



Research article

Antioxidant, α -glucosidase, antimicrobial activities chemical composition and *in silico* analysis of *eucalyptus camaldulensis* dehn

Abdulrahman Mahmoud Dogara¹, Ateeq Ahmed Al-Zahrani^{2,*}, Sarwan W. Bradosty³, Saber W. Hamad^{4,5}, Shorsh Hussein Bapir⁶ and Talar K. Anwar⁷

¹ Biology Education Department, Tishk International University, Erbil, Iraq

² Chemistry Department, University College at Al-Qunfudhah, Umm Al-Qura University, Saudi Arabia

³ Department of Medical Laboratory Science, College of Science, Cihan University-Erbil, Kurdistan Region, Iraq

⁴ Department of Field Crops and Medicinal Plants, College of Agricultural Engineering Sciences, Salahaddin University-Erbil, Erbil, Kurdistan Region, Iraq

⁵ Department of Medical Laboratory Science, College of Science, Knowledge University, Kirkuk Road, 44001 Erbil, Iraq

⁶ Department of Horticulture, College of Agricultural Engineering Sciences, University of Raparin, Rania, Kurdistan Region, Iraq

⁷ Department of Plant Protection, College of Agricultural Engineering Sciences, Salahaddin University-Erbil, Erbil, Kurdistan Region, Iraq

* **Correspondence:** Email: aaalzahrani@uqu.edu.sa.

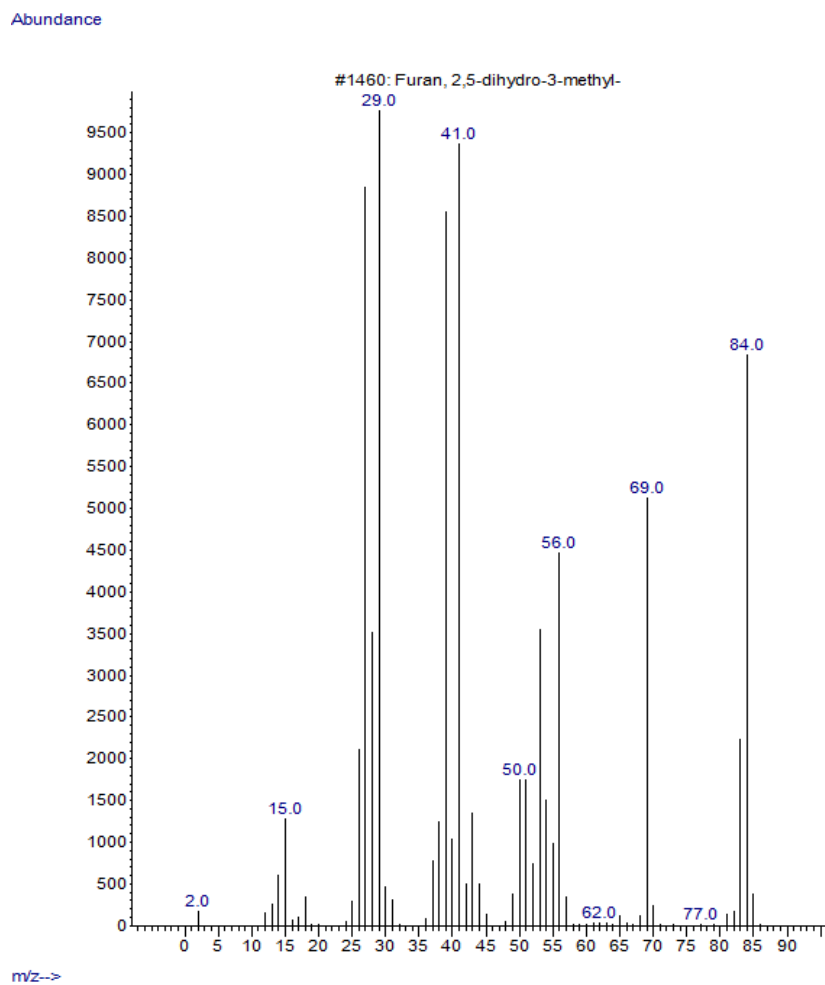
Supplemental information

Table S1. Phytochemicals of *Eucalyptus camaldulensis* leaves and their docking scores against α -glucosidase enzyme. N/A* = The number of rotatable bonds is 32. Too many rotatable bonds mean low docking accuracy. 12 phytochemicals gave docking score -5 or higher.

Compound	PubChem CID	Docking Score
alpha-D-glucopyranose (Native Inhibitor)	79025	-6.2
Quercetin	5280343	-8.6
Acarbose	41774	-8.3
Miglitol	441314	-5.8
Voglibose	444020	-6.4
Phytochemicals of <i>Eucalyptus camaldulensis</i>		
Furan, 2,5-dihydro-3-methyl-	533662	-4.1
6-Tridecene, 7-methyl-	5364660	-5.3
dl-Lysine	866	-5.3
3-Cyclohexylthiolane,S,S-dioxide	313687	-7.4
1-Isopropoxy-2,2,3-trimethylaziridine	538212	-5.2
1H-Cyclopropa[a]naphthalene, 1a,2,3,5,6,7,7a,7b-octahydro-1,1,7,7a-tetramethyl-, [1aR-(1a.alpha.,7.alpha.,7a.alpha.,7b.alpha.)]-	6432176	-7.2
Aromadendrin	122850	-8.5
Alloaromadendrene	10899740	-6.6
5.alpha.-Androstan-16-one	13963520	-8.6
(1S,2E,6E,10R)-3,7,11,11-Tetramethylbicyclo[8.1.0]undeca-2,6-diene	13894533	-7.5
Dodecanoic acid, methyl ester	8139	-8.0
1-Methylene-2b-hydroxymethyl-3,3-dimethyl-4b-(3-methylbut-2-enyl)-cyclohexane	550196	-7.3
1H-Cycloprop[e]azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, [1aR-(1a.alpha.,4a.alpha.,7.beta.,7a.beta.,7b.alpha.)]-	6432640	-7.4
Azulene, 1,2,3,3a,4,5,6,7-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1R-(1.alpha.,3a.beta.,4.alpha.,7.beta.)]-	90805	-6.7
Naphthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethenyl)-, [4aR-(4a.alpha.,7.alpha.,8a.beta.)]-	442393	-7.0
1-Tetradecene	14260	-5.1
2-Naphthalenemethanol, 2,3,4,4a,5,6,7,8-octahydro-.alpha.,.alpha.,4a,8-tetramethyl-, [2R-(2.alpha.,4a.beta.,8.beta.)]-	527256	-7.8
3-Tetradecanynoic acid	534441	-5.4
Methyl 10-oxo-8-decenoate	5362752	-5.4
9-Hexadecenoic acid, octadecyl ester	5363255	N/A*
cis-Z- α -Bisabolene epoxide	91753574	-7.0
Alpha-Phellandrene	7460	-6.3

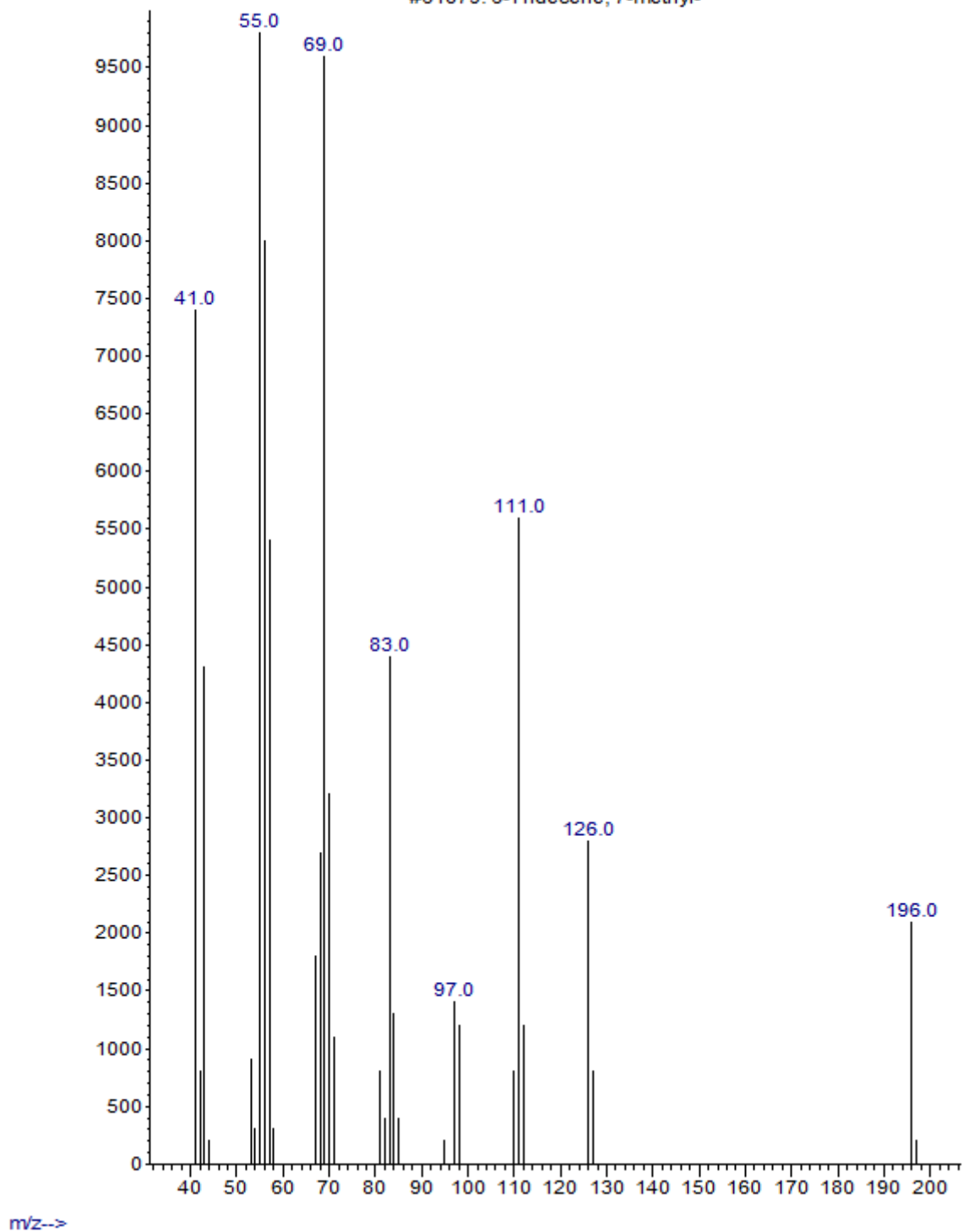
Continued on next page

Compound	PubChem CID	Docking Score
Gamma-Terpinene	7461	-6.4
Hexadecanoic acid, methyl ester	8181	-4.9
1,2-Benzenedicarboxylic acid, butyl 2-ethylhexyl ester	6818	-7.1
1-(+)-Ascorbic acid 2,6-dihexadecanoate	54722209	N/A*
7-Hexadecenal, (Z)-	5364438	-5.5
9,12-Octadecadienoic acid, methyl ester	5284421	-5.7
6-Octadecenoic acid, methyl ester, (Z)-	5362717	-5.9
9-Hexadecenoic acid	5282745	-6.1
Methyl stearate	8201	-5.2
1,19-Eicosadiene	519006	-5.3
9-Tetradecenal, (Z)-	5364471	-5.5
15-Hydroxypentadecanoic acid	78360	-5.6
E-9-Tetradecenal	5283368	-5.5
13-octadecadienol	17968622	-6.1
cis-Vaccenic acid	5282761	-5.8
trans-13-Octadecenoic acid	6161490	-6.1
Eicosane	8222	-5.0
cis-11-Hexadecenal	5364495	-5.2

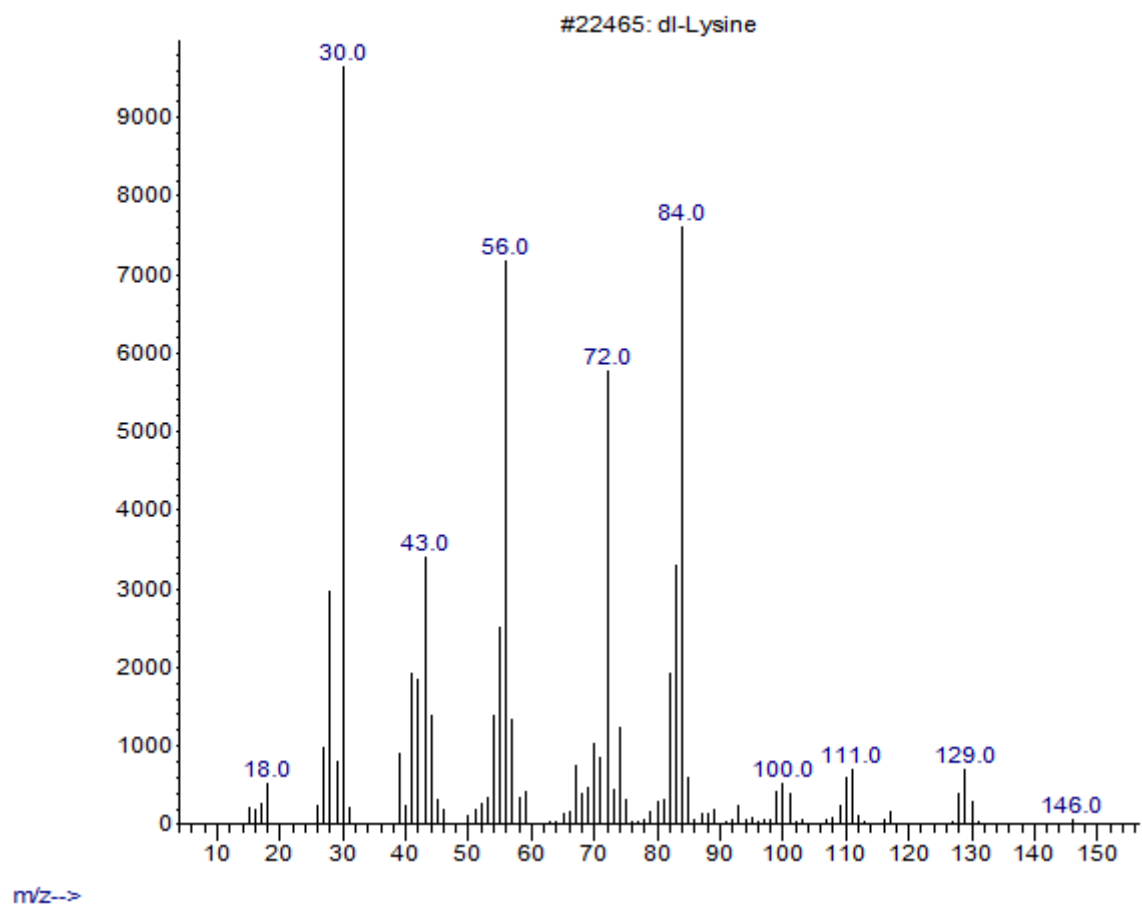
Table S2. Mass spectrum of each compound of the essential oil.

