



DEVELONUTRI BOOK

PART I - TOMATO

First Edition (June, 2010)

edited by

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FP6 - 036296

DEVELONUTRI

**Development of High Throughput Approaches to Optimise the
Nutritional Value of Crops and Crop-Based Foods**

Sixth Framework Program

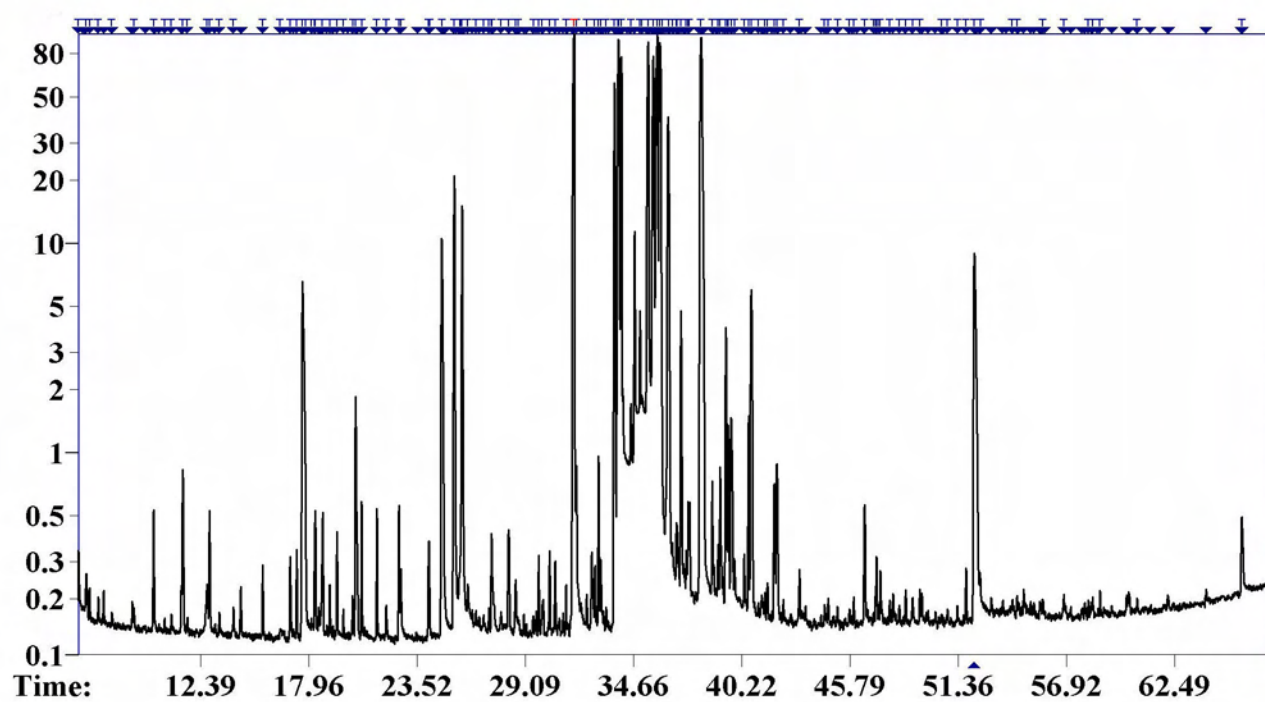
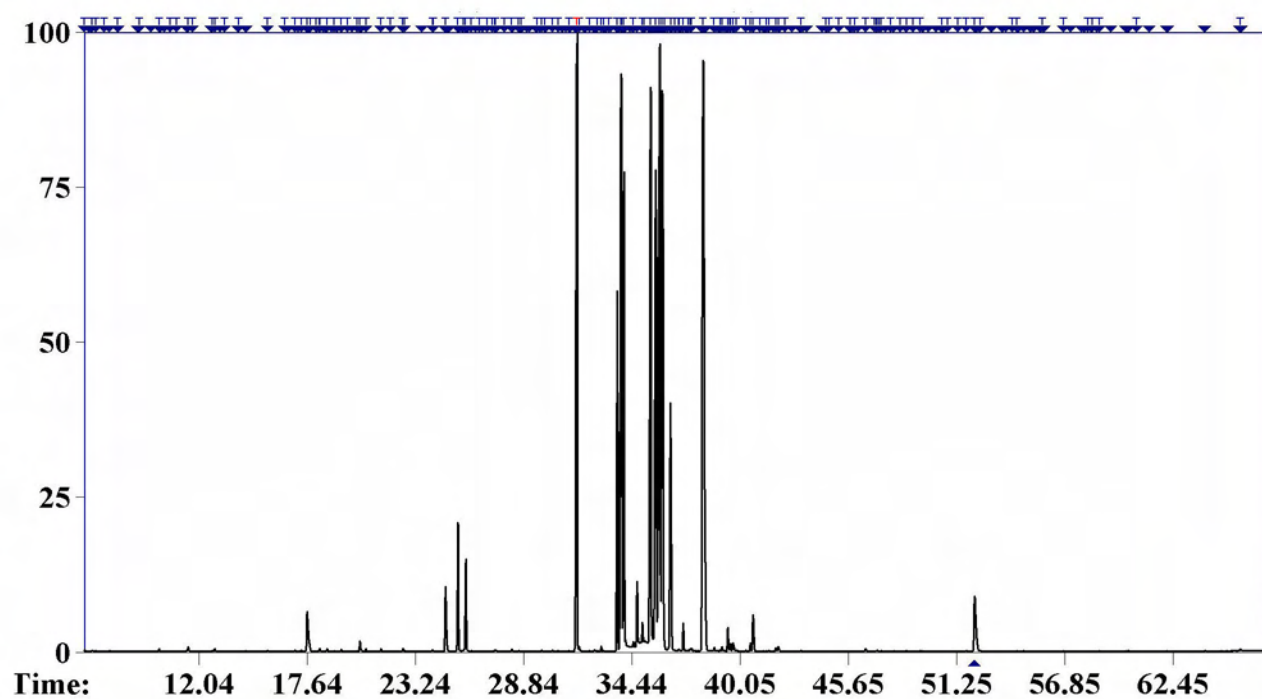
The **Develonutri Reference Book** is a database containing selected chromatographic, spectral and quantitative data collected during the project.

Edition I of the Book is constructed in Adobe Acrobat as a multi-platform publishing medium in order to facilitate inter-laboratory comparison of major analytical findings.

Although the current Edition is available on the internet and can be searched by readers, it is anticipated that future Editions will be available in html with potential for increased user interaction.

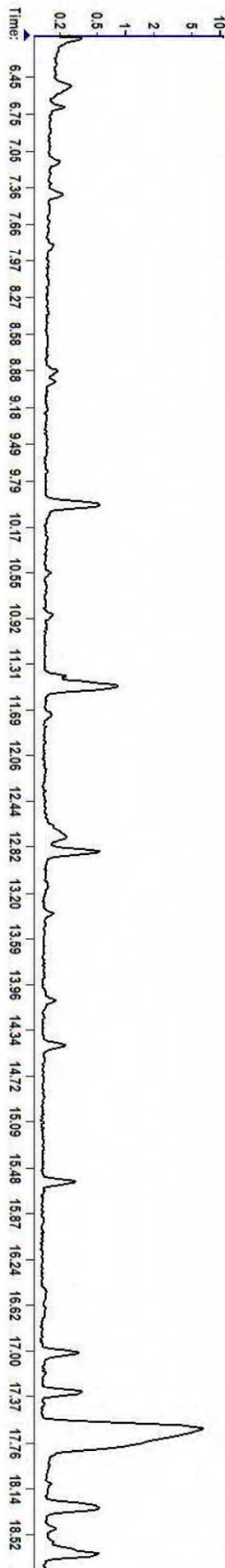
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RETENTION INDEX 900-1300

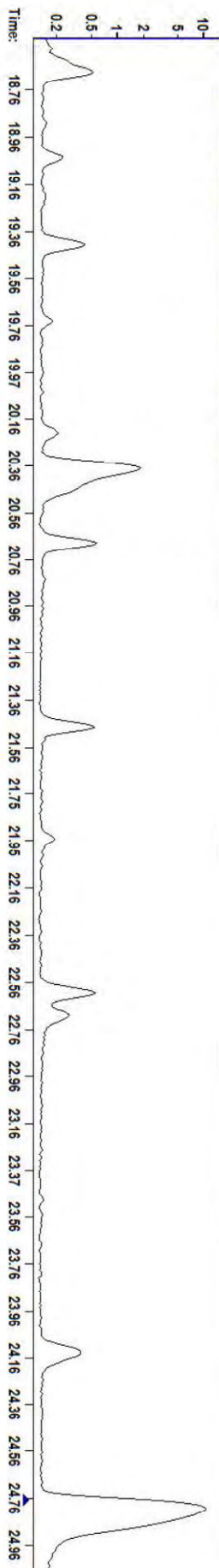
[return to main chromatogram](#)



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RETENTION INDEX 1300-1500

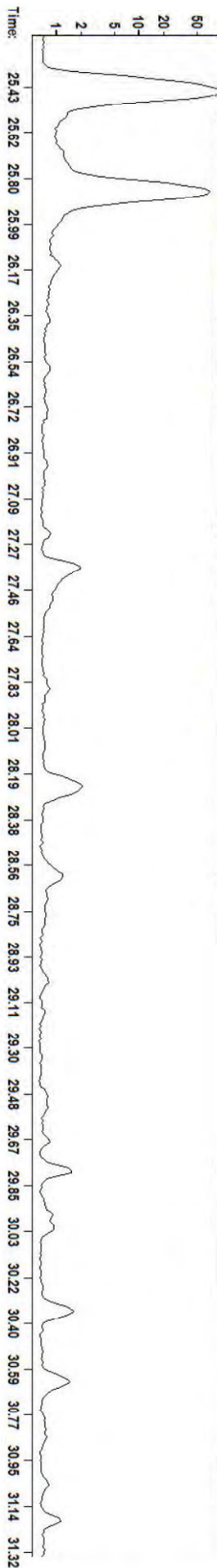
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RETENTION INDEX 1500-1700

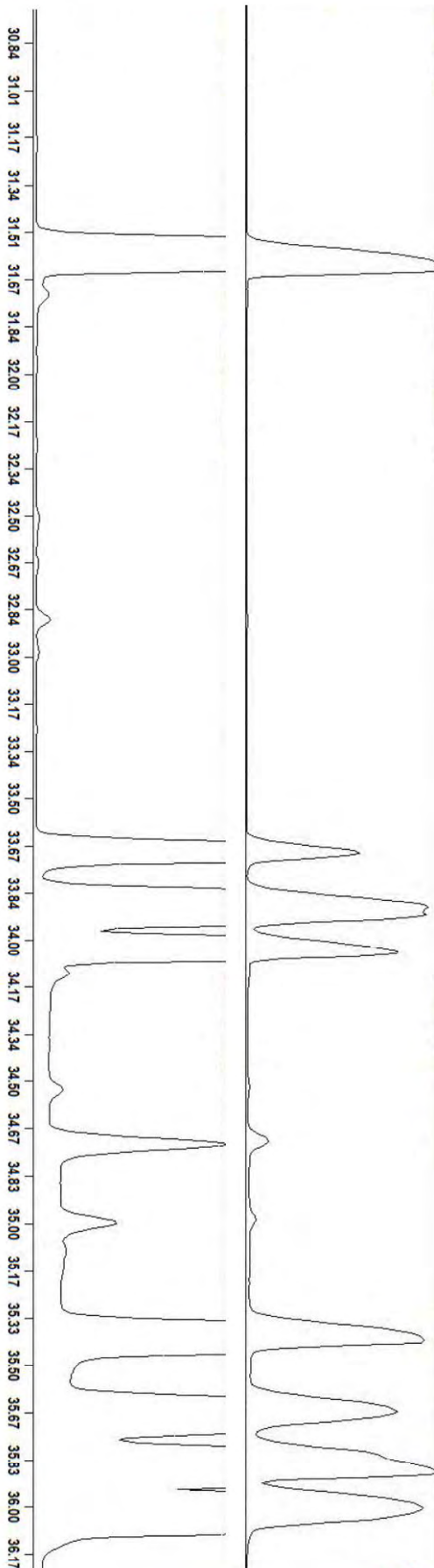
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RETENTION INDEX 1700-1900

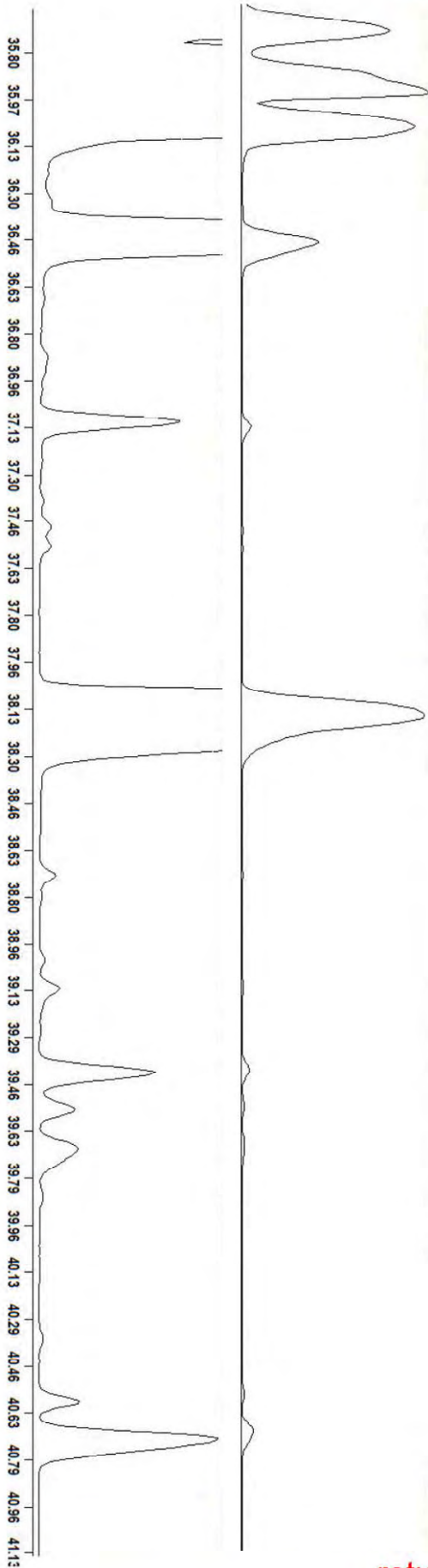
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[return to main chromatogram](#)

RETENTION INDEX 1900-2100

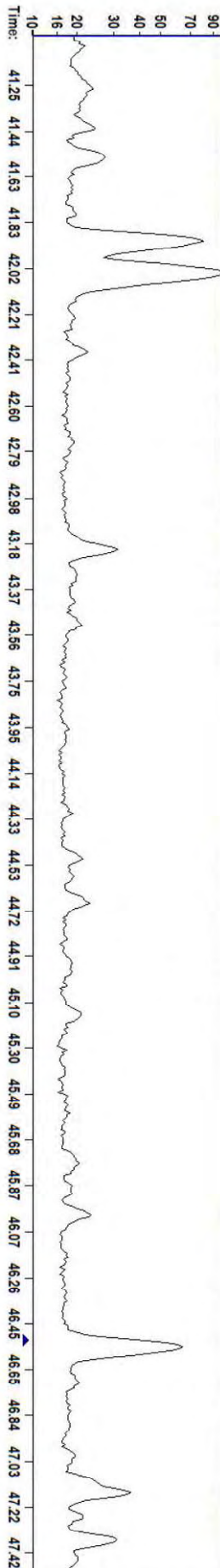
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RETENTION INDEX 2100-2400

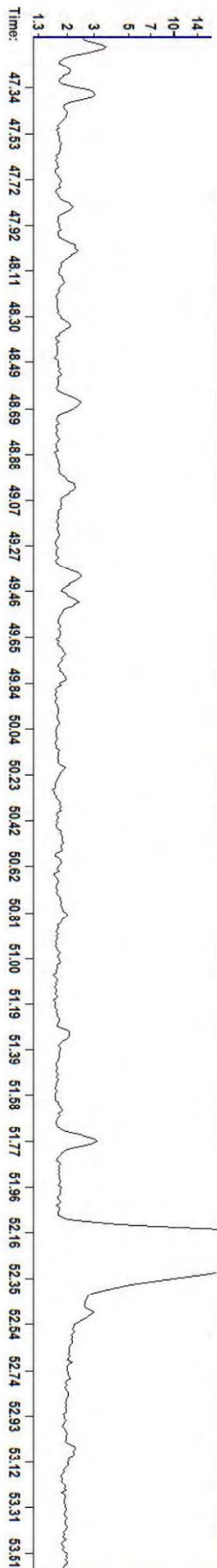
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[return to main chromatogram](#)

RETENTION INDEX 2400-2700

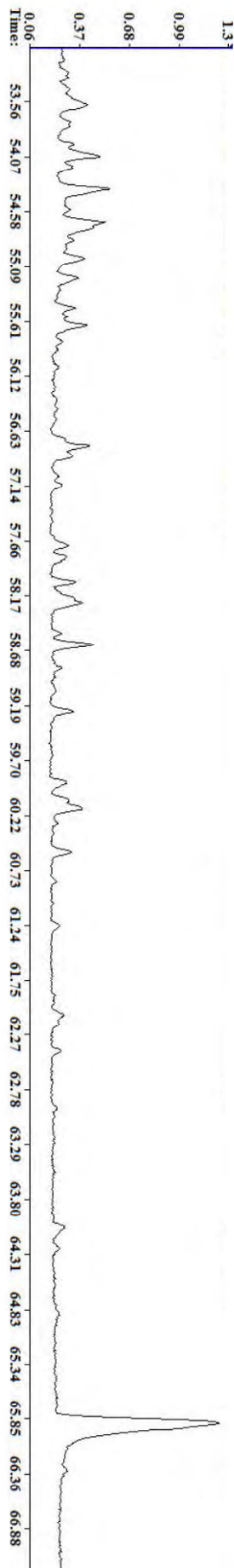
[return to main chromatogram](#)



[return to main chromatogram](#)

RETENTION INDEX 2700---

[return to main chromatogram](#)



[return to main chromatogram](#)

NIST GC/MS USER LIBRARY

compound naming convention

RH-T = Royal Holloway – Tomato (P=potato, W=wheat)

Retention Index DB-5MS (5% phenyl-methylpolysiloxane)

Abundance (AMDIS % total ion current)¹

Name

T=TMS, M=methoxime

CONF=confirmed, TENT=tentative²

CAS Registry – parent compound

GCMS method

RH-T-1142.9-0.05%-OXALIC ACID 2T-CONF-[144-62-7]-RH03

Best library match, N=NIST, G=Golm <http://csbdb.mpimp-golm.mpg.de/>

Unknown: major m/z (excluding m/z 73,147)

Weak spectrum – to be replaced

RH-T-1109.3-0.00%-[N: Tris(trimethylsilyl)hydroxylamine]-TENT-RH03-X

RH-T-1327.5-0.03%-[184,285,134, G: tms unk.hp: ARA COL. LEAF 014]-RH03

RH-T-1252.9-0.00%-BENZOIC ACID T-CONF-[65-85-0]- 8135A18-G

Comment/best library match on unknown

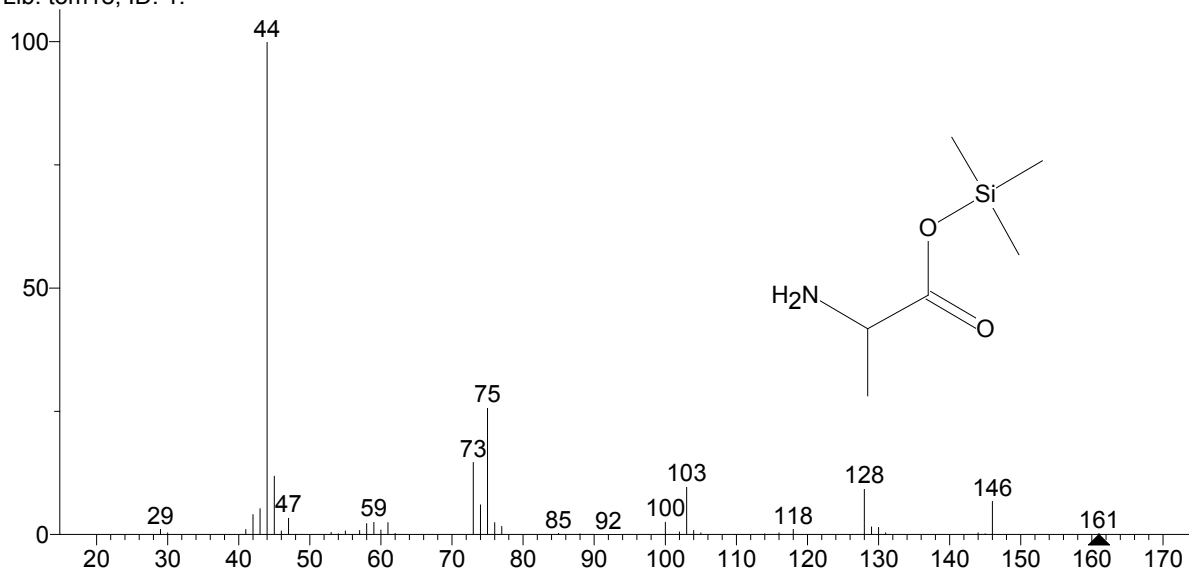
Non RHUL reference:
G=MPIMP,S=SCRI,F=ENEA

¹ A rough indication of compound abundance

² CONF=confirmed by standards or multiple library/RI matches

Hit 1 : RH-T-0954.2-0.01%-[N: L-Alanine, trimethylsilyl ester]-TENT-RH03

Lib: tom18; ID: 1.



(tom18) RH-T-0954.2-0.01%-[N: L-Alanine, trimethylsilyl ester]-TENT-RH03 RI:0954.2,

Name: RH-T-0954.2-0.01%-[N: L-Alanine, trimethylsilyl ester]-TENT-RH03

Formula: C₆H₁₅NO₂Si

MW: 161 ID#: 1 DB: tom18

RI: 0954.2,

Comment: RI=0954.2, 6.3419 min MG00244 [RI:954.2]

10 largest peaks:

44 999 | 75 257 | 73 146 | 45 118 | 103 97 | 128 93 | 146 67 | 74 60 | 43 52 | 42 40 |

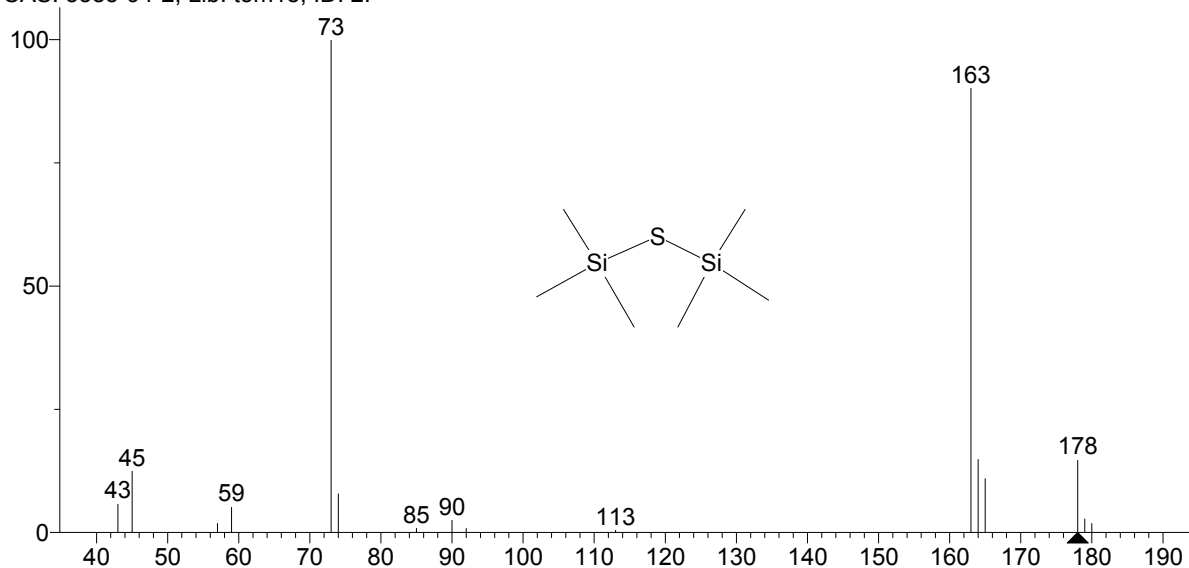
23 m/z Values and Intensities (19 low intensity peaks are not shown):

29 11	43 52	47 34	60 9	74 60	77 16	118 11	130 14
41 10	44 999	58 22	61 24	75 257	100 26	128 93	146 67
42 40	45 118	59 26	73 146	76 24	103 97	129 15	

Synonyms:

1. Alanine T;

Hit 2 : RH-T-0961.2-0.00%-[N:Bis(trimethylsilyl)sulfide]-TENT-RH03
CAS: 3385-94-2; Lib: tom18; ID: 2.



(tom18) RH-T-0961.2-0.00%-[N:Bis(trimethylsilyl)sulfide]-TENT-RH03 RI:961.2,

Name: RH-T-0961.2-0.00%-[N:Bis(trimethylsilyl)sulfide]-TENT-RH03

Formula: C₆H₁₈SSi₂

MW: 178 CAS#: 3385-94-2 ID#: 2 DB: tom18

Other DBs: None

RI: 961.2,

Comment: RI=961.2, 6.5829 min MG00244 |RI:961.2|

10 largest peaks:

73 999 | 163 901 | 164 148 | 178 148 | 45 124 | 165 109 | 74 78 | 43 58 | 59 52 | 179 27 |

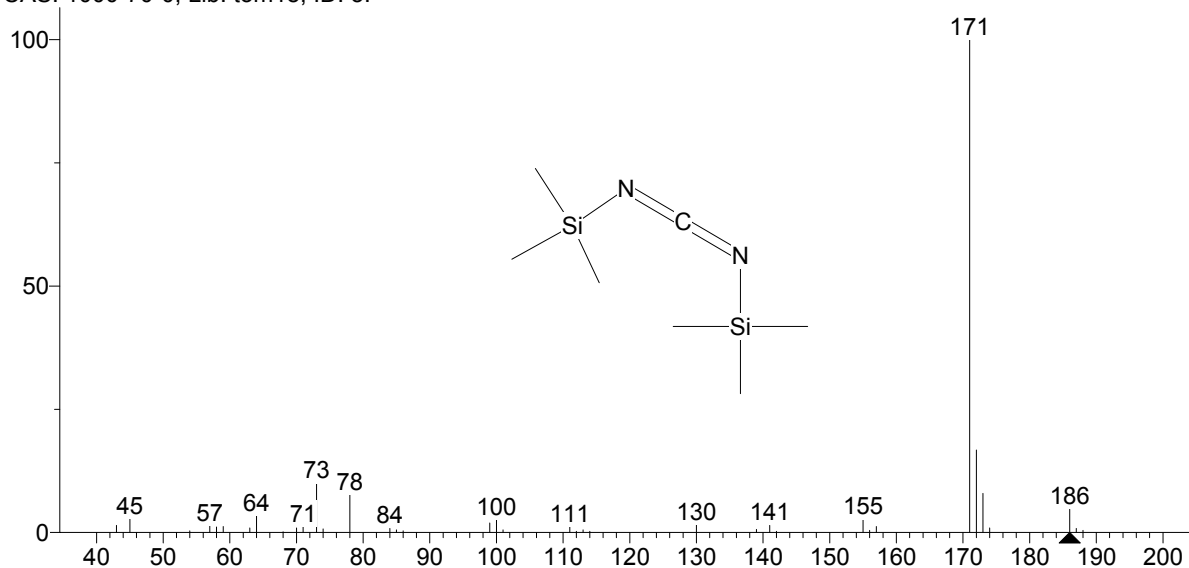
13 m/z Values and Intensities (3 low intensity peaks are not shown):

43 58 | 57 18 | 73 999 | 90 25 | 164 148 | 178 148 | 180 18 |
45 124 | 59 52 | 74 78 | 163 901 | 165 109 | 179 27 |

Synonyms:

1.Sulfide 2T-TENT;

Hit 3 : RH-T-0966.3-0.00%-[N:Carbodiimide, bis(trimethylsilyl)-]-TENT-RH03
CAS: 1000-70-0; Lib: tom18; ID: 3.



(tom18) RH-T-0966.3-0.00%-[N:Carbodiimide, bis(trimethylsilyl)-]-TENT-RH03 RI:966.3,

Name: RH-T-0966.3-0.00%-[N:Carbodiimide, bis(trimethylsilyl)-]-TENT-RH03

Formula: C₇H₁₈N₂Si₂

MW: 186 CAS#: 1000-70-0 ID#: 3 DB: tom18

Other DBs: None

RI: 966.3,

Comment: RI=966.3, 6.7616 min MG00244 [RI:966.3]

10 largest peaks:

171 999 | 172 167 | 73 99 | 173 79 | 78 76 | 186 47 | 64 33 | 45 27 | 155 26 | 100 25 |

23 m/z Values and Intensities (15 low intensity peaks are not shown):

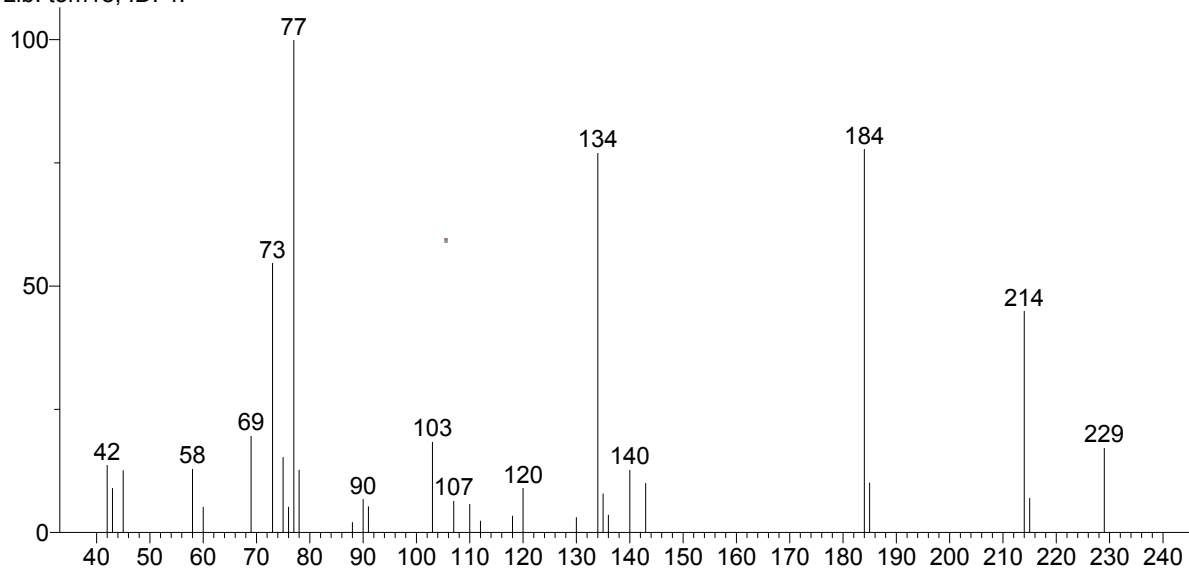
43 14 | 58 11 | 64 33 | 73 99 | 100 25 | 141 14 | 171 999 | 174 9 |
45 27 | 59 12 | 70 9 | 78 76 | 111 11 | 155 26 | 172 167 | 186 47 |
57 13 | 63 9 | 71 11 | 99 19 | 130 15 | 157 12 | 173 79 |

Synonyms:

1.Carbodiimide 2T-TENT;

Hit 4 : RH-T-0982.9-0.00%-[184,134,214,229,103]-RH03

Lib: tom18; ID: 4.



(tom18) RH-T-0982.9-0.00%-[184,134,214,229,103]-RH03 RI:982.9,

Name: RH-T-0982.9-0.00%-[184,134,214,229,103]-RH03

MW: N/A ID#: 4 DB: tom18

RI: 982.9,

Comment: RI=982.9, 7.3329 min MG00244 [RI:982.9]

10 largest peaks:

77 999 | 184 777 | 134 770 | 73 546 | 214 449 | 69 196 | 103 184 | 229 172 | 75 152 | 42 136 |

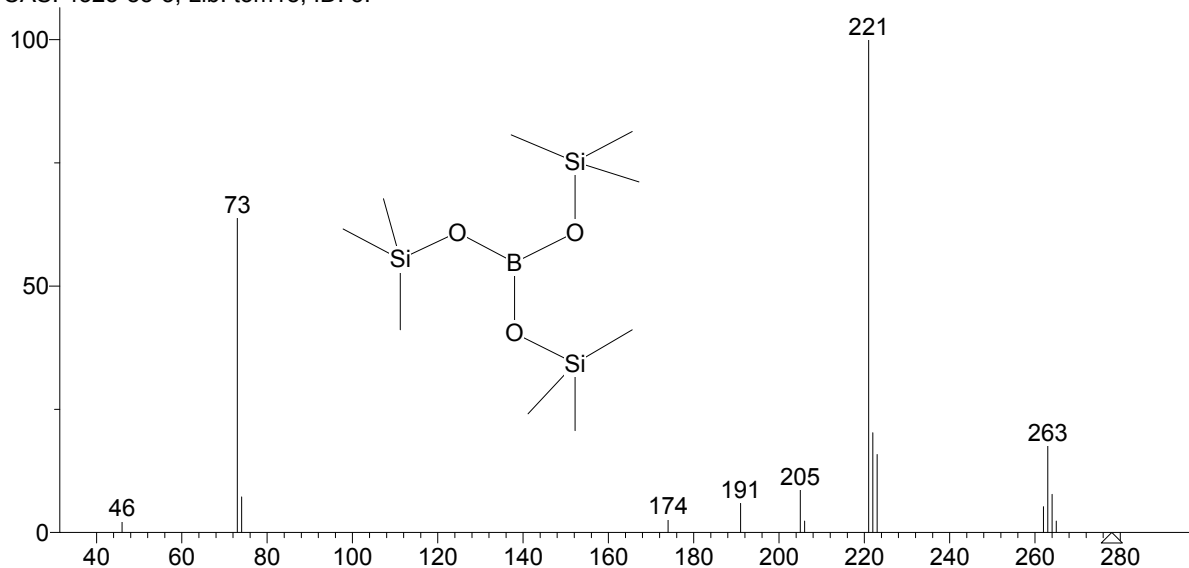
31 m/z Values and Intensities:

42 136 | 60 51 | 76 51 | 90 67 | 110 57 | 130 30 | 140 127 | 214 449 |
43 89 | 69 196 | 77 999 | 91 52 | 112 23 | 134 770 | 143 99 | 215 69 |
45 125 | 73 546 | 78 126 | 103 184 | 118 33 | 135 78 | 184 777 | 229 172 |
58 129 | 75 152 | 88 20 | 107 64 | 120 90 | 136 35 | 185 100 |

Synonyms:

1.m184,134,214,229,103;

Hit 5 : RH-T-0985.8-0.00%-[N:Tris(trimethylsilyl)borate]-TENT-RH03
CAS: 4325-85-3; Lib: tom18; ID: 5.



(tom18) RH-T-0985.8-0.00%-[N:Tris(trimethylsilyl)borate]-TENT-RH03 RI:985.8,

Name: RH-T-0985.8-0.00%-[N:Tris(trimethylsilyl)borate]-TENT-RH03

Formula: $C_9H_{27}BO_3Si_3$

MW: 278 CAS#: 4325-85-3 ID#: 5 DB: tom18

Other DBs: None

RI: 985.8,

Comment: RI=985.8, 7.4337 min MG00244 |RI:985.8|

10 largest peaks:

221 999 | 73 637 | 222 202 | 263 175 | 223 158 | 205 86 | 264 77 | 74 72 | 191 59 | 262 52 |

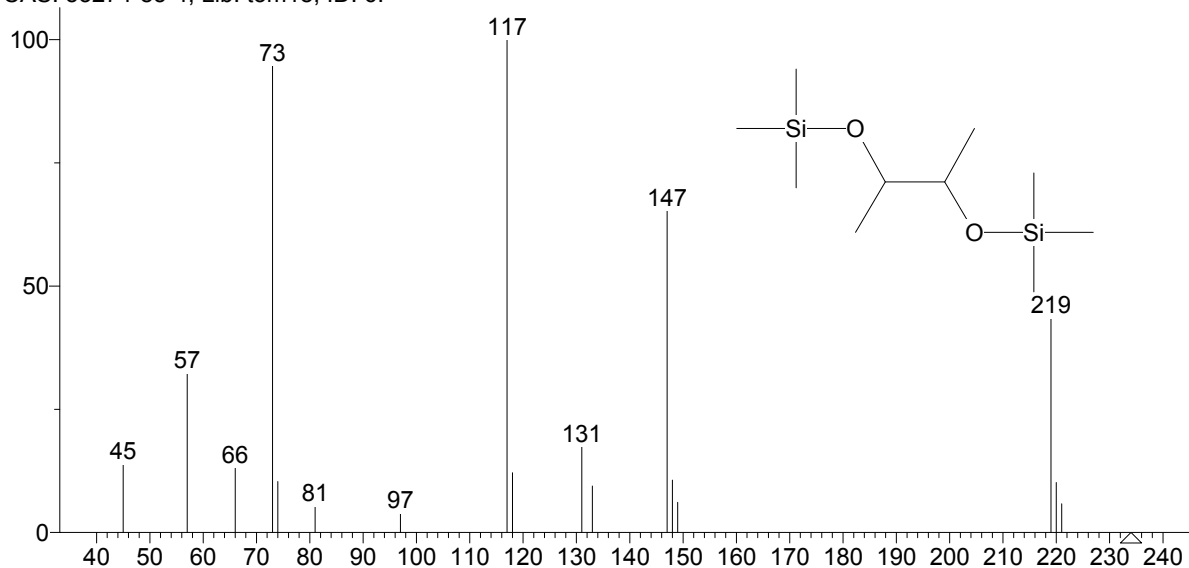
14 m/z Values and Intensities:

46 22 | 74 72 | 191 59 | 206 23 | 222 202 | 262 52 | 264 77 |
73 637 | 174 26 | 205 86 | 221 999 | 223 158 | 263 175 | 265 23 |

Synonyms:

1.Borate 3T-TENT;

Hit 6 : RH-T-0999.3-0.00%-[N: Butane, 2,3-bis(trimethylsiloxy)-]-TENT-RH03
CAS: 53274-85-4; Lib: tom18; ID: 6.



(tom18) RH-T-0999.3-0.00%-[N: Butane, 2,3-bis(trimethylsiloxy)-]-TENT-RH03 RI:999.3,

Name: RH-T-0999.3-0.00%-[N: Butane, 2,3-bis(trimethylsiloxy)-]-TENT-RH03

Formula: C₁₀H₂₆O₂Si₂

MW: 234 CAS#: 53274-85-4 ID#: 6 DB: tom18

Other DBs: None

RI: 999.3,

Comment: RI=999.3, 7.8980 min MG00244 [RI:999.3]

10 largest peaks:

117 999 | 73 946 | 147 652 | 219 433 | 57 322 | 131 173 | 45 137 | 66 130 | 118 121 | 148 106 |

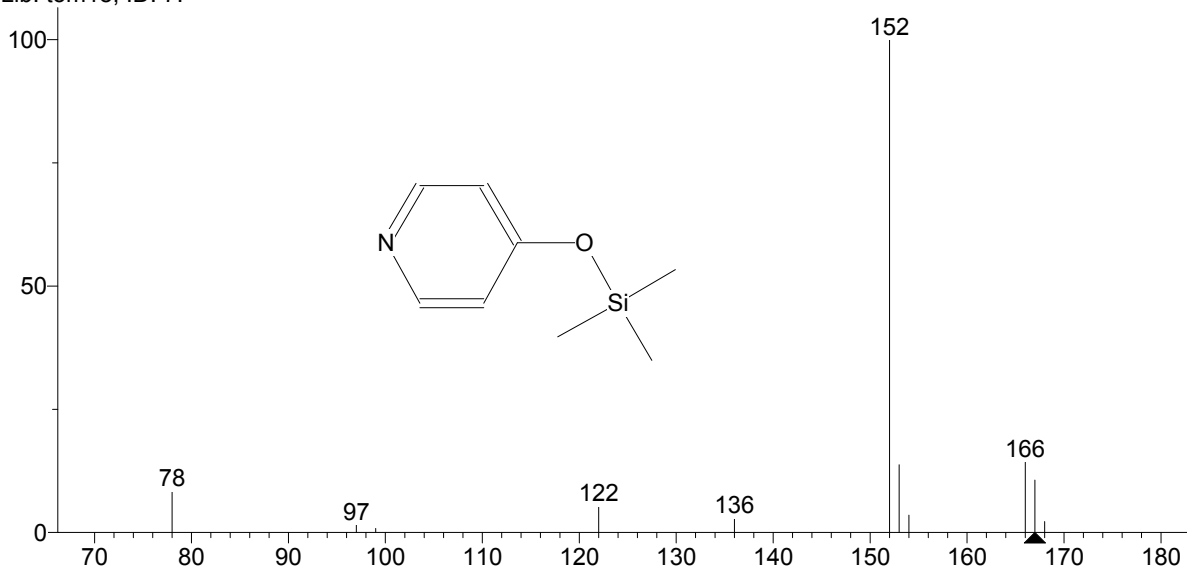
17 m/z Values and Intensities:

45 137 | 66 130 | 74 103 | 97 38 | 118 121 | 133 94 | 148 106 | 219 433 | 221 58 |
57 322 | 73 946 | 81 52 | 117 999 | 131 173 | 147 652 | 149 61 | 220 101 |

Synonyms:

1. Butane, 2,3-2T-TENT;

Hit 7 : RH-T-1032.1-0.00%-[N:4-Hydroxypyridine, trimethylsilyl ether]-TENT-RH03
Lib: tom18; ID: 7.



(tom18) RH-T-1032.1-0.00%-[N:4-Hydroxypyridine, trimethylsilyl ether]-TENT-RH03 RI:1032.1,

Name: RH-T-1032.1-0.00%-[N:4-Hydroxypyridine, trimethylsilyl ether]-TENT-RH03

Formula: C₈H₁₃NOSi

MW: 167 ID#: 7 DB: tom18

RI: 1032.1,

Comment: RI=1032.1, 9.0292 min MG00244 [RI:1032.1]

10 largest peaks:

152 999 | 166 143 | 153 137 | 167 106 | 78 83 | 122 52 | 154 35 | 136 28 | 168 22 | 97 15 |

10 m/z Values and Intensities (1 low intensity peak is not shown):

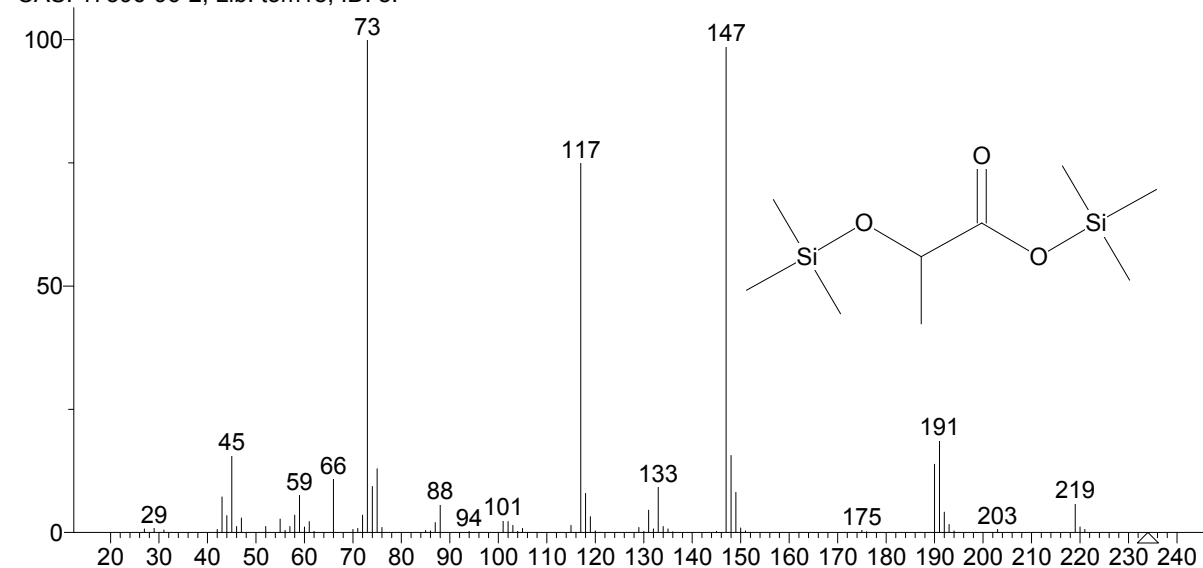
78 83 | 97 15 | 122 52 | 136 28 | 152 999 | 153 137 | 154 35 | 166 143 | 167 106 | 168 22 |

Synonyms:

1.Hydroxypyridine T TENT;

Hit 8 : RH-T-1063.0-0.02%-LACTIC ACID 2T-CONF-[50-21-5]-RH03

CAS: 17596-96-2; Lib: tom18; ID: 8.



(tom18) RH-T-1063.0-0.02%-LACTIC ACID 2T-CONF-[50-21-5]-RH03

Name: RH-T-1063.0-0.02%-LACTIC ACID 2T-CONF-[50-21-5]-RH03

Formula: C₉H₂₂O₃Si₂

MW: 234 CAS#: 17596-96-2 ID#: 8 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:1063|

10 largest peaks:

73 999 | 147 985 | 117 749 | 191 186 | 45 156 | 148 156 | 190 138 | 75 129 | 66 108 | 74 93 |

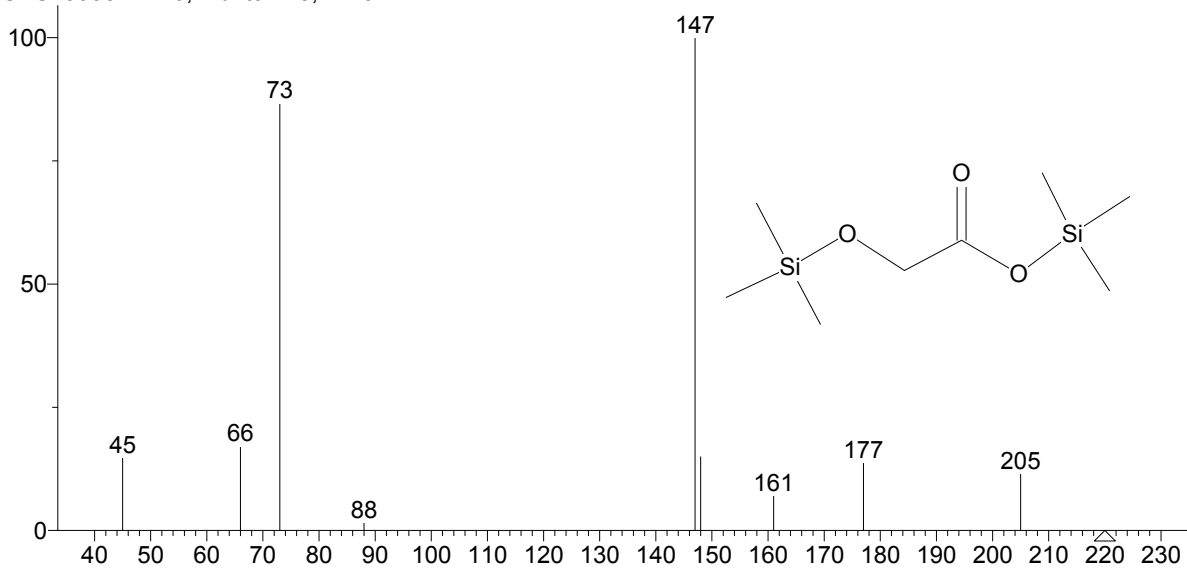
42 m/z Values and Intensities (24 low intensity peaks are not shown):

29	9	47	29	59	75	73	999	88	56	117	749	133	92	150	9	219	58
43	72	52	12	60	11	74	93	101	24	118	79	134	12	190	138	220	11
44	34	55	27	61	22	75	129	102	22	119	32	147	985	191	186		
45	156	57	12	66	108	76	10	103	14	129	10	148	156	192	41		
46	12	58	35	72	35	87	20	115	14	131	45	149	81	193	16		

Synonyms:

1.LACTIC ACID 2T-CONF-[50-21-5];

Hit 9 : RH-T-1079.0-0.00%-GLYCOLIC ACID 2T-CONF-[79-14-1]-RH03
CAS: 33581-77-0; Lib: tom18; ID: 9.



(tom18) RH-T-1079.0-0.00%-GLYCOLIC ACID 2T-CONF-[79-14-1]-RH03

Name: RH-T-1079.0-0.00%-GLYCOLIC ACID 2T-CONF-[79-14-1]-RH03

Formula: C₈H₂₀O₃Si₂

MW: 220 CAS#: 33581-77-0 ID#: 9 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:1079|

9 largest peaks:

147 999 | 73 865 | 66 170 | 148 149 | 45 147 | 177 136 | 205 114 | 161 69 | 88 15 |

9 m/z Values and Intensities:

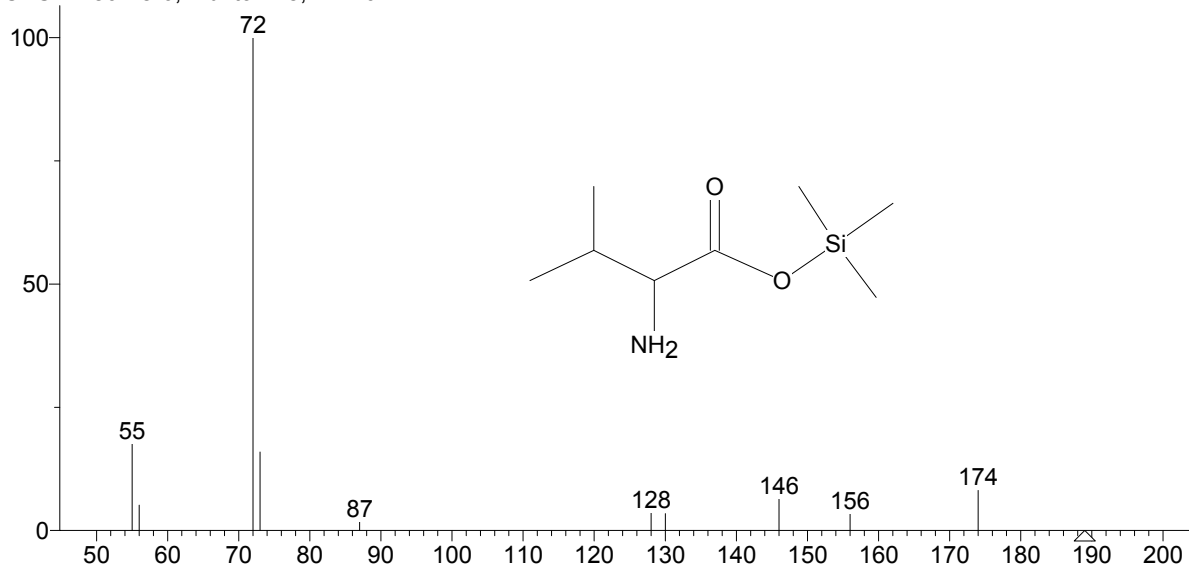
45 147 | 66 170 | 73 865 | 88 15 | 147 999 | 148 149 | 161 69 | 177 136 | 205 114 |

Synonyms:

1.GLYCOLIC ACID 2T-CONF-[79-14-1];

Hit 10 : RH-T-1089.4-0.00%-VALINE 1T-CONF-[516-06-3]-RH03

CAS: 7480-78-6; Lib: tom18; ID: 10.



(tom18) RH-T-1089.4-0.00%-VALINE 1T-CONF-[516-06-3]-RH03

Name: RH-T-1089.4-0.00%-VALINE 1T-CONF-[516-06-3]-RH03

Formula: C₈H₁₉NO₂Si

MW: 189 CAS#: 7480-78-6 ID#: 10 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:1089.4|

10 largest peaks:

72 999 | 55 175 | 73 159 | 174 81 | 146 63 | 56 51 | 128 35 | 130 34 | 156 33 | 87 17 |

10 m/z Values and Intensities:

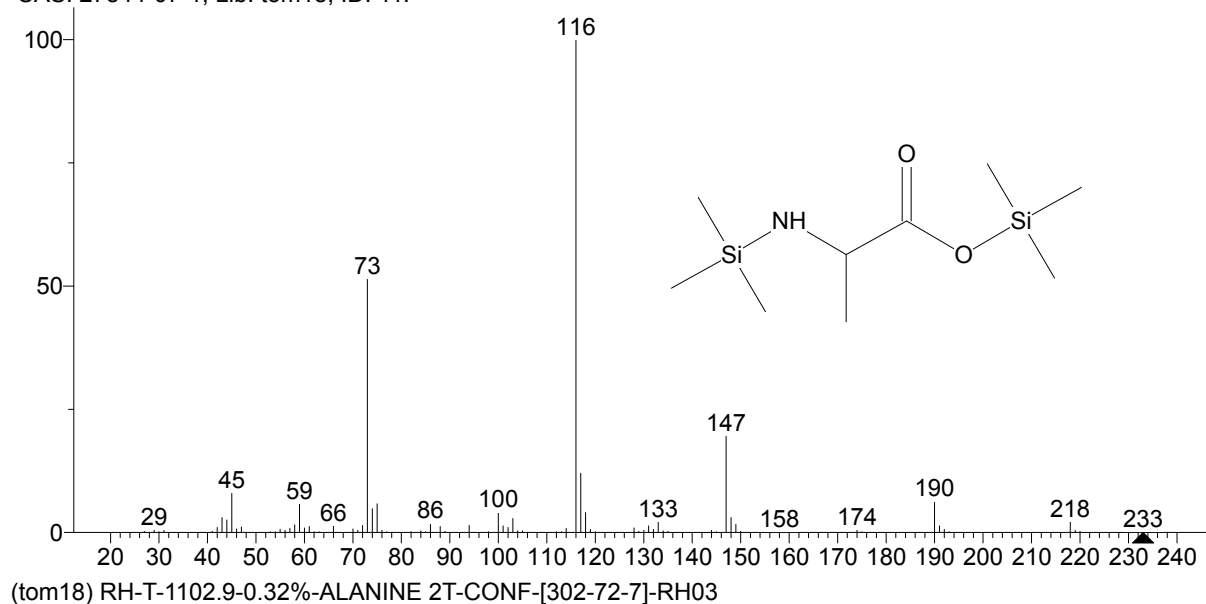
55 175 | 56 51 | 72 999 | 73 159 | 87 17 | 128 35 | 130 34 | 146 63 | 156 33 | 174 81 |

Synonyms:

1.VALINE 1T-CONF-[516-06-3];

Hit 11 : RH-T-1102.9-0.32%-ALANINE 2T-CONF-[302-72-7]-RH03

CAS: 27844-07-1; Lib: tom18; ID: 11.



Name: RH-T-1102.9-0.32%-ALANINE 2T-CONF-[302-72-7]-RH03

Formula: C₉H₂₃NO₂Si₂

MW: 233 CAS#: 27844-07-1 ID#: 11 DB: tom18

Other DBs: None

Comment: RI:MG00238 [RI:1102.9]

10 largest peaks:

116	999	73	513	147	195	117	120	45	79	190	62	75	58	59	57	74	48	100	40
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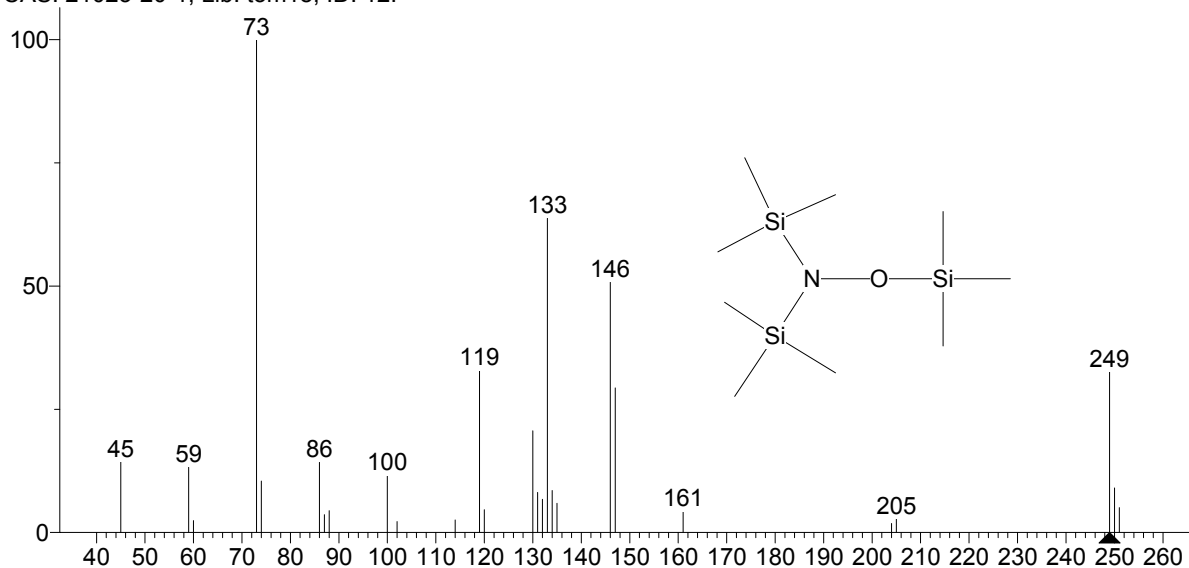
33 m/z Values and Intensities (46 low intensity peaks are not shown):

42	10	47	11	61	12	74	48	94	14	103	28	128	9	148	30	218	21
43	30	58	15	66	13	75	58	100	40	116	999	131	13	149	16		
44	25	59	57	72	14	86	18	101	13	117	120	133	21	190	62		
45	79	60	9	73	513	88	12	102	10	118	40	147	195	191	13		

Synonyms:

1.ALANINE 2T-CONF-[302-72-7];

Hit 12 : RH-T-1109.3-0.00%-[N: Tris(trimethylsilyl)hydroxylamine]-TENT-RH03
CAS: 21023-20-1; Lib: tom18; ID: 12.



(tom18) RH-T-1109.3-0.00%-[N: Tris(trimethylsilyl)hydroxylamine]-TENT-RH03 RI:1109.3,

Name: RH-T-1109.3-0.00%-[N: Tris(trimethylsilyl)hydroxylamine]-TENT-RH03

Formula: $C_9H_{27}NOSi_3$

MW: 249 CAS#: 21023-20-1 ID#: 12 DB: tom18

Other DBs: None

RI: 1109.3,

Comment: RI=1109.3, 11.7060 min MG00244 [RI:1109.3]

10 largest peaks:

73 999 | 133 637 | 146 507 | 119 328 | 249 325 | 147 293 | 130 206 | 45 143 | 86 142 | 59 132 |

27 m/z Values and Intensities:

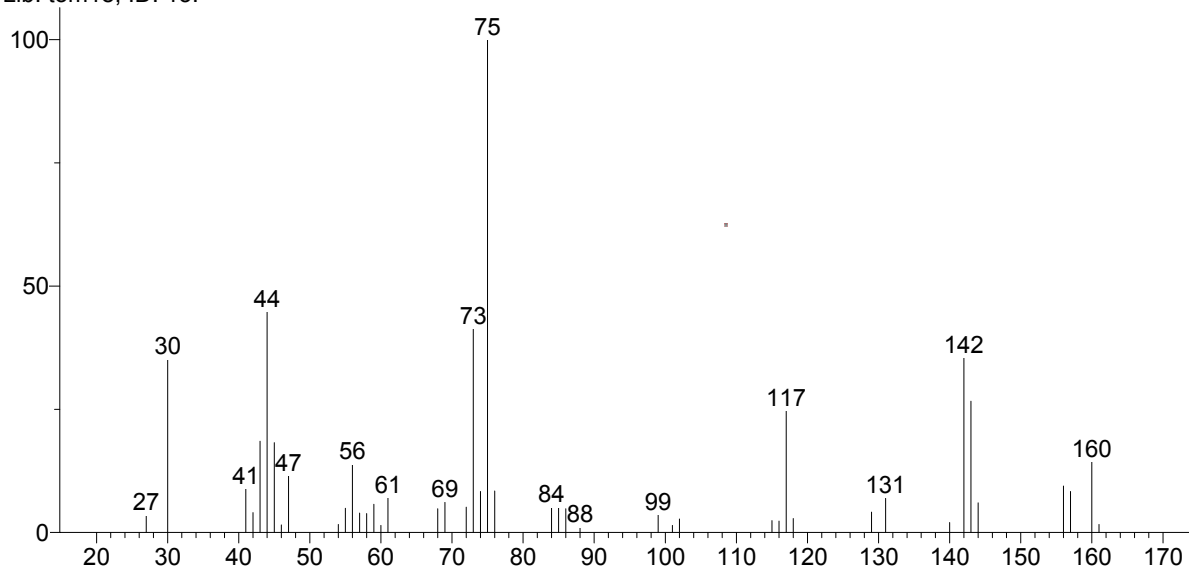
45 143 | 73 999 | 87 36 | 102 22 | 120 46 | 132 67 | 135 59 | 161 42 | 249 325 |
59 132 | 74 104 | 88 44 | 114 25 | 130 206 | 133 637 | 146 507 | 204 18 | 250 90 |
60 24 | 86 142 | 100 115 | 119 328 | 131 81 | 134 85 | 147 293 | 205 27 | 251 50 |

Synonyms:

1.Hydroxylamine 3T-TENT;

Hit 13 : RH-T-1117.4-0.01%-[142,143,117,160]-RH03

Lib: tom18; ID: 13.



(tom18) RH-T-1117.4-0.01%-[142,143,117,160]-RH03 RI:1117.4,

Name: RH-T-1117.4-0.01%-[142,143,117,160]-RH03

MW: N/A ID#: 13 DB: tom18

RI: 1117.4,

Comment: RI=1117.4, 11.9951 min MG00244 [RI:1117.4]

10 largest peaks:

75 999 | 44 447 | 73 412 | 142 354 | 30 350 | 143 266 | 117 246 | 43 185 | 45 182 | 160 143 |

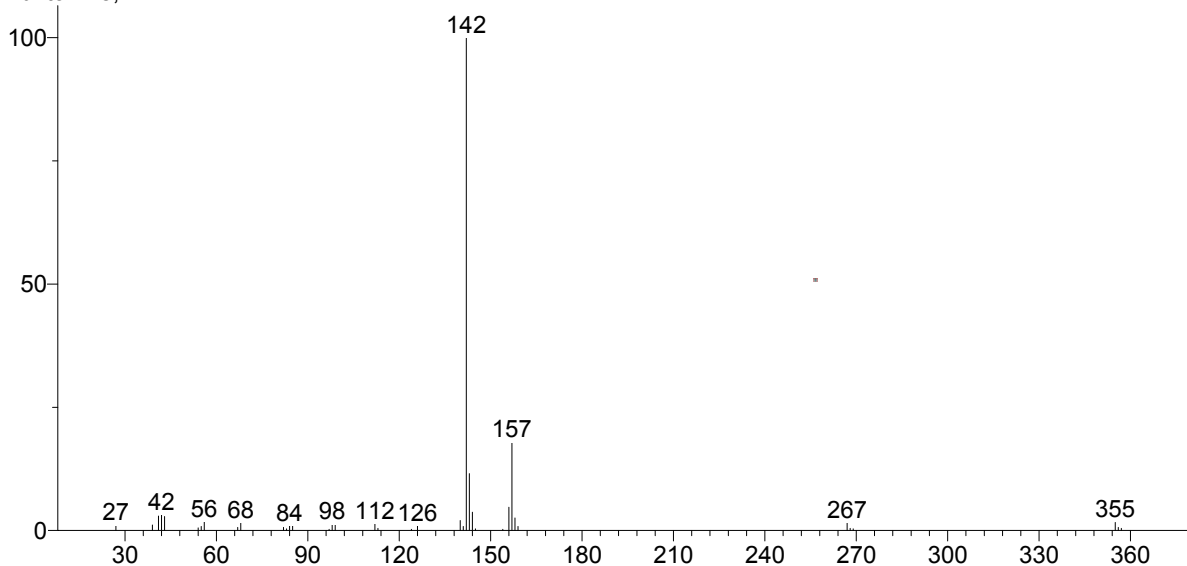
45 m/z Values and Intensities:

27 34	44 447	55 49	60 14	73 412	85 50	102 27	129 41	144 60
30 350	45 182	56 137	61 70	74 83	86 48	115 24	131 69	156 94
41 88	46 15	57 39	68 48	75 999	88 10	116 23	140 20	157 83
42 40	47 114	58 38	69 61	76 84	99 35	117 246	142 354	160 143
43 185	54 16	59 57	72 51	84 50	101 14	118 28	143 266	161 16

Synonyms:

1.m142,143,117,160;

Hit 14 : RH-T-1140.5-0.02%-[142,157, N: sim. 2-Pyrrolidinone, 1-(trimethylsilyl)]-RH03
Lib: tom18; ID: 14.



(tom18) RH-T-1140.5-0.02%-[142,157, N: sim. 2-Pyrrolidinone, 1-(trimethylsilyl)]-RH03 RI:1140.5,

Name: RH-T-1140.5-0.02%-[142,157, N: sim. 2-Pyrrolidinone, 1-(trimethylsilyl)]-RH03

MW: N/A ID#: 14 DB: tom18

RI: 1140.5,

Comment: RI=1140.5, 12.8301 min MG00244 [RI:1140.5]

10 largest peaks:

142 999 | 157 178 | 143 115 | 156 47 | 144 37 | 42 31 | 41 29 | 43 28 | 158 25 | 140 20 |

22 m/z Values and Intensities (16 low intensity peaks are not shown):

27 10 | 42 31 | 68 15 | 98 12 | 126 9 | 143 115 | 157 178 | 355 16 |

39 11 | 43 28 | 84 9 | 99 12 | 140 20 | 144 37 | 158 25 |

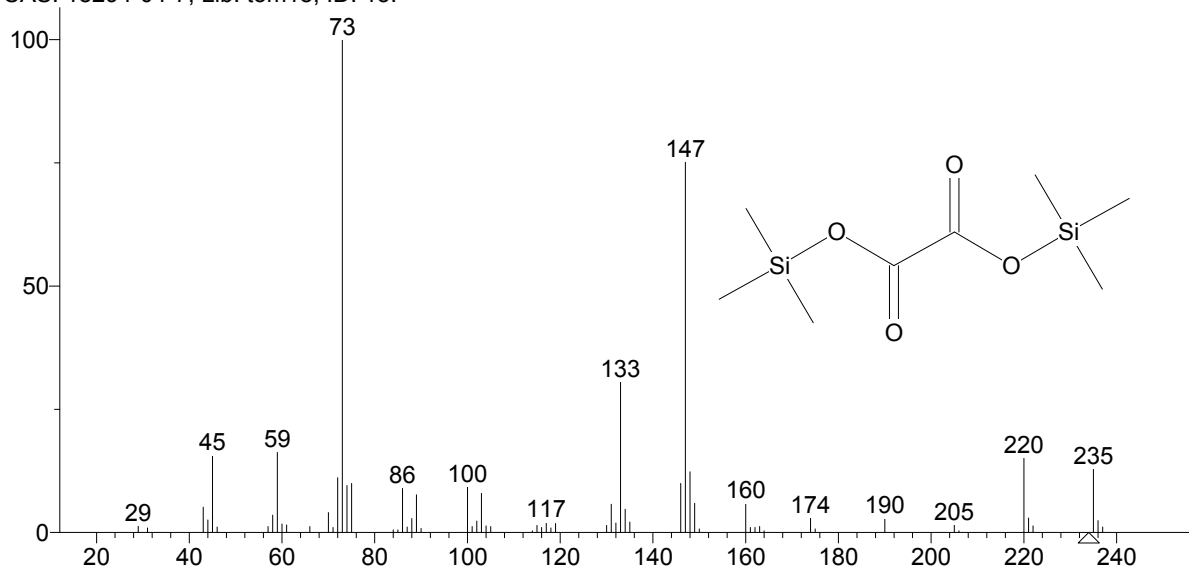
41 29 | 56 17 | 85 9 | 112 13 | 142 999 | 156 47 | 267 15 |

Synonyms:

1.m142,157, N: sim. 2-Pyrrolidinone, 1-(trimethylsilyl)-];

Hit 15 : RH-T-1142.9-0.05%-OXALIC ACID 2T-CONF-[144-62-7]-RH03

CAS: 18294-04-7; Lib: tom18; ID: 15.



(tom18) RH-T-1142.9-0.05%-OXALIC ACID 2T-CONF-[144-62-7]-RH03

Name: RH-T-1142.9-0.05%-OXALIC ACID 2T-CONF-[144-62-7]-RH03

Formula: C₈H₁₈O₄Si₂

MW: 234 CAS#: 18294-04-7 ID#: 15 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:1142.9|

10 largest peaks:

73 999 | 147 751 | 133 305 | 59 162 | 45 156 | 220 150 | 235 128 | 148 123 | 72 111 | 75 99 |

56 m/z Values and Intensities (8 low intensity peaks are not shown):

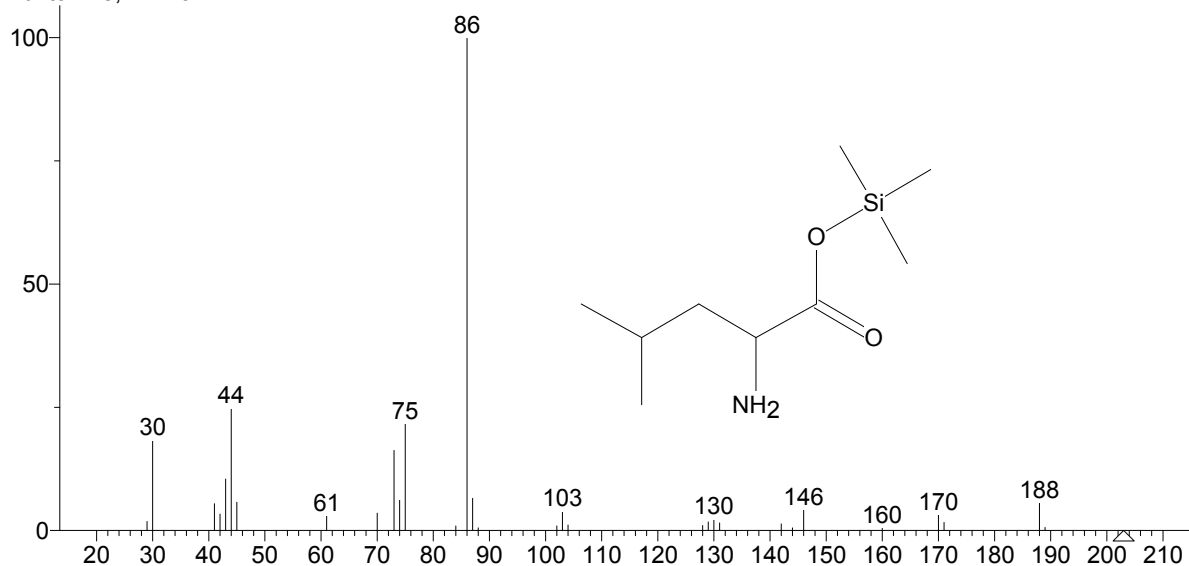
29 13	57 12	70 40	86 89	102 23	117 20	133 305	149 59	190 28	236 24
31 9	58 35	71 10	87 11	103 79	118 9	134 47	160 58	205 15	237 11
43 51	59 162	72 111	88 28	104 13	119 18	135 21	161 10	220 150	
44 25	60 17	73 999	89 76	105 12	130 14	146 99	162 10	221 29	
45 156	61 15	74 95	100 92	115 14	131 57	147 751	163 12	222 13	
46 11	66 12	75 99	101 12	116 10	132 19	148 123	174 29	235 128	

Synonyms:

1.OXALIC ACID 2T-CONF-[144-62-7];

Hit 16 : RH-T-1157.0-0.01%-LEUCINE 1T-TENT-[61-90-5]-RH03

Lib: tom18; ID: 16.



(tom18) RH-T-1157.0-0.01%-LEUCINE 1T-TENT-[61-90-5]-RH03 RI:1156.1,

Name: RH-T-1157.0-0.01%-LEUCINE 1T-TENT-[61-90-5]-RH03

Formula: C₉H₂₁NO₂Si

MW: 203 ID#: 16 DB: tom18

RI: 1156.1,

Comment: RI=1156.1, 12.6933 min AB2129 [RI:1157]

10 largest peaks:

86	999	44	247	75	216	30	182	73	162	43	104	87	65	74	61	45	57	188	55
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27 m/z Values and Intensities (4 low intensity peaks are not shown):

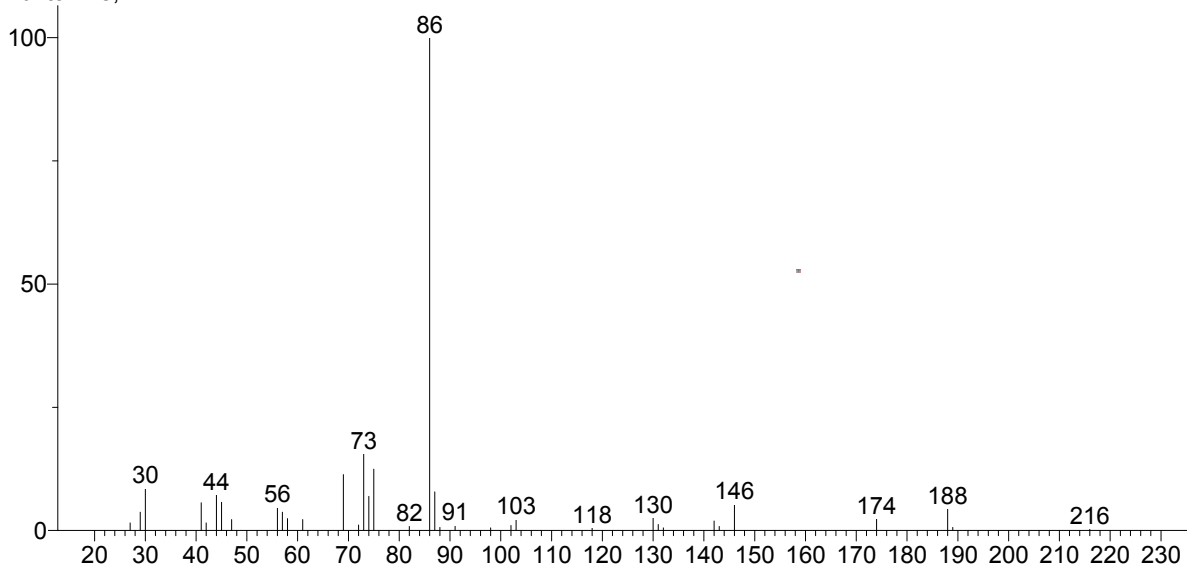
29	18	42	33	45	57	73	162	84	9	102	9	128	10	131	15	170	31
30	182	43	104	61	29	74	61	86	999	103	38	129	17	142	13	171	16
41	54	44	247	70	35	75	216	87	65	104	11	130	22	146	41	188	55

Synonyms:

1.LEUCINE 1T-TENT-[61-90-5];

Hit 17 : RH-T-1175.2-0.01%-[86,188,146,130]-RH03

Lib: tom18; ID: 17.



(tom18) RH-T-1175.2-0.01%-[86,188,146,130]-RH03

Name: RH-T-1175.2-0.01%-[86,188,146,130]-RH03

MW: N/A ID#: 17 DB: tom18

Comment: RI:MG00246 |RI:1175.2|

10 largest peaks:

86 999 | 73 155 | 75 124 | 69 113 | 30 85 | 87 78 | 44 72 | 74 69 | 45 57 | 41 56 |

28 m/z Values and Intensities (8 low intensity peaks are not shown):

27 15 | 41 56 | 45 57 | 57 37 | 69 113 | 74 69 | 87 78 | 103 22 | 142 19 | 188 43 |

29 37 | 42 15 | 47 22 | 58 24 | 72 11 | 75 124 | 91 10 | 130 25 | 146 52 |

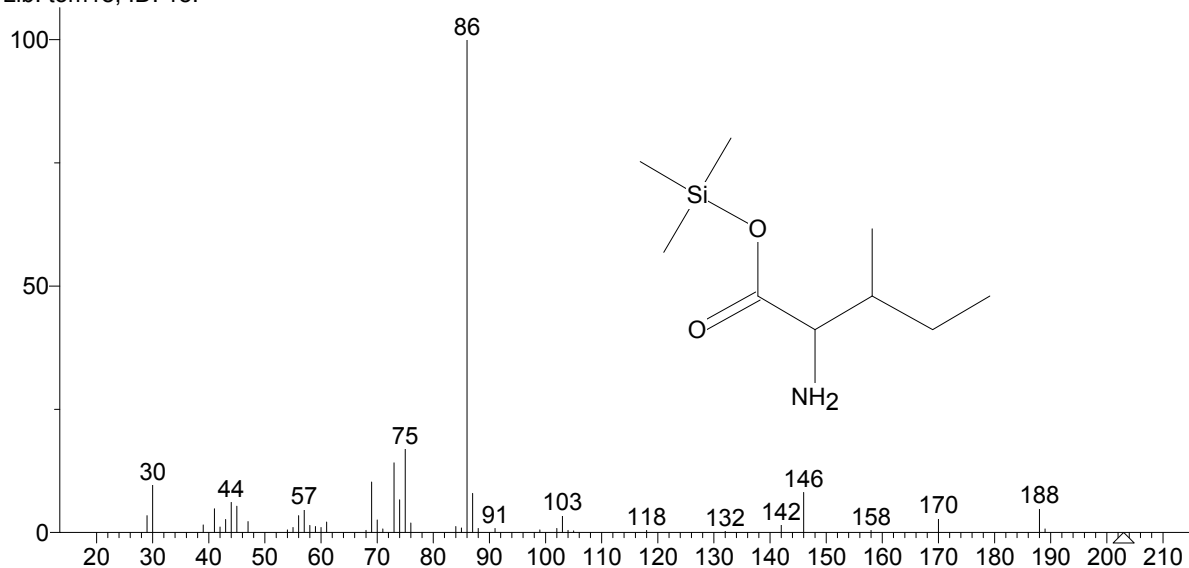
30 85 | 44 72 | 56 46 | 61 22 | 73 155 | 86 999 | 102 10 | 131 12 | 174 23 |

Synonyms:

1.m86,188,146,130;

Hit 18 : RH-T-1176.7-0.00%-[N: l-Isoleucine, trimethylsilyl ester]-TENT-RH03

Lib: tom18; ID: 18.



(tom18) RH-T-1176.7-0.00%-[N: l-Isoleucine, trimethylsilyl ester]-TENT-RH03 RI:1176.7,

Name: RH-T-1176.7-0.00%-[N: l-Isoleucine, trimethylsilyl ester]-TENT-RH03

Formula: C₉H₂₁NO₂Si

MW: 203 ID#: 18 DB: tom18

RI: 1176.7,

Comment: RI=1176.7, 14.1348 min MG00244 [RI:1176.7]

10 largest peaks:

86 999 | 75 169 | 73 141 | 69 102 | 30 96 | 146 81 | 87 79 | 74 66 | 44 61 | 45 53 |

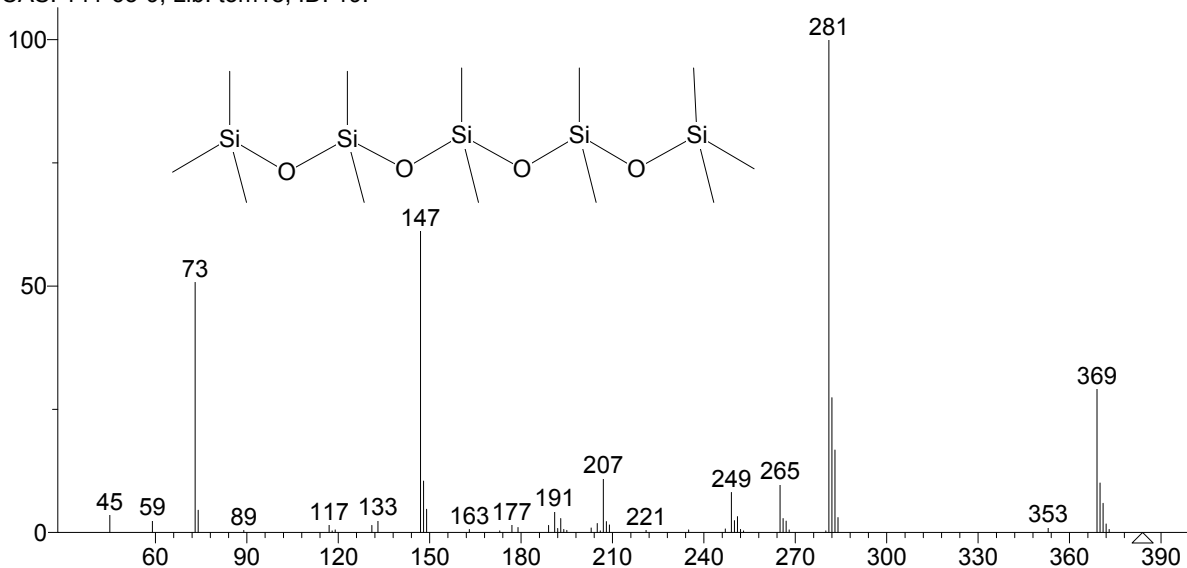
31 m/z Values and Intensities (13 low intensity peaks are not shown):

29 34 | 42 11 | 47 22 | 58 14 | 69 102 | 75 169 | 86 999 | 146 81 |
 30 96 | 43 26 | 55 10 | 59 12 | 70 25 | 76 19 | 87 79 | 170 28 |
 39 15 | 44 61 | 56 34 | 60 10 | 73 141 | 84 12 | 103 34 | 188 48 |
 41 48 | 45 53 | 57 46 | 61 21 | 74 66 | 85 9 | 142 15 |

Synonyms:

1.Isoleucine T-TENT;

Hit 19 : RH-T-1178.2-0.01%-[N: Pentasiloxane, dodecamethyl-]-TENT-RH03
CAS: 141-63-9; Lib: tom18; ID: 19.



(tom18) RH-T-1178.2-0.01%-[N: Pentasiloxane, dodecamethyl-]-TENT-RH03

Name: RH-T-1178.2-0.01%-[N: Pentasiloxane, dodecamethyl-]-TENT-RH03

Formula: C₁₂H₃₆O₄Si₅

MW: 384 CAS#: 141-63-9 ID#: 19 DB: tom18

Other DBs: None

Comment: 14.2172 min MG00244 [RI:1178.2]

10 largest peaks:

281 999 | 147 611 | 73 507 | 369 291 | 282 273 | 283 167 | 207 109 | 148 104 | 370 100 | 265 97 |

35 m/z Values and Intensities (17 low intensity peaks are not shown):

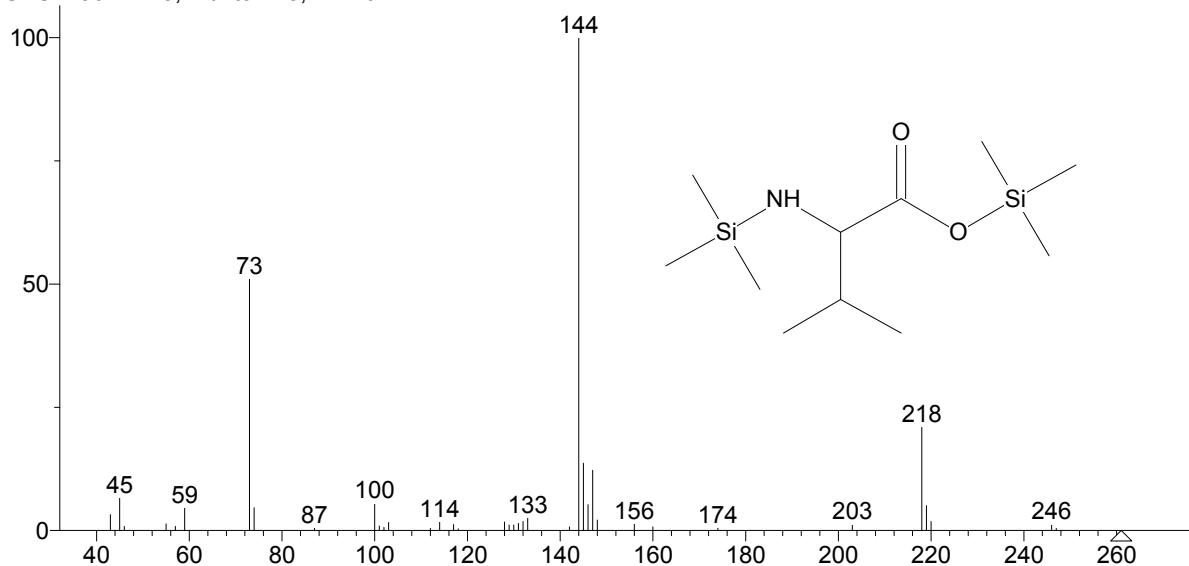
45 35	117 15	148 104	189 14	205 18	249 81	266 28	283 167	370 100
59 24	131 14	149 47	191 42	207 109	250 24	267 23	284 30	371 59
73 507	133 24	177 15	193 28	208 22	251 32	281 999	353 10	372 17
74 45	147 611	179 10	203 9	209 15	265 97	282 273	369 291	

Synonyms:

1.Pentasiloxane, dodecamethyl-]-TENT;

Hit 20 : RH-T-1217.4-0.02%-VALINE 2T-CONF-[516-06-3]-RH03

CAS: 7364-44-5; Lib: tom18; ID: 20.



