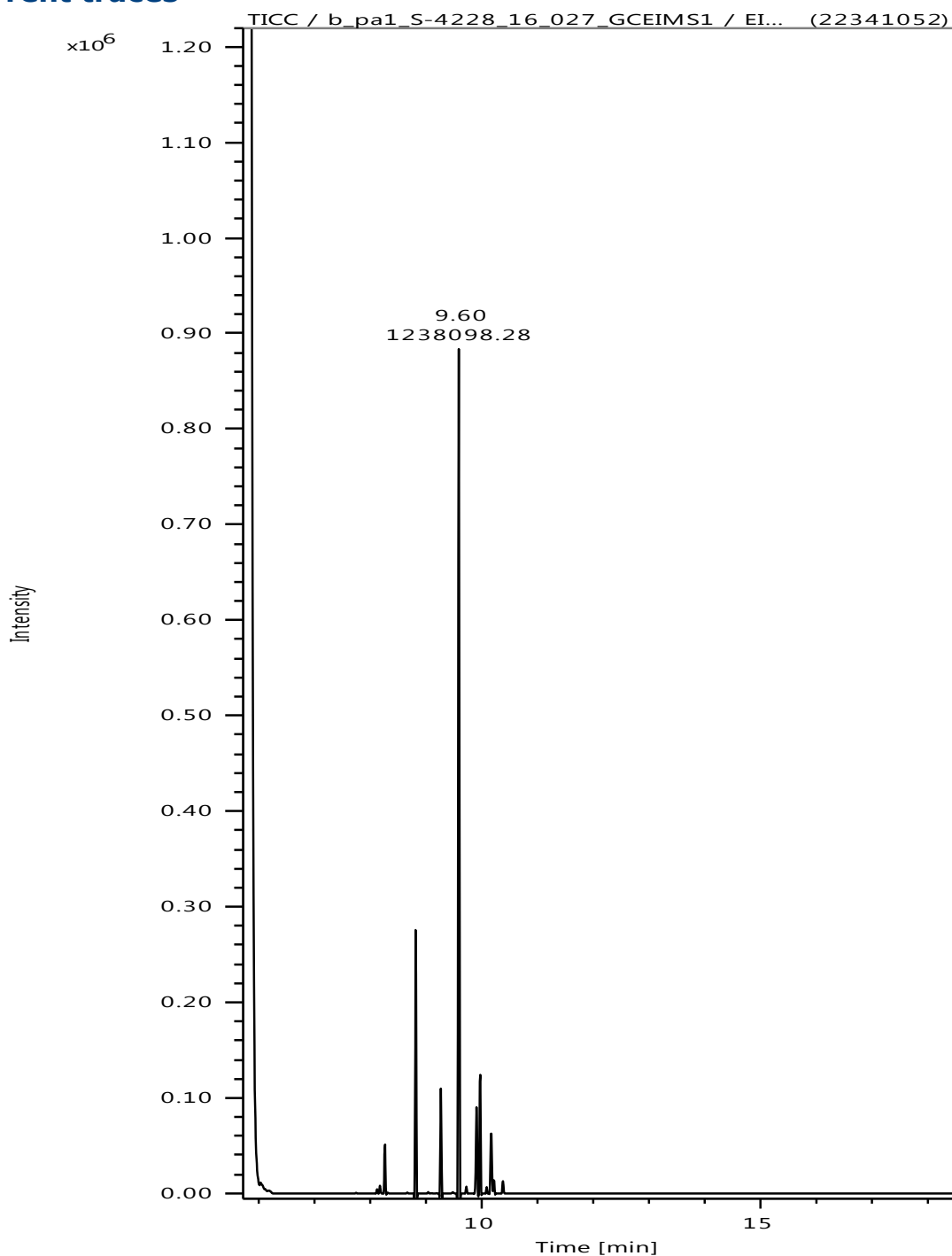


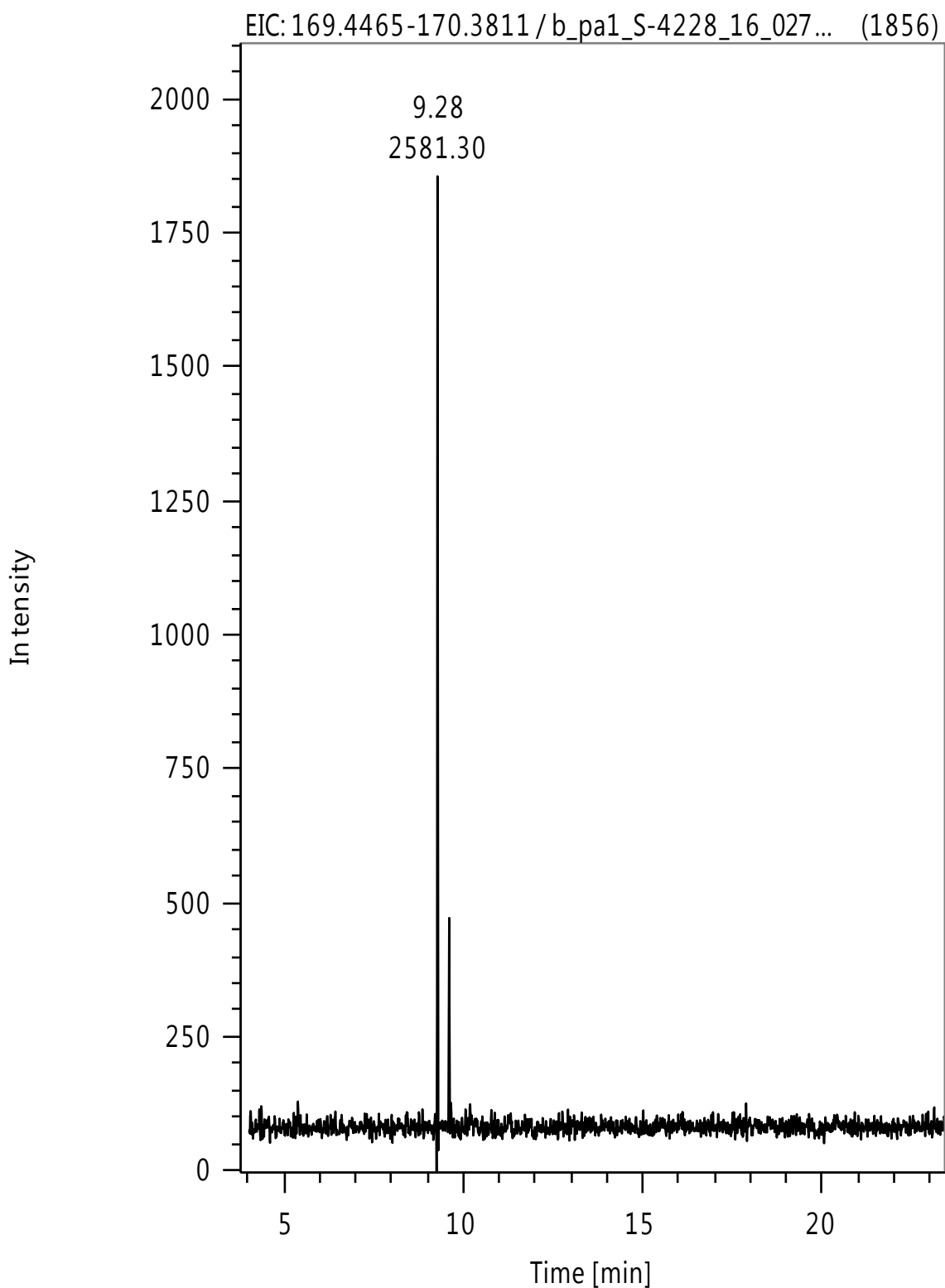
GC-EIMS analysis of 16-027

B Partridge

