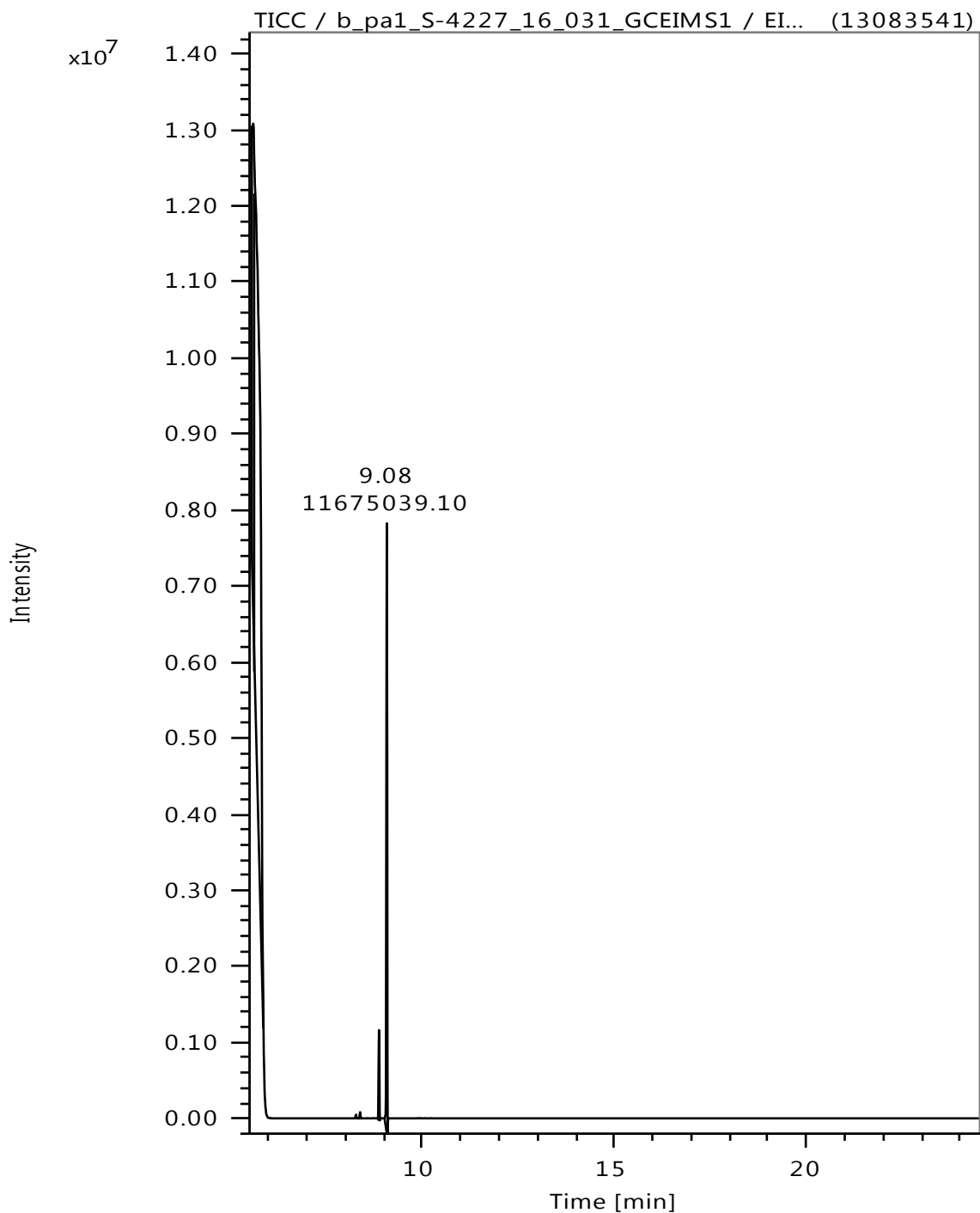


GC-EIMS analysis of 16-031

B Partridge

Ion Current traces

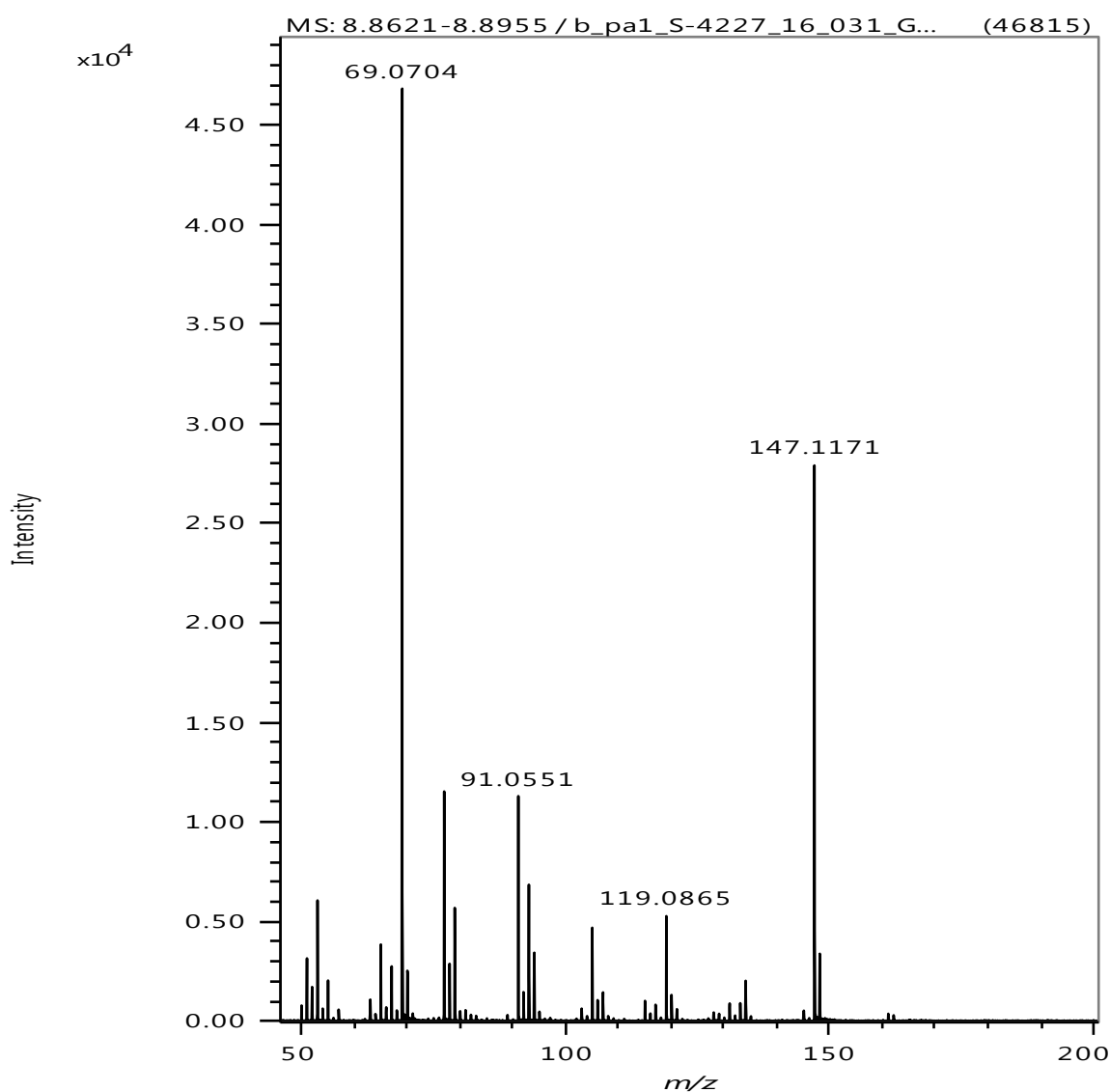


Total Ion Current (TIC) trace

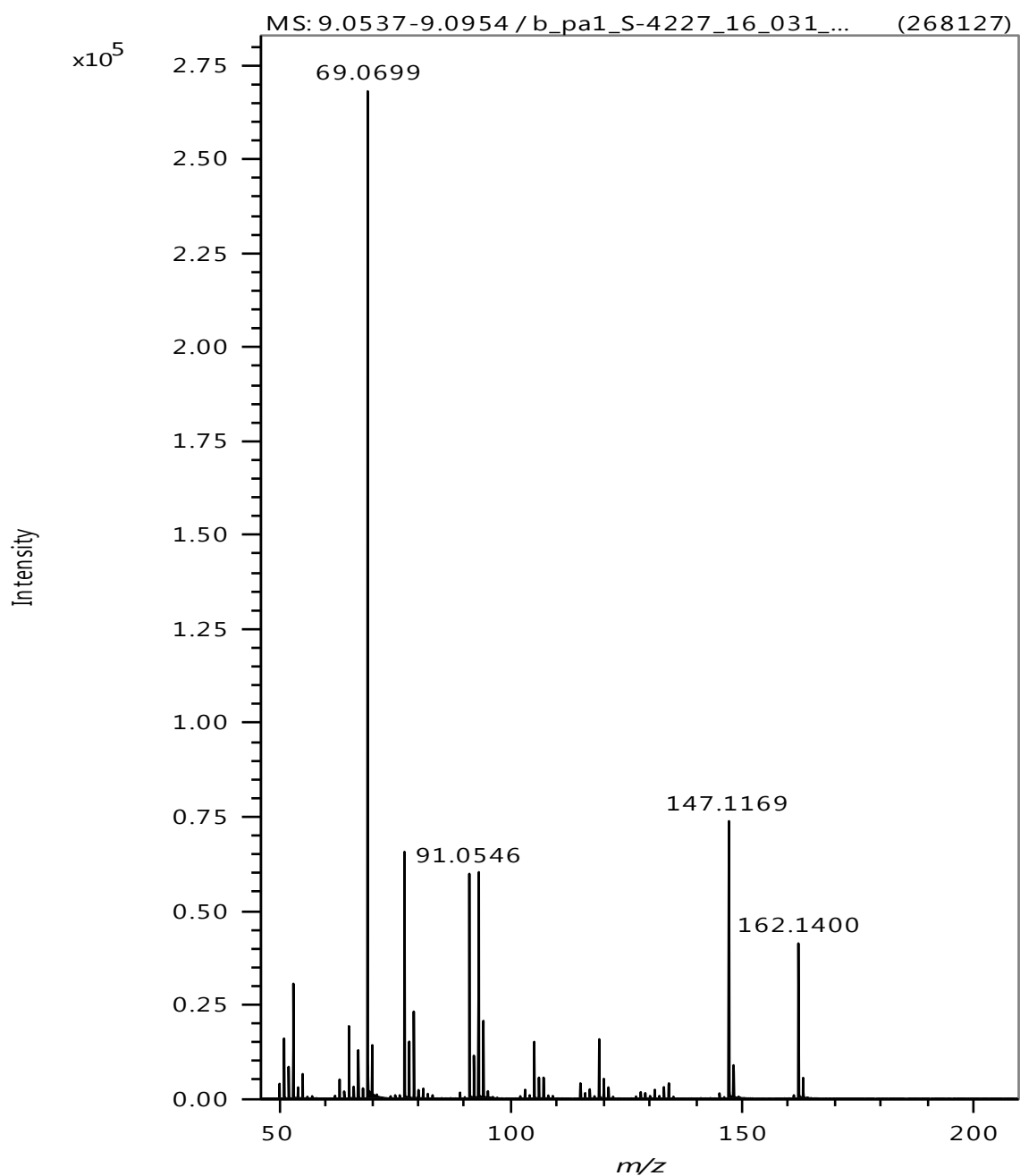
Chromatographic information

No.	Time [min]	Type	Area	Area [%]	Area [% of Total]	Height	Start [min]	End [min]
1	8.8788	BB	1640791.33	14.62	12.76	1182516.48	8.8538	8.9038
2	9.0787	BB	11220676.86	100.00	87.24	7827570.46	9.0204	9.1287

Mass spectral information



Mass	Formula	Calculated Mass	Mass Difference [ppm]	DBE
147.11713	C11 H15	147.11683	2.06	4.5



Mass	Formula	Calculated Mass	Mass Difference [ppm]	DBE
162.14000	C12 H18	162.14030	-1.88	4.0

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)