(tom18) RH-T-1217.4-0.02%-VALINE 2T-CONF-[516-06-3]-RH03

Name: RH-T-1217.4-0.02%-VALINE 2T-CONF-[516-06-3]-RH03

Formula: C₁₁H₂₇NO₂Si₂

MW: 261 CAS#: 7364-44-5 ID#: 20 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:1217.4|

10 largest peaks:

144 999 | 73 509 | 218 209 | 145 136 | 147 122 | 45 65 | 100 54 | 146 52 | 219 50 | 74 46 |

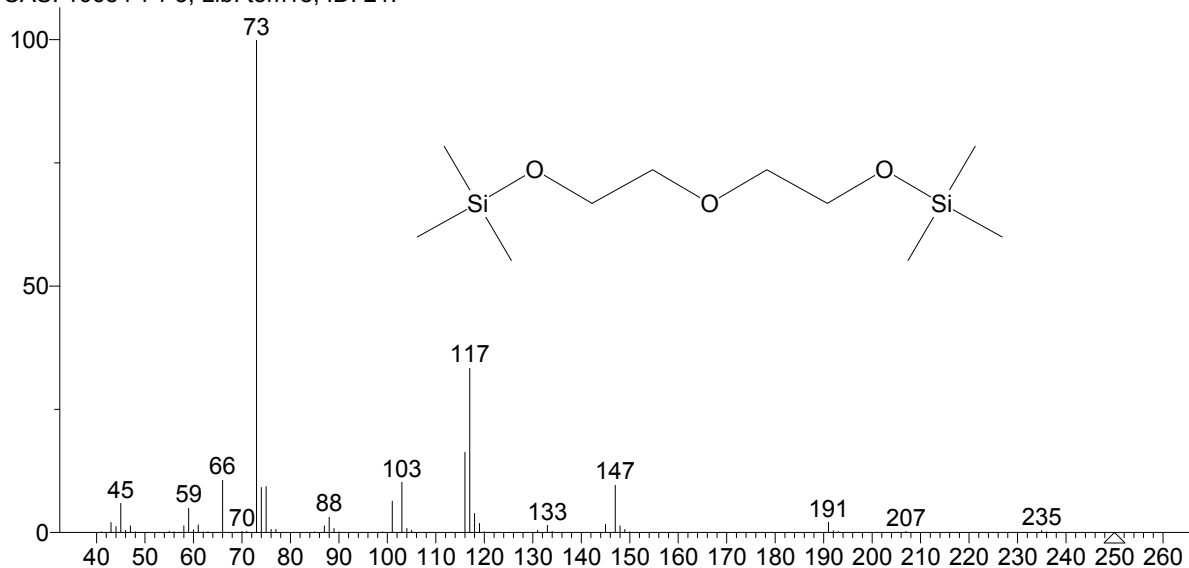
28 m/z Values and Intensities (10 low intensity peaks are not shown):

43 32	59 45	100 54	114 17	129 11	132 18	145 136	148 21	218 209	246 12
45 65	73 509	101 9	117 12	130 11	133 25	146 52	156 13	219 50	
55 13	74 46	103 16	128 17	131 14	144 999	147 122	203 12	220 18	

Synonyms:

1. VALINE 2T-CONF-[516-06-3];

Hit 21 : RH-T-1245.7-0.00%-DIETHYLENE GLYCOL 2T-CONF-[111-46-6]-8135A18-G
CAS: 16654-74-3; Lib: tom18; ID: 21.



(tom18) RH-T-1245.7-0.00%-DIETHYLENE GLYCOL 2T-CONF-[111-46-6]-8135A18-G RI:1245.7,

Name: RH-T-1245.7-0.00%-DIETHYLENE GLYCOL 2T-CONF-[111-46-6]-8135A18-G

Formula: C₁₀H₂₆O₃Si₂

MW: 250 CAS#: 16654-74-3 ID#: 21 DB: tom18

Other DBs: None

RI: 1245.7,

Comment: RI=1245.7, 15.2839 min 8135A18 |RI:1245.7|

10 largest peaks:

73 999 | 117 334 | 116 162 | 66 107 | 103 102 | 147 97 | 75 93 | 74 91 | 101 63 | 45 59 |

24 m/z Values and Intensities (28 low intensity peaks are not shown):

43 20 | 47 13 | 61 15 | 74 91 | 88 32 | 116 162 | 119 18 | 147 97 |

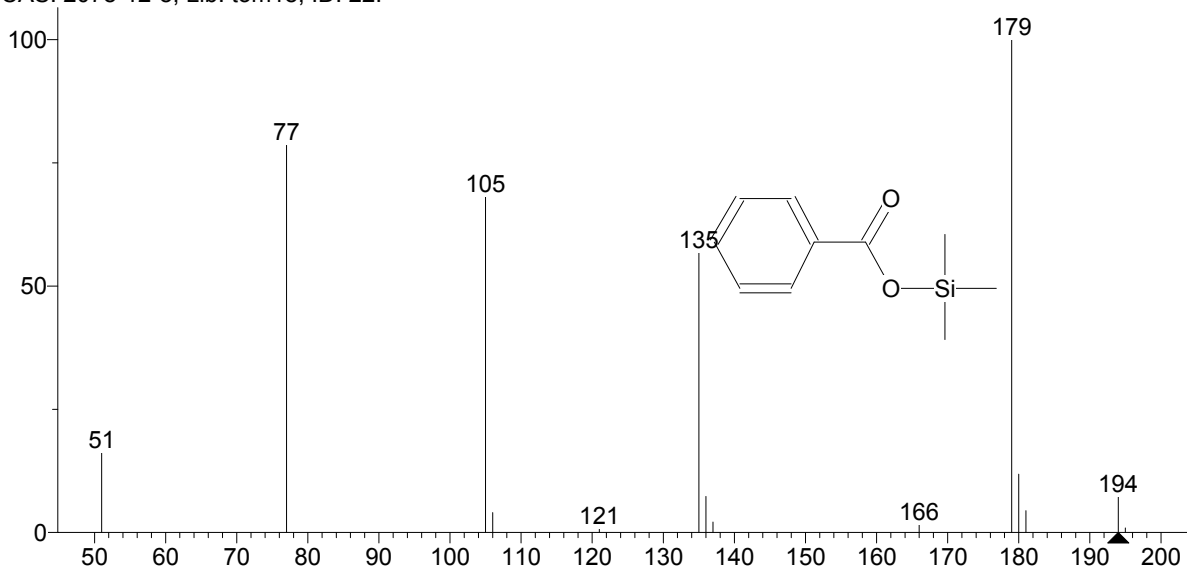
44 12 | 58 13 | 66 107 | 75 93 | 101 63 | 117 334 | 133 15 | 148 13 |

45 59 | 59 50 | 73 999 | 87 13 | 103 102 | 118 38 | 145 16 | 191 21 |

Synonyms:

1.DIETHYLENE GLYCOL 2T-CONF-[111-46-6];

Hit 22 : RH-T-1252.9-0.00%-BENZOIC ACID T-CONF-[65-85-0]- 8135A18-G
CAS: 2078-12-8; Lib: tom18; ID: 22.



(tom18) RH-T-1252.9-0.00%-BENZOIC ACID T-CONF-[65-85-0]- 8135A18-G RI:1252.9,

Name: RH-T-1252.9-0.00%-BENZOIC ACID T-CONF-[65-85-0]- 8135A18-G

Formula: C₁₀H₁₄O₂Si

MW: 194 CAS#: 2078-12-8 ID#: 22 DB: tom18

Other DBs: None

RI: 1252.9,

Comment: RI=1252.9, 15.4419 min 8135A18 |RI:1252.9|

10 largest peaks:

179 999 | 77 785 | 105 680 | 135 567 | 51 161 | 180 118 | 136 73 | 194 72 | 181 44 | 106 40 |

13 m/z Values and Intensities (1 low intensity peak is not shown):

51 161 | 105 680 | 135 567 | 137 21 | 179 999 | 181 44 | 195 9 |

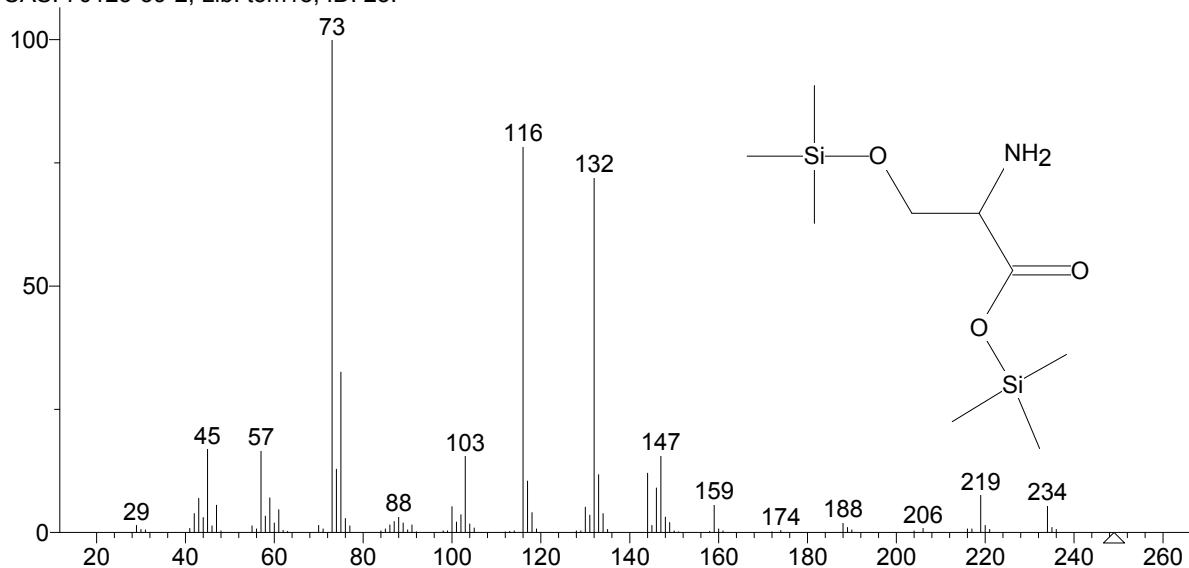
77 785 | 106 40 | 136 73 | 166 15 | 180 118 | 194 72 |

Synonyms:

1.BENZOIC ACID T-CONF-[65-85-0];

Hit 23 : RH-T-1258.1-0.19%-SERINE 2T-CONF-[302-84-1]-RH03

CAS: 70125-39-2; Lib: tom18; ID: 23.



(tom18) RH-T-1258.1-0.19%-SERINE 2T-CONF-[302-84-1]-RH03

Name: RH-T-1258.1-0.19%-SERINE 2T-CONF-[302-84-1]-RH03

Formula: C₉H₂₃NO₃Si₂

MW: 249 CAS#: 70125-39-2 ID#: 23 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:1258.1|

10 largest peaks:

73	999	116	782	132	719	75	325	45	169	57	166	147	156	103	155	74	128	144	120
----	-----	-----	-----	-----	-----	----	-----	----	-----	----	-----	-----	-----	-----	-----	----	-----	-----	-----

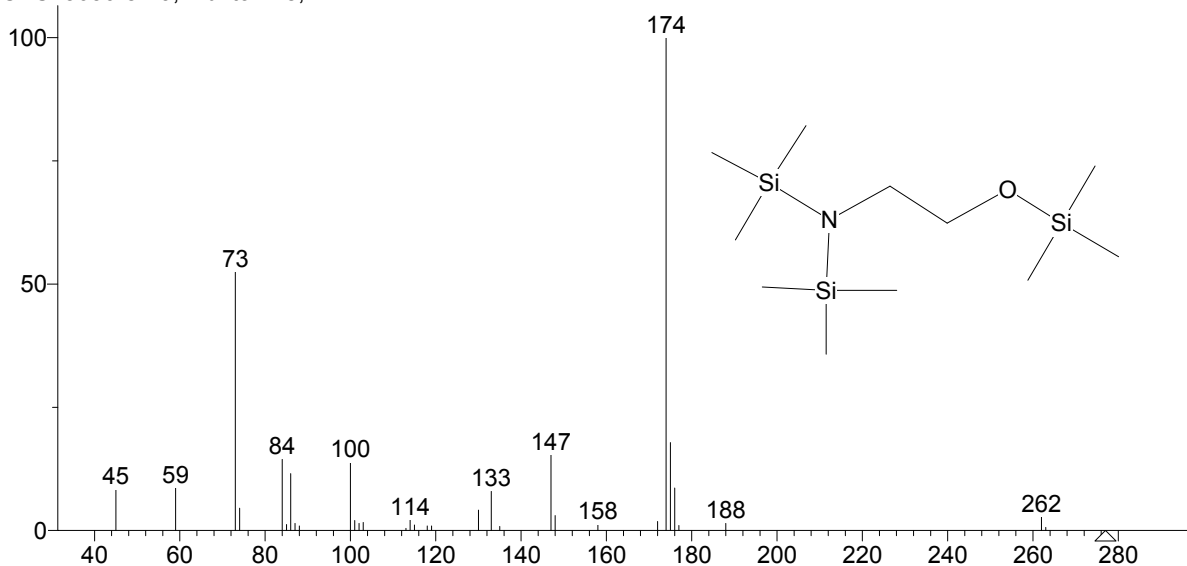
52 m/z Values and Intensities (34 low intensity peaks are not shown):

29	14	47	55	61	46	77	13	100	52	116	782	133	117	148	31	219	76
42	38	55	13	70	14	86	15	101	21	117	104	134	38	149	20	220	14
43	69	57	166	73	999	87	22	102	36	118	40	144	120	159	56	234	54
44	30	58	33	74	128	88	32	103	155	130	51	145	14	188	20	235	10
45	169	59	70	75	325	89	19	104	17	131	35	146	90	189	10		
46	13	60	19	76	28	91	15	105	9	132	719	147	156	206	9		

Synonyms:

1.SERINE 2T-CONF-[302-84-1];

Hit 24 : RH-T-1266.3-0.02%-ETHANOLAMINE 3T-CONF-[141-43-5]-RH02
CAS: 5630-81-9; Lib: tom18; ID: 24.



(tom18) RH-T-1266.3-0.02%-ETHANOLAMINE 3T-CONF-[141-43-5]-RH02

Name: RH-T-1266.3-0.02%-ETHANOLAMINE 3T-CONF-[141-43-5]-RH02

Formula: C₁₁H₃₁NOSi₃

MW: 277 CAS#: 5630-81-9 ID#: 24 DB: tom18

Other DBs: None

Comment: RI:MG00238 [RI:1266.3]

10 largest peaks:

174 999 | 73 524 | 175 178 | 147 153 | 84 144 | 100 137 | 86 115 | 59 86 | 176 86 | 45 83 |

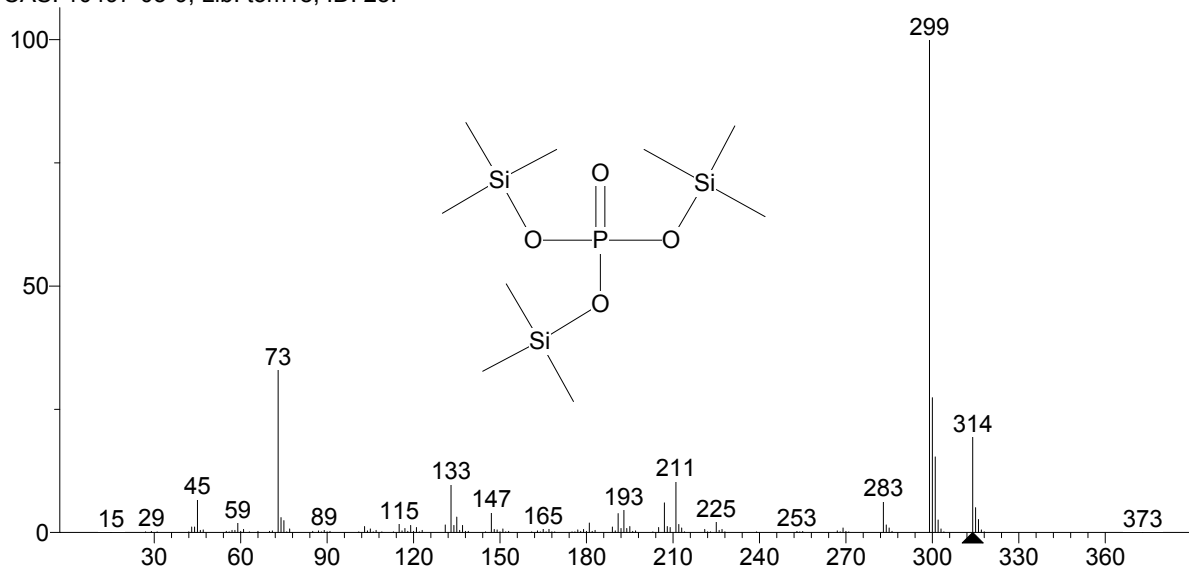
29 m/z Values and Intensities (3 low intensity peaks are not shown):

45 83 | 74 45 | 86 115 | 100 137 | 103 16 | 118 9 | 133 79 | 158 12 | 175 178 | 188 14 |
59 86 | 84 144 | 87 14 | 101 20 | 114 21 | 119 9 | 147 153 | 172 18 | 176 86 | 262 27 |
73 524 | 85 12 | 88 9 | 102 14 | 115 11 | 130 41 | 148 30 | 174 999 | 177 10 |

Synonyms:

1.ETHANOLAMINE 3T-CONF-[141-43-5];

Hit 25 : RH-T-1274.8-1.41%-PHOSPHORIC ACID 3T-CONF-[7664-38-2]-RH03
CAS: 10497-05-9; Lib: tom18; ID: 25.



(tom18) RH-T-1274.8-1.41%-PHOSPHORIC ACID 3T-CONF-[7664-38-2]-RH03

Name: RH-T-1274.8-1.41%-PHOSPHORIC ACID 3T-CONF-[7664-38-2]-RH03

Formula: C₉H₂₇O₄PSi₃

MW: 314 CAS#: 10497-05-9 ID#: 25 DB: tom18

Other DBs: None

Comment: RI:MG00238 [RI:1274.8]

10 largest peaks:

299 999 | 73 329 | 300 273 | 314 193 | 301 153 | 211 103 | 133 97 | 45 66 | 283 62 | 207 60 |

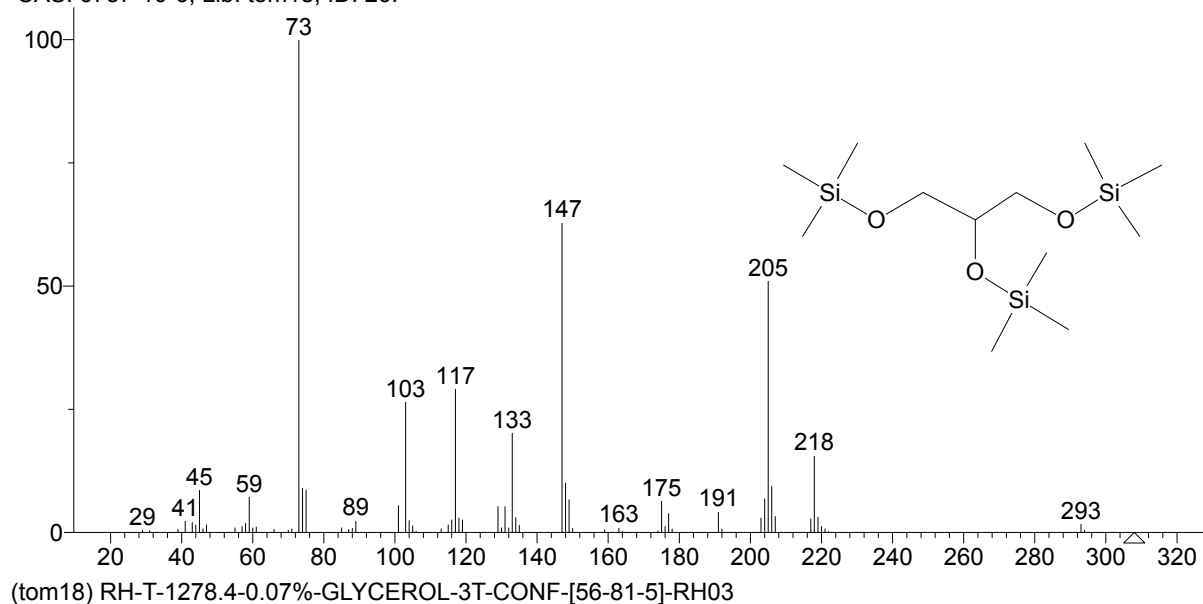
41 m/z Values and Intensities (91 low intensity peaks are not shown):

43	11	74	30	121	10	137	14	193	45	209	10	269	9	300	273	316	26
44	11	75	24	131	15	147	40	195	12	211	103	283	62	301	153		
45	66	103	12	133	97	181	19	205	10	212	16	284	15	302	25		
59	19	115	17	134	14	189	11	207	60	213	9	285	9	314	193		
73	329	119	14	135	31	191	38	208	12	225	21	299	999	315	50		

Synonyms:

1. PHOSPHORIC ACID 3T-CONF-[7664-38-2];

Hit 26 : RH-T-1278.4-0.07%-GLYCEROL-3T-CONF-[56-81-5]-RH03
CAS: 6787-10-6; Lib: tom18; ID: 26.



Name: RH-T-1278.4-0.07%-GLYCEROL-3T-CONF-[56-81-5]-RH03

Formula: C₁₂H₃₂O₃Si₃

MW: 308 CAS#: 6787-10-6 ID#: 26 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:1278.4|

10 largest peaks:

73 999 | 147 628 | 205 509 | 117 291 | 103 264 | 133 201 | 218 156 | 148 100 | 206 93 | 74 89 |

50 m/z Values and Intensities (20 low intensity peaks are not shown):

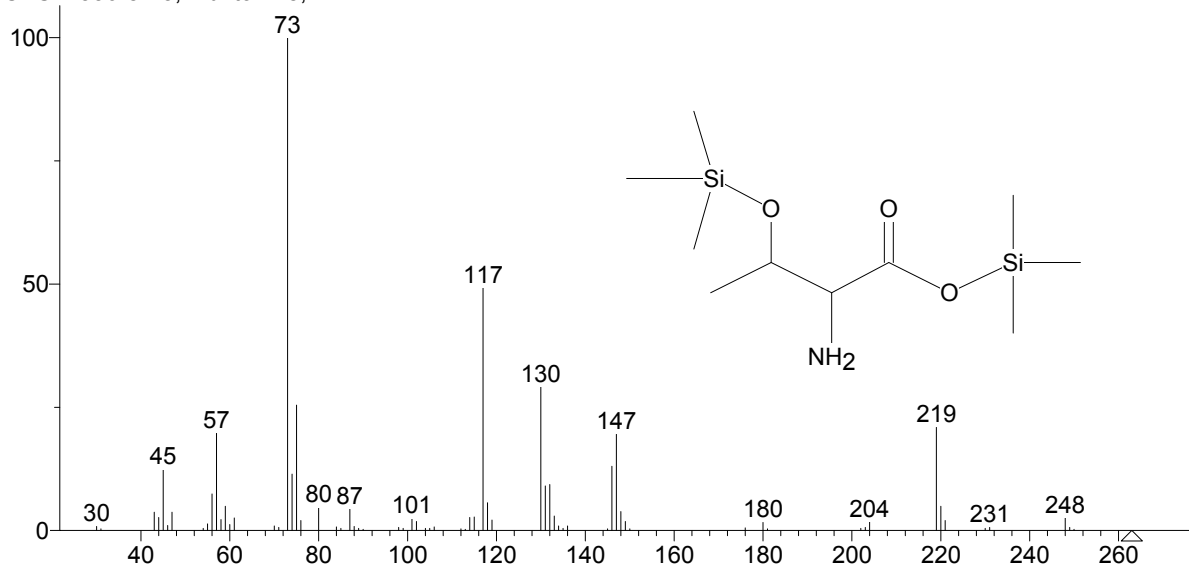
41	23	55	9	61	11	89	24	115	15	129	52	134	30	163	10	203	29	217	27
43	20	57	12	73	999	101	54	116	25	130	9	135	14	175	63	204	68	218	156
44	15	58	18	74	89	103	264	117	291	131	52	147	628	176	12	205	509	219	31
45	86	59	72	75	86	104	24	118	29	132	9	148	100	177	38	206	93	220	12
47	15	60	9	85	9	105	13	119	25	133	201	149	66	191	42	207	32	293	16

Synonyms:

1.GLYCEROL-3T-CONF-[56-81-5];

Hit 27 : RH-T-1293.6-0.13%-THREONINE 2T-TENT-[80-68-2]-RH03

CAS: 7536-82-5; Lib: tom18; ID: 27.



(tom18) RH-T-1293.6-0.13%-THREONINE 2T-TENT-[80-68-2]-RH03

Name: RH-T-1293.6-0.13%-THREONINE 2T-TENT-[80-68-2]-RH03

Formula: C₁₀H₂₅NO₃Si₂

MW: 263 CAS#: 7536-82-5 ID#: 27 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:1293.6|

10 largest peaks:

73 999 | 117 492 | 130 291 | 75 254 | 219 209 | 57 197 | 147 195 | 146 130 | 45 123 | 74 114 |

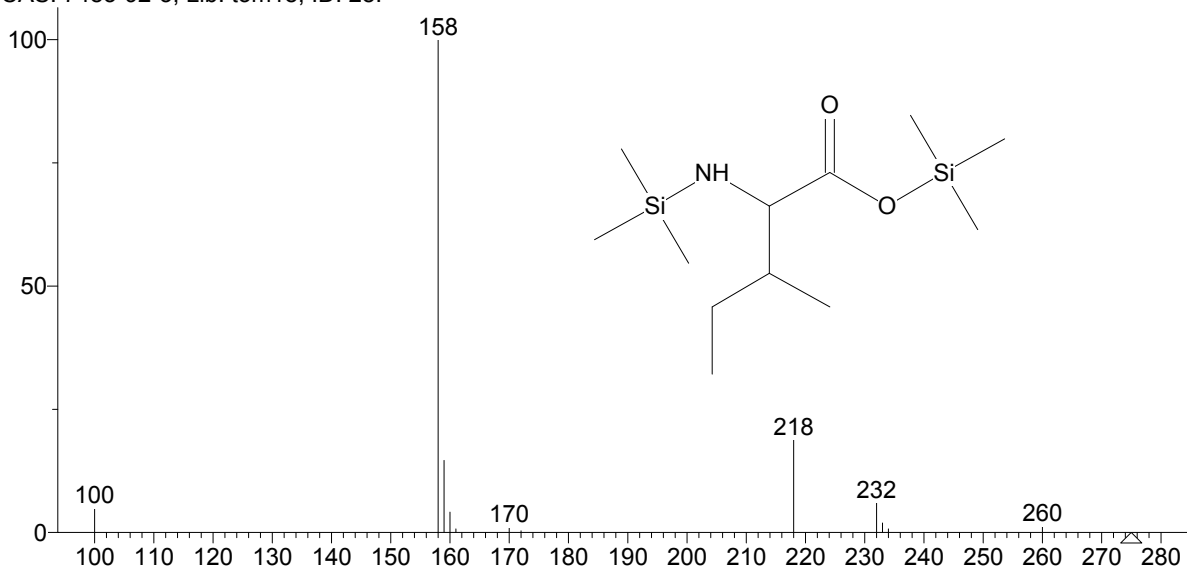
42 m/z Values and Intensities (27 low intensity peaks are not shown):

43 37	55 13	60 12	75 254	102 18	119 21	134 9	149 18	221 20
44 26	56 74	61 25	76 20	114 26	130 291	136 9	180 16	248 25
45 123	57 197	70 9	80 46	115 27	131 90	146 130	204 17	
46 10	58 22	73 999	87 43	117 492	132 93	147 195	219 209	
47 37	59 49	74 114	101 24	118 56	133 29	148 38	220 49	

Synonyms:

1.THREONINE 2T-TENT-[80-68-2];

Hit 28 : RH-T-1293.7-0.01%-ISOLEUCINE 2T-TENT-[73-32-5]-RH03-X
CAS: 7483-92-3; Lib: tom18; ID: 28.



(tom18) RH-T-1293.7-0.01%-ISOLEUCINE 2T-TENT-[73-32-5]-RH03-X

Name: RH-T-1293.7-0.01%-ISOLEUCINE 2T-TENT-[73-32-5]-RH03-X

Formula: C₁₂H₂₉NO₂Si₂

MW: 275 CAS#: 7483-92-3 ID#: 28 DB: tom18

Other DBs: None

Comment: RI:MG00238 [RI:1293.7]

10 largest peaks:

158 999 | 218 187 | 159 146 | 232 60 | 100 48 | 160 41 | 233 19 | 260 12 | 170 10 | 161 7 |

9 m/z Values and Intensities (3 low intensity peaks are not shown):

100 48 | 158 999 | 159 146 | 160 41 | 170 10 | 218 187 | 232 60 | 233 19 | 260 12 |

Synonyms:

1.ISOLEUCINE 2T-TENT-[73-32-5];

Hit 29 : RH-T-1294.8-0.00%-PROLINE 2T-TENT-[147-85-3]-RH03-X

Lib: tom18; ID: 29.



(tom18) RH-T-1294.8-0.00%-PROLINE 2T-TENT-[147-85-3]-RH03-X

Name: RH-T-1294.8-0.00%-PROLINE 2T-TENT-[147-85-3]-RH03-X

Formula: C₁₁H₂₅NO₂Si₂

MW: 259 ID#: 29 DB: tom18

Comment: RI:MG00238 [RI:1294.8]

3 largest peaks:

142 999 | 143 128 | 216 68 |

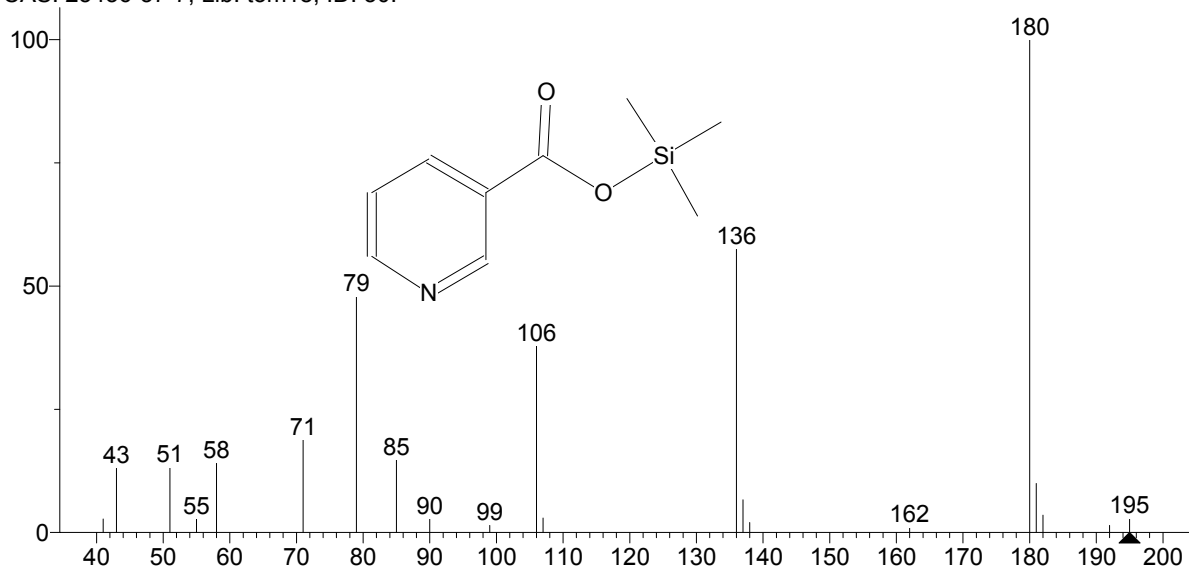
3 m/z Values and Intensities:

142 999 | 143 128 | 216 68 |

Synonyms:

1.PROLINE 2T-TENT-[147-85-3];

Hit 30 : RH-T-1302.3-0.00%-NICOTINIC ACID T-CONF-[59-67-6]-8135A18-G-X
CAS: 25436-37-7; Lib: tom18; ID: 30.



(tom18) RH-T-1302.3-0.00%-NICOTINIC ACID T-CONF-[59-67-6]-8135A18-G-X RI:1302.3,

Name: RH-T-1302.3-0.00%-NICOTINIC ACID T-CONF-[59-67-6]-8135A18-G-X

Formula: C₉H₁₃NO₂Si

MW: 195 CAS#: 25436-37-7 ID#: 30 DB: tom18

Other DBs: None

RI: 1302.3,

Comment: RI=1302.3, 16.5346 min 8135A18 |RI:1302.3|

10 largest peaks:

180 999 | 136 574 | 79 478 | 106 378 | 71 187 | 85 147 | 58 140 | 51 131 | 43 130 | 181 99 |

21 m/z Values and Intensities:

41 27 | 55 27 | 79 478 | 99 14 | 136 574 | 162 10 | 182 35 |

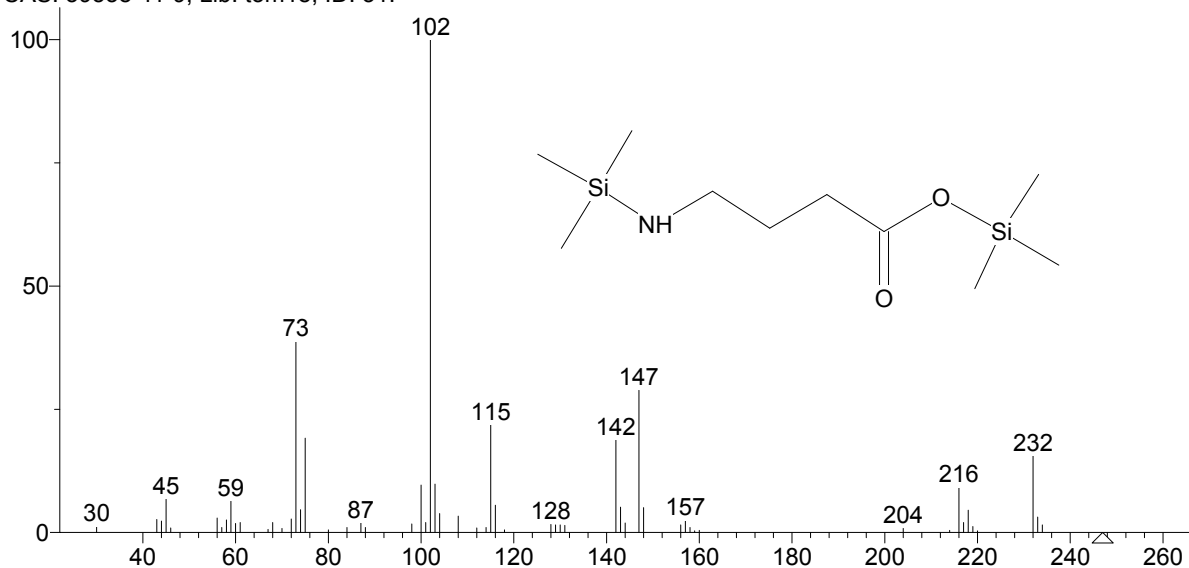
43 130 | 58 140 | 85 147 | 106 378 | 137 66 | 180 999 | 192 14 |

51 131 | 71 187 | 90 27 | 107 29 | 138 20 | 181 99 | 195 28 |

Synonyms:

1.NICOTINIC ACID T-CONF-[59-67-6];

Hit 31 : RH-T-1302.6-0.01%-[N: N,O-Bis-(trimethylsilyl)-4-aminobutyric acid]-TENT-RH03
CAS: 39538-11-9; Lib: tom18; ID: 31.



(tom18) RH-T-1302.6-0.01%-[N: N,O-Bis-(trimethylsilyl)-4-aminobutyric acid]-TENT-RH03 RI:1302.6,

Name: RH-T-1302.6-0.01%-[N: N,O-Bis-(trimethylsilyl)-4-aminobutyric acid]-TENT-RH03

Formula: C₁₀H₂₅NO₂Si₂

MW: 247 CAS#: 39538-11-9 ID#: 31 DB: tom18

Other DBs: None

RI: 1302.6,

Comment: RI=1302.6, 18.5692 min MG00244 [RI:1302.6]

10 largest peaks:

102 999 | 73 387 | 147 288 | 115 218 | 75 191 | 142 187 | 232 155 | 103 98 | 100 96 | 216 91 |

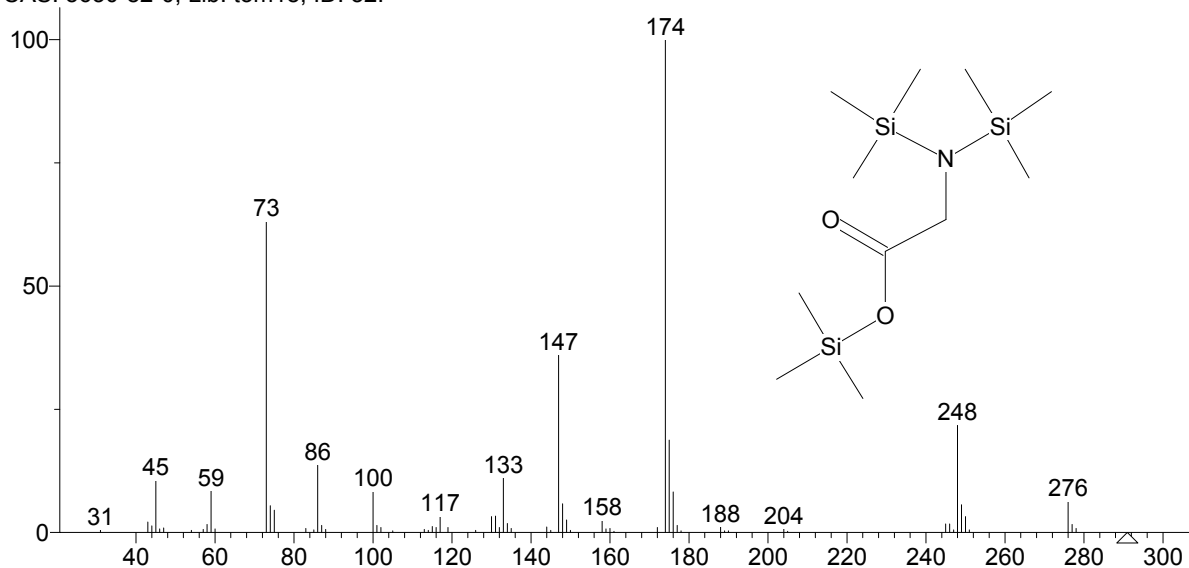
49 m/z Values and Intensities (9 low intensity peaks are not shown):

30 12	56 29	61 20	75 191	100 96	108 33	128 16	143 51	157 24	219 12
43 26	57 10	68 20	84 10	101 20	112 9	129 15	144 19	158 10	232 155
44 23	58 25	72 27	87 19	102 999	114 10	130 15	147 288	216 91	233 31
45 67	59 63	73 387	88 10	103 98	115 218	131 14	148 50	217 20	234 15
46 9	60 18	74 46	98 17	104 38	116 55	142 187	156 15	218 45	

Synonyms:

1,4-Aminobutyric acid 2T-TENT;

Hit 32 : RH-T-1304.5-0.06%-GLYCINE 3T-CONF-[56-40-6]-RH03
CAS: 5630-82-0; Lib: tom18; ID: 32.



(tom18) RH-T-1304.5-0.06%-GLYCINE 3T-CONF-[56-40-6]-RH03

Name: RH-T-1304.5-0.06%-GLYCINE 3T-CONF-[56-40-6]-RH03

Formula: C₁₁H₂₉NO₂Si₃

MW: 291 CAS#: 5630-82-0 ID#: 32 DB: tom18

Other DBs: None

Comment: RI:MG00238 [RI:1304.5]

10 largest peaks:

174 999 | 73 630 | 147 359 | 248 217 | 175 187 | 86 136 | 133 110 | 45 105 | 59 84 | 100 83 |

41 m/z Values and Intensities (26 low intensity peaks are not shown):

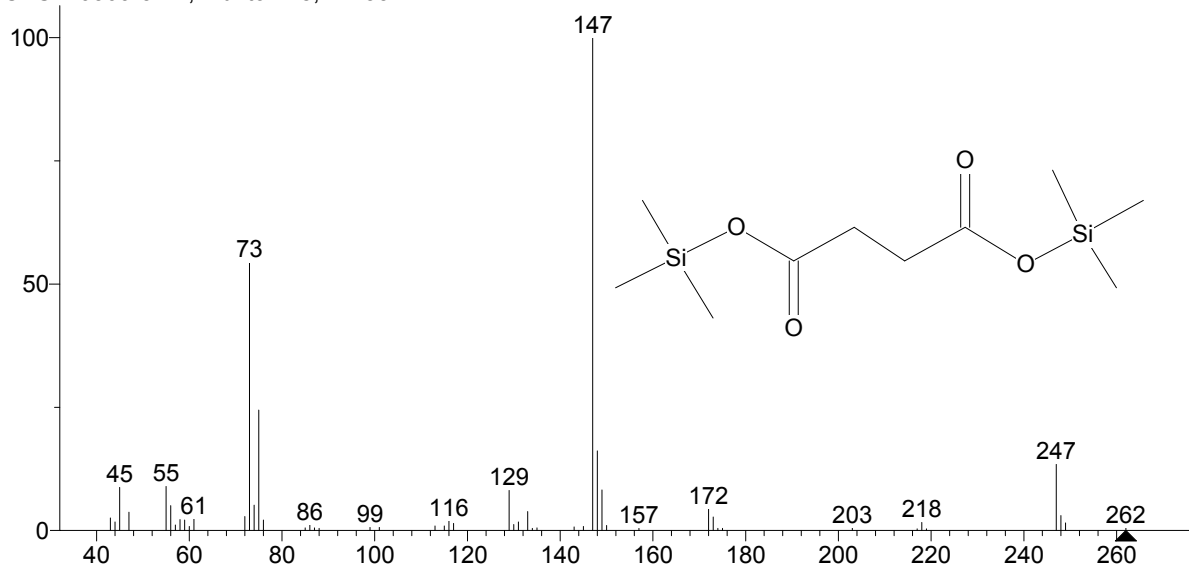
43 21	59 84	87 14	116 10	132 10	148 58	175 187	246 17	277 16
44 13	73 630	100 83	117 32	133 110	149 25	176 82	248 217	
45 105	74 54	101 14	119 10	134 18	158 24	177 14	249 56	
47 9	75 45	102 10	130 32	144 11	172 10	188 11	250 32	
58 16	86 136	115 12	131 33	147 359	174 999	245 17	276 62	

Synonyms:

1.GLYCINE 3T-CONF-[56-40-6];

Hit 33 : RH-T-1316.4-0.03%-SUCCINIC ACID 2T-CONF-[110-15-6]-RH03

CAS: 40309-57-7; Lib: tom18; ID: 33.



(tom18) RH-T-1316.4-0.03%-SUCCINIC ACID 2T-CONF-[110-15-6]-RH03

Name: RH-T-1316.4-0.03%-SUCCINIC ACID 2T-CONF-[110-15-6]-RH03

Formula: C₁₀H₂₂O₄Si₂

MW: 262 CAS#: 40309-57-7 ID#: 33 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:1316.4|

10 largest peaks:

147 999 | 73 543 | 75 244 | 148 161 | 247 134 | 55 89 | 45 87 | 149 82 | 129 81 | 74 51 |

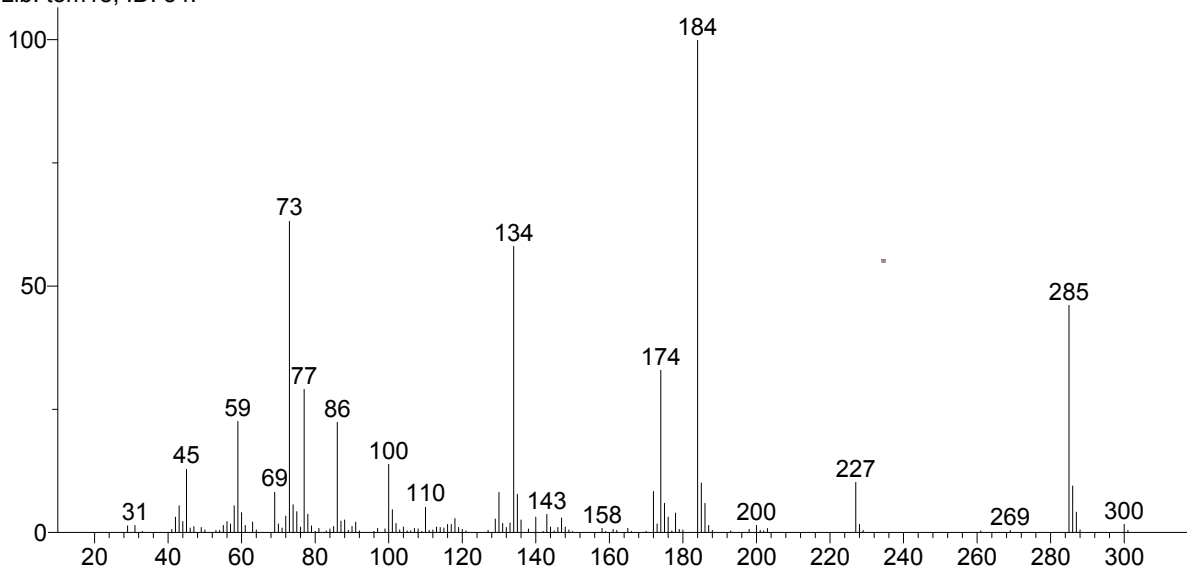
34 m/z Values and Intensities (17 low intensity peaks are not shown):

43 25	55 89	59 21	74 51	113 9	129 81	147 999	172 43	248 30
44 17	56 50	61 23	75 244	115 9	130 12	148 161	173 27	249 15
45 87	57 11	72 28	76 21	116 19	131 17	149 82	218 16	
47 37	58 22	73 543	86 11	117 14	133 38	150 10	247 134	

Synonyms:

1.SUCCINIC ACID 2T-CONF-[110-15-6];

Hit 34 : RH-T-1327.5-0.03%-[184,285,134, G: tms unk.hp: ARA COL. LEAF 014]-RH03
 Lib: tom18; ID: 34.



(tom18) RH-T-1327.5-0.03%-[184,285,134, G: tms unk.hp: ARA COL. LEAF 014]-RH03 RI:1327.5,

Name: RH-T-1327.5-0.03%-[184,285,134, G: tms unk.hp: ARA COL. LEAF 014]-RH03

MW: N/A ID#: 34 DB: tom18

RI: 1327.5,

Comment: RI=1327.5, 19.3999 min MG00244 [RI:1327.5]

10 largest peaks:

184 999 | 73 632 | 134 580 | 285 461 | 174 329 | 77 290 | 59 225 | 86 223 | 100 138 | 45 129 |

78 m/z Values and Intensities (51 low intensity peaks are not shown):

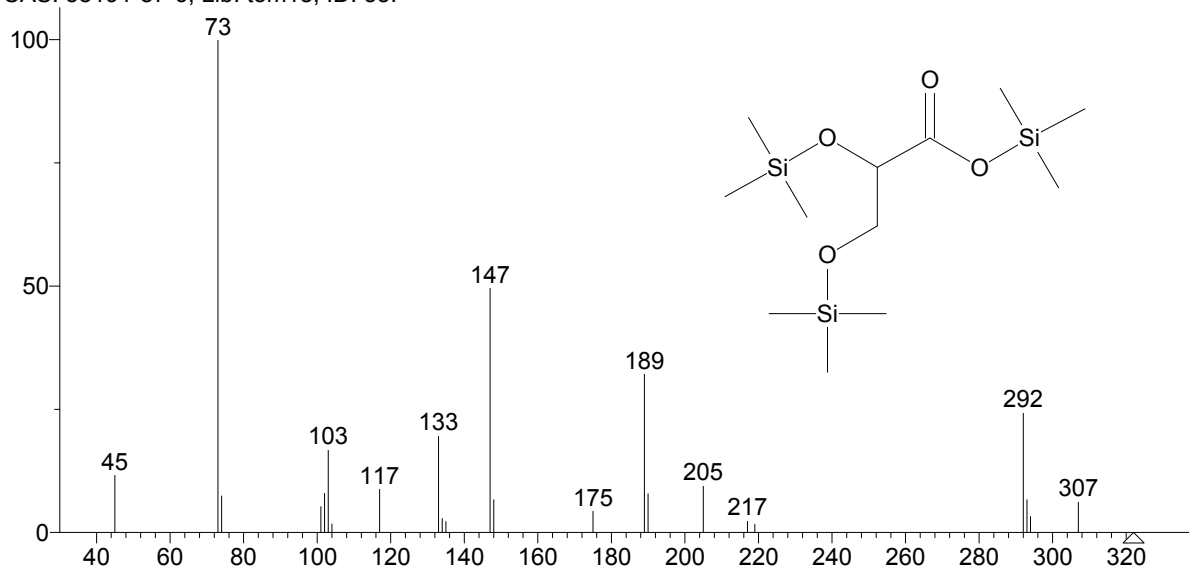
29 13	49 10	63 21	76 11	90 12	114 10	131 18	144 11	175 59	227 102
31 14	55 14	69 83	77 290	91 21	115 9	132 10	146 10	176 31	228 16
42 31	56 22	70 17	78 37	100 138	116 16	133 19	147 29	178 39	285 461
43 54	57 17	71 9	79 13	101 46	117 16	134 580	148 11	184 999	286 94
44 22	58 54	72 33	85 12	102 18	118 28	135 77	158 9	185 100	287 41
45 129	59 225	73 632	86 223	104 11	119 10	136 25	172 83	186 59	300 17
46 9	60 40	74 56	87 23	110 52	129 27	140 31	173 17	187 14	
47 12	61 14	75 42	88 25	113 11	130 81	143 37	174 329	200 14	

Synonyms:

1.m184,285,134, G: tms unk.hp: ARA COL. LEAF 014];

Hit 35 : RH-T-1337.5-0.01%-GLYCERIC ACID 3T-CONF-[473-81-4]-RH03

CAS: 38191-87-6; Lib: tom18; ID: 35.



(tom18) RH-T-1337.5-0.01%-GLYCERIC ACID 3T-CONF-[473-81-4]-RH03

Name: RH-T-1337.5-0.01%-GLYCERIC ACID 3T-CONF-[473-81-4]-RH03

Formula: C₁₂H₃₀O₄Si₃

MW: 322 CAS#: 38191-87-6 ID#: 35 DB: tom18

Other DBs: None

Comment: RI:MG00238 [RI:1337.5]

10 largest peaks:

73 999 | 147 495 | 189 321 | 292 243 | 133 196 | 103 168 | 45 116 | 205 95 | 117 87 | 102 79 |

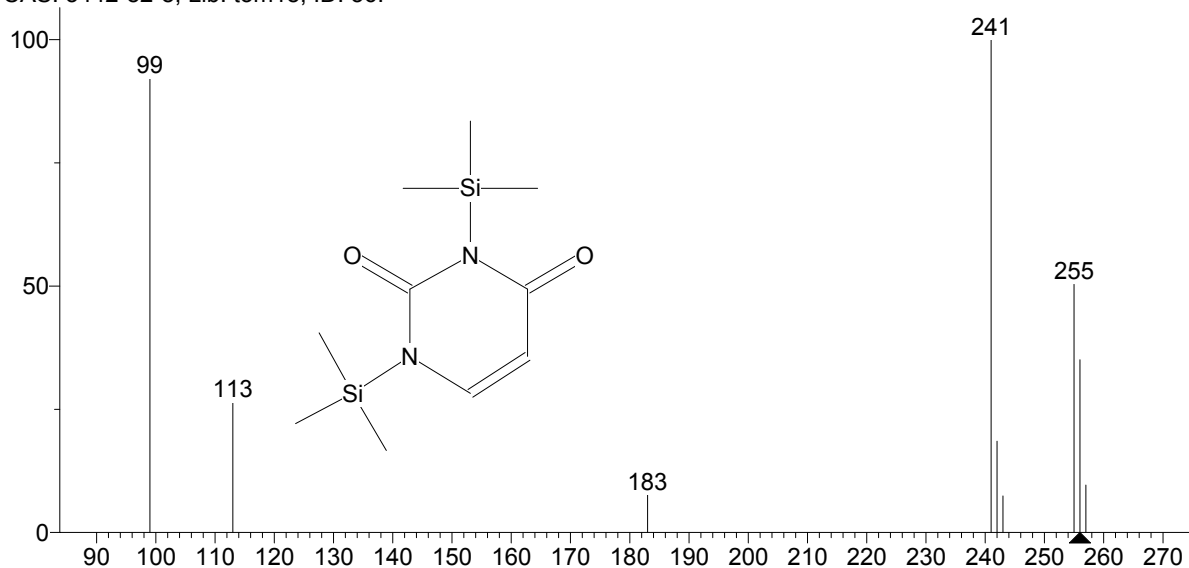
23 m/z Values and Intensities:

45 116 | 101 52 | 104 17 | 134 28 | 148 66 | 190 78 | 219 16 | 294 32 |
 73 999 | 102 79 | 117 87 | 135 22 | 175 43 | 205 95 | 292 243 | 307 62 |
 74 74 | 103 168 | 133 196 | 147 495 | 189 321 | 217 24 | 293 66 |

Synonyms:

1.GLYCERIC ACID 3T-CONF-[473-81-4];

Hit 36 : RH-T-1343.3-0.00%-URACIL T-CONF-[66-22-8]-8135A18-G-X
CAS: 3442-82-8; Lib: tom18; ID: 36.



(tom18) RH-T-1343.3-0.00%-URACIL T-CONF-[66-22-8]-8135A18-G-X RI:1343.3,

Name: RH-T-1343.3-0.00%-URACIL T-CONF-[66-22-8]-8135A18-G-X

Formula: C₁₀H₂₀N₂O₂Si₂

MW: 256 CAS#: 3442-82-8 ID#: 36 DB: tom18

Other DBs: None

RI: 1343.3,

Comment: RI=1343.3, 17.4480 min 8135A18 |RI:1343.3|

9 largest peaks:

241 999 | 99 920 | 255 503 | 256 350 | 113 263 | 242 185 | 257 96 | 183 76 | 243 74 |

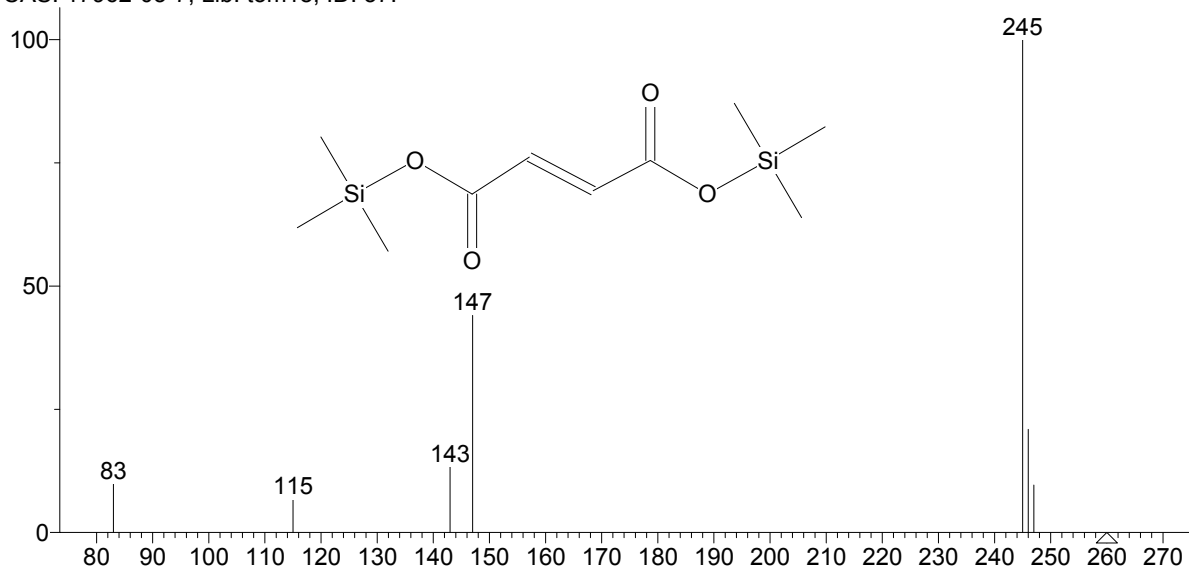
9 m/z Values and Intensities:

99 920 | 113 263 | 183 76 | 241 999 | 242 185 | 243 74 | 255 503 | 256 350 | 257 96 |

Synonyms:

1.URACIL T-CONF-[66-22-8];

Hit 37 : RH-T-1352.6-0.00%-FUMARIC ACID 2T-CONF-[110-17-8]-RH03-X
CAS: 17962-03-7; Lib: tom18; ID: 37.



(tom18) RH-T-1352.6-0.00%-FUMARIC ACID 2T-CONF-[110-17-8]-RH03-X

Name: RH-T-1352.6-0.00%-FUMARIC ACID 2T-CONF-[110-17-8]-RH03-X

Formula: C₁₀H₂₀O₄Si₂

MW: 260 CAS#: 17962-03-7 ID#: 37 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:1352.6|

7 largest peaks:

245 999 | 147 440 | 246 209 | 143 133 | 83 98 | 247 96 | 115 66 |

7 m/z Values and Intensities:

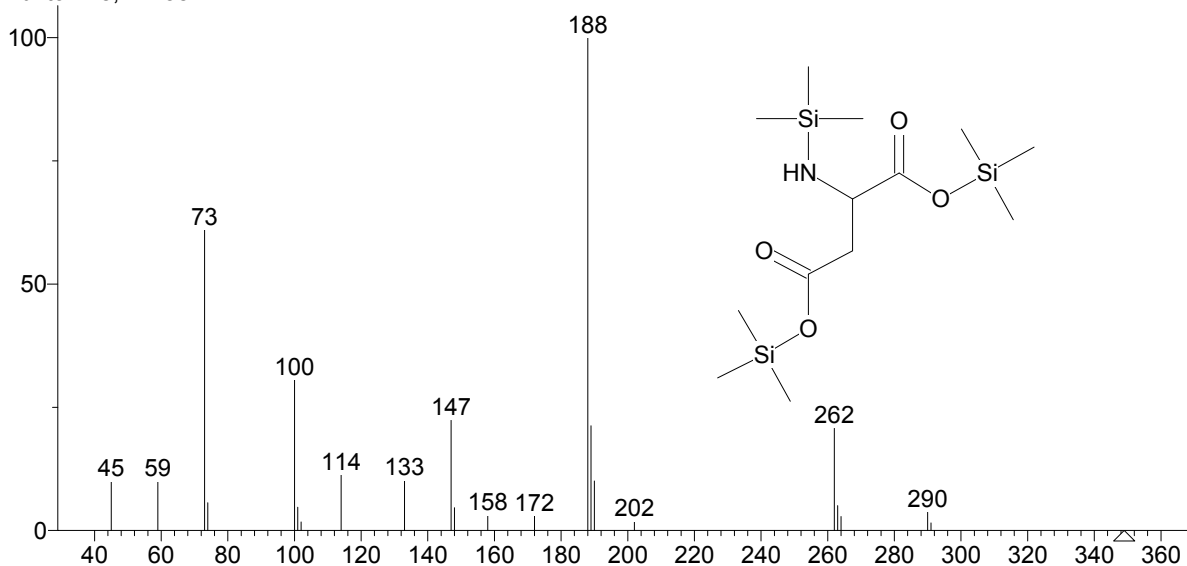
83 98 | 115 66 | 143 133 | 147 440 | 245 999 | 246 209 | 247 96 |

Synonyms:

1.FUMARIC ACID 2T-CONF-[110-17-8];

Hit 38 : RH-T-1355.4-0.01%-ALANINE 3T-PK1-TENT-[302-72-7]-RH03

Lib: tom18; ID: 38.



(tom18) RH-T-1355.4-0.01%-ALANINE 3T-PK1-TENT-[302-72-7]-RH03

Name: RH-T-1355.4-0.01%-ALANINE 3T-PK1-TENT-[302-72-7]-RH03

Formula: C₁₃H₃₁NO₄Si₃

MW: 349 ID#: 38 DB: tom18

Comment: RI:MG00238 |RI:1355.4|

10 largest peaks:

188 999 | 73 609 | 100 305 | 147 223 | 189 212 | 262 207 | 114 112 | 133 101 | 190 100 | 45 99 |

22 m/z Values and Intensities:

45 99 | 74 56 | 102 17 | 147 223 | 172 29 | 190 100 | 263 50 | 291 15 |

59 99 | 100 305 | 114 112 | 148 46 | 188 999 | 202 18 | 264 28 |

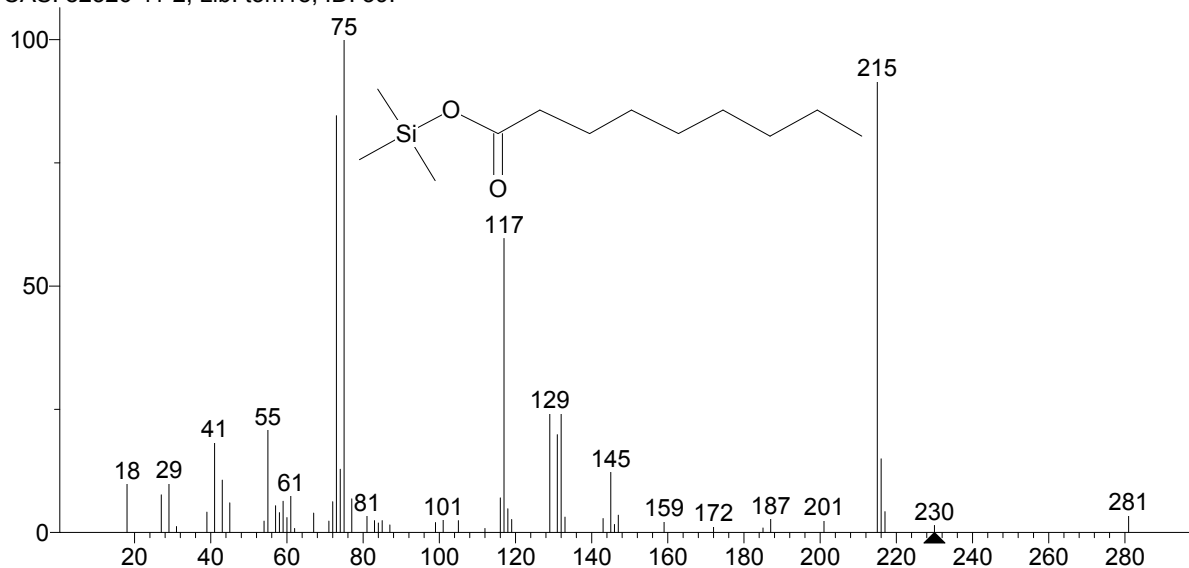
73 609 | 101 47 | 133 101 | 158 30 | 189 212 | 262 207 | 290 37 |

Synonyms:

1.ALANINE 3T-PK1-TENT-[302-72-7];

Hit 39 : RH-T-1361.1-0.02%-NONANOIC ACID T-CONF-[112-05-0]-RH03

CAS: 82326-11-2; Lib: tom18; ID: 39.



(tom18) RH-T-1361.1-0.02%-NONANOIC ACID T-CONF-[112-05-0]-RH03

Name: RH-T-1361.1-0.02%-NONANOIC ACID T-CONF-[112-05-0]-RH03

Formula: C₁₂H₂₆O₂Si

MW: 230 CAS#: 82326-11-2 ID#: 39 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:1361.1|

10 largest peaks:

75 999 | 215 914 | 73 845 | 117 596 | 129 241 | 132 241 | 55 208 | 131 198 | 41 182 | 216 149 |

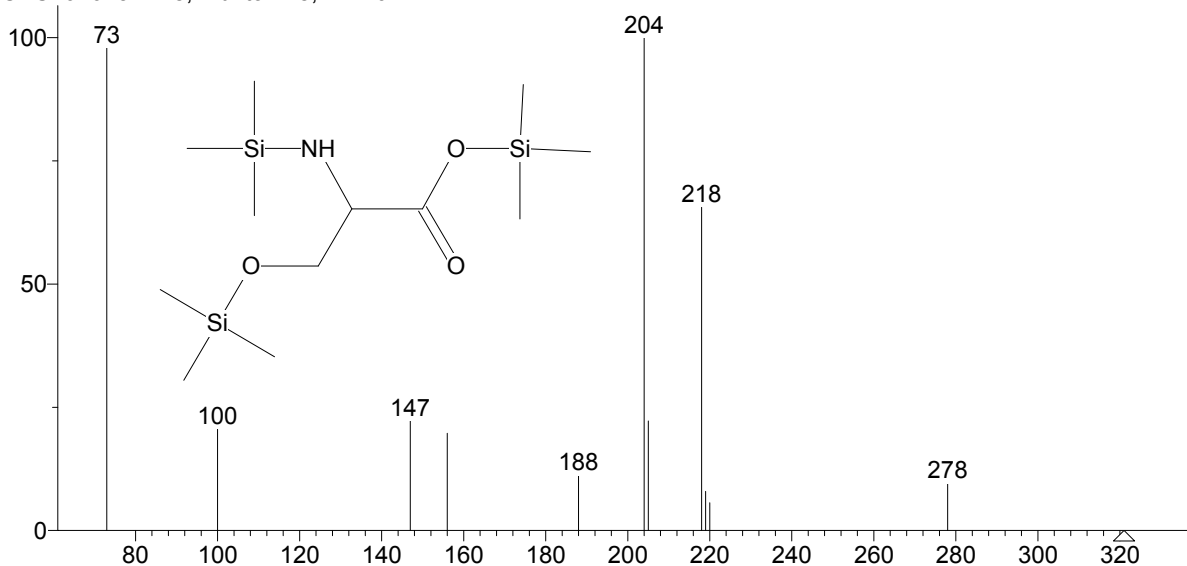
52 m/z Values and Intensities (2 low intensity peaks are not shown):

18 98	43 106	59 63	73 845	84 19	116 70	132 241	159 22	216 149
27 76	45 60	60 30	74 128	85 24	117 596	133 31	172 12	217 42
29 99	54 23	61 74	75 999	87 15	118 48	143 28	185 9	230 14
31 12	55 208	67 39	77 68	99 20	119 26	145 122	187 27	281 34
39 41	57 54	71 23	81 33	101 25	129 241	146 16	201 24	
41 182	58 40	72 62	83 24	105 24	131 198	147 35	215 914	

Synonyms:

1.NONANOIC ACID T-CONF-[112-05-0]-;

Hit 40 : RH-T-1365.8-0.05%-SERINE 3T-CONF-[302-84-1]-RH03-X
CAS: 64625-17-8; Lib: tom18; ID: 40.



(tom18) RH-T-1365.8-0.05%-SERINE 3T-CONF-[302-84-1]-RH03-X

Name: RH-T-1365.8-0.05%-SERINE 3T-CONF-[302-84-1]-RH03-X

Formula: C₁₂H₃₁NO₃Si₃

MW: 321 CAS#: 64625-17-8 ID#: 40 DB: tom18

Other DBs: None

Comment: RI:MG00238 [RI:1365.8]

10 largest peaks:

204 999 | 73 978 | 218 655 | 147 222 | 205 222 | 100 205 | 156 197 | 188 111 | 278 95 | 219 79 |

11 m/z Values and Intensities:

73 978 | 147 222 | 188 111 | 205 222 | 219 79 | 278 95 |
100 205 | 156 197 | 204 999 | 218 655 | 220 56 |

Synonyms:

1.SERINE 3T-CONF-[302-84-1];

Hit 41 : RH-T-1389.1-0.05%-THREONINE 3T-TENT-[80-68-2]-RH03-X
CAS: 7537-02-2; Lib: tom18; ID: 41.



(tom18) RH-T-1389.1-0.05%-THREONINE 3T-TENT-[80-68-2]-RH03-X

Name: RH-T-1389.1-0.05%-THREONINE 3T-TENT-[80-68-2]-RH03-X

Formula: C₁₃H₃₃NO₃Si₃

MW: 335 CAS#: 7537-02-2 ID#: 41 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:1389.1|

10 largest peaks:

73 999 | 218 417 | 219 355 | 117 328 | 291 165 | 101 132 | 292 128 | 220 104 | 74 90 | 203 77 |

16 m/z Values and Intensities:

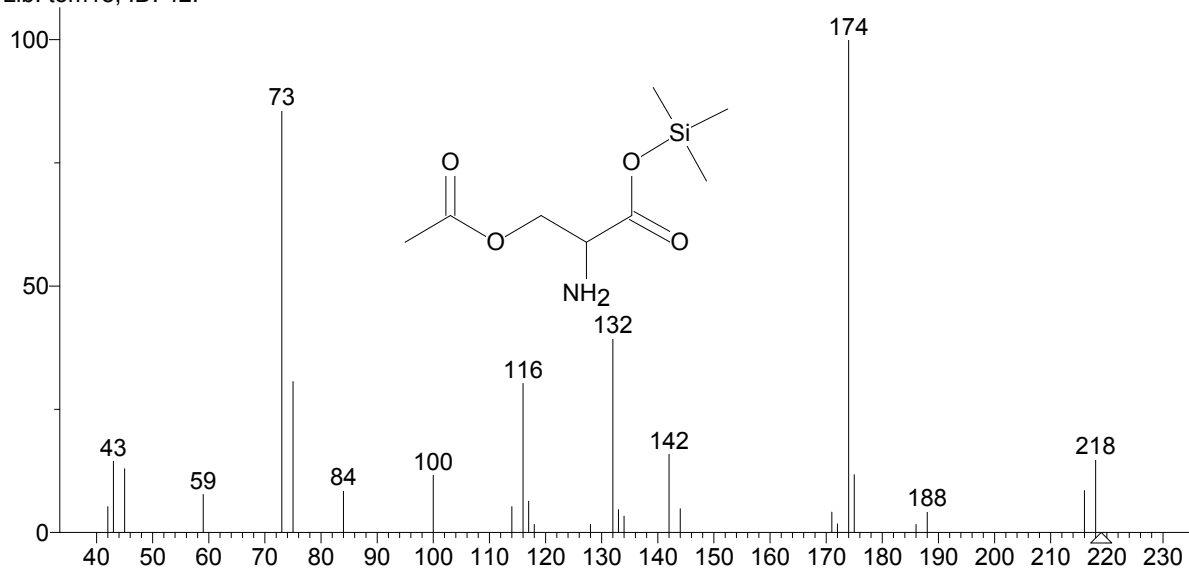
73 999 | 101 132 | 117 328 | 128 52 | 218 417 | 220 104 | 291 165 | 293 31 |
74 90 | 114 29 | 118 41 | 203 77 | 219 355 | 228 35 | 292 128 | 320 17 |

Synonyms:

1.THREONINE 3T-TENT-[80-68-2];

Hit 42 : RH-T-1400.0-0.00%-[G:O-ACETYL-SERINE-T]-TENT-8135A18-G

Lib: tom18; ID: 42.



(tom18) RH-T-1400.0-0.00%-[G:O-ACETYL-SERINE-T]-TENT-8135A18-G RI:1400.0,

Name: RH-T-1400.0-0.00%-[G:O-ACETYL-SERINE-T]-TENT-8135A18-G

Formula: C₈H₁₇NO₄Si

MW: 219 ID#: 42 DB: tom18

RI: 1400.0,

Comment: RI=1400.0, 18.7008 min 8135A18 [RI:1400]

10 largest peaks:

174 999 | 73 855 | 132 393 | 75 306 | 116 302 | 142 159 | 218 148 | 43 145 | 45 129 | 175 117 |

26 m/z Values and Intensities:

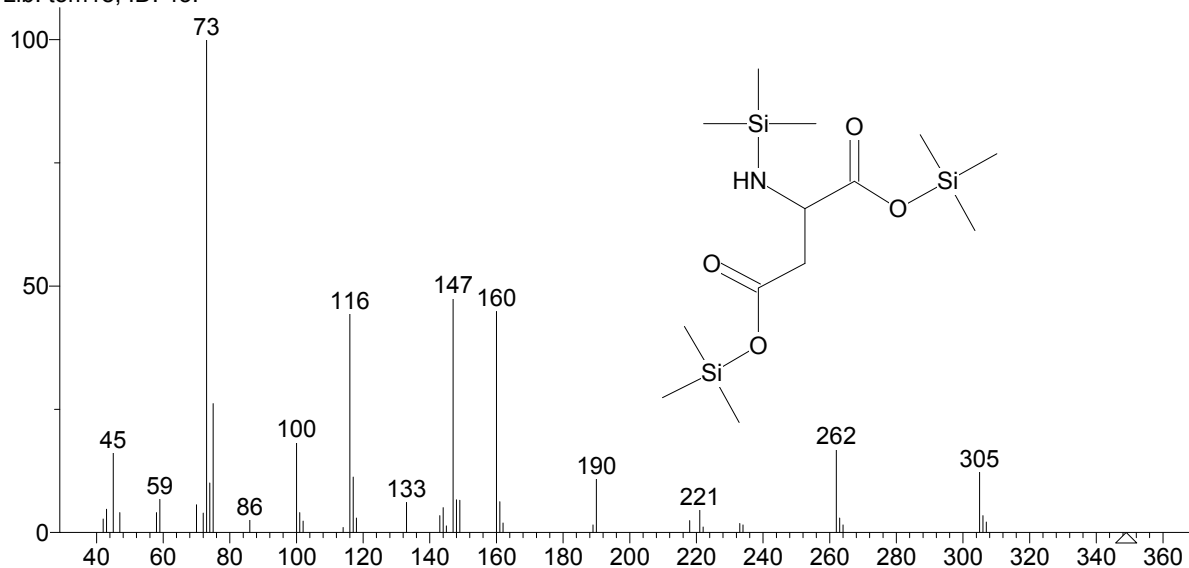
42 52	59 77	84 85	116 302	128 16	134 33	171 41	175 117	216 85
43 145	73 855	100 116	117 63	132 393	142 159	172 17	186 16	218 148
45 129	75 306	114 52	118 16	133 46	144 48	174 999	188 42	

Synonyms:

1.ACETYL-SERINE-T-TENT;

Hit 43 : RH-T-1403.5-0.01%-ALANINE 3T-PK2-TENT-[302-72-7]-RH03

Lib: tom18; ID: 43.



(tom18) RH-T-1403.5-0.01%-ALANINE 3T-PK2-TENT-[302-72-7]-RH03 RI:1403.5,

Name: RH-T-1403.5-0.01%-ALANINE 3T-PK2-TENT-[302-72-7]-RH03

Formula: C₁₃H₃₁NO₄Si₃

MW: 349 ID#: 43 DB: tom18

RI: 1403.5,

Comment: RI=1403.5, 21.9258 min MG00238 [RI:1403.5]

10 largest peaks:

73 999 | 147 474 | 160 448 | 116 443 | 75 261 | 100 182 | 262 168 | 45 161 | 305 122 | 117 112 |

42 m/z Values and Intensities:

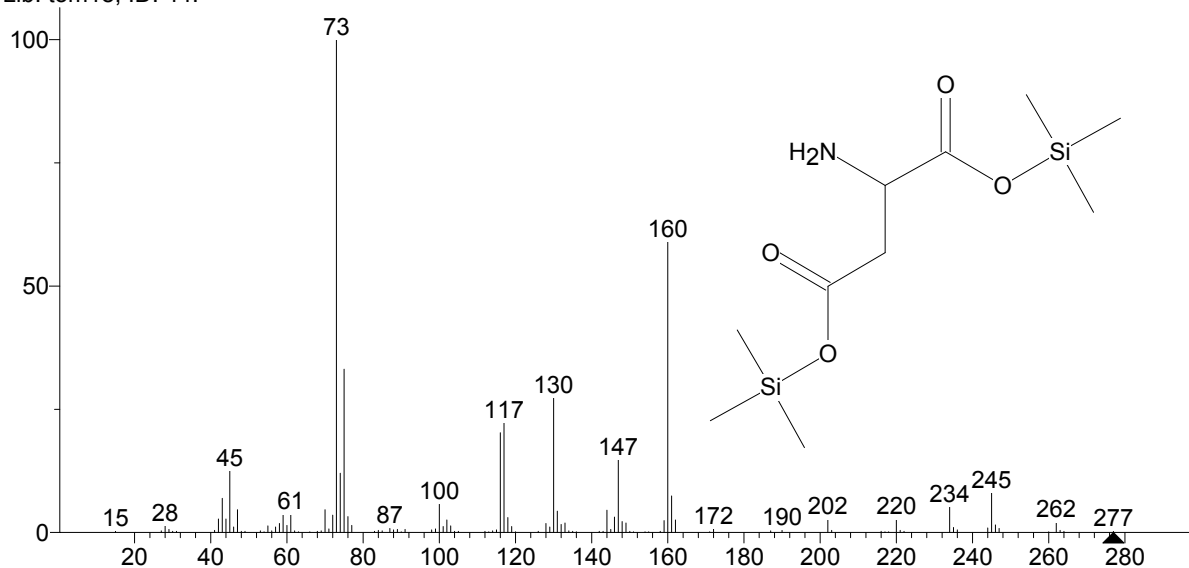
42 27	59 67	75 261	114 10	143 34	149 65	190 108	234 15	306 34
43 47	70 56	86 25	116 443	144 50	160 448	218 24	262 168	307 21
45 161	72 39	100 182	117 112	145 13	161 62	221 45	263 29	
47 40	73 999	101 40	118 29	147 474	162 19	222 11	264 15	
58 40	74 100	102 23	133 61	148 66	189 15	233 18	305 122	

Synonyms:

1.ALANINE 3T-PK2-TENT-[302-72-7];

Hit 44 : RH-T-1424.6-0.32%-ASPARTIC ACID 2T-CONF-[56-84-8]-RH03

Lib: tom18; ID: 44.



(tom18) RH-T-1424.6-0.32%-ASPARTIC ACID 2T-CONF-[56-84-8]-RH03

Name: RH-T-1424.6-0.32%-ASPARTIC ACID 2T-CONF-[56-84-8]-RH03

Formula: C₁₀H₂₃NO₄Si₂

MW: 277 ID#: 44 DB: tom18

Comment: RI:MG00238 [RI:1424.6]

10 largest peaks:

73 999 | 160 589 | 75 331 | 130 272 | 117 222 | 116 202 | 147 147 | 45 124 | 74 120 | 245 80 |

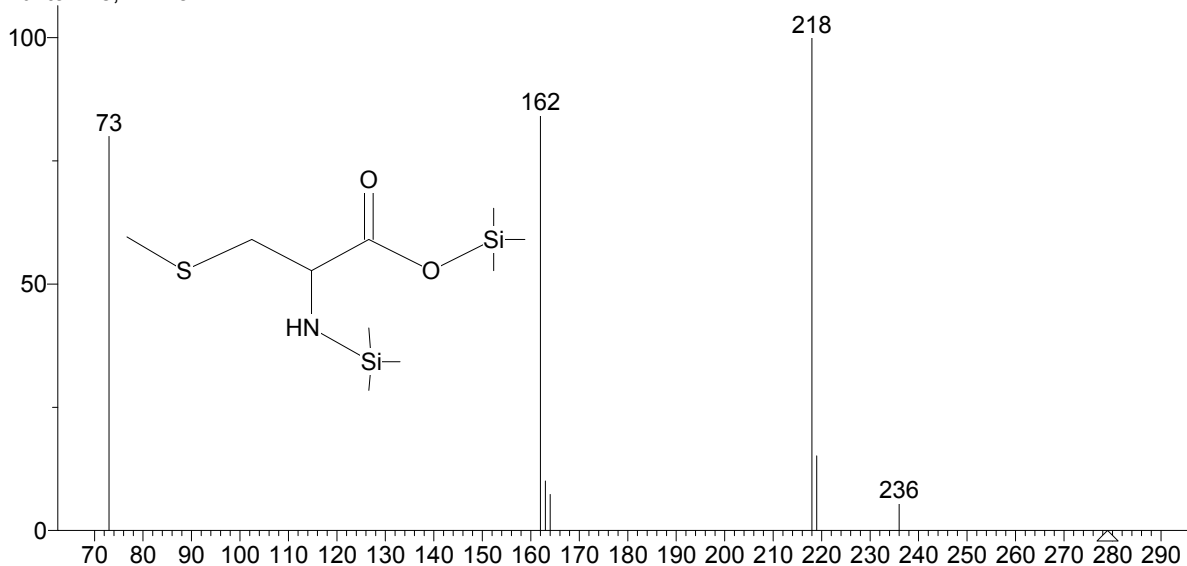
51 m/z Values and Intensities (62 low intensity peaks are not shown):

28 13	47 46	61 36	76 32	116 202	130 272	147 147	162 25	245 80
42 27	55 13	70 46	77 14	117 222	131 43	148 22	202 26	246 15
43 69	57 11	72 35	100 57	118 30	132 16	149 19	220 26	262 20
44 27	58 18	73 999	101 12	119 12	133 19	159 24	234 51	
45 124	59 35	74 120	102 25	128 18	144 45	160 589	235 10	
46 11	60 14	75 331	103 13	129 11	146 31	161 74	244 9	

Synonyms:

1.ASPARTIC ACID 2T-CONF-[56-84-8];

Hit 45 : RH-T-1427.3-0.00%-S-METHYL-CYSTEINE 2T-TENT-[7728-98-5]-8135A18-X
 Lib: tom18; ID: 45.



(tom18) RH-T-1427.3-0.00%-S-METHYL-CYSTEINE 2T-TENT-[7728-98-5]-8135A18-X RI:1427.3,

Name: RH-T-1427.3-0.00%-S-METHYL-CYSTEINE 2T-TENT-[7728-98-5]-8135A18-X

Formula: C₁₀H₂₅NO₂SSi₂

MW: 279 ID#: 45 DB: tom18

RI: 1427.3,

Comment: RI=1427.3, 19.2872 min 8135A18 |RI:1427.3|

7 largest peaks:

218 999 | 162 841 | 73 799 | 219 151 | 163 100 | 164 73 | 236 54 |

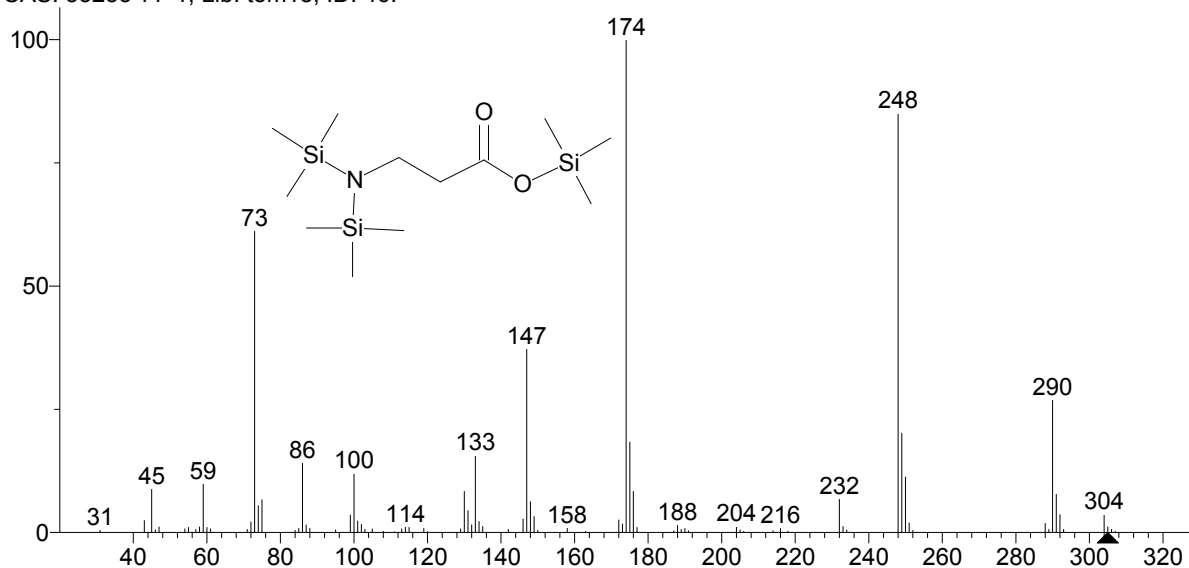
7 m/z Values and Intensities:

73 799 | 162 841 | 163 100 | 164 73 | 218 999 | 219 151 | 236 54 |

Synonyms:

1.S-METHYL-CYSTEINE 2T-TENT-[7728-98-5];

Hit 46 : RH-T-1427.9-0.03%-BETA-ALANINE 3T-CONF-[107-95-9]-RH03
CAS: 55255-77-1; Lib: tom18; ID: 46.



(tom18) RH-T-1427.9-0.03%-BETA-ALANINE 3T-CONF-[107-95-9]-RH03 RI:1427.9,

Name: RH-T-1427.9-0.03%-BETA-ALANINE 3T-CONF-[107-95-9]-RH03

Formula: C₁₂H₃₁NO₂Si₃

MW: 305 CAS#: 55255-77-1 ID#: 46 DB: tom18

Other DBs: None

RI: 1427.9,

Comment: RI=1427.9, 22.6977 min MG00238 |RI:1427.9|

10 largest peaks:

174 999 | 248 849 | 73 611 | 147 372 | 290 268 | 249 201 | 175 183 | 133 156 | 86 141 | 100 119 |

50 m/z Values and Intensities (36 low intensity peaks are not shown):

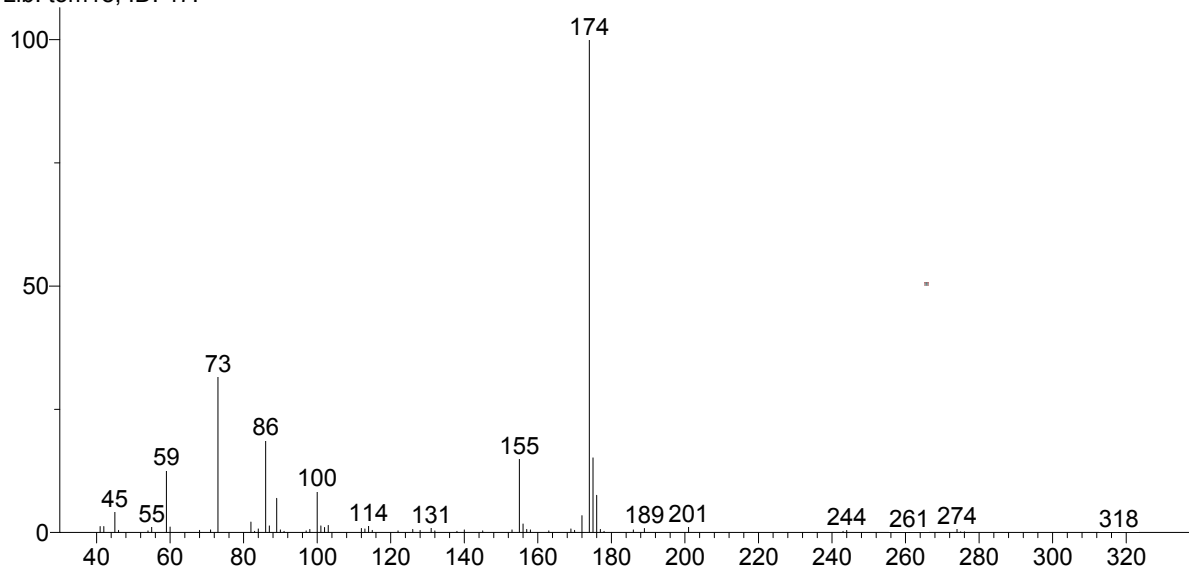
43	24	59	98	75	66	101	23	131	44	146	27	172	25	177	10	248	849	290	268
45	87	60	10	86	141	102	16	132	15	147	372	173	17	188	14	249	201	291	77
47	11	72	21	87	15	114	11	133	156	148	62	174	999	204	12	250	112	292	36
55	10	73	611	99	35	115	10	134	22	149	32	175	183	232	67	251	19	304	36
58	11	74	54	100	119	130	83	135	12	158	9	176	83	233	12	288	18	305	11

Synonyms:

1.BETA-ALANINE 3T-CONF-[107-95-9];

Hit 47 : RH-T-1435.1-0.02%-[174,155,86]-8135A18-G

Lib: tom18; ID: 47.