Abundance

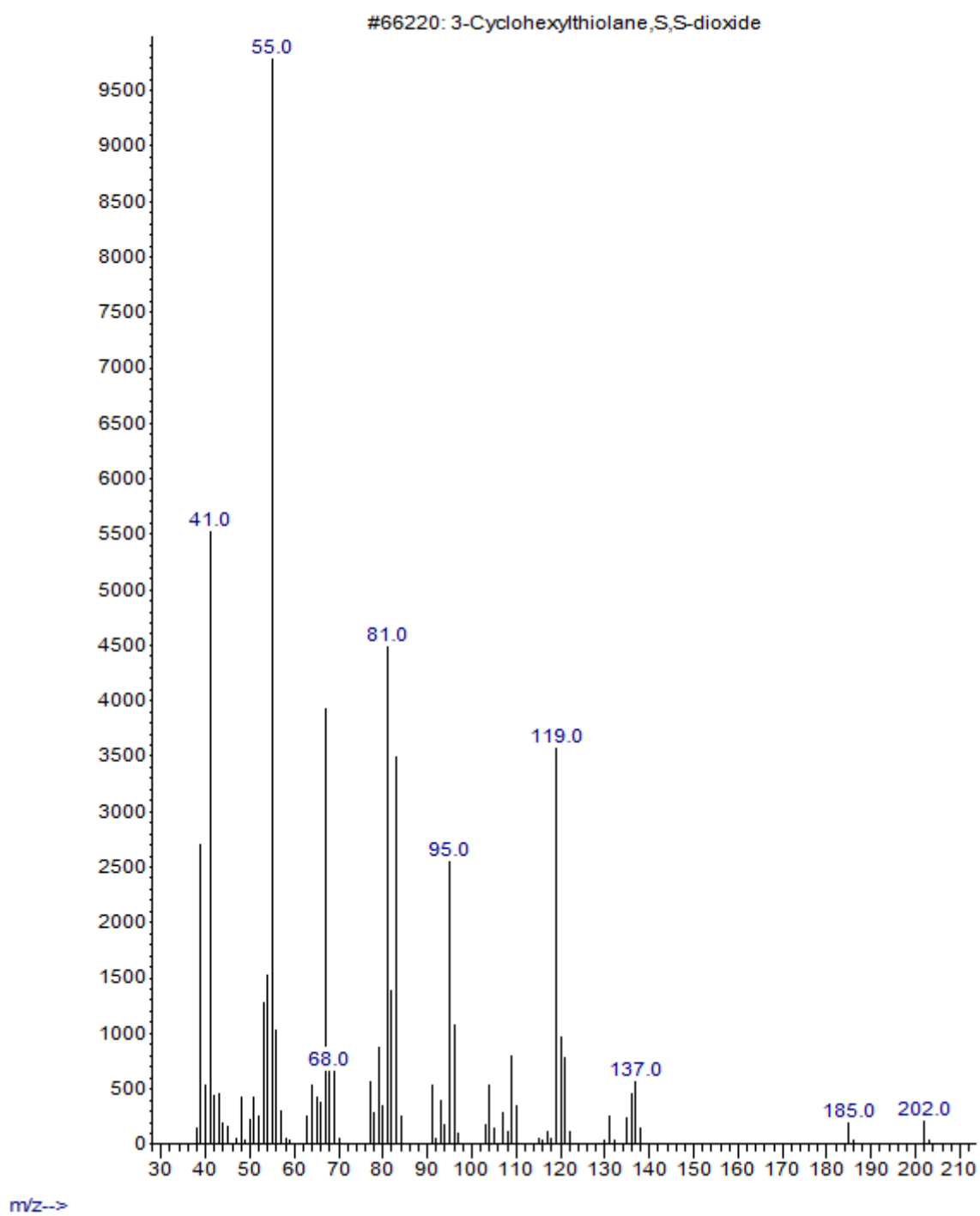
#61879: 6-Tridecene, 7-methyl-



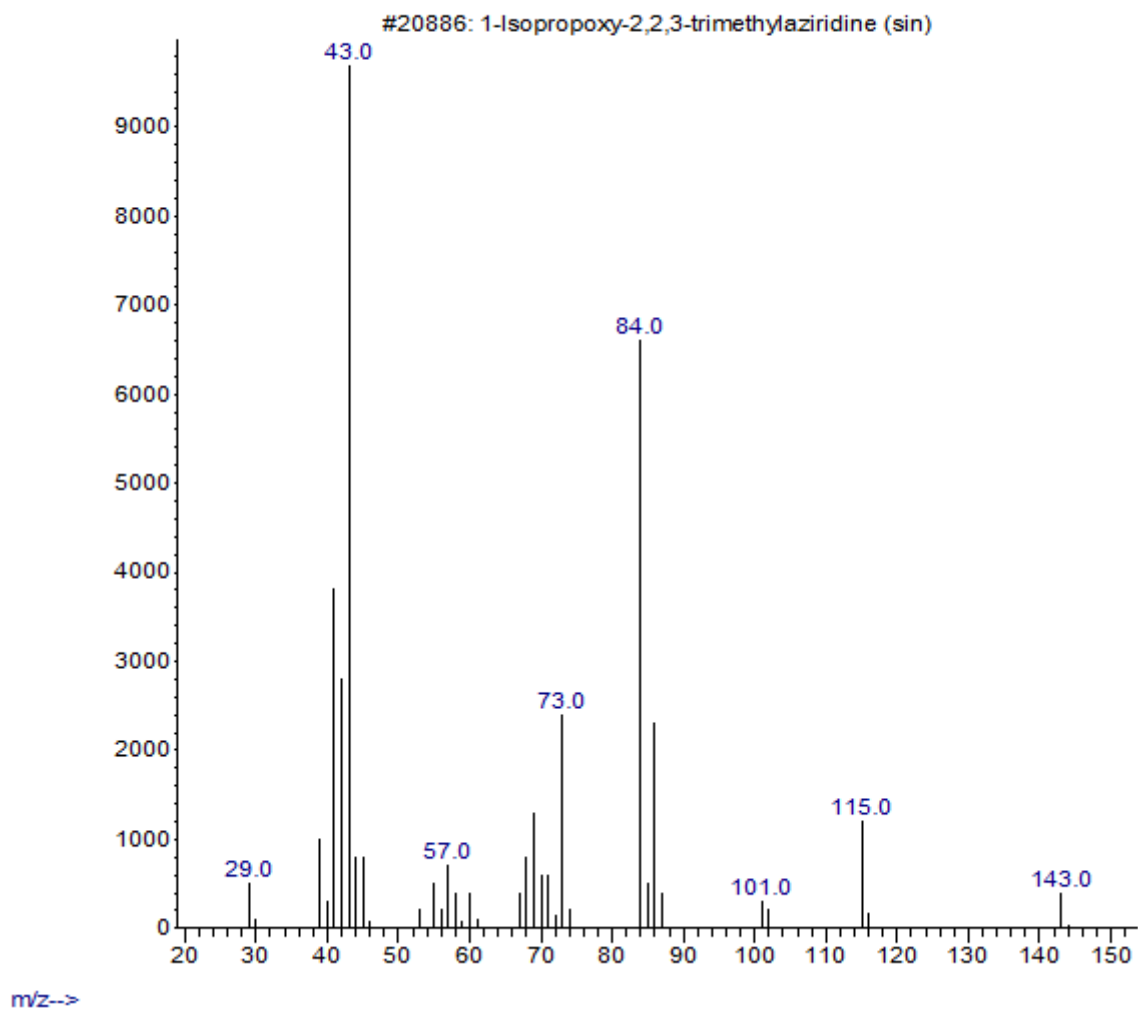
Abundance



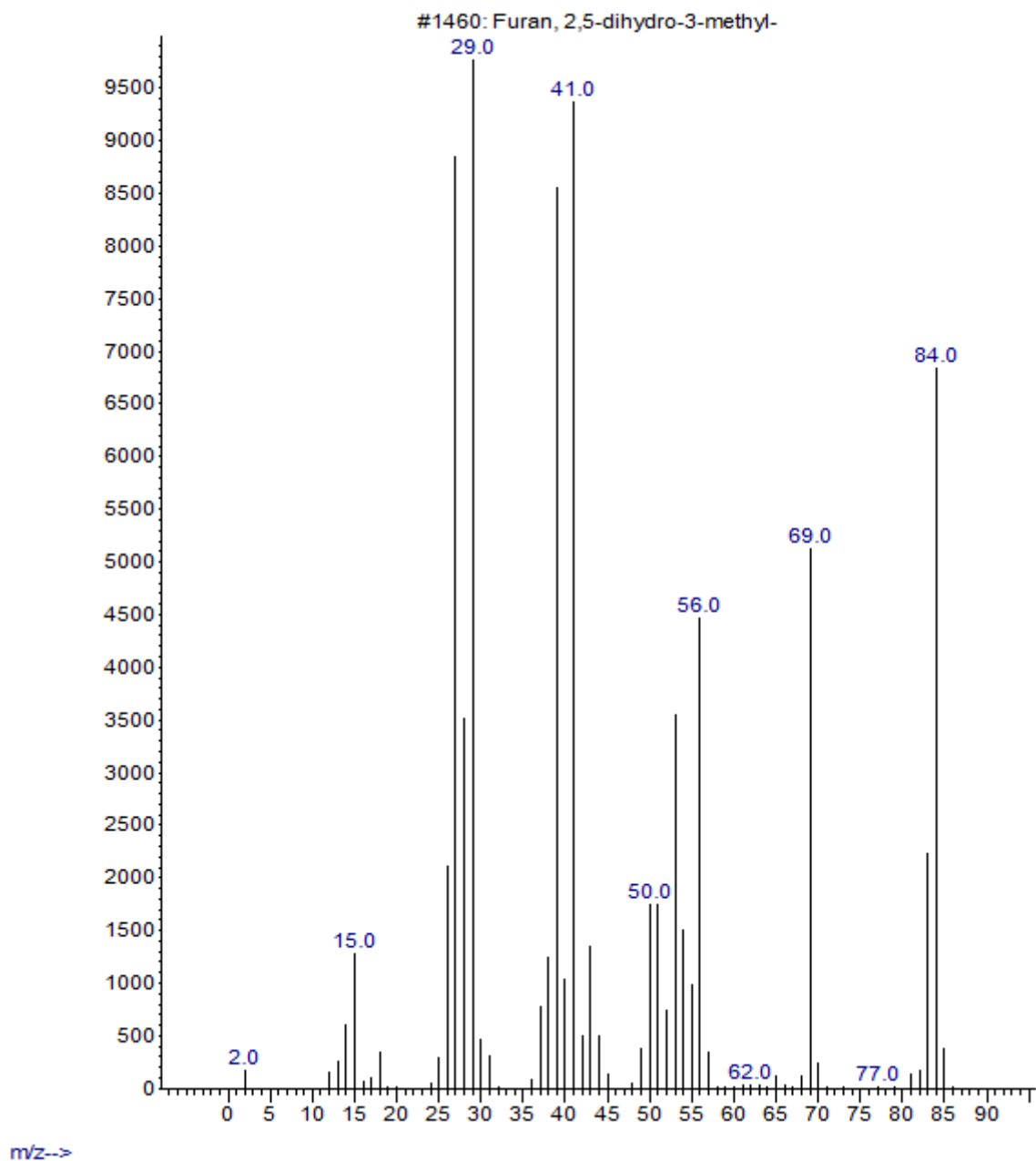
Abundance



Abundance

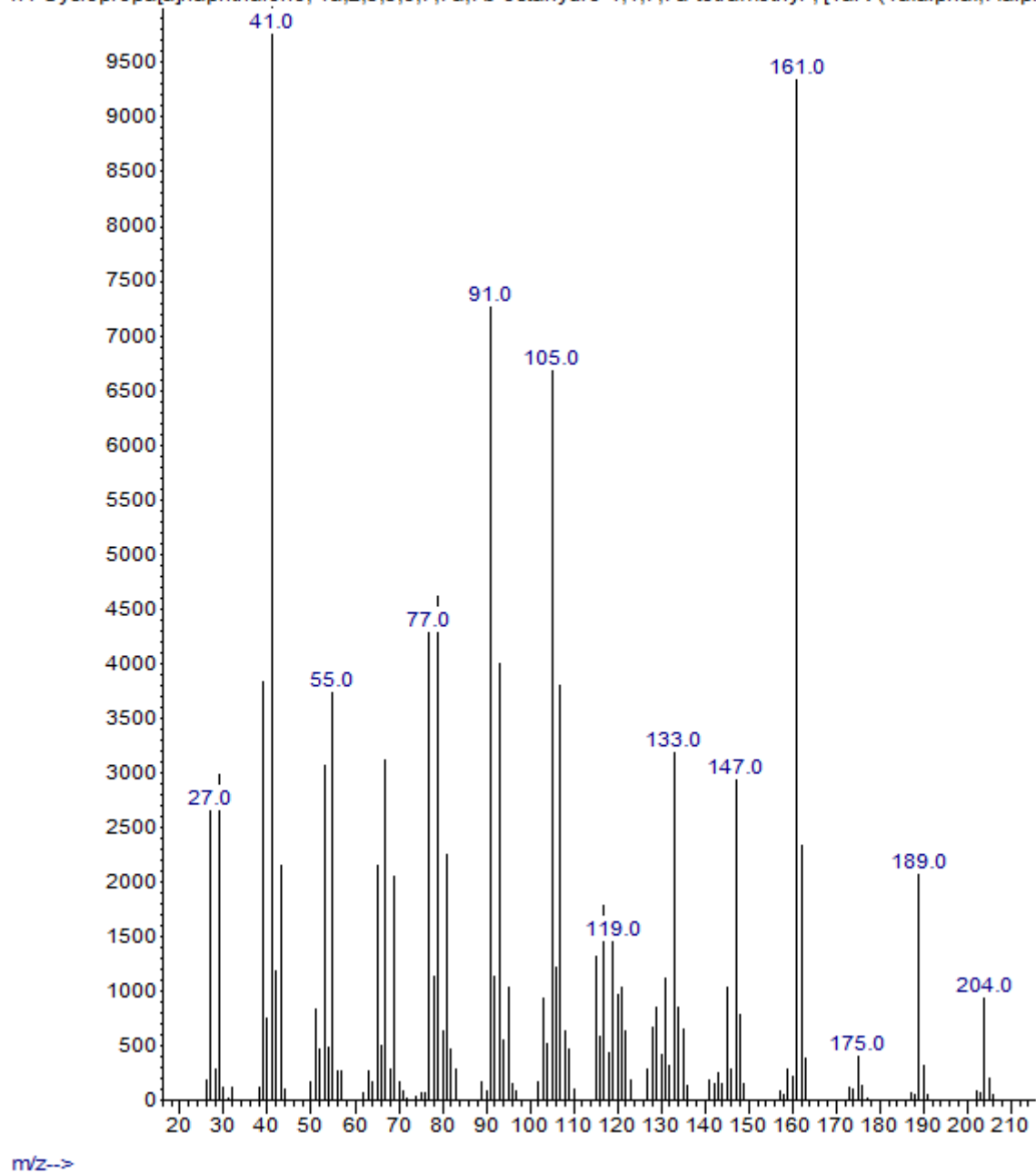


Abundance

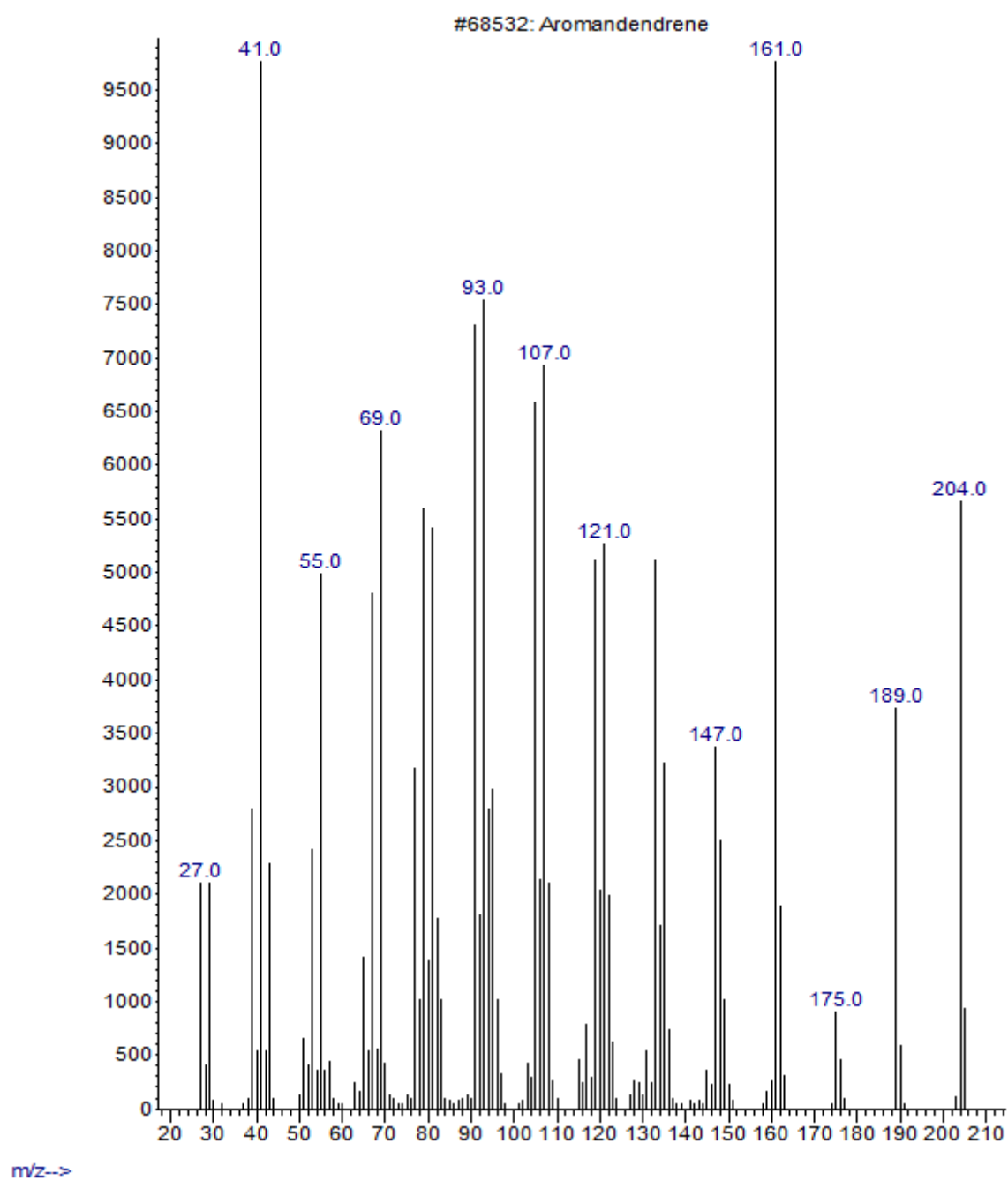


Abundance

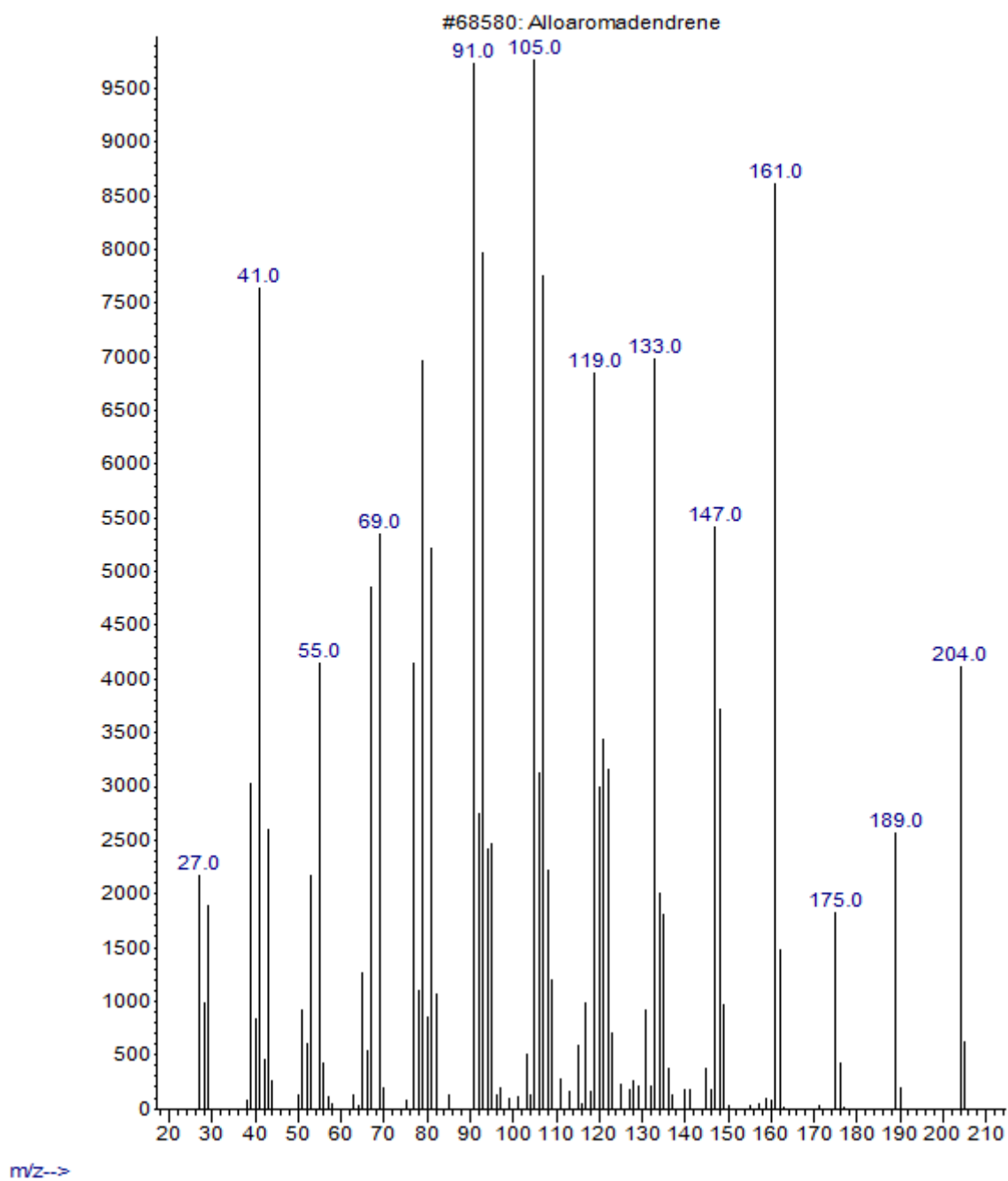
1H-Cyclopropa[a]naphthalene, 1a,2,3,5,6,7,7a,7b-octahydro-1,1,7,7a-tetramethyl-, [1aR-(1a.alpha.,7.alpha.



