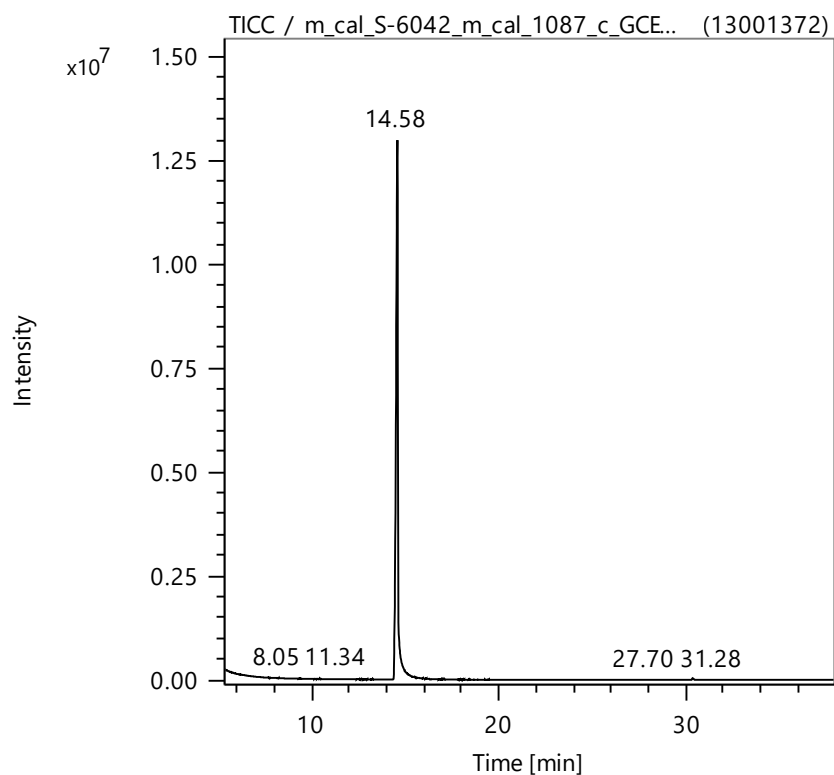


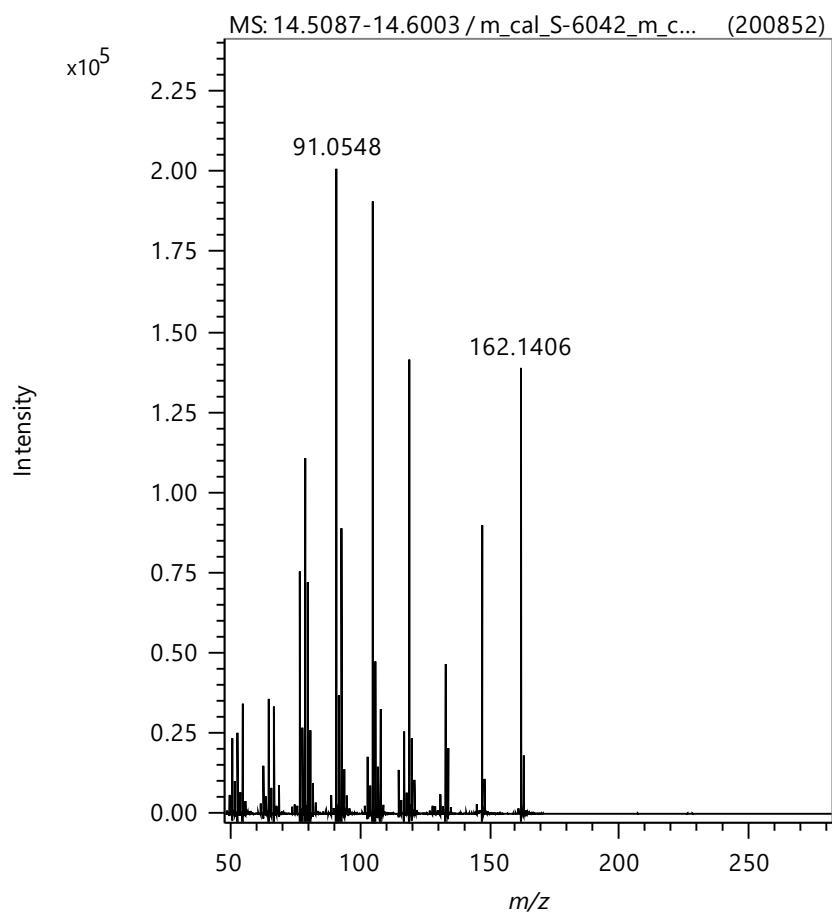
GC-EIMS analysis of m_cal 1087-c polar GC column