(tom18) RH-T-1435.1-0.02%-[174,155,86]-8135A18-G RI:1435.1,

Name: RH-T-1435.1-0.02%-[174,155,86]-8135A18-G

MW: N/A ID#: 47 DB: tom18

RI: 1435.1,

Comment: RI=1435.1, 19.4539 min 8135A18 |RI:1435.1|

10 largest peaks:

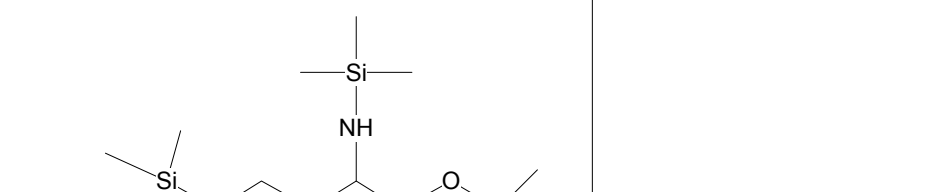
174	999	73	315	86	186	175	151	155	149	59	125	100	83	176	75	89	69	45	41
-----	-----	----	-----	----	-----	-----	-----	-----	-----	----	-----	-----	----	-----	----	----	----	----	----

24 m/z Values and Intensities (37 low intensity peaks are not shown):

41	12	55	11	73	315	87	13	101	13	114	13	156	17	175	151
42	12	59	125	82	21	89	69	102	10	131	9	172	34	176	75
45	41	60	11	86	186	100	83	103	14	155	149	174	999	201	11

Synonyms:

1.m174,155,86;

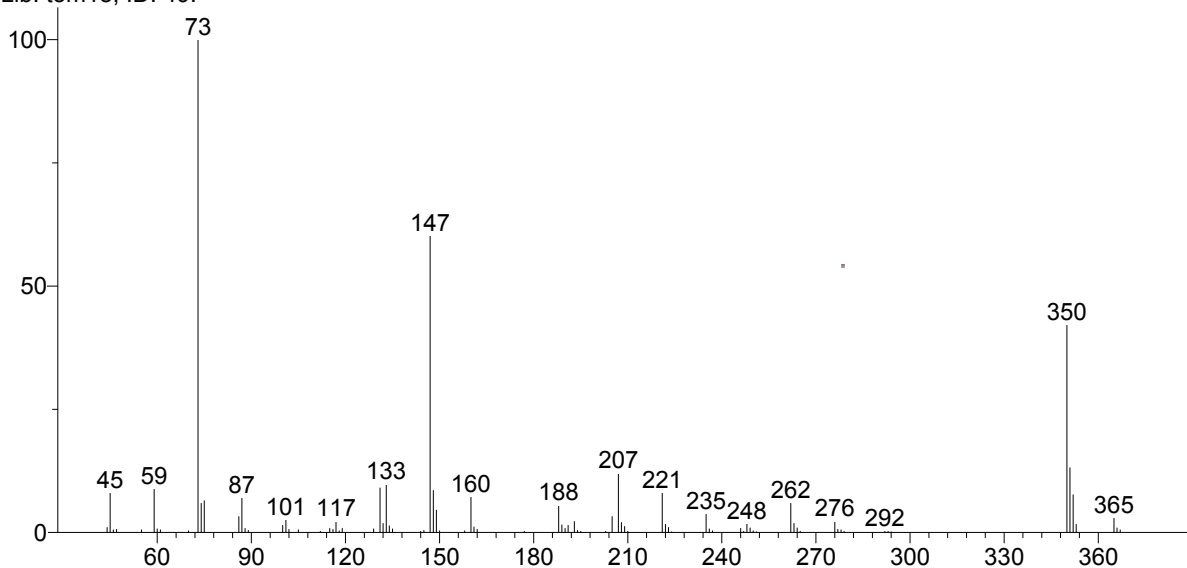


 Mass spectrum of compound 12b. The x-axis represents the mass-to-charge ratio (m/z) from 50 to 350, and the y-axis represents the relative intensity in percent from 0 to 100. The base peak is at m/z 218. Other labeled peaks include m/z 56, 73, 103, 128, 147, and 230. The chemical structure of 12b is shown above the spectrum.

1.HOMOSERINE-3T-TENT;

Hit 49 : RH-T-1455.9-0.01%-[350,262,207]-8135A18-G

Lib: tom18; ID: 49.



(tom18) RH-T-1455.9-0.01%-[350,262,207]-8135A18-G RI:1455.9,

Name: RH-T-1455.9-0.01%-[350,262,207]-8135A18-G

MW: N/A ID#: 49 DB: tom18

RI: 1455.9,

Comment: RI=1455.9, 19.9013 min 8135A18 [RI:1455.9]

10 largest peaks:

73 999 | 147 601 | 350 420 | 351 131 | 207 119 | 133 97 | 131 90 | 59 87 | 148 85 | 45 80 |

44 m/z Values and Intensities (43 low intensity peaks are not shown):

44 10 | 75 64 | 117 22 | 147 601 | 188 54 | 207 119 | 223 10 | 263 18 | 352 76 |

45 80 | 86 32 | 131 90 | 148 85 | 189 15 | 208 20 | 235 37 | 264 9 | 353 16 |

59 87 | 87 69 | 132 18 | 149 45 | 191 14 | 209 12 | 248 17 | 276 22 | 365 29 |

73 999 | 100 14 | 133 97 | 160 72 | 193 22 | 221 80 | 249 9 | 350 420 | 366 9 |

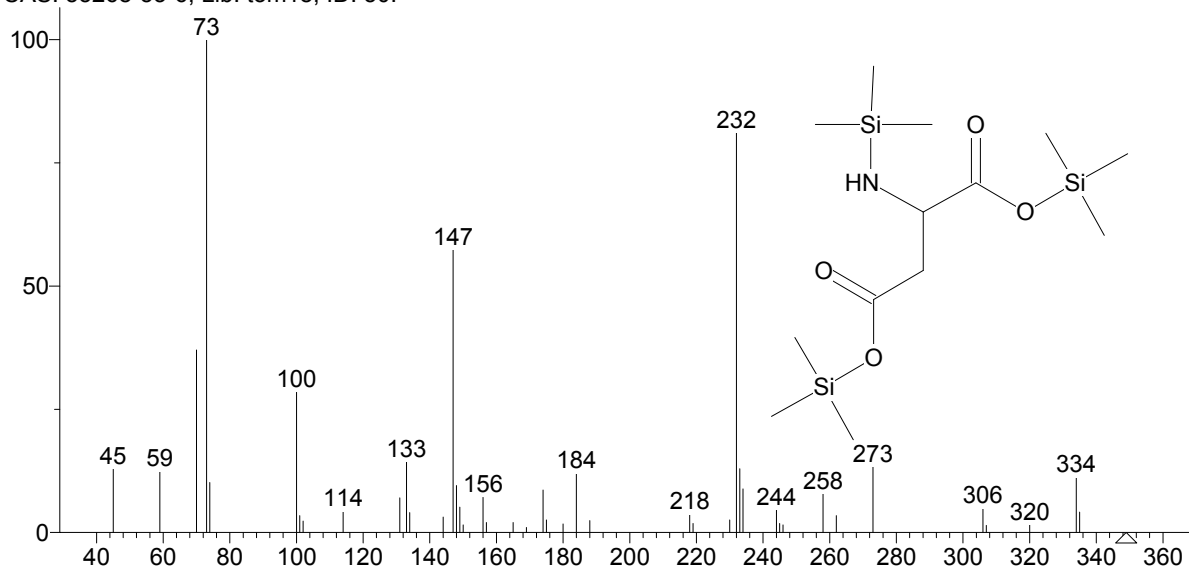
74 59 | 101 25 | 134 13 | 161 11 | 205 32 | 222 16 | 262 59 | 351 131 |

Synonyms:

1.m350,262,207;

Hit 50 : RH-T-1470.8-0.01%-ASPARTIC 3T PK1-TENT-[56-84-8]-RH03

CAS: 55268-53-6; Lib: tom18; ID: 50.



(tom18) RH-T-1470.8-0.01%-ASPARTIC 3T PK1-TENT-[56-84-8]-RH03

Name: RH-T-1470.8-0.01%-ASPARTIC 3T PK1-TENT-[56-84-8]-RH03

Formula: C₁₃H₃₁NO₄Si₃

MW: 349 CAS#: 55268-53-6 ID#: 50 DB: tom18

Other DBs: None

Comment: RI:MG00238 [RI:1470.8]

10 largest peaks:

73 999 | 232 810 | 147 573 | 70 370 | 100 284 | 133 143 | 273 133 | 233 129 | 45 128 | 59 123 |

43 m/z Values and Intensities:

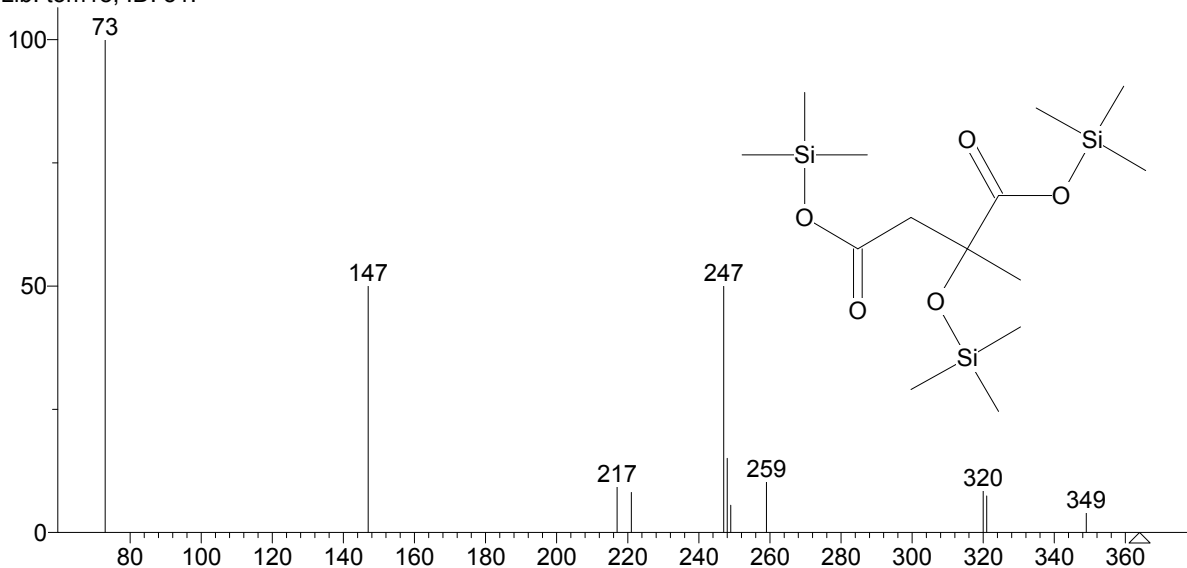
45 128 | 100 284 | 133 143 | 149 51 | 169 10 | 188 24 | 233 129 | 258 78 | 320 15 |
 59 123 | 101 34 | 134 40 | 150 15 | 174 86 | 218 36 | 234 88 | 262 34 | 334 111 |
 70 370 | 102 23 | 144 31 | 156 71 | 175 25 | 219 18 | 244 45 | 273 133 | 335 41 |
 73 999 | 114 42 | 147 573 | 157 20 | 180 17 | 230 25 | 245 18 | 306 48 |
 74 101 | 131 70 | 148 95 | 165 20 | 184 119 | 232 810 | 246 15 | 307 14 |

Synonyms:

1.ASPARTIC 3T PK1-TENT-[56-84-8];

Hit 51 : RH-T-1473.5-0.00%-CITRAMALIC ACID 2T-TENT-[6236-09-5]-RH03-X

Lib: tom18; ID: 51.



(tom18) RH-T-1473.5-0.00%-CITRAMALIC ACID 2T-TENT-[6236-09-5]-RH03-X

Name: RH-T-1473.5-0.00%-CITRAMALIC ACID 2T-TENT-[6236-09-5]-RH03-X

Formula: C₁₄H₃₂O₅Si₃

MW: 364 ID#: 51 DB: tom18

Comment: RI:MG00238 [RI:1473.5]

10 largest peaks:

73 999 | 147 499 | 247 499 | 248 150 | 259 102 | 217 92 | 320 84 | 221 81 | 321 74 | 249 55 |

11 m/z Values and Intensities:

73 999 | 217 92 | 247 499 | 249 55 | 320 84 | 349 39 |

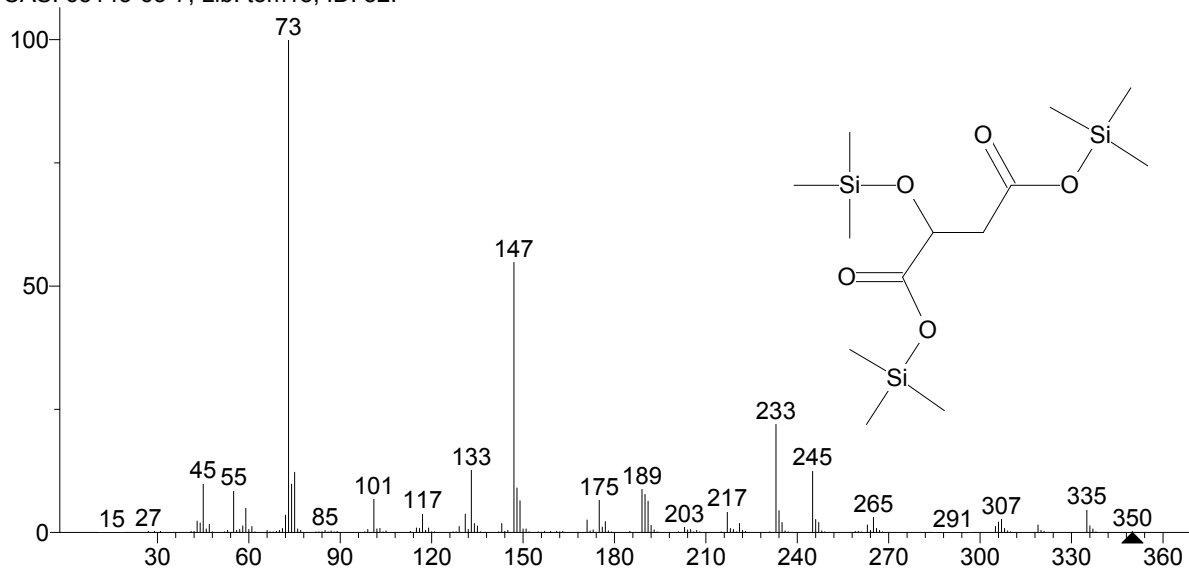
147 499 | 221 81 | 248 150 | 259 102 | 321 74 |

Synonyms:

1.CITRAMALIC ACID 2T-TENT-[6236-09-5];

Hit 52 : RH-T-1493.9-1.27%-MALIC ACID 3T-CONF-[617-48-1]-RH03

CAS: 65143-63-7; Lib: tom18; ID: 52.



(tom18) RH-T-1493.9-1.27%-MALIC ACID 3T-CONF-[617-48-1]-RH03

Name: RH-T-1493.9-1.27%-MALIC ACID 3T-CONF-[617-48-1]-RH03

Formula: C₁₃H₃₀O₅Si₃

MW: 350 CAS#: 65143-63-7 ID#: 52 DB: tom18

Other DBs: None

Comment: RI:MG00238 [RI:1493.9]

10 largest peaks:

73	999	147	548	233	219	133	126	245	125	75	122	45	99	74	98	148	90	189	87
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50 m/z Values and Intensities (98 low intensity peaks are not shown):

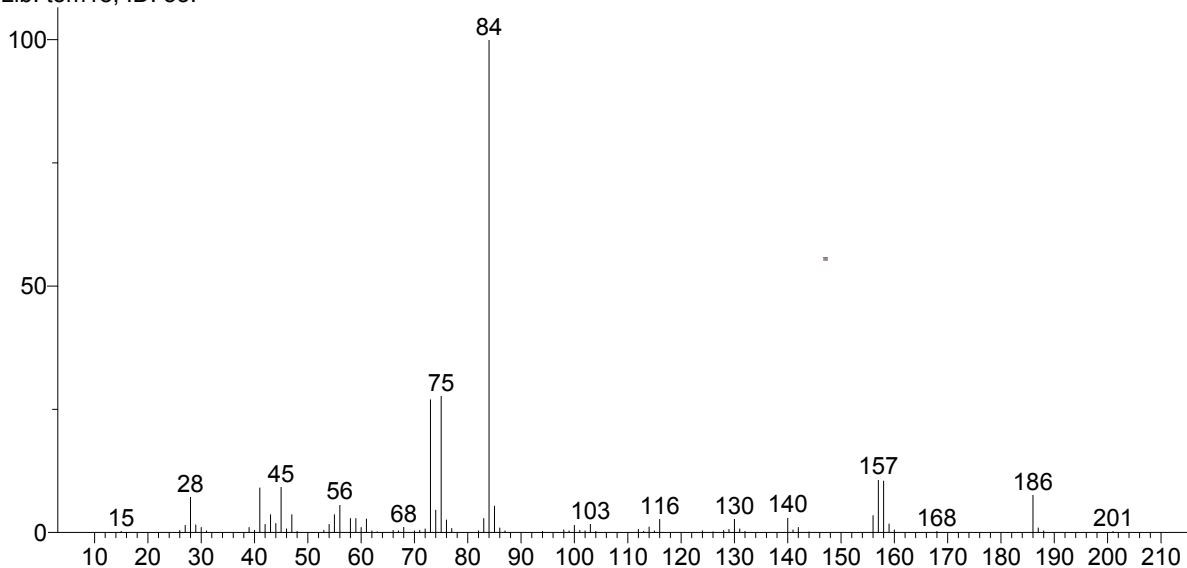
43	23	58	13	74	98	119	9	135	13	171	25	190	77	221	18	246	26	306	21
44	19	59	49	75	122	129	12	143	18	175	65	191	63	233	219	247	20	307	27
45	99	61	12	101	68	131	37	147	548	176	11	192	14	234	44	263	15	319	15
47	16	72	35	115	9	133	126	148	90	177	22	203	11	235	20	265	31	335	46
55	85	73	999	117	38	134	18	149	64	189	87	217	42	245	125	305	12	336	13

Synonyms:

1.MALIC ACID 3T-CONF-[617-48-1];

Hit 53 : RH-T-1497.3-0.10%-[84,186,158,157, sim. pipecolic]-RH03

Lib: tom18; ID: 53.



(tom18) RH-T-1497.3-0.10%-[84,186,158,157, sim. pipecolic]-RH03

Name: RH-T-1497.3-0.10%-[84,186,158,157, sim. pipecolic]-RH03

MW: N/A ID#: 53 DB: tom18

Comment: RI:MG00238 [RI:1497.3]

10 largest peaks:

84 999 | 75 276 | 73 269 | 157 107 | 158 104 | 45 92 | 41 90 | 186 76 | 28 72 | 56 56 |

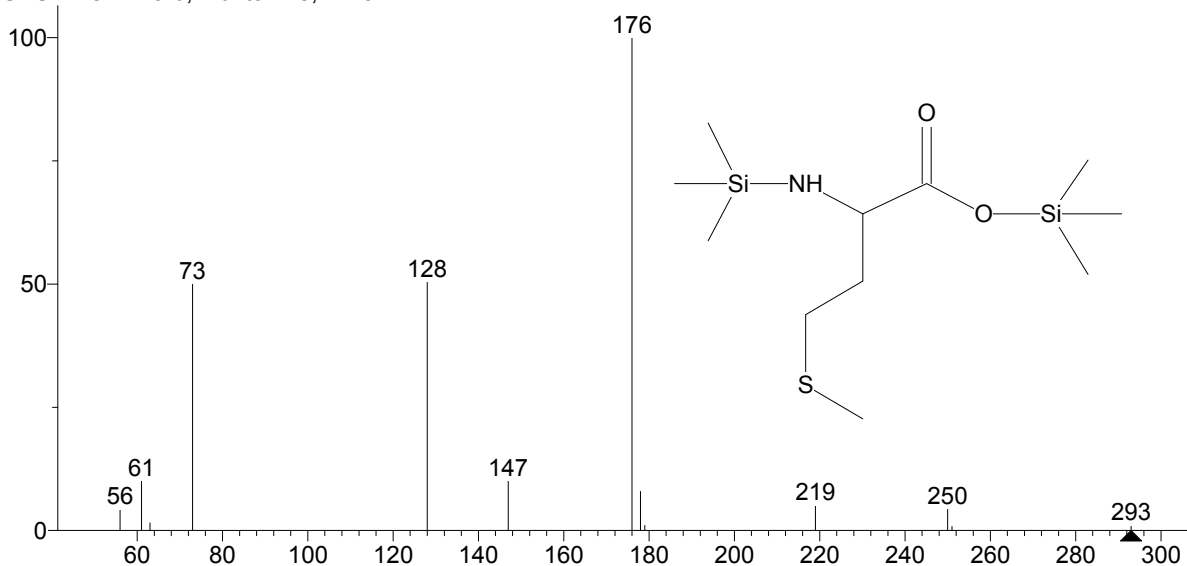
40 m/z Values and Intensities (38 low intensity peaks are not shown):

27 14 | 39 10 | 44 18 | 55 36 | 60 10 | 74 45 | 84 999 | 103 17 | 140 30 | 158 104 |
 28 72 | 41 90 | 45 92 | 56 56 | 61 27 | 75 276 | 85 53 | 114 11 | 142 10 | 159 17 |
 29 15 | 42 16 | 47 36 | 58 28 | 68 11 | 76 25 | 86 9 | 116 27 | 156 34 | 186 76 |
 30 10 | 43 36 | 54 16 | 59 28 | 73 269 | 83 28 | 100 14 | 130 27 | 157 107 | 187 9 |

Synonyms:

1.m84,186,158,157, sim. pipecolic;

Hit 54 : RH-T-1516.3-0.00%-[METHIONINE-2T-TENT-[59-51-8]-8135A18-G
CAS: 27844-10-6; Lib: tom18; ID: 54.



(tom18) RH-T-1516.3-0.00%-[METHIONINE-2T-TENT-[59-51-8]-8135A18-G RI:1516.3,

Name: RH-T-1516.3-0.00%-[METHIONINE-2T-TENT-[59-51-8]-8135A18-G

Formula: C₁₁H₂₇NO₂SSi₂

MW: 293 CAS#: 27844-10-6 ID#: 54 DB: tom18

Other DBs: None

RI: 1516.3,

Comment: RI=1516.3, 21.3471 min 8135A18 |RI:1516.3|

10 largest peaks:

176 999 | 128 503 | 73 499 | 61 100 | 147 100 | 178 79 | 219 50 | 250 43 | 56 42 | 63 15 |

12 m/z Values and Intensities (1 low intensity peak is not shown):

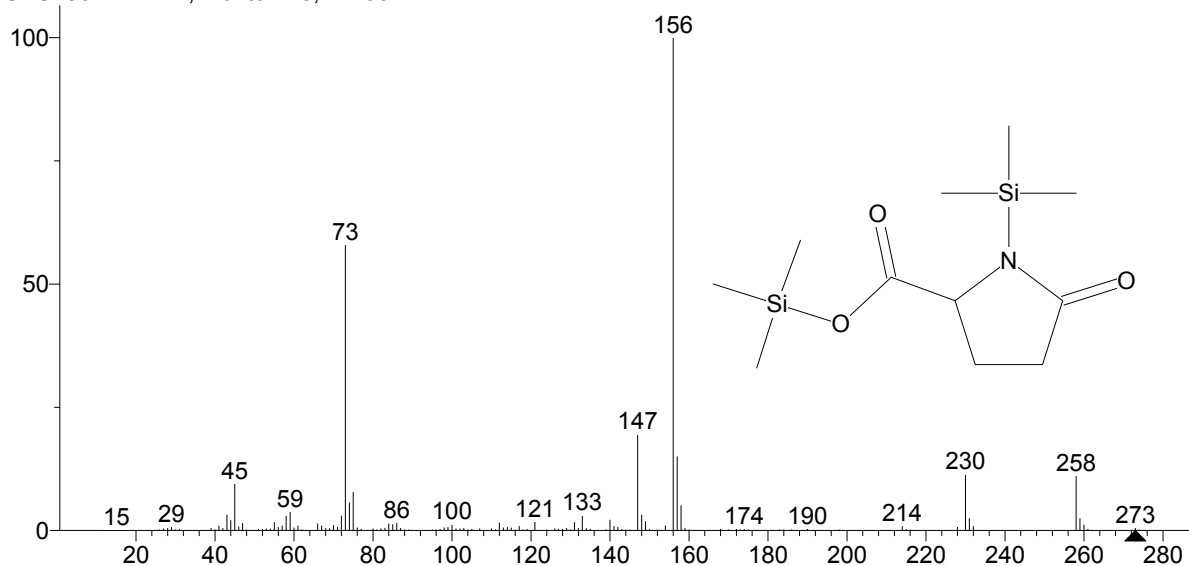
56 42 | 63 15 | 128 503 | 176 999 | 179 10 | 250 43 |
61 100 | 73 499 | 147 100 | 178 79 | 219 50 | 293 10 |

Synonyms:

1.METHIONINE-2T-TENT-[59-51-8];

Hit 55 : RH-T-1519.1-1.34%-OXOPROLINE 2T-CONF-[98-79-3]-RH03

CAS: 30274-77-2; Lib: tom18; ID: 55.



(tom18) RH-T-1519.1-1.34%-OXOPROLINE 2T-CONF-[98-79-3]-RH03

Name: RH-T-1519.1-1.34%-OXOPROLINE 2T-CONF-[98-79-3]-RH03

Formula: C₁₁H₂₃NO₃Si₂

MW: 273 CAS#: 30274-77-2 ID#: 55 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:1519.1|

10 largest peaks:

156 999 | 73 578 | 147 194 | 157 149 | 230 113 | 258 110 | 45 94 | 75 77 | 74 56 | 158 50 |

38 m/z Values and Intensities (89 low intensity peaks are not shown):

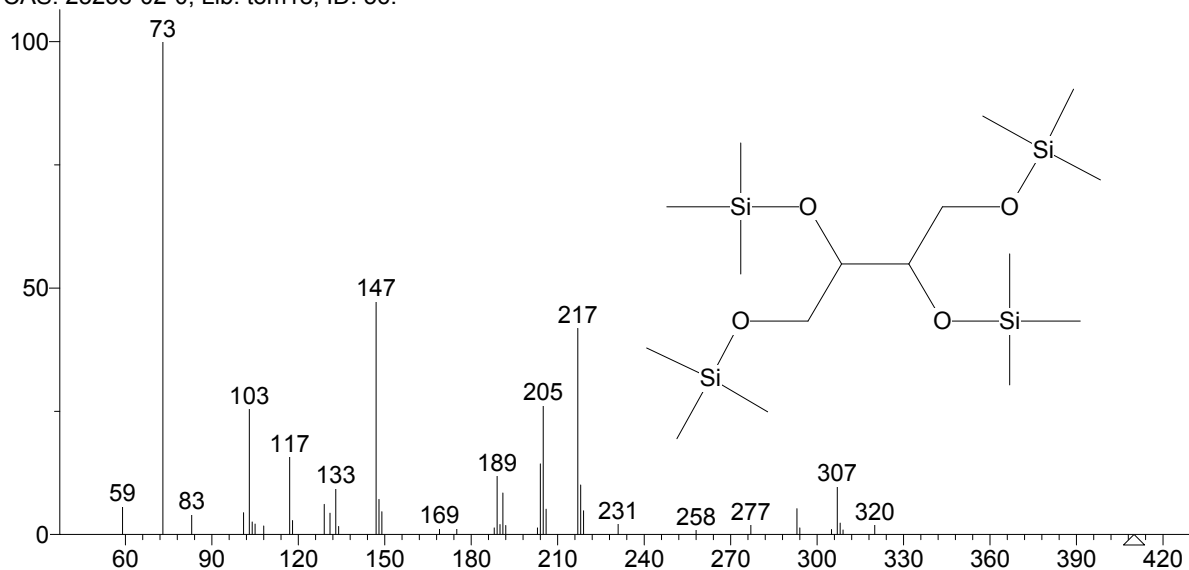
41 9	47 14	59 37	70 10	75 77	100 12	133 30	149 18	158 50	259 24
43 31	55 16	61 9	72 29	84 13	112 15	140 21	154 9	230 113	260 11
44 20	57 9	66 13	73 578	85 12	121 17	147 194	156 999	231 24	
45 94	58 29	67 9	74 56	86 15	131 16	148 31	157 149	258 110	

Synonyms:

1.OXOPROLINE 2T-CONF-[98-79-3];

Hit 56 : RH-T-1522.9-0.01%-ERYTHRITOL 3T-TENT-[149-32-6]-RH03

CAS: 25258-02-0; Lib: tom18; ID: 56.



(tom18) RH-T-1522.9-0.01%-ERYTHRITOL 3T-TENT-[149-32-6]-RH03

Name: RH-T-1522.9-0.01%-ERYTHRITOL 3T-TENT-[149-32-6]-RH03

Formula: C₁₆H₄₂O₄Si₄

MW: 410 CAS#: 25258-02-0 ID#: 56 DB: tom18

Other DBs: None

Comment: RI:MG00238 [RI:1522.9]

10 largest peaks:

73 999 | 147 472 | 217 418 | 205 261 | 103 254 | 117 157 | 204 143 | 189 118 | 218 100 | 307 97 |

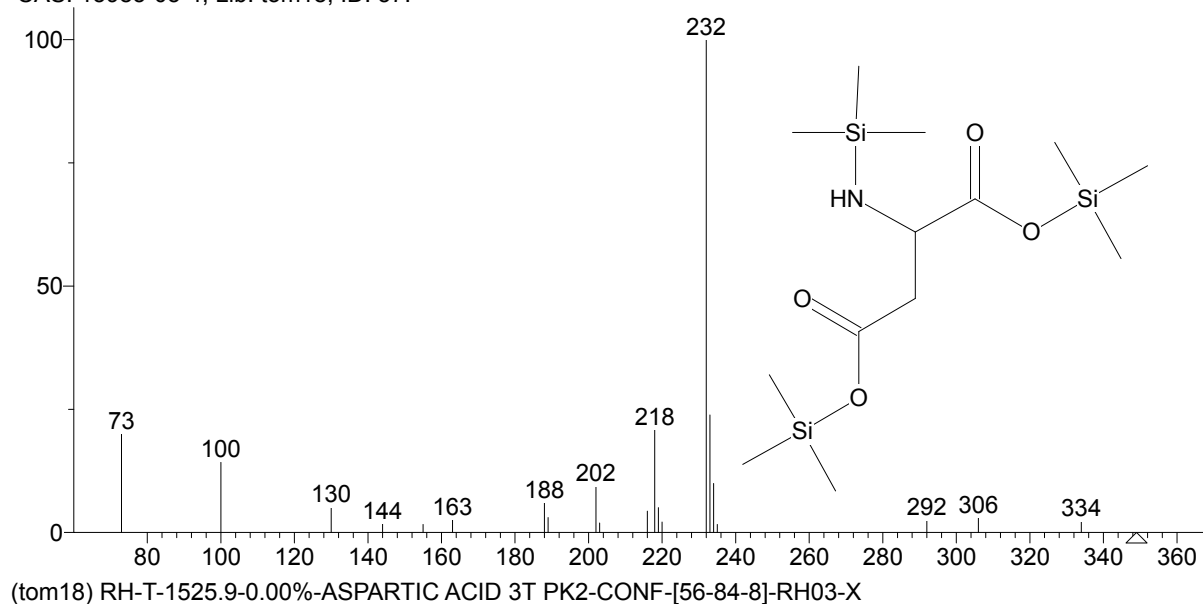
41 m/z Values and Intensities:

59	56	104	25	129	61	148	71	189	118	204	143	219	48	294	13	320	19
73	999	105	21	131	43	149	46	190	20	205	261	231	21	305	10		
83	40	108	17	133	93	169	12	191	84	206	51	258	9	307	97		
101	44	117	157	134	16	175	12	192	18	217	418	277	19	308	23		
103	254	118	28	147	472	188	13	203	13	218	100	293	52	309	9		

Synonyms:

1.ERYTHRITOL 3T-TENT-[149-32-6];

Hit 57 : RH-T-1525.9-0.00%-ASPARTIC ACID 3T PK2-CONF-[56-84-8]-RH03-X
CAS: 15985-05-4; Lib: tom18; ID: 57.



Name: RH-T-1525.9-0.00%-ASPARTIC ACID 3T PK2-CONF-[56-84-8]-RH03-X

Formula: C₁₃H₃₁NO₄Si₃

MW: 349 CAS#: 15985-05-4 ID#: 57 DB: tom18

Other DBs: None

Comment: RI:MG00238 [RI:1525.9]

10 largest peaks:

232 999 | 233 238 | 218 208 | 73 199 | 100 142 | 234 99 | 202 93 | 188 60 | 130 50 | 219 50 |

21 m/z Values and Intensities:

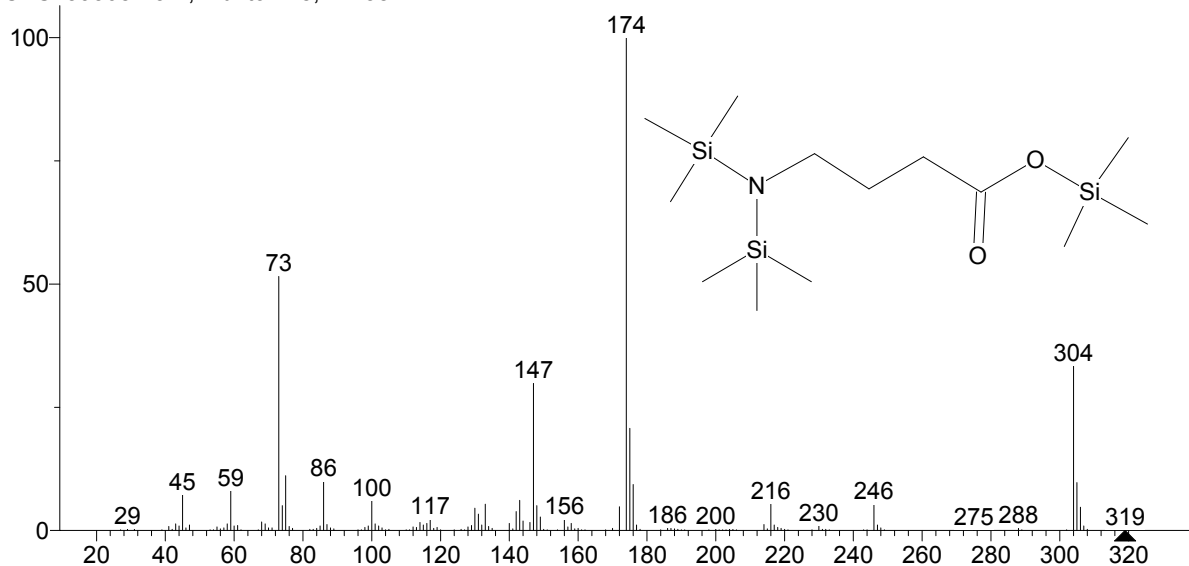
73 199 | 144 17 | 188 60 | 203 19 | 219 50 | 233 238 | 292 24 |
100 142 | 155 16 | 189 30 | 216 43 | 220 21 | 234 99 | 306 29 |
130 50 | 163 25 | 202 93 | 218 208 | 232 999 | 235 16 | 334 22 |

Synonyms:

1.ASPARTIC ACID 3T PK2-CONF-[56-84-8];

Hit 58 : RH-T-1528.1-1.68%-4-AMINOBTYRIC ACID 3T-CONF-[56-12-2]-RH02

CAS: 39508-23-1; Lib: tom18; ID: 58.



(tom18) RH-T-1528.1-1.68%-4-AMINOBTYRIC ACID 3T-CONF-[56-12-2]-RH02

Name: RH-T-1528.1-1.68%-4-AMINOBTYRIC ACID 3T-CONF-[56-12-2]-RH02

Formula: C₁₃H₃₃NO₂Si₃

MW: 319 CAS#: 39508-23-1 ID#: 58 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:1528.1|

10 largest peaks:

174 999 | 73 515 | 304 333 | 147 298 | 175 207 | 75 111 | 86 99 | 305 97 | 176 93 | 59 80 |

54 m/z Values and Intensities (88 low intensity peaks are not shown):

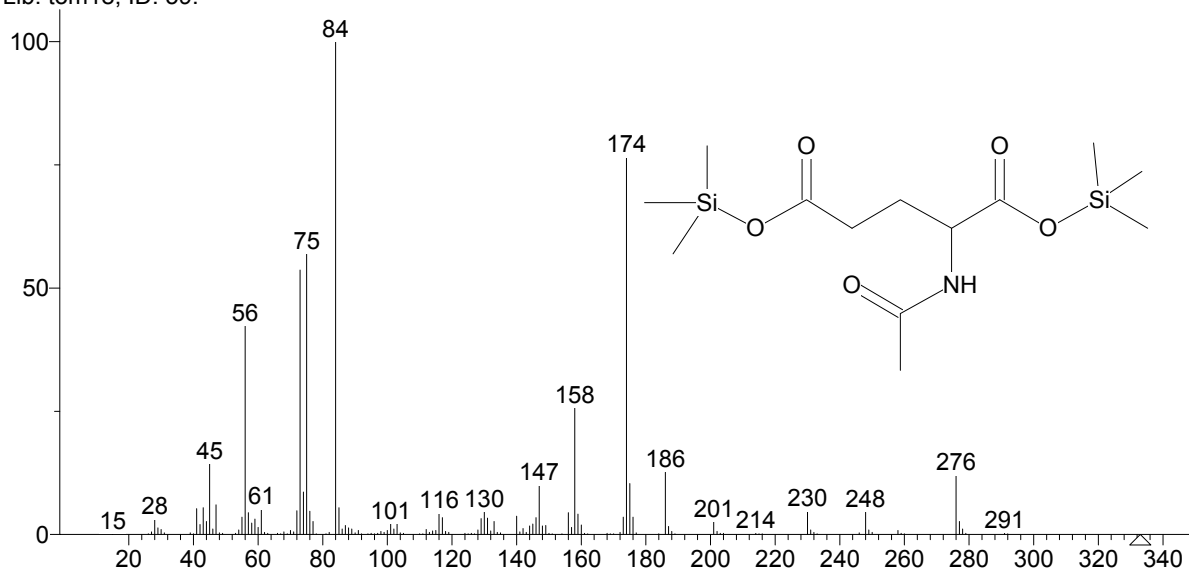
43	13	60	9	75	111	101	13	129	10	142	38	149	27	176	93	246	52
44	9	61	10	85	9	102	9	130	45	143	61	156	22	177	11	247	11
45	72	68	17	86	99	114	16	131	33	144	19	158	14	214	12	304	333
47	11	69	13	87	12	115	11	132	11	146	16	172	48	216	53	305	97
58	13	73	515	99	9	116	14	133	53	147	298	174	999	217	11	306	47
59	80	74	50	100	60	117	22	140	14	148	50	175	207	230	9	307	9

Synonyms:

1,4-AMINOBTYRIC ACID 3T-CONF-[56-12-2];

Hit 59 : RH-T-1531.0-1.34%-N-ACETYLGLUTAMIC ACID 2T-[1188-37-0]-TENT-RH01

Lib: tom18; ID: 59.



(tom18) RH-T-1531.0-1.34%-N-ACETYLGUTAMIC ACID 2T-[1188-37-0]-TENT-RH01 RI:1531.0,

Name: RH-T-1531.0-1.34%-N-ACETYLGUTAMIC ACID 2T-[1188-37-0]-TENT-RH01

Formula: C₁₃H₂₇NO₅Si₂

MW: 333 ID#: 59 DB: tom18

RI: 1531.0,

Comment: RI=1531.0, 22.9252 min AB2129 |RI:1531|

10 largest peaks:

84 999 | 174 764 | 75 568 | 73 536 | 56 422 | 158 256 | 45 143 | 186 126 | 276 119 | 175 103 |

68 m/z Values and Intensities (77 low intensity peaks are not shown):

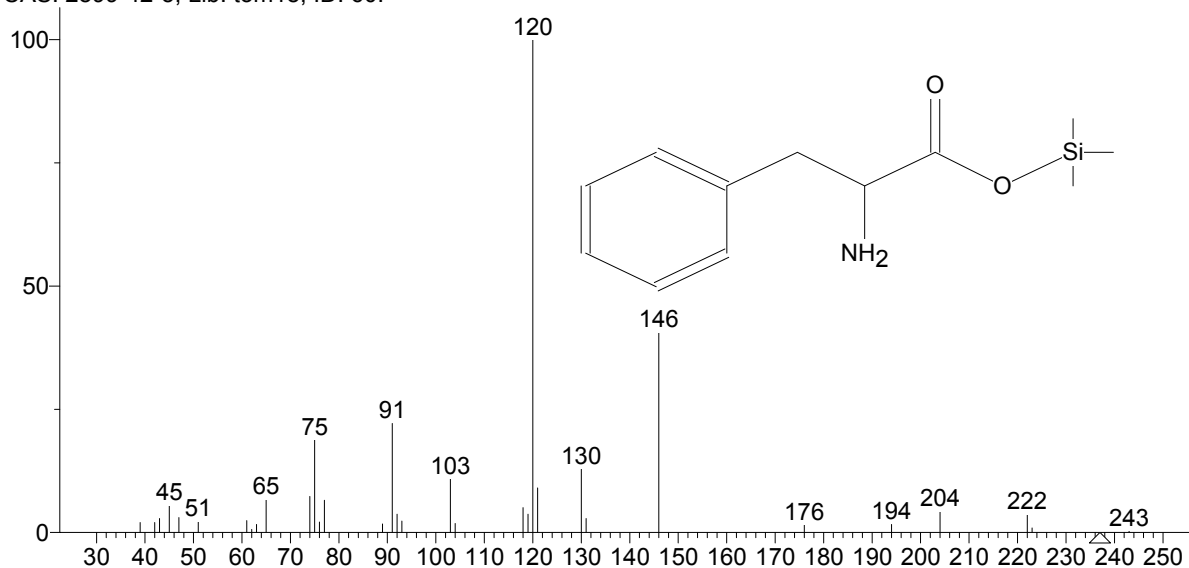
28 30	45 143	58 23	75 568	88 13	117 34	142 12	156 44	175 103	248 45
29 13	46 11	59 31	76 47	89 11	128 9	144 17	157 14	176 35	249 9
30 10	47 60	60 14	77 26	101 21	129 32	145 21	158 256	186 126	276 119
41 52	54 9	61 50	84 999	102 11	130 45	146 34	159 41	187 16	277 26
42 20	55 35	72 48	85 54	103 21	131 33	147 99	160 19	201 25	278 11
43 54	56 422	73 536	86 11	112 10	133 26	148 17	173 35	230 46	
44 26	57 44	74 86	87 18	116 42	140 37	149 18	174 764	231 9	

Synonyms:

1.N-ACETYLGUTAMIC ACID 2T-[1188-37-0]-TENT;

Hit 60 : RH-T-1539.9-0.03%-PHENYLALANINE 1T-CONF-[150-30-1]-RH03

CAS: 2899-42-5; Lib: tom18; ID: 60.



(tom18) RH-T-1539.9-0.03%-PHENYLALANINE 1T-CONF-[150-30-1]-RH03

Name: RH-T-1539.9-0.03%-PHENYLALANINE 1T-CONF-[150-30-1]-RH03

Formula: C₁₂H₁₉NO₂Si

MW: 237 CAS#: 2899-42-5 ID#: 60 DB: tom18

Other DBs: None

Comment: RI:MG00238 [RI:1539.9]

10 largest peaks:

120 999	146 405	91 221	75 187	130 128	103 108	121 90	74 73	65 66	77 65
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31 m/z Values and Intensities (2 low intensity peaks are not shown):

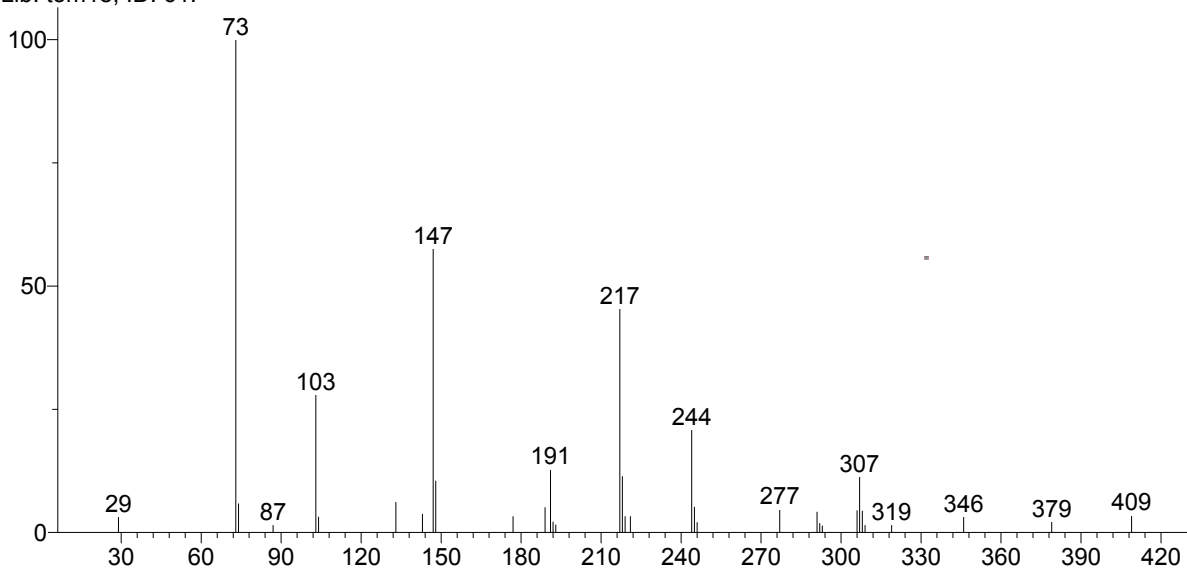
39 20	47 30	65 66	77 65	93 23	119 37	131 28	204 42
42 20	51 22	74 73	89 17	103 108	120 999	146 405	222 36
43 28	61 24	75 187	91 221	104 18	121 90	176 15	223 9
45 54	63 16	76 21	92 37	118 50	130 128	194 16	

Synonyms:

1.PHENYLALANINE 1T-CONF-[150-30-1];

Hit 61 : RH-T-1543.1-0.00%-[217,103,244G, :tms unkN.hp: TOMATO LEAF 005]-RH03

Lib: tom18; ID: 61.



(tom18) RH-T-1543.1-0.00%-[217,103,244G, :tms unkN.hp: TOMATO LEAF 005]-RH03 RI:1543.1,

Name: RH-T-1543.1-0.00%-[217,103,244G, :tms unkN.hp: TOMATO LEAF 005]-RH03

MW: N/A ID#: 61 DB: tom18

RI: 1543.1,

Comment: RI=1543.1, 26.2605 min MG00244 [RI:1543.1]

10 largest peaks:

73 999 | 147 575 | 217 453 | 103 278 | 244 207 | 191 127 | 218 113 | 307 112 | 148 104 | 133 61 |

34 m/z Values and Intensities:

29 31 | 103 278 | 147 575 | 191 127 | 218 113 | 245 51 | 292 18 | 308 43 | 379 21 |

73 999 | 104 31 | 148 104 | 192 21 | 219 32 | 246 20 | 293 13 | 309 14 | 409 34 |

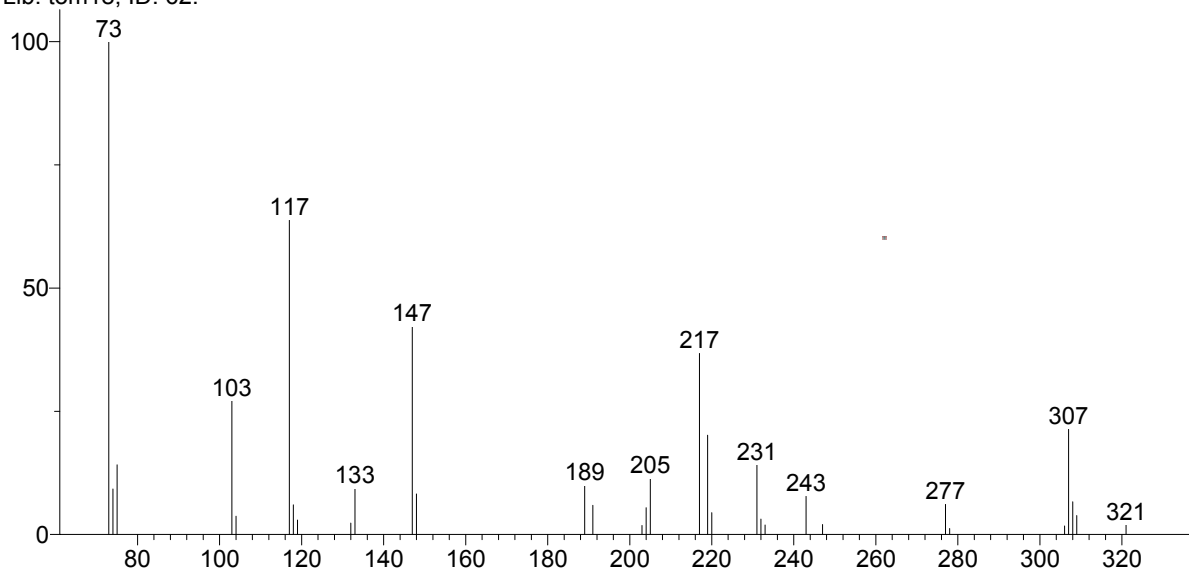
74 58 | 133 61 | 177 32 | 193 15 | 221 32 | 277 46 | 306 44 | 319 14 |

87 14 | 143 37 | 189 50 | 217 453 | 244 207 | 291 41 | 307 112 | 346 31 |

Synonyms:

1.m217,103,244G, :tms unkN.hp: TOMATO LEAF 005;

Hit 62 : RH-T-1550.1-0.00%-[117,217,307,103,231,N: sim. Pentitol, 1-desoxytetrakis-O-(trimethylsilyl)-]-RH03
Lib: tom18; ID: 62.



(tom18) RH-T-1550.1-0.00%-[117,217,307,103,231,N: sim. Pentitol, 1-desoxytetrakis-O-(trimethylsilyl)-]-RH03 RI:1550.1,

Name: RH-T-1550.1-0.00%-[117,217,307,103,231,N: sim. Pentitol, 1-desoxytetrakis-O-(trimethylsilyl)-]-RH03

MW: N/A ID#: 62 DB: tom18

RI: 1550.1,

Comment: RI=1550.1, 26.4673 min MG00244 [RI:1550.1]

10 largest peaks:

73 999 | 117 637 | 147 421 | 217 367 | 103 271 | 307 213 | 219 201 | 75 141 | 231 141 | 205 113 |

32 m/z Values and Intensities:

73 999	104 37	132 23	189 99	205 113	231 141	247 20	307 213
74 92	117 637	133 93	191 59	217 367	232 31	277 61	308 66
75 141	118 60	147 421	203 18	219 201	233 19	278 12	309 38
103 271	119 29	148 82	204 54	220 44	243 77	306 17	321 19

Synonyms:

1.m117,217,307,103,231, N:sim. Pentitol, 1-desoxytetrakis-O-(trimethylsilyl)-;

Hit 63 : RH-T-1554.9-0.10%-CYSTEINE 3T-CONF-[52-90-4]-8135A18-G
CAS: 56272-69-6; Lib: tom18; ID: 63.



(tom18) RH-T-1554.9-0.10%-CYSTEINE 3T-CONF-[52-90-4]-8135A18-G RI:1554.9,

Name: RH-T-1554.9-0.10%-CYSTEINE 3T-CONF-[52-90-4]-8135A18-G

Formula: C₁₂H₃₁NO₂SSi₃

MW: 337 CAS#: 56272-69-6 ID#: 63 DB: tom18

Other DBs: None

RI: 1554.9,

Comment: RI=1554.9, 22.0567 min 8135A18 |RI:1554.9|

10 largest peaks:

220 999 | 218 767 | 100 239 | 221 143 | 222 84 | 132 80 | 59 61 | 98 53 | 116 43 | 294 29 |

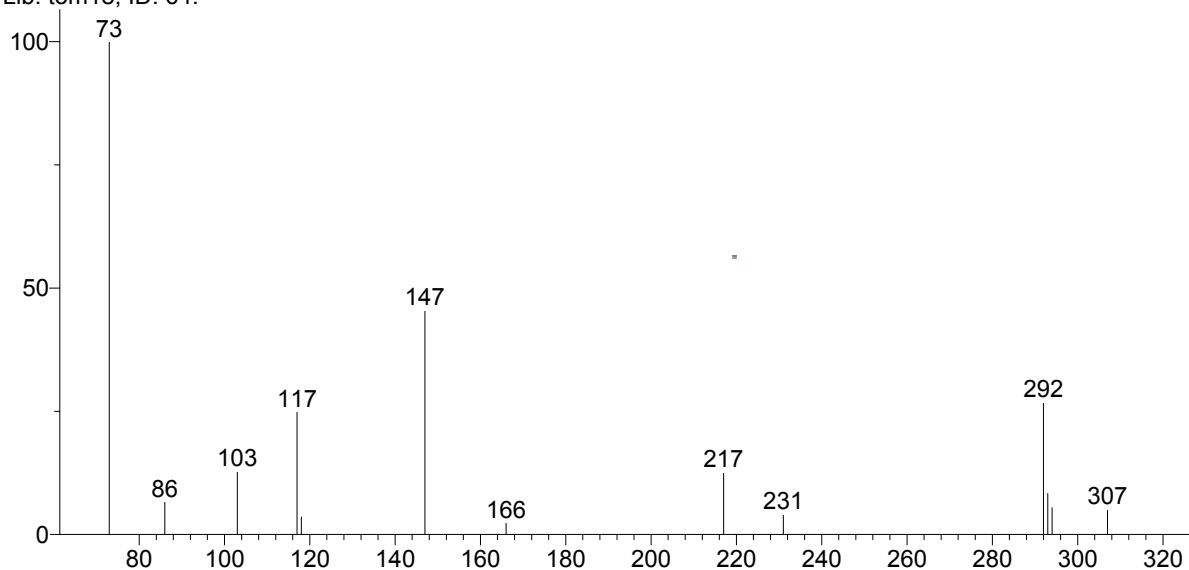
18 m/z Values and Intensities (5 low intensity peaks are not shown):

59 61 | 100 239 | 105 9 | 115 28 | 132 80 | 218 767 | 221 143 | 223 13 | 294 29 |
98 53 | 101 25 | 114 18 | 116 43 | 163 16 | 220 999 | 222 84 | 232 13 | 322 9 |

Synonyms:

1.CYSTEINE 3T-CONF-[52-90-4];

Hit 64 : RH-T-1555.7-0.00%-[292,217,117, G: sim. Threonic acid (4TMS)]-RH03-X
Lib: tom18; ID: 64.



(tom18) RH-T-1555.7-0.00%-[292,217,117, G: sim. Threonic acid (4TMS)]-RH03-X RI:1555.7,

Name: RH-T-1555.7-0.00%-[292,217,117, G: sim. Threonic acid (4TMS)]-RH03-X

MW: N/A ID#: 64 DB: tom18

RI: 1555.7,

Comment: RI=1555.7, 26.6364 min MG00244 [RI:1555.7]

10 largest peaks:

73 999 | 147 454 | 292 267 | 117 248 | 103 127 | 217 125 | 293 83 | 86 65 | 294 54 | 307 50 |

13 m/z Values and Intensities:

73 999 | 103 127 | 118 35 | 166 23 | 231 40 | 293 83 | 307 50 |

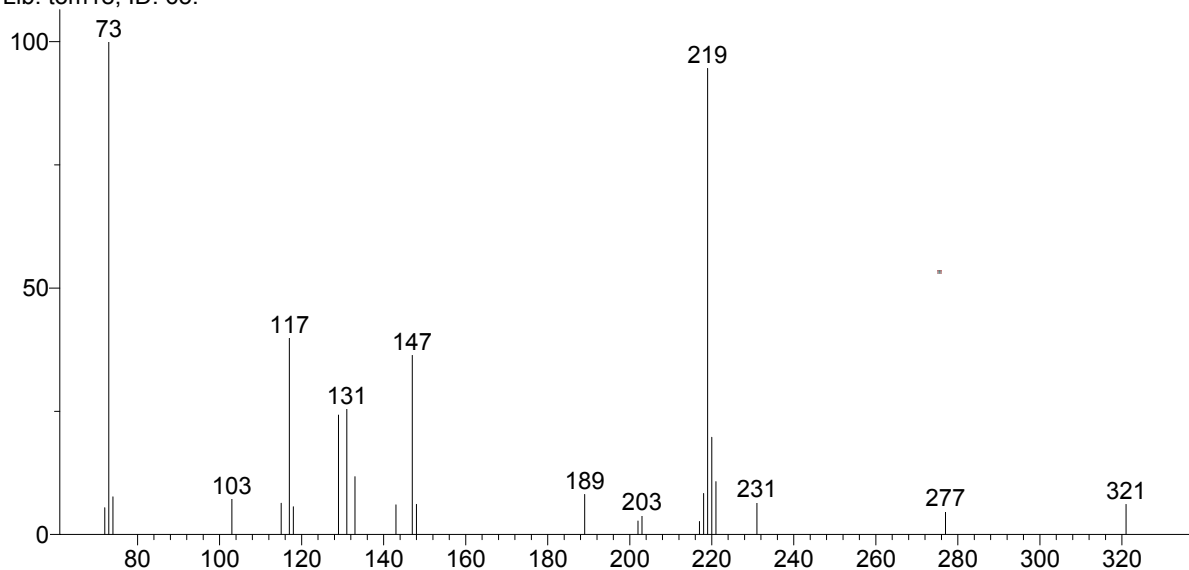
86 65 | 117 248 | 147 454 | 217 125 | 292 267 | 294 54 |

Synonyms:

1.m292,217,117, G: sim. Threonic acid (4TMS);

Hit 65 : RH-T-1563.4-0.01%-[219,117,131]-RH03

Lib: tom18; ID: 65.



(tom18) RH-T-1563.4-0.01%-[219,117,131]-RH03

Name: RH-T-1563.4-0.01%-[219,117,131]-RH03

MW: N/A ID#: 65 DB: tom18

Comment: RI:MG00238 |RI:1563.4|

10 largest peaks:

73 999 | 219 945 | 117 398 | 147 363 | 131 254 | 129 242 | 220 197 | 133 117 | 221 107 | 218 83 |

24 m/z Values and Intensities:

72 54 | 103 72 | 118 56 | 133 117 | 148 61 | 203 38 | 219 945 | 231 64 |

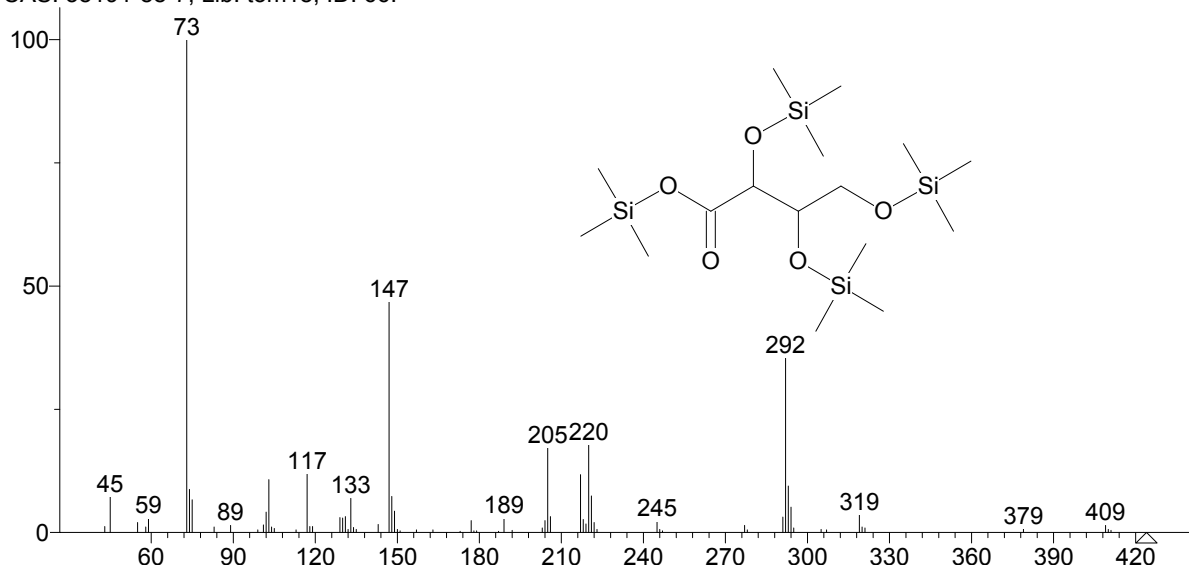
73 999 | 115 63 | 129 242 | 143 60 | 189 81 | 217 26 | 220 197 | 277 46 |

74 76 | 117 398 | 131 254 | 147 363 | 202 27 | 218 83 | 221 107 | 321 61 |

Synonyms:

1.m219,117,131;

Hit 66 : RH-T-1572.4-0.06%-2,3,4-TRIHYDROXYBUTYRIC ACID 4T-CONF-[7306-96-9]-RH03
CAS: 38191-88-7; Lib: tom18; ID: 66.



(tom18) RH-T-1572.4-0.06%-2,3,4-TRIHYDROXYBUTYRIC ACID 4T-CONF-[7306-96-9]-RH03

Name: RH-T-1572.4-0.06%-2,3,4-TRIHYDROXYBUTYRIC ACID 4T-CONF-[7306-96-9]-RH03

Formula: C₁₆H₄₀O₅Si₄

MW: 424 CAS#: 38191-88-7 ID#: 66 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:1572.4|

10 largest peaks:

73 999 | 147 467 | 292 353 | 220 177 | 205 171 | 117 118 | 217 117 | 103 107 | 293 94 | 74 87 |

49 m/z Values and Intensities (23 low intensity peaks are not shown):

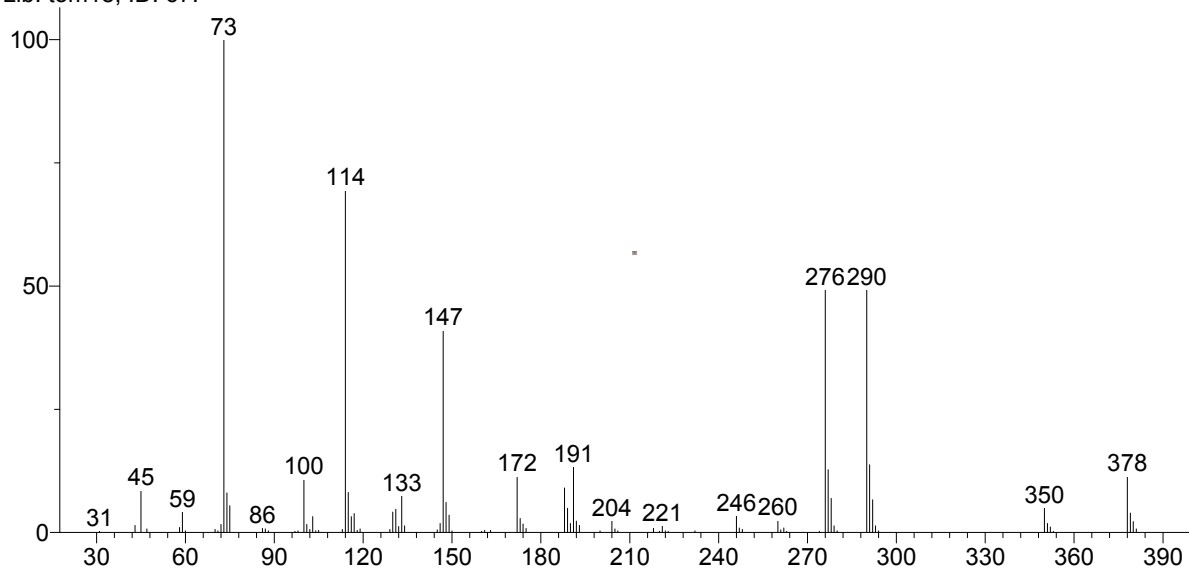
43	12	73	999	101	15	118	12	133	69	149	43	205	171	220	177	291	31	319	35
45	72	74	87	102	41	119	12	134	10	177	24	206	32	221	74	292	353	320	11
55	20	75	66	103	107	129	30	143	16	189	28	217	117	222	20	293	94	321	9
58	11	83	11	104	11	130	29	147	467	203	9	218	26	245	22	294	51	409	14
59	28	89	14	117	118	131	32	148	73	204	24	219	17	277	14	295	9		

Synonyms:

1,2,3,4-TRIHYDROXYBUTYRIC ACID 4T-CONF-[7306-96-9]; 2,3,4-THREONIC ACID 3T;

Hit 67 : RH-T-1577.8-0.03%-[114,290,276,378]-RH03

Lib: tom18; ID: 67.



(tom18) RH-T-1577.8-0.03%-[114,290,276,378]-RH03 RI:1577.8,

Name: RH-T-1577.8-0.03%-[114,290,276,378]-RH03

MW: N/A ID#: 67 DB: tom18

RI: 1577.8,

Comment: RI=1577.8, 27.2962 min MG00244 [RI:1577.8]

10 largest peaks:

73 999 | 114 693 | 276 492 | 290 491 | 147 409 | 291 137 | 191 133 | 277 127 | 172 113 | 378 113 |

53 m/z Values and Intensities (39 low intensity peaks are not shown):

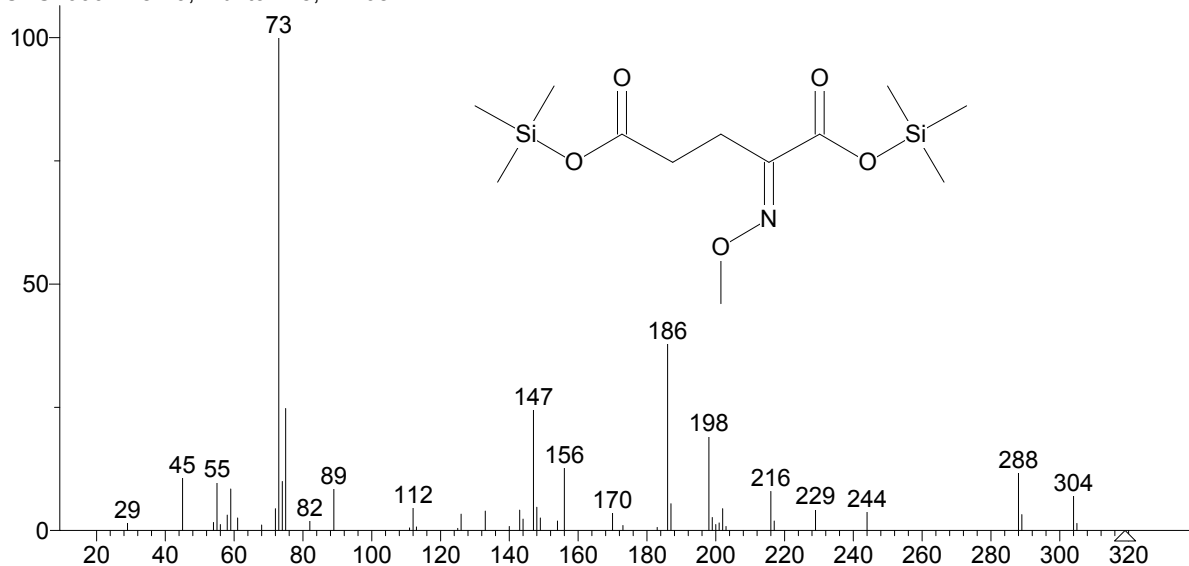
43 14	74 80	115 81	133 74	172 113	191 133	247 9	279 13	351 18
45 85	75 54	116 32	134 13	173 28	192 23	260 24	290 491	352 11
58 10	100 107	117 38	146 18	174 17	193 14	262 9	291 137	378 113
59 41	101 16	130 41	147 409	188 90	204 23	276 492	292 66	379 39
72 16	103 32	131 47	148 61	189 49	221 13	277 127	293 13	380 22
73 999	114 693	132 12	149 35	190 18	246 33	278 69	350 49	

Synonyms:

1.m114,290,276,378;

Hit 68 : RH-T-1580.6-0.00%-2-OXOGLUTARIC ACID M2T-CONF-[328-50-7]-RH03

CAS: 60022-87-9; Lib: tom18; ID: 68.



(tom18) RH-T-1580.6-0.00%-2-OXOGLUTARIC ACID M2T-CONF-[328-50-7]-RH03 RI:1580.6,

Name: RH-T-1580.6-0.00%-2-OXOGLUTARIC ACID M2T-CONF-[328-50-7]-RH03

Formula: C₁₂H₂₅NO₅Si₂

MW: 319 CAS#: 60022-87-9 ID#: 68 DB: tom18

Other DBs: None

RI: 1580.6,

Comment: RI=1580.6, 27.3803 min MG00244 [RI:1580.6]

10 largest peaks:

73 999 | 186 378 | 75 247 | 147 244 | 198 190 | 156 126 | 288 116 | 45 106 | 74 99 | 55 97 |

42 m/z Values and Intensities (6 low intensity peaks are not shown):

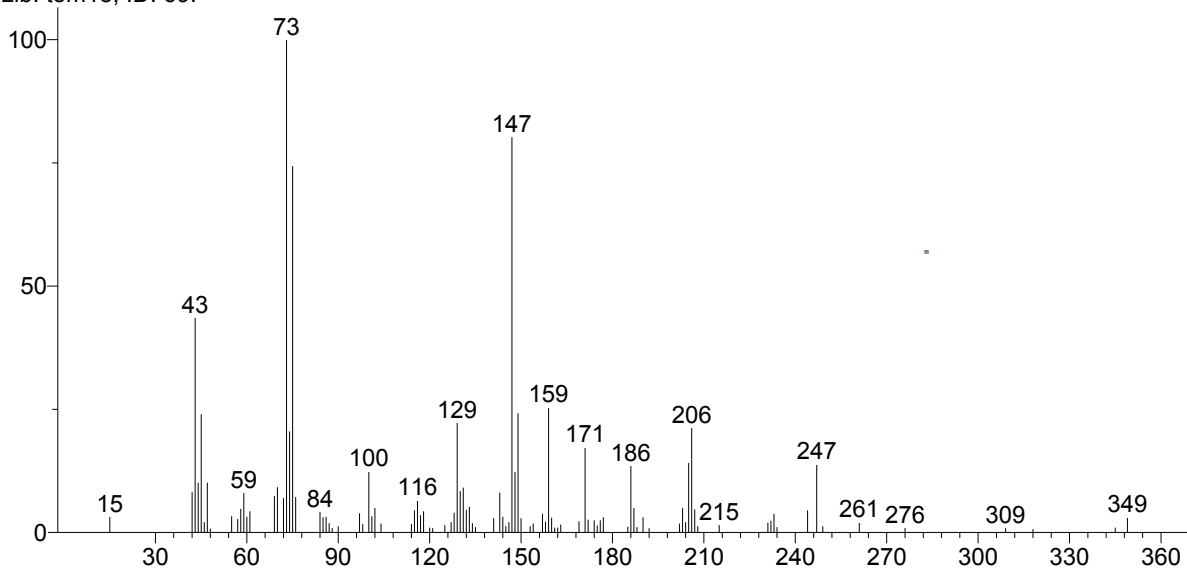
29 15	58 31	73 999	112 45	147 244	170 35	199 26	217 19	304 70
45 106	59 84	74 99	126 33	148 47	173 10	200 12	229 42	305 14
54 16	61 25	75 247	133 39	149 25	186 378	201 15	244 37	
55 97	68 11	82 19	143 41	154 19	187 54	202 44	288 116	
56 12	72 44	89 84	144 23	156 126	198 190	216 79	289 32	

Synonyms:

1,2-OXOGLUTARIC ACID M2T-CONF-[328-50-7];

Hit 69 : RH-T-1583.8-0.02%-[206,159,129, N: sim...-L-Asparagine, N2-TMS-, TMS ester]-RH03

Lib: tom18; ID: 69.



(tom18) RH-T-1583.8-0.02%-[206,159,129, N: sim...-L-Asparagine, N2-TMS-, TMS ester]-RH03 RI:1583.8,

Name: RH-T-1583.8-0.02%-[206,159,129, N: sim...-L-Asparagine, N2-TMS-, TMS ester]-RH03

MW: N/A ID#: 69 DB: tom18

RI: 1583.8,

Comment: RI=1583.8, 27.4765 min MG00238 [RI:1583.8]

10 largest peaks:

73 999 | 147 801 | 75 742 | 43 435 | 159 253 | 149 241 | 45 239 | 129 222 | 206 211 | 74 204 |

96 m/z Values and Intensities (6 low intensity peaks are not shown):

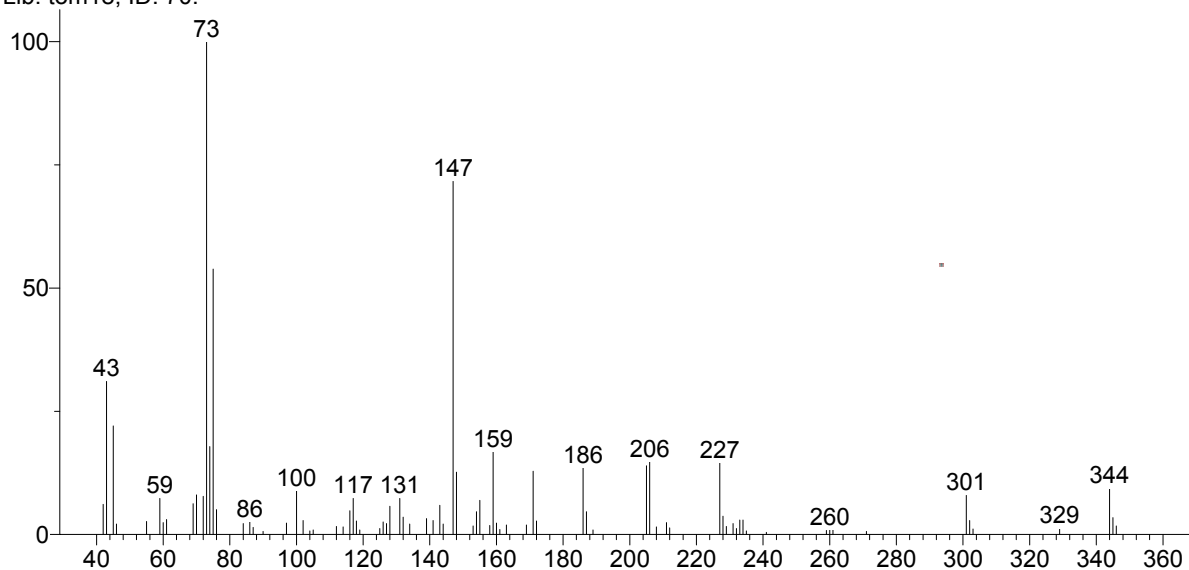
15 31	59 79	84 41	104 17	129 222	145 12	159 253	176 24	205 140	247 137
42 81	60 31	85 30	114 16	130 83	146 20	160 29	177 30	206 211	249 12
43 435	61 42	86 31	115 44	131 90	147 801	161 9	185 11	207 46	261 20
44 100	69 73	87 18	116 64	132 45	148 122	162 9	186 134	208 12	276 9
45 239	70 91	90 12	117 34	133 51	149 241	163 15	187 49	215 14	345 9
46 20	72 69	97 38	118 42	134 18	150 28	169 22	188 10	231 19	349 30
47 100	73 999	98 16	120 9	135 10	153 12	171 172	190 30	232 23	
55 32	74 204	100 123	125 14	141 28	154 17	172 25	202 17	233 37	
57 26	75 742	101 32	127 20	143 80	157 37	174 24	203 49	234 10	
58 47	76 71	102 49	128 39	144 31	158 21	175 13	204 20	244 44	

Synonyms:

1.m206,159,129, N: sim...-L-Asparagine, N2-TMS-, TMS ester;

Hit 70 : RH-T-1584.4-0.01%-[344,301,227,206,186,159, G: sim. Glutamine 4T]-RH03

Lib: tom18; ID: 70.



(tom18) RH-T-1584.4-0.01%-[344,301,227,206,186,159, G: sim. Glutamine 4T]-RH03 RI:1584.4,

Name: RH-T-1584.4-0.01%-[344,301,227,206,186,159, G: sim. Glutamine 4T]-RH03

MW: N/A ID#: 70 DB: tom18

RI: 1584.4,

Comment: RI=1584.4, 27.4924 min MG00244 [RI:1584.4]

10 largest peaks:

73 999 | 147 716 | 75 538 | 43 310 | 45 220 | 74 178 | 159 167 | 206 147 | 227 145 | 205 139 |

76 m/z Values and Intensities (6 low intensity peaks are not shown):

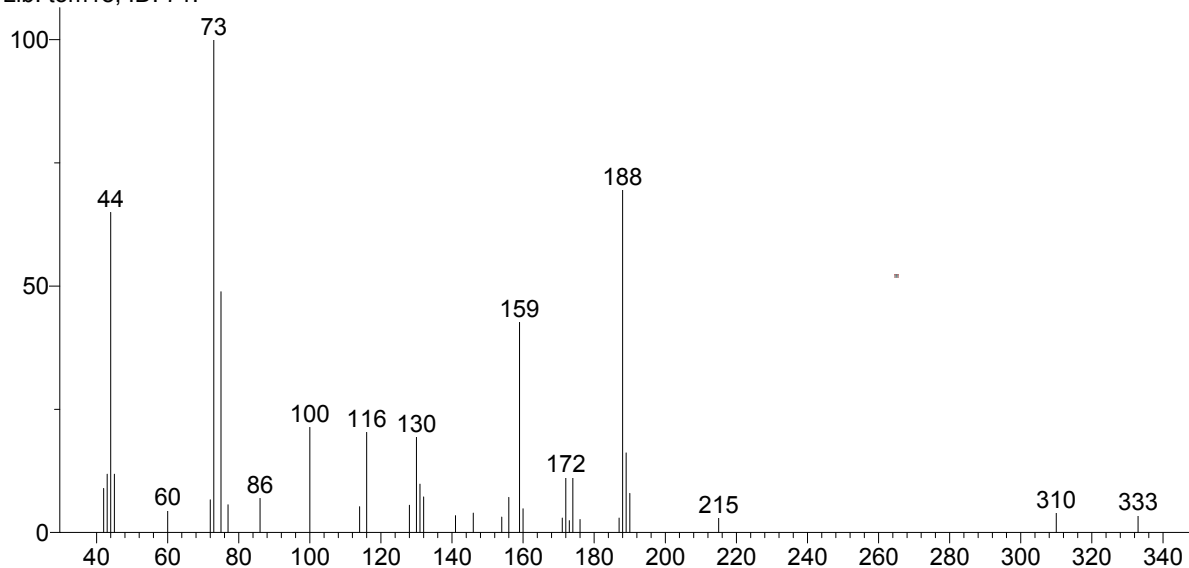
42 61	69 62	86 25	116 48	131 73	148 126	163 19	206 147	232 12	329 12
43 310	70 80	87 14	117 73	132 35	153 17	169 19	208 15	233 29	344 93
45 220	72 77	97 23	118 27	134 21	154 46	171 128	211 24	234 29	345 34
46 21	73 999	100 88	119 9	139 32	155 69	172 27	212 13	260 9	346 17
55 26	74 178	102 28	125 12	141 28	158 18	186 135	227 145	261 9	
59 73	75 538	105 9	126 25	143 59	159 167	187 46	228 37	301 79	
60 24	76 50	112 16	127 22	144 21	160 23	189 9	229 16	302 28	
61 30	84 22	114 15	128 57	147 716	161 10	205 139	231 22	303 11	

Synonyms:

1.m344,301,227,206,186,159, G: sim. Glutamine 4T;

Hit 71 : RH-T-1595.8-0.00%-[188,159,130,100, N: sim. propionylglycine T]-RH03

Lib: tom18; ID: 71.



(tom18) RH-T-1595.8-0.00%-[188,159,130,100, N: sim. propionylglycine T]-RH03 RI:1595.8,

Name: RH-T-1595.8-0.00%-[188,159,130,100, N: sim. propionylglycine T]-RH03

MW: N/A ID#: 71 DB: tom18

RI: 1595.8,

Comment: RI=1595.8, 27.8333 min MG00244 [RI:1595.8]

10 largest peaks:

73 999 | 188 694 | 44 649 | 75 488 | 159 426 | 100 213 | 116 203 | 130 193 | 189 161 | 43 118 |

35 m/z Values and Intensities:

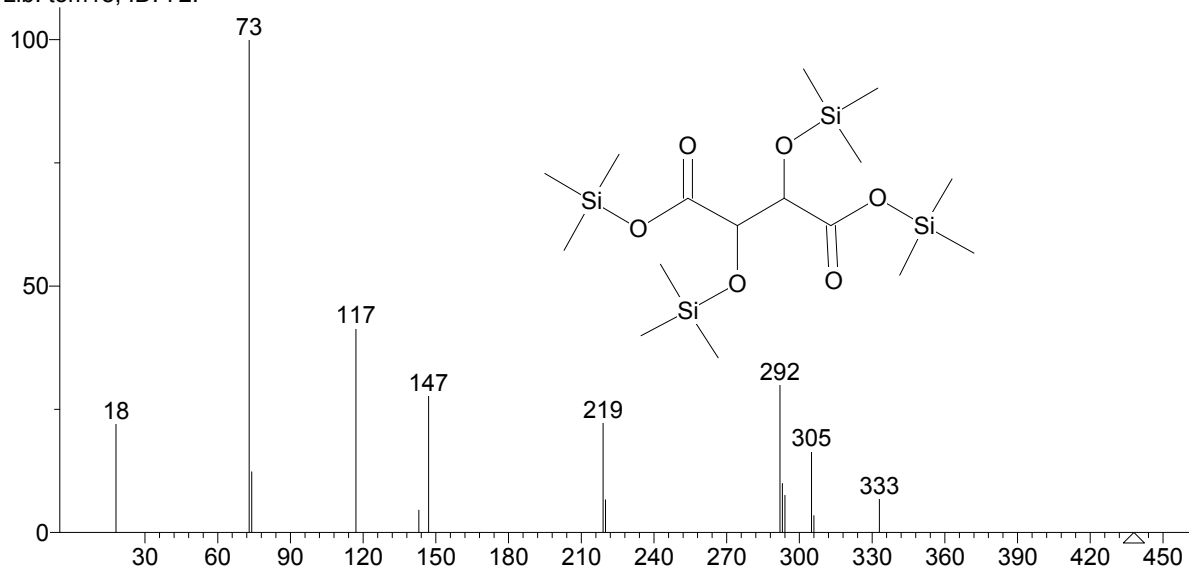
42 89 | 60 44 | 77 56 | 116 203 | 132 72 | 156 71 | 172 111 | 187 29 | 215 29 |
43 118 | 72 66 | 86 69 | 128 55 | 141 34 | 159 426 | 173 24 | 188 694 | 310 39 |
44 649 | 73 999 | 100 213 | 130 193 | 146 39 | 160 48 | 174 111 | 189 161 | 333 34 |
45 118 | 75 488 | 114 52 | 131 98 | 154 31 | 171 29 | 176 26 | 190 79 |

Synonyms:

1.m188,159,130,100, N: sim. propionylglycine T;

Hit 72 : RH-T-1607.2-0.00%-TARTARIC ACID 4T-CONF-[133-37-9]-RH03-X

Lib: tom18; ID: 72.



(tom18) RH-T-1607.2-0.00%-TARTARIC ACID 4T-CONF-[133-37-9]-RH03-X

Name: RH-T-1607.2-0.00%-TARTARIC ACID 4T-CONF-[133-37-9]-RH03-X

Formula: C₁₆H₃₈O₆Si₄

MW: 438 ID#: 72 DB: tom18

Comment: RI:MG00246 [RI:1607.2]

10 largest peaks:

73 999 | 117 413 | 292 299 | 147 276 | 219 222 | 18 220 | 305 164 | 74 123 | 293 99 | 294 75 |

14 m/z Values and Intensities:

18 220 | 74 123 | 143 45 | 219 222 | 292 299 | 294 75 | 306 34 |

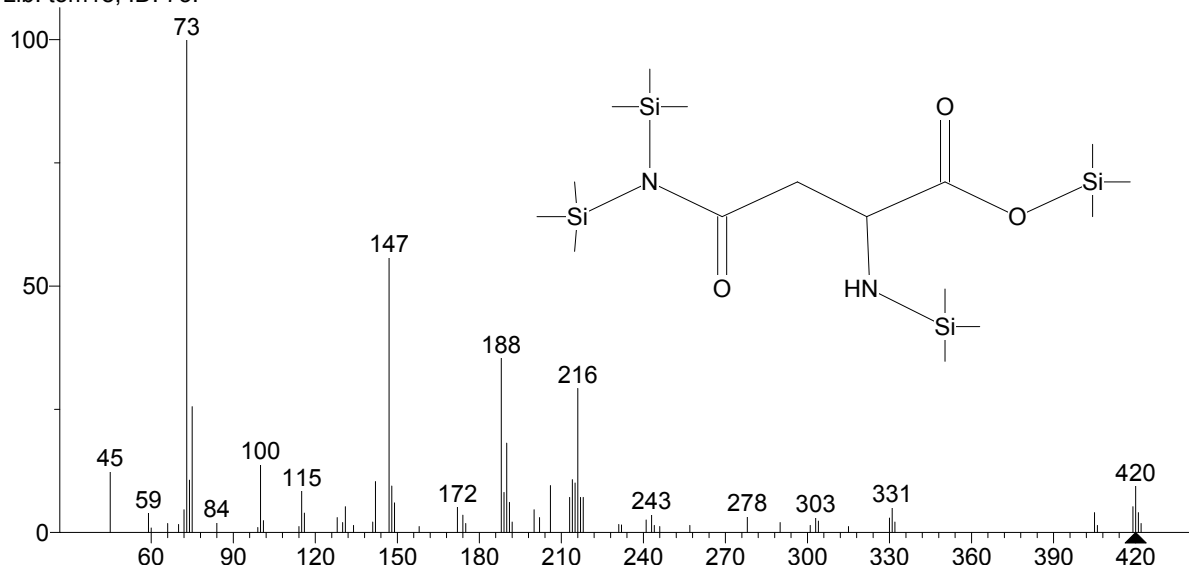
73 999 | 117 413 | 147 276 | 220 66 | 293 99 | 305 164 | 333 68 |

Synonyms:

no synonyms.