Ion Current traces



Total Ion Current (TIC) trace

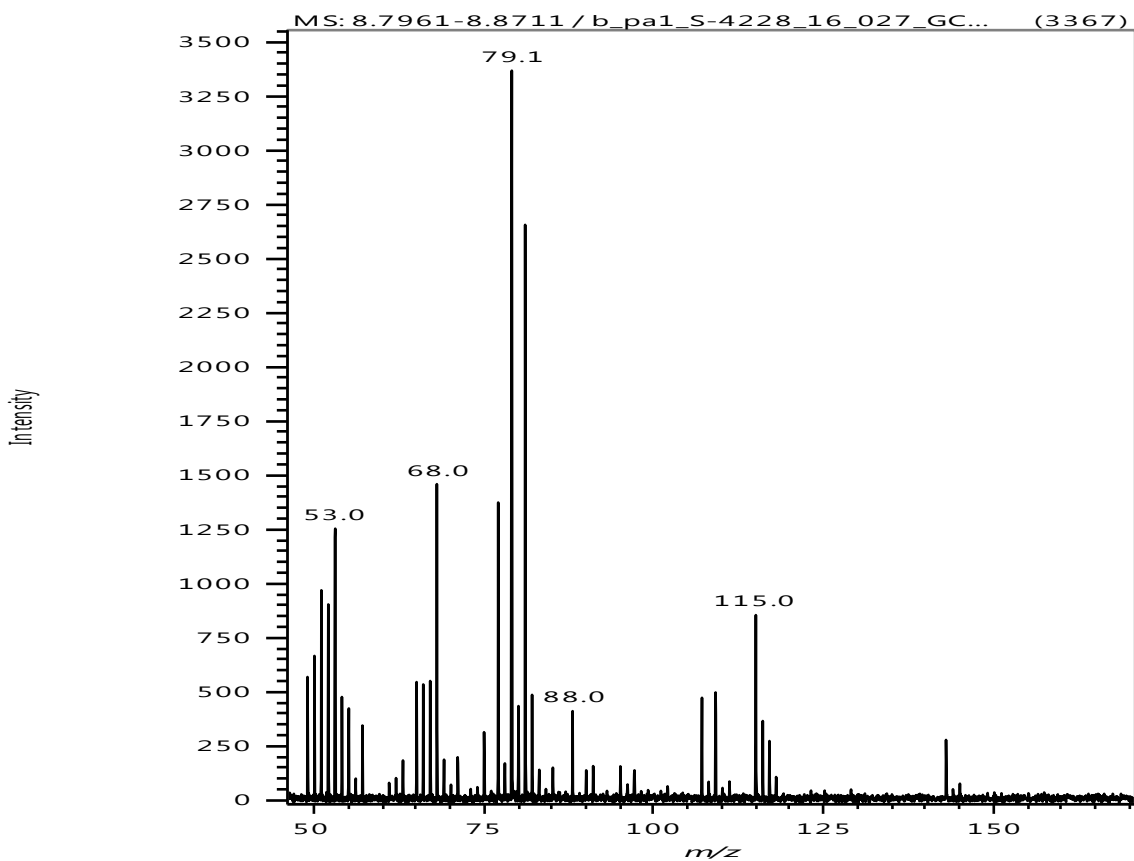
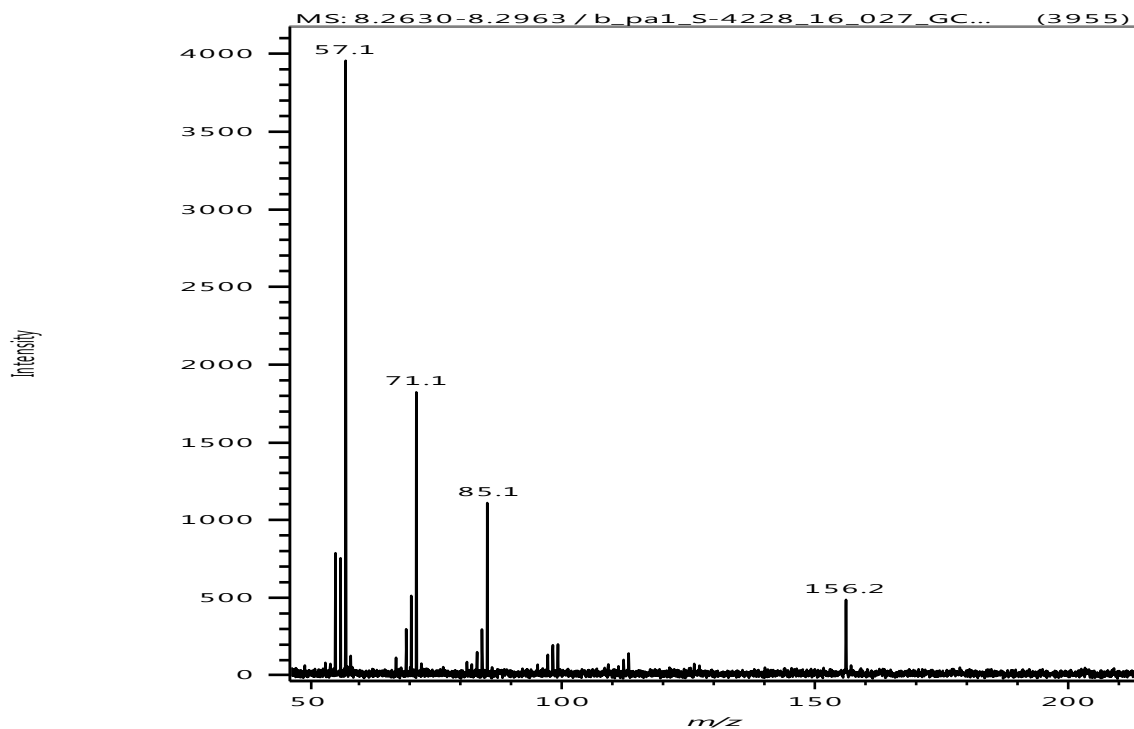