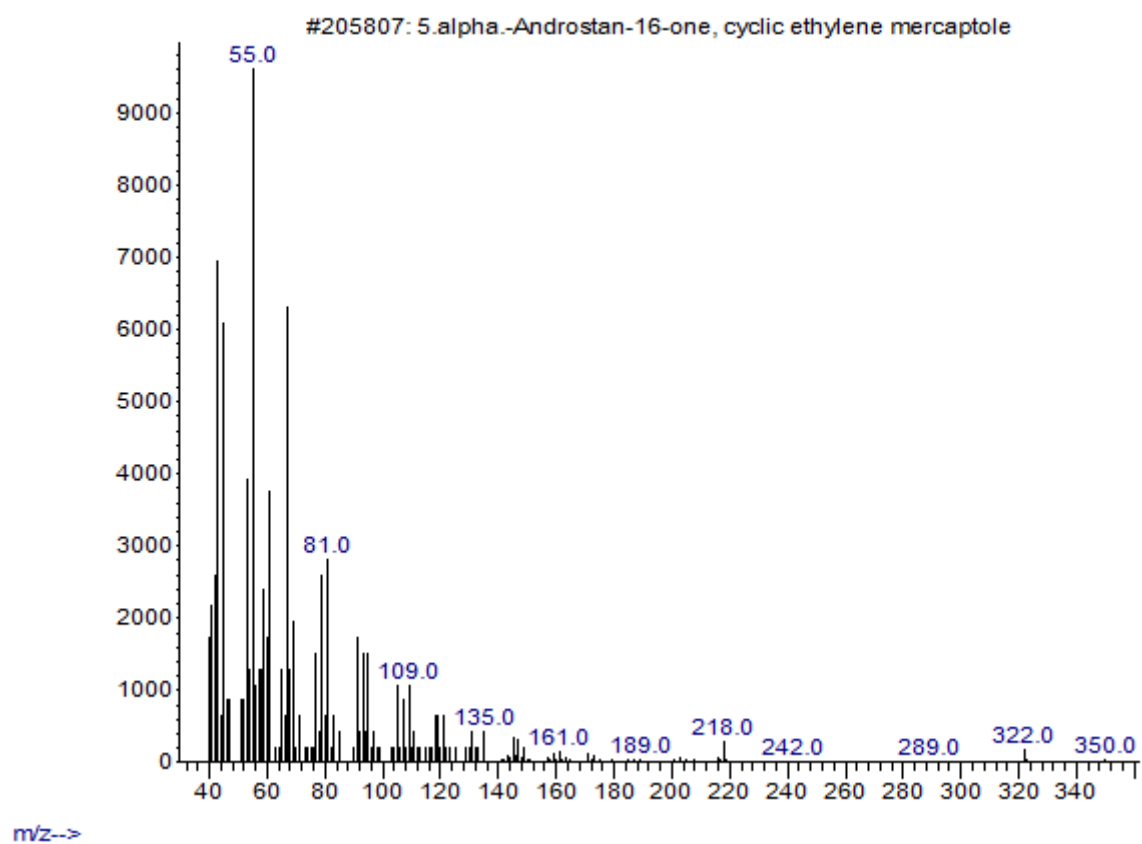
Abundance



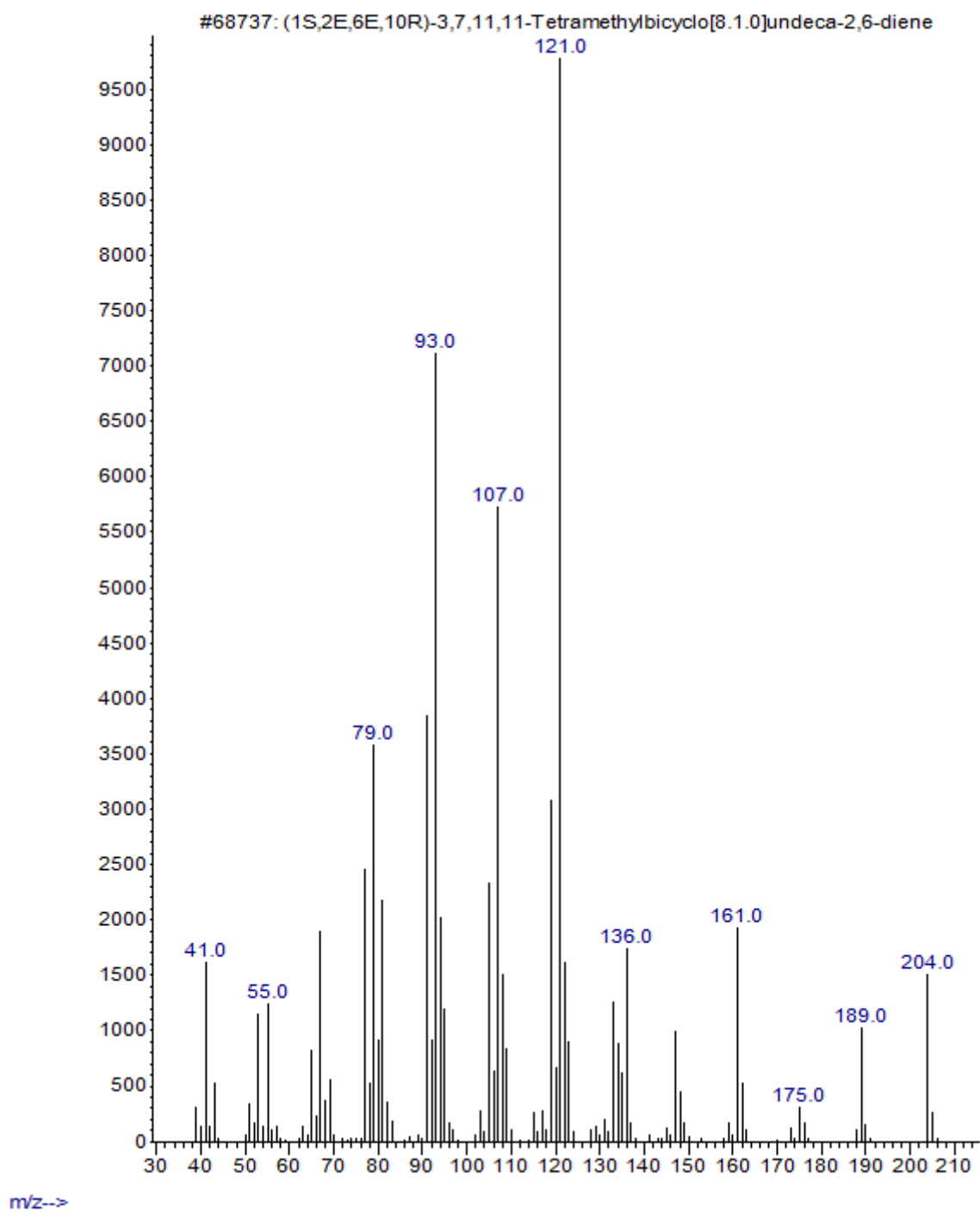
Abundance



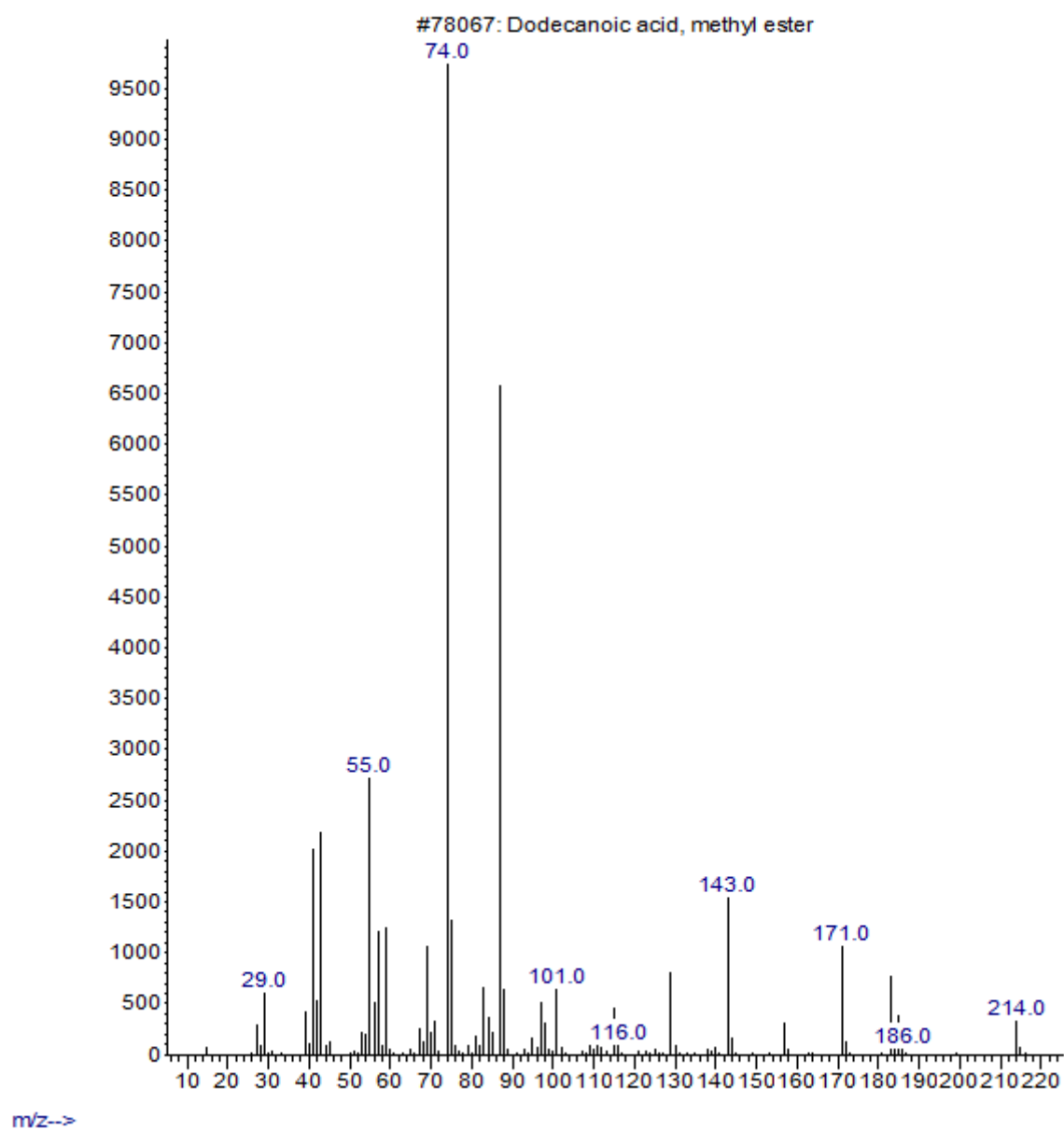
Abundance



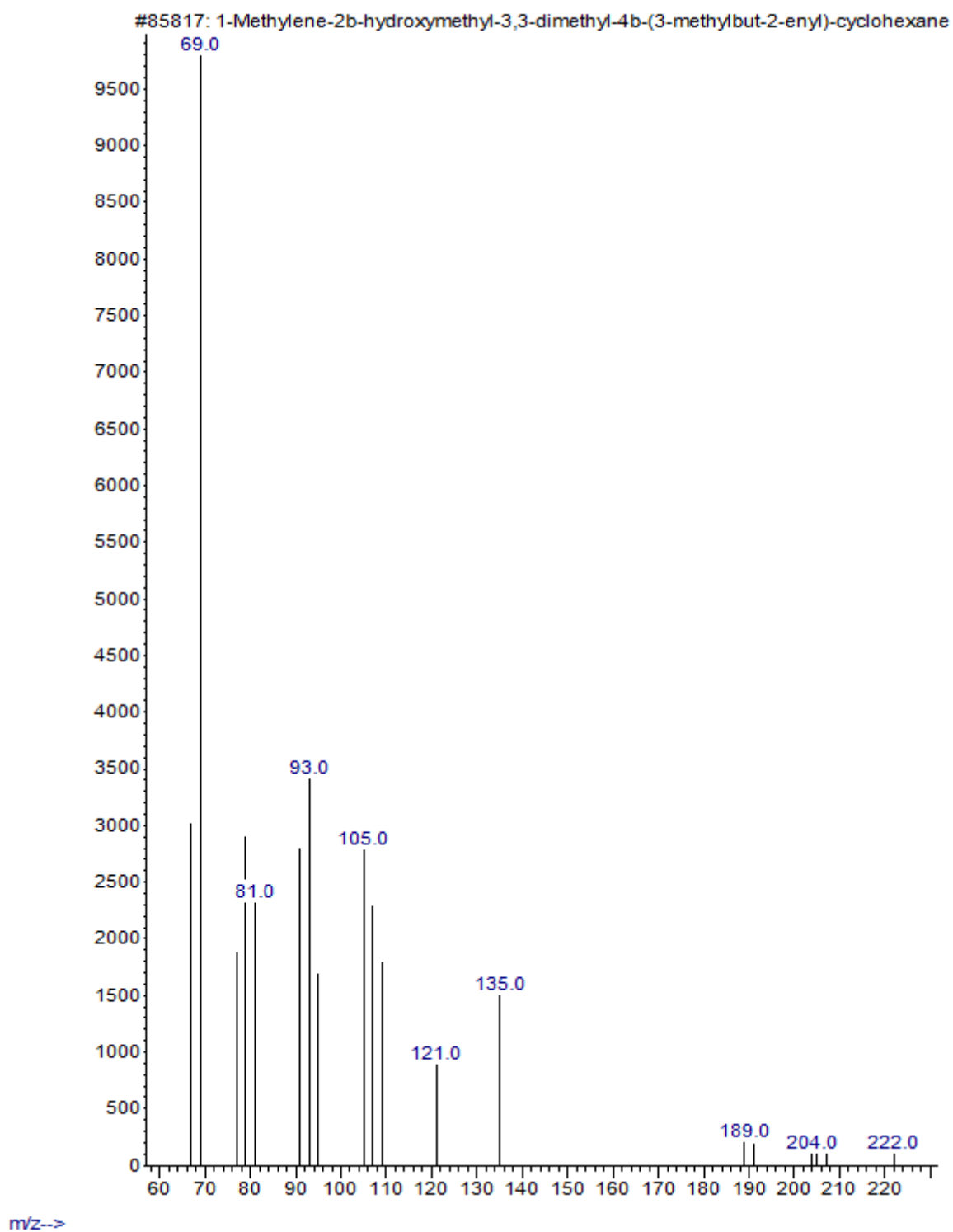
Abundance



Abundance

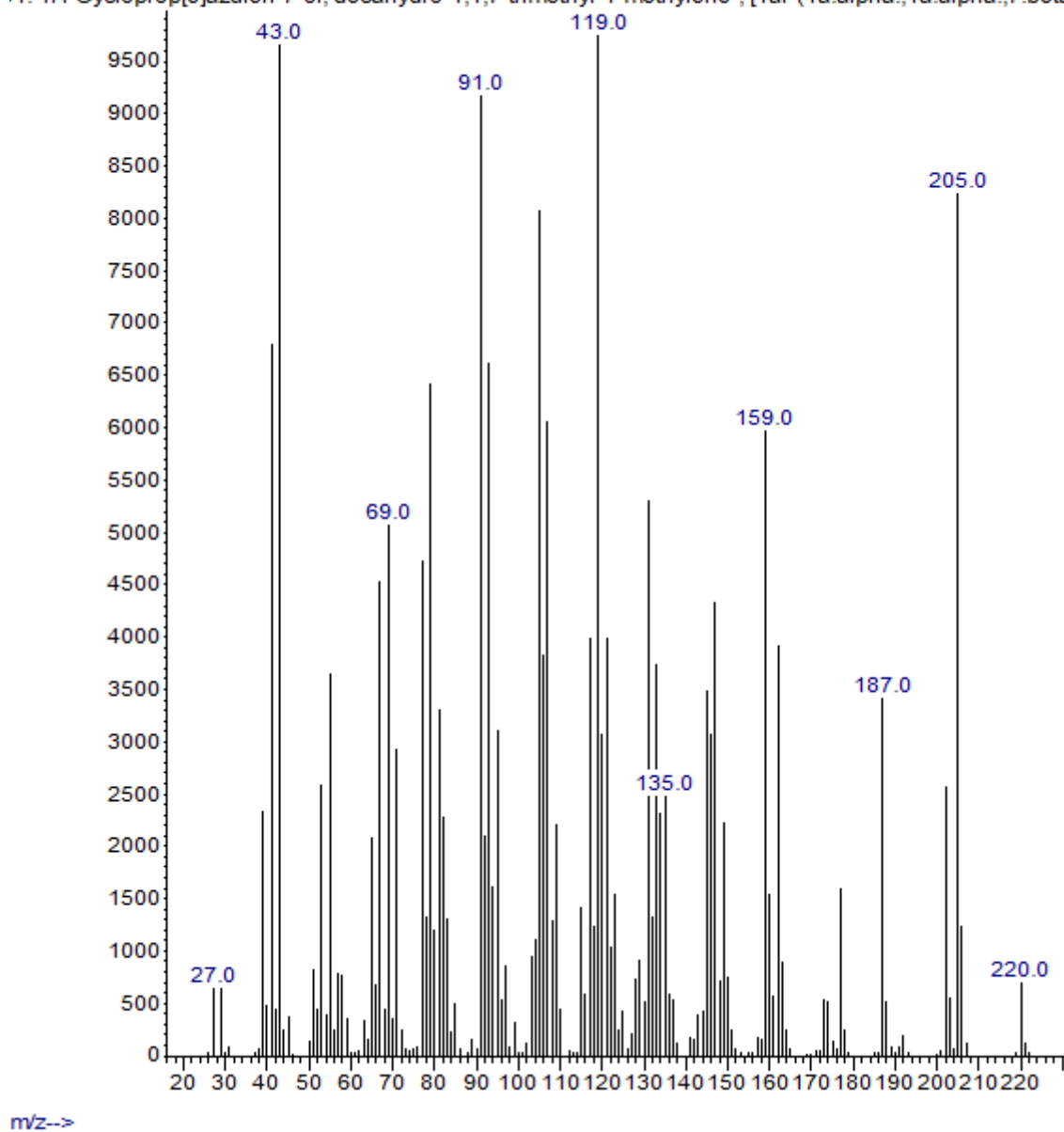


Abundance



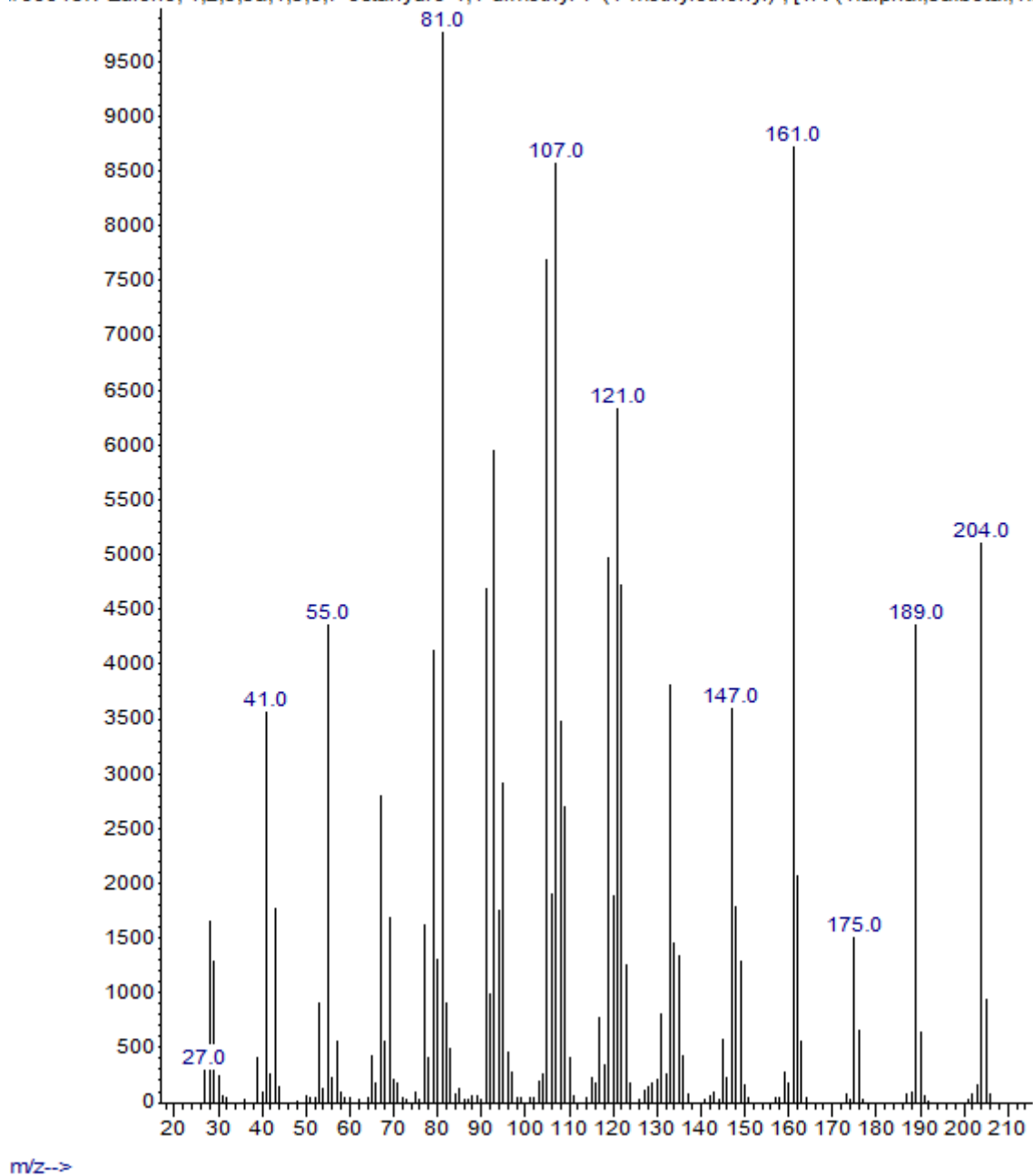
Abundance

14: 1H-Cycloprop[e]azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, [1ar-(1a.alpha.,4a.alpha.,7.beta.,7