Hit 73 : RH-T-1610.5-0.04%-ASPARAGINE 4T-CONF-[70-47-3]-RH03

Lib: tom18; ID: 73.



(tom18) RH-T-1610.5-0.04%-ASPARAGINE 4T-CONF-[70-47-3]-RH03 RI:1610.5,

Name: RH-T-1610.5-0.04%-ASPARAGINE 4T-CONF-[70-47-3]-RH03

Formula: C₁₆H₄₀N₂O₃Si₄

MW: 420 ID#: 73 DB: tom18

RI: 1610.5,

Comment: RI=1610.5, 28.2555 min MG00243 |RI:1610.5|

10 largest peaks:

73 999 | 147 557 | 188 354 | 216 292 | 75 255 | 190 181 | 100 137 | 45 123 | 214 107 | 74 106 |

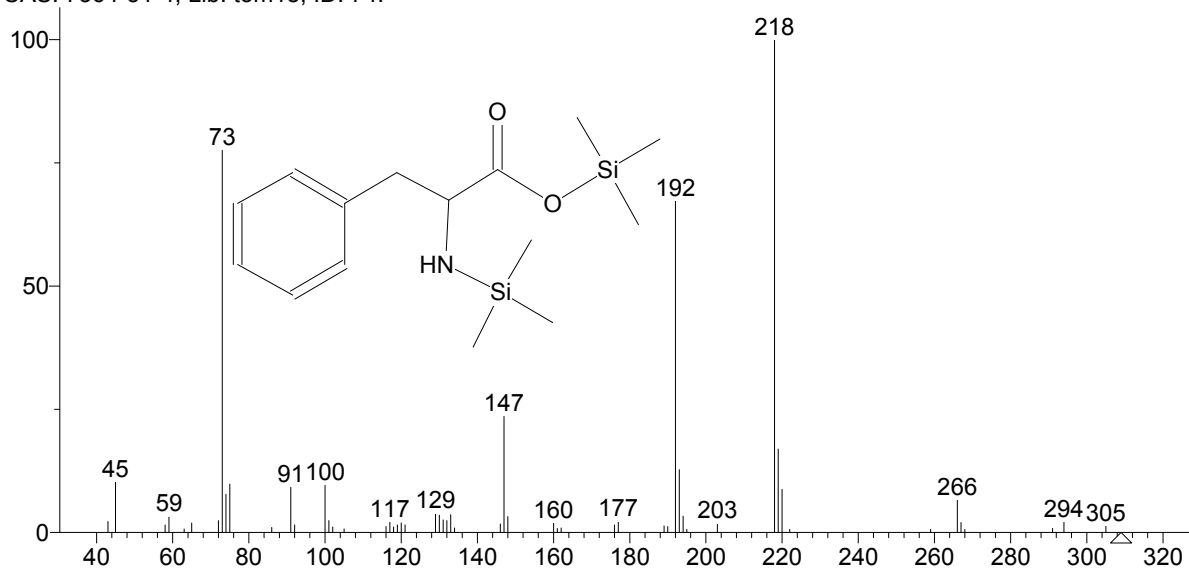
65 m/z Values and Intensities:

45 123	74 106	115 84	142 103	175 18	202 30	218 71	257 14	330 29	421 40
59 39	75 255	116 39	147 557	188 354	206 95	231 16	278 32	331 50	422 18
60 9	84 20	128 30	148 94	189 81	213 71	232 15	290 20	332 21	
66 18	99 10	130 20	149 60	190 181	214 107	241 25	301 14	405 40	
70 16	100 137	131 52	158 12	191 61	215 100	243 36	303 30	406 14	
72 46	101 24	134 14	172 51	192 21	216 292	244 14	304 23	419 52	
73 999	114 12	141 21	174 35	200 46	217 71	246 12	315 12	420 94	

Synonyms:

1.ASPARAGINE 4T-CONF-[70-47-3];

Hit 74 : RH-T-1621.6-0.01%-PHENYLALANINE 2T-CONF-[150-30-1]-RH03
CAS: 7364-51-4; Lib: tom18; ID: 74.



(tom18) RH-T-1621.6-0.01%-PHENYLALANINE 2T-CONF-[150-30-1]-RH03 RI:1621.6,

Name: RH-T-1621.6-0.01%-PHENYLALANINE 2T-CONF-[150-30-1]-RH03

Formula: C₁₅H₂₇NO₂Si₂

MW: 309 CAS#: 7364-51-4 ID#: 74 DB: tom18

Other DBs: None

RI: 1621.6,

Comment: RI=1621.6, 28.5702 min MG00244 |RI:1621.6|

10 largest peaks:

218 999 | 73 775 | 192 672 | 147 235 | 219 169 | 193 127 | 45 102 | 75 98 | 100 96 | 91 92 |

47 m/z Values and Intensities (8 low intensity peaks are not shown):

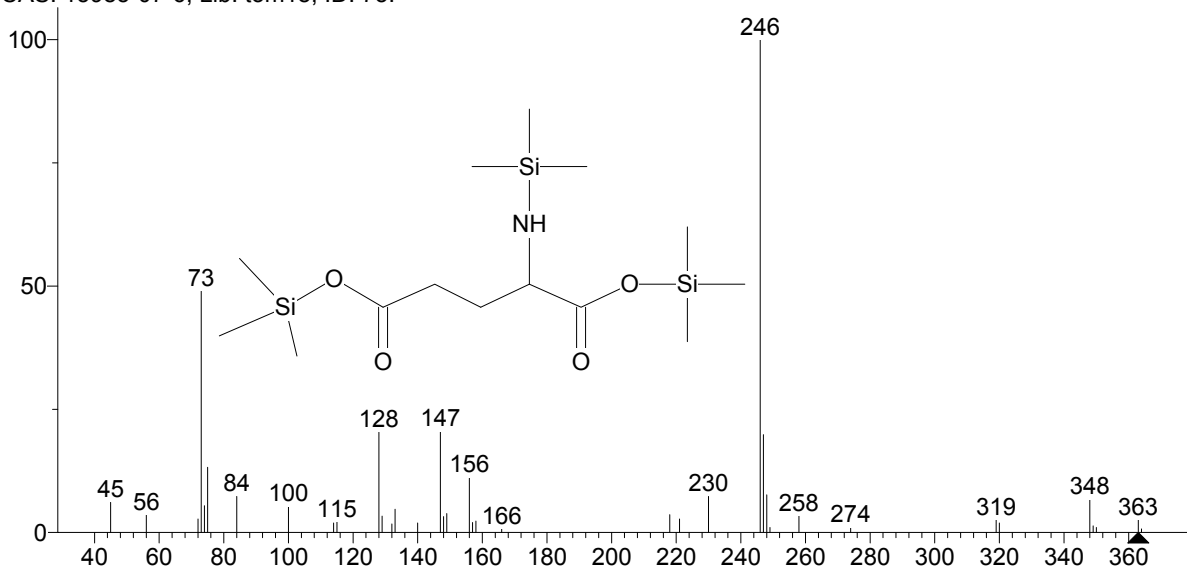
43 22	72 24	91 92	116 12	121 15	133 36	160 19	190 12	218 999	294 21
45 102	73 775	92 15	117 21	129 38	134 9	162 9	192 672	219 169	305 13
58 15	74 77	100 96	118 11	130 35	146 17	176 15	193 127	220 87	
59 32	75 98	101 24	119 15	131 25	147 235	177 22	194 33	266 65	
65 19	86 10	102 11	120 19	132 24	148 32	189 13	203 18	267 20	

Synonyms:

1.PHENYLALANINE 2T-CONF-[150-30-1];

Hit 75 : RH-T-1625.9-0.00%-GLUTAMIC ACID 3T-CONF-[56-86-0]-RH03

CAS: 15985-07-6; Lib: tom18; ID: 75.



(tom18) RH-T-1625.9-0.00%-GLUTAMIC ACID 3T-CONF-[56-86-0]-RH03 RI:1625.9,

Name: RH-T-1625.9-0.00%-GLUTAMIC ACID 3T-CONF-[56-86-0]-RH03

Formula: C₁₄H₃₃NO₄Si₃

MW: 363 CAS#: 15985-07-6 ID#: 75 DB: tom18

Other DBs: None

RI: 1625.9,

Comment: RI=1625.9, 28.6919 min MG00244 [RI:1625.9]

10 largest peaks:

246 999 | 73 489 | 147 204 | 128 203 | 247 198 | 75 132 | 156 111 | 248 76 | 84 73 | 230 73 |

36 m/z Values and Intensities (2 low intensity peaks are not shown):

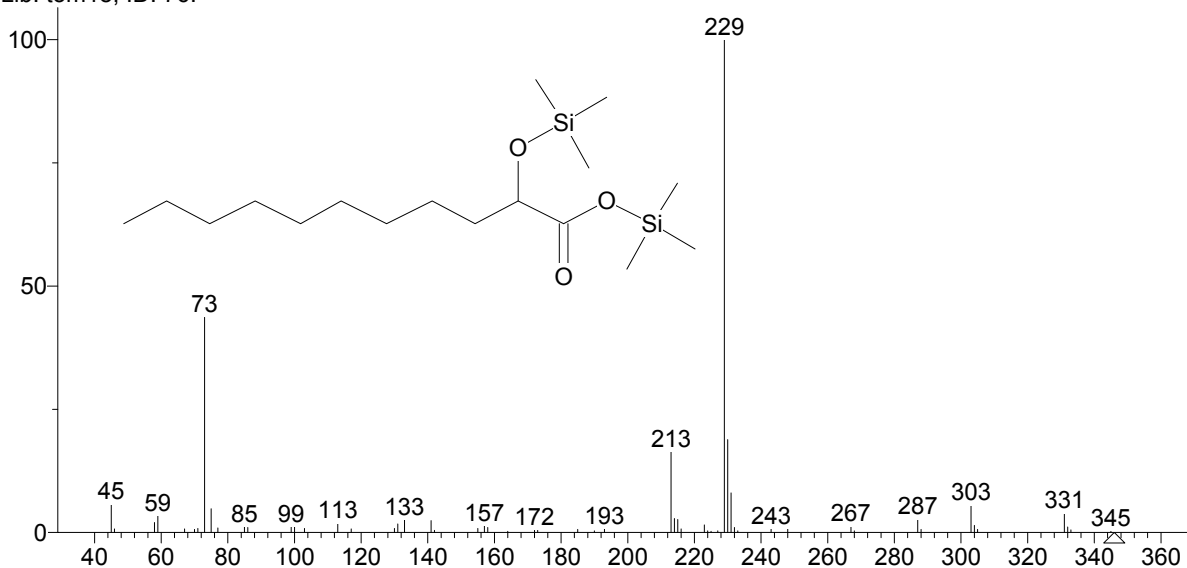
45 61	74 54	114 19	132 17	148 32	158 23	246 999	258 33	348 66
56 35	75 132	115 21	133 47	149 38	218 36	247 198	274 10	349 13
72 27	84 73	128 203	140 19	156 111	221 27	248 76	319 25	350 10
73 489	100 52	129 33	147 204	157 20	230 73	249 10	320 19	363 25

Synonyms:

1.GLUTAMIC ACID 3T-CONF-[56-86-0];

Hit 76 : RH-T-1635.8-0.00%-[N:2-Hydroxyundecanoic acid 2T-TENT]-8135A18-G-X

Lib: tom18; ID: 76.



(tom18) RH-T-1635.8-0.00%-[N:2-Hydroxyundecanoic acid 2T-TENT]-8135A18-G-X RI:1635.8,

Name: RH-T-1635.8-0.00%-[N:2-Hydroxyundecanoic acid 2T-TENT]-8135A18-G-X

Formula: C₁₇H₃₈O₃Si₂

MW: 346 ID#: 76 DB: tom18

RI: 1635.8,

Comment: RI=1635.8, 23.5434 min 8135A18 [RI:1635.8]

10 largest peaks:

229	999	73	436	230	188	213	163	231	80	45	56	303	54	75	48	331	38	59	33
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30 m/z Values and Intensities (27 low intensity peaks are not shown):

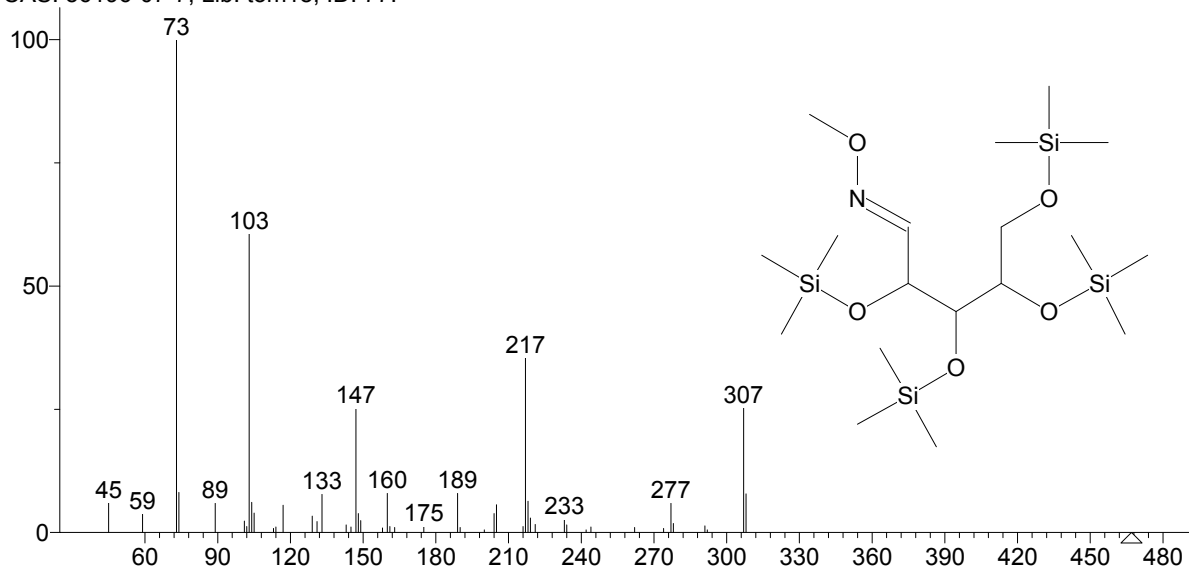
45	56	73	436	85	11	100	11	133	25	158	10	215	26	230	188	267	12	304	14
58	20	75	48	86	10	113	18	141	24	213	163	223	15	231	80	287	26	331	38
59	33	77	9	99	11	131	17	157	13	214	28	229	999	232	10	303	54	332	11

Synonyms:

1.2-Hydroxyundecanoic acid 2T-TENT;

Hit 77 : RH-T-1655.7-0.00%-XYLOSE M4T-TENT-[58-86-6]-RH03

CAS: 56196-07-7; Lib: tom18; ID: 77.



(tom18) RH-T-1655.7-0.00%-XYLOSE M4T-TENT-[58-86-6]-RH03

Name: RH-T-1655.7-0.00%-XYLOSE M4T-TENT-[58-86-6]-RH03

Formula: C₁₈H₄₅NO₅Si₄

MW: 467 CAS#: 56196-07-7 ID#: 77 DB: tom18

Other DBs: None

Comment: RI:MG00246 [RI:1655.7]

10 largest peaks:

73 999 | 103 605 | 217 354 | 307 252 | 147 251 | 74 81 | 160 79 | 189 79 | 308 78 | 133 77 |

43 m/z Values and Intensities (5 low intensity peaks are not shown):

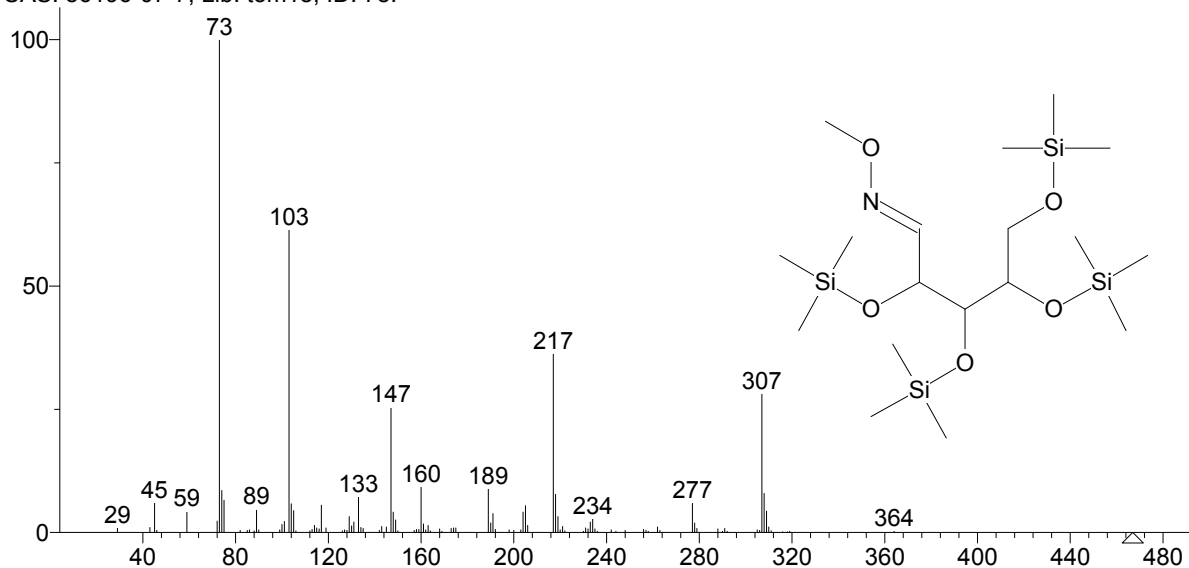
45	60	101	23	114	11	143	15	158	9	189	79	217	354	234	15	291	13
59	37	102	12	117	55	145	11	160	79	190	10	218	63	244	11	307	252
73	999	103	605	129	33	147	251	161	12	204	38	219	29	262	10	308	78
74	81	104	61	131	22	148	38	163	10	205	56	221	16	277	59		
89	59	105	39	133	77	149	24	175	12	216	12	233	26	278	18		

Synonyms:

1.XYLOSE M4T-TENT-[58-86-6];

Hit 78 : RH-T-1661.8-0.02%-XYLOSE M4T-TENT-[58-86-6]-RH03

CAS: 56196-07-7; Lib: tom18; ID: 78.



(tom18) RH-T-1661.8-0.02%-XYLOSE M4T-TENT-[58-86-6]-RH03

Name: RH-T-1661.8-0.02%-XYLOSE M4T-TENT-[58-86-6]-RH03

Formula: C₁₈H₄₅NO₅Si₄

MW: 467 CAS#: 56196-07-7 ID#: 78 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:1661.8|

10 largest peaks:

73 999 | 103 613 | 217 362 | 307 281 | 147 253 | 160 92 | 189 88 | 74 85 | 308 79 | 218 77 |

53 m/z Values and Intensities (54 low intensity peaks are not shown):

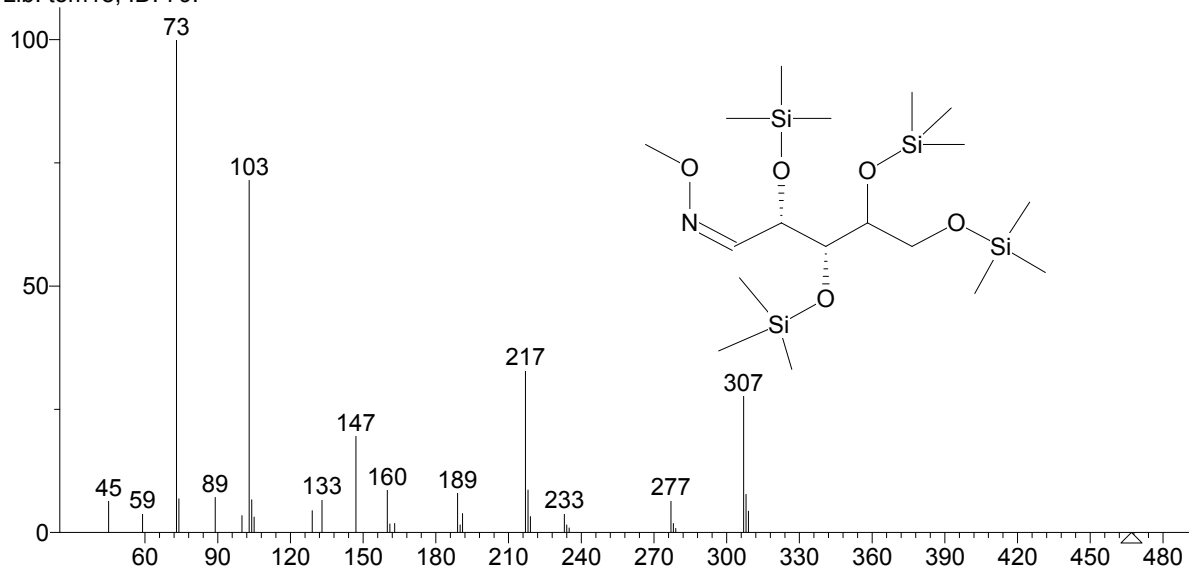
29	9	74	85	104	58	129	32	145	11	163	14	204	41	221	12	278	19
43	10	75	65	105	44	130	13	147	253	174	9	205	54	231	9	307	281
45	60	89	46	114	14	131	21	148	41	175	9	206	14	233	21	308	79
59	42	100	16	115	9	133	72	149	25	189	88	217	362	234	27	309	43
72	23	101	22	117	55	134	10	160	92	190	19	218	77	262	11	310	11
73	999	103	613	119	9	143	12	161	17	191	38	219	32	277	59		

Synonyms:

1.XYLOSE M4T-TENT-[58-86-6];

Hit 79 : RH-T-1668.3-0.01%-ARABINOSE M4T-TENT-[5328-37-0]-RH03

Lib: tom18; ID: 79.



(tom18) RH-T-1668.3-0.01%-ARABINOSE M4T-TENT-[5328-37-0]-RH03

Name: RH-T-1668.3-0.01%-ARABINOSE M4T-TENT-[5328-37-0]-RH03

Formula: C₁₈H₄₅NO₅Si₄

MW: 467 ID#: 79 DB: tom18

Comment: RI:MG00238 |RI:1668.3|

10 largest peaks:

73 999 | 103 714 | 217 328 | 307 276 | 147 195 | 160 86 | 218 86 | 189 80 | 308 77 | 89 71 |

29 m/z Values and Intensities (1 low intensity peak is not shown):

45 63 | 74 68 | 103 714 | 129 44 | 160 86 | 189 80 | 217 328 | 233 38 | 277 64 | 308 77 |

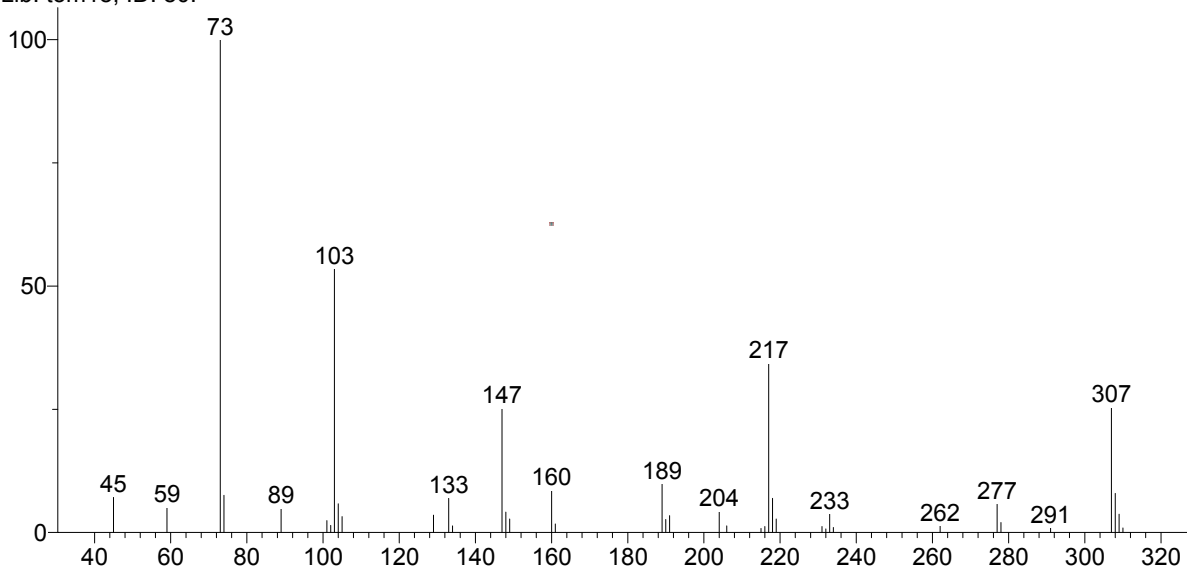
59 38 | 89 71 | 104 66 | 133 66 | 161 17 | 190 15 | 218 86 | 234 15 | 278 18 | 309 43 |

73 999 | 100 34 | 105 31 | 147 195 | 163 18 | 191 38 | 219 32 | 235 9 | 307 276 |

Synonyms:

1.ARABINOSE M4T-TENT-[5328-37-0];

Hit 80 : RH-T-1676.0-0.01%-[103,217,307,189,160, sim. ARABINOSE MX4T-TENT-[58-86-6]-RH01
Lib: tom18; ID: 80.



(tom18) RH-T-1676.0-0.01%-[103,217,307,189,160, sim. ARABINOSE MX4T-TENT-[58-86-6]-RH01 RI:1676.0,

Name: RH-T-1676.0-0.01%-[103,217,307,189,160, sim. ARABINOSE MX4T-TENT-[58-86-6]-RH01

MW: N/A ID#: 80 DB: tom18

RI: 1676.0,

Comment: RI=1676.0, 26.3171 min AB2129 [RI:1676]

10 largest peaks:

73 999 | 103 534 | 217 342 | 307 253 | 147 251 | 189 98 | 160 85 | 308 79 | 74 75 | 45 71 |

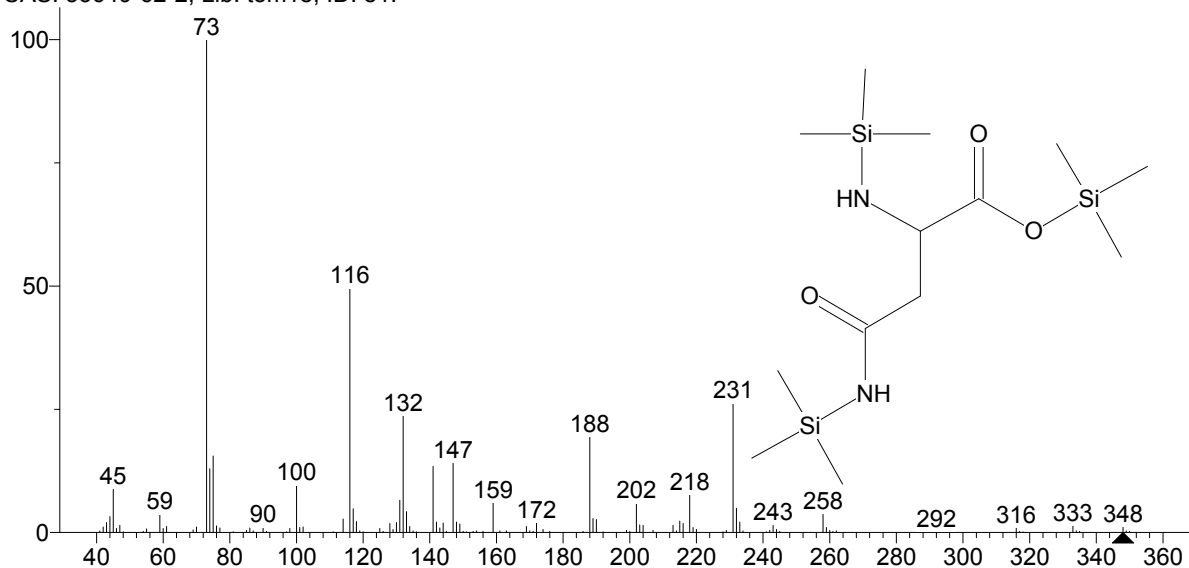
38 m/z Values and Intensities (2 low intensity peaks are not shown):

45 71 | 89 48 | 104 58 | 134 13 | 160 85 | 191 34 | 217 342 | 233 37 | 278 20 | 309 37 |
59 50 | 101 24 | 105 32 | 147 251 | 161 17 | 204 42 | 218 69 | 234 10 | 291 9 | 310 9 |
73 999 | 102 14 | 129 35 | 148 41 | 189 98 | 206 13 | 219 27 | 262 13 | 307 253 |
74 75 | 103 534 | 133 69 | 149 27 | 190 26 | 216 12 | 231 12 | 277 57 | 308 79 |

Synonyms:

1.m103,217,307,189,160, sim. ARABINOSE MX4T-TENT-[58-86-6];

Hit 81 : RH-T-1677.5-0.00%-ASPARAGINE 3T-CONF-[70-47-3]-8135A18-G
CAS: 55649-62-2; Lib: tom18; ID: 81.



(tom18) RH-T-1677.5-0.00%-ASPARAGINE 3T-CONF-[70-47-3]-8135A18-G RI:1677.5,

Name: RH-T-1677.5-0.00%-ASPARAGINE 3T-CONF-[70-47-3]-8135A18-G

Formula: C₁₃H₃₂N₂O₃Si₃

MW: 348 CAS#: 55649-62-2 ID#: 81 DB: tom18

Other DBs: None

RI: 1677.5,

Comment: RI=1677.5, 24.3069 min 8135A18 [RI:1677.5]

10 largest peaks:

73 999 | 116 494 | 231 261 | 132 236 | 188 193 | 75 155 | 147 140 | 141 134 | 74 129 | 100 95 |

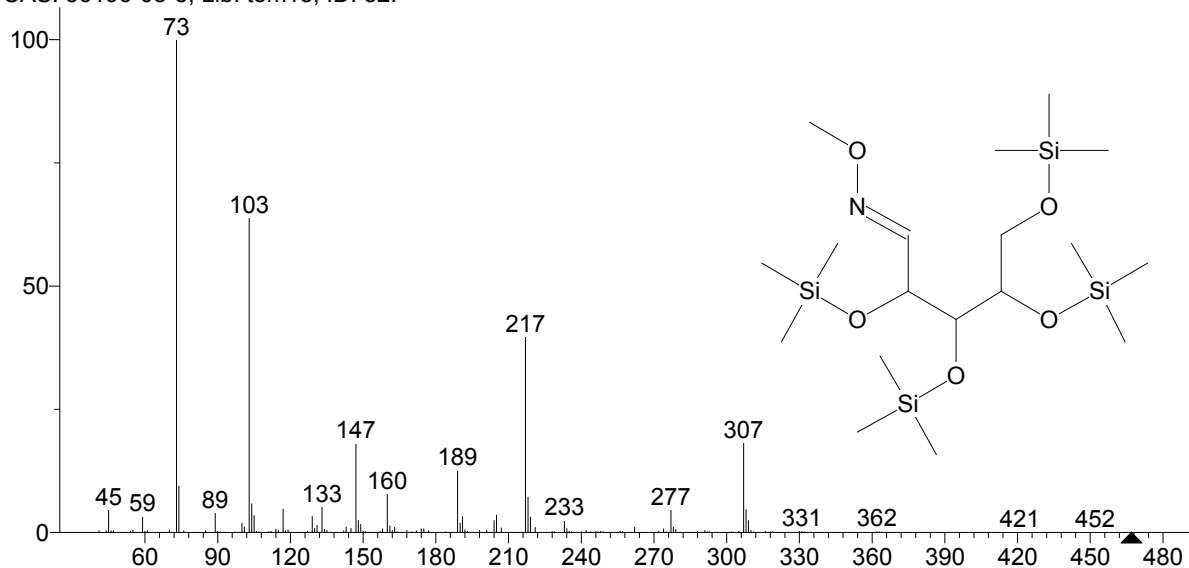
58 m/z Values and Intensities (57 low intensity peaks are not shown):

42	11	61	12	77	9	114	27	131	65	143	9	169	12	203	15	219	10	259	10
43	20	70	11	86	9	116	494	132	236	144	19	172	19	204	14	231	261	316	9
44	32	73	999	90	10	117	48	133	42	147	140	188	193	213	14	232	49	333	13
45	87	74	129	100	95	118	22	134	12	148	21	189	28	215	23	233	21	348	11
47	14	75	155	101	10	128	18	141	134	149	17	190	26	216	18	243	14		
59	36	76	13	102	11	130	20	142	21	159	60	202	58	218	75	258	37		

Synonyms:

1.ASPARAGINE 3T-CONF-[70-47-3];

Hit 82 : RH-T-1681.3-0.01%-RIBOSE M4T-TENT-[50-69-1]-8135A18-G
CAS: 56196-08-8; Lib: tom18; ID: 82.



(tom18) RH-T-1681.3-0.01%-RIBOSE M4T-TENT-[50-69-1]-8135A18-G RI:1681.3,

Name: RH-T-1681.3-0.01%-RIBOSE M4T-TENT-[50-69-1]-8135A18-G

Formula: C₁₈H₄₅NO₅Si₄

MW: 467 CAS#: 56196-08-8 ID#: 82 DB: tom18

Other DBs: None

RI: 1681.3,

Comment: RI=1681.3, 24.3759 min 8135A18 |RI:1681.3|

10 largest peaks:

73 999 | 103 637 | 217 396 | 307 181 | 147 180 | 189 125 | 74 94 | 160 77 | 218 71 | 104 58 |

38 m/z Values and Intensities (82 low intensity peaks are not shown):

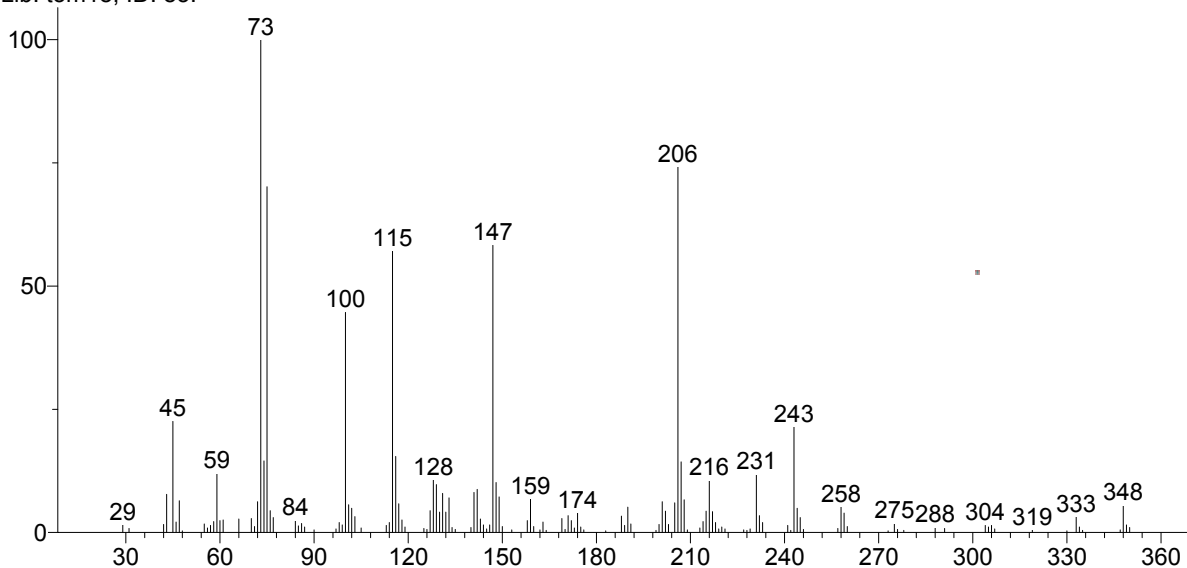
45 45 | 89 39 | 104 58 | 131 14 | 148 24 | 163 10 | 204 24 | 218 71 | 262 10 | 308 46 |
59 32 | 100 19 | 105 34 | 133 51 | 149 16 | 189 125 | 205 35 | 219 31 | 277 45 | 309 24 |
73 999 | 101 11 | 117 47 | 143 11 | 160 77 | 190 19 | 207 9 | 221 10 | 278 11 |
74 94 | 103 637 | 129 32 | 147 180 | 161 13 | 191 32 | 217 396 | 233 24 | 307 181 |

Synonyms:

1.RIBOSE M4T-TENT-[50-69-1];

Hit 83 : RH-T-1693.7-0.02%-[206,115,243,206,100, G: sim. L-Asparagine 3T]-RH02

Lib: tom18; ID: 83.



(tom18) RH-T-1693.7-0.02%-[206,115,243,206,100, G: sim. L-Asparagine 3T]-RH02 RI:1693.7,

Name: RH-T-1693.7-0.02%-[206,115,243,206,100, G: sim. L-Asparagine 3T]-RH02

MW: N/A ID#: 83 DB: tom18

RI: 1693.7,

Comment: RI=1693.7, 30.6108 min MG00244 [RI:1693.7]

10 largest peaks:

73 999 | 206 741 | 75 701 | 147 582 | 115 570 | 100 446 | 45 225 | 243 214 | 116 154 | 74 145 |

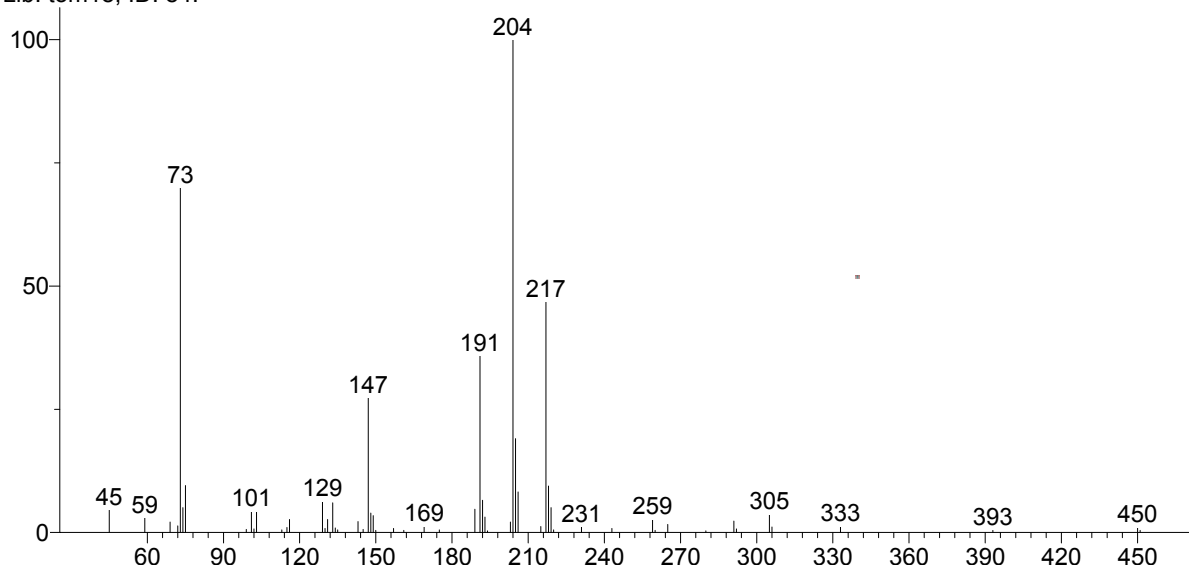
107 m/z Values and Intensities (33 low intensity peaks are not shown):

29 15	60 24	84 24	113 14	131 79	148 101	174 39	206 741	232 34	304 14
42 16	61 25	85 13	114 20	132 41	149 72	175 11	207 143	233 20	305 11
43 77	66 27	86 18	115 570	133 70	150 12	188 33	208 66	241 14	306 14
45 225	70 28	87 11	116 154	134 10	158 24	189 14	213 9	243 214	333 31
46 21	71 12	98 20	117 58	140 10	159 68	190 51	214 22	244 49	334 11
47 64	72 62	99 15	118 25	141 81	160 12	191 17	215 43	245 30	348 54
55 17	73 999	100 446	119 11	142 87	163 21	200 16	216 105	258 51	349 15
56 9	74 145	101 56	127 44	143 27	169 28	201 62	217 42	259 39	350 10
57 14	75 701	102 49	128 106	144 15	171 34	202 43	218 20	260 12	
58 22	76 44	103 32	129 97	146 15	172 24	203 16	220 11	275 18	
59 119	77 30	105 9	130 41	147 582	173 9	205 60	231 117	288 10	

Synonyms:

1.m206,115,243,206,100, G: sim. L-Asparagine 3T;

Hit 84 : RH-T-1712.5-0.01%-[204,217,191,305, N: sim. D-Xylose, tetrakis(trimethylsilyl)-]-RH03
 Lib: tom18; ID: 84.



(tom18) RH-T-1712.5-0.01%-[204,217,191,305, N: sim. D-Xylose, tetrakis(trimethylsilyl)-]-RH03 RI:1712.5,

Name: RH-T-1712.5-0.01%-[204,217,191,305, N: sim. D-Xylose, tetrakis(trimethylsilyl)-]-RH03

MW: N/A ID#: 84 DB: tom18

RI: 1712.5,

Comment: RI=1712.5, 31.1251 min MG00244 [RI:1712.5]

10 largest peaks:

204 999 | 73 698 | 217 467 | 191 358 | 147 272 | 205 190 | 75 95 | 218 94 | 206 82 | 192 65 |

40 m/z Values and Intensities (18 low intensity peaks are not shown):

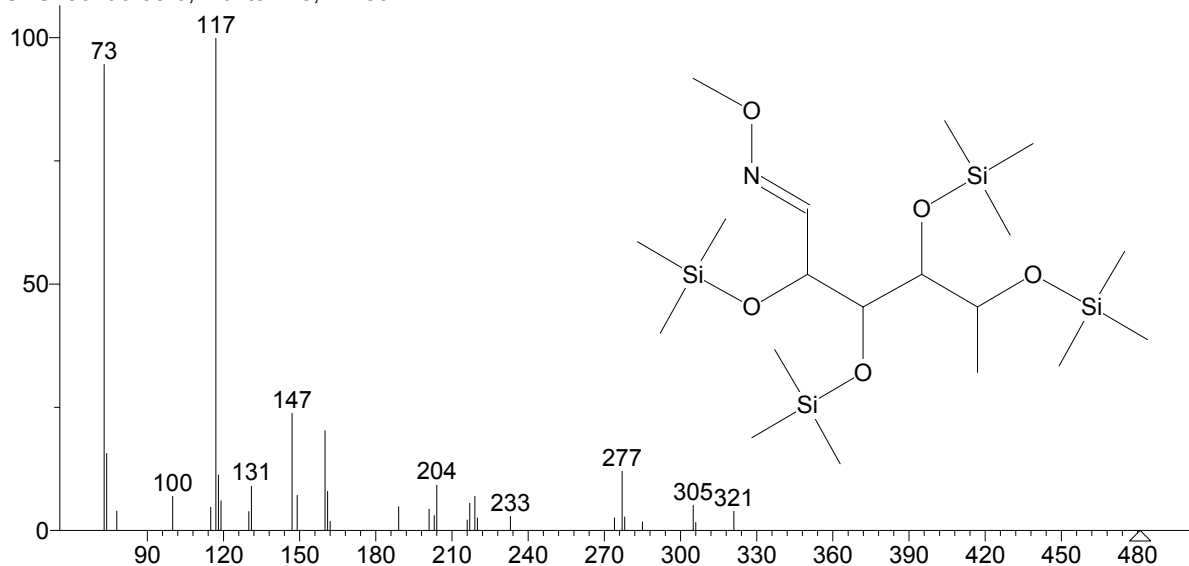
45 45	73 698	103 41	131 26	147 272	189 47	203 21	215 12	231 11	305 36
59 29	74 50	115 10	133 60	148 39	191 358	204 999	217 467	259 26	306 11
69 21	75 95	116 26	134 9	149 34	192 65	205 190	218 94	265 16	333 12
72 13	101 42	129 62	143 22	169 12	193 31	206 82	219 50	291 23	450 10

Synonyms:

1.m204,217,191,305, N: sim. D-Xylose, tetrakis(trimethylsilyl)-;

Hit 85 : RH-T-1717.4-0.00%-RHAMNOSE M4T-CONF-[10485-94-6]-RH03

CAS: 56196-05-5; Lib: tom18; ID: 85.



(tom18) RH-T-1717.4-0.00%-RHAMNOSE M4T-CONF-[10485-94-6]-RH03

Name: RH-T-1717.4-0.00%-RHAMNOSE M4T-CONF-[10485-94-6]-RH03

Formula: C₁₉H₄₇NO₅Si₄

MW: 481 CAS#: 56196-05-5 ID#: 85 DB: tom18

Other DBs: None

Comment: RI:MG00244 |RI:1717.4|

10 largest peaks:

117 999 | 73 945 | 147 238 | 160 202 | 74 156 | 277 120 | 118 112 | 204 93 | 131 91 | 161 79 |

31 m/z Values and Intensities:

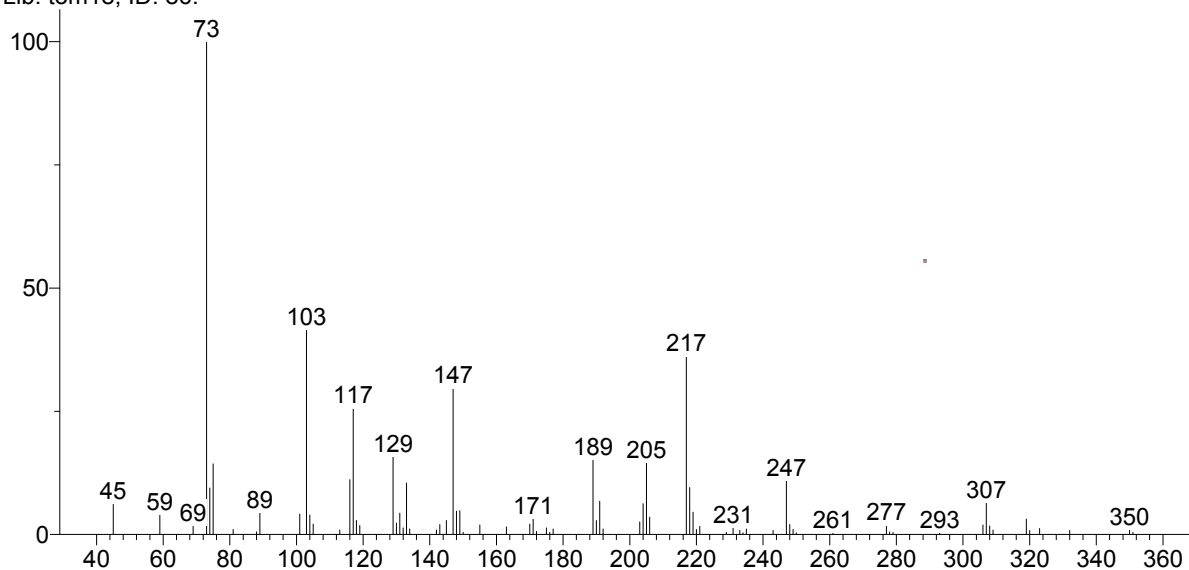
73 945 | 115 47 | 130 38 | 160 202 | 201 43 | 217 55 | 274 25 | 305 51 |
 74 156 | 117 999 | 131 91 | 161 79 | 203 30 | 219 69 | 277 120 | 306 16 |
 78 39 | 118 112 | 147 238 | 162 18 | 204 93 | 220 25 | 278 27 | 321 39 |
 100 70 | 119 60 | 149 71 | 189 48 | 216 21 | 233 29 | 285 17 |

Synonyms:

1.RHAMNOSE M4T-CONF-[10485-94-6];

Hit 86 : RH-T-1722.5-0.05%-[217,103,117,307, sim. XYLITOL 5T-TENT-RH03

Lib: tom18; ID: 86.



(tom18) RH-T-1722.5-0.05%-[217,103,117,307, sim. XYLITOL 5T-TENT-RH03

Name: RH-T-1722.5-0.05%-[217,103,117,307, sim. XYLITOL 5T-TENT-RH03

MW: N/A ID#: 86 DB: tom18

Comment: RI:MG00244 |RI:1722.5|

10 largest peaks:

73 999 | 103 414 | 217 360 | 147 296 | 117 255 | 129 157 | 189 150 | 205 145 | 75 143 | 116 111 |

61 m/z Values and Intensities (16 low intensity peaks are not shown):

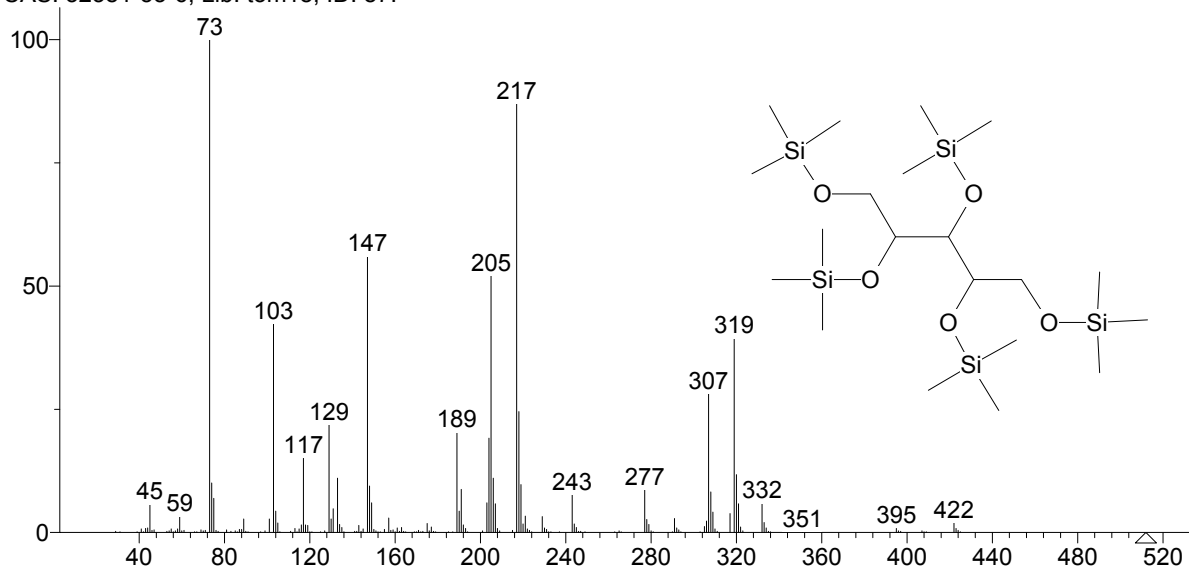
45	61	89	43	117	255	133	104	149	48	189	150	206	35	235	11	308	17
59	39	101	41	118	28	134	11	155	19	190	28	217	360	247	108	309	9
69	16	103	414	119	18	142	9	163	15	191	67	218	95	248	20	319	31
73	999	104	39	129	157	143	20	170	21	192	11	219	45	249	10	323	12
74	94	105	21	130	23	145	28	171	31	203	25	220	10	277	18	350	9
75	143	113	9	131	43	147	296	175	13	204	62	221	16	306	19		
81	10	116	111	132	13	148	47	177	11	205	145	231	13	307	63		

Synonyms:

1.m217,103,117,307, sim. XYLITOL 5T-TENT;

Hit 87 : RH-T-1728.2-5.08%-RIBITOL 5T-CONF-[488-81-3]-RH03

CAS: 32381-53-6; Lib: tom18; ID: 87.



(tom18) RH-T-1728.2-5.08%-RIBITOL 5T-CONF-[488-81-3]-RH03

Name: RH-T-1728.2-5.08%-RIBITOL 5T-CONF-[488-81-3]-RH03

Formula: C₂₀H₅₂O₅Si₅

MW: 512 CAS#: 32381-53-6 ID#: 87 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:1728.2|

10 largest peaks:

73 999 | 217 869 | 147 559 | 205 520 | 103 422 | 319 393 | 307 281 | 218 245 | 129 218 | 189 202 |

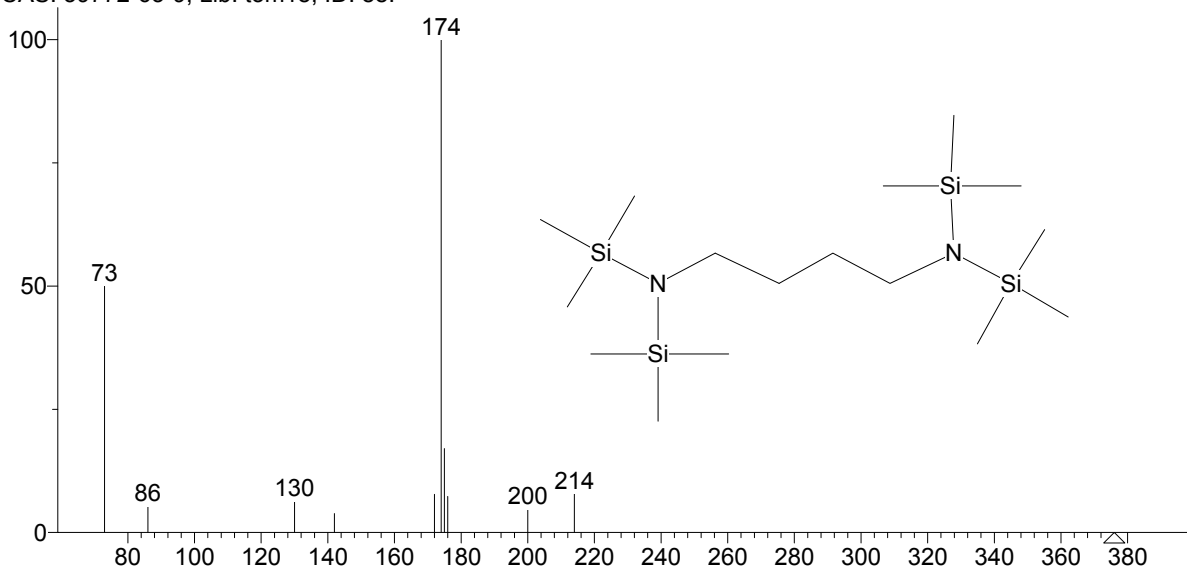
68 m/z Values and Intensities (108 low intensity peaks are not shown):

44	9	101	27	119	14	143	14	175	18	204	191	220	17	277	86	307	281	322	11
45	56	103	422	129	218	147	559	177	11	205	520	221	33	278	26	308	82	332	58
59	32	104	43	130	27	148	94	189	202	206	110	229	32	279	16	309	41	333	20
73	999	105	19	131	48	149	60	190	43	207	58	230	9	291	28	317	38	334	9
74	100	116	15	133	110	157	29	191	87	217	869	243	76	292	9	319	393	422	19
75	69	117	150	134	16	161	9	192	15	218	245	244	17	305	12	320	117		
89	27	118	15	135	10	163	10	203	60	219	97	245	10	306	23	321	58		

Synonyms:

1.RIBITOL 5T-CONF-[488-81-3];

Hit 88 : RH-T-1733.2-0.00%-PUTRESCINE 4T-TENT-[110-60-1]-RH03-X
CAS: 39772-63-9; Lib: tom18; ID: 88.



(tom18) RH-T-1733.2-0.00%-PUTRESCINE 4T-TENT-[110-60-1]-RH03-X

Name: RH-T-1733.2-0.00%-PUTRESCINE 4T-TENT-[110-60-1]-RH03-X

Formula: C₁₆H₄₄N₂Si₄

MW: 376 CAS#: 39772-63-9 ID#: 88 DB: tom18

Other DBs: None

Comment: RI:MG00238 [RI:1733.2]

10 largest peaks:

174 999 | 73 499 | 175 170 | 214 78 | 172 77 | 176 73 | 130 62 | 86 52 | 200 46 | 142 38 |

10 m/z Values and Intensities:

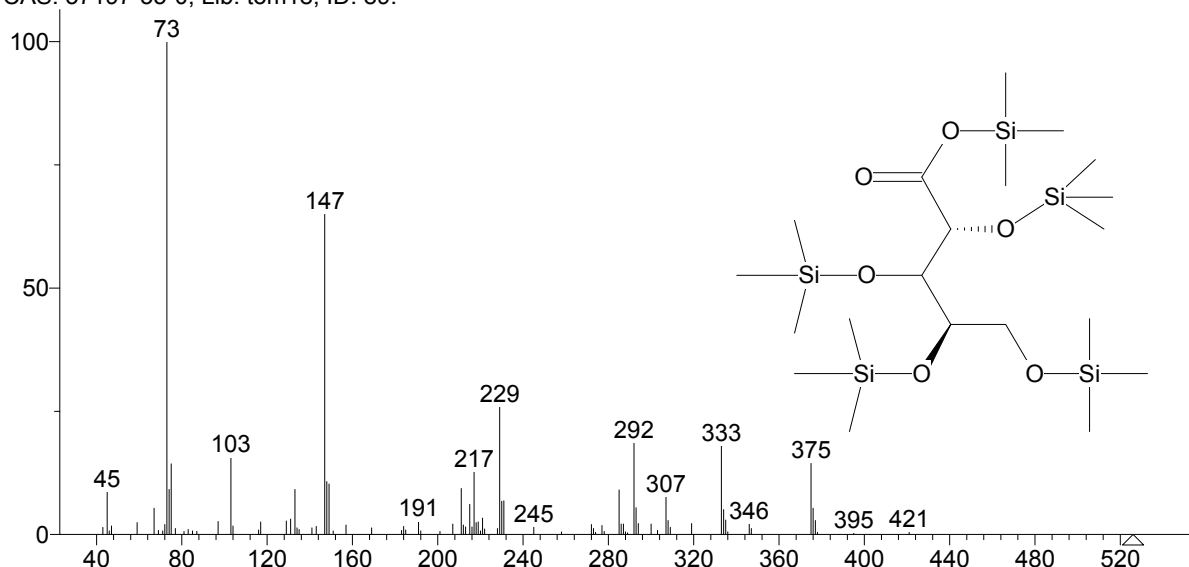
73 499 | 86 52 | 130 62 | 142 38 | 172 77 | 174 999 | 175 170 | 176 73 | 200 46 | 214 78 |

Synonyms:

1.PUTRESCINE 4T-TENT-[110-60-1];

Hit 89 : RH-T-1752.8-0.01%-[G: RIBONIC ACID 5T]-TENT-RH03

CAS: 57197-35-0; Lib: tom18; ID: 89.



(tom18) RH-T-1752.8-0.01%-[G-RIBONIC ACID 5T]-TENT-RH03 RI:1752.8,

Name: RH-T-1752.8-0.01%-[G-RIBONIC ACID 5T]-TENT-RH03

Formula: C₂₀H₅₀O₆Si₅

MW: 526 CAS#: 57197-35-0 ID#: 89 DB: tom18

Other DBs: None

RI: 1752.8,

Comment: RI=1752.8, 32.2099 min MG00244 [RI:1752.8]

10 largest peaks:

73 999 | 147 650 | 229 258 | 292 185 | 333 179 | 103 156 | 375 144 | 75 143 | 217 126 | 148 107 |

69 m/z Values and Intensities (21 low intensity peaks are not shown):

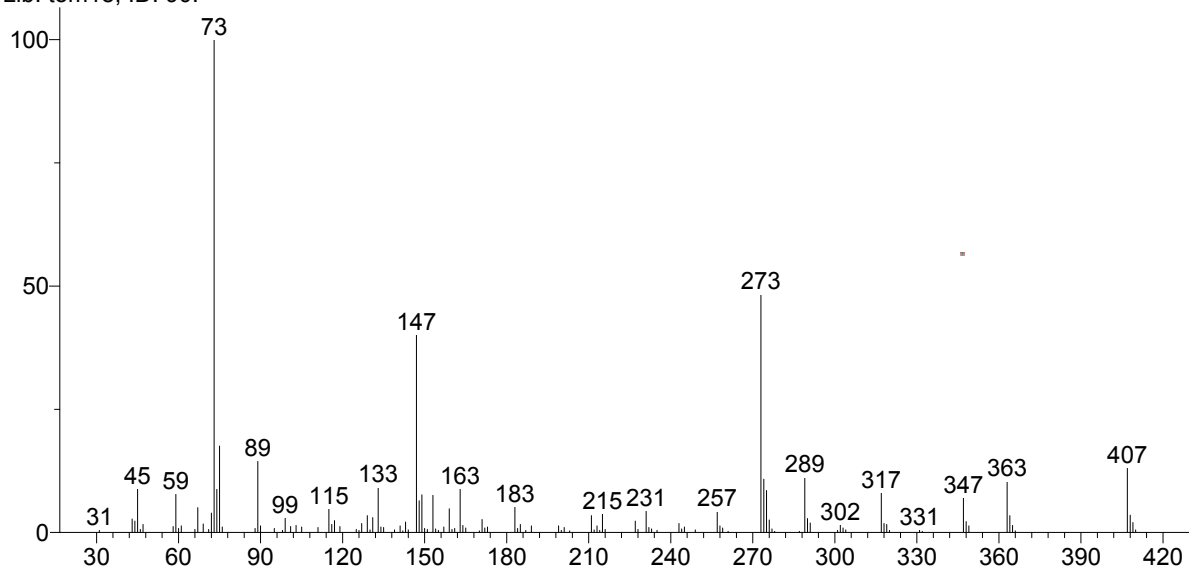
43	14	74	91	116	9	141	13	184	16	215	61	228	12	277	18	300	21	335	29
45	86	75	143	117	25	143	16	185	9	216	15	229	258	285	90	307	75	346	21
47	17	77	12	129	27	147	650	191	26	217	126	230	67	286	21	308	28	347	12
59	24	83	10	131	31	148	107	207	21	218	24	231	68	287	21	309	14	375	144
67	53	97	26	133	91	149	102	211	93	219	25	245	15	292	185	319	22	376	53
72	20	103	156	134	13	157	19	212	19	221	33	272	20	293	54	333	179	377	28
73	999	104	17	135	10	169	13	213	15	222	11	273	12	294	22	334	50		

Synonyms:

1.RIBONIC ACID 5T]-TENT;

Hit 90 : RH-T-1757.3-0.06%-[273,407,363-,289,347]-RH01

Lib: tom18; ID: 90.



(tom18) RH-T-1757.3-0.06%-[273,407,363-,289,347]-RH01 RI:1757.3,

Name: RH-T-1757.3-0.06%-[273,407,363-,289,347]-RH01

MW: N/A ID#: 90 DB: tom18

RI: 1757.3,

Comment: RI=1757.3, 28.1007 min AB2129 [RI:1757.3]

10 largest peaks:

73 999 | 273 482 | 147 400 | 75 175 | 89 144 | 407 130 | 289 111 | 274 108 | 363 103 | 133 91 |

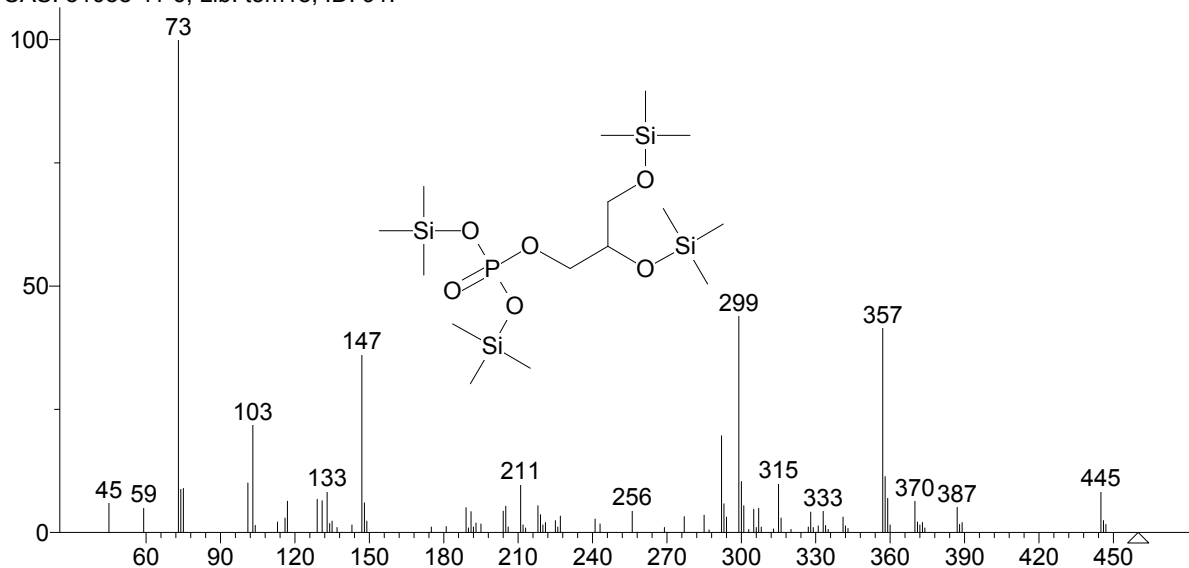
82 m/z Values and Intensities (44 low intensity peaks are not shown):

43 27	72 39	103 14	131 30	153 75	183 51	231 43	275 85	319 16	409 20
44 23	73 999	105 11	133 91	157 11	185 16	232 10	276 25	347 70	
45 88	74 87	111 10	134 11	159 48	189 13	243 18	289 111	348 22	
47 16	75 175	115 47	135 10	163 88	199 13	245 11	290 28	349 13	
58 12	76 11	116 16	141 13	164 14	201 10	257 42	291 19	363 103	
59 77	89 144	117 24	143 21	165 9	211 34	258 13	302 15	364 34	
61 13	90 13	119 12	147 400	171 26	213 13	259 9	303 9	365 14	
67 50	99 29	127 18	148 64	172 9	215 37	273 482	317 80	407 130	
69 17	101 12	129 34	149 76	173 11	227 23	274 108	318 18	408 35	

Synonyms:

1.m273,407,363-,289,347];

Hit 91 : RH-T-1764.3-0.02%-GLYCEROL-3-PHOSPHATE 4T-CONF-[57-03-4]-RH03
CAS: 31038-11-6; Lib: tom18; ID: 91.



(tom18) RH-T-1764.3-0.02%-GLYCEROL-3-PHOSPHATE 4T-CONF-[57-03-4]-RH03

Name: RH-T-1764.3-0.02%-GLYCEROL-3-PHOSPHATE 4T-CONF-[57-03-4]-RH03

Formula: C₁₅H₄₁O₆PSi₄

MW: 460 CAS#: 31038-11-6 ID#: 91 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:1764.3|

10 largest peaks:

73 999 | 299 438 | 357 414 | 147 360 | 103 218 | 292 196 | 358 113 | 300 103 | 101 100 | 315 99 |

83 m/z Values and Intensities (6 low intensity peaks are not shown):

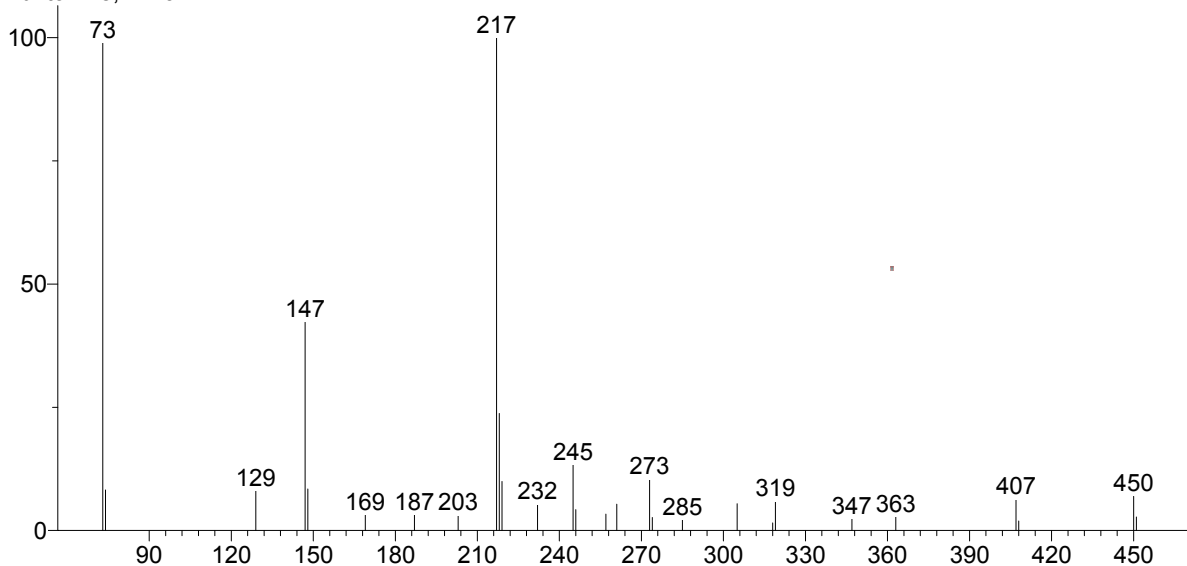
45	60	116	29	147	360	193	19	219	36	269	10	305	47	331	13	370	63	446	24
59	50	117	63	148	60	195	17	220	15	277	32	306	10	333	43	371	21	447	16
73	999	129	67	149	23	204	43	221	20	285	35	307	49	334	14	372	15		
74	87	131	64	175	11	205	53	225	24	292	196	308	11	341	31	373	20		
75	89	133	83	181	12	206	11	226	11	293	58	315	99	342	13	374	9		
101	100	134	18	189	50	211	97	227	33	294	31	316	29	357	414	387	51		
103	218	135	23	190	9	212	15	241	27	299	438	327	11	358	113	388	16		
104	14	137	10	191	42	213	9	243	17	300	103	328	41	359	69	389	20		
113	21	143	15	192	11	218	54	256	44	301	54	329	10	360	15	445	83		

Synonyms:

1.GLYCEROL-3-PHOSPHATE 4T-CONF-[57-03-4];

Hit 92 : RH-T-1769.3-0.01%-[217,245,450,407,273]-RH03

Lib: tom18; ID: 92.



(tom18) RH-T-1769.3-0.01%-[217,245,450,407,273]-RH03

Name: RH-T-1769.3-0.01%-[217,245,450,407,273]-RH03

MW: N/A ID#: 92 DB: tom18

Comment: RI:MG00238 |RI:1769.3|

10 largest peaks:

217 999 | 73 988 | 147 422 | 218 237 | 245 133 | 273 103 | 219 99 | 148 84 | 74 82 | 129 80 |

28 m/z Values and Intensities:

73 988 | 147 422 | 187 31 | 218 237 | 245 133 | 261 53 | 285 21 | 319 58 | 407 62 | 451 27 |

74 82 | 148 84 | 203 30 | 219 99 | 246 42 | 273 103 | 305 54 | 347 23 | 408 19 |

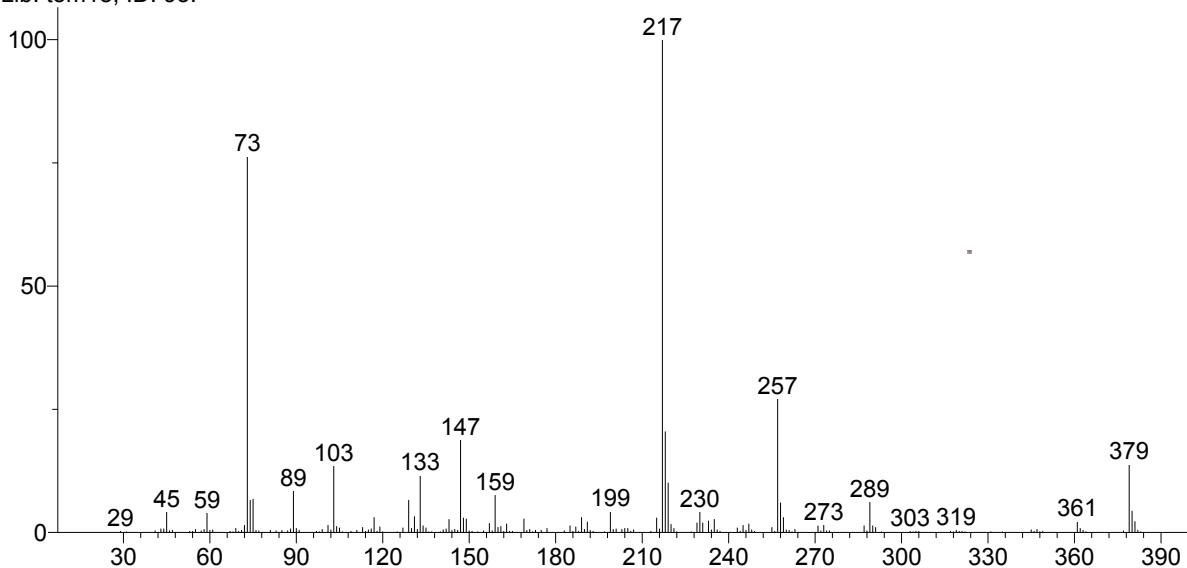
129 80 | 169 31 | 217 999 | 232 52 | 257 33 | 274 26 | 318 15 | 363 27 | 450 69 |

Synonyms:

1.m217,245,450,407,273;

Hit 93 : RH-T-1775.7-0.09%-[217,257,379,289,103]-RH03

Lib: tom18; ID: 93.



(tom18) RH-T-1775.7-0.09%-[217,257,379,289,103]-RH03 RI:1775.7,

Name: RH-T-1775.7-0.09%-[217,257,379,289,103]-RH03

MW: N/A ID#: 93 DB: tom18

RI: 1775.7,

Comment: RI=1775.7, 32.8250 min MG00244 [RI:1775.7]

10 largest peaks:

217 999 | 73 762 | 257 270 | 218 204 | 147 187 | 379 137 | 103 135 | 133 115 | 219 100 | 89 84 |

62 m/z Values and Intensities (124 low intensity peaks are not shown):

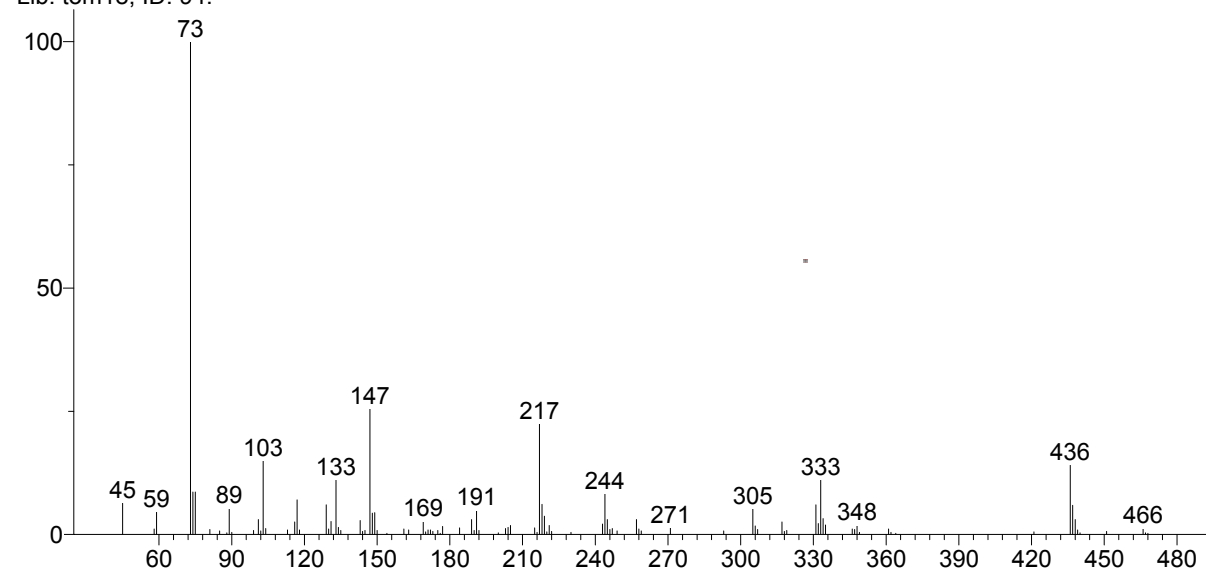
45	41	101	14	127	9	147	187	163	17	215	29	231	19	257	270	290	13
59	39	103	135	129	65	148	29	169	27	217	999	233	23	258	60	291	10
72	14	104	12	131	32	149	27	185	13	218	204	235	26	259	30	361	22
73	762	105	9	133	115	157	18	187	11	219	100	243	9	271	13	379	137
74	65	113	10	134	13	159	75	189	30	220	16	245	14	273	15	380	43
75	67	117	30	135	9	160	10	191	21	229	19	247	17	287	13	381	22
89	84	119	11	143	26	161	12	199	42	230	41	255	10	289	61		

Synonyms:

1.m217,257,379,289,103;

Hit 94 : RH-T-1780.7-0.04%-[217,436,333,244,305]-RH02

Lib: tom18; ID: 94.



(tom18) RH-T-1780.7-0.04%-[217,436,333,244,305]-RH02

Name: RH-T-1780.7-0.04%-[217,436,333,244,305]-RH02

MW: N/A ID#: 94 DB: tom18

Comment: RI:MG00238 [RI:1780.7]

10 largest peaks:

73 999 | 147 254 | 217 224 | 103 149 | 436 140 | 133 110 | 333 110 | 74 86 | 75 86 | 244 82 |

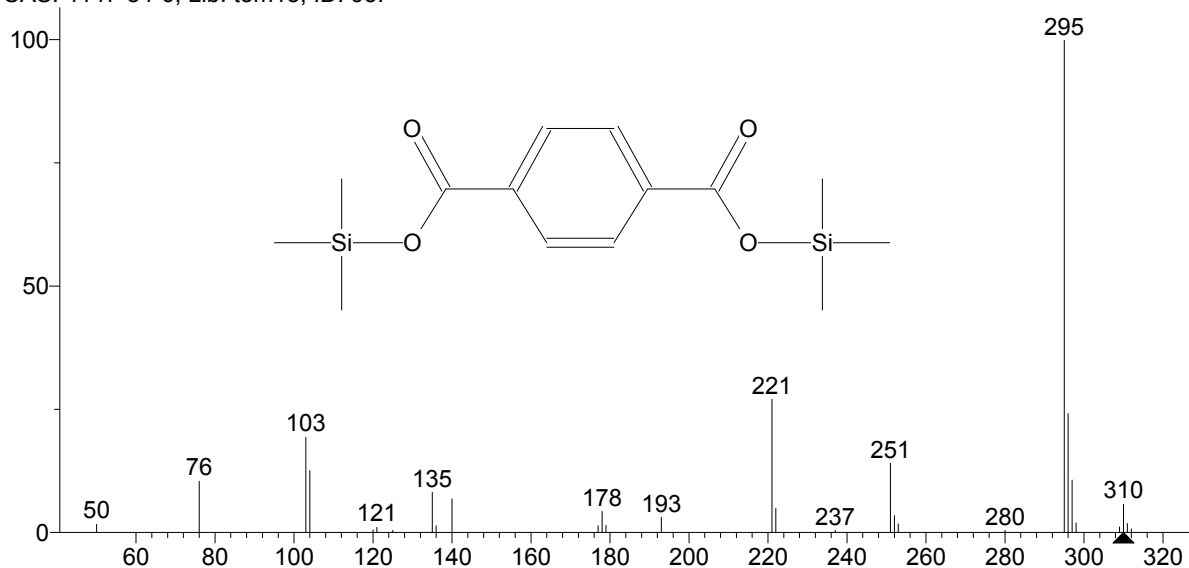
67 m/z Values and Intensities (34 low intensity peaks are not shown):

45	63	89	52	118	9	147	254	172	9	205	18	244	82	305	51	334	32	437	59
58	11	101	30	129	60	148	43	177	16	215	13	245	30	306	17	335	19	438	30
59	45	103	149	130	11	149	44	184	13	217	224	246	10	307	10	346	11	439	9
73	999	104	12	131	26	161	11	189	30	218	61	247	12	317	25	347	10	466	12
74	86	113	9	133	110	163	9	191	48	219	37	257	30	331	60	348	18		
75	86	116	25	134	14	169	26	203	12	221	18	258	11	332	22	361	11		
81	10	117	70	143	28	171	9	204	14	243	21	271	13	333	110	436	140		

Synonyms:

1.m217,436,333,244,305;

Hit 95 : RH-T-1783.2-0.00%-TEREPHTHALIC ACID 2T-CONF-CONTAM-[100-21-0]-RH01
CAS: 4147-84-6; Lib: tom18; ID: 95.



(tom18) RH-T-1783.2-0.00%-TEREPHTHALIC ACID 2T-CONF-CONTAM-[100-21-0]-RH01 RI:1783.2,

Name: RH-T-1783.2-0.00%-TEREPHTHALIC ACID 2T-CONF-CONTAM-[100-21-0]-RH01

Formula: C₁₄H₂₂O₄Si₂

MW: 310 CAS#: 4147-84-6 ID#: 95 DB: tom18

Other DBs: None

RI: 1783.2,

Comment: RI=1783.2, 28.6600 min AB2129 |RI:1783.2|

10 largest peaks:

295 999 | 221 270 | 296 241 | 103 194 | 251 141 | 104 125 | 297 106 | 76 105 | 135 81 | 140 68 |

24 m/z Values and Intensities (5 low intensity peaks are not shown):

50 18 | 104 125 | 136 13 | 178 43 | 221 270 | 252 34 | 296 241 | 309 11 |

76 105 | 121 12 | 140 68 | 179 14 | 222 49 | 253 17 | 297 106 | 310 58 |

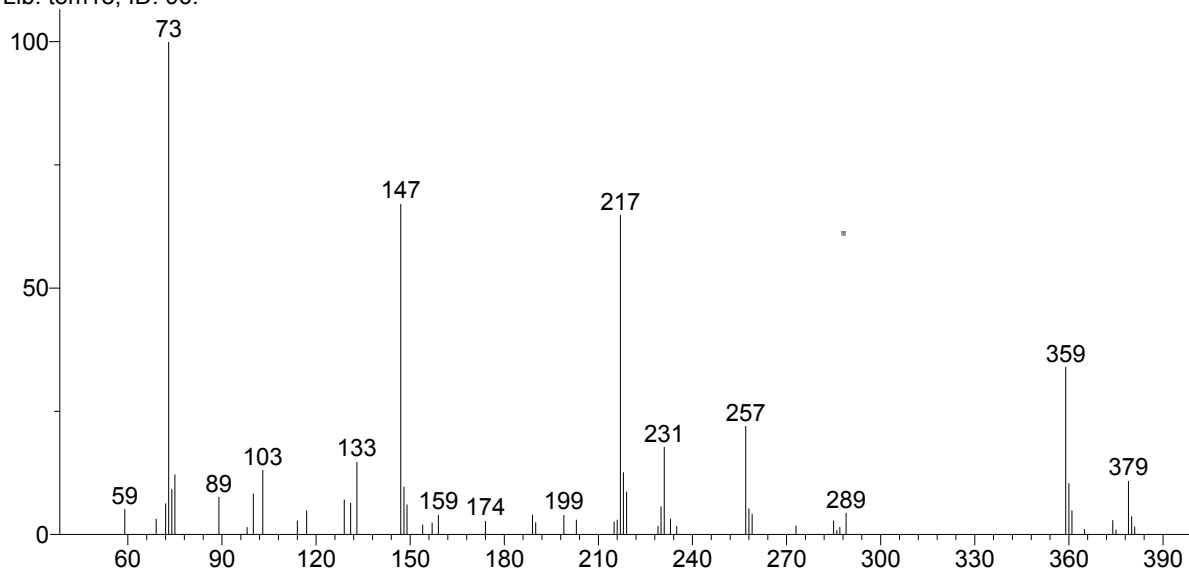
103 194 | 135 81 | 177 13 | 193 31 | 251 141 | 295 999 | 298 19 | 311 18 |

Synonyms:

1.TEREPHTHALIC ACID 2T-CONF-CONTAM;

Hit 96 : RH-T-1790.4-0.00%-[217,359,257,231,379]-RH03

Lib: tom18; ID: 96.