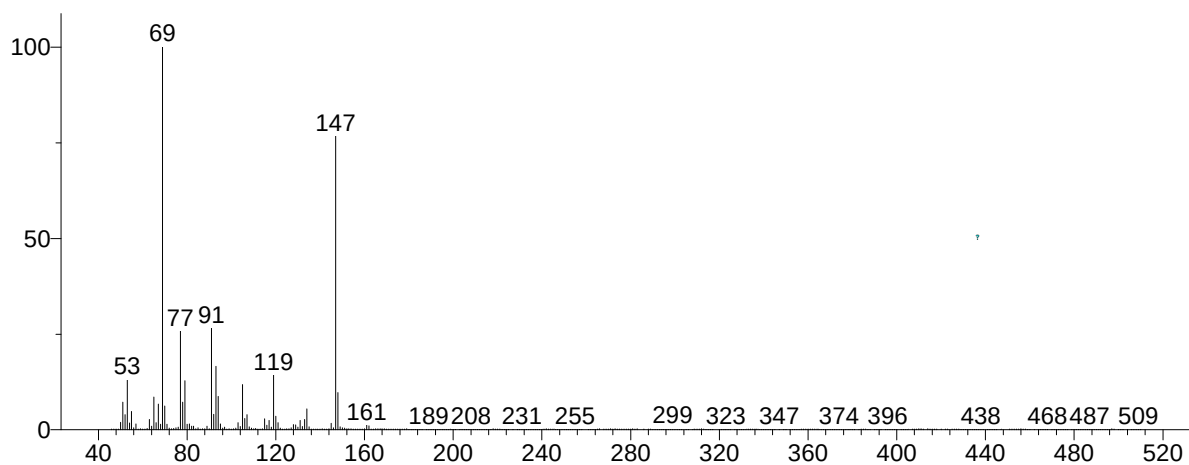
Library Search results

on following pages

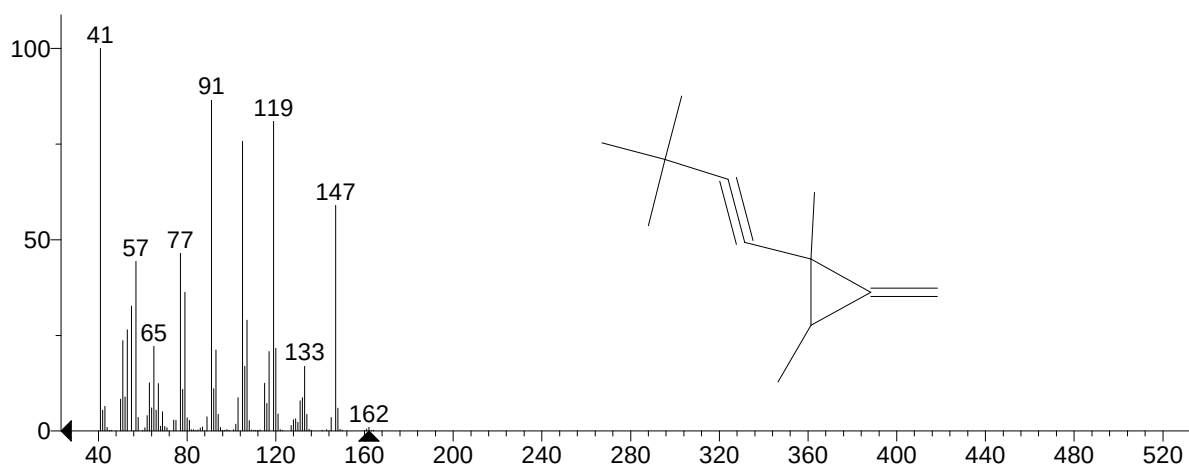
Notes

Some similarity in spectra from the 2 chromatographic peaks. One yields a molecular ion (9.0 min), but the other (8.8 min) doesn't, only showing the m/z 147 ion, C₁₁H₁₅.

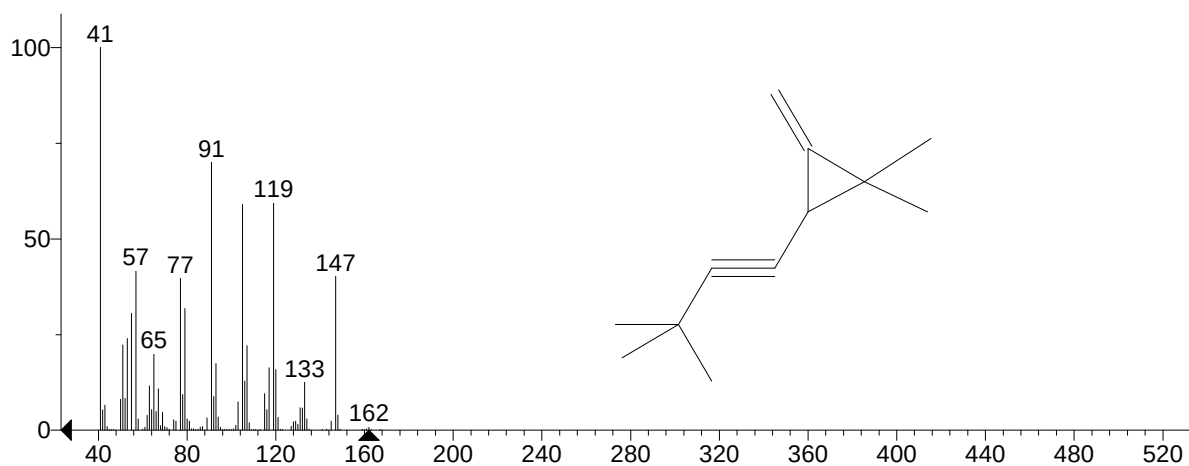
Unknown: MS: 8.8621-8.8955 / b_pa1_S-4227_16_031_GCEIMS1 / b_pa1 / Jan2016a
Compound in Library Factor = -639



