

Discovering the molecular basis for ligand pharmacological activity on β -adrenoceptors

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Abstract

G-protein coupled receptors (GPCRs) are the largest and most diverse family of membrane proteins in the human genome and play an important role in cellular signalling by transducing a variety of different external signals to the interior of the cell. Due to their association with numerous human diseases, GPCRs are targeted by almost 34% of approved drugs. Since the discovery of β -blockers by Sir James Black more than 60 years, β -adrenoceptors (β ARs) belonging to class A G-protein coupled receptor (GPCR) family have become important therapeutic target for the treatment of cardiovascular and respiratory diseases. Despite success of existing drugs, we still need to better address the needs of patients with both asthma (treated with β 2-AR agonists) and cardiovascular dysfunction (treated with β 1-AR antagonists), a multi-morbidity combination of conditions that results in two-fold increase in heart failure in asthma patients on medication. This can be achieved by improving sub-type selectivity of drugs, fine-tuning their signalling properties, and increasing their ligand residency times as this would reduce their sensitivity to endogenously secreted adrenalin. Therefore, the identification of the specific and common determinants of ligand pharmacological activity on β 1-ARs and β 2-ARs and the investigation of the kinetic process of ligand binding to β -adrenergic subtypes are crucial to understand to the molecular mechanism of ligand selectivity between the subtypes.

In the first part of this PhD thesis (Chapter 3), we were interested in answering four questions to elucidate the molecular properties of the ligand binding at human β 1-ARs and β 2-ARs: Can we determine the underlying factors mediating agonism and antagonism for human β 1-A at atomic level? Are atomic interactions between ligand

and the human β 1-AR responsible for their pharmacological properties? Which atomic interactions determine the agonism or antagonism at human β 1-ARs? What are the similarities and differences between human β 1-ARs and β 2-ARs? We aimed to answer these questions by applying molecular docking and machine learning (ML) approaches.

In the second part of the thesis (Chapter 4), we focused on the kinetic binding characterization studies at human β 1-AR to advance current understanding of the molecular basis for fast or slow ligand binding kinetics. We explored the possible answers to these critical questions for four known β -blockers (Nebivolol, Carvedilol, Bisoprolol and Esmolol): Can we characterize the optimal fluorescent tracer for determination of kinetic binding parameters of unlabelled ligands for human β 1-AR? Can we use TR-FRET based approach for the characterization studies for human β 1-AR? Can we find the correct ligand binding poses and determine the atomic interactions of these four ligands for human β 1-AR? Is there a connection between the atomic interactions and the kinetic binding parameters of these ligands for human β 1-AR? By using TR-FRET based approach as alternative to traditional radioligand binding assays, we investigated the ligand binding kinetic for human β 1-AR and also revealed the key interactions of the ligands at molecular level via computational experiments.

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Abbreviations

β1-AR	Beta 1 Adrenergic Receptor
β2-AR	Beta 2 Adrenergic Receptor
BRET	Bioluminescence Resonance Energy Transfer
BSA	Bovine Serum Albumin
3D	Three-Dimensional
DMSO	Dimethylsulfoxide
ECL	Extracellular Loop
GPCR	G Protein-Coupled Receptor
GPD	Guanosine Nucleoside Triphosphate
GTP	Guanosine Nucleoside Triphosphate
HEPES	4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid
k_{on}	Association Rate Constant
k_{off}	Dissociation Rate Constant
K_i	Inhibition Constant
K_d	Equilibrium Dissociation Constant
ICL	Intercellular Loop
MD	Molecular Dynamics
PCR	Polymerase Chain Reaction
PBS	Phosphate Buffered Saline
RMSD	Root Mean Square Deviation
RT	Residence Time
TM	Transmembrane
TR-FRET	Time resolved – Forster Resonance Energy Transfer

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Chapter 1. Introduction

1.1. G-protein coupled receptors (GPCRs)

G-protein coupled receptors (GPCRs) are, with more than 800 unique members, the largest and most diverse family of membrane proteins in human genome (Lappano and Maggiolini, 2011; Rosenbaum et al., 2009). The main function of GPCRs is transduction of extracellular stimuli into intracellular signals through activation of heterotrimeric G proteins. Hence, they play crucial role in regulation of many fundamental physiological processes. Due to their physiological importance, GPCRs have become important drug targets for treatment of various diseases such as asthma, hypertension, cancer, cardiovascular disease, and they are targeted by approximately 34% of approved drugs (Deganutti et al., 2019; Hauser et al., 2017; Yang et al., 2021)

1.2. History of GPCR Research

The term of ‘receptive substances’ was firstly introduced in 1905 by John Newport Langley in order to explain the action of chemicals along the sympathetic nervous system (Baker et al., 2011; Hill, 2006; Maehle, 2009). In 1906, Paul Ehrlich modified his own ‘side chain theory’ and proposed the term of ‘chemoreceptor’ to elucidate the chemical interactions between drugs and receptors. Their theories led to the development of the ‘receptor’ concept. In late 50s, first quantitative methods were developed (Arunlakshana and Schild, 1959; Stephenson, 1956) by applying law of mass action to functional response data obtained from isolated cells to measure affinity of antagonists and partial agonists bound to GPCRs. In 1958, adenylyl cyclase

enzyme which synthesizes cyclic AMP (cAMP) and cAMP which regulates the actions of many receptors were discovered by (Sutherland and Rall, 1958) and Nobel Prize in Physiology or Medicine 1971 for its discovery was awarded to Earl W Sutherland. These findings led to the development of functional cAMP assays based on measurement of cAMP production to study the receptor activation and signalling (Hill et al., 1981; Insel and Kennedy, 1978; Jacobson, 2015; Lappano and Maggiolini, 2011; Nahorski, 1977; Rosenbaum et al., 2009; Schultz and Daly, 1973; Seamon and Daly, 1982).

During late 1960s and early 1970s, radioligand binding approaches had extensively been used to study the binding of ligands to GPCRs (Hill, 2006; Lefkowitz, 2007). The first application of radioligand binding methods to GPCRs receptors was achieved by William Paton and Humphrey Rang (Paton and Rang, 1965) in order to investigate the binding of ^3H -atropine to muscarinic receptors. In 1974, Burgen and King (Burgen and King, 1974) performed the radioligand binding experiments to investigate whether ^3H -propylbenzilylcholine mustard binds to muscarinic receptors. In GPCRs research, radioligand binding methods are based on the detection of binding by performing competition between the ligand and the radiolabelled ligand for the target receptor.

In 1980, the ‘ternary complex model’ was proposed for the high and low affinity states of β -adrenoceptors by Andre De Lean and Robert Lefkowitz (De Lean et al., 1980) to explain the mechanism of GPCR signalling. In ternary complex models, the receptors have two different binding site for ligand binding and G-protein binding (Weiss et al., 1996). These model explains the receptor’s interaction with ligands and G-poteins. In the following years, collaborative studies in the GPCR drug discovery facilitated the

characterization of partial β -adrenoceptor agonist dichloroisoprenaline and the development of β -adrenoceptor antagonist propranolol (Baker et al., 2011). With the advances in recombinant DNA technology, in 1986, hamster β_2 adrenoceptor cDNA was cloned successfully (Dixon et al., 1986) and they revealed high sequence similarities between seven transmembrane (7TM) regions of bovine rhodopsin and β_2 adrenoceptor. Since the determination of the sequence homology, a variety of GPCRs have been cloned. In the year 2000, the first attempt to GPCR crystallization was made for bovine rhodopsin (Palczewski et al., 2000a). Since that time, the structural knowledge obtained from growing number of GPCR crystal structures (Cherezov et al., 2007; Palczewski et al., 2000a; Rasmussen et al., 2011) have provided many insights for GPCR-structure based drug design (Gacasan et al., 2017; Kobilka, 2011). Moreover, eight Nobel prizes have highlighted the importance of GPCR research to scientific area (Baker et al., 2011; Lin, 2013).

1.3. Structural characteristics of GPCRs

The first structural knowledge was obtained from the low resolution electron cryo-microscopy of bovine rhodopsin (Unger and Schertler, 1995). In 2000, the first high resolution crystal structure of rhodopsin was released by Palczewski et al. (Palczewski et al., 2000a) and the structure confirmed the similarity of structural characteristics among GPCRs. Furthermore, recent advances in membrane protein engineering and crystallography have facilitated the determination of several GPCR crystal structures (Thal et al., 2018). According to statistics data from the GPCRdb (Pandy-Szekeres et al., 2018), 1102 GPCR crystal structures have been deposited into the Protein Data Bank (PDB) to date (**Figure 1**).

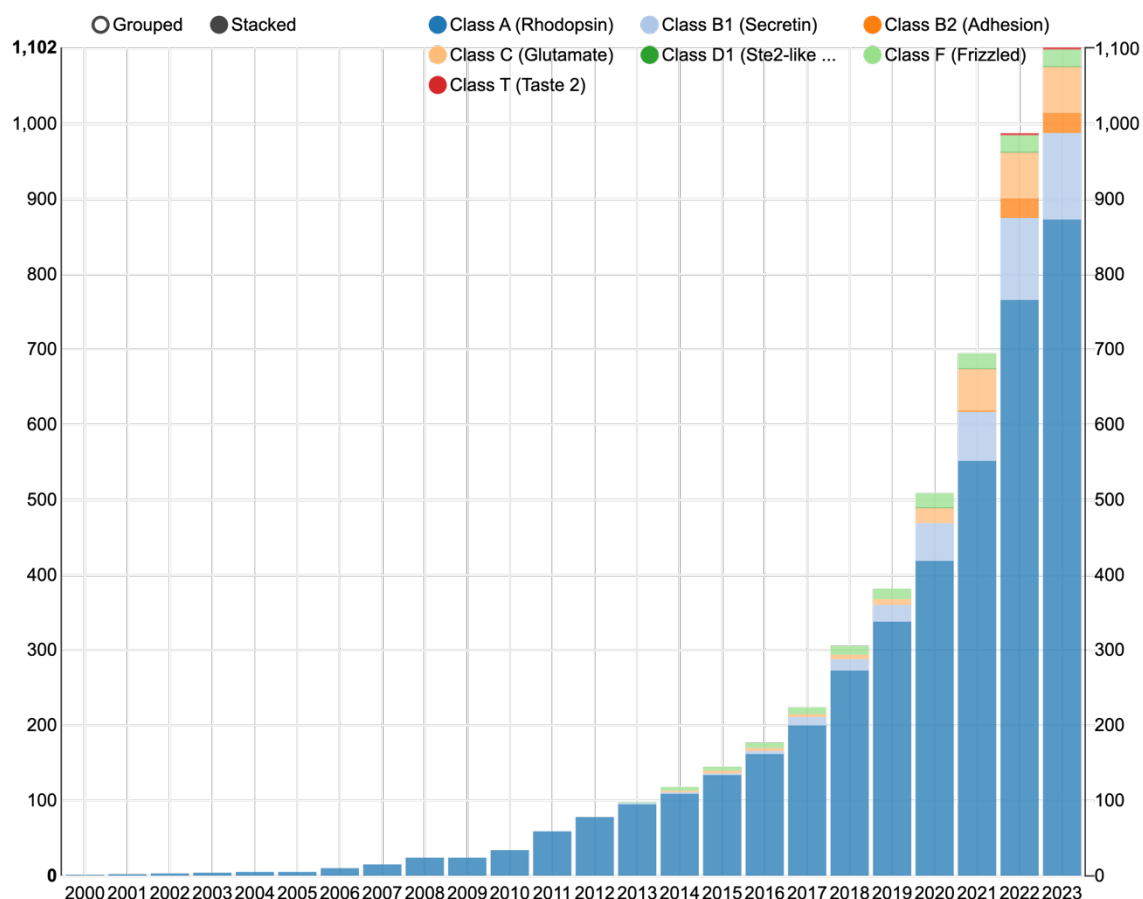


Figure 1. Number of the available structures for 23 years (Figure is downloaded from the GPCRdb (Pandy-Szekeres et al., 2018), <https://gpcrdb.org/structure/statistics>).

Available structures revealed that all GPCRs share common three dimensional (3D) structure (**Figure 2**) consisting a seven transmembrane (7 TMs) helices interconnected by three intracellular (ICL1, ICL2 and ICL3) and three extracellular (ECL1, ECL2 and ECL3) loops with an extracellular N-terminal region and an intracellular C-terminal region (Deganutti et al., 2019; Gacasan et al., 2017; Kobilka, 2007b; Kobilka, 2011; Palczewski et al., 2000a; Rasmussen et al., 2011). Besides, disulphide bond between two conserved cysteine residues in ECL2 and TM3 is common structural characteristic for GPCRs. The extracellular region is responsible for ligand binding whereas the intracellular region interacts with downstream effectors.

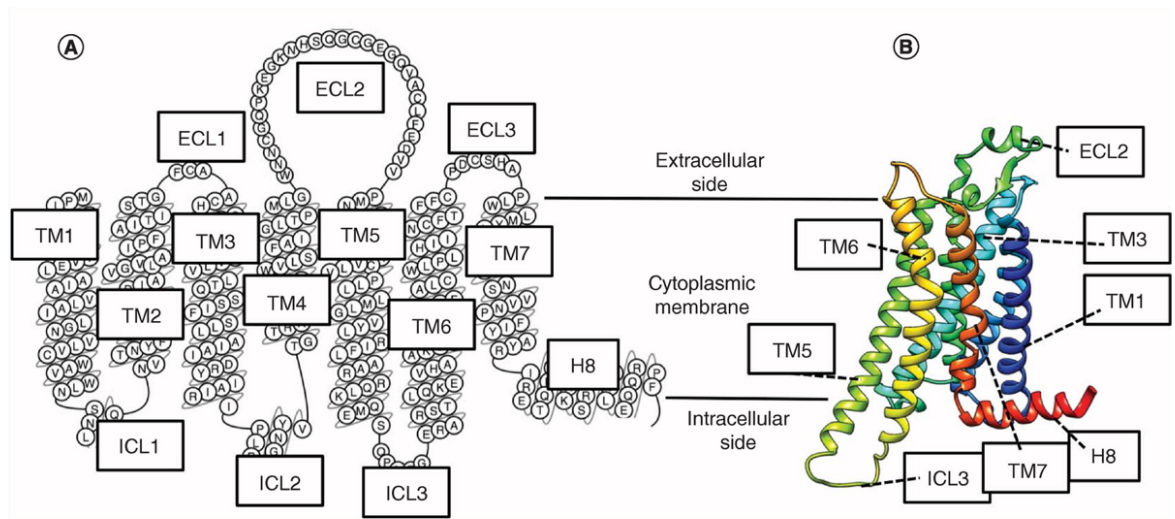


Figure 2. Schematic representation of the structure of a G-protein-coupled receptor. A) Snake map of the main structural characteristics of a GPCR. B) Ribbon representation of the tertiary organization of the structural elements. (Figures are adapted from (Deganutti et al., 2019))

1.3.1. Structural characteristics of Class A GPCRs

Of 1102 GPCRs in PDB, 873 are from the class A GPCRs (Pandy-Szekeres et al., 2018), <https://gpcrdb.org/structure/statistics>) and their ligands can bind either the orthosteric or allosteric binding sites (Chan et al., 2019; Congreve et al., 2017; DeVree et al., 2016; Flock et al., 2015; Katritch et al., 2014; Roth et al., 2017; Tautermann, 2014). The orthosteric ligand binding site is highly conserved and located within formed by residues in TM3, TM5, TM6 and TM7 (extracellular side of the 7 TM) (**Figure 3**) (Chan et al., 2019). On the contrary, the allosteric ligand binding site is highly diverse and can be located anywhere on the receptor (**Figure 4**) (Egyed et al., 2022).

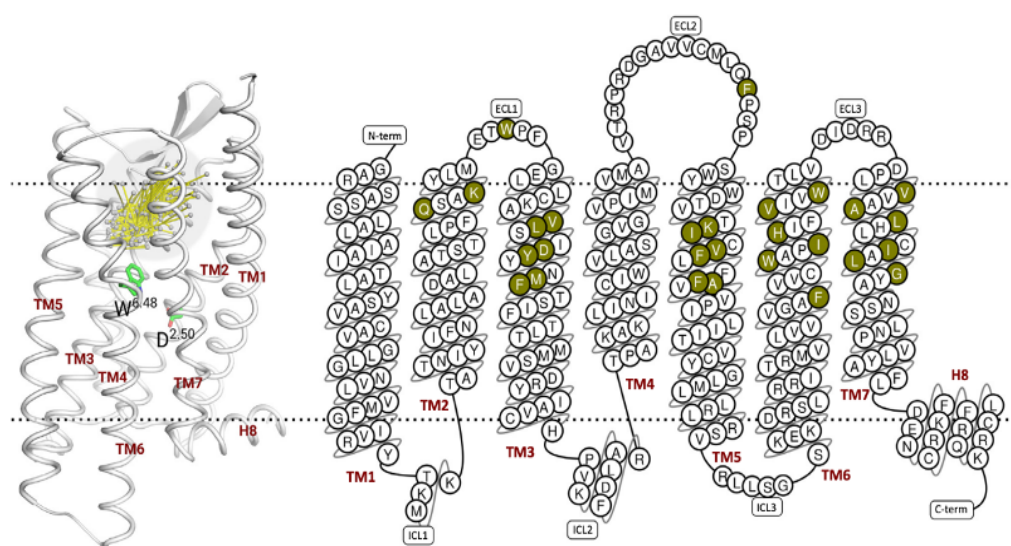


Figure 3. Schematic representation of the GPCR-ligand interactions in classical orthosteric binding sites and interacting residues with ligands in the crystal structure of the mOR (PDB ID: 4N6H) receptor. (Figure is adapted from the (Chan et al., 2019))

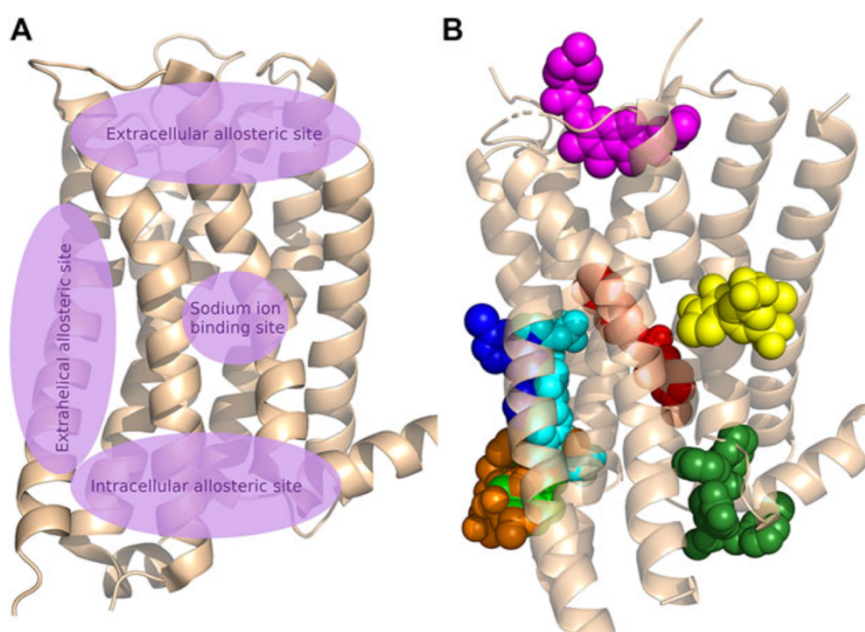


Figure 4. Cartoon representation of the allosteric binding sites and allosteric ligands in Class A GPCRs. A) Location of the major allosteric binding sites in Class A GPCRs. B) Allosteric binding sites of various ligands of Class A GPCRs: D1R (green, PDB ID: 7LJD), AP8 in FFAR1 (cyan, PDB ID: 5TZY), ORG27569 in CB1 (red, PDB ID: 6KQI), MIPS521 in A1R (yellow, PDB ID: 7LD3), LY2119620 in M2R (magenta, PDB ID: 4MQT), Cmpd-15PA in β 2AR (dark green, PDB ID: 5X7D), AS408 in β 2AR (dark blue, PDB ID: 6OBA), cmpd-6fa in β 2AR (orange, PDB ID: 8N48) (Figure is adapted from the (Egyed et al., 2022))

1.3.2. Conserved contacts and residues of GPCRs

The evolutionarily conserved structural scaffold of GPCRs is mediated by the consensus network of inter-TM contacts at the interfaces involving TM1-TM2, TM3-TM4, TM3-TM5 and TM3-TM6-TM7 (**Figure 5**) (Venkatakrishnan et al., 2013). Additionally, each TM helix have at least one highly conserved residue (Mirzadegan et al., 2003; Trzaskowski et al., 2012). Asn in TM1, Asp in TM2, Arg in TM3, Trp in TM4, Pro in TM5, Pro in TM6 and Pro in TM7 have been identified as highly conserved residues and these most conserved residues in each TM helix are designated as residue .50 by Ballesteros and Weinstein numbering system (Ballesteros and Weinstein, 2015).

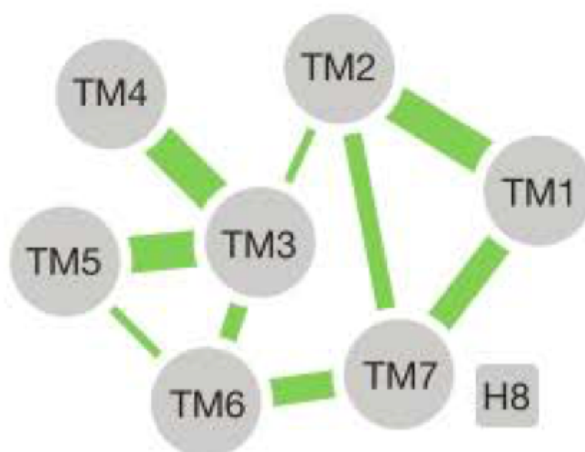


Figure 5. Schematic representation of consensus network of the inter-TM contacts at GPCRs. TM helices in consensus network are shown as circles and H8 is represented as a square. The green lines between the circles demonstrate the presence of consensus contacts, and the thickness of the green line is proportional to the number of contacts. (Figure is adapted from (Venkatakrishnan et al., 2013)).

1.4. Classification of GPCRs

The two classification systems are mostly in use to characterise GPCR families: the A-F and the GRAFS system. One of the first GPCR classification system, A-F classification was introduced by Kolakowski and classifies GPCRs into six main families according to their sequence homology (Kolakowski, 1994). These are the Class A (Rhodopsin-like receptors); Class B (Secretin/adhesion receptors); Class C (Metabotropic glutamate receptors); Class D (Fungal mating pheromone receptors); Class E (Cyclic AMP receptors); Class F (Frizzled/smoothed receptors). Due to the diversity of GPCRs, in 2003, Fredriksson modified A-F classification system and proposed another classification system called GRAFS based on the phylogenetic analysis of the human GPCR sequences (Fredriksson et al., 2003). According to GRAFS system, human GPCRs are divided into five main classes, named Glutamate, Rhodopsin, Adhesion, Frizzled/Taste2 and Secretin (**Figure 6**) (Stevens et al., 2013). The main difference between the A-F system and the GRAFS system is separation of the Class B (Secretin/adhesion receptors) into Secretin family and Adhesion family.

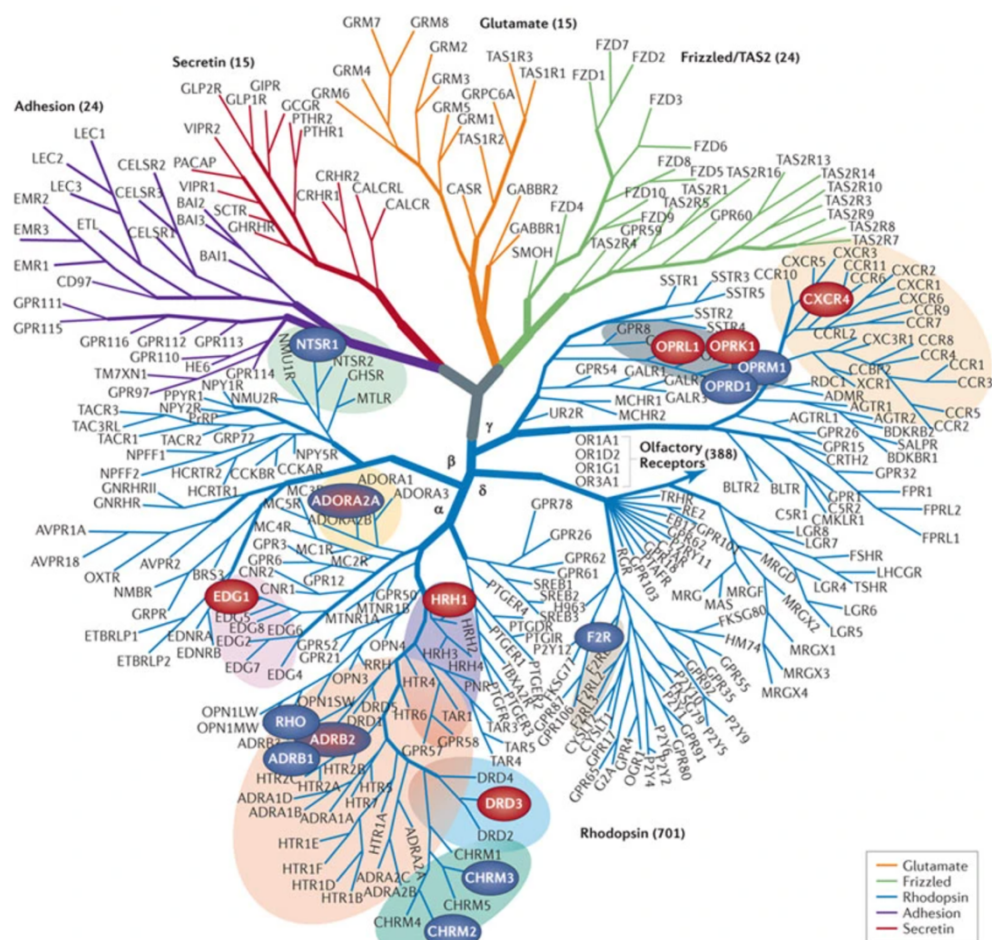


Figure 6. Phylogenetic tree of the GPCR family according to GRAFS system (Figure is adapted from (Stevens et al., 2013)). Family members with determined structures are highlighted within the tree.

The Class A, also known as the ‘Rhodopsin-like receptors’ is the largest family of the GPCRs in human genome with 873 members (**Figure 7**) ((Pandy-Szekeres et al., 2018), <https://gpcrdb.org/structure/statistics>). According to GRAFS classification system (Fredriksson et al., 2003), this family have been divided into four main subgroups, α , β , γ and δ . Due to the their crucial roles in human physiology, Class A GPCRs are the most extensively studied GPCR target for drug discovery (Bristow,

1.5. Affinity and Efficacy of GPCR Ligands

The majority of the GPCRs exhibit the basal (constitutive) activity in the ligand-free inactive state and they are activated by binding of ligands displaying different affinities and efficacies (Lefkowitz et al., 1993; Milligan, 2003; Samama et al., 1993). Affinity is described as the strength of the interaction between the receptor and the ligand while the efficacy is defined as the ability of a ligand to generate cellular responses when binds to the receptor (Kenakin, 2013; Vauquelin and Charlton, 2013; Vilardaga et al., 2009). Based on their efficacies, ligands can be classified into four classes: full agonists, partial agonists, antagonists and inverse agonists (**Figure 8**) (Wacker et al., 2017). Full agonists completely stimulate the receptor activation whereas partial agonists activate the receptor above basal level and below maximal level. On the contrary, inverse agonists reduce the level of receptor activation below basal level while antagonists bind to the receptor and compete with ligands for binding. Efficacy and affinity are the two most important determinants which influence the degree of the cellular response to agonists (Strange, 2008; Williams and Sewing, 2005). On the other hand, the binding of antagonists to receptor is only governed by affinity. Therefore, receptors are activated by agonists while antagonists do not have the ability to activate receptors.

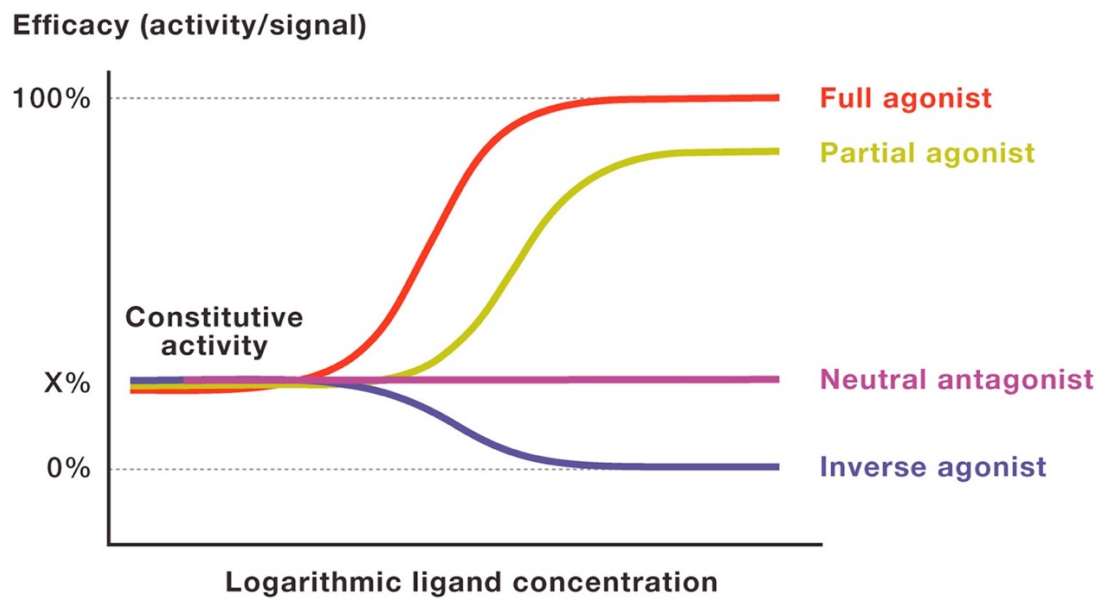


Figure 8. Schematic representation of classification of the ligand efficacy at GPCRs. Based on their efficacies, ligands can be classified into four classes: full agonist (red curve), partial agonist (yellow curve), neutral antagonist (magenta line), inverse agonist (purple curve). (Figure is adapted from (Wacker et al., 2017))

1.6. Intracellular Signalling by GPCRs

In signal transduction, GPCR activation is translated into various signals mediated through heterotrimeric G proteins, arrestins, ion channels, kinases and variety scaffolding proteins (**Figure 9**) (Benovic et al., 1989; Brown et al., 2003; Gainetdinov et al., 2004; Komolov et al., 2017; Luttrell et al., 1999; Rasmussen et al., 2011; Wootten et al., 2018).

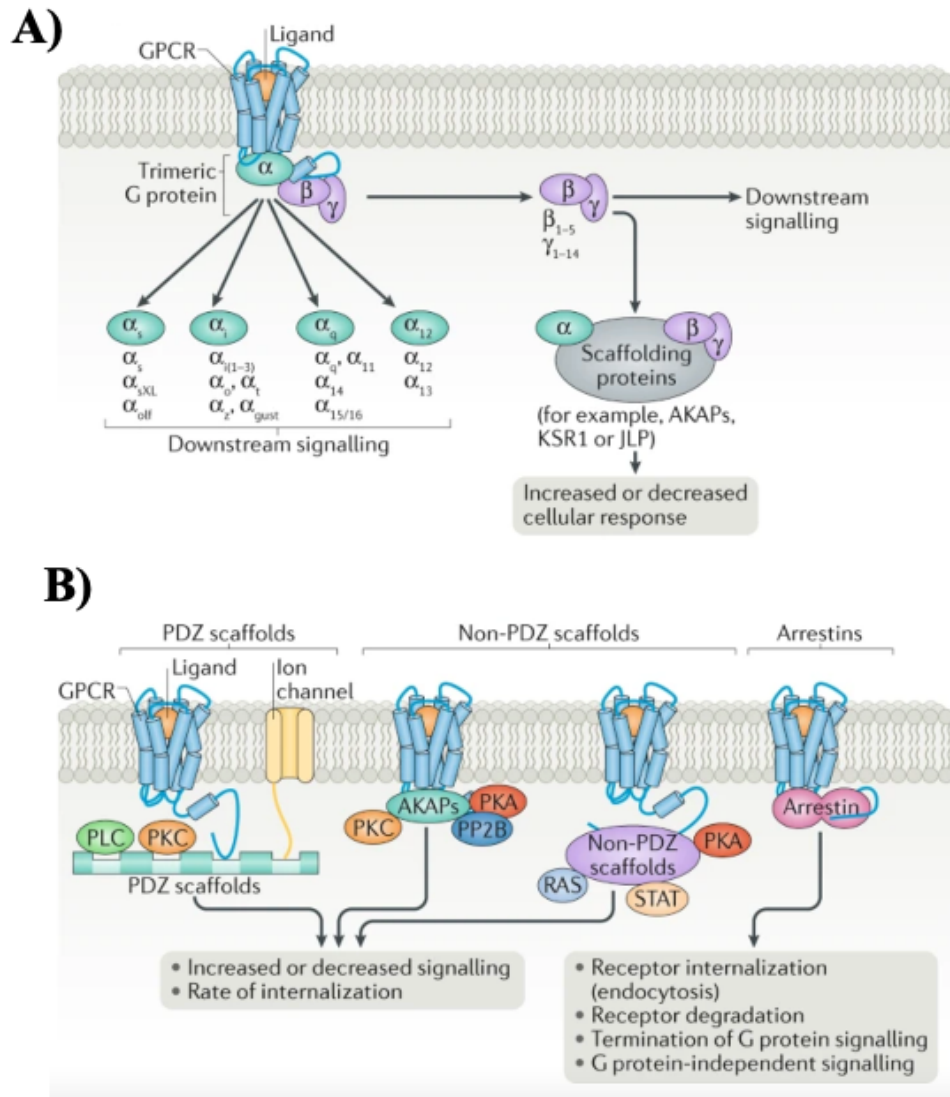


Figure 9. Schematic representation of the GPCR signalling. A) Schematic representation of the GPCR signalling through heterotrimeric G proteins ($G\alpha$, $G\beta$, and $G\gamma$). B) Schematic representation of GPCR scaffolding proteins which play important roles in the regulation of GPCR signalling. These scaffolds can be grouped into three classes: PDZ scaffolds, non-PDZ scaffolds and arrestins. (Figure is adapted from (Wootten et al., 2018))

The receptor mediated activation of heterotrimeric G proteins is also shown in **Figure 10** (Sutkeviciute and Vilardaga, 2020). Heterotrimeric guanine nucleotide binding proteins also known as G proteins consist of three subunits: α , β , and γ . $G\alpha$ subunits are subdivided into four main classes ($G\alpha_s$, $G\alpha_i$, $G\alpha_q$ and $G\alpha_{12}$) according to their

sequence homology and functional similarity. Conformational changes induced by binding of a ligand to GPCRs activate the heterotrimeric G proteins by promoting the exchange of guanosine diphosphate (GDP) for triphosphate (GTP) (Black et al., 2016; Hill et al., 2010; Leifert et al., 2005). Following the exchange, $G\alpha$ subunit dissociate from the β/γ subunits of G protein and the dissociated subunits initiate the different signal transduction cascades. Hydrolysis of GTP to GDP terminates the signalling cascades (Leifert et al., 2005). $G_{\alpha s}$ stimulates adenylyl cyclase enzyme to increase cyclic AMP (cAMP) production whereas $G_{\alpha i}$ decreases cAMP levels by inhibiting adenylyl cyclase enzyme. $G_{\alpha q}$ activates β -isoforms of phospholipase C which is responsible from the separation of phosphatidylinositol 4,5- bisphosphate (PIP₂) into inositol 1,4,5-trisphosphate (IP₃) and diacylglycerol (DAG). The fourth class, $G_{\alpha 12}$, increases the activity of Rho through guanine nucleotide exchange factor (RhoGEF).

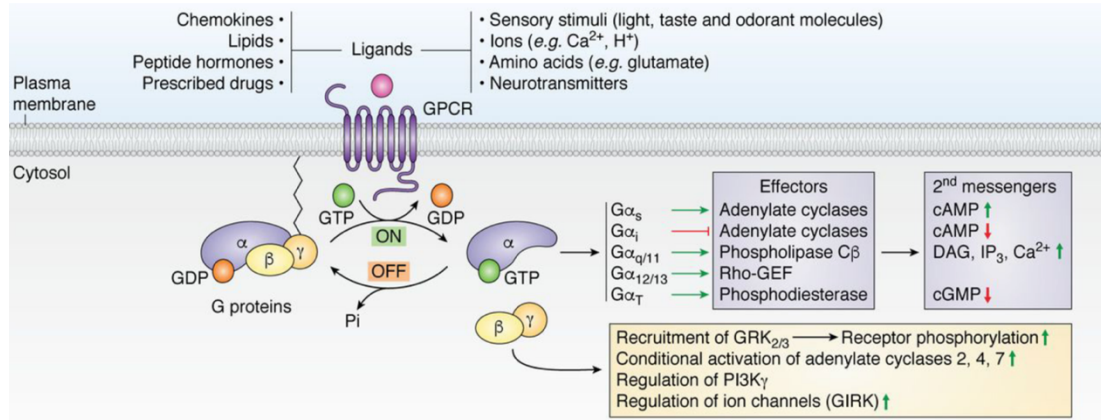


Figure 10. Schematic representation of the basic paradigm of GPCR signalling. (Figure is adapted from (Sutkeviciute and Vilardaga, 2020))

1.7. The Beta1 (β_1) and Beta2 (β_2) Adrenergic Receptors

The Adrenergic Receptors (ARs) belong to the Rhodopsin/Class A family of the GPCRs and targeted by endogenous ligands, epinephrine and norepinephrine (Ahlquist, 1948; Wu et al., 2021). The first classification of adrenoceptor into two major types, alpha (α) and beta (β), was developed by Ahluqist (Ahlquist, 1948) who investigated the effect of several agonists on immune response. In the later years, Ahluqist's classification was expanded (Minneman et al., 1981) and each major adrenoceptor type was divided into two subtypes: α_1/α_2 and β_1/β_2 (Bylund, 1992; Lands et al., 1967; Langer, 1980). In recent years, advances in gene cloning technology has enabled the characterization of receptors and nine subtypes have been identified : α_{1A} , α_{1B} , α_{1D} , α_{2A} , α_{2B} , α_{2C} , β_1 , β_2 and β_3 (Bylund, 1992; Bylund et al., 1994; Dixon et al., 1986; Emorine et al., 1989; Hein and Kobilka, 1995; Langer, 1980; Philipp and Hein, 2004; Qu et al., 2019; Stockigt et al., 2012).

β -Adrenergic receptors (β -ARs) have become one of the most widely studied model systems for GPCR studies (Brodde, 2008; Kolinski et al., 2012; Madamanchi, 2007). The β -ARs have been classified into three main subtypes, beta1 (β_1), beta2 (β_2) and beta3 (β_3) (Bylund, 1992; Bylund et al., 1994; Dixon et al., 1986; Emorine et al., 1989; Hein and Kobilka, 1995; Langer, 1980; Philipp and Hein, 2004; Qu et al., 2019; Stockigt et al., 2012). They are expressed in the variety of human tissues including the heart, lungs, liver, brain, vascular smooth muscle, pancreas, spleen and adipose tissue (Scanzano and Cosentino, 2015). The β -ARs are activated by the endogenous ligands, norepinephrine and epinephrine, and they play pivotal role in the regulation of cardiovascular, metabolic, pulmonary and central nervous systems (Brodde, 2007;

2008). In the present study, we will focus on β 1-ARs and β 2-ARs only as model receptors.

The β 1-ARs are expressed mainly in the heart, kidney, adipose tissue and they contribute to the regulation of heart rate, cardiac functions, renin release and lipolysis (Alhayek and Preuss, 2022). Although all three subtypes of β -ARs are expressed in human heart, the β 1-ARs are the predominant subtype accounting 75–80 % of the β -ARs (Madamanchi, 2007; Woo and Xiao, 2012). Therefore, the β 1-AR are widely used as target receptor for treatment of the cardiovascular diseases (Bristow, 2011). In addition, endogenous ligand norepinephrine has relatively higher affinity for β 1-ARs compared to other endogenous ligand, epinephrine (Wachter and Gilbert, 2012). The other β -AR subtype, β 2-ARs are mainly found in the lung (Carstairs et al., 1985) but is also expressed in kidney, blood vessels, liver and heart (Blair et al., 1979; Healy et al., 1985; Heitz et al., 1983). 25-20 % of the β -ARs in hearth belong to β 2-AR subtype (Madamanchi, 2007). β 2-ARs are major target for the treatment of asthma and mediation of smooth muscle relaxation in airways (Bai, 1992; Cazzola et al., 2011; Lin et al., 2012; Nguyen et al., 2017)

1.8. β -Adrenoceptor Antagonists (β -Blockers)

β -adrenoceptor antagonists, commonly known as β -blockers, are important class of drugs that inhibit the action of endogenous catecholamines epinephrine and norepinephrine by binding to β -adrenergic receptors (do Vale et al., 2019; Farzam and Jan, 2022). In clinical practice, β -blockers have been mostly used to treat variety cardiovascular diseases including ischemic heart disease, hypertension, heart failure as well as non-cardiovascular diseases such as tremor, glaucoma, anxiety,

hyperthyroidism and migraine. The invention of the first clinically successful β -blocker, propranolol, was done by Sir James Black for the treatment of cardiovascular diseases in 1965 (Baker et al., 2011; Black, 2010). For this discovery, he was awarded the Nobel Prize for Physiology or Medicine in 1988 (Ganellin and Duncan, 2010). Since the 1960s, more than twenty β -blockers have been introduced for clinical use (Baker et al., 2011; Frishman, 2008).

β -blockers are divided into three generations on the basis of their pharmacological properties, first generation, second generation and third generation (do Vale et al., 2019). The first generation β -blockers (propranolol, timolol, pindolol, nadolol, sotalol, alprenolol, bupranolol, carazolol) are nonselective β -blockers demonstrating similar binding affinities for β_1 -AR and β_2 -AR. The second generation β -blockers (atenolol, bisoprolol, metoprolol, betaxolol, acebutolol, xamoterol), also called as β_1 -selective blockers, have higher affinity for β_1 -ARs compared to β_2 -ARs. The third generation β -blockers, known as vasodilating β -blockers, are composed of β_1 -selective (nebivolol, celiprolol) and nonselective (carvedilol, labetalol) blockers having vasodilating properties. At the present time, propranolol, bisoprolol, nebivolol, atenolol, betaxolol have been widely used in treatment of hypertension whereas other antagonists include carvedilol, propranolol, metoprolol, esmolol, atenol, bisoprolol have been used in treatment of cardiac disorders (Alexander et al., 2019; Baker et al., 2011).

Despite the clinical success of β -blockers, as well as β_2 -AR agonists as bronchodilators in asthma, there is a need for more subtype selective drugs (Baker and Wilcox, 2017; Barisione et al., 2010; Bennett et al., 2021; Harrington, 2021; Jiménez-Rosés et al., 2022; Loth et al., 2014; Oliver et al., 2019; Wacker et al., 2017;

Zolotareva et al., 2019). This is important for co-morbidly conditions, such as asthma and heart conditions. Metanalysis clearly showed worse outcome for patients with heart disfunctions who are on asthma medication, a combination that affects approximately 10% of patients. (Morales et al., 2014). Improving selectivity of currently used drugs so that unavoidable systemic expose to β 2-AR agonists would not activate β 1 receptors in the heart may be very advantageous in this case (Baker et al., 2017). Another area of potential improvement of existing drugs are developing long residence time β 1-AR antagonists, as they are much less likely to be affected by dynamics changes in hormonal level in the body and provide better therapeutic efficacy (Copeland, 2015; 2021). The development of new drugs would be greatly facilitated by detailed understanding of the atomic interactions between the ligand and the receptor that determine their pharmacological activity and their residence time.

1.9. Computational Approaches for Drug Discovery

1.9.1. Homology Modelling

Because of the important roles of the GPCRs in human body, understanding the molecular basis of GPCR activation and ligand-receptor interactions is essential for GPCR structure-based drug design to develop new drugs (Congreve et al., 2011; Jozwiak and Plazinska, 2021; Lundstrom, 2009; Weis and Kobilka, 2018). Since determination of the first crystal structure of a GPCR molecule (Palczewski et al., 2000a), a variety of three dimensional (3D) structures of GPCR molecules have been determined (Congreve et al., 2020). On the other hand, 3D structure of many GPCRs is not available in Protein Data Bank (PDB) (Berman et al., 2000; Castleman et al., 2019; Isberg et al., 2014; Latorraca et al., 2017). Due to the expensive and time consuming experimental methods in drug discovery process, computational methods including homology modelling, molecular docking and molecular dynamics simulations have been extensively applied for GPCR structure-based drug design (Jiménez-Rosés et al., 2022; Kooistra et al., 2016; Leelananda and Lindert, 2016; Plazinska et al., 2015; Scharf et al., 2019; Selvam et al., 2012). In the absence of the 3D structure of GPCR, homology modelling approach has been used to produce desired receptor structures to investigate the ligand-receptor interactions (Cavasotto and Phatak, 2009; Costanzi, 2012). Homology modelling is computational method which predicts the 3D structure of a target protein from its amino acid sequence of the target (Muhammed and Aki-Yalcin, 2019; Vyas et al., 2012). In addition to sequence of the target protein with unknown 3D structure, the method uses the templates with known 3D structure to construct the model structure of the target (Blundell et al., 1987; Waterhouse et al., 2018). Homology modelling consists of four sequential steps: 1)

Identification of the suitable structural template(s); 2) Sequence alignment of target and template protein(s); 3) Model building; and 4) Model quality evaluation (Bordoli et al., 2009) (**Figure 11**). The quality of a homology model depends on several factors such as resolution of the template structure and sequence identity between template and target sequences.

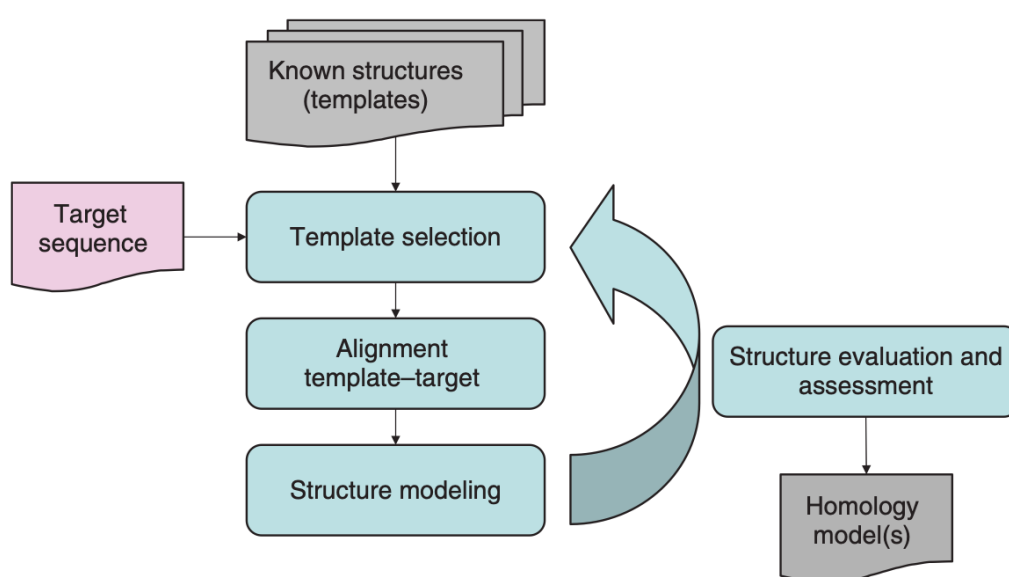


Figure 11. The schematic representation of the four sequential steps of homology modelling. (Figure is adapted from (Bordoli et al., 2009))

1.9.2. Molecular Dynamics (MD) Simulations

Molecular dynamics (MD) simulation is computational approach to investigate the physical movements of macromolecules (Alder and Wainwright, 1959). MD provides the opportunity for the exploration of the interaction between the ligands and receptor proteins, dynamics of binding, binding kinetics and functions (Adcock and McCammon, 2006; Cournia et al., 2015; Dror et al., 2012; Khalili-Araghi et al., 2009; Stansfeld and Sansom, 2011). MD simulation approaches have been commonly used

to study the mechanism of GPCR activation since the first MD simulation of a GPCR (Adcock and McCammon, 2006; Dror et al., 2011a; Dror et al., 2011b; Plazinska et al., 2013; Plazinska et al., 2015). The MD simulations have been extensively used in understanding structural, kinetic and thermodynamic characteristics of macromolecules at molecular level. In MD simulations, for each atom of the molecular system, Newton's equations of motion is solved numerically in order to obtain most detailed time dependent information about the dynamics of the system (Adcock and McCammon, 2006; Dodson et al., 2008). For the analysis of equilibrated MD simulation trajectories, typically, root mean square deviation (RMSD), root mean square fluctuation (RMSF) and principal component (PCA) analysis are calculated (Baltrukevich and Podlowska, 2022).

1.9.3. Molecular Docking

In the presence of 3D structure of GPCRs, molecular docking has been extensively used in drug discovery to predict ligand-receptor interactions at molecular level (Bartuzi et al., 2017; Peterson et al., 2018). Molecular docking is a structure-based method that predicts the most favourable ligand binding conformation in the binding site of a protein when they form the complex (**Figure 12**) (Morris and Lim-Wilby, 2008). Therefore, molecular docking is one of the most widely applied applications of molecular modelling approaches in structure-based drug discovery (Ferreira et al., 2015; Meng et al., 2011; Morris and Lim-Wilby, 2008). In the first part of the docking, large number of possible protein-ligand structures are generated from its unbound constituents using 3D structure of the receptor and the ligand of interest. In the second part, possible protein-ligand complex structure is ordered depends on the global minimum free energy of ligand-protein complex scoring functions and the structure

with the lowest score is chosen as near native conformation (Grinter and Zou, 2014; Meng et al., 2011).

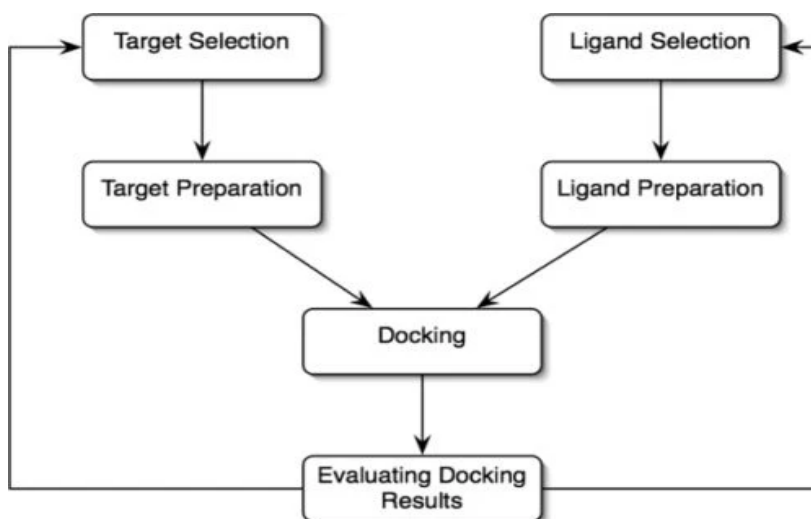


Figure 12. The typical workflow of the docking (Figure is adapted from (Morris and Lim-Wilby, 2008))

1.9.4. Interaction Fingerprint Analysis (IFP) and Machine Learning (ML)

Interactions between and within molecular structures play a significant role in many biological processes from molecular recognition and protein folding. The analysis of each interaction formed by residues of biomolecular complexes can provide fundamental insights for understanding structure–function relationships. Interaction fingerprints (IFs) provide the effective representation and analysis of 3D protein–ligand interactions and fast comparison of the similarity between different molecules. Molecular fingerprints are powerful tools in cheminformatics for structure-activity relationship studies, virtual screening and mapping chemical space (Capecchi et al., 2020). In structure-based drug discovery studies, characterization of the properties of each interactions can supply valuable information to medicinal chemists (Bouysset and Fiorucci, 2021; Fischer et al., 2021). Therefore, representing and analysing of the

3D protein-ligand interactions is a crucial step in drug discovery process (Deng et al., 2004). Molecular fingerprints are preferred for large-scale dataset screening to reduce the computational cost. In the first step of the process, interactions between ligand and protein are calculated from 3D structure. After then, the interaction information, where the presence or absence of specific interactions between the binding pocket residues and the ligand are represented as binary 1D form (Vass et al., 2016). Generally, the presence of the particular interaction is denoted as 1 whereas the absence of the particular interaction is denoted as 0 (Perez-Nueno et al., 2009). IFPs are also extremely popular in order to investigate the ligand-receptor interactions (Vass et al., 2016). Therefore, in recent years, novel protein-ligand interaction fingerprint approaches involving Machine Learning (ML) have been developed to identify the ligand binding site and ligand-receptor interactions of the GPCR structures (Jiménez-Rosés et al., 2022; Vass et al., 2016). Especially, machine learning approaches have been widely used for classification and regression of the GPCR ligand libraries (Ahmed et al., 2021; Jiménez-Rosés et al., 2022; Karimi et al., 2020; Oh et al., 2022). ML is the science, which it is part of artificial intelligence (AI) and computer science, focused on the use of data and statistical algorithms that gives computers the ability to learn from previous data and make decisions (also called predictions) (Sarker, 2021). ML models can be grouped into three main categories: supervised learning, unsupervised learning and reinforcement learning (Raschka and Kaufman, 2020). Supervised machine learning algorithms are generally used for solving classification and regression problems. In supervised learning, firstly, a labelled dataset is used to train the ML models. Then, the trained algorithm is then fed on the unlabelled test dataset to categorise them into similar groups. On the other hand, unsupervised learning uses a unlabelled dataset as training dataset.

Unsupervised learning is used for solving clustering and association problems. Unlabelled data does not have a fixed output variable. The model learns from the data, discovers the pattern and features in the data and returns the output. Reinforcement learning algorithms enables an agent to learn in an interactive environment by trial and error using feedback from its own actions and experiences; they are widely used in the gaming industries to build games (Raschka and Kaufman, 2020; Sarker, 2021).

1.10. Experimental Approaches for Studying Ligand Binding to GPCRs

1.10.1. Radioligand Binding Assays

Radioligand binding assays have traditionally been used to understand the properties of the receptors at molecular level in receptor pharmacology and drug development (Flanagan, 2016; Lefkowitz, 2004; Lefkowitz et al., 1970). The radioligand binding assay was first introduced by Lefkowitz et al. (Lefkowitz et al., 1970). Since 1970s, radioligand binding assays have been widely used to study the receptor-ligand binding affinity, GPCR expression and the binding kinetics in GPCR drug discovery and development. In radioligand binding assays, the target receptor is incubated together with a radiolabelled ligand for determined time and temperature. Subsequently, receptor-bound and unbound ligand are separated by filtration to measure the fraction of the ligand bound to the receptor using scintillation counter (Flanagan, 2016).

1.10.2. Resonance Energy Transfer-Based Approaches

During the last decade, as alternative to radioligand binding assays, resonance energy transfer-based approaches have been developed to study interactions of the ligand-receptor in living cells (**Figure 13**) (Ayoub, 2016; Kobayashi et al., 2019). Resonance energy transfer-based approaches can be grouped into fluorescence resonance energy transfer (FRET) and bioluminescence resonance energy transfer (BRET) technologies according to the fluorescent labels (Zhou et al., 2021). BRET technology uses a light emitting luciferase enzyme donor and a fluorescent acceptor whereas FRET technology requires extra excitation laser for the excitation of FRET donor fluorophores (Ayoub, 2016; Kobayashi et al., 2019; Zhou et al., 2021).

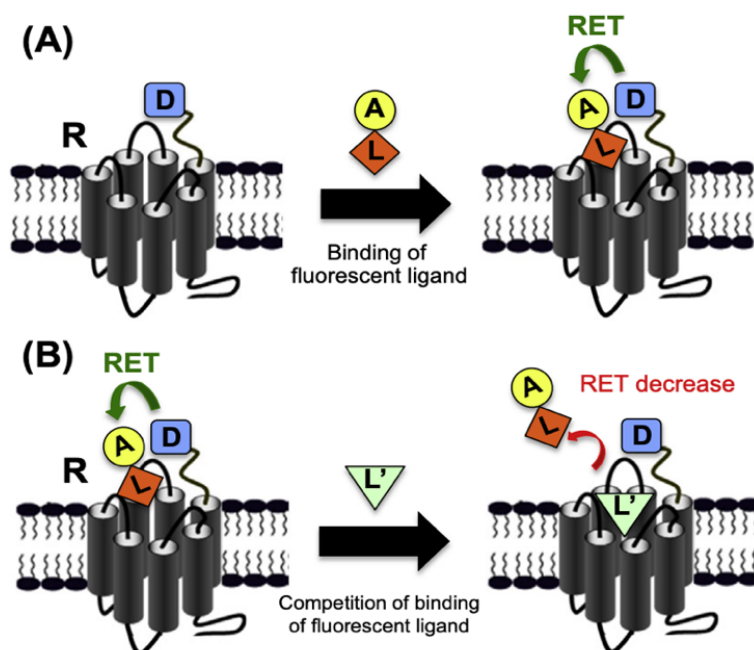


Figure 13. The measurement of the ligand-GPCR interaction via resonance energy transfer (RET)-based assays. A) The schematic representation demonstrates the measurement of the RET signals between the energy donor (D)-fused receptor and the energy acceptor (A)-conjugated ligand (L). B) The schematic representation shows the competition of the RET signals measured between donor-fused receptor (D-R) and the acceptor-conjugated ligand (A-L) by an unlabelled ligand (L'). (Figure is adapted from the (Ayoub, 2016))

1.11. Computational Studies of β 1 and β 2 Adrenergic Receptors

Binding and unbinding kinetics is relevant for predicting drug efficacy in living organisms (Copeland et al., 2006; Swinney, 2004). Therefore, some previous studies investigated the ligand binding and unbinding mechanism at β -ARs by performing molecular dynamics simulations. One previous study (Selvam et al., 2012) performed steered molecular dynamics simulations on selective antagonist Esmolol bound β 1-AR and ICI-118551 bound β 2-AR structures in order to study the molecular mechanism of unbinding events. It is demonstrated that preferred pathway is dependent on receptor type. As a result of their study, they observed that β 1-ARs show strong preference for membrane pathway while β 2-ARs use lateral pathway. For Esmolol, K347 is found to be important for unbinding process whereas aromatic and hydrophobic interactions seemed to be significant for ICI-118551. In 2015, another study (Plazinska et al., 2015) performed molecular dynamics simulations on agonist (fenoterol) and inverse agonist (carazolol) bound β 2-AR structures to investigate the kinetics of the ligand binding and unbinding mechanisms using GROMACS software (Abraham et al., 2015). Aromatic residues (H93, F194, H178 and H296) in the extracellular domain have been suggested to play important role for the ligand binding in the initial phases. They also observed that conformation of the receptors can change the ligand entry and exit pathways in the extracellular region.

In the recent years, docking of large-scale compound libraries have been applied to existing β 2-ARs to explore the effects of the receptor conformations on ligand efficacy. One of these studies investigated whether the active state β 2-AR can act as

a template to other active state GPCRs. Unlike the previous study, they revealed that large scale compound library into an agonist (BI-167107) bound active state β 2-AR structure predicted exclusively agonists. Another study by Scharf et al. (2019) explored whether comparative docking to different conformations of β 2-AR could preferentially detect novel compounds with agonist activity. As a result of their study, they obtained unique agonist ligands with pyrazole part for the β 2-AR and showed one of them had similar intrinsic efficacy to salbutamol which is known clinically used drug. Their study proposed that using different active state structures in molecular docking experiments can be effective for design and identification of agonist ligands. Their finding might be useful for modelling of other GPCRs with unknown 3D structures to study the mechanism of agonist binding. Findings obtained from above studies demonstrated that structure-based ligand design for β 2-ARs crucially depends on receptor conformation and hence their activation state. Comparison the docking results obtained with active and inactive receptor conformations provides valuable insights to discover new ligands for other GPCRs. Nevertheless, this approach is not efficient for some specific receptor subtypes when any structural information of the subtype for one particular organism are not available.

Several studies have investigated to link structural properties of the ligands and ligand- β -AR interactions to their functionality based on existing β -ARs via ligand docking or MD simulations (Chan et al., 2019; Jiménez-Rosés et al., 2022; Kooistra et al., 2015; Kooistra et al., 2016). These studies focused only targeted turkey β 1-ARs, turkey β 2-ARs and human β 2-ARs. One of these study (Kooistra et al., 2015) incorporated interaction fingerprints (IFPs) into molecular docking protocols of the ligands and identify important residues for the ligand binding using 31 β -AR crystal structures including 15 human β 2-AR and 16 turkey β 1-AR. Their study suggested

that IFPs can provide valuable knowledge for structure-based drug discovery by revealing efficacy of ligands. But, they did not investigate the differences between β 1-AR and β 2-AR in their study. Therefore, IFPs can be useful to explore the differences between β 1-ARs and β 2-ARs. In another study (Kooistra et al., 2016), docking scoring approach combining energy-based scoring function using PLANTS docking with a molecular IFPs approach was applied to β 2-AR crystal structures to identify new ligands. As a result of their study, they recommended that optimization of this combined approach needed for each targeted receptor using careful retrospective validation. This limits the application of their approach directly to β 1-ARs. Whereas the above two studies focused on only docking data, a study (Chan et al., 2019) generated IFPs from molecular dynamics simulations (MD). In their study, they docked 12 different ligands with known efficacy into β 2-AR via Glide docking software and 100 ns long MD simulations of these docked structures were performed using Desmond software in order to predict the effects of these ligands on β 2-AR. They revealed 16 important (W109, D113, V114, V117, F193, Y199, S203, S204, S207, W286, F289, F290, N293, Y308, I309 and N312) interacting β 2-AR residues with the ligands using IFPs. Their study also demonstrated that interaction profiles and movements of TM5 and TM6 helices are dependent on the bound ligand type. Due to the limited number of ligands, MD can be applied to obtain detailed ligand-receptor information. On the other hand, application of MD to each compound is impossible in any large-scale compound library. In our latest publication (Jiménez-Rosés et al., 2022), we have determined specific residues of the human β 2-AR and common atomic interactions mediating pharmacological actions of agonism and antagonism for each ligand by performing docking and ML approaches. In this study, 2683 known β -AR ligands were docked into three different human β 2-AR structures

and atomic interaction fingerprints (AIFs) were identified. As a result of the study, we found that K97, F194, S203, S204, S207, H296, and K305 residues mediate agonist ligand binding whereas the antagonist ligands interact with W286 and Y316 residues. This study suggested that ML approach can provide valuable knowledge for identification of the key interactions associated with agonism or antagonism of the ligands. Also, unlike other IFPs studies (Chan et al., 2019; Kooistra et al., 2015; Kooistra et al., 2016), this study provided to obtain AIFs. Therefore, our findings are promising to investigate interactions mediate agonism and antagonism at atomic level for other β 2-ARs and β 1-ARs.

On the other hand, computational applications to human β 1-AR have been limited due to the absence of the 3D structure (Beuming and Sherman, 2012; Ul-Haq et al., 2015). Previous computational studies have been used turkey β 1-AR and human β 2-AR structure as template to construct the homology model of human β 1-AR due to the high sequence similarity (Beuming and Sherman, 2012; Ul-Haq et al., 2015). One of these study (Beuming and Sherman, 2012) used only one inactive state template whereas the other one (Ul-Haq et al., 2015) used eight inactive state and two active state templates. Therefore, their studies can be developed using active state templates to investigate agonism and antagonism at human β 1-AR.

1.12. Experimental Studies of ligand binding to β 1 and β 2 Adrenergic Receptors

In 2010, Baker investigated the affinity and intrinsic efficacy of 31 β 1-, β 2-, and β 3-adrenoceptor agonists in order to determine subtype selectivity determinants by measuring whole-cell [^{3} H]-CGP 12177 radioligand binding and [^{3} H]-cAMP accumulation (Baker, 2010b). She observed that subtype selectivity of some agonists such as salmeterol and formoterol is more dependent on selective affinity for β 2 adrenoceptor compared to other agonists such as isoprenaline. On the other hand, salmeterol, formoterol and isoprenaline had comparable intrinsic efficacy values for three receptor subtypes. She found subtype selectivity of several ligands such as denopamine for β 1; Z40140d, clenbuterol, and salbutamol for β 2 is highly dependent on intrinsic efficacy. This study demonstrated that subtype selectivity of agonists is dependent on both selective affinity and selective intrinsic efficacy. Moreover, in the same year, Baker revealed that the highest similarity of any of the turkey β -ARs to human β -ARs is between the turkey β 3C-receptor and the human β 2-AR (Baker, 2010a). In 2015, a mutagenesis study was conducted in order to reveal important amino acids of the human β 2-AR for high affinity and selectivity of agonist salmeterol (Baker et al., 2015). For affinity measurements, whole-cell [^{3} H]-CGP12177 radioligand binding was used while [^{3} H]-cAMP accumulation was measured to determine the functional effects of the mutations. They found that K305 in ECL3 and H296 in TM6 are two most important residues in salmeterol's binding. Additionally, for all agonists, Y308 in TM7 was found to be important for binding. On the contrary, F194 in ECL2 and R304 in ECL3 did not have noticeable effect on the binding of salmeterol to human β 2-AR. Also, they observed that intrinsic efficacy and duration of action of salmeterol did not change with mutations. This study demonstrated that amino acids in extracellular loops and transmembrane regions of

human β 2-AR play important roles in high affinity and selectivity of agonist salmeterol. Furthermore, other mutagenesis study published in 2014, demonstrated that the importance of L195 and W199 in TM4 region for low affinity state of human β 1-AR (Baker et al., 2014).

In 2022, Sykes et al. published the radioligand binding assays to study the β 1-AR binding kinetics of several clinically relevant β 1/ β 2-AR using [^{3} H]-DHA for labelling. They revealed that the hydrophobic properties of a molecule directly affect its kinetic association rate (k_{on}) and affinity for the β 1-AR. Moreover, they demonstrated that the potential role kinetics plays in the on-target and off-target pharmacologically of clinically used β -blockers (Sykes et al., 2022).

In addition to radioligand binding assays, in recent years, BRET assays have been applied to human β 1-AR and β 2-AR. One study investigated the ligand binding characteristics of three fluorescent ligands to human β 1-AR using NanoBRET assay. They demonstrated NanoBRET assay can be applied to human β 1-AR to study ligand-receptor interactions. Nevertheless, they highlighted the importance of ensuring both the fluorescent probe and competing ligands are in true equilibrium before interpretations regarding probe dependence can be made (Soave et al., 2016). Similarly, another study focused on human β 2-AR to characterise the ligands using a fluorescent analogue of the β -adrenoceptor antagonist propranolol in NanoBRET assay (Stoddart et al., 2016). In 2021, TR-FRET assay was applied successfully to human β 2-AR to show the functional solubilization of the receptor (Harwood et al., 2021).

1.13. Aim of Thesis

Due to the significant role of β 1-AR and β 2-AR in the cardiovascular system, and the need to design more selective drugs with improved signalling profiles to address asthma and cardiovascular co-morbidity problem, identifying the key ligand-receptor interactions is crucial step to design of new agonist and antagonist ligands (Baker and Wilcox, 2017; Barisione et al., 2010; Bennett et al., 2021; Harrington, 2021; Jiménez-Rosés et al., 2022; Oliver et al., 2019; Wacker et al., 2017; Zolotareva et al., 2019). As mentioned above, in the past, large scale docking studies have been widely performed against human β 2-ARs and turkey β 1-ARs. However, for human β 1-AR, computational studies focused on the homology modelling of the human β 1-AR structure (Beuming and Sherman, 2012; Ul-Haq et al., 2015). Up to date, the mechanism underlying factors determining agonism and antagonism has not been investigated at atomic level for human β 1-AR via large scale docking. Being able to identify which atoms of the ligand mediate agonist and antagonist provide valuable molecular insights into the design of drug candidates for human β -ARs. Therefore, using same publicly available ligand dataset with known activity on β -ARs and computational approach (docking, AIFs and ML) in our previous study (Jiménez-Rosés et al., 2022), we decided to compare the results for human β 1-ARs and human β 2-ARs. In addition, in order to develop a detailed understanding of interactions between human β 1-AR and known four β -blockers (Nebivolol, Carvedilol, Bisoprolol and Esmolol) and ligand residency time, we studied their binding kinetics in living cells. Fluorescent based assays are now alternative to expensive, time consuming, hazardous and heterogenous radioligand binding assays and their application to another GPCRs needs optimization to characterize the ligands. Up to date, TR-FRET

assays have not been applied to human β 1-AR for characterization of ligands. Therefore, we decided to develop a TR-FRET based assay to understand interactions between human β 1-AR and four known β -blockers. Furthermore, we used computational approaches including docking and AIFs to complement experimental ligand binding kinetics to understand whether specific residues are linked to binding kinetic rate constants of these antagonists at human β 1-AR.

This main aim of this Doctoral Thesis is to investigate the molecular basis for ligand pharmacological activity on β -adrenoceptors. To this end, **Chapter 3** identifies specific and common determinants of ligand pharmacological activity on β 1-ARs and β 2-ARs using docking and ML. Particularly, this chapter will attempt to **(1)** determine the underlying factors mediating agonism and antagonism for human β 1-AR at atomic level, **(2)** explore the atomic interactions between ligand and the human β 1-AR responsible for their pharmacological properties, **(3)** reveal the which atomic interactions determine the agonism or antagonism at human β 1-Ars and **(4)** investigate the similarities and differences between human β 1-AR and β 2-AR. **Chapter 4** focuses on the ligand binding kinetic studies of the human β 1-adrenoceptor via Time-Resolved Fluorescence Resonance Energy Transfer (TR-FRET) approach and key interactions between the ligands and receptor via computational approaches. Specially, this chapter will attempt to **(1)** characterize the optimal fluorescent tracer for determination of kinetic binding parameters of unlabelled ligands for human β 1-AR, **(2)** develop a reliable method for characterization of binding kinetic properties at human β 1-AR, **(3)** determine the kinetic binding parameters of selected ligands, **(4)** predict the correct ligand binding poses and determine the atomic interactions of these four ligands for human β 1-AR and **(5)** investigate whether a connection between the

atomic interactions and the kinetic binding parameters of the ligands for human β 1-AR.

Chapter 2. Materials and Methods

2.1. Materials

Dulbecco's Modified Eagle Medium (DMEM), Hank's Balanced Salt Solution (HBSS), 5'-Guanylyl imidodiphosphate (GppNHp), Pluronic acid, HEPES solution (1M), Bovine Serum Albumin (BSA), DMSO, cell dissociation non-enzymatic solution was purchased from Sigma-Aldrich. 384-well Optiplates plates were purchased from Perkin Elmer. SNAP-Lumi4-Tb and LABMED Tag-lite labelling medium were purchased from Cisbio Bioassays. OptiMEM, Blasticidin HCL 10 mg/ml, Trypsin EDTA (0.25%) were purchased from Gibco. Zeocin was purchased from Invitrogen. β -AR compounds: Alprenolol, Nebivolol, Carvedilol, Bisoprolol and Esmolol were purchased from Sigma-Aldrich.

2.2. Methods

2.2.1. Human β 1-AR Template Selection and Homology Modelling

The human β 1-AR amino acid sequence was obtained from the UniProt database Bairoch et al. (2005) with accession number P08588. From the structural points of view, the GPCR structure is more conserved than sequence. For that reason, in this study, we used the Template Selection Tool in GPCRdb (Pandy-Szekeres et al., 2018) to select active state structures as homology modelling templates for human β 1-AR by performing structure-based alignments. According to GPCRdb structure-based alignment, three active state crystal β -AR structures were closest templates for homology modelling of human β 1-AR: One template from turkey β 1-AR (PDB ID:

6H7N (Warne et al., 2018), 2.5 Å resolution), and two templates from human β 2-AR (PDB ID: 3SN6 Rasmussen et al. (2011), 3.2 Å resolution and PDB ID: 4LDE (Ring et al., 2013), 2.8 Å resolution) (**Table 1**). Moreover, the sequence similarity of these high-resolution crystal structures where the turkey β 1-AR was 51 % with human β 1AR whereas the human β 2-ARs having 54 % and 52 % sequence similarity, respectively (**Table 1**).

Table 1. Active State β -AR Structures for Homology Modelling of the Human β 1-AR

PDB ID	Receptor Name	Species	Sequence Similarity	Sequence Identity	Resolution Å
3SN6	β 1-AR	Human	54	35	3.2
4LDE	β 2-AR	Human	52	34	2.8
6H7N	β 1-AR	Wild Turkey	51	36	2.5

For 3SN6 PDB file, artefacts were observed at position M96T^{2x66} – receptor expression, M98T^{23x49} – receptor expression and N187E (ECL2) – glycosylation site. Some atoms of R63^{2x49}, K97N(ECL1), M98^{23x49}, W99^{23x50}, F101^{23x52}, K149^{4x41}, R175(ECL2), D192^{45x51}, F193^{45x52}, F194 (ECL2), T195 (ECL2), K267^{6x29}, H269^{6x31}, K270^{6x32}, L272^{6x34}, Q299^{6x61}, N301(ECL3), L302(ECL3), R304^{7x30}, E306^{7x32} and R333^{8x51} were missing in the 3SN6 PDB file (Zhou et al., 2019).

For 4LDE PDB file, artefacts were observed at position 1-15 (Expression tag) and 176-177 (Linker). Some atoms of K60^{1x59}, E62^{12x48}, K149^{4x41}, F223^{5x62}, Q224^{5x63}, Q231^{5x70}, K263^{6x25}, F264^{6x26}, K270^{6x32} were missing in the 4LDE PDB file (Zhou et al., 2019). Mutations were introduced in the construct at M96T^{2x66} – receptor expression, M98T^{23x49} – receptor expression, N187E (ECL2) – glycosylation site, C265A^{6x27} – other effect positions (Pandy-Szekeres et al., 2018; Zhou et al., 2019).

For 6H7N PDB file, artefacts were observed at position 1-5 (Expression tag) and 303-307 (Expression tag). Mutations were introduced in the construct at R68S^{1x59} – thermostabilising, M90V^{2x53} – thermostabilising, C116L^{3x27} – receptor-expression, F327A^{7x36} – thermostabilising, F338M^{7x48} – thermostabilising and C358A^{8x59} – palmitoylation-site.

After alignment step, the FASTA sequence of these three templates were retrieved from RCSB Protein Data Bank (PDB) (Berman, 2000). Before the homology modelling, the third intracellular loop (ICL3), N- and C- terminal of human β 1-AR amino acid sequence were removed. Then, the human β 1-AR sequence was aligned with the sequence of the crystal structures of the three templates using Jalview 2.11.1.0 Waterhouse et al. (2009) for each different template separately. After the alignment step, three different homology models of human β 1-AR were generated based on each these templates using MODELLER (Webb and Sali, 2016). Construction of these homology models of human β 1-AR were carried out before experimental crystal structures of human β 1-AR were released. After one year of our study, experimental crystal structures of human β 1-AR were publicly available. Therefore, the generated three models of human β 1-AR were then compared to recently resolved two experimental crystal structures of human β 1-AR.

2.2.2. Preparation of Experimentally Determined Human β 1-AR Structures for Molecular Docking

The 3D crystal structures of human β 1-AR bound to antagonist carazolol (PDB ID: 7BVQ) Xu et al. (2021) in the inactive state and to the agonist BI-167107 and nanobody 6B9 (PDB ID: 7BU7) Xu et al. (2021) in the active state were obtained from the PDB. Subsequently, for docking process, the endolysin from both structures and the nanobody from the active state of human β 1-AR were deleted.

Table 2. Active State and Inactive State Experimental Human β 1-AR Structures

PDB ID	Receptor Name	Species	State	Resolution Å	Publication
7BU7	β 1-AR	Human	Active	2.6	(Xu et al., 2020)
7BVQ	β 1-AR	Human	Inactive	2.5	(Xu et al., 2020)

2.2.3. Preparation of Ligand Dataset

A total of 2683 unique β -AR ligands were selected from ZINC (Irwin and Shoichet, 2004), ChEMBL (Mendez et al., 2019), DrugBank (Wishart et al., 2006), GPCRdb (Pandy-Szekeres et al., 2018) and Guide to Pharmacology (Armstrong et al., 2020). Then, Excel files containing all ligand SMILES (Simplified Molecular Input Line Entry Specification) strings (internal representation of the molecular structure) and their chemical properties were retrieved from these databases. 1317 of these ligands have known pharmacological activity whereas the other 1366 ligands with unknown pharmacological activity have been reported as binders. In this study, partial and full agonist ligands were categorized as agonist ligands while inverse agonists were classified antagonists. For each ligand, an internal ID was designated and more than 2500 ligands were these enumerated from 1 to 2683. For each ligand, internal ID,

InChIKey, SMILES string and pharmacological action (agonist/antagonist/binder) were determined. For the conversion of ligand SMILES strings to International Chemical Identifier key (InChIKey), Open Babel software v3.1.1. software (O'Boyle et al., 2011) was used. Via Open Babel, duplicate molecules obtained from different databases were removed from the dataset and hydrogen atoms were added to each ligand at pH 7.4. Default stereoisomers/tautomers created by Open Babel was kept and only one single output molecule was generated for each ligand. For each ligand, physiochemical properties of the ligands were obtained. The SMILES representation of the ligands are shown in the **Appendix B**. For docking experiments, the 3D coordinates built from ligand SMILES strings via Open Babel v3.1.1. software (O'Boyle et al., 2011).

2.2.4. Molecular Docking

The semi-flexible molecular docking experiments of the studied ligands were carried out via AutoDock Vina software developed by Trott and Olson (2010) with default parameters. In semi-flexible molecular docking, ligands are flexible whereas receptor is rigid. To perform the molecular docking, firstly, the structures of the receptors and the ligands were converted into PDBQT format using UCSF Chimera developed by Pettersen et al. (2004). Secondly, the grid box was set to 22 x 22 x 32 Å around orthosteric binding site of β 1-AR by superimposing all receptor structures. After then, in the absence of human β 1-AR, all ligand structures were docked into the three homology models of human β 1-AR using AutoDock Vina. With the determination of crystal structures of human β 1-AR a few months ago, we expanded our study by docking the same ligand dataset into the two experimentally determined structures of human β 1-AR. For each ligand, a set of up to 10 possible poses were generated. As a

result of the molecular docking of 2683 ligands into the five β 1-AR structures, 125000 docking poses were generated.

2.2.5. Atomic Interaction Fingerprint Calculations and Filtering

Arpeggio software (Jubb et al., 2017) can be used to calculate interactions for homology models or docking poses. For this study the Arpeggio Python program was installed and run on MAC OSX. Then, the atomic receptor-ligand interaction fingerprints (AIFs) were calculated for all docking poses by running Arpeggio software (Jubb et al., 2017) via Docker (a software container platform). Firstly, all the interactions for all the poses were calculated and then, we applied a filter (explained in below) to eliminate wrong poses. Arpeggio calculates 13 different interatomic interaction types using the knowledge of atom type, distance and angle constraints. The interaction types are: Covalent, Van der Waals (VdW), Aromatic, Hydrophobic, Carbonyl, Polar, Weak Polar, Proximal, Ionic, Hydrogen Bond, Weak Hydrogen Bond, VdW Clash, Halogen Bond. It extracts nearest-neighbour atoms within a 5-Å radial cut off. Interactions between atoms are converted into binary format and stored as Structural Interaction Fingerprints (SIFts). SIFt is the binary representation of the presence or absence of special interactions between the ligand and the receptor's residues (Deng et al., 2004; Szulc et al., 2023).

In this particular study, before Arpeggio analysis, the python `clean_pdb.py` script provided from Arpeggio (<https://github.com/harryjubb/pdbtools>) was executed on the five human β 1-ARs in order to resolve a number of common errors in PDB files. After then, all ligand poses were combined with human β 1-ARs, obtaining the output files that were run in Arpeggio (Jubb et al., 2017). The Arpeggio output files, interatomic interactions were represented as binary indications but they do not include header

information for columns. Therefore, we modified these files and added headers for each columns to analyse the interactions easily. During cleaning process of the text in file, the 3D information of the structures were not modified. Only, the text part before atomic coordinates were removed and information related to each atom were extracted from original PDB files for analysis.

Subsequently, Arpeggio output files were analysed using Python programming language to exclude all irrelevant docking poses. The majority (CA 97%) of β 2-AR ligands possess a prevalent β -hydroxyamine motif interacting particular interactions with the receptor. Due to the structural similarity between β 1-ARs and β 2-ARs, we filtered the ligand poses including ionic contacts with D138^{3.32x32} residue and hydrogen bond with N363^{7.39x38} residue from Arpeggio outputs, as they are reported to be essentials for ligand binding. With filtering process, output files including two key interactions were separated from other output files. Therefore, the ligands do not contain β -hydroxyamine motif were eliminated.

2.2.6. Statistical Analysis

The frequencies of each atomic interaction were calculated using Python programming language. Then, the most frequently observed interactions at least 10% of all docking poses were extracted for further analysis. Common and unique interactions for agonist and antagonist ligands were identified. In the final step, Pearson's correlation coefficient (r) method was used in order to calculate pairwise correlations between the atomic interactions and pharmacological action for each human β 1-AR structure. Matthews correlation coefficient (MCC), accuracy and cut-off values were calculated for each dataset separately via Excel.

The MCC metric is described using below equation:

$$\text{MCC} = \frac{\text{TP} \times \text{TN} - \text{FP} \times \text{FN}}{\sqrt{(\text{TP} + \text{FP})(\text{TP} + \text{FN})(\text{TN} + \text{FP})(\text{TN} + \text{FN})}}$$

(Equation 1)

TP is the number of true positives, TN is the number of true negatives, FP is the number of false positives and FN is the number of false negatives. When the dataset is unbalanced, accuracy cannot be calculated correctly (Chicco and Jurman, 2020). In this study, the number of the agonists were higher than the number of the antagonists. Therefore, to solve the problems related to imbalance dataset, we calculated the MCC values for each structure. Plots and figures were generated with Excel and Prism 9 (GraphPad Software, San Diego, U.S.A.).