(tom18) RH-T-1790.4-0.00%-[217,359,257,231,379]-RH03 RI:1790.4,

Name: RH-T-1790.4-0.00%-[217,359,257,231,379]-RH03

MW: N/A ID#: 96 DB: tom18

RI: 1790.4,

Comment: RI=1790.4, 33.2210 min MG00244 [RI:1790.4]

10 largest peaks:

73 999 | 147 671 | 217 647 | 359 339 | 257 220 | 231 177 | 133 148 | 103 130 | 218 125 | 75 121 |

52 m/z Values and Intensities (1 low intensity peak is not shown):

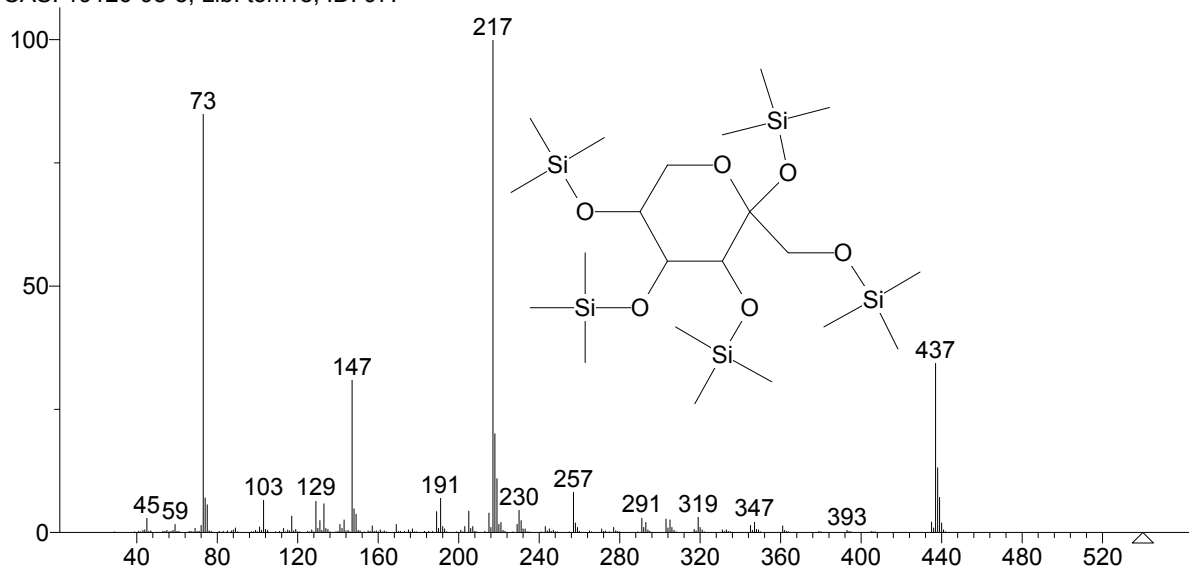
59 51	89 76	129 70	154 19	199 40	219 86	257 220	289 43	375 9
69 31	98 14	131 63	157 23	203 29	229 16	258 52	359 339	379 109
72 62	100 82	133 148	159 40	215 25	230 56	259 41	360 103	380 36
73 999	103 130	147 671	174 28	216 29	231 177	273 17	361 48	381 15
74 91	114 27	148 96	189 39	217 647	233 31	285 27	365 10	
75 121	117 48	149 60	190 24	218 125	235 16	287 14	374 28	

Synonyms:

1.m217,359,257,231,379;

Hit 97 : RH-T-1809.7-4.00%-FRUCTOSE 5T PK1-TENT-RH03

CAS: 19126-98-8; Lib: tom18; ID: 97.



(tom18) RH-T-1809.7-4.00%-FRUCTOSE 5T PK1-TENT-RH03

Name: RH-T-1809.7-4.00%-FRUCTOSE 5T PK1-TENT-RH03

Formula: C₂₁H₅₂O₆Si₅

MW: 540 CAS#: 19126-98-8 ID#: 97 DB: tom18

Other DBs: None

Comment: RI:MG00251 |RI:1808.4|

10 largest peaks:

217 999 | 73 848 | 437 343 | 147 309 | 218 200 | 438 131 | 219 109 | 257 82 | 439 71 | 74 70 |

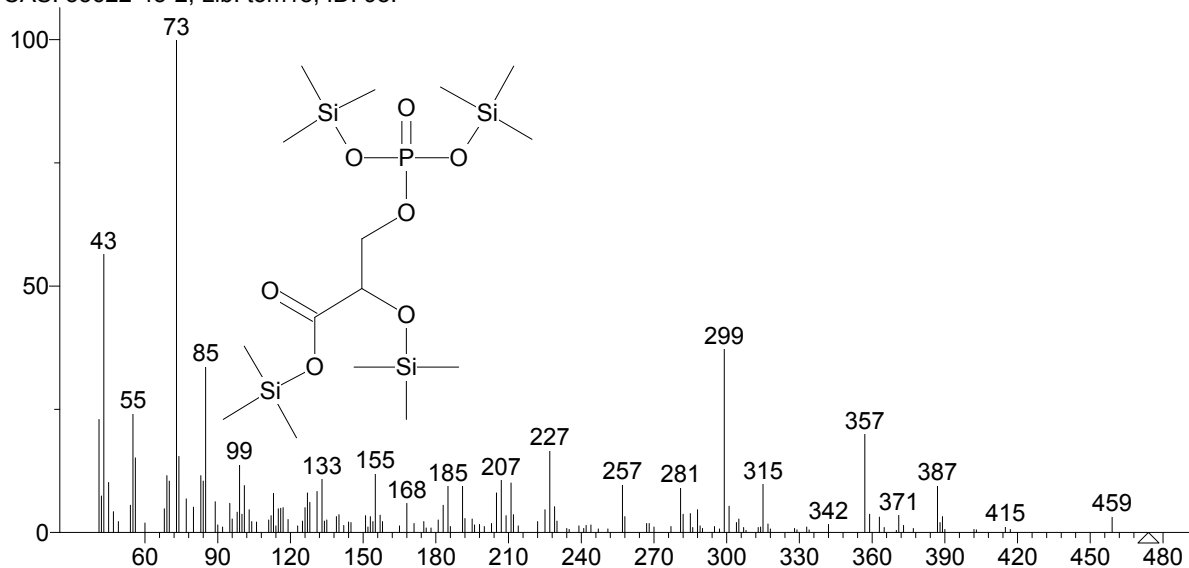
59 m/z Values and Intensities (151 low intensity peaks are not shown):

45	29	89	9	133	58	157	13	205	43	219	109	243	12	292	10	319	31	436	9
59	16	101	11	141	16	169	16	207	12	220	16	257	82	293	20	320	10	437	343
72	14	103	65	143	25	189	42	215	39	221	20	258	19	303	27	345	14	438	131
73	848	117	33	147	309	191	69	216	10	229	16	259	10	304	9	347	22	439	71
74	70	129	64	148	48	192	12	217	999	230	45	277	10	305	25	361	13	440	19
75	56	131	24	149	37	203	12	218	200	231	24	291	30	306	10	435	21		

Synonyms:

1.FRUCTOSE 5T PK1-TENT;

Hit 98 : RH-T-1812.2-0.00%-GLYCERIC ACID 3 PHOSPHATE 4T-8135A18-G-X
CAS: 55622-45-2; Lib: tom18; ID: 98.



(tom18) RH-T-1812.2-0.00%-GLYCERIC ACID 3 PHOSPHATE 4T-8135A18-G-X RI:1812.2,

Name: RH-T-1812.2-0.00%-GLYCERIC ACID 3 PHOSPHATE 4T-8135A18-G-X

Formula: C₁₅H₃₉O₇PSi₄

MW: 474 CAS#: 55622-45-2 ID#: 98 DB: tom18

Other DBs: None

RI: 1812.2,

Comment: RI=1812.2, 26.7877 min 8135A18 |RI:1812.2|

10 largest peaks:

73 999 | 43 565 | 299 372 | 85 336 | 55 241 | 41 229 | 357 199 | 227 166 | 74 154 | 56 151 |

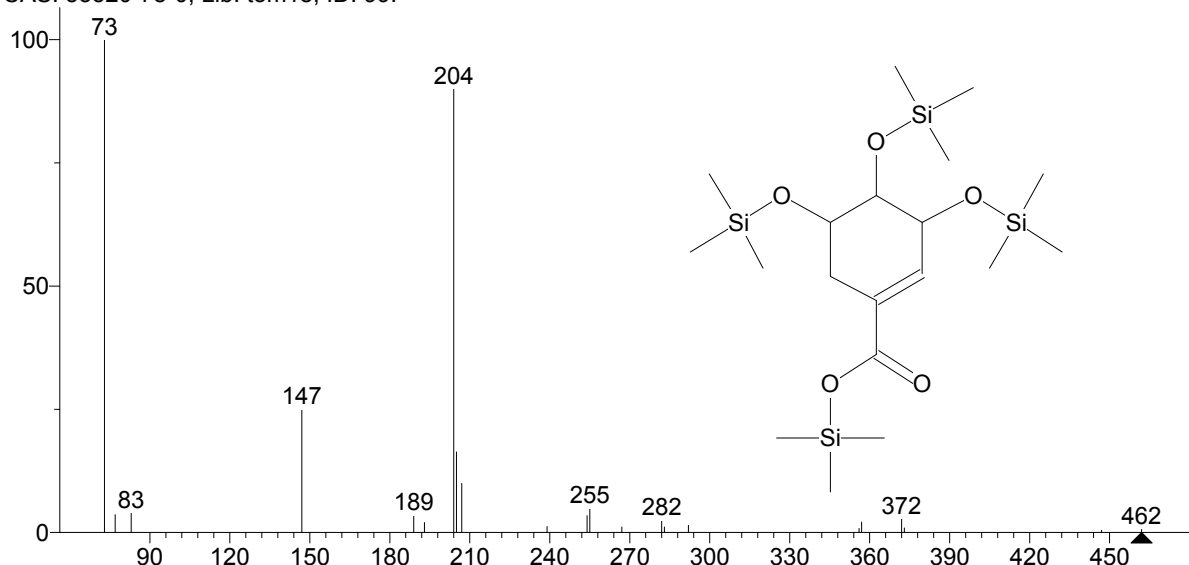
127 m/z Values and Intensities (18 low intensity peaks are not shown):

41 229	73 999	99 137	119 26	144 21	176 9	205 80	244 15	295 12	359 37
42 74	74 154	100 37	123 13	145 20	178 9	207 106	257 97	299 372	363 31
43 565	77 68	101 95	125 23	151 34	181 25	209 34	258 32	301 53	365 10
45 101	80 51	103 46	126 50	152 11	183 55	211 100	267 18	304 20	371 35
47 42	83 115	104 22	127 80	153 32	185 94	212 36	268 18	305 27	373 14
49 22	84 104	106 21	128 61	154 22	186 12	214 13	270 11	307 10	387 95
54 55	85 336	111 25	131 83	155 119	191 94	222 22	277 12	313 10	388 20
55 241	89 62	112 34	133 108	157 35	192 28	225 46	281 91	314 11	389 32
56 151	90 15	113 79	134 23	158 22	195 27	227 166	282 37	315 98	415 12
60 19	92 11	114 13	135 25	165 13	196 15	229 52	285 38	317 17	459 32
68 48	95 59	115 48	139 32	168 59	198 16	230 23	286 10	333 11	
69 115	96 27	116 49	140 36	171 18	200 12	239 13	288 46	342 16	
70 104	98 41	117 50	142 14	175 22	203 18	242 14	289 13	357 199	

Synonyms:

1. GLYCERIC ACID 3 PHOSPHATE 4T-;

Hit 99 : RH-T-1817.1-0.00%-SHIKIMIC ACID 4T-CONF-[138-59-0]-8135A18-G-X
CAS: 55520-78-0; Lib: tom18; ID: 99.



(tom18) RH-T-1817.1-0.00%-SHIKIMIC ACID 4T-CONF-[138-59-0]-8135A18-G-X RI:1817.1,

Name: RH-T-1817.1-0.00%-SHIKIMIC ACID 4T-CONF-[138-59-0]-8135A18-G-X

Formula: C₁₉H₄₂O₅Si₄

MW: 462 CAS#: 55520-78-0 ID#: 99 DB: tom18

Other DBs: None

RI: 1817.1,

Comment: RI=1817.1, 26.8794 min 8135A18 |RI:1817.1|

10 largest peaks:

73 999 | 204 899 | 147 249 | 205 163 | 207 99 | 255 48 | 83 39 | 77 36 | 189 34 | 254 34 |

19 m/z Values and Intensities (3 low intensity peaks are not shown):

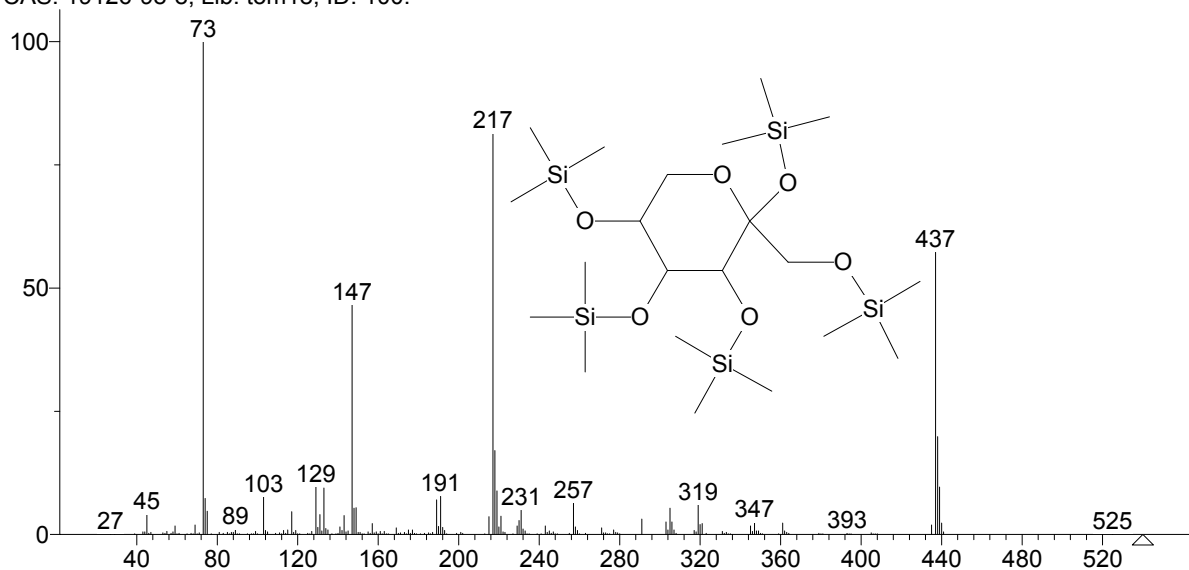
73 999 | 83 39 | 189 34 | 204 899 | 207 99 | 254 34 | 267 11 | 283 11 | 357 21 | 373 9 |
77 36 | 147 249 | 193 20 | 205 163 | 239 12 | 255 48 | 282 24 | 292 14 | 372 27 |

Synonyms:

1.SHIKIMIC ACID 4T-CONF-[138-59-0];

Hit 100 : RH-T-1817.7-0.20%-FRUCTOSE 5T PK2-TENT-RH03

CAS: 19126-98-8; Lib: tom18; ID: 100.



(tom18) RH-T-1817.7-0.20%-FRUCTOSE 5T PK2-TENT-RH03

Name: RH-T-1817.7-0.20%-FRUCTOSE 5T PK2-TENT-RH03

Formula: C₂₁H₅₂O₆Si₅

MW: 540 CAS#: 19126-98-8 ID#: 100 DB: tom18

Other DBs: None

Comment: RI:MG00251 |RI:1817.7|

10 largest peaks:

73 999 | 217 813 | 437 572 | 147 465 | 438 198 | 218 170 | 129 96 | 439 96 | 133 94 | 219 88 |

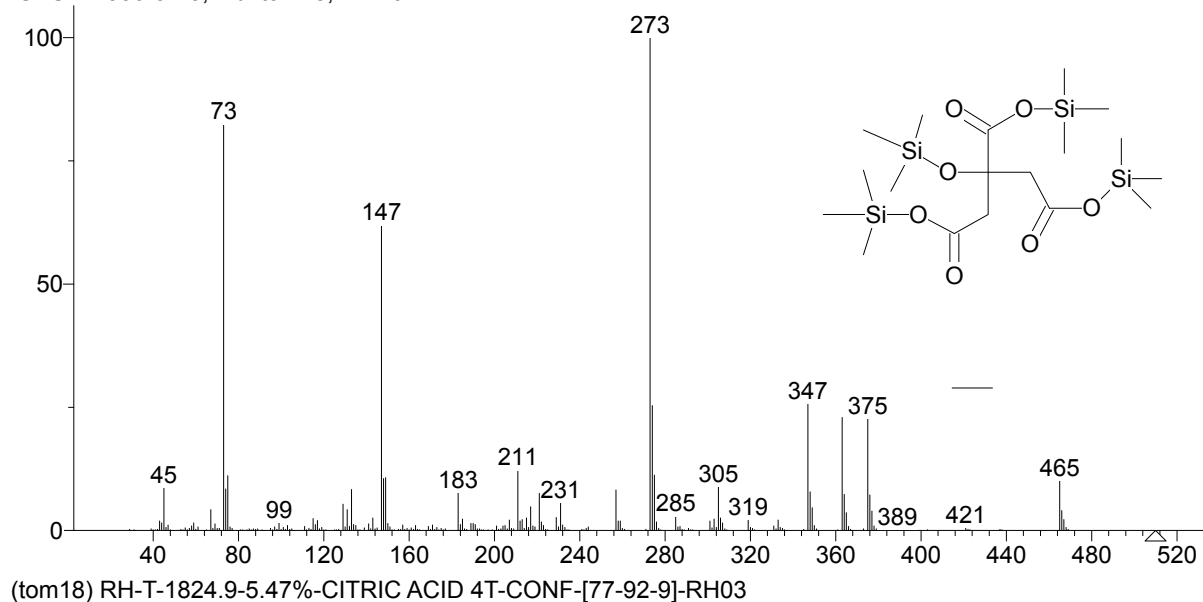
61 m/z Values and Intensities (141 low intensity peaks are not shown):

45	40	103	76	134	12	157	22	192	14	229	17	271	13	307	9	435	19
59	17	115	9	135	9	169	13	215	36	230	28	277	9	319	60	437	572
69	19	117	46	141	15	175	9	217	813	231	49	291	31	320	20	438	198
73	999	129	96	143	38	177	9	218	170	232	11	303	25	321	22	439	96
74	73	130	14	147	465	189	70	219	88	243	17	304	9	345	17	440	23
75	47	131	40	148	53	190	16	220	15	257	63	305	53	347	24		
89	10	133	94	149	54	191	77	221	37	258	15	306	25	361	23		

Synonyms:

1.FRUCTOSE 5T PK2-TENT;

Hit 101 : RH-T-1824.9-5.47%-CITRIC ACID 4T-CONF-[77-92-9]-RH03
CAS: 14330-97-3; Lib: tom18; ID: 101.



Name: RH-T-1824.9-5.47%-CITRIC ACID 4T-CONF-[77-92-9]-RH03

Formula: C₂₀H₄₆O₇Si₄

MW: 510 CAS#: 14330-97-3 ID#: 101 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:1824.9|

10 largest peaks:

273 999 | 73 823 | 147 618 | 347 256 | 274 253 | 363 229 | 375 226 | 211 121 | 275 112 | 75 111 |

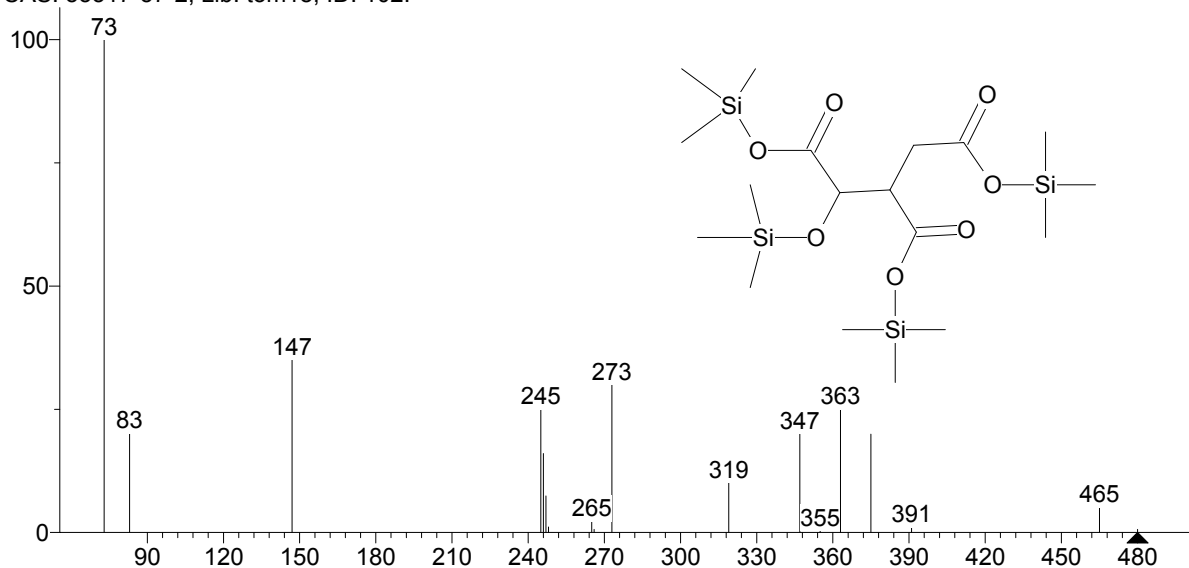
82 m/z Values and Intensities (147 low intensity peaks are not shown):

43 19	74 84	133 83	157 11	201 9	218 9	259 19	306 25	363 229	467 22
44 15	75 111	134 12	163 10	204 9	221 75	273 999	307 15	364 73	
45 86	99 15	135 10	171 11	205 10	222 17	274 253	319 21	365 36	
47 11	103 10	141 13	183 76	207 21	223 10	275 112	331 9	375 226	
58 9	115 24	143 25	184 12	211 121	229 26	276 17	333 21	376 72	
59 15	116 12	147 618	185 23	212 19	231 55	285 28	347 256	377 39	
67 42	117 20	148 105	189 14	213 22	232 11	301 19	348 78	378 9	
69 13	129 53	149 107	190 14	215 25	257 82	303 23	349 46	465 100	
73 823	131 42	150 14	191 12	217 48	258 19	305 88	350 10	466 40	

Synonyms:

1.CITRIC ACID 4T-CONF-[77-92-9];

Hit 102 : RH-T-1825.8-0.00%-ISOCITRIC ACID 4T-CONF-[320-77-4]-8135A18-G-X
CAS: 55517-57-2; Lib: tom18; ID: 102.



(tom18) RH-T-1825.8-0.00%-ISOCITRIC ACID 4T-CONF-[320-77-4]-8135A18-G-X RI:1825.8,

Name: RH-T-1825.8-0.00%-ISOCITRIC ACID 4T-CONF-[320-77-4]-8135A18-G-X

Formula: C₁₈H₄₀O₇Si₄

MW: 480 CAS#: 55517-57-2 ID#: 102 DB: tom18

Other DBs: None

RI: 1825.8,

Comment: RI=1825.8, 27.0414 min 8135A18 |RI:1825.8|

10 largest peaks:

73 999 | 147 349 | 273 299 | 245 249 | 363 249 | 83 200 | 347 199 | 375 199 | 246 160 | 319 100 |

15 m/z Values and Intensities (3 low intensity peaks are not shown):

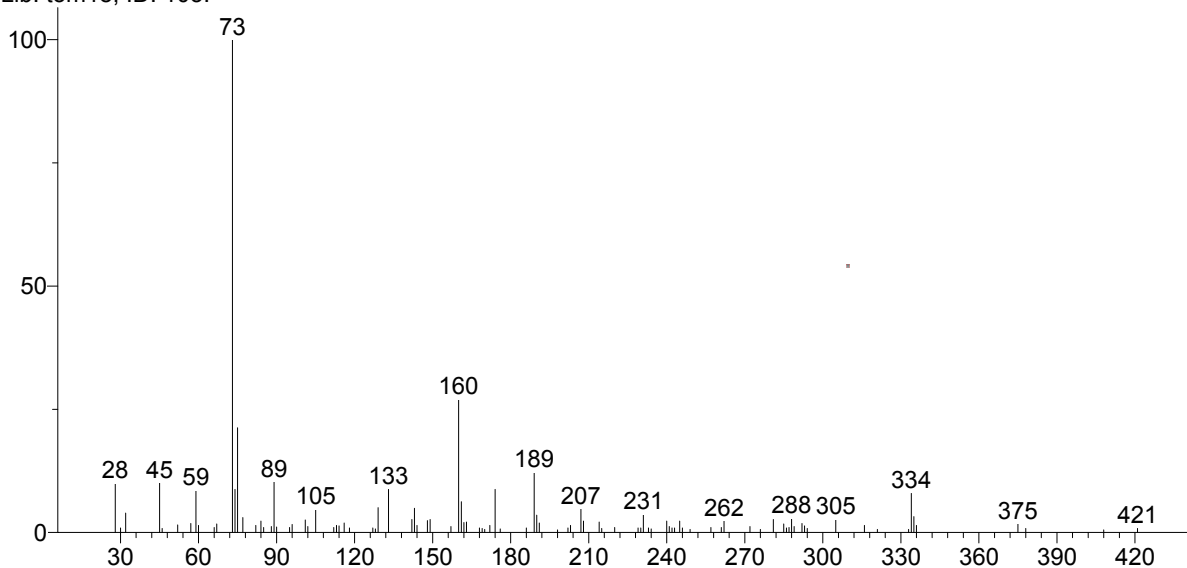
73 999 | 147 349 | 246 160 | 248 11 | 273 299 | 347 199 | 375 199 | 465 50 |
83 200 | 245 249 | 247 74 | 265 22 | 319 100 | 363 249 | 391 10 |

Synonyms:

1.ISOCITRIC ACID 4T-CONF-[320-77-4];

Hit 103 : RH-T-1832.1-0.02%-[160,189,334,133]-RH01

Lib: tom18; ID: 103.



(tom18) RH-T-1832.1-0.02%-[160,189,334,133]-RH01 RI:1832.1,

Name: RH-T-1832.1-0.02%-[160,189,334,133]-RH01

MW: N/A ID#: 103 DB: tom18

RI: 1832.1,

Comment: RI=1832.1, 29.6817 min AB2129 |RI:1832.1|

10 largest peaks:

73 999 | 160 269 | 75 212 | 189 121 | 89 102 | 45 100 | 28 99 | 74 87 | 133 87 | 174 87 |

84 m/z Values and Intensities (16 low intensity peaks are not shown):

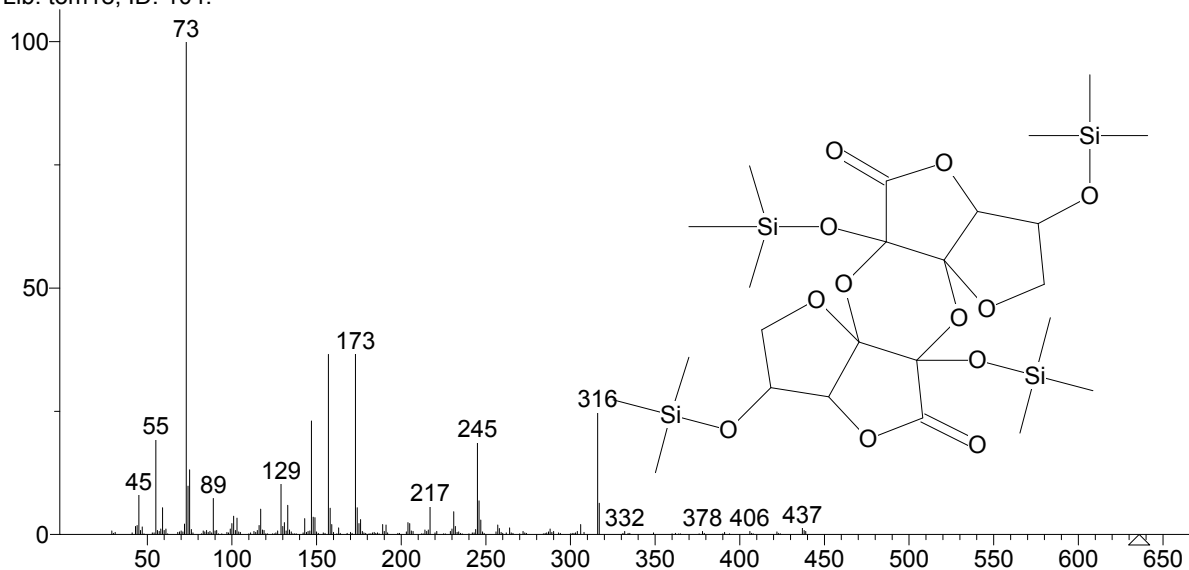
28 99	67 17	89 102	114 13	148 24	174 87	214 21	243 9	286 9	335 32
30 9	73 999	90 11	116 19	149 26	186 9	220 10	245 23	287 10	336 14
32 39	74 87	95 10	118 9	157 12	189 121	229 9	246 9	288 28	375 17
45 100	75 212	96 16	127 9	160 269	190 35	230 9	257 10	289 12	
52 15	77 30	101 25	129 50	161 62	191 19	231 36	261 10	292 18	
57 18	82 14	102 12	133 87	162 20	202 9	233 9	262 23	293 13	
59 85	84 23	105 46	142 26	163 21	203 14	240 23	272 12	305 26	
60 14	85 10	112 10	143 49	168 9	207 47	241 12	281 26	316 14	
66 10	88 12	113 14	144 14	172 14	208 23	242 9	285 17	334 79	

Synonyms:

1.m160,189,334,133;

Hit 104 : RH-T-1840.9-0.06%-DEHYDROASCORBIC ACID DIMER 4T-CONF-RH03

Lib: tom18; ID: 104.



(tom18) RH-T-1840.9-0.06%-DEHYDROASCORBIC ACID DIMER 4T-CONF-RH03 RI:1840.9,

Name: RH-T-1840.9-0.06%-DEHYDROASCORBIC ACID DIMER 4T-CONF-RH03

Formula: C₂₄H₄₄O₁₂Si₄

MW: 636 ID#: 104 DB: tom18

RI: 1840.9,

Comment: RI=1840.9, 34.5274 min MG00244 [RI:1840.9]

10 largest peaks:

73 999 | 173 366 | 157 365 | 316 247 | 147 230 | 55 192 | 245 186 | 75 131 | 129 102 | 74 98 |

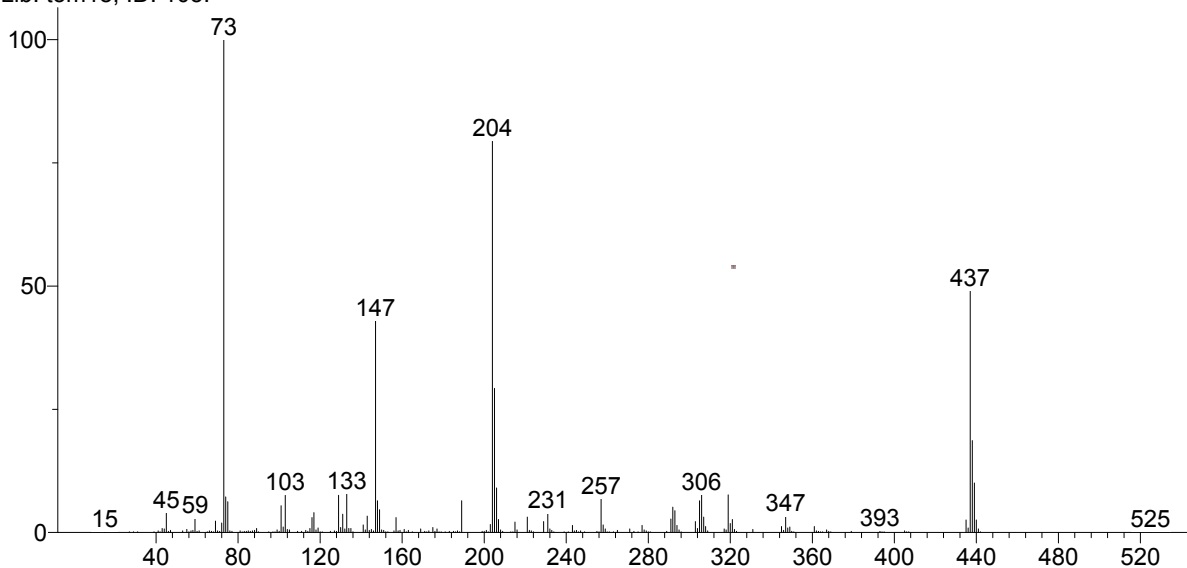
60 m/z Values and Intensities (145 low intensity peaks are not shown):

43 16	59 54	76 10	116 18	133 59	157 365	175 22	214 9	244 10	264 13
44 18	61 11	89 73	117 51	134 9	158 53	176 30	216 9	245 186	288 11
45 80	72 21	99 11	118 9	143 32	159 20	189 20	217 56	246 68	306 20
47 15	73 999	100 22	129 102	147 230	163 13	191 19	230 11	247 29	316 247
55 192	74 98	101 37	130 16	148 35	173 366	204 24	231 46	257 19	317 63
58 11	75 131	103 33	131 24	149 34	174 54	205 22	232 16	258 12	437 13

Synonyms:

1.DEHYDROASCORBIC ACID DIMER 4T-CONF;

Hit 105 : RH-T-1846.9-0.86%-[204,437,306,257, N: sim. D-Fructose 5T]-RH03
 Lib: tom18; ID: 105.



(tom18) RH-T-1846.9-0.86%-[204,437,306,257, N: sim. D-Fructose 5T]-RH03 RI:1846.9,

Name: RH-T-1846.9-0.86%-[204,437,306,257, N: sim. D-Fructose 5T]-RH03

MW: N/A ID#: 105 DB: tom18

RI: 1846.9,

Comment: RI=1846.9, 34.6816 min MG00244 [RI:1846.9]

10 largest peaks:

73 999 | 204 793 | 437 489 | 147 429 | 205 292 | 438 186 | 439 100 | 206 90 | 133 78 | 306 76 |

61 m/z Values and Intensities (153 low intensity peaks are not shown):

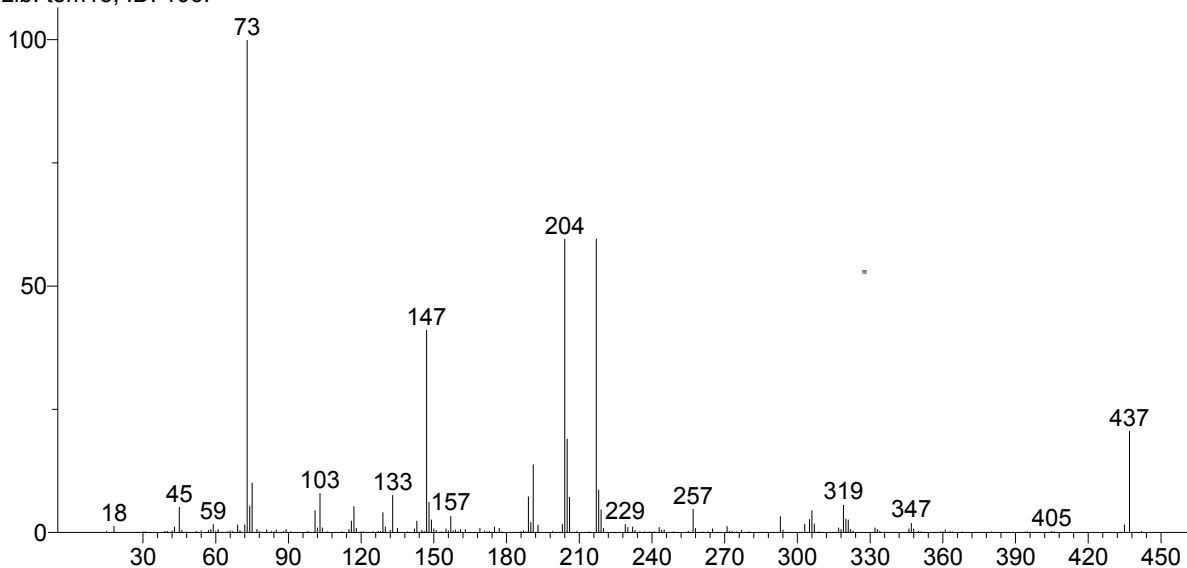
45	39	101	54	130	10	149	46	206	90	257	68	303	22	321	26	436	9
59	28	102	11	131	37	157	30	207	26	258	15	305	64	345	12	437	489
69	23	103	75	133	78	175	10	215	21	277	14	306	76	347	32	438	186
72	19	116	30	141	15	189	64	221	31	291	27	307	31	348	9	439	100
73	999	117	40	143	33	203	16	229	22	292	51	308	12	349	11	440	25
74	72	119	9	147	429	204	793	231	38	293	44	319	76	361	12		
75	62	129	75	148	64	205	292	243	14	294	14	320	18	435	25		

Synonyms:

1.m204,437,306,257, N: sim. D-Fructose 5T;

Hit 106 : RH-T-1850.2-0.31%-[204,217,437, N: D-Fructose T5]-RH03

Lib: tom18; ID: 106.



(tom18) RH-T-1850.2-0.31%-[204,217,437, N: D-Fructose T5]-RH03 RI:1850.2,

Name: RH-T-1850.2-0.31%-[204,217,437, N: D-Fructose T5]-RH03

MW: N/A ID#: 106 DB: tom18

RI: 1850.2,

Comment: RI=1850.2, 34.7640 min MG00251 |RI:1850.2|

10 largest peaks:

73 999 | 204 595 | 217 595 | 147 410 | 437 205 | 205 189 | 191 137 | 75 100 | 218 86 | 103 80 |

54 m/z Values and Intensities (108 low intensity peaks are not shown):

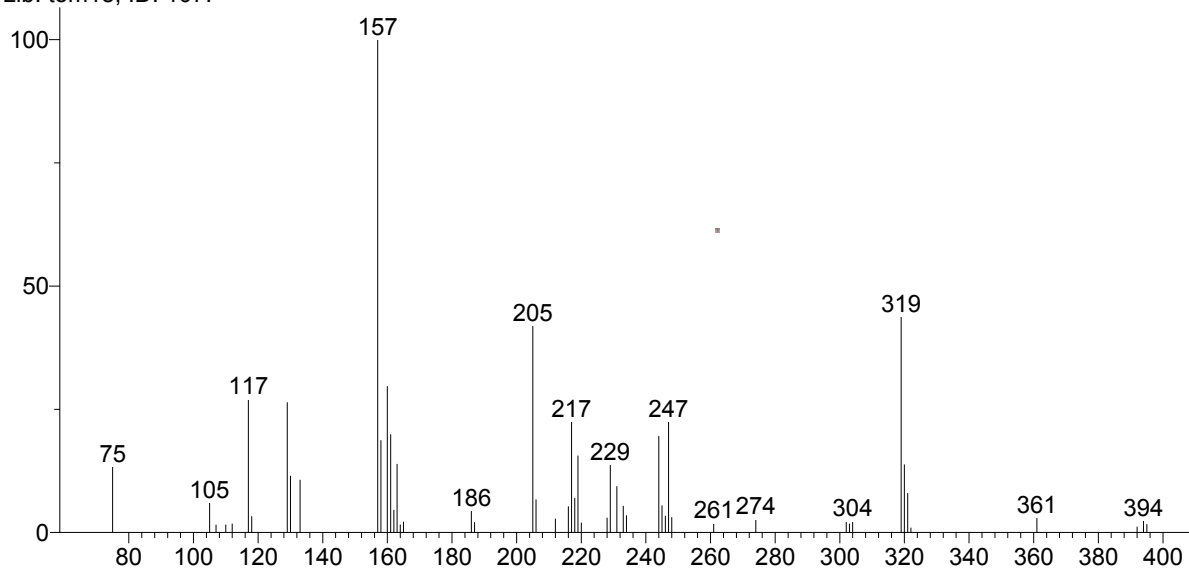
18	13	73	999	104	9	143	23	189	72	205	189	230	10	303	16	320	27
43	11	74	53	116	23	147	410	190	20	206	71	232	11	305	26	321	25
45	51	75	100	117	52	148	61	191	137	217	595	243	10	306	44	332	9
59	16	101	44	129	40	149	25	193	15	218	86	257	47	307	17	347	20
69	15	102	9	130	11	157	34	203	16	219	46	271	12	317	9	435	15
72	15	103	80	133	75	175	11	204	595	229	16	293	32	319	56	437	205

Synonyms:

1.m204,217,437, N: D-Fructose T5;

Hit 107 : RH-T-1850.5-0.02%-[157,319,205,244,117]-RH01-X

Lib: tom18; ID: 107.



(tom18) RH-T-1850.5-0.02%-[157,319,205,244,117]-RH01-X RI:1850.5,

Name: RH-T-1850.5-0.02%-[157,319,205,244,117]-RH01-X

MW: N/A ID#: 107 DB: tom18

RI: 1850.5,

Comment: RI=1850.5, 30.0586 min AB2129 |RI:1850.5|

10 largest peaks:

157 999 | 319 436 | 205 419 | 160 296 | 117 269 | 129 263 | 217 224 | 247 223 | 161 198 | 244 195 |

51 m/z Values and Intensities:

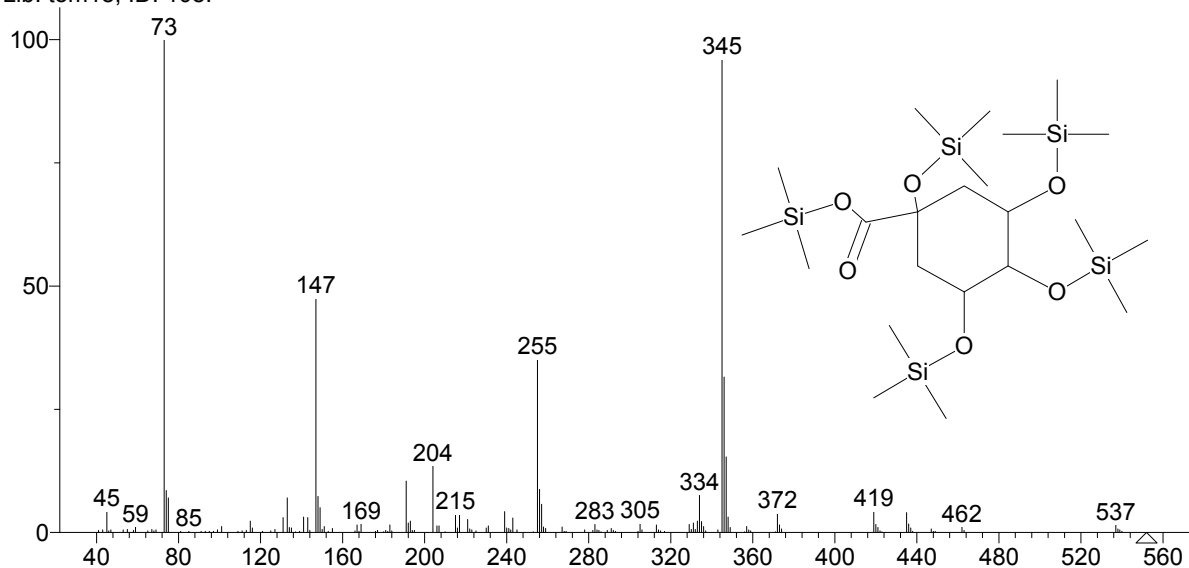
75 133 | 118 32 | 160 296 | 186 43 | 217 224 | 231 93 | 247 223 | 304 22 | 392 11 |
105 60 | 129 263 | 161 198 | 187 20 | 218 69 | 233 53 | 248 30 | 319 436 | 394 23 |
107 15 | 130 114 | 162 45 | 205 419 | 219 155 | 234 34 | 261 18 | 320 137 | 395 16 |
110 15 | 133 106 | 163 138 | 206 66 | 220 19 | 244 195 | 274 26 | 321 79 |
112 17 | 157 999 | 164 15 | 212 27 | 228 29 | 245 54 | 302 21 | 322 9 |
117 269 | 158 186 | 165 21 | 216 52 | 229 136 | 246 33 | 303 17 | 361 29 |

Synonyms:

1.m157,319,205,244,117;

Hit 108 : RH-T-1856.7-0.29%-QUINIC ACID 5T-CONF-[77-95-2]-RH03

Lib: tom18; ID: 108.



(tom18) RH-T-1856.7-0.29%-QUINIC ACID 5T-CONF-[77-95-2]-RH03

Name: RH-T-1856.7-0.29%-QUINIC ACID 5T-CONF-[77-95-2]-RH03

Formula: C₂₂H₅₂O₆Si₅

MW: 552 ID#: 108 DB: tom18

Comment: RI:MG00238 [RI:1856.7]

10 largest peaks:

73 999 | 345 959 | 147 474 | 255 350 | 346 315 | 347 153 | 204 135 | 191 104 | 256 87 | 74 85 |

66 m/z Values and Intensities (84 low intensity peaks are not shown):

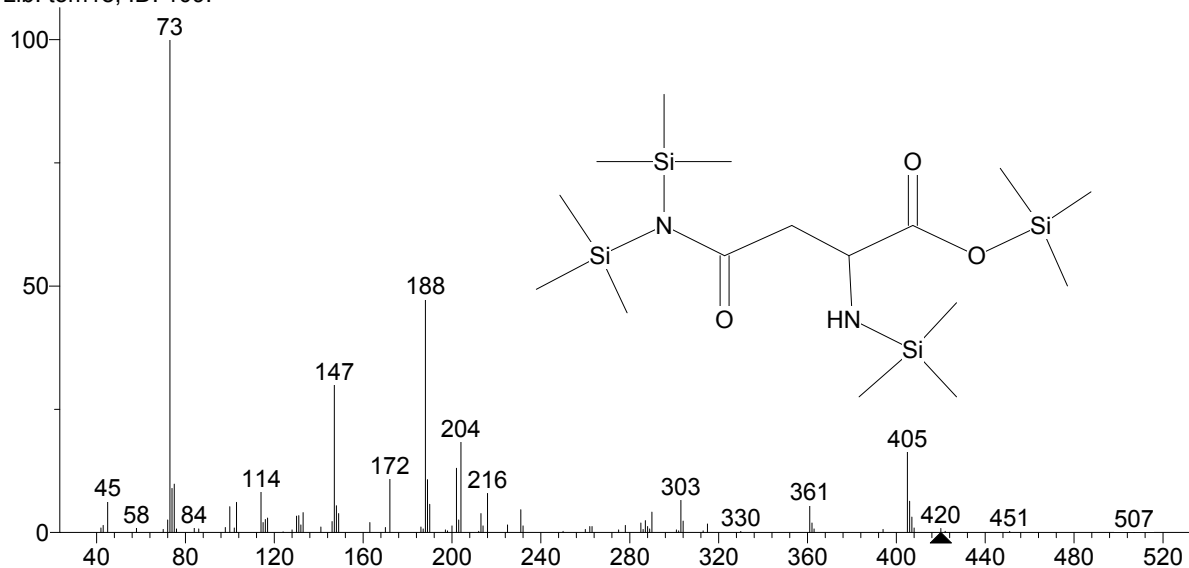
45	42	116	9	147	474	191	104	216	9	243	29	305	18	336	12	372	38	437	9
59	11	131	30	148	73	192	19	217	35	255	350	313	15	345	959	373	15	462	11
73	999	133	70	149	50	193	23	221	26	256	87	329	16	346	315	419	42	537	15
74	85	134	10	151	12	204	135	230	9	257	57	331	19	347	153	420	16		
75	70	135	9	167	15	206	13	231	13	258	11	333	23	348	31	421	10		
101	12	141	31	169	17	207	13	239	42	267	11	334	75	349	10	435	40		
115	23	143	30	183	15	215	36	240	9	283	16	335	22	357	12	436	17		

Synonyms:

1.QUINIC ACID 5T-CONF-[77-95-2];

Hit 109 : RH-T-1863.3-0.02%-[G:L-Asparagine (4TMS)]-TENT-RH03

Lib: tom18; ID: 109.



(tom18) RH-T-1863.3-0.02%-[G:L-Asparagine (4TMS)]-TENT-RH03 RI:1863.3,

Name: RH-T-1863.3-0.02%-[G:L-Asparagine (4TMS)]-TENT-RH03

Formula: C₁₆H₄₀N₂O₃Si₄

MW: 420 ID#: 109 DB: tom18

RI: 1863.3,

Comment: RI=1863.3, 35.0996 min MG00244 [RI:1863.3]

10 largest peaks:

73 999 | 188 472 | 147 299 | 204 183 | 405 163 | 202 130 | 172 108 | 189 107 | 75 98 | 74 89 |

59 m/z Values and Intensities (24 low intensity peaks are not shown):

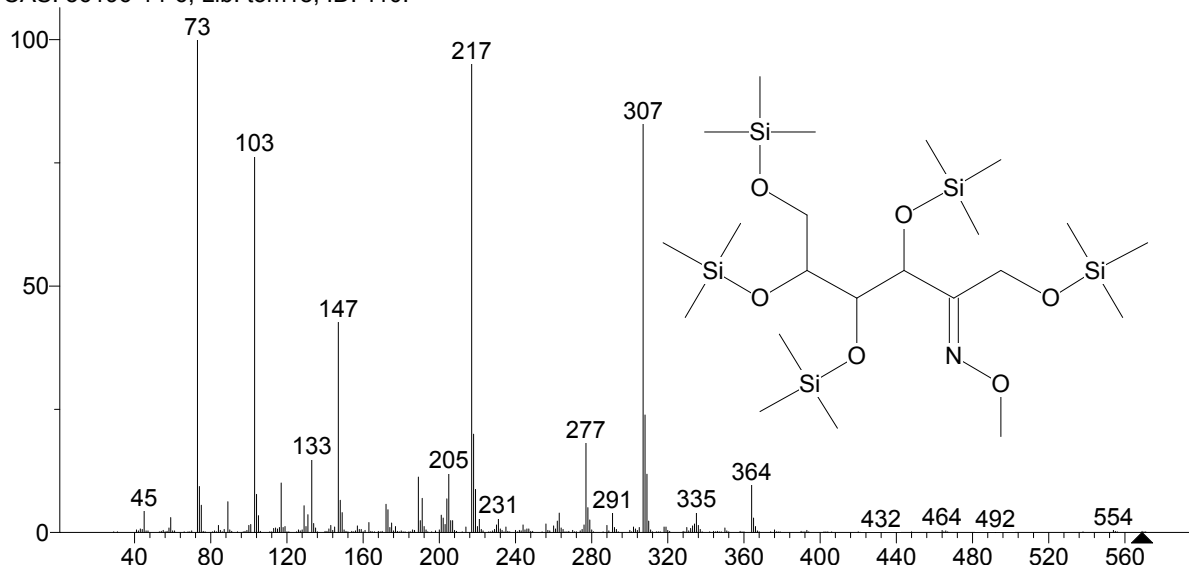
42	9	74	89	103	61	131	34	148	54	188	472	204	183	232	13	288	12	362	19
43	14	75	98	114	82	132	15	149	38	189	107	213	38	262	12	290	41	405	163
45	62	84	9	115	20	133	40	163	20	190	57	214	13	263	12	303	65	406	63
58	9	98	10	116	26	141	11	170	10	200	13	216	79	278	14	304	23	407	31
72	25	100	52	117	29	146	22	172	108	202	130	225	15	285	19	315	17	408	9
73	999	102	9	130	33	147	299	186	11	203	25	231	46	287	24	361	54		

Synonyms:

1.Asparagine 4T;

Hit 110 : RH-T-1876.3-9.44%-FRUCTOSE M5T PK1-CONF-[57-48-7]-RH03

CAS: 56196-14-6; Lib: tom18; ID: 110.



(tom18) RH-T-1876.3-9.44%-FRUCTOSE M5T PK1-CONF-[57-48-7]-RH03 RI:1876.1,

Name: RH-T-1876.3-9.44%-FRUCTOSE M5T PK1-CONF-[57-48-7]-RH03

Formula: C₂₂H₅₅NO₆Si₅

MW: 569 CAS#: 56196-14-6 ID#: 110 DB: tom18

Other DBs: None

RI: 1876.1,

Comment: RI=1876.1, 30.5853 min AB2129 [RI:1876.3]

10 largest peaks:

73 999 | 217 950 | 307 828 | 103 762 | 147 426 | 308 238 | 218 199 | 277 181 | 133 148 | 205 119 |

86 m/z Values and Intensities (182 low intensity peaks are not shown):

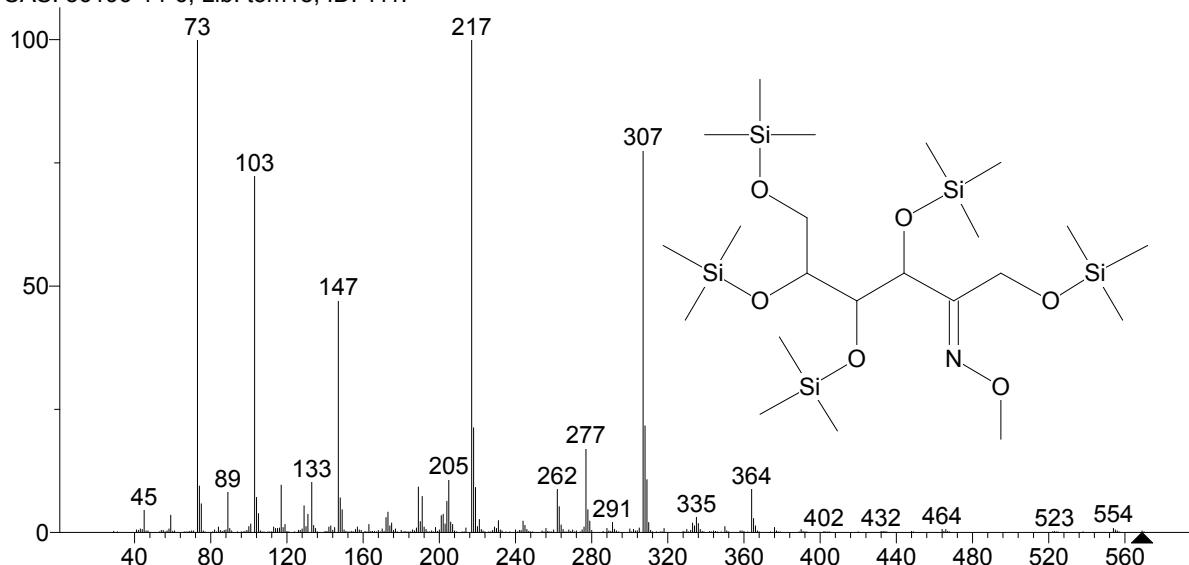
45	43	101	16	129	54	148	65	189	112	206	24	231	28	277	181	308	238	336	14
58	9	103	762	130	12	149	40	190	24	207	24	235	11	278	50	309	118	350	9
59	30	104	77	131	36	157	13	191	69	214	11	244	15	279	25	310	23	364	96
73	999	105	34	133	148	163	20	192	12	217	950	256	17	288	14	318	11	365	29
74	93	114	9	134	18	172	57	201	35	218	199	260	13	291	39	319	11	366	12
75	55	116	10	135	9	173	46	202	29	219	87	262	23	292	10	330	10		
84	14	117	100	143	14	174	10	203	16	220	12	263	39	302	11	333	13		
89	62	118	10	145	11	175	19	204	68	221	28	264	9	305	10	334	17		
100	14	119	12	147	426	177	12	205	119	230	15	276	15	307	828	335	40		

Synonyms:

1.FRUCTOSE M5T PK1-CONF;

Hit 111 : RH-T-1886.2-6.96%-FRUCTOSE M5T PK2-CONF-[57-48-7]-RH03

CAS: 56196-14-6; Lib: tom18; ID: 111.



(tom18) RH-T-1886.2-6.96%-FRUCTOSE M5T PK2-CONF-[57-48-7]-RH03 RI:1886.0,

Name: RH-T-1886.2-6.96%-FRUCTOSE M5T PK2-CONF-[57-48-7]-RH03

Formula: C₂₂H₅₅NO₆Si₅

MW: 569 CAS#: 56196-14-6 ID#: 111 DB: tom18

Other DBs: None

RI: 1886.0,

Comment: RI=1886.0, 30.7888 min AB2129 [RI:1886.2]

10 largest peaks:

73 999 | 217 998 | 307 774 | 103 723 | 147 470 | 308 216 | 218 212 | 277 170 | 205 107 | 309 107 |

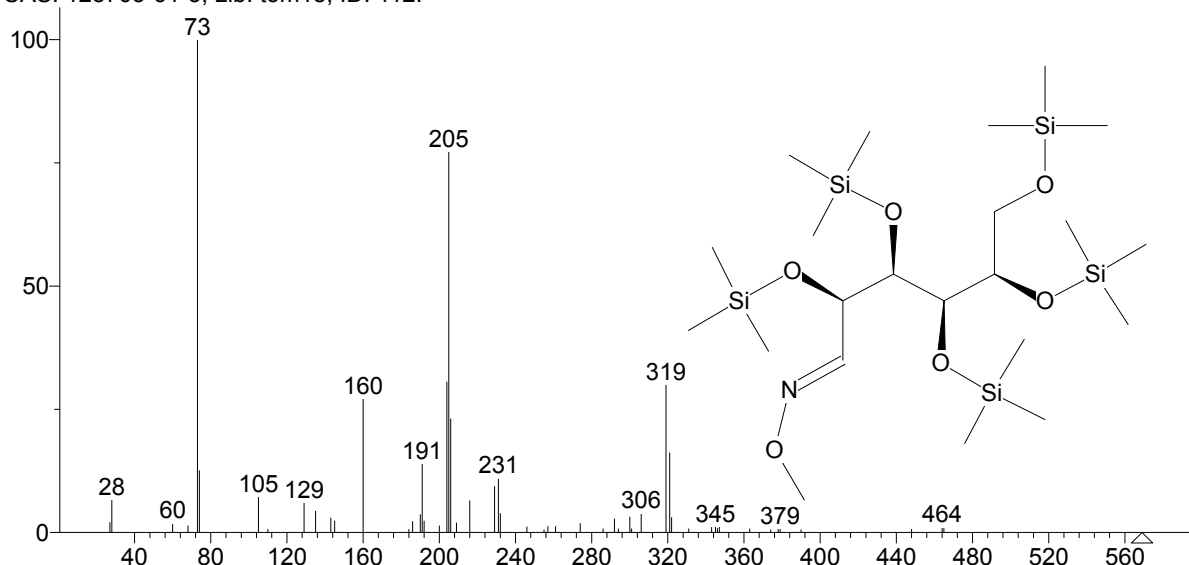
80 m/z Values and Intensities (210 low intensity peaks are not shown):

45	45	101	17	119	16	145	10	174	13	201	34	217	998	245	14	291	21	335	31
59	35	103	723	129	54	147	470	175	19	202	37	218	212	262	87	305	9	336	18
73	999	104	71	130	12	148	70	188	9	203	17	219	91	263	52	307	774	350	12
74	94	105	38	131	37	149	46	189	92	204	63	220	12	264	15	308	216	364	88
75	58	113	11	133	102	157	11	190	22	205	107	221	26	276	11	309	107	365	28
84	11	116	9	134	14	163	16	191	73	206	21	229	11	277	170	310	20	366	13
89	82	117	96	142	11	172	30	192	11	207	16	231	24	278	46	333	19	376	10
100	12	118	10	143	13	173	41	198	10	214	9	244	23	279	23	334	13	554	10

Synonyms:

1.FRUCTOSE M5T PK2;

Hit 112 : RH-T-1887.7-0.01%-MANNOSE M5T-TENT-RH01-X
CAS: 128705-61-3; Lib: tom18; ID: 112.



(tom18) RH-T-1887.7-0.01%-MANNOSE M5T-TENT-RH01-X RI:1887.7,

Name: RH-T-1887.7-0.01%-MANNOSE M5T-TENT-RH01-X

Formula: C₂₂H₅₅NO₆Si₅

MW: 569 CAS#: 128705-61-3 ID#: 112 DB: tom18

Other DBs: None

RI: 1887.7,

Comment: RI=1887.7, 30.8240 min AB2129 [RI:1887.7]

10 largest peaks:

73 999 | 205 771 | 204 305 | 319 299 | 160 271 | 206 230 | 321 161 | 191 138 | 74 125 | 231 109 |

39 m/z Values and Intensities (15 low intensity peaks are not shown):

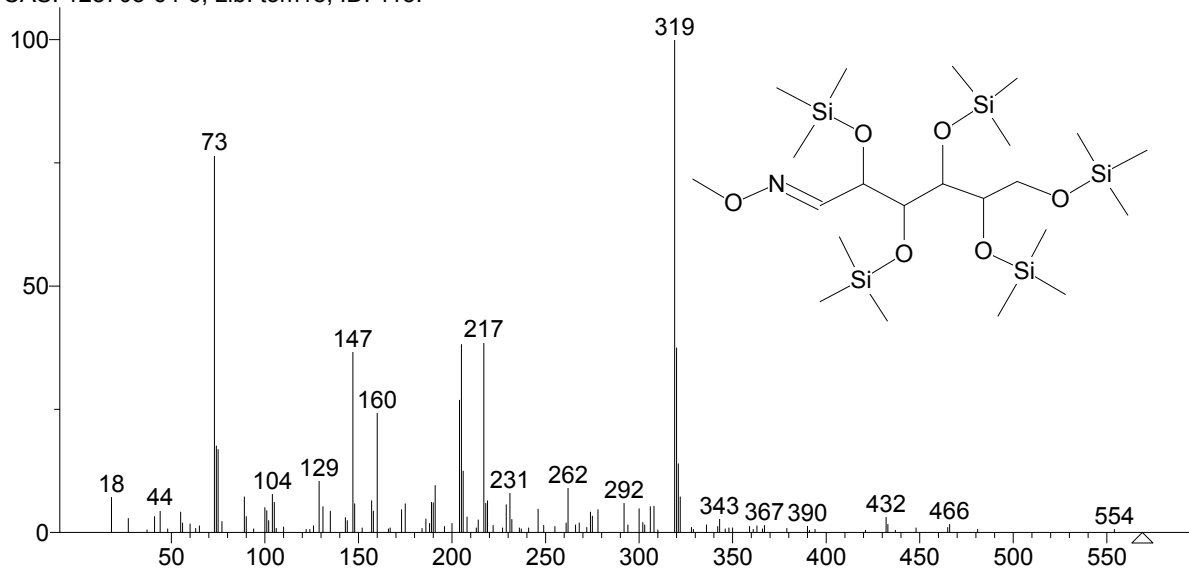
27	20	73	999	135	43	186	22	200	13	209	19	232	38	274	18	319	299	345	11
28	65	74	125	143	29	190	36	204	305	216	64	246	11	292	27	321	161	347	11
60	18	105	72	145	23	191	138	205	771	229	93	257	12	300	31	322	30	464	10
68	13	129	60	160	271	192	23	206	230	231	109	261	12	306	38	343	10		

Synonyms:

1.MANNOSE M5T;

Hit 113 : RH-T-1890.4-0.01%-GALACTOSE-M5T-TENT-RH01

CAS: 128705-64-6; Lib: tom18; ID: 113.



(tom18) RH-T-1890.4-0.01%-GALACTOSE-M5T-TENT-RH01 RI:1890.4,

Name: RH-T-1890.4-0.01%-GALACTOSE-M5T-TENT-RH01

Formula: C₂₂H₅₅NO₆Si₅

MW: 569 CAS#: 128705-64-6 ID#: 113 DB: tom18

Other DBs: None

RI: 1890.4,

Comment: RI=1890.4, 30.8795 min AB2129 |RI:1890.4|

10 largest peaks:

319 999 | 73 764 | 217 385 | 205 381 | 320 374 | 147 366 | 204 268 | 160 242 | 74 175 | 75 168 |

95 m/z Values and Intensities (22 low intensity peaks are not shown):

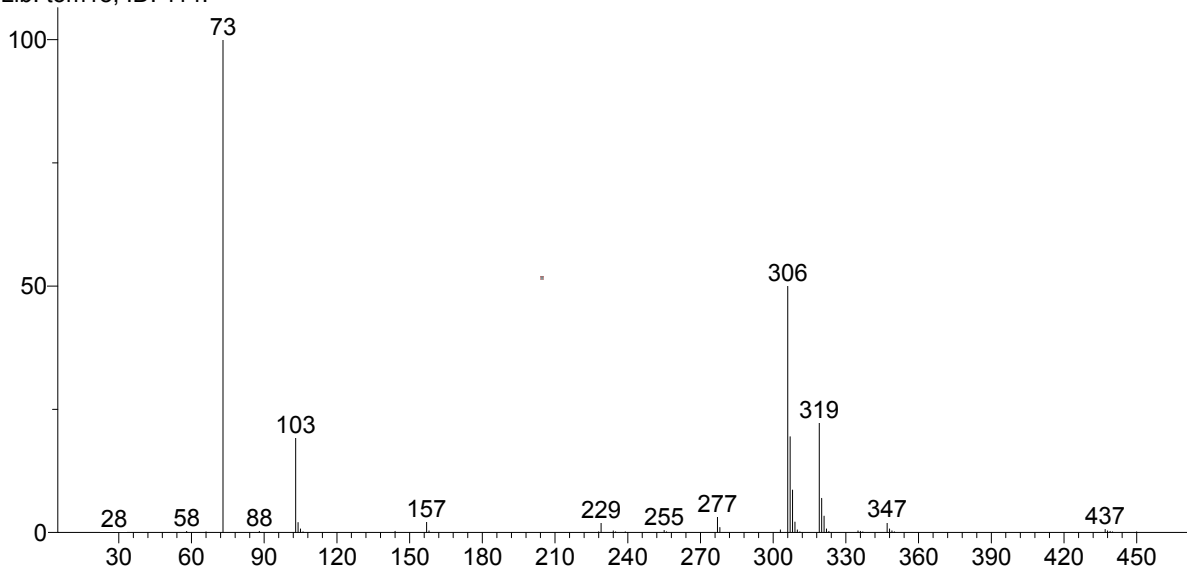
18 71	75 168	126 13	158 43	196 12	219 64	255 12	294 15	328 10	432 31
27 28	77 22	129 104	160 242	200 18	222 14	261 19	300 48	336 15	433 16
41 32	89 72	131 52	167 9	204 268	227 9	262 90	302 20	342 12	448 9
44 44	90 32	135 43	173 46	205 381	229 56	266 15	303 15	343 27	465 10
55 41	100 50	143 30	175 58	206 124	231 80	268 19	306 52	348 9	466 16
56 19	101 44	144 24	186 27	208 31	232 26	272 10	308 53	350 9	
60 17	102 24	147 366	188 18	213 9	236 9	274 41	319 999	359 12	
65 13	104 77	148 58	189 61	214 25	241 9	275 33	320 374	363 13	
73 764	105 61	152 9	190 60	217 385	246 47	278 46	321 139	367 14	
74 175	110 11	157 64	191 95	218 59	249 14	292 59	322 72	390 13	

Synonyms:

1.GALACTOSE-M5T-TENT;

Hit 114 : RH-T-1891.5-0.69%-[306,319,103, poorly resolved]-RH03-X

Lib: tom18; ID: 114.



(tom18) RH-T-1891.5-0.69%-[306,319,103, poorly resolved]-RH03-X RI:1891.5,

Name: RH-T-1891.5-0.69%-[306,319,103, poorly resolved]-RH03-X

MW: N/A ID#: 114 DB: tom18

RI: 1891.5,

Comment: RI=1891.5, 35.8232 min MG00246 [RI:1891.5]

10 largest peaks:

73 999 | 306 499 | 319 222 | 307 194 | 103 191 | 308 86 | 320 69 | 321 33 | 277 31 | 157 21 |

15 m/z Values and Intensities (30 low intensity peaks are not shown):

73 999 | 104 20 | 229 19 | 278 10 | 307 194 | 309 21 | 320 69 | 347 20 |

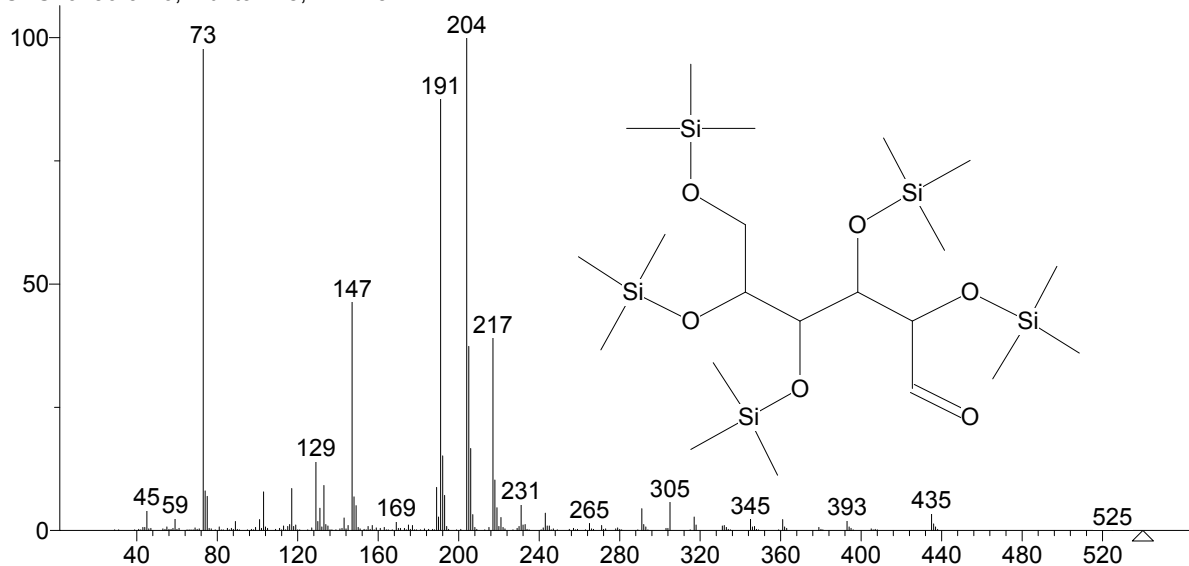
103 191 | 157 21 | 277 31 | 306 499 | 308 86 | 319 222 | 321 33 |

Synonyms:

1.m306,319,103, poorly resolved;

Hit 115 : RH-T-1894.6-5.00%-GLUCOSE 5T-TENT-RH03

CAS: 6736-97-6; Lib: tom18; ID: 115.



(tom18) RH-T-1894.6-5.00%-GLUCOSE 5T-TENT-RH03

Name: RH-T-1894.6-5.00%-GLUCOSE 5T-TENT-RH03

Formula: C₂₁H₅₂O₆Si₅

MW: 540 CAS#: 6736-97-6 ID#: 115 DB: tom18

Other DBs: None

Comment: RI:MG00251 |RI:1894.6|

10 largest peaks:

204 999 | 73 977 | 191 875 | 147 463 | 217 390 | 205 373 | 206 166 | 192 151 | 129 139 | 218 102 |

60 m/z Values and Intensities (148 low intensity peaks are not shown):

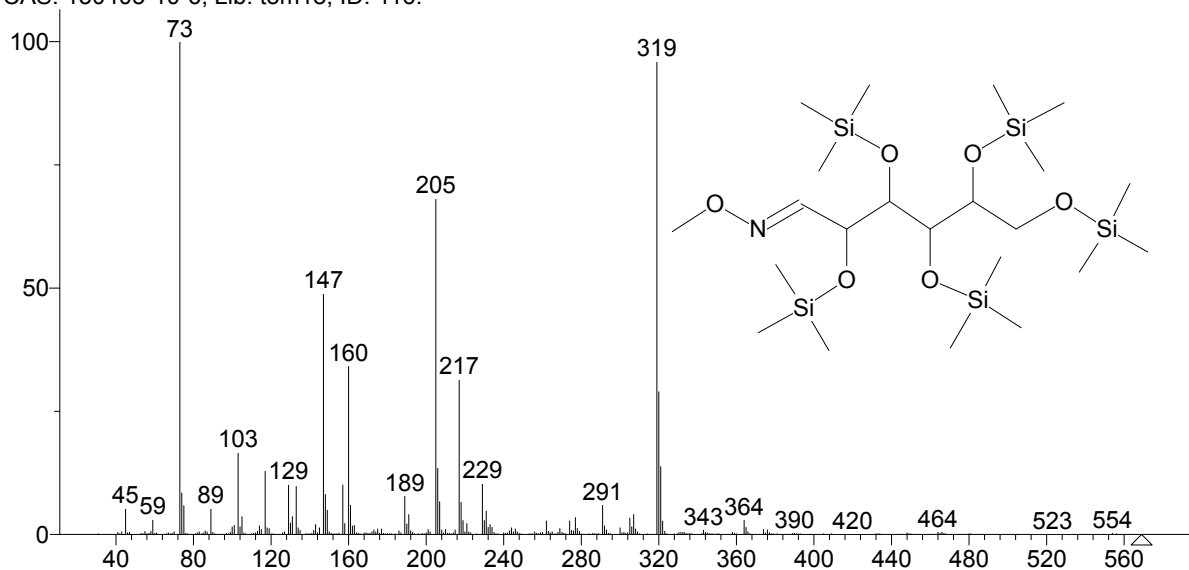
45	40	101	22	129	139	143	25	169	18	192	151	217	390	233	12	291	44	332	10
59	24	103	78	130	18	145	10	175	11	193	71	218	102	243	35	292	12	345	23
73	977	113	9	131	45	147	463	177	10	204	999	219	46	244	9	305	57	361	22
74	80	116	12	133	91	148	68	189	87	205	373	221	26	245	9	317	27	393	20
75	69	117	85	134	12	149	50	190	27	206	166	231	52	265	14	318	11	435	34
89	18	119	11	135	9	157	10	191	875	207	32	232	11	271	10	331	9	436	13

Synonyms:

1.GLUCOSE 5T;

Hit 116 : RH-T-1901.9-9.14%-GLUCOSE M5T PK1-CONF-[50-99-7]-RH01

CAS: 130405-10-6; Lib: tom18; ID: 116.



(tom18) RH-T-1901.9-9.14%-GLUCOSE M5T PK1-CONF-[50-99-7]-RH01 RI:1901.9,

Name: RH-T-1901.9-9.14%-GLUCOSE M5T PK1-CONF-[50-99-7]-RH01

Formula: C₂₂H₅₅NO₆Si₅

MW: 569 CAS#: 130405-10-6 ID#: 116 DB: tom18

Other DBs: None

RI: 1901.9,

Comment: RI=1901.9, 31.1138 min AB2129 [RI:1901.9]

10 largest peaks:

73 999 | 319 959 | 205 681 | 147 488 | 160 341 | 217 314 | 320 289 | 103 166 | 321 137 | 206 134 |

79 m/z Values and Intensities (191 low intensity peaks are not shown):

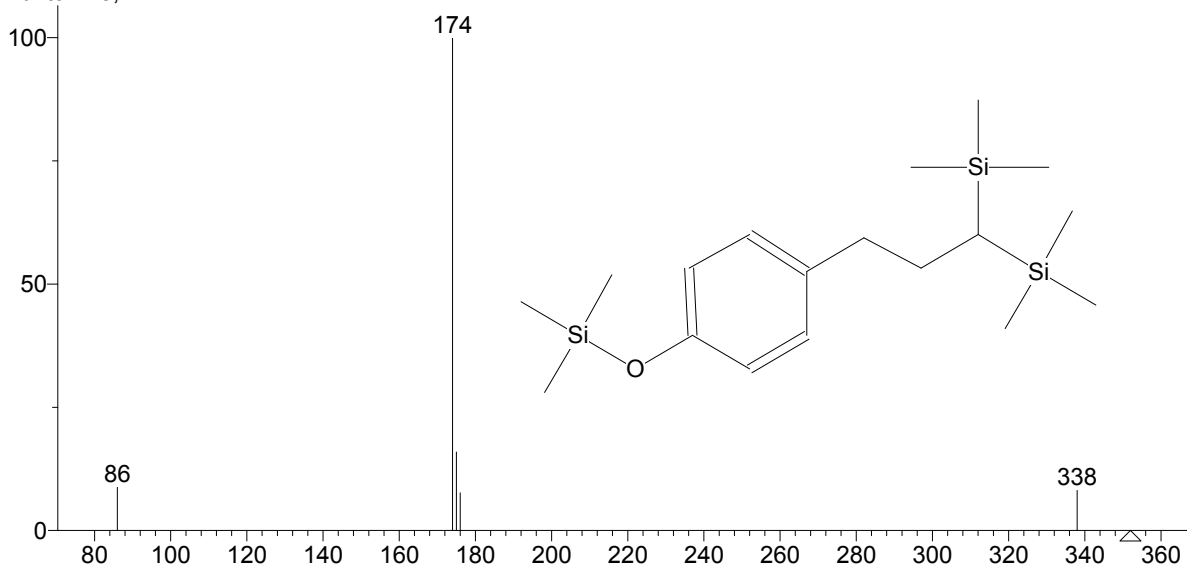
45	52	103	166	129	101	148	81	173	9	206	134	221	22	246	11	293	9	321	137
59	30	104	15	130	23	149	49	175	11	207	66	229	103	262	27	300	13	322	27
73	999	105	36	131	36	157	100	177	11	208	9	230	28	269	12	305	33	343	9
74	84	114	17	133	97	158	22	189	78	210	10	231	47	274	27	306	15	364	29
75	58	115	10	134	13	160	341	190	21	215	9	232	14	277	34	307	40	365	14
89	52	117	128	143	20	161	59	191	40	217	314	233	20	278	12	308	11	374	10
100	15	118	13	145	13	162	17	201	10	218	65	234	14	291	59	319	959	376	9
101	18	119	12	147	488	163	18	205	681	219	28	244	13	292	17	320	289		

Synonyms:

1.GLUCOSE M5T PK1-CONF-[50-99-7];

Hit 117 : RH-T-1905.6-0.00%-TYRAMINE 3T-TENT-[51-67-2]-RH03-X

Lib: tom18; ID: 117.



(tom18) RH-T-1905.6-0.00%-TYRAMINE 3T-TENT-[51-67-2]-RH03-X

Name: RH-T-1905.6-0.00%-TYRAMINE 3T-TENT-[51-67-2]-RH03-X

Formula: C₁₈H₃₆OSi₃

MW: 352 ID#: 117 DB: tom18

Comment: RI:MG00238 [RI:1905.6]

5 largest peaks:

174 999 | 175 159 | 86 88 | 338 81 | 176 76 |

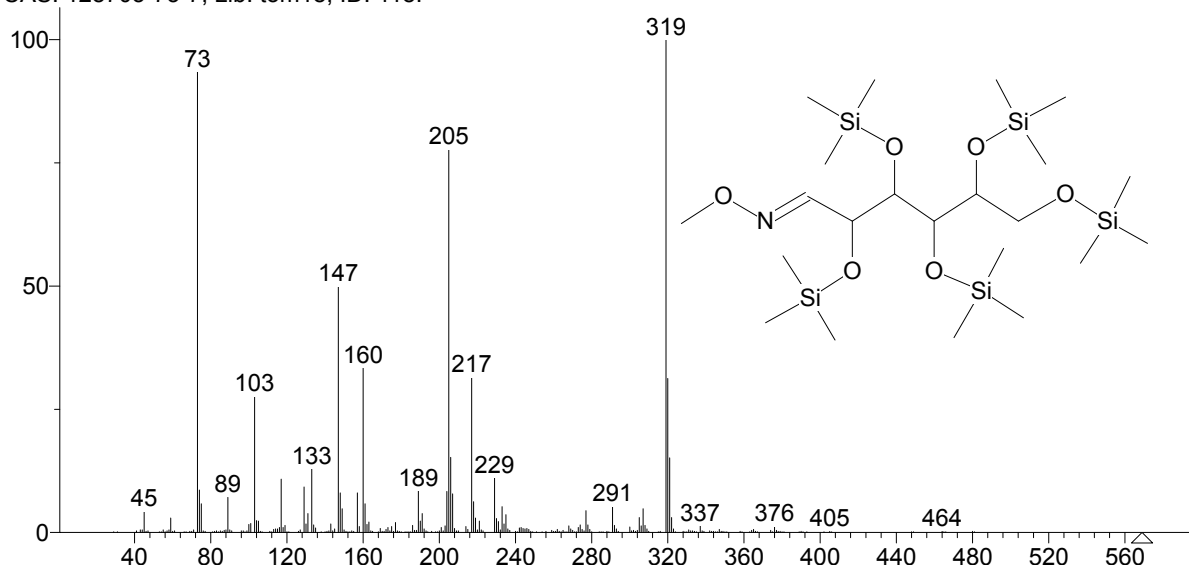
5 m/z Values and Intensities:

86 88 | 174 999 | 175 159 | 176 76 | 338 81 |

Synonyms:

1.TYRAMINE 3T-TENT;

Hit 118 : RH-T-1916.2-4.98%-GLUCOSE M5T PK2-CONF-[50-99-7]-RH01
CAS: 128705-73-7; Lib: tom18; ID: 118.



(tom18) RH-T-1916.2-4.98%-GLUCOSE M5T PK2-CONF-[50-99-7]-RH01 RI:1916.2,

Name: RH-T-1916.2-4.98%-GLUCOSE M5T PK2-CONF-[50-99-7]-RH01

Formula: C₂₂H₅₅NO₆Si₅

MW: 569 CAS#: 128705-73-7 ID#: 118 DB: tom18

Other DBs: None

RI: 1916.2,

Comment: RI=1916.2, 31.3948 min AB2129 [RI:1916.2]

10 largest peaks:

319 999 | 73 934 | 205 776 | 147 498 | 160 333 | 217 314 | 320 312 | 103 275 | 206 152 | 321 151 |

75 m/z Values and Intensities (188 low intensity peaks are not shown):

45 42	103 275	130 17	149 48	175 12	204 83	221 23	243 10	300 11	322 30
59 29	104 24	131 38	157 80	177 20	205 776	229 110	268 13	305 30	337 13
73 934	105 23	133 128	158 12	186 14	206 152	230 28	273 10	306 13	376 12
74 86	116 10	134 15	160 333	189 84	207 78	231 22	274 15	307 48	
75 58	117 108	135 9	161 58	190 23	214 12	233 52	277 44	308 14	
89 71	118 10	143 17	162 16	191 38	217 314	234 17	278 15	319 999	
100 16	119 14	147 498	163 21	201 10	218 62	235 36	291 52	320 312	
101 18	129 92	148 80	173 10	203 13	219 29	242 9	292 14	321 151	

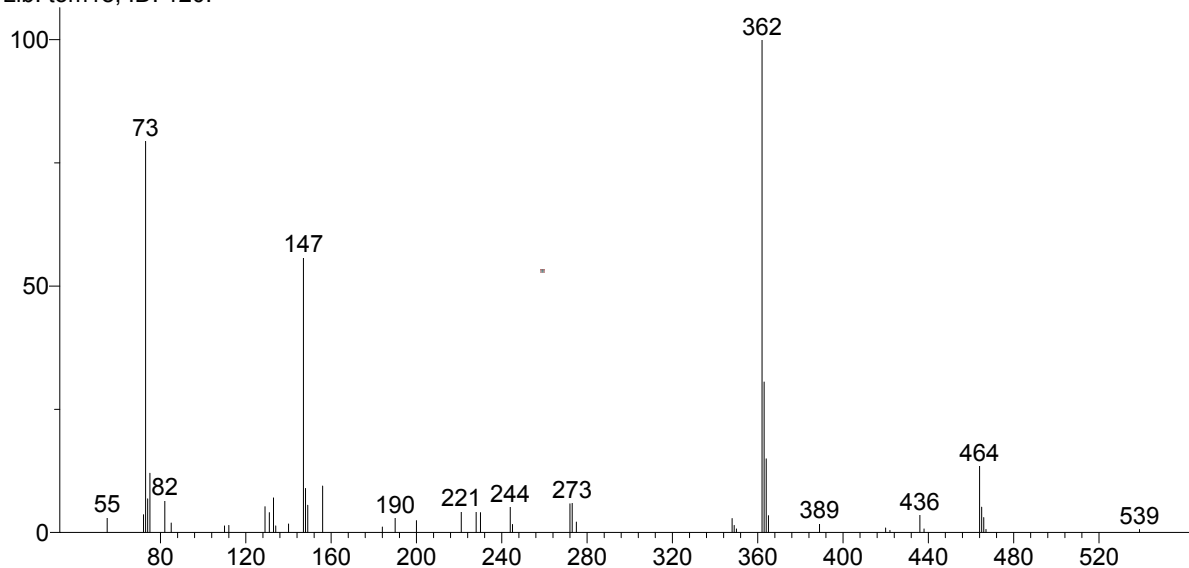
Synonyms:

1.GLUCOSE M5T PK2-CONF;

Mass spectrum of polydimethylsiloxane (PDMS) showing relative intensity versus m/z . The base peak is at m/z 73. Other significant peaks are labeled at m/z 45, 59, 86, 100, 128, 147, 156, 174, 186, 200, 218, 230, 244, 272, 301, 317, 329, 391, and 434. A chemical structure of a PDMS chain segment is shown above the spectrum.

1.Lysine 4T;

Hit 120 : RH-T-1926.0-0.00%-[362,464,273,539, G: EIQTMS_N12C_ATHL_1928.1_3161BN34_[NA]]-RH03
Lib: tom18; ID: 120.



(tom18) RH-T-1926.0-0.00%-[362,464,273,539, G: EIQTMS_N12C_ATHL_1928.1_3161BN34_[NA]]-RH03 RI:1926.0,

Name: RH-T-1926.0-0.00%-[362,464,273,539, G: EIQTMS_N12C_ATHL_1928.1_3161BN34_[NA]]-RH03

MW: N/A ID#: 120 DB: tom18

RI: 1926.0,

Comment: RI=1926.0, 36.6766 min MG00238 [RI:1926]

10 largest peaks:

362 999 | 73 793 | 147 557 | 363 305 | 364 149 | 464 135 | 75 120 | 156 94 | 148 89 | 133 70 |

41 m/z Values and Intensities (5 low intensity peaks are not shown):

55 30 | 82 64 | 131 40 | 148 89 | 200 24 | 245 16 | 349 14 | 389 18 | 466 30 |

72 36 | 85 19 | 133 70 | 149 55 | 221 42 | 272 58 | 362 999 | 420 9 |

73 793 | 110 13 | 134 13 | 156 94 | 228 41 | 273 59 | 363 305 | 436 35 |

74 68 | 112 14 | 140 17 | 184 11 | 230 40 | 275 21 | 364 149 | 464 135 |

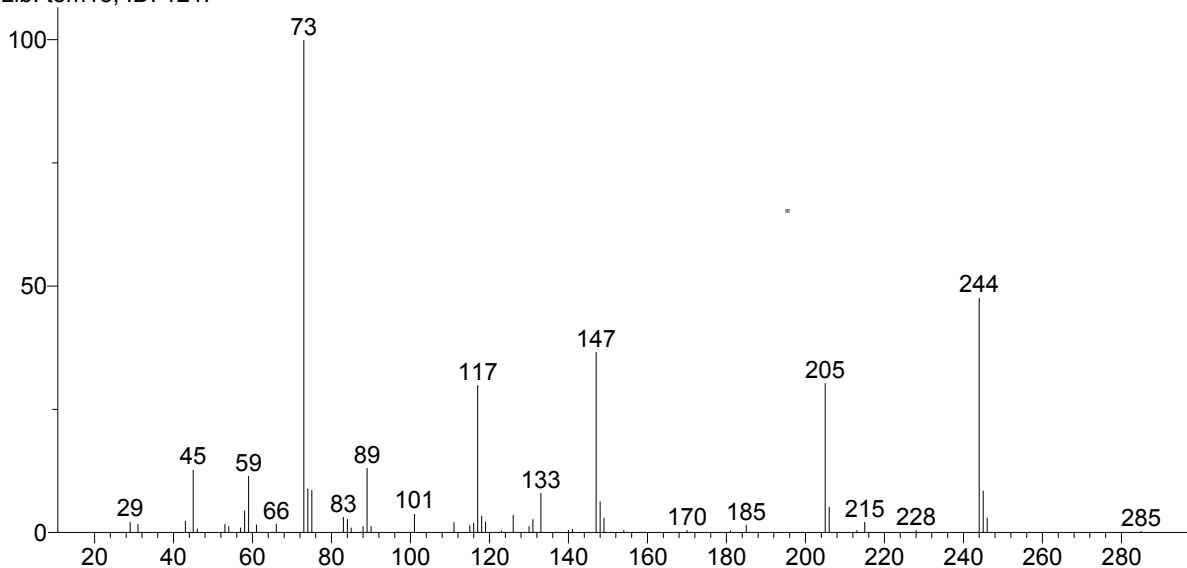
75 120 | 129 52 | 147 557 | 190 29 | 244 51 | 348 28 | 365 34 | 465 51 |

Synonyms:

1.m362,464,273,539, G: EIQTMS_N12C_ATHL_1928.1_3161BN34_[NA];

Hit 121 : RH-T-1929.8-0.04%-[244,205,117]-RH01

Lib: tom18; ID: 121.