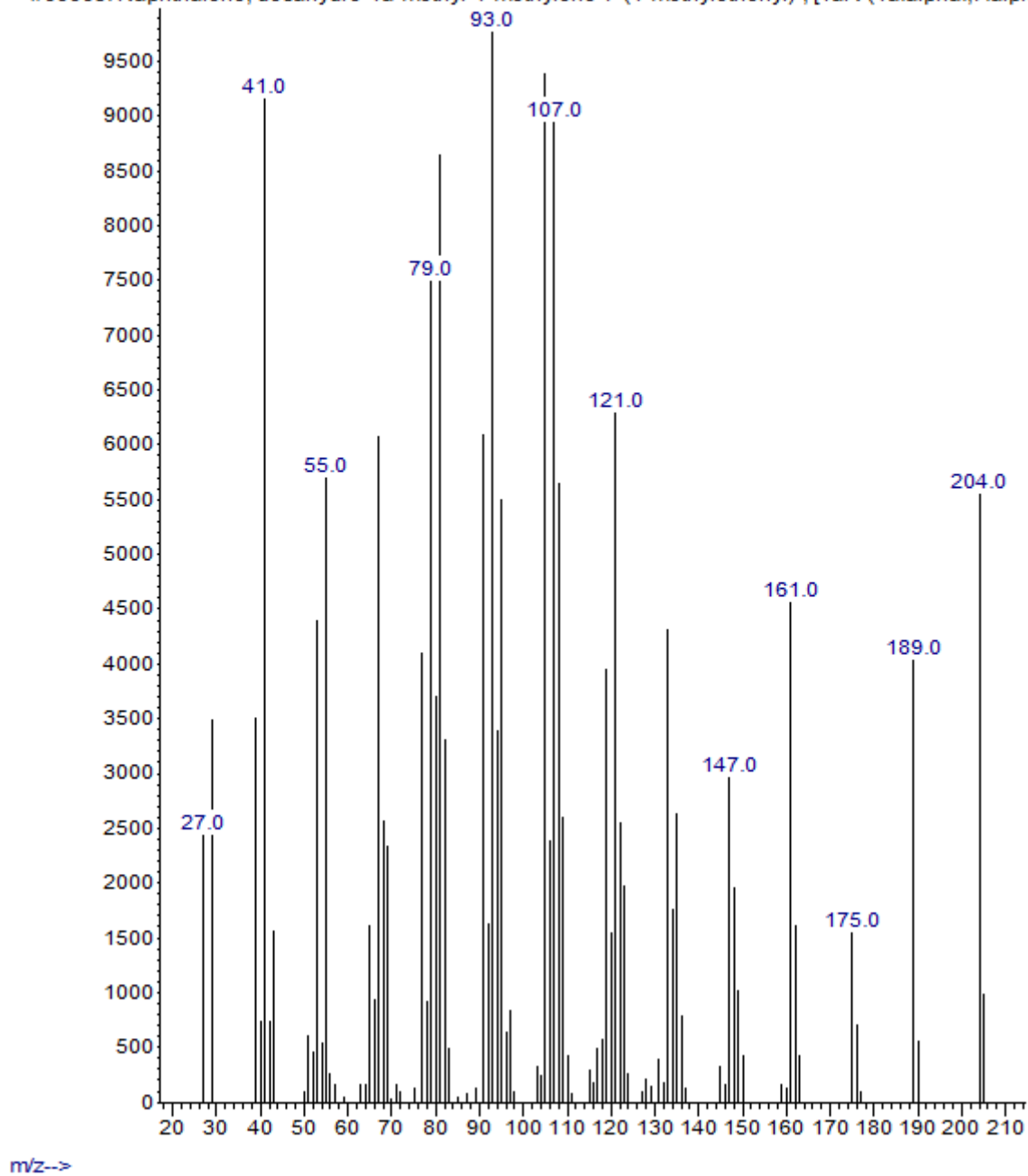
Abundance

#68913: Azulene, 1,2,3,3a,4,5,6,7-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1R-(1.alpha.,3a.beta.,4.alpha.)]

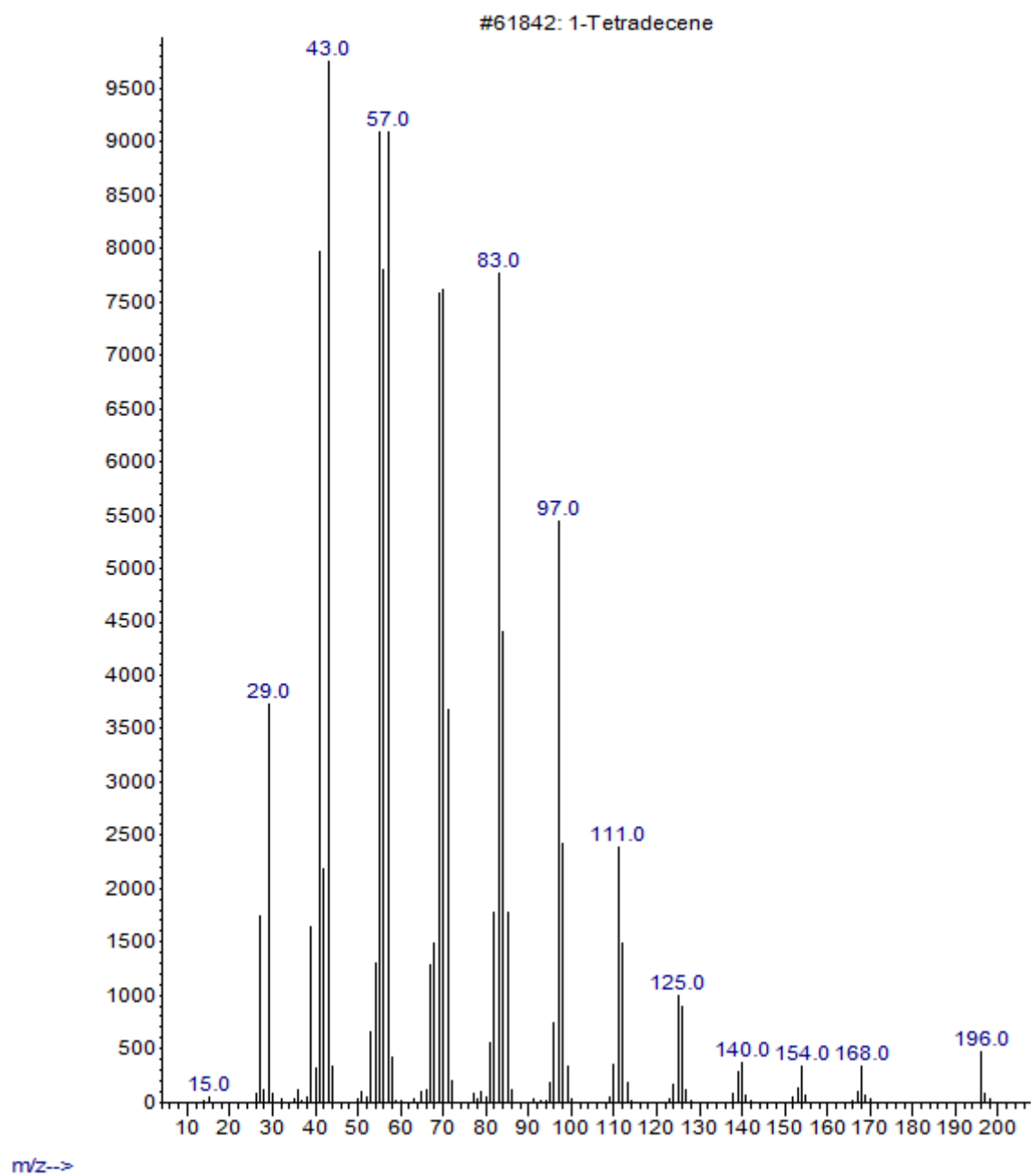


Abundance

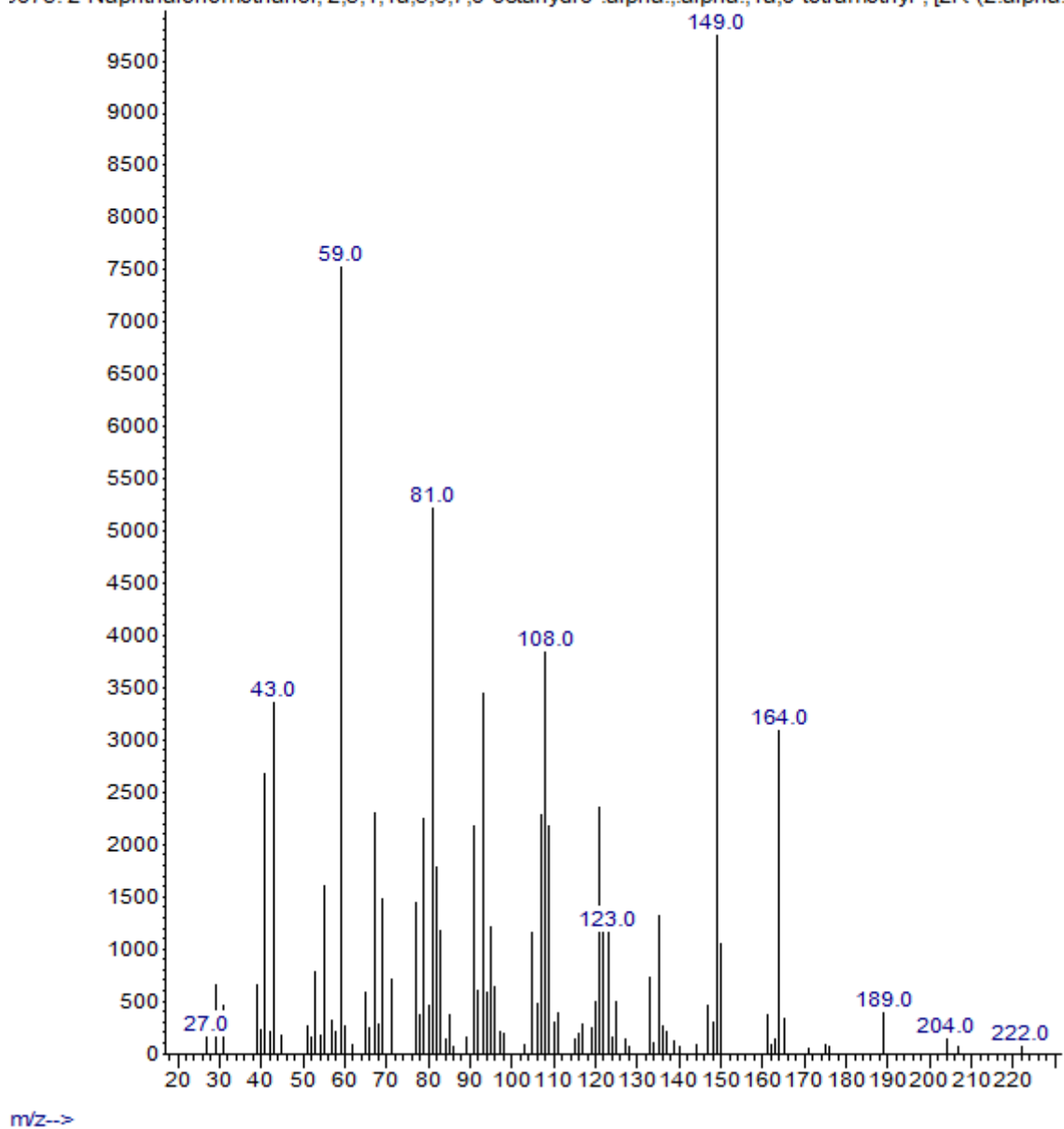
#68863: Naphthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethenyl)-, [4aR-(4a.alpha.,7.alpha.



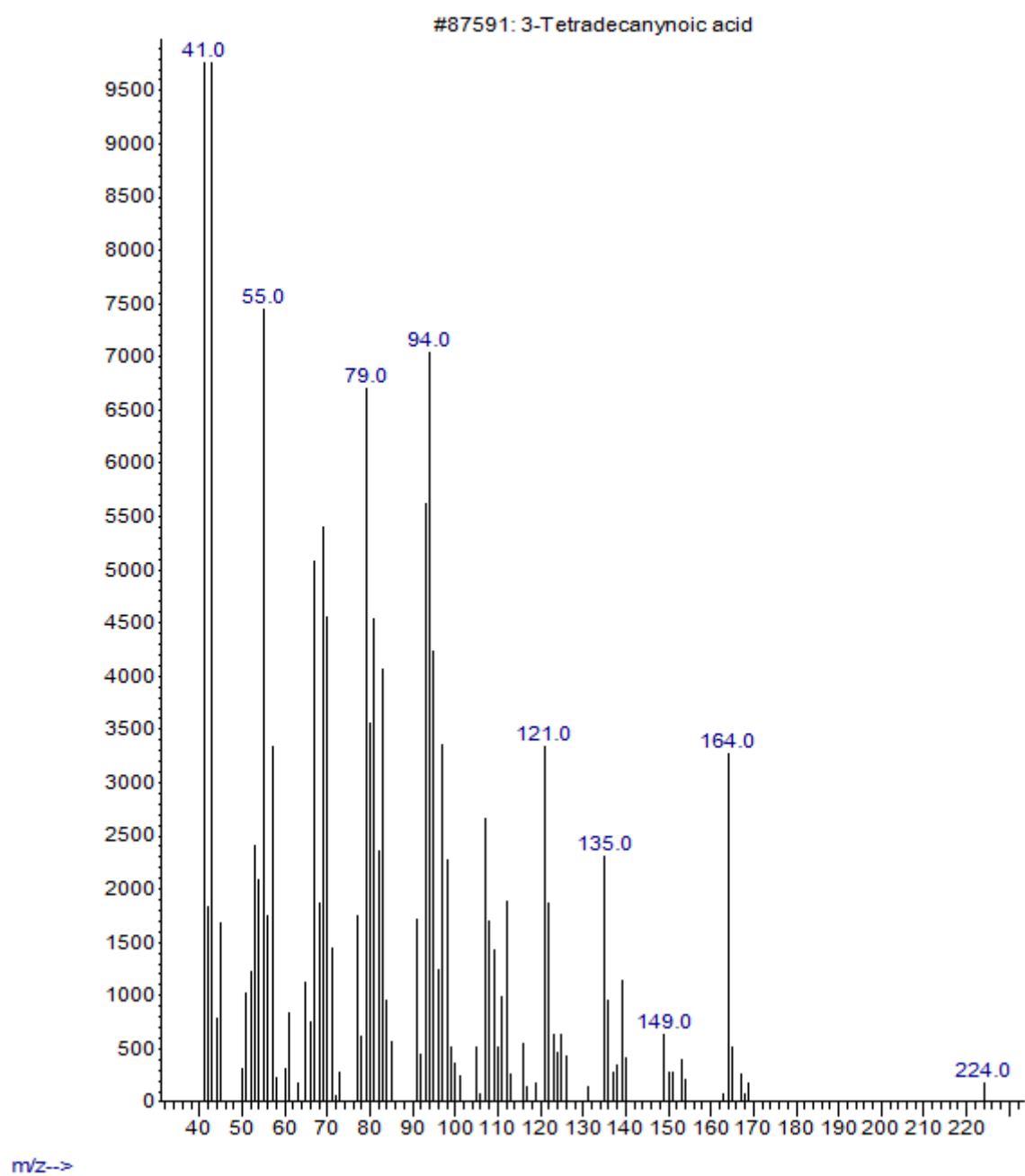
Abundance



Abundance

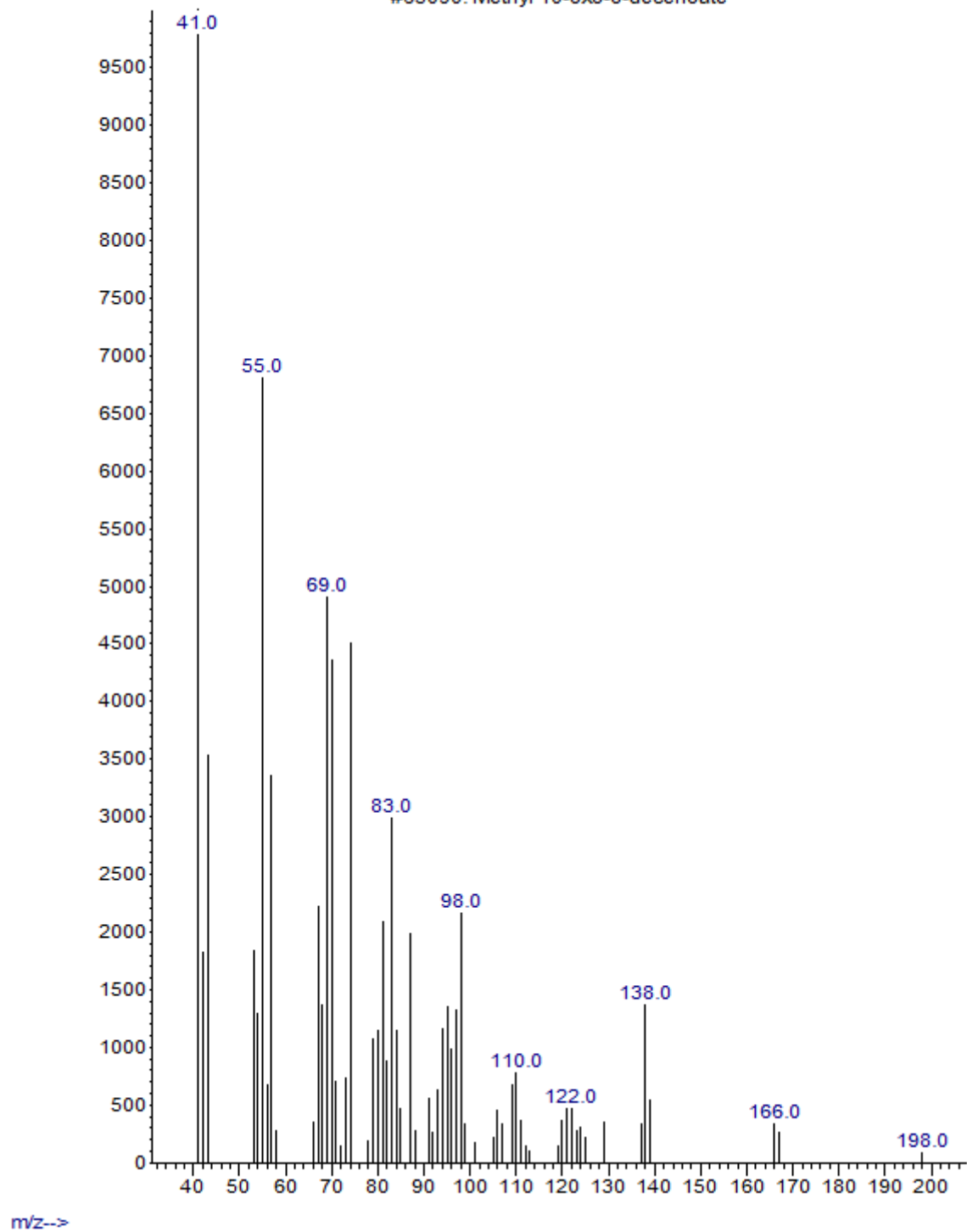
5873: 2-Naphthalenemethanol, 2,3,4,4a,5,6,7,8-octahydro- $\alpha,\alpha,4a,8$ -tetramethyl-, [2R-(2 $\alpha,4$ 