2.2.7. Machine Learning (ML)

Machine Learning models were trained and validated using Categorical Boosting (CatBoost) classifier (Prokhorenkova et al. 2018). In this study, for each structures, filtered datasets were analysed. To train the CatBoost classifier, we used labelled the dataset including ligand pharmacological activity knowledge. As input, Excel files containing ligand ID number, ligand pose number, interacting residues of the receptor, interacting atom type of the ligand and interaction type were used for agonists and antagonists. Presence of the specific interaction were labelled as 1 whereas absence of these interaction were labelled as 0. CatBoost is effective for handling of categorical variables in the dataset (Prokhorenkova et al. 2018). Before training the classifier, the

dataset were separated into training and test datasets. After then, supervised ML approach was applied to the training datasets to train the model and it was evaluated on the test datasets. Matthews correlation coefficient (MCC) was used as the performance metric for each structure to classify the ligands as agonist or antagonist. In final step, the most important atomic interactions were determined via Shapley Additive Explanations (SHAP) value method (Lundberg and Lee, 2017). Experiments were performed using Python packages and figures were generated with Prism 9 (GraphPad Software, San Diego, U.S.A.).

2.2.8. RMSD Calculations for 7TMs and binding site region

2.2.8.1. Ligand Binding Region Residues

Using Arpeggio Jubb et al. (2017), we identified binding region residues of the active state human β 1-AR (PDB ID 7BU7) as follows: I118^{2.64x63}, V119^{2.65x64}, W134^{3.28x28}, T135^{3.29x29}, D138^{3.32x32}, V139^{3.33x33}, V142^{3.36x36}, T143^{3.37x37}, D217^{45.51x51}, F218^{45.52x52}, S228^{5.42x43}, S229^{5.43x44}, S232^{5.46x46}, W337^{6.48x48}, F340^{6.51x51}, F341^{6.52x52}, N344^{6.55x55}, R357^{7.33x32}, D356^{7.32x31}, F359^{7.35x34}, V360^{7.36x35}, N363^{7.39x38}, W364^{7.40x39} and Y367^{7.43x42}.

2.2.8.2. 7 TM Residue Ranges

In this study, the seven transmembrane (7 TM) regions are defined in **Table 3**:

Table 3. 7 TM residue range for comparison with active state experimental human β 1-AR (PDB ID: 7BU7) or the inactive state experimental human β 1-AR (PDB ID: 7BVQ).

	PDB ID: 7BU7 or 7BVQ	hm3SN6	hm4LDE	hm6H7N
TM1	54 - 86	55 - 86	54 - 86	61 - 86
TM2	91 - 122	91 - 122	91 - 122	91 - 122
TM3	127 - 162	127 - 162	127 - 162	127 - 162
TM4	171 - 197	171 - 197	171 - 197	171 - 197
TM5	221 – 256 / 221-260	221 - 260	221 - 256	221 - 260
TM6	319 - 350	316 - 350	314 - 350	315 - 350
TM7	355 - 379	355 - 379	355 - 379	355 - 379

2.2.8.3. Protein structure RMSD Calculations

Calculations of RMSD of 7TM regions for modelled structures from the experimental structures were performed after superposition of Carbon alpha ($C\alpha$) of the residues in each TM regions using PyMol (Schrödinger). For calculations of RMSD of binding site region, 24 important ligand binding site residues (listed in above) of homology models and experimental structures of human β 1-AR were superposed via PyMol and RMSD values were calculated.

2.2.9. Computational Experiments of Four Selected Ligands for Human β 1-AR

Semi-flexible molecular docking experiments with homology model of human β 1-AR, active state experimental structure of human β 1-AR and inactive state experimental structure of human β 1-AR were performed to reveal the most important atomic interactions of Nebivolol, Carvedilol, Bisoprolol and Esmolol for human β 1-AR, we performed using Audock Vina (Trott and Olson, 2010). Five independent docking experiments were carried out for each receptor structure, Firstly, we calculated the RMSD between 9 ligands in known 15 experimental β -ARs (Appendix Table A1) and the docked version of the same ligands obtained in **Chapter 3** to find suitable poses bound to homology model of human β 1-AR and experimental human β 1-ARs for analysing binding poses of Nebivolol, Carvedilol, Bisoprolol and Esmolol. This calculation was performed via an open source python code which is named isoRMSD.py measures RMSD differences between two conformation with different atom names (<https://github.com/OutOfcontrol/isoRMSD/blob/master/isoRMSD.py>). Then, we checked ligand binding poses having optimal RMSD using Pymol again and we observed that this code accurately detected best ligand binding poses. Thus, in addition to known experimental turkey β 1-ARs and human β 2-ARs, we obtained best binding poses of 9 known ligands bound homology model human of β 1-AR and experimental human β 1-ARs to compare Nebivolol, Carvedilol, Bisoprolol and Esmolol bound human β 1-ARs. After then, we tried to predict possible correct ligand binding poses of Nebivolol, Carvedilol, Bisoprolol and Esmolol and their contacts with the receptor residues using these β -AR structures.

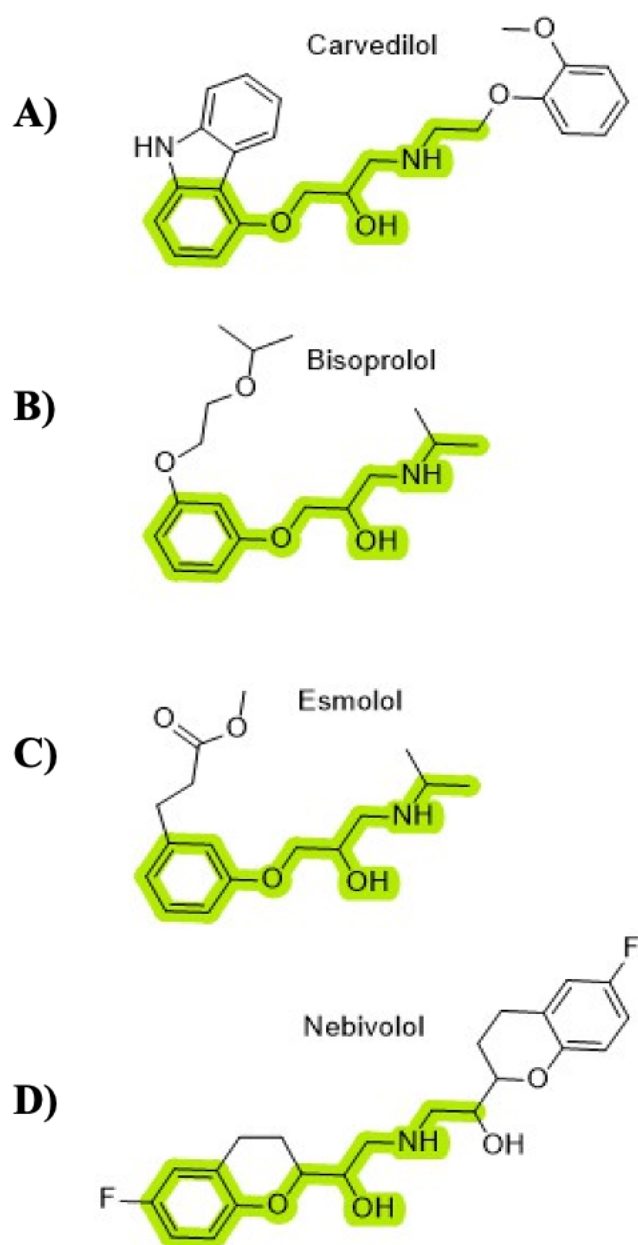


Figure 14. Ligands used in both computational and experimental studies in **Chapter 4**. A) Carvedilol B) Bisoprolol C) Esmolol D) Nebivolol. The common parts of the four ligands were represented as green colour.

2.2.10. Primer Design and Polymerase Chain Reactions (PCR)

To construct the pcDNA4TO-TS-SNAP- β 1-AR, the first 24 amino acids were deleted from β 1-AR sequence and the sequence between 25. and 477. amino acids were inserted to sequence of the pCDNA4 via Serial Cloner. Then, primers were designed using AAscan PCR cloning software (Sun et al., 2013) and primer sequences were shown in **Table 4**.

Table 4. Forward and reverse primers for Polymerase Chain Reactions (PCR)

Forward Primer (SNAP - β2-AR)	TGTAAAAGCTTAAGTTTAAAAAGGCTCGAGTCTAGAGG
Reverse Primer (SNAP - β2-AR)	GCCGCGCCGGTACCTGCAGGACCCAGCCCAG
Forward Primer (β1-AR)	CAGGTACCGGCGCGGCCACCGCGGCGCGGCTG
Reverse Primer (β1-AR)	AACTTAAGCTTTTACACCTTGGATTCCGAGGCGAAGC

After obtaining primers, two fragments (insert and backbone) were made by performing Polymerase Chain Reactions (PCR). SNAP was obtained from the SNAP- β 2-AR and β 1-AR was amplified for Gibson assembly experiments. The following reagents are mixed on ice into 200 μ L PCR tubes (**Table 5**).

Table 5. Reagents for PCR experiments

Insert PCR mix (β1-AR)	Backbone PCR mix (SNAP-β2-AR)
1 μ L Forward Primer	1 μ L Forward Primer
1 μ L Reverse Primer	1 μ L Reverse Primer
1 μ L Insert DNA	1 μ L Backbone DNA
7 μ L Deionised Water	7 μ L Deionised Water
10 μ L Primestar HS Polymerase Master Mix	10 μ L Q5 Polymerase Master Mix
Total Volume = 20 μL	Total Volume = 20 μL

All PCR experiments were performed using PCR MAX-Alpha Cyclor 2: Initial polymerase activation at 98°C for 30 s, then 20 thermal cycles, each with denaturation at 98 °C for 10 s, annealing from 70 °C down to 67.5 °C at a 0.5 °C decrement each cycle, and elongation at 72 °C for 2 mins for backbone and 1 mins for insert, then 10 cycles each with denaturation at 98 °C for 10 s, annealing at 67.5 °C for 20 s, and elongation at 72 °C for 7 mins for backbone and 1.30 mins for insert, followed by a final elongation at 72 °C for 7 min 72 °C for 7 mins for backbone, 1.30 mins for insert and a hold at 10 °C.

2.2.11. Agarose Gel Electrophoresis

A 0.75% agarose gel was prepared by combining 0.375 g agarose powder and 50 mL 1xTAE buffer and microwaved until the agarose was completely dissolved. After mixture was cooled down to 50 °C for 5 min, 5 µL SybrSafe was added to the mixture to visualise the DNA under ultraviolet (UV) light. The agarose gel was then poured into a gel casting tray to form wells. After the gel was completely solidified, agarose gel was placed into a Fisherbrand™ Sub-Gel Midi Horizontal Gel Electrophoresis Unit and covered with 1xTAE buffer until wells were submerged. After preparing agarose gel, for each PCR product, a mixture containing 2 µL of PCR product, 2 µL of deionised water and 1 µL of 5xloading dye was prepared for electrophoresis. Firstly, for reference, 2 µL of GeneRuler™ 1kb DNA ladder was loaded to first well. Secondly, all mixtures were loaded to other wells from left to right of the gel. In final step of the loading process, DNA ladder was loaded to the next well. After loading the ladder and the mixtures, the gel was run at 90 Volt for 40 minutes using a Fischer Scientific nanoPAC-300P Power Supply (300 V, 400 mA, 60 W). The gel was analysed by comparing each band to the DNA ladder via Clare Chemical Research DR-45M Dark Reader Transilluminator.

2.2.12. DNA Purification

Methylated DNA templates were digested by adding 0.3 µL restriction enzyme DpnI to each PCR product in order to reduce background of the original DNA template. The reactions were incubated at 37 °C for 48 hr for DpnI digestion. After then, digested DNAs were purified using MinElute Reaction Cleanup Kit (Qiagen) following the manufacturer's directions. Once DNA purification was completed, concentration of each purified DNA was measured using a spectrophotometer.

2.2.13. Molecular Cloning via Gibson Assembly

The purified backbone DNA (SNAP) and insert DNA (β 1-AR) fragments were assembled in vitro via recombination-based molecular cloning method, also known as ‘Gibson Assembly’. For the study, 50 ng total amount DNA was used and molar ratio of insert: backbone was set as 7:1. The following reagents were mixed in PCR tube (Table 6):

Table 6. The amount of the reagents for Gibson Assembly

Reagents
0.26 μ L Backbone DNA (SNAP)
0.47 μ L Insert DNA (β 1-AR)
1.77 μ L Deionised Water
7.5 μ L Gibson Assembly Mix
Total Volume = 10 μL

Gibson Assembly mixtures were then incubated at 50 °C for 15 mins followed by 45°C for 1 hr using PCR MAX.

2.2.14. Cell Transformation

In the beginning of the cell transformation, all equipment was sterilised using 70% ethanol and chemically competent *Escherichia coli* Top10 cells were thawed on ice. The mixture for cell transformation was prepared by adding 2 μ L of assembled DNA fragments to 20 μ L of chemically competent *Escherichia coli* Top10 cells in PCR tube and the mixture was incubated on ice for 20 mins. Then, the cells were firstly heat shocked 42 °C for 30 s using PCR MAX and put back on ice for 2 mins. In final step, the transformed cells were spread onto Luria-Broth (LB) agar plate containing 100 μ g/mL carbenicillin and incubated at 37 °C for 16 hr.

2.2.15. Colony Selection

Next day, after transformation, six cell colonies were selected from the LB agar plate using sterile pipette tips and the tips with bacteria on it were into the cell culture tubes containing 5 mL liquid LB and 0.5 μ L carbenicillin (100 μ g/mL). After then, the bacterial cultures were incubated at 37 °C and 220 rpm for 18 hr in a Stuart SI600 Large Shaking Incubator.

2.2.16. Plasmid DNA Purification and DNA Sequencing

The bacterial cultures were centrifuged at 4122g for 30 min in ThermoFisher Multifuge X3 F3 to obtain pellet of cells. After then, the plasmid DNAs were isolated from bacterial cultures using a QIAprep Spin Miniprep Kit (Qiagen) following the manufacturer's directions. Once isolation protocol was completed, the concentration of the purified plasmid DNAs was determined via a spectrophotometer. In final step, 700 ng total amount DNA was mixed with two different DNA sequencing primers (BGHR and SNAPf) in a PCR tube for each sample and then the samples were sent to GENEWIZ© for DNA sequencing.

2.2.17. Cell Culture

HEKTR cells expressing the β 1-AR were cultured in high glucose Dulbecco's Modified Eagle's Medium (DMEM) supplemented with 10 % foetal bovine serum (FBS), 5 μ g/ μ L blasticidin and 20 μ g/ μ L zeocin. All cells were grown in 75 cm² tissue culture flasks (T75) at 37° C and 5 % CO². When the cell confluency reached to 80 %, cells were passaged to new flasks using cell culture techniques. To perform the cell passaging, medium was aspirated from the flasks and firstly cells were washed with 10 ml of Phosphate Buffer Saline (PBS). After aspiration of the PBS, the cells were

detached from the flasks with 1 ml of Trypsin-ethylenediaminetetraacetic acid (Trypsin-EDTA). Then, cells were resuspended in 9 ml of DMEM and 0.5 ml of the cell suspension were added to a new flask containing 15 ml of DMEM. After adding antibiotics, the flasks were incubated at 37°C and 5 % CO². Remaining cell suspension were added to a falcon tube and cells were centrifugated for 3 min at 400 rpm. After centrifugation, supernatants were aspirated, and cell pellets were frozen at -80 °C. pcDNA4TO-TS-SNAP-β1-AR was transfected into HEK293-TR using polyethylenimine (PEI). By adding 5 µg/µl blasticidin and 20 µg/µl zeocin, stable cell line was generated. Stable cell lines were maintained in high glucose DMEM with 10% fetal bovine serum (FBS), 5mg/mL blasticidin and 20mg/mL zeocin, at 37 °C. and 5% CO². After one week, to obtain large number of cells for ligand binding assays, HEKTR cells expressing the TS-SNAP-β1-AR were passaged to 175 cm² tissue culture flasks (T175). When the cell confluency reached to 70 %, to induce TS-SNAP-β1-AR expression, 40 µl tetracycline (1 µg/ml) were added to the flasks 48 h before labelling.

2.2.18. Terbium Labelling of SNAP tagged β1-AR cells

HEK293 cells stably expressing SNAP-β1 were cultured in T175 flasks using DMEM supplement 10 % FBS and the selection antibiotics (blasticidin and zeocin). The receptor expression was induced by addition of tetracycline (1 µg/ml) to the cell culture when the cells had reached 80% confluency to induce receptor expression prior to labelling with terbium. After 48 h of tetracycline addition, medium was aspirated from the flasks, and the cells were firstly washed with 5 ml of PBS and then washed again with 5 ml of Tag-lite labelling medium (LABMED). After washing steps, 10 ml

LABMED containing 100 nM Lumi4-Tb was added to flasks and incubated for 1 h at 37 °C under 5 % CO₂ to label receptor with terbium cryptate (FRET donor).

2.2.19. Membrane Preparation

Cell pellets were thawed on ice and resuspended in 20mL Buffer B. The suspensions were homogenised using 6 x 1 sec pulses of a Polytron tissue homogeniser (Werke, Ultra-Turrax) and subsequently centrifuged at 48.000g at 4 °C for 30 min. The supernatant was discarded and the pellet, resuspended and centrifuged as explained above. The final pellet was resuspended in Buffer C. Protein concentration was determined using the bicinchoninic acid assay kit (Sigma-Aldrich), using BSA as a standard with membrane aliquots maintained at -80 °C for ligand binding assays.

2.2.20. TR-FRET Ligand Binding Assays

All TR-FRET ligand binding experiments were performed in 384 well OptiPlates using assay binding buffer and non-selective β 2-AR antagonist alprenolol was preferred to determine non-specific binding (NSB). In the final step, membranes in assay binding buffer containing GppNHp were added to plates to dissociate G proteins that may be stabilising the high-affinity state of the receptor and the plates were incubated at room temperature for 30 mins prior to signal detection. For the characterization of fluorescent ligands, S-propranolol-red and S-propranolol-green, (Hello Bio, UK, cat no. HB7817 and HB7816, respectively), signal detection measurements were performed in PHERAstar FSX (BMG Labtech, Offenburg, Germany) using standard HTRF filter settings. After characterization of the kinetic binding parameters of fluorescent ligands, competition binding assays were conducted using optimal tracer green propranolol.

2.2.21. Data Analysis of Experimental Data

All experimental data were analysed by non-regression using Prism 9 (GraphPad Software, San Diego, U.S.A.). Firstly, the fluorescent ligand (tracer) association data were globally fitted to the Equation 2 to determine the binding kinetic parameters of the tracer.

$$k_{\text{ob}} = [L] \cdot k_{\text{on}} + k_{\text{off}} \quad \text{(Equation 2)}$$

which in, k_{on} is the association rate constant of the tracer ($\text{M}^{-1} \text{min}^{-1}$), k_{off} is dissociation of the tracer (min^{-1}) and L is the concentration of fluorescent ligand (nM).

Secondly, association and dissociation rate constants of unlabelled ligands were determined using Motulsky–Mahan model (Motulsky and Mahan, 1984). Data from competition kinetic experiments globally fitted to the Equation 2 :

$$K_A = k_1[L] + k_2$$

$$K_B = k_3[I] + k_4$$

$$S = \sqrt{((K_A - K_A)^2 + 4 \cdot k_1 \cdot k_3 \cdot L \cdot I \cdot 10^{-18})}$$

$$K_F = 0.5 * (K_A + K_B + S)$$

$$K_S = 0.5 * (K_A + K_B - S)$$

$$Q = \frac{B_{\text{max}} * K_1 * L * 10^{-9}}{K_F - K_S}$$

$$Y = Q \cdot \left(\frac{k_4 \cdot (K_F - K_S)}{K_F \cdot K_S} + \frac{k_4 - K_F}{K_F} \exp^{(-K_F \cdot X)} - \frac{k_4 \cdot K_S}{K_S} \exp^{(-K_S \cdot X)} \right)$$

(Equation 3)

where, k_1 is the k_{on} of the tracer ($M^{-1} min^{-1}$), k_2 is k_{off} of the tracer (min^{-1}), k_3 is the k_{on} of the unlabelled ligand ($M^{-1} min^{-1}$), k_4 is k_{off} of the unlabelled ligand (min^{-1}), L is the concentration of the tracer used (nM), I is the concentration of the unlabelled ligand (nM), X is the time (min) and Y is the specific binding (nM).

Chapter 3. Discovering specific and common determinants of ligand pharmacological activity on β 1- and β 2-adrenergic receptors using docking and machine learning

3.1. Introduction

As the largest and most diverse most family of membrane proteins in the human genome, G-protein coupled receptors (GPCRs) play an important role in cellular signalling by transducing a variety of different external signals to the interior of the cell (Lappano and Maggiolini, 2011; Rosenbaum et al., 2009). Due to their association with numerous human diseases, GPCRs are targeted by almost 34% of approved drugs (Deganutti et al., 2019; Hauser et al., 2017; Yang et al., 2021).

From the GPCR structure-based drug design points of view, understanding the structural basis of GPCR drug selectivity is critical to develop new compounds to target a specific receptor (Congreve et al., 2011; Jozwiak and Plazinska, 2021; Lundstrom, 2009; Weis and Kobilka, 2018; Yang et al., 2021). As a result, there has been great interest in the understanding of GPCRs structurally and computationally (Lee et al., 2018; Rosenbaum et al., 2009). In 2007, the determination of the first crystal structures of the ligand-activated human GPCR β 2-adrenoceptor (Cherezov et al., 2007; Rasmussen et al., 2007; Rosenbaum et al., 2007) provided the important knowledge about structural perspective, revealing that all GPCRs share a common 3D structure, consisting of extracellular N-terminal region, intracellular C-terminal region and seven transmembrane (TMs) helices interconnected by three intracellular (ICL1, ICL2 and ICL3) and three extracellular (ECL1, ECL2 and ECL3) loops (Deganutti et

al., 2019; Gacasan et al., 2017; Kobilka, 2007b; Kobilka, 2011; Palczewski et al., 2000b; Rasmussen et al., 2011)).

Since the discovery of β -blockers by Sir James Black more than 60 years, β -adrenoceptors (β ARs) belonging to class A G-protein coupled receptor (GPCR) family have become important therapeutic target for the treatment of cardiovascular and respiratory diseases (Baker et al., 2011; Bristow, 2011; Cazzola et al., 2011). β 1-ARs and β 2-ARs are highly structurally similar GPCRs and activated by endogenous catecholamines epinephrine and noradrenaline. However, they perform different functions in different tissues. Due to the significant role of β 1-AR and β 2-AR in the cardiovascular system, identifying the key ligand-receptor interactions is crucial step to design of new agonist ligands. Since 2007, there has been significant progress in structural studies of GPCRs, as for example the demonstration that GPCR ligands govern GPCR activity by altering their conformations (Deupi and Kobilka, 2007; Kobilka and Deupi, 2007; Weis and Kobilka, 2018). Nonetheless the underlying factors that determine ligand selectivity at β 1-AR and β 2-AR are still an open fundamental question in GPCR structure-based drug design.

When we commenced our investigation on August 2020, there were 24 turkey β 1-AR and 34 human β 2-AR crystal structures in the Protein Data Bank (PDB) (Berman, 2000) to select suitable templates for homology modelling of the human β 1-AR structure. Therefore, in the absence of the experimental structure of human β 1-AR, until December 2020, turkey β 1-AR and human β 2-AR crystal structures have been used as templates for homology modelling of human β 1-AR due to the high sequence similarity (Beuming and Sherman, 2012; Ul-Haq et al., 2015). Although, findings obtained from these previous homology modelling studies have provided useful

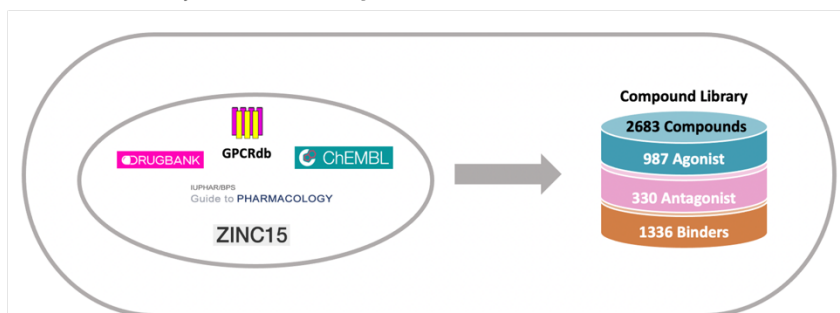
knowledge to understand ligand-human β 1-AR interactions, the underlying factors determining β 1-AR-ligand interactions at atomic level still not clearly understood. With the determination of the active and inactive state of human β 1-AR crystal structures (PDB ID: 7BU7 and 7BVQ, respectively) in 2021 by Xu et al. (2021) 3D structures have become available to investigate the structural basis of ligand selectivity for human β 1-AR.

In our latest publication (Jiménez-Rosés et al., 2022), we have successfully identified specific residues of the human β 2-AR and common atomic interactions with the ligands which exert pharmacological actions of agonism and antagonism. This was achieved by docking of 2683 known β -AR ligands, calculating atomic interaction fingerprints (AIFs) and applying Machine Learning (ML) approach. Therefore, the study motivated us to apply the same methodology to homology models and experimental structures of the human β 1-AR. However, it is not clear to what degree the observation made for β 2-AR would translate to the closely related β 1-AR and whenever the residues mediating the agonism are the same or different in two receptors. Therefore, here, we have asked is whether the ligands have common or specific interactions with β 1-AR to exert their pharmacological actions on them.

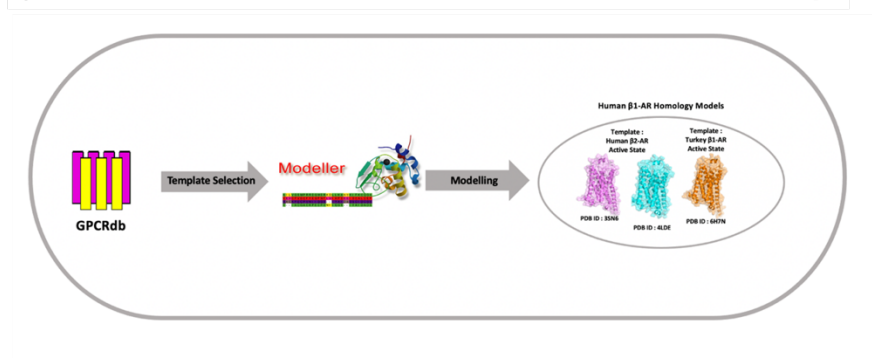
In this study, we focused on the molecular docking of a large dataset of different ligands with known pharmacological activity at β -ARs into a homology model of human β 1-AR and two experimental human β 1-AR structures in order to investigate the structural basis of ligand selectivity (**Figure 15**). For this aim, firstly, homology models of the human β 1-AR were built based on the three active state β 1-AR structures. Secondly, 2683 known β -AR ligands were docked into the three homology models and two experimental structures. Thirdly, atomic receptor-ligand interaction

fingerprints (AIFs) were calculated for all 125000 docking poses to investigate whether common interacting atoms within the ligand binding region. We have found that in general both experimentally determined structures and the homology models yielded the similar results and that the key mediators of agonism and antagonism are the similar in these two receptors using statistical analysis and ML approaches. However, we also identified specific differences between β 1-AR and β 2-AR that could be exploited to design selective for one or the other receptor.

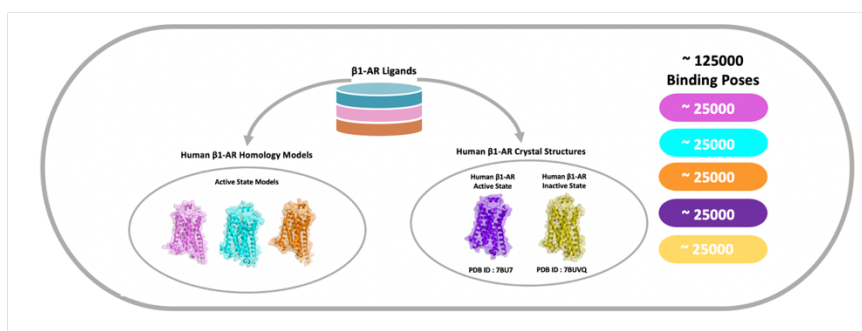
1) DATASET OF β 1-ADRENOCEPTOR LIGANDS



2) TEMPLATE SELECTION and HOMOLOGY MODELLING OF HUMAN β 1-AR



3) MOLECULAR DOCKING - AutoDock Vina



4) ATOMIC INTERACTIONS - ARPEGGIO

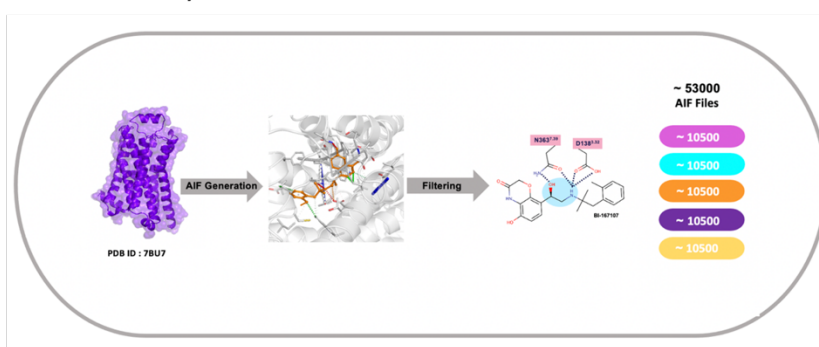


Figure 15. Workflow of the study. (1) Source of β 1-AR ligands available at open access repositories which comprise our 2683 compound dataset. (2) Template selection was performed via GPCRdb and three homology models of human were generated using MODELLER. (3) Molecular docking of β 1-AR ligands into three homology models of human β 1-AR and two experimental structures of human β 1-AR was performed via Autodock Vina (4) Interatomic interaction fingerprint (AIF) were calculated using Arpeggio.

3.2. Results and Discussion

3.2.1. Comparison of Homology Models with Experimental Structures

In the beginning of the study, we decided to construct homology models for generating the 3D structure of the human β 1-AR because of the absence of the experimentally determined human β 1-AR structure. Template selection were performed via GPCRdb structure-based alignment (Pandy-Szekeres et al., 2018) and three different homology models of human β 1-AR were generated based on different active state templates (one Turkey β 1-AR template (PDB ID: 6H7N (Warne et al., 2018)) and two Human β 2-AR templates (PDB ID: 3SN6 Rasmussen et al. (2011) and PDB ID: 4LDE (Ring et al., 2013)) using MODELLER (Webb and Sali, 2016). After, the experimental structures of active (PDB ID: 7BU7) and inactive state (PDB ID: 7BVQ) human β 1-AR were resolved by Xu et al. (2021), we evaluated the structural accuracy of our homology models by performing structural analysis (**Figure 16**).

To investigate the structural similarities and differences between three different homology models and two experimental structures, we firstly compared each transmembrane (TM) regions using PyMOL (Schrödinger). For this aim, we calculated RMSD (Root Mean Square Deviation) of 7TM regions for modelled structures from the experimental structures after superposition of Carbon alpha ($C\alpha$) of the residues in each TM regions. As shown in **Figure 16A**, it is noteworthy that all RMSD values for 7TM regions of the three homology models are less than 2 Å compared with the active state experimental structure of human β 1-AR (PDB ID: 7BU7). Therefore, RMSD values ranging from 0.27 to 1.52 Å suggest that all homology models of human β 1-AR are in good agreement with active state experimental structure of human β 1-AR. In particular, for TM1, TM2, TM3, TM5 and

TM6 regions, the lowest RMSD values are achieved by modelled structure from turkey β 1-AR template (PDB ID: 6H7N). Notably, these findings revealed that modelled structure from active state turkey β 1-AR template has high structural similarity to the active state experimental human β 1-AR.

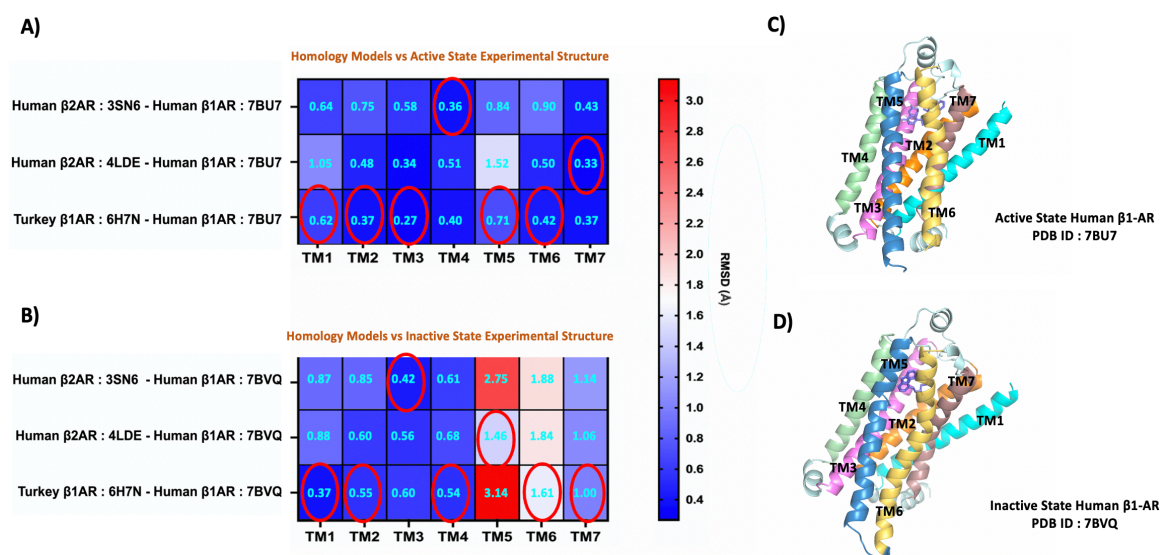


Figure 16. TM regions of experimental human β 1-ARs and TM RMSD calculations of homology models against experimental human β 1-ARs. (A) TM RMSD calculations of three homology models against experimental active state human β 1-AR. (B) TM RMSD calculations of three homology models against experimental inactive state human β 1-AR. Red circles represent the lowest RMSD values for each TM region. (C) TM regions of experimental active state human β 1-AR (PDB ID: 7BU7) (D) TM regions of experimental inactive state human β 1-AR (PDB ID: 7BVQ).

Similar to the structural comparison of our modelled structures to the active state experimental structure of human β 1-AR (PDB ID: 7BU7 Xu et al. (2021)), we measured RMSD values of 7TM regions for our modelled structures from the inactive state experimental structure of human β 1-AR (PDB ID: 7BVQ Xu et al. (2021)). As presented in **Figure 16B**, among the three homology models, only the modelled structure from human β 1-AR template (PDB ID: 4LDE) has a lower RMSD value, less than 2 Å for all TM regions. On the other hand, the most significant differences were observed in TM5 regions for the other two modelled structures having higher

RMSD (2.75 Å and 3.14 Å, respectively). In addition to TM5 region, TM6 exhibited larger RMSD differences for all three homology models. For TM6, the RMSD values from the inactive state experimental structure of human β 1-AR were observed in the range of 1.61 – 1.88 Å. On the contrary, for all three homology models, we found RMSD values for TM6 were lower than 1 Å with respect to active state experimental structure of human β 1-AR. Our results clearly revealed that TM5 and TM6 have important effect on the inactive state experimental structure of the human β 1-AR as state determinant. These findings are in line with the previous study (Hauser et al., 2021) demonstrating that toggle switch TM6 stabilizes only the inactive state whilst TM5 plays a significant role on GPCR activation as the other universal switch. Moreover, 7TM RMSD comparisons with respect to active and inactive state experimental human β 1-AR structures (**Figure 16A and 16B**) revealed that TM7 is the third functionally important region for the inactive state. This is consistent with previous homology model study showing TM5, TM6 and TM7 having slightly higher RMSD in the inner membrane side for most of the compared pairs of inactive GPCR structures (Mobarec et al., 2009). Based on the above structural analysis (**Figure 16A and 16B**), we concluded that active state turkey β 1-AR and human β 2-AR templates are more accurate starting structures for modelling of the active state human β 1-AR instead of modelling of the inactive state human β 1-AR.

To further elucidate the structural accuracy of our modelled structures, we compared protein structures in terms of binding site RMSD (**Figure 17A**). For this aim, we firstly attempted to identify which residues of active state human β 1-AR (PDB ID: 7BU7 Xu et al. (2021)) interact with ligand using Arpeggio (Jubb et al., 2017). These 24 important residues in the binding site of the active state human β 1-AR are as follows:

I118^{2.64x63}, V119^{2.65x64}, W134^{3.28x28}, T135^{3.29x29}, D138^{3.32x32}, V139^{3.33x33}, V142^{3.36x36}, T143^{3.37x37}, D217^{45.51x51}, F218^{45.52x52}, S228^{5.42x43}, S229^{5.43x44}, S232^{5.46x46}, W337^{6.48x48}, F340^{6.51x51}, F341^{6.52x52}, N344^{6.55x55}, D356^{7.32x31}, R357^{7.33x32}, F359^{7.35x34}, V360^{7.36x35}, N363^{7.39x38}, W364^{7.40x39} and Y367^{7.43x42} (**Figure 17B and 18**).

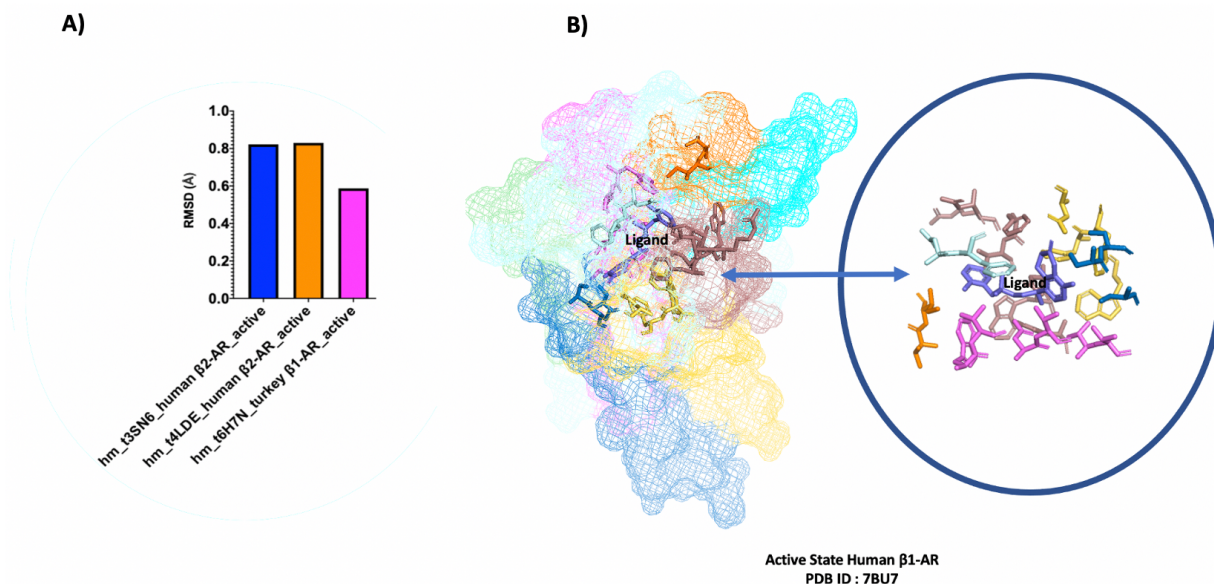


Figure 17. (A) RMSD comparisons for the 24 residues, calculated relative to the active state experimental human β1-AR structure (PDB ID: 7BU7) (B) 24 important binding site residues of active state human β1-AR.

Then, we calculated RMSD of these 24 important residues (**Figure 17A and 18**) in the binding site to select the best homology model for further analysis using PyMol (Schrödinger). In this study, three homology models were compared with the crystal structure of the active state human β1-AR. As shown in **Figure 17A**, the RMSD value (0.58 Å) of the homology model of human β1-AR generated from turkey β1-AR were lowest compared to the other two models (0.82 Å and 0.83 Å) generated from human β2-AR. Therefore, it is clear that the best template is active state turkey β1-AR (PDB ID: 6H7N) for homology modelling of active state human β1-AR.

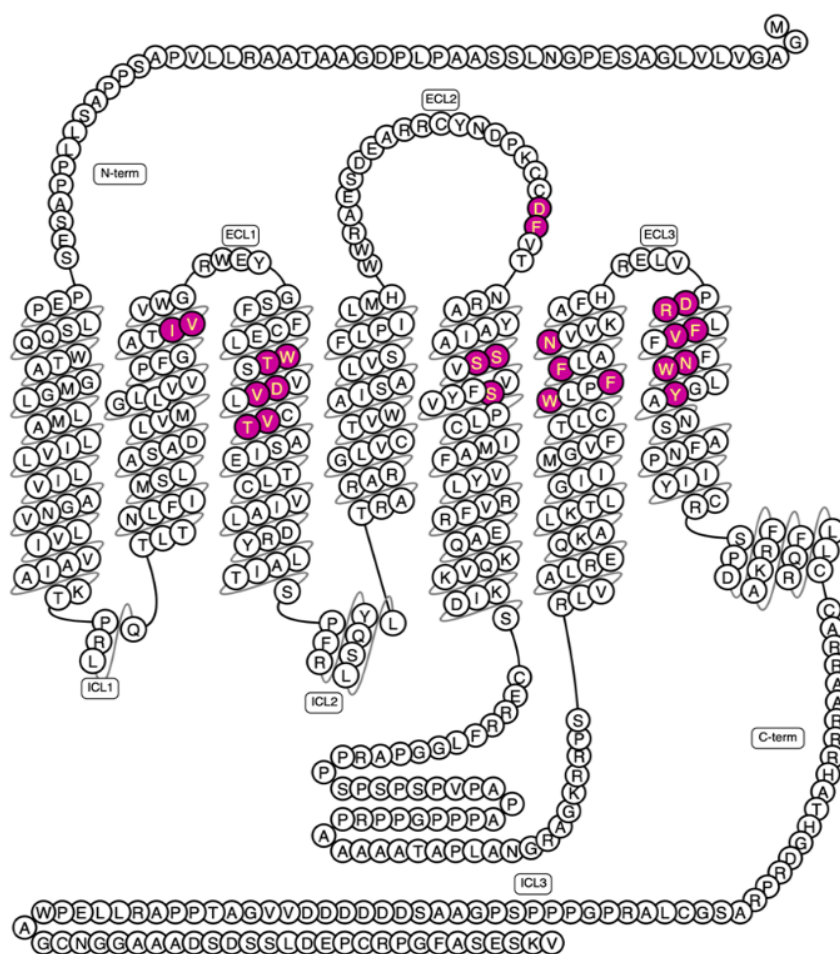


Figure 18. The snake map of 24 important binding site residues (magenta coloured) on active state experimental human β 1-AR (PDB ID: 7BU7) (Figure is generated via GPCRdb (Pandy-Szekeres et al., 2018))

As a result, based on the RMSD analysis of the modelled human β 1-AR structures (**Figure 16 and 17**), the structure of the active state turkey β 1-AR provides the more accurate basis for homology modelling studies of the human β 1-AR compared to the active state human β 2-AR structures. Therefore, among the three models, the modelled structure based on the turkey β 1-AR template was selected for molecular docking studies. As mentioned in previous sections, before experimental structures of human β 1-AR were released, we performed homology model studies. Then we expanded our study using the experimental structures. Due to the limited number of

experimental structure of human β 1-AR, we tried to find useful information using homology modelling of β -ARs for future studies. So, we compared the models and experimental structures and then we used them for further studies.

3.2.2. Identification of Key Interactions Mediate Agonism and Antagonism of Ligands

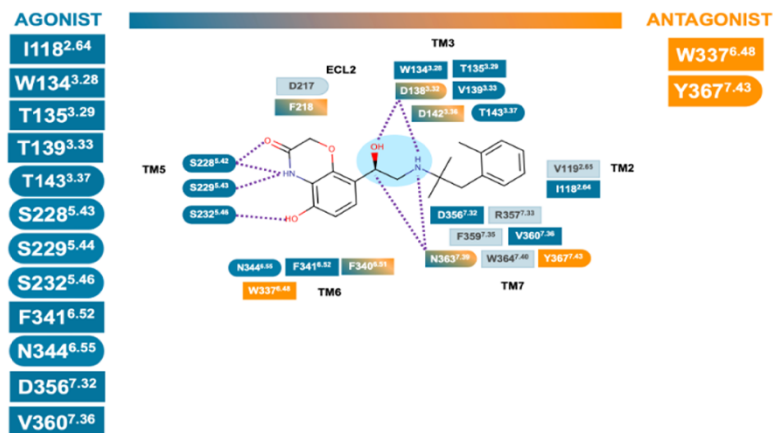
After the construction of the three human β 1-AR homology models and selection of the best homology model, we carried out molecular docking of known 2683 β -AR ligands into the best homology model and two experimental structures of the human β 1AR via Autodock Vina (Trott and Olson, 2010). For each structure, we obtained ~25,000 poses (totally ~125000 binding poses) from molecular docking. In order to investigate the ligand-receptor interactions for the three structures, we used each ligand binding poses to generate atomic interaction fingerprints (AIFs) via Arpeggio (Jubb et al., 2017). We calculated all inter-atomic interactions for each ligand binding pose, including the type of the non-covalent bond (proximity, ionic, hydrogen, hydrophobic, etc), the nature of the atoms (N, C, O, H, F) and the ID of the atoms. In total, we identified about 10,000 different interaction types that occurred in our dataset that were used for subsequent analysis.

In all existing crystallographic structures of β 1-ARs and β 2-ARs, the ligands occupy an identical binding site and adopt very similar binding poses. Importantly, the β -AR hydroxylamine motif that is present in ca 97% of all ligands in our dataset interacts with D113^{3.32x32} and N312^{7.39x38} in β 2-AR, and structurally equivalent to D138^{3.32x32} and N363^{7.39x38} in β 1-AR. For this aim, we extracted the ligand binding poses including ionic contacts with D138^{3.32x32} residue and hydrogen bond with N363^{7.39x38}

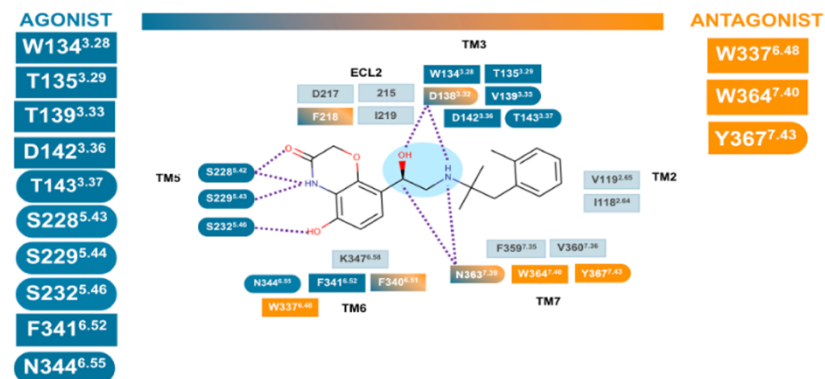
residue by applying filter to all docking poses of three human β 1-AR structures. This filtering process facilitated to analyse the interactions between human β 1-AR and ligands resulting in a reduction of the number of ligand binding poses (**Figure 15**).

To reveal the most important atomic interactions mediating pharmacological properties of ligands, we firstly performed statistical analysis on the filtered dataset using Pearson's pairwise correlation (**Figure 19**). In these figures, important residues and atomic interactions between ligands and the human β 1-ARs were coloured according to their pharmacological activity. Blue to orange colour indicates increasing antagonist properties of the interactions. In this study, BI-167107 ligand was selected to demonstrate atomic interactions between ligands and human β 1-ARs for adaptation of the presentation of figures to our previous study. The ethanolamine moiety of the BI-167107 ligands was highlighted in light blue. The blue coloured and orange coloured boxes corresponds to the important atomic interactions for agonism and antagonism, respectively. The residues involved in the interactions with both agonists and antagonists were displayed two coloured boxes (blue and orange). The shape of boxes represents the interaction types. The squared shape represents the hydrophobic and aromatic contacts, round shape represents the polar, ionic and hydrogen bond contacts, and the combination of both. Ionic and/or hydrogen bond contacts were displayed as dotted purple line. Interactions with residues on TM2, TM3, TM5, TM6, TM7 and ECL2 were grouped separately and displayed according to their regions. Therefore, from these figures, it can be seen the locations of interacting residues. Our statistical analysis on β 1-AR structures indicates that there are several common residues for homology model (**Figure 19A**), active state experimental structure (**Figure 19B**) and inactive state experimental structure (**Figure 19C**) of human β 1-AR.

A)



B)



C)

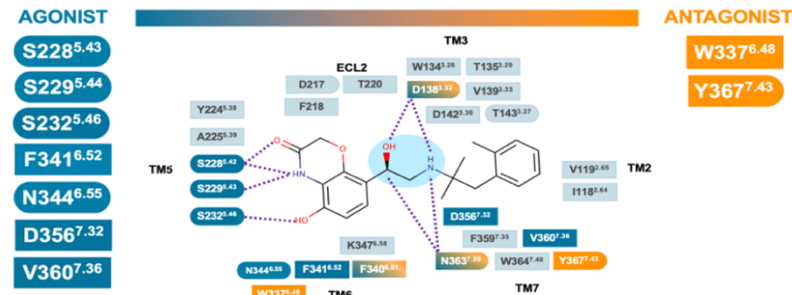


Figure 19. Schematic representation of the interactions predicted using the pairwise correlation approach. (A) AIF of best homology model of human β 1-AR (turkey β 1-AR template - PDB ID: 6H7N) (B) AIF of experimental active state human β 1-AR (PDB ID: 7BU7) (C) AIF of experimental inactive state human β 1-AR (PDB ID: 7BVQ) The type of interaction is summarised in squared shape for hydrophobic and aromatic contacts, round shape for the polar, ionic and hydrogen bond contacts, and the combination of both. The dotted purple line represents ionic and/or hydrogen bond contacts. The ethanolamine moiety of the BI-167107 ligands is highlighted in light blue.

We found that the most crucial agonist ligand interactions are aromatic/hydrophobic contacts with F341^{6.52x52} residue and ionic/polar/hydrogen bond contacts with S228^{5.42x43}, S229^{5.43x44}, S232^{5.46x461}, F341^{6.52x52}, and N344^{6.55x55} residues. On the other hand, aromatic/hydrophobic contacts with W337^{6.48x48}, Y367^{7.43x42} residues and ionic/polar/hydrogen bond contacts with Y367^{7.43x42} residue is the most significant interactions for the antagonist ligands. Although there are several residues in TM2 and TM3 contribute to ligand binding for active state homology model and active state experimental structure of human β 1-AR; for the inactive state experimental structure of human β 1-AR, the most important residues were only observed in TM5, TM6 and TM7. These findings confirmed the previous study displaying residues in TM5, TM6 and TM7 play important role for inactive state GPCRs (Mobarec et al., 2009). Also, our results revealing the effect of two universal switches, at the TM5 and TM6 which are consistent with the previous study (Hauser et al., 2021). As expected, the most representative interactions are similar for crystal structure of the active state human β 1-AR and the best homology modelled based on active state turkey β 1-AR. However, the AIF of the homology model of β 1-AR is different from the AIF of inactive state crystal structure of human β 1-AR. In 2008, inactive state β 2-AR structure was shown to be suitable not only for retrieving antagonists but also for identifying agonists with docking-based in silico screening methods (de Graaf and Rognan, 2008). More recently, another study (Scharf et al., 2019) suggested that different active state structures in molecular docking experiments can be effective for design and identification of agonists. On the other hand, they discovered one agonist from large scale docking against inactive β 2-AR structure. In addition, neutral antagonists/partial agonists can bind to both the active and inactive state of the receptor. Due to the

neutral antagonist/partial agonist nature of some ligands, ligand-receptor interactions can be analysed in both the active and inactive state. Taken together, our large-scale docking of agonists and antagonists to both inactive and active state human β 1-ARs can provide opportunity to discover new compounds and understand activation mechanism of the receptor.

Previously, we have shown for human β 2-AR that over a thousand ligands of diverse structures interact with a few specific residues of the receptor and form the same type of chemical bonds to exert their pharmacological action of agonism or antagonism (Jiménez-Rosés et al., 2022). Therefore, in order to investigate similarities and differences between AIFs of β 1-AR and AIFs of β 2-AR, we compared our findings for β 1-AR with our previous results obtained from β 2-AR structures (**Figure 20**).

For both subtypes, we found there are 5 important common residues. S228/203^{5.42x43}, S229/204^{5.43x44}, S232/207^{5.46x461} residues in TM5 make ionic/polar/hydrogen bond contacts with agonist ligands whereas antagonist ligands forms aromatic/hydrophobic contacts with W337/286^{6x48} in TM6 and ionic/polar/hydrogen contacts with Y367/316^{7x43} in TM7. . Hydrophobic interactions with W286^{6x48} of human β 2-AR were found be important for antagonists and inverse agonists compared to agonists by one MD study (Chan et al., 2016). 203^{5.42x43}, 204^{5.43x44} and 207^{5.46x461} have previously been identified as critical for agonist binding and receptor activation at human β 2-AR by mutagenesis studies (Sato et al., 1999; Strader et al., 1989)

However, considering all the interacting residues in binding site, we observed that the AIF of $\beta 1$ -AR is overall slightly different from AIF of $\beta 2$ -AR which it could be link to ligand selectivity. According to our findings, more residues in TM3 and TM6 especially F341^{6.52x52} and N344^{6.55x55} are important for $\beta 1$ -AR agonism but not for $\beta 2$ -AR, although these residues are conserved in both subtypes. In 2003, one study (Baker et al., 2003) demonstrated both F341^{6.52x52} and N344^{6.55x55} are crucial for high affinity binding of potent antagonist CGP 12177 and classic antagonist CGP 20712A for the ‘catecholamine’ site of the human $\beta 1$ -AR whereas this finding was not observed for binding of another antagonist propranolol. However, they observed mutations at F341^{6.52x52} and N344^{6.55x55} have any effect on the agonist actions of CGP 12177 at the secondary ‘CGP 12177’ site of the human $\beta 1$ -AR. It is not possible to generalize their observation obtained from agonist effect measurement of β -blockers to all agonists bind to human $\beta 1$ -AR. Existing experimental structures of the human $\beta 1$ -AR with bound agonists (Adrenaline (PDB ID : 7BTS), Noradrenaline (PDB ID : 7BU6), CHEMBL1615159 (PDB ID : 7BU7) and inverse agonist (Carazolol (PDB ID : 7BVQ) contact residue N344^{6.55x55} whereas only agonist CHEMBL1615159 do not interact with F341^{6.52x52}. On the other hand, there are no experimental human $\beta 1$ -AR bound antagonist to obtain detailed features of antagonist binding. Therefore, according to literature, it is less apparent whether F341^{6.52x52} and N344^{6.55x55} in TM3 play decisive role in agonism at human $\beta 1$ -AR. Furthermore, the other residue D138^{3.32x32} in TM3 and also N363^{7.39x38} in TM7 were previously reported as key residues for both agonism and antagonism at human $\beta 1$ -AR (Baker et al., 2003). Our results were also consistent with this finding, and we observed D138^{3.32x32} and N363^{7.39x38} are not specific determinants for agonism at human $\beta 1$ -AR.

To confirm the performance of the Pearson's pairwise correlation approach, we calculated the maximum Matthews Correlation Coefficient (MCC) which is described as the measure of the quality of binary classifications. The real interaction values in the [0:1] interval can be converted into zeros and ones using heuristic cut-off thresholds (Chicco and Jurman, 2023). According to cut-off values, predictions below cut-off values are considered as zeros and the predictions equal or above cut-off value are considered ones. In the present study, agonist predictions were represented as ones whereas antagonist predictions were represented as zeros for each ligand. Applying heuristic cut-offs, we calculated maximum accuracy and highest MCC values for each structure. We computed MCC values as 0.64, 0.70 and 0.60 while accuracy values were calculated as 86%, 90%, and 84% in the homology model of human β 1-AR, active state human β 1-AR (PDB ID: 7BU7) and inactive state human β 1-AR (PDB ID: 7BVQ), respectively (**Figure 21**). The accuracy values (blue lines) and MCC values (red lines) based on cut-off values can be seen from the **Figure 21**. Using the data obtained from Pearson's pairwise correlation approach, we classified ligands as agonist and antagonist and produced confusion matrixes (**Figure 21**). In confusion matrixes, the number of true positives (TP) was shown in green box at top left corner whereas the number of false positives (FP) was displayed in yellow box at top right corner. The number of true negatives (TN) was indicated in at lower left corner and the number of false negatives (FN) was demonstrated in at lower right corner. Our analysis revealed that most of ligands showed agonist activity for human β 1-AR compared to antagonists.

To compare the results of the human β 1-AR and β 2-AR, in this study, we calculated the MCC and accuracy values of human β 2-AR structures separately for each structure. According to our previous study, MCC values were measured as 0.49, 0.37 and 0.33 whereas accuracy values were estimated as 82%, 79%, 73% in the active state human β 2-AR (PDB ID: 3SN6), another active state human β 2-AR (PDB ID: 4LDE) and inactive state human β 2-AR (PDB ID: 5JQH), respectively (**Figure 22**). According to confusion matrixes, most of ligands displayed agonist activity for human β 1-AR. It is not surprising that the results were similar for classification for both human β 1-AR and human β 2-AR (Jiménez-Rosés et al., 2022). Because we used same ligand library, same methodology, and also β 1-ARs and β 2-ARs have higher structural similarity.

For each structure, we classified ligands as agonists and antagonists using Categorical Boosting (CatBoost) classifier (Prokhorenkova et al. 2018) (**Figure 23 and 24**) and extracted ligand-receptor interaction information from feature importance predictions by applying Shapley Additive Explanations (SHAP) value method (Lundberg and Lee (2017) separately (**Figure 25 and 26**). The SHAP value of the 40 important features for the each structure were plotted in (**Figure 25 and 26**). The y-axis indicates the feature and the x-axis represents the SHAP value. The features were ordered according to their importance. The color of the points on the figures shows the value of the feature from low to high. In our case, blue color indicates the agonist properties whereas red color represents the antagonist properties. Pairwise interactions between atoms or residues and interaction types were demonstrated in the left side of the figures. The interaction information were divided into two parts in texts. The interaction information related to the receptor were demonstrated on the left side while interaction information related to the ligand were showed on the right side.

Our matrix results demonstrated ML approach significantly reduced wrong estimations for classification (**Figure 21, 22, 23 and 24**). In addition, SHAP value results generally verified some important interactions obtained from pairwise correlation analysis (**Figure 27 and 28**). As a result, we revealed that key mediators of agonism and antagonism for β 1-AR and β 2-AR by applying pairwise correlation analysis and ML approaches.

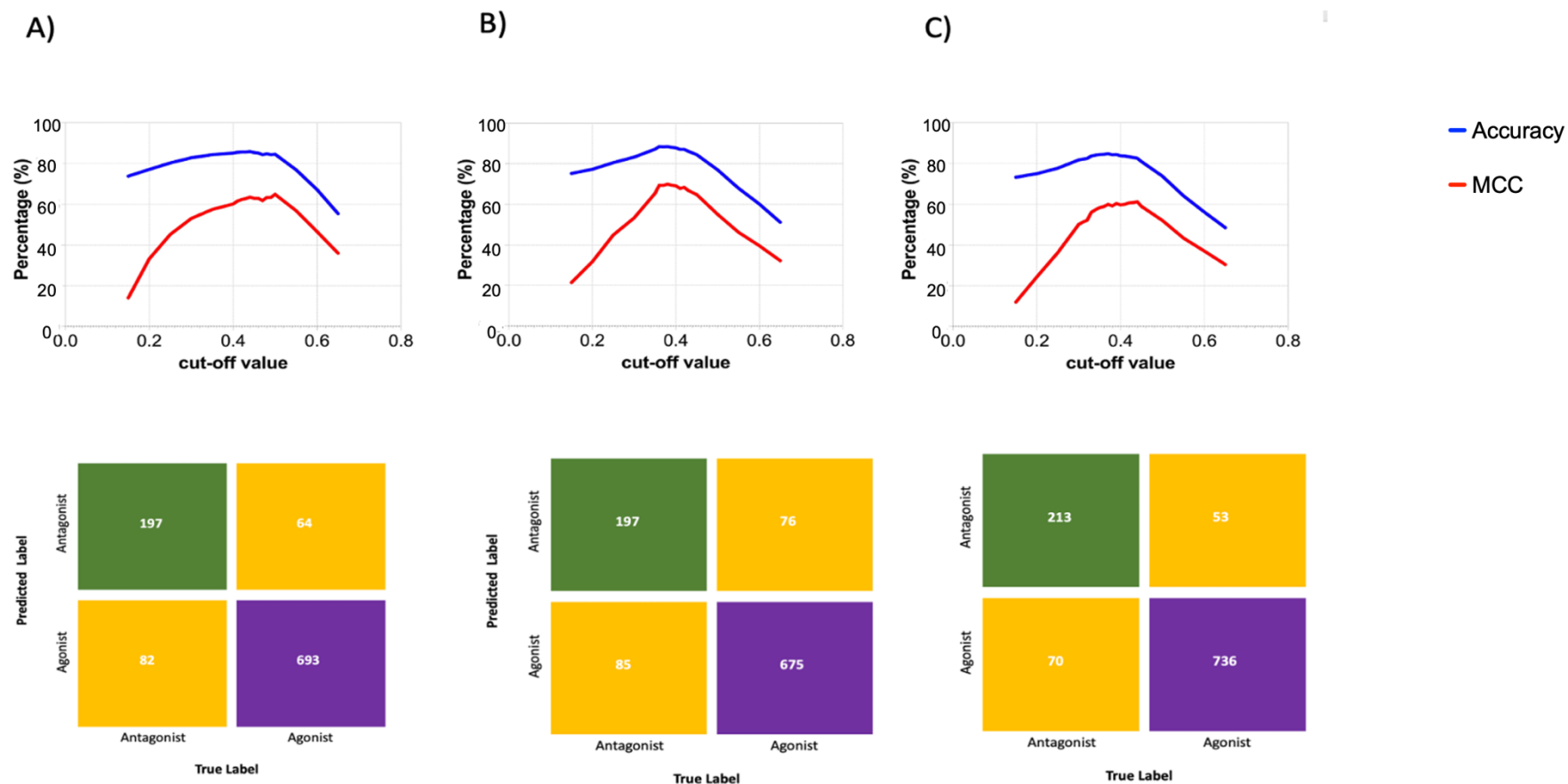


Figure 21. Cut-off graph to obtain the maximum MCC value for the Pearson's correlation approach and the corresponding confusion matrix to differentiate agonist and antagonist. (A) Homology model of human β 1-AR (turkey β 2-AR template - PDB ID: 6H7N) dataset, above: cut-off and below: confusion matrix MCC. (B) Active state experimental human β 1-AR (PDB ID: 7BU7) dataset, above: cut-off and below: confusion matrix MCC (C) Inactive state experimental human β 1-AR (PDB ID: 7BVQ) dataset, above: cut-off and below: confusion matrix MCC.

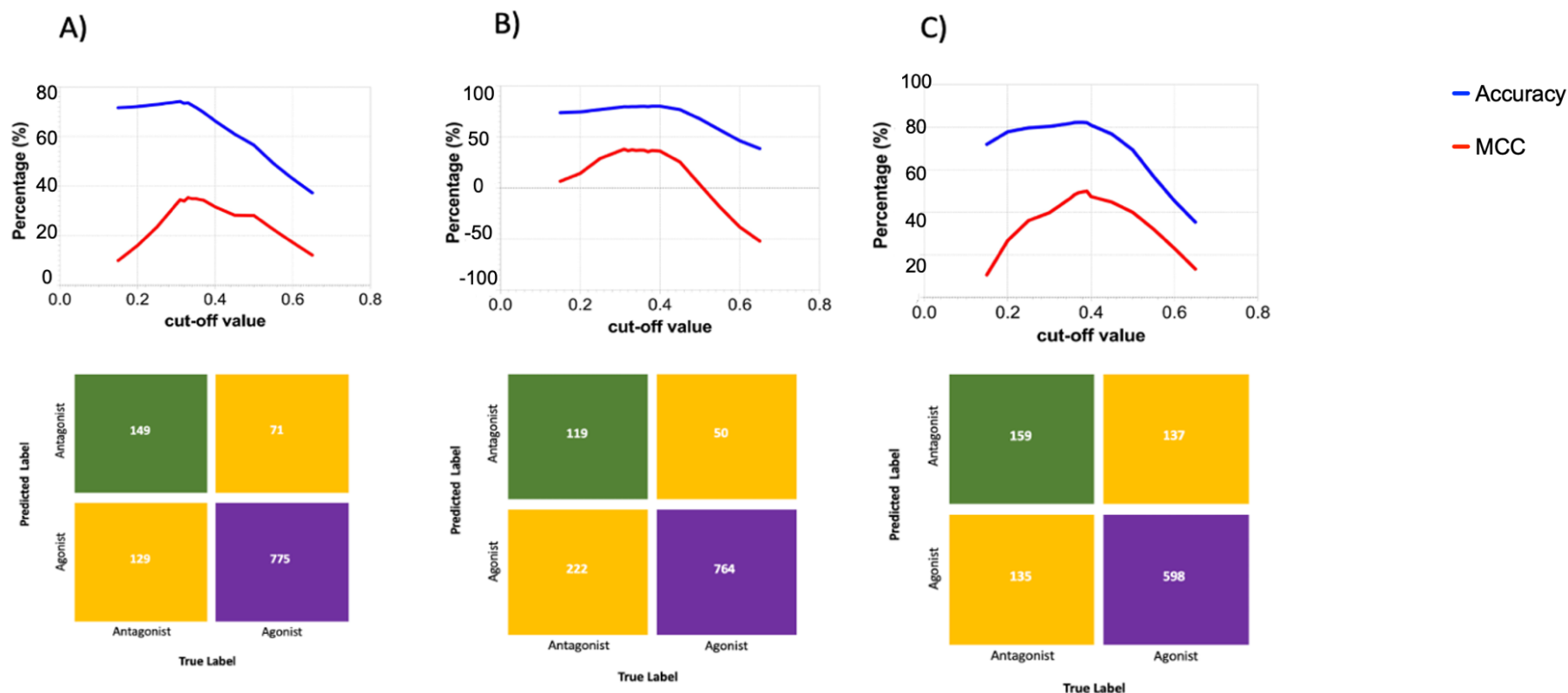


Figure 22. Cut-off graph to obtain the maximum MCC value for the Pearson's correlation approach and the corresponding confusion matrix to differentiate agonist and antagonist. (A) Active state human β 2-AR (PDB ID: 3SN6) dataset, above: cut-off and below: confusion matrix MCC. (B) Active state human β 2-AR (PDB ID: 4LDE) dataset, above: cut-off and below: confusion matrix MCC. (C) Inactive state human β 2-AR (PDB ID: 5JQH) dataset, above: cut-off and below: confusion matrix MCC.

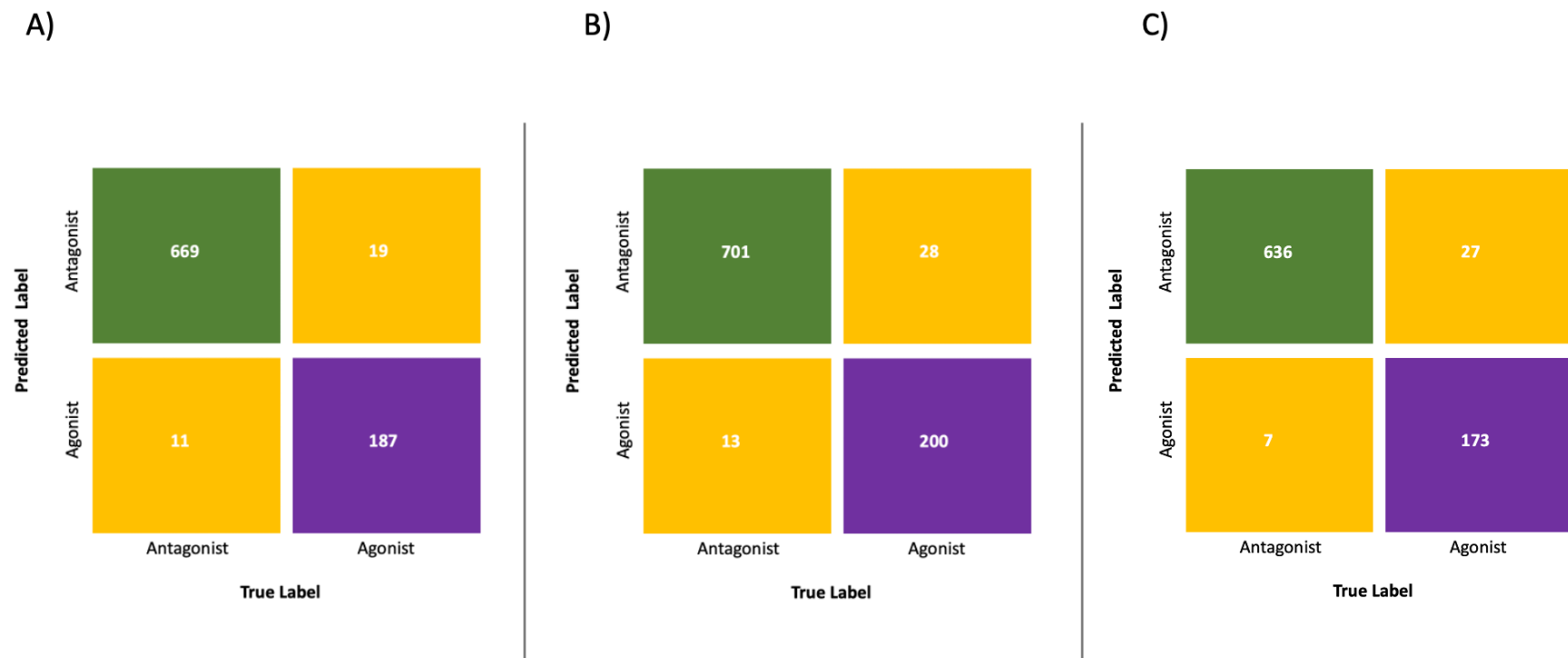


Figure 23. Catboost Classification Confusion Matrix for Cross Validation for the filtered dataset. The figures show the median confusion matrix across all K-folds and repeats. Y-axis shows the frequency of classes predicted by the model, across all samples. The x-axis shows the true known class label. Overall, the confusion matrix provides insight into the ratios of false positive & negatives made by the model across samples for the filtered data. (A) Homology model of human β 1-AR (turkey β 2-AR template - PDB ID: 6H7N) (B) Active state experimental human β 1-AR (PDB ID: 7BU7) (C) Inactive state experimental human β 1-AR (PDB ID: 7BVQ).

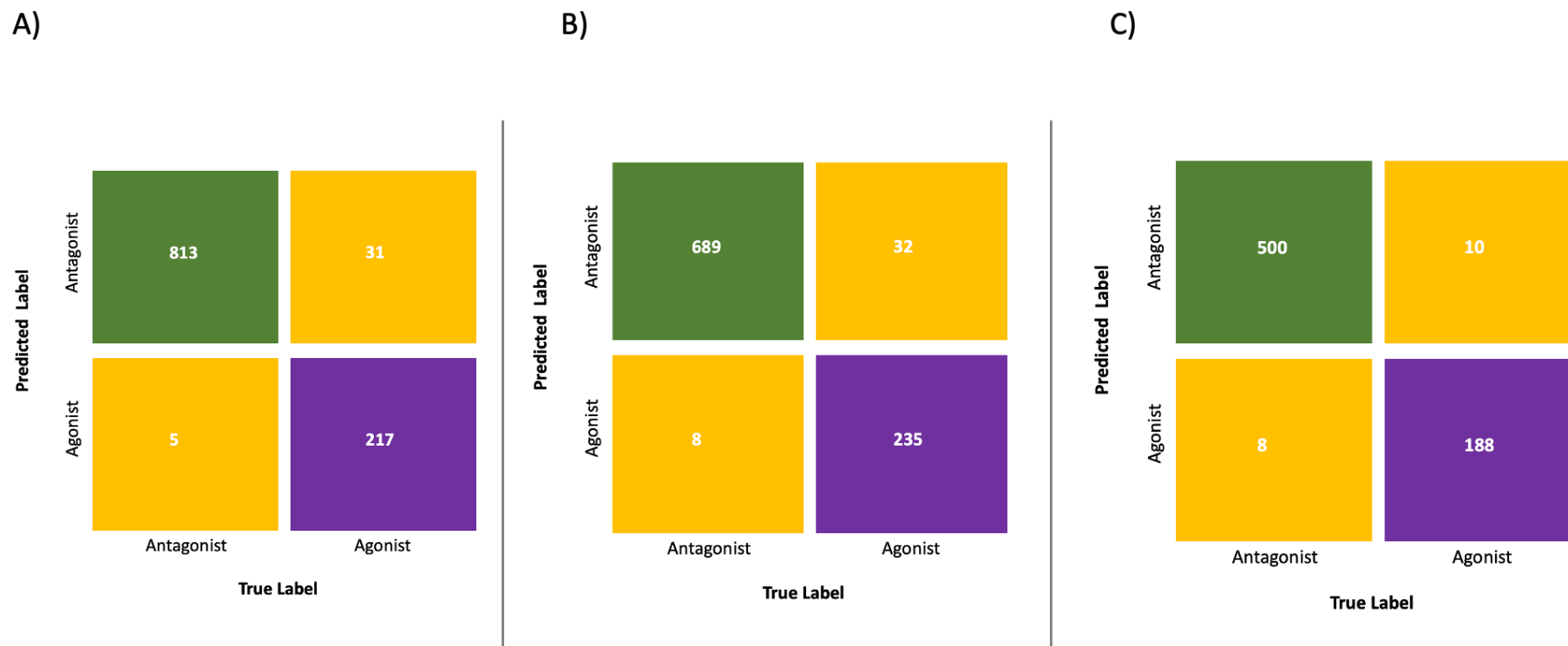


Figure 24. Catboost Classification Confusion Matrix for Cross Validation for the filtered dataset. The figures show the median confusion matrix across all K-folds and repeats. Y-axis shows the frequency of classes predicted by the model, across all samples. The x-axis shows the true known class label. Overall, the confusion matrix provides insight into the ratios of false positive & negatives made by the model across samples for the filtered dataset. (A) Active state human β 2-AR (PDB ID: 3SN6) (B) Active state human β 2-AR (PDB ID: 4LDE) (C) Inactive state human β 2-AR (PDB ID: 5JQH).

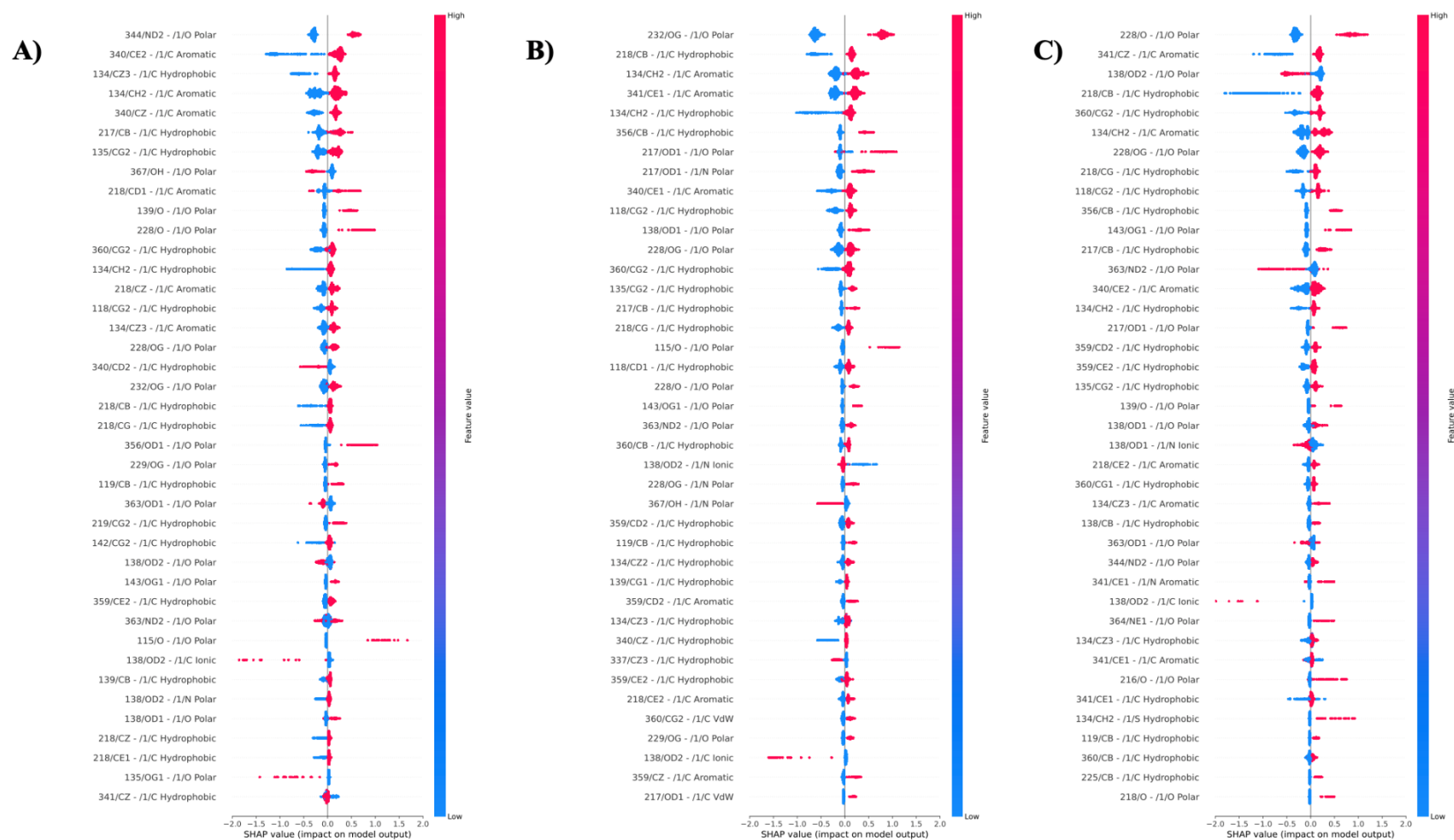


Figure 25. Feature importance of the Catboost model applying the SHAP value method. (A) Local SHAP values per sample (each ligand pose) are sorted by the mean absolute SHAP value method for homology model of human $\beta 1$ -AR (turkey $\beta 2$ -AR template - PDB ID: 6H7N) (B) Local SHAP values per sample (each ligand pose) are sorted by the mean absolute SHAP value method for active state experimental human $\beta 1$ -AR (PDB ID: 7BU7) (C) Local SHAP values per sample (each ligand pose) are sorted by the mean absolute SHAP value method for inactive state experimental human $\beta 1$ -AR (PDB ID: 7BVQ).