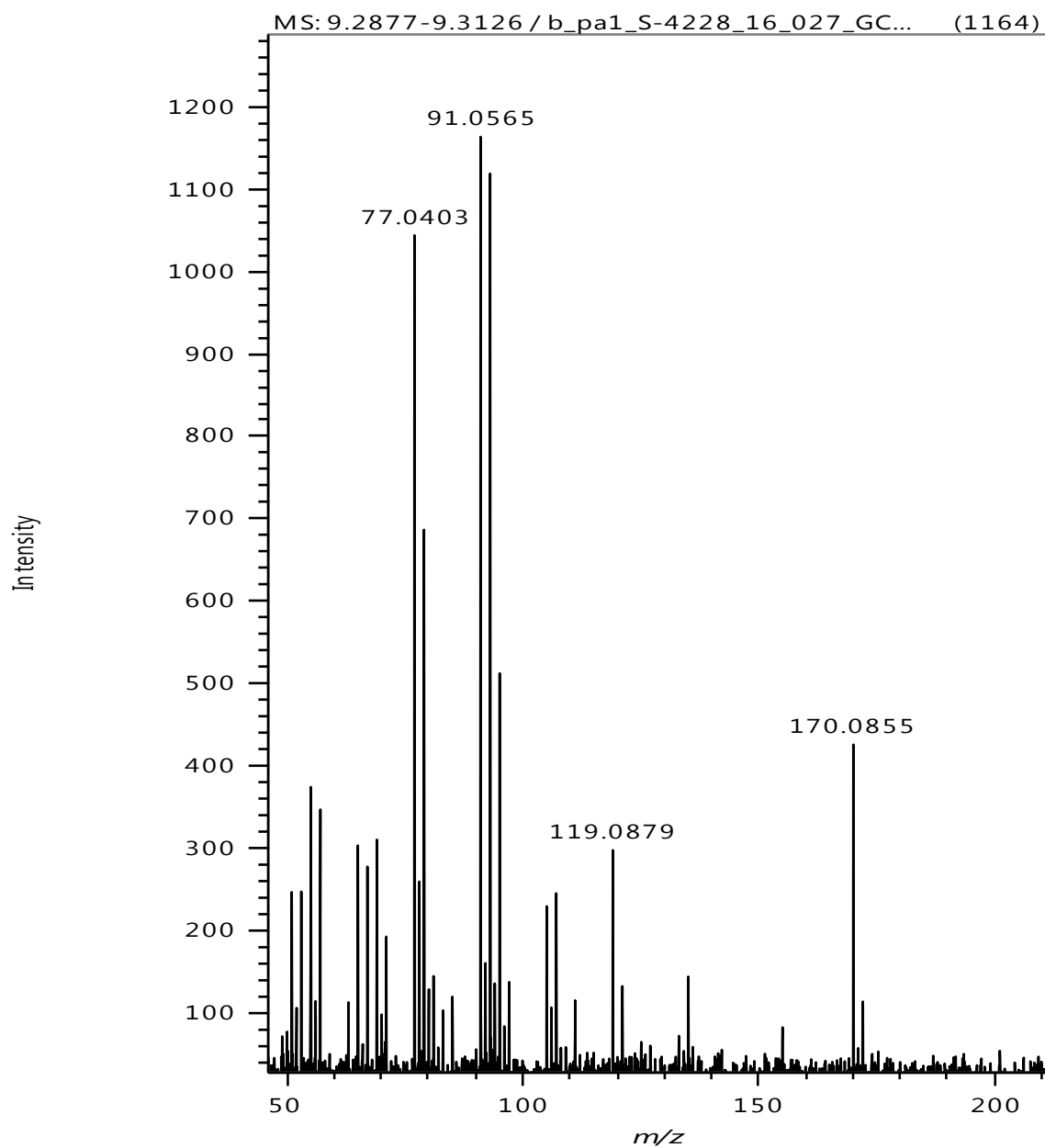
Extracted Ion Current (EIC) trace for target m/z 170 $C_{10}H_{15}Cl$

Chromatographic information

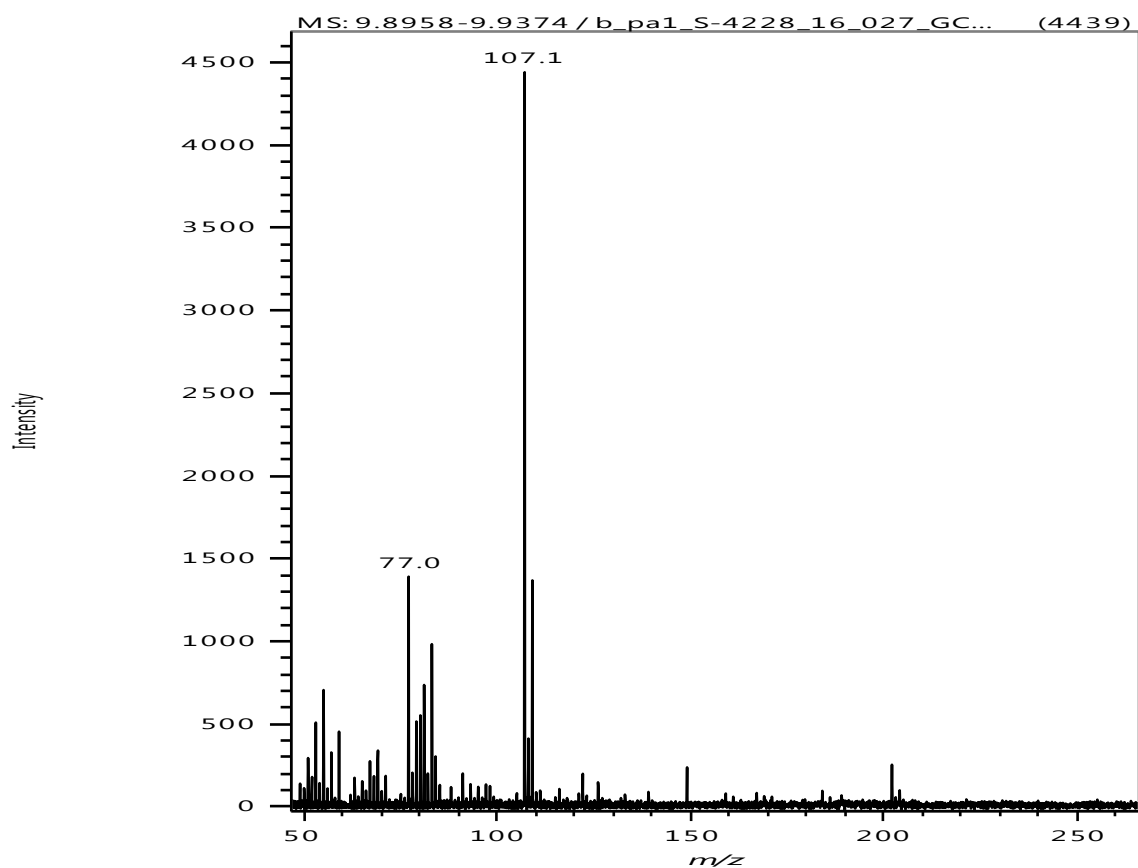
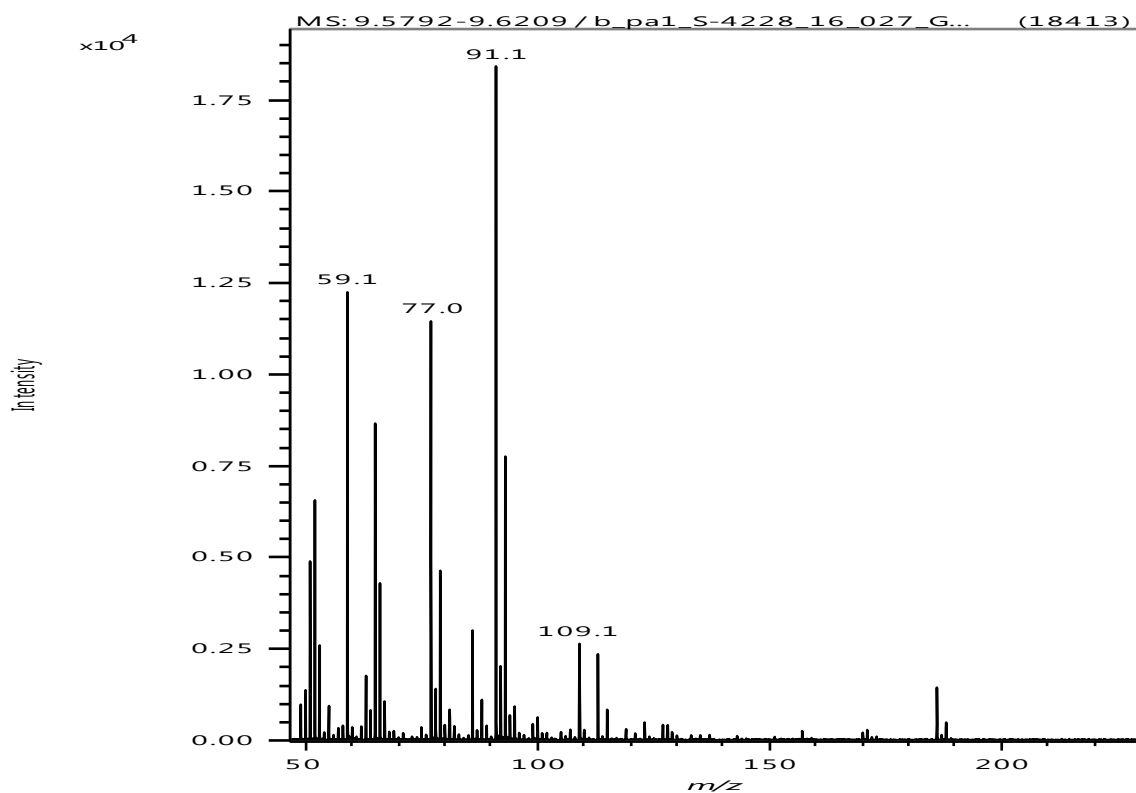
No.	Time [min]	Type	Area	Area [%]	Area [% of Total]	Height	Start [min]	End [min]
1	8.2796	BB	73317.72	6.02	3.22	51965.68	8.2547	8.3046
2	8.8295	BB	384693.72	31.59	16.87	278395.67	8.7961	8.8545
3	9.2793	BB	151557.90	12.45	6.65	113976.99	9.2543	9.3043
4	9.6042	BB	1217684.75	100.00	53.40	901396.70	9.5709	9.6292
5	9.9208	BB	140988.73	11.58	6.18	91828.79	9.8791	9.9458
6	9.9874	BB	170629.40	14.01	7.48	123017.35	9.9624	10.0041
7	10.1790	BB	106394.70	8.74	4.67	61651.83	10.1540	10.2124
8	10.2290	BB	16992.89	1.40	0.75	12892.19	10.2124	10.2540
9	10.3956	BB	17908.43	1.47	0.79	12662.23	10.3706	10.4206