Abundance

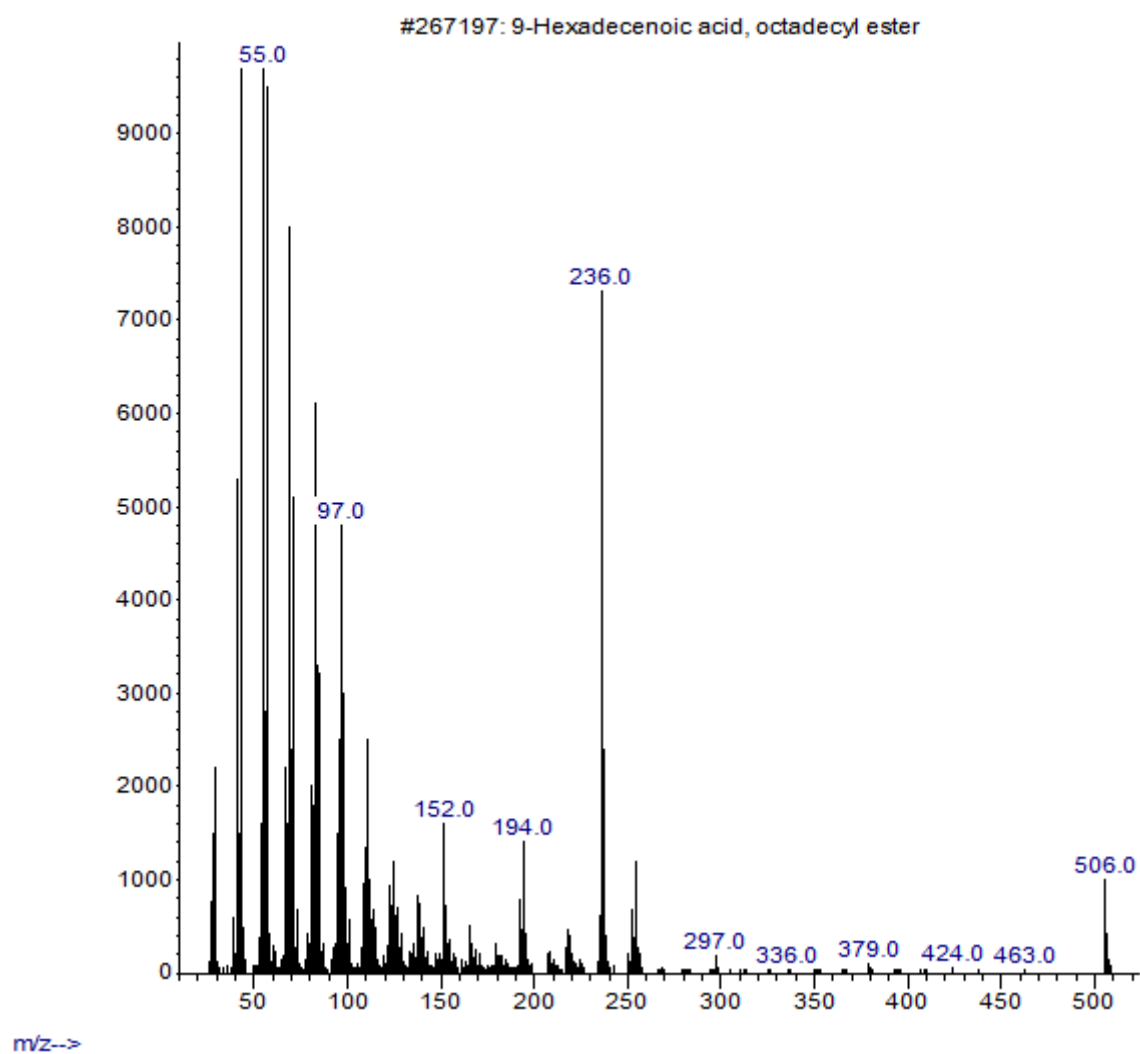


Abundance

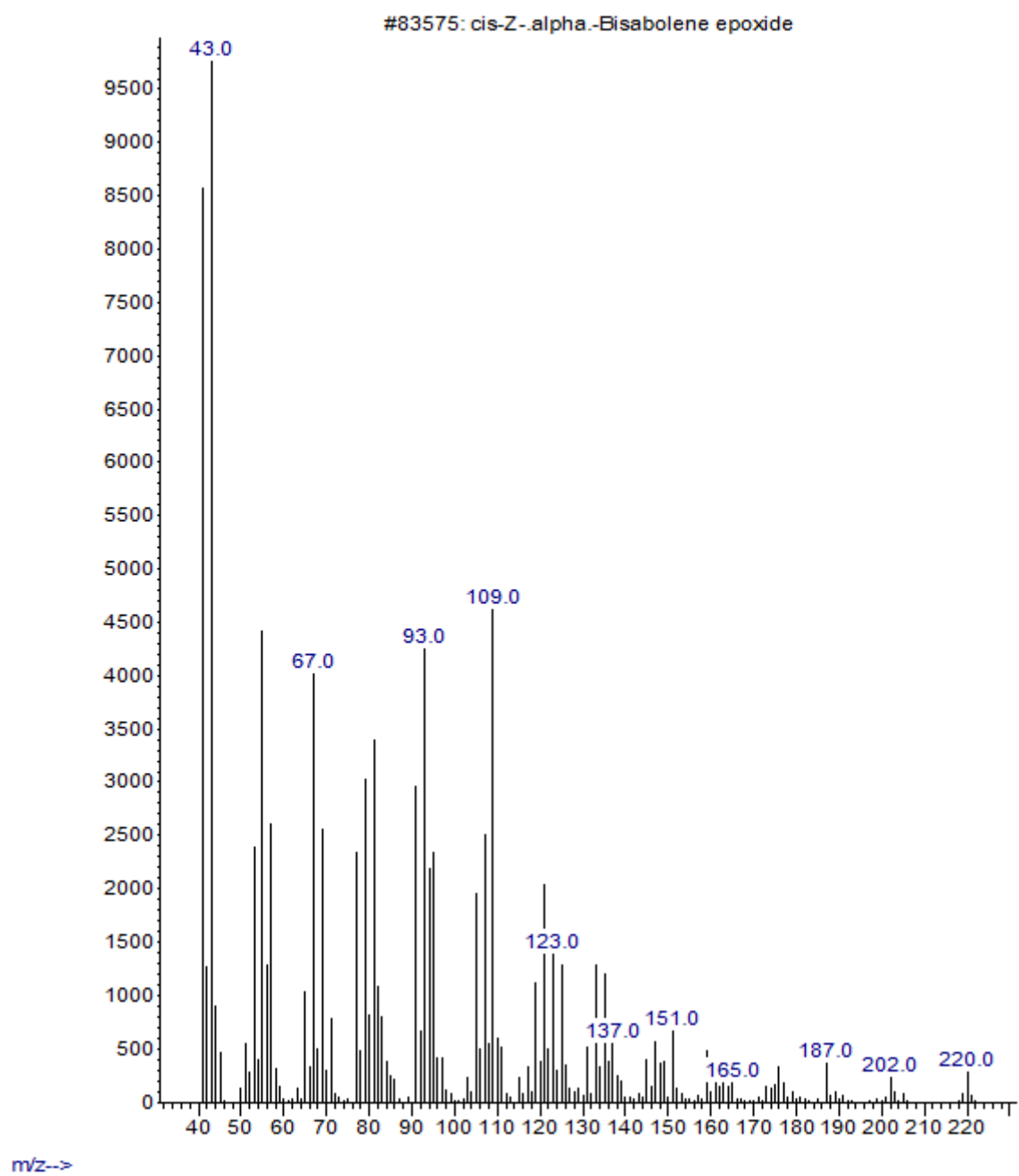
#63090: Methyl 10-oxo-8-decenoate



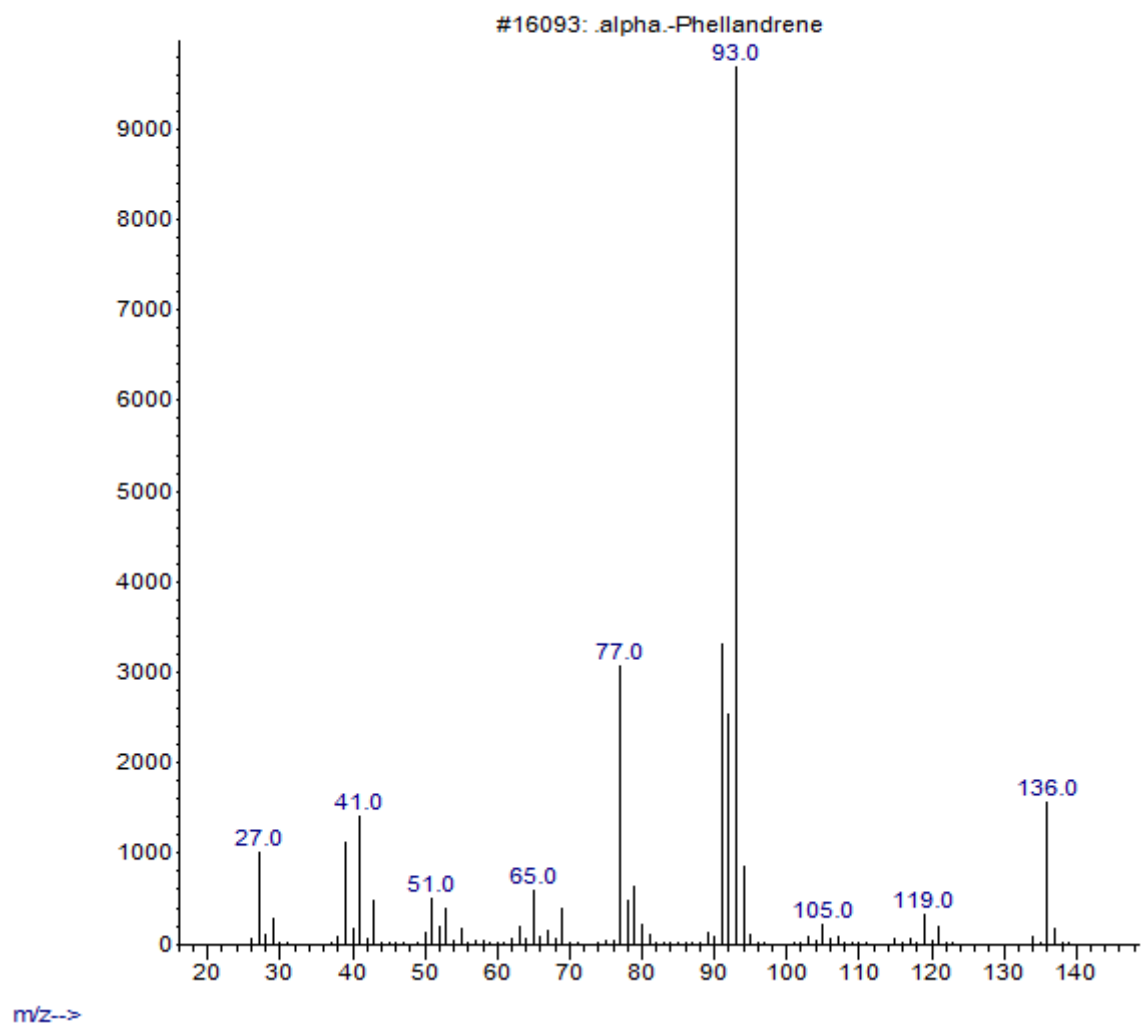
Abundance



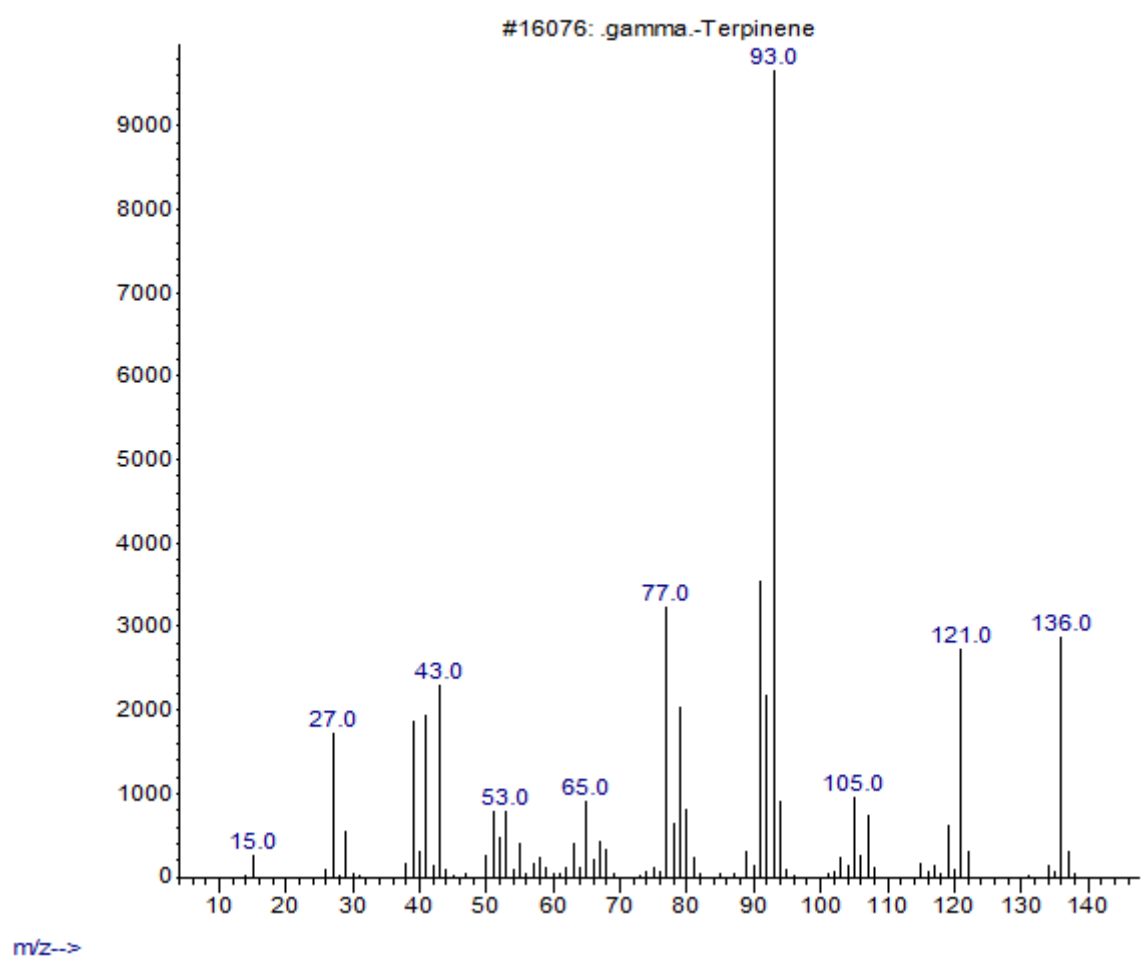
Abundance



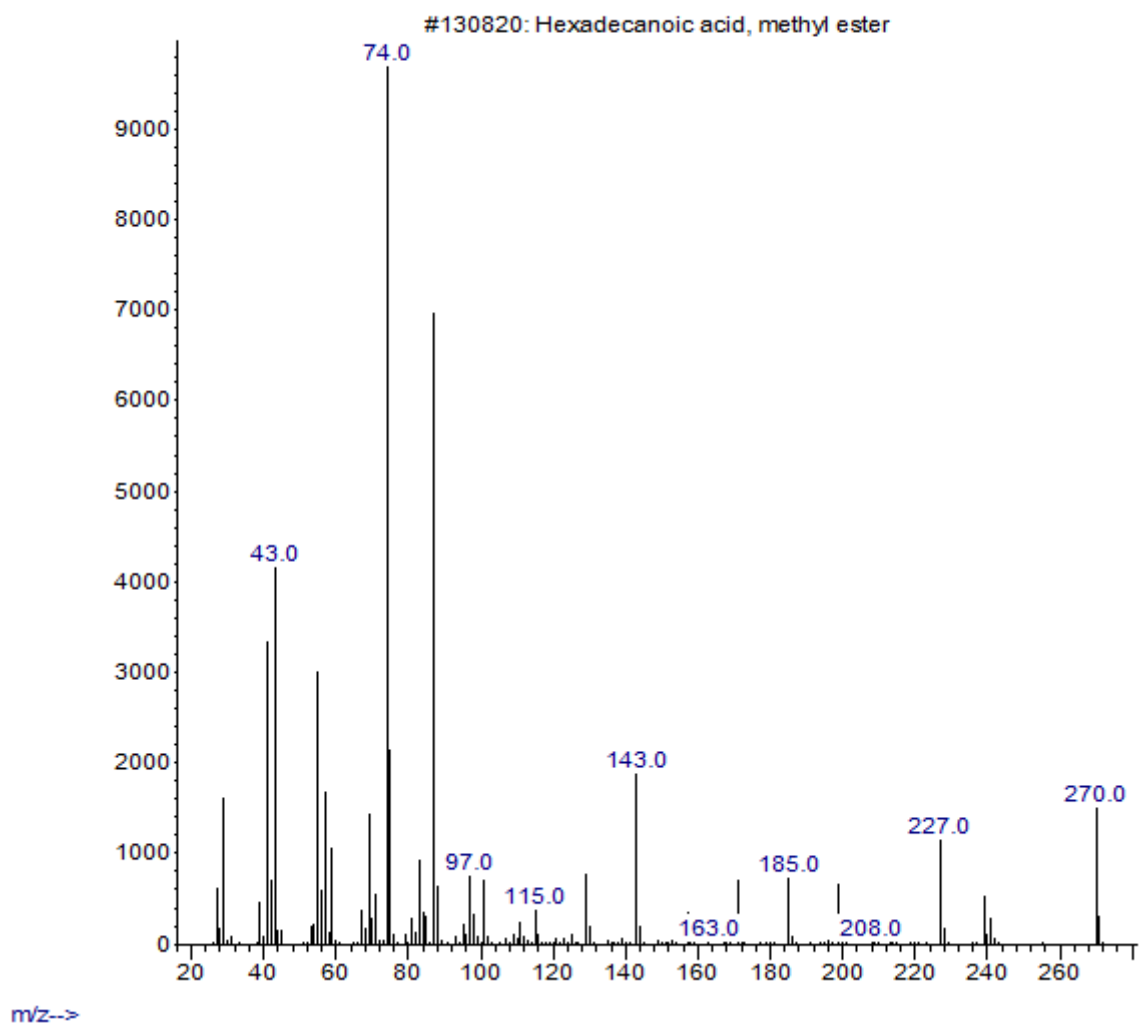
Abundance



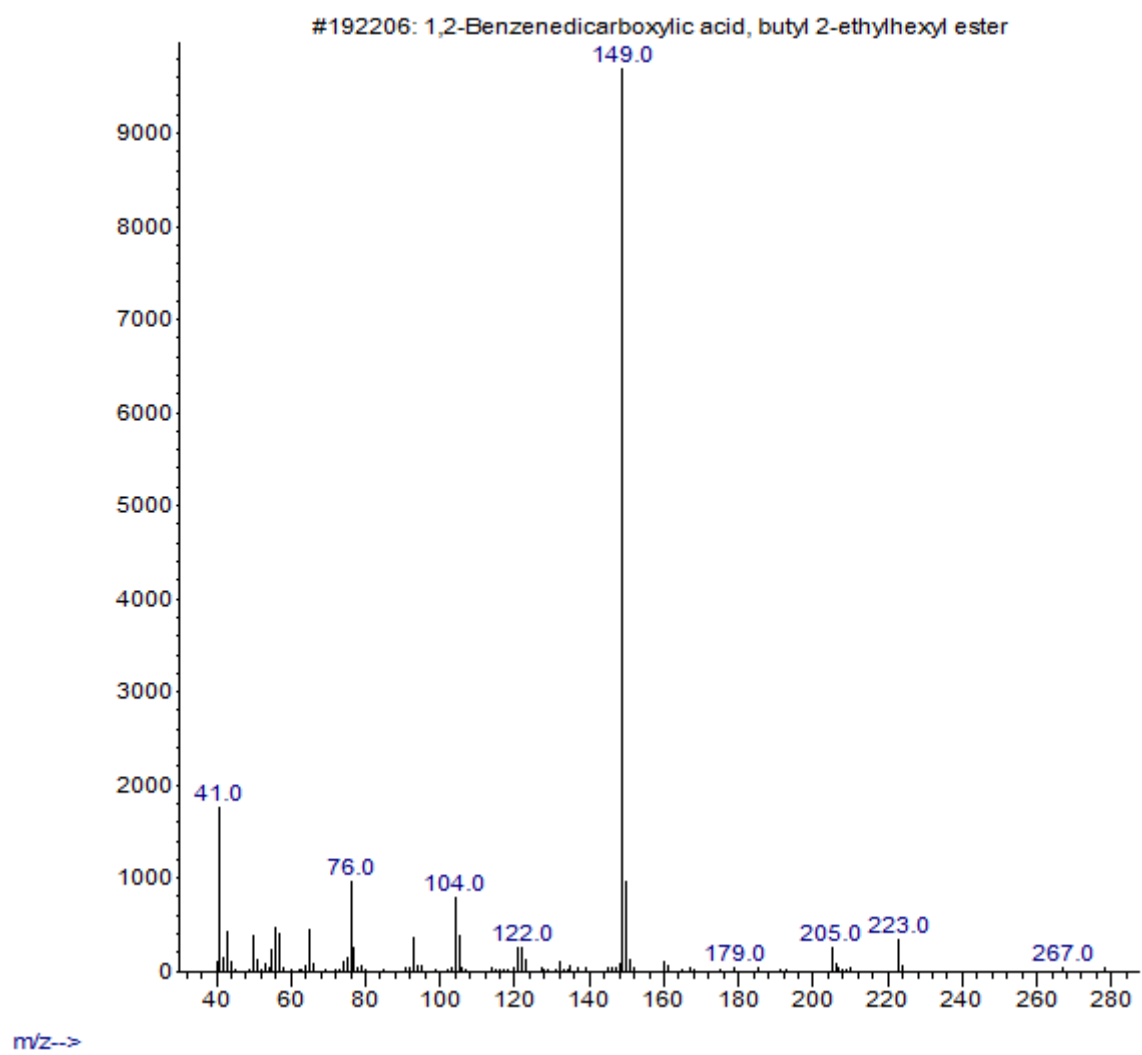
Abundance



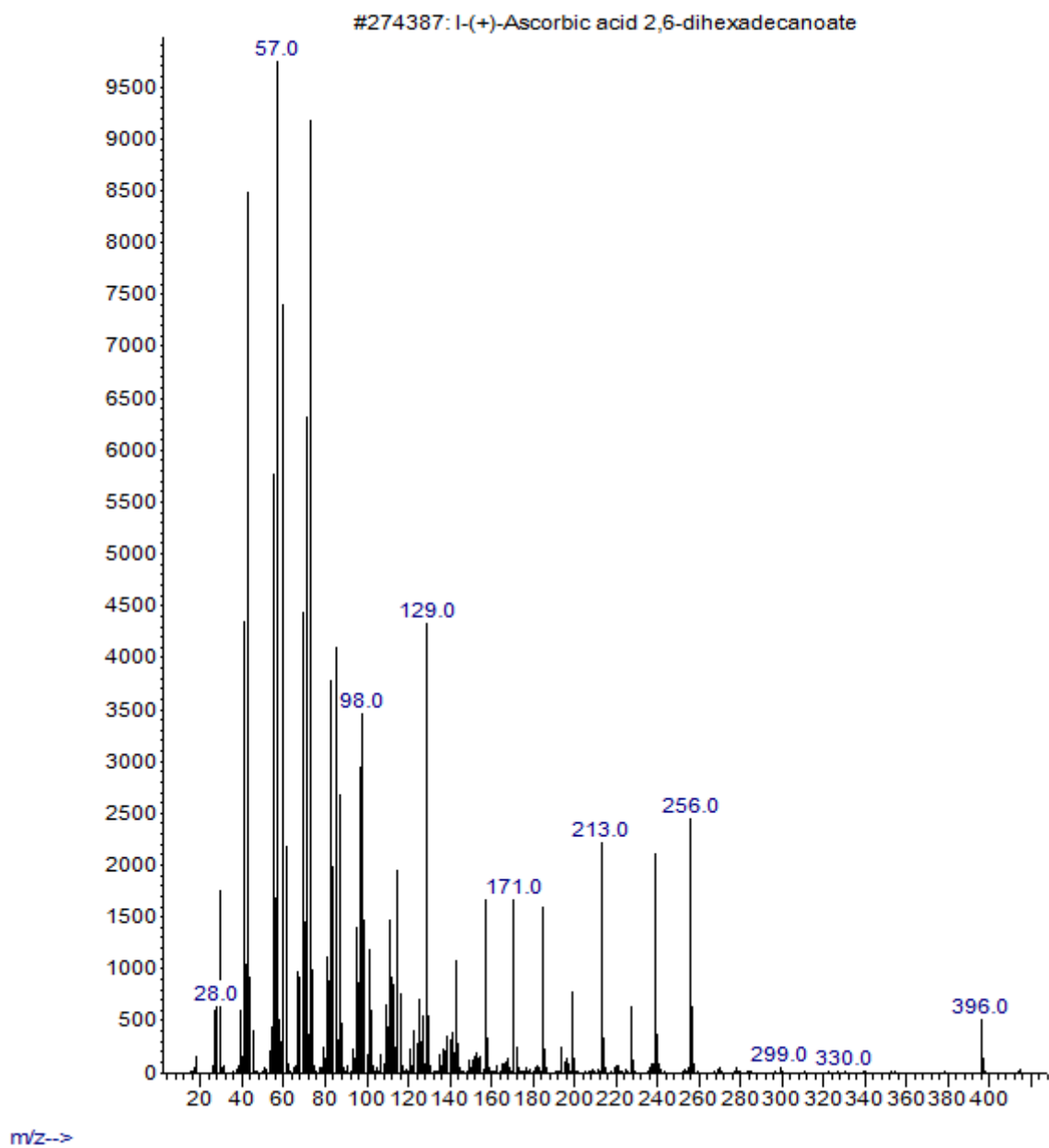