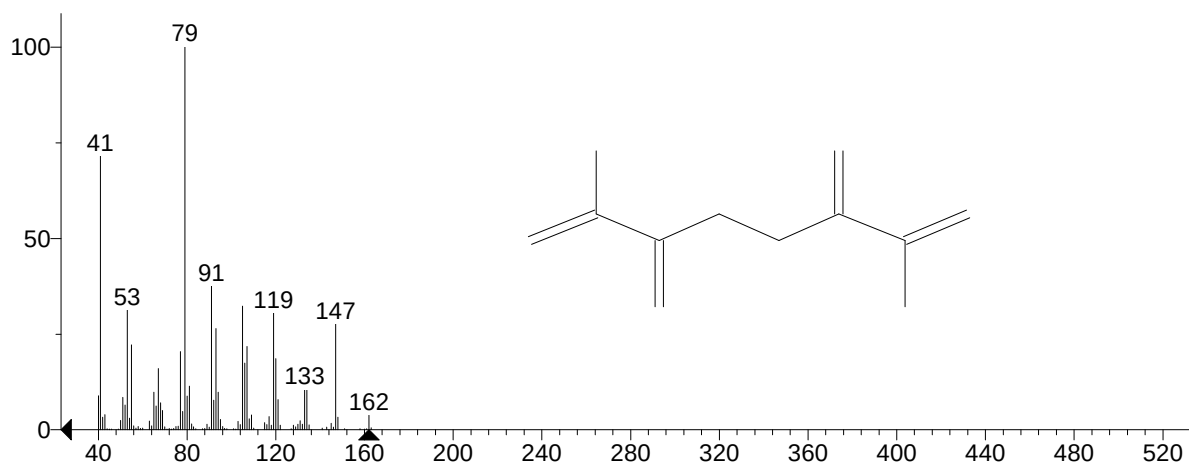
Hit 1 : 1-(3,3-Dimethyl-but-1-ynyl)-1,2-dimethyl-3-methylene-cyclopropane
C₁₂H₁₈; MF: 724; RMF: 724; Prob 21.8%; Lib: mainlib; ID: 3773.



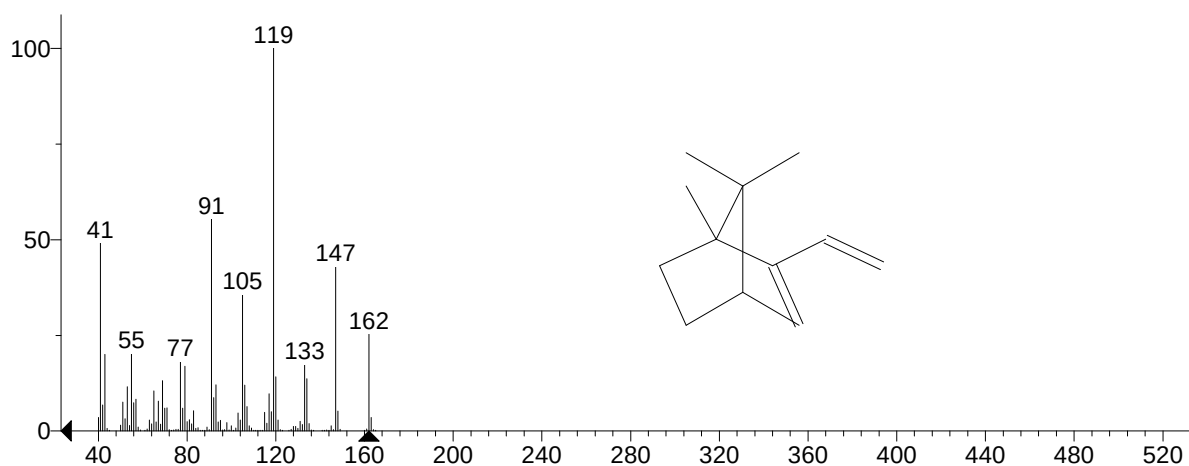
Hit 2 : 2-(3,3-Dimethyl-but-1-ynyl)-1,1-dimethyl-3-methylene-cyclopropane
C₁₂H₁₈; MF: 722; RMF: 722; Prob 20.1%; Lib: mainlib; ID: 3774.