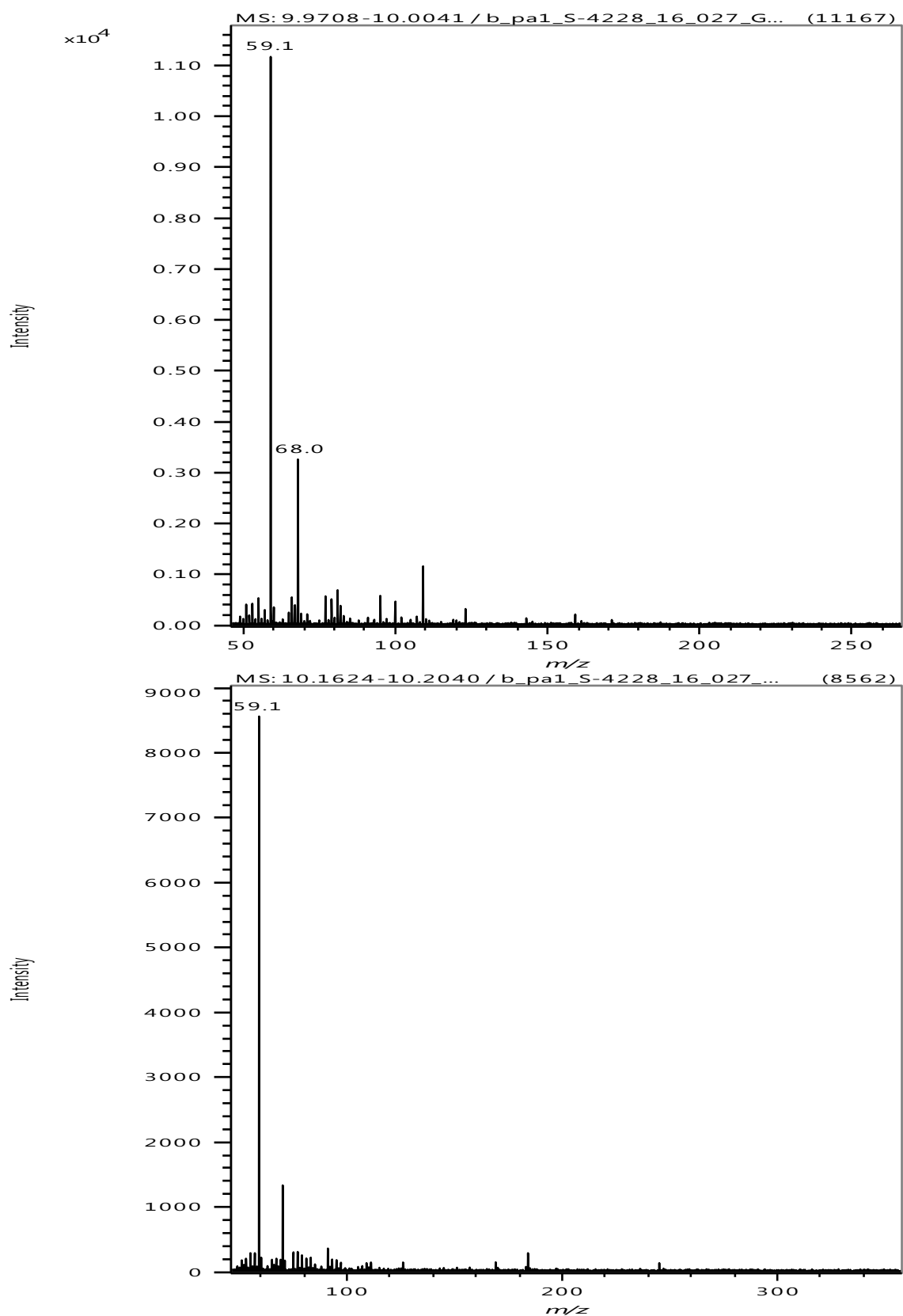
Mass spectral information





Mass	Formula	Calculated Mass	Mass Difference [ppm]	DBE
170.08555	C ₁₀ H ₁₅ Cl	170.08568	-0.78	3.0
	C ₉ H ₁₄ O ₃	170.09375	-48.21	3.0