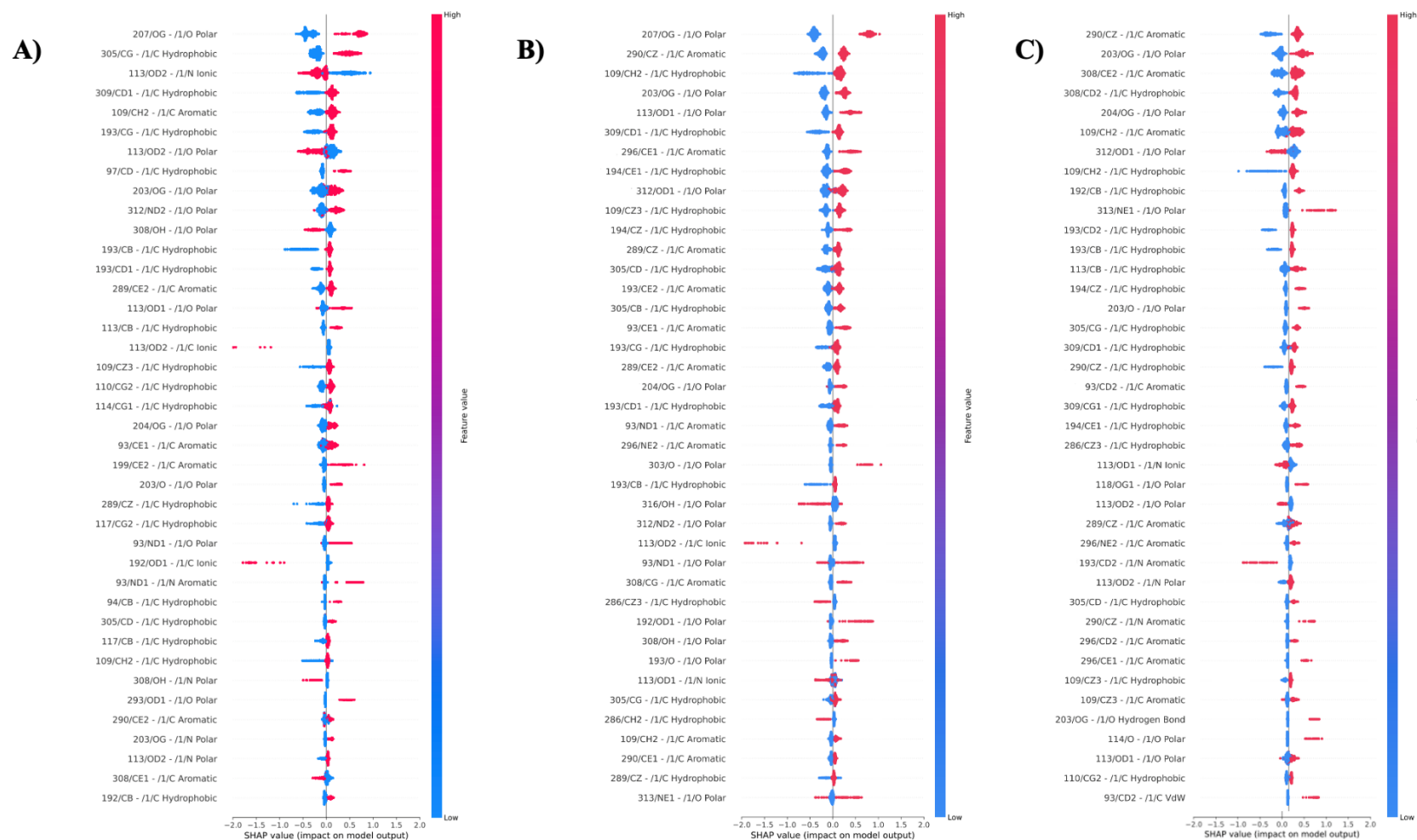
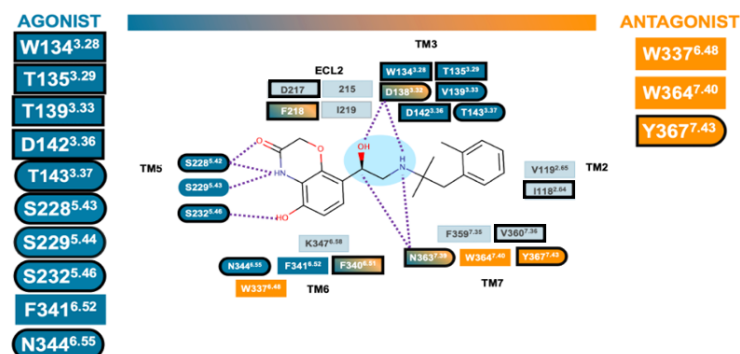
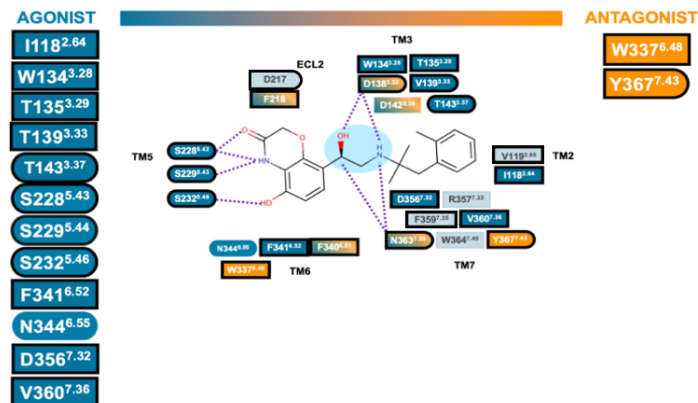


Figure 26. Feature importance of the Catboost model applying the SHAP value method. (A) Local SHAP values per sample (each ligand pose) are sorted by the mean absolute SHAP value method for active state human $\beta 2$ -AR (PDB ID: 3SN6) (B) Local SHAP values per sample (each ligand pose) are sorted by the mean absolute SHAP value method for active state human $\beta 2$ -AR (PDB ID: 4LDE) (C) Local SHAP values per sample (each ligand pose) are sorted by the mean absolute SHAP value method for inactive state human $\beta 2$ -AR (PDB ID: 5JQH) .

A)



B)



C)

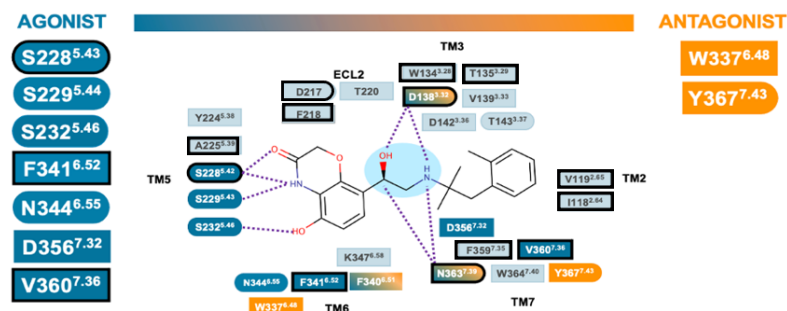
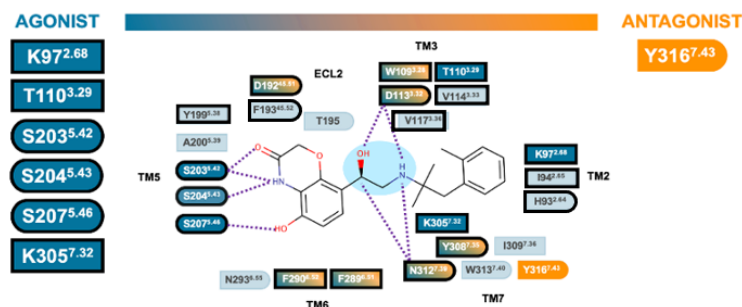
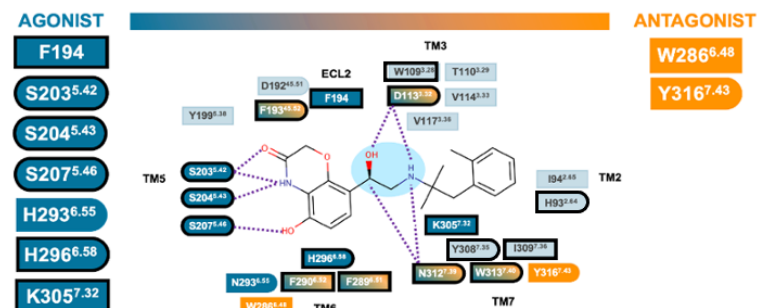


Figure 27. Schematic representation of the interactions for the machine learning approach (A) AIF of best homology model of human β 1-AR (turkey β 2-AR template - PDB ID: 6H7N (B) AIF of active state experimental human β 1-AR (PDB ID: 7BU7) (C) AIF of inactive state experimental human β 1-AR (PDB ID: 7BVQ) The type of interaction is summarised in squared shape for hydrophobic and aromatic contacts, round shape for the polar, ionic and hydrogen bond contacts, and the combination of both. The dotted purple line represents ionic and/or hydrogen bond contacts. The black outlines represent the atomic interactions with higher feature importance. The ethanolamine moiety of the BI-167107 ligands is highlighted in light blue.

A)



B)



C)

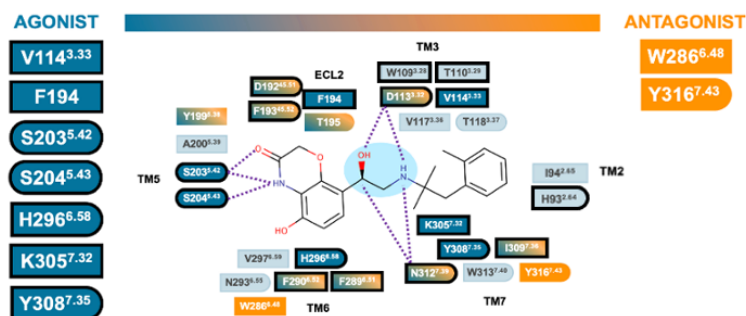


Figure 28. Schematic representation of the interactions for the machine learning approach (A) (A) AIF of active state human β 2-AR (PDB ID: 3SN6) (B) AIF of active state human β 2-AR (PDB ID: 4LDE) (C) AIF of inactive state human β 2-AR (PDB ID: 45JQH). The type of interaction is summarised in squared shape for hydrophobic and aromatic contacts, round shape for the polar, ionic and hydrogen bond contacts, and the combination of both. The dotted purple line represents ionic and/or hydrogen bond contacts. The black outlines represent the atomic interactions with higher feature importance. The ethanolamine moiety of the BI-167107 ligands is highlighted in light blue.

3.3. Chapter 3 Summary

The aim of the study was to identify specific and common determinants of ligand pharmacological activity on β 1- and β 2-ARs using docking and ML approaches. For this aim, firstly, we built the three homology models of the human β 1-AR based on different active state β -AR structures via MODELLER (Webb and Sali, 2016). Secondly, we docked 2683 known β -AR ligands into the three homology models and two experimental human β 1-AR structures via Autodock Vina (Trott and Olson, 2010). After the molecular docking of large dataset of β -AR ligands into three homology models of human β 1-AR and two crystal structure of human β 1-AR structures, we revealed that specific interaction fingerprints for agonist and antagonist ligands via Arpeggio (Jubb et al., 2017). Despite the structural similarity between homology models and crystal structures of human β 1-AR, our comparative analysis on RMSD and statistical analysis on frequency values revealed that the best template for modelling of human β 1-AR is turkey β 1-AR (**Figure 16 and 17**). According to our statistical analysis, interaction fingerprints are highly similar for active state homology model of human β 1-AR and active state experimental structure of human β 1-AR compared to inactive state experimental structure of human β 1-AR (**Figure 19**). After molecular docking and interaction pattern analysis, a ML predictor of the ligand activity (agonist or antagonist) based on interaction fingerprints were developed (**Figure 21**). Then, we have successfully determined specific residues of human β 1-AR and common atomic interactions mediating pharmacological actions of agonism and antagonism for each ligand. According to our results, general both experimentally determined structures and the homology model yielded the similar results (**Figure 19 and 27**) and that the key mediators of agonism and antagonism are

the similar in β 1-AR and β 2-AR receptors by using pairwise correlation analysis and ML approaches (**Figure 20 and 28**). Understanding the molecular basis of ligand activity at β -ARs by performing docking studies of ligands with known pharmacological activity in combination with ML approaches can have major impact on targeting β -AR structure-based drug discovery.

Chapter 4. Determination of the ligand binding kinetics of the human β 1-adrenoceptor via Time-Resolved Fluorescence Resonance Energy Transfer (TR-FRET) approach

4.1. Introduction

The β -adrenergic receptors (β -ARs) are members of class A G protein-coupled receptors (GPCRs) and are activated by the endogenous catecholamines epinephrine and noradrenaline (Ahlquist, 1948; Wu et al., 2021). As part of the sympathetic nervous system, β -ARs are involved in the regulation of cardiovascular, pulmonary and metabolic functions (Brodde, 2007; 2008). To date, three β -AR subtypes have been characterised: β 1-AR, β 2-AR, and β 3-AR (Bylund, 1992; Bylund et al., 1994; Dixon et al., 1986; Emorine et al., 1989; Hein and Kobilka, 1995; Langer, 1980; Philipp and Hein, 2004; Qu et al., 2019; Stockigt et al., 2012). Of the three β -AR subtypes, β 1-AR is the predominant subtype expressed in the heart (Madamanchi, 2007; Woo and Xiao, 2012). Thus, the β 1-ARs are the target of β -adrenergic receptor antagonists (β -blockers) widely clinically used in treatment of cardiovascular diseases such as chronic heart failure, coronary artery disease, hypertension and arrhythmias (Alhayek and Preuss, 2022; Bristow, 2011). However, β -blockers also antagonize β 2-ARs, as few are truly selective based on affinity which can lead to many adverse effects, especially in people with asthma (Morales et al., 2011; Morales et al., 2017). Vice versa, β 2-AR agonists used for treatment of asthma can activate β 1-ARs, leading to adverse reactions in patients with cardiovascular conditions (Salpeter et al., 2004). In addition to equilibrium selectivity of drugs, the importance of the ligand binding kinetics in receptor subtype selectivity has recently been demonstrated for dopamine

receptors. Therefore, an investigation of the kinetic process of ligand binding to β adrenergic subtypes is crucial to understand the molecular mechanism of ligand selectivity between the subtypes (Sykes et al., 2022). For *in vivo* efficacy, a common approach is based on affinity or potency values (Guo et al., 2017; Jansson-Lofmark et al., 2020). On the other hand, binding kinetics parameters have been generally neglected in drug discovery process (Guo et al., 2017). Previous studies suggested that the binding kinetics of drug-receptor interactions are more important determinants than equilibrium binding parameters in determining the efficacy of the drugs *in vivo* (Copeland et al., 2006; Swinney, 2004; Tummino and Copeland, 2008; Zhang and Monsma, 2009). Hence, in drug discovery, the characterization of the drug-receptor binding kinetics has gained popularity for the development of new GPCR targeted therapeutics. The characterization of binding kinetics of ligands at GPCRs has traditionally been performed via radioligand binding assays. On the other hand, during the last decade, fluorescence-based methods have become an alternative to expensive, time consuming, hazardous and heterogenous radioligand binding assays (Ciruela et al., 2014; Cottet et al., 2012; Stoddart et al., 2016; Sykes et al., 2017; Vernall et al., 2014; Zwier et al., 2010). However, application of fluorescent ligands to specific GPCRs generally requires an optimization process to generate a suitable ligand binding assay (Stoddart et al., 2018). Time-resolved fluorescence resonance energy transfer (TR-FRET) ligand-binding assays provide to monitor real-time kinetics of the ligand binding to GPCR on membranes and intact cells and easy collection of larger dataset (Kobayashi et al., 2019; Soave et al., 2020; Swinney et al., 2015). In this assays, ligands are labeled red or green acceptors and time resolved FRET emission are measured via terbium cryptate (Zhang and Xie, 2012). To date, few studies have used TR-FRET ligand-binding assays to determine the kinetics of

unlabelled ligands for GPCRs (Soave et al., 2020). More recently, TR-FRET ligand-binding assays have been successfully applied to various GPCR, including dopamine D2 receptor (Klein Herenbrink et al., 2016; Sykes et al., 2017), gonadotropin releasing hormone receptor (Nederpelt et al., 2016), and the histamine H1 receptor (Bosma et al., 2019; Schiele et al., 2015).

A kinetic binding study for human β 1-ARs in the literature has recently been reported by (Sykes et al., 2022) and was based on radioligand binding assays, using [^{3} H]-DHA as a tracer compound. To date, the time-resolved fluorescence resonance energy transfer (TR-FRET) approach has never been applied to human β 1-ARs and ligand binding characteristics have not been investigated for β 1-adrenoceptor antagonists at the physiological temperature (37°C) via this approach. Therefore, in the present study, we have developed the first novel homogenous TR-FRET based assay to determine the kinetic binding characteristics of unlabelled ligands for human β 1-AR.

Nebivolol and Carvedilol are the third-generation β -blockers with vasodilating properties (AlHabeeb et al., 2022; Howlett, 2014; Remme, 2010). Both Nebivolol and Carvedilol have been used in the treatment of heart failure (HF) (Remme, 2010). Bisoprolol, a second generation β -blocker, has been also used for the treatment of the HF (Metra et al., 2007; Remme, 2010). Esmolol is short acting second-generation β -blocker and generally used in the anaesthesia (Blanski et al., 1988; Gray et al., 1985). Compared to second generation β -blockers, third generation β -blockers (Nebivolol and Carvedilol) with vasodilating properties may have more beneficial for cardiovascular diseases (Chan You et al., 2021; Cheng, 2009; Ferri, 2021; Manrique et al., 2009). Due to the differences between β -blockers, the binding characterization of β -blockers can provide valuable insights for designing of the new effective β -

blockers with fewer side effects (Ferri, 2021; Fongemie and Felix-Getzik, 2015). For this study, Nebivolol and Carvedilol were selected from third-generation β -blockers whereas Bisoprolol and Esmolol were selected from second generation-generation β -blockers to compare the binding kinetic parameters at human β 1-AR.

In this study, firstly, association assays were performed to characterise the tracer kinetic binding parameters of two different fluorescent ligands for human β 1-AR. Secondly, we determined the binding kinetics of unlabelled four different unknown β -blocker Nebivolol, Carvedilol, Bisoprolol and Esmolol (**Figure 14**) using the optimal fluorescent tracer using the competition kinetic binding approach first documented by Motulsky and Mahan (Motulsky and Mahan, 1984). Thirdly, molecular docking of these four β -blocker were carried out using our homology models of the human β 1-AR and two experimental determined human β 1-AR structures. In the final step, we investigated the ligand-receptor interactions through Arpeggio (Jubb et al., 2017) and compared our computational and experimental results. We revealed that dissociation rate constant (k_{off}) is the most important determinant for determination of the kinetic binding characteristics of unlabelled ligands for human β 1-AR. This study has demonstrated that the TR-FRET based ligand-binding assay allows us to accurately study ligand binding kinetics of ligands for human β 1-AR at physiological conditions. Consequently, the findings and the TR-FRET based methodology developed in the study could be useful for future drug discovery studies as an alternative to the radioligand binding assays.

4.2. Results and Discussion

4.2.1. Characterization of the Fluorescent Ligands for Tracer Selection

Investigations into drug-receptor binding kinetics have been the subject of intensive research in drug discovery fields, particularly respiratory diseases in the case of GPCRs with the aim of developing new therapeutics with increased receptor selectivity and fewer side effects (Bosma et al., 2019; Sykes et al., 2012). For that purpose, radioligand tracers have been generally used in competition association experiments (Dowling and Charlton, 2006; Gillard et al., 2002; Guo et al., 2013; Ramsey et al., 2011; Sullivan et al., 2006; Sykes et al., 2022; Unett et al., 2013). However, it is still not fully understood whether the kinetic characteristic of the tracer has an effect on the measurement of kinetic binding parameters of unlabelled ligands (Bosma et al., 2019). Although one previous study by (Sykes et al., 2022) determined the binding kinetics of a radioligand tracer for human β 1-AR, to date the binding kinetics of any fluorescent tracer has never been characterized for human β 1-AR using the TR-FRET methodology. Hence, before the determination of association and dissociation rate constants of any unlabelled ligands, we performed the binding association assays to measure of the kinetic properties of the tracer.

Propranolol is a typical competitive non-selective beta-receptor antagonist. For competition assays, fluorescent propranolol derivatives can be used as acceptors to signal collect. Red acceptors emit light at 665 nm and 620 nm whereas green acceptors emit light at 520 nm and 620 nm (Zwier et al., 2010). Terbium cryptate (Lumi4®-Tb) has energetic compatibility with both green and red fluorescent dyes. Therefore, we initially, characterised tracer kinetic binding characteristics for human β 1-AR based on the non-selective β -AR antagonist alprenolol using two different competitive

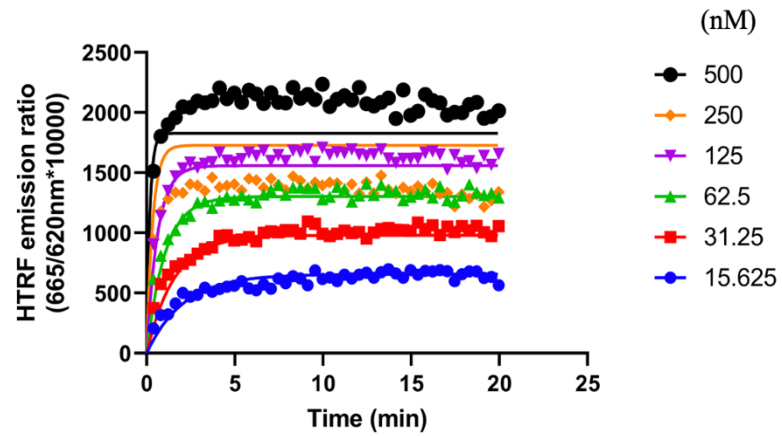
fluorescent β 2-AR antagonists: (S)-propranolol-green and (S)-propranolol-red. All competition kinetic association assays were performed by using membranes expressing a human N-terminally SNAP-tagged β 1-AR, incubated in HEPES buffered Hanks Balanced Salt Solution (HBSS) at 37 °C for 20 mins. For each fluorescent ligand, the observed association rates were monitored at six different concentrations of each ligand. **Figure 29** displays the representative plots of kinetic association binding curves for (S)-propranolol-red and (S)-propranolol-green, respectively. In this study, association binding kinetic curve of red propranolol was generated over the range 500 - 31.25 nM concentrations whereas association kinetic binding curve of green propranolol was calculated using 62.5 - 1.95 nM. Data obtained from kinetic association binding assays were fitted to the Motulsky–Mahan model (Motulsky and Mahan, 1984) to measure the association (k_{on}) and dissociation (k_{off}) rate constants of the both fluorescent ligands. For each fluorescent ligands, the kinetic parameters including association rate constant (k_{on}), dissociation rate constant (k_{off}), residence time (min), and kinetic binding affinity (pKd) were calculated by fitting the data derived from kinetic association binding assays (**Figure 29**) to Motulsky-Mahan model (Motulsky and Mahan, 1984) and the values are given in **Table 7**.

Table 7. Kinetic binding parameters of red and green propranolol for human $\beta 1$ -AR. Data are mean $\pm$ S.E.M. form 3 different experiments performed in singlet.

Tracer	Tracer k_{off} (min^{-1})	Tracer k_{on} ($\text{M}^{-1} \text{min}^{-1}$)	Tracer Residence time (min)	Tracer pKd
(S)- propranolol- red	0.30 ± 0.18	$9.40 \pm 0.27 \times 10^6$	4.54 ± 2.24	7.63 ± 0.19
(S)- propranolol- green	0.48 ± 0.11	$2.43 \pm 0.27 \times 10^7$	1.66 ± 0.44	7.73 ± 0.06

According to our tracer kinetic binding parameters (**Table 7 and Figure 29**), (S)-propranolol-green has relatively higher association and dissociation rates ($k_{\text{on}} = 2.43 \pm 0.27 \times 10^7 \text{ M}^{-1} \text{ min}^{-1}$ and $k_{\text{off}} = 0.48 \pm 0.11 \text{ min}^{-1}$, respectively) compared to (S)-propranolol-red kinetic rates ($k_{\text{on}} = 9.40 \pm 0.27 \times 10^6 \text{ M}^{-1} \text{ min}^{-1}$ and $k_{\text{off}} = 0.30 \pm 0.18 \text{ min}^{-1}$). It is also clear that (S)-propranolol-green dissociated rapidly from the $\beta 1$ -AR with a mean residence time of 1.66 min while (S)-propranolol-red dissociation was relatively slow (mean residence time of 4.54 min). **Figure 29** demonstrates the deviation for the 250 nM (S)-propranolol-red ligand concentration. However, the (S)-propranolol-green ligand accurately discriminated the concentration differences in determining the binding kinetics.

A) (S)-propranolol-red binding



B) (S)-propranolol-green binding

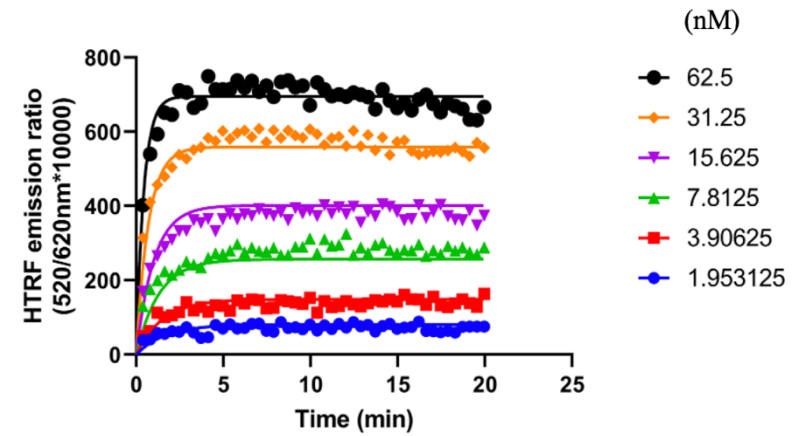


Figure 29: (S)-propranolol-red and (S)-propranolol-green kinetic association binding curves for human β 1-AR at 37° C.

Moreover, at the same time, we also observed the effect of tracer kinetics on the kinetic determinations of Alprenolol, the β -AR antagonist ligand, used to define non-specific binding (NSB). The kinetic parameters (k_{on} , k_{off} , residence time and pK_i) were obtained from the kinetic association binding curves are given in **Table 8**. In the presence of (S)-propranolol-green, Alprenolol has relatively higher association and dissociation rates ($k_{on} = 1.37 \pm 0.28 \times 10^8 \text{ M}^{-1} \text{ min}^{-1}$ and $k_{off} = 0.65 \pm 0.28 \text{ min}^{-1}$, respectively). In the presence of (S)-propranolol-red, very similar association and dissociation rates were observed for alprenolol ($k_{on} = 1.52 \pm 0.42 \times 10^8 \text{ M}^{-1} \text{ min}^{-1}$ and $k_{off} = 0.82 \pm 0.25 \text{ min}^{-1}$). Our apparent affinity values demonstrated that in the (S)-propranolol-green, NSB had a higher binding affinity ($pK_i = 8.42 \pm 0.16$) for the human β 1-AR when compared to (S)-propranolol-red ($pK_i = 8.28 \pm 0.15$).

Table 8. Kinetic binding parameters of the non-selective β -AR antagonist Alprenolol for human β 1-AR in the presence of both fluorescent ligands. All data are mean $\pm$ S.E.M. of 3 different experiments performed in singlet.

NSB	k_{off} (min^{-1})	k_{on} ($\text{M}^{-1} \text{ min}^{-1}$)	Residence time (min)	pK_i
(S)- propranolol- red	0.65 ± 0.28	$1.37 \pm 0.28 \times 10^8$	2.01 ± 1.18	8.42 ± 0.16
(S)- propranolol- green	0.82 ± 0.25	$1.52 \pm 0.42 \times 10^8$	1.05 ± 0.34	8.28 ± 0.15

4.2.2. Characterization of Unlabelled β -AR Ligands for Human β 1-AR

Although binding of Nebivolol, Carvedilol and Bisoprolol to human β 1-AR were studied in previous radioligand binding assays (Baker, 2010b; Sykes et al., 2022), TR-FRET assays had not previously been performed for the kinetic characterization of these ligands for human β 1-AR. Hence, in the present study, we performed the competition kinetic binding association assays using Motulsky-Mahan model (Motulsky and Mahan, 1984) to measure of the kinetic properties of the four β -AR antagonist; Nebivolol, Carvedilol, Bisoprolol and Esmolol.

As detailed above, all competition kinetic association assays for human β 1-AR were performed using the rapidly dissociating tracer (S)-propranolol-green to determine the kinetic binding parameters accurately. For each unlabelled compounds the kinetic parameters (association rate constant (k_{on}), dissociation (k_{off}) rate constant, residence time (RT) and kinetic binding affinity (pK_d) were calculated by fitting the data derived from kinetic association binding assays to Motulsky-Mahan model (Motulsky and Mahan, 1984) and the values are shown in **Table 9**.

Table 9. Kinetic binding parameters of four unlabelled compounds for human β 1-AR. All data are mean $\pm$ S.E.M. of 4 different experiments performed in singlet.

β -AR antagonist	k_{off} (min^{-1})	k_{on} ($\text{M}^{-1} \text{min}^{-1}$)	Residence time (min)	Kinetic pK_d
Nebivolol	0.0025 ± 0.001	$3.08 \pm 0.67 \times 10^7$	732.25 ± 334.10	10.26 ± 0.32
Carvedilol	0.02 ± 0.01	$1.44 \pm 2.96 \times 10^8$	32.99 ± 7.18	9.78 ± 0.18
Bisoprolol	0.06 ± 0.02	$1.16 \pm 0.41 \times 10^7$	16.11 ± 4.75	8.29 ± 0.06
Esmolol	0.89 ± 0.49	$7.29 \pm 4.65 \times 10^6$	1.58 ± 0.62	6.83 ± 0.06

According to binding kinetics analysis, Nebivolol had the slowest dissociation rate ($k_{\text{off}} = 0.0025 \pm 0.001 \text{ min}^{-1}$) whereas Esmolol displayed the fastest dissociation rate ($k_{\text{off}} = 0.89 \pm 0.49 \text{ min}^{-1}$). Carvedilol and Bisoprolol had similar moderate dissociation rates ($k_{\text{off}} = 0.02 \pm 0.01 \text{ min}^{-1}$ and $k_{\text{off}} = 0.06 \pm 0.02 \text{ min}^{-1}$, respectively).

According to residence time values, the fastest dissociating compound was Esmolol with residence time of 1.58 min while the slowest dissociating compound was Nebivolol having residence time of 732.25 min. Carvedilol was the second slowest dissociating compound (residence time = 32.99) followed by Bisoprolol (residence time = 16.11)

Our kinetic pK_d results also revealed that Nebivolol showed the highest affinity for human β_1 -AR ($pK_d = 10.26$) whereas Esmolol had lowest affinity for human β_1 -AR ($pK_d = 6.83$). Nebivolol is followed by Carvedilol demonstrating higher affinity ($pK_d = 9.78$). Bisoprolol also showed higher affinity as the third most effective ligand ($pK_d = 8.29$).

Our findings are in good agreement with previous studies determining the equilibrium binding properties of Nebivolol, Bisoprolol and Carvedilol for human β_1 -AR using radioligand binding assays. As reported in one previous study by (Baker, 2010b), we also found Nebivolol had highest affinity for human β_1 -AR. Moreover, our findings confirmed the previous radioligand binding study (Sykes et al., 2022) revealing the kinetic characterization of Bisoprolol ($k_{\text{off}} = 0.14 \pm 0.06 \text{ min}^{-1}$, residence time = 7.14, $pK_d = 8.20$). However, our findings for Carvedilol were slightly different from the previous study (Sykes et al., 2022) (Carvedilol, $k_{\text{off}} = 0.09 \pm 0.02 \text{ min}^{-1}$, residence

time = 11.11, $pK_d = 10.36$). The ~ 4 difference in k_{off} may be due to the differences in assay conditions and the use of a different, faster dissociating tracer in the present study. However, it is worth noting that differences of this magnitude are common when comparing values reported in different studies. Previous studies (Convents et al., 1987; McPherson et al., 1985; Muntz et al., 1986) demonstrated that adrenoceptor binding constants differ significantly depending on the assay conditions, including incubation time and temperature, assay buffer and the studied tissues. In this study, we incubated fluorescent ligand with $\beta 1$ -AR HEKTR cell membranes for 20 min in assay buffer whereas previous study (Sykes et al., 2022) incubated radioligand with $\beta 1$ -AR CHO cell membranes for 180 min. This might explain the differences for binding kinetics of investigated ligands at human $\beta 1$ -AR.

As expected, we observed significant differences in the association constant rate (k_{off}), residence time (RT) and kinetic pK_d values for each ligand. Observed differences in RT values are the results of differences in k_{off} . Therefore, we observed that RT values is correlated to k_{off} values. According to our results, k_{off} is the most important parameter to determine the kinetic binding profile of antagonists for human $\beta 1$ -AR. For the first time, we developed a novel TR-FRET assay to characterise the four selected β -blockers: Nebivolol, Carvedilol, Bisoprolol and Esmolol for human $\beta 1$ -AR. Consequently, using a rapidly dissociating fluorescent tracer, reported previously (Sykes et al., 2022), we correctly characterized the unlabelled ligands for human $\beta 1$ -AR using TR-FRET methodology.

4.2.3. Identification of Key Interactions of the Ligands for Human β 1-AR

To identify the most important atomic interactions of Nebivolol, Carvedilol, Bisoprolol and Esmolol for human β 1-AR, we performed semi-flexible molecular docking experiments with homology model of human β 1-AR, active state experimental structure of human β 1-AR and inactive state experimental structure of human β 1-AR using Audock Vina (Trott and Olson, 2010). For each receptor structure, five independent docking experiments were carried out and generated up to 10 poses for each ligand in every experiment. By increasing experiment number, we tried to increase the accuracy of our docking experiments. In total, 600 docking poses (200 poses for each receptor) were obtained for three different human β 1-AR structures.

We firstly calculated the RMSD between 9 ligands in known 15 experimental β -ARs (Appendix Table A1) and the docked version of the same ligands obtained in **Chapter 3** to find suitable poses bound to homology model of human β 1-AR and experimental human β 1-ARs for analysing binding poses of Nebivolol, Carvedilol, Bisoprolol and Esmolol. This calculation was performed via an open source python code which is named isoRMSD.py measures RMSD differences between two conformation with different atom names (<https://github.com/Out0fcontrol/isoRMSD/blob/master/isoRMSD.py>). Then, we checked ligand binding poses having optimal RMSD using PyMol again and we observed that this code accurately detected best ligand binding poses. Thus, in addition to known experimental turkey β 1-ARs and human β 2-ARs, we obtained best binding poses of 9 known ligands bound homology model human of β 1-AR and

experimental human β 1-ARs to compare Nebivolol, Carvedilol, Bisoprolol and Esmolol bound human β 1-ARs. After then, we tried to predict possible correct ligand binding poses of Nebivolol, Carvedilol, Bisoprolol and Esmolol and their contacts with the receptor residues using these β -AR structures.

We determined the possible correct binding poses of Nebivolol for homology model of human β 1-AR, active state experimental structure of human β 1-AR and inactive state experimental structure of human β 1-AR, correct binding poses of Carvedilol for active state experimental structure and inactive state experimental structure of human β 1-AR, correct binding poses of Bisoprolol for inactive state experimental structure of human β 1-AR. Unfortunately, we did not find any plausible binding poses for Esmolol.

After finding correct ligand binding poses, we obtained the atomic interactions of Nebivolol, Carvedilol and Bisoprolol from Arpeggio (Jubb et al., 2017) and analysed the data. Hence, as expected, we observed that Nebivolol in inactive state experimental structure interacts with more receptor residues than active state homology model and experimental structure. On the other hand, Bisoprolol showed a clear preference to bind to the inactive state. To date, the structures of Carvedilol bound inactive state turkey β 1-AR (PDB ID : 4AMJ (Warne et al., 2012)) and human β 2-AR (PDB ID : 6PS3 (Ishchenko et al., 2019)) provided significant insight into the interactions of Carvedilol at β -ARs. Interestingly, interactions with four residues, S229^{5.43x44}, N344^{6.55x55}, W337^{6x48} and F359^{7.35x34}, that are present in both inactive state turkey β 1-AR and human β 2-AR were not observed in inactive state human β 1-AR. Moreover, interactions with T135^{3.29x29}, C216, D217 in inactive state turkey β 1-

AR and interactions with T143, A225 in inactive state human β 2-AR were not observed in inactive state human β 1-AR.

According to our analysis, we found that 6 residues are common for all correct binding poses of the Nebivolol, Carvedilol and Bisoprolol at human β 1-AR. These 6 important residues are as follows: W134^{3.28x28}, D138^{3.32x32}, V139^{3.33x33}, F218^{45.52x52}, F340^{6.51x51}, N363^{7.39x38} (**Figure 30**). For Nebivolol and Carvedilol, we revealed that similar atomic interactions play important role in ligand binding of human β 1-AR. Except two residues (T220 in ECL2 and F359^{7.35x34} in TM7), all interacting residues (I118^{2.64x63}, V119^{2.65x64}, W134^{3.28x28}, D138^{3.32x32}, D139, V142^{3.36x36}, F218^{45.52x52}, Y224, S228^{5.42x43}, F340^{6.51x51}, F341^{6.52x52}, V360^{7.36x35}, N363^{7.39x38}, W364^{7.40x39} and Y367^{7.43x42}) were identical in Carvedilol bound inactive state human β 1-AR. Unlike interactions of larger antagonist Nebivolol and Carvedilol, smaller antagonist Bisoprolol having lower affinity does not interact with I118^{2.64x63}, V119^{2.65x64}, V142^{3.36x36}, Y224, S228^{5.42x43}, V360^{7.36x35}, W364^{7.40x39} and Y367^{7.43x42}. Interestingly, only Bisoprolol prefers to form hydrophobic/aromatic contacts with T135^{3.29x29} instead of V142^{3.36x36} in TM3. It is clear that number of the interacting residues for Bisoprolol are less than Nebivolol and Carvedilol. Therefore, we suggested that differences in the number of interacting residues which it could be link to differences in binding kinetic parameters. In the experimental section, we demonstrated that Nebivolol and Carvedilol have higher affinity and slower dissociation rates for human β 1-AR compared to Bisoprolol. I118^{2.64x63} and V119^{2.65x64}, in TM2, V360^{7.36x35}, W364^{7.40x39} and Y367^{7.43x42} in TM7 has been previously shown in the vicinity of the ligands during the dissociation process that form extraction channel at β 1-AR (Gonzalez et al., 2011). In consistent with these findings, we observed that in the absence of hydrophobic/aromatic interactions with these residues, Bisoprolol can

dissociate more rapidly than larger antagonists Carvedilol and Nebivolol. Also, the presence of hydrophobic/aromatic interactions with T135^{3.29x29} in TM3 can contribute to the differences in stability, affinity, kinetic parameters with other two ligands interact V142^{3.36x36} in TM3. Previous study (Hauser et al., 2021) demonstrating TM3 is stabilization hub to maintain the common GPCR fold and crucial for the stability of GPCR supports our findings. On the other hand, we observed that lack of the hydrophobic/aromatic contacts with T220 in ECL2 and F359^{7.35x34} in TM7 could explain why Carvedilol relatively faster dissociates than Nebivolol. The ECL2 was found to be critical to ligand-binding kinetics due to the its conformational flexibility (Avlani et al., 2007) and its interactions with the proximal helices contributes to the stability of the inactive state GPCR (Jager et al., 2007; Klco et al., 2005). The role of F359^{7.35x34} in forming a junction between ECL2 and TM7 has been highlighted in the allosteric/orthosteric binding and activation cooperativity (Avlani et al., 2007). Therefore, our findings are consistent with these previous studies. Moreover, differences in binding kinetics of Nebivolol and Bisoprolol might also be driven hydrophobic/aromatic contacts with I118^{2.64x63} in TM2 (Lim et al., 2023). To summarise our findings, the affinity and dissociation rate constants are governed by specific ligand-receptor interactions for Nebivolol, Carvedilol and Bisoprolol. In the future, new ligands could be developed to maximise the interaction leading to long residency time. Also, the quality of docking can be improved by consideration of flexibility of the human β 1-ARs or by incorporating MD simulations. Overall, the analysis of the ligand-receptor interactions leading to the long residency times can be used to guide the design of novel β 1-AR long-acting ligands.

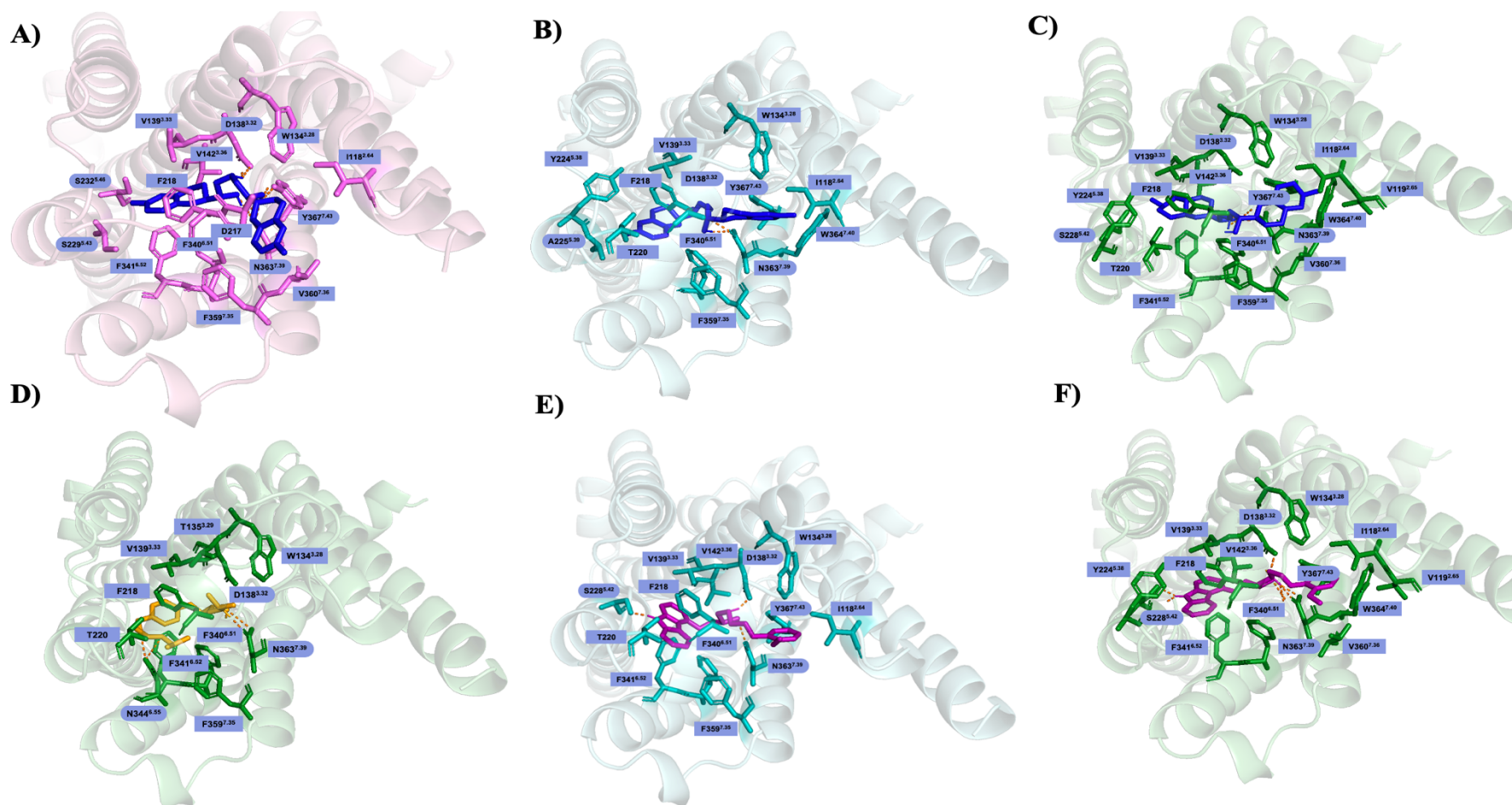


Figure 30. Atomic interactions of the possible correct ligand binding poses for the human β 1-AR (A) Interactions of Nebivolol bound to homology model of human β 1-AR (B) Interactions of Nebivolol bound to active state experimental structure of human β 1-AR (PDB ID: 7BU7) (C) Interactions of Nebivolol bound to inactive state experimental structure of human β 1-AR (PDB ID: 7BVQ) (D) Interactions of Bisoprolol bound to inactive state experimental structure of human β 1-AR (PDB ID: 7BVQ) (E) Interactions of Carvedilol bound to active state experimental structure of human β 1-AR (PDB ID: 7BU7) (F) Interactions of Carvedilol bound to inactive state experimental structure of human β 1-AR (PDB ID: 7BVQ). The type of interaction is summarised in squared shape for hydrophobic and aromatic contacts, round shape for the polar, ionic and hydrogen bond contacts, and the combination of both. The dotted orange line represents polar contacts of the ligands.

4.3. Chapter 4 Summary

The aim of the study was to determine the unlabelled ligand binding kinetics of the human β 1-AR using the TR-FRET approach. For this aim, firstly, we performed competition kinetic binding association assays using Motulsky-Mahan model (Motulsky and Mahan, 1984) to characterise the tracer kinetic binding characteristics of two different fluorescent ligands for the human β 1-AR. Our tracer kinetic binding parameters indicated that (S)-propranolol-green displaying fast binding kinetic profile can be used as an ideal tracer for the reliable determination of the kinetic and equilibrium parameters of unlabelled ligands binding the human β 1-AR (**Table 7 and Figure 29**). Secondly, using this ideal fluorescent tracer in competition kinetic binding association assays, we investigated the binding kinetics of four different known β -blockers: Nebivolol, Carvedilol, Bisoprolol and Esmolol. Our results (**Table 9**) revealed that, among the ligands we studied, Nebivolol is the slowest dissociating ligand and has the highest affinity for human β 1-AR. In contrast, Esmolol is the fastest dissociating ligand and showed the lowest affinity for human β 1-AR. Also, according to our results, Carvedilol was the second slowest dissociating ligand and followed by third slowest dissociating ligand Bisoprolol. Our findings for Nebivolol, Bisoprolol and Carvedilol are consistent with the previous radioligand binding assays described in the literature (Baker, 2010b; Sykes et al., 2022). To best our knowledge, this is the first TR-FRET based study determining the kinetic binding characteristics of ligands for human β 1-AR. The use of an optimal tracer having fast binding kinetics previously suggested, allowed us to accurately determine the binding kinetics of unlabelled ligands for human β 1-AR. Moreover, we suggest that dissociation rate constant (k_{off}) could be used as a determinant of the kinetic binding characteristics of unlabelled

ligands for human β 1-AR. Furthermore, we determined the most crucial interactions (**Figure 30**) for Nebivolol, Carvedilol and Bisoprolol using Arpeggio (Jubb et al., 2017) and observed the link between the specific ligand-human β 1-AR interactions and the kinetic ligand binding parameters (**Table 9 and Figure 30**). In conclusion, our findings contribute to the understanding of ligand-receptor binding kinetics at human β 1-AR and the methodology developed in the study could be used to study kinetic binding of other ligands of human β 1-AR.

Chapter 5. General Discussion and Future Directions

The identification of the specific and common determinants of ligand pharmacological activity on β 1- and β 2-ARs and the investigation of kinetic process of ligand binding to β -adrenergic subtypes are crucial to understand to the molecular mechanism of ligand selectivity between the subtypes, as well for development of long-residency ligands that may have favourable therapeutic properties.

In this thesis, we focused on answering the following key questions: Can we determine the underlying factors mediating agonism and antagonism for human β 1-A at atomic level? Are atomic interactions between ligand and the human β 1-AR responsible for their pharmacological properties? Which atomic interactions determine the agonism or antagonism at human β 1-ARs? What are the similarities and differences between human β 1-ARs and β 2-ARs? The answer to these questions is important for discovering new drugs with higher selectivity and fewer side effects.

We performed docking experiments on both homology model and experimental structures with a large-scale ligand library. We observed a very good agreement between the results obtained using homology model and experimentally determined structures (**Figure 19 and Figure 21**). This strongly suggests that homology models provide a good model for the atomic interaction fingerprint analysis. In this particular case, closely related template structure was used, increasing the quality of the homology model.

The study identified the most important atomic interactions of human β 1-AR and explored the similarities and differences between human β 1-ARs and β 2-ARs (**Figure 19 and Figure 20**). We found that for β -AR agonism ionic/polar/hydrogen bond

contacts with S228/203^{5.42x43}, S229/204^{5.43x44}, S232/207^{5.46x461} residues in TM5 are crucial whereas for β -AR antagonism the most important interactions were observed with aromatic/hydrophobic contacts with W337/286^{6x48} in TM6 and ionic/polar/hydrogen contacts with Y367/316^{7x43} in TM7. The importance of these residues for ligand binding have also been reported in the literature (Chan et al., 2016; Jiménez-Rosés et al., 2022; Sato et al., 1999; Strader et al., 1989). Interestingly, β 1-AR agonism is specifically linked to residues in TM3 and TM6 especially F341^{6.52x52} and N344^{6.55x55}, unlike β 2-AR agonism (Jiménez-Rosés, Morgan et al. 2022). Early previous studies indicated F341/290^{6.52x52} in TM6 is important for the interactions including aromatic catechol ring of catecholamine agonist in the human β 2-AR and has been proposed to be involved in the rotamer “toggle switch” allows receptor activation (Kobilka, 2007a; Shi et al., 2002; Swaminath et al., 2005). Moreover, N344/293^{6.55x55} in TM6 has been proposed to be crucial for the stereospecific agonist recognition and activation of the human β 2-AR (Wieland et al., 1996). On the other hand, existing agonist and antagonist bound human β 2-AR interacts with except one agonist bound human β 2-AR (PDB ID : 4QKX (Weichert et al., 2014)). This might explain why interactions with N344/293^{6.55x55} were not specific for agonist for human β 2-AR and interactions with F341/290^{6.52x52} were not captured by some active state human β 2-AR. One previous study (Baker et al., 2003) investigating agonist effect measurement of β -blockers at human β 1-AR demonstrated that mutations at F341^{6.52x52} and N344^{6.55x55} effected agonist action of some antagonist not all antagonist in their study suggesting that these interactions are key modulators of β 1-AR activity and can be explored to design novel ligands. Moreover, in the absence of inactive state human β 1-AR bound antagonist ligand it is hard to determine whether F341^{6.52x52} and N344^{6.55x55} in TM3 play decisive role in agonism at human β 1-AR. Our study

provides preliminary data for the differences between β 1-AR and β 2-AR agonism. Being able to identify which atoms of the ligand mediate agonist and antagonist activity could be used to improve the quality of further docking studies of human β 1-AR, by incorporating the ligand activity in the scoring function (Jiménez-Rosés et al., 2022). On the other hand, existing scoring functions are not capable of determining the possible correct binding poses in large-scale docking studies. Currently, we exactly know binding sites of these four GPCR structure bound to adrenaline (PDB ID : 7BTS, active state (Xu et al. (2021))), carazolol (PDB ID: 7BVQ, inactive state (Xu et al. (2021))), BI-167107 (PDB ID: 7BU7, active state (Xu et al. (2021))), noradrenaline (PDB ID: 7BU6, active state (Xu et al. (2021))) in literature. Therefore, future structural studies with other ligands may expand the detailed analysis of important interactions at human β 1-AR.

The study also classified the large-scale ligand library as agonist and antagonist for human β 1-ARs using statistical analysis and classifier (**Figure 23**). Interestingly, the differences for the accurate prediction of classification between pairwise correlation analysis and machine learning approach were clearly observed in classification matrixes (**Figure 21**). Like our previous computational study on human β 2-ARs (Jiménez-Rosés et al., 2022), we observed that ML approach significantly reduced wrong classification estimations for human β 1-ARs. Therefore, the study suggests that application of machine learning approach can provide better predictions than pairwise correlation analysis for classification of ligands at human β 1-ARs and also other GPCRs. In this study, we used smaller grid box for molecular docking experiments and knowledge of the specific contacts (ionic contacts with D138^{3.32x32} residue and hydrogen bond with N363^{7.39x38} residue) to eliminate wrong ligand poses. However, we did not optimize the docking process to obtain the correct orientation of the ligand

binding poses. Therefore, the inaccuracy in the orientation of the ligand binding poses affects the quality of our classification predictions. Nevertheless, important ligand-receptor interactions of agonism and antagonism for human β 2-AR in literature (were captured as crucial by this study focused on human β 1-ARs (**Figure 19 and Figure 20**). Hence, from large dataset of ligand binding poses, we were able to observe that our data support the hypothesis that ligand pharmacological activity are driven by specific atomic ligand-receptor interactions. Using ML approaches, we were able to average ‘wrong’ poses themselves out and identify the structure-activity relationship for human β 1-ARs (**Figure 23**)

In addition to computational study (**Chapter 3**), this thesis (in **Chapter 4**) investigated the answers to several questions related to kinetic binding characterization of four known β -blockers, Nebivolol, Carvedilol, Bisoprolol and Esmolol, at human β 1-AR: Can we characterize the optimal fluorescent tracer for determination of kinetic binding parameters of unlabelled ligands for human β 1-AR? Can we use TR-FRET based approach for the characterization studies for human β 1-AR? Can we find the correct ligand binding poses and determine the atomic interactions of these four ligands for human β 1-AR? Is there a connection between the atomic interactions and the kinetic binding parameters of these four ligands for human β 1-AR?

Initially, we developed a fluorescence-based TR-FRET kinetic ligand binding assay, as a modern, environmentally safe and higher throughput alternative to radioligand binding assays employed earlier. We identified a fluorescent ligand with favourable kinetic characteristics, to be used a tracer for subsequent characterisation of kinetics of binding and dissociation of the unlabelled ligands. The study revealed (S)-propranolol-green tracer has faster binding kinetics than (S)-propranolol-red

(**Table 7 and Figure 29**), hence it is optimal tracer to accurately determine the binding kinetics of unlabelled ligands for human β 1-AR. Then, we characterized the binding kinetics of four known β -blockers (Nebivolol, Carvedilol, Bisoprolol and Esmolol). According to our results (**Table 9**), β 1-selective Nebivolol was the slowest dissociating β -blocker and had the highest affinity for human β 1-AR. In contrast, Esmolol was the fastest dissociating β -blocker and showed the lowest affinity for human β 1-AR. Carvedilol was the second slowest dissociating β -blocker and followed by third slowest dissociating β -blocker β 1-selective Bisoprolol. Our findings are consistent with previous studies determining the equilibrium binding properties of Nebivolol, Bisoprolol and Carvedilol for human β 1-AR using radioligand binding assays (Baker, 2010b; Sykes et al., 2022). From our data, it is clear that dissociation rates of the third-generation β -blockers (Nebivolol and Carvedilol) more slower than the dissociation rates of the second-generation generation β -blockers (Bisoprolol and Esmolol). β -blockers do not show homogenous properties and Nebivolol is highly selective β -AR antagonist with a novel pharmacologic profile compared to others (Ferri, 2021; Fongemie and Felix-Getzik, 2015; Munzel and Gori, 2009). Our findings elucidated also the difference between Nebivolol and the others (Carvedilol, Bisoprolol and Esmolol). We revealed that dissociation rate constant (k_{off}) plays key role for determination of kinetic binding characteristics of unlabelled ligands at human β 1-AR.

Moreover, molecular docking studies also allowed us to unravel the possible interaction between investigated antagonists and human β 1-AR. Our approach could generate possible correct poses for Nebivolol, Carvedilol and Bisoprolol (**Figure 30**). An antagonist has higher binding affinity to inactive state; thus, we were able to obtain inactive state human β 1-ARs bound Nebivolol, Carvedilol and Bisoprolol. The role of

interactions with ECL2 and TM7 in binding kinetics were reported on other GPCRs (Jager et al., 2007; Klco et al., 2005). In consistent with these findings, we revealed that dissociation of the Carvedilol might mainly drive by hydrophobic/aromatic interactions with T220 in ECL2 and F359 in TM7. Therefore, presence of hydrophobic/aromatic interactions with ECL2 and TM7 in Nebivolol might led more stable binding and relatively slower dissociation rate constants compared to Carvedilol. Especially, the differences in flexibility of ECL2 loop may influence binding kinetics of Nebivolol and Carvedilol at human β 1-AR. On the other hand, we revealed that dissociation of Bisoprolol might be affected by interactions with specific residues in TM2, TM3, TM5 and TM7. The five residues (I118^{2.64x63} and V119^{2.65x64}, in TM2, V360^{7.36x35}, W364^{7.40x39} and Y367^{7.43x42} in TM7) in observed our study were previously shown to be involved in the dissociation at β 1-AR (Gonzalez et al., 2011). Additionally, we revealed that hydrophobic/aromatic interactions with V142^{3.36x36} in TM3 and Y224^{5.38x39} in TM5 and polar/ionic/hydrogen bond with S228^{5.42x43} in TM5 might be critical also for stable binding of Bisoprolol and preference of interactions with T135^{3.29x29} in TM3 instead of V142^{3.36x36} influence the binding kinetics. Interestingly, a previous radioligand binding study (Lim et al., 2023) indicated that I118^{2.64x63} in TM2 is responsible for the selective binding of Nebivolol for the human β 1-AR. On the other hand, in their computational studies they did not observe any interaction between I118^{2.64x63} and Bisoprolol. Therefore, presence of hydrophobic/aromatic interaction with I118^{2.64x63} may influence stable binding of Nebivolol compared to Bisoprolol. All β -blockers used in the treatment of the cardiovascular disease have at least one chiral centre (Siebert et al., 2008). Compared to other β -blockers, Nebivolol possess four chiral centres. It is not surprising to obtain possible correct ligand poses of Nebivolol for three structures due to the relative

rigidity of larger Nebivolol. According to our data, differences between dissociation rate or residence time in Nebivolol, Carvedilol and Bisoprolol might be the results of specific ligand-receptor interactions. Our findings might provide a new rationale for further studies aim to discover new drugs with less side effects.

Although tremendous efforts have been made, determination of possible correct poses in docking is very challenging. Due to the high number of chiral centres, one recent study (Lim et al., 2023) did not even attempt to dock Nebivolol into human β 1-AR models or experimental human β 1-ARs. On the other hand, they preferred to dock smaller antagonists Bisoprolol and Esmolol into inactive state homology model of human β 1-AR derived from turkey β 1-AR template (PDB ID: 2VT4 (Warne et al., 2008)). Interestingly, although human β 1-ARs have been available since 2020 they did not use existing human β 1-ARs. Especially, the high-resolution inactive state experimental human β 1-AR allows us to predict possible correct poses of known antagonists and reveal their detailed ligand-receptor interaction information. One of our most important findings in **Chapter 4** is that we revealed specific atomic interactions between three known β -blockers Nebivolol, Carvedilol and Bisoprolol and human β 1-AR (**Figure 30**). Another most important finding is that our interaction data obtained from computational studies might be explain differences in binding kinetics of these ligands at human β 1-AR. In contrast, our approach failed to create possible correct poses for Esmolol. As mentioned above, larger antagonists with similar structure, Nebivolol and Carvedilol, can have similar interactions with binding site of human β 1-AR. Considering similar interactions of structurally similar but larger ligands, it is reasonable to suppose that antagonist Esmolol might interact with similar residues of human β 1-AR as the structurally similar antagonist Bisoprolol. However, it is difficult to predict which residues of human β 1-AR might interact with

Esmolol accurately. Esmolol is the ultra-short acting β -blocker and its molecular structure is smaller than other three β -blocker used in this study, but it have a methyl butyrate (Blanski et al., 1988). These properties of Esmolol might explain the difficulties in obtaining the possible correct ligand poses from docking experiments. This limitation can be overcome by employing flexible docking and adding water molecules for ligand binding site or increasing the number of experiments.

In future, computational studies will be carried out with experimental human β 1-ARs to study interactions between human β 1-ARs and their ligands. Especially, agonist bound active state human β 1-ARs will provide structural information for discovery of new agonists whereas inverse agonists bound inactive state human β 1-AR will be preferred to detect new antagonist. The application of ML may make a tremendous contribution to finding new GPCR-targeted therapeutics from large-scale compound libraries for human β 1-AR and uncovering atomic interactions between ligands and the receptor. Mutagenesis studies can also test the predicted interacting residues. Future research taking advantage of flexible docking may be able to provide a possible solution to limitation in our study. However, our computational approach can be applied to other GPCRs, especially less studied β -AR subtype β 3-AR to obtain preliminary interaction data for agonism and antagonism. On the other hand, association and dissociation kinetics are important descriptors for the optimization of the drug binding to GPCRs (Swinney et al., 2015) and being able to optimize ligand binding at human β 1-AR facilitates drug discovery. TR-FRET technology can be applied with S-propranolol-green tracer to characterize the binding kinetics of other known β -blockers for human β 1-AR. Thus, a detailed understanding of interactions between human β 1-AR and known β -blockers in living cells can be captured through affinity of ligands and association/dissociation rate constants. Complementary

computational studies can be also performed to investigate relation of atomic interactions between kinetic binding rate constants, ultimately guiding the design of novel ligands with improved ligand residency time.

Chapter 6. General Conclusion

In this thesis (**Chapter 3**), we have investigated the hypothesis that ligands have common or specific interactions with β 1-AR to exert their pharmacological actions on them. The study began in 2019 before the determination of the experimental human β 1-ARs. Therefore, homology modelling studies were aimed as first step of the study. With the determination of the experimental human β 1-ARs (Xu et al., 2021), we expanded our study. Our structural analysis on three different homology models revealed that active state turkey β 1-AR template is highly structurally similar to the active state experimental human β 1-AR structure (**Figure 16 and Figure 17**). We applied same methodology in our previous study (Jiménez-Rosés et al., 2022) focused on human β 2-ARs to human β 1-ARs and docked the same large-scale ligand dataset. For molecular docking experiments, using smaller grid box, we limited the search area for ligand binding. Molecular docking aims to predict both the binding mode of a ligand and the affinity of the complex but does not reveal the key interactions for agonism or antagonism (Ballante et al., 2021; Wu et al., 2021). Interaction fingerprints derived from large scale ligand dataset bound to human β 1-ARs would thus enable determination of ligand pharmacological activity. Comparability of the results derived human β 1-ARs and human β 2-ARs facilitated to detect common and specific atomic interactions from agonism and antagonism (**Figure 19 and Figure 20**). For both subtypes, we found that the most important residues that contribute to the ligand receptor interactions of agonists are located on

TM5 while the decisive residues of antagonists are gathered on TM6 and TM7. This finding was consistent with the previous studies. Chan et al., 2016; Jiménez-Rosés et al., 2022; Sato et al., 1999; Strader et al., 1989). However it is not clear the roles of the F341^{6.52x52} and N344^{6.55x55} residues in agonist binding at human β 1-AR in literature (Baker et al., 2003; Xu et al., 2021), we observed that residues in TM3 and TM6 especially F341^{6.52x52} and N344^{6.55x55} are important for human β 1-AR agonism compared to human β 2-AR (Jiménez-Rosés et al., 2022). We have also shown that ML approach provides better predictions for classification of ligands than pairwise correlation approach by reducing the number of the wrong poses (**Figure 23**). Availability of both active and inactive state experimental human β 1-ARs provided us to capture the differences between the mechanism of agonism and antagonism. Moreover, our study implies that closely related homology model can provide similar predictions like active state experimental human β 1-AR (**Figure 21A and Figure 21B**). Despite the limitations of the study, our findings shown that specific atomic interactions mediate the mechanism of agonism and antagonism at human β 1-AR. Our findings provides a preliminary picture of ligand pharmacological activity in human β 1-ARs for further structure-based drug design studies.

In this thesis (**Chapter 4**), we have investigated whether TR-FRET assays can be alternative to radioligand binding assays for the measurement of the four known β -blockers, Nebivolol, Carvedilol, Bisoprolol and Esmolol, at human β 1-AR. We revealed that (S)-propranolol-green fluorescent tracer has faster binding kinetics than (S)-propranolol-red (**Table 7 and Figure 29**). After then, we found significant differences between second generation β -blockers (Nebivolol and Carvedilol) and third generation β -blockers (Bisoprolol and Esmolol). Among the ligands we studied, β 1-selective blocker Nebivolol was the slowest dissociating ligand whereas non-

selective Carvedilol was the second slowest dissociating β -blocker (**Table 9**). On the other hand, other β 1-selective blocker Bisoprolol had faster dissociation rate than non-selective β -blocker Carvedilol. The fastest dissociation rate constant were observed for other β 1-selective blocker Esmolol. Our findings for Nebivolol, Bisoprolol and Carvedilol are consistent with the previous radioligand binding assays described in the literature (Baker, 2010b; Sykes et al., 2022). Our findings imply that dissociation rate constant (k_{off}) is the most important determinant for the kinetic binding characteristics of unlabelled ligands at human β 1-AR. Moreover, these findings also mean that differences in kinetic binding parameters of them might be dependent on generation of the β -blocker and their chemical structures. According to our study, fluorescent β 2-AR antagonist (S)-propranolol-green can also be used for kinetic binding studies at human β 1-ARs in the absence of specific β 1-AR fluorescent tracer. As complementary to binding kinetics experiments, we have performed computational experiments to test whether the specific interactions mediate binding kinetics of the β -blockers used in the study (**Figure 30**). The availability of inactive state experimental human β 1-AR structure enhanced the probability of formation of antagonist bound human β 1-AR complex. We found that the lack of hydrophobic/aromatic interactions with T220 in ECL2 and F359^{7.35x34} in TM7 might lead to relatively faster dissociation of Carvedilol compared to Nebivolol. On the other hand, the absence of the hydrophobic/aromatic interactions with I118^{2.64x63} and V119^{2.65x64}, in TM2, V360^{7.36x35}, W364^{7.40x39} and 367^{7.43x42} in in TM7 might play important role in the relatively slower dissociation of Bisoprolol. The importance of these interactions has previously been demonstrated for another ligands by several studies (Avlani et al., 2007; Gonzalez et al., 2011; Hauser et al., 2021; Jager et al., 2007; Klco et al., 2005; Lim et al., 2023). Our findings imply that specific

atomic interactions might explain the differences in binding kinetic rates of the known β -blockers at atomic level although prediction of the correct binding of ligand binding poses remains a great challenge. Moreover, our findings indicate that molecular interactions can differ according to the chemical structure of the ligands. Therefore, our interaction data derived from larger antagonists Nebivolol and Carvedilol can be used for designing of another larger antagonist whereas the interaction information obtained from smaller antagonist Bisoprolol can be useful for developing of another smaller ligands at human β 1-AR. Despite the limitations of the computational part, our findings have shown that the combination of binding kinetics assays and computational experiments can provide detailed picture of the kinetic mechanism of the antagonists at human β 1-ARs. Taken together, the experimental and computational data in **Chapter 4** can be used as starting point for further studies to capture

Chapter 7. References

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Chapter 8. APPENDIX A

Table A1: Analysis of the correct binding poses information of 9 ligand for each human structure according to RMSD values. Green check mark represents the correct binding poses, red cross represents the wrong binding poses and orange box represents the best binding poses.

Ligand Name	Reference PDB IDs	Homology Model Human β 1-AR										Active State Human β 1-AR										Inactive State Human β 1-AR									
		1	2	3	4	5	6	7	8	9	10	1	2	3	4	5	6	7	8	9	10	1	2	3	4	5	6	7	8	9	10
Dobutamin	2Y00,2Y01,6H7L	✓	✓	✗	✗	✓	✗	✗	✗	✗	✓	✗	✗	✗	✗	✗	✓	✗	✗	✓	✗	✓	✓	✗	✓	✗	✗	✗	✗	✗	✗
Carmoterol	2Y02	✗	✗	✗	✓	✓	✗	✓	✗	✗	✗	✓	✓	✓	✓	✓	✓	✗	✗	✗	✗	✓	✓	✓	✓	✓	✓	✗	✓	✗	✗
Isoprenaline	2Y03,6H7J,7JJ0	✓	✓	✗	✓	✗	✗	✗	✗	✗	✗	✓	✓	✗	✗	✗	✗	✓	✓	✗	✓	✓	✓	✗	✗	✗	✗	✗	✗	✗	✗
Salbutamol	2Y04,6H7N	✓	✓	✗	✗	✗	✗	✗	✗	✗	✗	✓	✓	✓	✓	✗	✗	✗	✓	✗	✗	✓	✓	✓	✓	✗	✗	✓	✗	✗	✗
(S)-Carvedilol	4AMJ	✗	✗	✗	✗	✗	✗	✗	✗	✓	✗	✓	✓	✓	✓	✗	✓	✗	✗	✗	✗	✓	✓	✓	✓	✓	✓	✗	✓	✓	✗
Xamoterol	6H7N	✓	✓	✓	✓	✗	✗	✗	✗	✗	✗	✓	✗	✓	✗	✓	✓	✗	✓	✗	✗	✓	✓	✗	✗	✗	✗	✗	✓	✗	✗
(S)-Carazolol	7YCW	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✓	✗	✓	✓	✗	✗	✗	✗	✓	✗	✓	✗	✗	✓	✓	✗	✓	✗	✗	✗
(S)-Carazolol	7BVQ	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✓	✗	✓	✓	✗	✗	✗	✗	✓	✗	✓	✗	✗	✓	✓	✗	✗	✗	✗	✗
BI-167107	7BU7	✓	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✓	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗
L-Epinephrine	7BTS	✗	✓	✗	✓	✓	✗	✗	✗	✓	✗	✓	✗	✗	✓	✓	✗	✗	✗	✗	✗	✗	✗	✓	✗	✓	✓	✗	✗	✓	✗

Chapter 9. APPENDIX B

SMILES	Target
<chem>CCN(C)[C@@H](C)[C@@H](C1=CC=CC=C1)O</chem>	β_2
<chem>COc1cc(CCNCC(COc2ccc(c(c2)O)O)O)ccc1OC</chem>	β_1
<chem>CC(COC1=CC=CC=C1)NC(C)C(C2=CC=C(C=C2)O)O</chem>	β_2
<chem>CC(C)(C)NC[C@H](C1=CC(=CC(=C1)O)O)O</chem>	β_2
<chem>COC1=CC(=CC(=C1OC)OC)CC2C3=CC(=C(C=C3CCN2)O)O</chem>	β_1/β_2
<chem>CC(C)(C)NCC(C1=CC(=CC(=C1)OC(=O)N(C)C)OC(=O)N(C)C)O</chem>	β_2
<chem>CCN(CC)C(=O)NC1=CC(=C(C=C1)OCC(CNC(C)(C)C)O)C(=O)C</chem>	β_1/β_2
<chem>CC(C)(C)NCC(C1=CC(=C(C(=C1)Cl)N)Cl)O</chem>	β_2
<chem>CC(C)(C)NCC(C1=CC(=C(C=C1)O)O)O</chem>	β_2
<chem>C[C@H](CCC1=CC=C(C=C1)O)NCCC2=CC(=C(C=C2)O)O</chem>	β_1
<chem>CC(C)(C)NCC(C1=CC(=C(C(=C1)Cl)N)C(F)(F)F)O</chem>	β_2
<chem>CC(C)NCC(C1=CC(=CC(=C1)O)O)O</chem>	β_2
<chem>C1=CC=C(C=C1)CCCCOCCCCCNCC(C2=CC(=C(C=C2)O)CO)O</chem>	β_2
<chem>CC(C)(C)NCC(C1=CC(=CC(=C1)O)O)O</chem>	β_2
<chem>CC(CC1=CC=C(C=C1)O)NCC(C2=CC(=CC(=C2)O)O)O</chem>	β_1/β_2
<chem>CC1=CC=C(C=C1)C(=O)OC2=C(C=C(C=C2)C(CNC(C)(C)C)O)OC(=O)C3=CC=C(C=C3)C</chem>	β_2
<chem>CC(CCC1=CC=C(C=C1)O)NCCC2=CC(=C(C=C2)O)O</chem>	β_1/β_2
<chem>C1=CC(=C(C=C1C(CN)O)O)O</chem>	β_1
<chem>C[C@H](CC1=CC=C(C=C1)O)NC[C@H](C2=CC(=CC(=C2)O)O)O</chem>	β_2
<chem>C[C@@H](CC1=CC=C(C=C1)O)NC[C@H](C2=CC(=CC(=C2)O)O)O</chem>	β_2
<chem>O=c1ccc2c([nH]1)c(O)ccc2[C@H](CNCCCCCOCC(c1cccc1)(F)F)O</chem>	β_2
<chem>C1=CC(=CC=C1CCCCNC[C@@H](C2=CC(=C(C=C2)O)O)O)O</chem>	β_1
<chem>O=CNc1cc(ccc1O)[C@H](CN[C@@H](Cc1ccc(cc1)OC)C)O</chem>	β_2
<chem>CCN(CC)CCN(CCNCCC1=C2C(=C(C=C1)O)NC(=O)S2)C(=O)CCOCCC3=CC=CC4=CC=CC=C43</chem>	β_2
<chem>COc1cc(NC(=O)CCN2CCC(OC(=O)Nc3ccccc3-c3ccccc3)CC2)c(Cl)cc1CNC[C@H](O)c1ccc(O)c2[nH]c(=O)ccc12</chem>	β_2
<chem>CN(C)C(=O)COc1ccc2c(c1)C[C@@H](NC[C@H](O)c1ccc(O)c(CCO)c1)CC2</chem>	β_2
<chem>CC1=CC=CC=C1CC(C)(C)NCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O</chem>	β_2
<chem>Cc1ccc(C(=O)Oc2ccc(C(O)CNC(C)(C)C)cc2OC(=O)c2ccc(C)cc2)cc1</chem>	β_2

COc1ccc(C[C@@H](C)NC[C@H](O)c2ccc(O)c3[nH]c(=O)ccc23)cc1	β2
CCN(CC)C(=O)Nc1ccc(OCC(O)CNC(C)(C)C)c(C(C)=O)c1	β1/β2
CC(C)NCC(C1=CC(=C(C=C1)N)C#N)O	β1/β2
CC(C)(C)NCC(O)c1cc(Cl)c(N)c(Cl)c1	β2
CC(C)NCC(C1=CC(=C(C(=C1)Cl)N)Cl)O	β2
CC(C)NCC(C1=CC=C(C=C1)O)O	β1/β2
C[C@H](CCc1ccccc1)NC[C@H](O)c1ccc(O)c(C(N)=O)c1	β2
CNCC(c1ccc(c(c1)O)O)O	β1/β2
NCC(c1ccc(c(c1)O)O)O	β1
CC(CCc1ccc(cc1)O)NCCc1ccc(c(c1)O)O	β1/β2
NCCc1ccc(O)c(O)c1	β1
CN1C2=C(C(=O)N(C1=O)C)N(C=N2)CC3OCCO3	β2
C1=CC(=C(C=C1[C@H]([C@@H](C(=O)O)N)O)O)O	β1/β2
CC(Cc1ccc(cc1)O)NCC(c1cc(O)cc(c1)O)O	β1/β2
O=CNc1cc(ccc1O)C(CNC(Cc1ccc(cc1)OC)C)O	β2
C1=CC(=CC(=C1)S(=O)(=O)N)CCCCOCCCCCNC[C@@H](C2=CC(=C(C=C2)O)CO)O	β2
CC1=NCCC2=C1NC3=CC=CC=C23	β2
C1CN[C@H](C2=CC(=C(C=C21)O)O)CC3=CC=C(C=C3)O[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)CO)O)O)O	β2
CCc1cc2CC(Cc2cc1CC)NC[C@@H](c1ccc(c2c1ccc(=O)[nH]2)O)O	β2
CCC(C(C1=CC(=C(C=C1)O)O)O)NC(C)C	β2
CCC(NC(C)C)C(O)c1ccc(O)c(O)c1	β2
CCC(C(C1=CC(=C(C=C1)O)O)O)NC(C)C.CS(=O)(=O)O	β2
CC(NCC(c1ccc(c(c1)O)O)O)C	β1/β2
CC(COc1ccccc1)NC(C)C(O)c1ccc(O)cc1	β2
CNC[C@@H](c1ccc(c(c1)O)O)O	β1/β2
CNC[C@@H](C1=CC(=C(C=C1)O)O)O.C(C(C(=O)O)O)(C(=O)O)O	β1/β2
CN[C@H]([C@@H](c1ccccc1)O)C	β1/β2
CC(C)NC[C@@H](C1=CC(=C(C=C1)O)O)O	β2
OCc1cc(ccc1O)[C@H](CNC(C)(C)C)O	β2

NC[C@@H](c1ccc(c(c1)O)O)O	β1
C[C@@H]([C@@H](C1=CC=CC=C1)O)N(C)C	β1/β2
O=CNc1cc([C@@H](O)CNCCc2ccc(NC[C@H](O)c3ccccc3)cc2)ccc1O	β2
COc1ccc(cc1)CC(NC[C@@H](c1cc(O)cc2c1OCC(=O)N2)O)(C)C	β2
CC(C)NCC(O)c1cc(O)cc(O)c1	β2
CC(C)(C)NCC(C1=NC(=C(C=C1)O)CO)O	β2
CC(C)(C)NCC(O)c1ccc(O)c(CO)n1	β2
CCC(C(c1ccc(c2c1ccc(=O)[nH]2)O)O)NC(C)C	β2
CC[C@@H]([C@@H](C1=C2C=CC(=O)NC2=C(C=C1)O)O)NC(C)C	β2
CC(CC1=CC2=C(C=C1)OCO2)NCC(C3=CC(=C(C=C3)O)O)O	β1/β2
CC(Cc1ccc2c(c1)OCO2)NCC(O)c1ccc(O)c(O)c1	β1/β2
COc1cc(CCNC[C@@H](c2ccc(cc2)O)O)ccc1OC	β1
C[C@H](CC1=CC=C(C=C1)O)NC[C@@H](C2=CC(=CC(=C2)O)O)O	β2
CC(NCC(c1ccc(cc1)O)O)CCc1ccc(cc1)O	β1/β2
CC(C(C1=CC=C(C=C1)O)O)NCCC2=CC=C(C=C2)O	β2
CC(NCCc1ccc(O)cc1)C(O)c1ccc(O)cc1	β2
COC1=C(C=C(C=C1)CCNCC(COC2=CC(=C(C=C2)O)O)O)OC	β1
OCc1cc(ccc1O)C(CNC(C)(C)C)O	β2
OCc1cc(ccc1O)C(CNCCCCCOCCCCc1ccccc1)O	β2
C1=CC=C(C=C1)CCCCOCCCCCNCC(C2=CC(=C(C=C2)O)CO)O.C1=CC=C2C(=C1)C=CC(=C2O)C(=O)O	β2
C1=CC=C(C=C1)CCOCCCS(=O)(=O)CCNCCC2=C3C(=C(C=C2)O)NC(=O)S3	β2
COc1cc(CCNCC(c2ccc(c(c2)O)O)O)ccc1OC	β1
COC1=C(C=C(C=C1)CCNCC(C2=CC(=C(C=C2)O)O)O)OC	β1
OC(c1cc(O)cc(c1)O)CNC(C)(C)C	β2
CC(C)(C)NCC(C1=CC=CC=C1Cl)O	β2
CC(CC1=CC=C(C=C1)OC)NCC(C2=CC(=C(C=C2)O)NC=O)O	β2
OCc1cc(ccc1O)[C@H](CNCCCCCOCCOCc1c(Cl)ccccc1Cl)O	β2
OC(COc1ccc(cc1)O)CNCCNC(=O)N1CCOCC1	β1
C1COCCN1C(=O)NCCNCC(COC2=CC=C(C=C2)O)O	β1

CC(C)N[C@@H]1CCN2C3=C([C@H]1O)C=CC=C3NC2=O	β2
OC(c1ccc(c(c1)NS(=O)(=O)C)O)CNC(Cc1cccc1)(C)C	β1/β2
CC(C)(CC1=CC=CC=C1)NCC(C2=CC(=C(C=C2)O)NS(=O)(=O)C)O	β1/β2
CC(C)NCC(C1=CC2=C(C=C1)N=CN2)O	β1
B(O)(O)OC1=C(C=C(C=C1))[C@@H](CNC(C)(C)C)O)CO	β2
C1=CC(=C(C=C1C(CNCCCCNC2=C3C(=NC=N2)N(C=N3)[C@H]4[C@@H]([C@@H]([C@H](O4)CO)O)O)O)NC=O)O	β2
C1=CC(=C(C=C1C(CNCCNC2=C3C(=NC=N2)N(C=N3)[C@H]4[C@@H]([C@@H]([C@H](O4)CO)O)O)O)NC=O)O	β2
C1=CC=C(C=C1)C(=O)NC2=CC=C(C=C2)C(=O)C[N+](=O)C3=CC=CC(=C3)NC(=O)C4=CC=CC=C4.[Br-]	β2
CC1(CC2=C(CO1)C(=NC3=C2C4=C(S3)C(=NC=N4)NCCC5CCCO5)C6=CC=CO6)C	β2
C1=CC(=C(C=C1C(CNCCCCNC2=C3C(=NC=N2)N(C=N3)[C@H]4[C@@H]([C@@H]([C@H](O4)CO)O)O)O)N)O	β2
CC1(CC2=C(CO1)C(=NC3=C2C4=C(S3)C(=NC=N4)NCCCO)C5=CC=CO5)C	β2
CN(C)C1=CC=C(C=C1)CN2C/C=C\C(N(C(=O)C2)CC3=CC=C(C=C3)F)C4=CC=C(C=C4)OC	β2
CC1(CC2=C(CO1)C(=NC3=C2C4=C(S3)C(=NC=N4)NCCN(C)C)N5CCCC5)C	β2
COC1=CC=C(C=C1)CSC2=C(C=C(C=C2)C3=C(N4C=CC=CC4=N3)NCC5=CC=CC=C5)OC.C(=O)(C(F)(F)F)O	β2
C[C@@H](C1=CC=C(C=C1)OC)NC[C@@H](C2=CC(=C(C=C2)O)NC=O)O.C(=C/C(=O)O)\C(=O)O	β2
CCC(=O)N1CCC2=C1C(=CC(=C2)Br)S(=O)(=O)N(C)C3=CC=C(C=C3)OC	β2
CC[C@H](CC1=CC=C(C=C1)O)NC[C@@H](C2=CC(=CC(=C2)O)O)O	β2
CCC1=CC=C(C=C1)OCC(=O)NC2=CC(=C(C=C2)C3=NC4=CC=CC=C4O3)O	β2
C[C@H](CC1=CC=C(C=C1)OCCCCCN2C(=O)C3CCCCC3C(=N2)C4=CC(=C(C=C4)OC)OC)NC[C@@H](C5=CC(=C(C=C5)O)NC=O)O	β2
C1=CC=C2C(=C1)C(=NC(=N2)NC3=CC=CC=C3O)NCC4=CC=CO4.C1	β2
CC1(CC2=C(CO1)C(=NC3=C2C4=C(S3)C(=NC(=N4)SC)SCCO)C5=CC=CO5)C	β2
CC1=NCCC2=C1NC3=CC=CC=C23.C1=C(C=C(C=C1[N+](=O)[O-])O)[N+](=O)[O-][N+](=O)[O-]	β2
CCOC(=O)C1=CC=C(C=C1)NC(=O)CC2=COC3=C2C=C4CCCC4=C3	β2
CC1=NN(C(=O)C1N=NC2=CC=C(C=C2)F)C(=S)N	β2
CCN(CCO)C1=NC=NC2=C1SC3=C2C4=C(COC(C4)(C)C)C(=N3)CC(C)C	β2
CC1(CC2=C(CO1)C(=NC3=C2C4=C(S3)C(=NC=N4)N5CCN(CC5)CCO)N6CCCC6)C	β2
C1=CC(=C(C=C1C(CNCCCCCNC2=C3C(=NC=N2)N(C=N3)[C@H]4[C@@H]([C@@H]([C@H](O4)CO)O)O)O)NC=O)O	β2
CCCCCN1C(=C(C(=O)NC1=O)C=NC2=C(N(N(C2=O)C3=CC=CC=C3)C)C)O	β2