M Callingham

Chromatographic information



Mass spectral information



Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
162.14057	C12 H18	162.14030	0.27	1.68	4.0
	C8 H18 O3	162.12505	15.53	95.77	0.0
	C11 H14 O	162.10392	36.66	226.08	5.0

Library Search results

On following pages

Analysis information

Instrument

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

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

Acquisition mass range: 40-300Da

Mass Calibration by PFTBA

MS Ion Source conditions:

Electron Ionisation

Ionisation energy: 70eV Temperature: 150°C

Chromatography conditions:

GC column: Thermo Scientific TG POLAR 30m x 0.25mm x 25um

Column temperature programme: 50°C (4min) to 260°C @ 5°C min⁻¹

Carrier gas: Helium

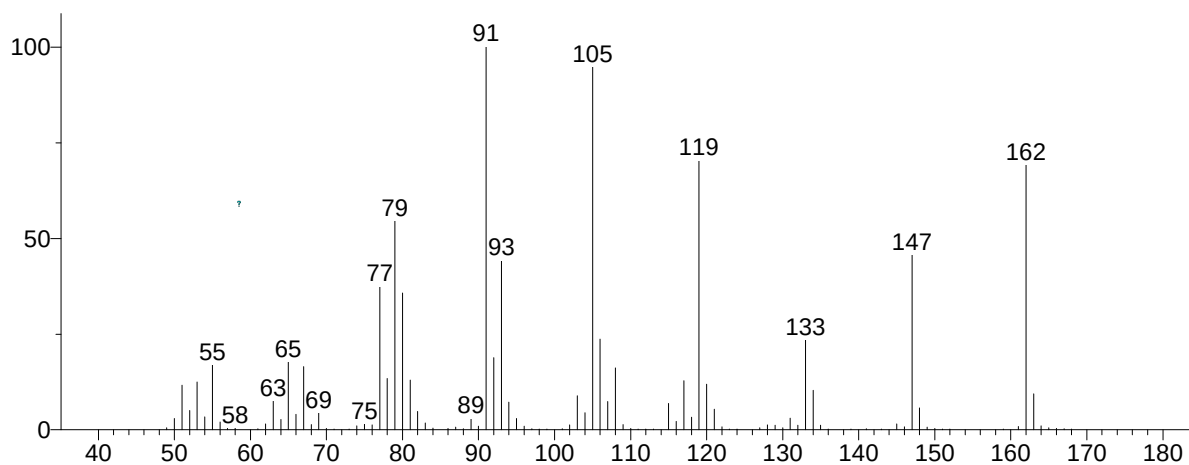
Inlet temperature: 200°C

Transfer line temperature: 180°C

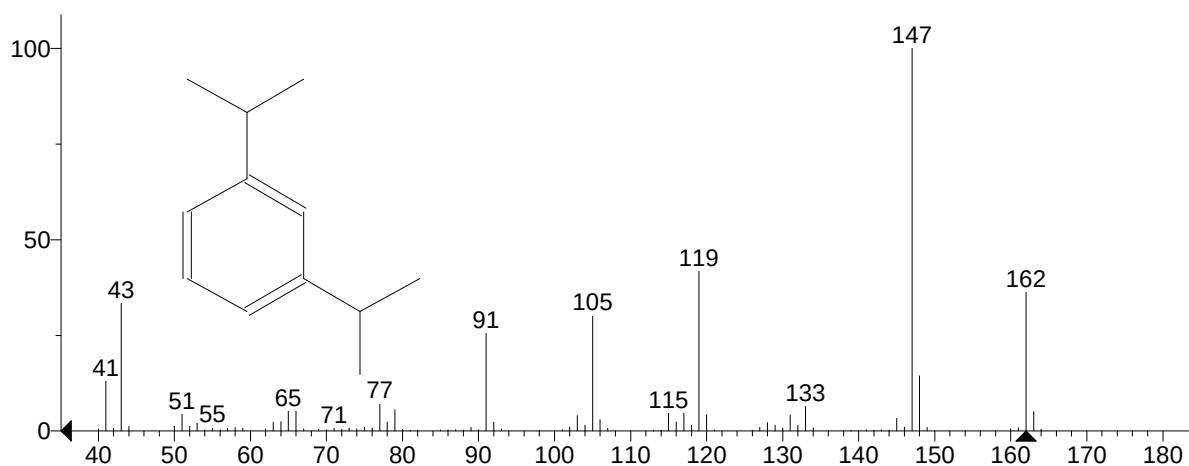
Notes

** Search Report Page 1 of 2 **

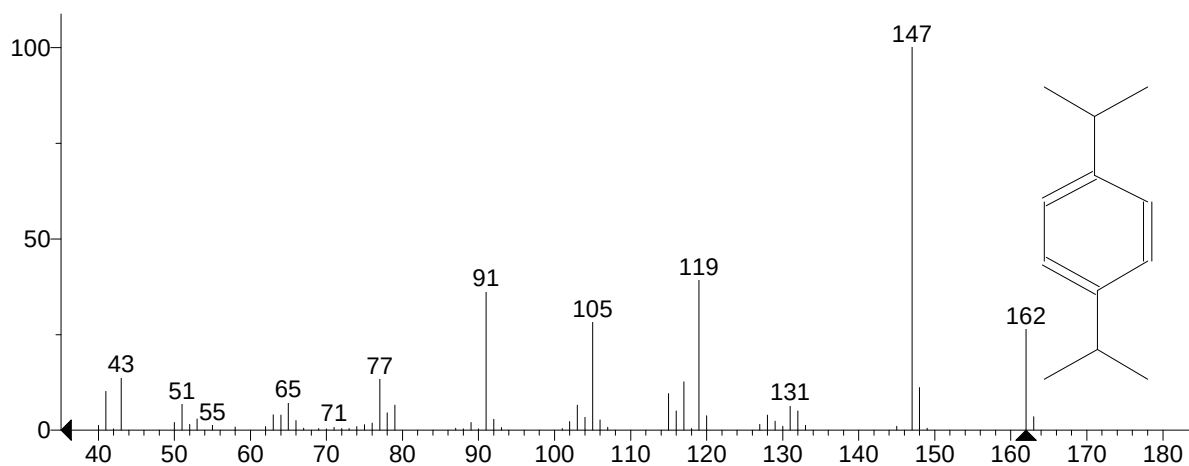
Unknown: MS: 14.5087-14.6003 / m_cal_S-6042_m_cal_1087_c_GCEIMS1 / m_cal / August2017
Compound in Library Factor = -521