Instrument Parameters

Electron Ionisation

Acquisition mass range 50-500Da

MS Ion Source conditions:

Temperature: 150°C

Ionisation energy: 70eV

Mass Calibration by PFK

Chromatography conditions:

GC column: J&W DB-5MS 30m x 0.25mm x 25um

Column temperature programme: 40°C to 350°C @ 25°C min⁻¹

Carrier gas: Helium

Inlet temperature: 150°C

Transfer line temperature: 150°C

Instrument:

Mass Spectrometer: JEOL AccuTOF GCX (JEOL Ltd., Tokyo, Japan)

Gas Chromatograph: Agilent 7890B (Agilent Technologies Inc, Wilmington, USA)

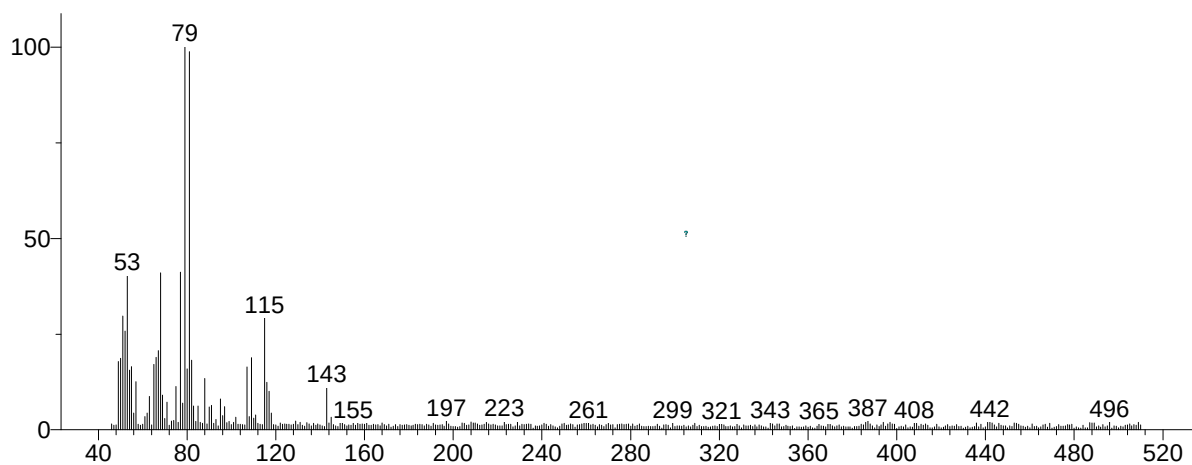
Library Search results

on following pages

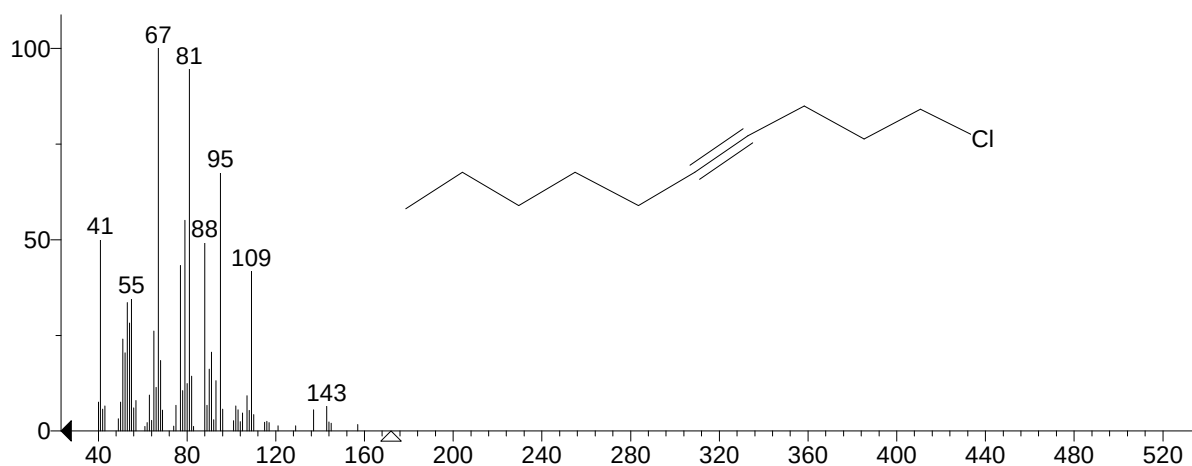
Notes

Generally a weak chromatogram. Target molecule observed and accurately mass measured. Some other components have library search results, some were too indeterminate to give sensible matches. Some components also contain Cl (8.8, 9.3 [target], 9.6 & 9.9 min

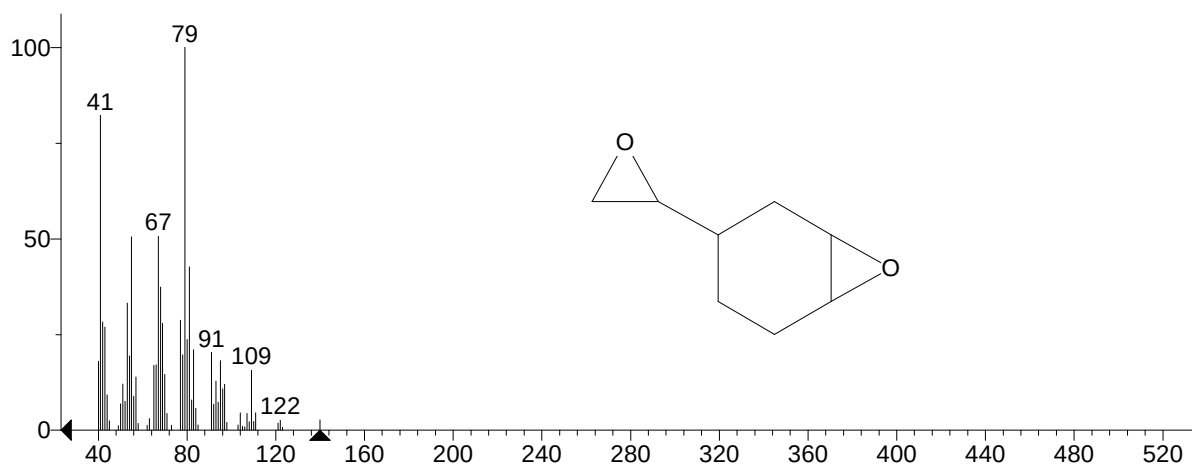
Unknown: MS: 8.7961-8.8711 / b_pa1_S-4228_16_027_GCEIMS1 / b_pa1 / Jan2016a
Compound in Library Factor = -441



Hit 1 : 1-Chloro-4-decyne
C₁₀H₁₇Cl; MF: 750; RMF: 772; Prob 41.4%; CAS: 26817-65-2; Lib: mainlib; ID: 32863.