Abundance



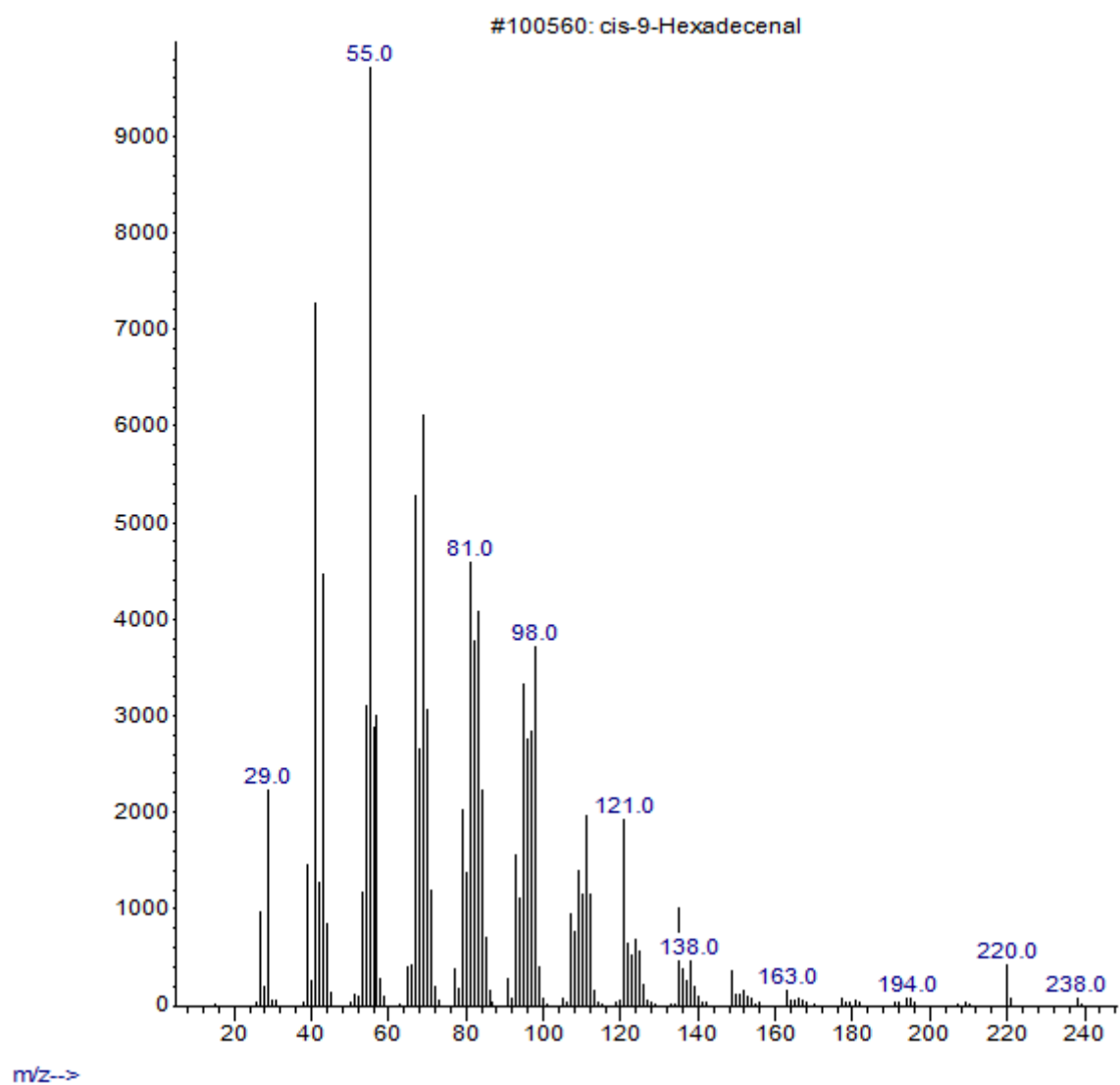
Abundance



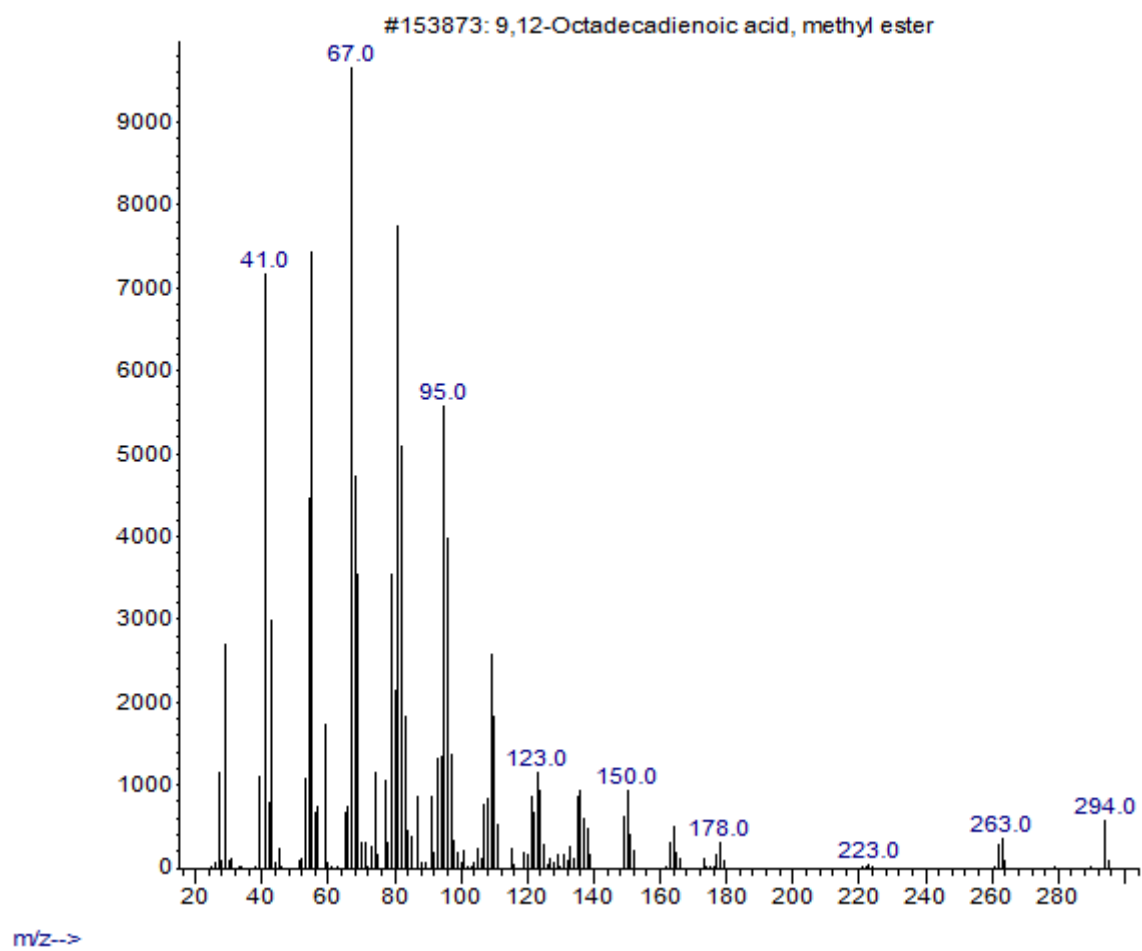
Abundance



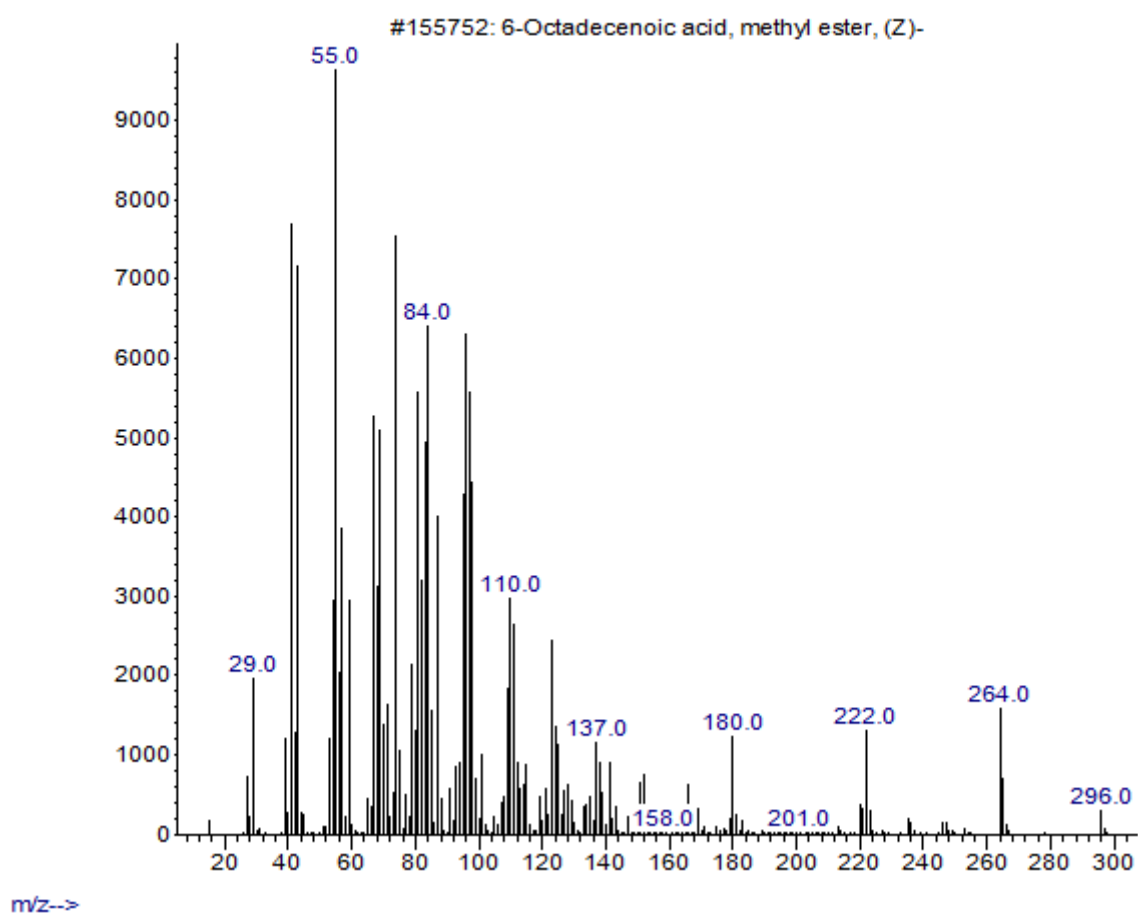
Abundance



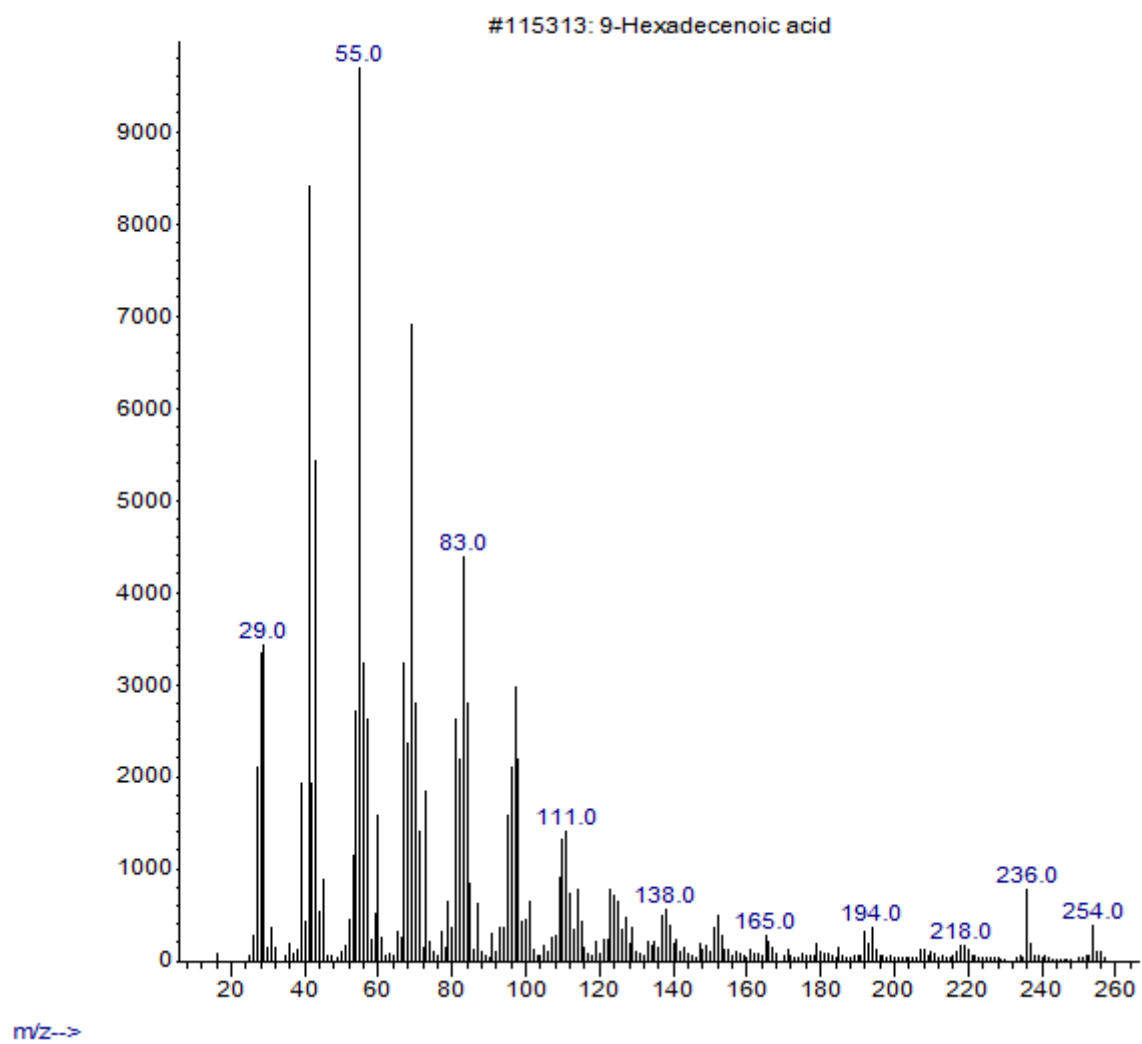
Abundance



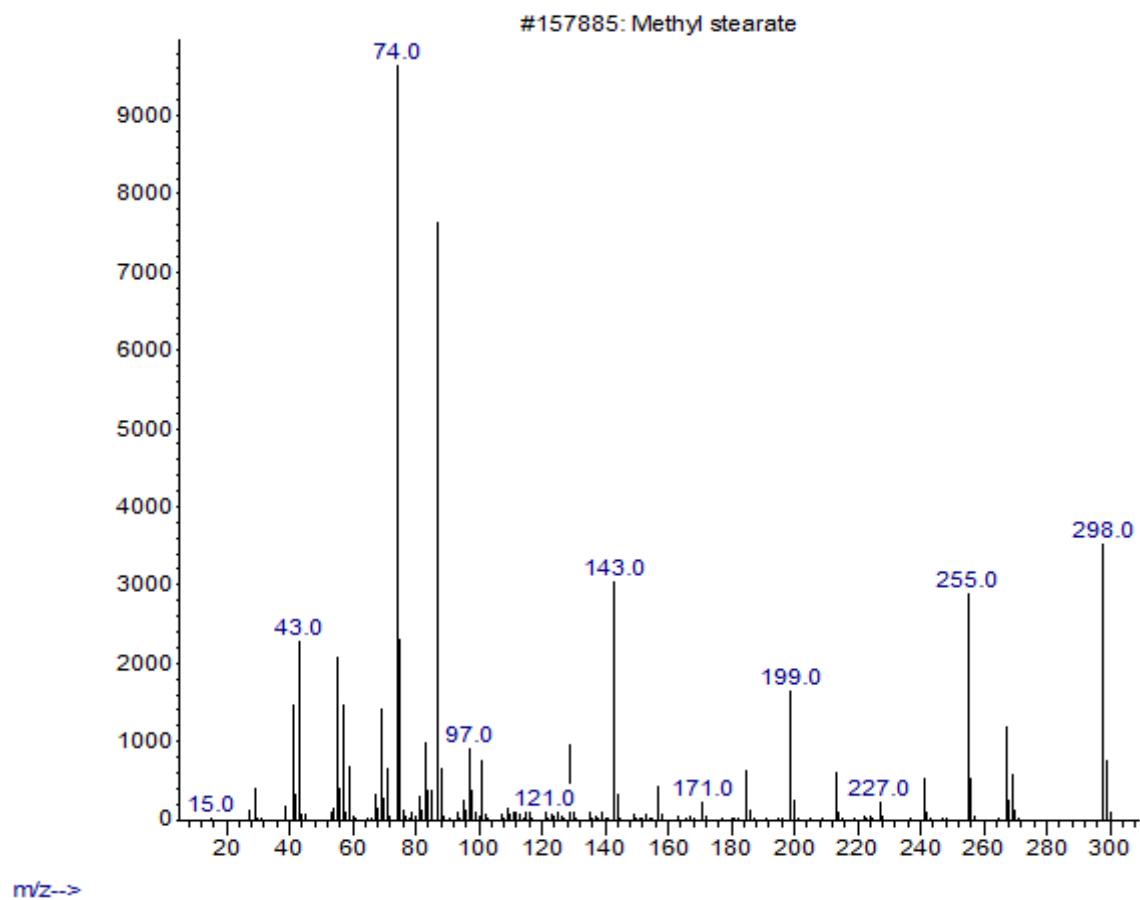
Abundance



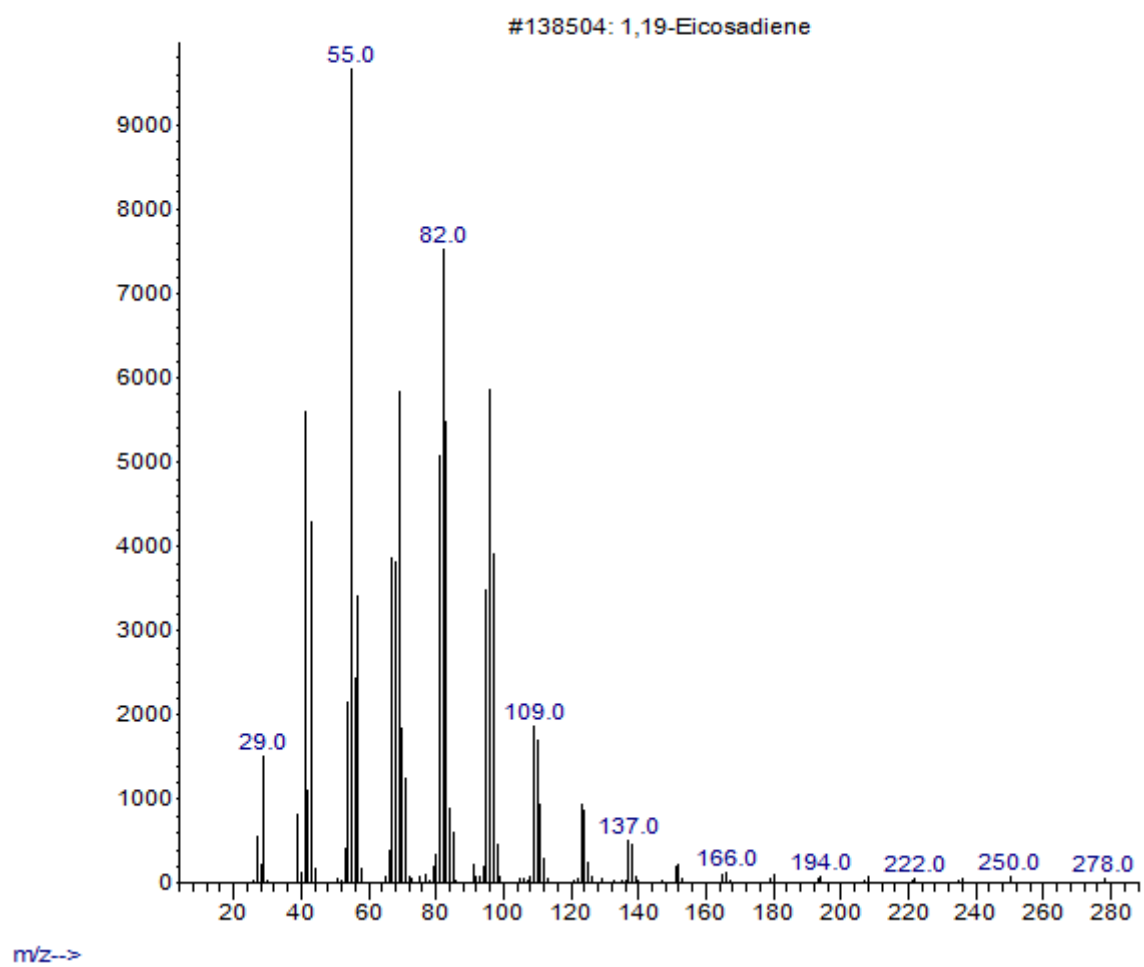
Abundance



Abundance