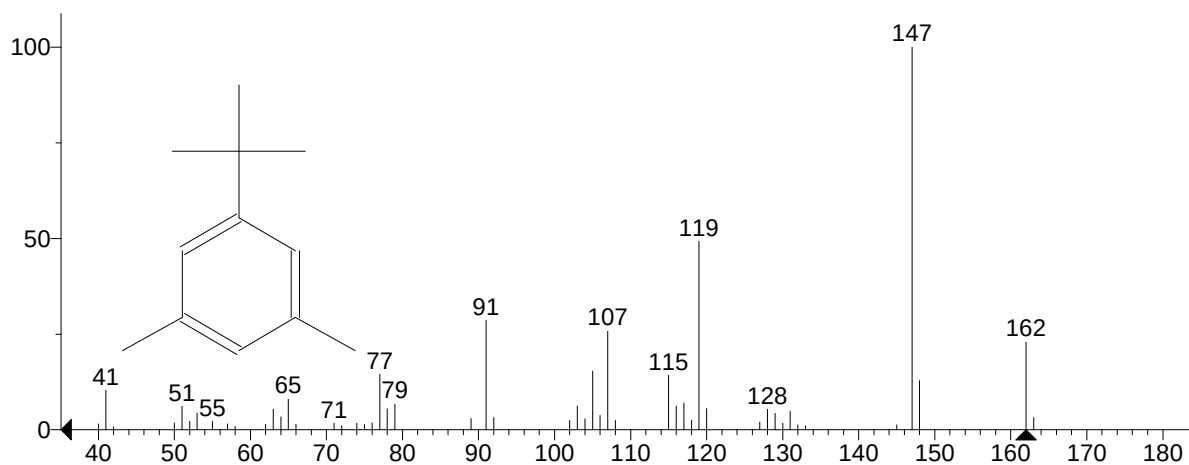
Hit 1 : Benzene, 1,3-bis(1-methylethyl)-
C₁₂H₁₈; MF: 734; RMF: 750; Prob 60.5%; CAS: 99-62-7; Lib: nistdemo; ID: 424.



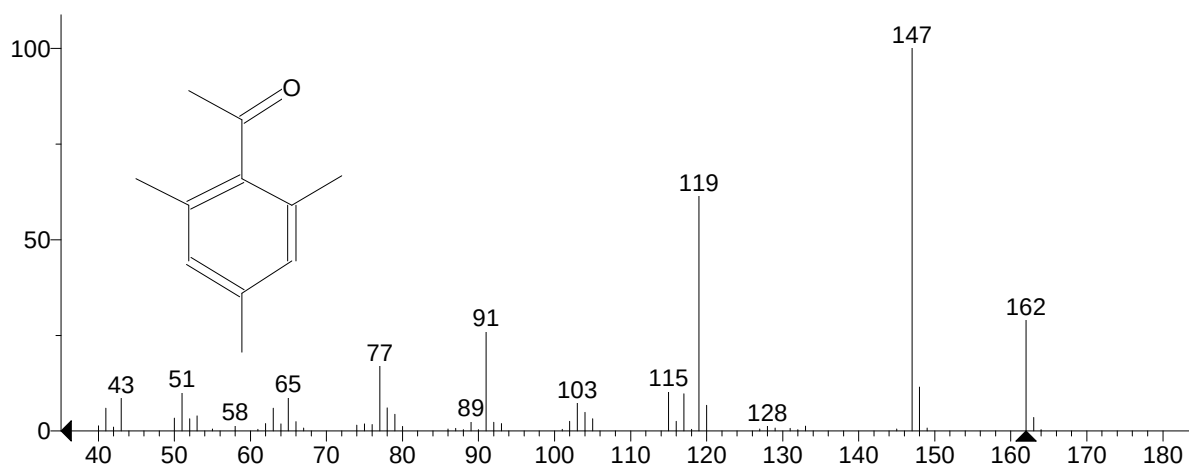
Hit 2 : Benzene, 1,4-bis(1-methylethyl)-
C₁₂H₁₈; MF: 694; RMF: 744; Prob 14.0%; CAS: 100-18-5; Lib: nistdemo; ID: 833.



Hit 3 : Benzene, 1-(1,1-dimethylethyl)-3,5-dimethyl-
C₁₂H₁₈; MF: 688; RMF: 759; Prob 11.0%; CAS: 98-19-1; Lib: nistdemo; ID: 1335.



Hit 4 : Ethanone, 1-(2,4,6-trimethylphenyl)-
C₁₁H₁₄O; MF: 681; RMF: 731; Prob 8.45%; CAS: 1667-01-2; Lib: nistdemo; ID: 1835.



Hit 5 : 4-t-Butyl-o-xylene
C₁₂H₁₈; MF: 639; RMF: 672; Prob 1.89%; CAS: 7397-06-0; Lib: nistdemo; ID: 1840.