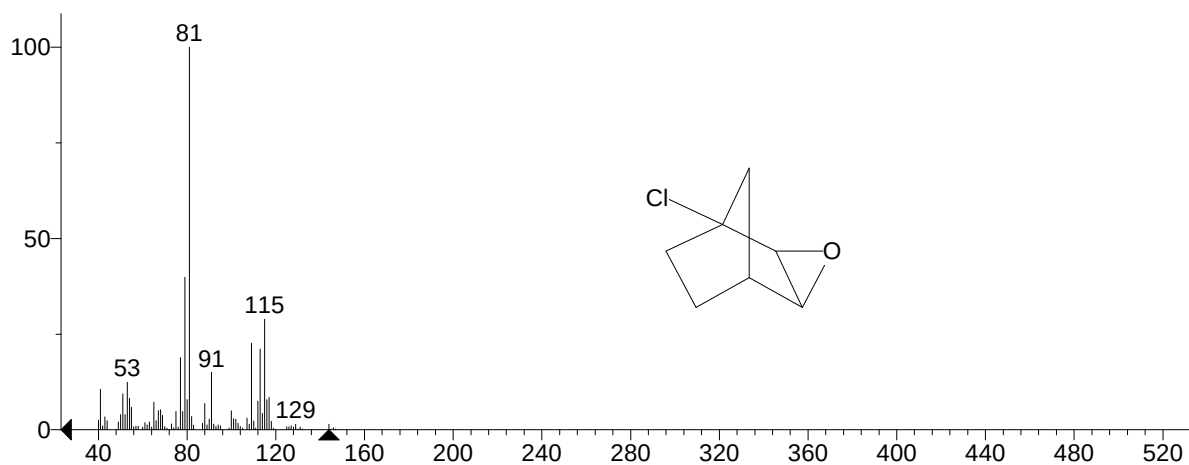


Hit 2 : 7-Oxabicyclo[4.1.0]heptane, 3-oxiranyl-
C₈H₁₂O₂; MF: 700; RMF: 790; Prob 8.42%; CAS: 106-87-6; Lib: mainlib; ID: 48494.



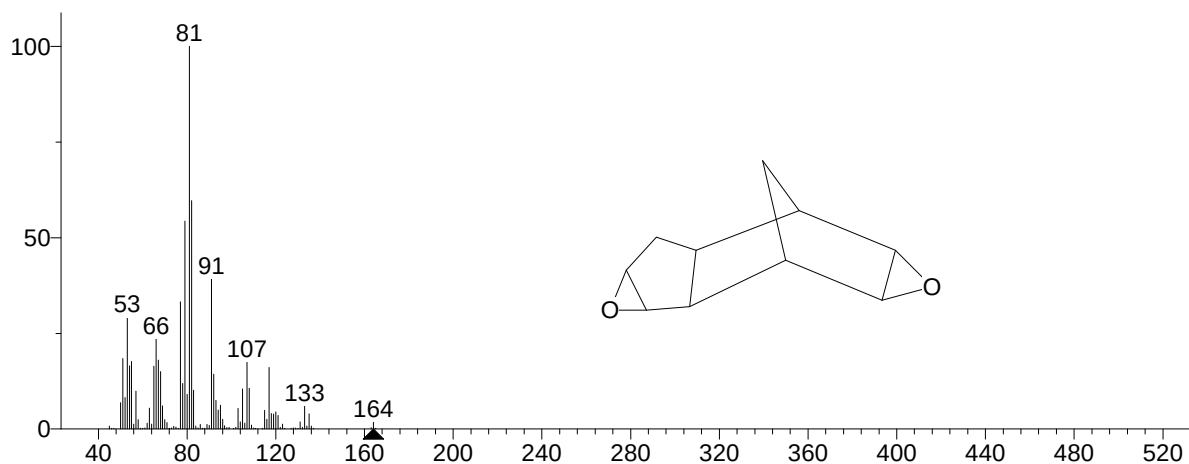
Hit 3 : 1-Chloro-3-oxatricyclo[3.2.1.0(2,4)]octane

C₇H₉ClO; MF: 698; RMF: 727; Prob 7.76%; Lib: mainlib; ID: 50281.



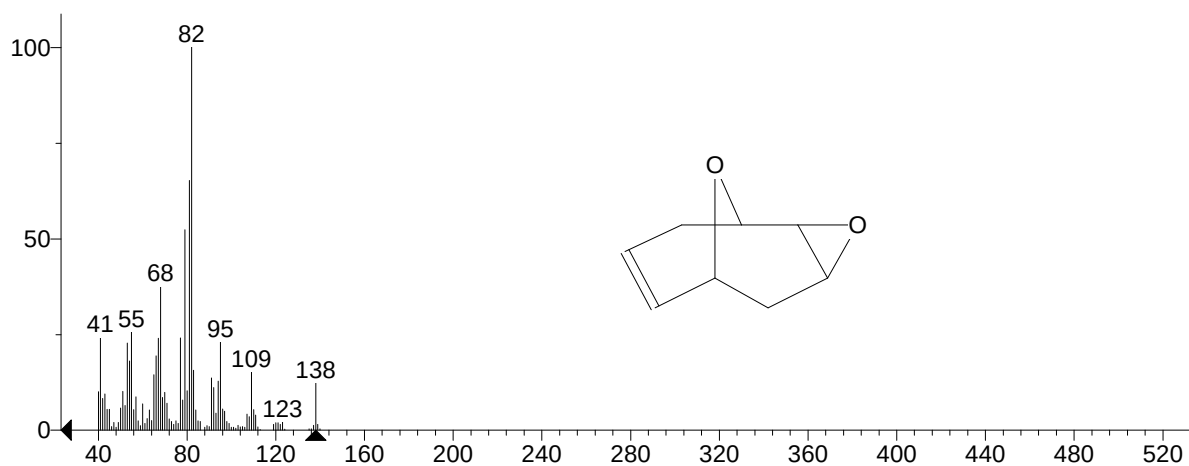
Hit 4 : Dicyclopentadiene diepoxide

C₁₀H₁₂O₂; MF: 694; RMF: 719; Prob 6.56%; CAS: 81-21-0; Lib: mainlib; ID: 50379.