COC(=O)C1=C(C[C@@H]2CC[C@H]1N2C(=O)NCC3=CC(=CC=C3)F)C4=CC(=CC=C4)OCC5=CC=CC=C5	β2
CC1(CC2=C(CO1)C(=NC3=C2C4=C(S3)C(=NC=N4)NCCN)N5CCOCC5)C	β2
CC1=CC(=CC=C1)NC2=NN=C(C3=CC=CC=C32)C4=CC=C(C=C4)C(=O)N5C[C@H]6C[C@@H](C5)C7=CC=CC(=O)N7C6	β2
CC1(CC2=C(CO1)C(=NC3=C2C4=C(S3)C(=NC=N4)NCCO)C5=CC=CO5)C	β2
CC(CC1=CC=C(C=C1)O)NCC(C2=CC(=C(C=C2)O)O)O.C1=CC=C(C=C1)C(=O)O	β2
C1=CC(=C(C=C1C(CNCCOCCOCCNC2=C3C(=NC=N2)N(C=N3)[C@H]4[C@@H]([C@@H]([C@H](O4)CO)O)O)O)NC=O)O	β2
CC1(CC2=C(CO1)C(=NC3=C2C4=C(S3)C(=NC=N4)NCCCOC)C5=CC=CO5)C	β2
C1C2=C(C(=CC(=C2)[N+](=O)[O-])CSC3=NC(=CC(=N3)N)N)OCO1	β2
CC(C)NC[C@H](C1=CC(=C(C=C1)O)O)O.C(C(C(=O)O)O)(C(=O)O)O	β2
CC(C)CC1=NC2=C(C3=C1COC(C3)(C)C)C4=C(S2)C(=NC=N4)NCC5=CC=CO5	β2
C1CC2=C(C1)C(=NC3=C2C4=C(S3)C(=NC=N4)NCCN5CCOCC5)N6CCOCC6	β2
CC(CNC1=CC=CC(=C1)C2=C(C=C(C=C2)C(=O)O)C(=O)O)NCC(C3=CC(=CC=C3)C1)O	β1
C1=CC(=CC(=C1)NCCNCC(C2=CC(=CC=C2)C1)O)C3=C(C=CN=C3)C(=O)O	β1
CC(C)(C)NCC(COC1=C(C=C(C(=C1)O)O)F)O	β1
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNC2CCN(CC2)C3=CC=C(C=C3)C(=O)O)O)O	β1
CC(C)(C)C1=CC=C(C=C1)CNC(=O)NC2=CC=CC(=C2)CCNCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O	β2
CC(CC1=CC=C(C=C1)OCC2=NO[N+](=C2C(=O)N)[O-])NCC(C3=CC(=CC(=C3)O)O)O	β2
COCCNCC1=CC=CC(=C1)CCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O	β2
CC1=C2C(=C3C=CC=CC3=N2)CCN1	β2
CCCC1=CC=C(C=C1)CCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O	β2
CCCCN(CC(=O)O)C(=O)C1=CC=C(C=C1)N2CCC(CC2)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O	β2
CCC1=C(C=C2CC(CC2=C1)NCC(C3=C4CCC(=O)NC4=C(C=C3)O)O)CC	β2
C1=CC=C(C=C1)CCNC(=O)NC2=CC=CC(=C2)CCNCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O	β2
CCOC1=CC=C(C=C1)NC2=CC=C(C=C2)CCNCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O	β2
COC1=C(C=C(C=C1)C2=NN(C(=O)C3C2CCCC3)CCCCNCC(C4=CC(=C(C=C4)O)NC=O)O)OC	β2
C1C(C1NCC2=CC=CC(=C2)CCNCCC3=C4C(=C(C=C3)O)NC(=O)S4)C5=CC=CC=C5	β2
COC1=C(C=C(C=C1)C2=NN(C(=O)C3C2CCCC3)CCCCCNCC(C4=CC(=C(C=C4)O)NC=O)O)OC	β2
CCOC1=CC=C(C=C1)NC2=CC=C(C=C2)CCNCC(C3=CC(=C(C=C3)O)CO)O	β2
C1=CC(=C(C=C1C(CNCCCCCNC2=NC=NC3=C2N=CN3C4C(C(C(O4)CO)O)O)O)NC=O)O	β2

CC(CC1=CC=C(C=C1)OCCCCN2C(=O)C3CCCCC3C(=N2)C4=CC(=C(C=C4)OC)OC)NCC(C5=CC(=C(C=C5)O)NC=O)O	β2
CC(CC1=CC=C(C=C1)OCC2=NON=C2C(=O)N)NCC(C3=CC(=CC(=C3)O)O)O	β2
CC1=CC=C(C=C1)NC(=O)CCCC(C)NCC(COC2=CC=CC3=CC=CC=C32)O	β2
C1C(CC2=CC=CC=C21)NCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O	β2
C1=CC=C(C(=C1)CCNCC2=CC=CC(=C2)CCNCC(C3=C4C(=C(C=C3)O)NC(=O)S4)O)F	β2
CC1=CC=CC2=C1NC=C2CCNCC3=CC=C(C=C3)CCNCC(C4=C5C(=C(C=C4)O)NC(=O)S5)O	β2
CCOC1=NO[N+](=C1S(=O)(=O)C2=CC=CC=C2)[O-]	β2
C1=CC=C(C=C1)CNCC2=CC=CC(=C2)C3=CC(=CC=C3)CCNCC(C4=C5C(=C(C=C4)O)NC(=O)S5)O	β2
C1CCC(CC1)C2CCCC2NCC(C3=C4C(=C(C=C3)O)NC(=O)S4)O	β2
C1CC(C(C1)NCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O)C4=CC=CC=C4	β2
COC1=C(C=CC(=C1Cl)NC(=O)CCN2CCC(CC2)OC(=O)NC3=CC=CC=C3C4=CC=CC=C4)CNCC(C5=C6C=CC(=O)NC6=C(C=C5)O)O	β2
C(C1=NO[N+](=C1C(=O)N)[O-])O	β2
COC1=C(C=C(C=C1)C(=O)NC2=C(C=NC=C2Cl)Cl)OCCCCNCC(C3=CC(=C(C=C3)O)CO)O	β2
CC(CC1=CC=C(C=C1)OC2=NON=C2S(=O)(=O)C3=CC=CC=C3)NCC(C4=CC(=CC(=C4)O)O)O	β2
COC1=C(C=C(C=C1)C(=O)NC2=C(C=NC=C2Cl)Cl)OCCCCCNCC(C3=CC(=C(C=C3)O)CO)O	β2
COC1=C(C=C(C=C1)C(=O)NC2=C(C=NC=C2Cl)Cl)OCCCNCC(C3=CC(=C(C=C3)O)CO)O	β2
COC1=C(C=C(C=C1)C(=O)NC2=C(C=NC=C2Cl)Cl)OCCCCCNCC(C3=CC(=C(C=C3)O)CO)O	β2
C1CN(CCC1OC(=O)NC2=CC=CC=C2C3=CC=CC=C3)CCCCCNCC(C4=C5C=CC(=O)NC5=C(C=C4)O)O	β2
CC(CC1=CC=C(C=C1)OCCCCCN2C(=O)C3CCCCC3C(=N2)C4=CC(=C(C=C4)OC)OC)NCC(C5=CC(=C(C=C5)O)NC=O)O	β2
CC(CC1=CC2=CC=CC=C2C=C1)NCC(C3=CC(=CC(=C3)O)O)O	β2
C1=CC=NC(=C1)CCNCC2=CC=C(C=C2)CCNCC(C3=C4C(=C(C=C3)O)NC(=O)S4)O	β2
C1CCC(C1)C2CCCC2NCC(C3=C4C(=C(C=C3)O)NC(=O)S4)O	β2
COC1=C(C=C(C=C1)C2=NN(C(=O)C3C2CCCC3)CCCCNCC(C4=CC(=C(C=C4)O)CO)O)OC	β2
C1=CC=C(C=C1)NC(=O)NC2=CC=CC(=C2)CCNCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O	β2
CC1=CC=C(C=C1)NC(=O)CCCC(C)NCC(COC2=CC=C(C=C2)NC(=O)C)O	β2
C1=CC(=C(C=C1C(CNCCCCNC2=NC=NC3=C2N=CN3C4C(C(C(O4)CO)O)O)O)O)NC=O)O	β2
CC(CC1=CC=C(C2=CC=CC=C12)OC)NCC(C3=CC(=CC(=C3)O)O)O	β2
COC1=C(C=C(C=C1)C2=NN(C(=O)C3C2CCCC3)CCCCCNCC(C4=CC(=C(C=C4)O)CO)O)OC	β2
C1=CC(=CC(=C1)NC(=O)NCC2=CC=CC(=C2)C(=O)N)CCNCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O	β2
CC(CCCCC(=O)NC1=CC=C(C=C1)C(F)(F)F)NCC(COC2=CC=CC3=CC=CC=C32)O	β2

<chem>COC1=C(C=C(C=C1)C2=NN(C(=O)C3C2CCCC3)CCCCNCC(C4=CC(=C(C=C4)O)NC(=O)O)OC</chem>	β2
<chem>COC1=C(C=C(C=C1)C2=NN(C(=O)C3C2CCCC3)CCNCC(C4=CC(=C(C=C4)O)NC(=O)O)OC</chem>	β2
<chem>CC(C1=CC=CC=C1)NCC2=CC=CC=C2C3=CC=C(C=C3)CCNCCC4=C5C(=C(C=C4)O)NC(=O)S5</chem>	β2
<chem>CCCCOC1=CC=CC(=C1)CCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O</chem>	β2
<chem>CC1=CC=CC(=C1)C2CCCC2NCC(C3=C4C(=C(C=C3)O)NC(=O)S4)O</chem>	β2
<chem>CCC1=CC=CC(=C1)C2CCCC2NCC(C3=C4C(=C(C=C3)O)NC(=O)S4)O</chem>	β2
<chem>CCCCC1=CC(=CC=C1)CCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O</chem>	β2
<chem>CS(=O)(=O)NC1=C(C=CC(=C1)C(CNC2CCN(CC2)C3=CC=C(C=C3)C(=O)N4CCCC4C(=O)O)O)O</chem>	β2
<chem>C1=CC=C(C=C1)CCCN(C(=O)NC2=CC=CC(=C2)CCNCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O</chem>	β2
<chem>COC1=C(C=C(C=C1)C2=NN(C(=O)C3C2CCCC3)CCCCNCC(C4=CC(=C(C=C4)O)CO)O)OC</chem>	β2
<chem>CC1=NON=C1COC2=CC=C(C=C2)CC(C)NCC(C3=CC(=CC(=C3)O)O)O</chem>	β2
<chem>CC1=[N+](ON=C1COC2=CC=C(C=C2)CC(C)NCC(C3=CC(=CC(=C3)O)O)O)[O-]</chem>	β2
<chem>C1CN(CCC1C2=CC=CC=C2)CC3=CC=CC(=C3)CCNCC(C4=C5C(=C(C=C4)O)NC(=O)S5)O</chem>	β2
<chem>C1CC(C(C1)OCC2=CC=CC=C2)NCC(C3=C4C(=C(C=C3)O)NC(=O)S4)O</chem>	β2
<chem>CC(CC1=CC=C(C=C1)OC2=NO[N+](=C2S(=O)(=O)C3=CC=CC=C3)[O-])NCC(C4=CC(=CC(=C4)O)O)O</chem>	β2
<chem>C1CN(CC1C(C2=CC=CC=C2)(C3=CC=CC=C3)C(=O)N)CCCCCCCCNCC(C4=C5C=CC(=O)NC5=C(C=C4)O)O</chem>	β2
<chem>C1CN(CCC1OC(=O)NC2=CC=CC=C2C3=CC=CC=C3)CCCNCC(C4=C5C=CC(=O)NC5=C(C=C4)O)O</chem>	β2
<chem>CCCC1=CC(=CC=C1)CCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O</chem>	β2
<chem>C1CN(CCC1OC(=O)NC2=CC=CC=C2C3=CC=CC=C3)CCCCCCCCNCC(C4=CC(=C(C=C4)O)NC(=O)O</chem>	β2
<chem>C1=CC=C(C=C1)CNCC2=CC=CC(=C2)C3=CC(=CC=C3)CCNCCC4=C5C(=C(C=C4)O)NC(=O)S5</chem>	β2
<chem>C1=CC(=C(C=C1C(CNCCCCNC2=NC=NC3=C2N=CN3C4C(C(C(O4)CO)O)O)O)N)O</chem>	β2
<chem>C[N+](C2CC(CC1C3C2O3)OC(=O)C(C4=CC=CS4)(C5=CC=CS5)O)CCCCCCCCNCC(C6=C7C=CC(=O)NC7=C(C=C6)O)O</chem>	β2
<chem>COC1=CC=CC=C1CNCC2=CC=CC(=C2)CCNCC(C3=C4C(=C(C=C3)O)NC(=O)S4)O</chem>	β2
<chem>COC1=C(C=C(C=C1)C2=NN(C(=O)C3C2CCCC3)CCNCC(C4=CC(=C(C=C4)O)CO)O)OC</chem>	β2
<chem>CC(CCCCC(=O)NC1=CC=C(C=C1)C(F)(F)F)NCC(COC2=CC=C(C=C2)NC(=O)C)O</chem>	β2
<chem>C1=CC=NC(=C1)CCNCC2=CC=CC(=C2)CCNCC(C3=C4C(=C(C=C3)O)NC(=O)S4)O</chem>	β2
<chem>CC(CNC1=CC=CC(=C1)CC(=O)O)NCC(C2=CC(=CC=C2)Cl)O</chem>	β2
<chem>CC(C1=CC=CC=C1)NCC2=CC=CC=C2C3=CC=C(C=C3)CCNCC(C4=C5C(=C(C=C4)O)NC(=O)S5)O</chem>	β2
<chem>C1CN(CCC1OC(=O)NC2=CC=CC=C2C3=CC=CC=C3)CCCCCCCCNCC(C4=C5C=CC(=O)NC5=C(C=C4)O)O</chem>	β2
<chem>CC(CCC1=CC=C(C=C1)O)NCC(C2=CC=C(C=C2)O)O</chem>	β2

CC(C(C1=CC=C(C=C1)O)O)NCCC2=CC(=C(C=C2)OCC(=O)O)C1	β2
CC(CC1=CC=C(C=C1)O)CCCCN2C(=O)C3CCCCC3C(=N2)C4=CC(=C(C=C4)OC)OC)NCC(C5=CC(=C(C=C5)O)NC=O)O	β2
CC1=CC=C(C=C1)C(CNC2=CC=C(C=C2)CCNCC(C3=CC(=C(C=C3)O)CO)O)O	β2
C1=CC(=C(C=C1)C(CNCCOCCOCCNC2=NC=NC3=C2N=CN3C4C(C(C(O4)CO)O)O)O)NC=O)O	β2
CCC1=C(C=C2CC(CC2=C1)NCCC3=C4C=CC(=O)NC4=C(C=C3)O)CC	β2
CC(C)NC1CCN2C3=C(C1O)C=CC=C3NC2=O	β2
C1=CC(=CC(=C1)NC(=O)NCC2=C(C=CC=C2C1)Cl)CCNCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O	β1/β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNC2CCN(CC2)C3=CC=C(C=C3)NC(=O)CC(=O)O)O)O	β1/β2
CC(CNC1=CC=C(C=C1)CC(=O)NS(=O)(=O)C)NCC(C2=CC(=CC=C2)Cl)O	β1/β2
C1=CC=C(C=C1)CNC(=O)NC2=CC=CC(=C2)CCNCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O	β1/β2
C1=CC(=C(C=C1)C(CN)O)F)O)O	β1/β2
CC(C)(C)NCC(COC1=CC(=C(C=C1)O)O)O	β1/β2
CC(CNC1=CC=CC=C1)NCC(C2=CC(=CC=C2)Cl)O	β1/β2
C1=CC=C(C=C1)OC2=CC=CC(=C2)NC(=O)NC3=CC=CC(=C3)CCNCC(C4=C5C=CC(=O)NC5=C(C=C4)O)O	β1/β2
CC(CNC1=CC=C(C=C1)CNS(=O)(=O)C)NCC(C2=CC(=CC=C2)Cl)O	β1/β2
CCCCN(C1=CC=C(C=C1)N2CCC(CC2)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O)C(=O)CC(=O)O	β1/β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNC2CCN(CC2)C3=CC=C(C=C3)C(=O)NCC(=O)O)O)O	β1/β2
CC(C)(C)NCC(COC1=C(C(=C(C=C1)O)O)F)O	β1/β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNC2CCN(CC2)C3=CC=C(C=C3)CCC(=O)O)O)O	β1/β2
CC(CNC1=CC=C(C=C1)C(=O)O)NCC(C2=CC(=CC=C2)Cl)O	β1/β2
CC(CNC1=CC=C(C=C1)CNC(=O)C)NCC(C2=CC(=CC=C2)Cl)O	β1/β2
CC1=CC=C(C=C1)CNC(=O)CC2=CC=C(C=C2)NCC(C)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
CCCCN(C1=CC=C(C=C1)N2CCC(CC2)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O)S(=O)(=O)CC(=O)O	β1/β2
CC1=CC=C(C=C1)S(=O)(=O)NCCC2=CC=C(C=C2)NCC(C)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
C1=CC(=CC(=C1)NC(=O)NCC2=CC=C(C=C2)F)CCNCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O	β1/β2
C1=CC=C(C=C1)C(C2=CC=CC=C2)NC(=O)NC3=CC=CC(=C3)CCNCC(C4=C5C=CC(=O)NC5=C(C=C4)O)O	β1/β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNC2CCN(CC2)C3=CC=C(C=C3)COCC(=O)O)O)O	β1/β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNC2CCN(CC2)C3=CC=C(C=C3)C(=O)N)O)O	β1/β2
C1C2CC3CC1CC(C2)(C3)CNC(=O)NC4=CC=CC(=C4)CCNCC(C5=C6C=CC(=O)NC6=C(C=C5)O)O	β1/β2
CCOC(=O)CNC(=O)C1=CC=C(C=C1)N2CCC(CC2)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O	β1/β2

CC(C)CC(C(=O)O)NC(=O)C1=CC=C(C=C1)N2CCC(CC2)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O	β1/β2
CC1=CC=C(C=C1)S(=O)(=O)NC(=O)CC2=CC=C(C=C2)NCC(C)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNC2CCN(CC2)C3=CC=C(C=C3)C(=O)NC(CC4=CC=CC=C4)C(=O)O)O)O	β1/β2
CC(CNC1=CC=C(C=C1)CC(=O)NC2=NC=CS2)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
CC(CNC1=CC=C(C=C1)CC(=O)NS(=O)(=O)C2=CC=CC=C2)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
COC1=CC=CC=C1CNC(=O)NC2=CC=CC(=C2)CCNCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O	β1/β2
C1=CC=C(C=C1)C2=CC=CC=C2NC(=O)NC3=CC=CC(=C3)CCNCC(C4=C5C=CC(=O)NC5=C(C=C4)O)O	β1/β2
C1CCC(CC1)(CC2=CC=C(C=C2)O)NC(=O)C3=CC=CC=C3	β2
CN(C)C1=CC=C(C=C1)C2=NOC(=N2)C3CCN(CC3)S(=O)(=O)C4=CC(=CC=C4)Cl	β2
CN(CC1=CC=CC=C1)S(=O)(=O)C2=CC=C(C=C2)NS(=O)(=O)CC3=CC=CC=C3	β2
C1CC(=O)N(C1)CCCN2=C(C=C(C=C2)C(CC(=O)N)NC(=O)CC3=CC=C(C=C3)Cl)[N+](=O)[O-]	β2
CC1=CC=C(O1)C2=NOC(=N2)C3CCCN(C3)S(=O)(=O)C4=CC=CC(=C4)C(=O)C	β2
C1CC(OC1)COCC(CN2CCN(CC2)S(=O)(=O)C3=C(C=CC(=C3)C(F)(F)F)Cl)O	β2
CN1C2=C(N=C1N3CCN(CC3)C4=CC=CC=N4)N(C(=O)N(C2=O)CC5=CC=C(C=C5)Cl)C	β2
CC1=CC=C(C=C1)S(=O)(=O)N(C)CC(=O)N2CCN(CC2)C3=CC=CC=N3	β2
C1CC(=O)N(C1=O)CC(=O)NC2=NC(=CS2)C3=NC4=CC=CC=C4S3	β2
CC1=NC=C(S1)CN2CCCC(C2)C(=O)NC3=CC=C(C=C3)C4=CC(=CC=C4)F	β2
C1CN(CCN1C2=CC=CC=N2)C(=O)C(C3=CC=CC=C3)C4=CC=CC=C4	β2
CN(CC1=CC=CC=C1F)C2=NC(=NC3=CC=CC=C32)C4=CN=CC=C4	β2
C1=CC=C2C(=C1)NC(=N2)CSC3=NN=C(N3CC4=CC=CO4)C5=CC(=CC=C5)Cl	β2
C1CN(CCN1C2=C(C=C(C=C2)C(CC(=O)N)NC(=O)C3=CC(=CC=C3)Br)[N+](=O)[O-])C4=CC=CC=N4	β2
C1CCN(CC1)C(=O)C2=CC=C(C=C2)OC3CCN(CC3)CC4=CC=C(C=C4)C(F)(F)F	β2
COC(=O)C1=CC=C(C=C1)NC(=O)COC2=CC=C(C=C2)S(=O)(=O)N3CCCCC3	β2
C1=CC(=CC=C1CNC(=O)CCCCCN2C(=O)C3=C(C=CS3)NC2=O)F	β2
CCOC1=CC2=C(C=C1)N=C(S2)NC(=O)CSC3=NC4=C(N3C)N=CC=C4	β2
CCCCN(CCCC)C1=NC2=CC=CC=C2N=C1NS(=O)(=O)C3=CC=C(C=C3)NC(=O)C	β2
CCCCC(=O)NC1=CC=C(C=C1)C(=O)N2CCCC(C2)C(=O)OCC	β2
C1CCN(C(C1)C2=CN=CC=C2)S(=O)(=O)C3=CC=C(C=C3)NC(=O)C4=C(C=CC=C4F)F	β2
CSC1=CC=C(C=C1)CN2CCC(CC2)OC3=CC=C(C=C3)C(=O)N4CCCC4	β2
C1CCN(C1)C(=O)C2=CC=C(C=C2)OC3CCN(CC3)CC4=CC=C(C=C4)F	β2

CC1=NC=C(C=C1)OCC2=CC(=NO2)C(=O)NCC3=CC=C(C=C3)OC(F)(F)F	β2
CCCC1=CC=C(C=C1)OCC2=NC(=NO2)C3=CC=C(C=C3)NC(=O)C4=CC=CO4	β2
CC(=O)NC1=CC=C(C=C1)S(=O)(=O)N(CC2=CN=CC=C2)CC3=CC4=CC=CC=C4NC3=O	β2
C1=CC=C(C=C1)C2=CC=C(C=C2)S(=O)(=O)NC3=CC=CC(=C3)C4=CN5C=CC=NC5=N4	β2
CCOC1=CC=C(C=C1)CNC(=O)C2=CC=C(C=C2)NC(=O)C3=CSCCO3	β2
CCC1=CC=C(C=C1)CN2CCC(CC2)OC3=CC=C(C=C3)C(=O)N4CCCC4	β2
C1=CC=C(C=C1)CCC2=CC=CC=C2C(=O)NC3=CC=CC=C3	β2
CN(CC1=CC=CS1)C2=NC(=NC3=CC=CC=C32)C4=CN=CC=C4	β2
CC1=C(OC2=C1C=C(C=C2)S(=O)(=O)N3CCCCC3)C(=O)N4CCC5=CC=CC=C5C4	β2
CC1=CC=C(C=C1)CSC2=NN=C(N2C)C3=CC=C(C=C3)NC(=O)C	β2
C1=CC=C2C(=C1)C(=O)C3=C(O2)C=C(C=C3)C#CC4=CC(=CC=C4)N	β2
CC(=CCC(C)(C)C1N(CC01)C(=O)C2=CC=CC=C2)C	β2
CCN1CCN(CC1)C2=C(C=C(C=C2)NC(=O)C3=CC=C(O3)[N+](=O)[O-])C1	β2
CN(CC(=O)N1CCN(CC1)C2=NC=CC=N2)S(=O)(=O)C3=CC=C(C=C3)C1	β2
C=CCN1C(=NN=C1SCC(=O)C2=CC(=CC=C2)[N+](=O)[O-])CCNC(=O)C3=CC=CS3	β2
CC1=CC=C(C=C1)N(C)S(=O)(=O)C2=C(C=CC(=C2)C3=CN=C(O3)C4CC4)C	β2
COC1=CC(=NC(=N1)NC(=O)CSC2=NN=C(N2C3CCCCC3)C4=CC=CC=C4)OC	β2
C1COCCN1C(=O)C2=CC=CC=C2C(=O)NC3=CC4=C(C=C3)N=C(S4)SCC5=CC=C(C=C5)C1	β2
CCOC(=O)C1(C=C(C(=O)N1C2=CC=C(C=C2)O)NC3=CC=C(C=C3)O)C	β2
C=CCN1C(=NN=C1SCC(=O)C2=CC=C(C=C2)Br)CCNC(=O)C3=CC=CS3	β2
CCOC(=O)N1CCN(CC1)C(=O)CN(C)S(=O)(=O)C2=CC=C(C=C2)C1	β2
CC1C(=O)N(C(C=CCN1CC2=CC=C(C=C2)N(C)C)C3=CC=C(C=C3)OC)CC4=CC=C(C=C4)F	β2
CCC1=CC=C(C=C1)CNC(=O)C2=CC=C(C=C2)NC(=O)C3=CSCCO3	β2
CC1=C(C=C(C=C1)C2=NC3=C(O2)C=CC=N3)NC(=O)C4=C(C5=CC=CC=C5S4)C1	β2
CCCCCN1C(=O)C(=CNC2=C(N(N(C2=O)C3=CC=CC=C3)C)C)C(=O)NC1=O	β2
CCCNC(=O)C1=C(SN=N1)S(=O)(=O)C2=CC=C(C=C2)C1	β2
C1CC(=O)N(C1)CCNC2=C(C=C(C=C2)C(CC(=O)N)NC(=O)C3=CC=CC=C3)[N+](=O)[O-]	β2
CC1=C(C=C(C=C1)C(=O)OC(C2=CC=CC=C2)C(=O)C3=CC=CC=C3)NC(=O)C	β2
C1COCCN1S(=O)(=O)C2=CC=C(C=C2)CCC(=O)NC3=NC(=CS3)COC4=CC=CC=C4	β2
CCN1C(=NN=C1SCC(=O)N2CCCC2)C3=CC=C(C=C3)N	β2

CC1=CC(=C(C=C1)OCC(=O)NC2=CC=C(C=C2)C3=NC4=C(O3)C=CC=N4)C	β2
CC1=CC=C(C=C1)NC(=O)C(C2=CC=C(C=C2)Cl)N3CCOCC3	β2
C1=CC=C2C(=C1)NC(=N2)CSC3=NN=C(N3CC4=CC=CO4)COC5=CC=C(C=C5)C1	β2
CC(C(=O)N1CCOCC1)SC2=NC(=CC(=N2)C(F)(F)F)C3=CC=CC=C3	β2
CCOC1=C(C=CC(=C1)C=NN2C=NN=C2)OCCOC3=C(C=C(C=C3)CC=C)OC	β2
C1CN(CCN1CC2=CC3=C(C=C2)OCO3)C(=O)C4=CC5=C(S4)N=C6C=CC=CN6C5=O	β2
CCOC(=O)C1=CC=C(C=C1)NC(=O)CN2N=C(N=N2)C3=CC=C(C=C3)C	β2
C1CCC(CC1)(CC2=CC=C(C=C2)O)NC(=O)CC3=CC=CC=C3	β2
CC(C(=O)N1CCCCC1)SC2=NC(=CC(=N2)C(F)(F)F)C3=CC=CC=C3	β2
CC(C1=NC(=NO1)C2=CC=C(C=C2)NC(=O)C3=CC=CO3)OC4=C(C=C(C=C4)Cl)C1	β2
CC(=O)N1C2=CC=CC=C2C(CC1(C)C)(C)C3=CC=CC=C3	β2
CCCC1=CC=C(C=C1)OCC2=NC(=NO2)C3=CC=C(C=C3)NC(=O)C4=CC=CS4	β2
CC1=NC=C(C=C1)OCC2=CC(=NO2)C(=O)NCC3=CN(N=C3)C4=CC(=CC=C4)F	β2
COC1=CC(=C(C=C1)OC)CCNC(=O)C2CCN(CC2)C3=NN=C(S3)N4C=CC=C4	β2
C1COC2=C(O1)C=CC(=C2)C(=O)NC3=CC4=C(C=C3)OC(=N4)C5=CC6=CC=CC=C6C=C5	β2
CC1=CC(=C(C=C1)O)NC(=O)C2=CC(=CC=C2)NC(=O)C3=CC=CO3	β2
C1=CC2=C(N=C1)N=C(O2)C3=CC=C(C=C3)NC(=O)C4=CC=C(O4)[N+](=O)[O-]	β2
CC1=CC=C(C=C1)CN2C=CC(=N2)NC(=O)C3=NN4C(=CC(=NC4=C3)C5=CC=CO5)C(F)(F)F	β2
CC1=CC=C(C=C1)OCCN(C)C(=O)C2=NOC(=C2)COC3=CC=C(C=C3)C(=O)C	β2
C1CC(=O)N(C1)CCCN2=C(C=C(C=C2)C(CC(=O)N)NC(=O)CC3=CC=CC4=CC=CC=C43)[N+](=O)[O-]	β2
CCN1C(=NN=C1SCC2=CC=C(C=C2)C#N)COC3=CC=C(C=C3)Cl	β2
COC1=CC=C(C=C1)CC(=O)NC2=CC=C(C=C2)C3=CN4C=CC=CC4=N3	β2
CC1=CC=C(C=C1)SCC(=O)NC2=CC=C(C=C2)C3=NC4=CC=CC=C4N3	β2
CCOC(=O)C1=CN(C2=C(C(=C(C=C2)C1=O)F)NCCCN(C)C)F)C3CC3	β2
COC1=CC=CC=C1OCCCC(=O)NC2=NC=CS2	β2
CN(CC(=O)N1CCN(CC1)C2=CC=CC=N2)S(=O)(=O)C3=CC=CC=C3	β2
C1CC(CN(C1)S(=O)(=O)C2=C(C=CC(=C2)Cl)Cl)C(=O)NCCCN3C=CN=C3	β2
C1=CC=C2C(=C1)C=CC=C2N3C(=NN=N3)SCC4=CC=CC=N4	β2
CN(CC(=O)N1CCN(CC1)C2=CC=CC=N2)S(=O)(=O)C3=CC=C(C=C3)Cl	β2
CC(=O)NC1=CC=C(C=C1)S(=O)(=O)NCCC2=CSC(=N2)C3=CN=CC=C3	β2

<chem>CC1=CC=C(C=C1)SCC(=O)NC2=CC=C(C=C2)C3=NN=C(O3)C4=CC=CO4</chem>	β2
<chem>CC1=NC=C(C=C1)OCC2=CC(=NO2)C(=O)N(C)CC3=CN(N=C3)C4=CC=CC=C4C</chem>	β2
<chem>C1=CC=C(C=C1)C2=NN(C(=O)C=C2)CC(=O)NC3=CC=C(C=C3)NC(=O)C4=CC=CC=N4</chem>	β2
<chem>CC1=CC=CC=C1N2CCN(CC2)C3=NC=NC4=C3C=NN4CC5=CC=C(C=C5)C1</chem>	β2
<chem>C1CCN2C(C1)C(=O)N(C2=O)CCCCN3CCN(CC3)C4=CC=CC(=C4)C(F)(F)F</chem>	β2
<chem>CSC1=CC=C(C=C1)C(=O)C2CCCN(C2)CC3=CC=CN3C4=CN=CC=C4</chem>	β2
<chem>CN(CCOC1=CC=C(C=C1)C2=NN(C=C2)S(=O)(=O)C3=CC=CC4=CC=CC=C43)C5=CC=CC=N5</chem>	β2
<chem>CCCCOC1=CC=CC(=C1)C(=O)NC2=CC=C(C=C2)NC(=O)C3=CC=CO3</chem>	β2
<chem>CCCCOC1=CC=CC(=C1)C(=O)NC2=CC=C(C=C2)NC(=O)C3=CC=CS3</chem>	β2
<chem>CN1C(=NN=N1)SC2=NC=NC3=C2C(=CS3)C4=CC=C(C=C4)Br</chem>	β2
<chem>CC1=CC=C(C=C1)C2=C(SC(=N2)NC(=O)C3=NN(C=C3[N+](=O)[O-])C)C</chem>	β2
<chem>C1=CC=C2C(=C1)N(C3=C(S2)C=CC(=C3)Cl)C(=O)CSC4=NN=C(N4CC5=CC=CO5)C6=CC=NC=C6</chem>	β2
<chem>CC(C1=NC(=NO1)C2=CC=C(C=C2)NC(=O)C3=CC=CC=N3)OC4=C(C=C(C=C4)Cl)Cl</chem>	β2
<chem>C1=CC=C(C=C1)C2=NN=C(C(=C2)C#N)OC3=CC=CC=C3Cl</chem>	β2
<chem>CC(C)(C)C1=CC=C(C=C1)OCC(=O)NC2=CC=C(C=C2)C3=NC4=C(O3)N=CC=C4</chem>	β2
<chem>CCC(=O)C1=CC=C(C=C1)OCC(=O)N2CCN(CC2)CC(=O)NC3=CC=C(C=C3)C</chem>	β2
<chem>COC1=CC=C(C=C1)C2CC(=NN2C(=O)C3=CC=CS3)C4=CC=C(C=C4)OC</chem>	β2
<chem>CCC1=CC=C(C=C1)OCC(=O)NC2=CC(=O)C(=C3NC4=CC=CC=C4O3)C=C2</chem>	β2
<chem>C1=CC=C(C=C1)C2=NC(=NC(=C2)C#N)OC3=CC=C(C=C3)Cl</chem>	β2
<chem>CCC1=CC=CC=C1N(C)S(=O)(=O)C2=CC3=C(C=C2)NC=C(C3=O)C(=O)O</chem>	β2
<chem>CN(CC(=O)N1CCN(CC1)C2=CC=CC=N2)S(=O)(=O)C3=CC=C(C=C3)Br</chem>	β2
<chem>CC1=CC=C(C=C1)OCC(=O)NC2=CC=C(C=C2)C3=NC4=C(O3)C=CC=N4</chem>	β2
<chem>COCCC1=NC=C(C=N1)CN2CCC(CC2)C(=O)NC3=CC=C(C=C3)N4C=CC=N4</chem>	β2
<chem>CCC(=O)NC1=C(C=C(C=C1)C2=NN3C(=NN=C3S2)C)C</chem>	β2
<chem>CCN(CC)S(=O)(=O)C1=C(C=CC(=C1)NC(=O)C2=COCCO2)Cl</chem>	β2
<chem>C1OC2=C(O1)C=C(C=C2)CNC(=O)CCCCCN3C(=O)C4=C(C=CS4)NC3=O</chem>	β2
<chem>CC1=CC(=NC2=C1C(=C(S2)C3=NN=C(N3CC=C)SCC4=CC=C(C=C4)F)N)C</chem>	β2
<chem>CCC1=CC=C(C=C1)CN2CCC(CC2)OC3=CC=C(C=C3)C(=O)N4CCCCC4</chem>	β2
<chem>CC(=O)NC1=CC=C(C=C1)S(=O)(=O)N2CCCCC2C3=CN=CC=C3</chem>	β2
<chem>CC1=CC(=NC2=C1C(=C(S2)C3=NN=C(N3CC=C)SCC4=CC=CC=C4Cl)N)C</chem>	β2

C1CN(CCC1C(=O)N2CCN(CC2)CC3=CC=CC=C3)C(=O)C4=CC(=CC=C4)Cl	β2
CCOC(=O)N1CCN(CC1)C2=NN=C(C3=CC=CC=C32)C4=CC=C(C=C4)C	β2
CC1=C(C=C(C=C1)C(=O)OCC(=O)NC2=NC(=CS2)C3=CC=CC=C3)NC(=O)C4=CC=CO4	β2
CC1=NC=C(C=N1)CN2CCCC(C2)C(=O)NC3=CC=C(C=C3)C4=CC(=CC=C4)F	β2
CC(C(=O)N1CCCC1)SC2=NC(=CC(=N2)C(F)(F)F)C3=CC=CC=C3	β2
CCOC(=O)C1=CC=C(C=C1)N2C(C3=C(NN=C3C2=O)C4=CC=CO4)C5=CC(=CC=C5)[N+](=O)[O-]	β2
C1CC2=CC=CC=C2N(C3=CC=CC=C31)C(=O)COC4=CC=CC=C4F	β2
CCOC(=O)C1=CC=C(C=C1)NC(=O)COC2=CC=C(C=C2)S(=O)(=O)N3CCCC3	β2
COC(=O)C1=C(CC2CCC1N2C(=O)NCC3=CC(=CC=C3)F)C4=CC(=CC=C4)OCC5=CC=CC=C5	β2
CC1=C(SCCO1)C(=O)NC2=CC=C(C=C2)C(=O)N3CCN(CC3)C4=CC=CC=C4F	β2
CN1C(=NN=C1SCC(=O)N2CCC3=CC=CC=C32)CNC4=NC(=CS4)C5=CC=CC=C5	β2
CN1C(=NN=N1)SC2=NC=NC3=C2C(=CS3)C4=CC=C(C=C4)Cl	β2
C1=CC2=C(N=C1)N=C(O2)C3=CC=C(C=C3)NC(=O)CSC4=CC=C(C=C4)Cl	β2
CC1CCC(CC1)NC(=O)CCS(=O)(=O)C2=CC3=C(C=C2)N(CC3)C(=O)C4CC4	β2
CC1=CC(=NC2=NC(=NN12)C(=O)NC3=CC(=CC=C3)S(=O)(=O)N(C)C4=CC=CC=C4)C	β2
CCCCN(C1=CC=CC=C1)C(=O)C2=CC=C(C=C2)NC(=O)C(C)C	β2
CC(=O)N1CCC2=C1C=CC(=C2)C(=O)CN3CCN(CC3)C4=CC(=CC=C4)Cl	β2
CC(C)NC(=O)CCCS(=O)(=O)C1=NC(=CC(=N1)C(F)(F)F)C2=CC=CC=C2OC	β2
CC(=O)C1=CC(=C(C=C1)OC)COC2=C(C=C(C=C2)Cl)Cl	β2
CC1=CC=CC2=NC(=CN12)COC3=C(C4=CC=CC=C4C=C3)Br	β2
CCOC(=O)C1=CC=C(C=C1)NC(=O)CN2N=C(N=N2)C3=CC=CC=C3	β2
CC(=O)NC1=CC=C(C=C1)S(=O)(=O)N2CCC(CC2)OC3=CC=C(C=C3)N4C=NN=N4	β2
CC1=CC=C(C=C1)CS(=O)(=O)C2=NC3=C(CCCC3)C(=N2)N(C)C	β2
CC1=CC=C(C=C1)SC2=NC(=NC(=C2)N3CCOCC3)C4=CC=CC=C4	β2
CC(=O)NC1=CC=C(C=C1)S(=O)(=O)N(CC2=CC=CO2)CC3=CC4=CC=CC=C4NC3=O	β2
CC1CCCN(C1)C2=C(C=NC3=CC(=C(C=C32)OC)OC)S(=O)(=O)C4=CC=CC=C4	β2
CSC1=CC=C(C=C1)CNC(=O)C2=CC=C(C=C2)NC(=O)C3=CSCCO3	β2
CC1=CC(=CC(=C1)C(=O)NC(CC(=O)N)C2=CC(=C(C=C2)N3CCN(CC3)C4=CC=CC=N4)[N+](=O)[O-])C	β2
CCN(CC1=CC=CC=C1)S(=O)(=O)C2=C(C=CC(=C2)C(=O)NC(C)C3CC4CCC3C4)OC	β2
COC1=CC=C(C=C1)CNC(=O)CCCCCNC2=NC(=S)NC3=CC=CC=C32	β2

COC1=CC=C(C=C1)S(=O)(=O)N2CCCC(C2)C(=O)NC3=CC=C(C=C3)NC(=O)C4=CC=CC=N4	β2
C=CCN1C(=NN=C1SCC(=O)C2=CC=C(C=C2)Cl)CCNC(=O)C3=CC=CS3	β2
CC1=CC(=NC2=C1C(=C(S2)C3=NN=C(N3C)SCC4=CC=C(C=C4)Cl)N)C	β2
CC1=CC=C(C=C1)NC(=O)C(C2=CC=C(C=C2)Cl)N3CCCCC3	β2
CCOC1=CC=CC=C1C(=O)NCC(=O)OCC2=CSC(=N2)CC(=O)NC3=CC=C(C=C3)C	β2
CC1=CC=C(C=C1)OCC2=NN=C(N2CC3=CC=CO3)SCC4=NC5=CC=CC=C5N4	β2
CCCCC(=O)NC1=CC=C(C=C1)S(=O)(=O)N2CCCCC2C3=CN=CC=C3	β2
C1CN(CCN1C2=C(C=C(C=C2)C(CC(=O)N)NC(=O)C3=CC=C(C=C3)Br)[N+](=O)[O-])C4=CC=CC=N4	β2
COC1=CC(=C(C=C1)CN2CCC(CC2)OC3=CC=C(C=C3)C(=O)N4CCCC4)F	β2
CCOC1=CC=C(C=C1)NC(=O)CNC(=O)C2=NN(C(=O)C3=CC=CC=C32)C4=CC(=C(C=C4)OC)OC	β2
CN(C1=CC=CC=C1)S(=O)(=O)C2=CC=CC(=C2)C(=O)NC3=CC=CC(=C3)C(=O)NC4CC4	β2
C1OC2=C(O1)C=C(C=C2)CNC(=O)CCCCCN3C(=O)C4=CC=CC=C4NC3=S	β2
C1CCC(CC1)NC(=O)N2CCC(CC2)NC3=CC=C(C=C3)CCNCC(COC4=CC=C(C=C4)O)O	β1
C1=CC=C2C(=C1)C3=C(N2)C=CC=C3OCC(CNCCC4=CC=C(C=C4)NC(=O)CC5=CC=CC=N5)O	β1
COC1=CC=CC(=C1)NC(=O)NC2=CC=C(C=C2)CC(CO)NCC(COC3=CC=CC=C3)O	β1
C1=CC=NC(=C1)CC(=O)NC2=CC=C(C=C2)CCNCC(COC3=CN=CC=C3)O	β1
COC1=CC=C(C=C1)CC(=O)NC2=CC=C(C=C2)CCNCC(COC3=CC=C(C=C3)O)O	β1
CC(C)OC1=C(C=CC(=C1)C2=CC=C(C=C2)CCNCC(C3=CC(=CC=C3)F)O)C(=O)O	β1
C1CN(CCC1NC2=CC=C(C=C2)CCNCC(COC3=CC=C(C=C3)O)O)C(=O)NCC4=C(C=CC(=C4)F)F	β1
C1=CC=C(C=C1)C(=O)NC2=C(C=C(C=C2)OC3=CC=CC(=C3)CCNCC(C4=CC(=CC=C4)Cl)O)C(=O)O	β1
CCCOC1=C(C=CC(=C1)C2=CC=C(C=C2)CCNC(C)C(C3=CC=CC=C3)O)C(=O)O	β1
C1CCC(C1)CCCN(C(=O)N2CCC(CC2)NC3=CC=C(C=C3)CCNCC(COC4=CC=C(C=C4)O)O	β1
CCN(CC)C(=O)N1CCC(CC1)NC2=CC=C(C=C2)CCNCC(COC3=CC=C(C=C3)O)O	β1
C1CN(CCC1NC2=CC=C(C=C2)CCNCC(COC3=CC=C(C=C3)O)O)C(=O)N	β1
CC(CC1=CC=C(C=C1)C2=CC(=C(C=C2)C(=O)O)OC3CCCCC3)NCC(C4=CC=CC=C4)O	β1
CC(=O)NC1=CC(=CC(=C1)C(=O)O)OC2=CC=CC(=C2)CCNCC(C3=CC(=CC=C3)Cl)O	β1
CC(C)(CC1=CC=C(C=C1)OC2=NC=C(C=C2)C(=O)N)NCC(COC3=CC=CC4=C3N(C(=O)N4)C)O	β1
COC1=CC=C(C=C1)NC(=O)NC2=CC=C(C=C2)CC(CO)NCC(COC3=CC=CC=C3)O	β1
C1=CC=NC(=C1)CC(=O)NC2=CC=C(C=C2)CCNCC(COC3=CC=CC4=C3C=CN4)O	β1
C1=CC=C(C=C1)COC2=CC=CC(=N2)CC(=O)NC3=CC=C(C=C3)CCNCC(COC4=CC=CC=C4)O	β1

C1=CC(=CC(=C1)Cl)C(CNCCC2=CC=C(C=C2)C3=CC=C(S3)C(=O)O)O	β1
C1=CC(=CC=C1CCNCC(COC2=CC=C(C=C2)O)O)NC(=O)CC3=CSC=C3	β1
C1CC2=C(CC1NCC(C3=CC(=CC=C3)Cl)O)C=C(C=C2)OC4=NC=C(C=C4)C(=O)O	β1
CS(=O)(=O)NC1=C(C=CC(=C1)OC(CNC2CCN(CC2)C3=CC=C(C=C3)CC4C(=O)NC(=O)S4)O)O	β1
C1CN(CCC1NCC(O)OC2=CC=CC3=C2C=CC(=O)N3)C4=CC=C(C=C4)CC5C(=O)NC(=O)S5	β1
C1CN(CCC1NCC(COC2=CC=CC3=NC(=O)N=C32)O)C4=CC=C(C=C4)CC5C(=O)NC(=O)S5	β1
C1=CC=C(C=C1)N2C=CN=C2CC(=O)NC3=CC=C(C=C3)CCNCC(COC4=CC=CC=C4)O	β1
CCCCCCCCNC(=O)N1CCC(CC1)NC2=CC=C(C=C2)CCNCC(COC3=C4CCC(=O)NC4=C(C=C3)O)O	β1
COC1=C(C=CC(=C1)CCNCC(C2=CC(=CC=C2)Cl)O)C3=CC=C(C=C3)C(=O)O	β1
CC(C)COC1=C(C=CC(=C1)C2=CC=C(C=C2)CCNCC(C3=CC(=CC=C3)Cl)O)C(=O)O	β1
CC(C)OC1=C(C=CC(=C1)C2=CC=C(C=C2)CCNC(C)C(C3=CC=C(C=C3)O)O)C(=O)O	β1
C1=CC=C(C=C1)C(C2=CC=CC=C2)C(=O)NC3=CC=C(C=C3)CCNCC(COC4=CC=C(C=C4)O)O	β1
C1=CC=C(C=C1)CN2C3=CC=CC=C3N=C2CC(=O)NC4=CC=C(C=C4)CCNCC(COC5=CC=CC=C5)O	β1
CC(C)OC1=C(C=CC(=C1)C2=CC=C(C=C2)OCCNCC(C3=CC(=CC=C3)Cl)O)C(=O)O	β1
C1CN(CCC1NC2=CC=C(C=C2)CCNCC(COC3=CC=C(C=C3)O)O)C(=O)NCC4=C(C=C(C=C4)Cl)Cl	β1
C1=CC=C(C=C1)OCC(CNC(CC2=CC=C(C=C2)NC(=O)NC3=CC(=CC=C3)[N+](=O)[O-])CO)O	β1
C1CC2=C(CC1NCC(C3=CC(=CC=C3)Cl)O)C=C(C=C2)C4=NC=C(C=C4)C(=O)O	β1
CCC1=CC=C(C=C1)CC(C)(C)NCC(C2=CC(=C(C=C2)Cl)N)Cl)O	β1
COC1=CC=C(C=C1)S(=O)(=O)N2CCC(CC2)NCC(COC3=CC=C(C=C3)O)O	β1
C1=CC=C(C=C1)OCC(CNCCC2=CC=C(C=C2)NS(=O)(=O)C3=CC=CC=C3)O	β1
CC(C)OC1=C(C=CC(=C1)C2=CC=C(C=C2)CCNCC(C3=CC(=CC=C3)Cl)O)C(=O)O	β1
CN(C1=CC=C(C=C1)CCNCC(COC2=CC=CC=C2)O)C(=O)CC3=NC=CN3CC4=CC=CC=C4	β1
CC1=C(C=CC(=C1)C(=O)O)C2=CC=C(C=C2)CCNCC(C3=CC(=CC=C3)Cl)O	β1
CC1=CC(=NC(=C1)CC(=O)NC2=CC=C(C=C2)CCNCC(COC3=CC=CC=C3)O)C	β1
C1=CC=NC(=C1)CC(=O)NC2=CC=C(C=C2)CCNCC(COC3=CC=C(C=C3)O)O	β1
C1CN(CCC1NCC(COC2=CC=C(C=C2)O)O)C3=CC=C(C=C3)CC4C(=O)NC(=O)S4	β1
CCOC1=C(C=CC(=C1)C2=CC=C(C=C2)CC(C)NCC(C3=CC=CC=C3)O)C(=O)O	β1
C1CN(CCC1NC2=CC=C(C=C2)CCNCC(COC3=CC=C(C=C3)O)O)C(=O)NCC4=C(C=C(C=C4)F)F	β1
CC(C)OC1=C(C=CC(=C1)C2=CC3=C(CCC(C3)NCC(C4=CC=C(C=C4)Cl)O)C=C2)C(=O)O	β1
C1CC2=C(CC1NCC(C3=CN=C(C=C3)Cl)O)C=C(C=C2)C4=CC=C(C=C4)C(=O)O	β1

CC(C)(CC1=CC(=CC(=C1)F)F)NCC(C2=CC(=C(C(=C2)Cl)N)Cl)O	β1
C1=CC(=CC(=C1)OC2=CC(=C(C(=C2)F)C(=O)O)CCNCC(C3=CC(=CC(=C3)Cl)O	β1
C1CN(CCC1NC2=CC=C(C(=C2)CCNCC(COC3=CC=C(C(=C3)O)O)C(=O)NCC4=CC=C(C(=C4)F	β1
CC(C)OC1=C(C=CC(=C1)C2=CC=C(C(=C2)OCCNCC(C3=CC=CC(=C3)O)C(=O)O	β1
C1=CC=C2C=NC(=CC2=C1)CC(=O)NC3=CC=C(C(=C3)CCNCC(COC4=CC=C(C(=C4)O)O	β1
CCCCCCCCNC(=O)N1CCC(CC1)NC2=CC=C(C(=C2)CCNCC(COC3=CC=C(C(=C3)O)O	β1
CS(=O)(=O)NC1=C(C=CC(=C1)OCC(CNCCC2=CC=C(C(=C2)NC3CCN(CC3)C(=O)NCC4=C(C=CC(=C4)F)F)O)O	β1
CC(C)CC1=C(C=CC(=C1)C2=CC=C(C(=C2)CC(C)NCC(C3=CC=CC(=C3)O)C(=O)NS(=O)(=O)C	β1
CC1=C(C=CC(=C1)C2=CC=C(C(=C2)CCNCC(C3=CC(=CC(=C3)Cl)O)C(=O)O	β1
CC1=C(C=CC(=C1)C(=O)O)C2=CC3=C(CCC(C3)NCC(C4=CC=C(C(=C4)Cl)O)C=C2	β1
C1=CC(=CC(=C1)Cl)C(CNCCC2=CC=C(C(=C2)C3=C(C=C(C(=C3)C(=O)O)Cl)O	β1
COC1=C(C=CC(=C1)C2=CC=C(C(=C2)CCNCC(C3=CC(=CC(=C3)Cl)O)C(=O)O	β1
C1CCC(CC1)OC2=C(C=CC(=C2)C3=CC=C(C(=C3)OCCNCC(C4=CC=CC(=C4)O)C(=O)O	β1
C1CC2=C(CC1NCC(C3=CC(=CC(=C3)Cl)O)C=C(C(=C2)OC4=CC=C(S4)C(=O)O	β1
C1CCC(CC1)NC(=O)NC2=CC=C(C(=C2)S(=O)(=O)N3CCC(CC3)CNCC(COC4=CC=C(C(=C4)O)O	β1
C1CCC(CC1)OC2=C(C=CC(=C2)C3=CC=C(C(=C3)OCCNCC(C4=CC(=CC(=C4)Cl)O)C(=O)O	β1
C1=CC=C(C(=C1)OCC(CNCCC2=CC=C(C(=C2)NC(=O)CC3=NC=CN3)O	β1
CC(C)OC1=C(C=CC(=C1)C2=CC=C(C(=C2)CCNCC(C3=CC(=C(C(=C3)O)NS(=O)(=O)C)O)C(=O)NS(=O)(=O)C	β1
COC1=C(C=CC(=C1)C(=O)O)C2=CC=C(C(=C2)CCNCC(C3=CC(=CC(=C3)Cl)O	β1
CC(C)OC1=C(C=CC(=C1)C2=CC=C(C(=C2)CCNCC(C3=CC=C(C(=C3)Cl)O)C(=O)O	β1
C1=CC=C2C(=C1)C=CC=C2CC(=O)NC3=CC=C(C(=C3)CCNCC(COC4=CC=C(C(=C4)O)O	β1
C1=CC(=CC(=C1)Cl)C(CNCCC2=CC=C(C(=C2)C3=CC=C(C(=C3)C(=O)O)Cl)O	β1
COC1=C(C=C(C(=C1)OC2=CC=CC(=C2)CCNCC(C3=CC(=CC(=C3)Cl)O)C(=O)O	β1
C1CN(CCC1CNCC(COC2=CC=C(C(=C2)O)O)S(=O)(=O)C3=CC=C(C(=C3)NC(=O)NC4=CC=CC(=C4	β1
C1=CC(=CC(=C1)Cl)C(CNCCC2=CC=C(C(=C2)NC3=CC=C(C(=C3)C(=O)O)O	β1
C1=CC=C(C(=C1)C(C(=O)NC2=CC=C(C(=C2)CCNCC(COC3=CC=C(C(=C3)O)O)O	β1
C1=CC(=CC(=C1)Cl)C(CNCCC2=CC=C(C(=C2)C3=NC=C(C(=C3)C(=O)O)O	β1
C1=CC=C(C(=C1)C(=O)NC2=CC(=CC(=C2)C(=O)O)OC3=CC=CC(=C3)CCNCC(C4=CC(=CC(=C4)Cl)O	β1
CC(C)OC1=C(C=CC(=C1)C2=CC=C(C(=C2)CC(C)NCC(C3=CC(=CC(=C3)Cl)O)C(=O)O	β1
CC(C)OC1=C(C=CC(=C1)C2=CC=C(C(=C2)CC(C)NCC(C3=CC=CC(=C3)O)C(=O)O	β1

C1=CC=C(C=C1)NC(=O)NC2=CC=C(C=C2)CC(NCC(COC3=CC=CC=C3)O)O	β1
COC1=C(C=C(C=C1)OC2=CC=CC(=C2)CCNCC(C3=CN=CC=C3)O)C(=O)O	β1
CC(C)COC1=C(C=CC(=C1)C2=CC=C(C=C2)CC(C)NCC(C3=CC=CC=C3)O)C(=O)O	β1
CC(CC1=CC=C(C=C1)C2=CC(=C(C=C2)C(=O)O)OC3CCCCC3)NCC(C4=CN=CC=C4)O	β1
CC(C)OC1=C(C=C(C=C1)OC2=CC=CC(=C2)CCNCC(C3=CC(=CC=C3)Cl)O)C(=O)O	β1
C1CN(CCC1CNCC(COC2=CC=C(C=C2)O)O)S(=O)(=O)C3=CC=C(C=C3)NC(=O)NCCCC4=CC=CS4	β1
CC(C)(C)C(=O)NC1=C(C=C(C=C1)OC2=CC=CC(=C2)CCNCC(C3=CC(=CC=C3)Cl)O)C(=O)O	β1
CC(C)OC1=C(C=CC(=C1)C2=CC=C(C=C2)CC(C)NCC(C3=CN=CC=C3)O)C(=O)O	β1
C1CN(CCC1CNCC(COC2=CC=CC3=C2C4=CC=CC=C4N3)O)CCC(F)(F)F	β1
C1CN(CCC1NC2=CC=C(C=C2)CCNCC(COC3=CC=C(C=C3)O)O)C(=O)NCC4=C(C=CC=C4F)F	β1
C1CC2=C(CC1NCC(C3=CC=CC=C3Cl)O)C=C(C=C2)C4=CC=C(C=C4)C(=O)O	β1
C1=CC(=CC(=C1)OC2=CC(=C(C=C2)Cl)C(=O)O)CCNCC(C3=CC(=CC=C3)Cl)O	β1
CC(=O)NC1=C(C=C(C=C1)OC2=CC=CC(=C2)CCNCC(C3=CC(=CC=C3)Cl)O)C(=O)O	β1
C1CC2=C(CC1NCC(C3=CC=C(C=C3)Cl)O)C=C(C=C2)C4=CC=C(C=C4)C(=O)O	β1
C1CN(CCC1NC2=CC=C(C=C2)CCNCC(COC3=CC=C(C=C3)O)O)C(=O)NCC4=CC=CC=C4F	β1
C1=CC(=CC(=C1)Cl)C(CNCCC2=CC=C(C=C2)NC3=CC=CC(=C3)C(=O)O)O	β1
CC(CC1=CC=C(C=C1)C2=CC=C(C=C2)C(=O)O)NCC(C3=CC=CC=C3)O	β1
CCOC1=C(C=CC(=C1)C2=CC=C(C=C2)CCNCC(C3=C(C=CN=C3)N)O)C(=O)NS(=O)(=O)C	β1
C1CC2=C(CC1NCC(C3=CN=C(C=C3)Cl)O)C=C(C=C2)OC4=CC=CC(=C4)C(=O)O	β1
C1=CSC(=C1)CC(=O)NC2=CC=C(C=C2)CCNCC(COC3=CC=C(C=C3)O)O	β1
C1=CC=C(C=C1)CN2C=CN=C2CC(=O)NC3=CC=C(C=C3)CCNCC(COC4=CC=CC=C4)O	β1
CC(C)CC1=C(C=CC(=C1)C2=CC=C(C=C2)CCNC(C)C(C3=CC=CC=C3)O)C(=O)O	β1
C1=CC(=CC(=C1)Cl)C(CNCCC2=CC=C(C=C2)OC3=NC=C(C=C3)C(=O)O)O	β1
C1CC2=C(CC1NCC(C3=CC=C(C=C3)C(F)(F)F)O)C=C(C=C2)C4=CC=C(C=C4)C(=O)O	β1
CCCOC1=C(C=CC(=C1)C2=CC=C(C=C2)CCCNCC(C3=CC(=CC=C3)Cl)O)C(=O)O	β1
C1=CC=C(C=C1)C(CNCCC2=CC=C(C=C2)C3=CC(=C(C=C3)C(=O)O)OC4=CC=CC=C4)O	β1
C1=CC(=CC(=C1)Cl)C(CNCCC2=CC=C(C=C2)C3=CC=C(C=C3)C(=O)O)O	β1
CCCCCNC(=O)NC1=CC=C(C=C1)S(=O)(=O)N2CCC(CC2)CNCC(COC3=CC=C(C=C3)O)O	β1
C1=CC(=CC(=C1)Cl)CC(=O)NC2=CC=C(C=C2)CCNCC(COC3=CC=C(C=C3)O)O	β1
CN(C)C1=CC(=CC(=C1)C(=O)O)OC2=CC3=C(CCC(C3)NCC(C4=CN=C(C=C4)Cl)O)C=C2	β1

C1=CC=C(C=C1)OCC(CNCCC2=CC=C(C=C2)NC(=O)CC3=NC(=CC=C3)Cl)O	β1
C1=CC(=CC=C1CCNCC(COC2=CC=C(C=C2)O)O)NC(=O)CC3=CC=NC=C3	β1
CNC(=O)N1CCC(CC1)NC2=CC=C(C=C2)CCNCC(COC3=CC=C(C=C3)O)O	β1
CC(CC1=CC=C(C=C1)C2=CC=C(C=C2)C(=O)O)NCC(C3=CN=CC=C3)O	β1
CC(C)COC1=C(C=CC(=C1)C2=CC=C(C=C2)OCCNCC(C3=CC(=CC=C3)Cl)O)C(=O)O	β1
CCCNC1=CC(=CC(=C1)C(=O)O)OC2=CC3=C(CCC(C3)NCC(C4=CC(=CC=C4)Cl)O)C=C2	β1
C1CC(CC2=C(C1)C=CC(=C2)OC3=CC=CC(=C3)C(=O)O)NCC(C4=CC(=CC=C4)Cl)O	β1
CCCOC1=C(C=CC(=C1)C2=CC=C(C=C2)CC(C)NCC(C3=CN=CC=C3)O)C(=O)O	β1
CC(C(C1=CC=C(C=C1)O)O)NCCC2=CC=C(C=C2)C3=CC(=C(C=C3)C(=O)NS(=O)(=O)C)OC4CCCCC4	β1
C1CN(CCC1NCC(COC2=CC=CC=C2)O)C3=CC=C(C=C3)CC4C(=O)NC(=O)S4	β1
C1CC2=C(CC1NCC(C3=CC(=CC=C3)Cl)O)C=C(C=C2)OCC(=O)O	β1
C1CC2=C(CC1NCC(C3=CC(=CC=C3)Cl)O)C=C(C=C2)OC4=CC(=CC(=C4)N)C(=O)O	β1
C1=CC=C(C=C1)OCC(CNCCC2=CC=C(C=C2)NC(=O)CC3=NC=CN3CC4=CC=C(C=C4)Cl)O	β1
CC(C)COC1=C(C=CC(=C1)C2=CC=C(C=C2)OCCNCC(C3=CC=CC=C3)O)C(=O)O	β1
C1CN(CCC1CNCC(COC2=CC=C(C=C2)O)O)S(=O)(=O)C3=CC=C(C=C3)NC(=O)NCC4=C(C=CC(=C4)F)F	β1
C1CC2=C(CC1NCC(C3=CC=C(C=C3)Cl)O)C=C(C=C2)C4=CC(=C(C=C4)C(=O)O)F	β1
C1=CC(=CN=C1)CC(=O)NC2=CC=C(C=C2)CCNCC(COC3=CC=C(C=C3)O)O	β1
C1=CC=C(C=C1)NC(=O)NC2=CC=C(C=C2)CC(CO)NCC(COC3=CC=CC=C3)O	β1
COC1=CC=CC=C1CC(=O)NC2=CC=C(C=C2)CCNCC(COC3=CC=C(C=C3)O)O	β1
C1=CC=C(C=C1)OCC(CNCCC2=CC=C(C=C2)NC(=O)CC3=NC=CN3CC4=CC5=CC=CC=C5C=C4)O	β1
C1=CC=C2C(=C1)C(C=N2)CC(=O)NC3=CC=C(C=C3)CCNCC(COC4=CC=C(C=C4)O)O	β1
CC(C)OC1=C(C=CC(=C1)C2=CC=C(C=C2)CC(C)(C)NCC(C3=CC=CC=C3)O)C(=O)O	β1
CCCOC1=C(C=CC(=C1)C2=CC=C(C=C2)OCCNCC(C3=CC=CC=C3)O)C(=O)O	β1
CCCNC(=O)NC1=CC=C(C=C1)CC(CO)NCC(COC2=CC=CC=C2)O	β1
CC(C)OC1=C(C=CC(=C1)C2=CC=C(C=C2)CCNC(C)C(C3=CC=C(C=C3)O)O)C(=O)NS(=O)(=O)C	β1
C1CCC(CC1)OC2=C(C=CC(=C2)C3=CC=C(C=C3)CCNCC(C4=CC(=CC=C4)Cl)O)C(=O)O	β1
CC(CC1=CC(=CC=C1)OC2=CC=CC(=C2)C(=O)O)NCC(C3=CC(=CC=C3)Cl)O	β1
COC1=CC=CC(=C1)CC(=O)NC2=CC=C(C=C2)CCNCC(COC3=CC=C(C=C3)O)O	β1
C1CC2=C(CC1NCC(C3=CC=C(C=C3)Cl)O)C=C(C=C2)OC4=CC=CC(=C4)C(=O)O	β1
CC(CC1=CNC2=C1C=CC=C2OCCN)NCC(C3=CC(=CC=C3)NS(=O)(=O)C4=CC=CS4)O	β1

CC(C)NC(=O)N1CCC(CC1)NC2=CC=C(C=C2)CCNCCC(COC3=CC=C(C=C3)O)O	β1
COC1=CC=CC=C1NC(=O)NC2=CC=C(C=C2)CC(CO)NCCC(COC3=CC=CC=C3)O	β1
CC(C)OC1=C(C=CC(=C1)C2=CC=C(C=C2)CCNCCC(C3=C(C=CN=C3)N)O)C(=O)O	β1
CC(CC1=CC=C(C=C1)C2=CC=C(C=C2)C(=O)O)NCCC(C3=CC(=CC=C3)Cl)O	β1
C1=CC=C(C=C1)CN2C=C(N=C2)CC(=O)NC3=CC=C(C=C3)CCNCCC(COC4=CC=CC=C4)O	β1
C1CN(CCC1CNCC(COC2=CC(=C(C=C2)O)F)O)S(=O)(=O)C3=CC=C(C=C3)NC(=O)NCCC4=C(C=CC(=C4)F)F	β1
CC1=C(C=CC(=C1)C2=CC3=C(CCC(C3)NCCC(C4=CC=C(C=C4)Cl)O)C=C2)C(=O)O	β1
C1=CC=C2C=C(C=CC2=C1)CC(=O)NC3=CC=C(C=C3)CCNCCC(COC4=CC=C(C=C4)O)O	β1
C1CC2=C(CC1NCCC(C3=CC=C(C=C3)Cl)O)C=C(C=C2)C4=C(C=C(C=C4)C(=O)O)F	β1
C1CC2=C(CC1NCCC(C3=CC(=CC=C3)Cl)O)C=C(C=C2)OC4=CC(=CC(=C4)NC5CCOCC5)C(=O)O	β1
CCCOC1=C(C=CC(=C1)C2=CC=C(C=C2)OCCNCCC(C3=CC(=CC=C3)Cl)O)C(=O)O	β1
C1CCC(CC1)NC2=CC(=CC(=C2)C(=O)O)OC3=CC4=C(CCC(C4)NCCC(C5=CC(=CC=C5)Cl)O)C=C3	β1
C1=CC(=CC=C1CCNCCC(COC2=CC=C(C=C2)O)O)NC(=O)CC3=CC=C(C=C3)Cl	β1
CC1=C(N=CC=C1)CC(=O)NC2=CC=C(C=C2)CCNCCC(COC3=CC=CC=C3)O	β1
C1=CC=C(C(=C1)CC(=O)NC2=CC=C(C=C2)CCNCCC(COC3=CC=C(C=C3)O)O)Cl	β1
C1=CC=C(C=C1)C(C(=O)NC2=CC=C(C=C2)CCNCCC(COC3=CC=C(C=C3)O)O)N	β1
C1CCC(CC1)OC2=C(C=CC(=C2)C3=CC=C(C=C3)CCNCCC(C4=CC=CC=C4)O)C(=O)O	β1
CC(=O)NC1=CC(=CC(=C1)C(=O)O)OC2=CC3=C(CCC(C3)NCCC(C4=CC(=CC=C4)Cl)O)C=C2	β1
C1=CC(=CC(=C1)Cl)C(CNCCC2=CC=C(C=C2)C3=CC(=C(C=C3)C(=O)O)F)O	β1
CC(C)OC1=C(C=CC(=C1)C2=CC=C(C=C2)CCNC(C)C(C3=CC(=CC=C3)O)O)C(=O)NS(=O)(=O)C	β1
C1=CC(=CC(=C1)Cl)C(CNCCC2=CC=C(C=C2)C3=CC(=C(C=C3)C(=O)O)Cl)O	β1
CC(C)NC(=O)NC1=CC=C(C=C1)CC(CO)NCCC(COC2=CC=CC=C2)O	β1
C1CCC(CC1)OC2=C(C=CC(=C2)C3=CC=C(C=C3)CCNCCC(C4=CN=CC=C4)O)C(=O)O	β1
C1=CC=C(C=C1)OCC(CNCCC2=CC=C(C=C2)NC(=O)CC3=NC=CN3CC4=CC=C(C=C4)Br)O	β1
C1=CC=C(C=C1)CC(=O)NC2=CC=C(C=C2)CCNCCC(COC3=CC=C(C=C3)O)O	β1
CC(C)C1=CC=C(C=C1)CC(C)(C)NCCC(C2=CC(=C(C(=C2)Cl)N)Cl)O	β1
CC(C)OC1=C(C=CC(=C1)C2=CC=C(C=C2)CCNC(C)C(C3=CC=CC=C3)O)C(=O)O	β1
C1=CC=C2C(=C1)C=CC(=N2)CC(=O)NC3=CC=C(C=C3)CCNCCC(COC4=CC=C(C=C4)O)O	β1
CC(CC1=CC=C(C=C1)C2=CC(=C(C=C2)C(=O)O)OC)NCCC(C3=CC=CC=C3)O	β1
C1=CC(=CC=C1CCNCCC(COC2=CC=C(C=C2)O)O)NC(=O)CC3=NC=CN=C3	β1

C1=CC(=CC(=C1)Cl)C(CNCCC2=CC=C(C=C2)C3=C(C=C(C=C3)C(=O)O)F)O	β1
CC(C)OC1=C(C=CC(=C1)C2=CC=C(C=C2)CCNCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O)C(=O)O	β1
C1=CC=NC(=C1)CC(=O)NC2=CC=C(C=C2)CCNCC(COC3=CC=CC4=C3NC(=O)N4)O	β1
C1=CC(=CC(=C1)Cl)C(CNCCC2=CC=C(C=C2)CC3=CC=C(C=C3)OCC(=O)O)O	β1
CC(C)OC1=C(C=CC(=C1)C2=CC=C(C=C2)CCNCC(C3=CN=C(C=C3)N)O)C(=O)O	β1
C1=CC(=CC(=C1)OC2=CC(=C(C=C2)F)C(=O)O)CCNCC(C3=CN=CC=C3)O	β1
C1CCC(CC1)NC(=O)NC2=CC=C(C=C2)CC(CO)NCC(COC3=CC=CC=C3)O	β1
CC(C)CC1=C(C=CC(=C1)C2=CC=C(C=C2)OCCNCC(C3=CN=C(C=C3)N)O)C(=O)O	β1
CCCOC1=C(C=CC(=C1)C2=CC=C(C=C2)NCCNCC(C3=CC(=CC=C3)Cl)O)C(=O)O	β1
CC1=C(C=C(C=C1)OC2=CC=CC(=C2)CCNCC(C3=CC(=CC=C3)Cl)O)C(=O)O	β1
C1CC2=C(C=CC(=C2)CCNCC(COC3=CC=CC=C3)O)N(C1)C(=O)CC4=NC=CN4CC5=CC=CC=C5	β1
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCCC2=CC=C(C=C2)NC3CCN(CC3)C(=O)NCC4=C(C=CC(=C4)F)F)O)O	β1
CC(C)CC1=C(C=CC(=C1)C2=CC=C(C=C2)OCCNCC(C3=CC(=CC=C3)Cl)O)C(=O)O	β1
C1=CC(=CC(=C1)Cl)C(CNCCC2=CC=C(C=C2)C3=CC=C(C=C3)CC(=O)O)O	β1
CC(C)OC1=C(C=CC(=C1)C2=CC=C(C=C2)CCNCC(C3=C(C=CN=C3)N)O)C(=O)NS(=O)(=O)C	β1
COC1=CC=C(C=C1)S(=O)(=O)N2CCC(CC2)NCC(COC3=CC=CC4=C3C5=CC=CC=C5N4)O	β1
CCCN(C1=CC=C(C=C1)CCNCC(COC2=CC=CC=C2)O)C(=O)CC3=NC=CN3CC4=CC=CC=C4	β1
CC(C)OC1=C(C=CC(=C1)C2=CC=C(C=C2)CCNCC(C3=CC(=CC=C3)O)O)C(=O)O	β1
CN(CCN1CCC(CC1)OC(=O)NC2=CC=CC=C2C3=CC=CC=C3)C(=O)C4=CC=C(C=C4)CNCC(C5=C6C=CC(=O)NC6=C(C=C5)O)O	β2
CC(CC1=CC=CC(=C1)CC(=O)NCC2=CC=CC=C2OC)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O	β2
CCN(CC)CCN(CCNCCC1=C2C(=C(C=C1)O)NC(=O)S2)C(=O)CCOCCC3=CC(=CC=C3)F	β2
CC(C)N(CCC(C1=CC=CC=C1)C2=C(C=CC(=C2)CCCCOC3=CC=C(C=C3)CCNCC(C4=CC(=C(C=C4)O)NS(=O)(=O)C)O)O)C(C)C	β2
COC1=CC=CC=C1OCCNCC(C2=CC(=C(C=C2)O)O)O	β2
CC(CC1=CC=CC(=C1)CC(=O)NC23CC4CC(C2)CC(C4)C3)NCC(C5=CC(=C(C=C5)O)CO)O	β2
CC(CC1=CC=CC(=C1)CC(=O)NCC2=CC(=C(C=C2)Cl)Cl)NCC(C3=CC(=C(C=C3)O)CO)O	β2
CC1=C(C=CC(=C1OC)CNCC(C2=C3C=CC(=O)NC3=C(C=C2)O)O)NC(=O)CCN4CCC(CC4)OC(=O)NC5=CC=CC=C5C6=CC=CC=C6	β2
COC1=C(C=CC(=C1)NC(=O)CCN2CCC(CC2)OC(=O)NC3=CC=CC=C3C4=CC=CC=C4)CNCC(C5=C6C=CC(=O)NC6=C(C=C5)O)O	β2
C1CCN(CC1)CCN(CCNCCC2=C3C(=C(C=C2)O)NC(=O)S3)C(=O)CCOCCC4=CC(=CC=C4)Cl	β2
CC(C)CCC1=CC=C(C=C1)C(CNC2=CC=C(C=C2)CCNCC(C3=CC(=C(C=C3)O)CO)O)O	β2
CC(CC1=CC2=C(C=C1)NC(=C2)C(=O)NCC3CCC3)NCC(C4=CC(=C(C=C4)O)CO)O	β2

CC(C)N(CCC(C1=CC=CC=C1)C2=C(C=CC(=C2)CCCCOC3=CC=C(C=C3)CCNCC(C4=CC(=C(C=C4)O)CO)O)O)C(C)C	β2
CC(C)N(CCNCCC1=C2C(=C(C=C1)O)NC(=O)S2)C(=O)CCOCCC3=CC=CC=C3	β2
CC(CC1=CC=CC(=C1)CC(=O)NCC2=CC=CC=C2)NCC(C3=CC(=C(C=C3)O)CO)O	β2
COC1=CC=C(C=C1)CN2CCN(CC2)C3=CC=C(C=C3)CCNCC(C4=CC(=C(C=C4)O)CO)O	β2
CN(C)CCCN(CCNCCC1=C2C(=C(C=C1)O)NC(=O)S2)C(=O)CCOCCC3=CC=CC=C3	β2
CCN(CC)CCN(CCNCCC1=C2C(=C(C=C1)O)NC(=O)S2)C(=O)CCOCCC3=CC4=CC=CC=C4C=C3	β2
CC(C)N(CCC(C1=CC=CC=C1)C2=C(C=CC(=C2)CCCN(C=O)CCCCCCCCCNCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O)O)C(C)C	β2
C1=CC=C2C(=C1)C=CC=C2CCOCCOCCCNCC(C3=C4C(=C(C=C3)O)NC(=O)S4)O	β2
CC(CC1=CC=CC(=C1)CC(=O)NCC2CCCC2)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O	β2
COC1=CC=C(C=C1)CCNCC(C2=CC(=CC(=C2)O)O)O	β2
COC1=C(C=C(C=C1)NC2=CC=C(C=C2)CCNCC(C3=CC(=C(C=C3)O)CO)O)C4=CC=CC=C4	β2
C1=CC=C2C(=C1)C=CC=C2NC3=CC=C(C=C3)CCNCC(C4=CC(=C(C=C4)O)CO)O	β2
CCN(CC1=C(C=C(C=C1)O)C1)C(=O)CC2=CC(=CC=C2)CC(C)(C)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O	β2
C1=CC=C(C=C1)CCOCCC(=O)NCCNCCC2=C3C(=C(C=C2)O)NC(=O)S3	β2
CCC(CC1=CC2=C(C=C1)NC(=C2)C(=O)NCC3=C(C=CC=C3OC)OC)NCC(C4=CC(=C(C=C4)O)CO)O	β2
CCN1C2=C(C=C(C=C2)CC(C)NCC(C3=CC(=C(C=C3)O)CO)O)C=C1C(=O)NCC4=C(C=CC=C4OC)OC	β2
C1=CC=C(C=C1)C2=CC=C(C=C2)C(CNC3=CC=C(C=C3)CCNCC(C4=CC(=C(C=C4)O)CO)O)O	β2
C1=CC=C(C=C1)CNC(=O)CC2=CC(=CC=C2)CCNCC(C3=CC(=C(C=C3)O)CO)O	β2
C1=CC(=CC=C1CCNCC(C2=CC(=C(C=C2)O)CO)O)NCC(C3=CC=C(C=C3)C1)O	β2
CC#CCNC1=CC=CC(=C1)C(CNC(C)CC2=CNC3=C2C=CC=C3OS(=O)(=O)C)O	β2
CC(C)N(CCC(C1=CC=CC=C1)C2=C(C=CC(=C2)CCCN(C=O)CC3=CC(=CC=C3)CC(C)(C)NCC(C4=CC(=C(C=C4)O)NS(=O)(=O)C)O)O)C(C)C	β2
CC(C)N(CCC(C1=CC=CC=C1)C2=C(C=CC(=C2)CCCCOC3=CC=C(C=C3)CCNCC(C4=CC(=C(C=C4)O)O)O)O)C(C)C	β2
C1CN(CCC1OC(=O)NC2=CC=CC=C2C3=CC=CC=C3)CCCCCCCCCNCC(C4=CC(=C(C=C4)O)CO)O	β2
C1CN(CCC1OC(=O)NC2=CC=CC=C2C3=CC=CC=C3)CCC(=O)NC4=CC=CC(=C4)CCNCC(C5=C6C=CC(=O)NC6=C(C=C5)O)O	β2
C1=CC=C2C(=C1)C=CC=C2CCOCCSCCCNCC(C3=C4C(=C(C=C3)O)NC(=O)S4)O	β2
CC(CC1=CC2=C(C=C1)NC(=C2)C(=O)NCCC3=CC(=CC=C3)OC)NCC(C4=CC(=C(C=C4)O)CO)O	β2
CC(C)(CC1=CC=CC(=C1)CC(=O)NCC2=CC3=C(C=C2)C=C(C=C3)O)NCC(C4=CC(=C(C=C4)O)NS(=O)(=O)C)O	β2
C1=CC(=CC(=C1)C(F)(F)F)CCNCCSCCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O	β2
C1=CC=C(C=C1)CCOCCOCCCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O	β2

C1=CC=C(C=C1)CCNCCCSCCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O	β2
COC1=C(C=CC(=C1)CCNCCC2=CC(=C(C=C2)O)O)OCCCC3=CC=CC=C3	β2
C1CN(CCC1OC(=O)NC2=CC=CC=C2C3=CC=CC=C3)CCC(=O)NCCCCCNCC(C4=C5C=CC(=O)NC5=C(C=C4)O)O	β2
CC(CC1=CC=CC(=C1)CC(=O)NCC2=CC=CC=C2)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O	β2
CC1=C(C=CC(=C1)CNCC(C2=C3C=CC(=O)NC3=C(C=C2)O)O)NC(=O)CCN4CCC(CC4)OC(=O)NC5=CC=CC=C5C6=CC=CC=C6	β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCCCCCCCCCN2CC3CC3(C2)COC(=O)NC4=CC=CC=C4C5=CC(=C(C=C5)O)Cl)O)O	β2
C1=CC=C(C=C1)CCOCCSCCCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O	β2
CN(C1=CC(=C(C=C1)CNCC(C2=C3C=CC(=O)NC3=C(C=C2)O)O)OC)C(=O)CCN4CCC(CC4)OC(=O)NC5=CC=CC=C5C6=CC=CC=C6	β2
C1CN(CCN1C2=CC=CC=C2)C3=CC=C(C=C3)CCNCC(C4=CC(=C(C=C4)O)CO)O	β2
CC(C)OC1=CC=CC2=C1NC=C2CC(C)NCC(C3=CC(=CC=C3)NS(=O)(=O)C4=CC=CS4)O	β2
CCN(CC)CCN(CCNCC(C1=C2C(=C(C=C1)O)NC(=O)S2)O)C(=O)CCOCCC3=CC(=CC=C3)Cl	β2
CN(CCNCC(C1=C2C(=C(C=C1)O)NC(=O)S2)O)C(=O)CCOCCC3=CC=CC=C3	β2
COC1=CC=CC(=C1)NC2=CC=C(C=C2)CCNCC(C3=CC(=C(C=C3)O)CO)O	β2
CC(C)N(CCC(C1=CC=CC=C1)C2=C(C=CC(=C2)CCCNC(=O)CC3=CC(=CC=C3)CC(C)(C)NCC(C4=CC(=C(C=C4)O)CO)O)O)C(C)C	β2
C1CN(CCC1CN2C=NC(=N2)C(C3=CC=CC=C3)(C4=CC=CC=C4)O)CCC5=CC=C(C=C5)CCNCC(C6=C7C=CC(=O)NC7=C(C=C6)O)O	β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCCCCCCCCCN2CCC(CC2)OC(=O)NC3=CC=CC=C3C4=CC=CC=C4O)O)O	β2
C1=CC(=CC(=C1)Cl)CCNCCCS(=O)(=O)CCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O	β2
CCCC(CC1=CC=C(C=C1)OC)NCC(C2=CC(=CC(=C2)O)O)O	β2
CCOC1=CC=CC2=C1NC=C2CC(C)NCC(C3=CC(=CC=C3)NS(=O)(=O)C4=CC=CS4)O	β2
CN(C1=C(C=C(C(=C1)OC)CNCC(C2=C3C=CC(=O)NC3=C(C=C2)O)O)Cl)C(=O)CCN4CCC(CC4)OC(=O)NC5=CC=CC=C5C6=CC=CC=C6	β2
C1=CC=C(C=C1)C2=CC=C(C=C2)NC3=CC=C(C=C3)CCNCC(C4=CC(=C(C=C4)O)CO)O	β2
CCCCN(CCNCCC1=C2C(=C(C=C1)O)NC(=O)S2)C(=O)CCOCCC3=CC=CC=C3	β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCCCCCCCCCN2CCC(CC2)OC(=O)NC3=C(C=C(C=C3)F)C4=CC(=C(C=C4)O)Cl)O)O	β2
CC(C)N(C)CCN(CCNCCC1=C2C(=C(C=C1)O)NC(=O)S2)C(=O)CCOCCC3=CC(=CC=C3)Cl	β2
COC1=C(C=C(C=C1)CCNCC(C2=C3C=CC(=O)NC3=C(C=C2)O)O)NC(=O)CCN4CCC(CC4)OC(=O)NC5=CC=CC=C5C6=CC=CC=C6	β2
CC(CC1=CNC2=C1C=CC=C2OS(=O)(=O)C)NCC(C3=CC(=CC=C3)NCC(=C)C)O	β2
CCC1=CC=C(C=C1)CC(C)(C)NCC(C2=CC(=C(C=C2)O)CO)O	β2
CC(CC1=CNC2=C1C=CC=C2OS(=O)(=O)C)NCC(C3=CC(=CC=C3)NCC=CC4=CC=CC=C4)O	β2
CC1=C(C=CC(=C1)NC(=O)CCN2CCC(CC2)OC(=O)NC3=CC=CC=C3C4=CC=CC=C4)CNCC(C5=C6C=CC(=O)NC6=C(C=C5)O)O	β2