(tom18) RH-T-1929.8-0.04%-[244,205,117]-RH01 RI:1929.8,

Name: RH-T-1929.8-0.04%-[244,205,117]-RH01

MW: N/A ID#: 121 DB: tom18

RI: 1929.8,

Comment: RI=1929.8, 31.6616 min AB2129 [RI:1929.8]

10 largest peaks:

73 999 | 244 476 | 147 366 | 205 302 | 117 298 | 89 130 | 45 127 | 59 114 | 74 88 | 75 85 |

41 m/z Values and Intensities (10 low intensity peaks are not shown):

29 22 | 54 12 | 66 17 | 84 26 | 101 38 | 118 33 | 133 79 | 205 302 | 246 29 |

31 16 | 57 9 | 73 999 | 85 9 | 111 20 | 119 21 | 147 366 | 206 51 |

43 23 | 58 43 | 74 88 | 88 12 | 115 14 | 126 35 | 148 62 | 215 21 |

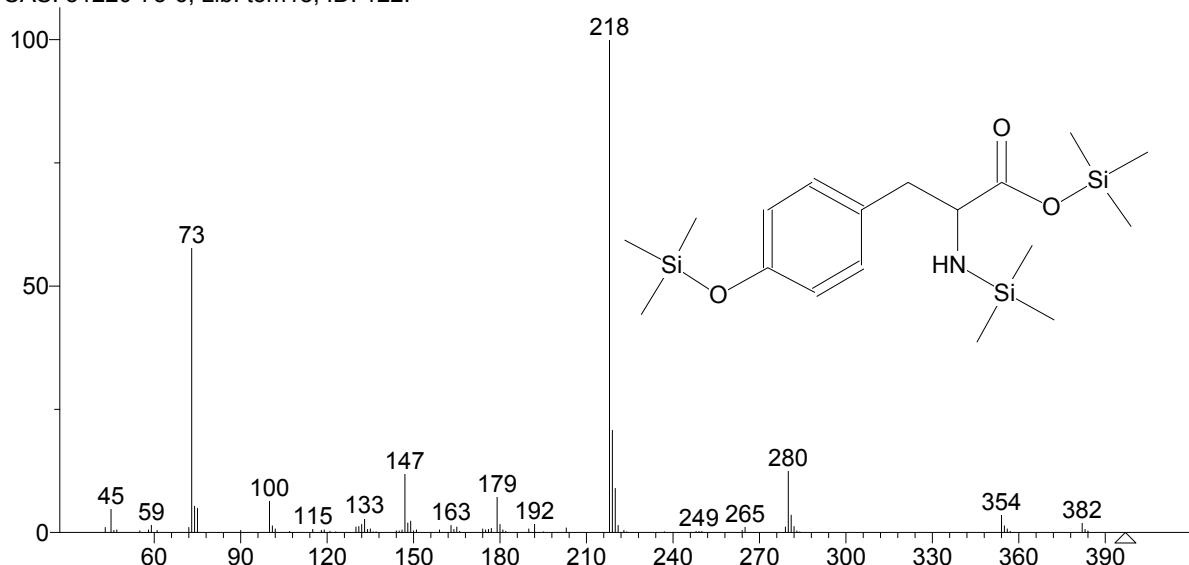
45 127 | 59 114 | 75 85 | 89 130 | 116 19 | 130 12 | 149 29 | 244 476 |

53 16 | 61 15 | 83 31 | 90 12 | 117 298 | 131 26 | 185 15 | 245 84 |

Synonyms:

1.m244,205,117;

Hit 122 : RH-T-1934.7-0.01%-[N: L-Tyrosine, N,O-bis(trimethylsilyl)-, TMS ester]-TENT-RH03
CAS: 51220-73-6; Lib: tom18; ID: 122.



(tom18) RH-T-1934.7-0.01%-[N: L-Tyrosine, N,O-bis(trimethylsilyl)-, TMS ester]-TENT-RH03 RI:1934.7,

Name: RH-T-1934.7-0.01%-[N: L-Tyrosine, N,O-bis(trimethylsilyl)-, TMS ester]-TENT-RH03

Formula: C₁₈H₃₅NO₃Si₃

MW: 397 CAS#: 51220-73-6 ID#: 122 DB: tom18

Other DBs: None

RI: 1934.7,

Comment: RI=1934.7, 36.8888 min MG00244 [RI:1934.7]

10 largest peaks:

218 999 | 73 576 | 219 207 | 280 124 | 147 118 | 220 89 | 179 72 | 100 63 | 74 53 | 75 49 |

34 m/z Values and Intensities (46 low intensity peaks are not shown):

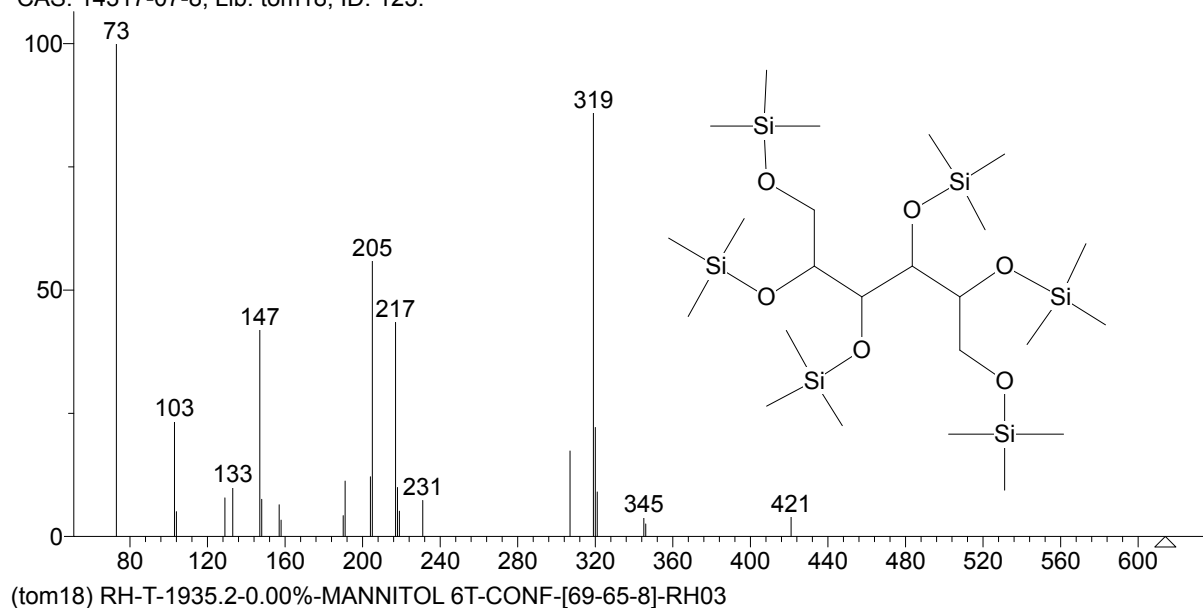
43 10	73 576	101 13	133 28	163 14	192 17	220 89	280 124	355 13
45 47	74 53	130 11	147 118	165 11	203 9	221 14	281 35	382 19
59 15	75 49	131 12	148 19	179 72	218 999	265 11	282 12	
72 10	100 63	132 16	149 23	180 16	219 207	279 11	354 35	

Synonyms:

1.Tyrosine, N,O-bis(trimethylsilyl)-, TMS ester TENT;

Hit 123 : RH-T-1935.2-0.00%-MANNITOL 6T-CONF-[69-65-8]-RH03

CAS: 14317-07-8; Lib: tom18; ID: 123.



Name: RH-T-1935.2-0.00%-MANNITOL 6T-CONF-[69-65-8]-RH03

Formula: C₂₄H₆₂O₆Si₆

MW: 614 CAS#: 14317-07-8 ID#: 123 DB: tom18

Other DBs: None

Comment: RI:MG00238 [RI:1935.2]

10 largest peaks:

73 999 | 319 859 | 205 558 | 217 434 | 147 419 | 103 233 | 320 221 | 307 173 | 204 121 | 191 112 |

24 m/z Values and Intensities:

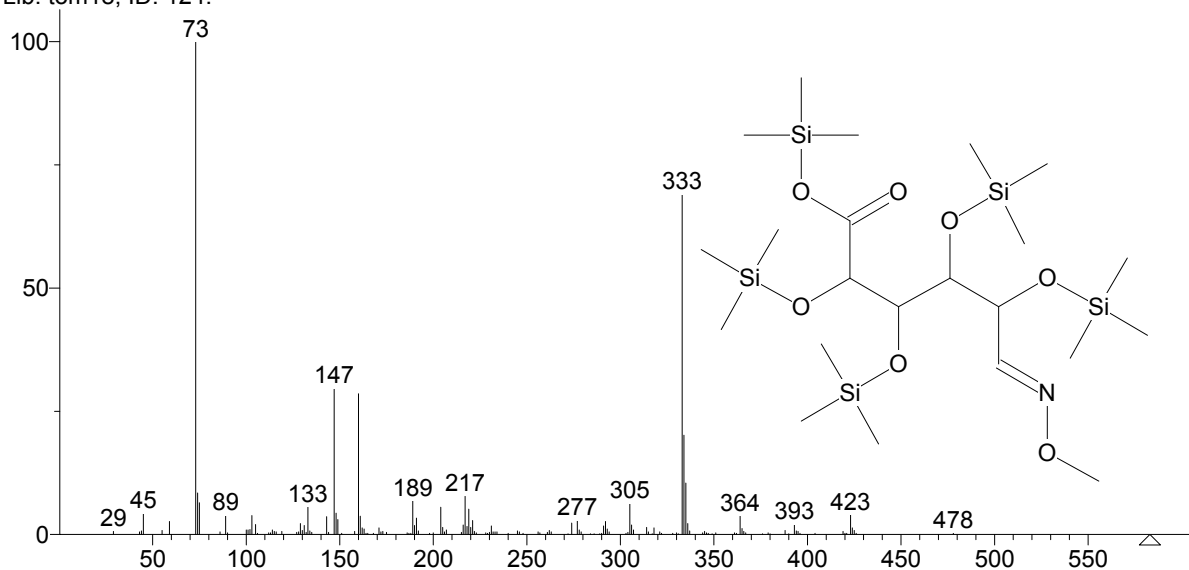
73 999 | 129 78 | 148 75 | 190 42 | 205 558 | 219 51 | 319 859 | 345 38 |
 103 233 | 133 99 | 157 64 | 191 112 | 217 434 | 231 73 | 320 221 | 346 25 |
 104 50 | 147 419 | 158 33 | 204 121 | 218 99 | 307 173 | 321 90 | 421 39 |

Synonyms:

1.MANNITOL 6T-CONF;

Hit 124 : RH-T-1942.0-0.11%-GALACTURONIC ACID M5T-PK1-CONF-[473-81-4]-RH03

Lib: tom18; ID: 124.



(tom18) RH-T-1942.0-0.11%-GALACTURONIC ACID M5T-PK1-CONF-[473-81-4]-RH03

Name: RH-T-1942.0-0.11%-GALACTURONIC ACID M5T-PK1-CONF-[473-81-4]-RH03

Formula: C₂₂H₅₃NO₇Si₅

MW: 583 ID#: 124 DB: tom18

Comment: RI:MG00238 |RI:1942|

10 largest peaks:

73 999 | 333 689 | 147 296 | 160 285 | 334 201 | 335 104 | 74 84 | 217 77 | 189 68 | 75 64 |

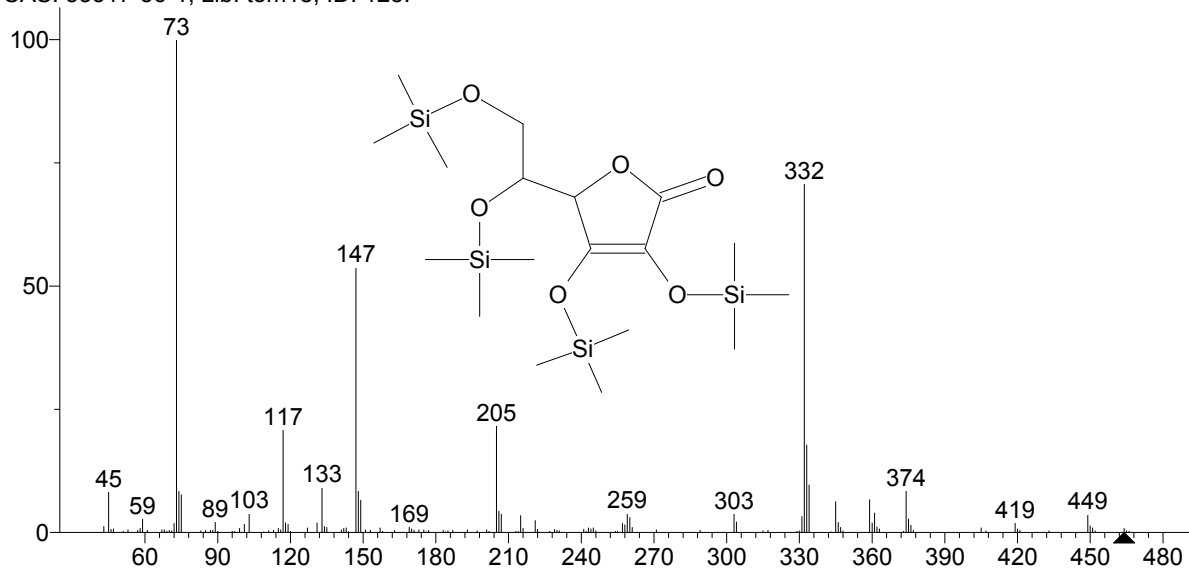
57 m/z Values and Intensities (94 low intensity peaks are not shown):

45	42	100	9	129	22	149	30	189	68	216	19	231	17	293	11	333	689	393	20
59	26	101	9	131	18	160	285	190	18	217	77	274	23	305	62	334	201	423	39
73	999	102	10	133	55	161	37	191	33	218	16	277	28	306	19	335	104	424	13
74	84	103	38	143	36	162	13	204	55	219	51	278	9	307	9	336	22		
75	64	105	20	147	296	163	11	205	14	220	14	291	17	314	14	364	37		
89	38	114	9	148	43	171	13	207	9	221	28	292	26	318	13	365	12		

Synonyms:

1.GALACTURONIC ACID M5T-PK1-CONF;

Hit 125 : RH-T-1944.2-0.12%-[L-ASCORBIC ACID 4T-CONF-[50-81-7]]-RH03
CAS: 55517-56-1; Lib: tom18; ID: 125.



(tom18) RH-T-1944.2-0.12%-[L-ASCORBIC ACID 4T-CONF-[50-81-7]]-RH03 RI:1944.2,

Name: RH-T-1944.2-0.12%-[L-ASCORBIC ACID 4T-CONF-[50-81-7]]-RH03

Formula: C₁₈H₄₀O₆Si₄

MW: 464 CAS#: 55517-56-1 ID#: 125 DB: tom18

Other DBs: None

RI: 1944.2,

Comment: RI=1944.2, 37.1218 min MG00251 |RI:1944.2|

10 largest peaks:

73 999 | 332 706 | 147 537 | 205 216 | 117 207 | 333 177 | 334 96 | 133 91 | 374 84 | 74 83 |

57 m/z Values and Intensities (80 low intensity peaks are not shown):

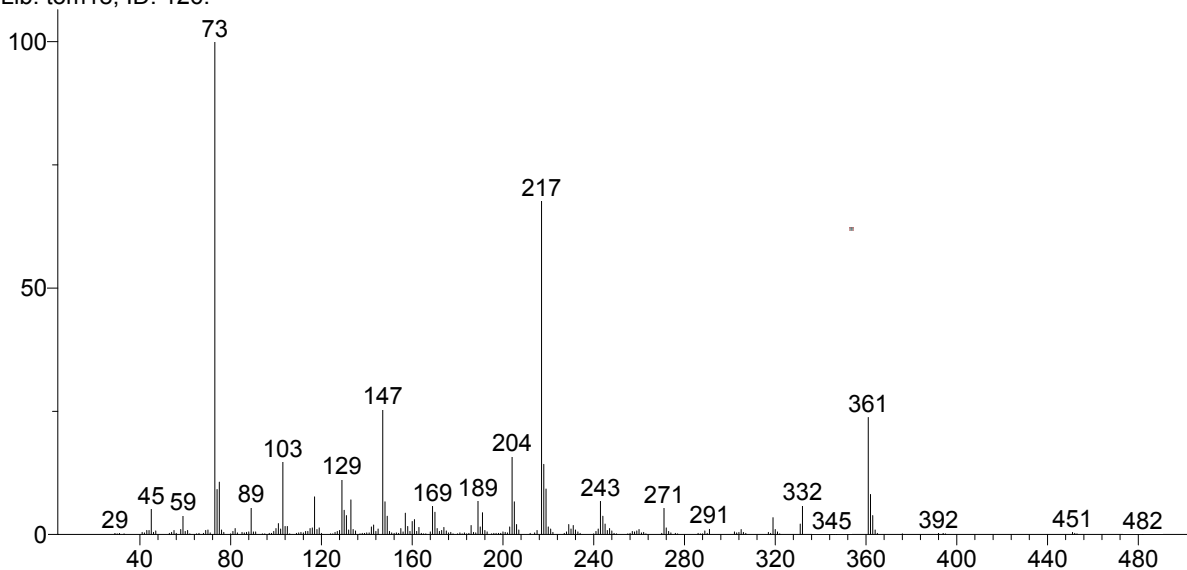
43 12	75 76	119 16	143 9	205 216	245 9	303 37	345 62	362 11	449 36
45 82	89 21	127 9	147 537	206 43	257 18	304 21	346 20	374 84	450 13
59 27	101 16	131 19	148 83	207 37	258 15	331 32	347 10	375 27	451 9
72 18	103 38	133 91	149 65	215 34	259 38	332 706	359 66	376 14	
73 999	117 207	134 12	157 9	221 24	260 30	333 177	360 19	405 9	
74 83	118 19	135 10	169 11	243 9	261 10	334 96	361 39	419 19	

Synonyms:

1.ASCORBIC ACID 4T-CONF-[50-81-7];

Hit 126 : RH-T-1955.0-0.10%-[217,361,103]-RH03

Lib: tom18; ID: 126.



(tom18) RH-T-1955.0-0.10%-[217,361,103]-RH03 RI:1953.8,

Name: RH-T-1955.0-0.10%-[217,361,103]-RH03

MW: N/A ID#: 126 DB: tom18

RI: 1953.8,

Comment: RI=1953.8, 32.1320 min AB2129 [RI:1955]

10 largest peaks:

73 999 | 217 676 | 147 253 | 361 237 | 204 158 | 103 147 | 218 142 | 129 111 | 75 106 | 219 92 |

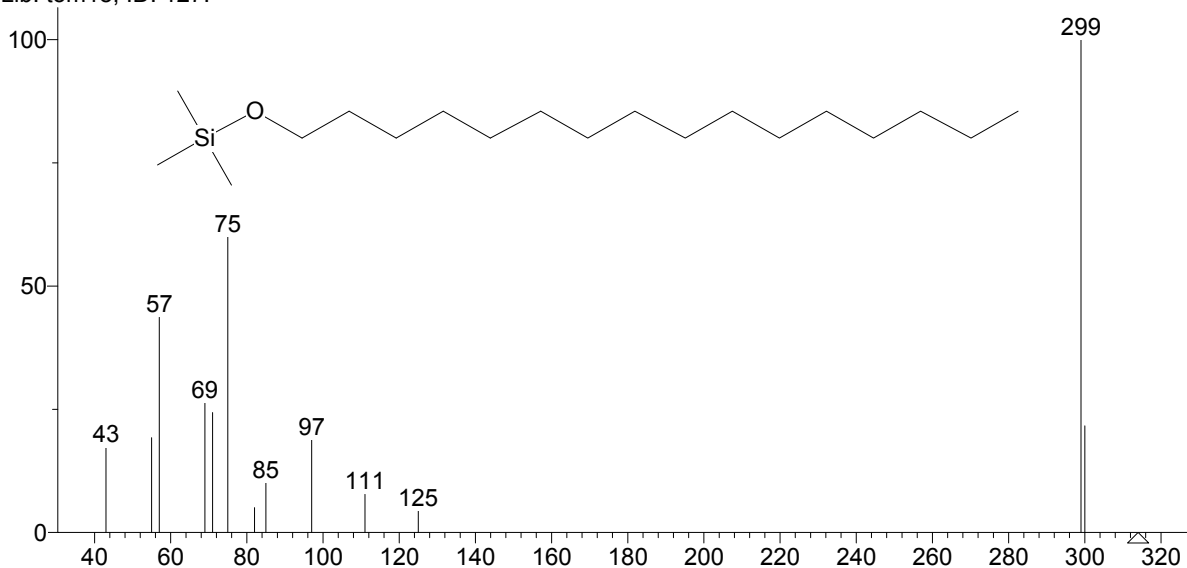
79 m/z Values and Intensities (146 low intensity peaks are not shown):

45	51	82	12	115	12	132	9	149	37	170	45	204	158	221	11	245	21	320	10
58	10	89	54	116	13	133	70	155	12	171	12	205	66	229	20	247	12	331	21
59	38	100	12	117	76	134	10	157	43	174	14	206	20	230	11	260	10	332	58
70	9	101	22	118	10	142	15	158	16	186	18	207	9	231	18	271	53	361	237
73	999	102	11	119	13	143	19	160	26	189	68	217	676	232	9	272	13	362	81
74	91	103	147	129	111	145	11	161	30	190	15	218	142	242	11	291	12	363	38
75	106	104	16	130	49	147	253	163	14	191	44	219	92	243	67	305	10	364	9
76	9	105	16	131	38	148	66	169	57	203	15	220	15	244	37	319	34		

Synonyms:

1.m217,361,103;

Hit 127 : RH-T-1958.5-0.00%-HEXADECANOL T-CONF-[36653-82-4]-TENT-G-X
Lib: tom18; ID: 127.



(tom18) RH-T-1958.5-0.00%-HEXADECANOL T-CONF-[36653-82-4]-TENT-G-X RI:1958.5,

Name: RH-T-1958.5-0.00%-HEXADECANOL T-CONF-[36653-82-4]-TENT-G-X

Formula: C₁₉H₄₂OSi

MW: 314 ID#: 127 DB: tom18

RI: 1958.5,

Comment: RI=1958.5, 29.4810 min 8135A18 |RI:1958.5|

10 largest peaks:

299 999	75 599	57 436	69 262	71 243	300 216	55 192	97 187	43 172	85 100
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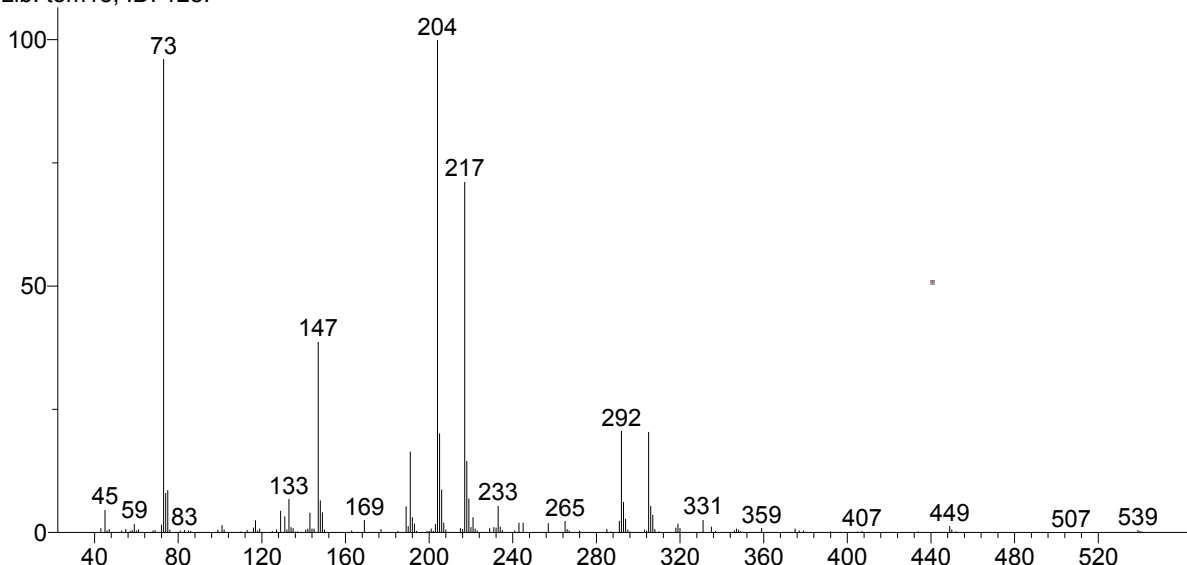
13 m/z Values and Intensities:

43 172	57 436	71 243	82 50	97 187	125 43	300 216
55 192	69 262	75 599	85 100	111 77	299 999	

Synonyms:

1. HEXADECANOL T;

Hit 128 : RH-T-1958.8-[204,217,305,292, N: sim. Galacturonic acid, 2,3,4,5-O-(TMS)-, TMS ester]-RH03
Lib: tom18; ID: 128.



(tom18) RH-T-1958.8-[204,217,305,292, N: sim. Galacturonic acid, 2,3,4,5-O-(TMS)-, TMS ester]-RH03 RI:1955.7,

Name: RH-T-1958.8-[204,217,305,292, N: sim. Galacturonic acid, 2,3,4,5-O-(TMS)-, TMS ester]-RH03

MW: N/A ID#: 128 DB: tom18

RI: 1955.7,

Comment: RI=1955.7, 37.4022 min MG00244 [RI:1958.8]

10 largest peaks:

204 999 | 73 960 | 217 711 | 147 387 | 292 206 | 305 203 | 205 200 | 191 163 | 218 144 | 206 86 |

54 m/z Values and Intensities (79 low intensity peaks are not shown):

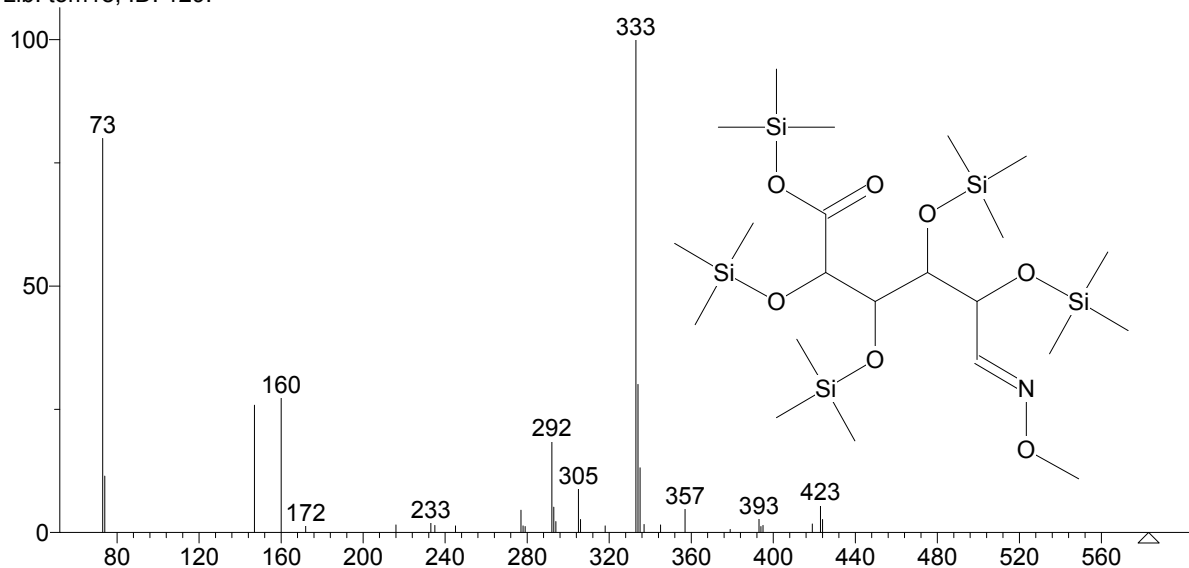
45	46	101	14	134	10	189	52	204	999	219	68	234	11	292	206	318	9
59	18	116	9	143	39	190	12	205	200	220	10	243	19	293	61	319	17
72	15	117	24	147	387	191	163	206	86	221	30	245	19	294	27	331	26
73	960	129	43	148	64	192	30	207	19	231	10	257	18	305	203	335	11
74	79	131	32	149	40	193	17	217	711	232	9	265	23	306	53	359	9
75	85	133	68	169	25	203	16	218	144	233	54	291	23	307	35	449	13

Synonyms:

1.m204,217,305,292, N: sim. Galacturonic acid, 2,3,4,5-O-(TMS)-, TMS ester;

Hit 129 : RH-T-1959.2-0.01%-GALACTURONIC ACID M5T PK2-CONF-[473-81-4]-RH03-X

Lib: tom18; ID: 129.



(tom18) RH-T-1959.2-0.01%-GALACTURONIC ACID M5T PK2-CONF-[473-81-4]-RH03-X

Name: RH-T-1959.2-0.01%-GALACTURONIC ACID M5T PK2-CONF-[473-81-4]-RH03-X

Formula: C₂₂H₅₃NO₇Si₅

MW: 583 ID#: 129 DB: tom18

Comment: RI:MG00238 [RI:1959.2]

10 largest peaks:

333	999	73	799	334	300	160	272	147	258	292	184	335	131	74	114	305	88	423	54
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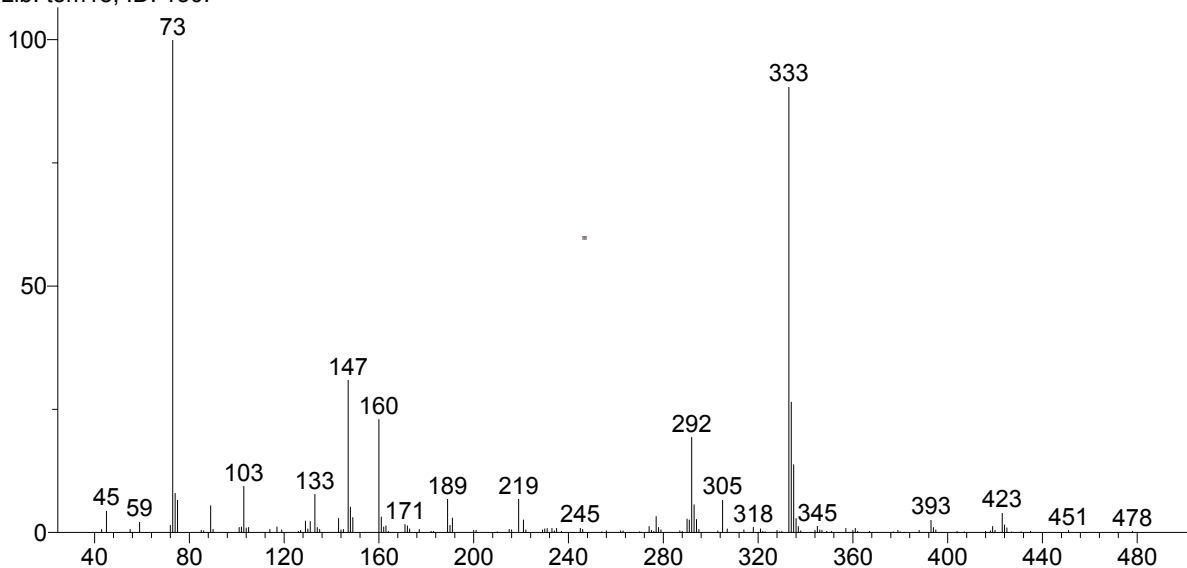
30 m/z Values and Intensities (1 low intensity peak is not shown):

73	799	160	272	233	19	277	45	292	184	305	88	333	999	337	16	393	27	419	17
74	114	172	13	235	14	278	13	293	51	306	26	334	300	345	15	394	12	423	54
147	258	216	15	245	13	279	12	294	22	318	13	335	131	357	47	395	14	424	26

Synonyms:

1.GALACTURONIC ACID M5T PK2-CONF;

Hit 130 : RH-T-1959.3-0.04%-[333,292,160,219,189,423,393, N: sim. Glucaric acid, 2,3,4,5-O-(TMS)-, bis(TMS) e
Lib: tom18; ID: 130.



(tom18) RH-T-1959.3-0.04%-[333,292,160,219,189,423,393, N: sim. Glucaric acid, 2,3,4,5-O-(TMS)-, bis(TMS) ester]-RH03 RI:1959.3

Name: RH-T-1959.3-0.04%-[333,292,160,219,189,423,393, N: sim. Glucaric acid, 2,3,4,5-O-(TMS)-, bis(TMS) ester]-RH03

MW: N/A ID#: 130 DB: tom18

RI: 1959.3,

Comment: RI=1959.3, 37.4916 min MG00244 [RI:1959.3]

10 largest peaks:

73 999 | 333 904 | 147 309 | 334 264 | 160 229 | 292 193 | 335 137 | 103 94 | 74 79 | 133 78 |

55 m/z Values and Intensities (78 low intensity peaks are not shown):

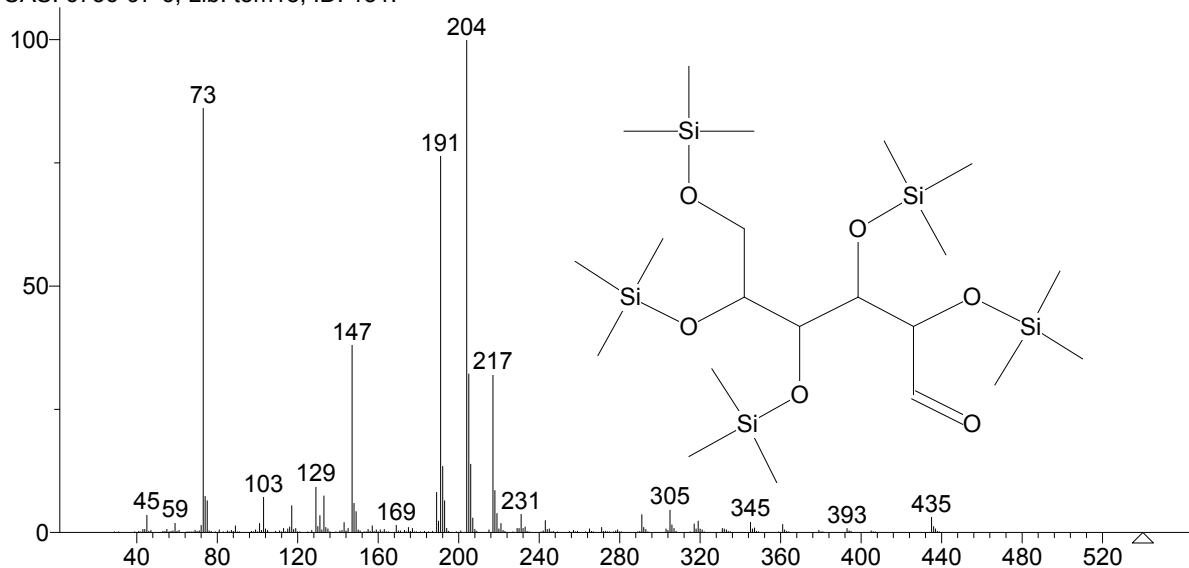
45	44	89	54	117	11	147	309	163	13	219	68	290	27	318	11	345	13	425	9
59	22	101	10	129	23	148	51	171	16	221	25	291	25	333	904	393	26		
72	14	102	11	131	22	149	30	172	13	245	10	292	193	334	264	394	10		
73	999	103	94	133	78	160	229	189	68	274	12	293	56	335	137	419	12		
74	79	104	9	134	10	161	31	190	14	277	32	294	26	336	28	423	40		
75	65	105	10	143	28	162	11	191	29	278	10	305	66	337	12	424	15		

Synonyms:

1.m333,292,160,219,189,423,393, N: sim. Glucaric acid, 2,3,4,5-O-(TMS)-, bis(TMS) ester;

Hit 131 : RH-T-1980.0-1.00%-GLUCOSE 5T-TENT-[50-99-7]-PK2-RH03

CAS: 6736-97-6; Lib: tom18; ID: 131.



(tom18) RH-T-1980.0-1.00%-GLUCOSE 5T-TENT-[50-99-7]-PK2-RH03 RI:1986.1,

Name: RH-T-1980.0-1.00%-GLUCOSE 5T-TENT-[50-99-7]-PK2-RH03

Formula: C₂₁H₅₂O₆Si₅

MW: 540 CAS#: 6736-97-6 ID#: 131 DB: tom18

Other DBs: None

RI: 1986.1,

Comment: RI=1986.1, 38.1460 min MG00246 [RI:1986.1]

10 largest peaks:

204 999 | 73 860 | 191 763 | 147 380 | 205 321 | 217 320 | 206 138 | 192 134 | 129 93 | 218 85 |

51 m/z Values and Intensities (165 low intensity peaks are not shown):

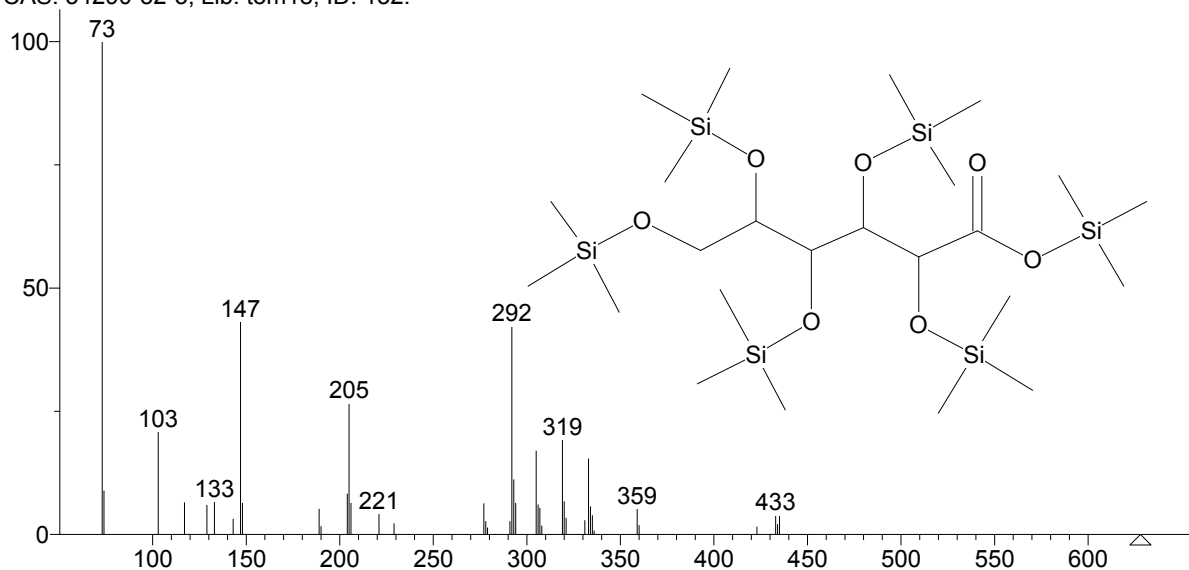
45	36	89	13	130	12	148	59	190	23	206	138	231	37	305	46	361	16
59	20	101	18	131	34	149	42	191	763	207	29	233	11	306	15	435	31
72	14	103	72	133	74	157	13	192	134	217	320	243	24	317	17	436	12
73	860	116	11	134	10	169	15	193	64	218	85	271	10	319	23		
74	73	117	54	143	20	175	10	204	999	219	38	291	36	345	22		
75	64	129	93	147	380	189	81	205	321	221	18	292	10	347	9		

Synonyms:

1.GLUCOSE 5T-TENT-[50-99-7]-PK2;

Hit 132 : RH-T-2004.3-0.01%-GLUCONIC ACID 6T-TENT-RH03

CAS: 34290-52-3; Lib: tom18; ID: 132.



(tom18) RH-T-2004.3-0.01%-GLUCONIC ACID 6T-TENT-RH03

Name: RH-T-2004.3-0.01%-GLUCONIC ACID 6T-TENT-RH03

Formula: C₂₄H₆₀O₇Si₆

MW: 628 CAS#: 34290-52-3 ID#: 132 DB: tom18

Other DBs: None

Comment: RI:MG00238 [RI:2004.3]

10 largest peaks:

73 999 | 147 431 | 292 421 | 205 265 | 103 208 | 319 191 | 305 169 | 333 153 | 293 111 | 74 88 |

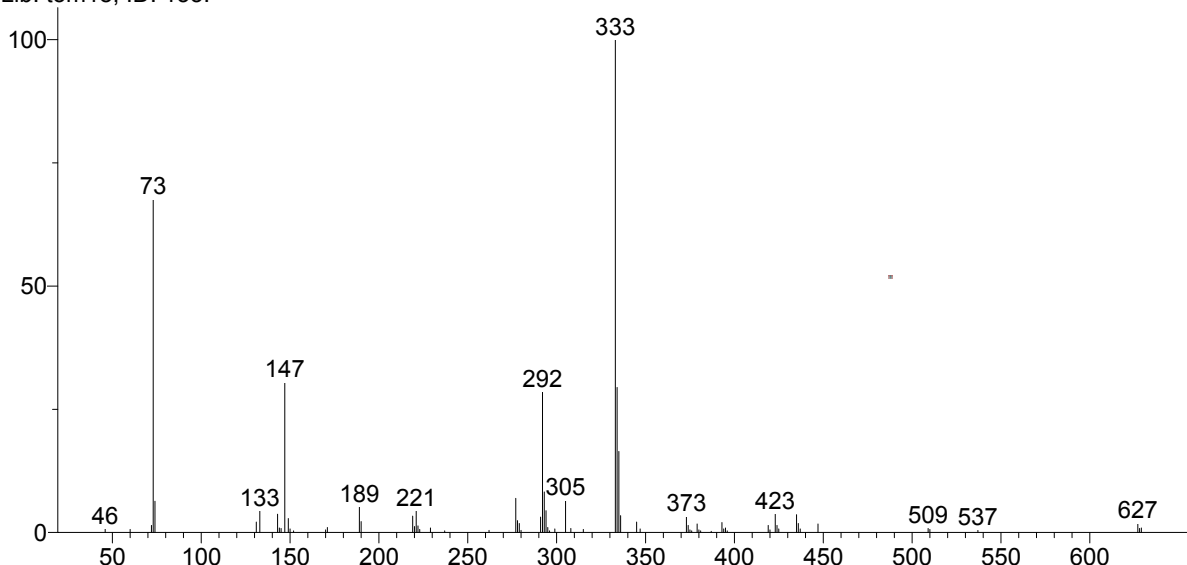
40 m/z Values and Intensities (1 low intensity peak is not shown):

73 999	129 59	148 63	205 265	277 62	292 421	306 60	320 66	334 56	423 15
74 88	133 65	189 51	206 63	278 26	293 111	307 53	321 33	335 38	433 38
103 208	143 31	190 16	221 41	279 13	294 63	308 17	331 28	359 51	434 20
117 64	147 431	204 82	229 22	291 26	305 169	319 191	333 153	360 18	435 37

Synonyms:

1. GLUCONIC ACID 6T-TENT;

Hit 133 : RH-T-2017.1-0.02%-[333,292, N: sim. Glucaric acid, 2,3,4,5-O-(TMS)-, bis(TMS) ester]-RH03
Lib: tom18; ID: 133.



(tom18) RH-T-2017.1-0.02%-[333,292, N: sim. Glucaric acid, 2,3,4,5-O-(TMS)-, bis(TMS) ester]-RH03 RI:2017.1,

Name: RH-T-2017.1-0.02%-[333,292, N: sim. Glucaric acid, 2,3,4,5-O-(TMS)-, bis(TMS) ester]-RH03

MW: N/A ID#: 133 DB: tom18

RI: 2017.1,

Comment: RI=2017.1, 38.8874 min MG00244 [RI:2017.1]

10 largest peaks:

333 999 | 73 675 | 147 304 | 334 294 | 292 284 | 335 164 | 293 82 | 277 69 | 305 64 | 74 63 |

44 m/z Values and Intensities (29 low intensity peaks are not shown):

72 14 | 143 37 | 189 51 | 222 13 | 291 31 | 305 64 | 345 21 | 395 9 | 436 18 |

73 675 | 144 9 | 190 22 | 229 9 | 292 284 | 333 999 | 373 32 | 419 14 | 447 17 |

74 63 | 147 304 | 219 33 | 277 69 | 293 82 | 334 294 | 374 14 | 423 37 | 627 18 |

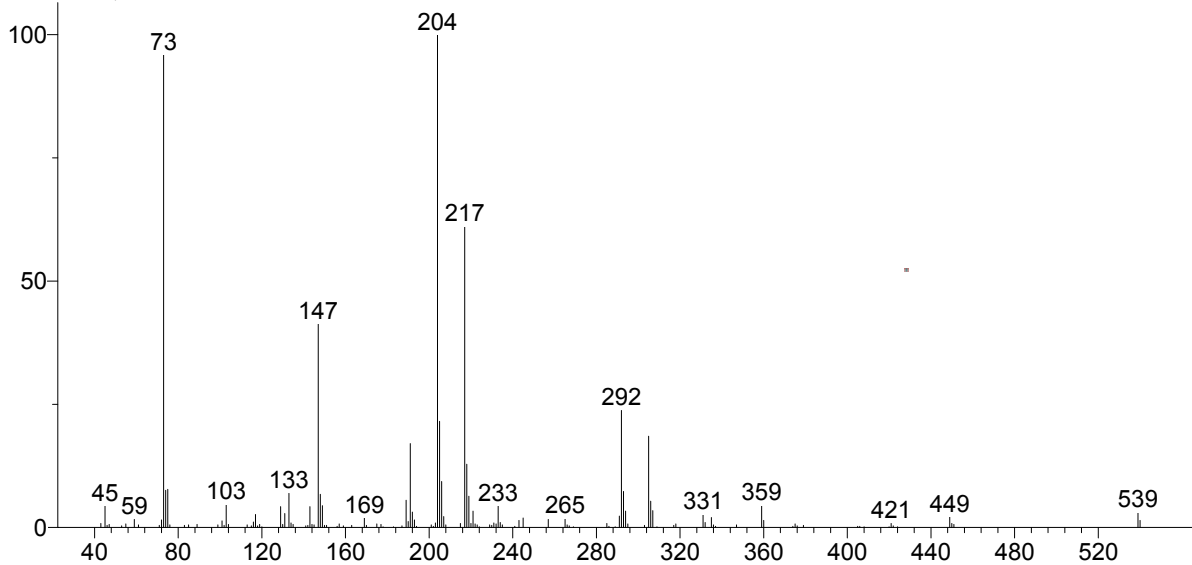
131 21 | 149 28 | 220 12 | 278 24 | 294 44 | 335 164 | 379 17 | 424 14 | 629 9 |

133 43 | 171 10 | 221 43 | 279 18 | 295 10 | 336 34 | 393 20 | 435 36 |

Synonyms:

1.m333,292, N: sim. Glucaric acid, 2,3,4,5-O-(TMS)-, bis(TMS) ester;

Hit 134 : RH-T-2023.1-0.08%-[204,217,292,305, N: sim. Galacturonic acid, 2,3,4,5-O-(TMS)-, TMS ester]-RH03
Lib: tom18; ID: 134.



(tom18) RH-T-2023.1-0.08%-[204,217,292,305, N: sim. Galacturonic acid, 2,3,4,5-O-(TMS)-, TMS ester]-RH03 RI:2023.1,

Name: RH-T-2023.1-0.08%-[204,217,292,305, N: sim. Galacturonic acid, 2,3,4,5-O-(TMS)-, TMS ester]-RH03

MW: N/A ID#: 134 DB: tom18

RI: 2023.1,

Comment: RI=2023.1, 39.0258 min MG00244 [RI:2023.1]

10 largest peaks:

204 999 | 73 958 | 217 610 | 147 412 | 292 237 | 205 215 | 305 185 | 191 170 | 218 128 | 206 93 |

55 m/z Values and Intensities (78 low intensity peaks are not shown):

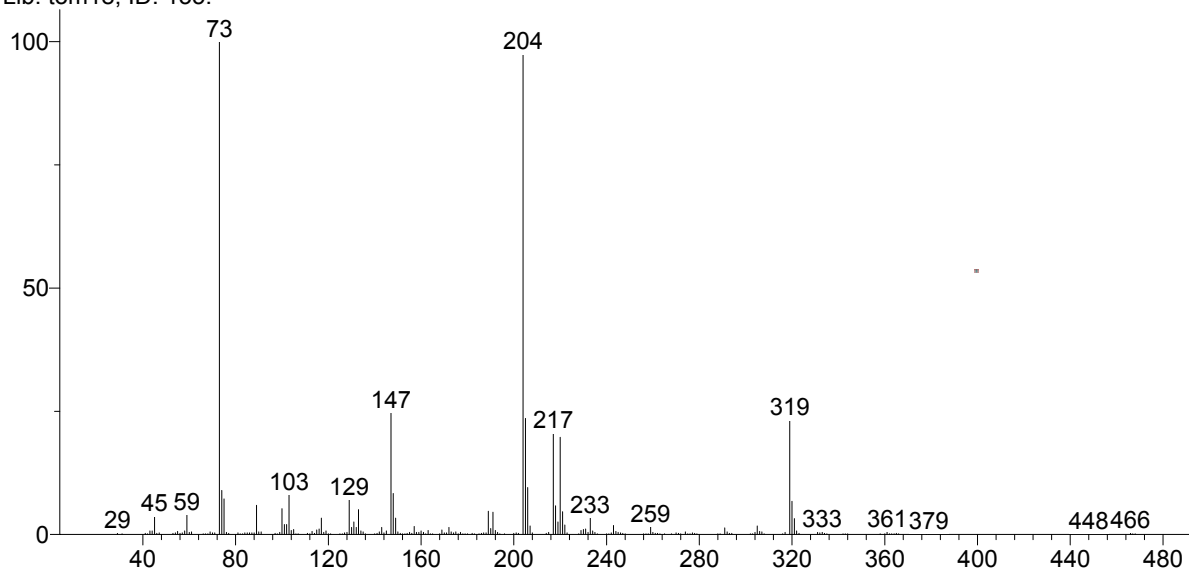
45	43	101	13	133	69	169	19	203	9	218	128	243	14	293	73	332	10	540	14
59	16	103	46	134	9	189	55	204	999	219	63	245	19	294	33	335	20		
72	15	116	11	143	42	190	12	205	215	221	33	257	16	305	185	359	44		
73	958	117	26	147	412	191	170	206	93	231	9	265	18	306	53	360	14		
74	75	129	42	148	67	192	31	207	22	233	43	291	23	307	34	449	21		
75	77	131	28	149	44	193	15	217	610	234	10	292	237	331	26	539	30		

Synonyms:

1.m204,217,292,305, N: sim. Galacturonic acid, 2,3,4,5-O-(TMS)-, TMS ester;

Hit 135 : RH-T-2036.7-0.70%-[204,319,220,217]-RH03

Lib: tom18; ID: 135.



(tom18) RH-T-2036.7-0.70%-[204,319,220,217]-RH03

Name: RH-T-2036.7-0.70%-[204,319,220,217]-RH03

MW: N/A ID#: 135 DB: tom18

Comment: RI:MG00238 [RI:2036.7]

10 largest peaks:

73 999 | 204 973 | 147 246 | 205 235 | 319 231 | 217 204 | 220 197 | 206 95 | 74 89 | 148 83 |

49 m/z Values and Intensities (172 low intensity peaks are not shown):

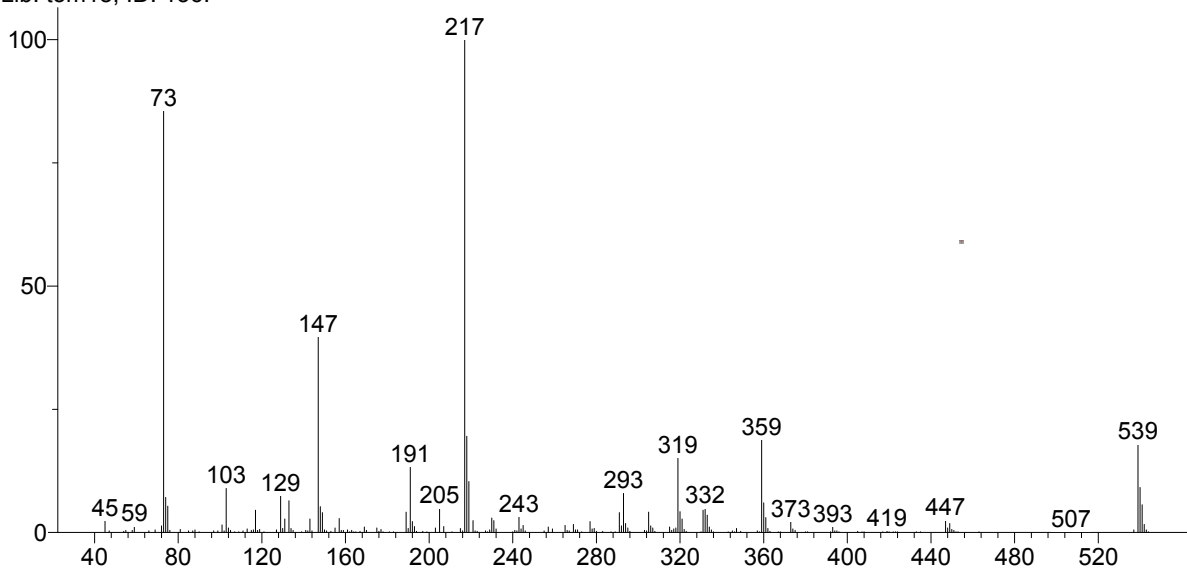
45 36 | 89 59 | 105 10 | 130 14 | 147 246 | 172 14 | 205 235 | 219 25 | 231 11 | 305 17 |
59 39 | 100 52 | 115 9 | 131 25 | 148 83 | 189 47 | 206 95 | 220 197 | 233 33 | 319 231 |
73 999 | 101 20 | 116 11 | 132 14 | 149 33 | 190 12 | 207 17 | 221 46 | 243 18 | 320 67 |
74 89 | 102 20 | 117 33 | 133 50 | 157 16 | 191 45 | 217 204 | 222 19 | 259 15 | 321 32 |
75 72 | 103 80 | 129 70 | 143 14 | 169 9 | 204 973 | 218 58 | 230 10 | 291 13 |

Synonyms:

1.m204,319,220,217;

Hit 136 : RH-T-2040.7-0.07%-[217,539,359,319,191]-RH03

Lib: tom18; ID: 136.



(tom18) RH-T-2040.7-0.07%-[217,539,359,319,191]-RH03 RI:2040.7,

Name: RH-T-2040.7-0.07%-[217,539,359,319,191]-RH03

MW: N/A ID#: 136 DB: tom18

RI: 2040.7,

Comment: RI=2040.7, 39.4385 min MG00244 [RI:2040.7]

10 largest peaks:

217 999 | 73 854 | 147 396 | 218 195 | 359 187 | 539 178 | 319 150 | 191 132 | 219 103 | 540 91 |

69 m/z Values and Intensities (131 low intensity peaks are not shown):

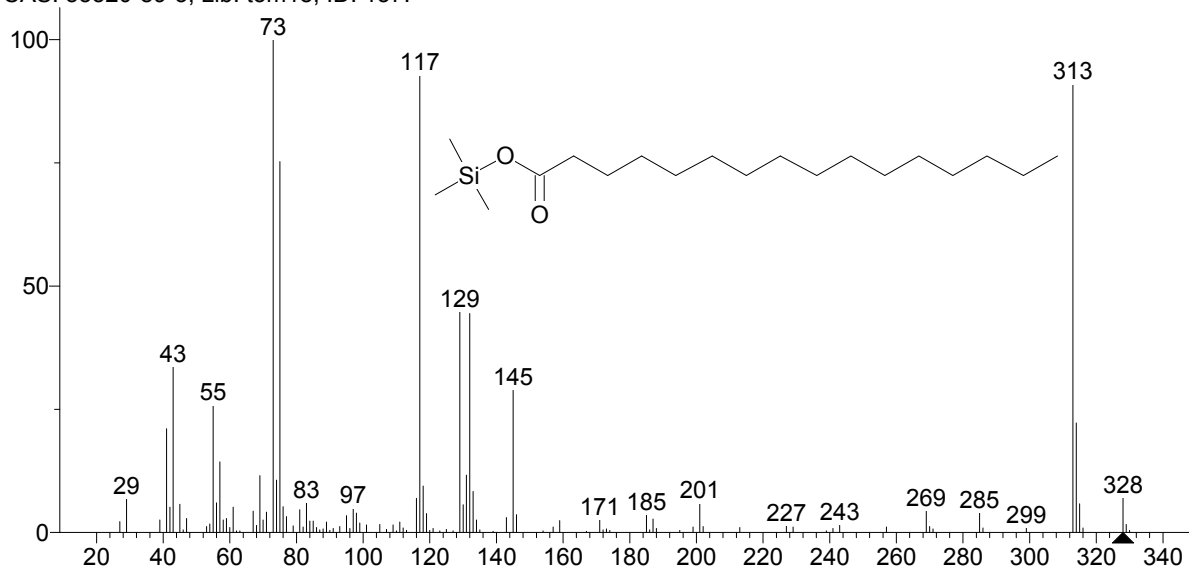
45	23	103	89	147	396	189	41	217	999	245	14	293	79	318	9	334	11	448	9
59	12	104	9	148	52	191	132	218	195	257	11	294	18	319	150	359	187	449	18
72	13	117	45	149	40	192	22	219	103	265	14	295	9	320	42	360	60	539	178
73	854	129	74	155	9	193	12	221	24	269	16	305	41	321	27	361	30	540	91
74	71	131	27	157	28	203	9	230	29	277	22	306	13	331	45	373	21	541	56
75	53	133	64	169	11	205	48	231	24	291	40	307	9	332	48	393	11	542	16
101	15	143	27	175	9	207	12	243	31	292	13	315	11	333	35	447	24		

Synonyms:

1.m217,539,359,319,191;

Hit 137 : RH-T-2044.9-0.12%-PALMITIC ACID 1T-CONF-[57-10-3]-RH03

CAS: 55520-89-3; Lib: tom18; ID: 137.



(tom18) RH-T-2044.9-0.12%-PALMITIC ACID 1T-CONF-[57-10-3]-RH03 RI:2043.9,

Name: RH-T-2044.9-0.12%-PALMITIC ACID 1T-CONF-[57-10-3]-RH03

Formula: C₁₉H₄₀O₂Si

MW: 328 CAS#: 55520-89-3 ID#: 137 DB: tom18

Other DBs: None

RI: 2043.9,

Comment: RI=2043.9, 33.8645 min AB2129 |RI:2044.9|

10 largest peaks:

73 999 | 117 926 | 313 908 | 75 752 | 129 447 | 132 444 | 43 335 | 145 288 | 55 257 | 314 222 |

82 m/z Values and Intensities (30 low intensity peaks are not shown):

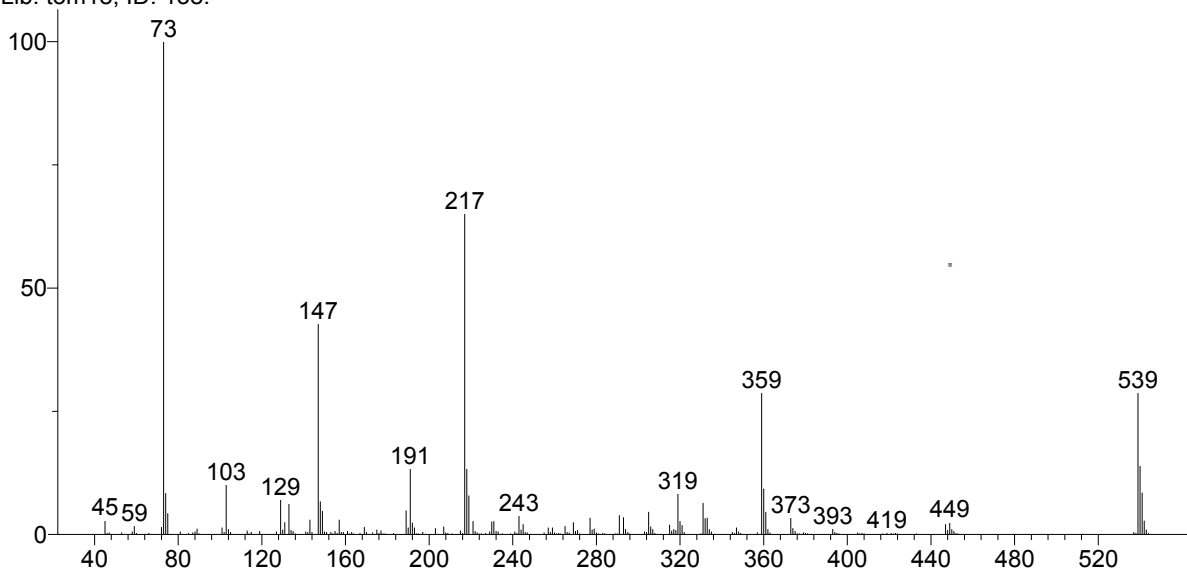
27 22	54 17	68 14	79 13	95 34	116 69	134 25	199 11	270 12	329 16
29 67	55 257	69 115	81 46	97 48	117 926	143 30	201 58	285 39	
39 25	56 60	70 25	82 11	98 39	118 94	145 288	202 12	286 9	
41 210	57 143	71 41	83 59	99 19	119 38	146 36	213 10	299 9	
42 51	58 25	73 999	84 23	101 15	129 447	157 11	227 13	313 908	
43 335	59 28	74 106	85 23	105 16	130 56	159 24	229 11	314 222	
45 57	60 10	75 752	86 10	109 15	131 116	171 25	243 14	315 58	
47 28	61 51	76 52	89 21	111 21	132 444	185 35	257 11	316 9	
53 12	67 43	77 32	93 12	112 9	133 83	187 27	269 43	328 70	

Synonyms:

1.PALMITIC ACID 1T-CONF-[57-10-3];

Hit 138 : RH-T-2047.2-0.21%-[217,539,359,191,319]-RH03

Lib: tom18; ID: 138.



(tom18) RH-T-2047.2-0.21%-[217,539,359,191,319]-RH03 RI:2047.2,

Name: RH-T-2047.2-0.21%-[217,539,359,191,319]-RH03

MW: N/A ID#: 138 DB: tom18

RI: 2047.2,

Comment: RI=2047.2, 39.5901 min MG00244 [RI:2047.2]

10 largest peaks:

73 999 | 217 650 | 147 427 | 359 287 | 539 286 | 540 138 | 191 132 | 218 132 | 103 100 | 360 92 |

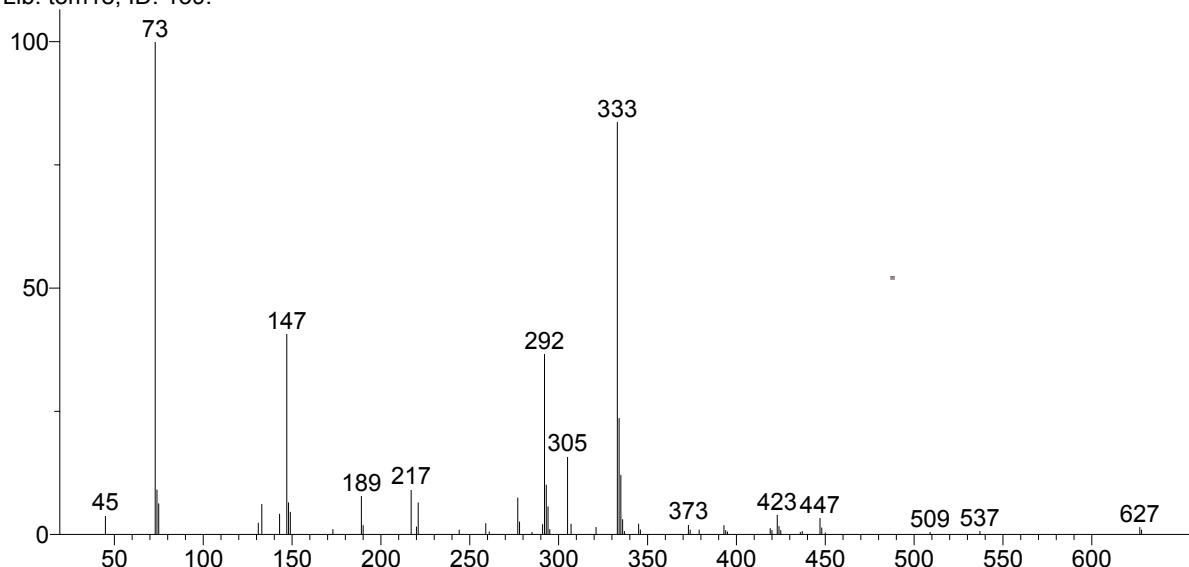
75 m/z Values and Intensities (126 low intensity peaks are not shown):

45	28	103	100	148	66	192	23	230	25	269	24	306	15	332	32	373	33	541	84
59	16	104	10	149	47	193	13	231	26	277	33	307	10	333	33	374	12	542	27
72	14	129	70	157	29	203	12	243	37	278	9	315	19	334	10	393	11	543	9
73	999	130	9	169	14	207	15	244	9	279	11	317	10	347	13	447	20		
74	83	131	24	175	9	217	650	245	20	291	38	319	82	359	287	449	24		
75	42	133	61	189	48	218	132	257	13	293	34	320	26	360	92	450	10		
89	11	143	29	190	13	219	78	259	13	294	10	321	18	361	45	539	286		
101	13	147	427	191	132	221	26	265	16	305	45	331	63	362	10	540	138		

Synonyms:

1.m217,539,359,191,319;

Hit 139 : RH-T-2053.9-0.01%-[333,292, N: sim. Glucaric acid, 2,3,4,5-O-(TMS)-, bis(TMS) ester]-TENT-RH03
Lib: tom18; ID: 139.



(tom18) RH-T-2053.9-0.01%-[333,292, N: sim. Glucaric acid, 2,3,4,5-O-(TMS)-, bis(TMS) ester]-TENT-RH03 RI:2053.9,

Name: RH-T-2053.9-0.01%-[333,292, N: sim. Glucaric acid, 2,3,4,5-O-(TMS)-, bis(TMS) ester]-TENT-RH03

MW: N/A ID#: 139 DB: tom18

RI: 2053.9,

Comment: RI=2053.9, 39.7452 min MG00244 |RI:2053.9|

10 largest peaks:

73 999 | 333 836 | 147 406 | 292 366 | 334 235 | 305 158 | 335 120 | 293 100 | 217 91 | 74 90 |

45 m/z Values and Intensities (12 low intensity peaks are not shown):

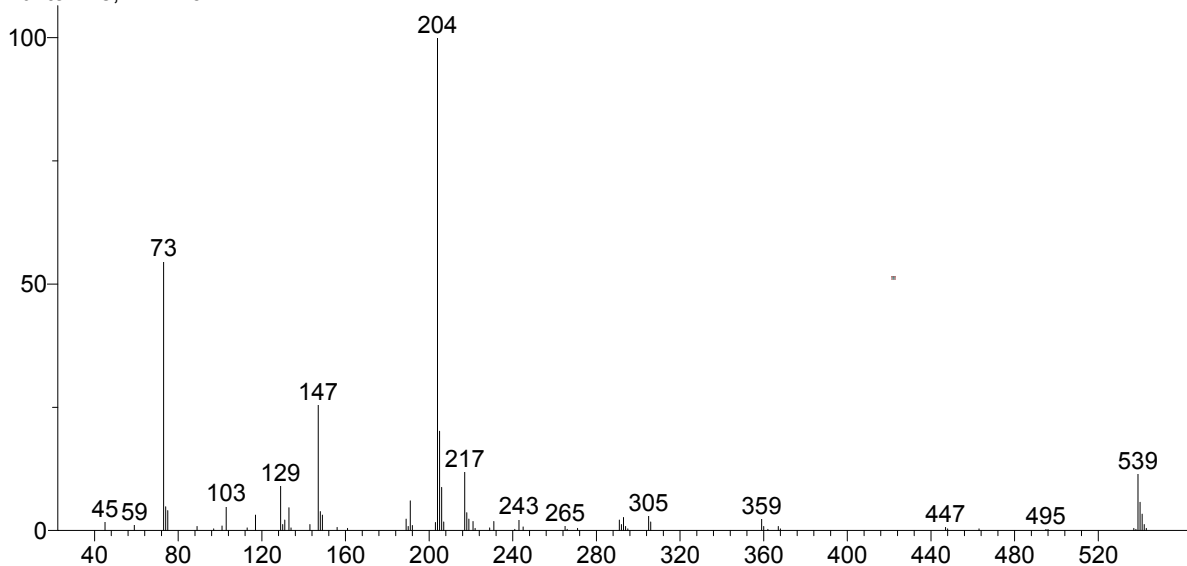
45	38	133	61	173	10	221	64	291	20	305	158	335	120	374	9	424	16
73	999	143	41	189	78	244	9	292	366	307	21	336	30	379	9	447	33
74	90	147	406	190	18	259	22	293	100	321	14	345	21	393	18	448	13
75	62	148	64	217	91	277	74	294	56	333	836	346	9	419	12	627	14
131	23	149	45	220	15	278	25	295	10	334	235	373	20	423	39	628	9

Synonyms:

1.m333,292, N: sim. Glucaric acid, 2,3,4,5-O-(TMS)-, bis(TMS) ester;

Hit 140 : RH-T-2076.3-0.02%-[204,539,359,217]-RH03

Lib: tom18; ID: 140.



(tom18) RH-T-2076.3-0.02%-[204,539,359,217]-RH03 RI:2076.3,

Name: RH-T-2076.3-0.02%-[204,539,359,217]-RH03

MW: N/A ID#: 140 DB: tom18

RI: 2076.3,

Comment: RI=2076.3, 40.2691 min MG00244 [RI:2076.3]

10 largest peaks:

204 999 | 73 545 | 147 254 | 205 201 | 217 118 | 539 114 | 129 90 | 206 87 | 191 60 | 540 57 |

41 m/z Values and Intensities (27 low intensity peaks are not shown):

45 17 | 101 9 | 131 21 | 149 31 | 204 999 | 218 36 | 265 9 | 306 17 | 542 12 |

59 11 | 103 48 | 133 46 | 189 23 | 205 201 | 219 23 | 291 21 | 359 23 |

73 545 | 117 31 | 143 12 | 191 60 | 206 87 | 221 18 | 292 12 | 539 114 |

74 48 | 129 90 | 147 254 | 192 10 | 207 17 | 231 18 | 293 26 | 540 57 |

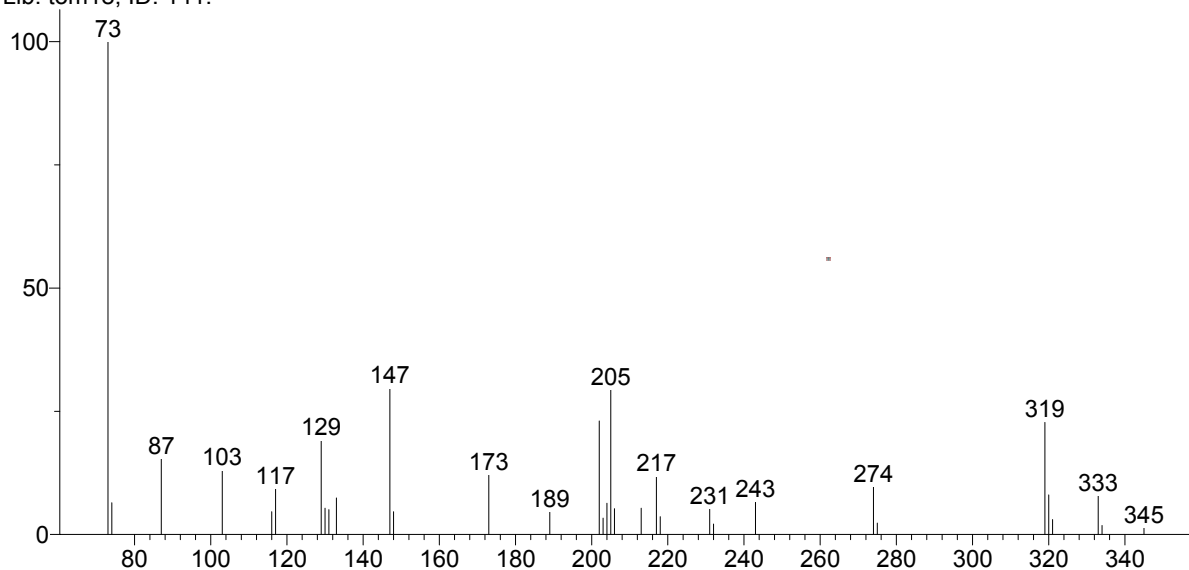
75 40 | 130 12 | 148 38 | 203 16 | 217 118 | 243 22 | 305 29 | 541 33 |

Synonyms:

1.m204,539,359,217;

Hit 141 : RH-T-2080.7-0.01%-[205,319,205,202,129]-RH03

Lib: tom18; ID: 141.



(tom18) RH-T-2080.7-0.01%-[205,319,205,202,129]-RH03

Name: RH-T-2080.7-0.01%-[205,319,205,202,129]-RH03

MW: N/A ID#: 141 DB: tom18

Comment: RI:MG00244 [RI:2072.7]

10 largest peaks:

73 999 | 147 296 | 205 293 | 202 230 | 319 227 | 129 190 | 87 153 | 103 129 | 173 120 | 217 117 |

33 m/z Values and Intensities:

73 999 | 116 46 | 131 50 | 173 120 | 204 63 | 217 117 | 243 65 | 320 80 | 345 13 |

74 64 | 117 92 | 133 74 | 189 45 | 205 293 | 218 36 | 274 96 | 321 30 |

87 153 | 129 190 | 147 296 | 202 230 | 206 52 | 231 51 | 275 23 | 333 78 |

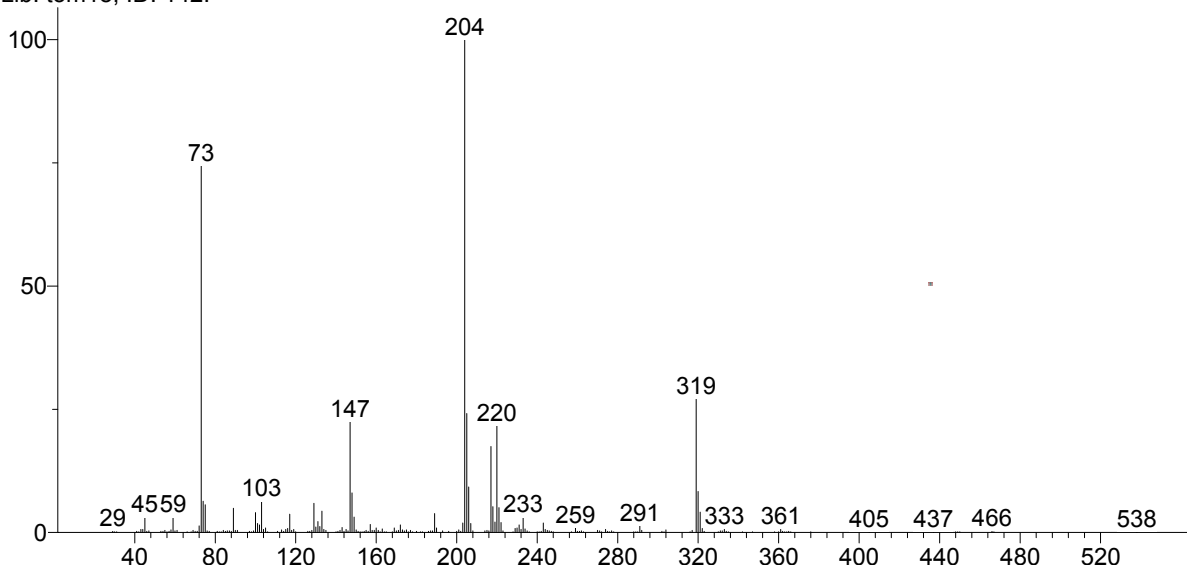
103 129 | 130 53 | 148 46 | 203 33 | 213 53 | 232 21 | 319 227 | 334 18 |

Synonyms:

1.m205,319,205,202,129;

Hit 142 : RH-T-2086.8-0.15%-[204,319,220,217]-RH03

Lib: tom18; ID: 142.



(tom18) RH-T-2086.8-0.15%-[204,319,220,217]-RH03 RI:2086.8,

Name: RH-T-2086.8-0.15%-[204,319,220,217]-RH03

MW: N/A ID#: 142 DB: tom18

RI: 2086.8,

Comment: RI=2086.8, 40.5136 min MG00244 [RI:2086.8]

10 largest peaks:

204 999 | 73 743 | 319 270 | 205 241 | 147 224 | 220 216 | 217 174 | 206 92 | 320 83 | 148 80 |

48 m/z Values and Intensities (160 low intensity peaks are not shown):

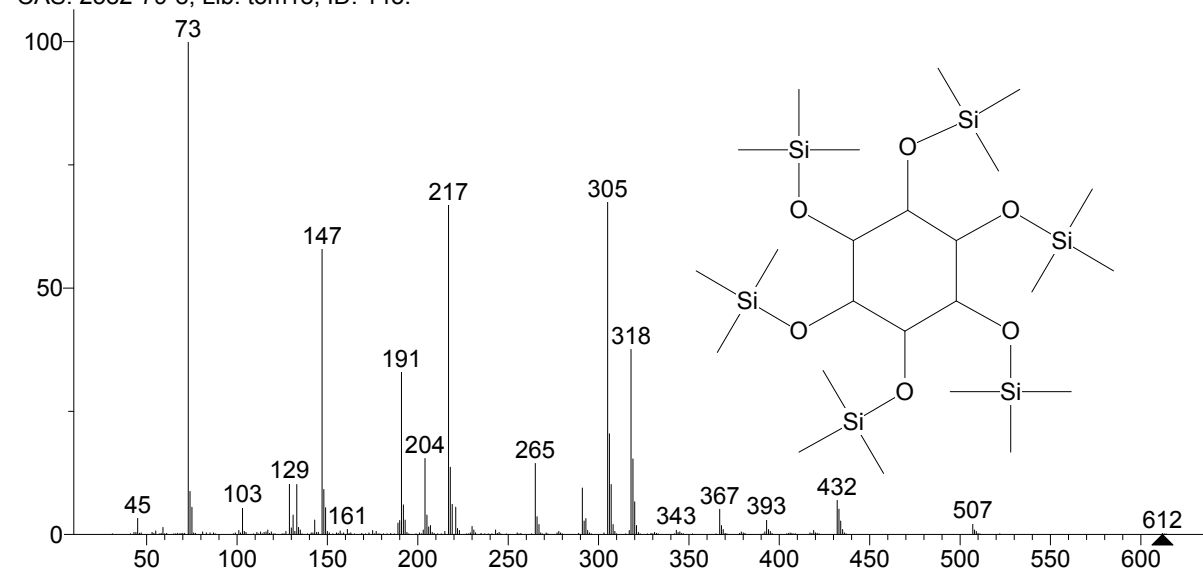
45 30	75 56	103 62	131 22	148 80	172 15	205 241	219 21	231 15	319 270
59 30	89 49	105 9	132 12	149 31	189 38	206 92	220 216	233 30	320 83
72 13	100 40	117 37	133 43	157 16	190 9	207 18	221 50	243 19	321 41
73 743	101 18	129 59	143 10	160 9	203 19	217 174	222 20	259 9	
74 63	102 15	130 11	147 224	169 9	204 999	218 52	230 9	291 13	

Synonyms:

1.m204,319,220,217;

Hit 143 : RH-T-2092.7-0.93%-myo-INOSITOL 6T-CONF-[87-89-8]-RH03

CAS: 2582-79-8; Lib: tom18; ID: 143.



(tom18) RH-T-2092.7-0.93%-myo-INOSITOL 6T-CONF-[87-89-8]-RH03

Name: RH-T-2092.7-0.93%-myo-INOSITOL 6T-CONF-[87-89-8]-RH03

Formula: C₂₄H₆₀O₆Si₆

MW: 612 CAS#: 2582-79-8 ID#: 143 DB: tom18

Other DBs: None

Comment: RI:MG00238 [RI:2092.7]

10 largest peaks:

73 999 | 305 674 | 217 668 | 147 579 | 318 375 | 191 329 | 306 204 | 204 154 | 319 153 | 265 144 |

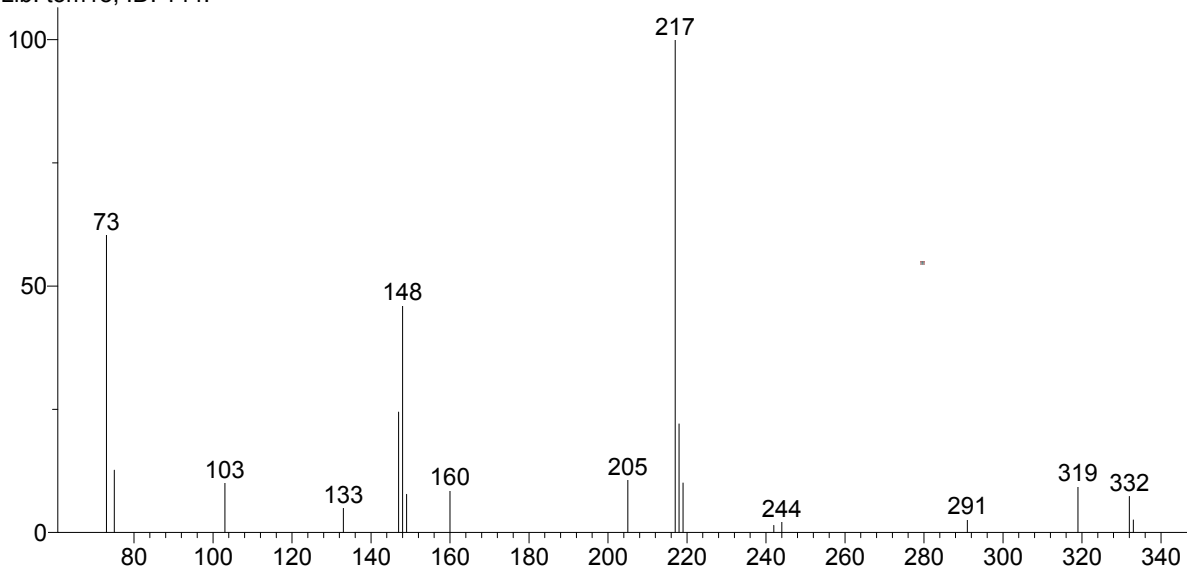
62 m/z Values and Intensities (167 low intensity peaks are not shown):

45	33	129	103	147	579	192	60	217	668	243	9	305	674	321	18	432	69
59	14	130	13	148	91	193	29	218	136	265	144	306	204	343	10	433	51
73	999	131	39	149	54	203	9	219	61	266	36	307	101	367	51	434	27
74	87	133	101	161	11	204	154	221	55	267	20	308	20	368	18	435	10
75	55	134	14	189	23	205	39	222	12	291	94	318	375	369	10	507	22
103	54	135	9	190	28	206	15	230	16	292	27	319	153	393	30	508	9
117	9	143	29	191	329	207	18	231	9	293	32	320	66	394	10		

Synonyms:

1.INOSITOL, MYO 6T-CONF-[87-89-8];

Hit 144 : RH-T-2107.1-0.00%-[217,319, N: sim..D-Galactofuranose 5T]-RH03-X
Lib: tom18; ID: 144.



(tom18) RH-T-2107.1-0.00%-[217,319, N: sim..D-Galactofuranose 5T]-RH03-X RI:2107.1,

Name: RH-T-2107.1-0.00%-[217,319, N: sim..D-Galactofuranose 5T]-RH03-X

MW: N/A ID#: 144 DB: tom18

RI: 2107.1,

Comment: RI=2107.1, 40.9824 min MG00244 [RI:2107.1]

10 largest peaks:

217 999 | 73 603 | 148 460 | 147 244 | 218 220 | 75 126 | 205 106 | 103 100 | 219 100 | 319 93 |

18 m/z Values and Intensities:

73 603 | 103 100 | 147 244 | 149 77 | 205 106 | 218 220 | 242 14 | 291 26 | 332 73 |

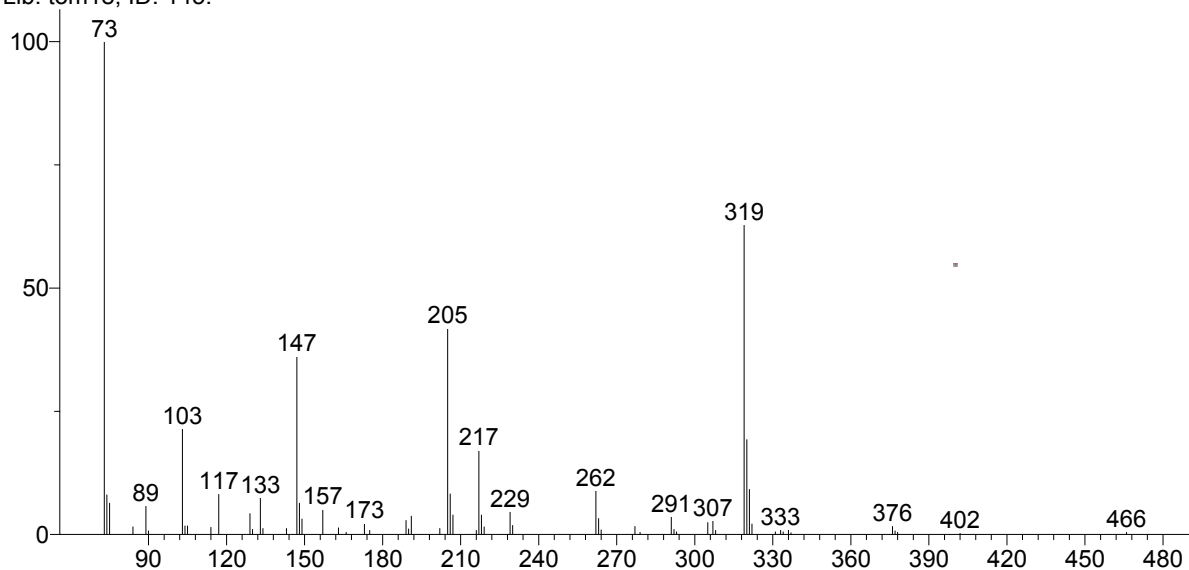
75 126 | 133 49 | 148 460 | 160 85 | 217 999 | 219 100 | 244 21 | 319 93 | 333 25 |

Synonyms:

1.m217,319, N: sim..D-Galactofuranose 5T;

Hit 145 : RH-T-2125.5-0.04%-[319,205,103,217,262, N: sim. GALACTOSE 6T]-RH03

Lib: tom18; ID: 145.