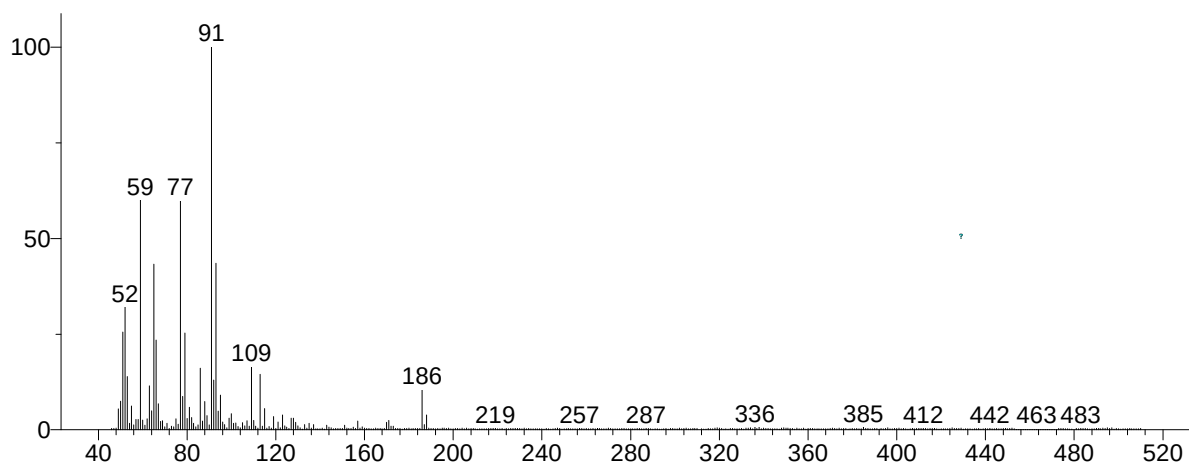


Hit 5 : 3,10-Dioxatricyclo[4.3.1.0(2,4)]dec-7-ene

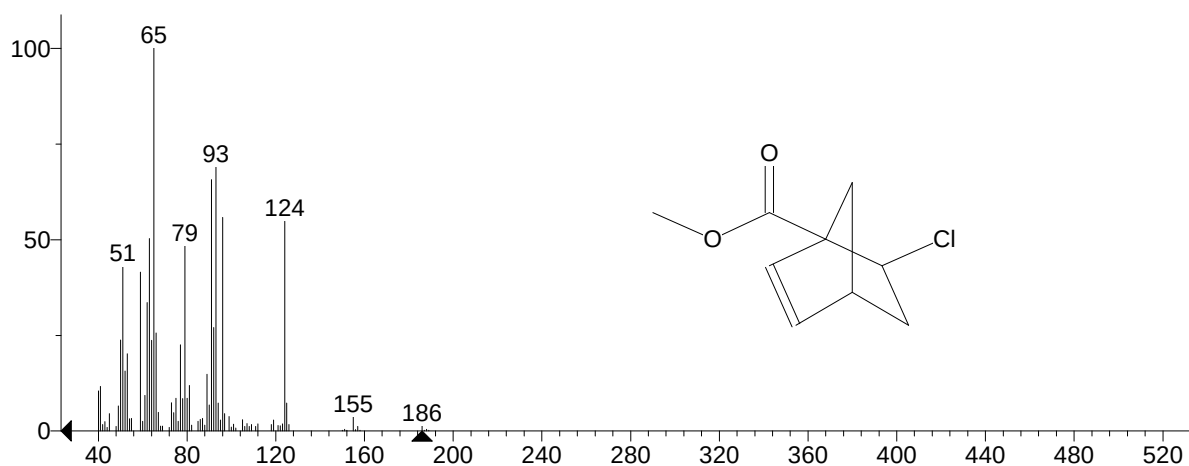
C₈H₁₀O₂; MF: 685; RMF: 744; Prob 4.76%; Lib: mainlib; ID: 51425.



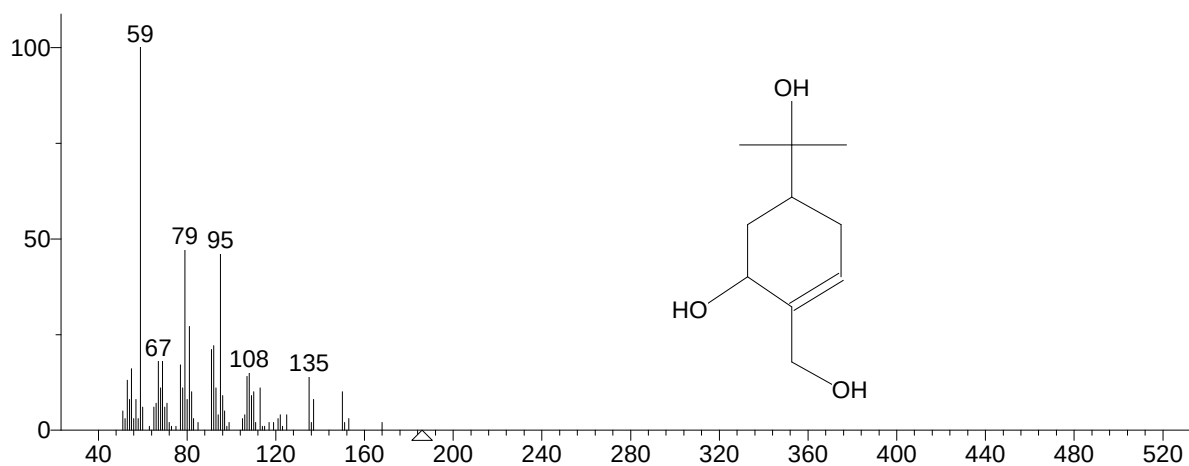
Unknown: MS: 9.5792-9.6209 / b_pa1_S-4228_16_027_GCEIMS1 / b_pa1 / Jan2016a
Compound in Library Factor = -188



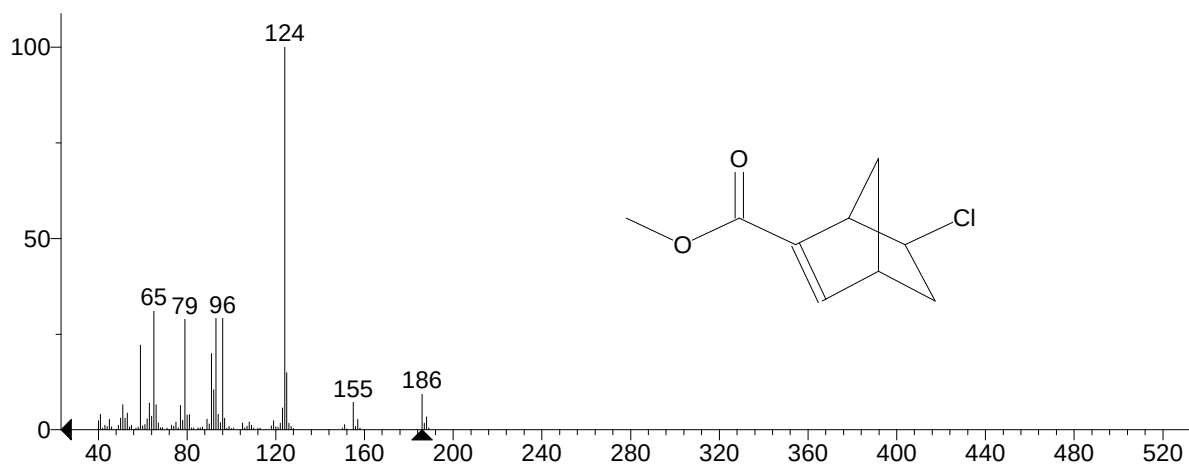
Hit 1 : Bicyclo[2.2.1]hept-2-ene-1-carboxylic acid, 6-chloro-, methyl ester, endo-
C₉H₁₁ClO₂; MF: 620; RMF: 657; Prob 76.8%; CAS: 85173-64-4; Lib: mainlib; ID: 31841.