CC(C)(CNCCC1=C2C(=C(C=C1)O)NC(=O)S2)NC(=O)CCOCCCC3=CC=CC=C3	β2
CCC=CCNC1=CC=CC(=C1)C(CNC(C)CC2=CNC3=C2C=CC=C3OS(=O)(=O)C)O	β2
CN(CC(C1=CC=CC=C1)O)C2=CC=C(C=C2)CCNCC(C3=CC(=C(C=C3)O)CO)O	β2
C1CCC(CC1)C(C2=CC=CC=C2)(C3=NN(C=N3)CC4CCN(CC4)CCCCCCCCCNCC(C5=C6C=CC(=O)NC6=C(C=C5)O)O)O	β2
CC(CC1=CC2=C(C=C1)NC(=C2)C(=O)NCC3=CC=CC=C3OC)NCC(C4=CC(=C(C=C4)O)CO)O	β2
C1=CC=C(C=C1)C(CNC2=CC=C(C=C2)CCNCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O)O	β2
CCCC1=C(C=C2CC(CC2=C1)NCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O)CCC	β2
CCN(CC)CCN(CCNCCC1=C2C(=C(C=C1)O)NC(=O)S2)C(=O)CCOCCCC3=CC(=CC=C3)OC	β2
COC1=C(C=CC(=C1)C(=O)NCCN2CCC(CC2)OC(=O)NC3=CC=CC=C3C4=CC=CC=C4)CNCC(C5=C6C=CC(=O)NC6=C(C=C5)O)O	β2
C1CC2=C(C1)C=C(C=C2)NC3=CC=C(C=C3)CCNCC(C4=CC(=C(C=C4)O)CO)O	β2
CN(C)CCN(CCNCCC1=C2C(=C(C=C1)O)NC(=O)S2)C(=O)CCOCCCC3=CC=CC=C3	β2
CCC(CC1=CC=C(C=C1)O)NCC(C2=CC(=CC(=C2)O)O)O	β2
CC(CC1=CNC2=C1C=CC=C2OS(=O)(=O)C)NCC(C3=CC(=CC=C3)NCC=C)O	β2
CC(CC1=CC=CC(=C1)CC(=O)NCCC2=CC=CC=C2)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O	β2
CC(CC1=CNC2=C1C=CC=C2OS(=O)(=O)C)NCC(C3=CC(=CC=C3)NCC4=CC=CC=C4)O	β2
CC(C)N(CCC(C1=CC=CC=C1)C2=C(C=CC(=C2)CCCNC(=O)CC3=CC(=CC=C3)CC(C)NCC(C4=CC(=CC(=C4)O)O)O)O)C(C)C	β2
CC(CC1=CC2=C(C=C1)NC(=C2)C(=O)NCC3=CC=C(C=C3)O)NCC(C4=CC(=C(C=C4)O)CO)O	β2
C1CN(CCC1OC(=O)NC2=CC=CC=C2C3=CC=CC=C3)CCC(=O)NC4=C(C=C(C=C4)CNCC(C5=C6C=CC(=O)NC6=C(C=C5)O)O)C1	β2
CC1=CC(=CC(=C1CNC(=O)CC2=CC(=CC=C2)CC(C)(C)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O)C)O	β2
CN(CCCN(CCNCCC1=C2C(=C(C=C1)O)NC(=O)S2)C(=O)CCOCCCC3=CC(=CC=C3)Cl)C4CC4	β2
CCN(CC1=CC=NC=C1)CC2=CC=CC(=C2)C3=CC=C(C=C3)CCNCCC4=C5C(=C(C=C4)O)NC(=O)S5	β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCCCCCCCCCN2CCC(CC2)OC(=O)NC3=CC=CC=C3C4=CC(=C(C=C4)O)Cl)O)O	β2
CCOC1=CC=C(C=C1)CCNCCSCCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O	β2
C1=CC=C(C=C1)CCNCC2=CC=C(C=C2)CCNCC(C3=CC(=C(C=C3)O)CO)O	β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCCCCCCCCCN2CCC(CC2)OC(=O)NC3=CC=CC=C3C4=CC=CC=C4)O)O	β2
CC(=O)N1CCN(CC1)C2=CC=C(C=C2)CCNCC(C3=CC(=C(C=C3)O)CO)O	β2
C1CN(CCC1OC(=O)NC2=CC=CC=C2C3=CC=CC=C3)CCNC(=O)C4=CC=C(C=C4)CNCC(C5=C6C=CC(=O)NC6=C(C=C5)O)O	β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCCCCCCCCCN2CCC(CC2)OC(=O)NC3=CC=CC=C3C4=CC(=C(C=C4)O)Cl)O)O	β2
C1CN(CCC1NC(=O)CC2=CC=CC=C2)C3=CC=C(C=C3)CCNCC(C4=CC(=C(C=C4)O)CO)O	β2

C1CCC2=C(C1)C(=NN2C3=C(C=CC=C3F)O)OC4CCN(CC4)CCCCCCCCCNCC(C5=C6C=CC(=O)NC6=C(C=C5)O)O	β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCCCCCCCCCN2CCC(CC2)OC(=O)NC3=CC=CC=C3C4=CC(=C(C=C4)O)Cl)O)O	β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCCCCCCCCCN2CCC(CC2)OC(=O)NC3=CC=CC=C3C4=CC(=C(C=C4)O)Cl)O)O	β2
CC(CC1=CNC2=C1C=CC=C2OS(=O)(=O)C)NCC(C3=CC(=CC=C3)OCC4=CC=CC=C4)O	β2
C1CN(CCC1C(=O)C2=CC=CC=C2)C3=CC=C(C=C3)CCNCC(C4=CC(=C(C=C4)O)CO)O	β2
CC(CC1=CC2=C(C=C1)N(C(=C2)C(=O)NCC3=C(C=CC=C3OC)OC)CC4=CC=CC=C4)NCC(C5=CC(=C(C=C5)O)CO)O	β2
C1=CC=C(C(=C1)CCNCC2=CC=C(C=C2)CCNCCC3=C4C(=C(C=C3)O)NC(=O)S4)F	β2
C1CN(CCC1OC(=O)NC2=CC=CC=C2C3=CC=CC=C3)CCC(=O)NC4=CC(=C(C=C4)CNCC(C5=C6C=CC(=O)NC6=C(C=C5)O)O)Cl	β2
C1CN(CCC1OC(=O)NC2=CC=CC=C2C3=CC=CC=C3)CCCCCCCCCNCC(C4=C5C=CC(=O)NC5=C(C=C4)O)O	β2
CN(CCNCCC1=C2C(=C(C=C1)O)NC(=O)S2)C(=O)CCOCCC3=CC=CC=C3	β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCCCCCCCCCN2CC3C(C2)C3COC(=O)NC4=CC=CC=C4C5=CC(=C(C=C5)O)Cl)O)O	β2
COC1=CC=CC=C1CNCC2=CC=C(C=C2)CCNCC(C3=C4C(=C(C=C3)O)NC(=O)S4)O	β2
CC(C)N(CCC(C1=CC=CC=C1)C2=C(C=CC(=C2)CCNCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O)O)C(C)C	β2
C1C[N+](C(C1)OC(=O)NC3=CC=CC=C3C4=CC=CC=C4)CCCCCCCCCNCC(C5=C6C=CC(=O)NC6=C(C=C5)O)O	β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCCCCCCCCCN2CCC(CC2)OC(=O)NC3=C(C=CC(=C3)F)C4=CC(=C(C=C4)O)Cl)O)O	β2
CC(CC1=CC2=C(C=C1)NC(=C2)C(=O)NCC3=NC=CS3)NCC(C4=CC(=C(C=C4)O)CO)O	β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCCC2=CC=C(C=C2)OCCCN3CCC(CC3)OC(=O)NC4=CC=CC=C4C5=CC(=C(C=C5)O)Cl)O)O	β2
C1CCC(CC1)C(C2=CC=CC=C2)(C3=NN(C=N3)CC4CCN(CC4)CCC5=CC=C(C=C5)CCNCC(C6=C7C=CC(=O)NC7=C(C=C6)O)O)O	β2
CC(C)(C)C1=CC=C(C=C1)C(CNC2=CC=C(C=C2)CCNCC(C3=CC(=C(C=C3)O)CO)O)O	β2
CC(C)C(CC1=CC=C(C=C1)OC)NCC(C2=CC(=CC(=C2)O)O)O	β2
CCN(C)CCCN(CCNCCC1=C2C(=C(C=C1)O)NC(=O)S2)C(=O)CCOCCC3=CC(=CC=C3)Cl	β2
C1CN(CCC1CN2C=NC(=N2)C(C3=CC=CC=C3)(C4=CC=CC=C4)O)CCCCCCCCCNCC(C5=C6C=CC(=O)NC6=C(C=C5)O)O	β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCCCCCCCCCN2CCC(CC2)OC(=O)NC3=CC=CC=C3C4=CC(=C(C=C4F)O)F)O)O	β2
COC1=C(C=CC(=C1)CCNCC(C2=CC(=C(C=C2)O)O)O)OCCCC3=CC=CC=C3	β2
CC(C)(CC1=CC=CC(=C1)CC(=O)NCC2=C(C=CC(=C2)Cl)O)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O	β2
CCC1=CC=C(C=C1)CCNCCSCCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O	β2
COC1=C(C=CC(=C1)CCNCC(C2=C3C=CC(=O)NC3=C(C=C2)O)O)OCCCC4=CC=CC=C4	β2
C1=CC(=CC=C1CCNCC(C2=CC(=C(C=C2)O)CO)O)NCC(C3=CC=C(C=C3)F)O	β2
CC(CC1=CC2=C(C=C1)NC(=C2)C(=O)NCC3=CC=C(C=C3)S(=O)(=O)N)NCC(C4=CC(=C(C=C4)O)CO)O	β2

CC1=C(C=C2CC(CC2=C1)NCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O)C	β2
C1=CC(=CC=C1CCNCC(C2=CC(=C(C=C2)O)CO)O)NCC3=CC(=C(C=C3)Cl)Cl	β2
CC(CC1=CC2=C(C=C1)NC(=C2)C(=O)NCC3=CC=CC=C3)NCC(C4=CC(=C(C=C4)O)CO)O	β2
CC(C)N(CCC(C1=CC=CC=C1)C2=C(C=CC(=C2)CCCCOCCCCCNCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O)O)C(C)C	β2
CC(CC1=CC=CC2=CC=CC=C2)NCC(C3=CC(=CC(=C3)O)O)O	β2
CC(CC1=CC2=C(C=C1)NC(=C2)C(=O)NC(C)C3=CC=CC=C3)NCC(C4=CC(=C(C=C4)O)CO)O	β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCCCCCCCCCN2CCC(CC2)OC(=O)NC3=CC=CC=C3C4=CC(=C(C=C4)O)Cl)O)O	β2
C1=CC(=CC=C1CCNCC(C2=CC(=C(C=C2)O)CO)O)NC3=CC=C(C=C3)F	β2
CC1=CC(=C(C=C1)C2=CC(=C(C=C2)O)Cl)NC(=O)OC3CCN(CC3)CCCCCCCCCNCC(C4=CC(=C(C=C4)O)NS(=O)(=O)C)O	β2
COC1=CC(=C(C=C1)OC)C(CNC2=CC=C(C=C2)CCNCC(C3=CC(=C(C=C3)O)CO)O)O	β2
C1=CC=C(C=C1)CCOCCC(=O)N(CCCN)CCNCCC2=C3C(=C(C=C2)O)NC(=O)S3	β2
C1CC(CCC1CNCC(C2=C3C=CC(=O)NC3=C(C=C2)O)O)NC(=O)CCN4CCC(CC4)OC(=O)NC5=CC=CC=C5C6=CC=CC=C6	β2
C1CN(CCC1CC2=CC=CC=C2)C3=CC=C(C=C3)CCNCC(C4=CC(=C(C=C4)O)CO)O	β2
CC(C)(CC1=CC=CC(=C1)CC(=O)NCC2=CC=CC=C2)NCC(C3=CC(=C(C=C3)O)CO)O	β2
COC1=CC=CC=C1OCCNCCC2=CC(=C(C=C2)O)O	β2
CC(CC1=CC2=C(C=C1)NC(=C2)C(=O)N(C)CC3=CC=CC=C3)NCC(C4=CC(=C(C=C4)O)CO)O	β2
CCC1=C2CC(CC2=C(C=C1)CC)NCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O	β2
C1CN(CCC1OC(=O)NC2=CC=CC=C2C3=CC=CC=C3)CCC(=O)NC4=CC=C(C=C4)CNCC(C5=C6C=CC(=O)NC6=C(C=C5)O)O	β2
COC1=C(C=C(C=C1)NC(=O)CCN2CCC(CC2)OC(=O)NC3=CC=CC=C3C4=CC=CC=C4)CCNCC(C5=C6C=CC(=O)NC6=C(C=C5)O)O	β2
C1CN(CCC1C2=CC=CC=C2)C3=CC=C(C=C3)CCNCC(C4=CC(=C(C=C4)O)CO)O	β2
CCCCN(CCNCC(C1=C2C(=C(C=C1)O)NC(=O)S2)O)C(=O)CCOCCC3=CC=CC=C3	β2
CCCN(CCNCCC1=C2C(=C(C=C1)O)NC(=O)S2)C(=O)CCOCCC3=CC=CC=C3	β2
C1CN(CCC1OC(=O)NC2=CC=CC=C2C3=CC(=C(C=C3)O)Cl)CCCCCCCCCNCC(C4=C5C=CC(=O)NC5=C(C=C4)O)O	β2
C1CN(CCC1CCCC2=CC=CC=C2)C3=CC=C(C=C3)CCNCC(C4=CC(=C(C=C4)O)CO)O	β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCCCCCCCCCN2CCC(CC2)OC(=O)NC3=CC=CC=C3C4=CC(=CC(=C4O)F)F)O)O	β2
CC(C)(CC1=CC=CC(=C1)CC(=O)NCC2=C(C=C(C=C2)O)Cl)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O	β2
CC(C)(CC1=CC=CC(=C1)CC(=O)NCC2=CC(=C(C=C2)Cl)O)Cl)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O	β2
CCC(CC1=CC=C(C=C1)OC)NCC(C2=CC(=CC(=C2)O)O)O	β2
C1=CC=NC(=C1)CCNCCC2=CC=C(C=C2)CCNCCC3=C4C(=C(C=C3)O)NC(=O)S4	β2

CC(C)N(CCC(C1=CC=CC=C1)C2=C(C=CC(=C2)CCCCOC3=CC=C(C=C3)CCNCC(C4=C5C=CC(=O)NC5=C(C=C4)O)O)O)C(C)C	β2
CCN(CCNCCC1=C2C(=C(C=C1)O)NC(=O)S2)C(=O)CCOCCC3=CC=CC=C3	β2
CCN(CC)CCN(CCNCCC1=C2C(=C(C=C1)O)NC(=O)S2)C(=O)CCOCCC3=CC=CC=C3	β2
CC(CC1=CC2=C(C=C1)NC(=C2)C(=O)NCC3=CC=CC=C3SC)NCC(C4=CC(=C(C=C4)O)CO)O	β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCCCCCCCCCN2CCC(CC2)OC(=O)NC3=CC=CC=C3C4=CC(=C(C=C4)O)F)O)O	β2
CCN(CC)CCN(CCNCCC1=C2C(=C(C=C1)O)NC(=O)S2)C(=O)CCOCCC3=CC(=CC=C3)Cl	β2
CCCCC1=C(C=C2CC(CC2=C1)NCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O)CCCC	β2
C1=CC=C(C=C1)CCOCCSCCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O	β2
C1CN(CCC1NC(=O)NC2=CC=CC=C2C3=CC=CC=C3)CCCCCCCCCNCC(C4=C5C=CC(=O)NC5=C(C=C4)O)O	β2
CC(C)(CC1=CC=CC(=C1)CC(=O)NCC2=CC(=CC(=C2O)Cl)Cl)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O	β2
CC(C)(CC1=CC(=CC(=C1)F)NCC(C2=CC(=CC3=C2OCC(=O)N3)O)O	β2
C1=CC=C2C=C(C=CC2=C1)C(CNC3=CC=C(C=C3)CCNCC(C4=CC(=C(C=C4)O)CO)O)O	β2
COC1=C(C=CC(=C1)CCNCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O)OCCCC4=CC=CC=C4	β2
C1=CC=C(C=C1)C(COC2=CC=C(C=C2)CCNCC(C3=CC(=C(C=C3)O)CO)O)O	β2
CC1=C(C=CC(=C1)CNCC(C2=C3C=CC(=O)NC3=C(C=C2)O)O)N(C)C(=O)CCN4CCC(CC4)OC(=O)NC5=CC=CC=C5C6=CC=CC=C6	β2
C1=CC=C2C=C(C=CC2=C1)CNC3=CC=C(C=C3)CCNCC(C4=CC(=C(C=C4)O)CO)O	β2
CC(CC1=CC2=C(C=C1)NC(=C2)C(=O)NCC3=C(C=CC=C3F)F)NCC(C4=CC(=C(C=C4)O)CO)O	β2
COC1=C(C=CC(=C1)CNCC(C2=C3C=CC(=O)NC3=C(C=C2)O)O)NC(=O)CCN4CCC(CC4)OC(=O)NC5=CC=CC=C5C6=CC=CC=C6	β2
CCCCN(CCN(C)CCC1=C2C(=C(C=C1)O)NC(=O)S2)C(=O)CCOCCC3=CC=CC=C3	β2
CC(C)(CC1=CC=CC=C1)NCC(C2=CC(=C(C=C2)O)CO)O	β2
CC(C)(CC1=CC=CC(=C1)CC(=O)NCC2=CC=CC=C2)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O	β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCCCCCCCCCN2CCC(CC2)OC(=O)NC3=CC=CC=C3C4=CC=C(C=C4)O)O)O	β2
C1=CC(=CC=C1CCNCC(C2=CC(=C(C=C2)O)CO)O)Br	β2
C1=CC(=C(C=C1)Cl)CCNCC2=CC=C(C=C2)CCNCCC3=C4C(=C(C=C3)O)NC(=O)S4)Cl	β2
C1=CC(=CC=C1CCNCC(C2=CC(=C(C=C2)O)CO)O)NCC(C3=CC=C(C=C3)O)O	β2
CC(CC1=CC=C(C=C1)OC)NCC(C2=CC(=CC(=C2)O)O)O	β2
CC(C)(CC1=CC=C(C=C1)OC2=NC=C(C=C2)C(=O)N)NCC(COC3=CC=CC4=C3N(C(=O)N4)CCCC5CCCC5)O	β2
CC(CC1=CC=CC(=C1)CC(=O)NCCCC2=CC=CC=C2)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O	β2
CC(CC1=CC(=CC=C1)CNCCC2=C(C=CC=C2Cl)Cl)NCC(C3=C4C(=C(C=C3)O)NC(=O)S4)O	β2

CC(C)(CC1=CC=C(C=C1)NCC(C2=CC=CC=C2)O)NCC(C3=CC(=C(C=C3)O)CO)O	β2
CC(CC1=CC2=C(C=C1)NC(=C2)C(=O)NCC3=C(C=CC=C3OC)OC)NCC(C4=CC(=C(C=C4)O)CO)O	β2
CC1=CC(=C(C=C1C(=O)NCCN2CCC(CC2)OC(=O)NC3=CC=CC=C3C4=CC=CC=C4)C)CNCC(C5=C6C=CC(=O)NC6=C(C=C5)O)O	β2
CC1=C(C=C(C=C1)CNC(=O)CC2=CC(=CC=C2)CC(C)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O)C	β2
CCOC1=CC=CC=C1CNC(=O)CC2=CC(=CC=C2)CC(C)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O	β2
C1=CC=C(C=C1)OC2=CC=C(C=C2)NC3=CC=C(C=C3)CCNCC(C4=CC(=C(C=C4)O)CO)O	β2
C1=CC(=CC=C1CCNCC(C2=CC(=C(C=C2)O)CO)O)NC3=CC=C(C=C3)O	β2
CC1=CC(=C(C(=C1)C2=CC(=C(C=C2)O)Cl)NC(=O)OC3CCN(CC3)CCCCCCCCCNCC(C4=CC(=C(C=C4)O)NS(=O)(=O)C)O)C	β2
C1C(CC2=C1C=CC(=C2)NCC(C3=CC=CC=C3)O)NCC(C4=CC(=C(C=C4)O)CO)O	β2
COC1=CC(=C(C=C1)C(CNC2=CC=C(C=C2)CCNCC(C3=CC(=C(C=C3)O)CO)O)O)OC	β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCCCCCCCCCN2CCC(CC2)OC(=O)NC3=CC=CC=C3C4=CC(=CC=C4)O)O)O	β2
COC1=C(C=C2CC(CC2=C1)NCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O)OC	β2
C1=CC=C(C=C1)C(CNC2=CC=C(C=C2)CCNCC(C3=CC(=C(C(=C3)Cl)N)Cl)O)O	β2
C1C2=CC=CC=C2CN1CC3=CC=CC(=C3)C4=CC=C(C=C4)CCNCC(C5=C6C(=C(C=C5)O)NC(=O)S6)O	β2
C1CCN(C1)CC2=CC=C(C=C2)CCNCC(C3=C4C(=C(C=C3)O)NC(=O)S4)O	β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCCCCCCCCCN2CCC(CC2)OC(=O)NC3=CC=CC=C3C4=CC(=CC(=C4)F)O)O)O	β2
C1CN(CC1OC2=CC=C(C=C2)Cl)CC3=CC=C(C=C3)CCNCCC4=C5C(=C(C=C4)O)NC(=O)S5	β2
CC(C)(CC1=CC=CC(=C1)CC(=O)NCC2=CC=C(C=C2)C3=CC=C(C=C3)O)NCC(C4=CC(=C(C=C4)O)NS(=O)(=O)C)O	β2
CC(CC1=CC2=C(C=C1)NC(=C2)C(=O)NCC3=CC=CC=N3)NCC(C4=CC(=C(C=C4)O)CO)O	β2
CC(C)(CC1=CC=CC(=C1)CC(=O)NCC2=CC=CC(=C2)C3=CC=C(C=C3)O)NCC(C4=CC(=C(C=C4)O)NS(=O)(=O)C)O	β2
CC1=CC(=C(C=C1)NC(=O)CCN2CCC(CC2)OC(=O)NC3=CC=CC=C3C4=CC=CC=C4)OC)CNCC(C5=C6C=CC(=O)NC6=C(C=C5)O)O	β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCCCCCCCCCN2C3CCC2CC(C3)OC(=O)NC4=CC=CC=C4C5=CC(=C(C=C5)O)Cl)O)O	β2
COCCNCC1=CC=C(C=C1)CCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O	β2
CCN(CC)CCN(CCNCC(C1=C2C(=C(C=C1)O)NC(=O)S2)O)C(=O)CCOCCC3=CC=CC=C3	β2
CC(CC1=CC2=C(C=C1)N(C(=C2)C(=O)NCC3=C(C=CC=C3OC)OC)C)NCC(C4=CC(=C(C=C4)O)CO)O	β2
CC(C)(CC1=CC=CC(=C1)CC(=O)NCC2=CC(=C(C=C2)Cl)Cl)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O	β2
CC(C)(C)OC(=O)NCCOC1=CC=C(C=C1)NC2=CC=C(C=C2)CCNCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O	β1/β2
CCN(CC)C(=O)COC1=CC=CC2=C1NC=C2CC(C)NCC(C3=CC(=CC=C3)NS(=O)(=O)C4=CC=CS4)O	β1/β2
COC(=O)C1=CC=CC(=C1)C2=CC(=CC=C2)NCCNCC(C3=CC(=CC=C3)Cl)O	β1/β2

CC(CC1=CNC2=CC=CC=C21)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
CN(CCC1=CC=CC=C1)CCOCCCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O	β1/β2
CC(C)(CC1=CC=C(C=C1)NC(=O)CCCNCCS(=O)(=O)O)NCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O	β1/β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCC2CCN(CC2)S(=O)(=O)C3=CC=C(C=C3)N4C=CC5=C(C=CC=C54)C(=O)O)O)O	β1/β2
CC(C)(CC1=CC(=CC=C1)C(F)(F)F)NCC(C2=CC(=CC3=C2OCC(=O)N3)O)O	β1/β2
CC(CC1=CNC2=C1C=CC=C2OS(=O)(=O)C)NCC(C3=CC(=CC=C3)NS(=O)(=O)C4=CC=CS4)O	β1/β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCC2CCN(CC2)S(=O)(=O)C3=CC=C(C=C3)N4C=C(C=N4)C(=O)O)O)O	β1/β2
CC(C)NC1=C(C=CC(=C1)C2=CC=C(C=C2)CCNCC(C3=CC=CC=C3)O)C(=O)O	β1/β2
COC1=C(C=C(C=C1)NC2=CC=C(C=C2)CCNCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O)C5=CC(=CC=C5)CN	β1/β2
CC(CNC1=CC=CC(=C1)C2=CC=C(C=C2)C(=O)O)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
CC1=CC(=CC=C1)CC(C)(C)NCC(C2=CC(=CC3=C2OCC(=O)N3)O)O	β1/β2
CC(CNC1=CC=CC(=C1)C2=C(C=CS2)C(=O)O)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
CS(=O)(=O)NC1=C(C=CC(=C1)OCC(CNCC2CCN(CC2)S(=O)(=O)C3=CC=C(C=C3)NC(=O)NCC4=C(C=CC(=C4)F)F)O)O	β1/β2
CC(C)(CC1=CC=C(C=C1)NC(=O)CCCNCC(=O)CCN)NCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O	β1/β2
C1=CC=C(C=C1)C(CNC2=CC=C(C=C2)CCNCC(C3=CC(=C(C=C3)O)NC(=O)O)O)O	β1/β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCC2CCN(CC2)C3=CC=C(C=C3)C(=O)NC(CC4=CC=CC=C4)C(=O)O)O)O	β1/β2
C1CCC(CC1)OC2=C(C=CC(=C2)C3=CC=C(C=C3)CCNCC(C4=C(C=CN=C4)N)O)C(=O)O	β1/β2
CC(C)(COC1=CC=C(C=C1)NC2=CC=C(C=C2)CCNCC(C3=CC(=C(C=C3)O)NC(=O)O)O)N	β1/β2
CC(CC1=CNC2=C1C=CC=C2OS(=O)(=O)C)NCC(C3=CC(=CC=C3)NS(=O)(=O)C4=CC=CC=C4)O	β1/β2
CCCCCCCCN1C(=O)N(N=N1)C2=CC=C(C=C2)S(=O)(=O)NC3=CC=C(C=C3)CCNCC(C4=CN=CC=C4)O	β1/β2
C1=CC=C(C=C1)C(CNC2=CC=C(C=C2)CCNCC(C3=CC(=C(C=C3)O)CO)O)O	β1/β2
CC(C)(CC1=CC=CC=C1C(F)(F)F)NCC(C2=CC(=CC3=C2OCC(=O)N3)O)O	β1/β2
CC(C)(CC1=CC=CC=C1)NCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O	β1/β2
CC(CNC1=CC=CC(=C1)C2=C(C=CO2)C(=O)O)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
CC(CC1=CNC2=C1C=CC=C2OS(=O)(=O)C3=CC=C(C=C3)C(=O)O)NCC(C4=CC(=CC=C4)NS(=O)(=O)C5=CC=CS5)O	β1/β2
CC(C)(CC1=CC=C(C=C1)C(F)(F)F)NCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O	β1/β2
C1=CC(=CC=C1CCNCC(C2=C3C=CC(=O)NC3=C(C=C2)O)O)NC4=CC=C(C=C4)OCCCN	β1/β2
C1CN(CCC1CN2C(=O)C3=CC=CC4=CC(=CC(=C43)C2=O)O)CC(COC5=CC=CC6=C5C7=CC=CC=C7N6)O	β1/β2
CCOC(=O)S(=O)(=O)OC1=CC=CC2=C1NC=C2CC(C)NCC(C3=CC(=CC=C3)NS(=O)(=O)C4=CC=CS4)O	β1/β2
CC(C)(CC1=CC=C(C=C1)C(=O)O)NCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O	β1/β2

CC(CNC1=CC=C(C=C1)C2=NC(=CO2)C(=O)O)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
C1=CC(=CC(=C1)NCCNCC(C2=CC(=CC=C2)Cl)O)C3=NC(=CC=C3)C(=O)O	β1/β2
C1=CC(=CC(=C1)Cl)CCNCCOCCCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O	β1/β2
CC(C)(CC1=CC=C(C=C1)Br)NCC(C2=CC(=CC3=C2OCC(=O)N3)O)O	β1/β2
C1CC(NC1CC2=CC=C(C=C2)NS(=O)(=O)C3=CC=C(C=C3)C4=NC(=CS4)C5=CC=C(C=C5)C(F)(F)F)C(C6=CC=CC=C6)O	β1/β2
C1CN(CCC1NCC(COC2=CC=C(C=C2)O)O)C3=C4C(=CSC4=NC=N3)C5=CC=CS5	β1/β2
CC(C)(CC1=CC(=CC=C1)C(F)(F)F)NCC(C2=CC(=C(C=C2)O)CO)O	β1/β2
CC(CC1=CNC2=C1C=CC=C2OS(=O)(=O)C)NCC(C3=CC(=CC=C3)NS(=O)(=O)C4=CC=CC(=C4)N)O	β1/β2
C1CCC(CC1)OC2=C(C=CC(=C2)C3=CC=C(C=C3)CCNCC(C4=CN=C(C=C4)N)O)C(=O)O	β1/β2
CC(CC1=CN2CCCOC3=CC=CC1=C32)NCC(C4=CC(=CC=C4)NS(=O)(=O)C5=CC=CS5)O	β1/β2
CC(CNC1=CC=CC(=C1)C2=C(C=CC=N2)C(=O)O)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
CC(CNC1=CC=CC(=C1)C2=CSC(=N2)C(=O)O)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
CC(C)(CC1=CC(=CC=C1)OC)NCC(C2=CC(=CC3=C2OCC(=O)N3)O)O	β1/β2
C1CN(CCC1NCC(COC2=CC=CC(=C2)CO)O)C3=C4C(=CSC4=NC=N3)C5=CC=CC=C5	β1/β2
CC(C)(CC1=CC=C(C=C1)C2=CC=CC=C2)NCC(C3=C4C(=C(C=C3)O)NC(=O)CO4)O	β1/β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCC2CCN(CC2)S(=O)(=O)C3=CC=C(C=C3)NC(=O)NCC4=C(C=CC(=C4)F)F)O)O	β1/β2
CC(CC1=CNC2=C1C=CC=C2OCC3=CC=CC=C3)NCC(C4=CC(=CC=C4)NS(=O)(=O)C5=CC=CS5)O	β1/β2
CC(C)(CC1=CC=CC=C1)NCC(C2=CC(=CC3=C2OCC(=O)N3)O)O	β1/β2
CC(CC1=CNC2=C1C=CC=C2OCC(=O)O)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
CC(CNC1=CC=C(C=C1)CC(=O)O)NCC(C2=CC(=CC=C2)Cl)O	β1/β2
CCCCCCCCNC(=O)NC1=CC=C(C=C1)S(=O)(=O)N2CCC(CC2)CNCC(COC3=CC=C(C=C3)O)O	β1/β2
CC(CC1=CNC2=C1C=CC=C2OS(=O)(=O)C3=CC=CC=C3)NCC(C4=CC(=CC=C4)NS(=O)(=O)C5=CC=CS5)O	β1/β2
C1CCC(C1)CCCN2C(=O)N(N=N2)C3=CC=C(C=C3)S(=O)(=O)NC4=CC=C(C=C4)CCNCC(C5=CN=CC=C5)O	β1/β2
CC(CC1=CNC2=C1C=CC=C2OC)NCC(C3=CC(=CC=C3)NS(=O)(=O)C4=CC=CS4)O	β1/β2
C1C(=O)N(C(=O)N1)C2=CC=CC=C2CCCCOCCCCCNCC(C3=CC(=C(C=C3)O)CO)O	β1/β2
CC(C)CC(C(=O)O)NC(=O)C1=CC=C(C=C1)N2CCC(CC2)CNCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O	β1/β2
CC1=CC=CC=C1CC(C)(C)NCC(C2=CC(=C(C=C2)O)CO)O	β1/β2
C1COCCN1CCOC2=CC=C(C=C2)NC3=CC=C(C=C3)CCNCC(C4=C5C=CC(=O)NC5=C(C=C4)O)O	β1/β2
CC(C)(CC1=CC(=CC(=C1)F)F)NCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O	β1/β2
C1CN(CCC1NCC(COC2=CC=CC(=C2)NC(=O)N)O)C3=C4C(=CSC4=NC=N3)C5=CC=CC=C5	β1/β2

C1=CC(=CC(=C1)NC(=O)NCC(=O)O)CCCCOCCCCCNCC(C2=CC(=C(C=C2)O)CO)O	β1/β2
C1=CC=C(C(=C1)CCNCCSCCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O)C1	β1/β2
CC(CC1=CC=C(C=C1)NC(=O)CC2=NC=CN2CC3=CC=CC=C3)NCC(COC4=CC=CC=C4)O	β1/β2
CC(C)(COC1=C(C=C(C=C1)NC2=CC=C(C=C2)CCNCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O)C5=CC=CC=C5)N	β1/β2
CC(CNC1=CC=CC(=C1)C2=C(N=CO2)C(=O)O)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
CC(C)(CC1=CC=C(C=C1)NC(=O)CCCNCC(=O)CN(C)C)NCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O	β1/β2
C1=CC(=CC(=C1)NCCNCC(C2=CC(=CC=C2)Cl)O)C3=C(C=CO3)C(=O)O	β1/β2
C1=CC(=CC(=C1)Cl)CCNCCCS(=O)CCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O	β1/β2
CC(C)(CC1=CC=C(C=C1)NC(=O)CCCNCC(=O)CN2CCN(CC2)C)NCC(C3=C4C(=C(C=C3)O)NC(=O)CO4)O	β1/β2
CCCCCNC(=O)NC1=CC=C(C=C1)S(=O)(=O)N2CCC(CC2)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O	β1/β2
C1=CC(=CC(=C1)Cl)CCNCCSCCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O	β1/β2
CC(C)(C)C1=CC=C(C=C1)CC(C)(C)NCC(C2=CC(=CC3=C2OCC(=O)N3)O)O	β1/β2
CC(CC1=CNC2=C1C=CC=C2OS(=O)(=O)C3=CN=CC=C3)NCC(C4=CC(=CC=C4)NS(=O)(=O)C5=CC=CS5)O	β1/β2
CC1=CC=CC=C1CC(C)(C)NCC(C2=CC(=CC3=C2OCC(=O)N3)O)O	β1/β2
CC(CC1=CNC2=C1C=CC=C2OS(=O)(=O)C)NCC(C3=CC=C(C=C3)C(=O)NC4=CC=CC=C4)O	β1/β2
CC(CC1=CNC2=C1C=CC=C2OCC(=O)N(C)C)NCC(C3=CC(=CC=C3)NS(=O)(=O)C4=CC=CS4)O	β1/β2
CCOC1=CC=C(C=C1)CC(C)(C)NCC(C2=CC(=CC3=C2OCC(=O)N3)O)O	β1/β2
C1CN(CCC1NCC(COC2=CC=C(C=C2)O)O)C3=C4C(=CSC4=NC=N3)C5=CC=C(C=C5)F	β1/β2
CC(C)(CC1=CC=C(C=C1)Cl)NCC(C2=CC(=CC3=C2OCC(=O)N3)O)O	β1/β2
C1=CC(=CC(=C1)Cl)CCNCCSCCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O	β1/β2
CC(C)(COC1=CC=C(C=C1)NC2=CC=C(C=C2)CCNCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O)N	β1/β2
C1CN(CCC1C(=O)C2=CC=C(C=C2)F)CC(COC3=CC=CC4=C3C5=CC=CC=C5N4)O	β1/β2
CC(C)NCC(COC1=CC2=C(C=C1)N(CCC2)CC3=CC=CC=C3)O	β1/β2
C1=CC=C(C=C1)S(=O)(=O)NC2=CC=C(C=C2)CCNCC(COC3=CC=C(C=C3)O)O	β1/β2
C1=CC=C(C=C1)CCOCCSCCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O	β1/β2
CC(C)(CC1=CC=C(C=C1)NC(=O)CCCN=C(N)N)NCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O	β1/β2
C1CN(CCC1NCC(COC2=CC(=C(C=C2)O)CO)O)C3=C4C(=CSC4=NC=N3)C5=CC=CC=C5	β1/β2
COC1=CC(=CC=C1)OCC(CNC2CCN(CC2)C3=C4C(=CSC4=NC=N3)C5=CC=CC=C5)O	β1/β2
CC(C)CC1=C(C=CC(=C1)C2=CC=C(C=C2)CCNCC(C3=C(C=CN=C3)N)O)C(=O)O	β1/β2
CCCCCCCCC(=O)NC1=CC=C(C=C1)S(=O)(=O)N2CCC(CC2)CNCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O	β1/β2

<chem>COC1=C(C=C(C=C1)NC2=CC=C(C=C2)CCNCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O)C5=CC=CC=C5</chem>	$\beta 1/\beta 2$
<chem>C1CN(CCC1NCC(COC2=CC=CC=C2F)O)C3=C4C(=CSC4=NC=N3)C5=CC=CC=C5</chem>	$\beta 1/\beta 2$
<chem>CCC1=CC=C(C=C1)CC(C)(C)NCC(C2=CC(=CC3=C2OCC(=O)N3)O)O</chem>	$\beta 1/\beta 2$
<chem>CC(C)N(CC1=C(C=CC(=C1)F)F)C(=O)NC2=CC=C(C=C2)S(=O)(=O)N3CCC(CC3)CNCC(C4=CC(=C(C=C4)O)NS(=O)(=O)C)O</chem>	$\beta 1/\beta 2$
<chem>CC(C)(CC1=CC=C(C=C1)OC(F)(F)F)NCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O</chem>	$\beta 1/\beta 2$
<chem>CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCC2CCN(CC2)C3=CC=C(C=C3)C(=O)NC(CC(=O)O)C(=O)O)O)O</chem>	$\beta 1/\beta 2$
<chem>CS(=O)(=O)NC1=C(C=CC(=C1)C(CNC2CCN(CC2)C3=CC=C(C=C3)CC4C(=O)NC(=O)S4)O)O</chem>	$\beta 1/\beta 2$
<chem>C1=CC=C(C=C1)C(=O)NCCOC2=CC=C(C=C2)NC3=CC=C(C=C3)CCNCC(C4=C5C=CC(=O)NC5=C(C=C4)O)O</chem>	$\beta 1/\beta 2$
<chem>CC=CCNC1=CC=CC(=C1)C(CNC(C)CC2=CNC3=C2C=CC=C3OS(=O)(=O)C)O</chem>	$\beta 1/\beta 2$
<chem>CC(CC1=CNC2=CC=CC=C21)NCC(C3=CC(=CC=C3)NS(=O)(=O)C4=CC=CS4)O</chem>	$\beta 1/\beta 2$
<chem>CC(CC1=CNC2=C1C=CC=C2OS(=O)(=O)C3=CC=CS3)NCC(C4=CC(=CC=C4)NS(=O)(=O)C5=CC=CS5)O</chem>	$\beta 1/\beta 2$
<chem>CC(CNC1=CC=C(C=C1)C2=C(C=CS2)C(=O)O)NCC(C3=CC(=CC=C3)Cl)O</chem>	$\beta 1/\beta 2$
<chem>CC(CNC1=CC=CC(=C1)C2=CC=CC=C2C(=O)O)NCC(C3=CC(=CC=C3)Cl)O</chem>	$\beta 1/\beta 2$
<chem>C1=CC(=CC=C1COCCOCCCCCNCC(C2=CC(=C(C=C2)O)CO)O)S(=O)(=O)N</chem>	$\beta 1/\beta 2$
<chem>CC(C)CC1=C(C=CC(=C1)C2=CC=C(C=C2)CCNCC(C3=CN=C(C=C3)N)O)C(=O)O</chem>	$\beta 1/\beta 2$
<chem>CC(CC1=CNC2=C1C=CC=C2OS(=O)(=O)C)NCC(C3=CC=C(C=C3)S(=O)(=O)NC4=CC=CC=C4)O</chem>	$\beta 1/\beta 2$
<chem>CC(C)C1=CC=C(C=C1)CC(C)(C)NCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O</chem>	$\beta 1/\beta 2$
<chem>CC(CNC1=CC=CC(=C1)C2=NC(=CS2)C(=O)O)NCC(C3=CC(=CC=C3)Cl)O</chem>	$\beta 1/\beta 2$
<chem>C1CN(CCC1NCC(COC2=CC=CC(=C2)O)O)C3=C4C(=CSC4=NC=N3)C5=CC=CC=C5</chem>	$\beta 1/\beta 2$
<chem>CC1=C(C=C(C=C1)C(=O)O)C2=CC(=CC=C2)NCCNCC(C3=CC(=CC=C3)Cl)O</chem>	$\beta 1/\beta 2$
<chem>C1=CC(=CC=C1CCNCC(C2=C3C=CC(=O)NC3=C(C=C2)O)O)NC4=CC=C(C=C4)OCCCCN</chem>	$\beta 1/\beta 2$
<chem>C1=CC(=C(C(=C1)Cl)Cl)CCNCCOCCCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O</chem>	$\beta 1/\beta 2$
<chem>C1=CC(=CC=C1COCCOCCCCCNCC(C2=CC(=C(C=C2)O)CO)O)O</chem>	$\beta 1/\beta 2$
<chem>C1=CC=C(C(=C1)CCNCCCSNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O)Cl</chem>	$\beta 1/\beta 2$
<chem>CCCCCCCCS(=O)(=O)OC1=CC=CC2=C1NC=C2CC(C)NCC(C3=CC(=CC=C3)NS(=O)(=O)C4=CC=CS4)O</chem>	$\beta 1/\beta 2$
<chem>CC(CNC1=CC=C(C=C1)CCC(=O)O)NCC(C2=CC(=CC=C2)Cl)O</chem>	$\beta 1/\beta 2$
<chem>C1=CC(=C(C(=C1)Cl)Cl)CCNCCSCCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O</chem>	$\beta 1/\beta 2$
<chem>COC1=CC=C(C=C1)CCNCC(COC2=CC3=C(C=C2)N(CCC3)CC4=CC=CC=C4)O</chem>	$\beta 1/\beta 2$
<chem>C1=CC=C(C(=C1)S(=O)(=O)NC2=CC=C(C=C2)CCNCC(COC3=CC=C(C=C3)O)O)Cl</chem>	$\beta 1/\beta 2$
<chem>CC(C)SC1=C(C=CC(=C1)C2=CC=C(C=C2)CCNCC(C3=C(C=CN=C3)N)O)C(=O)NS(=O)(=O)C</chem>	$\beta 1/\beta 2$

C1=CC(=CC=C1CCNCC(C2=C3C=CC(=O)NC3=C(C=C2)O)O)NC4=CC=C(C=C4)OCCN	β1/β2
COC1=C(C=C(C=C1)NC2=CC=C(C=C2)CCNCC(C3=CC(=C(C=C3)O)NC=O)O)C4=CC=CC=C4	β1/β2
CC1=CC(=CC=C1)CC(C)(C)NCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O	β1/β2
CCCCS(=O)(=O)OC1=CC=CC2=C1NC=C2CC(C)NCC(C3=CC(=CC=C3)NS(=O)(=O)C4=CC=CS4)O	β1/β2
CC(CNC1=CC=C(C=C1)C2=NC(=CS2)C(=O)O)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
CC(C)(CC1=CC=C(C=C1)NC(=O)CCCN=C(N)N)NCC(C2=CC(=CC3=C2OCC(=O)N3)O)O	β1/β2
CC(CNC1=CC=CC(=C1)C2=CC(=CC=C2)C(=O)O)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
COC1=C(C=C(C=C1)NC2=CC=C(C=C2)CCNCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O)C5=CC=CC=C5CN	β1/β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCC2CCN(CC2)S(=O)(=O)C3=CC=C(C=C3)N4C=C(C5=CC=CC=C54)CC(=O)O)O)O	β1/β2
CC(CC1=CNC2=C1C=CC=C2OS(=O)(=O)C)NCC(C3=CC(=CC=C3)NCC#C)O	β1/β2
CC(CC1=CNC2=C1C=CC=C2S(=O)(=O)C)NCC(C3=CC(=CC=C3)NS(=O)(=O)C4=CC=CC(=C4)N)O	β1/β2
C1=CC(=CC(=C1)NCCNCC(C2=CC(=CC=C2)Cl)O)C3=C(C=CS3)C(=O)O	β1/β2
CC(CNC1=CC=CC(=C1)C2=NC(=CO2)C(=O)O)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
CS(=O)(=O)N1CCN(CC1)CCOC2=CC=C(C=C2)NC3=CC=C(C=C3)CCNCC(C4=C5C=CC(=O)NC5=C(C=C4)O)O	β1/β2
CC(C)(CC1=CC=C(C=C1)O)NCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O	β1/β2
CCCCOC1=CC=C(C=C1)S(=O)(=O)N2CC(C2)NCC(C3=CC=C(C=C3)O)O	β1/β2
C1CN(CCN1)CCOC2=CC=C(C=C2)NC3=CC=C(C=C3)CCNCC(C4=C5C=CC(=O)NC5=C(C=C4)O)O	β1/β2
C1CN(CCC1NCC(C2=CC(=C(C=C2)O)NS(=O)(=O)C3=CC=CC=C3)O)C4=CC=C(C=C4)CC5C(=O)NC(=O)S5	β1/β2
C1=CC(=CC(=C1)N2C(=O)C=CNC2=O)CCCCOCCCCCNCC(C3=CC(=C(C=C3)O)CO)O	β1/β2
CC(C)C1=CC=C(C=C1)CC(C)(C)NCC(C2=CC(=CC3=C2OCC(=O)N3)O)O	β1/β2
C1=CC=C(C=C1)C(CNCCC2=CC=C(C=C2)NS(=O)(=O)C3=CC=C(C=C3)C4=NC(=CS4)C5=CC=C(C=C5)C(F)(F)F)O	β1/β2
COC1=C(C=C(C=C1)NC2=CC=C(C=C2)CCNCC(C3=C4C=CC(=O)NC4=C(C=C3)O)O)C5=CC=C(C=C5)CN	β1/β2
CC(C)(C)C1=CC=C(C=C1)CC(C)(C)NCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O	β1/β2
COC1=CC=CC=C1OCC(CNC2CCN(CC2)C3=C4C(=CSC4=NC=N3)C5=CC=CC=C5)O	β1/β2
CCCCCCCCNC(=O)NC1=CC=C(C=C1)S(=O)(=O)N2CCC(CC2)CNCC(COC3=C4CCC(=O)NC4=C(C=C3)O)O	β1/β2
C1=CC(=CC(=C1)Cl)CCNCCCOCCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O	β1/β2
CC(C)(CC1=CC=C(C=C1)NC(=O)CCCN)NCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O	β1/β2
CC(CC1=CNC2=C1C=CC=C2OS(=O)(=O)C)NCC(C3=CC(=CC=C3)NCC=C(C)C)O	β1/β2
CC(C)(CC1=CC=CC(=C1)C(=O)O)NCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O	β1/β2
C1=CC(=CC(=C1)NCCNCC(C2=CC(=CC=C2)Cl)O)C3=CC(=CN=C3)C(=O)O	β1/β2

CC1=CSC2=NC=NC(=C12)N3CCC(CC3)NCC(COC4=CC=C(C=C4)O)O	β1/β2
CC(CNC1=CC=C(C=C1)C2=CSC(=N2)C(=O)O)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
CC(C)(CC1=CC=C(C=C1)F)NCC(C2=CC(=CC3=C2OCC(=O)N3)O)O	β1/β2
C1CN(CCC1NCC(COC2=CC=CC=C2)O)C3=C4C(=CSC4=NC=N3)C5=CC=C(C=C5)F	β1/β2
C1=CC(=C(C(=C1)Cl)Cl)CCNCCSCCCNCC(C2=C3C(=C(C=C2)O)NC(=O)S3)O	β1/β2
CC(CC1=CNC2=C1C=CC=C2OCC(=O)O)NCC(C3=CC(=CC=C3)NS(=O)(=O)C4=CC=CS4)O	β1/β2
CC(CC1=CN(C2=C1C=CC=C2OC)CC3=CC=CC=C3)NCC(C4=CC(=CC=C4)NS(=O)(=O)C5=CC=CS5)O	β1/β2
CCOC(=O)C1=CC=C(C=C1)S(=O)(=O)OC2=CC=CC3=C2NC=C3CC(C)NCC(C4=CC(=CC=C4)NS(=O)(=O)C5=CC=CS5)O	β1/β2
CS(=O)(=O)NC1=C(C=CC(=C1)C(CNCC2CCN(CC2)S(=O)(=O)C3=CC=C(C=C3)NC(=O)NC(CC4=CC=CC=C4)C(=O)O)O)O	β1/β2
CC(C)(CC1=CC=C(C=C1)OC2=NC=C(C=C2)C(=O)N)NCC(COC3=CC=CC4=C3C5(CC5)C(=O)N4)O	β1/β2
CC(C)(CC1=CC=C(C=C1)C2=CC=CC=C2)NCC(C3=CC(=CC4=C3OCC(=O)N4)O)O	β1/β2
CC(CC1=CNC2=C1C=CC=C2OS(=O)(=O)C)NCC(C3=CC(=CC=C3)NC(=O)C4=CC=CC=C4)O	β1/β2
CC(C)(CC1=CC(=CC=C1)C(F)(F)F)NCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O	β1/β2
CC(C)(CC1=CC=C(C=C1)OC(F)(F)F)NCC(C2=CC(=CC3=C2OCC(=O)N3)O)O	β1/β2
C1CN(CCC1NCC(COC2=CC=CC=C2)O)C3=C4C=CSC4=NC=N3	β1/β2
CC(C)(CC1=CC=C(C=C1)NC(=O)CCCNC(=O)CN)NCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O	β1/β2
CC(C)(CC1=CC=C(C=C1)NC(=O)CCCN)NCC(C2=CC(=CC3=C2OCC(=O)N3)O)O	β1/β2
CC(CNC1=CC=C(C=C1)C2=C(C=CO2)C(=O)O)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
CCC1=CC=C(C=C1)CC(C)(C)NCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O	β1/β2
CC(CC1=CNC2=C1C=CC=C2OC)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
CC(CC1=CNC2=C1C=CC=C2OS(=O)(=O)C)NCC(C3=CC(=CC=C3)NCC4=CC5=CC=CC=C5C=C4)O	β1/β2
CC(C)S(=O)(=O)OC1=CC=CC2=C1NC=C2CC(C)NCC(C3=CC(=CC=C3)NS(=O)(=O)C4=CC=CS4)O	β1/β2
CC(C)(CC1=CC=C(C=C1)C(F)(F)F)NCC(C2=CC(=CC3=C2OCC(=O)N3)O)O	β1/β2
CC(CC1=CC=C(C=C1)OCC(=O)O)NCC(C2=CC(=CC=C2)Cl)O	β1/β2
CC(CNC1=CC=C(C=C1)C2=C(N=CO2)C(=O)O)NCC(C3=CC(=CC=C3)Cl)O	β1/β2
CC(C)(CC1=CC=C(C=C1)NC(=O)CCCNC(=O)C(CCCN)N)NCC(C2=C3C(=C(C=C2)O)NC(=O)CO3)O	β1/β2
C1=CC(=CC=C1CCNCC(C2=C3C=CC(=O)NC3=C(C=C2)O)O)NC4=CC=C(C=C4)OCCOCCN	β1/β2
C1=CC(=CC(=C1)CS(=O)(=O)N)CCCCOCCCCCNCC(C2=CC(=C(C=C2)O)CO)O	β1/β2
CCCC(=O)NC1=CC(=C(C=C1)OCC(CNC(C)C)O)C(=O)C	β1
CC(C)NCC(COC1=CC=C(C=C1)CCOC)O	β1

CC(C)NCC(COC1=CC=C(C=C1)CC(=O)N)O	β1
CC(=O)C1=CN=C(N1)CC2=CC=C(C=C2)OC[C@@H](CNCCC3=CC(=C(C=C3)OC)OC)O	β1
CC(C)NCC(COC1=CC=C(C=C1)COCCOC(C)C)O	β1
CC1(C(N1)C(C2=CC=CC=C2)O)C	β2
CC1=C(C=CC(=C1)C(=O)N)C2=C(C=CN2C3=CC(=C(C=C3)C(=O)O)O)C4=CC=C(C=C4)OC	β2
CC1(C(N1)C(C2=CC3=CC=CC=C3C=C2)O)C	β2
CC(C)(C)NC[C@@H](CON=C1C2=CC=CC=C2C3=CC=CC=C31)O	β2
COC1=CC(=C(C=C1)OC)C2=NN=C3N2N=C(CS3)C4=CC(=C(C=C4)OC)O[C@@H]5CCOC5	β2
COC1(COC2=CC=CC=C2O1)C3=NCCN3	β2
COC1=CC(=C(C=C1)OC)C2=NN=C3N2N=C(C=C3)C4=CC(=C(C=C4)OC)O[C@@H]5CCOC5	β2
CC(C)(C)NCC(COC1=CC=CC2=C1SCCC2)O	β1/β2
CC(C)(C)NC[C@@H](COC1=CC=CC2=C1CCCC2=O)O	β1/β2
C1CN(CCN1CCCCC2=CN(N=C2)C3=CC=C(C=C3)Cl)C4=CC=CC=C4	β2
COCC1=CN=C(N1)C2=CC=C(C=C2)OCC(CNCCC3=CC(=C(C=C3)OC)OC)O	β2
CC(C)NCC(C1=CC(=C(C=C1)Cl)Cl)O	β1/β2
CC(C)(C)NC[C@@H](COC1=CC=CC2=C1CC3(C2=O)CCCCC3)O	β1/β2
CC(C)NCC(COC1=CC=C(C=C1)CCC(=O)OC)O	β1
CC1=CC(=C(C=C1OC(=O)C)C)OCC(CNC(C)C)O	β1/β2
CC(C)NCC(COC1=CC=CC=C1OCC=C)O	β1/β2
CC(C)NCC(C1=CC2=CC=CC=C2C=C1)O	β1/β2
C1CC2=C(C=CC(=C2)F)OC1C(CNCC(C3CCC4=C(O3)C=CC(=C4)F)O)O	β1
CC(C)(C)NCC(COC1=CC=CC2=C1C[C@@H]([C@@H](C2)O)O)O	β1/β2
CC(C)NCC(C1=CC=C(C=C1)NS(=O)(=O)C)O	β1/β2
CCCNCC(COC1=CC=CC=C1C(=O)CCC2=CC=CC=C2)O	β1/β2
C1C(=O)NC2=C(S1)C(=CC=C2)OCC(CNCCNS(=O)(=O)C3=CC(=C(C=C3)Cl)S(=O)(=O)N)O	β1
CC(C)(C)C1=CC=C(C=C1)NCC(CON=C(C2CC2)C3CC3)O	β1
CC(CCC1=CC=C(C=C1)F)NCC(COC2=CC=C(C=C2)CCOCC3CCC3)O	β1
CC(CCC1=CC=CC=C1)NCC(C2=CC(=C3C(=C2)C=CN3)C(=O)N)O	β1
C1CCC(CC1)NC2=NC=CC(=C2)C3=NC(=C4C=CN=CC4=C3)N5CCNCC5	β1

C1CC(=O)NC2=C1C(=CC=C2)OCC(CNCCNS(=O)(=O)C3=CC(=C(C=C3)Cl)S(=O)(=O)N)O	β1
CC(C)NCC(COC1=CC=C(C=C1)C(=O)N)O	β1
CC=CC1=CC(=C(C=C1)OCC(CNC(C)C)O)OC	β1
CC(CCC1=CC=CC=C1)NCC(COC2=CC=C(C=C2)CCOCC3CCCC3)O	β1
CC(C)(C)NCC(COC1=CC=CC2=C1C(=C(N2)C#N)I)O	β1
CC1=C2CCCC2=C(C=C1)OCC(CNC(C)C)O	β1
C1=CC=C2C(=C1)C=CC=C2OCC(CNCCNS(=O)(=O)C3=CC(=C(C=C3)Cl)S(=O)(=O)N)O	β1
CC(C)NCC(COC1=CC=C(C=C1)CS(=O)CC2CC2)O	β1
C1C(=O)NC2=C(S1)C(=CC=C2)OCC(CNCCNC3=CC(=C(C=C3)Cl)S(=O)(=O)N)O	β1
CC(C)NCC(COC1=CC2=C(C=C1)C(=O)NCCO2)O	β1
CCOCCOC1=CC=C(C=C1)OCC(CNCCC2=CC(=C(C=C2)OC)OC)O	β1
C1=CC=C2C(=C1)C=CC=C2OCC(CNCCNC3=CC(=C(C=C3)Cl)S(=O)(=O)N)O	β1
CC(C)(C)NC1=CC=CC2=C1SC(C(=O)N2)OCCCO	β1
CCC1=CC=C(C=C1)OCC(CNC(C)C)O	β1
C1CN(CCN1CC(COC2=CC=CC3=CC=CC=C32)O)C4=CC(=C(C=C4)Cl)S(=O)(=O)N	β1
CC(C)NCC(COC1=CC=C(C=C1)CCOC2CCCCC2)O	β1
C1=CC=C2C(=C1)C=CC=C2OCC(CNCCNC(=O)C3=CC(=C(C=C3)Cl)S(=O)(=O)N)O	β1
CC1=CC=C(C=C1)NCC(CON=C(C2CC2)C3CC3)O	β1
CC(C)NCC(COC1=CC=C(C=C1)CCOCC2CCCC2)O	β1
CCN(CC)C(=O)C1CN(C2CC3=CNC4=CC=CC(=C34)C2=C1)C(=O)NC5=CC=CC=C5	β1
CC(C)NCC(COC1=CC=C(C=C1)CCSCC2CCC2)O	β1
CC(C)NCC(COC1=CC=C(C=C1)CCOC2CCCC2)O	β1
C1C(=O)NC2=C(S1)C(=CC=C2)OCC(CNCCNC(=O)C3=CC(=C(C=C3)Cl)S(=O)(=O)N)O	β1
CC(C)NCC(COC1=CC=C(C=C1)COCC2CC2)O	β1
CC(C)NCC(COC1=CC=C(C=C1)C(=O)NC)O	β1
C1CCC(CC1)NC2=NC=CC(=C2)C3=NC(=CC(=C3)C(=O)N)N4CCNCC4	β1
C1CC(=O)NC2=C1C(=CC=C2)OCC(CNCCNC(=O)C3=CC(=C(C=C3)Cl)S(=O)(=O)N)O	β1
C1CN(CCN1CC(COC2=CC=CC3=C2SCC(=O)N3)O)C4=CC(=C(C=C4)Cl)S(=O)(=O)N	β1
C1CC1C(=NOCC(CNC2=NC3=CC=CC=C3N2)O)C4CC4	β1
CC(=NOCC(CNC(C)(C)C)O)C	β2

<chem>COC(=O)CCC1=CC=C(C=C1)OCC(CNCC2=CC=CC=C2)O</chem>	β2
<chem>CC(C)NCC(COC1=CC=CC=C1CCC(=O)OC)O</chem>	β2
<chem>COCCC1=CN=C(N1)C2=CC=C(C=C2)OCC(CNCCC3=CC(=C(C=C3)OC)OC)O</chem>	β2
<chem>CCOC(=O)CCNCC(COC1=CC=C(C=C1)OC)O</chem>	β2
<chem>CC(C)(C)NCC(CON=C1C2=CC=CC=C2C3C1(CCCCC3)OCCO)O</chem>	β2
<chem>CC(C)(C)C(=O)CC(=NOCC(CNC(C)(C)C)O)C1CC1</chem>	β2
<chem>CC(C)CNCC(COC1=CC=CC2=CC=CC=C21)O</chem>	β2
<chem>CC(C)NCC(COC1=CC=CC(=C1)C(=O)OC=C)O</chem>	β2
<chem>COC1=C(C=C(C=C1)CCNCC(COC2=CC=C(C=C2)C3=NC=CN3)O)OC</chem>	β2
<chem>CCOC(=O)CCNCC(COC1=CC=CC=C1)O</chem>	β2
<chem>COC1=CC(=CC(=C1OC)OC)CC2C3=CC(=C(C(=C3CCN2)C(F)(F)F)O)O</chem>	β2
<chem>CCOC(=O)CCNCC(COC1=CC=CC=C1Cl)O</chem>	β2
<chem>C1=CC=C2C(=C1)C=CC=C2OCC(CNCC(=O)N)O</chem>	β2
<chem>CC(C)OCC(CNC(C)(C)C)O</chem>	β2
<chem>COC1=C(C=C(C=C1)CCNCC(COC2=CC=C(C=C2)C3=NC=C(N3)C(F)(F)F)O)OC</chem>	β2
<chem>CCOC(=O)CCC1=CC=C(C=C1)OCC(CNC(C)C)O</chem>	β2
<chem>CC(C)(C)NCC(CON=C1C2=CC=CC=C2C3C1(CCCCC3)O)O</chem>	β2
<chem>C1=CC=C(C=C1)CCNCC(COC2=CC=C(C=C2)C3=NC=C(N3)C4=CC=CS4)O</chem>	β2
<chem>CC(C)(CO)NCC(COC1=CC=CC=C1C(=O)OC)O</chem>	β2
<chem>COC1=C(C=C(C=C1)CCNCC(COC2=NC=C(C=C2)C3=NC=C(N3)C4=CC=CS4)O)OC</chem>	β2
<chem>C1CCN(CC1)CC(C2=COC3=CC=CC=C3O2)O</chem>	β2
<chem>CCC(=O)OCC(CNC(C)(C)C)O</chem>	β2
<chem>CC(C)NCC(COC1=CC=C(C2=CC=CC=C21)O)O</chem>	β2
<chem>CCOC(=O)C1=CN=C(N1)C2=CC=C(C=C2)OCC(CNCCC3=CC(=C(C=C3)OC)OC)O</chem>	β2
<chem>CS(=O)(=O)NC1=CC=C(C=C1)C(CNCCOC2=CC=C(C=C2)N3C=CN=C3)O</chem>	β2
<chem>CC(C)C1=CN=C(N1)C2=CC=C(C=C2)OCC(CNC(C)C)O</chem>	β2
<chem>COC(=O)CCNCC(COC1=CC=CC2=CC=CC=C21)O</chem>	β2
<chem>CC1=CC=CC=C1OCC(CNCCC(=O)OC)O</chem>	β2
<chem>CC(C)C(=O)OCC(CNC(C)(C)C)O</chem>	β2
<chem>COC1=C(C=C(C=C1)CCNCC(COC2=CC=C(C=C2)C3=NC=C(N3)C4=CC=CS4)O)OC</chem>	β2

CC1=CC=CC=C1OCC(CNCC(=O)OC)O	β2
COC1=C(C=C(C=C1))CCNCC(COC2=CC=C(C=C2)CCC3=NC=C(N3)C4=CC=CS4)O)OC	β2
CCOC(=O)CCNCC(COC1=CC=CC2=CC=CC=C21)O	β2
CC(C)NCC(COC1=CC=C(C=C1)CC(=O)OC)O	β2
CC(C)(C)NCC(CON=C(C1CC1)C2CC2)O	β2
CCOCCNCC(COC1=CC=C(C=C1)C2=NC=C(N2)C3=CC=CS3)O	β2
CC(C)NCC(COC1=C(C=C2CCCCC2=C1)OCC(CNC(C)C)O)O	β2
CC(C)NCC(COC(=O)C1CCCCC1)O	β2
CC1=C(N=C(N1)C2=CC=C(C=C2)OCC(CNCCC3=CC(=C(C=C3)OC)OC)O)C1	β2
COC1=C(C=C(C=C1))CCNCC(COC2=CC=C(C=C2)C3=NC=CO3)O)OC	β2
C1CC1NCC(COC2=CC=C(C=C2)C3=NC=C(N3)C4=CC=CS4)O	β2
CC1=C(C=CC(=C1)C2=NC=C(N2)C3=CC=CS3)OCC(CNCCC4=CC(=C(C=C4)OC)OC)O	β2
CCCOC(=O)CCC1=CC=C(C=C1)OCC(CNC(C)C)O	β2
CCC(C)(C)NCC(CON=C1C2=CC=CC=C2C3=CC=CC=C31)O	β2
CC1=C(N=C(N1)C2=CC=C(C=C2)OCC(CNCCC3=CC(=C(C=C3)OC)OC)O)Br	β2
CC(C)(CC1=CC(=C(C=C1)OC)OC)NCC(COC2=CC=C(C=C2)C3=NC=C(N3)C4=CC=CS4)O	β2
CC(C)(C)NCC(COC(=O)C1=CC=CS1)O	β2
CC(C)NCC(COC1=CC=C(C=C1)CC2=NC=C(N2)Br)O	β2
CC(=NOCC(CNC(C)(C)C)O)CC1CC1	β2
CC(C)(C)NCC(COC1=CC=C(C=C1)C2=NC=CN2)O	β2
CC1=CC=CC=C1OCC(CN2CCN(CC2)C3=CC=C(C=C3)NS(=O)(=O)C)O	β2
CC(C)(C)NCC(COC1=CC=C(C=C1)CC2=NC=C(N2)C3=CC=CS3)O	β2
CC(C)(C)NCC(CON=C1C2=C(C=CC(=C2)F)C3C1(CCCC3)OC)O	β2
CC(C)(C)NCC(COC(C)(C)C=C)O	β2
CC(CC1=CC(=C(C=C1)OC)OC)NCC(COC2=CC=C(C=C2)C3=NC=C(N3)C4=CC=CS4)O	β2
C1CC1C(=NOCC(CNC2=CC=C(C=C2)I)O)C3CC3	β2
CC(C)NCC(C1=CC(=CC=C1)Br)O	β2
CC(C)NCC(COC1=CC=C(C=C1)C(=O)OC)O	β2
CC(C)NCC(COC1=CC(=O)C(=O)C2=CC=CC=C21)O	β2
COC1=C(C=C(C=C1))CCNCC(C2=COC3=CC=CC=C3O2)O)OC	β2

<chem>CCOC(=O)CCCNCC(COC1=CC=CC=C1C)O</chem>	β_2
<chem>CC1=CN=C(N1)C2=CC=C(C=C2)OCC(CNC3CC3)O</chem>	β_2
<chem>CC(=NOCC(CNC(C)(C)C)O)C1CC1</chem>	β_2
<chem>COCCCC1=CC=C(C=C1)OCC(CNCC2=CC=C(C=C2)NS(=O)(=O)C)O</chem>	β_2
<chem>CCOC(=O)CCNCC(COC1=CC=CCC1(C)C)O</chem>	β_2
<chem>COC1=C(C=C(C=C1)CCNCC(COC2=CC=C(C=C2)C3=NC=C(N3)CN4CCOCC4)O)OC</chem>	β_2
<chem>CC(C)(C)NCC(CON=C1C2=CC=CC=C2C3C1(CCCC3)OCCO)O</chem>	β_2
<chem>COC1=CC(=CC(=C1OC)OC)CC2C3=C(CCN2)C(=C(C(=C3F)O)O)F</chem>	β_2
<chem>COC(=O)CCC1=CC=C(C=C1)OCC(CNCCCC2=CC=CC=C2)O</chem>	β_2
<chem>CCCC1=CC=CC=C1OCC(CNC(C)C)O</chem>	β_1/β_2
<chem>CC(C)NCC(COC1=CC=C(C=C1)C=CC(=O)OC)O</chem>	β_2
<chem>C1=CC=C(C=C1)OCC(CN)O</chem>	β_2
<chem>CCOC(=O)CCCNCC(COC1=CC=CC=C1)O</chem>	β_2
<chem>CC(C)(C)NCC(CON=C1C2=CC=CC=C2C3C1(CCCCC3)OC)O</chem>	β_2
<chem>CCOC(=O)CCNCC(COC1=CC(=CC=C1)Cl)O</chem>	β_2
<chem>CC1=CN=C(N1)CC2=CC=C(C=C2)OCC(CNC(C)(C)C)O</chem>	β_2
<chem>CS(=O)(=O)NC1=CC=C(C=C1)OCC(CNCC2=CC=C(C=C2)N3C=CN=C3)O</chem>	β_2
<chem>COCCCC1=CC=C(C=C1)OCC(CNCCOC2=CC=C(C=C2)N3C=CN=C3)O</chem>	β_2
<chem>CC1=CN=C(N1)CC2=CC=C(C=C2)OCC(CNCCC3=CC(=C(C=C3)OC)OC)O</chem>	β_2
<chem>C1CCCN(CC1)CC(C2=COC3=CC=CC=C3O2)O</chem>	β_2
<chem>CCOC(=O)CCNCC(COC1=CC=C(C=C1)Cl)O</chem>	β_2
<chem>COC1=CC(=CC(=C1OC)OC)CC2C3=C(C(=C(C=C3CCN2)O)O)F</chem>	β_2
<chem>COC1=C(C=C(C=C1)CCNCC(COC2=C(C=C(C=C2)C3=NC=C(N3)C4=CC=CS4)Cl)O)OC</chem>	β_2
<chem>CCCNCC(COC1=CC=C(C=C1)C2=NC=C(N2)C3=CC=CS3)O</chem>	β_2
<chem>CC(C)(C)NCC(COC(=O)C1CCCCC1)O</chem>	β_2
<chem>CC1=C(N=C(N1)C2=CC=C(C=C2)OCC(CNCCC3=CC(=C(C=C3)OC)OC)O)COC</chem>	β_2
<chem>CC(C)NCC(C1=COC2=CC=CC=C2O1)O</chem>	β_2
<chem>CC(C1CC1)NOCC(CNC(C)(C)C)O</chem>	β_2
<chem>CC(C)(C)COCC(CNC(C)(C)C)O</chem>	β_2
<chem>CC(C)(C)NCC(COC1=CC=C(C=C1)C2=NC=C(N2)C3=CC=CS3)O</chem>	β_2

<chem>CC(C)NCC(COC(=O)C1=CC=CS1)O</chem>	β2
<chem>CCOC(=O)CCNCC(COC1=CC=CC=C1C)O</chem>	β2
<chem>CCOC(=O)CNCC(COC1=CC=CC=C1C)O</chem>	β2
<chem>CC(C)(C)NCC(COC1=CC=CC=C1C(=O)OC)O</chem>	β2
<chem>CC1=CC=CC=C1OCC(CNCC2=CC=C(C=C2)N3C=CN=C3)O</chem>	β2
<chem>COC1=C(C=C(C=C1)CCNCC(COC2=CC=C(C=C2)OCC3=NC=CN3)O)OC</chem>	β2
<chem>CC(C)NCC(COC1=CC2=C(C=C1)N=CN2)O</chem>	β2
<chem>CC(C)(C)NCC(COC1=CC=C(C=C1)C2=NC=C(N2)C(F)(F)F)O</chem>	β2
<chem>CC(C)(CC1=CC=C(C=C1)N)NCC(CON=C(C2CC2)C3CC3)O</chem>	β2
<chem>CC(C)NCC(CON=C1C2=CC=CC=C2C3C1(CCCCC3)OC)O</chem>	β2
<chem>CC1=CC(=CC=C1)OCC(CNCC2=CC=C(C=C2)NS(=O)(=O)C)O</chem>	β2
<chem>CC1=CC=CC=C1OCC(CNC(C)C)O</chem>	β2
<chem>CC1=CC=C(C=C1)C(CNC(C)C)O</chem>	β2
<chem>CCOC(=O)CCNCC(COC1=CC=CC=C1C(=O)OC)O</chem>	β2
<chem>COC1=C(C=C(C=C1)CCNCC(COC2=CC=C(C=C2)C3=NC=C(N3)Br)O)OC</chem>	β2
<chem>CC(C)NCC(COC1=CC=C(C=C1)CCCC(=O)OC)O</chem>	β2
<chem>CCOC(=O)CC(C)(C)NCC(COC1=CC=CC=C1C)O</chem>	β2
<chem>CC(C)(C)NCCC(=O)N=C(C1CC1)C2CC2</chem>	β2
<chem>CC(C)(C)NCC(CON=C1C2=CC=CC=C2C3C1(CCCCC3)O)O</chem>	β2
<chem>CC(C)NCC(COC1=CC=CC=C1C(=O)OC=C)O</chem>	β2
<chem>CC(=O)C1=CN=C(N1)C2=CC=C(C=C2)OCC(CNCCC3=CC(=C(C=C3)OC)OC)O</chem>	β2
<chem>CC(C)NCC(COC1=CC=C(C=C1)C2=NC=C(N2)C3=CC=CS3)O</chem>	β2
<chem>CC1=CN=C(N1)C2=CC=C(C=C2)OCC(CNC(C)(C)C)O</chem>	β2
<chem>CC(C)COCC(CNC(C)(C)C)O</chem>	β2
<chem>CC(C)(C)NCC(CON=C1C2=CC=CC=C2C3C1(CCCCC3)OC)O</chem>	β2
<chem>C1=CSC(=C1)C2=CN=C(N2)C3=CC=C(C=C3)OCC(CNCCC4=CC=NC=C4)O</chem>	β2
<chem>CC(C1CC1)OCC(CNC(C)(C)C)O</chem>	β2
<chem>CC1=CC(=CC=C1)OCC(CN2CCN(CC2)C3=CC=C(C=C3)NS(=O)(=O)C)O</chem>	β2
<chem>CC(C)NCC(COC1=CC=CC2=C1N=CN2)O</chem>	β2
<chem>CC(C)NCC(CON=C1C2=CC=CC=C2C3C1(CCCCC3)OC)O</chem>	β2

<chem>CS(=O)(=O)NC1=CC=C(C=C1)OCC(CNCCOC2=CC=C(C=C2)N3C=CN=C3)O</chem>	β1/β2
<chem>CC(C)NCC(COC1=CC=C(C=C1)C(=O)OC=C)O</chem>	β2
<chem>CC(C)(C)NCC(COCC1CC1)O</chem>	β2
<chem>C1CC1NCC(COC2=CC=C(C=C2)C3=NC=C(N3)C(F)(F)F)O</chem>	β2
<chem>COC1=CC(=CC(=C1OC)OC)CC2C3=C(C(=C(C=C3CCN2)O)O)I</chem>	β2
<chem>CCOC(=O)C(C)(C)NCC(COC1=CC=CC=C1C(=O)OC)O</chem>	β2
<chem>CC(C)NCC(C1=CC=CC=C1OC)O</chem>	β2
<chem>CC(C)NCC(COC(=O)CC1=CC=CS1)O</chem>	β2
<chem>CC(C)NCC(COC1=CC=CC=C1C2CC2)O</chem>	β1/β2
<chem>CC1=CN=C(N1)C2=CC(=C(C=C2)OCC(CNCCC3=CC(=C(C=C3)OC)OC)O)OC</chem>	β2
<chem>CCOC(=O)CNCC(COC1=CC=CC2=CC=CC=C21)O</chem>	β2
<chem>CC(C)C(=O)OCC(CNC(C)C)O</chem>	β2
<chem>CC(C)NCC(C1=CC=C(C=C1)Br)O</chem>	β2
<chem>CCOC(=O)C1=CC=C(C=C1)OCC(CNC(C)C)O</chem>	β2
<chem>CC(C)NCC(CON=C1C2=C(C=CC(=C2)F)C3C1(CCCC3)OC)O</chem>	β2
<chem>CC1CC(CC(C1)(C)C)OCC(CNC(C)(C)C)O</chem>	β2
<chem>CC(C)(C)NCC(COC1=CC=C(C=C1)C(=O)OC)O</chem>	β2
<chem>CC(C(C1=C(C=CC(=C1)OC)OC)O)NC(C)(C)C</chem>	β2
<chem>CC(C)NCC(COC1=CC=CC=C1OCC(CNC(C)C)O)O</chem>	β2
<chem>CC(C)NCC(C1=CC=C(C=C1)[N+](=O)[O-])O</chem>	β1/β2
<chem>C1=CC=C(C=C1)NC(=O)NCCNCC(COC2=CC=C(C=C2)C3=NC=CN3)O</chem>	β2
<chem>CC1=CN=C(N1)C2=CC(=C(C=C2)OCC(CNCCC3=CC(=C(C=C3)OC)OC)O)Br</chem>	β2
<chem>CC(C)(C)NCC(COC(C1CC1)C2CC2)O</chem>	β2
<chem>CC1=C2CCCC2=C(C=C1)OCC(C(C)NC(C)C)O</chem>	β2
<chem>CC1=CC(=CC=C1)C(CNC(C)C)O</chem>	β2
<chem>CC(C)(C)NCC(CON=CC1CC1)O</chem>	β2
<chem>CC1(C(N1)C(C2=CC(=C(C=C2)Cl)Cl)O)C</chem>	β2
<chem>CCOC(=O)CCNCC(COC1=CC=CC(=C1)OC)O</chem>	β2
<chem>COC1=C(C=C(C=C1)CCNCC(COC2=CC=C(C=C2)COCC3=NC=CN3)O)OC</chem>	β2
<chem>COC1=C(C=C(C=C1)CCNCC(COC2=CC=CC=C2C(=O)OC)O)OC</chem>	β2

<chem>COC1=CC(=CC(=C1OC)OC)CC2C3=CC(=C(C(=C3CCN2)I)O)O</chem>	β2
<chem>CC(C)C(=NOCC(CNC(C)(C)C)O)C</chem>	β2
<chem>CCOC(=O)CCNCC(COC1=CC=CC(=C1)C)O</chem>	β2
<chem>CC1=C(N=C(N1)C2=CC=C(C=C2)OCC(CNCCC3=CC(=C(C=C3)OC)OC)O)C(=O)C</chem>	β2
<chem>CC(CC1=CC=C(C=C1)OCCF)NCC(C2=CC(=CC(=C2)O)O)O</chem>	β2
<chem>CC1=CC=CC=C1OCC(CNCC(C)C)O</chem>	β2
<chem>COC1=C(C=C(C=C1)CCNCC(COC2=CC=C(C=C2)C3=NC=C(N3)Cl)O)OC</chem>	β2
<chem>CC1=C(N=C(N1)C2=CC=C(C=C2)OCC(CNCCC3=CC(=C(C=C3)OC)OC)O)C</chem>	β2
<chem>CCOCC1=CN=C(N1)C2=CC=C(C=C2)OCC(CNCCC3=CC(=C(C=C3)OC)OC)O</chem>	β2
<chem>CC(C)NCC(COC1=CC=C(C=C1)C2=NC=CN2)O</chem>	β2
<chem>C1=CC=C(C=C1)OCC(CNCCOC2=CC=C(C=C2)N3C=CN=C3)O</chem>	β2
<chem>CC(C)(C)C1=CN=C(N1)C2=CC=C(C=C2)OCC(CNCCC3=CC(=C(C=C3)OC)OC)O</chem>	β2
<chem>CCOC(=O)CNCC(COC1=CC=CC=C1)O</chem>	β2
<chem>CCOC(=O)CCCCNCC(COC1=CC=CC=C1C)O</chem>	β2
<chem>COC1=C(C=C(C=C1)CCNCC(COC2=CC=C(C=C2)CCC(=O)OC)O)OC</chem>	β2
<chem>CC(C)(CC1=CC=C(C=C1)NCC(CON=C(C2CC2)C3CC3)O)NCC(CON=C(C4CC4)C5CC5)O</chem>	β2
<chem>CC1CC(=NOCC(CNC(C)(C)C)O)CC(C1)(C)C</chem>	β2
<chem>COC1=C(C=C(C=C1)CCNCC(COC2=CC=C(C=C2)C3=NC=C(N3)C(=O)N)O)OC</chem>	β2
<chem>CC1=CC(=CC=C1)OCC(CNCCOC2=CC=C(C=C2)N3C=CN=C3)O</chem>	β2
<chem>CC(C)CNCC(COC1=CC=CC=C1)O</chem>	β2
<chem>C1=CC=C2C(=C1)C=CC=C2OCC(CN)O</chem>	β2
<chem>CC(C)(C)NCC(C1=COC2=CC=CC=C2O1)O</chem>	β2
<chem>CC(C)NCC(COC1=CC=CC=C1C(=O)OC)O</chem>	β2
<chem>COC1=C(C=C(C=C1)CCNCC(COC2=C(C=C(C=C2)C3=NC=C(N3)Br)Cl)O)OC</chem>	β2
<chem>CC(C)(C)NCC(COC1=CC=C(C=C1)CCC(=O)OC)O</chem>	β2
<chem>CCOC(=O)C1=CC=CC=C1OCC(CNC(C)(C)C)O</chem>	β2
<chem>CCCCCNC(=O)NC1=CC=C(C=C1)S(=O)(=O)NC2=CC3=C(C=C2)C=C(C=C3)CC4C5=CC(=C(C=C5CCN4)O)O</chem>	β1/β2
<chem>CC(C)NCC1C2=CC(=C(C=C2CCO1)O)O</chem>	β1/β2
<chem>CCCCCNC(=O)NC1=CC=C(C=C1)S(=O)(=O)NC2=CC=CC(=C2)C3=CC(=CC=C3)CC4C5=CC(=C(C=C5CCN4)O)O</chem>	β1/β2
<chem>C1CCC(CC1)S(=O)(=O)NC2=CC=C(C=C2)CCNCC(COC3=CC=C(C=C3)O)O</chem>	β1/β2