(tom18) RH-T-2125.5-0.04%-[319,205,103,217,262, N: sim. GALACTOSE 6T]-RH03

Name: RH-T-2125.5-0.04%-[319,205,103,217,262, N: sim. GALACTOSE 6T]-RH03

MW: N/A ID#: 145 DB: tom18

Comment: RI:MG00238 [RI:2125.5]

10 largest peaks:

73 999 | 319 627 | 205 417 | 147 360 | 103 213 | 320 192 | 217 170 | 321 91 | 262 88 | 206 82 |

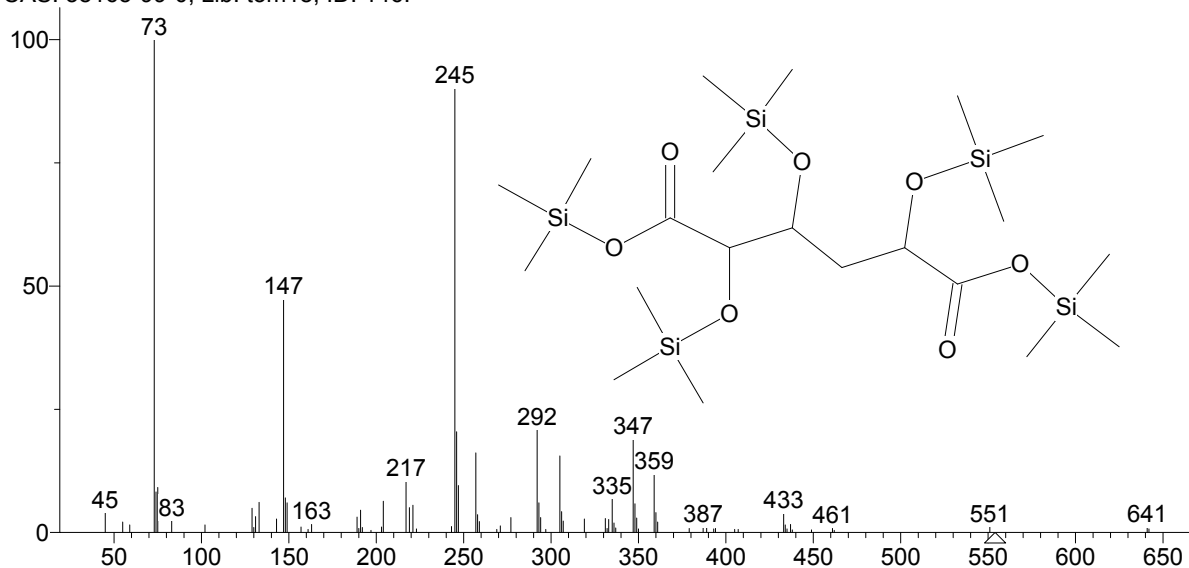
48 m/z Values and Intensities (14 low intensity peaks are not shown):

73 999 | 103 213 | 129 42 | 147 360 | 173 22 | 205 417 | 219 15 | 264 9 | 307 27 | 333 9 |
74 80 | 104 17 | 130 10 | 148 63 | 189 28 | 206 82 | 229 45 | 277 16 | 319 627 | 336 9 |
75 63 | 105 17 | 133 74 | 149 31 | 190 11 | 207 39 | 230 18 | 291 35 | 320 192 | 376 16 |
84 15 | 114 14 | 134 12 | 157 50 | 191 37 | 217 170 | 262 88 | 292 10 | 321 91 |
89 57 | 117 81 | 143 12 | 163 13 | 202 12 | 218 39 | 263 32 | 305 24 | 322 21 |

Synonyms:

1.m319,205,103,217,262, N: sim. GALACTOSE 6T;

Hit 146 : RH-T-2129.0-0.02%-[N: 3-Deoxy-arabino-hexaric acid 5T]-TENT-RH03
CAS: 38165-99-0; Lib: tom18; ID: 146.



(tom18) RH-T-2129.0-0.02%-[N: 3-Deoxy-arabino-hexaric acid 5T]-TENT-RH03 RI:2129.0,

Name: RH-T-2129.0-0.02%-[N: 3-Deoxy-arabino-hexaric acid 5T]-TENT-RH03

Formula: C₂₁H₅₀O₇Si₅

MW: 554 CAS#: 38165-99-0 ID#: 146 DB: tom18

Other DBs: None

RI: 2129.0,

Comment: RI=2129.0, 41.4739 min MG00244 [RI:2129]

10 largest peaks:

73 999 | 245 900 | 147 472 | 292 208 | 246 204 | 347 188 | 257 161 | 305 155 | 359 117 | 217 103 |

60 m/z Values and Intensities (19 low intensity peaks are not shown):

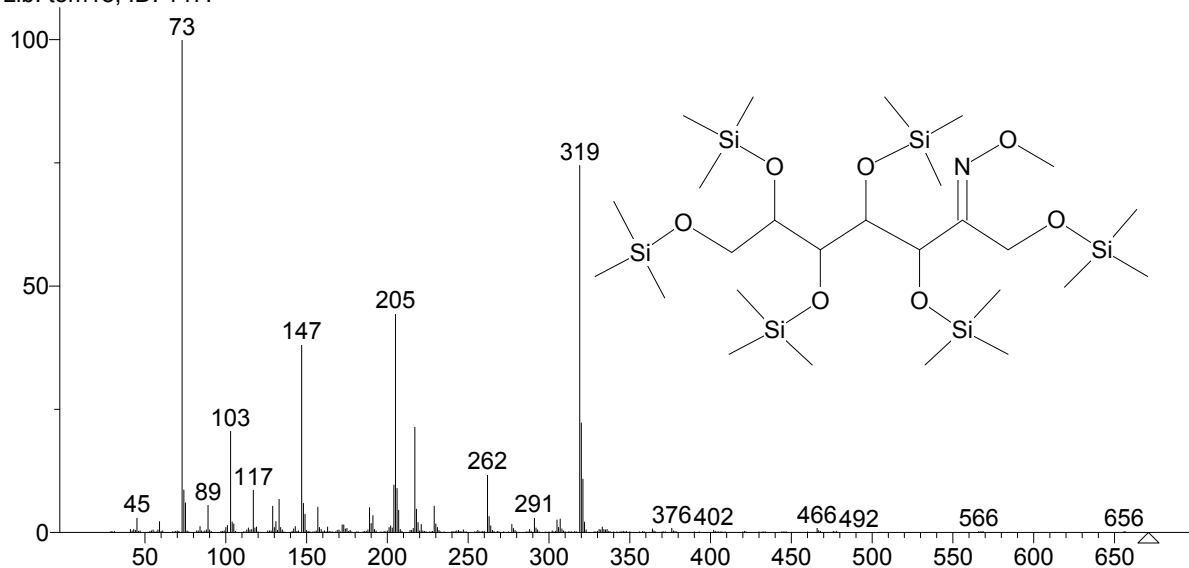
45	39	83	23	143	27	189	31	219	50	257	161	293	60	331	28	348	58	389	10
55	21	102	15	147	472	191	45	221	55	258	36	294	30	333	26	349	29	433	38
59	15	129	49	148	70	192	10	243	12	259	22	305	155	335	67	359	117	434	15
73	999	130	10	149	60	203	11	245	900	271	13	306	42	336	19	360	40	437	16
74	82	131	32	157	11	204	63	246	204	277	30	307	23	337	9	361	21	551	11
75	91	133	61	163	16	217	103	247	95	292	208	319	27	347	188	387	10	641	10

Synonyms:

1,3-Deoxy-arabino-hexaric acid 5T;

Hit 147 : RH-T-2146.3-0.48%-SEDOHEPTULOSE MX6T PK1-TENT-[3019-74-7]-RH03

Lib: tom18; ID: 147.



(tom18) RH-T-2146.3-0.48%-SEDOHEPTULOSE MX6T PK1-TENT-[3019-74-7]-RH03

Name: RH-T-2146.3-0.48%-SEDOHEPTULOSE MX6T PK1-TENT-[3019-74-7]-RH03

Formula: C₂₆H₆₅NO₇Si₆

MW: 671 ID#: 147 DB: tom18

Comment: RI:MG00238 [RI:2146.3]

10 largest peaks:

73 999 | 319 744 | 205 444 | 147 381 | 320 222 | 217 213 | 103 205 | 262 117 | 321 108 | 204 96 |

63 m/z Values and Intensities (211 low intensity peaks are not shown):

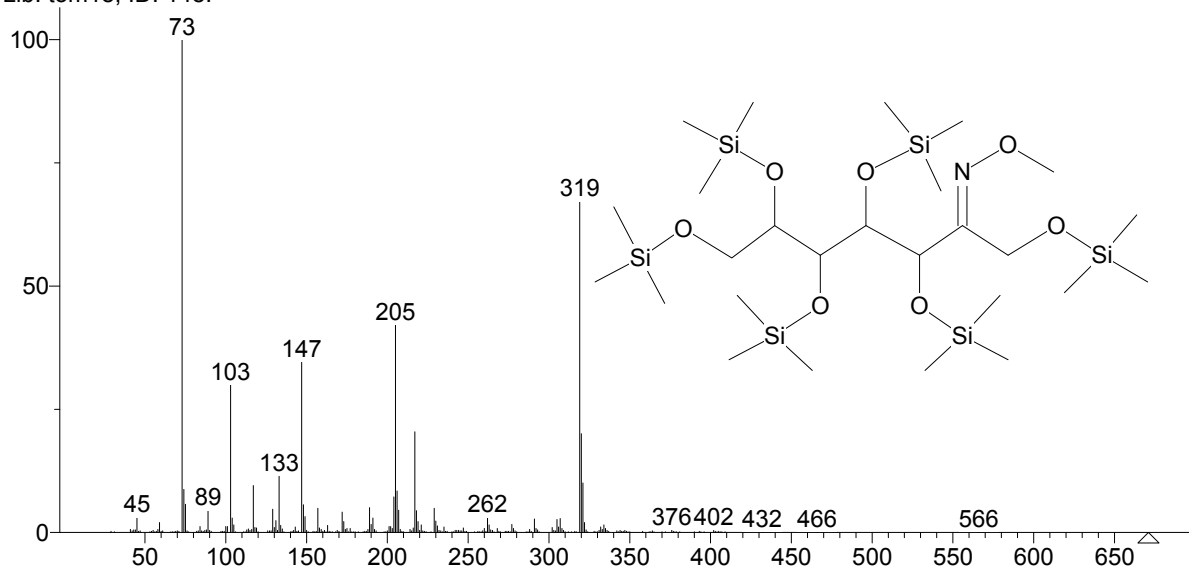
45	30	100	10	118	9	143	12	172	15	203	9	219	20	264	13	319	744
59	22	101	14	119	11	147	381	173	15	204	96	221	16	277	16	320	222
73	999	103	205	129	53	148	59	189	50	205	444	229	53	291	30	321	108
74	86	104	21	130	10	149	37	190	18	206	89	230	17	292	9	322	21
75	60	105	17	131	22	157	51	191	34	207	45	231	10	305	25	333	11
84	12	114	9	133	67	158	10	201	10	217	213	262	117	306	10	376	9
89	55	117	86	134	10	163	11	202	13	218	47	263	32	307	27	466	9

Synonyms:

1.SEDOHEPTULOSE MX6T PK1-TENT-[3019-74-7];

Hit 148 : RH-T-2151.8-0.74%-SEDOHEPTULOSE M6T PK2-TENT-[3019-74-7]-RH03

Lib: tom18; ID: 148.



(tom18) RH-T-2151.8-0.74%-SEDOHEPTULOSE M6T PK2-TENT-[3019-74-7]-RH03

Name: RH-T-2151.8-0.74%-SEDOHEPTULOSE M6T PK2-TENT-[3019-74-7]-RH03

Formula: C₂₆H₆₅NO₇Si₆

MW: 671 ID#: 148 DB: tom18

Comment: RI:MG00238 [RI:2151.8]

10 largest peaks:

73 999 | 319 671 | 205 420 | 147 345 | 103 299 | 217 204 | 320 200 | 133 114 | 321 100 | 117 95 |

62 m/z Values and Intensities (200 low intensity peaks are not shown):

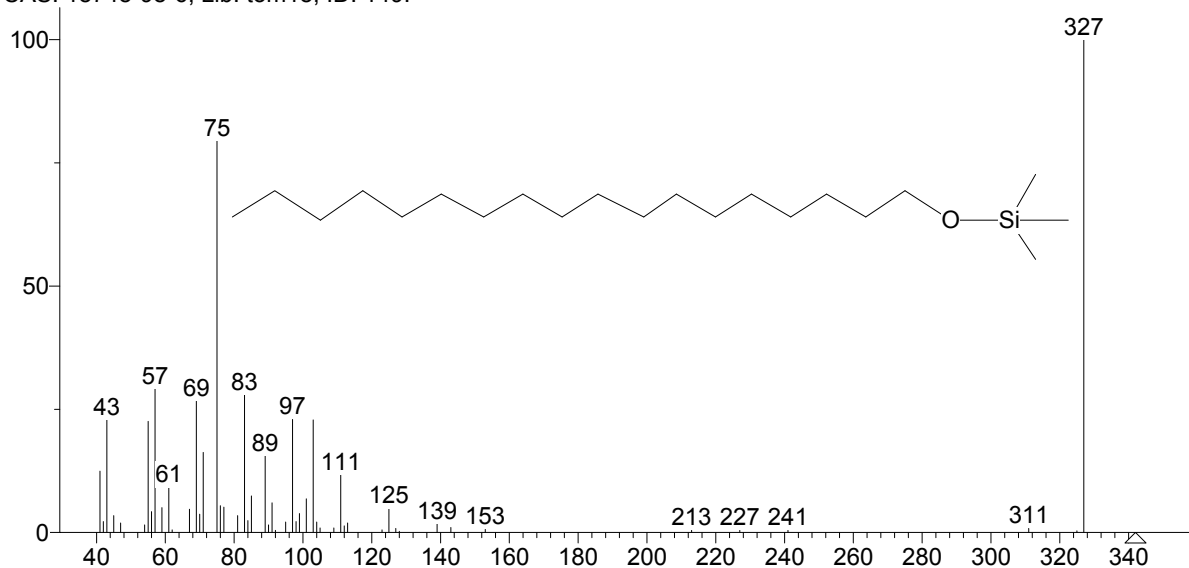
45	30	100	12	119	9	147	345	173	22	205	420	221	15	263	15	319	671
59	20	101	12	129	47	148	56	189	50	206	84	229	49	277	16	320	200
73	999	103	299	130	10	149	32	190	16	207	45	230	23	291	27	321	100
74	87	104	29	131	24	157	49	191	29	216	9	231	13	302	10	322	20
75	57	105	15	133	114	158	9	201	12	217	204	235	11	305	26	332	11
84	12	117	95	134	14	163	14	202	12	218	44	247	9	306	11	334	15
89	44	118	10	143	11	172	41	204	72	219	22	262	30	307	28		

Synonyms:

1.SEDOHEPTULOSE M6T PK2-TENT-[3019-74-7];

Hit 149 : RH-T-2153.5-0.00%-OCTADECANOL T-TENT-8135A18-G

CAS: 18748-98-6; Lib: tom18; ID: 149.



(tom18) RH-T-2153.5-0.00%-OCTADECANOL T-TENT-8135A18-G RI:2153.5,

Name: RH-T-2153.5-0.00%-OCTADECANOL T-TENT-8135A18-G

Formula: C₂₁H₄₆OSi

MW: 342 CAS#: 18748-98-6 ID#: 149 DB: tom18

Other DBs: None

RI: 2153.5,

Comment: RI=2153.5, 32.5186 min 8135A18 |RI:2153.5|

10 largest peaks:

327 999 | 75 794 | 57 291 | 83 279 | 69 266 | 97 229 | 43 228 | 103 228 | 55 225 | 71 162 |

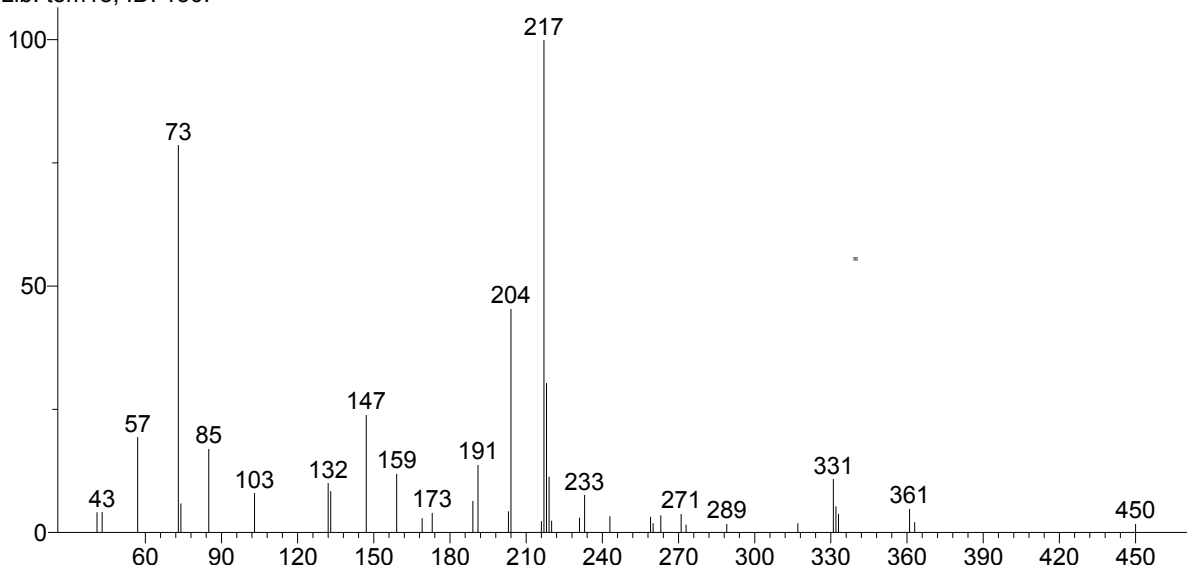
41 m/z Values and Intensities (11 low intensity peaks are not shown):

41 124	54 15	61 91	75 794	84 24	95 21	103 228	112 13	327 999
42 22	55 225	67 47	76 54	85 74	97 229	104 21	113 19	
43 228	56 42	69 266	77 51	89 155	98 22	105 9	125 48	
45 34	57 291	70 37	81 34	90 15	99 38	109 9	139 17	
47 19	59 50	71 162	83 279	91 60	101 68	111 116	143 10	

Synonyms:

1.OCTADECANOL T-TENT;

Hit 150 : RH-T-2167.2-0.00%-[217,204,191,331,159,85,450, N:sim. Lyxofuranoside, methyl 2,3,5-tris-O-(T)-]RH0:
Lib: tom18; ID: 150.



(tom18) RH-T-2167.2-0.00%-[217,204,191,331,159,85,450, N:sim. Lyxofuranoside, methyl 2,3,5-tris-O-(T)-]RH03 RI:2167.2,

Name: RH-T-2167.2-0.00%-[217,204,191,331,159,85,450, N:sim. Lyxofuranoside, methyl 2,3,5-tris-O-(T)-]RH03

MW: N/A ID#: 150 DB: tom18

RI: 2167.2,

Comment: RI=2167.2, 42.3317 min MG00244 [RI:2167.2]

10 largest peaks:

217 999 | 73 785 | 204 454 | 218 302 | 147 239 | 57 193 | 85 170 | 191 137 | 159 119 | 219 112 |

38 m/z Values and Intensities:

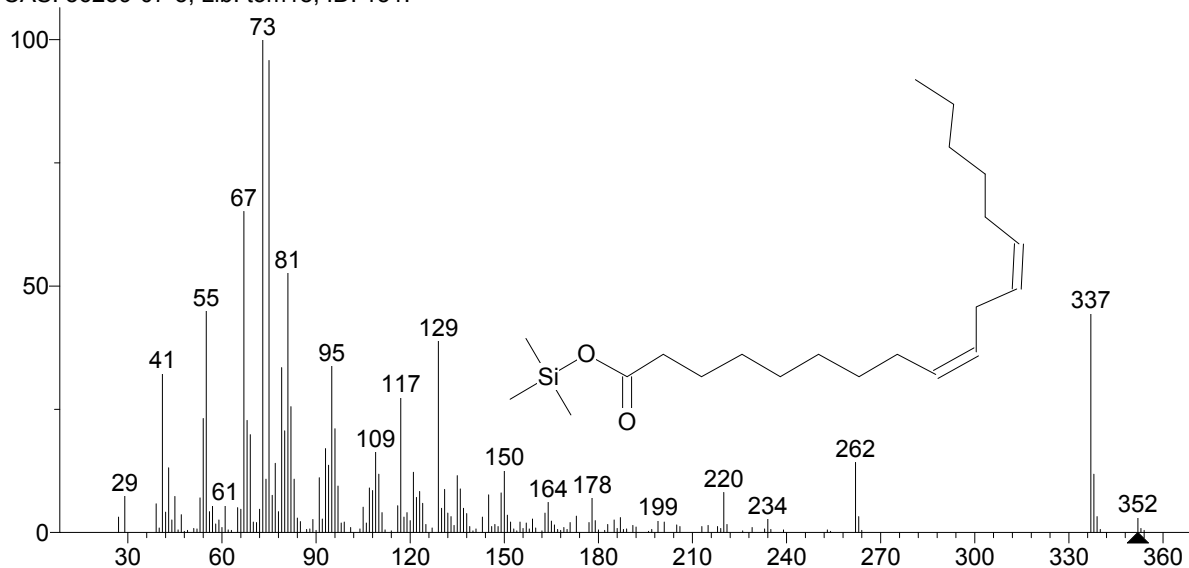
41 40	74 58	133 83	173 40	204 454	219 112	243 32	271 38	331 108	363 20
43 41	85 170	147 239	189 63	216 22	220 23	259 31	273 15	332 52	450 18
57 193	103 80	159 119	191 137	217 999	231 29	260 18	289 18	333 37	
73 785	132 100	169 28	203 42	218 302	233 76	263 34	317 18	361 48	

Synonyms:

1.m217,204,191,331,159,85,450, N:sim. Lyxofuranoside, methyl 2,3,5-tris-O-(T)-;

Hit 151 : RH-T-2205.8-0.16%-LINOLEIC ACID 1T-CONF-[60-33-3]-RH03

CAS: 56259-07-5; Lib: tom18; ID: 151.



(tom18) RH-T-2205.8-0.16%-LINOLEIC ACID 1T-CONF-[60-33-3]-RH03

Name: RH-T-2205.8-0.16%-LINOLEIC ACID 1T-CONF-[60-33-3]-RH03

Formula: C₂₁H₄₀O₂Si

MW: 352 CAS#: 56259-07-5 ID#: 151 DB: tom18

Other DBs: None

Comment: RI:MG00238 [RI:2205.8]

10 largest peaks:

73 999	75 957	67 651	81 526	55 449	337 444	129 388	95 337	79 334	41 322
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125 m/z Values and Intensities (41 low intensity peaks are not shown):

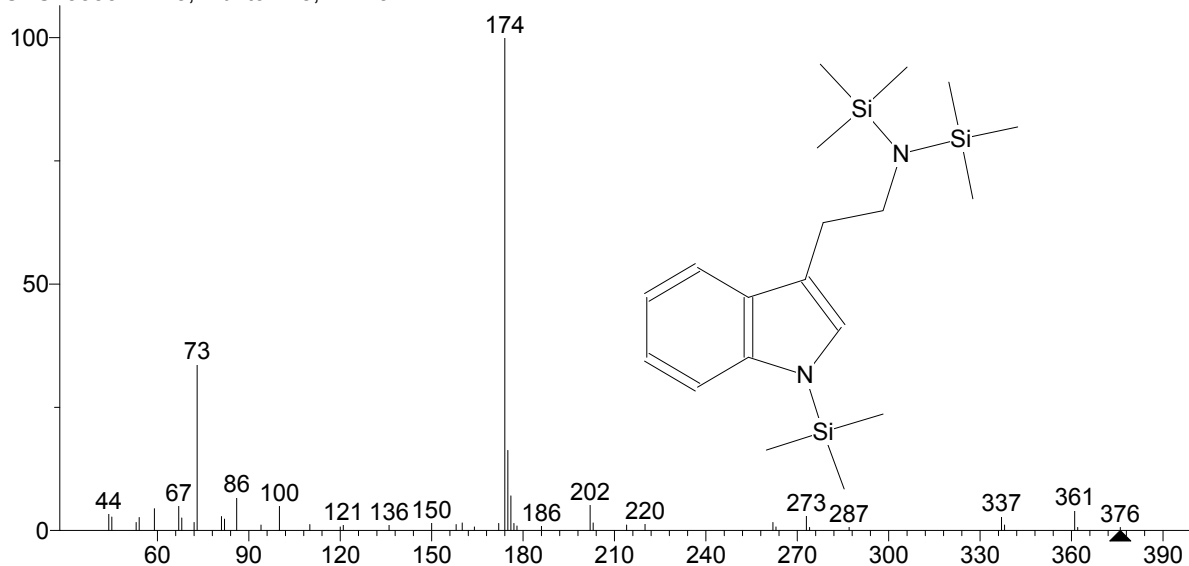
27 31	56 42	72 47	85 22	106 19	123 83	138 38	159 27	185 25	229 10
29 74	57 53	73 999	89 26	107 90	124 59	139 12	160 9	187 30	234 27
39 58	58 17	74 108	91 111	108 85	125 16	143 31	163 39	191 14	262 142
40 9	59 25	75 957	92 27	109 163	127 9	145 76	164 61	192 11	263 32
41 322	60 10	76 75	93 170	110 118	129 388	146 12	165 23	199 24	337 444
42 41	61 54	77 140	94 136	111 40	130 49	147 16	166 15	201 21	338 118
43 131	65 50	78 42	95 337	116 54	131 87	148 12	169 10	205 15	339 32
44 25	66 47	79 334	96 210	117 273	132 39	149 80	171 20	206 12	352 30
45 73	67 651	80 206	97 94	118 31	133 32	150 125	173 33	213 12	
47 36	68 227	81 526	98 19	119 40	134 14	151 35	177 20	215 14	
53 70	69 198	82 255	99 21	120 24	135 115	152 21	178 70	218 12	
54 231	70 21	83 108	101 10	121 122	136 88	155 21	179 24	220 81	
55 449	71 20	84 29	105 51	122 71	137 49	157 19	183 16	221 16	

Synonyms:

1.LINOLEIC ACID 1T-CONF-[60-33-3];

Hit 152 : RH-T-2206.6-0.01%TRYPTAMINE 3T-TENT-[61-54-1]-RH03

CAS: 55334-17-3; Lib: tom18; ID: 152.



(tom18) RH-T-2206.6-0.01%TRYPTAMINE 3T-TENT-[61-54-1]-RH03

Name: RH-T-2206.6-0.01%TRYPTAMINE 3T-TENT-[61-54-1]-RH03

Formula: C₁₉H₃₆N₂Si₃

MW: 376 CAS#: 55334-17-3 ID#: 152 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:2206.6|

10 largest peaks:

174	999	73	336	175	162	176	70	86	66	202	51	67	49	100	49	59	44	361	40
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36 m/z Values and Intensities (7 low intensity peaks are not shown):

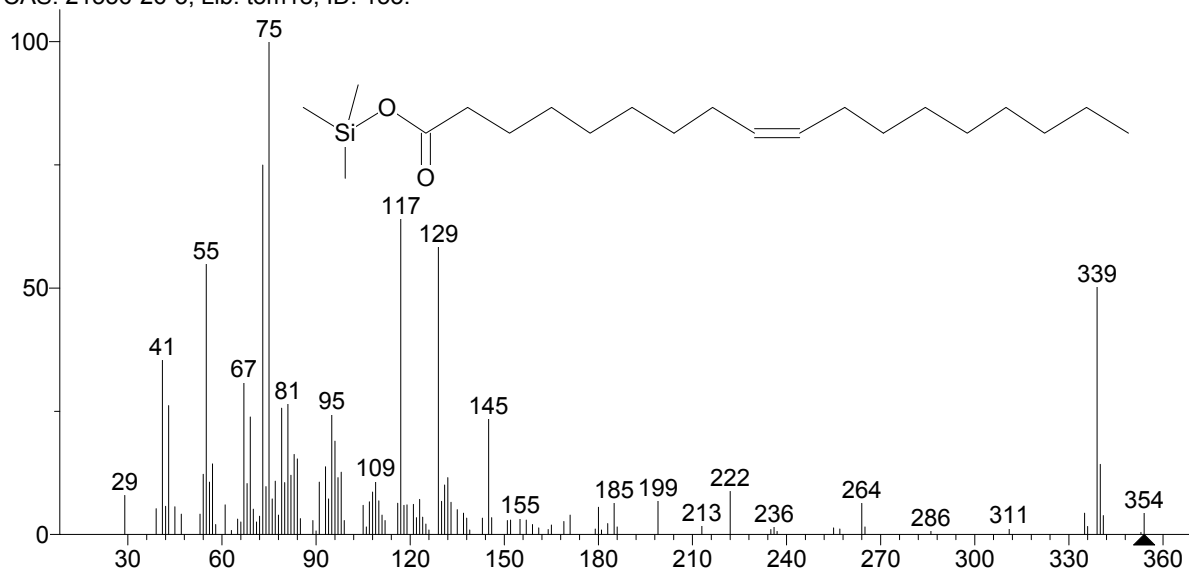
44	33	59	44	73	336	94	11	136	11	172	14	177	14	203	15	273	29
45	27	67	49	81	28	100	49	150	15	174	999	178	9	214	11	337	28
53	16	68	25	82	23	110	12	158	12	175	162	186	9	220	13	338	11
54	26	72	16	86	66	121	11	160	15	176	70	202	51	262	16	361	40

Synonyms:

1.TRYPTAMINE 3T-TENT-[61-54-1];

Hit 153 : RH-T-2212.4-0.05%-OLEIC ACID 1T-CONF-[112-80-1]-RH03

CAS: 21556-26-3; Lib: tom18; ID: 153.



(tom18) RH-T-2212.4-0.05%-OLEIC ACID 1T-CONF-[112-80-1]-RH03

Name: RH-T-2212.4-0.05%-OLEIC ACID 1T-CONF-[112-80-1]-RH03

Formula: C₂₁H₄₂O₂Si

MW: 354 CAS#: 21556-26-3 ID#: 153 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:2212.4|

10 largest peaks:

75 999	73 749	117 640	129 583	55 548	339 502	41 353	67 308	81 264	43 261
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106 m/z Values and Intensities (5 low intensity peaks are not shown):

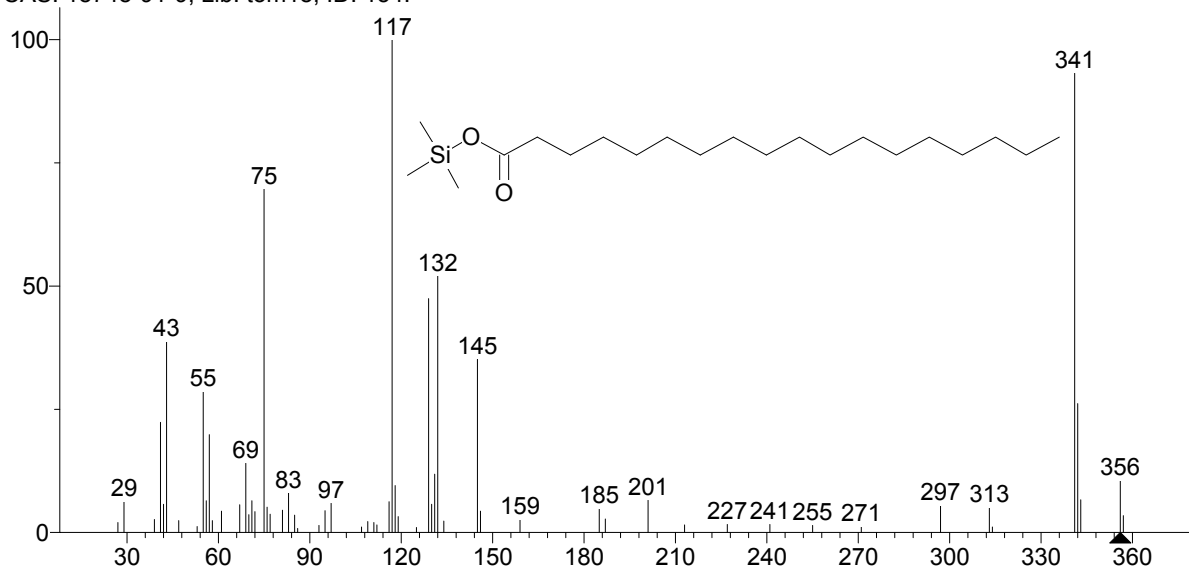
29 79	57 143	73 749	84 153	105 59	119 60	133 65	157 29	185 63	311 12
39 52	58 20	74 97	85 32	106 15	121 61	135 50	159 20	186 15	335 43
41 353	61 60	75 999	89 28	107 66	122 34	137 43	161 13	199 68	336 16
42 57	65 31	76 72	91 106	108 86	123 71	138 33	164 10	213 17	339 502
43 261	66 25	77 108	93 137	109 107	124 35	139 9	165 19	222 87	340 142
45 56	67 308	78 39	94 72	110 68	125 21	143 33	169 26	235 10	341 38
47 41	68 103	79 256	95 243	111 39	126 9	145 234	171 39	236 15	354 43
53 41	69 238	80 105	96 189	112 28	129 583	146 34	179 11	255 13	
54 122	70 51	81 264	97 115	116 63	130 67	151 28	180 55	257 11	
55 548	71 25	82 120	98 126	117 640	131 100	152 29	181 9	264 63	
56 106	72 37	83 162	99 28	118 59	132 115	155 32	183 22	265 15	

Synonyms:

1.OLEIC ACID 1T-CONF-[112-80-1];

Hit 154 : RH-T-2241.7-0.06%-STEARIC ACID 1T-CONF-[57-11-4]-RH03

CAS: 18748-91-9; Lib: tom18; ID: 154.



(tom18) RH-T-2241.7-0.06%-STEARIC ACID 1T-CONF-[57-11-4]-RH03

Name: RH-T-2241.7-0.06%-STEARIC ACID 1T-CONF-[57-11-4]-RH03

Formula: C₂₁H₄₄O₂Si

MW: 356 CAS#: 18748-91-9 ID#: 154 DB: tom18

Other DBs: None

Comment: RI:MG00238 [RI:2241.7]

10 largest peaks:

117 999	341 931	75 696	132 520	129 474	43 387	145 351	55 285	342 261	41 223
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60 m/z Values and Intensities (1 low intensity peak is not shown):

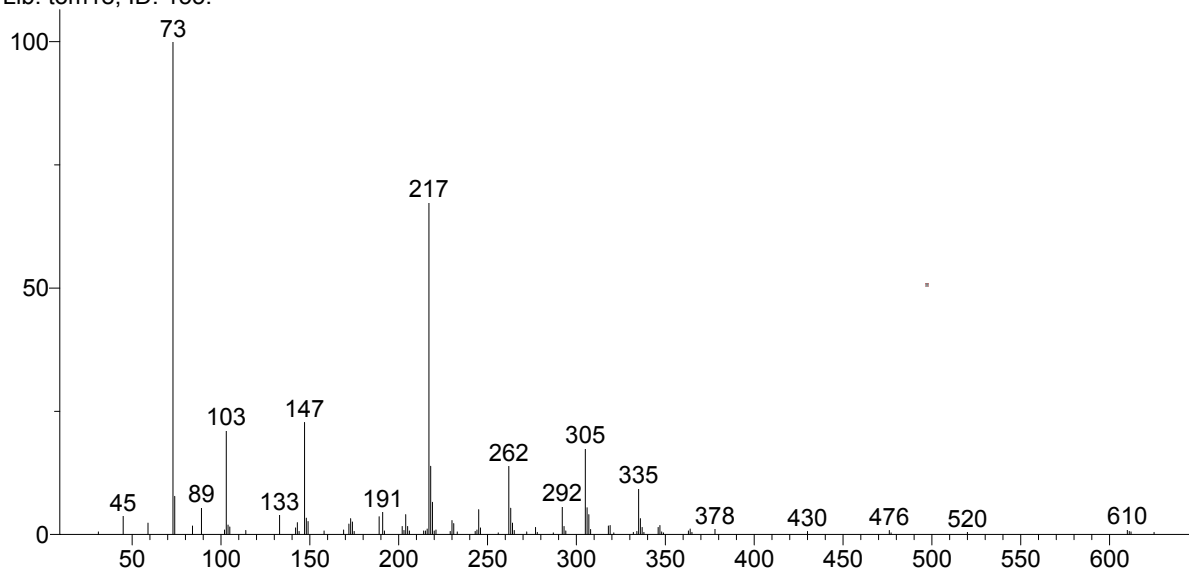
27 20	47 24	61 43	75 696	93 14	112 15	129 474	146 43	227 16	314 11
29 62	53 12	67 56	76 51	95 44	116 62	130 57	159 26	241 16	341 931
39 26	55 285	69 140	77 37	97 59	117 999	131 118	185 48	255 14	342 261
41 223	56 64	70 36	81 45	107 11	118 95	132 520	187 27	271 12	343 66
42 57	57 198	71 64	83 80	109 22	119 32	134 23	201 65	297 54	356 105
43 387	58 24	72 42	85 35	111 20	125 10	145 351	213 15	313 50	357 34

Synonyms:

1.STEARIC ACID 1T-CONF-[57-11-4];

Hit 155 : RH-T-2244.2-0.03%-[217,305,103,262,610]-RH01

Lib: tom18; ID: 155.



(tom18) RH-T-2244.2-0.03%-[217,305,103,262,610]-RH01 RI:2244.2,

Name: RH-T-2244.2-0.03%-[217,305,103,262,610]-RH01

MW: N/A ID#: 155 DB: tom18

RI: 2244.2,

Comment: RI=2244.2, 37.4809 min AB2129 [RI:2244.2]

10 largest peaks:

73 999 | 217 673 | 147 227 | 103 210 | 305 174 | 218 138 | 262 138 | 335 93 | 74 77 | 219 65 |

55 m/z Values and Intensities (35 low intensity peaks are not shown):

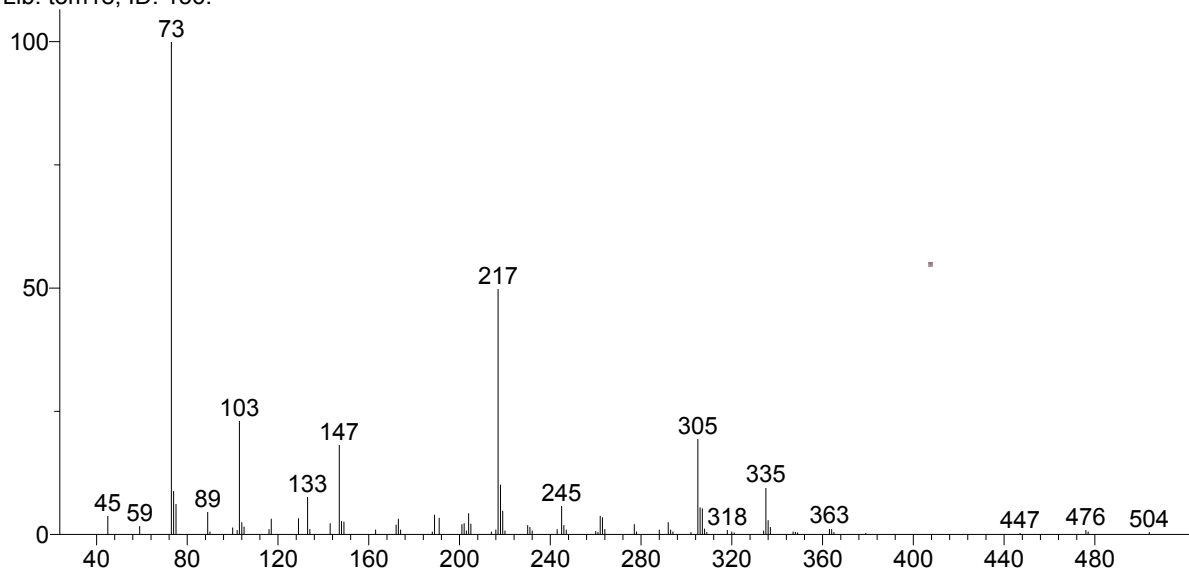
45 37	102 9	143 24	173 32	205 16	230 28	263 53	306 54	336 32	610 10
59 23	103 210	147 227	174 25	216 11	231 22	264 23	307 40	337 14	
73 999	104 19	148 33	189 36	217 673	244 9	277 14	308 10	346 14	
74 77	105 15	149 26	191 45	218 138	245 50	292 56	318 17	347 18	
84 17	133 39	169 9	202 16	219 65	246 13	293 16	319 18	364 11	
89 54	142 13	172 21	204 40	221 9	262 138	305 174	335 93	378 11	

Synonyms:

1.m217,305,103,262,610;

Hit 156 : RH-T-2253.9-0.04%-[217,305,103,335,245]-RH01

Lib: tom18; ID: 156.



(tom18) RH-T-2253.9-0.04%-[217,305,103,335,245]-RH01 RI:2253.9,

Name: RH-T-2253.9-0.04%-[217,305,103,335,245]-RH01

MW: N/A ID#: 156 DB: tom18

RI: 2253.9,

Comment: RI=2253.9, 37.6483 min AB2129 [RI:2253.9]

10 largest peaks:

73	999	217	497	103	230	305	193	147	181	218	100	335	95	74	87	133	75	75	61
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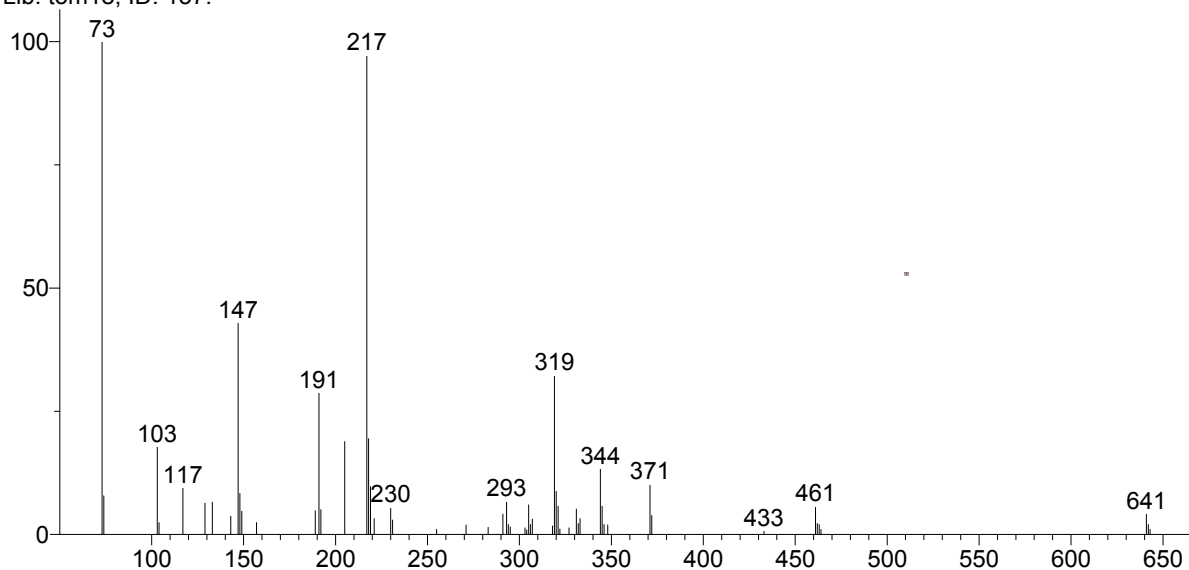
57 m/z Values and Intensities (24 low intensity peaks are not shown):

45	37	100	13	129	32	149	25	191	33	217	497	245	57	277	20	307	52	363	12
59	17	103	230	133	75	163	9	201	20	218	100	246	18	288	9	308	11	364	10
73	999	104	24	134	10	172	19	202	22	219	47	247	9	292	24	318	9	476	9
74	87	105	15	143	22	173	31	204	42	230	18	262	37	293	9	335	95		
75	61	116	10	147	181	174	9	205	21	231	14	263	34	305	193	336	28		
89	45	117	31	148	26	189	39	216	9	243	10	264	10	306	54	337	14		

Synonyms:

1.m217,305,103,335,245;

Hit 157 : RH-T-2260.6-0.00%-[217,319,191,344,371,205,461,641, N: sim.D-Galactofuranose 5T]-RH03
 Lib: tom18; ID: 157.



(tom18) RH-T-2260.6-0.00%-[217,319,191,344,371,205,461,641, N: sim.D-Galactofuranose 5T]-RH03 RI:2260.6,

Name: RH-T-2260.6-0.00%-[217,319,191,344,371,205,461,641, N: sim.D-Galactofuranose 5T]-RH03

MW: N/A ID#: 157 DB: tom18

RI: 2260.6,

Comment: RI=2260.6, 44.3715 min MG00244 [RI:2260.6]

10 largest peaks:

73 999 | 217 971 | 147 428 | 319 322 | 191 287 | 218 194 | 205 188 | 103 177 | 344 132 | 371 101 |

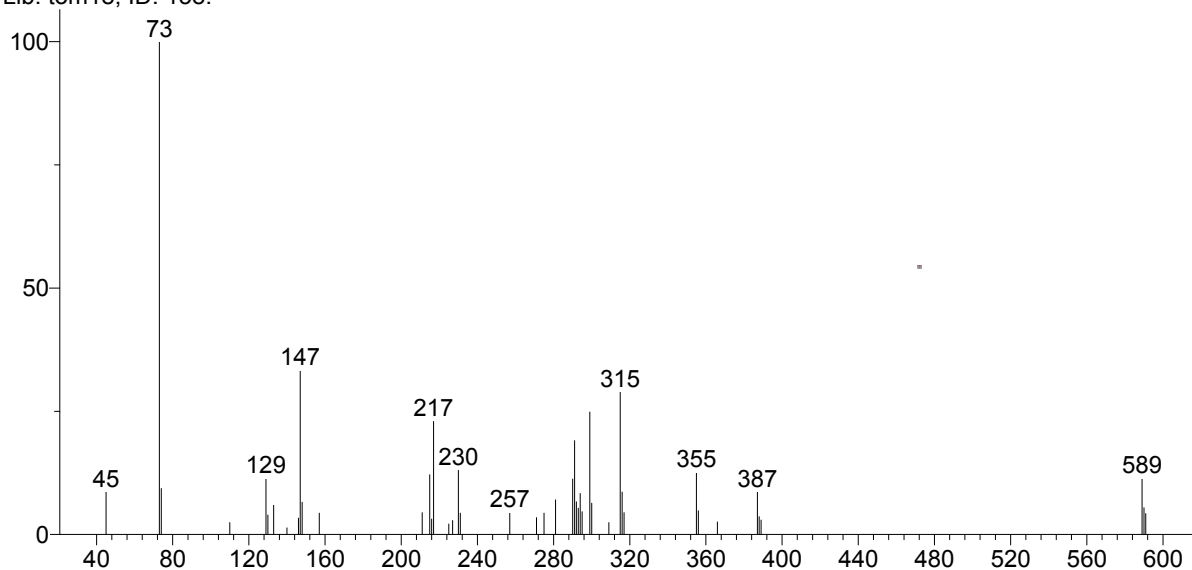
56 m/z Values and Intensities (1 low intensity peak is not shown):

73 999	133 65	189 48	219 97	283 14	304 9	320 87	333 32	372 38	642 20
74 78	143 37	191 287	221 32	291 41	305 60	321 57	344 132	461 56	643 10
103 177	147 428	192 50	230 54	293 66	306 20	322 11	345 57	462 22	
104 24	148 83	205 188	231 29	294 20	307 31	327 13	346 20	463 20	
117 94	149 47	217 971	255 10	295 15	318 17	331 51	348 19	464 10	
129 63	157 24	218 194	271 19	303 13	319 322	332 22	371 101	641 41	

Synonyms:

1.m217,319,191,344,371,205,461,641, N: sim.D-Galactofuranose 5T;

Hit 158 : RH-T-2265.6-0.00%-[315,217,299,589,291,355,387, N:sim. D-Fructose, 6-phosphate 6T]-RH03
Lib: tom18; ID: 158.



(tom18) RH-T-2265.6-0.00%-[315,217,299,589,291,355,387, N:sim. D-Fructose, 6-phosphate 6T]-RH03 RI:2265.6,

Name: RH-T-2265.6-0.00%-[315,217,299,589,291,355,387, N:sim. D-Fructose, 6-phosphate 6T]-RH03

MW: N/A ID#: 158 DB: tom18

RI: 2265.6,

Comment: RI=2265.6, 44.4801 min MG00244 [RI:2265.6]

10 largest peaks:

73 999 | 147 332 | 315 288 | 299 248 | 217 229 | 291 190 | 230 130 | 355 125 | 215 121 | 129 113 |

45 m/z Values and Intensities:

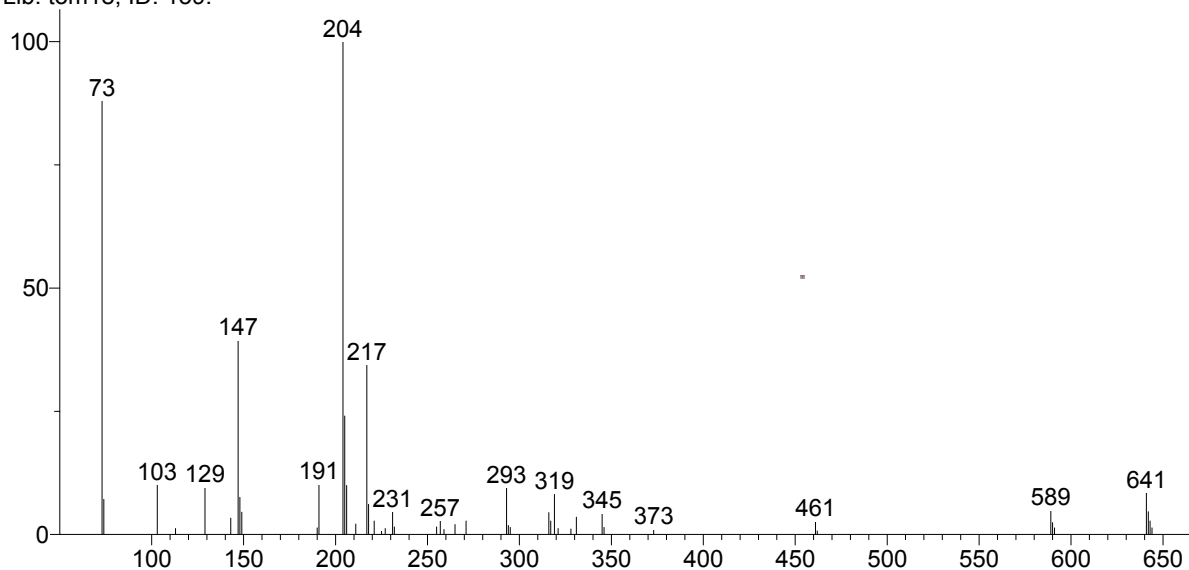
45	86	130	39	148	65	217	229	257	44	291	190	299	248	317	44	388	36
73	999	133	59	157	43	225	21	271	34	292	66	300	63	355	125	389	29
74	93	140	13	211	44	227	28	275	43	293	53	309	24	356	48	589	113
110	24	146	33	215	121	230	130	281	70	294	83	315	288	366	25	590	54
129	113	147	332	216	31	231	43	290	112	295	46	316	86	387	86	591	42

Synonyms:

1.m315,217,299,589,291,355,387, N:sim. D-Fructose, 6-phosphate 6T;

Hit 159 : RH-T-2269.7-0.01%-[204,217,293,641,589,345]-RH03

Lib: tom18; ID: 159.



(tom18) RH-T-2269.7-0.01%-[204,217,293,641,589,345]-RH03 RI:2269.7,

Name: RH-T-2269.7-0.01%-[204,217,293,641,589,345]-RH03

MW: N/A ID#: 159 DB: tom18

RI: 2269.7,

Comment: RI=2269.7, 44.5678 min MG00244 [RI:2269.7]

10 largest peaks:

204 999 | 73 878 | 147 393 | 217 343 | 205 240 | 191 101 | 103 100 | 206 99 | 129 95 | 293 94 |

46 m/z Values and Intensities (2 low intensity peaks are not shown):

73 878 | 143 33 | 191 101 | 217 343 | 232 15 | 271 27 | 317 27 | 345 42 | 590 24 | 644 13 |

74 71 | 147 393 | 204 999 | 218 61 | 255 15 | 293 94 | 319 81 | 346 14 | 591 13 |

103 100 | 148 75 | 205 240 | 221 27 | 257 27 | 294 18 | 321 12 | 373 10 | 641 84 |

113 12 | 149 45 | 206 99 | 227 12 | 259 10 | 295 14 | 328 11 | 461 26 | 642 46 |

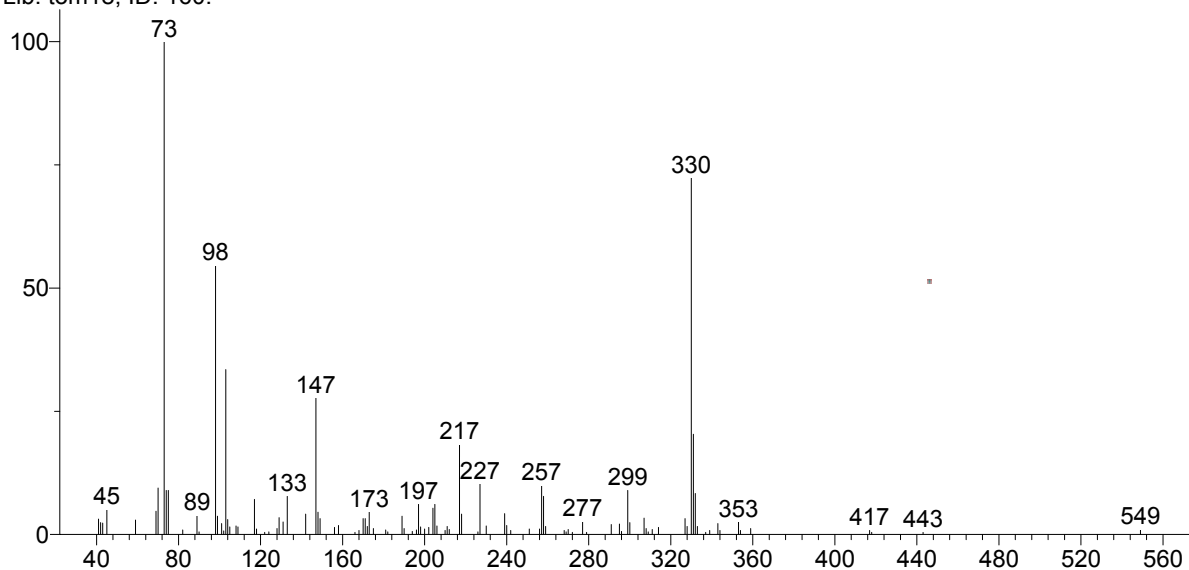
129 95 | 190 13 | 211 21 | 231 45 | 265 20 | 316 44 | 331 35 | 589 48 | 643 27 |

Synonyms:

1.m204,217,293,641,589,345;

Hit 160 : RH-T-2282.7-0.06%-[330,98,103,217,299,257,549]-RH01

Lib: tom18; ID: 160.



(tom18) RH-T-2282.7-0.06%-[330,98,103,217,299,257,549]-RH01 RI:2282.7,

Name: RH-T-2282.7-0.06%-[330,98,103,217,299,257,549]-RH01

MW: N/A ID#: 160 DB: tom18

RI: 2282.7,

Comment: RI=2282.7, 38.1459 min AB2129 [RI:2282.7]

10 largest peaks:

73 999 | 330 723 | 98 545 | 103 334 | 147 276 | 331 203 | 217 182 | 227 102 | 257 99 | 70 94 |

81 m/z Values and Intensities (24 low intensity peaks are not shown):

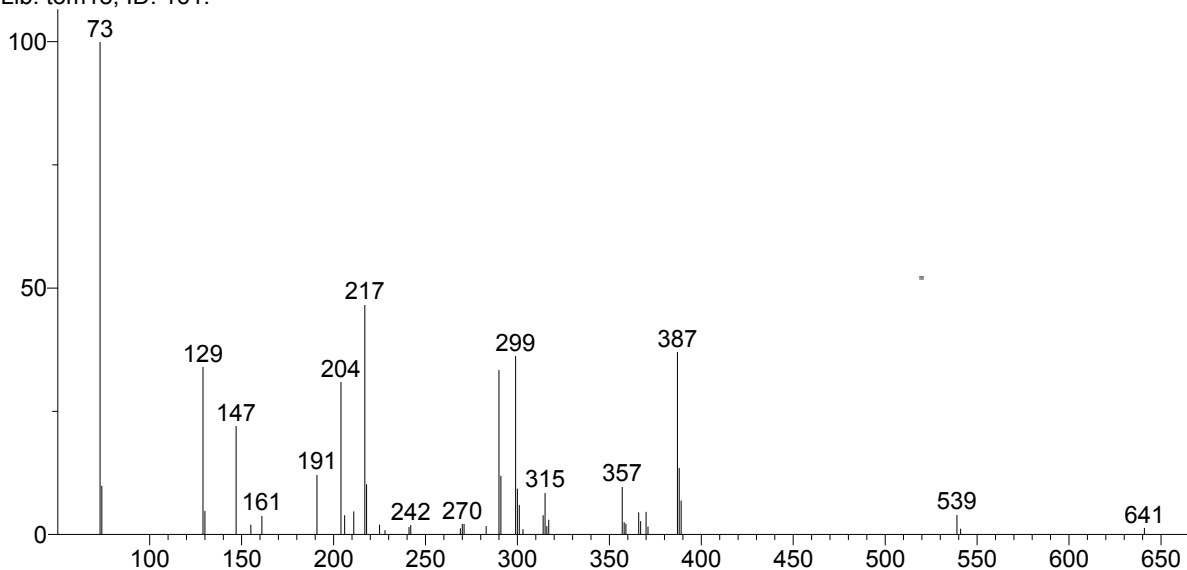
41	31	75	89	108	17	147	276	175	12	204	53	239	42	291	20	328	16
42	24	82	9	109	15	148	45	181	9	205	61	240	18	295	21	330	723
43	23	89	38	117	71	149	32	189	37	206	17	251	11	299	89	331	203
45	50	98	545	118	11	156	14	190	12	211	16	256	11	300	24	332	83
59	29	99	37	128	12	158	18	196	9	212	10	257	99	307	33	333	16
69	47	101	22	129	34	170	32	197	61	217	182	258	77	308	12	343	22
70	94	103	334	131	25	171	32	198	15	218	41	259	16	311	10	353	25
73	999	104	30	133	77	172	16	200	11	227	102	270	10	314	14	359	12
74	89	105	15	142	41	173	45	202	14	230	17	277	26	327	32	549	10

Synonyms:

1.m330,98,103,217,299,257,549;

Hit 161 : RH-T-2293.0-0.00%-[217,387,299,290,129,204,539, phosphate]-RH03

Lib: tom18; ID: 161.



(tom18) RH-T-2293.0-0.00%-[217,387,299,290,129,204,539, phosphate]-RH03 RI:2293.0,

Name: RH-T-2293.0-0.00%-[217,387,299,290,129,204,539, phosphate]-RH03

MW: N/A ID#: 161 DB: tom18

RI: 2293.0,

Comment: RI=2293.0, 45.0681 min MG00244 [RI:2293]

10 largest peaks:

73 999 | 217 466 | 387 370 | 299 361 | 129 339 | 290 333 | 204 309 | 147 220 | 388 134 | 191 121 |

43 m/z Values and Intensities (1 low intensity peak is not shown):

73 999 | 155 19 | 211 46 | 242 19 | 290 333 | 303 10 | 357 97 | 370 45 | 539 40 |

74 98 | 161 38 | 217 466 | 269 12 | 291 118 | 314 38 | 358 24 | 371 15 | 541 11 |

129 339 | 191 121 | 218 101 | 270 21 | 299 361 | 315 85 | 359 21 | 387 370 | 641 13 |

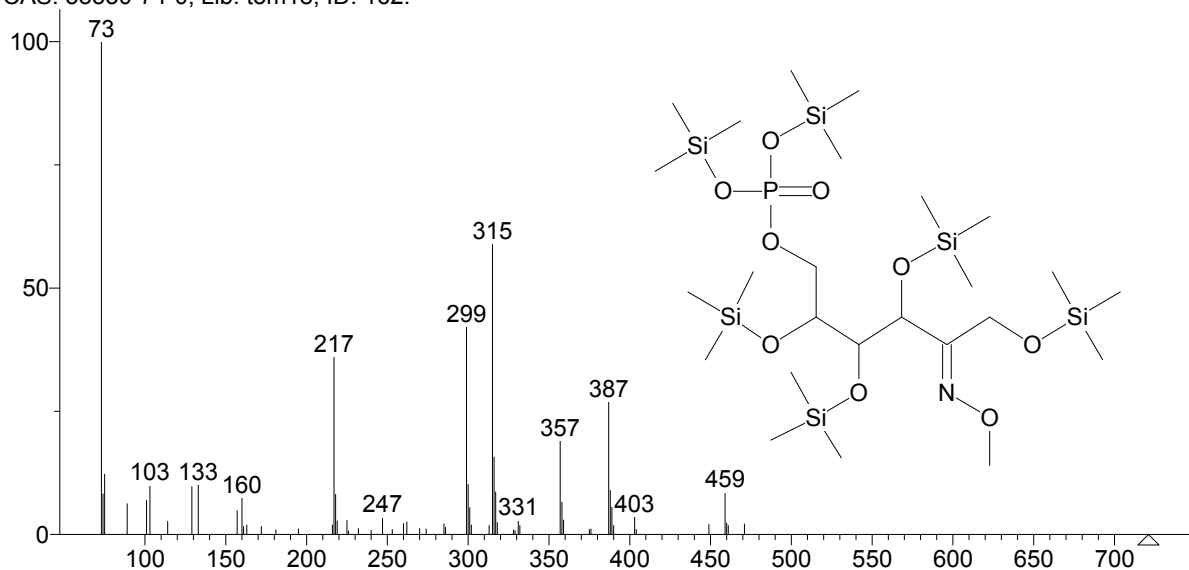
130 47 | 204 309 | 225 19 | 271 21 | 300 92 | 316 16 | 366 44 | 388 134 |

147 220 | 206 38 | 241 14 | 283 16 | 301 59 | 317 29 | 367 26 | 389 68 |

Synonyms:

1.m217,387,299,290,129,204,539, phosphate;

Hit 162 : RH-T-2322.5-0.01%-FRUCTOSE-6-PHOSPHATE M6T-CONF-[643-13-0]-RH03
CAS: 55530-74-0; Lib: tom18; ID: 162.



(tom18) RH-T-2322.5-0.01%-FRUCTOSE-6-PHOSPHATE M6T-CONF-[643-13-0]-RH03

Name: RH-T-2322.5-0.01%-FRUCTOSE-6-PHOSPHATE M6T-CONF-[643-13-0]-RH03

Formula: C₂₅H₆₄NO₉PSi₆

MW: 721 CAS#: 55530-74-0 ID#: 162 DB: tom18

Other DBs: None

Comment: RI:MG00238 [RI:2322.5]

10 largest peaks:

73 999 | 315 588 | 299 420 | 217 359 | 387 268 | 357 189 | 316 157 | 75 122 | 300 101 | 133 100 |

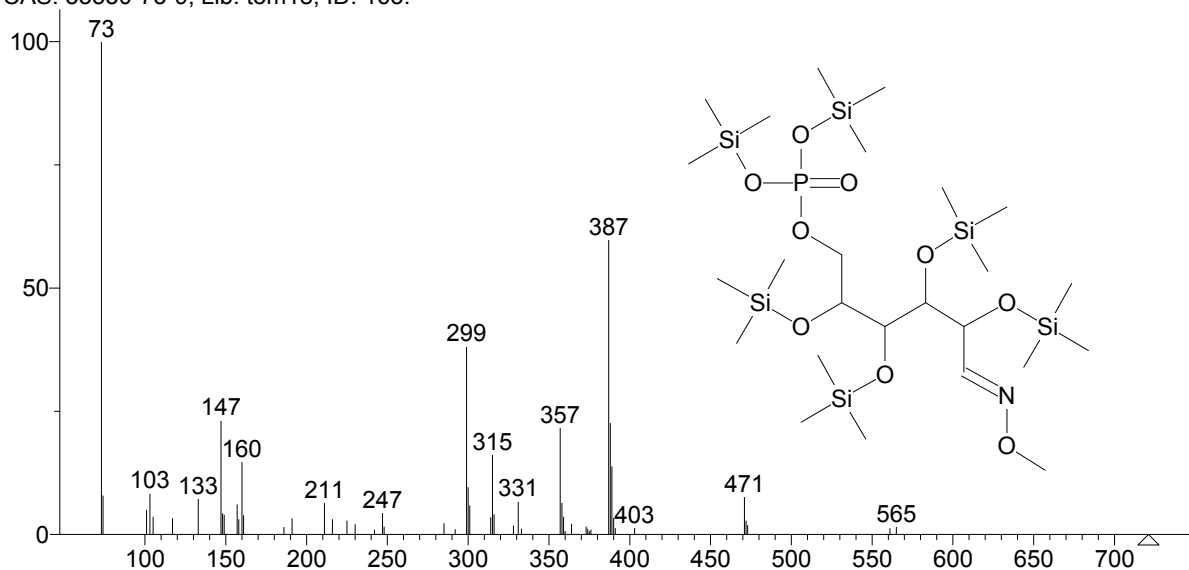
58 m/z Values and Intensities (3 low intensity peaks are not shown):

73	999	114	26	163	19	218	81	260	22	299	420	316	157	357	189	388	89	459	85
74	82	129	97	172	16	219	27	262	25	300	101	317	86	358	65	389	55	460	23
75	122	133	100	181	9	225	28	270	12	301	54	318	24	359	29	390	18	461	18
89	62	157	48	195	11	232	12	274	11	302	19	328	9	375	10	403	35	471	21
101	69	160	74	216	19	247	34	285	21	313	18	331	28	376	11	404	10		
103	99	161	16	217	359	253	10	286	14	315	588	332	18	387	268	449	20		

Synonyms:

1.FRUCTOSE-6-PHOSPHATE M6T-CONF-[643-13-0];

Hit 163 : RH-T-2332.6-0.02%-GLUCOSE-6-PHOSPHATE M6T PK1-CONF-[56-73-5]-RH03
CAS: 55530-73-9; Lib: tom18; ID: 163.



(tom18) RH-T-2332.6-0.02%-GLUCOSE-6-PHOSPHATE M6T PK1-CONF-[56-73-5]-RH03

Name: RH-T-2332.6-0.02%-GLUCOSE-6-PHOSPHATE M6T PK1-CONF-[56-73-5]-RH03

Formula: C₂₅H₆₄NO₉PSi₆

MW: 721 CAS#: 55530-73-9 ID#: 163 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:2332.6|

10 largest peaks:

73 999 | 387 597 | 299 381 | 147 231 | 388 225 | 357 215 | 315 161 | 160 146 | 389 137 | 300 95 |

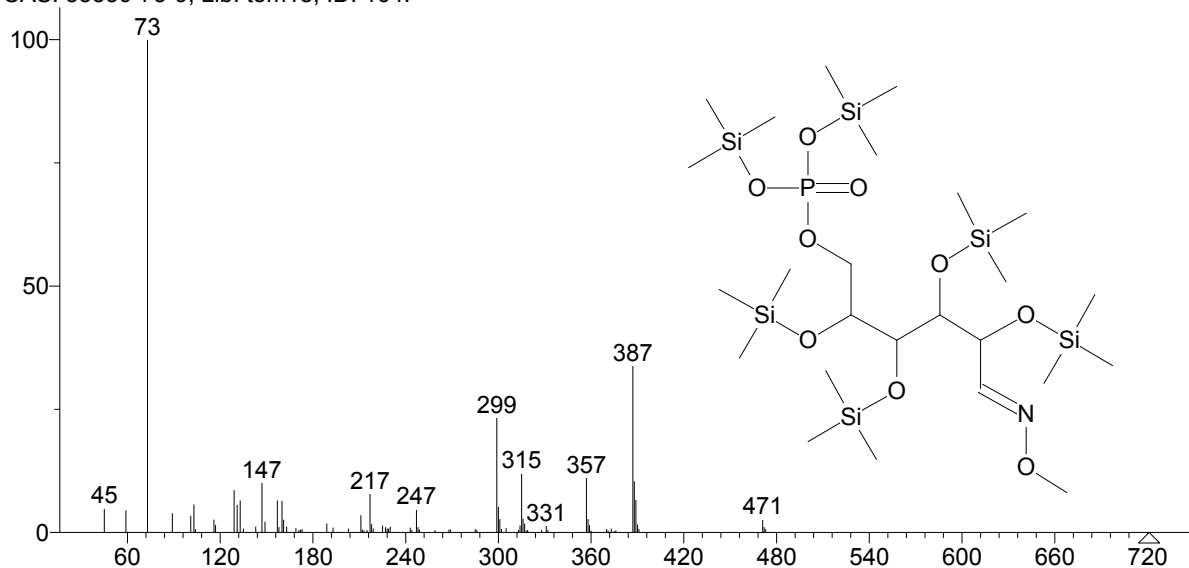
52 m/z Values and Intensities (2 low intensity peaks are not shown):

73	999	133	72	160	146	225	27	292	10	316	40	359	35	388	225	472	27
74	78	147	231	161	38	230	20	299	381	328	17	364	21	389	137	473	18
101	49	148	42	186	14	242	9	300	95	331	66	373	15	390	33	561	12
103	83	149	39	191	32	247	43	301	58	333	11	374	11	391	12	565	15
105	35	157	60	211	63	248	15	314	34	357	215	376	9	403	13		
117	32	158	30	216	30	285	22	315	161	358	63	387	597	471	75		

Synonyms:

1.GLUCOSE-6-PHOSPHATE M6T PK1-CONF-[56-73-5];

Hit 164 : RH-T-2344.2-0.01%-GLUCOSE-6-PHOSPHATE-M6T-PK2-CONF-8135A18-G-X
CAS: 55530-73-9; Lib: tom18; ID: 164.



(tom18) RH-T-2344.2-0.01%-GLUCOSE-6-PHOSPHATE-M6T-PK2-CONF-8135A18-G-X RI:2344.2,

Name: RH-T-2344.2-0.01%-GLUCOSE-6-PHOSPHATE-M6T-PK2-CONF-8135A18-G-X

Formula: C₂₅H₆₄NO₉PSi₆

MW: 721 CAS#: 55530-73-9 ID#: 164 DB: tom18

Other DBs: None

RI: 2344.2,

Comment: RI=2344.2, 34.9652 min 8135A18 |RI:2344.2|

10 largest peaks:

73 999 | 387 337 | 299 232 | 315 119 | 357 110 | 388 103 | 147 100 | 129 85 | 217 78 | 389 65 |

47 m/z Values and Intensities (35 low intensity peaks are not shown):

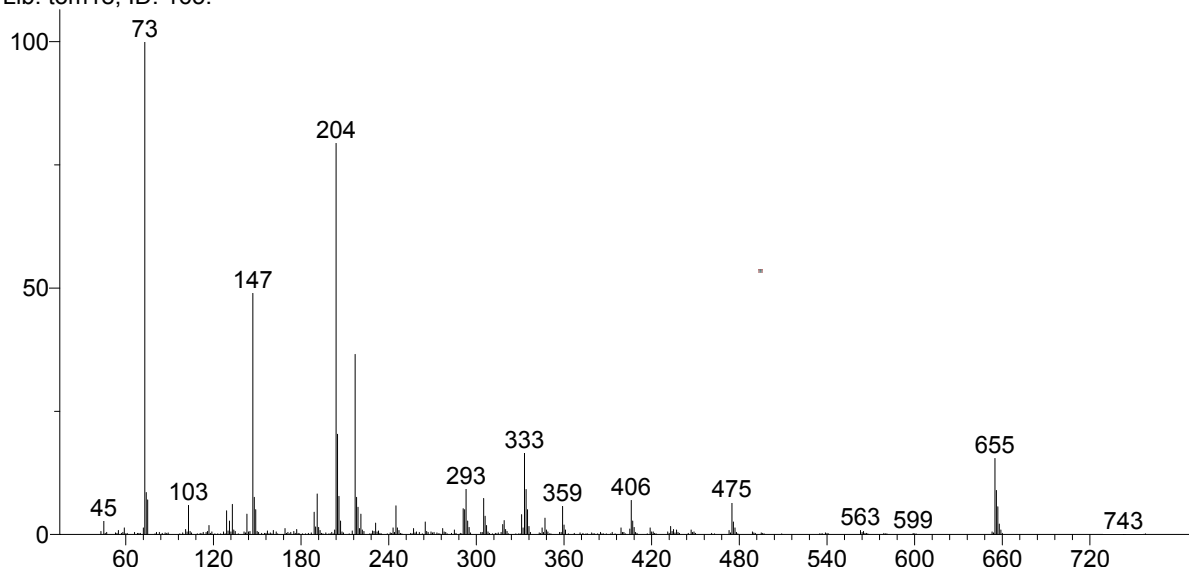
45	48	103	56	133	64	158	10	193	9	227	10	299	232	316	27	359	14	471	26
59	44	116	25	143	11	160	63	211	34	230	11	300	51	317	17	387	337	472	10
73	999	117	14	147	100	161	25	217	78	243	9	301	26	331	13	388	103		
89	38	129	85	149	21	163	11	218	16	247	46	314	13	357	110	389	65		
101	33	131	55	157	64	189	17	225	13	248	10	315	119	358	26	390	15		

Synonyms:

1.GLUCOSE-6-PHOSPHATE-M6T-PK2-CONF;

Hit 165 : RH-T-2359.4-0.10%-[204,217,655,333,475,406,743, N: sim. Galacturonic T5]-RH03

Lib: tom18; ID: 165.



(tom18) RH-T-2359.4-0.10%-[204,217,655,333,475,406,743, N: sim. Galacturonic T5]-RH03 RI:2359.4,

Name: RH-T-2359.4-0.10%-[204,217,655,333,475,406,743, N: sim. Galacturonic T5]-RH03

MW: N/A ID#: 165 DB: tom18

RI: 2359.4,

Comment: RI=2359.4, 46.4472 min MG00244 [RI:2359.4]

10 largest peaks:

73 999 | 204 793 | 147 489 | 217 365 | 205 203 | 333 165 | 655 154 | 293 92 | 334 91 | 656 89 |

83 m/z Values and Intensities (218 low intensity peaks are not shown):

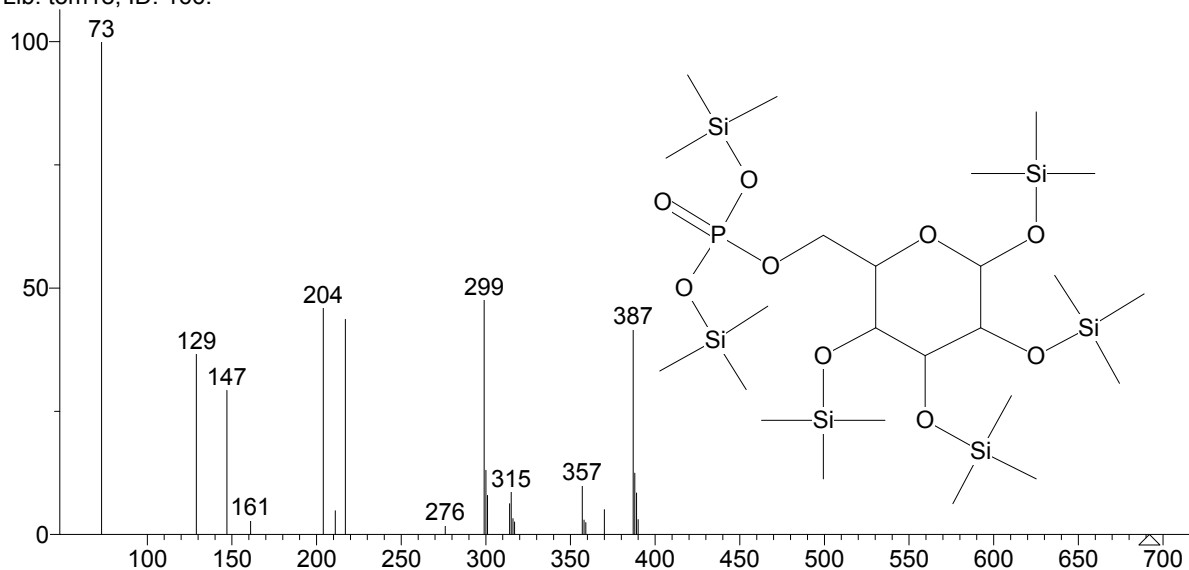
45	27	129	48	177	10	207	27	245	58	294	27	332	13	360	19	435	10	658	21
59	13	131	27	189	45	217	365	246	13	295	14	333	165	361	9	437	9	659	9
72	13	133	61	190	15	218	75	257	12	305	73	334	91	399	13	447	9		
73	999	134	9	191	82	219	55	265	25	306	37	335	50	405	11	475	64		
74	85	143	41	192	14	220	12	277	12	307	18	336	16	406	69	476	25		
75	70	147	489	203	9	221	41	285	9	318	20	345	13	407	27	477	13		
101	10	148	75	204	793	222	9	291	52	319	28	347	33	408	14	655	154		
103	59	149	50	205	203	231	23	292	50	320	10	348	9	419	13	656	89		
117	18	169	12	206	77	243	13	293	92	331	40	359	57	433	16	657	56		

Synonyms:

1.m204,217,655,333,475,406,743, N: sim. Galacturonic T5;

Hit 166 : RH-T-2368.2-0.00%-[N:Glucopyranose, 1,2,3,4-O-(T)-, bis(T) phos]-TENT-RH03

Lib: tom18; ID: 166.



(tom18) RH-T-2368.2-0.00%-[N:Glucopyranose, 1,2,3,4-O-(T)-, bis(T) phos]-TENT-RH03 RI:2368.2,

Name: RH-T-2368.2-0.00%-[N:Glucopyranose, 1,2,3,4-O-(T)-, bis(T) phos]-TENT-RH03

Formula: C₂₄H₆₁O₉PSi₆

MW: 692 ID#: 166 DB: tom18

RI: 2368.2,

Comment: RI=2368.2, 46.6295 min MG00244 [RI:2368.2]

10 largest peaks:

73 999 | 299 475 | 204 459 | 217 436 | 387 415 | 129 366 | 147 292 | 300 130 | 388 124 | 357 99 |

23 m/z Values and Intensities:

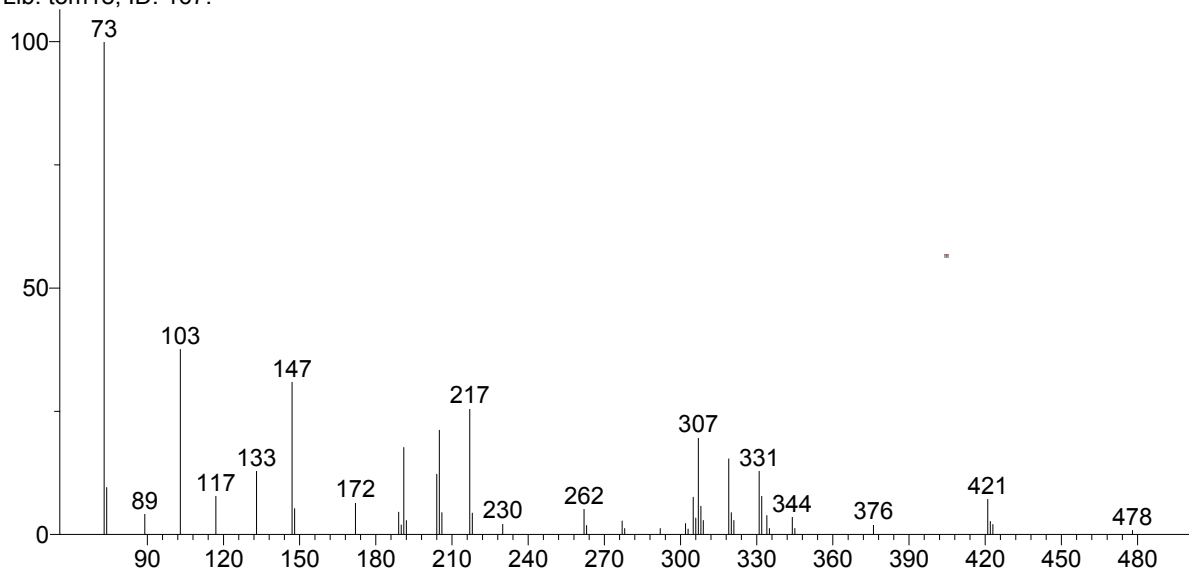
73 999 | 161 28 | 217 436 | 300 130 | 315 86 | 357 99 | 370 50 | 389 84 |
 129 366 | 204 459 | 276 18 | 301 79 | 316 32 | 358 29 | 387 415 | 390 30 |
 147 292 | 211 48 | 299 475 | 314 62 | 317 25 | 359 24 | 388 124 |

Synonyms:

1.Glucopyranose, 1,2,3,4-O-(T)-, bis(T) phos]-TENT;

Hit 167 : RH-T-2375.8-0.01%-[103,217,307,205,191]-RH03

Lib: tom18; ID: 167.



(tom18) RH-T-2375.8-0.01%-[103,217,307,205,191]-RH03

Name: RH-T-2375.8-0.01%-[103,217,307,205,191]-RH03

MW: N/A ID#: 167 DB: tom18

Comment: RI:MG00238 [RI:2375.8]

10 largest peaks:

73 999 | 103 375 | 147 309 | 217 255 | 205 211 | 307 196 | 191 176 | 319 153 | 133 128 | 331 128 |

44 m/z Values and Intensities (1 low intensity peak is not shown):

73 999 | 133 128 | 190 19 | 206 44 | 263 18 | 303 11 | 309 28 | 332 77 | 376 20 |

74 95 | 147 309 | 191 176 | 217 255 | 277 27 | 305 75 | 319 153 | 334 38 | 421 71 |

89 41 | 148 52 | 192 28 | 218 43 | 278 12 | 306 33 | 320 44 | 335 12 | 422 26 |

103 375 | 172 64 | 204 122 | 230 22 | 292 12 | 307 196 | 321 28 | 344 35 | 423 20 |

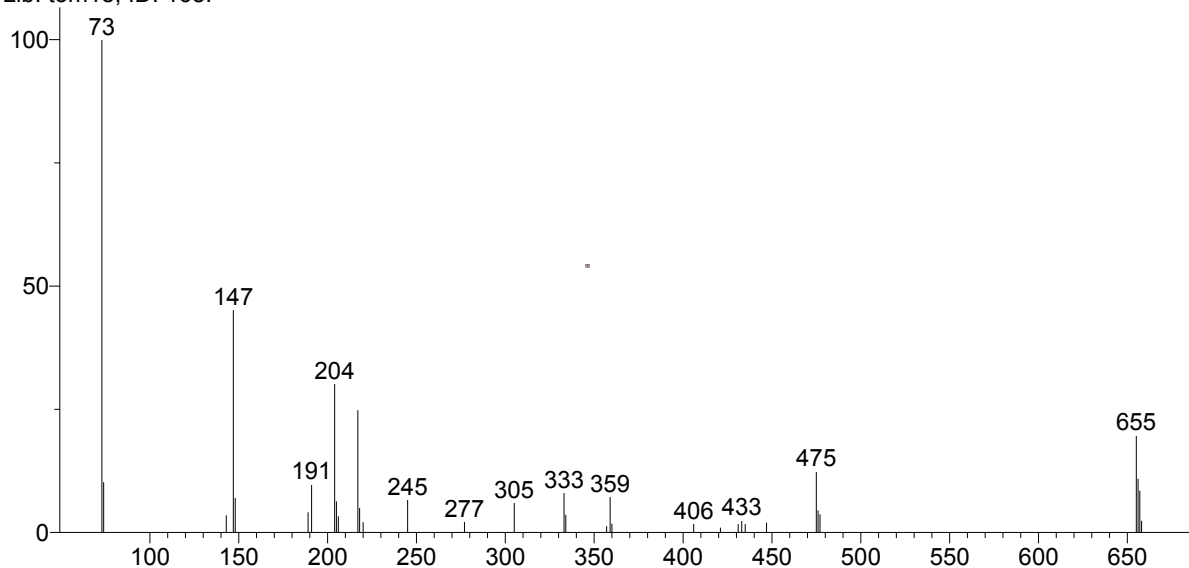
117 77 | 189 45 | 205 211 | 262 51 | 302 22 | 308 57 | 331 128 | 345 12 |

Synonyms:

1.m103,217,307,205,191;

Hit 168 : RH-T-2382.1-0.00%-[204,655,217,475,333,359]-RH03

Lib: tom18; ID: 168.