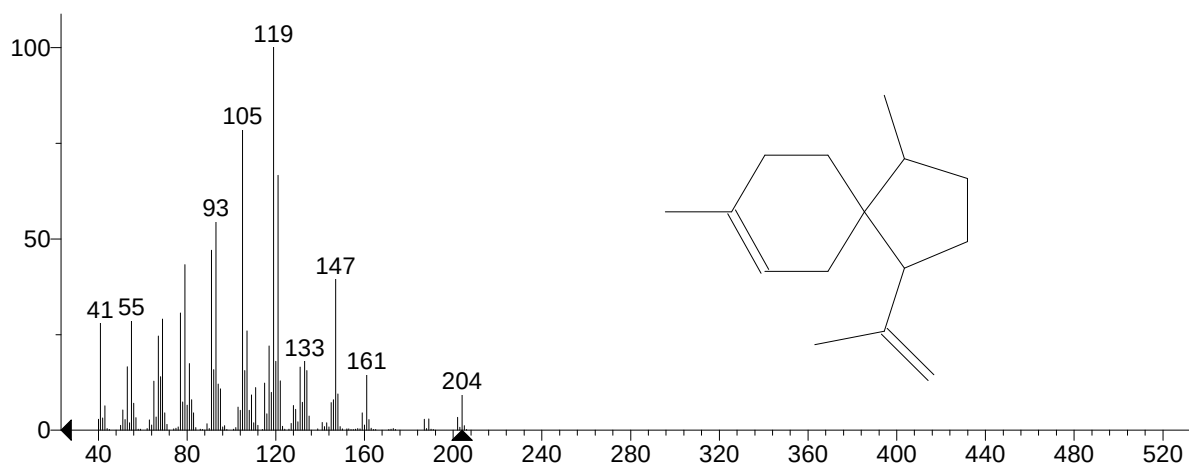
Hit 3 : 1,7-Octadiene, 2,7-dimethyl-3,6-bis(methylene)-
C₁₂H₁₈; MF: 691; RMF: 691; Prob 5.47%; CAS: 16714-60-6; Lib: mainlib; ID: 48493.



Hit 4 : 1,7,7-Trimethyl-2-vinylbicyclo[2.2.1]hept-2-ene
C₁₂H₁₈; MF: 681; RMF: 681; Prob 3.86%; CAS: 130930-56-2; Lib: mainlib; ID: 99054.

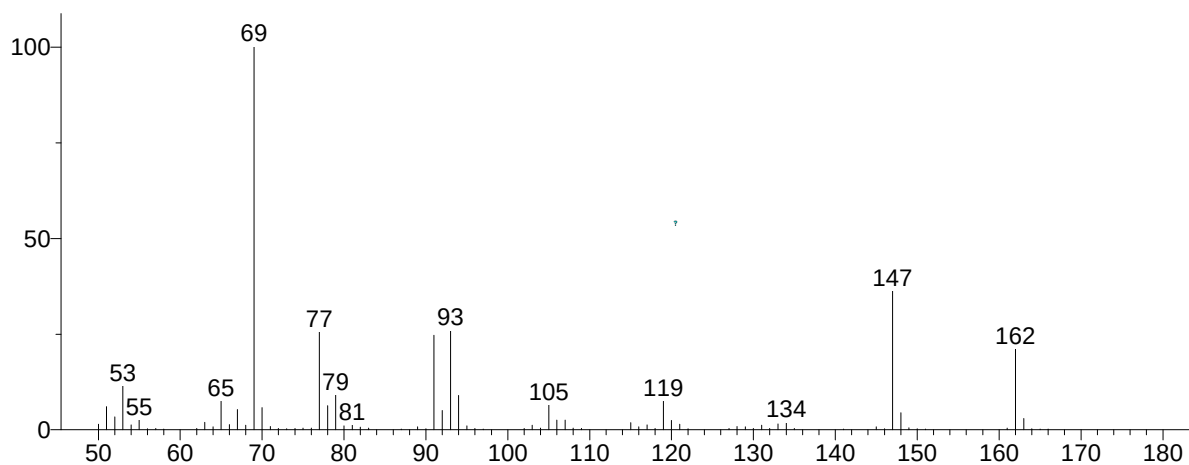


Hit 5 : (1R,4S,5S)-1,8-Dimethyl-4-(prop-1-en-2-yl)spiro[4.5]dec-7-ene
C₁₅H₂₄; MF: 681; RMF: 681; Prob 3.86%; CAS: 43219-80-3; Lib: mainlib; ID: 100091.