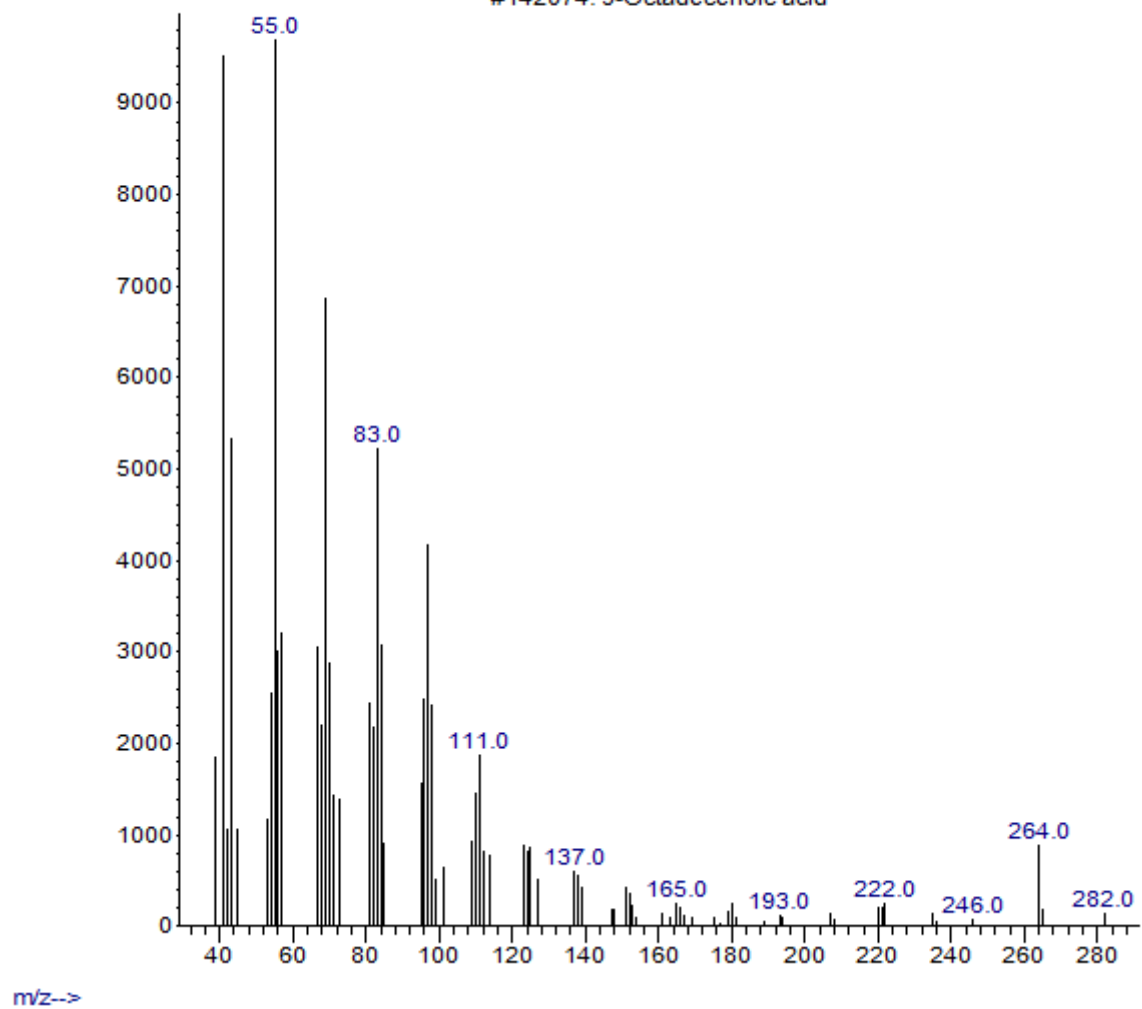


Abundance

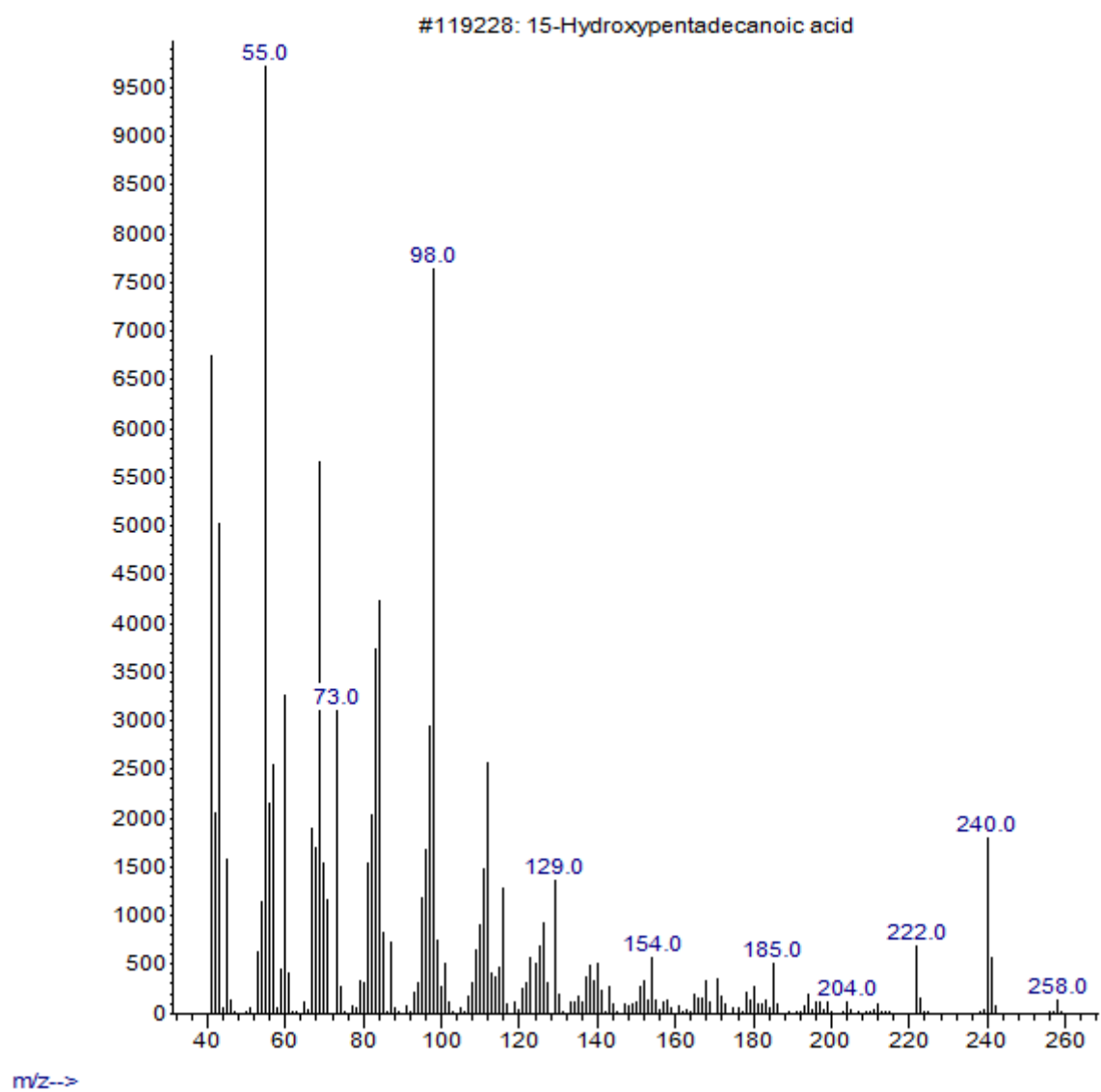


Abundance

#142074: 9-Octadecenoic acid

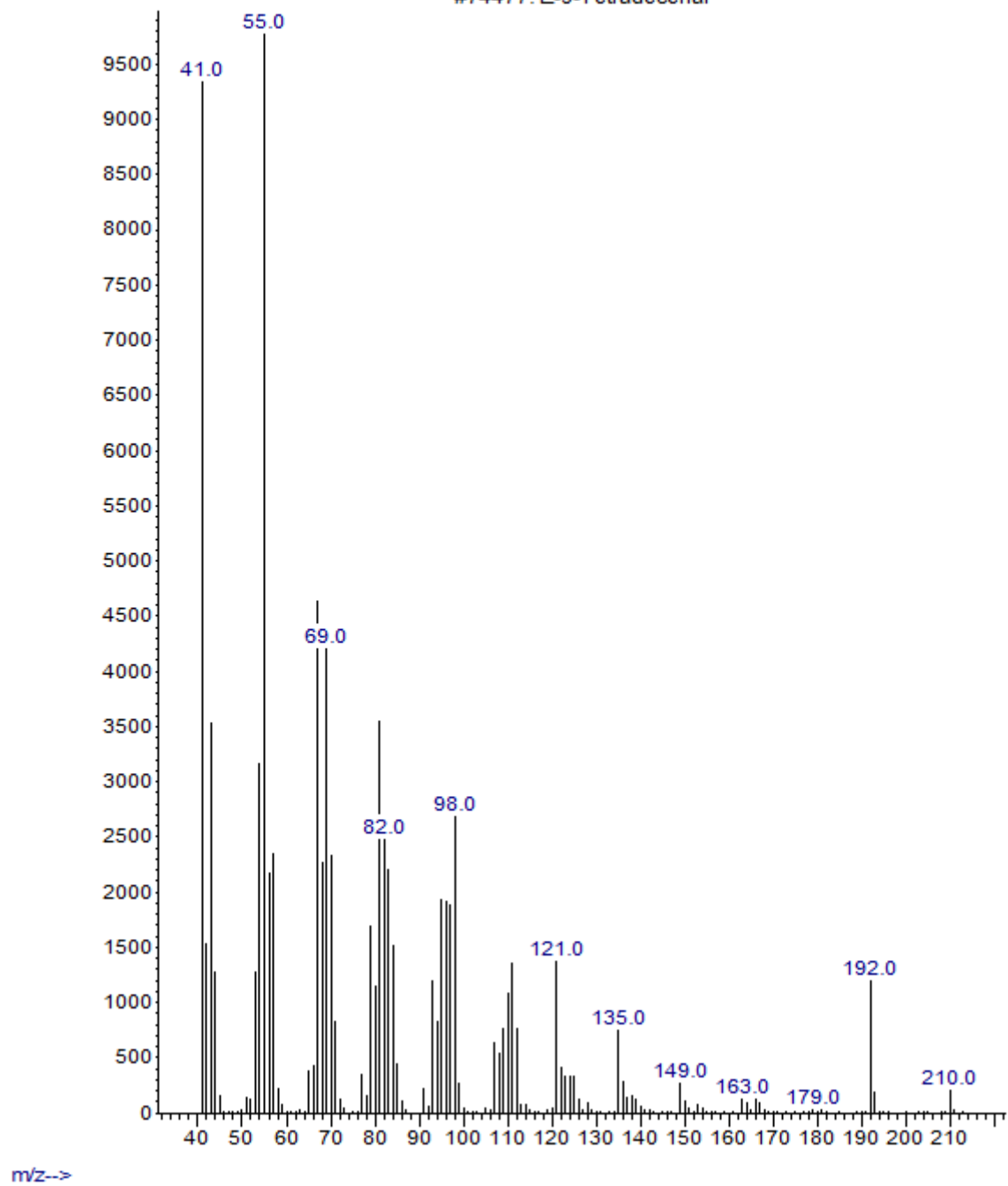


Abundance

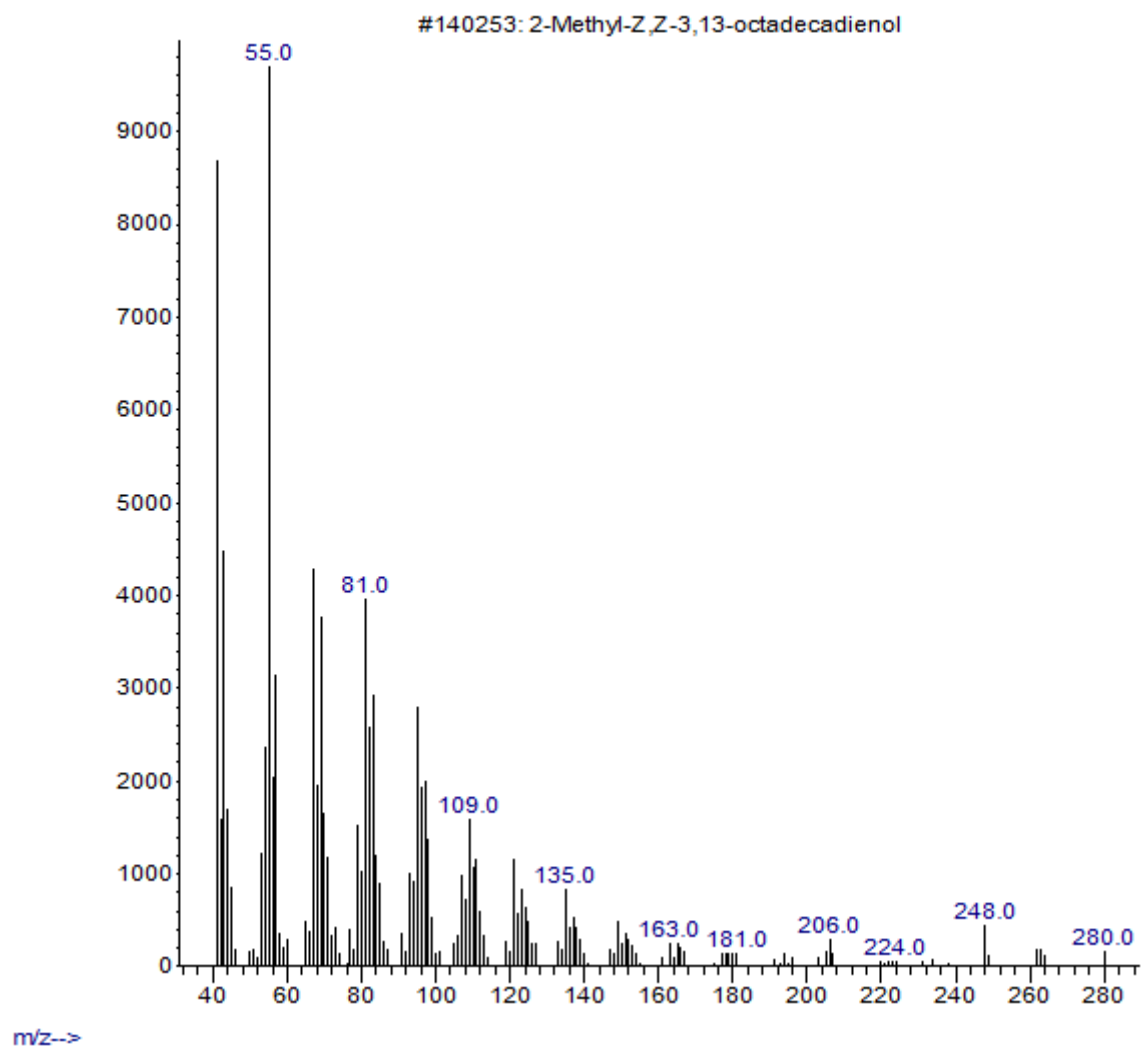


Abundance

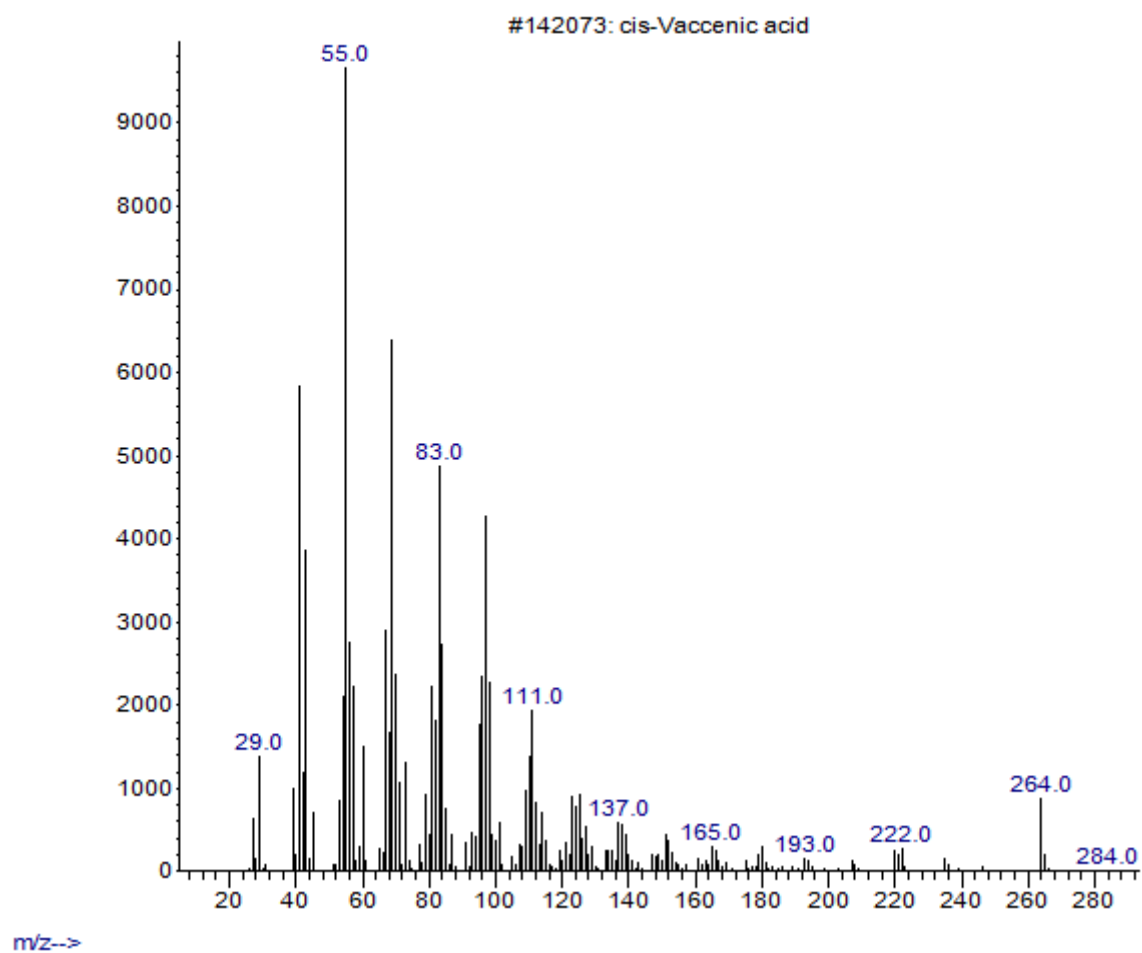
#74477: E-9-Tetradecenal



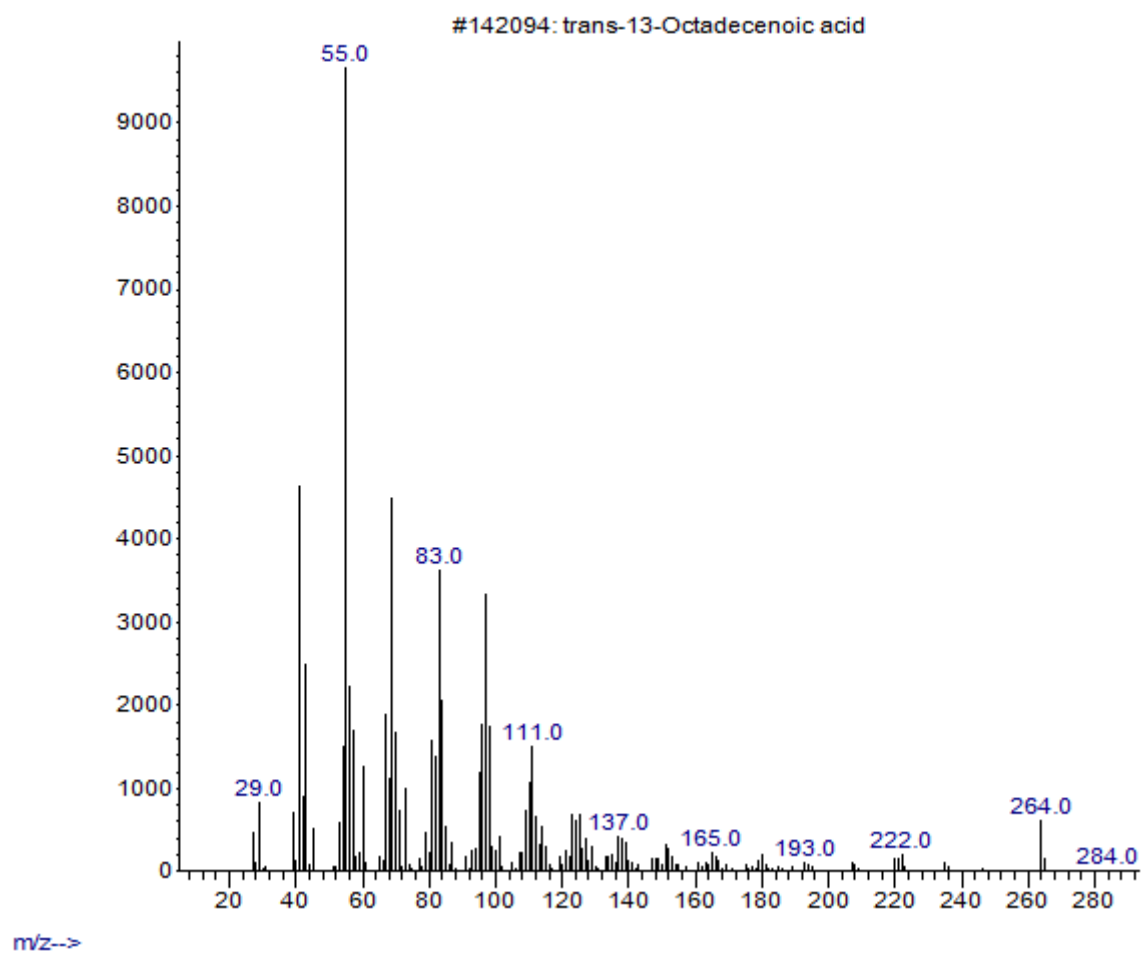
Abundance



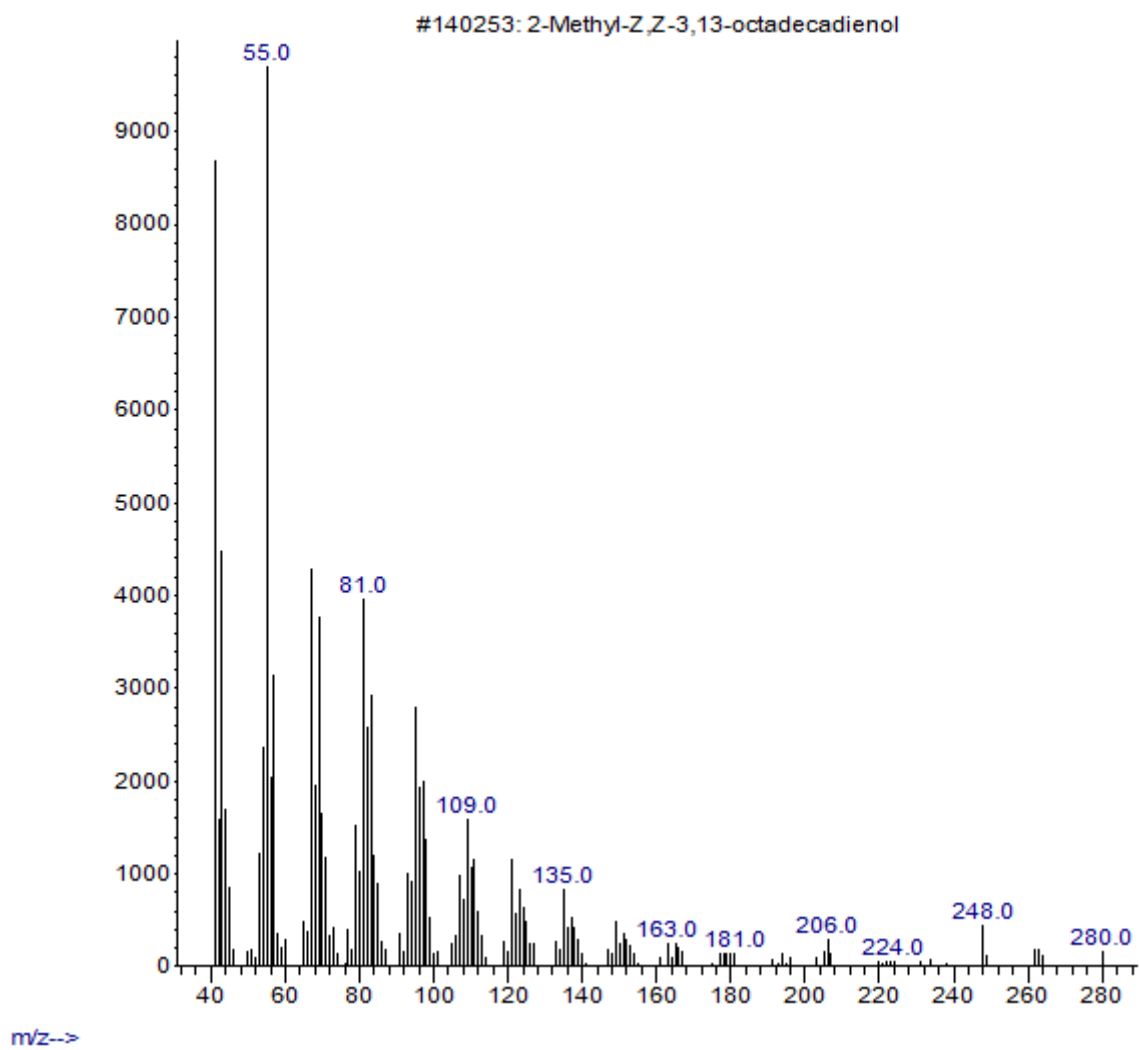