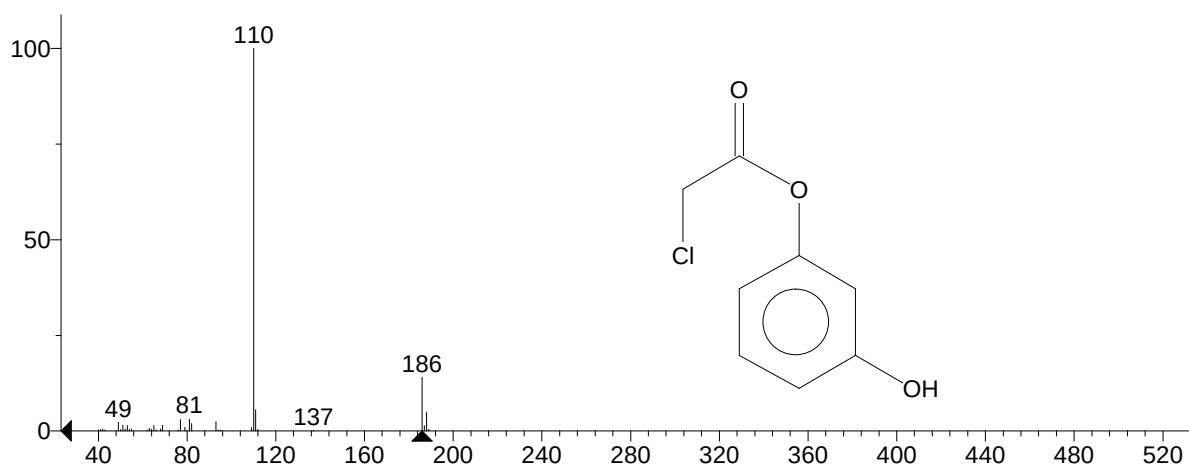
Hit 2 : 5-Hydroxy-4-hydroxymethyl-1-(1-hydroxy-1-isopropyl)cyclohex-3-ene
C₁₀H₁₈O₃; MF: 572; RMF: 614; Prob 15.9%; CAS: 87096-72-8; Lib: mainlib; ID: 30212.



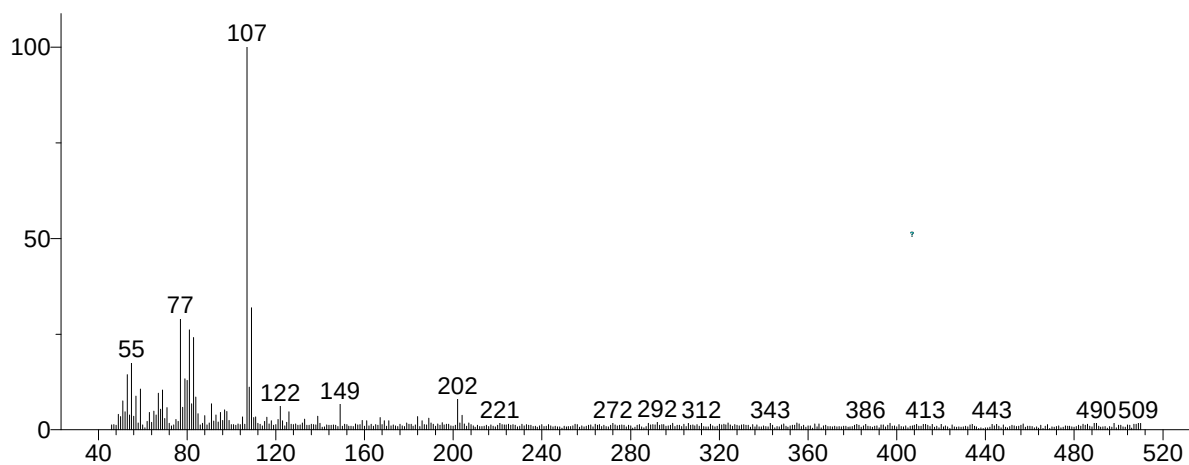
Hit 3 : 6-Chlorobicyclo[2.2.1]hept-2-ene-2-carboxylic acid, methyl ester
C₉H₁₁ClO₂; MF: 552; RMF: 559; Prob 7.24%; Lib: mainlib; ID: 107913.



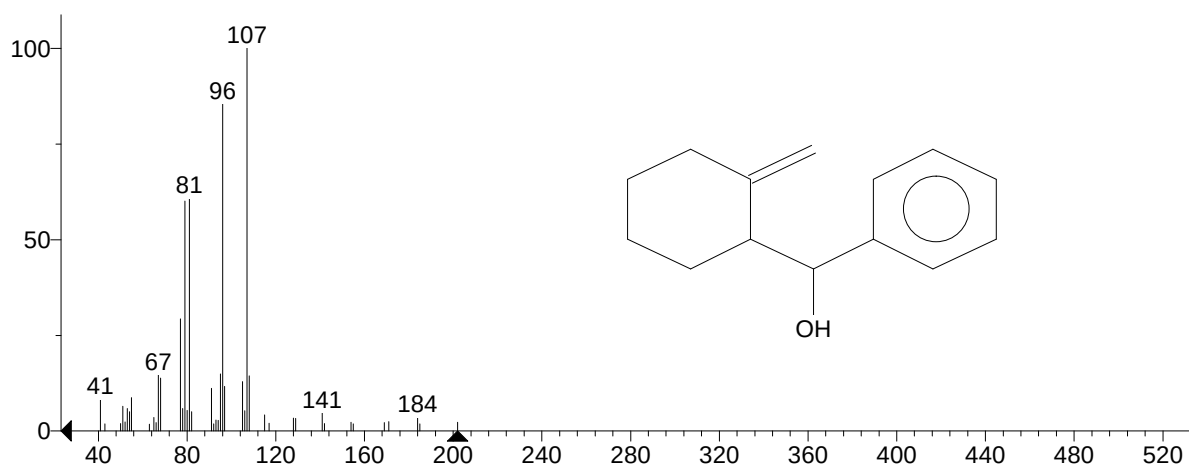
Hit 4 : 1,3-Benzenediol, O-chloroacetyl-
C₈H₇ClO₃; MF: 335; RMF: 397; Prob 0.07%; Lib: mainlib; ID: 87596.



Unknown: MS: 9.8958-9.9374 / b_pa1_S-4228_16_027_GCEIMS1 / b_pa1 / Jan2016a
Compound in Library Factor = -308



Hit 1 : (2-Methylene-cyclohexyl)-phenyl-methanol
C₁₄H₁₈O; MF: 564; RMF: 740; Prob 96.9%; CAS: 130447-40-4; Lib: mainlib; ID: 83845.



Hit 2 : (2,2-Dichlorocyclopropoxy)benzene
C₉H₈Cl₂O; MF: 421; RMF: 604; Prob 3.06%; CAS: 13764-07-3; Lib: mainlib; ID: 85812.