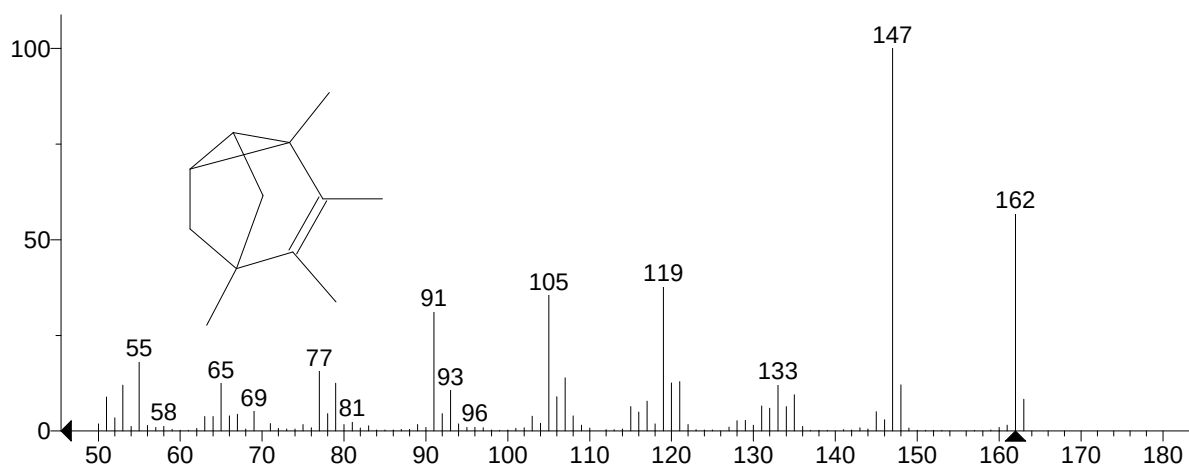


**** Search Report Page 1 of 2 ****

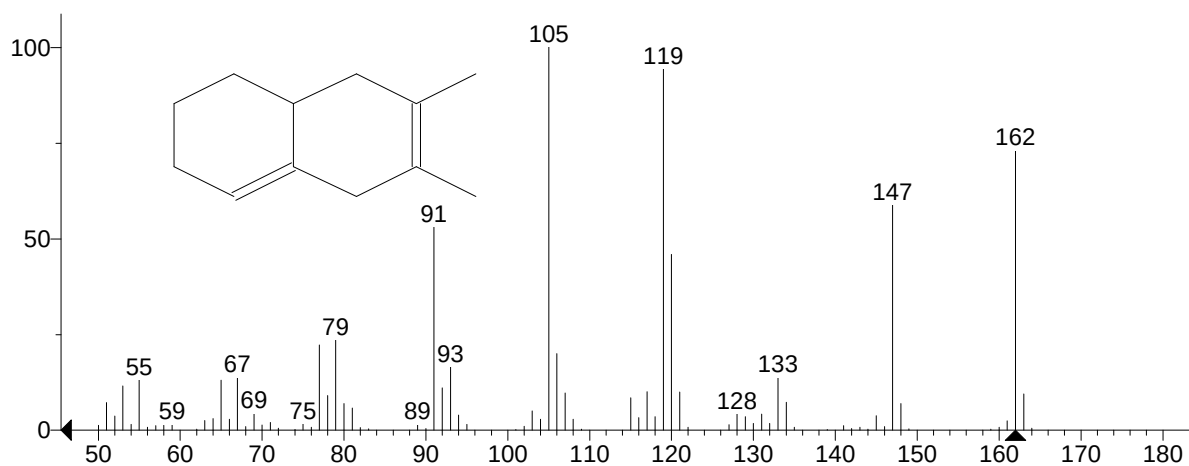
Unknown: MS: 9.0537-9.0954 / b_pa1_S-4227_16_031_GCEIMS1 / b_pa1 / Jan2016a
Compound in Library Factor = -984