<chem>CC(CCC1=CC=C(C=C1)OC)NCC(COC2=CC=C(C=C2)O)O</chem>	$\beta 1/\beta 2$
<chem>CCCCCNC(=O)NC1=CC=C(C=C1)S(=O)(=O)NC2=CC3=C(C=C2)C=C(C=C3)OCC4C5=CC(=C(C=C5CCN4)O)O</chem>	$\beta 1/\beta 2$
<chem>CCCCCNC(=O)NC1=CC=C(C=C1)S(=O)(=O)NC2=CC=C(C=C2)C3=CC=C(C=C3)CC4C5=CC(=C(C=C5CCN4)O)O</chem>	$\beta 1/\beta 2$
<chem>C1CC(N(C1)C(=O)CNCC(COC2=CC=CC=C2)O)C#N</chem>	$\beta 1/\beta 2$
<chem>CCCCCNC(=O)NC1=CC=C(C=C1)S(=O)(=O)NC2=CC=CC(=C2)C3=CC=C(C=C3)CC4C5=CC(=C(C=C5CCN4)O)O</chem>	$\beta 1/\beta 2$
<chem>COC1=CC=C(C=C1)CCCNCC(COC2=CC=C(C=C2)O)O</chem>	$\beta 1/\beta 2$
<chem>C1=CC(=CC=C1CCNCC(COC2=CC=C(C=C2)O)O)NS(=O)(=O)C3=CC=C(C=C3)C1</chem>	$\beta 1/\beta 2$
<chem>CS(=O)(=O)C1=CC=CC2=C1NC=C2CCNCC(C3=CC(=CC=C3)NS(=O)(=O)C4=CC=CC(=C4)N)O</chem>	$\beta 1/\beta 2$
<chem>CC1=CC(=CC=C1)OCC(CNC(C)C)O</chem>	$\beta 1/\beta 2$
<chem>CCCCCNC(=O)NC1=CC=C(C=C1)S(=O)(=O)NC2=CC=C(C=C2)CCNCC(COC3=CC=C(C=C3)O)O</chem>	$\beta 1/\beta 2$
<chem>CCCCCNC(=O)NC1=CC=C(C=C1)S(=O)(=O)NC2=CC=C(C=C2)C3=CC=C(C=C3)OCC4C5=CC(=C(C=C5CCN4)O)O</chem>	$\beta 1/\beta 2$
<chem>CCCCCNC(=O)NC1=CC=C(C=C1)S(=O)(=O)NC2=CC=C(C=C2)C3=CC(=CC=C3)CC4C5=CC(=C(C=C5CCN4)O)O</chem>	$\beta 1/\beta 2$
<chem>CCCCCNC(=O)NC1=CC=C(C=C1)S(=O)(=O)NC2=CC=C(C=C2)OCC3C4=CC(=C(C=C4CCN3)O)O</chem>	$\beta 1/\beta 2$
<chem>CS(=O)(=O)OC1=CC=CC2=C1NC=C2CCNCC(C3=CC(=CC=C3)NS(=O)(=O)C4=CC=CS4)O</chem>	$\beta 1/\beta 2$
<chem>COC1=CC(=CC(=C1OC)OC)C2=CC=C(C=C2)CC3C4=CC(=C(C=C4CCN3)O)O</chem>	$\beta 1/\beta 2$
<chem>CN(C)C(=NC1=NC(=O)C(=CC2=CC=C(C=C2)N3CCC(CC3)NCC(COC4=CC=CC5=C4NC(=O)N5)O)S1)N</chem>	$\beta 1/\beta 2$
<chem>C1=CC(=CC=C1CCNCC(COC2=CC=C(C=C2)O)O)NS(=O)(=O)C3=CC=C(C=C3)Br</chem>	$\beta 1/\beta 2$
<chem>C1=CC=C2C(=C1)C=C(C=N2)S(=O)(=O)NC3=CC=C(C=C3)CCNCC(COC4=CC=C(C=C4)O)O</chem>	$\beta 1/\beta 2$
<chem>CCCCCNC(=O)NC1=CC=C(C=C1)S(=O)(=O)NC2=CC=CC(=C2)C3=CC=C(C=C3)OCC4C5=CC(=C(C=C5CCN4)O)O</chem>	$\beta 1/\beta 2$
<chem>CS(=O)(=O)NC1=C(C=CC(=C1)C(CNC2CCN(CC2)C3=CC=C(C=C3)CC4C(=O)N(C(=O)S4)CC(=O)O)O)O</chem>	$\beta 1/\beta 2$
<chem>CCCCCN1C(=O)N(N=N1)C2=CC=C(C=C2)S(=O)(=O)NC3=CC=C(C=C3)CCNCC(C4=CN=CC=C4)O</chem>	$\beta 1/\beta 2$
<chem>CCCCCNC(=O)NC1=CC=C(C=C1)S(=O)(=O)NC2=CC=C(C=C2)CC3C4=CC(=C(C=C4CCN3)O)O</chem>	$\beta 1/\beta 2$
<chem>C1=CC(=CC=C1CCNCC(COC2=CC=C(C=C2)O)O)NS(=O)(=O)C3=CC=C(C=C3)I</chem>	$\beta 1/\beta 2$
<chem>CS(=O)(=O)NC1=C(C=CC(=C1)C(CNC2CCN(CC2)C3=CC=C(C=C3)CN4C(=O)NC(=O)O4)O)O</chem>	$\beta 1/\beta 2$
<chem>CC1=NN2C(=NC3=C(C2=N1)CCNCC3)CC4=CC=CC=C4</chem>	$\beta 2$
<chem>CC(C)C(C(=O)O)NC(=O)C1=CC=C(C=C1)N2CCC(CC2)NCC(C3=CC(=C(C=C3)O)NS(=O)(=O)C)O</chem>	$\beta 2$
<chem>CC1=C(C=CC(=C1)C2=CC=CC=C2C(C)OCC(CNC(C)(C)CC3=CC(=C(C=C3)Cl)F)O)C(=O)O</chem>	$\beta 2$
<chem>COC(=O)CCc1ccc(cc1)OCC(CNC(C)C)O</chem>	$\beta 1$
<chem>CC(=O)Oc1c(C)cc(OCC(O)CNC(C)C)c(C)c1C</chem>	$\beta 1/\beta 2$

<chem>C=CCOc1cccc1OCC(O)CNC(C)C</chem>	$\beta 1/\beta 2$
<chem>OC(COc1ccc(cc1)NC(=O)C)CNC(C)C</chem>	$\beta 1$
<chem>OC(COc1ccc(cc1)c1nc(en1C)C(F)(F)F)CNCCOc1ccc(c(c1)C(=O)N)O</chem>	$\beta 1$
<chem>CCCC(=Nc1ccc(c(c1)C(=O)C)OCC(CNC(C)C)O)O</chem>	$\beta 1$
<chem>OC(COc1cc(C)ccc1Cl)CNC(C)(C)C</chem>	$\beta 1/\beta 2$
<chem>CC(C)NCC(O)c1ccc2ccccc2c1</chem>	$\beta 1$
<chem>COCCc1ccc(cc1)OCC(CNC(C)C)O</chem>	$\beta 1$
<chem>OC(COc1ccc(cc1)OCCOCC1CC1)CNC(C)C</chem>	$\beta 1/\beta 2$
<chem>CCCNCC(COc1ccccc1C(=O)CCc1ccccc1)O</chem>	$\beta 1/\beta 2$
<chem>OC(C1CCc2c(O1)ccc(c2)F)CNCC(C1CCc2c(O1)ccc(c2)F)O</chem>	$\beta 1$
<chem>OC(COc1ccc(cc1)CC(=O)N)CNC(C)C</chem>	$\beta 1$
<chem>O[C@H](COc1ccc(cc1)CCOCC1CC1)CNC(C)C</chem>	$\beta 1$
<chem>OC(COc1ccc(cc1)CCOCC1CC1)CNC(C)C</chem>	$\beta 1$
<chem>COc1ccccc1OCCNCC(COc1ccccc2c1c1ccccc1[nH]2)O</chem>	$\beta 1$
<chem>OC(COc1ccccc1)CNC(C)C</chem>	$\beta 1$
<chem>OCCc1ccc(cc1)OCC(CNC(C)C)O</chem>	$\beta 1/\beta 2$
<chem>CC(CCc1ccccc1)NCC(c1ccc(c(c1)C(=N)O)O)O</chem>	$\beta 1$
<chem>N#Cc1cc(OCCOCC2CC2)ccc1OCC(CNCCNC(=O)Nc1ccc(cc1)O)O</chem>	$\beta 1$
<chem>CC(C)NCC(O)COc1ccc(COCCOC(C)C)cc1</chem>	$\beta 1$
<chem>OC(COc1ccccc2c1C[C@H](O)[C@@H](C2)O)CNC(C)(C)C</chem>	$\beta 1/\beta 2$
<chem>OC(COc1ccccc2c1c([125I])c([nH]2)C#N)CNC(C)C</chem>	$\beta 1$
<chem>CC(NCC(c1ccc(cc1)NS(=O)(=O)C)O)C</chem>	$\beta 1/\beta 2$
<chem>OC(COc1ccccc2c1ccccc2)CNC(C)C</chem>	$\beta 1/\beta 2$
<chem>C=CCc1ccccc1OCC(CNC(C)C)O</chem>	$\beta 2$
<chem>O[C@H](COc1ccccc2c1ccccc2)CNC(C)C</chem>	$\beta 1/\beta 2$
<chem>CC(C)(C)NC[C@H](O)COc1nsnc1N1CCOCC1</chem>	$\beta 1/\beta 2$
<chem>O[C@H](COc1ccccc2c1CCCC2=O)CNC(C)(C)C</chem>	$\beta 1/\beta 2$
<chem>CC(C)(C)NC[C@H](O)COc1ccccc1C1CCCC1</chem>	$\beta 1/\beta 2$

CC(C)(Cc1ccc(Oc2ccc(C(N)=O)cn2)cc1)NC[C@H](O)COc1ccccc2[nH]c3ccccc3c12	β1/β2
O[C@H](COc1ccccc2c1[nH]c(=O)[nH]2)CNC(C)(C)C	β1/β2
OC(COc1ccccc2c1[nH]c(=O)[nH]2)CNC(C)(C)C	β1/β2
C1CCC(C1)OCCOC2=CC=C(C=C2)OCC(CNCCNC(=O)NC3=CC=C(C=C3)O)O	β1/β2
C1CCC(C1)OCCOC2=CC=C(C=C2)OCC(CNCCNC(=O)NC3=CC(=CC=C3)Cl)O	β1/β2
CC1=CC(=C(C=C1)C(C)C)OCC(CN2CCC(CC2)CN3C(=O)C4=CC=CC5=C4C(=CC=C5)C3=O)O	β1/β2
CCOCCOC1=CC=C(C=C1)OCC(CNCCNC(=O)NC2=CC=C(C=C2)O)O	β1/β2
C1=CC(=CC=C1CCOCCOC2=CC=C(C=C2)OCC(CNCCNC(=O)NC3=CC=C(C=C3)O)O)F	β1/β2
C1CCC(C1)OCCOC2=CC=C(C=C2)OCC(CNCCNC(=O)NC3=CC=CC=C3)O	β1/β2
C1CC1COCCOC2=CC(=C(C=C2)OCC(CNCCNC(=O)NC3=CC=C(C=C3)O)O)C#N	β1
CN1C=C(N=C1C2=CC=C(C=C2)OCC(CNCCOC3=CC(=C(C=C3)O)C(=O)N)O)C(F)(F)F	β1
CC1=CC(=CC=C1)OCC(CNCCC2=CC(=C(C=C2)OC)OC)O	β1
COC1=CC=CC=C1OCCNCC(COC2=CC=CC3=C2C4=CC=CC=C4N3)O	β1
CC1(OC[C@H](O1)COC(=O)CCC2=CC=C(C=C2)OC[C@H](CNCCNC(=O)N3CCOCC3)O)C	β1
CC(C)NCC(COC1=CC=C(C=C1)OCCOCC2CC2)O	β1/β2
CC(C)NCC(COC1=CC=CC=C1)O	β2
CC(C)NCC(COC1=CC=C(C=C1)CCCO)O	β1/β2
CC(C)NCC(COC1=CC=CC2=C1C(=C(N2)C#N)[125I])O	β2
CC(C)(C)NCC(CSC1=NC(=CS1)C2=CC=C(S2)C(=O)N)O	β1/β2
CC(C)(C)NC[C@H](COC1=NSN=C1N2CCOCC2)O	β1/β2
CC(C)NC[C@H](COC1=CC=C(C=C1)CCOC)O	β1
CC(C)(C)NCC(COC1=CC=CC2=C1CCC(=O)N2)O	β1/β2
CC(C)NC[C@H](COC1=CC=C(C=C1)CC(=O)N)O	β1
CC(C)NC[C@H](COC1=CC=C(C=C1)CCOCC2CC2)O	β1
CC(CCC1=CC=CC=C1)NCC(C2=CC(=C(C=C2)O)C(=O)N)O	β1/β2
CC(C)[C@@]1(C(=O)N2[C@H](C(=O)N3CCC[C@H]3[C@@]2(O1)O)CC4=CC=CC=C4)NC(=O)[C@@H]5C[C@@H]6[C@@H](CC7=CNC8=CC=CC6=C78)N(C5)C	β1/β2
CC(C)[C@H]1C(=O)N2CCC[C@H]2[C@]3(N1C(=O)[C@](O3)(C(C)C)NC(=O)[C@@H]4C[C@H]5[C@@H](CC6=CNC7=CC=CC5=C67)N(C4)C)O	β1/β2
CCCCC1=C(C2=CC=CC=C2O1)C(=O)C3=CC(=C(C=C3)I)OCCN(CC)CC)I	β1/β2

CC(C)NCC(COC1=CC=CC2=C1C=CN2)O	β1/β2
CC(C)NC[C@@H](COC1=CC=C(C=C1)OCCOC)O	β1
CC(=O)C1=CN=C(N1)C2=CC=C(C=C2)OC[C@H](CNCCC3=CC(=C(C=C3)OC)OC)O	β1
CCC1=CC=CC2=C1OC(=C2)C(CNC(C)(C)C)O	β1/β2
CC1=CC2=C(N1)C=CC=C2OCC(CNC(C)C)O	β1/β2
CC(C)(C)NCC(COC1=CC=CC=C1C#N)O	β1/β2
O[C@H](COc1ccc(cc1)O)CNC(C)C	β1
OC(COc1cccc2c1cc[nH]2)CNC(C)C	β1/β2
CC1=CC2=C(N1)C=CC=C2OCC(CNC(C)(C)C)OC(=O)C3=CC=CC=C3	β1/β2
OC(COc1cccc2c1c1cccc1[nH]2)CNC(C)C	β1/β2
CC(N[C@H])([C@H](COc1ccc(c2c1CCC2)C)O)C	β2
CC(C)NCC(COC1=CC=CC2=C1C3=CC=CC=C3N2)O	β1/β2
O=C(Cc1csc(n1)N)Nc1ccc(cc1)CCNC[C@@H](c1cccc1)O	β3
C1c1cccc(c1)[C@H](CNCCNc1cccc(c1)c1cccc(c1)C(=O)O)O	β3
CCc1cccc1OC[C@H](CN[C@H]1CCCc2c1cccc2)O	β3
C1CN(CC1C(C2=CC=CC=C2)(C3=CC=CC=C3)C(=O)N)CCC4=CC5=C(C=C4)OCC5	M3
C[C@@]1(C(=O)N2[C@H](C(=O)N3CCC[C@H]3[C@@]2(O1)O)CC4=CC=CC=C4)NC(=O)[C@H]5CN([C@@H]6CC7=CNC8=CC=CC(=C78)C6=C5)C	A

SMILES	Target	ZINC ID
<chem>C=CCc1ccccc1OC[C@H](O)CNC(C)C</chem>	β 1	ZINC0000000000 23
<chem>CC(C)(C)NC[C@@H](O)COc1cccc2c1CCC(=O)N2</chem>	β 1	ZINC0000000001 28
<chem>CC(C)NC[C@@H](O)c1ccccc1Cl</chem>	β 1	ZINC0000000001 78
<chem>COC(=O)CCc1ccc(OC[C@H](O)CNC(C)C)cc1</chem>	β 1	ZINC0000000002 57
<chem>CC[C@H](NC(C)C)[C@@H](O)c1ccc(O)c(O)c1</chem>	β 2	ZINC0000000004 01
<chem>C[C@H](CCc1ccccc1)NC[C@@H](O)c1ccc(O)c(C(N)=O)c1</chem>	β 1	ZINC0000000004 16
<chem>CC(C)NC[C@@H](O)c1cc(O)cc(O)c1</chem>	β 2	ZINC0000000004 69
<chem>C[C@H](CCc1ccc(O)cc1)NC[C@@H](O)c1ccc(O)cc1</chem>	β 2	ZINC0000000006 94
<chem>COc1cc(C[C@@H]2NCCc3cc(O)c(O)cc32)cc(OC)c1OC</chem>	β 1	ZINC0000000008 02
<chem>COc1ccc(C[C@H](C)NC[C@@H](O)c2ccc(O)c(NC=O)c2)cc1</chem>	β 1	ZINC0000000008 56
<chem>C[C@H](CCc1ccc(O)cc1)NC[C@H](O)c1ccc(O)cc1</chem>	β 2	ZINC0000000010 78
<chem>c1ccc2nc(N3CCNCC3)ccc2c1</chem>	β 1	ZINC0000000020 20
<chem>CC(C)NC[C@@H](O)c1ccc(N)c(C#N)c1</chem>	β 1	ZINC0000000023 07
<chem>CC(C)N[C@H]1CCn2c(=O)[nH]c3cccc(c32)[C@@H]1O</chem>	β 2	ZINC0000000040 10
<chem>CC(C)NC[C@@H](O)c1ccc(NS(C)(=O)=O)cc1</chem>	β 1	ZINC0000000041 66
<chem>Clc1cccc(N2CCNCC2)c1</chem>	β 1	ZINC0000000042 85
<chem>C[C@H](Cc1c[nH]c2ccccc12)NC[C@H](O)c1cccc(Cl)c1</chem>	β 1	ZINC0000000066 35

<chem>COc1ccccc1N1CCNCC1</chem>	$\beta 1$	ZINC0000000126 87
<chem>CC(C)(C)NC[C@@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 2$	ZINC0000000202 30
<chem>CC(C)NC[C@@H](O)COc1cccc2ccccc12</chem>	$\beta 1$	ZINC0000000202 40
<chem>C[C@H](Cc1c[nH]c2ccccc12)NC[C@@H](O)c1cccc(Cl)c1</chem>	$\beta 1$	ZINC0000000212 28
<chem>CC(C)NC[C@@H](O)COc1cccc2[nH]ccc12</chem>	$\beta 1$	ZINC0000000566 46
<chem>CC(C)NC[C@@H](O)c1ccc(O)c(O)c1</chem>	$\beta 1$	ZINC0000000566 53
<chem>CC(C)(C)NC[C@@H](O)c1cc(Cl)c(N)c(Cl)c1</chem>	$\beta 1$	ZINC0000000572 62
<chem>C[C@@H](NCCc1ccc(O)cc1)[C@@H](O)c1ccc(O)cc1</chem>	$\beta 2$	ZINC0000000574 83
<chem>COc1cccc(N2CCNCC2)c1</chem>	$\beta 1$	ZINC0000000660 34
<chem>Cc1cccc(N2CCNCC2)c1C</chem>	$\beta 1$	ZINC0000000660 69
<chem>Cc1ccc(N2CCNCC2)cc1C</chem>	$\beta 1$	ZINC0000000660 72
<chem>Cc1cc(N2CCNCC2)c2ccccc2n1</chem>	$\beta 1$	ZINC0000000842 12
<chem>C=CCc1ccccc1OC[C@@H](O)CNC(C)C</chem>	$\beta 1$	ZINC0000000865 99
<chem>c1ccc(N2CCNCC2)cc1</chem>	$\beta 1$	ZINC0000001202 71
<chem>Clc1cncc(Cl)c1N1CCNCC1</chem>	$\beta 2$	ZINC0000001272 19
<chem>CCCC(=O)Nc1ccc(OC[C@@H](O)CNC(C)C)c(C(C)=O)c1</chem>	$\beta 1$	ZINC0000001567 92
<chem>FC(F)(F)c1cc(N2CCNCC2)c2ccccc2n1</chem>	$\beta 2$	ZINC0000001706 53

<chem>Cc1ccc2nc(C(F)(F)F)cc(N3CCNCC3)c2c1</chem>	$\beta 2$	ZINC0000001707 19
<chem>Clc1ccc2c(N3CCNCC3)ccnc2c1</chem>	$\beta 2$	ZINC0000001715 26
<chem>Cc1ccc(C(C)C)c(OC[C@H](O)CN2CCCCC2)c1</chem>	$\beta 2$	ZINC0000002458 41
<chem>Cc1ccc(C(C)C)c(OC[C@@H](O)CN2CCCCC2)c1</chem>	$\beta 2$	ZINC0000002458 43
<chem>FC(F)(F)c1cc(N2CCNCC2)cc(C(F)(F)F)c1</chem>	$\beta 1$	ZINC0000002525 16
<chem>COc1cc2c3c(c1OC)-c1cc4c(cc1C[C@@H]3N(C)CC2)OCO4</chem>	$\beta 1$	ZINC0000003381 36
<chem>COc1cc2c3c(c1OC)-c1cc4c(cc1C[C@H]3N(C)CC2)OCO4</chem>	$\beta 1$	ZINC0000003381 40
<chem>Clc1cccc(N2CCNCC2)c1Cl</chem>	$\beta 1$	ZINC0000003867 29
<chem>CC[C@@H](NC(C)C)[C@H](O)c1ccc(O)c(O)c1</chem>	$\beta 2$	ZINC0000004029 80
<chem>CC[C@@H](NC(C)C)[C@@H](O)c1ccc(O)c(O)c1</chem>	$\beta 2$	ZINC0000004029 81
<chem>C[C@@H](CCc1ccccc1)NC[C@@H](O)c1ccc(O)c(C(N)=O)c1</chem>	$\beta 1$	ZINC0000004030 11
<chem>C[C@H](N)Cc1c[nH]c2ccccc12</chem>	$\beta 1$	ZINC0000004044 50
<chem>C[C@@H](N)Cc1c[nH]c2ccccc12</chem>	$\beta 1$	ZINC0000004044 51
<chem>Clc1ccc(N2CCNCC2)cc1Cl</chem>	$\beta 1$	ZINC0000004101 39
<chem>CN(C)C(=O)C(CCN1CCC(O)(c2ccc(Cl)cc2)CC1)(c1ccccc1)c1ccccc1</chem>	$\beta 2$	ZINC0000005379 28
<chem>COC(=O)COc1ccc(C[C@@H](C)NC[C@H](O)c2cccc(Cl)c2)cc1</chem>	$\beta 1$	ZINC0000005752 32
<chem>Clc1ccc(CO[C@H](Cn2ccnc2)c2ccc(Cl)cc2Cl)cc1</chem>	$\beta 1$	ZINC0000005968 81

<chem>Clc1ccc(CO[C@H](Cn2ccnc2)c2ccc(Cl)cc2Cl)c(Cl)c1</chem>	$\beta 1$	ZINC0000006079 71
<chem>Clc1ccc(CO[C@@H](Cn2ccnc2)c2ccc(Cl)cc2Cl)cc1</chem>	$\beta 1$	ZINC0000006430 55
<chem>C[C@H](CNc1ccc(CC(=O)O)cc1)NC[C@H](O)c1cccc(Cl)c1</chem>	$\beta 1$	ZINC0000008361 82
<chem>Clc1ccc(CO[C@@H](Cn2ccnc2)c2ccc(Cl)cc2Cl)c(Cl)c1</chem>	$\beta 1$	ZINC0000008967 40
<chem>COc1ccc(C[C@@H](C)NC[C@@H](O)c2ccc(O)c(NC=O)c2)cc1</chem>	$\beta 1$	ZINC0000008972 58
<chem>CC(C)(C)NC[C@H](O)COc1cccc2[nH]cc(CC(N)=O)c12</chem>	$\beta 2$	ZINC0000013222 22
<chem>CC(C)(C)NC[C@@H](O)COc1cccc2[nH]cc(CC(N)=O)c12</chem>	$\beta 2$	ZINC0000013222 23
<chem>COc1cccc2c(C[C@@H](C)NC[C@H](O)c3cccc(Cl)c3)c[nH]c12</chem>	$\beta 1$	ZINC0000014861 49
<chem>COc1ccc([C@@H](Cc2ccccc2)NC[C@@H](O)Cc2ccc(O)c(NS(C)(=O)=O)c2)cc1OC</chem>	$\beta 1$	ZINC0000014908 62
<chem>COc1cccc1OCCNC[C@@H](O)COc1cccc2[nH]c3ccccc3c12</chem>	$\beta 1$	ZINC0000015305 80
<chem>CC/C(=C(\c1cccc1)c1ccc(OCCN(C)C)cc1)c1cccc1</chem>	$\beta 1$	ZINC0000015306 89
<chem>CCCNC[C@@H](O)COc1cccc1C(=O)CCc1cccc1</chem>	$\beta 1$	ZINC0000015307 60
<chem>O=C(NCCNC[C@@H](O)COc1ccc(O)cc1)N1CCOCC1</chem>	$\beta 1$	ZINC0000015323 64
<chem>O=C(O)COc1ccc(OCCNC[C@H](O)COc2ccccc2)cc1</chem>	$\beta 1$	ZINC0000015333 80
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)COc2ccc(O)cc2)cc1)c1ccc2ccccc2c1</chem>	$\beta 1$	ZINC0000015394 19
<chem>Cc1cc2c(OC[C@H](CNC(C)(C)C)OC(=O)c3ccccc3)cccc2[nH]1</chem>	$\beta 1$	ZINC0000015429 01
<chem>C[C@H](Cc1ccc(OCS(=O)(=O)O)cc1)NC[C@H](O)c1cccc(Cl)c1</chem>	$\beta 1$	ZINC0000015438 94

<chem>CC(C)NC[C@H](O)c1ccccc1Cl</chem>	$\beta 1$	ZINC0000015763 50
<chem>CC(C)(Cc1ccccc1)NC[C@@H](O)c1ccc(O)c(NS(C)(=O)=O)c1</chem>	$\beta 2$	ZINC0000018656 07
<chem>O[C@@H](CNCCc1ccc(NC(=S)Nc2ccc(F)cc2)cc1)COc1ccccc1</chem>	$\beta 1$	ZINC0000019024 91
<chem>Cc1nc(-c2ccc(OCCNC[C@H](O)c3ccnc3)cc2)c(C)o1</chem>	$\beta 1$	ZINC0000019117 76
<chem>CC(C)NC[C@@H](O)COc1cccc2[nH]c3ccccc3c12</chem>	$\beta 2$	ZINC0000019992 43
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)COc2ccnc2)cc1)c1ccc(I)cc1</chem>	$\beta 1$	ZINC0000020045 98
<chem>C[C@@H](CCc1ccc(O)cc1)NC[C@@H](O)c1ccc(O)cc1</chem>	$\beta 2$	ZINC0000020141 85
<chem>CC[C@H](NC1CCCC1)[C@H](O)c1ccc(O)c(O)c1</chem>	$\beta 2$	ZINC0000020194 82
<chem>CC[C@@H](NC1CCCC1)[C@H](O)c1ccc(O)c(O)c1</chem>	$\beta 2$	ZINC0000020194 83
<chem>CC[C@H](NC1CCCC1)[C@@H](O)c1ccc(O)c(O)c1</chem>	$\beta 2$	ZINC0000020194 84
<chem>CC[C@@H](NC1CCCC1)[C@@H](O)c1ccc(O)c(O)c1</chem>	$\beta 2$	ZINC0000020194 85
<chem>CS(=O)(=O)Nc1ccc(OC[C@@H](O)CNCCOc2ccc(-n3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000020227 43
<chem>CS(=O)(=O)Nc1ccc([C@@H](O)CNCCOc2ccc(-n3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000020227 45
<chem>Cc1cccc(OC[C@@H](O)CNC(C)C)c1</chem>	$\beta 1$	ZINC0000020331 45
<chem>Clc1cc(Cl)cc(N2CCNCC2)c1</chem>	$\beta 1$	ZINC0000021684 54
<chem>COc1cc(OC)cc(N2CCNCC2)c1</chem>	$\beta 1$	ZINC0000023899 95
<chem>Cc1ccc(OC[C@@H](O)[C@@H](C)NC(C)C)c2c1CCC2</chem>	$\beta 1$	ZINC0000025306 99

<chem>FC(F)(F)c1ccnc(N2CCNCC2)n1</chem>	$\beta 1$	ZINC0000025575 59
<chem>N#Cc1cccc1OC[C@H](O)CNCCNC(=O)Nc1cccc1</chem>	$\beta 1$	ZINC0000025682 37
<chem>C[C@H](O)CNCCOc1cccc1-c1cccc1</chem>	$\beta 2$	ZINC0000028808 12
<chem>C[C@@H](O)CNCCOc1cccc1-c1cccc1</chem>	$\beta 2$	ZINC0000028808 13
<chem>CC(C)(C)NC[C@H](O)COc1cccc2oc3ccccc3c12</chem>	$\beta 2$	ZINC0000031092 33
<chem>CC(C)(C)NC[C@@H](O)COc1cccc2oc3ccccc3c12</chem>	$\beta 2$	ZINC0000031092 34
<chem>CC(C)(C)NC[C@@H](O)CON=C1c2cccc2-c2cccc21</chem>	$\beta 1$	ZINC0000033314 13
<chem>OCc1cc([C@H](O)CNCCCCCOCCCCc2cccc2)ccc1O</chem>	$\beta 1$	ZINC0000037852 68
<chem>CS(=O)(=O)Nc1ccc(OC[C@@H]2CN(c3ccccc3)CCN2)cc1</chem>	$\beta 1$	ZINC0000037966 05
<chem>COc1cccc1N1CCN[C@H](CNC(=O)c2ccc(NS(C)(=O)=O)cc2)C1</chem>	$\beta 1$	ZINC0000037966 13
<chem>CS(=O)(=O)Nc1ccc(C(=O)NC[C@@H]2CN(c3cccc(Cl)c3)CCN2)cc1</chem>	$\beta 1$	ZINC0000037966 17
<chem>CN(c1ccc(C(=O)NC[C@@H]2CN(c3ccccc3)CCN2)cc1)S(C)(=O)=O</chem>	$\beta 1$	ZINC0000037966 26
<chem>O=C(NC[C@H]1CN(c2ccccc2)CCN1)c1ccc(-n2ccnc2)cc1</chem>	$\beta 1$	ZINC0000037966 30
<chem>Clc1cccc1C(c1cccc1)(c1cccc1)n1ccnc1</chem>	$\beta 1$	ZINC0000038078 04
<chem>O=S(=O)(CCc1cccc1)Nc1ccc(CCNC[C@H](O)COc2ccc(O)cc2)cc1</chem>	$\beta 1$	ZINC0000038080 32
<chem>O=C(O)COc1ccc2c(c1)C[C@@H](NC[C@H](O)c1cccc(Cl)c1)CC2</chem>	$\beta 1$	ZINC0000038094 22
<chem>Cc1cc(CCCCOCCCCCN[C@H](O)c2ccc(O)c(CO)c2)cc(NC(N)=O)c1</chem>	$\beta 1$	ZINC0000038175 99

<chem>NC(=O)Nc1cccc(CCCCOCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)c1</chem>	$\beta 1$	ZINC0000038176 02
<chem>CCN(CC)C(=O)N[C@H]1C=C2c3cccc4[nH]cc(c34)C[C@H]2N(C)C1</chem>	$\beta 1$	ZINC0000038310 01
<chem>CC(C)(O)c1cccc1CC[C@@H](SCC1(CC(=O)O)CC1)c1cccc(/C=C/c2ccc3ccc(Cl)cc3n2)c1</chem>	$\beta 2$	ZINC0000038311 51
<chem>C[C@H](Cc1ccc(OC(=O)O)cc1)NC[C@H](O)c1cccc(Cl)c1</chem>	$\beta 1$	ZINC0000038717 71
<chem>Cn1cc(C(F)(F)F)nc1-c1ccc(OC[C@@H](O)CNCCOc2ccc(O)c(C(N)=O)c2)cc1</chem>	$\beta 1$	ZINC0000038720 10
<chem>Cc1ccc(OC[C@@H](O)[C@H](C)NC(C)C)c2c1CCC2</chem>	$\beta 1$	ZINC0000038728 81
<chem>C[C@H](Cc1ncc(CCCC(=O)O)s1)NC[C@H](O)COc1cccc1</chem>	$\beta 1$	ZINC0000039191 97
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2cnc(CCC3CCCC3)o2)cc1</chem>	$\beta 1$	ZINC0000039199 76
<chem>O=C1N(CCCC2CCCC2)CCN1c1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000039199 88
<chem>CCCCCNC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(-c3ccc(C[C@H]4NCCc5cc(O)c(O)cc54)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000039238 56
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-n2ncc(Cc3ccc(C(F)(F)F)cc3)n2)cc1</chem>	$\beta 2$	ZINC0000039239 69
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2noc(Cc3ccc(OC(F)(F)F)cc3)n2)cc1</chem>	$\beta 1$	ZINC0000039240 84
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(-c3ccc(C(F)(F)F)cc3)cs2)cc1</chem>	$\beta 1$	ZINC0000039241 72
<chem>COc1cc(-c2ccc(C[C@@H](C)NC[C@H](O)c3ccccc3)cc2)ccc1C(=O)O</chem>	$\beta 1$	ZINC0000039333 66
<chem>NCCCCOC[C@H]1O[C@@H](OCCc2c[nH]c3ccccc23)[C@H](OCC2ccccc2)[C@@H](OCC2ccccc2)[C@@H]1OCc1ccccc1</chem>	$\beta 2$	ZINC0000039363 09
<chem>CCCCCNC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000039393 88
<chem>COc1c(I)cc(C[C@H]2NCCc3nc(N)sc32)cc1I</chem>	$\beta 1$	ZINC0000039408 87

<chem>Cc1c(C(=O)c2ccc(Cl)cc2)c2ccc(OC(F)(F)F)cc2n1Cc1cccc(O[C@H](C)C(=O)O)c1</chem>	$\beta 1$	ZINC0000039426 00
<chem>CS(=O)(=O)Nc1cccc(COCCOCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)c1</chem>	$\beta 1$	ZINC0000039444 70
<chem>COc1cccc1CNC(=O)c1cc2cc(C[C@@H](C)NC[C@H](O)c3ccc(O)c(CO)c3)ccc2[nH]1</chem>	$\beta 2$	ZINC0000039483 44
<chem>COc1cccc(OC)c1CNC(=O)c1cc2cc(C[C@@H](C)NC[C@H](O)c3ccc(O)c(CO)c3)ccc2[nH]1</chem>	$\beta 2$	ZINC0000039483 47
<chem>C[C@H](Cc1ccc2[nH]c(C(=O)N(C)Cc3cccc3)cc2c1)NC[C@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 2$	ZINC0000039483 50
<chem>N#C/N=C(\Nc1cccc1)Nc1ccc(CCNC[C@H](O)COc2cccc2)cc1</chem>	$\beta 1$	ZINC0000039510 48
<chem>C[C@H](Cc1c[nH]c2c(OCC(=O)O)cccc12)NC[C@H](O)c1cccc(Cl)c1</chem>	$\beta 1$	ZINC0000039527 25
<chem>CC(C)(Cc1ccc2cccc2c1)NC[C@@H](O)COc1cccc(Cl)c1C#N</chem>	$\beta 2$	ZINC0000039756 68
<chem>CC(C)(C)NC[C@@H](O)COc1cccc2[nH]c(=O)[nH]c12</chem>	$\beta 1$	ZINC0000039791 34
<chem>C[C@H](Cc1ccc2[nH]c(C(=O)N[C@H](C)c3cccc3)cc2c1)NC[C@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 2$	ZINC0000039876 32
<chem>C[C@H](Cc1ccc2[nH]c(C(=O)NCC3CCC3)cc2c1)NC[C@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 2$	ZINC0000039876 33
<chem>C[C@H](Cc1ccc2[nH]c(C(=O)NCc3ccc(S(N)(=O)=O)cc3)cc2c1)NC[C@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 2$	ZINC0000039876 36
<chem>O=S(=O)(c1cccc(CCCOCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)c1)N1CCOCC1</chem>	$\beta 1$	ZINC0000039892 30
<chem>NS(=O)(=O)c1cccc(CCCOCCCCCNC[C@@H](O)c2ccc(O)c(CO)c2)c1</chem>	$\beta 1$	ZINC0000039892 34
<chem>O=C1CNC(=O)N1c1cccc(CCCOCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)c1</chem>	$\beta 1$	ZINC0000039894 97
<chem>NS(=O)(=O)c1cccc(COCCOCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)c1</chem>	$\beta 1$	ZINC0000039916 25
<chem>N#Cc1cccc1OC[C@@H](O)CNCCNC(=O)Nc1cccc1</chem>	$\beta 1$	ZINC0000039957 21

<chem>CCOC(=O)c1oc2cccc(OC[C@@H](O)CNC(C)C)c2c1C</chem>	$\beta 2$	ZINC0000040082 95
<chem>c1cc(N2CCNCC2)c2cc[nH]c2c1</chem>	$\beta 1$	ZINC0000046394 56
<chem>Cc1nc(N2CCNCC2)c2c3c(sc2n1)C[C@H](C)CC3</chem>	$\beta 1$	ZINC0000048487 07
<chem>Cc1nc(N2CCNCC2)c2c3c(sc2n1)C[C@@H](C)CC3</chem>	$\beta 1$	ZINC0000048487 08
<chem>Cc1ccc(C)c(OC[C@H](O)CNC2CCCC2)c1</chem>	$\beta 2$	ZINC0000050503 15
<chem>Cc1ccc(C)c(OC[C@@H](O)CNC2CCCC2)c1</chem>	$\beta 2$	ZINC0000050503 16
<chem>CS(=O)(=O)Nc1ccc(OC[C@H]2CN(c3ccccc3)CCN2)cc1</chem>	$\beta 1$	ZINC0000060133 93
<chem>COc1ccccc1N1CCN[C@@H](CNC(=O)c2ccc(NS(C)(=O)=O)cc2)C1</chem>	$\beta 1$	ZINC0000060133 95
<chem>CS(=O)(=O)Nc1ccc(C(=O)NC[C@H]2CN(c3ccccc3)CCN2)cc1</chem>	$\beta 1$	ZINC0000060133 96
<chem>CN(c1ccc(C(=O)NC[C@H]2CN(c3ccccc3)CCN2)cc1)S(C)(=O)=O</chem>	$\beta 1$	ZINC0000060133 98
<chem>C[C@@H](CCc1ccccc1)NC[C@H](O)c1cc(C(N)=O)c2[nH]ccc2c1</chem>	$\beta 1$	ZINC0000060206 79
<chem>C[C@H](CCc1ccccc1)NC[C@H](O)c1cc(C(N)=O)c2[nH]ccc2c1</chem>	$\beta 1$	ZINC0000060364 96
<chem>C[C@H](CCc1ccccc1)NC[C@@H](O)c1cc(C(N)=O)c2[nH]ccc2c1</chem>	$\beta 1$	ZINC0000060364 99
<chem>c1ccc2c(N3CCNCC3)ccnc2c1</chem>	$\beta 2$	ZINC0000060626 46
<chem>O[C@@H](CNC1CCCCC1)COc1cccc2[nH]ccc12</chem>	$\beta 1$	ZINC0000060942 38
<chem>CSc1nc(N2CCNCC2)c2sc3c(c2n1)CCCC3</chem>	$\beta 1$	ZINC0000066613 23
<chem>C[C@H](Cc1cccc(CC(=O)NCc2ccc(Cl)c(Cl)c2)c1)NC[C@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 2$	ZINC0000067180 01

<chem>C[C@H](Cc1c[nH]c2c(OS(C)(=O)=O)cccc12)NC[C@H](O)c1cccc(NC/C=C/c2cccc2)c1</chem>	β2	ZINC0000067184 52
<chem>COc1ccc(OC[C@H](O)CNC2CCN(c3ncnc4ccc(-c5cccc5)c34)CC2)cc1</chem>	β2	ZINC0000086166 35
<chem>COc1ccc(OC[C@@H](O)CNC2CCN(c3ncnc4ccc(-c5cccc5)c34)CC2)cc1</chem>	β2	ZINC0000086166 37
<chem>Cc1ccc(C(C)C)c(OC[C@@H](O)CN2CCC(CN3C(=O)c4cccc5cccc(c45)C3=O)CC2)c1</chem>	β1	ZINC0000097817 88
<chem>C=CCc1cccc1OC[C@H](O)CN1CCC(CN2C(=O)c3cccc4cccc(c34)C2=O)CC1</chem>	β1	ZINC0000097817 90
<chem>C=CCc1cccc1OC[C@@H](O)CN1CCC(CN2C(=O)c3cccc4cccc(c34)C2=O)CC1</chem>	β1	ZINC0000097817 93
<chem>O=C(NC[C@@H]1CN(c2cccc2)CCN1)c1cccc1</chem>	β1	ZINC0000114223 26
<chem>O=C(NC[C@H]1CN(c2cccc2)CCN1)c1cccc1</chem>	β1	ZINC0000114223 27
<chem>O=C(NC[C@@H]1CN(c2cccc2)CCN1)c1ccc(-n2ccnc2)cc1</chem>	β1	ZINC0000114223 32
<chem>C[C@@H](Cc1c[nH]c2cccc12)NC[C@@H](O)c1cccc(Cl)c1</chem>	β1	ZINC0000114223 92
<chem>C=CCc1ccc(OC[C@@H](O)CN2CCC(CN3C(=O)c4cccc5cccc(c45)C3=O)CC2)c(OC)c1</chem>	β1	ZINC0000118473 20
<chem>C=CCc1ccc(OC[C@H](O)CN2CCC(CN3C(=O)c4cccc5cccc(c45)C3=O)CC2)c(OC)c1</chem>	β1	ZINC0000118473 21
<chem>COc1ccc(OC[C@@H](O)CN2CCC(CN3C(=O)c4cccc5cccc(c45)C3=O)CC2)c(C(C)(C)C)c1</chem>	β1	ZINC0000118475 07
<chem>COc1ccc(OC[C@H](O)CN2CCC(CN3C(=O)c4cccc5cccc(c45)C3=O)CC2)c(C(C)(C)C)c1</chem>	β1	ZINC0000118475 08
<chem>CC(C)c1cccc1OC[C@@H](O)CN1CCC(CN2C(=O)c3cccc4cccc(c34)C2=O)CC1</chem>	β1	ZINC0000121705 48
<chem>CC(C)c1cccc1OC[C@H](O)CN1CCC(CN2C(=O)c3cccc4cccc(c34)C2=O)CC1</chem>	β1	ZINC0000121705 58
<chem>N#Cc1cc(OCCOCC2CC2)ccc1OC[C@@H](O)CNCCNC(=O)Nc1ccc(O)cc1</chem>	β1	ZINC0000134905 95

<chem>C[C@H]1C[C@@H](C)N1C(=O)[C@@H]1C=C2c3cccc4[nH]cc(c34)C[C@H]2N(C)C1</chem>	$\beta 1$	ZINC0000134913 58
<chem>C[C@H]1C[C@H](C)N1C(=O)[C@@H]1C=C2c3cccc4[nH]cc(c34)C[C@H]2N(C)C1</chem>	$\beta 1$	ZINC0000134913 60
<chem>COc1cccc1N1CCN(CCCn2c(O)nc3c([nH]c4cccc43)c2=O)CC1</chem>	$\beta 2$	ZINC0000138221 90
<chem>COc1ccc(NC(=O)NCCNC[C@H](O)COc2cccc2C#N)cc1</chem>	$\beta 1$	ZINC0000138406 72
<chem>NS(=O)(=O)c1cc(C(=O)NCCNC[C@H](O)COc2cccc3c2SCC(=O)N3)ccc1Cl</chem>	$\beta 1$	ZINC0000138612 02
<chem>NS(=O)(=O)c1cc(C(=O)NCCNC[C@H](O)COc2cccc3c2CCC(=O)N3)ccc1Cl</chem>	$\beta 1$	ZINC0000138612 04
<chem>NS(=O)(=O)c1cc(C(=O)NCCNC[C@H](O)COc2cccc3cccc23)ccc1Cl</chem>	$\beta 1$	ZINC0000138612 06
<chem>NS(=O)(=O)c1cc(S(=O)(=O)NCCNC[C@H](O)COc2cccc3cccc23)ccc1Cl</chem>	$\beta 1$	ZINC0000138612 12
<chem>NS(=O)(=O)c1cc(NCCNC[C@H](O)COc2cccc3c2SCC(=O)N3)ccc1Cl</chem>	$\beta 1$	ZINC0000138612 14
<chem>NS(=O)(=O)c1cc(NCCNC[C@H](O)COc2cccc3cccc23)ccc1Cl</chem>	$\beta 1$	ZINC0000138612 18
<chem>NS(=O)(=O)c1cc(N2CCN(C[C@@H](O)COc3cccc4c3SCC(=O)N4)CC2)ccc1Cl</chem>	$\beta 1$	ZINC0000138612 19
<chem>NS(=O)(=O)c1cc(N2CCN(C[C@@H](O)COc3cccc4cccc34)CC2)ccc1Cl</chem>	$\beta 1$	ZINC0000138612 23
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNC2CCN(c3ccc(CCC(=O)O)cc3)CC2)ccc1O</chem>	$\beta 1$	ZINC0000138626 47
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNC2CCN(c3ccc(COCC(=O)O)cc3)CC2)ccc1O</chem>	$\beta 1$	ZINC0000138626 48
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNC2CCN(c3ccc(C(N)=O)cc3)CC2)ccc1O</chem>	$\beta 1$	ZINC0000138626 49
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNC2CCN(c3ccc(C(=O)NCC(=O)O)cc3)CC2)ccc1O</chem>	$\beta 1$	ZINC0000138626 50
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNC2CCN(c3ccc(NC(=O)CC(=O)O)cc3)CC2)ccc1O</chem>	$\beta 1$	ZINC0000138626 52

<chem>O=C1NCN(c2ccccc2)C12CCN(Cc1cccc(Oc3ccccc3)c1)CC2</chem>	$\beta 1$	ZINC0000138643 23
<chem>CNC[C@H](O)c1ccc(O)c2[nH]c(=O)sc12</chem>	$\beta 1$	ZINC0000139131 41
<chem>Nc1c(Cl)cc([C@@H](O)CNCCc2ccc(NC[C@H](O)c3ccccc3)cc2)cc1Cl</chem>	$\beta 2$	ZINC0000139188 06
<chem>O=S1(=O)CCc2ccc(CCCOCCCCCNC[C@H](O)c3ccc(O)c(CO)c3)cc21</chem>	$\beta 1$	ZINC0000139838 55
<chem>O=S1(=O)CCCc2ccc(CCCOCCCCCNC[C@H](O)c3ccc(O)c(CO)c3)cc21</chem>	$\beta 1$	ZINC0000139838 58
<chem>COc1c(I)cc(C[C@@H]2NCCc3nc(N)sc32)cc1I</chem>	$\beta 1$	ZINC0000141143 87
<chem>CCCCCCCCc1esc(N2CCc3cc(S(=O)(=O)Nc4ccc(CCNC[C@H](O)c5ccnc5)cc4)ccc32)n1</chem>	$\beta 1$	ZINC0000141144 95
<chem>CCCCCNC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(C[C@@H]3NCCc4cc(O)c(O)cc43)cc2)cc1</chem>	$\beta 1$	ZINC0000141152 97
<chem>CCCCCCCCc1esc(N2CCc3c(N/C(=N/c4ccc(CCNC[C@H](O)c5ccnc5)cc4)NC#N)cccc32)n1</chem>	$\beta 1$	ZINC0000141284 59
<chem>NC(=O)C(c1ccccc1)(c1ccccc1)[C@@H]1CCN(CCCCCCCCCNC[C@@H](O)c2ccc(O)c3[nH]c(=O)ccc23)C1</chem>	$\beta 2$	ZINC0000141921 00
<chem>C=CCc1ccccc1OC[C@H](O)CN1CCOCC1</chem>	$\beta 1$	ZINC0000192287 63
<chem>C=CCc1ccccc1OC[C@@H](O)CN1CCOCC1</chem>	$\beta 1$	ZINC0000192287 65
<chem>CS(=O)(=O)Nc1ccc(CNC[C@@H]2CN(c3ccccc3)CCN2)cc1</chem>	$\beta 1$	ZINC0000193668 34
<chem>FC(F)(F)c1ccnc(N2CCNCC2)c1</chem>	$\beta 1$	ZINC0000202868 31
<chem>Cc1c[nH]c2cccc(OC[C@@H](O)CN3CCN(C(c4ccccc4)c4ccccc4)CC3)c12</chem>	$\beta 2$	ZINC0000204618 66
<chem>Cc1c[nH]c2cccc(OC[C@H](O)CN3CCN(C(c4ccccc4)c4ccccc4)CC3)c12</chem>	$\beta 2$	ZINC0000204618 68
<chem>CS(=O)(=O)Nc1ccc(CNC[C@H]2CN(c3ccccc3)CCN2)cc1</chem>	$\beta 1$	ZINC0000224428 66

<chem>CC(C)c1ccccc1OC[C@@H](O)CN1CCOCC1</chem>	$\beta 1$	ZINC0000236335 12
<chem>CC(C)c1ccccc1OC[C@H](O)CN1CCOCC1</chem>	$\beta 1$	ZINC0000236335 14
<chem>c1csc(-c2cccc3ccc(N4CCNCC4)nc23)c1</chem>	$\beta 1$	ZINC0000248943 65
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(-c3ccc(F)c(F)c3)cs2)cc1</chem>	$\beta 1$	ZINC0000254191 31
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCC2CCN(S(=O)(=O)c3ccc(-n4cc(C(=O)O)cn4)cc3)CC2)ccc1O</chem>	$\beta 1$	ZINC0000254191 52
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCC2CCN(c3ccc(C(=O)N[C@@H](CC(=O)O)C(=O)O)cc3)CC2)ccc1O</chem>	$\beta 1$	ZINC0000254191 57
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(-c3cccc(F)c3F)cs2)cc1</chem>	$\beta 1$	ZINC0000254216 31
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(-c3ccc(F)cc3F)cs2)cc1</chem>	$\beta 1$	ZINC0000254216 36
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(-c3cc(F)c(F)c(F)c3)cs2)cc1</chem>	$\beta 1$	ZINC0000254216 41
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(-c3cccc(C(F)(F)F)c3)cs2)cc1</chem>	$\beta 1$	ZINC0000254216 46
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(-c3cccc3C(F)(F)F)cs2)cc1</chem>	$\beta 1$	ZINC0000254216 52
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNC2CCN(c3ccc(C(=O)N[C@@H](Cc4ccccc4)C(=O)O)cc3)CC2)ccc1O</chem>	$\beta 2$	ZINC0000254219 87
<chem>COc1cccc2c1CC[C@H]1CN(CCN3c(O)nc4c(sc5ccnc54)c3=O)C[C@@H]21</chem>	$\beta 2$	ZINC0000254220 25
<chem>Oc1cc2c(cc1O)[C@H]1c3ccccc3CN[C@@H]1CC2</chem>	$\beta 1$	ZINC0000257585 12
<chem>Cc1ncn1-c1ccc(OCCNC[C@@H](O)COc2ccc(NS(C)(=O)=O)cc2)cc1</chem>	$\beta 1$	ZINC0000260227 04
<chem>Cc1ncn1-c1ccc(OCCNC[C@H](O)COc2ccc(NS(C)(=O)=O)cc2)cc1</chem>	$\beta 1$	ZINC0000260227 12
<chem>CC(C)(COc1ccc(-n2ccnc2)cc1)NC[C@@H](O)COc1ccc(NS(C)(=O)=O)cc1</chem>	$\beta 1$	ZINC0000260249 30

<chem>CC(C)(COc1ccc(-n2ccnc2)cc1)NC[C@H](O)COc1ccc(NS(C)(=O)=O)cc1</chem>	$\beta 1$	ZINC0000260249 38
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(-c3ccc(O)cc3)cs2)cc1</chem>	$\beta 1$	ZINC0000261462 89
<chem>CC(C)(C)c1ccc(-c2csc(-c3ccc(S(=O)(=O)Nc4ccc(CCNC[C@H](O)c5ccnc5)cc4)cc3)n2)cc1</chem>	$\beta 1$	ZINC0000261462 96
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(Cc2nc(Cc3ccc4ccccc4c3)cs2)cc1</chem>	$\beta 1$	ZINC0000261470 84
<chem>CC(=O)Nc1ccc(-c2csc(-c3ccc(S(=O)(=O)Nc4ccc(CCNC[C@H](O)c5ccnc5)cc4)cc3)n2)cc1</chem>	$\beta 1$	ZINC0000261470 97
<chem>Nc1ccc(OC[C@@H](O)CNCCc2ccc(NS(=O)(=O)c3ccc(I)cc3)cc2)cn1</chem>	$\beta 1$	ZINC0000261631 75
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(I)cc1</chem>	$\beta 1$	ZINC0000261651 99
<chem>CC(C)c1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(N)nc3)cc2)cc1</chem>	$\beta 1$	ZINC0000261675 21
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-n2ncc(Cc3ccc(F)c(F)c3)n2)cc1</chem>	$\beta 1$	ZINC0000261830 62
<chem>Nc1ccc(OC[C@@H](O)CNCCc2ccc(NS(=O)(=O)c3ccc(Br)cc3)cc2)cn1</chem>	$\beta 1$	ZINC0000261834 09
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)COc2ccnc2)cc1)c1ccc(Br)cc1</chem>	$\beta 1$	ZINC0000261834 87
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)COc2ccnc2)cc1)c1ccc(Cl)cc1</chem>	$\beta 1$	ZINC0000261834 92
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)COc2ccnc2)cc1)c1ccc(F)cc1</chem>	$\beta 1$	ZINC0000261839 71
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-n2ncc(Cc3ccc(F)c3)n2)cc1</chem>	$\beta 1$	ZINC0000261849 44
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)COc2ccnc2)cc1)c1ccc(Cl)c(Cl)c1</chem>	$\beta 1$	ZINC0000261863 86
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-n2ncc(-c3ccc(F)cc3)n2)cc1</chem>	$\beta 2$	ZINC0000261865 22
<chem>CC(C)c1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000261866 09

<chem>COc1ccc(-c2cnn(-c3ccc(S(=O)(=O)Nc4ccc(CCNC[C@H](O)c5ccnc5)cc4)cc3)n2)cc1F</chem>	$\beta 1$	ZINC0000261869 79
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)COc2ccccc2)cc1)c1ccc(I)cc1</chem>	$\beta 1$	ZINC0000261875 83
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-n2ncc(-c3ccc(OC(F)(F)F)cc3)n2)cc1</chem>	$\beta 1$	ZINC0000261876 92
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-n2ncc(-c3ccc(F)c(F)c3)n2)cc1</chem>	$\beta 1$	ZINC0000261876 97
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)COc2ccc(F)cc2)cc1)c1ccc(I)cc1</chem>	$\beta 1$	ZINC0000261877 11
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-n2ncc(COc3ccc(OC(F)(F)F)cc3)n2)cc1</chem>	$\beta 1$	ZINC0000261889 26
<chem>CCc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000261897 08
<chem>Nc1ccc(OC[C@@H](O)CNCCc2ccc(NS(=O)(=O)c3ccc(F)cc3)cc2)cn1</chem>	$\beta 1$	ZINC0000261897 16
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)COc2ccnc2)cc1)c1cnc2ccccc2c1</chem>	$\beta 1$	ZINC0000261897 59
<chem>CCc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(N)nc3)cc2)cc1</chem>	$\beta 1$	ZINC0000261897 70
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)COc2ccnc2)cc1)c1ccccc1</chem>	$\beta 1$	ZINC0000261901 63
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-n2ncc(Cc3c(F)cccc3F)n2)cc1</chem>	$\beta 2$	ZINC0000262475 82
<chem>Nc1ccc(OC[C@@H](O)CNCCc2ccc(NS(=O)(=O)c3ccc(Cl)cc3)cc2)cn1</chem>	$\beta 1$	ZINC0000262482 14
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-n2ncc(COc3ccc(C(F)(F)F)cc3)n2)cc1</chem>	$\beta 1$	ZINC0000262487 42
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-n2ncc(COc3ccc(F)c(F)c3)n2)cc1</chem>	$\beta 1$	ZINC0000262495 31
<chem>CCCCCNC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(N)nc3)cc2)cc1</chem>	$\beta 1$	ZINC0000262499 92
<chem>COc1ccc(OC[C@@H](O)CNCCc2ccc(NS(=O)(=O)c3ccc(I)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000262506 49

<chem>Nc1ccc(OC[C@@H](O)CNCCc2ccc(NS(=O)(=O)c3ccc(Cl)c(Cl)c3)cc2)cn1</chem>	$\beta 1$	ZINC0000262509 66
<chem>CCCCCNC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000262515 25
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-n2ncc(Cc3ccc(OC(F)(F)F)cc3)n2)cc1</chem>	$\beta 1$	ZINC0000262521 23
<chem>Nc1ccc(OC[C@@H](O)CNCCc2ccc(NS(=O)(=O)c3ccccc3)cc2)cn1</chem>	$\beta 1$	ZINC0000262522 61
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-n2ncc(Cc3ccc(F)cc3)n2)cc1</chem>	$\beta 1$	ZINC0000262527 97
<chem>COc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(N)nc3)cc2)cc1</chem>	$\beta 1$	ZINC0000262535 16
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-n2ncc(Cc3c(F)cc(F)cc3F)n2)cc1</chem>	$\beta 1$	ZINC0000262548 40
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-n2ncc(-c3cccc(F)c3)n2)cc1</chem>	$\beta 1$	ZINC0000262549 66
<chem>Nc1ccc(OC[C@@H](O)CNCCc2ccc(NS(=O)(=O)c3cnc4ccccc4c3)cc2)cn1</chem>	$\beta 1$	ZINC0000262550 18
<chem>COc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000262557 31
<chem>C[C@H](Cc1ncc(CCCC(=O)O)s1)NC[C@@H](O)c1cccc(Cl)c1</chem>	$\beta 1$	ZINC0000263759 25
<chem>C[C@H](Cc1ncc(CCCC(=O)O)s1)NC[C@H](O)c1cccc(Cl)c1</chem>	$\beta 1$	ZINC0000263759 26
<chem>C[C@H](Cc1ncc(CCCCC(=O)O)s1)NC[C@H](O)COc1ccccc1</chem>	$\beta 1$	ZINC0000263766 38
<chem>COc1cc(-c2ccc(C[C@@H]3NCCc4cc(O)c(O)cc43)cc2)cc(OC)c1OC</chem>	$\beta 1$	ZINC0000263769 92
<chem>C[C@H](Cc1ncc(CCC(=O)O)s1)NC[C@H](O)COc1ccccc1</chem>	$\beta 1$	ZINC0000263787 46
<chem>CCCCCNC(=O)Nc1ccc(S(=O)(=O)Nc2ccc3cc(C[C@@H]4NCCc5cc(O)c(O)cc54)ccc3c2)cc1</chem>	$\beta 1$	ZINC0000263838 85
<chem>CCCCCNC(=O)Nc1ccc(S(=O)(=O)Nc2cccc(-c3ccc(C[C@@H]4NCCc5cc(O)c(O)cc54)cc3)c2)cc1</chem>	$\beta 1$	ZINC0000263847 05

CCCCCNC(=O)Nc1ccc(S(=O)(=O)Nc2cccc(-c3ccc(OC[C@@H]4NCCc5cc(O)c(O)cc54)cc3)c2)cc1	β1	ZINC0000263850
CCCCCNC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(OC[C@@H]3NCCc4cc(O)c(O)cc43)cc2)cc1	β1	ZINC0000263851
CCCCCNC(=O)Nc1ccc(S(=O)(=O)Nc2ccc3cc(OC[C@@H]4NCCc5cc(O)c(O)cc54)ccc3c2)cc1	β1	ZINC0000263853
CCCCCNC(=O)Nc1ccc(S(=O)(=O)Nc2cccc(-c3cccc(C[C@@H]4NCCc5cc(O)c(O)cc54)c3)c2)cc1	β1	ZINC0000263873
CCCCCNC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(-c3ccc(OC[C@@H]4NCCc5cc(O)c(O)cc54)cc3)cc2)cc1	β1	ZINC0000263889
O=C1N(CCCC(F)(F)F)CCN1c1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1	β1	ZINC0000264952
CCCCCN1cnn(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)c1=O	β1	ZINC0000264966
CCCCCN1c(C)cn(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)c1=O	β1	ZINC0000264991
O=C1N(CCCC(F)(F)C(F)(F)F)CCN1c1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1	β1	ZINC0000264991
CCCCCN1ncn(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)c1=O	β2	ZINC0000265002
CCCCCN1CCN(c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)C1=O	β1	ZINC0000265022
CCCCCN1C(=O)CN(c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)C1=O	β1	ZINC0000265025
Cc1cccc1OC[C@@H](O)CN1CCN(c2ccc(NS(C)(=O)=O)cc2)CC1	β1	ZINC0000267234
Cc1cccc(OC[C@@H](O)CNCCOc2ccc(-n3ccnc3)cc2)c1	β1	ZINC0000267265
COCCc1ccc(OC[C@@H](O)CNCCOc2ccc(-n3ccnc3)cc2)cc1	β1	ZINC0000267265
COCCc1ccc(OC[C@@H](O)CNCc2ccc(NS(C)(=O)=O)cc2)cc1	β1	ZINC0000267274
Cc1cccc(OC[C@@H](O)CNCc2ccc(NS(C)(=O)=O)cc2)c1	β1	ZINC0000267274

<chem>Cc1ccccc1OC[C@@H](O)CNCCc1ccc(-n2ccnc2)cc1</chem>	$\beta 1$	ZINC0000267345 71
<chem>O[C@@H](CNCCOc1ccc(-n2ccnc2)cc1)COc1ccccc1</chem>	$\beta 1$	ZINC0000267372 80
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCC2CCN(c3ccc(C(=O)N[C@@H](Cc4ccccc4)C(=O)O)cc3)CC2)ccc1O</chem>	$\beta 1$	ZINC0000267387 23
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCC2CCN(S(=O)(=O)c3ccc(NC(=O)NCc4cc(F)ccc4F)cc3)CC2)ccc1O</chem>	$\beta 1$	ZINC0000267423 84
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCC2CCN(S(=O)(=O)c3ccc(-n4cc(CC(=O)O)c5ccccc54)cc3)CC2)ccc1O</chem>	$\beta 1$	ZINC0000267441 86
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCC2CCN(S(=O)(=O)c3ccc(NC(=O)N[C@@H](Cc4ccccc4)C(=O)O)cc3)CC2)ccc1O</chem>	$\beta 1$	ZINC0000267454 43
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCC2CCN(S(=O)(=O)c3ccc(-n4ccc5c(C(=O)O)cccc54)cc3)CC2)ccc1O</chem>	$\beta 1$	ZINC0000267497 35
<chem>CS(=O)(=O)Nc1cc(OC[C@@H](O)CNCC2CCN(S(=O)(=O)c3ccc(NC(=O)NCc4cc(F)ccc4F)cc3)CC2)ccc1O</chem>	$\beta 1$	ZINC0000267515 25
<chem>CCCCC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1</chem>	$\beta 2$	ZINC0000268309 11
<chem>CCCCCOC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000268313 10
<chem>CC(C)c1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1</chem>	$\beta 2$	ZINC0000268321 17
<chem>O=C(Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1)OCCc1ccccc1</chem>	$\beta 1$	ZINC0000268335 68
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccccc1</chem>	$\beta 2$	ZINC0000268345 94
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc2ccccc2c1</chem>	$\beta 1$	ZINC0000268345 98
<chem>O=S(=O)(CCc1ccccc1)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 2$	ZINC0000268354 02
<chem>O=C(NCCc1ccccc1)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000268355 06
<chem>CS(=O)(=O)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000268364 75

<chem>CCCNC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000268366 35
<chem>CNC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000268367 93
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(Cl)cc1</chem>	$\beta 2$	ZINC0000268369 31
<chem>O=C(CCCc1cccc1)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000268371 05
<chem>CCCOC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1</chem>	$\beta 2$	ZINC0000268378 01
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1cnc2cccc2c1</chem>	$\beta 2$	ZINC0000268400 40
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(Br)cc1</chem>	$\beta 1$	ZINC0000268490 35
<chem>N#CN/C(=N\c1ccc(I)cc1)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000272107 03
<chem>N#CN/C(=N\c1cccc(I)c1)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000272107 07
<chem>N#CN/C(=N\c1cc(Cl)cc(Cl)c1)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000272110 40
<chem>N#CN/C(=N\c1cccc(F)c1)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000272110 43
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(-c3ccc(OC(F)(F)F)cc3)cs2)cc1</chem>	$\beta 1$	ZINC0000272125 96
<chem>N#CN/C(=N\c1cccc(Oc2cccc2)c1)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000272128 73
<chem>N#CN/C(=N\c1ccc2c(c1)CCN2c1nc(-c2ccc(OC(F)(F)F)cc2)cs1)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000272137 62
<chem>N#CN/C(=N\c1ccc(CCNC[C@H](O)c2ccnc2)cc1)Nc1cccc(C(N)=O)c1</chem>	$\beta 1$	ZINC0000272142 49
<chem>N#CN/C(=N\c1cccc2cccc12)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000272148 49
<chem>N#CN/C(=N\c1ccc2c(c1)N(c1nc(-c3ccc(OC(F)(F)F)cc3)cs1)CC2)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000272153 46

<chem>N#CN/C(=N\c1cccc2c1CCN2c1nc(-c2ccc(OC(F)(F)F)cc2)cs1)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000272168 92
<chem>N#CN/C(=N\c1ccc2ccccc2c1)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000273013 14
<chem>C[C@H]1C[C@H](C)N1C(=O)[C@@H]1C=C2c3cccc4[nH]cc(c34)C[C@@H]2N(C)C1</chem>	$\beta 1$	ZINC0000274316 36
<chem>C[C@H]1C[C@@H](C)N1C(=O)[C@@H]1C=C2c3cccc4[nH]cc(c34)C[C@@H]2N(C)C1</chem>	$\beta 1$	ZINC0000274319 14
<chem>Cc1ccc(S(=O)(=O)/N=C(\O)Cc2ccc(NC[C@@H](C)NC[C@H](O)c3cccc(Cl)c3)c2)cc1</chem>	$\beta 1$	ZINC0000276571 05
<chem>O=C1N(CCC2CCCC2)CCN1c1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000277645 15
<chem>CCCCCn1c(=O)[nH]n(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)c1=O</chem>	$\beta 1$	ZINC0000278545 36
<chem>O=C1NC(=O)[C@H](Cc2ccc(N3CCC(NC[C@H](O)Oc4cccc5[nH]c(=O)ccc45)CC3)cc2)S1</chem>	$\beta 1$	ZINC0000278551 48
<chem>O=C1NC(=O)[C@@H](Cc2ccc(N3CCC(NC[C@H](O)Oc4cccc5[nH]c(=O)ccc45)CC3)cc2)S1</chem>	$\beta 1$	ZINC0000278551 57
<chem>O=C1N(Cc2ccc(F)c(F)c2)CCN1c1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000278552 96
<chem>O=c1n(CCCC(F)(F)F)ccn1-c1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1</chem>	$\beta 2$	ZINC0000278558 98
<chem>O=C1N(CCCc2ccc(Cl)cc2)CCN1c1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000278560 34
<chem>O=C1NC(=O)[C@@H](Cc2ccc(N3CCC(NC[C@H](O)COc4cccc4)CC3)cc2)S1</chem>	$\beta 1$	ZINC0000278615 07
<chem>CCCCN1CCN(c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)C1=O</chem>	$\beta 1$	ZINC0000278619 45
<chem>O=c1n(CCCC2CCCC2)ccn1-c1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000278623 86
<chem>O=C1N(CCCC2CCCC2)CCN1c1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000278633 93
<chem>O=C1N(CCC2CCCC2)CCN1c1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000278634 00

<chem>O=C1NC(=O)[C@@H](Cc2ccc(N3CCC(NC[C@H](O)COc4ccc(O)cc4)CC3)cc2)S1</chem>	$\beta 1$	ZINC0000278637 85
<chem>CCCCC(C)(C)CN1CCN(c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)C1=O</chem>	$\beta 1$	ZINC0000278652 03
<chem>CCCCCN1CCN(c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)C1=O</chem>	$\beta 1$	ZINC0000278653 08
<chem>O=C1NC(=O)[C@@H](Cc2ccc(N3CCC(NC[C@H](O)c4ccc(O)c(NS(=O)(=O)c5ccccc5)c4)CC3)cc2)S1</chem>	$\beta 1$	ZINC0000278717 16
<chem>CS(=O)(=O)Nc1cc(O[C@@H](O)CNC2CCN(c3ccc(C[C@@H]4SC(=O)NC4=O)cc3)CC2)ccc1O</chem>	$\beta 1$	ZINC0000278755 14
<chem>CS(=O)(=O)Nc1cc(O[C@@H](O)CNC2CCN(c3ccc(C[C@@H]4SC(=O)NC4=O)cc3)CC2)ccc1O</chem>	$\beta 1$	ZINC0000278755 22
<chem>CN1CCN(c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)C1=O</chem>	$\beta 1$	ZINC0000278763 20
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNC2CCN(c3ccc(C[C@@H]4SC(=O)N(CC(=O)O)C4=O)cc3)CC2)ccc1O</chem>	$\beta 1$	ZINC0000280214 77
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNC2CCN(c3ccc(C[C@@H]4SC(=O)N(CC(=O)O)C4=O)cc3)CC2)ccc1O</chem>	$\beta 1$	ZINC0000280214 82
<chem>CN(C)C(=N)NC1=NC(=O)/C=C/c2ccc(N3CCC(NC[C@H](O)COc4cccc5[nH]c(=O)[nH]c45)CC3)cc2)S1</chem>	$\beta 1$	ZINC0000281072 61
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNC2CCN(c3ccc(Cn4oc(=O)nc4O)cc3)CC2)ccc1O</chem>	$\beta 1$	ZINC0000281090 21
<chem>C/C=C/CNc1cccc([C@@H](O)CN[C@H](C)Cc2c[nH]c3c(OS(C)(=O)=O)cccc23)c1</chem>	$\beta 1$	ZINC0000283350 90
<chem>C#CCNc1cccc([C@@H](O)CN[C@H](C)Cc2c[nH]c3c(OS(C)(=O)=O)cccc23)c1</chem>	$\beta 1$	ZINC0000283455 62
<chem>C[C@H](Cc1c[nH]c2c(OS(C)(=O)=O)cccc12)NC[C@H](O)c1cccc(NCc2ccc3ccccc3c2)c1</chem>	$\beta 1$	ZINC0000283470 94
<chem>O=C(Nc1ccc(C[C@@H](CO)NC[C@H](O)COc2ccccc2)cc1)Nc1cccc(C(=O)O)c1</chem>	$\beta 1$	ZINC0000283472 50
<chem>O=C(Nc1ccc(C[C@@H](CO)NC[C@H](O)COc2ccccc2)cc1)Nc1cccc([N+](=O)[O-])c1</chem>	$\beta 1$	ZINC0000283475 04
<chem>C=CCNc1cccc([C@@H](O)CN[C@H](C)Cc2c[nH]c3c(OS(C)(=O)=O)cccc23)c1</chem>	$\beta 2$	ZINC0000283546 47

<chem>O=C(Nc1ccccc1)Nc1ccc(CCNC[C@H](O)COc2ccccc2)cc1</chem>	$\beta 1$	ZINC0000283560 77
<chem>C=C(C)CNc1cccc([C@@H](O)CN[C@H](C)Cc2c[nH]c3c(OS(C)(=O)=O)cccc23)c1</chem>	$\beta 2$	ZINC0000283574 65
<chem>C[C@H](Cc1c[nH]c2c(OS(C)(=O)=O)cccc12)NC[C@H](O)c1cccc(NC(=O)c2ccccc2)c1</chem>	$\beta 1$	ZINC0000283611 46
<chem>C[C@H](Cc1c[nH]c2c(OS(C)(=O)=O)cccc12)NC[C@H](O)c1cccc(NS(=O)(=O)c2ccccc2)c1</chem>	$\beta 1$	ZINC0000283611 70
<chem>CC#CCNc1cccc([C@@H](O)CN[C@H](C)Cc2c[nH]c3c(OS(C)(=O)=O)cccc23)c1</chem>	$\beta 2$	ZINC0000283616 21
<chem>CC/C=C/CNc1cccc([C@@H](O)CN[C@H](C)Cc2c[nH]c3c(OS(C)(=O)=O)cccc23)c1</chem>	$\beta 2$	ZINC0000283623 48
<chem>CC(C)=CCNc1cccc([C@@H](O)CN[C@H](C)Cc2c[nH]c3c(OS(C)(=O)=O)cccc23)c1</chem>	$\beta 1$	ZINC0000283659 40
<chem>C[C@H](Cc1c[nH]c2c(OS(C)(=O)=O)cccc12)NC[C@H](O)c1cccc(OCc2ccccc2)c1</chem>	$\beta 2$	ZINC0000283660 31
<chem>C[C@H](Cc1c[nH]c2c(OS(C)(=O)=O)cccc12)NC[C@H](O)c1cccc(NCc2ccccc2)c1</chem>	$\beta 2$	ZINC0000283697 05
<chem>O=CNc1cc([C@@H](O)CNCCc2ccc(OCCCCc3ccccc3)cc2)ccc1O</chem>	$\beta 2$	ZINC0000283706 55
<chem>O=CNc1cc([C@@H](O)CNCCc2ccc(OCCc3ccccc3)cc2)ccc1O</chem>	$\beta 2$	ZINC0000283713 26
<chem>O=CNc1cc([C@@H](O)CNCCc2ccc(Oc3ccccc3)cc2)ccc1O</chem>	$\beta 2$	ZINC0000283720 31
<chem>O=CNc1cc([C@@H](O)CNCCc2ccc(OC3Cc4ccccc4C3)cc2)ccc1O</chem>	$\beta 2$	ZINC0000283772 16
<chem>O=CNc1cc([C@@H](O)CNCCc2cccc(OCCCCc3ccccc3)c2)ccc1O</chem>	$\beta 2$	ZINC0000283825 57
<chem>O=CNc1cc([C@@H](O)CNCCc2cccc(OCCCOc3ccccc3)c2)ccc1O</chem>	$\beta 2$	ZINC0000283828 54
<chem>O=CNc1cc([C@@H](O)CNCCc2ccc(OCCCc3ccccc3)cc2)ccc1O</chem>	$\beta 2$	ZINC0000283828 86
<chem>C[C@H](Cc1c[nH]c2c(OS(C)(=O)=O)cccc12)NC[C@H](O)c1cccc(NS(=O)(=O)c2cccs2)c1</chem>	$\beta 1$	ZINC0000283837 17

<chem>C[C@H](Cc1c[nH]c2c(OCCN)cccc12)NC[C@H](O)c1cccc(NS(=O)(=O)c2cccs2)c1</chem>	β 1	ZINC0000283843 70
<chem>C[C@H](Cc1c[nH]c2ccccc12)NC[C@H](O)c1cccc(NS(=O)(=O)c2cccs2)c1</chem>	β 1	ZINC0000284556 10
<chem>C[C@H](Cc1c[nH]c2c(OS(=O)(=O)c3ccc(C(=O)O)cc3)cccc12)NC[C@H](O)c1cccc(NS(=O)(=O)c2cccs2)c1</chem>	β 1	ZINC0000284562 05
<chem>C[C@H](Cc1c[nH]c2c(OS(=O)(=O)c3ccccc3)cccc12)NC[C@H](O)c1cccc(NS(=O)(=O)c2cccs2)c1</chem>	β 1	ZINC0000284562 08
<chem>C[C@H](Cc1c[nH]c2c(OS(=O)(=O)c3cccs3)cccc12)NC[C@H](O)c1cccc(NS(=O)(=O)c2cccs2)c1</chem>	β 1	ZINC0000284564 50
<chem>C[C@H](Cc1c[nH]c2c(OCC(=O)N(C)C)cccc12)NC[C@H](O)c1cccc(NS(=O)(=O)c2cccs2)c1</chem>	β 1	ZINC0000284573 94
<chem>C[C@H](Cc1c[nH]c2c(OCc3ccccc3)cccc12)NC[C@H](O)c1cccc(NS(=O)(=O)c2cccs2)c1</chem>	β 1	ZINC0000284579 14
<chem>COc1cccc2c(C[C@@H](C)NC[C@H](O)c3cccc(NS(=O)(=O)c4cccs4)c3)c[nH]c12</chem>	β 1	ZINC0000284583 28
<chem>C[C@H](Cc1c[nH]c2c(OS(=O)(=O)c3cccn3)cccc12)NC[C@H](O)c1cccc(NS(=O)(=O)c2cccs2)c1</chem>	β 1	ZINC0000284588 81
<chem>C[C@H](Cc1c[nH]c2c(OCC(=O)O)cccc12)NC[C@H](O)c1cccc(NS(=O)(=O)c2cccs2)c1</chem>	β 1	ZINC0000284599 62
<chem>C[C@H](Cc1c[nH]c2c(S(C)(=O)=O)cccc12)NC[C@H](O)c1cccc(NS(=O)(=O)c2cccc(N)c2)c1</chem>	β 1	ZINC0000284634 70
<chem>C[C@H](Cc1ccc(OCC(=O)O)cc1)NC[C@H](O)c1cc(Br)no1</chem>	β 1	ZINC0000286472 35
<chem>C[C@H](Cc1ccc(OCC(=O)O)cc1)NC[C@@H](O)c1cc(Br)no1</chem>	β 1	ZINC0000286472 38
<chem>CCOC(=O)COc1ccc(C[C@@H](C)NC[C@H](O)c2cc(Br)no2)cc1</chem>	β 1	ZINC0000286472 46
<chem>CCOC(=O)COc1ccc(C[C@@H](C)NC[C@@H](O)c2cc(Br)no2)cc1</chem>	β 1	ZINC0000286472 48
<chem>CCCCOc1ccc(C[C@@H](C)NC[C@H](O)c2cc(Br)no2)cc1</chem>	β 1	ZINC0000286472 51
<chem>CCCCOc1ccc(C[C@@H](C)NC[C@@H](O)c2cc(Br)no2)cc1</chem>	β 1	ZINC0000286472 53

<chem>COc1ccc(C[C@@H](C)NC[C@H](O)c2cc(O)cc(O)c2)cc1</chem>	$\beta 2$	ZINC0000286521 26
<chem>COc1ccc(C[C@@H](C)NC[C@@H](O)c2cc(O)cc(O)c2)cc1</chem>	$\beta 2$	ZINC0000286521 42
<chem>COc1ccc(C[C@H](C)NC[C@@H](O)c2cc(O)cc(O)c2)cc1</chem>	$\beta 2$	ZINC0000286521 60
<chem>C[C@H](Cc1ccccc1)NC[C@H](O)c1cc(O)cc(O)c1</chem>	$\beta 2$	ZINC0000286521 67
<chem>C[C@@H](Cc1ccccc1)NC[C@H](O)c1cc(O)cc(O)c1</chem>	$\beta 2$	ZINC0000286521 71
<chem>C[C@H](Cc1ccc(N)cc1)NC[C@H](O)c1cc(O)cc(O)c1</chem>	$\beta 2$	ZINC0000286521 85
<chem>C[C@@H](Cc1ccc(N)cc1)NC[C@H](O)c1cc(O)cc(O)c1</chem>	$\beta 2$	ZINC0000286521 89
<chem>C[C@H](Cc1cccc2ccccc12)NC[C@H](O)c1cc(O)cc(O)c1</chem>	$\beta 2$	ZINC0000286522 00
<chem>C[C@H](Cc1cccc2ccccc12)NC[C@@H](O)c1cc(O)cc(O)c1</chem>	$\beta 2$	ZINC0000286522 07
<chem>C[C@@H](Cc1cccc2ccccc12)NC[C@@H](O)c1cc(O)cc(O)c1</chem>	$\beta 2$	ZINC0000286522 11
<chem>CCCC[C@@H](C)NC[C@H](O)c1cc(O)cc(O)c1</chem>	$\beta 2$	ZINC0000286522 15
<chem>C[C@H](Cc1cccc(CC(=O)NCc2ccccc2)c1)NC[C@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 2$	ZINC0000287037 25
<chem>Cc1ccc(OC[C@@H](O)CNC(C)C)c2c1CCC2</chem>	$\beta 1$	ZINC0000287653 94
<chem>NCCCCCOC[C@H]1O[C@@H](OCCc2c[nH]c3ccccc23)[C@H](OCc2ccccc2)C[C@@H]1OCc1ccccc1</chem>	$\beta 2$	ZINC0000287718 37
<chem>C[C@H](Cc1ccc2[nH]c(C(=O)NCc3nccs3)cc2c1)NC[C@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 2$	ZINC0000288237 75
<chem>O[C@@H](CNC12CC3CC(CC(C3)C1)C2)COc1cccc2[nH]ccc12</chem>	$\beta 1$	ZINC0000288238 62
<chem>CC[C@H](Cc1ccc2[nH]c(C(=O)NCc3c(OC)cccc3OC)cc2c1)NC[C@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 2$	ZINC0000288250 94