Abundance



Abundance

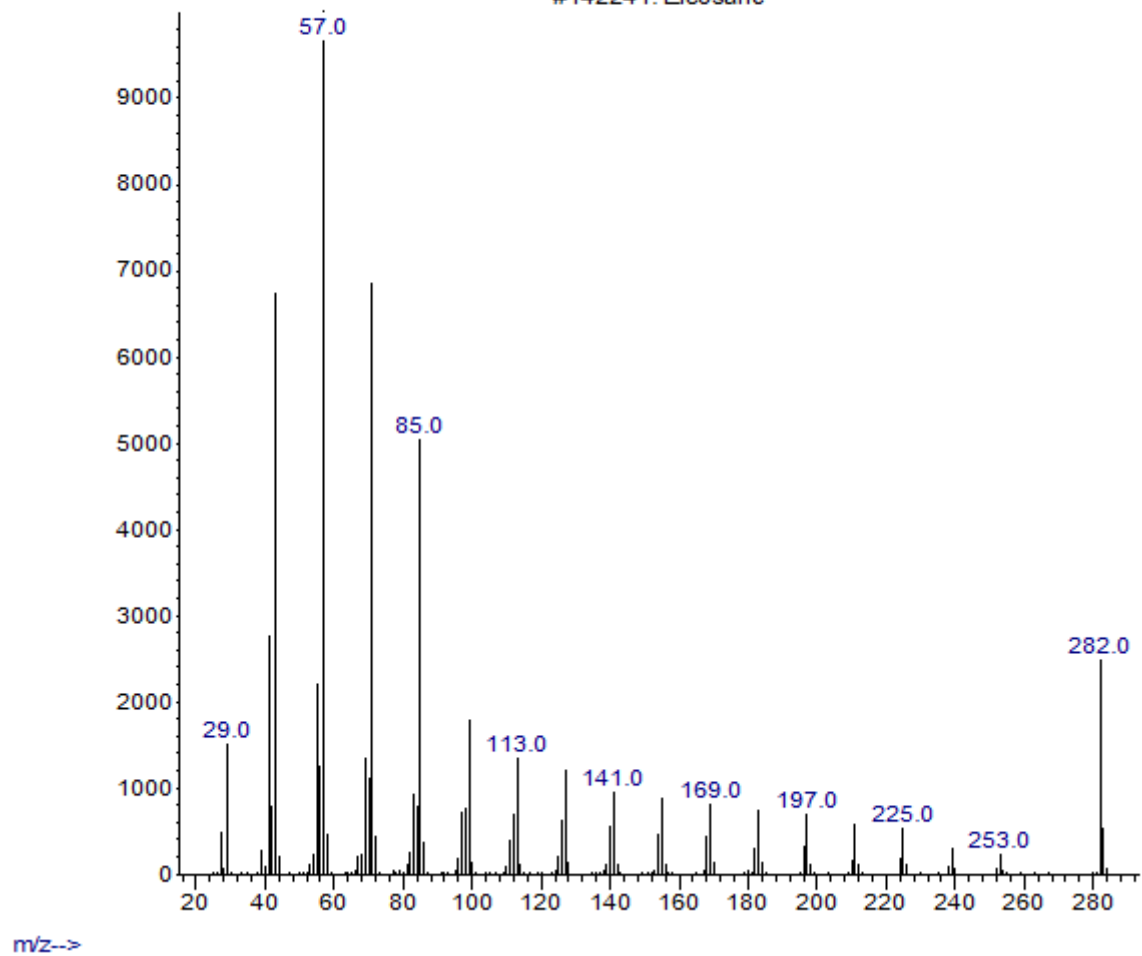


Abundance

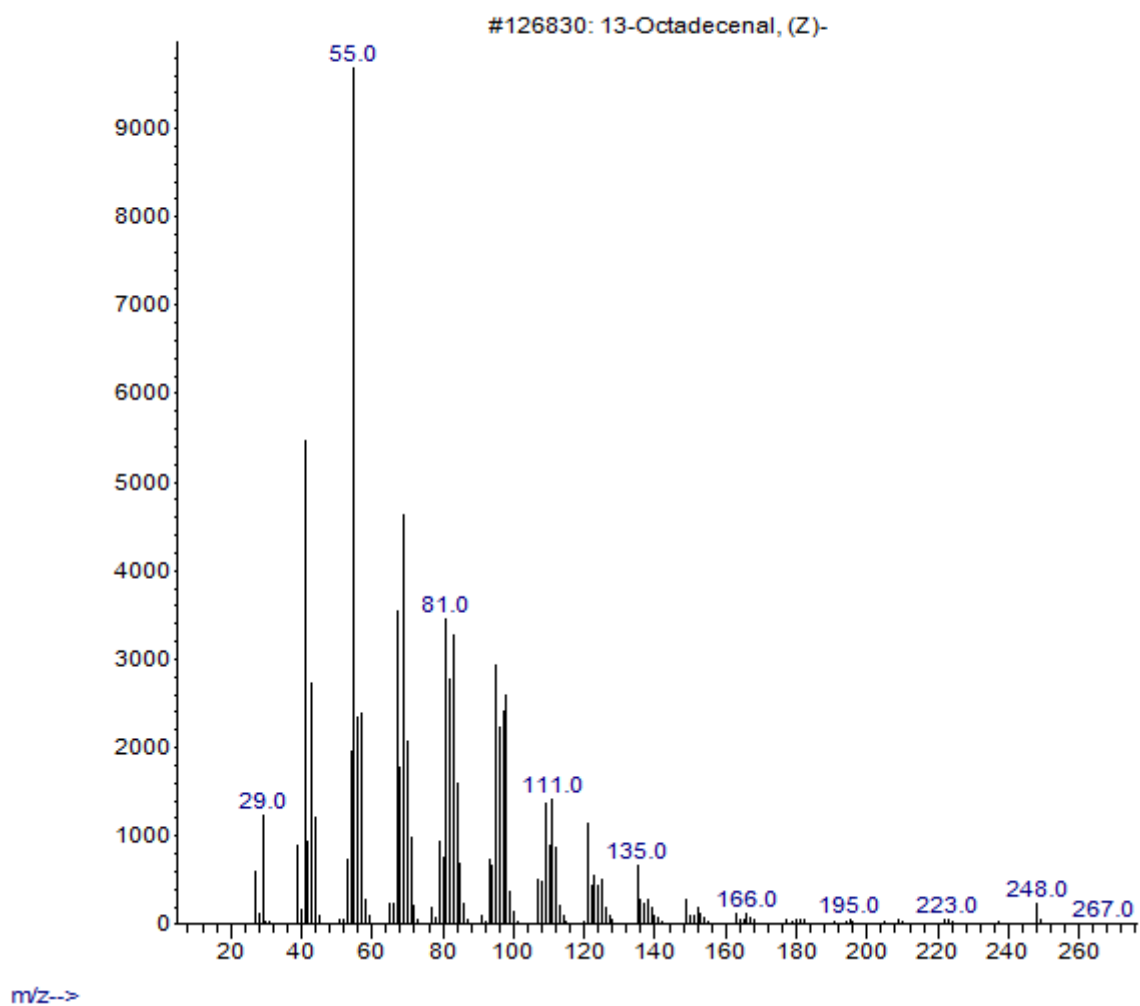


Abundance

#142241: Eicosane



Abundance



AIMS Press

© 2024 the Author(s), licensee AIMS Press. This is an open access article distributed under the terms of the Creative Commons Attribution License (<http://creativecommons.org/licenses/by/4.0>)