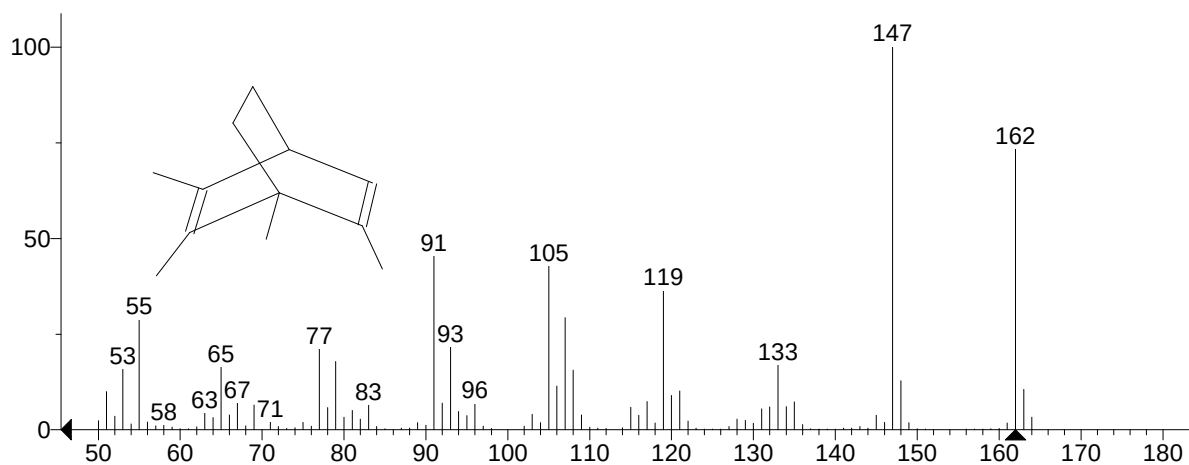
Hit 1 : Tricyclo[3.2.1.02,7]oct-3-ene, 2,3,4,5-tetramethyl-
C₁₂H₁₈; MF: 703; RMF: 707; Prob 14.3%; CAS: 62338-44-7; Lib: mainlib; ID: 135502.



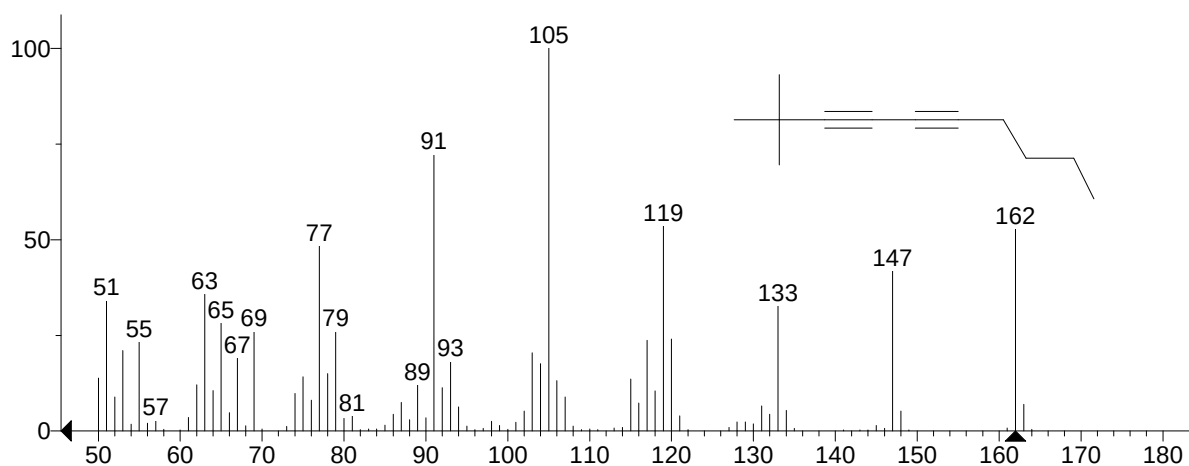
Hit 2 : 6,7-Dimethyl-1,2,3,5,8,8a-hexahydronaphthalene
C₁₂H₁₈; MF: 693; RMF: 693; Prob 10.1%; CAS: 107914-92-1; Lib: mainlib; ID: 80865.



Hit 3 : Bicyclo[2.2.2]octa-2,5-diene, 1,2,3,6-tetramethyl-
C₁₂H₁₈; MF: 692; RMF: 696; Prob 9.73%; CAS: 62338-43-6; Lib: mainlib; ID: 135497.



Hit 4 : 3,5-Decadiyne, 2,2-dimethyl-
C₁₂H₁₈; MF: 687; RMF: 687; Prob 7.84%; CAS: 55682-73-0; Lib: mainlib; ID: 80322.



Hit 5 : 2(1H)-Naphthalenone, 4a,5,8,8a-tetrahydro-4a-methyl-, trans-
C₁₁H₁₄O; MF: 682; RMF: 682; Prob 6.32%; CAS: 17429-21-9; Lib: mainlib; ID: 49586.