<chem>COc1cccc(OC)c1CNC(=O)c1cc2cc(C[C@@H](C)NC[C@H](O)c3ccc(O)c(CO)c3)ccc2n1C</chem>	$\beta 2$	ZINC0000288250 95
<chem>COc1cccc(OC)c1CNC(=O)c1cc2cc(C[C@@H](C)NC[C@H](O)c3ccc(O)c(CO)c3)ccc2n1Cc1cccc1</chem>	$\beta 2$	ZINC0000288250 98
<chem>C[C@H](Cc1ccc2[nH]c(C(=O)NCc3ccccc3)cc2c1)NC[C@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 2$	ZINC0000288251 05
<chem>CSc1cccc1CNC(=O)c1cc2cc(C[C@@H](C)NC[C@H](O)c3ccc(O)c(CO)c3)ccc2[nH]1</chem>	$\beta 2$	ZINC0000288251 06
<chem>C[C@H](Cc1ccc2[nH]c(C(=O)NCc3c(F)cccc3F)cc2c1)NC[C@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 2$	ZINC0000288251 07
<chem>C[C@H](Cc1ccc2[nH]c(C(=O)NCc3ccc(O)cc3)cc2c1)NC[C@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 2$	ZINC0000288251 08
<chem>C[C@H](Cc1ccc2[nH]c(C(=O)NCc3cccn3)cc2c1)NC[C@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 2$	ZINC0000288251 09
<chem>COc1cccc(CCNC(=O)c2cc3cc(C[C@@H](C)NC[C@H](O)c4ccc(O)c(CO)c4)ccc3[nH]2)c1</chem>	$\beta 2$	ZINC0000288251 10
<chem>COc1cccc2c1C[C@H]1C[C@@H](C(=O)N3CCN(c4ccc([N+](=O)[O-])cc4)CC3)CN(C)[C@@H]1C2</chem>	$\beta 1$	ZINC0000289498 59
<chem>COc1cccc([C@@H](Cc2ccccc2)NC[C@H](O)Cc2ccc(O)c(NS(C)(=O)=O)c2)c1</chem>	$\beta 2$	ZINC0000289580 25
<chem>COc1cccc([C@@H](Cc2ccccc2)NC[C@@H](O)Cc2ccc(O)c(NS(C)(=O)=O)c2)c1</chem>	$\beta 1$	ZINC0000289580 33
<chem>COc1ccc([C@@H](Cc2ccccc2)NC[C@H](O)Cc2ccc(O)c(NS(C)(=O)=O)c2)cc1</chem>	$\beta 2$	ZINC0000289580 38
<chem>COc1ccc([C@@H](Cc2ccccc2)NC[C@@H](O)Cc2ccc(O)c(NS(C)(=O)=O)c2)cc1</chem>	$\beta 1$	ZINC0000289580 41
<chem>COc1ccc([C@@H](Cc2ccccc2)NC[C@H](O)Cc2ccc(O)c(NS(C)(=O)=O)c2)cc1OC</chem>	$\beta 2$	ZINC0000289580 51
<chem>COc1ccc([C@H](Cc2ccccc2)NC[C@@H](O)Cc2ccc(O)c(NS(C)(=O)=O)c2)cc1OC</chem>	$\beta 1$	ZINC0000289580 76
<chem>COc1ccc([C@H](Cc2ccccc2)NC[C@H](O)Cc2ccc(O)c(NS(C)(=O)=O)c2)cc1OC</chem>	$\beta 2$	ZINC0000289580 79
<chem>CS(=O)(=O)Nc1cc(C[C@H](O)CN[C@H](Cc2ccccc2)c2ccc(Cl)c(Cl)c2)ccc1O</chem>	$\beta 1$	ZINC0000289580 84

<chem>COc1ccc([C@@H](Cc2ccccc2)NC[C@@H](O)Cc2ccc(O)c(NS(C)(=O)=O)c2)cc1O</chem>	β 1	ZINC0000289580 87
<chem>CS(=O)(=O)Nc1cc(C[C@H](O)CN[C@H](Cc2ccccc2)c2ccc(OC(F)F)c(OC(F)F)c2)ccc1O</chem>	β 1	ZINC0000289580 89
<chem>COc1ccc([C@H](Cc2ccccc2)NC[C@H](O)Cc2ccc(O)c(NS(C)(=O)=O)c2)cc1OC</chem>	β 1	ZINC0000289581 26
<chem>COc1ccc([C@H](Cc2ccccc2)NC[C@H](O)Cc2ccc(O)c(NS(C)(=O)=O)c2)cc1</chem>	β 1	ZINC0000289581 29
<chem>COc1cccc([C@H](Cc2ccccc2)NC[C@H](O)Cc2ccc(O)c(NS(C)(=O)=O)c2)c1</chem>	β 1	ZINC0000289581 38
<chem>CS(=O)(=O)Nc1cc(C[C@@H](O)CN[C@@H](Cc2ccccc2)c2ccc(OC(F)F)c(OC(F)F)c2)ccc1O</chem>	β 1	ZINC0000289581 41
<chem>COc1ccc([C@H](Cc2ccccc2Cl)NC[C@H](O)Cc2ccc(O)c(NS(C)(=O)=O)c2)cc1OC</chem>	β 1	ZINC0000289581 45
<chem>COc1ccc([C@H](Cc2ccccc(Cl)c2)NC[C@H](O)Cc2ccc(O)c(NS(C)(=O)=O)c2)cc1OC</chem>	β 1	ZINC0000289581 50
<chem>COc1ccc([C@H](Cc2ccc(Cl)cc2)NC[C@H](O)Cc2ccc(O)c(NS(C)(=O)=O)c2)cc1OC</chem>	β 1	ZINC0000289581 56
<chem>O[C@@H](CNCCOc1ccc(-c2cscn2)cc1)c1ccnc1</chem>	β 1	ZINC0000289589 43
<chem>Cc1nc(-c2ccc(OCCNC[C@H](O)c3ccnc3)cc2)cs1</chem>	β 1	ZINC0000289589 50
<chem>O[C@@H](CNCCOc1ccc(-c2csc(C(F)(F)F)n2)cc1)c1ccnc1</chem>	β 1	ZINC0000289589 54
<chem>CCc1nc(-c2ccc(OCCNC[C@H](O)c3ccnc3)cc2)cs1</chem>	β 1	ZINC0000289589 87
<chem>O[C@@H](CNCCOc1ccc(-c2csc(C3CCCC3)n2)cc1)c1ccnc1</chem>	β 1	ZINC0000289589 98
<chem>O[C@@H](CNCCOc1ccc(-c2csc(-c3ccccc3)n2)cc1)c1ccnc1</chem>	β 1	ZINC0000289590 05
<chem>O[C@@H](CNCCOc1ccc(-c2csc(-c3ccnc3)n2)cc1)c1ccnc1</chem>	β 1	ZINC0000289590 30
<chem>O[C@@H](CNCCOc1ccc(-c2csc(-c3ccncc3)n2)cc1)c1ccnc1</chem>	β 1	ZINC0000289590 34

<chem>CCc1nc(-c2ccc(OCCNC[C@H](O)c3ccnc3)cc2)co1</chem>	$\beta 1$	ZINC0000289590 64
<chem>CC(C)c1nc(-c2ccc(OCCNC[C@H](O)c3ccnc3)cc2)co1</chem>	$\beta 1$	ZINC0000289591 64
<chem>O[C@@H](CNCCOc1ccc(-c2coc(COCc3ccccc3)n2)cc1)c1ccnc1</chem>	$\beta 1$	ZINC0000289592 28
<chem>OCc1nc(-c2ccc(OCCNC[C@H](O)c3ccnc3)cc2)co1</chem>	$\beta 1$	ZINC0000289592 62
<chem>Cc1ocnc1-c1ccc(OCCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000289592 82
<chem>C[C@H](Cc1cccc(CC(=O)NC23CC4CC(CC(C4)C2)C3)c1)NC[C@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 2$	ZINC0000291310 23
<chem>O=C(O)COc1ccc(Cc2ccc(CCNC[C@H](O)c3cccc(Cl)c3)cc2)cc1</chem>	$\beta 1$	ZINC0000291316 51
<chem>O=C(O)c1ccc(-c2ccc(CCNC[C@H](O)c3ccccc3)cc2)cc1Oc1ccccc1</chem>	$\beta 1$	ZINC0000291317 05
<chem>CN(c1ccc(CCNC[C@H](O)c2cccc(Cl)c2)cc1)c1ccc(OCC(=O)O)cc1</chem>	$\beta 1$	ZINC0000291317 09
<chem>O=C(O)COc1ccc(Nc2ccc(CCNC[C@H](O)c3cccc(Cl)c3)cc2)cc1</chem>	$\beta 1$	ZINC0000291317 13
<chem>O=C(O)COc1ccc(Oc2ccc(CCNC[C@H](O)c3cccc(Cl)c3)cc2)cc1</chem>	$\beta 1$	ZINC0000291317 82
<chem>O=C(O)c1ccc(-c2ccc(CCNC[C@H](O)c3cccc(Cl)c3)cc2Cl)cc1</chem>	$\beta 1$	ZINC0000291319 90
<chem>O=C(O)c1ccc(-c2ccc(CCNC[C@H](O)c3cccc(Cl)c3)cc2)c(Cl)c1</chem>	$\beta 1$	ZINC0000291319 94
<chem>O=C(O)c1ccc(-c2ccc(CCNC[C@H](O)c3cccc(Cl)c3)cc2)c(F)c1</chem>	$\beta 1$	ZINC0000291320 00
<chem>O=C(O)c1ccc(-c2ccc(CCNC[C@H](O)c3cccc(Cl)c3)cc2)cc1Cl</chem>	$\beta 1$	ZINC0000291320 83
<chem>O=C(O)c1ccc(-c2ccc(CCNC[C@H](O)c3cccc(Cl)c3)cc2)cc1F</chem>	$\beta 1$	ZINC0000291321 50
<chem>O=C(O)c1ccc(Oc2ccc(CCNC[C@H](O)c3cccc(Cl)c3)cc2)nc1</chem>	$\beta 1$	ZINC0000291323 34

<chem>O=C(O)c1ccc(-c2ccc(CCNC[C@H](O)c3cccc(Cl)c3)cc2)s1</chem>	$\beta 1$	ZINC0000291324 34
<chem>O=C(O)c1ccc(-c2ccc(CCNC[C@H](O)c3cccc(Cl)c3)cc2)nc1</chem>	$\beta 1$	ZINC0000291325 28
<chem>O=C(O)c1cccc(Nc2ccc(CCNC[C@H](O)c3cccc(Cl)c3)cc2)c1</chem>	$\beta 1$	ZINC0000291325 30
<chem>O=C(O)c1ccc(Nc2ccc(CCNC[C@H](O)c3cccc(Cl)c3)cc2)cc1</chem>	$\beta 1$	ZINC0000291326 28
<chem>O=C(O)c1ccc(-c2ccc(CCNC[C@H](O)c3cccc(Cl)c3)cc2)cc1</chem>	$\beta 1$	ZINC0000291328 00
<chem>O=C(O)Cc1ccc(-c2ccc(CCNC[C@H](O)c3cccc(Cl)c3)cc2)cc1</chem>	$\beta 1$	ZINC0000291328 05
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2noc(Cc3ccc4ccccc4c3)n2)cc1</chem>	$\beta 1$	ZINC0000292185 45
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2noc(Cc3ccc(-c4cccn4)cc3)n2)cc1</chem>	$\beta 1$	ZINC0000292185 50
<chem>CCCc1nc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)no1</chem>	$\beta 1$	ZINC0000292194 97
<chem>CCCCc1nc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)no1</chem>	$\beta 2$	ZINC0000292198 44
<chem>Cc1nc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)no1</chem>	$\beta 1$	ZINC0000292203 12
<chem>CCCCC1nc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)no1</chem>	$\beta 1$	ZINC0000292207 66
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(COc3ccc(F)cc3)no2)cc1</chem>	$\beta 1$	ZINC0000292209 39
<chem>C[C@@H](O)CCCC1nc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)no1</chem>	$\beta 1$	ZINC0000292210 55
<chem>C[C@H](O)CCCC1nc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)no1</chem>	$\beta 1$	ZINC0000292210 61
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2noc(COC3CCCC3)n2)cc1</chem>	$\beta 1$	ZINC0000292211 17
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(COc3ccc(F)c(F)c3)no2)cc1</chem>	$\beta 1$	ZINC0000292216 10

<chem>CNC(=O)N[C@@H](c1ccc(F)cc1)c1nc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4cccnc4)cc3)cc2)no1</chem>	$\beta 1$	ZINC0000292221 18
<chem>CNC(=O)N[C@H](c1ccc(F)cc1)c1nc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4cccnc4)cc3)cc2)no1</chem>	$\beta 1$	ZINC0000292221 23
<chem>CC(C)CCCc1nc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4cccnc4)cc3)cc2)no1</chem>	$\beta 2$	ZINC0000292221 77
<chem>N[C@@H](c1ccc(F)cc1)c1nc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4cccnc4)cc3)cc2)no1</chem>	$\beta 1$	ZINC0000292221 88
<chem>N[C@H](c1ccc(F)cc1)c1nc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4cccnc4)cc3)cc2)no1</chem>	$\beta 1$	ZINC0000292221 93
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2cccnc2)cc1)c1ccc(-c2noc(Cc3ccc(F)cc3)n2)cc1</chem>	$\beta 1$	ZINC0000292221 98
<chem>CCCCCc1nc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4cccnc4)cc3)cc2)no1</chem>	$\beta 1$	ZINC0000292225 68
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2cccnc2)cc1)c1ccc(-c2noc(CCCC3CCCC3)n2)cc1</chem>	$\beta 1$	ZINC0000292227 98
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2cccnc2)cc1)c1ccc(-c2noc(Cc3cccc(OC(F)(F)F)c3)n2)cc1</chem>	$\beta 1$	ZINC0000292228 60
<chem>CS(=O)(=O)Nc1ccc(Cc2nc(-c3ccc(S(=O)(=O)Nc4ccc(CCNC[C@H](O)c5cccnc5)cc4)cc3)no2)cc1</chem>	$\beta 1$	ZINC0000292229 29
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2cccnc2)cc1)c1ccc(-c2noc(Cc3ccc(C(F)(F)F)cc3)n2)cc1</chem>	$\beta 1$	ZINC0000292229 34
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2cccnc2)cc1)c1ccc(-c2noc(Cc3cccc(F)c3)n2)cc1</chem>	$\beta 1$	ZINC0000292229 39
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2cccnc2)cc1)c1ccc(-c2noc([C@@H](O)c3ccc(F)cc3)n2)cc1</chem>	$\beta 2$	ZINC0000292229 45
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2cccnc2)cc1)c1ccc(-c2noc([C@H](O)c3ccc(F)cc3)n2)cc1</chem>	$\beta 2$	ZINC0000292229 51
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2cccnc2)cc1)c1ccc(-c2nc(Cc3ccc(F)c(F)c3)no2)cc1</chem>	$\beta 1$	ZINC0000292229 56
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2cccnc2)cc1)c1ccc(-c2noc(CCCC3CCCCC3)n2)cc1</chem>	$\beta 1$	ZINC0000292229 74
<chem>COc1ccc(OCc2nc(-c3ccc(S(=O)(=O)Nc4ccc(CCNC[C@H](O)c5cccnc5)cc4)cc3)no2)cc1</chem>	$\beta 1$	ZINC0000292233 99

<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2noc(COc3ccc(OC(F)(F)F)cc3)n2)cc1</chem>	$\beta 1$	ZINC0000292237 09
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2noc(COc3ccc4ccccc4c3)n2)cc1</chem>	$\beta 1$	ZINC0000292237 77
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(Cc3ccc(F)cc3)no2)cc1</chem>	$\beta 1$	ZINC0000292238 34
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2noc(COc3ccccc3O)n2)cc1</chem>	$\beta 1$	ZINC0000292238 67
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2noc(COc3ccc(F)cc3)n2)cc1</chem>	$\beta 1$	ZINC0000292238 78
<chem>CS(=O)(=O)N[C@@H](c1ccc(F)cc1)c1nc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)no1</chem>	$\beta 1$	ZINC0000292239 80
<chem>CS(=O)(=O)N[C@H](c1ccc(F)cc1)c1nc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)no1</chem>	$\beta 1$	ZINC0000292239 85
<chem>COC(=O)N[C@@H](c1ccc(F)cc1)c1nc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)no1</chem>	$\beta 1$	ZINC0000292239 94
<chem>COC(=O)N[C@H](c1ccc(F)cc1)c1nc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)no1</chem>	$\beta 1$	ZINC0000292239 99
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2noc(Cc3ccc(F)c(F)c3)n2)cc1</chem>	$\beta 1$	ZINC0000292240 27
<chem>O=C(c1ccc(F)cc1)c1nc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)no1</chem>	$\beta 1$	ZINC0000292250 86
<chem>CC(=O)Nc1ccc(Cc2nc(-c3ccc(S(=O)(=O)Nc4ccc(CCNC[C@H](O)c5ccnc5)cc4)cc3)no2)cc1</chem>	$\beta 1$	ZINC0000292250 92
<chem>CC(=O)Nc1ccc(OCc2nc(-c3ccc(S(=O)(=O)Nc4ccc(CCNC[C@H](O)c5ccnc5)cc4)cc3)no2)cc1</chem>	$\beta 1$	ZINC0000292251 65
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2noc(COc3ccc(F)c(F)c3)n2)cc1</chem>	$\beta 1$	ZINC0000292253 82
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2noc(COc3ccc(C4N=NN=N4)cc3)n2)cc1</chem>	$\beta 1$	ZINC0000292255 66
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2noc(Cc3cc(F)c(F)c(F)c3)n2)cc1</chem>	$\beta 1$	ZINC0000292260 70
<chem>CSc1ccc(Cc2nc(-c3ccc(S(=O)(=O)Nc4ccc(CCNC[C@H](O)c5ccnc5)cc4)cc3)no2)cc1</chem>	$\beta 2$	ZINC0000292260 77

<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNC2CCN(c3ccc(C(=O)N4CCC[C@H]4C(=O)O)cc3)CC2)ccc1O</chem>	β2	ZINC0000292338 03
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2coc(COc3ccc(F)cc3)n2)cc1</chem>	β1	ZINC0000293110 14
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2coc(Cc3ccc(F)c(F)c3)n2)cc1</chem>	β1	ZINC0000293110 18
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2coc(COc3ccc(F)c(F)c3)n2)cc1</chem>	β1	ZINC0000293111 20
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2coc(Cc3ccc(F)cc3)n2)cc1</chem>	β1	ZINC0000293176 94
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2cnc(CCCC3CCCC3)o2)cc1</chem>	β1	ZINC0000293178 15
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2coc(Cc3ccc(C(F)(F)F)cc3)n2)cc1</chem>	β1	ZINC0000293178 89
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2cnc(CC3CCCC3)o2)cc1</chem>	β1	ZINC0000293203 41
<chem>CCCCCc1ncc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)o1</chem>	β1	ZINC0000293203 51
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2cnc(Cc3ccc(F)c(F)c3)o2)cc1</chem>	β1	ZINC0000293258 83
<chem>CC(C)(C)CCCCc1ncc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)o1</chem>	β1	ZINC0000293264 70
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2coc(-c3ccc(F)c(F)c3)n2)cc1</chem>	β1	ZINC0000293265 25
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2coc(-c3ccc(C(F)(F)F)cc3)n2)cc1</chem>	β1	ZINC0000293265 29
<chem>CCCCCc1ncc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)o1</chem>	β1	ZINC0000293276 73
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2coc(CCC3CCCC3)n2)cc1</chem>	β1	ZINC0000293303 98
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2cnc(Cc3cc(F)c(F)c3)o2)cc1</chem>	β1	ZINC0000293304 03
<chem>Cc1ncc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)o1</chem>	β1	ZINC0000293308 48

<chem>C[C@H](Cc1ccc(OCC(=O)NO)cc1)NC[C@H](O)c1cccc(Cl)c1</chem>	$\beta 1$	ZINC0000293318 24
<chem>C[C@H](Cc1ccc(OCC(N)=O)cc1)NC[C@H](O)c1cccc(Cl)c1</chem>	$\beta 1$	ZINC0000293331 72
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2cnc(-c3ccc(F)c(F)c3)o2)cc1</chem>	$\beta 2$	ZINC0000293343 25
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2cnc(-c3ccc(F)cc3)o2)cc1</chem>	$\beta 1$	ZINC0000293343 29
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2cnc(-c3ccccc3)o2)cc1</chem>	$\beta 1$	ZINC0000293343 35
<chem>NS(=O)(=O)c1cc(S(=O)(=O)NCCNC[C@H](O)COc2cccc3c2CCC(=O)N3)ccc1Cl</chem>	$\beta 1$	ZINC0000293399 95
<chem>C[C@H](Cc1ccc(OCCO)cc1)NC[C@H](O)c1cccc(Cl)c1</chem>	$\beta 1$	ZINC0000293406 00
<chem>NS(=O)(=O)c1cc(S(=O)(=O)NCCNC[C@H](O)COc2cccc3c2SCC(=O)N3)ccc1Cl</chem>	$\beta 1$	ZINC0000293406 67
<chem>CC(C)(C)Nc1cccc2c1S[C@@H](OCCCO)C(=O)N2</chem>	$\beta 1$	ZINC0000293416 33
<chem>O=S(=O)(Nc1ccccc1)c1ccc2c(c1)CCN2c1noc(CCCC2CCCC2)n1</chem>	$\beta 1$	ZINC0000294874 69
<chem>CN(CCc1ccccc1)C(=O)N1CCc2cc(S(=O)(=O)Nc3ccccc3)ccc21</chem>	$\beta 1$	ZINC0000294880 23
<chem>CNC(=O)N1CCc2cc(S(=O)(=O)Nc3ccccc3)ccc21</chem>	$\beta 2$	ZINC0000295446 77
<chem>O=S(=O)(Nc1ccccc1)c1ccc2c(c1)CCN2c1cccc(CCCC2CCCC2)c1</chem>	$\beta 1$	ZINC0000295470 34
<chem>CCCCCNC(=O)N(C)c1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000295488 06
<chem>CN(C)C(=O)N1CCc2cc(S(=O)(=O)Nc3ccccc3)ccc21</chem>	$\beta 1$	ZINC0000295488 27
<chem>CCCCCc1ccnc(N2CCc3cc(S(=O)(=O)Nc4ccccc4)ccc32)n1</chem>	$\beta 1$	ZINC0000295492 66
<chem>O=S(=O)(Nc1ccccc1)c1ccc2c(c1)CCN2c1nc(CCCC2CCCC2)cs1</chem>	$\beta 1$	ZINC0000295492 77

<chem>CN(C(=O)N1CCc2cc(S(=O)(=O)Nc3ccccc3)ccc21)C(C)(C)Cc1ccccc1</chem>	$\beta 1$	ZINC0000295499 61
<chem>CCCCCc1csc(N2CCc3cc(S(=O)(=O)Nc4ccccc4)ccc32)n1</chem>	$\beta 1$	ZINC0000295519 06
<chem>Cc1csc(N2CCc3cc(S(=O)(=O)Nc4ccccc4)ccc32)n1</chem>	$\beta 1$	ZINC0000295522 40
<chem>CCCCCN(C)C(=O)N1CCc2cc(S(=O)(=O)Nc3ccccc3)ccc21</chem>	$\beta 1$	ZINC0000295526 08
<chem>CCCCCc1ccc(N2CCc3cc(S(=O)(=O)Nc4ccccc4)ccc32)nc1</chem>	$\beta 1$	ZINC0000295533 00
<chem>CCCCCc1nc(N2CCc3cc(S(=O)(=O)Nc4ccccc4)ccc32)no1</chem>	$\beta 1$	ZINC0000295536 02
<chem>CCCCCc1cccc(N2CCc3cc(S(=O)(=O)Nc4ccccc4)ccc32)c1</chem>	$\beta 1$	ZINC0000295537 76
<chem>O=S(=O)(Nc1ccccc1)c1ccc2c(c1)CCN2c1cccc(CCCC2CCCC2)n1</chem>	$\beta 1$	ZINC0000295537 79
<chem>CCCCCc1cccc(N2CCc3cc(S(=O)(=O)Nc4ccccc4)ccc32)n1</chem>	$\beta 1$	ZINC0000295540 35
<chem>CCCCCCC(=O)N1CCc2cc(S(=O)(=O)Nc3ccccc3)ccc21</chem>	$\beta 1$	ZINC0000295554 92
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(Cc3ccc(F)cc3)cs2)cc1</chem>	$\beta 1$	ZINC0000295665 37
<chem>CCCCCc1csc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)n1</chem>	$\beta 2$	ZINC0000295671 23
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(-c3ccc(F)cc3)cs2)cc1</chem>	$\beta 1$	ZINC0000295677 03
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(-c3cccn3)cs2)cc1</chem>	$\beta 1$	ZINC0000295681 47
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(-c3ccnc3)cs2)cc1</chem>	$\beta 1$	ZINC0000295681 51
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(Cc3ccc4ccccc4c3)cs2)cc1</chem>	$\beta 1$	ZINC0000295684 01
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(CCc3ccccc3)cs2)cc1</chem>	$\beta 1$	ZINC0000295684 05

<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(-c3ccc4ccccc4c3)cs2)cc1</chem>	$\beta 2$	ZINC0000295691 64
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(-c3ccc4ncccc4c3)cs2)cc1</chem>	$\beta 1$	ZINC0000295695 11
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2nc(CCCC3CCCC3)cs2)cc1</chem>	$\beta 1$	ZINC0000295710 67
<chem>COc1ccc(CC(C)(C)NC[C@@H](O)COc2cccc(Cl)c2Cl)cc1</chem>	$\beta 2$	ZINC0000339652 97
<chem>NS(=O)(=O)c1cccc(CCCCOCCCCCNC[C@H](O)c2ccc(O)c(NC=O)c2)c1</chem>	$\beta 1$	ZINC0000339911 89
<chem>O=c1ccn(-c2cccc(CCCCOCCCCCNC[C@H](O)c3ccc(O)c(CO)c3)c2)c(=O)[nH]1</chem>	$\beta 1$	ZINC0000340163 47
<chem>COc1ccc(CC(C)(C)NC[C@H](O)COc2cccc(Cl)c2C#N)cc1</chem>	$\beta 2$	ZINC0000340350 24
<chem>COc1ccc(CC(C)(C)NC[C@@H](O)COc2cccc(Cl)c2C#N)cc1</chem>	$\beta 2$	ZINC0000340350 25
<chem>Cc1ccc(Sc2ccccc2N2CCNCC2)c(C)c1</chem>	$\beta 1$	ZINC0000340518 48
<chem>C[C@H](Cc1ccc(-c2ccc(C(=O)O)cc2)cc1)NC[C@H](O)c1cccc(Cl)c1</chem>	$\beta 1$	ZINC0000342839 20
<chem>OCc1cc([C@@H](O)CNCCc2ccc(Nc3cccc(-c4ccccc4)c3)cc2)ccc1O</chem>	$\beta 2$	ZINC0000343244 60
<chem>OCc1cc([C@@H](O)CNCCc2ccc(NC[C@H](O)c3ccccc3)cc2)ccc1O</chem>	$\beta 1$	ZINC0000343911 59
<chem>COc1ccc2nc(-c3ccc(OC[C@@H](O)CNC(C)C)cc3)n(C)c(=O)c2c1</chem>	$\beta 1$	ZINC0000345929 42
<chem>COc1ccc2nc(-c3ccc(OC[C@H](O)CNC(C)C)cc3)n(C)c(=O)c2c1</chem>	$\beta 1$	ZINC0000345929 43
<chem>CC(C)(Cc1ccc(Br)cc1)NC[C@@H](O)c1cc(O)cc2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000346308 45
<chem>N#Cc1ccccc1OC[C@@H](O)CNCCNC(=O)Nc1ccc(OCCF)cc1</chem>	$\beta 1$	ZINC0000346614 00
<chem>O=C(Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1)c1ccccc1</chem>	$\beta 1$	ZINC0000348015 48

<chem>CCCCCS(=O)(=O)Nc1ccc(CCNC[C@H](O)COc2ccc(O)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 49
<chem>COc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 50
<chem>Cc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 52
<chem>Oc1ccc(CCNC[C@H](O)COc2ccc(O)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 54
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)COc2ccc(O)cc2)cc1)c1ccc(Cl)c(Cl)c1</chem>	$\beta 2$	ZINC0000348015 57
<chem>C[C@@H](Cc1ccc(O)cc1)NC[C@H](O)COc1ccc(O)cc1</chem>	$\beta 1$	ZINC0000348015 58
<chem>C[C@@H](CCc1ccc(O)cc1)NC[C@H](O)COc1ccc(O)cc1</chem>	$\beta 1$	ZINC0000348015 60
<chem>O=S(=O)(Cc1ccccc1)Nc1ccc(CCNC[C@H](O)COc2ccc(O)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 61
<chem>CCCS(=O)(=O)Nc1ccc(CCNC[C@H](O)COc2ccc(O)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 62
<chem>Nc1ccc(CCNC[C@H](O)COc2ccc(O)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 63
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)COc2ccc(O)cc2)cc1)c1cccc(Cl)c1</chem>	$\beta 1$	ZINC0000348015 64
<chem>CCCCCN(C)C(=O)N(C)c1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 65
<chem>CCCCCOC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 66
<chem>CC(C)C(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 67
<chem>CC(=O)Nc1ccc(CCNC[C@H](O)COc2ccc(O)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 68
<chem>O=C(Nc1ccc(CCNC[C@H](O)COc2ccc(O)cc2)cc1)c1ccccc1</chem>	$\beta 1$	ZINC0000348015 69
<chem>CCC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 70

<chem>O=C(Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1)OCc1ccccc1</chem>	$\beta 1$	ZINC0000348015 71
<chem>CC(C)OC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 73
<chem>CCOC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 74
<chem>COC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 75
<chem>CCCCCNC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 76
<chem>CCCCCCNC(=O)N(C)c1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 77
<chem>CCCCCCN(C)C(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 78
<chem>O=C(Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1)NC1CCCCC1</chem>	$\beta 1$	ZINC0000348015 79
<chem>COCCCNc(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 80
<chem>CNC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 81
<chem>CCCCCCCCNC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 82
<chem>CC(C)NC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 83
<chem>CCCC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 84
<chem>CC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 85
<chem>CCCCCCC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 86
<chem>CCCCCCCNC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 87
<chem>CCCNc(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)COc3ccc(O)cc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348015 88

<chem>CCCCCCCCc1nc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)no1</chem>	$\beta 1$	ZINC0000348015 90
<chem>CCCCCCCCc1nc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)no1</chem>	$\beta 1$	ZINC0000348015 91
<chem>CCCCCCCCc1ncc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)o1</chem>	$\beta 1$	ZINC0000348015 92
<chem>CCCCCCCCc1ccnc(N2CCc3cc(S(=O)(=O)Nc4ccccc4)ccc32)n1</chem>	$\beta 1$	ZINC0000348015 93
<chem>CCCCCCCCc1nc(N2CCc3cc(S(=O)(=O)Nc4ccccc4)ccc32)no1</chem>	$\beta 1$	ZINC0000348015 94
<chem>CCCCCCCCc1cccc(N2CCc3cc(S(=O)(=O)Nc4ccccc4)ccc32)c1</chem>	$\beta 1$	ZINC0000348015 95
<chem>CCCCCCCCc1csc(N2CCc3cc(S(=O)(=O)Nc4ccccc4)ccc32)n1</chem>	$\beta 1$	ZINC0000348015 96
<chem>CCCCCCCCC(=O)N1CCc2cc(S(=O)(=O)Nc3ccccc3)ccc21</chem>	$\beta 1$	ZINC0000348015 97
<chem>CCCCCCCCc1enc(N2CCc3cc(S(=O)(=O)Nc4ccccc4)ccc32)o1</chem>	$\beta 1$	ZINC0000348015 98
<chem>CCCCCCCCc1csc(Nc2ccc(S(=O)(=O)Nc3ccccc3)cc2)n1</chem>	$\beta 1$	ZINC0000348015 99
<chem>CCCCCCCCc1csc(N(C)c2ccc(S(=O)(=O)Nc3ccccc3)cc2)n1</chem>	$\beta 1$	ZINC0000348016 00
<chem>CCCCCCCCc1cccc(N2CCc3cc(S(=O)(=O)Nc4ccccc4)ccc32)n1</chem>	$\beta 1$	ZINC0000348016 01
<chem>CCCCCCCCN(C)C(=O)N1CCc2cc(S(=O)(=O)Nc3ccccc3)ccc21</chem>	$\beta 1$	ZINC0000348016 02
<chem>CCCCCCCCNC(=O)N1CCc2cc(S(=O)(=O)Nc3ccccc3)ccc21</chem>	$\beta 1$	ZINC0000348016 03
<chem>CCCCCCCCc1csc(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)n1</chem>	$\beta 1$	ZINC0000348016 04
<chem>CCCCCCCCc1csc(Cc2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)n1</chem>	$\beta 1$	ZINC0000348016 05
<chem>CCCCCCCCN1CC(=O)N(c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)C1=O</chem>	$\beta 1$	ZINC0000348016 06

<chem>CCCCCCCCn1c(=O)[nH]n(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)c1=O</chem>	$\beta 1$	ZINC0000348016 07
<chem>CCCCCCCCn1c(C)cn(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)c1=O</chem>	$\beta 1$	ZINC0000348016 08
<chem>CCCCCCCCN1CCN(c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)C1=O</chem>	$\beta 1$	ZINC0000348016 09
<chem>CCCCCCCCn1ccn(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)c1=O</chem>	$\beta 1$	ZINC0000348016 10
<chem>CCCCCCCCN1C(=O)CN(c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)C1=O</chem>	$\beta 1$	ZINC0000348016 11
<chem>CCCCCCCCNC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348016 13
<chem>CCCCCCCC(=O)Nc1ccc(S(=O)(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1</chem>	$\beta 1$	ZINC0000348016 14
<chem>CCCCCCCCc1esc(N2CCc3cc(NC(=S)Nc4ccc(CCNC[C@H](O)c5ccnc5)cc4)ccc32)n1</chem>	$\beta 1$	ZINC0000348016 26
<chem>CCCCCCCCc1esc(N2CCc3cc(N/C(=N/c4ccc(CCNC[C@H](O)c5ccnc5)cc4)NC#N)ccc32)n1</chem>	$\beta 1$	ZINC0000348016 27
<chem>CCCCCCCCc1esc(N2CCc3ccc(N/C(=N/c4ccc(CCNC[C@H](O)c5ccnc5)cc4)NC#N)cc32)n1</chem>	$\beta 1$	ZINC0000348016 28
<chem>CCCCCCCCn1ncn(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)c1=O</chem>	$\beta 1$	ZINC0000348016 29
<chem>CCCCCCCCn1cnn(-c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)c1=O</chem>	$\beta 1$	ZINC0000348016 30
<chem>CCCCCCCCN1CCN(c2ccc(S(=O)(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)cc2)C1=O</chem>	$\beta 1$	ZINC0000348016 31
<chem>CCN(CC)C(=O)[C@@H]1C=C2c3ccc4[nH]cc(c34)C[C@H]2N(C(=O)Nc2ccccc2)C1</chem>	$\beta 1$	ZINC0000348376 17
<chem>COc1ccc(CC(C)(C)NC[C@@H](O)c2cc(O)cc3c2OCC(=O)N3)cc1</chem>	$\beta 1$	ZINC0000348922 66
<chem>CC(C)c1ccc(CC(C)(C)NC[C@@H](O)c2cc(O)cc3c2OCC(=O)N3)cc1</chem>	$\beta 1$	ZINC0000349975 45
<chem>CC(C)(Cc1ccc(F)cc1)NC[C@@H](O)c1cc(O)cc2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000358269 21

<chem>CC(C)(Cc1cccc1)NC[C@H](O)c1ccc(O)c2[nH]c(=O)sc12</chem>	$\beta 1$	ZINC0000359422 89
<chem>Cc1c(C)c(C)c2c(c1C)CC(NC[C@H](O)c1ccc(O)c3[nH]c(=O)ccc13)C2</chem>	$\beta 1$	ZINC0000359509 86
<chem>CCOc1ccc(CC(C)(C)NC[C@@H](O)c2cc(O)cc3c2OCC(=O)N3)cc1</chem>	$\beta 1$	ZINC0000359511 38
<chem>CCc1cc2c(cc1CC)CC(C)(NC[C@H](O)c1ccc(O)c3[nH]c(=O)ccc13)C2</chem>	$\beta 1$	ZINC0000359512 68
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CN[C@H]3CCC[C@@H]3OCc3cccc3)c2s1</chem>	$\beta 1$	ZINC0000359971 48
<chem>CNC[C@@H](O)c1ccc(O)c2[nH]c(=O)sc12</chem>	$\beta 1$	ZINC0000361079 23
<chem>CC(C)Cc1ccc(CCNC[C@H](O)c2ccc(O)c3[nH]c(=O)sc23)cc1</chem>	$\beta 1$	ZINC0000364001 77
<chem>COc1ccc(CC[C@@H](C)NC[C@H](O)COc2ccc(O)cc2)cc1</chem>	$\beta 2$	ZINC0000381529 35
<chem>COc1ccc(CC[C@@H](C)NC[C@@H](O)COc2ccc(O)cc2)cc1</chem>	$\beta 2$	ZINC0000381529 41
<chem>CCc1ccc(CC(C)(C)NC[C@@H](O)c2cc(O)cc3c2OCC(=O)N3)cc1</chem>	$\beta 1$	ZINC0000382153 27
<chem>CC(C)(Cc1ccc(Cl)cc1)NC[C@@H](O)c1cc(O)cc2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000382795 61
<chem>CCC1=C(CC)CC2=C(C1)CC(NC[C@H](O)c1ccc(O)c3[nH]c(=O)ccc13)C2</chem>	$\beta 1$	ZINC0000383462 33
<chem>CC(C)(Cc1ccc(C(F)(F)F)cc1)NC[C@@H](O)c1cc(O)cc2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000383469 63
<chem>COc1ccc(Nc2ccc(CCNC[C@H](O)c3ccc(O)c(CO)c3)cc2)cc1</chem>	$\beta 2$	ZINC0000383889 86
<chem>OCc1cc([C@H](O)CNCCc2ccc(NC[C@H](O)c3cccc3)cc2)ccc1O</chem>	$\beta 2$	ZINC0000383967 26
<chem>Cc1cc(C)cc(COCCOCCCCCN[C@H](O)c2ccc(O)c(CO)c2)c1</chem>	$\beta 1$	ZINC0000384000 54
<chem>COc1ccc(Nc2ccc(CCNC[C@@H](O)c3ccc(O)c(CO)c3)cc2)cc1</chem>	$\beta 2$	ZINC0000384600 67

<chem>NS(=O)(=O)c1cccc(CCCOCCCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)c1</chem>	$\beta 1$	ZINC0000384618 06
<chem>OCc1cc([C@H](O)CNCCc2ccc(NC[C@@H](O)c3ccccc3)cc2)ccc1O</chem>	$\beta 2$	ZINC0000384684 20
<chem>CCOc1ccc(Nc2ccc(CCNC[C@@H](O)c3ccc(O)c(CO)c3)cc2)cc1</chem>	$\beta 2$	ZINC0000384801 25
<chem>OCc1cc([C@H](O)CNCCc2ccc(Nc3ccccc3)cc2)ccc1O</chem>	$\beta 2$	ZINC0000384807 73
<chem>COc1ccc(Nc2ccc(CCNC[C@@H](O)c3ccc(O)c(CO)c3)cc2)cc1-c1ccccc1</chem>	$\beta 2$	ZINC0000384813 89
<chem>OCc1cc([C@@H](O)CNCCCCCCCCCCCCc2ccccc2)ccc1O</chem>	$\beta 1$	ZINC0000388388 19
<chem>OCc1cc([C@H](O)CNCCCCCCCCCCCCc2ccccc2)ccc1O</chem>	$\beta 1$	ZINC0000388388 20
<chem>O=C(O)c1ccc(-c2ccc3c(c2)C[C@@H](NC[C@H](O)c2ccc(Cl)cc2)CC3)cc1</chem>	$\beta 1$	ZINC0000389006 30
<chem>CC(C)Oc1cc(-c2ccc3c(c2)C[C@@H](NC[C@H](O)c2ccc(Cl)cc2)CC3)ccc1C(=O)O</chem>	$\beta 1$	ZINC0000403804 81
<chem>COc1ccc(CC(C)(C)NC[C@H](O)COc2ccccc2C#N)cc1</chem>	$\beta 2$	ZINC0000403807 40
<chem>COc1ccc(CC(C)(C)NC[C@@H](O)COc2ccccc2C#N)cc1</chem>	$\beta 2$	ZINC0000403807 41
<chem>O=C(Nc1cccc(Cn2ncc(N3CCNCC3)c(Cl)c2=O)c1)c1ccc(-c2ccccc2)cc1</chem>	$\beta 2$	ZINC0000403911 74
<chem>O=C(O)c1ccc(-c2ccc3c(c2)C[C@@H](NC[C@H](O)c2ccc(Cl)nc2)CC3)cc1</chem>	$\beta 1$	ZINC0000403914 92
<chem>CC(C)NC[C@@H](O)COc1ccc2c(c1)CCCN2Cc1ccccc1</chem>	$\beta 1$	ZINC0000403918 53
<chem>O=C(Cc1ncc[nH]1)Nc1ccc(CCNC[C@H](O)COc2ccccc2)cc1</chem>	$\beta 1$	ZINC0000403945 57
<chem>CNS(=O)(=O)c1cccc(CCCOCCCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)c1</chem>	$\beta 1$	ZINC0000404092 04
<chem>NS(=O)(=O)c1ccccc1CCCCOCCCCCCCNC[C@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 1$	ZINC0000404134 95

<chem>CC(=O)Nc1ccc(Oc2cccc(CCNC[C@H](O)c3ccnc3)c2)cc1C(=O)O</chem>	$\beta 1$	ZINC0000404223 94
<chem>C[C@H](Cc1cccc(Oc2cccc(C(=O)O)c2)c1)NC[C@H](O)c1cccc(Cl)c1</chem>	$\beta 1$	ZINC0000404224 00
<chem>COc1ccc(CCNC[C@@H](O)COc2ccc3c(c2)CCCN3Cc2ccccc2)cc1</chem>	$\beta 1$	ZINC0000404225 79
<chem>COc1ccc(CC(C)(C)NC[C@H](O)COc2cccc(Cl)c2Cl)cc1</chem>	$\beta 2$	ZINC0000404238 26
<chem>Cc1ccc2c(OCCN3CCC(Cc4cccc(NS(C)(=O)=O)c4)CC3)cccc2n1</chem>	$\beta 2$	ZINC0000404241 80
<chem>O=C(O)c1ccc(Oc2ccc3c(c2)C[C@@H](NC[C@H](O)c2cccc(Cl)c2)CC3)s1</chem>	$\beta 1$	ZINC0000404248 18
<chem>Cc1ccc2c(OCCN3CCC(Cc4cccc(N5CCCS5(=O)=O)c4)CC3)cccc2n1</chem>	$\beta 2$	ZINC0000404249 20
<chem>O=C(O)c1cccc(Oc2ccc3c(c2)C[C@@H](NC[C@H](O)c2cccc(Cl)c2)CCC3)c1</chem>	$\beta 1$	ZINC0000404252 32
<chem>C[C@H](Cc1ccc(-c2ccc(C(=O)O)cc2)cc1)NC[C@H](O)c1ccccc1</chem>	$\beta 1$	ZINC0000408341 61
<chem>C[C@H](Cc1ccc(-c2ccc(C(=O)O)c(OC3CCCCC3)c2)cc1)NC[C@H](O)c1ccccc1</chem>	$\beta 1$	ZINC0000408356 55
<chem>C[C@H](Cc1ccc(-c2ccc(C(=O)O)cc2)cc1)NC[C@H](O)c1ccnc1</chem>	$\beta 1$	ZINC0000408364 60
<chem>O=C(O)c1ccc(-c2ccc3c(c2)C[C@@H](NC[C@H](O)c2ccccc2Cl)CC3)cc1</chem>	$\beta 1$	ZINC0000408365 50
<chem>O=C(O)c1ccc(-c2ccc3c(c2)C[C@@H](NC[C@H](O)c2ccc(Cl)cc2)CC3)cc1F</chem>	$\beta 1$	ZINC0000408479 33
<chem>COc1cc(Oc2ccc3c(c2)C[C@@H](NC[C@H](O)c2cccc(Cl)c2)CC3)cc(C(=O)O)c1</chem>	$\beta 1$	ZINC0000408481 31
<chem>O=C(O)c1cccc(Oc2ccc3c(c2)C[C@@H](NC[C@H](O)c2ccc(Cl)cc2)CC3)c1</chem>	$\beta 1$	ZINC0000408481 39
<chem>Nc1cc(Oc2ccc3c(c2)C[C@@H](NC[C@H](O)c2cccc(Cl)c2)CC3)cc(C(=O)O)c1</chem>	$\beta 1$	ZINC0000408482 58
<chem>CC(=O)Nc1cc(Oc2ccc3c(c2)C[C@@H](NC[C@H](O)c2cccc(Cl)c2)CC3)cc(C(=O)O)c1</chem>	$\beta 1$	ZINC0000408482 59

<chem>CS(=O)(=O)/N=C(\O)c1ccc(-c2ccc(CCNC[C@H](O)c3ccccc3)cc2)cc1NC1CCCCC1</chem>	$\beta 1$	ZINC0000408488 98
<chem>O=C(O)c1ccc(-c2ccc3c(c2)C[C@@H](NC[C@H](O)c2ccc(C(F)(F)F)cc2)CC3)cc1</chem>	$\beta 1$	ZINC0000408601 79
<chem>O=C(O)c1ccc(-c2ccc3c(c2)C[C@@H](NC[C@H](O)c2ccc(Cl)cc2)CC3)c(F)c1</chem>	$\beta 1$	ZINC0000408614 20
<chem>CCCNc1cc(Oc2ccc3c(c2)C[C@@H](NC[C@H](O)c2ccc(Cl)c2)CC3)cc(C(=O)O)c1</chem>	$\beta 1$	ZINC0000408633 19
<chem>Cc1ccc(Cn2ncc(N3CCNCC3)c(Cl)c2=O)cc1NC(=O)c1ccc(-c2ccccc2)cc1</chem>	$\beta 2$	ZINC0000408635 75
<chem>CN(C)c1cc(Oc2ccc3c(c2)C[C@@H](NC[C@H](O)c2ccc(Cl)nc2)CC3)cc(C(=O)O)c1</chem>	$\beta 1$	ZINC0000408673 26
<chem>O=C(O)c1cccc(Oc2ccc3c(c2)C[C@@H](NC[C@H](O)c2ccc(Cl)nc2)CC3)c1</chem>	$\beta 1$	ZINC0000408673 28
<chem>C[C@H](Cc1ccc(NC(=O)Cc2nccn2Cc2ccccc2)cc1)NC[C@H](O)COc1ccccc1</chem>	$\beta 1$	ZINC0000408748 62
<chem>O=C(Cc1ccccc1)Nc1ccc(CCNC[C@H](O)COc2ccccc3[nH]c4ccccc4c23)cc1</chem>	$\beta 1$	ZINC0000408758 15
<chem>O=C(Cc1nccn1Cc1ccc(Cl)cc1)Nc1ccc(CCNC[C@H](O)COc2ccccc2)cc1</chem>	$\beta 1$	ZINC0000408787 85
<chem>O=C(Cc1cccc(Cl)n1)Nc1ccc(CCNC[C@H](O)COc2ccccc2)cc1</chem>	$\beta 1$	ZINC0000408803 13
<chem>CCCCCOc1cc(-c2ccc(CCNC[C@H](O)c3ccccc3)cc2)ccc1/C(O)=N/S(C)(=O)=O</chem>	$\beta 1$	ZINC0000408917 36
<chem>CS(=O)(=O)/N=C(\O)c1ccc(-c2ccc(CCNC[C@H](O)c3ccccc3)cc2)cc1OC1CCCC1</chem>	$\beta 1$	ZINC0000408917 37
<chem>CC(C)Oc1cc(-c2ccc(CCNC[C@H](O)c3ccccc3)cc2)ccc1/C(O)=N/S(C)(=O)=O</chem>	$\beta 1$	ZINC0000408925 05
<chem>CC(C)Nc1cc(-c2ccc(CCNC[C@H](O)c3ccccc3)cc2)ccc1/C(O)=N/S(C)(=O)=O</chem>	$\beta 1$	ZINC0000408926 22
<chem>COc1cc(-c2ccc(CCNC[C@H](O)c3ccccc3)cc2)ccc1/C(O)=N/S(C)(=O)=O</chem>	$\beta 1$	ZINC0000408946 20
<chem>NS(=O)(=O)c1ccc(CCCCOCCCCCN[C@H](O)c2ccc(O)c(CO)c2)cc1</chem>	$\beta 1$	ZINC0000409137 06

<chem>CN(C)S(=O)(=O)c1cccc(CCCCOCCCCCN[C@H](O)c2ccc(O)c(CO)c2)c1</chem>	β 1	ZINC0000409142 28
<chem>CC(C)NS(=O)(=O)c1cccc(CCCOCCCCCN[C@H](O)c2ccc(O)c(CO)c2)c1</chem>	β 1	ZINC0000409146 30
<chem>CS(=O)(=O)/N=C(\O)c1ccc(-c2ccc(CCNC[C@H](O)c3ccccc3)cc2)cc1CC1CCCCC1</chem>	β 1	ZINC0000409146 51
<chem>CC(C)Cc1cc(-c2ccc(CCNC[C@H](O)c3ccnc3)cc2)ccc1/C(O)=N/S(C)(=O)=O</chem>	β 1	ZINC0000409154 38
<chem>CC(C)Nc1cc(-c2ccc(CCNC[C@H](O)c3ccnc3)cc2)ccc1/C(O)=N/S(C)(=O)=O</chem>	β 1	ZINC0000409190 35
<chem>NS(=O)(=O)c1cccc(CCCCOCCCCCN[C@H](O)c2ccc(O)c(CO)c2)c1</chem>	β 1	ZINC0000409389 15
<chem>O=C(O)c1ccc(-c2ccc3c(c2)C[C@@H](NC[C@H](O)c2cccc(Cl)c2)CC3)nc1</chem>	β 1	ZINC0000409744 36
<chem>O=C(O)c1ccc(Oc2ccc3c(c2)C[C@@H](NC[C@H](O)c2cccc(Cl)c2)CC3)nc1</chem>	β 1	ZINC0000409750 32
<chem>C[C@H](Cc1ccc(-c2ccc(C(=O)O)c(OC3CCCCC3)c2)cc1)NC[C@H](O)c1ccnc1</chem>	β 1	ZINC0000409808 60
<chem>O=S(=O)(NC1CCCCC1)c1cccc(CCCOCCCCCN[C@H](O)c2ccc(O)c(CO)c2)c1</chem>	β 1	ZINC0000428044 59
<chem>O=S(=O)(c1cccc(CCCOCCCCCN[C@H](O)c2ccc(O)c(CO)c2)c1)N1CCCCC1</chem>	β 1	ZINC0000428343 57
<chem>O=C(O)c1cc(NC2CCCCC2)cc(Oc2ccc3c(c2)C[C@@H](NC[C@H](O)c2cccc(Cl)c2)CC3)c1</chem>	β 1	ZINC0000428508 38
<chem>O=C(O)c1cc(NC2CCOCC2)cc(Oc2ccc3c(c2)C[C@@H](NC[C@H](O)c2cccc(Cl)c2)CC3)c1</chem>	β 1	ZINC0000428522 24
<chem>OC[C@@H](CNCCc1ccc(Nc2ccccc2)cc1)COc1ccccc1</chem>	β 1	ZINC0000429212 40
<chem>OC[C@@H](CNCCc1ccc(NC(=S)NCc2ccccc2)cc1)COc1ccccc1</chem>	β 1	ZINC0000429896 89
<chem>OC[C@@H](CNCCc1ccc(NC(=S)Nc2ccc(I)cc2)cc1)COc1ccccc1</chem>	β 1	ZINC0000430105 76
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)COc2ccccc2)cc1)c1ccccc1</chem>	β 1	ZINC0000430107 45

<chem>COC(=O)c1ccc(NC(=S)Nc2ccc(CCNC[C@H](O)COc3ccccc3)cc2)cc1</chem>	β 1	ZINC0000430112 19
<chem>Cc1ccc(NC(=S)Nc2ccc(CCNC[C@H](O)COc3ccccc3)cc2)cc1</chem>	β 1	ZINC0000430119 60
<chem>O[C@@H](CNCCc1ccc(NC(=S)Nc2ccc(Br)cc2)cc1)COc1ccccc1</chem>	β 1	ZINC0000430125 11
<chem>N[C@@H](C(=O)Nc1ccc(CCNC[C@H](O)COc2ccc(O)cc2)cc1)c1ccccc1</chem>	β 1	ZINC0000430133 95
<chem>COc1cccc(NC(=S)Nc2ccc(CCNC[C@H](O)COc3ccccc3)cc2)c1</chem>	β 1	ZINC0000430173 51
<chem>COc1cccc1NC(=S)Nc1ccc(CCNC[C@H](O)COc2ccccc2)cc1</chem>	β 1	ZINC0000430177 20
<chem>O=[N+](O)c1ccccc1NC(=S)Nc1ccc(CCNC[C@H](O)COc2ccccc2)cc1</chem>	β 1	ZINC0000430199 66
<chem>COc1ccc(NC(=S)Nc2ccc(CCNC[C@H](O)COc3ccccc3)cc2)cc1</chem>	β 1	ZINC0000430214 75
<chem>O=C(Nc1ccc(CCNC[C@H](O)COc2ccc(O)cc2)cc1)[C@H](O)c1ccccc1</chem>	β 1	ZINC0000430218 08
<chem>O=C(Nc1ccc(CCNC[C@H](O)COc2ccccc2)cc1)Oc1ccccc1</chem>	β 1	ZINC0000430218 66
<chem>O=S(=O)(Nc1ccccc1)c1ccc(CCNC[C@@H](O)COc2ccccc2)cc1</chem>	β 1	ZINC0000430225 26
<chem>O[C@@H](CNCCc1ccc(NC(=S)Nc2ccccc2Cl)cc1)COc1ccccc1</chem>	β 1	ZINC0000430242 44
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CN[C@@H]3CCCC[C@H]3OCc3ccccc3)c2s1</chem>	β 1	ZINC0000430282 90
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CN[C@H]3CCC[C@H]3C3CCCC3)c2s1</chem>	β 1	ZINC0000430282 94
<chem>O=C(C[C@@H]1C=Nc2ccccc21)Nc1ccc(CCNC[C@H](O)COc2ccc(O)cc2)cc1</chem>	β 1	ZINC0000430588 80
<chem>O=C(Nc1ccc(CCNC[C@H](O)COc2ccccc2)cc1)c1ccccc1</chem>	β 1	ZINC0000430610 85
<chem>O[C@@H](CNCCc1ccc(NC(=S)Nc2ccc(Cl)cc2)cc1)COc1ccccc1</chem>	β 1	ZINC0000430628 80

<chem>NS(=O)(=O)c1ccc(NC(=S)Nc2ccc(CCNC[C@H](O)COc3ccccc3)cc2)cc1</chem>	$\beta 1$	ZINC0000430735 53
<chem>O[C@@H](CNCCc1ccc(NC(=S)NCCc2ccccc2)cc1)COc1ccccc1</chem>	$\beta 1$	ZINC0000430765 77
<chem>O=[N+](O-)[c1ccc(NC(=S)Nc2ccc(CCNC[C@H](O)COc3ccccc3)cc2)c1</chem>	$\beta 1$	ZINC0000430772 19
<chem>O=[N+](O-)[c1ccc(NC(=S)Nc2ccc(CCNC[C@H](O)COc3ccccc3)cc2)cc1</chem>	$\beta 1$	ZINC0000430788 68
<chem>O[C@@H](CNCCc1ccc(NC(=S)NC2CCCCC2)cc1)COc1ccccc1</chem>	$\beta 1$	ZINC0000431182 25
<chem>O[C@@H](CNCCc1ccc(NC(=S)Nc2cccc(Cl)c2)cc1)COc1ccccc1</chem>	$\beta 1$	ZINC0000431203 82
<chem>CC(C)N[C@H]1CCn2c(=O)[nH]c3cccc(c32)[C@H]1O</chem>	$\beta 2$	ZINC0000431638 30
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCCc3cccc(CNCc4ccccc4Cl)c3)c2s1</chem>	$\beta 1$	ZINC0000431714 30
<chem>COc1ccccc1CNCCc1cccc(CCNC[C@H](O)c2ccc(O)c3[nH]c(=O)sc23)c1</chem>	$\beta 1$	ZINC0000431714 35
<chem>N#Cc1ccccc1OC[C@@H](O)CNCCNC(=O)Nc1ccc(OCCCF)cc1</chem>	$\beta 1$	ZINC0000431972 34
<chem>OCc1cc(OC[C@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)ccc1O</chem>	$\beta 1$	ZINC0000431973 10
<chem>COCc1cc(OC[C@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)ccc1O</chem>	$\beta 1$	ZINC0000431973 13
<chem>COCc1cc(OC[C@@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)ccc1O</chem>	$\beta 1$	ZINC0000431973 14
<chem>CCc1cc(OC[C@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)ccc1O</chem>	$\beta 1$	ZINC0000431973 15
<chem>CCc1cc(OC[C@@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)ccc1O</chem>	$\beta 1$	ZINC0000431973 16
<chem>CS(=O)(=O)/N=C(\O)c1ccc(-c2ccc(CCNC[C@H](O)c3ccnc3)cc2)cc1OC1CCCCC1</chem>	$\beta 1$	ZINC0000443054 91
<chem>CS(=O)(=O)/N=C(\O)c1ccc(-c2ccc(CCNC[C@H](O)c3cnccc3N)cc2)cc1OC1CCCCC1</chem>	$\beta 1$	ZINC0000443061 87

<chem>O=C(Cc1nccn1Cc1ccc(Br)cc1)Nc1ccc(CCNC[C@H](O)COc2ccccc2)cc1</chem>	$\beta 1$	ZINC0000444054 39
<chem>O=C(Cc1nccn1Cc1ccc2ccccc2c1)Nc1ccc(CCNC[C@H](O)COc2ccccc2)cc1</chem>	$\beta 1$	ZINC0000444054 43
<chem>CS(=O)(=O)/N=C(\O)c1ccc(-c2ccc(CCNC[C@H](O)c3ccccc3)cc2)cc1OC1CCCCC1</chem>	$\beta 1$	ZINC0000444309 10
<chem>CS(=O)(=O)/N=C(\O)c1ccc(-c2ccc(CCNC[C@H](O)c3ccccc3)cc2)cc1SC1CCCC1</chem>	$\beta 1$	ZINC0000444309 12
<chem>FC(F)(F)c1ccc2c(N3CCNCC3)ccnc2c1</chem>	$\beta 2$	ZINC0000446287 43
<chem>CCc1ccc(CC(C)(C)NC[C@@H](O)c2ccc(O)c(CO)c2)cc1</chem>	$\beta 2$	ZINC0000452449 12
<chem>Cc1ccccc1CC(C)(C)NC[C@@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 1$	ZINC0000452449 96
<chem>CC(C)(Cc1cccc(C(F)(F)F)c1)NC[C@@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 1$	ZINC0000452450 99
<chem>CC(C)(Cc1ccc(NC(=O)CCCNC(=N)N)cc1)NC[C@@H](O)c1cc(O)cc2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000452451 89
<chem>CCc1ccc(CC(C)(C)NC[C@@H](O)c2cc(Cl)c(N)c(Cl)c2)cc1</chem>	$\beta 1$	ZINC0000452452 20
<chem>CC(C)(Cc1cccc(C(=O)O)c1)NC[C@@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000452454 97
<chem>CCc1ccc(CC(C)(C)NC[C@@H](O)c2ccc(O)c3c2OCC(=O)N3)cc1</chem>	$\beta 1$	ZINC0000452455 10
<chem>CC(C)(Cc1ccc(C(C)(C)C)cc1)NC[C@@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000452530 22
<chem>CC(C)(Cc1ccc(-c2ccccc2)cc1)NC[C@@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000452530 26
<chem>CC(C)(Cc1cc(F)cc(F)c1)NC[C@@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000452531 99
<chem>Cc1cccc(CC(C)(C)NC[C@@H](O)c2ccc(O)c3c2OCC(=O)N3)c1</chem>	$\beta 1$	ZINC0000452543 29
<chem>CC(C)(Cc1ccc(O)cc1)NC[C@@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000452549 58

<chem>CC(C)(Cc1cccc(C(F)(F)F)c1)NC[C@@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000452549 62
<chem>CC(C)c1ccc(CC(C)(C)NC[C@@H](O)c2cc(Cl)c(N)c(Cl)c2)cc1</chem>	$\beta 1$	ZINC0000452552 65
<chem>CC(C)(Cc1cc(F)cc(F)c1)NC[C@@H](O)c1cc(Cl)c(N)c(Cl)c1</chem>	$\beta 1$	ZINC0000452552 98
<chem>CC(C)(Cc1ccc(NC(=O)CCCN)cc1)NC[C@@H](O)c1cc(O)cc2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000452571 72
<chem>CC(C)(Cc1ccc(NC(=O)CCCNCC(=O)CCN)cc1)NC[C@@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000452584 91
<chem>CC(C)(Cc1cccc1)NC[C@@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 2$	ZINC0000452585 48
<chem>CC(C)(Cc1cccc1)NC[C@@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000452589 35
<chem>CC(C)(Cc1ccc(OC(F)(F)F)cc1)NC[C@@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000452612 40
<chem>CC(C)(Cc1ccc(NC(=O)CCCN)cc1)NC[C@@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000452889 04
<chem>CC(C)(Cc1ccc(NC(=O)CCCNCC(=O)N)cc1)NC[C@@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000452987 34
<chem>CC(C)c1ccc(CC(C)(C)NC[C@@H](O)c2ccc(O)c3c2OCC(=O)N3)cc1</chem>	$\beta 1$	ZINC0000452989 88
<chem>CC(C)(Cc1ccc(C(=O)O)cc1)NC[C@@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000453004 04
<chem>Cc1cccc1CC(C)(C)NC[C@@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000453024 47
<chem>CC(C)(Cc1ccc(NC(=O)CCCNCC(=O)CN)cc1)NC[C@@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000453147 28
<chem>CCOC(=O)CCc1ccc(OC[C@H](O)CNC(C)(C)Cc2ccc3ccccc3c2)c(C#N)c1</chem>	$\beta 2$	ZINC0000453157 21
<chem>CC(C)(Cc1ccc(C(F)(F)F)cc1)NC[C@@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000453176 37
<chem>CC(C)(Cc1cccc1)NC[C@@H](O)c1cc(O)cc2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000453520 68

<chem>CC(C)(Cc1ccc(-c2ccccc2)cc1)NC[C@@H](O)c1cc(O)cc2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000453676 66
<chem>Cc1cccc(CC(C)(C)NC[C@@H](O)c2cc(O)cc3c2OCC(=O)N3)c1</chem>	$\beta 1$	ZINC0000453677 43
<chem>CC(C)(Cc1ccccc1C(F)(F)F)NC[C@@H](O)c1cc(O)cc2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000453700 86
<chem>Cc1ccccc1CC(C)(C)NC[C@@H](O)c1cc(O)cc2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000453701 46
<chem>CC(C)(Cc1cc(F)cc(F)c1)NC[C@@H](O)c1cc(O)cc2c1OCC(=O)N2</chem>	$\beta 2$	ZINC0000453707 10
<chem>CC(C)(Cc1ccc(OC(F)(F)F)cc1)NC[C@@H](O)c1cc(O)cc2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000453715 54
<chem>CC(C)(Cc1cccc(C(F)(F)F)c1)NC[C@@H](O)c1cc(O)cc2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000453869 82
<chem>COc1cccc(CC(C)(C)NC[C@@H](O)c2cc(O)cc3c2OCC(=O)N3)c1</chem>	$\beta 1$	ZINC0000453886 10
<chem>CC(C)(Cc1ccc(C(C)(C)C)cc1)NC[C@@H](O)c1cc(O)cc2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000453888 49
<chem>COc1ccc(CC(C)(C)NC[C@H](O)COc2ccccc3[nH]c(=O)[nH]c23)cc1</chem>	$\beta 1$	ZINC0000454846 10
<chem>CC(C)Sc1cc(-c2ccc(CCNC[C@H](O)c3ccccc3)cc2)ccc1/C(O)=N/S(C)(=O)=O</chem>	$\beta 1$	ZINC0000455059 95
<chem>O=C(Nc1ccc(CCNC[C@H](O)c2ccccc2)cc1)c1ccccc1COc1ccccc1</chem>	$\beta 1$	ZINC0000490136 59
<chem>O=C(Nc1ccc(CCNC[C@H](O)c2ccccc2)cc1)c1ccccc1CCn1ccccc1</chem>	$\beta 2$	ZINC0000490137 29
<chem>O=C(Nc1ccc(CCNC[C@H](O)c2ccccc2)cc1)c1cccc(-c2ncc[nH]2)c1</chem>	$\beta 1$	ZINC0000490138 72
<chem>O=C(Nc1ccc(CCNC[C@H](O)c2ccccc2)cc1)c1ccccc1CCc1ccccc1</chem>	$\beta 1$	ZINC0000490140 76
<chem>O=C(Nc1ccc(CCNC[C@H](O)c2ccccc2)cc1)c1ccc(CCc2ccccc2)cc1</chem>	$\beta 1$	ZINC0000490152 12
<chem>O=C(Nc1ccc(CCNC[C@H](O)c2ccccc2)cc1)c1cccc(CCc2ccccc2)c1</chem>	$\beta 1$	ZINC0000490152 43

<chem>O=C(c1cccc1)C1CCN(C[C@H](O)COc2cccc3[nH]c4cccc4c23)CC1</chem>	β 1	ZINC0000490346 13
<chem>O=C(c1cccc1)C1CCN(C[C@@H](O)COc2cccc3[nH]c4cccc4c23)CC1</chem>	β 1	ZINC0000490346 14
<chem>COc1ccc(C(=O)C2CCN(C[C@H](O)COc3cccc4[nH]c5cccc5c34)CC2)cc1</chem>	β 1	ZINC0000490348 98
<chem>COc1ccc(C(=O)C2CCN(C[C@@H](O)COc3cccc4[nH]c5cccc5c34)CC2)cc1</chem>	β 1	ZINC0000490349 00
<chem>O=C(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1cccc1-c1nc2cccc2s1</chem>	β 1	ZINC0000490349 74
<chem>O=C(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1cccc1C1CCCC1</chem>	β 1	ZINC0000490349 76
<chem>O=C(Cc1nc(-c2cccc2)cs1)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	β 1	ZINC0000490350 04
<chem>C=CCc1cccc1OC[C@H](O)CN1CCC(CN2C(=O)CCCC2=O)CC1</chem>	β 1	ZINC0000490350 78
<chem>C=CCc1cccc1OC[C@@H](O)CN1CCC(CN2C(=O)CCCC2=O)CC1</chem>	β 1	ZINC0000490350 80
<chem>COc1ccc(CC2CCN(C[C@H](O)COc3cccc4[nH]c5cccc5c34)CC2)cc1</chem>	β 1	ZINC0000490351 94
<chem>COc1ccc(CC2CCN(C[C@@H](O)COc3cccc4[nH]c5cccc5c34)CC2)cc1</chem>	β 1	ZINC0000490351 96
<chem>OCc1cc([C@@H](O)CNCCCCCOCCOCc2cc(Cl)ccc2Cl)ccc1O</chem>	β 1	ZINC0000490353 33
<chem>CC(C)c1cccc1OC[C@H](O)CN1CCC(CN2C(=O)CCCC2=O)CC1</chem>	β 1	ZINC0000490353 56
<chem>CC(C)c1cccc1OC[C@@H](O)CN1CCC(CN2C(=O)CCCC2=O)CC1</chem>	β 1	ZINC0000490353 58
<chem>C=CCc1cccc1OC[C@H](O)CN1CCC(CN2C(=O)c3cccc4cc(O)cc(c34)C2=O)CC1</chem>	β 1	ZINC0000490353 60
<chem>C=CCc1cccc1OC[C@@H](O)CN1CCC(CN2C(=O)c3cccc4cc(O)cc(c34)C2=O)CC1</chem>	β 1	ZINC0000490353 62
<chem>Cc1sc2ncn(CC(=O)Nc3ccc(CCNC[C@H](O)c4ccnc4)cc3)c(=O)c2c1C</chem>	β 1	ZINC0000490355 80

<chem>Cc1ccc(COCCOCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)cc1</chem>	$\beta 2$	ZINC0000490356 17
<chem>C=CCc1ccccc1OC[C@H](O)CN1CCC(CN2C(=O)c3ccccc3C2=O)CC1</chem>	$\beta 1$	ZINC0000490356 53
<chem>C=CCc1ccccc1OC[C@@H](O)CN1CCC(CN2C(=O)c3ccccc3C2=O)CC1</chem>	$\beta 1$	ZINC0000490356 55
<chem>OCc1cc([C@@H](O)CNCCCCCOCCOCc2ccc(Cl)cc2)ccc1O</chem>	$\beta 2$	ZINC0000490359 38
<chem>CC(C)c1ccccc1OC[C@H](O)CN1CCC(CN2C(=O)c3ccccc3C2=O)CC1</chem>	$\beta 1$	ZINC0000490359 92
<chem>CC(C)c1ccccc1OC[C@@H](O)CN1CCC(CN2C(=O)c3ccccc3C2=O)CC1</chem>	$\beta 1$	ZINC0000490359 94
<chem>OCCOCCCCCNC[C@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 2$	ZINC0000490364 59
<chem>O=C1c2cccc3cccc(c23)C(=O)N1CC1CCN(C[C@H](O)COc2ccc3[nH]ccc3c2)CC1</chem>	$\beta 1$	ZINC0000490365 11
<chem>O=C1c2cccc3cccc(c23)C(=O)N1CC1CCN(C[C@@H](O)COc2ccc3[nH]ccc3c2)CC1</chem>	$\beta 1$	ZINC0000490365 13
<chem>C=CCc1ccccc1OC[C@H](O)CN1CCC(N2C(=O)c3cccc4cccc(c34)C2=O)CC1</chem>	$\beta 1$	ZINC0000490370 66
<chem>C=CCc1ccccc1OC[C@@H](O)CN1CCC(N2C(=O)c3cccc4cccc(c34)C2=O)CC1</chem>	$\beta 1$	ZINC0000490370 68
<chem>COc1cc2c3c(cccc3c1)C(=O)N(CC1CCN(C[C@@H](O)COc3ccccc3C(C)C)CC1)C2=O</chem>	$\beta 1$	ZINC0000490370 91
<chem>COc1cc2c3c(cccc3c1)C(=O)N(CC1CCN(C[C@H](O)COc3ccccc3C(C)C)CC1)C2=O</chem>	$\beta 1$	ZINC0000490370 93
<chem>C=CCc1ccccc1OC[C@@H](O)CNC1CCN(C)CC1</chem>	$\beta 1$	ZINC0000490370 95
<chem>C=CCc1ccccc1OC[C@H](O)CNC1CCN(C)CC1</chem>	$\beta 1$	ZINC0000490370 97
<chem>CC(C)c1ccccc1OC[C@H](O)CNC1CCN(C)CC1</chem>	$\beta 1$	ZINC0000490370 99
<chem>CC(C)c1ccccc1OC[C@@H](O)CNC1CCN(C)CC1</chem>	$\beta 1$	ZINC0000490371 01

<chem>C=CCc1cccc1OC[C@@H](O)CN1CCC(CN2C(=O)c3cccc4cc(OC)cc(c34)C2=O)CC1</chem>	$\beta 1$	ZINC0000490373 92
<chem>C=CCc1cccc1OC[C@H](O)CN1CCC(CN2C(=O)c3cccc4cc(OC)cc(c34)C2=O)CC1</chem>	$\beta 1$	ZINC0000490373 93
<chem>O=C1c2cccc3cccc(c23)C(=O)N1CC1CCN(C[C@H](O)COc2cccc3[nH]ccc23)CC1</chem>	$\beta 1$	ZINC0000490376 73
<chem>O=C1c2cccc3cccc(c23)C(=O)N1CC1CCN(C[C@@H](O)COc2cccc3[nH]ccc23)CC1</chem>	$\beta 1$	ZINC0000490376 75
<chem>O=C(CN1C[C@H](c2ccccc2)CC1=O)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000490462 94
<chem>O=C(CN1C[C@@H](c2ccccc2)CC1=O)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000490463 00
<chem>O=C(Cc1n[nH]c2ccccc12)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000490474 98
<chem>NC(=O)Nc1cccc(COCCOCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)c1</chem>	$\beta 1$	ZINC0000490476 10
<chem>O=C(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)OCc1nc2ccccc2[nH]1</chem>	$\beta 1$	ZINC0000490487 38
<chem>O=C(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1nc2ccccc2[nH]1</chem>	$\beta 1$	ZINC0000490491 54
<chem>O=C(Cn1nc(-c2ccccc2)cc1-c1ccccc1)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 2$	ZINC0000490494 36
<chem>O[C@H](COc1cccc2[nH]c3ccccc3c12)CN1CCC(Cc2ccccc2)CC1</chem>	$\beta 1$	ZINC0000490507 04
<chem>O[C@@H](COc1cccc2[nH]c3ccccc3c12)CN1CCC(Cc2ccccc2)CC1</chem>	$\beta 1$	ZINC0000490507 08
<chem>O=C(c1ccc(F)cc1)C1CCN(C[C@@H](O)COc2cccc3[nH]c4ccccc4c23)CC1</chem>	$\beta 1$	ZINC0000490535 42
<chem>OCc1cc([C@@H](O)CNCCCCCOCCOCc2cccc3ccccc23)ccc1O</chem>	$\beta 1$	ZINC0000490538 92
<chem>O=C(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccccc2ccnn12</chem>	$\beta 2$	ZINC0000490549 08
<chem>O=C(Cc1nc2ccccc2o1)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000490664 07

<chem>O=C(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1cccc1N1CCCC1</chem>	$\beta 2$	ZINC0000490667 01
<chem>O=C(Cn1cc2ccccc2n1)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000490671 05
<chem>O=C(Cn1nc2ccccc2n1)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000490671 07
<chem>CNc1nc(CC(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cs1</chem>	$\beta 1$	ZINC0000490672 35
<chem>O=C(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1cccc(-c2ccccc2)c1</chem>	$\beta 1$	ZINC0000490674 00
<chem>Nc1nc(CC(=O)Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)cs1</chem>	$\beta 1$	ZINC0000490710 79
<chem>O=C(Cc1csc(-c2ccccc2)n1)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000490710 95
<chem>O=C(Cc1nc2ccccc2[nH]1)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 2$	ZINC0000490894 02
<chem>O=C(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1cccc1-c1nc2ccccc2[nH]1</chem>	$\beta 1$	ZINC0000490894 91
<chem>O=C(Cn1c(=O)nc2ccccc21)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000490896 99
<chem>O=C(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1cccc(Cc2ccccc2)c1</chem>	$\beta 2$	ZINC0000490897 29
<chem>OC[C@H](COc1cccc2[nH]c3ccccc3c12)CN1CCC(Cc2ccccc2)CC1</chem>	$\beta 1$	ZINC0000490900 65
<chem>OC[C@H](COc1cccc2[nH]c3ccccc3c12)CN1CCC(Cc2ccccc2)CC1</chem>	$\beta 1$	ZINC0000490900 66
<chem>OCc1cc([C@@H](O)CNCCCCCOCCOCc2ccccc2)ccc1O</chem>	$\beta 1$	ZINC0000491096 53
<chem>O=C(Cc1cccc1)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000491111 87
<chem>CC(C)c1cccc1OC[C@H](O)CN1CCC(N2C(=O)c3cccc4cccc(c34)C2=O)CC1</chem>	$\beta 1$	ZINC0000491122 00
<chem>CC(C)c1cccc1OC[C@@H](O)CN1CCC(N2C(=O)c3cccc4cccc(c34)C2=O)CC1</chem>	$\beta 1$	ZINC0000491122 01

<chem>OCc1cc([C@@H](O)CNCCCCCOCCOCc2cccc(O)c2)ccc1O</chem>	$\beta 1$	ZINC0000491132 12
<chem>O=C(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)c1ccc(-c2ccccc2)cc1</chem>	$\beta 1$	ZINC0000491246 01
<chem>O=C(Cn1cnc2ccccc2c1=O)Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1</chem>	$\beta 1$	ZINC0000495257 68
<chem>CC(C)(Cc1ccc(NC(=O)CCCNC(=O)[C@@H](N)CCCN)cc1)NC[C@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000496779 86
<chem>CC(C)(Cc1ccc(NC(=O)CCCNC(=O)[C@H](N)CCCN)cc1)NC[C@@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000496779 89
<chem>CC(C)(Cc1ccc(NC(=O)CCCNC(=O)[C@@H](N)CCCN)cc1)NC[C@@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000496779 92
<chem>CN1CCN(CC(=O)NCCCC(=O)Nc2ccc(CC(C)(C)NC[C@@H](O)c3ccc(O)c4c3OCC(=O)N4)cc2)CC1</chem>	$\beta 1$	ZINC0000496948 14
<chem>CN(C)CC(=O)NCCCC(=O)Nc1ccc(CC(C)(C)NC[C@@H](O)c2ccc(O)c3c2OCC(=O)N3)cc1</chem>	$\beta 1$	ZINC0000497094 96
<chem>CC(C)(Cc1ccc(NC(=O)CCCNCCCS(=O)(=O)O)cc1)NC[C@@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000497451 39
<chem>CC(C)(Cc1ccc(NC(=O)CCCNC(=O)C[N+](C)(C)C)cc1)NC[C@H](O)c1cc(O)cc2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000497453 37
<chem>CC(C)(Cc1ccc(NC(=O)CCCNC(=O)C[N+](C)(C)C)cc1)NC[C@@H](O)c1cc(O)cc2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000497453 39
<chem>CC(C)(Cc1ccc(NC(=O)CCCNC(=O)C[N+](C)(C)C)cc1)NC[C@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000497454 88
<chem>CC(C)(Cc1ccc(NC(=O)CCCNC(=O)C[N+](C)(C)C)cc1)NC[C@@H](O)c1ccc(O)c2c1OCC(=O)N2</chem>	$\beta 1$	ZINC0000497454 90
<chem>O=C1c2cccc3cccc(c23)C(=O)N1CC1CCN(C[C@@H](O)COc2cccc3[nH]c4cccc4c23)CC1</chem>	$\beta 1$	ZINC0000497755 93
<chem>O=C1c2cccc3cccc(c23)C(=O)N1CC1CCN(C[C@H](O)COc2cccc3[nH]c4cccc4c23)CC1</chem>	$\beta 1$	ZINC0000497755 96
<chem>COc1cc2c3c(cccc3c1)C(=O)N(CC1CCN(C[C@H](O)COc3cccc4[nH]c5cccc5c34)CC1)C2=O</chem>	$\beta 1$	ZINC0000497756 48
<chem>COc1cc2c3c(cccc3c1)C(=O)N(CC1CCN(C[C@@H](O)COc3cccc4[nH]c5cccc5c34)CC1)C2=O</chem>	$\beta 1$	ZINC0000497756 50

<chem>O=C1c2cccc3cc(O)cc(c23)C(=O)N1CC1CCN(C[C@@H](O)COc2cccc3[nH]c4cccc4c23)CC1</chem>	β 1	ZINC0000497805 50
<chem>O=C1c2cccc3cccc(c23)C(=O)N1C1CCN(C[C@@H](O)COc2cccc3[nH]c4cccc4c23)CC1</chem>	β 1	ZINC0000497859 13
<chem>O=C1c2cccc3cccc(c23)C(=O)N1C1CCN(C[C@H](O)COc2cccc3[nH]c4cccc4c23)CC1</chem>	β 1	ZINC0000497859 14
<chem>CS(=O)(=O)Nc1cc(OC[C@@H](O)CNCCc2ccc(NC3CCN(C(=O)NCc4cc(F)ccc4F)CC3)cc2)ccc1O</chem>	β 1	ZINC0000498648 95
<chem>CS(=O)(=O)Nc1ccc(C(=O)NC[C@@H]2CN(c3cccc3)CCN2)cc1</chem>	β 1	ZINC0000499254 27
<chem>CS(=O)(=O)Nc1ccc(C(=O)NC[C@H]2CN(c3cccc3)CCN2)cc1</chem>	β 1	ZINC0000499254 28
<chem>CS(=O)(=O)Nc1ccc(NC[C@@H]2CN(c3cccc3)CCN2)cc1</chem>	β 1	ZINC0000499254 29
<chem>CS(=O)(=O)Nc1ccc(NC[C@H]2CN(c3cccc3)CCN2)cc1</chem>	β 1	ZINC0000499254 30
<chem>COc1cccc(N2CCN[C@H](CNC(=O)c3ccc(NS(C)(=O)=O)cc3)C2)c1</chem>	β 1	ZINC0000499254 53
<chem>COc1cccc(N2CCN[C@@H](CNC(=O)c3ccc(NS(C)(=O)=O)cc3)C2)c1</chem>	β 1	ZINC0000499254 54
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNC2CCN(c3ccc(C[C@H]4SC(=O)NC4=O)cc3)CC2)ccc1O</chem>	β 1	ZINC0000499254 55
<chem>CS(=O)(=O)Nc1cc([C@H](O)CNC2CCN(c3ccc(C[C@@H]4SC(=O)NC4=O)cc3)CC2)ccc1O</chem>	β 1	ZINC0000499254 56
<chem>O[C@@H](CNCCOc1ccc(-c2coen2)cc1)c1ccnc1</chem>	β 1	ZINC0000499470 18
<chem>Cc1nc(-c2ccc(OCCNC[C@H](O)c3ccnc3)cc2)co1</chem>	β 1	ZINC0000499496 20
<chem>COCc1nc(-c2ccc(OCCNC[C@H](O)c3ccnc3)cc2)co1</chem>	β 1	ZINC0000499496 73
<chem>CN1C[C@H](C(=O)N[C@]2(C)O[C@@]3(O)[C@@H]4CCCN4C(=O)[C@H](Cc4cccc4)N3C2=O)C=C2c3cccc4[nH]c c(c34)C[C@H]21</chem>	β 1	ZINC0000529557 54
<chem>CC(C)C[C@H]1C(=O)N2CCC[C@H]2[C@]2(O)O[C@](NC(=O)[C@@H]3C=C4c5cccc6[nH]c(Br)c(c56)C[C@H]4N(C))C3)(C(C)C)C(=O)N12</chem>	β 1	ZINC0000536831 51

<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNC3CCCCC3)c2s1</chem>	β 1	ZINC0000585753 53
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCCCCc3ccccc3)c2s1</chem>	β 1	ZINC0000585756 01
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CN[C@@H]3CCC[C@H]3OCc3ccccc3)c2s1</chem>	β 1	ZINC0000585756 05
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CN[C@H]3CCCC[C@@H]3OCc3ccccc3)c2s1</chem>	β 1	ZINC0000585757 98
<chem>C[C@@H](NC[C@H](O)c1ccc(O)c2[nH]c(=O)sc12)c1ccc2ccccc2c1</chem>	β 1	ZINC0000585810 66
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CN[C@@H]3CCC[C@@H]3C3CCCC3)c2s1</chem>	β 1	ZINC0000585816 89
<chem>CC1(C)[C@@H]2CC[C@@]1(C)[C@@H](NC[C@H](O)c1ccc(O)c3[nH]c(=O)sc13)C2</chem>	β 1	ZINC0000585816 92
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CN[C@@H]3CCCc4ccccc43)c2s1</chem>	β 1	ZINC0000585819 44
<chem>C[C@H](NC[C@H](O)c1ccc(O)c2[nH]c(=O)sc12)c1ccc2ccccc2c1</chem>	β 1	ZINC0000585819 95
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCCc3ccccc3)c2s1</chem>	β 1	ZINC0000585823 34
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CN[C@H]3CCCc4ccccc43)c2s1</chem>	β 1	ZINC0000585824 78
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CN[C@@H]3CCC[C@H]3C3CCCC3)c2s1</chem>	β 1	ZINC0000585830 31
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCCOc3ccccc3)c2s1</chem>	β 1	ZINC0000585832 35
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCCSc3ccc(Cl)cc3)c2s1</chem>	β 1	ZINC0000585832 56
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CN[C@H]3CCC[C@H]3C3CCCC3)c2s1</chem>	β 1	ZINC0000585832 92
<chem>C[C@@H](NC[C@H](O)c1ccc(O)c2[nH]c(=O)sc12)C1CCCC1</chem>	β 1	ZINC0000585836 60
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCC34CC5CC(CC(C5)C3)C4)c2s1</chem>	β 1	ZINC0000585839 59

<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCCC3ccccc3)c2s1</chem>	$\beta 1$	ZINC0000585839 64
<chem>C[C@H](NC[C@H](O)c1ccc(O)c2[nH]c(=O)sc12)C1CCCCC1</chem>	$\beta 1$	ZINC0000585905 29
<chem>CC(C)(C)CC(C)(C)NC[C@H](O)c1ccc(O)c2[nH]c(=O)sc12</chem>	$\beta 1$	ZINC0000585914 37
<chem>CCCCN(CCCC)CCNC[C@H](O)c1ccc(O)c2[nH]c(=O)sc12</chem>	$\beta 1$	ZINC0000585926 61
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CN[C@@H]3CCCC[C@@H]3C3CCCCC3)c2s1</chem>	$\beta 1$	ZINC0000585928 44
<chem>CN(CCCNC[C@H](O)c1ccc(O)c2[nH]c(=O)sc12)c1ccccc1</chem>	$\beta 1$	ZINC0000586040 30
<chem>CCC(CC)CNC[C@H](O)c1ccc(O)c2[nH]c(=O)sc12</chem>	$\beta 1$	ZINC0000586040 97
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNC3CCN(CCN4CCCCC4)CC3)c2s1</chem>	$\beta 1$	ZINC0000586391 74
<chem>Cc1onc(-c2ccccc2)c1CNC[C@H](O)c1ccc(O)c2[nH]c(=O)sc12</chem>	$\beta 1$	ZINC0000586497 97
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CN[C@@H]3CCC[C@@H]3C3CCCCC3)c2s1</chem>	$\beta 1$	ZINC0000622249 19
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CN[C@@H]3CCC[C@H]3C3CCCCC3)c2s1</chem>	$\beta 1$	ZINC0000622249 27
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CN[C@H]3CCCC[C@@H]3C3CCCCC3)c2s1</chem>	$\beta 1$	ZINC0000622249 28
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CN[C@@H]3CCCC[C@H]3C3CCCCC3)c2s1</chem>	$\beta 1$	ZINC0000622249 32
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CN[C@H]3CCCC[C@H]3C3CCCCC3)c2s1</chem>	$\beta 1$	ZINC0000622249 36
<chem>O[C@@H](CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1)COc1cccc(OC(F)(F)F)c1</chem>	$\beta 1$	ZINC0000645135 51
<chem>O[C@H](CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1)COc1cccc(OC(F)(F)F)c1</chem>	$\beta 1$	ZINC0000645135 54
<chem>OCc1cc(OC[C@@H](O)CNC2CCN(c3ncnc4scc(-c5cccs5)c34)CC2)ccc1O</chem>	$\beta 1$	ZINC0000645135 57

<chem>OCc1cc(OC[C@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)ccc1O</chem>	$\beta 1$	ZINC0000645135 59
<chem>O[C@@H](CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1)COc1ccccc1</chem>	$\beta 1$	ZINC0000645273 92
<chem>O[C@H](CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1)COc1ccccc1</chem>	$\beta 1$	ZINC0000645273 93
<chem>O[C@H](CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1)COc1ccccc1</chem>	$\beta 1$	ZINC0000645392 22
<chem>O[C@@H](CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1)COc1ccccc1</chem>	$\beta 1$	ZINC0000645392 23
<chem>O=C(O)c1ccc(O)cc1OC[C@@H](O)CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1</chem>	$\beta 2$	ZINC0000645394 19
<chem>O=C(O)c1ccc(O)cc1OC[C@H](O)CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1</chem>	$\beta 2$	ZINC0000645394 20
<chem>Oc1ccc(OC[C@@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)cc1O</chem>	$\beta 1$	ZINC0000645394 21
<chem>Oc1ccc(OC[C@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)cc1O</chem>	$\beta 1$	ZINC0000645394 22
<chem>OCc1ccc(OC[C@@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)cc1O</chem>	$\beta 2$	ZINC0000645395 42
<chem>OCc1ccc(OC[C@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)cc1O</chem>	$\beta 2$	ZINC0000645395 44
<chem>O[C@@H](CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1)COc1ccc(F)cc1</chem>	$\beta 1$	ZINC0000645396 12
<chem>O[C@H](CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1)COc1ccc(F)cc1</chem>	$\beta 1$	ZINC0000645396 14
<chem>O=C(c1cccc(OC[C@@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)c1)N1CCOCC1</chem>	$\beta 1$	ZINC0000645397 64
<chem>O=C(c1cccc(OC[C@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)c1)N1CCOCC1</chem>	$\beta 1$	ZINC0000645397 67
<chem>C=CCc1ccccc1OC[C@H](O)CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1</chem>	$\beta 1$	ZINC0000645397 74
<chem>C=CCc1ccccc1OC[C@@H](O)CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1</chem>	$\beta 1$	ZINC0000645397 75

<chem>OCc1cc(OC[C@H](O)CNC2CCN(c3ncnc4secc34)CC2)ccc1O</chem>	$\beta 1$	ZINC0000645397 76
<chem>OCc1cc(OC[C@@H](O)CNC2CCN(c3ncnc4secc34)CC2)ccc1O</chem>	$\beta 1$	ZINC0000645397 77
<chem>OCc1cccc(OC[C@H](O)CNC2CCN(c3ncnc4sec(-c5ccccc5)c34)CC2)c1</chem>	$\beta 2$	ZINC0000645398 08
<chem>O[C@H](CNC1CCN(c2ncnc3ccsc23)CC1)COc1ccccc1</chem>	$\beta 1$	ZINC0000645399 39
<chem>O[C@@H](CNC1CCN(c2ncnc3ccsc23)CC1)COc1ccccc1</chem>	$\beta 1$	ZINC0000645399 40
<chem>N#Cc1cccc(OC[C@@H](O)CNC2CCN(c3ncnc4sec(-c5ccccc5)c34)CC2)c1</chem>	$\beta 1$	ZINC0000645399 43
<chem>N#Cc1cccc(OC[C@H](O)CNC2CCN(c3ncnc4sec(-c5ccccc5)c34)CC2)c1</chem>	$\beta 1$	ZINC0000645399 44
<chem>Oc1ccc(OC[C@H](O)CNC2CCN(c3ncnc4ccsc34)CC2)cc1</chem>	$\beta 1$	ZINC0000645399 45
<chem>Oc1ccc(OC[C@@H](O)CNC2CCN(c3ncnc4ccsc34)CC2)cc1</chem>	$\beta 1$	ZINC0000645399 46
<chem>OCc1cc(OC[C@H](O)CNC2CCN(c3ncnc4ccsc34)CC2)ccc1O</chem>	$\beta 1$	ZINC0000645399 47
<chem>OCc1cc(OC[C@@H](O)CNC2CCN(c3ncnc4ccsc34)CC2)ccc1O</chem>	$\beta 1$	ZINC0000645399 48
<chem>Cc1csc2ncnc(N3CCC(NC[C@@H](O)COc4ccc(O)cc4)CC3)c12</chem>	$\beta 1$	ZINC0000645400 65
<chem>OCc1ccc(OC[C@@H](O)CNC2CCN(c3ncnc4sec(-c5ccccc5)c34)CC2)cc1</chem>	$\beta 2$	ZINC0000645400 90
<chem>OCc1ccc(OC[C@H](O)CNC2CCN(c3ncnc4sec(-c5ccccc5)c34)CC2)cc1</chem>	$\beta 2$	ZINC0000645400 92
<chem>CCc1ccc(OC[C@H](O)CNC2CCN(c3ncnc4sec(-c5ccccc5)c34)CC2)cc1</chem>	$\beta 1$	ZINC0000645402 31
<chem>CCc1ccc(OC[C@@H](O)CNC2CCN(c3ncnc4sec(-c5ccccc5)c34)CC2)cc1</chem>	$\beta 1$	ZINC0000645402 32
<chem>CC(=O)Nc1cccc(OC[C@H](O)CNC2CCN(c3ncnc4sec(-c5ccccc5)c34)CC2)c1</chem>	$\beta 1$	ZINC0000645404 60

<chem>CC(=O)Nc1cccc(OC[C@@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)c1</chem>	β 1	ZINC0000645404 62
<chem>CC(C)c1cccc1OC[C@H](O)CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1</chem>	β 1	ZINC0000645405 06
<chem>CC(C)c1cccc1OC[C@@H](O)CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1</chem>	β 1	ZINC0000645405 09
<chem>Oc1cccc(OC[C@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)c1</chem>	β 1	ZINC0000645407 68
<chem>Oc1ccc(OC[C@@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)cc1</chem>	β 1	ZINC0000645407 70
<chem>Oc1ccc(OC[C@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)cc1</chem>	β 1	ZINC0000645407 71
<chem>Cc1c(-c2ccccc2)sc2ncnc(N3CCC(NC[C@H](O)COc4ccccc4)CC3)c12</chem>	β 1	ZINC0000645409 22
<chem>Cc1c(-c2ccccc2)sc2ncnc(N3CCC(NC[C@@H](O)COc4ccccc4)CC3)c12</chem>	β 1	ZINC0000645409 23
<chem>O[C@H](CNC1CCN(c2ncnc3scc(-c4ccc(F)cc4)c23)CC1)COc1cccc1</chem>	β 1	ZINC0000645410 47
<chem>Oc1ccc(OC[C@H](O)CNC2CCN(c3ncnc4scc(-c5ccc(F)cc5)c34)CC2)cc1</chem>	β 1	ZINC0000645410 53
<chem>COc1cccc1OC[C@@H](O)CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1</chem>	β 1	ZINC0000645411 97
<chem>COc1cccc(OC[C@@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)c1</chem>	β 1	ZINC0000645412 02
<chem>Oc1ccc(OC[C@H](O)CNC2CCN(c3ncnc4scc(-c5cccs5)c34)CC2)cc1</chem>	β 1	ZINC0000645483 28
<chem>Cc1csc2ncnc(N3CCC(NC[C@H](O)COc4ccccc4)CC3)c12</chem>	β 1	ZINC0000645484 12
<chem>Cc1csc2ncnc(N3CCC(NC[C@@H](O)COc4ccccc4)CC3)c12</chem>	β 1	ZINC0000645484 13
<chem>OCc1cc(O)ccc1OC[C@@H](O)CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1</chem>	β 1	ZINC0000645486 00
<chem>OCc1cc(O)ccc1OC[C@H](O)CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1</chem>	β 1	ZINC0000645486 01

<chem>O=C(O)c1cc(OC[C@@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)ccc1O</chem>	β 1	ZINC0000645486 03
<chem>O=C(O)c1cc(OC[C@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)ccc1O</chem>	β 1	ZINC0000645486 04
<chem>O[C@H](CNC1CCN(c2ncnc3sccc23)CC1)COc1ccccc1</chem>	β 1	ZINC0000645486 66
<chem>CNC(=O)c1cccc(OC[C@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)c1</chem>	β 1	ZINC0000645487 67
<chem>CNC(=O)c1cccc(OC[C@@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)c1</chem>	β 1	ZINC0000645487 68
<chem>Oc1ccc(OC[C@H](O)CNC2CCN(c3ncnc4sccc34)CC2)cc1</chem>	β 1	ZINC0000645489 24
<chem>Oc1ccc(OC[C@@H](O)CNC2CCN(c3ncnc4sccc34)CC2)cc1</chem>	β 1	ZINC0000645489 25
<chem>CCc1cc(O)ccc1OC[C@H](O)CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1</chem>	β 1	ZINC0000645489 42
<chem>CCc1cc(O)ccc1OC[C@@H](O)CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1</chem>	β 1	ZINC0000645489 43
<chem>CCc1cccc(OC[C@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)c1</chem>	β 1	ZINC0000645490 14
<chem>CCc1cccc(OC[C@@H](O)CNC2CCN(c3ncnc4scc(-c5ccccc5)c34)CC2)c1</chem>	β 1	ZINC0000645490 15
<chem>Cc1c(-c2ccccc2)sc2ncnc(N3CCC(NC[C@H](O)COc4ccc(O)c(CO)c4)CC3)c12</chem>	β 1	ZINC0000645491 17
<chem>Cc1c(-c2ccccc2)sc2ncnc(N3CCC(NC[C@@H](O)COc4ccc(O)c(CO)c4)CC3)c12</chem>	β 1	ZINC0000645491 18
<chem>Cc1csc2ncnc(N3CCC(NC[C@H](O)COc4ccc(O)c(CO)c4)CC3)c12</chem>	β 1	ZINC0000645491 94
<chem>Cc1csc2ncnc(N3CCC(NC[C@@H](O)COc4ccc(O)c(CO)c4)CC3)c12</chem>	β 1	ZINC0000645491 95
<chem>O[C@H](CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1)COc1ccccc1F</chem>	β 1	ZINC0000645494 64
<chem>O[C@@H](CNC1CCN(c2ncnc3scc(-c4ccccc4)c23)CC1)COc1ccccc1F</chem>	β 1	ZINC0000645494 65

<chem>O[C@H](CNC1CCN(c2ncnc3ccc(-c4ccccc4)c23)CC1)COc1cccc(F)c1</chem>	$\beta 1$	ZINC0000645494 66
<chem>Cc1c(-c2ccccc2)sc2ncnc(N3CCC(NC[C@H](O)COc4ccc(O)cc4)CC3)c12</chem>	$\beta 1$	ZINC0000645494 67
<chem>Cc1c(-c2ccccc2)sc2ncnc(N3CCC(NC[C@@H](O)COc4ccc(O)cc4)CC3)c12</chem>	$\beta 1$	ZINC0000645494 68
<chem>COc1cccc1CNC(=O)Cc1cccc(C[C@@H](C)NC[C@H](O)c2ccc(O)c(NS(C)(=O)=O)c2)c1</chem>	$\beta 2$	ZINC0000645645 90
<chem>C[C@H](Cc1cccc(CC(=O)NCCc2ccccc2)c1)NC[C@H](O)c1ccc(O)c(NS(C)(=O)=O)c1</chem>	$\beta 2$	ZINC0000645646 71
<chem>C[C@H](Cc1cccc(CC(=O)NCC2CCCCC2)c1)NC[C@H](O)c1ccc(O)c(NS(C)(=O)=O)c1</chem>	$\beta 2$	ZINC0000645647 35
<chem>C[C@H](Cc1cccc(CC(=O)NCCCc2ccccc2)c1)NC[C@H](O)c1ccc(O)c(NS(C)(=O)=O)c1</chem>	$\beta 2$	ZINC0000645647 68
<chem>NC(=O)Nc1cccc(OC[C@H](O)CNC2CCN(c3ncnc4ccc(-c5ccccc5)c34)CC2)c1</chem>	$\beta 1$	ZINC0000647503 85
<chem>O=C(Nc1cccc1-c1cccc1)OC1CCN(CCCCCCCCNC[C@@H](O)c2ccc(O)c3[nH]c(=O)ccc23)CC1</chem>	$\beta 2$	ZINC0000660739 41
<chem>O=C(Nc1cccc1-c1cccc1)NC1CCN(CCCCCCCCNC[C@@H](O)c2ccc(O)c3[nH]c(=O)ccc23)CC1</chem>	$\beta 2$	ZINC0000660739 43
<chem>O=S(=O)(Nc1ccc(CCNC[C@H](O)c2ccccc2)cc1)c1ccc(-c2nc(-c3ccc(C(F)(F)F)cc3)cs2)cc1</chem>	$\beta 1$	ZINC0000660790 96
<chem>CC(C)N(CC[C@H](c1cccc1)c1cc(CCCCOc2ccc(CCNC[C@H](O)c3ccc(O)c4[nH]c(=O)ccc34)cc2)ccc1O)C(C)C</chem>	$\beta 2$	ZINC0000680876 87
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCCCCCCCCCN2CCC(OC(=O)Nc3ccccc3-c3ccc(O)c(Cl)c3)CC2)ccc1O</chem>	$\beta 2$	ZINC0000681060 40
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCCCCCCCCCN2CCC(OC(=O)Nc3ccc(F)cc3-c3ccc(O)c(Cl)c3)CC2)ccc1O</chem>	$\beta 2$	ZINC0000681060 49
<chem>CC(C)N(CC[C@H](c1cccc1)c1cc(CCNC[C@H](O)c2ccc(O)c(NS(C)(=O)=O)c2)ccc1O)C(C)C</chem>	$\beta 2$	ZINC0000713175 67
<chem>O=C1NC(=O)N(Cc2cccc(CCCCOCCCCCCCNC[C@H](O)c3ccc(O)c(CO)c3)c2)C1=O</chem>	$\beta 1$	ZINC0000721046 34
<chem>NC(=O)Nc1cc(CCCCOCCCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)cc(C(F)(F)F)c1</chem>	$\beta 1$	ZINC0000721046 77

<chem>O=C(CNC(=O)Nc1cccc(CCCCOCCCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)c1)NC1CCCC1</chem>	$\beta 1$	ZINC0000721048 19
<chem>CCNC(=O)NCc1cccc(CCCCOCCCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)c1</chem>	$\beta 1$	ZINC0000721053 05
<chem>CCNC(=O)Nc1cccc(CCCCOCCCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)c1</chem>	$\beta 1$	ZINC0000721054 34
<chem>NC(=O)CNC(=O)Nc1cccc(CCCCOCCCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)c1</chem>	$\beta 1$	ZINC0000721060 95
<chem>NC(=O)NCc1cccc(CCCCOCCCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)c1</chem>	$\beta 1$	ZINC0000721062 50
<chem>O=C(Nc1cccc(CCCCOCCCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)c1)NC1CCCCC1</chem>	$\beta 1$	ZINC0000721065 64
<chem>CCNC(=O)Nc1ccc(CCCCOCCCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)cc1</chem>	$\beta 1$	ZINC0000721067 16
<chem>C[C@H](Cc1ccc2ccccc2c1)NC[C@H](O)c1cc(O)cc(O)c1</chem>	$\beta 2$	ZINC0000721101 24
<chem>COc1ccc(C[C@@H](C)NC[C@H](O)c2cc(O)cc(O)c2)c2ccccc12</chem>	$\beta 2$	ZINC0000721101 26
<chem>O=C1CNC(=O)N1c1ccc(CCCCOCCCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)cc1</chem>	$\beta 1$	ZINC0000721104 13
<chem>NC(=O)CN1C(=O)CN(c2cccc(CCCCOCCCCCCCNC[C@H](O)c3ccc(O)c(CO)c3)c2)C1=O</chem>	$\beta 1$	ZINC0000721119 94
<chem>O=C1CN(c2cccc(CCCCOCCCCCCCNC[C@H](O)c3ccc(O)c(CO)c3)c2)C(=O)N1</chem>	$\beta 1$	ZINC0000721123 53
<chem>O=C1CNC(=O)N1Cc1cccc(CCCCOCCCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)c1</chem>	$\beta 1$	ZINC0000721123 54
<chem>CC1(C)NC(=O)N(c2cccc(CCCCOCCCCCCCNC[C@H](O)c3ccc(O)c(CO)c3)c2)C1=O</chem>	$\beta 1$	ZINC0000721126 69
<chem>O=C1CN(Cc2cccc(CCCCOCCCCCCCNC[C@H](O)c3ccc(O)c(CO)c3)c2)C(=O)N1</chem>	$\beta 1$	ZINC0000721126 70
<chem>O=C(Nc1cccc1-c1cccc1)O[C@H]1C[N+]2(CCCCCCCCCNC[C@H](O)c3ccc(O)c4[nH]c(=O)ccc34)CCC1CC2</chem>	$\beta 2$	ZINC0000721212 09
<chem>O=C(Nc1cccc1-c1cccc1)O[C@H]1C[N+]2(CCCCCCCCCNC[C@@H](O)c3ccc(O)c4[nH]c(=O)ccc34)CCC1CC2</chem>	$\beta 2$	ZINC0000721212 10

<chem>O=S(=O)(Nc1ccc(C[C@H]2CC[C@H]([C@H](O)c3ccccc3)N2)cc1)c1ccc(-c2nc(-c3ccc(C(F)(F)F)cc3)cs2)cc1</chem>	$\beta 1$	ZINC0000721221 07
<chem>O=S(=O)(Nc1ccc(C[C@@H]2CC[C@H]([C@H](O)c3ccccc3)N2)cc1)c1ccc(-c2nc(-c3ccc(C(F)(F)F)cc3)cs2)cc1</chem>	$\beta 1$	ZINC0000721221 08
<chem>O=S(=O)(Nc1ccc(C[C@H]2CC[C@@H]([C@@H](O)c3ccccc3)N2)cc1)c1ccc(-c2nc(-c3ccc(C(F)(F)F)cc3)cs2)cc1</chem>	$\beta 1$	ZINC0000721268 00
<chem>O=S(=O)(Nc1ccc(C[C@@H]2CC[C@@H]([C@@H](O)c3ccccc3)N2)cc1)c1ccc(-c2nc(-c3ccc(C(F)(F)F)cc3)cs2)cc1</chem>	$\beta 1$	ZINC0000721268 01
<chem>O=S(=O)(Nc1ccc(C[C@H]2CC[C@@H]([C@H](O)c3ccccc3)N2)cc1)c1ccc(-c2nc(-c3ccc(C(F)(F)F)cc3)cs2)cc1</chem>	$\beta 1$	ZINC0000721268 02
<chem>O=S(=O)(Nc1ccc(C[C@H]2CC[C@H]([C@@H](O)c3ccccc3)N2)cc1)c1ccc(-c2nc(-c3ccc(C(F)(F)F)cc3)cs2)cc1</chem>	$\beta 1$	ZINC0000721268 04
<chem>O=S(=O)(Nc1ccc(C[C@@H]2CC[C@H]([C@@H](O)c3ccccc3)N2)cc1)c1ccc(-c2nc(-c3ccc(C(F)(F)F)cc3)cs2)cc1</chem>	$\beta 1$	ZINC0000721268 05
<chem>CC(C)N(CC[C@H](c1ccccc1)c1cc(CCCCOc2ccc(CCNC[C@H](O)c3ccc(O)c(NS(C)(=O)=O)c3)cc2)ccc1O)C(C)C</chem>	$\beta 2$	ZINC0000721317 01
<chem>CC(C)N(CC[C@H](c1ccccc1)c1cc(CCCNC(=O)Cc2cccc(CC(C)(C)NC[C@H](O)c3ccc(O)c(CO)c3)c2)ccc1O)C(C)C</chem>	$\beta 2$	ZINC0000721317 14
<chem>CC(C)N(CC[C@H](c1ccccc1)c1cc(CCCCOc2ccc(CCNC[C@H](O)c3ccc(O)c(O)c3)cc2)ccc1O)C(C)C</chem>	$\beta 2$	ZINC0000721340 09
<chem>CC(C)N(CC[C@H](c1ccccc1)c1cc(CCCCOCCCCCNC[C@H](O)c2ccc(O)c(NS(C)(=O)=O)c2)ccc1O)C(C)C</chem>	$\beta 2$	ZINC0000721340 10
<chem>CC(C)N(CC[C@H](c1ccccc1)c1cc(CCCNC(=O)Cc2cccc(C[C@@H](C)NC[C@H](O)c3cc(O)cc(O)c3)c2)ccc1O)C(C)C</chem>	$\beta 2$	ZINC0000721340 26
<chem>CC(C)N(CC[C@H](c1ccccc1)c1cc(CCCCOc2ccc(CCNC[C@H](O)c3ccc(O)c(CO)c3)cc2)ccc1O)C(C)C</chem>	$\beta 2$	ZINC0000721340 27
<chem>COc1ccc2nc(-c3ccc(OC[C@@H](O)CN[C@@H](C)CF)cc3)n(C)c(=O)c2c1</chem>	$\beta 1$	ZINC0000721412 17
<chem>COc1ccc2nc(-c3ccc(OC[C@@H](O)CN[C@H](C)CF)cc3)n(C)c(=O)c2c1</chem>	$\beta 1$	ZINC0000721412 18
<chem>COc1ccc2nc(-c3ccc(OC[C@H](O)CN[C@@H](C)CF)cc3)n(C)c(=O)c2c1</chem>	$\beta 1$	ZINC0000721412 19
<chem>COc1ccc2nc(-c3ccc(OC[C@H](O)CN[C@H](C)CF)cc3)n(C)c(=O)c2c1</chem>	$\beta 1$	ZINC0000721412 20

<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCC[S@@](=O)CCCNCCc3cccc(Cl)c3)c2s1</chem>	$\beta 1$	ZINC0000721777 96
<chem>C[C@@H](CNCc1ccc(CCNC[C@H](O)c2ccc(O)c3[nH]c(=O)sc23)cc1)c1cccc1</chem>	$\beta 1$	ZINC0000731973 11
<chem>C[C@H](CNCc1ccc(CCNC[C@H](O)c2ccc(O)c3[nH]c(=O)sc23)cc1)c1cccc1</chem>	$\beta 1$	ZINC0000731973 12
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCCc3cccc(CNCCCc4cccc4)c3)c2s1</chem>	$\beta 1$	ZINC0000731973 13
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCCc3cccc(CNCCCc4cccc4)c3)c2s1</chem>	$\beta 1$	ZINC0000731973 14
<chem>O=c1[nH]c2c(O)ccc(CCNCCc3cccc(CNCCc4c(Cl)cccc4Cl)c3)c2s1</chem>	$\beta 2$	ZINC0000731973 18
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCCc3cccc3CNCCc3cccc3F)c2s1</chem>	$\beta 1$	ZINC0000731974 94
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCCc3cccc(CNCc4cccc4F)c3)c2s1</chem>	$\beta 1$	ZINC0000731975 94
<chem>O=c1[nH]c2c(O)ccc(CCNCCc3cccc(CN[C@H]4C[C@@H]4c4cccc4)c3)c2s1</chem>	$\beta 2$	ZINC0000731978 03
<chem>COc1cccc1CCNCc1ccc(CCNCCc2ccc(O)c3[nH]c(=O)sc23)cc1</chem>	$\beta 2$	ZINC0000731978 05
<chem>COc1cccc1CN(C)Cc1cccc(CCNC[C@H](O)c2ccc(O)c3[nH]c(=O)sc23)c1</chem>	$\beta 1$	ZINC0000731982 12
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCCc3cccc(CN4CCCC4)c3)c2s1</chem>	$\beta 1$	ZINC0000731982 15
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCCCc3cccc(CNCCc4c(Cl)cccc4Cl)c3)c2s1</chem>	$\beta 1$	ZINC0000731982 17
<chem>CCOc1cccc1CNCc1cccc(CCNC[C@H](O)c2ccc(O)c3[nH]c(=O)sc23)c1</chem>	$\beta 1$	ZINC0000731985 36
<chem>Cc1cccc2c(CCNCCc3cccc(CCNC[C@H](O)c4ccc(O)c5[nH]c(=O)sc45)c3)c[nH]c12</chem>	$\beta 1$	ZINC0000731993 88
<chem>C[C@H](Cc1cccc(CNCCc2c(Cl)cccc2Cl)c1)NC[C@H](O)c1ccc(O)c2[nH]c(=O)sc12</chem>	$\beta 1$	ZINC0000731995 09
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCCOc3cccc(CNCCc4cccc4F)c3)c2s1</chem>	$\beta 1$	ZINC0000731995 11

<chem>OCc1cc([C@H](O)CNC[C@@H]2CCC[C@H](CNC[C@H](O)c3ccc(O)c(CO)c3)C2)ccc1O</chem>	β 2	ZINC0000732210 44
<chem>OCc1cc([C@@H](O)CNCCc2ccc(NC[C@H](O)c3ccc(O)c(CO)c3)cc2)ccc1O</chem>	β 2	ZINC0000732219 89
<chem>OCc1cc([C@H](O)CNCCc2ccc(NC[C@H](O)c3ccc(O)c(CO)c3)cc2)ccc1O</chem>	β 2	ZINC0000732219 92
<chem>OCc1cc([C@H](O)CNc2ccc(CCNC[C@H](O)c3ccc(O)c(CO)c3)cc2)ccc1O</chem>	β 2	ZINC0000732219 95
<chem>OCc1cc([C@H](O)CNCCc2ccc(NC[C@@H](O)c3ccc(O)c(CO)c3)cc2)ccc1O</chem>	β 2	ZINC0000732219 99
<chem>O[C@H](CNCCc1ccc(NC[C@H](O)c2ccccc2)cc1)c1ccccc1</chem>	β 2	ZINC0000732220 02
<chem>O[C@@H](CNCCc1ccc(NC[C@H](O)c2ccccc2)cc1)c1ccccc1</chem>	β 2	ZINC0000732220 04
<chem>O[C@H](CNCCc1ccc(NC[C@@H](O)c2ccccc2)cc1)c1ccccc1</chem>	β 2	ZINC0000732220 07
<chem>O[C@H](CNc1ccc(CCNC[C@H](O)c2ccccc2)cc1)c1ccccc1</chem>	β 2	ZINC0000732220 11
<chem>Cc1ccc([C@@H](O)CNc2ccc(CCNC[C@H](O)c3ccc(O)c(CO)c3)cc2)cc1</chem>	β 2	ZINC0000732226 64
<chem>Cc1ccc([C@H](O)CNc2ccc(CCNC[C@@H](O)c3ccc(O)c(CO)c3)cc2)cc1</chem>	β 2	ZINC0000732226 66
<chem>Cc1ccc([C@@H](O)CNc2ccc(CCNC[C@@H](O)c3ccc(O)c(CO)c3)cc2)cc1</chem>	β 2	ZINC0000732226 68
<chem>CC(C)CCc1ccc([C@@H](O)CNc2ccc(CCNC[C@H](O)c3ccc(O)c(CO)c3)cc2)cc1</chem>	β 2	ZINC0000732226 73
<chem>CC(C)CCc1ccc([C@H](O)CNc2ccc(CCNC[C@@H](O)c3ccc(O)c(CO)c3)cc2)cc1</chem>	β 2	ZINC0000732226 74
<chem>CC(C)CCc1ccc([C@@H](O)CNc2ccc(CCNC[C@@H](O)c3ccc(O)c(CO)c3)cc2)cc1</chem>	β 2	ZINC0000732226 76
<chem>CC(C)(C)c1ccc([C@@H](O)CNc2ccc(CCNC[C@H](O)c3ccc(O)c(CO)c3)cc2)cc1</chem>	β 2	ZINC0000732230 10
<chem>CC(C)(C)c1ccc([C@H](O)CNc2ccc(CCNC[C@@H](O)c3ccc(O)c(CO)c3)cc2)cc1</chem>	β 2	ZINC0000732230 12

<chem>CC(C)(C)c1ccc([C@@H](O)CNc2ccc(CCNC[C@@H](O)c3ccc(O)c(CO)c3)cc2)cc1</chem>	β 2	ZINC0000732230 14
<chem>OCc1cc([C@@H](O)CNCCc2ccc(NC[C@H](O)c3ccc(-c4cccc4)cc3)cc2)ccc1O</chem>	β 2	ZINC0000732240 34
<chem>OCc1cc([C@H](O)CNCCc2ccc(NC[C@@H](O)c3ccc(-c4cccc4)cc3)cc2)ccc1O</chem>	β 2	ZINC0000732240 35
<chem>OCc1cc([C@H](O)CNCCc2ccc(NC[C@H](O)c3ccc(-c4cccc4)cc3)cc2)ccc1O</chem>	β 2	ZINC0000732240 36
<chem>OCc1cc([C@@H](O)CNCCc2ccc(NC[C@H](O)c3ccc4cccc4c3)cc2)ccc1O</chem>	β 2	ZINC0000732240 38
<chem>OCc1cc([C@H](O)CNCCc2ccc(NC[C@@H](O)c3ccc4cccc4c3)cc2)ccc1O</chem>	β 2	ZINC0000732240 39
<chem>OCc1cc([C@H](O)CNCCc2ccc(NC[C@H](O)c3ccc4cccc4c3)cc2)ccc1O</chem>	β 2	ZINC0000732240 40
<chem>CN(C[C@@H](O)c1cccc1)c1ccc(CCNC[C@H](O)c2ccc(O)c(CO)c2)cc1</chem>	β 2	ZINC0000732240 84
<chem>OCc1cc([C@H](O)CNCCc2ccc(NC[C@H](O)c3ccc(Cl)cc3)cc2)ccc1O</chem>	β 2	ZINC0000732240 90
<chem>OCc1cc([C@@H](O)CNCCc2ccc(NC[C@@H](O)c3ccc(Cl)cc3)cc2)ccc1O</chem>	β 2	ZINC0000732240 91
<chem>OCc1cc([C@H](O)CNCCc2ccc(NC[C@@H](O)c3ccc(Cl)cc3)cc2)ccc1O</chem>	β 2	ZINC0000732240 92
<chem>OCc1cc([C@H](O)CNCCc2ccc(NC[C@H](O)c3ccc(F)cc3)cc2)ccc1O</chem>	β 2	ZINC0000732240 94
<chem>OCc1cc([C@@H](O)CNCCc2ccc(NC[C@@H](O)c3ccc(F)cc3)cc2)ccc1O</chem>	β 2	ZINC0000732240 95
<chem>OCc1cc([C@H](O)CNCCc2ccc(NC[C@@H](O)c3ccc(F)cc3)cc2)ccc1O</chem>	β 2	ZINC0000732240 96
<chem>OCc1cc([C@@H](O)CNCCc2ccc(NC[C@H](O)c3ccc(O)c(CO)c3)cc2)ccc1O</chem>	β 2	ZINC0000732246 83
<chem>OCc1cc([C@H](O)CNCCc2ccc(NC[C@H](O)c3ccc(O)c(CO)c3)cc2)ccc1O</chem>	β 2	ZINC0000732246 84
<chem>OCc1cc([C@H](O)CNc2ccc(CNC[C@H](O)c3ccc(O)c(CO)c3)cc2)ccc1O</chem>	β 2	ZINC0000732246 85

<chem>OCc1cc([C@H](O)CNCCc2ccc(NC[C@@H](O)c3ccc(O)c(CO)c3)cc2)ccc1O</chem>	$\beta 2$	ZINC0000732246 86
<chem>OCc1cc([C@@H](O)CNCCc2ccc(OC[C@H](O)c3ccccc3)cc2)ccc1O</chem>	$\beta 2$	ZINC0000732401 25
<chem>OCc1cc([C@H](O)CNCCc2ccc(OC[C@@H](O)c3ccccc3)cc2)ccc1O</chem>	$\beta 2$	ZINC0000732401 28
<chem>OCc1cc([C@H](O)CNCCc2ccc(OC[C@H](O)c3ccccc3)cc2)ccc1O</chem>	$\beta 2$	ZINC0000732401 32
<chem>CC(C)(Cc1ccc(NC[C@@H](O)c2ccccc2)cc1)NC[C@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 2$	ZINC0000732401 39
<chem>CC(C)(Cc1ccc(NC[C@H](O)c2ccccc2)cc1)NC[C@@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 2$	ZINC0000732401 41
<chem>CC(C)(Cc1ccc(NC[C@@H](O)c2ccccc2)cc1)NC[C@@H](O)c1ccc(O)c(CO)c1</chem>	$\beta 2$	ZINC0000732401 45
<chem>OCc1cc([C@H](O)CNCCCCNC[C@H](O)c2ccc(O)c(CO)c2)ccc1O</chem>	$\beta 2$	ZINC0000732406 98
<chem>OCc1cc([C@@H](O)CNCCCCNC[C@H](O)c2ccc(O)c(CO)c2)ccc1O</chem>	$\beta 2$	ZINC0000732406 99
<chem>OCc1cc([C@H](O)CNCCCCNC[C@@H](O)c2ccc(O)c(CO)c2)ccc1O</chem>	$\beta 2$	ZINC0000732407 01
<chem>COc1ccc([C@@H](O)CNc2ccc(CCNC[C@H](O)c3ccc(O)c(CO)c3)cc2)c(OC)c1</chem>	$\beta 2$	ZINC0000732407 80
<chem>COc1ccc([C@H](O)CNc2ccc(CCNC[C@@H](O)c3ccc(O)c(CO)c3)cc2)c(OC)c1</chem>	$\beta 2$	ZINC0000732407 82
<chem>COc1ccc([C@@H](O)CNc2ccc(CCNC[C@@H](O)c3ccc(O)c(CO)c3)cc2)c(OC)c1</chem>	$\beta 2$	ZINC0000732407 84
<chem>COc1ccc(OC)c([C@@H](O)CNc2ccc(CCNC[C@H](O)c3ccc(O)c(CO)c3)cc2)c1</chem>	$\beta 2$	ZINC0000732407 88
<chem>COc1ccc(OC)c([C@H](O)CNc2ccc(CCNC[C@@H](O)c3ccc(O)c(CO)c3)cc2)c1</chem>	$\beta 2$	ZINC0000732407 91
<chem>COc1ccc(OC)c([C@@H](O)CNc2ccc(CCNC[C@@H](O)c3ccc(O)c(CO)c3)cc2)c1</chem>	$\beta 2$	ZINC0000732407 92
<chem>OCc1cc([C@H](O)CNCCc2ccc(NC[C@H](O)c3ccc(O)cc3)cc2)ccc1O</chem>	$\beta 2$	ZINC0000732407 96

<chem>OCc1cc([C@@H](O)CNCCc2ccc(NC[C@@H](O)c3ccc(O)cc3)cc2)ccc1O</chem>	$\beta 2$	ZINC0000732407 97
<chem>OCc1cc([C@H](O)CNCCc2ccc(NC[C@@H](O)c3ccc(O)cc3)cc2)ccc1O</chem>	$\beta 2$	ZINC0000732407 99
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCCc3cccc(CNCCc4ccccn4)c3)c2s1</chem>	$\beta 1$	ZINC0000733859 66
<chem>OCc1cc([C@H](O)CNCCCCCN[C@H](O)c2ccc(O)c(CO)c2)ccc1O</chem>	$\beta 2$	ZINC0000733892 77
<chem>OCc1cc([C@@H](O)CNCCCCCN[C@H](O)c2ccc(O)c(CO)c2)ccc1O</chem>	$\beta 2$	ZINC0000733892 81
<chem>OCc1cc([C@H](O)CNCCCCCN[C@@H](O)c2ccc(O)c(CO)c2)ccc1O</chem>	$\beta 2$	ZINC0000733892 84
<chem>O=c1ccc2c([C@@H](O)CNCCc3cccc(CNCCc4ccccn4)c3)ccc(O)c2[nH]1</chem>	$\beta 1$	ZINC0000821492 92
<chem>COc1cccc1CNCc1ccc(CCNC[C@@H](O)c2ccc(O)c3[nH]c(=O)sc23)cc1</chem>	$\beta 1$	ZINC0000821492 95
<chem>COc1ccc(CNCc2cccc(CCNC[C@H](O)c3ccc(O)c4[nH]c(=O)sc44)c2)cc1</chem>	$\beta 1$	ZINC0000821493 29
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCCc3ccc(CNCCc4c(Cl)cccc4Cl)cc3)c2s1</chem>	$\beta 1$	ZINC0000821516 50
<chem>O=c1[nH]c2c(O)ccc(CCNCc3cccc(CN4CCC(c5ccccc5)CC4)c3)c2s1</chem>	$\beta 2$	ZINC0000821525 45
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCCc3ccc(CNCCc4cccc4F)cc3)c2s1</chem>	$\beta 1$	ZINC0000821537 93
<chem>COc1cccc1CCNCc1cccc(CCNC[C@H](O)c2ccc(O)c3[nH]c(=O)sc23)c1</chem>	$\beta 1$	ZINC0000821537 96
<chem>COc1cccc1CCNCc1ccc(CCNC[C@H](O)c2ccc(O)c3[nH]c(=O)sc23)cc1</chem>	$\beta 1$	ZINC0000821548 24
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCCc3ccc(CNCCc4cccc4)cc3)c2s1</chem>	$\beta 1$	ZINC0000821548 30
<chem>C[C@@H](NCc1cccc1-c1ccc(CCNC[C@H](O)c2ccc(O)c3[nH]c(=O)sc23)cc1)c1cccc1</chem>	$\beta 2$	ZINC0000821556 86
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCCc3cccc(CNCCc4c(Cl)cccc4Cl)c3)c2s1</chem>	$\beta 1$	ZINC0000821556 95

<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CNCCc3cccc(CNCCc4cccc4Cl)c3)c2s1</chem>	$\beta 1$	ZINC0000821568 46
<chem>O=c1ccc2c([C@@H](O)CNCCc3ccc(NC[C@H](O)c4cccc4)cc3)ccc(O)c2[nH]1</chem>	$\beta 2$	ZINC0000821578 72
<chem>O=c1[nH]c2c(O)ccc(CCNCCc3ccc(-c4cccc(CN5Cc6cccc6C5)c4)cc3)c2s1</chem>	$\beta 2$	ZINC0000821588 58
<chem>COc1cccc(CNCc2cccc(CCNC[C@H](O)c3ccc(O)c4[nH]c(=O)sc34)c2)c1</chem>	$\beta 1$	ZINC0000821598 34
<chem>C[C@@H](NCc1cccc1-c1ccc(CCNCCc2ccc(O)c3[nH]c(=O)sc23)cc1)c1cccc1</chem>	$\beta 2$	ZINC0000821598 92
<chem>CC(C)c1cccc1OC[C@H](O)CN1CCN(CCN2C(=O)c3cccc4cccc(c34)C2=O)CC1</chem>	$\beta 1$	ZINC0000844662 38
<chem>CC(C)c1cccc1OC[C@@H](O)CN1CCN(CCN2C(=O)c3cccc4cccc(c34)C2=O)CC1</chem>	$\beta 1$	ZINC0000844662 39
<chem>N#Cc1cccc1OC[C@@H](O)CNCCNC(=O)c1ccc(F)nc1</chem>	$\beta 1$	ZINC0000845970 98
<chem>N#Cc1cccc1OC[C@@H](O)CNCCCC(=O)Nc1ccc(F)nc1</chem>	$\beta 1$	ZINC0000845970 99
<chem>N#Cc1cccc1OC[C@@H](O)CNCCNC(=O)Cc1ccc(F)cc1</chem>	$\beta 1$	ZINC0000845971 00
<chem>N#Cc1cccc1OC[C@@H](O)CNCCNS(=O)(=O)c1cccc1F</chem>	$\beta 1$	ZINC0000845971 01
<chem>N#Cc1cccc1OC[C@@H](O)CNCCNC(=O)Nc1cccc(OCCF)c1</chem>	$\beta 1$	ZINC0000846023 23
<chem>N#Cc1cccc1OC[C@@H](O)CNCCNC(=O)Nc1ccc(C(=O)O)c(F)c1</chem>	$\beta 1$	ZINC0000846044 00
<chem>N#Cc1cccc1OC[C@@H](O)CNCCNC(=O)N1CCOCC1</chem>	$\beta 1$	ZINC0000846046 80
<chem>N#Cc1cccc1OC[C@@H](O)CNCCNC(=O)Nc1nccs1</chem>	$\beta 1$	ZINC0000846047 01
<chem>N#Cc1cccc1OC[C@@H](O)CNCCNC(=O)Nc1ccc(Br)nc1</chem>	$\beta 1$	ZINC0000846146 00
<chem>N#Cc1cccc1OC[C@@H](O)CNCCNC(=O)Nc1cccc1F</chem>	$\beta 1$	ZINC0000846149 29

N#Cc1cccc1OC[C@@H](O)CNCCNC(=O)Nc1ccc(F)cc1	β 1	ZINC0000846149 33
C[C@@H](CF)Nc1ccc(NC(=O)NCCNC[C@H](O)COc2ccccc2C#N)cc1	β 1	ZINC0000846151 94
C[C@H](CF)Nc1ccc(NC(=O)NCCNC[C@H](O)COc2ccccc2C#N)cc1	β 1	ZINC0000846151 97
N#Cc1c(F)cccc1OC[C@@H](O)CNCCNC(=O)Nc1ccc(C(=O)O)cc1	β 1	ZINC0000846152 01
N#Cc1ccc(F)cc1OC[C@@H](O)CNCCNC(=O)Nc1ccc(C(=O)O)cc1	β 1	ZINC0000846152 04
N#Cc1cccc1OC[C@@H](O)CNCCNC(=O)Nc1ccc(OCCF)nc1	β 1	ZINC0000846171 06
N#Cc1cccc1OC[C@@H](O)CNCCNC(=O)Nc1ccc(F)nc1	β 1	ZINC0000846171 07
N#Cc1cccc1OC[C@@H](O)CNCCNC(=O)Nc1ccc(I)nc1	β 1	ZINC0000846175 85
N#Cc1cccc1OC[C@@H](O)CNCCNC(=O)Nc1cnc(Br)cn1	β 1	ZINC0000846175 86
N#Cc1cccc1OC[C@@H](O)CNCCNC(=O)Nc1nnn(CCF)n1	β 1	ZINC0000846175 88
CCOc1ccc(NC(=O)NCCNC[C@H](O)COc2cccc(F)c2C#N)cc1	β 1	ZINC0000846340 87
CCCCc1ccc2c(c1)C[C@H](NC[C@H](O)c1ccc(O)c3[nH]c(=O)ccc13)C2	β 1	ZINC0000846903 33
CCCCc1ccc2c(c1)C[C@@H](NC[C@H](O)c1ccc(O)c3[nH]c(=O)ccc13)C2	β 1	ZINC0000846903 34
CCc1cc2c(cc1CC)CC(NC[C@H](O)c1c(C)cc(O)c3[nH]c(=O)ccc13)C2	β 2	ZINC0000847049 79
CCc1cc2c(cc1CC)CC(NC[C@@H](O)c1c(C)cc(O)c3[nH]c(=O)ccc13)C2	β 2	ZINC0000847049 81
CCc1cc2c(cc1CC)CC(NC[C@H](O)c1ccc(O)c3[nH]c(=O)c(C)cc13)C2	β 1	ZINC0000847423 25
CCc1cc2c(cc1CC)CC(NC[C@@H](O)c1ccc(O)c3[nH]c(=O)c(C)cc13)C2	β 1	ZINC0000847423 27

<chem>COc1cc2nc(N3CCN(C(=O)[C@@H]4COc5ccccc5O4)CC3)nc(N)c2cc1OC</chem>	β2	ZINC0000945660 92
<chem>COc1cc2nc(N3CCN(C(=O)[C@H]4COc5ccccc5O4)CC3)nc(N)c2cc1OC</chem>	β2	ZINC0000945660 93
<chem>Cc1cc(N2CCNCC2)nc2ccccc12</chem>	β1	ZINC0000950678 45
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCCc2ccc(NC3CCN(C(=O)NCc4cc(F)ccc4F)CC3)cc2)ccc1O</chem>	β1	ZINC0000955417 97
<chem>CC(C)N(CC[C@H](c1ccccc1)c1cc(CCCNC(=O)CCCCCCCCCNC[C@H](O)c2ccc(O)c(NS(C)(=O)=O)c2)ccc1O)C(C)C</chem>	β2	ZINC0000955478 34
<chem>N#CN/C(=N\c1ccc2c(c1)CCN2c1nc(-c2ccc(OC(F)(F)F)cc2)cs1)Nc1ccc2cc(CCN[C@H](O)c3ccnc3)ccc2c1</chem>	β1	ZINC0000955482 64
<chem>COc1ccc(N2CCN(CC[C@@H](OC(N)=O)c3ccccc3)CC2)cc1</chem>	β1	ZINC0000955784 28
<chem>O=C(NCCNC[C@H](O)COc1ccc(OCCOCC2CC2)cc1)Nc1ccc(O)cc1</chem>	β1	ZINC0000955986 93
<chem>O=C(NCCNC[C@@H](O)COc1ccc(OCCOCC2CC2)cc1)Nc1ccc(O)cc1</chem>	β1	ZINC0000955986 94
<chem>O=C(NCCNC[C@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1ccccc1Br</chem>	β1	ZINC0000956010 23
<chem>O=C(NCCNC[C@@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1ccccc1Br</chem>	β1	ZINC0000956010 24
<chem>O=C(NCCNC[C@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1ccc(O)cc1</chem>	β1	ZINC0000956011 74
<chem>O=C(NCCNC[C@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1ccc(C(F)(F)F)cc1</chem>	β1	ZINC0000956014 22
<chem>O=C(NCCNC[C@@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1ccc(C(F)(F)F)cc1</chem>	β1	ZINC0000956014 23
<chem>O=C(NCCNC[C@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1ccc(Cl)cc1</chem>	β1	ZINC0000956014 71
<chem>O=C(NCCNC[C@@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1ccc(Cl)cc1</chem>	β1	ZINC0000956014 72
<chem>O=C(NCCNC[C@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1ccc(F)cc1</chem>	β1	ZINC0000956014 85

<chem>O=C(NCCNC[C@@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1ccc(F)cc1</chem>	$\beta 1$	ZINC0000956014 86
<chem>COc1ccc(NC(=O)NCCNC[C@H](O)COc2ccc(OCCOC3CCCC3)cc2)cc1</chem>	$\beta 1$	ZINC0000956017 62
<chem>COc1ccc(NC(=O)NCCNC[C@@H](O)COc2ccc(OCCOC3CCCC3)cc2)cc1</chem>	$\beta 1$	ZINC0000956017 63
<chem>O=C(NCCNC[C@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1ccc(Br)cc1</chem>	$\beta 1$	ZINC0000956018 80
<chem>O=C(NCCNC[C@@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1ccc(Br)cc1</chem>	$\beta 1$	ZINC0000956018 81
<chem>CCOCCOc1ccc(OC[C@@H](O)CNCCNC(=O)Nc2ccc(O)cc2)cc1</chem>	$\beta 1$	ZINC0000956021 58
<chem>O=C(NCCNC[C@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1cccc(O)c1</chem>	$\beta 1$	ZINC0000956021 99
<chem>O=C(NCCNC[C@@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1cccc(O)c1</chem>	$\beta 1$	ZINC0000956022 00
<chem>COc1cccc1NC(=O)NCCNC[C@H](O)COc1ccc(OCCOC2CCCC2)cc1</chem>	$\beta 1$	ZINC0000956022 16
<chem>COc1cccc1NC(=O)NCCNC[C@@H](O)COc1ccc(OCCOC2CCCC2)cc1</chem>	$\beta 1$	ZINC0000956022 17
<chem>O=C(NCCNC[C@H](O)COc1ccc(OCCOCCc2ccc(F)cc2)cc1)Nc1ccc(O)cc1</chem>	$\beta 1$	ZINC0000956024 33
<chem>O=C(NCCNC[C@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1cccc1O</chem>	$\beta 1$	ZINC0000956024 35
<chem>O=C(NCCNC[C@@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1cccc1O</chem>	$\beta 1$	ZINC0000956024 36
<chem>O=C(NCCNC[C@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1cccc(F)c1</chem>	$\beta 1$	ZINC0000956028 87
<chem>O=C(NCCNC[C@@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1cccc(F)c1</chem>	$\beta 1$	ZINC0000956028 88
<chem>O=C(NCCNC[C@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1cccc1Cl</chem>	$\beta 1$	ZINC0000956029 47
<chem>O=C(NCCNC[C@@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1cccc1Cl</chem>	$\beta 1$	ZINC0000956029 48

<chem>O=C(NCCNC[C@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1ccccc1C(F)(F)F</chem>	$\beta 1$	ZINC0000956032 55
<chem>O=C(NCCNC[C@@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1ccccc1C(F)(F)F</chem>	$\beta 1$	ZINC0000956032 56
<chem>Cc1cccc(NC(=O)NCCNC[C@H](O)COc2ccc(OCCOC3CCCC3)cc2)c1</chem>	$\beta 1$	ZINC0000956034 79
<chem>Cc1cccc(NC(=O)NCCNC[C@@H](O)COc2ccc(OCCOC3CCCC3)cc2)c1</chem>	$\beta 1$	ZINC0000956034 80
<chem>O=C(NCCNC[C@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1ccccc1F</chem>	$\beta 1$	ZINC0000956035 36
<chem>O=C(NCCNC[C@@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1ccccc1F</chem>	$\beta 1$	ZINC0000956035 37
<chem>Cc1ccccc1NC(=O)NCCNC[C@H](O)COc1ccc(OCCOC2CCCC2)cc1</chem>	$\beta 1$	ZINC0000956035 83
<chem>Cc1ccccc1NC(=O)NCCNC[C@@H](O)COc1ccc(OCCOC2CCCC2)cc1</chem>	$\beta 1$	ZINC0000956035 84
<chem>O=C(NCCNC[C@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1cccc(C(F)(F)F)c1</chem>	$\beta 1$	ZINC0000956043 76
<chem>O=C(NCCNC[C@@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1cccc(C(F)(F)F)c1</chem>	$\beta 1$	ZINC0000956043 77
<chem>Cc1ccc(NC(=O)NCCNC[C@H](O)COc2ccc(OCCOC3CCCC3)cc2)cc1</chem>	$\beta 1$	ZINC0000956046 79
<chem>Cc1ccc(NC(=O)NCCNC[C@@H](O)COc2ccc(OCCOC3CCCC3)cc2)cc1</chem>	$\beta 1$	ZINC0000956046 80
<chem>O=C(NCCNC[C@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1cccc(Br)c1</chem>	$\beta 1$	ZINC0000956050 09
<chem>O=C(NCCNC[C@@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1cccc(Br)c1</chem>	$\beta 1$	ZINC0000956050 10
<chem>O=C(NCCNC[C@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1ccccc1</chem>	$\beta 1$	ZINC0000956052 79
<chem>O=C(NCCNC[C@H](O)COc1ccc(OCCOC2CCCC2)cc1)Nc1cccc(Cl)c1</chem>	$\beta 1$	ZINC0000956053 21
<chem>COc1cccc(NC(=O)NCCNC[C@H](O)COc2ccc(OCCOC3CCCC3)cc2)c1</chem>	$\beta 1$	ZINC0000956055 84

<chem>COc1cccc(NC(=O)NCCNC[C@@H](O)COc2ccc(OCCOC3CCCC3)cc2)c1</chem>	$\beta 1$	ZINC0000956055 85
<chem>CC(C)N(CC[C@H](c1cccc1)c1cc(CCCNC(=O)Cc2cccc(CC(C)(C)NC[C@H](O)c3ccc(O)c(NS(C)(=O)=O)c3)c2)ccc1O)C(C)C</chem>	$\beta 2$	ZINC0000956173 24
<chem>N#Cc1cc2c(OC[C@@H](O)CN3CCN(C(c4cccc4)c4cccc4)CC3)cccc2[nH]1</chem>	$\beta 2$	ZINC0000956288 24
<chem>N#Cc1cc2c(OC[C@H](O)CN3CCN(C(c4cccc4)c4cccc4)CC3)cccc2[nH]1</chem>	$\beta 2$	ZINC0000956288 25
<chem>C=CCc1cccc1OC[C@H](O)CN1CCN(CCN2C(=O)c3cccc4cccc(c34)C2=O)CC1</chem>	$\beta 1$	ZINC0000958630 72
<chem>C=CCc1cccc1OC[C@@H](O)CN1CCN(CCN2C(=O)c3cccc4cccc(c34)C2=O)CC1</chem>	$\beta 1$	ZINC0000958630 73
<chem>Cc1ccc(C(C)C)c(OC[C@@H](O)CN2CCN(CCN3C(=O)c4cccc5cccc(c45)C3=O)CC2)c1</chem>	$\beta 2$	ZINC0000961720 10
<chem>Cc1ccc(C(C)C)c(OC[C@H](O)CN2CCN(CCN3C(=O)c4cccc5cccc(c45)C3=O)CC2)c1</chem>	$\beta 2$	ZINC0000963000 85
<chem>CS(=O)(=O)Nc1ccc(CCNC[C@H](O)COc2ccc(O)cc2)cc1</chem>	$\beta 1$	ZINC0000968808 58
<chem>O=S(=O)(CCCc1cccc1)Nc1ccc(CCNC[C@H](O)COc2ccc(O)cc2)cc1</chem>	$\beta 1$	ZINC0000968808 65
<chem>CC(C)S(=O)(=O)Nc1ccc(CCNC[C@H](O)COc2ccc(O)cc2)cc1</chem>	$\beta 1$	ZINC0000968808 70
<chem>CCN(CC)C(=O)[C@@H]1C=C2c3cccc4[nH]cc(c34)C[C@H]2N(C)C1</chem>	$\beta 1$	ZINC0000969038 03
<chem>Cc1ccc2nc(C(F)(F)F)cc(N3CCN(C)CC3)c2c1</chem>	$\beta 2$	ZINC0000969387 19
<chem>O=[N+](O-)/C=C(\Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)Nc1cccc(Oc2ccccc2)c1</chem>	$\beta 1$	ZINC0001000431 47
<chem>O=[N+](O-)/C=C(\Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)Nc1cccc(F)c1</chem>	$\beta 1$	ZINC0001000431 78
<chem>O=[N+](O-)/C=C(\Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)Nc1cccc2ccccc12</chem>	$\beta 1$	ZINC0001000431 86
<chem>O=[N+](O-)/C=C(\Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)Nc1ccc2ccccc2c1</chem>	$\beta 1$	ZINC0001000431 89

<chem>O=[N+](O-)/C=C(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)Nc1cc(Cl)cc(Cl)c1</chem>	$\beta 1$	ZINC0001000431 99
<chem>O=[N+](O-)/C=C(Nc1ccc(CCNC[C@H](O)c2ccnc2)cc1)Nc1cccc(I)c1</chem>	$\beta 1$	ZINC0001000432 06
<chem>NC(=O)c1cccc(N/C(=C/[N+](=O)[O-])Nc2ccc(CCNC[C@H](O)c3ccnc3)cc2)c1</chem>	$\beta 1$	ZINC0001000432 12
<chem>O=C1N=c2cccc(OC[C@@H](O)CNC3CCN(c4ccc(C[C@H]5SC(=O)NC5=O)cc4)CC3)c2=N1</chem>	$\beta 1$	ZINC0001008782 63
<chem>CC1(C)[C@@H]2CC[C@]1(C)[C@@H](NC[C@H](O)c1ccc(O)c3[nH]c(=O)sc13)C2</chem>	$\beta 1$	ZINC0001013614 62
<chem>COc1ccc(CCNC[C@@H](O)c2cc(O)cc(O)c2)cc1</chem>	$\beta 2$	ZINC0001032312 61
<chem>CC[C@H](Cc1ccc(OC)cc1)NC[C@H](O)c1cc(O)cc(O)c1</chem>	$\beta 2$	ZINC0001032312 63
<chem>CCC[C@H](Cc1ccc(OC)cc1)NC[C@H](O)c1cc(O)cc(O)c1</chem>	$\beta 2$	ZINC0001032312 74
<chem>O=S(=O)(c1cccc(CCCCOCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)c1)C1CCCC1</chem>	$\beta 1$	ZINC0001032398 58
<chem>CS(=O)(=O)c1ccc(CCCCOCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)cc1</chem>	$\beta 1$	ZINC0001032398 61
<chem>Cc1cc(CCCCOCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)cc(S(=O)(=O)C2CCCC2)c1</chem>	$\beta 1$	ZINC0001032398 65
<chem>O=S(=O)(c1ccc(CCCCOCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)cc1)C1CCCC1</chem>	$\beta 1$	ZINC0001032398 69
<chem>O=S(=O)(c1cccc(CCCCOCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)c1)C1CCCCC1</chem>	$\beta 1$	ZINC0001032398 73
<chem>O=S(=O)(c1cccc(CCCCOCCCCCNC[C@H](O)c2ccc(O)c(CO)c2)c1)C1CC=CC1</chem>	$\beta 1$	ZINC0001032517 44
<chem>O=C(Nc1ccc(C[C@@H]2CC[C@H]([C@H](O)c3ccccc3)N2)cc1)[C@@H]1CCc2sc(-c3ccc(F)cc3)nc21</chem>	$\beta 1$	ZINC0001032521 31
<chem>O=C(Nc1ccc(C[C@@H]2CC[C@H]([C@H](O)c3ccnc3)N2)cc1)[C@@H]1CCc2sc(-c3ccc(F)cc3)nc21</chem>	$\beta 2$	ZINC0001032521 33
<chem>Nc1nc2c(s1)CC[C@H]2C(=O)Nc1ccc(C[C@@H]2CC[C@H]([C@H](O)c3cccc(Cl)c3)N2)cc1</chem>	$\beta 2$	ZINC0001032521 63

<chem>C[C@H](Cc1c[nH]c2c(OS(C)(=O)=O)cccc12)NC[C@H](O)c1cccc(NS(=O)(=O)c2cccc(N)c2)c1</chem>	$\beta 1$	ZINC0001032919 03
<chem>COc1cccc2c(C[C@@H](C)NC[C@H](O)c3cccc(NS(=O)(=O)c4cccs4)c3)cn(Cc3ccccc3)c12</chem>	$\beta 1$	ZINC0001032920 13
<chem>C[C@H](Cc1c[nH]c2c(OS(C)(=O)=O)cccc12)NC[C@H](O)c1ccc(S(=O)(=O)Nc2ccccc2)cc1</chem>	$\beta 1$	ZINC0001032933 79
<chem>C[C@H](Cc1c[nH]c2c(OS(C)(=O)=O)cccc12)NC[C@H](O)c1ccc(C(=O)Nc2ccccc2)cc1</chem>	$\beta 1$	ZINC0001032933 81
<chem>C[C@H](Cc1cn2c3c(cccc13)OCCC2)NC[C@H](O)c1cccc(NS(=O)(=O)c2cccs2)c1</chem>	$\beta 1$	ZINC0001032934 38
<chem>CNc1nc(C(F)(F)c2ccccc2)nc2c1CCNCCC2</chem>	$\beta 2$	ZINC0001166954 99
<chem>OCc1cc([C@H](O)CNC[C@@H]2CCC[C@@H](CNC[C@H](O)c3ccc(O)c(CO)c3)C2)ccc1O</chem>	$\beta 2$	ZINC0001687416 03
<chem>OCc1cc([C@H](O)CNC[C@@H]2CCC[C@@H](CNC[C@@H](O)c3ccc(O)c(CO)c3)C2)ccc1O</chem>	$\beta 2$	ZINC0001687416 94
<chem>OCc1cc([C@H](O)CNC[C@H]2CCC[C@@H](CNC[C@@H](O)c3ccc(O)c(CO)c3)C2)ccc1O</chem>	$\beta 2$	ZINC0001687418 00
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCCCCCCCCCN2CCC(OC(=O)Nc3ccccc3-c3ccccc3)CC2)ccc1O</chem>	$\beta 2$	ZINC0001693216 29
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCCCCCCCCCN2CCC(OC(=O)Nc3ccccc3-c3ccc(O)cc3)CC2)ccc1O</chem>	$\beta 2$	ZINC0001693216 32
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCCCCCCCCCN2CCC(OC(=O)Nc3ccccc3-c3cccc(O)c3)CC2)ccc1O</chem>	$\beta 2$	ZINC0001693216 33
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCCCCCCCCCN2CCC(OC(=O)Nc3ccccc3-c3ccccc3O)CC2)ccc1O</chem>	$\beta 2$	ZINC0001693216 36
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCCCCCCCCCN2CCC(OC(=O)Nc3ccccc3-c3cc(F)cc(F)c3O)CC2)ccc1O</chem>	$\beta 2$	ZINC0001693216 46
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCCCCCCCCCN2CCC(OC(=O)Nc3ccccc3-c3cc(O)cc(F)c3)CC2)ccc1O</chem>	$\beta 2$	ZINC0001693216 47
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCCCCCCCCCN2CCC(OC(=O)Nc3ccccc3-c3cc(F)c(O)cc3F)CC2)ccc1O</chem>	$\beta 2$	ZINC0001693216 52
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCCCCCCCCCN2CCC(OC(=O)Nc3cc(F)ccc3-c3ccc(O)c(Cl)c3)CC2)ccc1O</chem>	$\beta 2$	ZINC0001693233 18

<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCCCCCCCCCN2CCC(OC(=O)Nc3ccccc3-c3ccc(O)c(Cl)c3)CC2)ccc1O</chem>	β 2	ZINC0001693233 21
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCCCCCCCCCN2CCC(OC(=O)Nc3ccccc3-c3ccc(O)c(Cl)c3)CC2)ccc1O</chem>	β 2	ZINC0001693233 22
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCCCCCCCCCN2CCC(OC(=O)Nc3ccccc3-c3ccc(O)c(Cl)c3)CC2)ccc1O</chem>	β 2	ZINC0001693233 24
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCCCCCCCCCN2CC[C@@H](OC(=O)Nc3ccccc3-c3ccc(O)c(Cl)c3)C2)ccc1O</chem>	β 2	ZINC0001693233 26
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCCCCCCCCCN2C[C@H]3C[C@@]3(COC(=O)Nc3ccccc3-c3ccc(O)c(Cl)c3)C2)ccc1O</chem>	β 2	ZINC0001693233 30
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCCCCCCCCCN2C[C@@H]3[C@@H](COC(=O)Nc4ccccc4-c4ccc(O)c(Cl)c4)[C@@H]3C2)ccc1O</chem>	β 2	ZINC0001693233 33
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCCCCCCCCCN2[C@H]3CC[C@H]2CC(OC(=O)Nc2ccccc2-c2ccc(O)c(Cl)c2)C3)ccc1O</chem>	β 2	ZINC0001693233 42
<chem>CS(=O)(=O)Nc1cc([C@@H](O)CNCCc2ccc(OCCCN3CCC(OC(=O)Nc4ccccc4-c4ccc(O)c(Cl)c4)CC3)cc2)ccc1O</chem>	β 2	ZINC0001693233 49
<chem>OCc1cc([C@H](O)CNCCc2ccc(Br)cc2)ccc1O</chem>	β 2	ZINC0001693507 70
<chem>OCc1cc([C@H](O)CNCCc2ccc(NC3ccc(Cl)c(Cl)c3)cc2)ccc1O</chem>	β 2	ZINC0001693511 93
<chem>OCc1cc([C@H](O)CNCCc2ccc(NC3ccc4ccccc4c3)cc2)ccc1O</chem>	β 2	ZINC0001693511 95
<chem>OCc1cc([C@H](O)CNCCc2ccc(N3CCC(c4ccccc4)CC3)cc2)ccc1O</chem>	β 2	ZINC0001693511 98
<chem>OCc1cc([C@H](O)CNCCc2ccc(N3CCC(Cc4ccccc4)CC3)cc2)ccc1O</chem>	β 2	ZINC0001693512 02
<chem>OCc1cc([C@H](O)CNCCc2ccc(N3CCC(CCCc4ccccc4)CC3)cc2)ccc1O</chem>	β 2	ZINC0001693512 06
<chem>O=C(c1ccccc1)C1CCN(c2ccc(CCNC[C@@H](O)c3ccc(O)c(CO)c3)cc2)CC1</chem>	β 2	ZINC0001693512 08
<chem>OCc1cc([C@H](O)CNCCc2ccc(N3CCN(c4ccccc4)CC3)cc2)ccc1O</chem>	β 2	ZINC0001693512 11
<chem>COc1ccc(CN2CCN(c3ccc(CCNC[C@@H](O)c4ccc(O)c(CO)c4)cc3)CC2)cc1</chem>	β 2	ZINC0001693512 12

<chem>CC(=O)N1CCN(c2ccc(CCNC[C@@H](O)c3ccc(O)c(CO)c3)cc2)CC1</chem>	$\beta 2$	ZINC0001693512 14
<chem>O=C(Cc1ccccc1)NC1CCN(c2ccc(CCNC[C@@H](O)c3ccc(O)c(CO)c3)cc2)CC1</chem>	$\beta 2$	ZINC0001693512 17
<chem>OCc1cc([C@H](O)CNCCc2ccc(Nc3ccc(Oc4ccccc4)cc3)cc2)ccc1O</chem>	$\beta 1$	ZINC0001693512 23
<chem>OCc1cc([C@@H](O)CNCCc2ccc(Nc3ccc4ccccc4c3)cc2)ccc1O</chem>	$\beta 2$	ZINC0001693512 26
<chem>OCc1cc([C@H](O)CNCCc2ccc(Nc3ccc4ccccc4c3)cc2)ccc1O</chem>	$\beta 2$	ZINC0001693512 27
<chem>OCc1cc([C@H](O)CNCCc2ccc(Nc3ccc4ccccc4c3)cc2)ccc1O</chem>	$\beta 2$	ZINC0001693512 29
<chem>OCc1cc([C@H](O)CNCCc2ccc(Nc3ccc4c(c3)CCC4)cc2)ccc1O</chem>	$\beta 2$	ZINC0001693512 31
<chem>OCc1cc([C@H](O)CNCCc2ccc(Nc3ccc(-c4ccccc4)cc3)cc2)ccc1O</chem>	$\beta 2$	ZINC0001693512 33
<chem>COc1cccc(Nc2ccc(CCNC[C@@H](O)c3ccc(O)c(CO)c3)cc2)c1</chem>	$\beta 2$	ZINC0001693512 34
<chem>CSc1ccc(Nc2ccc(CCNC[C@@H](O)c3ccc(O)c(CO)c3)cc2)cc1</chem>	$\beta 1$	ZINC0001693512 36
<chem>CSc1ccc(Nc2ccc(CCNC[C@H](O)c3ccc(O)c(CO)c3)cc2)cc1</chem>	$\beta 1$	ZINC0001693512 37
<chem>CC(C)Oc1ccc(Nc2ccc(CCNC[C@@H](O)c3ccc(O)c(CO)c3)cc2)cc1</chem>	$\beta 2$	ZINC0001693512 38
<chem>CC(C)Oc1ccc(Nc2ccc(CCNC[C@H](O)c3ccc(O)c(CO)c3)cc2)cc1</chem>	$\beta 2$	ZINC0001693512 39
<chem>OCc1cc([C@H](O)CNCCc2ccc(Nc3ccc(O)cc3)cc2)ccc1O</chem>	$\beta 2$	ZINC0001693512 41
<chem>OCc1cc([C@H](O)CNCCc2ccc(Nc3ccc(F)cc3)cc2)ccc1O</chem>	$\beta 1$	ZINC0001693512 45
<chem>COC(=O)c1ccc(Nc2ccc(CCNC[C@@H](O)c3ccc(O)c(CO)c3)cc2)cc1</chem>	$\beta 1$	ZINC0001693512 47
<chem>COC(=O)c1ccc(Nc2ccc(CCNC[C@H](O)c3ccc(O)c(CO)c3)cc2)cc1</chem>	$\beta 1$	ZINC0001693512 49

<chem>CN(C[C@@H](O)c1cccc1)c1ccc(CCNC[C@@H](O)c2ccc(O)c(CO)c2)cc1</chem>	$\beta 2$	ZINC0001697291 82
<chem>CN(C[C@H](O)c1cccc1)c1ccc(CCNC[C@@H](O)c2ccc(O)c(CO)c2)cc1</chem>	$\beta 2$	ZINC0001697291 83
<chem>OCc1cc([C@H](O)CN[C@@H]2Cc3ccc(NC[C@@H](O)c4cccc4)cc3C2)ccc1O</chem>	$\beta 2$	ZINC0001697291 84
<chem>OCc1cc([C@H](O)CN[C@H]2Cc3ccc(NC[C@@H](O)c4cccc4)cc3C2)ccc1O</chem>	$\beta 2$	ZINC0001697291 85
<chem>CC(C)(C)NC[C@H](O)c1ccc2c(c1)CO[B-](O)(O)O2</chem>	$\beta 2$	ZINC0001701438 38
<chem>C=CCc1cccc1OC[C@@H](O)CNCCOCCOCCNC(=O)CCCCNC(=O)COc1ccc(/C=C/c2ccc3n2[B-](F)(F)[N+]2=C(c4cccs4)C=CC2=C3)cc1</chem>	$\beta 1$	ZINC0001701815 76
<chem>C=CCc1cccc1OC[C@H](O)CNCCOCCOCCNC(=O)CCCCNC(=O)COc1ccc(/C=C/c2ccc3n2[B-](F)(F)[N+]2=C(c4cccs4)C=CC2=C3)cc1</chem>	$\beta 1$	ZINC0001701815 79
<chem>C=CCc1cccc1OC[C@@H](O)CNCCNC(=O)CCCCNC(=O)COc1ccc(/C=C/c2ccc3n2[B-](F)(F)[N+]2=C(c4cccs4)C=CC2=C3)cc1</chem>	$\beta 1$	ZINC0001701815 82
<chem>C=CCc1cccc1OC[C@H](O)CNCCNC(=O)CCCCNC(=O)COc1ccc(/C=C/c2ccc3n2[B-](F)(F)[N+]2=C(c4cccs4)C=CC2=C3)cc1</chem>	$\beta 1$	ZINC0001701815 85
<chem>O=C(CCCCCNC(=O)COc1ccc(/C=C/c2ccc3n2[B-](F)(F)[N+]2=C(c4cccs4)C=CC2=C3)cc1)NCCCCCCCCNC[C@H](O)COc1cccc2cccc12</chem>	$\beta 1$	ZINC0001701815 89
<chem>O=C(CCCCCNC(=O)COc1ccc(/C=C/c2ccc3n2[B-](F)(F)[N+]2=C(c4cccs4)C=CC2=C3)cc1)NCCCCNC[C@H](O)COc1cccc2cccc12</chem>	$\beta 1$	ZINC0001701815 92
<chem>O=C(CCCCCNC(=O)COc1ccc(/C=C/c2ccc3n2[B-](F)(F)[N+]2=C(c4cccs4)C=CC2=C3)cc1)NCCOCCOCCNC[C@@H](O)COc1cccc2[nH]ccc12</chem>	$\beta 1$	ZINC0001701815 95
<chem>O=C(CCCCCNC(=O)COc1ccc(/C=C/c2ccc3n2[B-](F)(F)[N+]2=C(c4cccs4)C=CC2=C3)cc1)NCCOCCOCCNC[C@H](O)COc1cccc2[nH]ccc12</chem>	$\beta 1$	ZINC0001701815 99
<chem>O=C(CCCCCNC(=O)COc1ccc(/C=C/c2ccc3n2[B-](F)(F)[N+]2=C(c4cccs4)C=CC2=C3)cc1)NCCNC[C@@H](O)COc1cccc2[nH]ccc12</chem>	$\beta 1$	ZINC0001701816 02
<chem>O=C(CCCCCNC(=O)COc1ccc(/C=C/c2ccc3n2[B-](F)(F)[N+]2=C(c4cccs4)C=CC2=C3)cc1)NCCNC[C@H](O)COc1cccc2[nH]ccc12</chem>	$\beta 1$	ZINC0001701816 05
<chem>O=C(CCCCCNC(=O)COc1ccc(/C=C/c2ccc3n2[B-](F)(F)[N+]2=C(c4cccs4)C=CC2=C3)cc1)NCCOCCOCCNC[C@@H](O)COc1cccc2cccc12</chem>	$\beta 1$	ZINC0001701816 11
<chem>O=C(CCCCCNC(=O)COc1ccc(/C=C/c2ccc3n2[B-](F)(F)[N+]2=C(c4cccs4)C=CC2=C3)cc1)NCCOCCOCCNC[C@H](O)COc1cccc2cccc12</chem>	$\beta 1$	ZINC0001701816 13

O=C(CCCCCNC(=O)COc1ccc(/C=C/c2ccc3n2[B-](F)(F)[N+]2=C(c4cccs4)C=CC2=C3)cc1)NCCNC[C@@H](O)COc1cccc2ccccc12	β1	ZINC0001701816
O=C(CCCCCNC(=O)COc1ccc(/C=C/c2ccc3n2[B-](F)(F)[N+]2=C(c4cccs4)C=CC2=C3)cc1)NCCNC[C@H](O)COc1cccc2ccccc12	β1	ZINC0001701816
O=C(CCCCCNC(=O)COc1ccc(/C=C/c2ccc3n2[B-](F)(F)[N+]2=C(c4cccs4)C=CC2=C3)cc1)NCCCCCCCCNC[C@@H](O)COc1cccc2ccccc12	β1	ZINC0001953492
O=C(CCCCCNC(=O)COc1ccc(/C=C/c2ccc3n2[B-](F)(F)[N+]2=C(c4cccs4)C=CC2=C3)cc1)NCCCCNC[C@@H](O)COc1cccc2ccccc12	β1	ZINC0001953647
OCc1cc([C@H](O)CN[C@@H]2CC[C@@H](NC[C@@H](O)c3ccc(O)c(CO)c3)CC2)ccc1O	β2	ZINC0002541123
OCc1cc([C@H](O)CN[C@@H]2CC[C@@H](NC[C@H](O)c3ccc(O)c(CO)c3)CC2)ccc1O	β2	ZINC0002541123
OCc1cc([C@@H](O)CN[C@@H]2CC[C@@H](NC[C@H](O)c3ccc(O)c(CO)c3)CC2)ccc1O	β2	ZINC0002541123
CC(C)(C)NC[C@H](O)c1ccc2c(c1)CO[B@-](O)(c1ccccc1)O2	β2	ZINC0002541246
CC(C)(C)NC[C@H](O)c1ccc2c(c1)CO[B@@-](O)(c1ccccc1)O2	β2	ZINC0002541246
OCc1cc([C@H](O)CN[C@H]2Cc3ccc(NC[C@H](O)c4ccccc4)cc3C2)ccc1O	β2	ZINC0002541943
OCc1cc([C@H](O)CN[C@@H]2Cc3ccc(NC[C@H](O)c4ccccc4)cc3C2)ccc1O	β2	ZINC0002541943
C[N@+]1(CCCCCCCCCNC[C@H](O)c2ccc(O)c3nc(O)ccc23)[C@@H]2C[C@H](OC(=O)C(O)(c3cccs3)c3cccs3)C[C@@H]1[C@H]1O[C@H]12	β2	ZINC0002611752
C[N@@+]1(CCCCCCCCCNC[C@H](O)c2ccc(O)c3nc(O)ccc23)[C@@H]2C[C@H](OC(=O)C(O)(c3cccs3)c3cccs3)C[C@@H]1[C@H]1O[C@H]12	β2	ZINC0002611752
Cc1ccc(CCNC[C@H](O)c2ccc(O)c3[nH]c(=O)sc23)cc1C	β1	ZINC0002998246
CCCCOc1ccc(CCNC[C@H](O)c2ccc(O)c3[nH]c(=O)sc23)cc1	β1	ZINC0002998270
CCOc1cccc([C@H]2CCC[C@H]2NC[C@H](O)c2ccc(O)c3[nH]c(=O)sc23)c1	β1	ZINC0002998278
Cc1ccccc1[C@H]1CCC[C@H]1NC[C@H](O)c1ccc(O)c2[nH]c(=O)sc12	β1	ZINC0002998284

<chem>Cc1ccc([C@H]2CCC[C@H]2NC[C@H](O)c2ccc(O)c3[nH]c(=O)sc23)cc1</chem>	β 1	ZINC0002998299 86
<chem>Cc1cccc([C@H]2CCC[C@H]2NC[C@H](O)c2ccc(O)c3[nH]c(=O)sc23)c1</chem>	β 1	ZINC0002998306 71
<chem>CCc1cccc([C@H]2CCC[C@H]2NC[C@H](O)c2ccc(O)c3[nH]c(=O)sc23)c1</chem>	β 1	ZINC0002998306 89
<chem>CC(C)[C@H]1CCC[C@H]1NC[C@H](O)c1ccc(O)c2[nH]c(=O)sc12</chem>	β 1	ZINC0002998307 20
<chem>O=c1[nH]c2c(O)ccc([C@@H](O)CN[C@@H]3CCC[C@@H]3CCc3ccccc3)c2s1</chem>	β 1	ZINC0002998327 98
<chem>O=C(CCN1CCC(OC(=O)Nc2ccccc2-c2ccccc2)CC1)N[C@@H]1CC[C@@H](CNC[C@H](O)c2ccc(O)c3nc(O)ccc23)CC1</chem>	β 2	ZINC0002998682 07