(tom18) RH-T-2382.1-0.00%-[204,655,217,475,333,359]-RH03 RI:2382.1,

Name: RH-T-2382.1-0.00%-[204,655,217,475,333,359]-RH03

MW: N/A ID#: 168 DB: tom18

RI: 2382.1,

Comment: RI=2382.1, 46.9160 min MG00244 [RI:2382.1]

10 largest peaks:

73 999 | 147 450 | 204 301 | 217 247 | 655 196 | 475 123 | 656 108 | 74 101 | 191 97 | 657 84 |

34 m/z Values and Intensities:

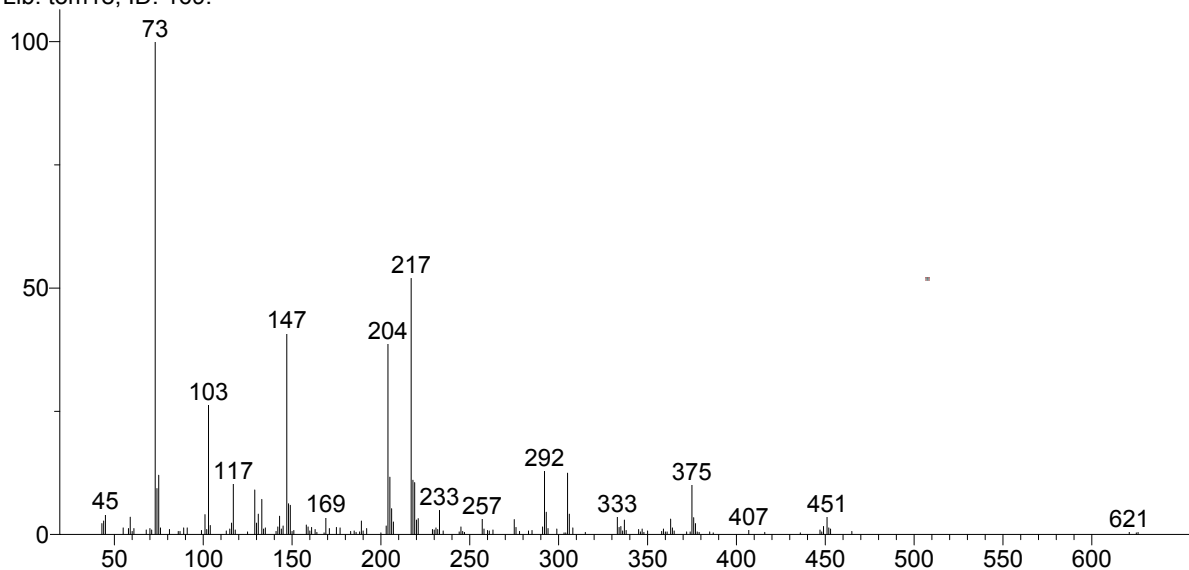
73 999 | 148 69 | 205 62 | 220 20 | 333 79 | 360 17 | 433 24 | 476 44 | 657 84 |
74 101 | 189 40 | 206 32 | 245 65 | 334 35 | 406 17 | 435 16 | 477 36 | 658 23 |
143 34 | 191 97 | 217 247 | 277 21 | 357 12 | 421 9 | 447 19 | 655 196 |
147 450 | 204 301 | 218 49 | 305 60 | 359 71 | 431 16 | 475 123 | 656 108 |

Synonyms:

1.m204,655,217,475,333,359;

Hit 169 : RH-T-2391.0-0.05%-[217,204,103,375,292,305,451,621]-RH03

Lib: tom18; ID: 169.



(tom18) RH-T-2391.0-0.05%-[217,204,103,375,292,305,451,621]-RH03

Name: RH-T-2391.0-0.05%-[217,204,103,375,292,305,451,621]-RH03

MW: N/A ID#: 169 DB: tom18

Comment: RI:MG00238 |RI:2391|

10 largest peaks:

73 999 | 217 519 | 147 407 | 204 386 | 103 262 | 292 128 | 305 124 | 75 120 | 205 116 | 218 110 |

95 m/z Values and Intensities (52 low intensity peaks are not shown):

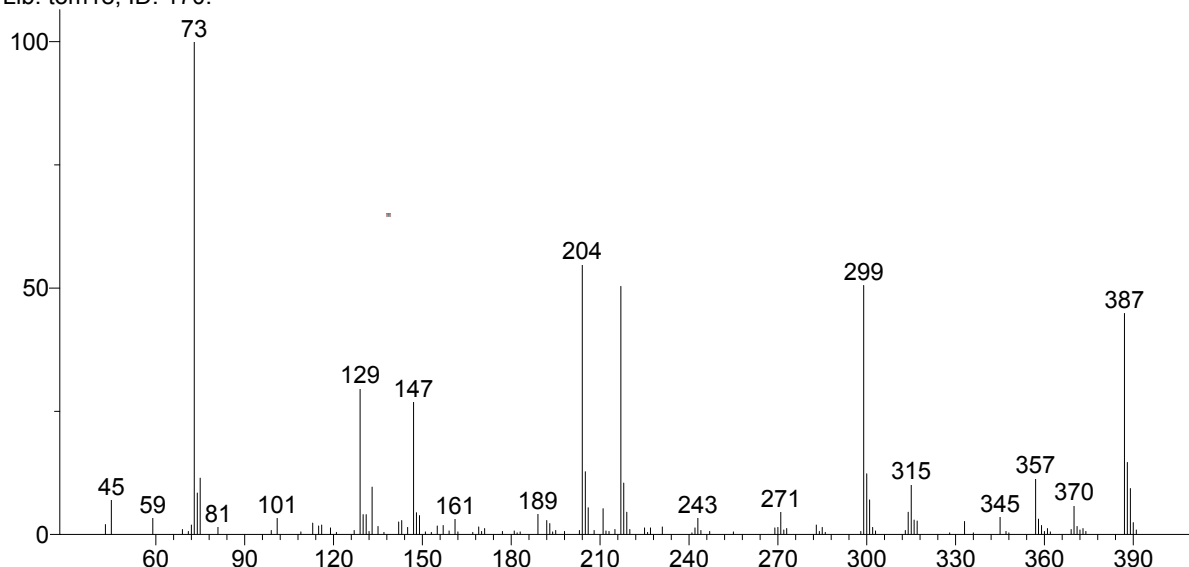
43	22	73	999	104	18	135	13	161	14	205	116	231	13	292	128	337	29	447	9
44	27	74	93	115	11	142	15	163	10	206	52	232	10	293	45	345	10	449	16
45	40	75	120	116	23	143	37	169	34	207	25	233	49	294	12	347	11	451	35
55	13	76	13	117	102	144	11	171	12	217	519	245	15	299	11	359	11	452	13
58	12	81	10	118	9	145	17	175	14	218	110	257	31	305	124	363	31	453	11
59	35	89	13	129	90	147	407	177	13	219	105	258	11	306	41	364	13		
61	12	91	13	130	23	148	62	189	27	220	29	263	9	308	13	375	100		
68	9	101	40	131	41	149	59	192	12	221	32	275	30	333	35	376	34		
70	12	102	10	133	71	158	19	203	17	229	10	276	14	334	14	377	22		
71	9	103	262	134	11	159	15	204	386	230	9	291	15	335	16	407	9		

Synonyms:

1.m217,204,103,375,292,305,451,621;

Hit 170 : RH-T-2401.1-0.02%-[204,217,299,387,129,357,315, N: sim. Mannose 6 phos.]-RH03

Lib: tom18; ID: 170.



(tom18) RH-T-2401.1-0.02%-[204,217,299,387,129,357,315, N: sim. Mannose 6 phos.]-RH03 RI:2401.1,

Name: RH-T-2401.1-0.02%-[204,217,299,387,129,357,315, N: sim. Mannose 6 phos.]-RH03

MW: N/A ID#: 170 DB: tom18

RI: 2401.1,

Comment: RI=2401.1, 47.3094 min MG00244 [RI:2401.1]

10 largest peaks:

73 999 | 204 547 | 299 505 | 217 503 | 387 448 | 129 296 | 147 268 | 388 146 | 205 127 | 300 123 |

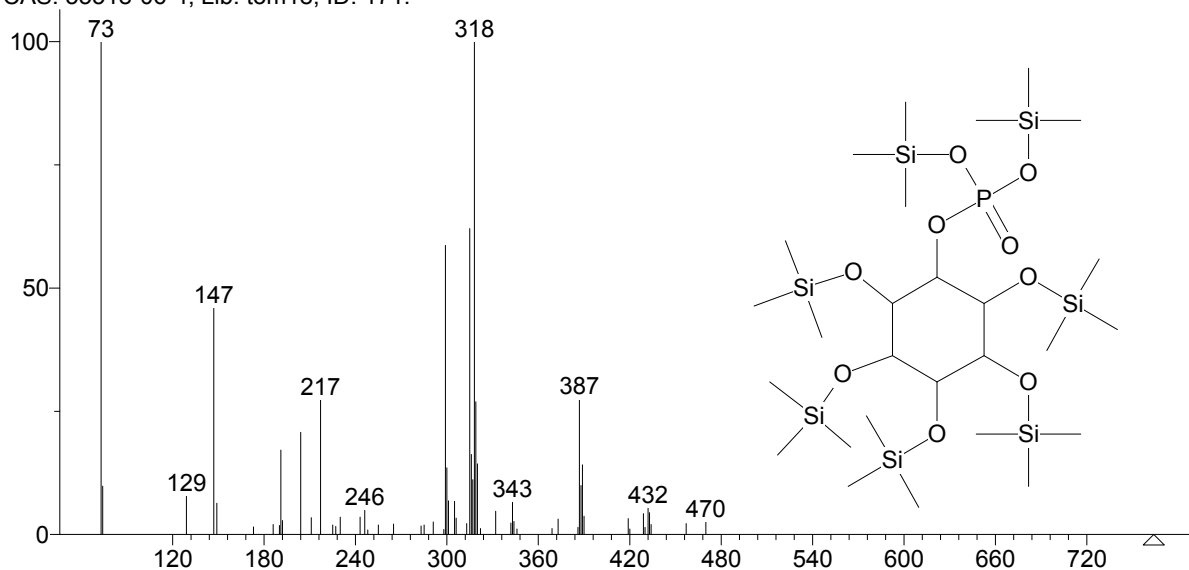
78 m/z Values and Intensities (41 low intensity peaks are not shown):

43	20	81	15	131	40	149	38	193	22	219	45	270	14	301	70	357	113	373	12
45	70	101	33	133	96	155	17	204	547	220	10	271	45	302	14	358	31	387	448
59	33	113	23	135	16	157	18	205	127	225	13	272	9	314	45	359	18	388	146
69	10	115	17	142	25	161	31	206	54	227	13	273	12	315	101	361	12	389	93
72	19	116	19	143	28	169	15	211	52	231	15	283	19	316	29	369	10	390	24
73	999	119	13	145	14	171	12	215	10	242	13	285	14	317	27	370	58	391	9
74	84	129	296	147	268	189	41	217	503	243	33	299	505	333	26	371	16		
75	114	130	40	148	44	192	28	218	104	269	13	300	123	345	35	372	9		

Synonyms:

1.m204,217,299,387,129,357,315, N: sim. Mannose 6 phos;

Hit 171 : RH-T-2423.8-0.01%-[N: Myo-Inositol, 1,3,4,5,6-O-(T)-bis(T)phosphate]-TENT-RH03
CAS: 55518-06-4; Lib: tom18; ID: 171.



(tom18) RH-T-2423.8-0.01%-[N: Myo-Inositol, 1,3,4,5,6-O-(T)-bis(T)phosphate]-TENT-RH03 RI:2423.8,

Name: RH-T-2423.8-0.01%-[N: Myo-Inositol, 1,3,4,5,6-O-(T)-bis(T)phosphate]-TENT-RH03

Formula: C₂₇H₆₉O₉PSi₇

MW: 764 CAS#: 55518-06-4 ID#: 171 DB: tom18

Other DBs: None

RI: 2423.8,

Comment: RI=2423.8, 47.7615 min MG00244 [RI:2423.8]

10 largest peaks:

73 999 | 318 999 | 315 620 | 299 586 | 147 459 | 387 273 | 217 272 | 319 269 | 204 207 | 191 171 |

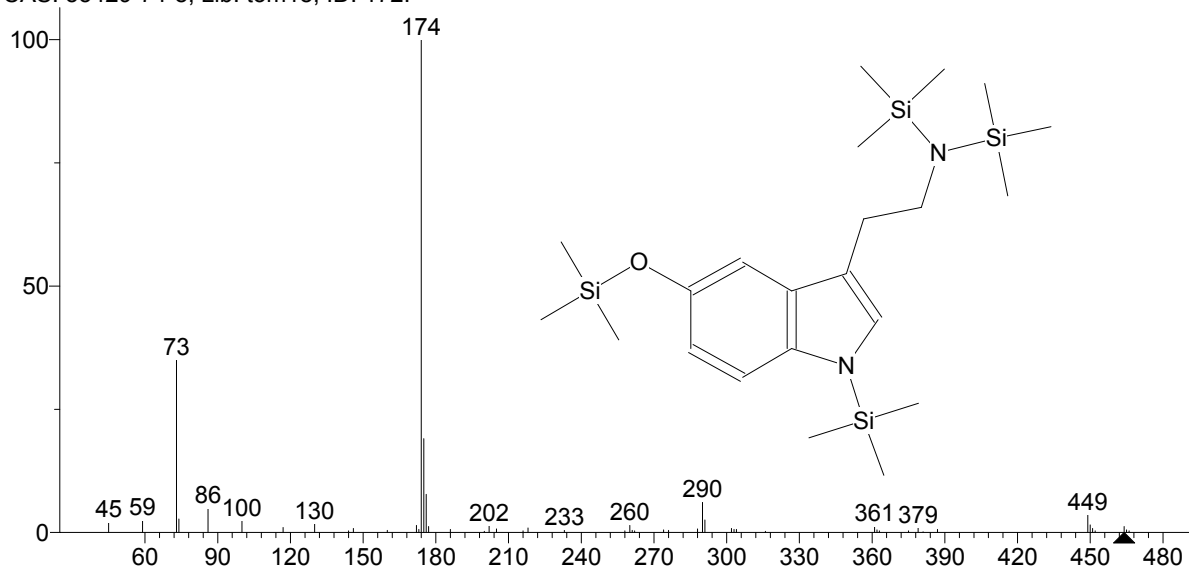
59 m/z Values and Intensities:

73 999	186 20	217 272	248 9	298 10	313 22	320 143	346 11	389 141	432 53
74 98	190 18	225 19	255 19	299 586	315 620	322 12	369 12	390 37	433 44
129 77	191 171	227 16	265 21	300 135	316 162	332 47	373 31	419 32	434 20
147 459	192 28	230 35	283 17	301 68	317 111	342 23	386 14	420 11	457 22
149 63	204 207	243 35	285 19	305 67	318 999	343 65	387 273	429 42	470 25
173 15	211 34	246 49	291 25	306 33	319 269	344 26	388 99	430 14	

Synonyms:

1. Myo-Inositol, 1,3,4,5,6-O-(T)-bis(T)phosphate]-TENT;

Hit 172 : RH-T-2451.9-0.01%-[N: Serotonin, tetra(trimethylsilyl)-]-TENT-RH03
CAS: 55429-74-8; Lib: tom18; ID: 172.



(tom18) RH-T-2451.9-0.01%-[N: Serotonin, tetra(trimethylsilyl)-]-TENT-RH03 RI:2451.9,

Name: RH-T-2451.9-0.01%-[N: Serotonin, tetra(trimethylsilyl)-]-TENT-RH03

Formula: C₂₂H₄₄N₂OSi₄

MW: 464 CAS#: 55429-74-8 ID#: 172 DB: tom18

Other DBs: None

RI: 2451.9,

Comment: RI=2451.9, 48.3214 min MG00244 |RI:2451.9|

10 largest peaks:

174 999 | 73 349 | 175 190 | 176 77 | 290 61 | 86 48 | 449 35 | 74 27 | 291 25 | 59 24 |

23 m/z Values and Intensities (28 low intensity peaks are not shown):

45 20 | 74 27 | 117 10 | 174 999 | 177 12 | 260 14 | 361 12 | 450 15 |

59 24 | 86 48 | 130 17 | 175 190 | 202 13 | 290 61 | 379 9 | 464 12 |

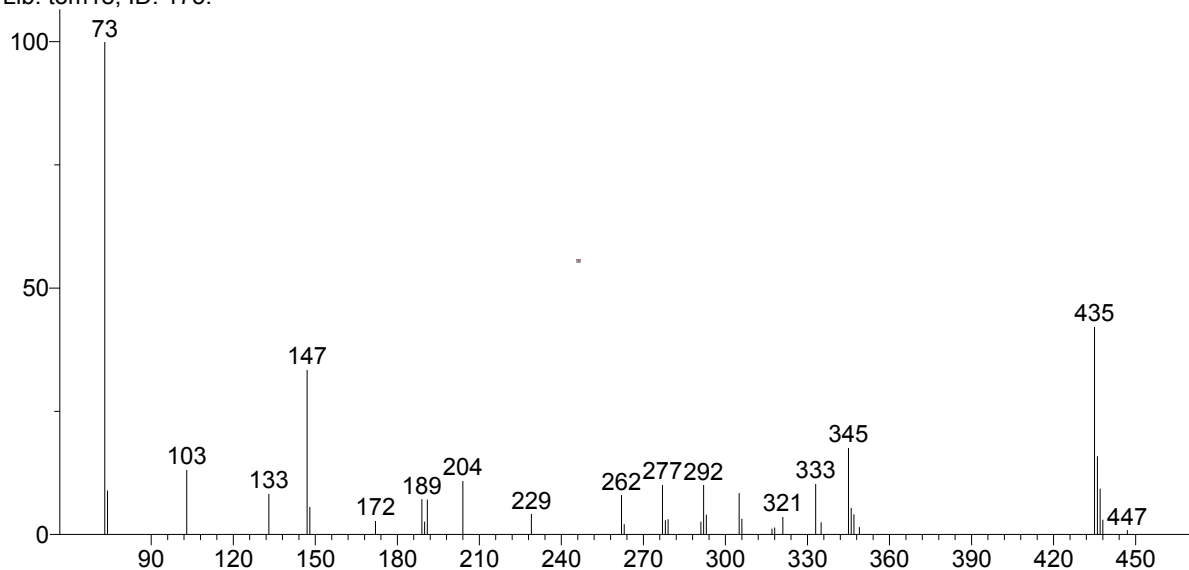
73 349 | 100 23 | 172 14 | 176 77 | 218 9 | 291 25 | 449 35 |

Synonyms:

1.Serotonin, tetra(trimethylsilyl)-]-TENT;

Hit 173 : RH-T-2464.9-0.01%-[435,345,333,305,292,277,103]-RH03

Lib: tom18; ID: 173.



(tom18) RH-T-2464.9-0.01%-[435,345,333,305,292,277,103]-RH03

Name: RH-T-2464.9-0.01%-[435,345,333,305,292,277,103]-RH03

MW: N/A ID#: 173 DB: tom18

Comment: RI:MG00238 [RI:2464.9]

10 largest peaks:

73 999 | 435 421 | 147 334 | 345 176 | 436 158 | 103 131 | 204 109 | 333 103 | 277 101 | 292 100 |

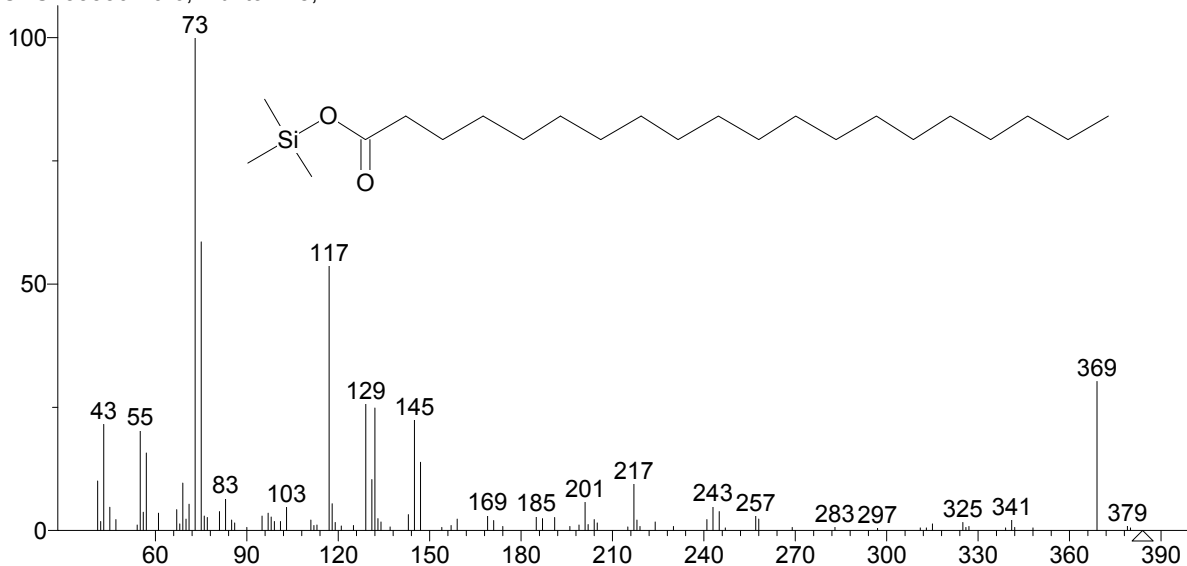
35 m/z Values and Intensities (1 low intensity peak is not shown):

73 999 | 147 334 | 190 25 | 262 80 | 279 30 | 305 83 | 321 36 | 346 53 | 436 158 |
74 88 | 148 55 | 191 70 | 263 20 | 291 25 | 306 31 | 333 103 | 347 40 | 437 92 |
103 131 | 172 28 | 204 109 | 277 101 | 292 100 | 317 11 | 335 24 | 349 14 | 438 29 |
133 83 | 189 71 | 229 41 | 278 28 | 293 39 | 318 13 | 345 176 | 435 421 |

Synonyms:

1.m435,345,333,305,292,277,103;

73

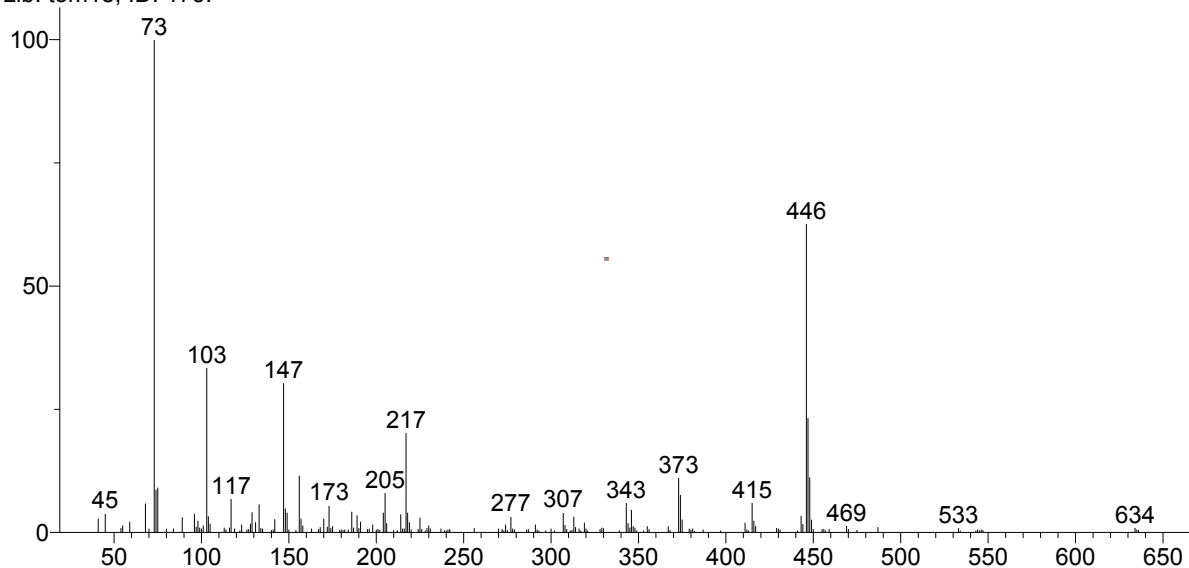


41	100	56	37	71	53	85	21	103	47	121	9	143	32	185	28	205	15	257	29
42	18	57	157	73	999	86	15	111	21	125	10	145	224	187	24	217	94	258	23
43	215	61	35	75	585	95	29	112	10	129	256	147	138	191	26	218	21	315	13
45	47	67	42	76	29	97	35	113	11	131	103	157	10	199	11	224	17	325	16
47	22	68	13	77	26	98	27	117	536	132	248	159	23	201	57	241	22	341	21
54	11	69	96	81	38	99	18	118	54	133	24	169	30	202	12	243	48	369	302
55	202	70	23	83	64	101	18	119	16	134	17	171	20	204	22	245	38	379	9

1.EICOSANOIC ACID-T-TENT-[506-30-9];

Hit 175 : RH-T-2480.2-0.09%-[446,103,217,373,415,634]-RH03

Lib: tom18; ID: 175.



(tom18) RH-T-2480.2-0.09%-[446,103,217,373,415,634]-RH03

Name: RH-T-2480.2-0.09%-[446,103,217,373,415,634]-RH03

MW: N/A ID#: 175 DB: tom18

Comment: RI:MG00238 |RI:2480.2|

10 largest peaks:

73 999 | 446 625 | 103 333 | 147 302 | 447 231 | 217 201 | 156 114 | 448 111 | 373 110 | 75 90 |

84 m/z Values and Intensities (101 low intensity peaks are not shown):

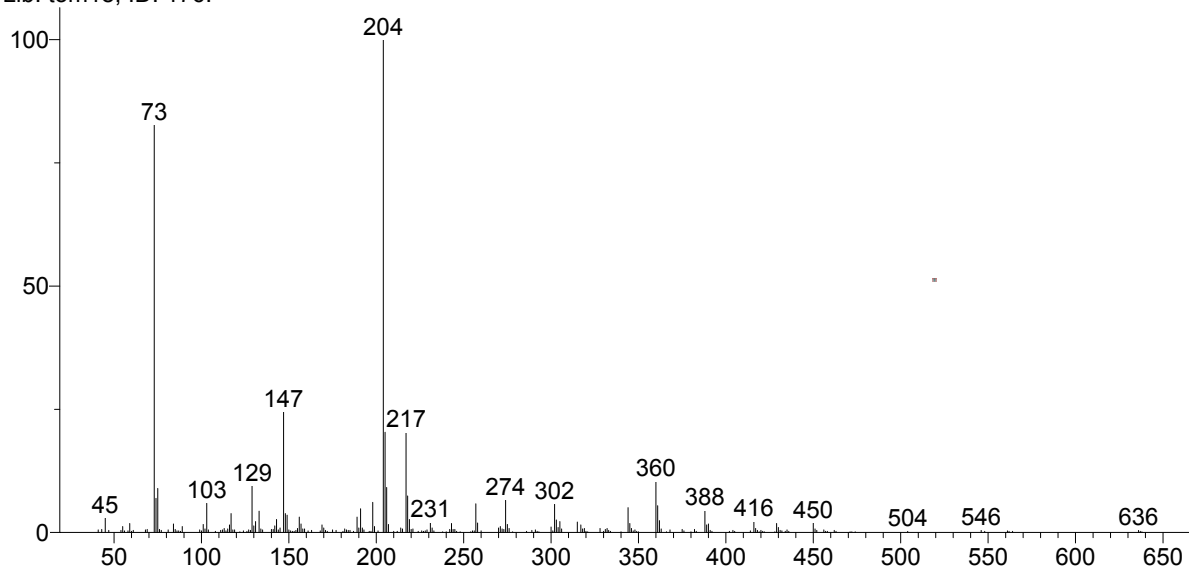
41	27	96	37	116	9	148	48	175	12	214	36	307	40	346	45	415	60	469	13
45	38	97	11	117	68	149	39	186	41	217	201	308	14	347	12	416	23	487	10
55	13	98	23	123	15	156	114	187	9	218	39	313	31	348	9	417	12	634	9
59	21	99	9	128	17	157	27	189	34	219	20	314	10	355	12	443	33		
68	58	101	13	129	40	158	13	191	21	225	29	319	19	367	12	444	16		
73	999	103	333	131	20	168	10	198	15	230	13	329	9	373	110	446	625		
74	86	104	32	133	56	170	27	204	39	274	15	343	59	374	75	447	231		
75	90	105	17	142	26	172	11	205	79	277	32	344	18	375	25	448	111		
89	30	113	9	147	302	173	54	206	18	291	15	345	9	411	19	449	25		

Synonyms:

1.m446,103,217,373,415,634;

Hit 176 : RH-T-2483.5-0.21%-[204,217,360,388,274]-RH03

Lib: tom18; ID: 176.



(tom18) RH-T-2483.5-0.21%-[204,217,360,388,274]-RH03

Name: RH-T-2483.5-0.21%-[204,217,360,388,274]-RH03

MW: N/A ID#: 176 DB: tom18

Comment: RI:MG00238 [RI:2483.5]

10 largest peaks:

204	999	73	826	147	244	205	203	217	202	360	103	129	94	206	91	75	89	218	74
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68 m/z Values and Intensities (158 low intensity peaks are not shown):

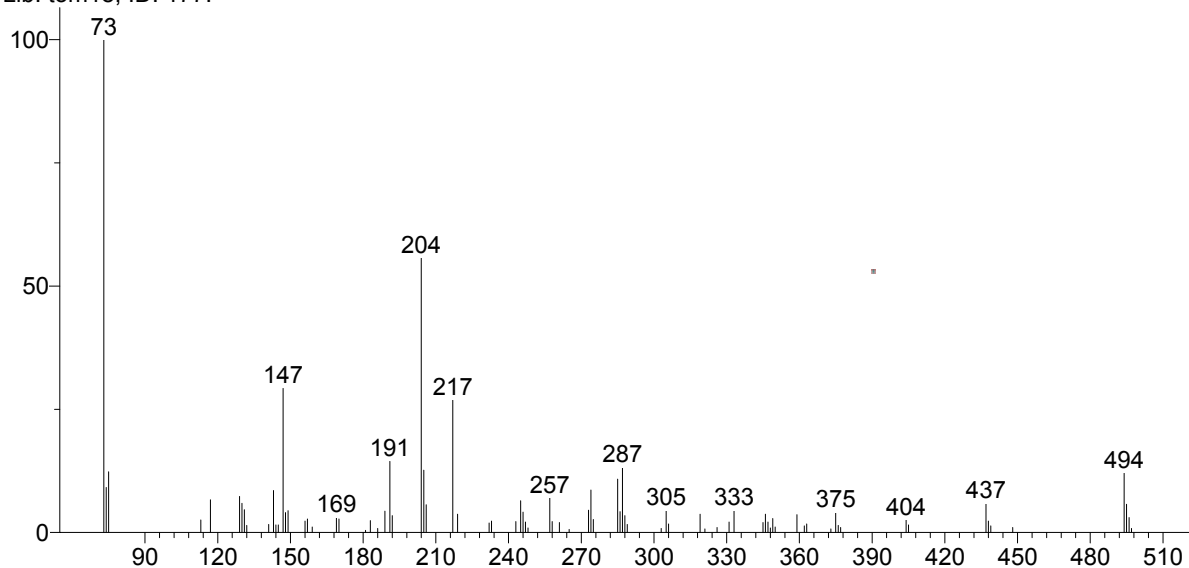
45	29	89	12	131	22	149	35	191	48	207	16	243	18	300	11	344	50	390	17
55	12	101	16	133	43	156	31	192	9	214	9	257	58	302	57	345	18	416	22
59	18	103	59	142	13	157	17	198	61	217	202	258	19	303	25	360	103	429	18
73	826	116	15	143	26	169	15	199	12	218	74	270	9	304	10	361	54	430	10
74	69	117	38	145	9	170	9	204	999	219	26	271	12	305	22	362	24	450	19
75	89	129	94	147	244	189	31	205	203	231	20	274	65	315	21	388	44		
84	17	130	13	148	38	190	9	206	91	232	9	275	16	317	15	389	15		

Synonyms:

1.m204,217,360,388,274;

Hit 177 : RH-T-2484.3-0.01%-[204,217,494,287,285,437]-RH03

Lib: tom18; ID: 177.



(tom18) RH-T-2484.3-0.01%-[204,217,494,287,285,437]-RH03 RI:2484.3,

Name: RH-T-2484.3-0.01%-[204,217,494,287,285,437]-RH03

MW: N/A ID#: 177 DB: tom18

RI: 2484.3,

Comment: RI=2484.3, 48.9671 min MG00244 [RI:2484.3]

10 largest peaks:

73 999 | 204 556 | 147 292 | 217 268 | 191 144 | 287 131 | 205 126 | 75 123 | 494 120 | 285 108 |

75 m/z Values and Intensities (7 low intensity peaks are not shown):

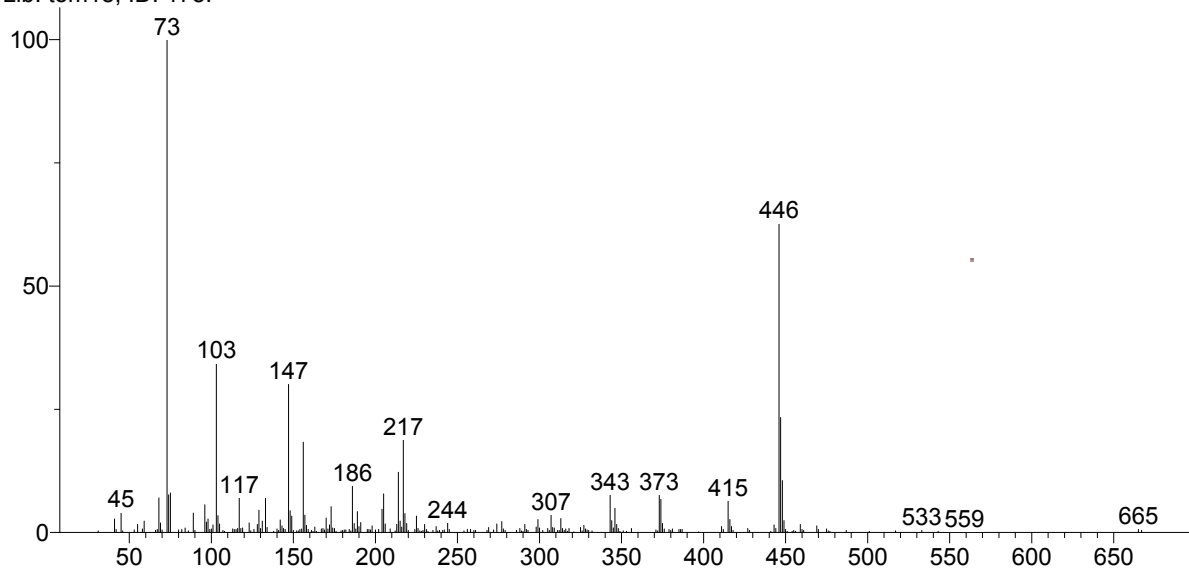
73 999	132 14	156 23	192 34	243 22	273 45	305 44	347 21	376 14	494 120
74 91	141 16	157 27	204 556	245 64	274 86	306 17	348 9	377 10	495 57
75 123	143 85	159 11	205 126	246 41	275 26	319 37	349 28	404 25	496 30
113 25	144 15	169 30	206 56	247 21	285 108	326 10	350 11	405 15	
117 66	145 15	170 27	217 268	248 9	286 42	331 21	359 36	437 58	
129 73	147 292	183 24	219 37	257 70	287 131	333 44	362 13	438 23	
130 59	148 40	189 43	232 19	258 22	288 34	345 20	363 17	439 13	
131 46	149 44	191 144	233 23	261 20	289 16	346 37	375 40	448 10	

Synonyms:

1.m204,217,494,287,285,437;

Hit 178 : RH-T-2494.7-0.14%-[446,103,217,214,373,343]-RH01

Lib: tom18; ID: 178.



(tom18) RH-T-2494.7-0.14%-[446,103,217,214,373,343]-RH01 RI:2494.7,

Name: RH-T-2494.7-0.14%-[446,103,217,214,373,343]-RH01

MW: N/A ID#: 178 DB: tom18

RI: 2494.7,

Comment: RI=2494.7, 41.5959 min AB2129 [RI:2494.7]

10 largest peaks:

73 999 | 446 626 | 103 342 | 147 300 | 447 233 | 217 187 | 156 183 | 214 122 | 448 105 | 186 94 |

91 m/z Values and Intensities (143 low intensity peaks are not shown):

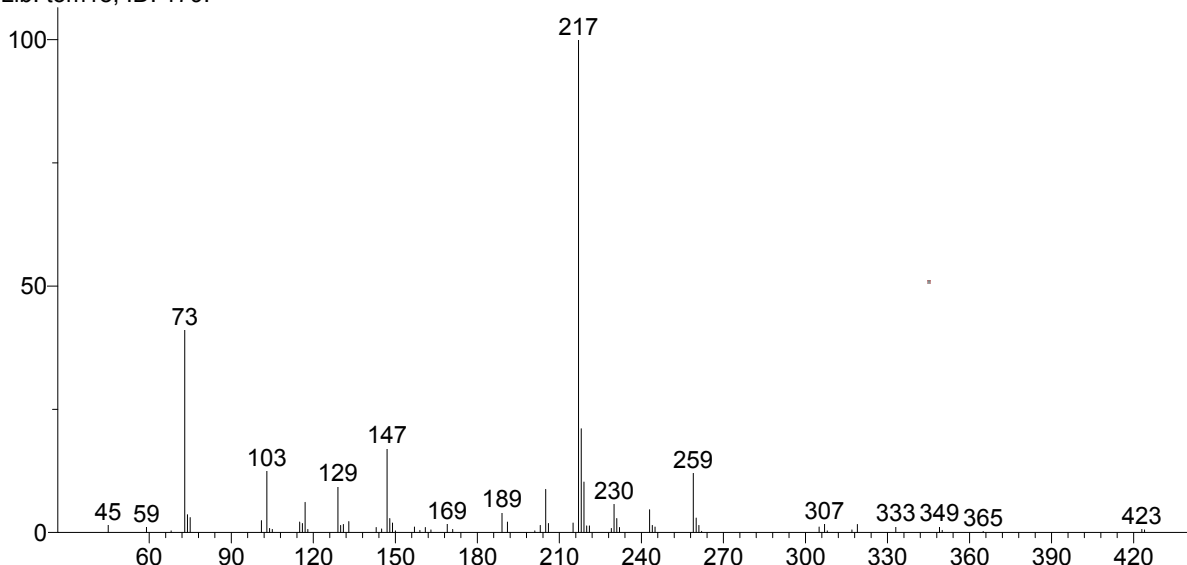
41	27	89	39	123	19	149	33	187	18	215	23	274	17	325	10	411	12	469	13
45	40	96	56	128	16	156	183	189	42	216	11	277	22	327	14	415	63		
55	16	97	21	129	45	157	35	190	12	217	187	291	16	343	76	416	26		
59	23	98	27	131	23	158	14	191	20	218	38	298	11	344	24	417	12		
68	70	101	15	133	69	163	11	198	13	219	18	299	26	345	9	443	15		
69	19	103	342	134	10	170	29	204	47	225	33	300	9	346	49	446	626		
73	999	104	34	142	25	172	15	205	78	230	16	307	35	347	16	447	233		
74	76	105	17	143	13	173	52	206	17	237	12	308	10	373	75	448	105		
75	80	117	70	147	300	174	9	213	16	244	19	309	9	374	67	449	24		
84	9	119	9	148	44	186	94	214	122	269	10	313	28	375	18	459	16		

Synonyms:

1.m446,103,217,214,373,343;

Hit 179 : RH-T-2501.6-0.01%-[217,259,103,205,129,243,230, N: sim. uridine 4T]-RH03

Lib: tom18; ID: 179.



(tom18) RH-T-2501.6-0.01%-[217,259,103,205,129,243,230, N: sim. uridine 4T]-RH03 RI:2501.6,

Name: RH-T-2501.6-0.01%-[217,259,103,205,129,243,230, N: sim. uridine 4T]-RH03

MW: N/A ID#: 179 DB: tom18

RI: 2501.6,

Comment: RI=2501.6, 49.3089 min MG00244 [RI:2501.6]

10 largest peaks:

217 999 | 73 410 | 218 210 | 147 170 | 103 124 | 259 120 | 219 102 | 129 93 | 205 87 | 117 61 |

46 m/z Values and Intensities (18 low intensity peaks are not shown):

45 15 | 101 24 | 129 93 | 147 170 | 169 17 | 206 18 | 220 13 | 243 46 | 261 14 | 349 12 |

59 11 | 103 124 | 130 14 | 148 28 | 189 40 | 215 19 | 221 13 | 244 14 | 305 11 |

73 410 | 115 21 | 131 16 | 149 19 | 191 21 | 217 999 | 230 57 | 245 11 | 307 17 |

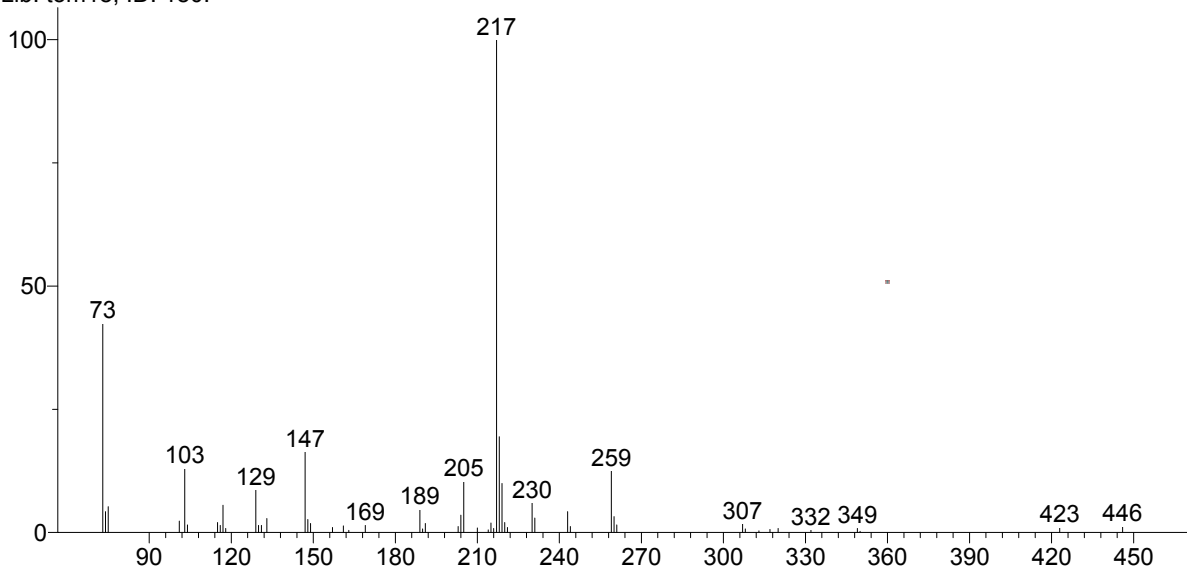
74 36 | 116 18 | 133 22 | 157 11 | 203 14 | 218 210 | 231 28 | 259 120 | 319 16 |

75 30 | 117 61 | 143 10 | 161 10 | 205 87 | 219 102 | 232 10 | 260 29 | 333 12 |

Synonyms:

1.m217,259,103,205,129,243,230, N: sim. uridine 4T;

Hit 180 : RH-T-2507.0-0.01%-[217,259,103,205,129,446, N: sim uridine 3T]-RH03
Lib: tom18; ID: 180.



(tom18) RH-T-2507.0-0.01%-[217,259,103,205,129,446, N: sim uridine 3T]-RH03 RI:2507.0,

Name: RH-T-2507.0-0.01%-[217,259,103,205,129,446, N: sim uridine 3T]-RH03

MW: N/A ID#: 180 DB: tom18

RI: 2507.0,

Comment: RI=2507.0, 49.4123 min MG00244 [RI:2507]

10 largest peaks:

217 999 | 73 423 | 218 194 | 147 163 | 103 129 | 259 124 | 205 103 | 219 99 | 129 86 | 230 60 |

41 m/z Values and Intensities (12 low intensity peaks are not shown):

73 423 | 104 15 | 130 14 | 149 18 | 191 18 | 215 19 | 221 10 | 259 124 | 446 12 |

74 42 | 115 20 | 131 14 | 157 10 | 203 12 | 217 999 | 230 60 | 260 32 |

75 52 | 116 14 | 133 28 | 161 13 | 204 35 | 218 194 | 231 29 | 261 15 |

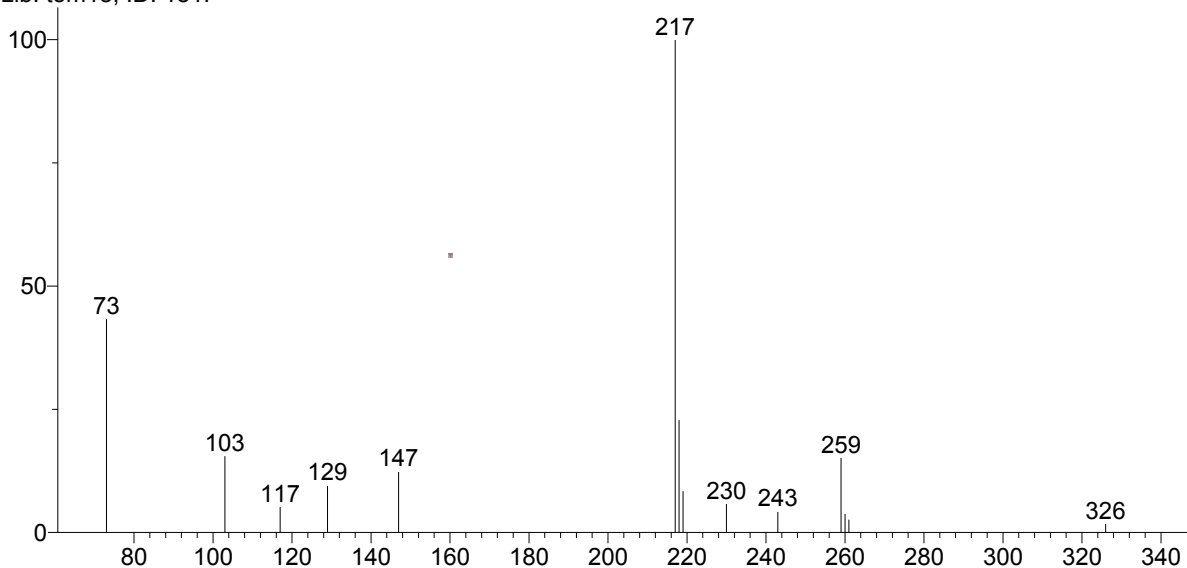
101 23 | 117 55 | 147 163 | 169 14 | 205 103 | 219 99 | 243 42 | 307 17 |

103 129 | 129 86 | 148 26 | 189 46 | 210 9 | 220 20 | 244 12 | 423 10 |

Synonyms:

1.m217,259,103,205,129,446, N: sim uridine 3T;

Hit 181 : RH-T-2519.0-0.00%-[217,259,103,129,230, N: sim uridine 3T]-RH03
Lib: tom18; ID: 181.



(tom18) RH-T-2519.0-0.00%-[217,259,103,129,230, N: sim uridine 3T]-RH03 RI:2519.0,

Name: RH-T-2519.0-0.00%-[217,259,103,129,230, N: sim uridine 3T]-RH03

MW: N/A ID#: 181 DB: tom18

RI: 2519.0,

Comment: RI=2519.0, 49.6427 min MG00244 [RI:2519]

10 largest peaks:

217 999 | 73 432 | 218 227 | 103 154 | 259 151 | 147 123 | 129 95 | 219 83 | 230 57 | 117 51 |

14 m/z Values and Intensities:

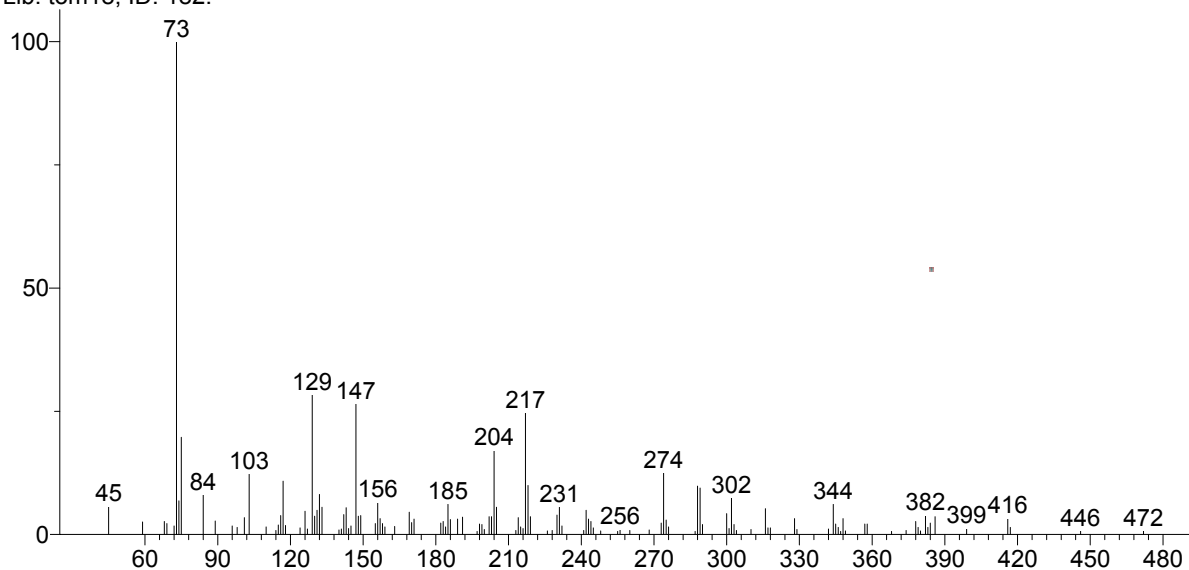
73 432 | 117 51 | 147 123 | 218 227 | 230 57 | 259 151 | 261 25 |
103 154 | 129 95 | 217 999 | 219 83 | 243 42 | 260 37 | 326 16 |

Synonyms:

1.m217,259,103,129,230, N: sim uridine 3T;

Hit 182 : RH-T-2523.0-0.02%-[217,129,204,274,344,416]-RH01

Lib: tom18; ID: 182.



(tom18) RH-T-2523.0-0.02%-[217,129,204,274,344,416]-RH01 RI:2523.0,

Name: RH-T-2523.0-0.02%-[217,129,204,274,344,416]-RH01

MW: N/A ID#: 182 DB: tom18

RI: 2523.0,

Comment: RI=2523.0, 42.0398 min AB2129 [RI:2523]

10 largest peaks:

73 999 | 129 283 | 147 264 | 217 246 | 75 197 | 204 170 | 274 124 | 103 122 | 117 108 | 218 99 |

107 m/z Values and Intensities (18 low intensity peaks are not shown):

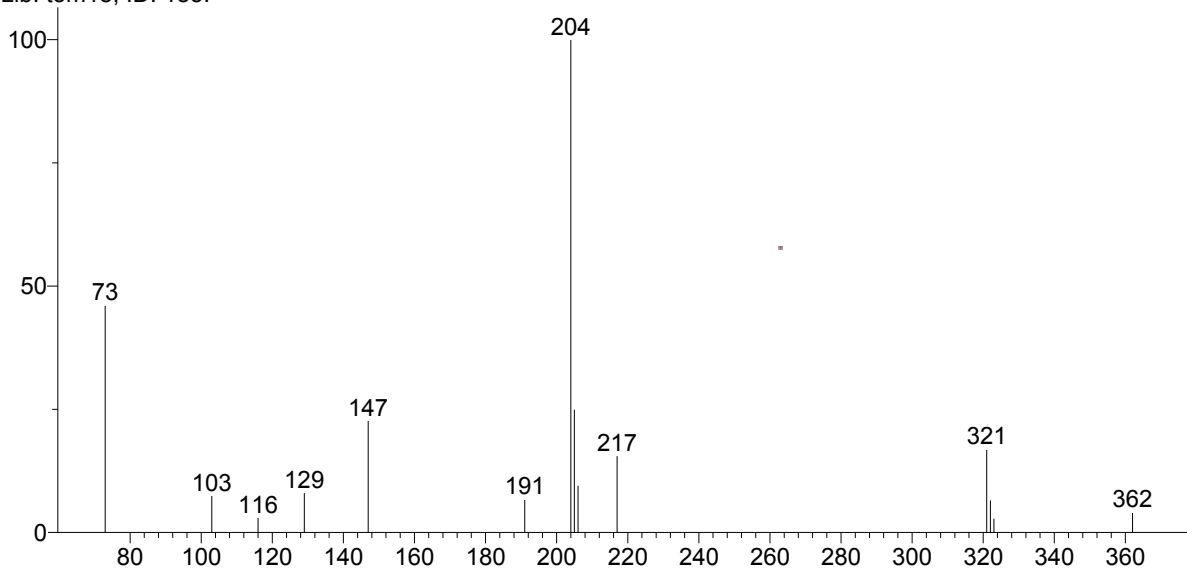
45	56	98	14	129	283	147	264	171	31	202	36	231	55	276	15	318	13	379	14
59	25	101	34	130	37	148	37	182	23	203	36	232	17	288	98	328	32	382	38
68	26	103	122	131	49	149	38	183	26	204	170	242	49	289	94	329	10	383	14
69	22	110	15	132	81	155	22	184	15	205	55	243	31	290	20	342	11	384	23
72	17	115	19	133	55	156	64	185	61	214	34	244	26	300	42	344	61	386	36
73	999	116	38	140	9	157	32	186	30	215	15	245	13	301	12	345	21	399	12
74	68	117	108	141	11	158	22	189	31	216	12	256	10	302	74	346	14	416	32
75	197	118	18	142	40	159	15	191	35	217	246	268	9	303	20	348	32	417	14
84	80	124	13	143	54	163	16	198	21	218	99	273	23	310	10	357	21		
89	27	126	47	144	12	169	45	199	20	219	36	274	124	316	52	358	21		
96	17	127	11	145	17	170	24	200	10	230	39	275	29	317	13	378	26		

Synonyms:

1.m217,129,204,274,344,416;

Hit 183 : RH-T-2523.9-0.00%-[204,321,191,129,103]-RH03

Lib: tom18; ID: 183.



(tom18) RH-T-2523.9-0.00%-[204,321,191,129,103]-RH03 RI:2523.9,

Name: RH-T-2523.9-0.00%-[204,321,191,129,103]-RH03

MW: N/A ID#: 183 DB: tom18

RI: 2523.9,

Comment: RI=2523.9, 49.7373 min MG00244 |RI:2523.9|

10 largest peaks:

204 999 | 73 460 | 205 248 | 147 226 | 321 168 | 217 154 | 206 94 | 129 79 | 103 74 | 191 66 |

14 m/z Values and Intensities:

73 460 | 116 29 | 147 226 | 204 999 | 206 94 | 321 168 | 323 27 |

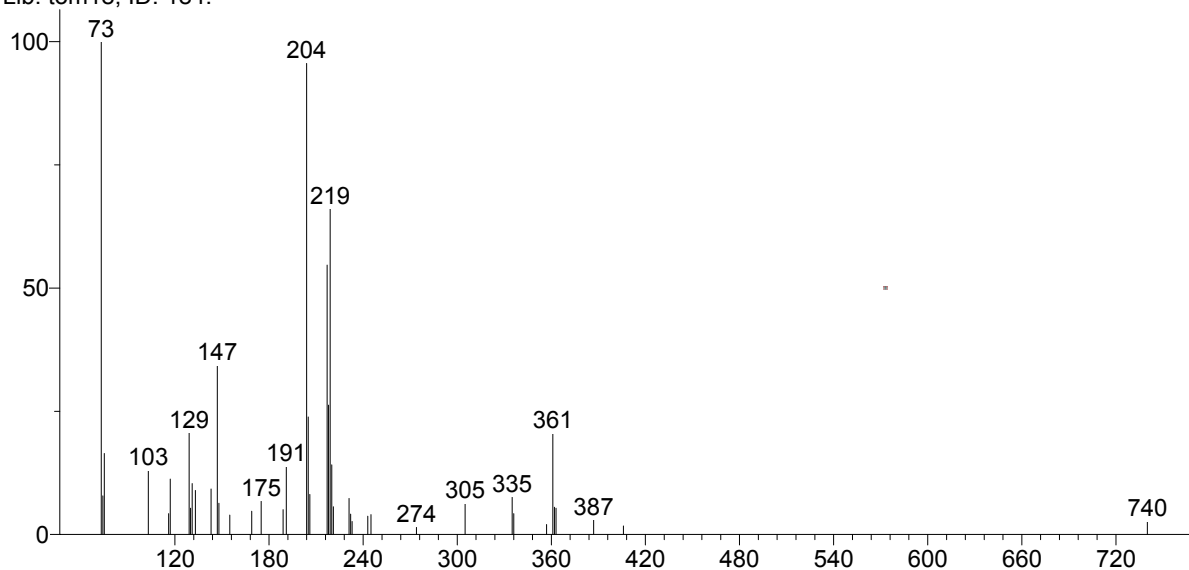
103 74 | 129 79 | 191 66 | 205 248 | 217 154 | 322 64 | 362 40 |

Synonyms:

1.m204,321,191,129,103;

Hit 184 : RH-T-2560.9-0.00%-[204,219,217,361,305,740]-RH03

Lib: tom18; ID: 184.



(tom18) RH-T-2560.9-0.00%-[204,219,217,361,305,740]-RH03 RI:2560.9,

Name: RH-T-2560.9-0.00%-[204,219,217,361,305,740]-RH03

MW: N/A ID#: 184 DB: tom18

RI: 2560.9,

Comment: RI=2560.9, 50.4462 min MG00244 |RI:2560.9|

10 largest peaks:

73 999 | 204 955 | 219 660 | 217 546 | 147 342 | 218 262 | 205 238 | 129 206 | 361 204 | 75 164 |

42 m/z Values and Intensities:

73 999 | 117 112 | 143 92 | 175 67 | 206 81 | 221 56 | 245 40 | 357 20 | 406 17 |

74 78 | 129 206 | 147 342 | 189 50 | 217 546 | 231 73 | 274 14 | 361 204 | 740 26 |

75 164 | 130 53 | 148 63 | 191 137 | 218 262 | 232 41 | 305 62 | 362 55 |

103 129 | 131 103 | 155 39 | 204 955 | 219 660 | 233 26 | 335 75 | 363 53 |

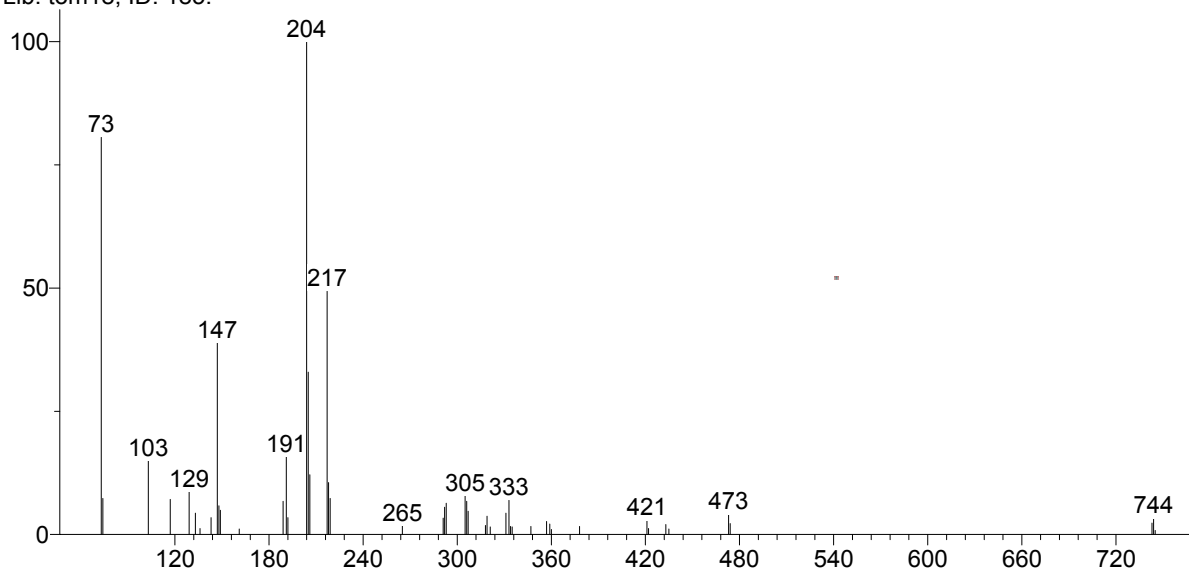
116 42 | 133 89 | 169 47 | 205 238 | 220 141 | 243 37 | 336 42 | 387 29 |

Synonyms:

1.m204,219,217,361,305,740;

Hit 185 : RH-T-2575.1-0.00%-[204,217,191,103,305,333,473]-RH03

Lib: tom18; ID: 185.



(tom18) RH-T-2575.1-0.00%-[204,217,191,103,305,333,473]-RH03 RI:2575.1,

Name: RH-T-2575.1-0.00%-[204,217,191,103,305,333,473]-RH03

MW: N/A ID#: 185 DB: tom18

RI: 2575.1,

Comment: RI=2575.1, 50.7187 min MG00244 [RI:2575.1]

10 largest peaks:

204	999	73	805	217	493	147	388	205	329	191	157	103	149	206	121	218	105	129	86
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48 m/z Values and Intensities (1 low intensity peak is not shown):

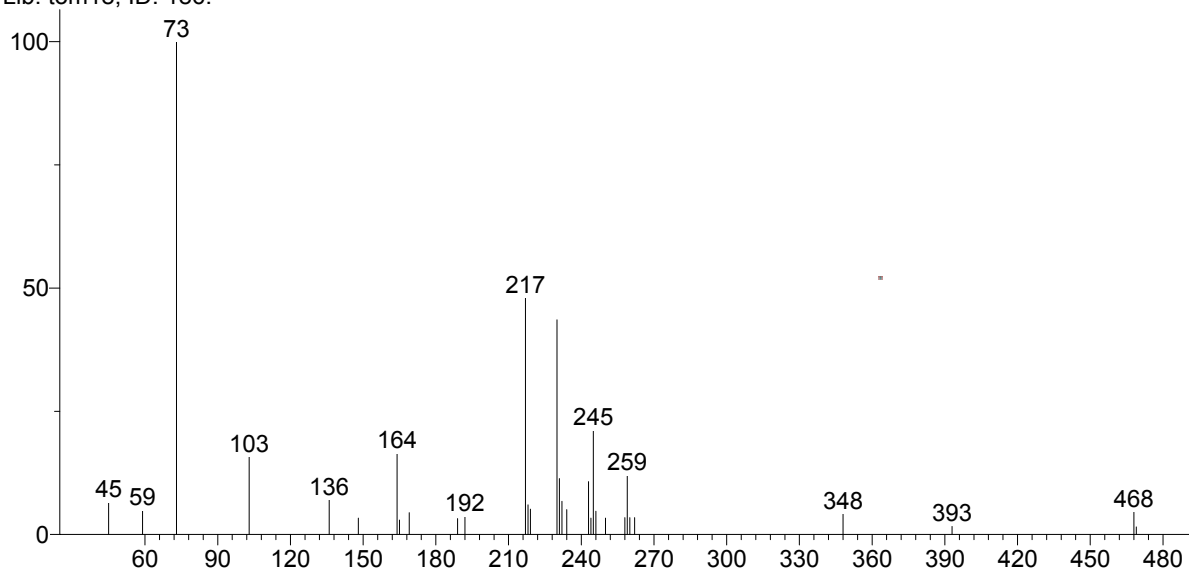
73	805	133	43	149	49	204	999	219	73	305	78	321	15	347	16	421	28	474	22
74	73	136	12	161	11	205	329	265	17	306	67	331	43	357	26	422	12	743	23
103	149	143	34	189	67	206	121	291	33	307	47	333	69	359	21	433	20	744	32
117	71	147	388	191	157	217	493	292	55	318	18	334	16	360	10	435	11		
129	86	148	58	192	34	218	105	293	63	319	37	335	15	378	16	473	40		

Synonyms:

1.m204,217,191,103,305,333,473;

Hit 186 : RH-T-2579.5-0.01%-[217,230,245,164,103,468]-RH01

Lib: tom18; ID: 186.



(tom18) RH-T-2579.5-0.01%-[217,230,245,164,103,468]-RH01 RI:2579.5,

Name: RH-T-2579.5-0.01%-[217,230,245,164,103,468]-RH01

MW: N/A ID#: 186 DB: tom18

RI: 2579.5,

Comment: RI=2579.5, 42.9267 min AB2129 |RI:2579.5|

10 largest peaks:

73 999 | 217 479 | 230 435 | 245 210 | 164 164 | 103 157 | 259 119 | 231 113 | 243 107 | 136 70 |

31 m/z Values and Intensities:

45 64 | 136 70 | 169 44 | 218 60 | 232 67 | 245 210 | 259 119 | 393 16 |

59 48 | 148 33 | 189 32 | 219 51 | 234 50 | 246 47 | 260 34 | 468 45 |

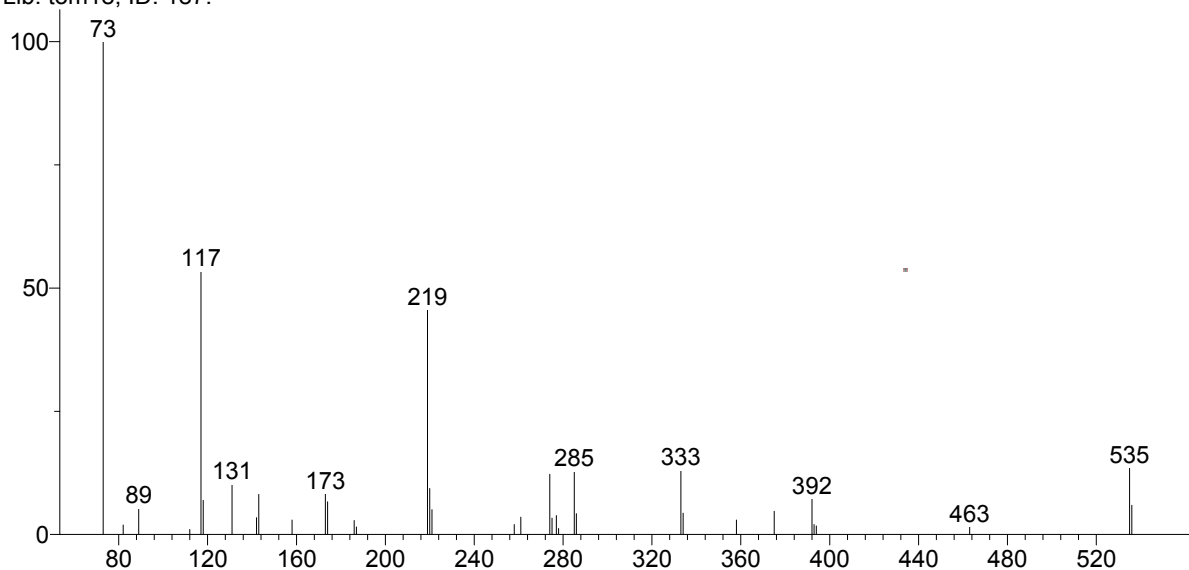
73 999 | 164 164 | 192 36 | 230 435 | 243 107 | 250 33 | 262 34 | 469 15 |

103 157 | 165 29 | 217 479 | 231 113 | 244 33 | 258 34 | 348 41 |

Synonyms:

1.m217,230,245,164,103,468;

Hit 187 : RH-T-2603.2-0.00%-[117,219,535,333,285,274, G: _LJAN_2610.8_2233BN14_[NA]-RH03
 Lib: tom18; ID: 187.



(tom18) RH-T-2603.2-0.00%-[117,219,535,333,285,274, G: _LJAN_2610.8_2233BN14_[NA]-RH03 RI:2603.2,

Name: RH-T-2603.2-0.00%-[117,219,535,333,285,274, G: _LJAN_2610.8_2233BN14_[NA]-RH03

MW: N/A ID#: 187 DB: tom18

RI: 2603.2,

Comment: RI=2603.2, 51.2540 min MG00244 [RI:2603.2]

10 largest peaks:

73 999 | 117 533 | 219 455 | 535 134 | 333 129 | 285 127 | 274 122 | 131 101 | 220 93 | 173 82 |

35 m/z Values and Intensities:

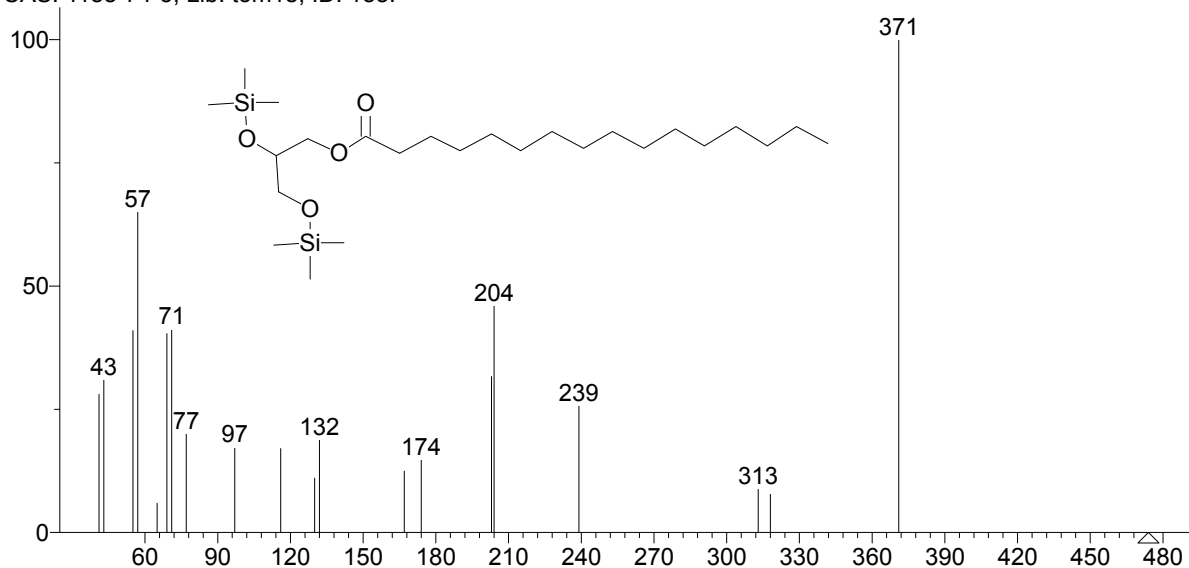
73 999 | 117 533 | 143 81 | 186 28 | 221 50 | 275 33 | 286 42 | 375 47 | 463 15 |
 82 19 | 118 69 | 158 29 | 187 15 | 258 20 | 277 38 | 333 129 | 392 72 | 535 134 |
 89 52 | 131 101 | 173 82 | 219 455 | 261 35 | 278 12 | 334 43 | 393 20 | 536 59 |
 112 10 | 142 34 | 174 66 | 220 93 | 274 122 | 285 127 | 358 29 | 394 17 |

Synonyms:

1.m117,219,535,333,285,274, G: _LJAN_2610.8_2233BN14_[NA];

Hit 188 : RH-T-2615.6-0.00%-MONOPALMITIN T-TENT-8135A18-G-X

CAS: 1188-74-5; Lib: tom18; ID: 188.



(tom18) RH-T-2615.6-0.00%-MONOPALMITIN T-TENT-8135A18-G-X RI:2615.6,

Name: RH-T-2615.6-0.00%-MONOPALMITIN T-TENT-8135A18-G-X

Formula: C₂₅H₅₄O₄Si₂

MW: 474 CAS#: 1188-74-5 ID#: 188 DB: tom18

Other DBs: None

RI: 2615.6,

Comment: RI=2615.6, 38.4199 min 8135A18 |RI:2615.6|

10 largest peaks:

371 999 | 57 650 | 204 459 | 71 411 | 55 409 | 69 403 | 203 316 | 43 309 | 41 280 | 239 256 |

20 m/z Values and Intensities:

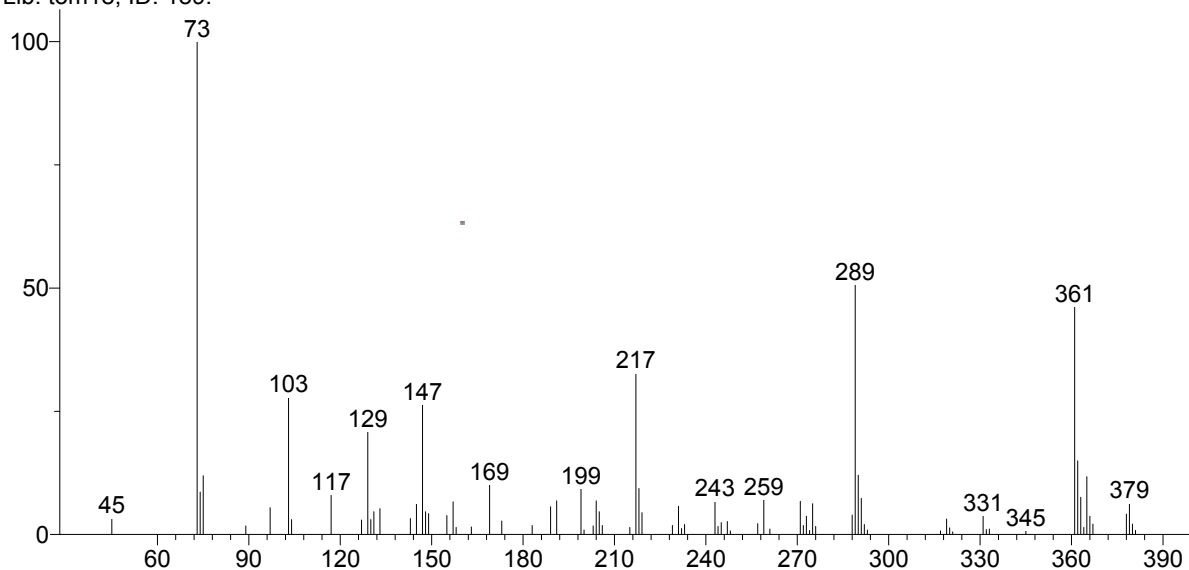
41 280	55 409	65 59	71 411	97 172	130 110	167 124	203 316	239 256	318 77
43 309	57 650	69 403	77 199	116 170	132 187	174 147	204 459	313 87	371 999

Synonyms:

1.MONOPALMITIN T-TENT;

Hit 189 : RH-T-2617.2-0.03%-[289,361,217,103,379, N: -sim. trehalose]-RH01

Lib: tom18; ID: 189.



(tom18) RH-T-2617.2-0.03%-[289,361,217,103,379, N: -sim. trehalose]-RH01 RI:2617.2,

Name: RH-T-2617.2-0.03%-[289,361,217,103,379, N: -sim. trehalose]-RH01

MW: N/A ID#: 189 DB: tom18

RI: 2617.2,

Comment: RI=2617.2, 43.5001 min AB2129 [RI:2617.2]

10 largest peaks:

73 999 | 289 506 | 361 461 | 217 326 | 103 277 | 147 262 | 129 207 | 362 149 | 290 120 | 75 119 |

75 m/z Values and Intensities (6 low intensity peaks are not shown):

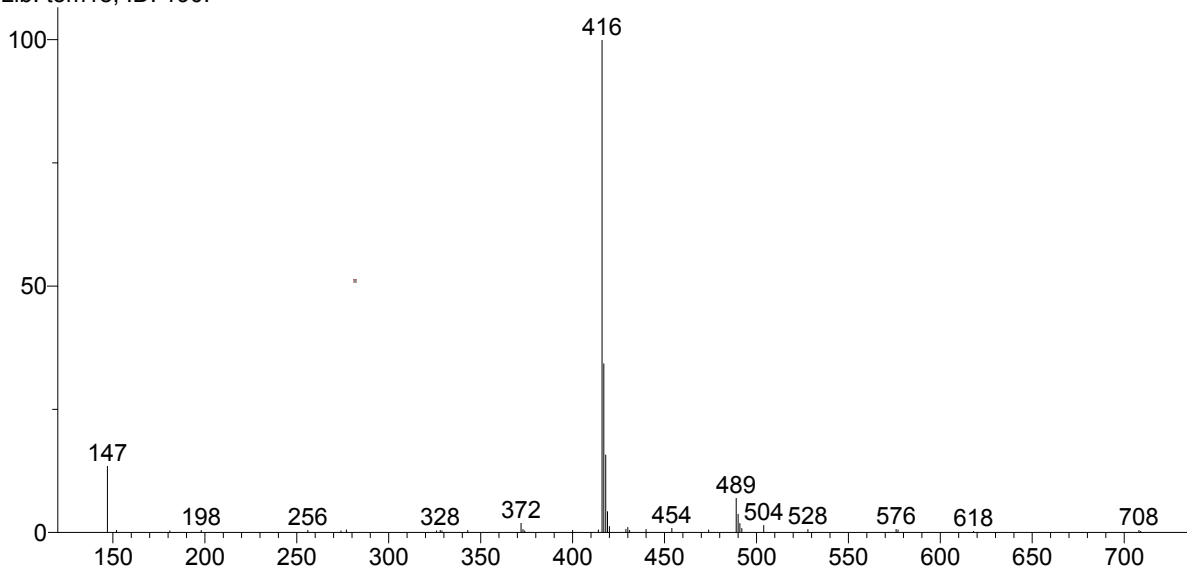
45 32	117 79	147 262	173 27	205 46	232 12	261 11	290 120	333 11	378 41
73 999	127 29	148 46	183 18	206 18	233 20	271 67	291 73	361 461	379 62
74 86	129 207	149 42	189 56	215 14	243 66	272 18	292 20	362 149	380 21
75 119	130 30	155 38	191 68	217 326	244 16	273 37	293 9	363 75	
89 17	131 46	157 66	199 92	218 93	245 24	275 62	319 31	364 14	
97 54	133 52	158 14	200 9	219 44	247 26	276 16	320 13	365 117	
103 277	143 32	163 15	203 17	229 18	257 22	288 39	331 37	366 37	
104 30	145 61	169 100	204 68	231 57	259 70	289 506	332 10	367 21	

Synonyms:

1.m289,361,217,103,379, N: -sim. trehalose;

Hit 190 : RH-T-2628.6-0.01%-[416,489,708]-RH03-X

Lib: tom18; ID: 190.



(tom18) RH-T-2628.6-0.01%-[416,489,708]-RH03-X RI:2628.6,

Name: RH-T-2628.6-0.01%-[416,489,708]-RH03-X

MW: N/A ID#: 190 DB: tom18

RI: 2628.6,

Comment: RI=2628.6, 51.7167 min MG00244 [RI:2628.6]

10 largest peaks:

416 999 | 417 342 | 418 157 | 147 135 | 489 70 | 419 42 | 490 37 | 372 19 | 491 18 | 504 14 |

13 m/z Values and Intensities (25 low intensity peaks are not shown):

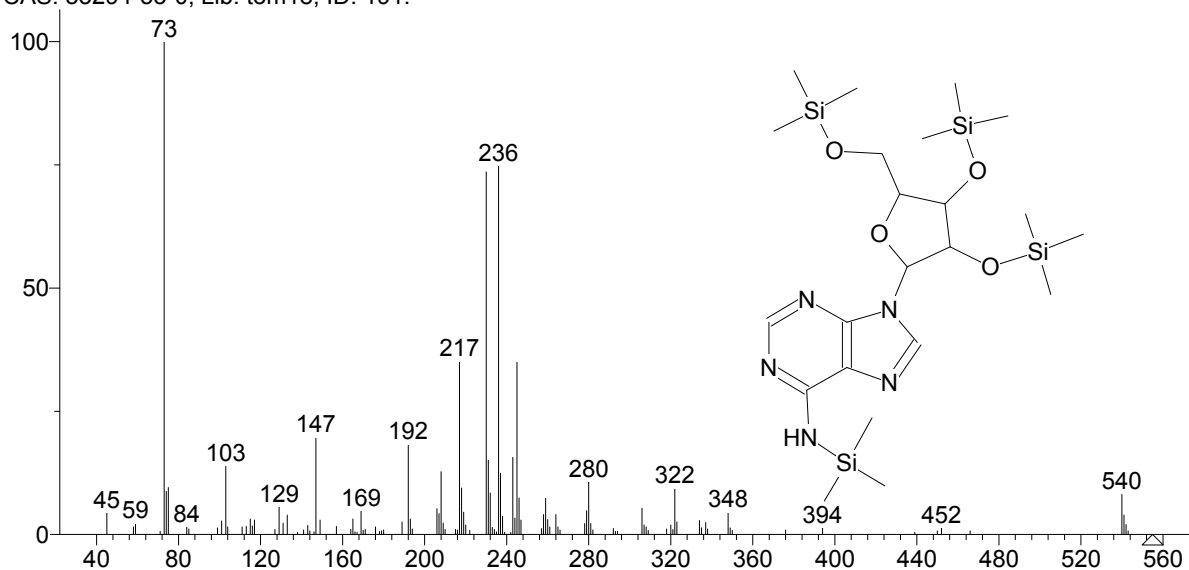
147 135 | 416 999 | 418 157 | 420 12 | 454 9 | 490 37 | 504 14 |

372 19 | 417 342 | 419 42 | 430 10 | 489 70 | 491 18 |

Synonyms:

1.m416,489,708;

Hit 191 : RH-T-2630.7-0.01%-[N: Adenosine-tetrakis(trimethylsilyl)-]-TENT-RH03
CAS: 53294-33-0; Lib: tom18; ID: 191.



(tom18) RH-T-2630.7-0.01%-[N: Adenosine-tetrakis(trimethylsilyl)-]-TENT-RH03 RI:2630.7,

Name: RH-T-2630.7-0.01%-[N: Adenosine-tetrakis(trimethylsilyl)-]-TENT-RH03

Formula: C₂₂H₄₅N₅O₄Si₄

MW: 555 CAS#: 53294-33-0 ID#: 191 DB: tom18

Other DBs: None

RI: 2630.7,

Comment: RI=2630.7, 51.7543 min MG00244 [RI:2630.7]

10 largest peaks:

73 999 | 236 747 | 230 735 | 217 350 | 245 349 | 147 196 | 192 182 | 243 156 | 231 150 | 103 138 |

94 m/z Values and Intensities (21 low intensity peaks are not shown):

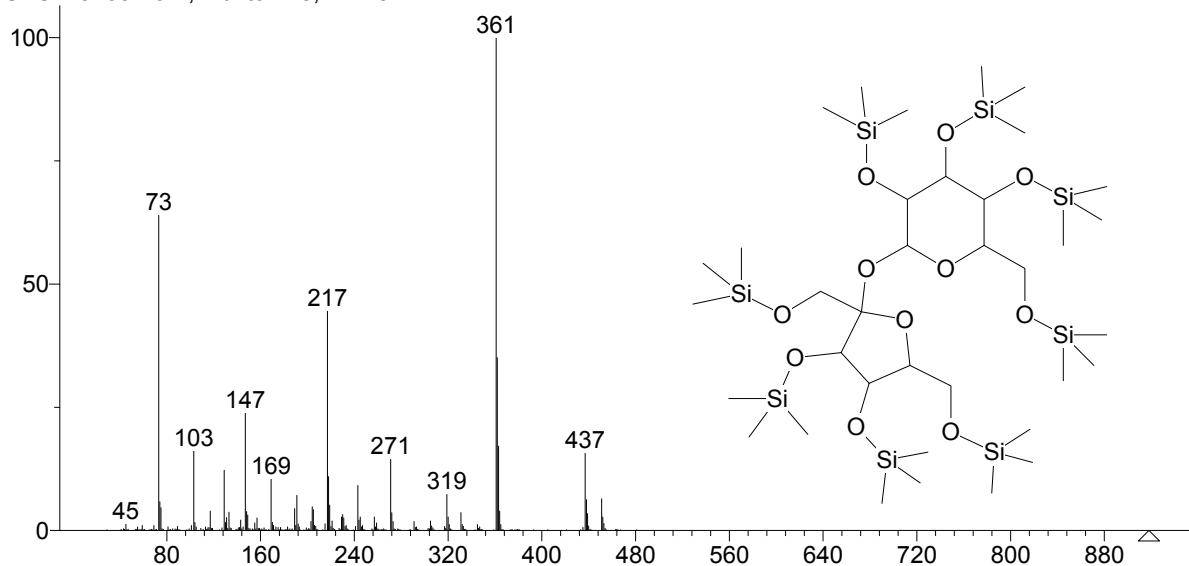
45	43	103	138	133	39	176	15	210	10	233	14	257	12	280	106	322	93	452	13
58	15	104	15	141	9	180	9	215	10	234	10	258	40	281	22	323	25	540	81
59	22	111	15	143	18	189	25	216	9	236	747	259	73	282	9	334	28	541	39
73	999	113	16	147	196	192	182	217	350	237	124	260	30	292	12	335	13	542	20
74	87	115	31	149	29	193	31	218	94	238	37	261	15	306	53	337	24		
75	95	116	17	157	16	194	11	219	45	243	156	264	40	307	19	338	11		
84	15	117	29	164	10	206	52	220	19	244	33	265	15	308	15	348	44		
85	11	127	10	165	31	207	42	230	735	245	349	266	9	318	11	349	13		
99	13	129	55	169	47	208	127	231	150	246	74	278	22	320	19	376	9		
101	27	131	23	171	10	209	23	232	84	247	29	279	48	321	10	394	13		

Synonyms:

1. Adenosine-tetrakis(trimethylsilyl)-TENT;

Hit 192 : RH-T-2648.9-2.59%-SUCROSE-8T-CONF- [57-50-1]-RH03

CAS: 19159-25-2; Lib: tom18; ID: 192.



(tom18) RH-T-2648.9-2.59%-SUCROSE-8T-CONF- [57-50-1]-RH03

Name: RH-T-2648.9-2.59%-SUCROSE-8T-CONF- [57-50-1]-RH03

Formula: C₃₆H₈₆O₁₁Si₈

MW: 918 CAS#: 19159-25-2 ID#: 192 DB: tom18

Other DBs: None

Comment: RI:MG00238 [RI:2648.9]

10 largest peaks:

361 999 | 73 639 | 217 445 | 362 350 | 147 238 | 363 171 | 103 161 | 437 157 | 271 144 | 129 122 |

70 m/z Values and Intensities (168 low intensity peaks are not shown):

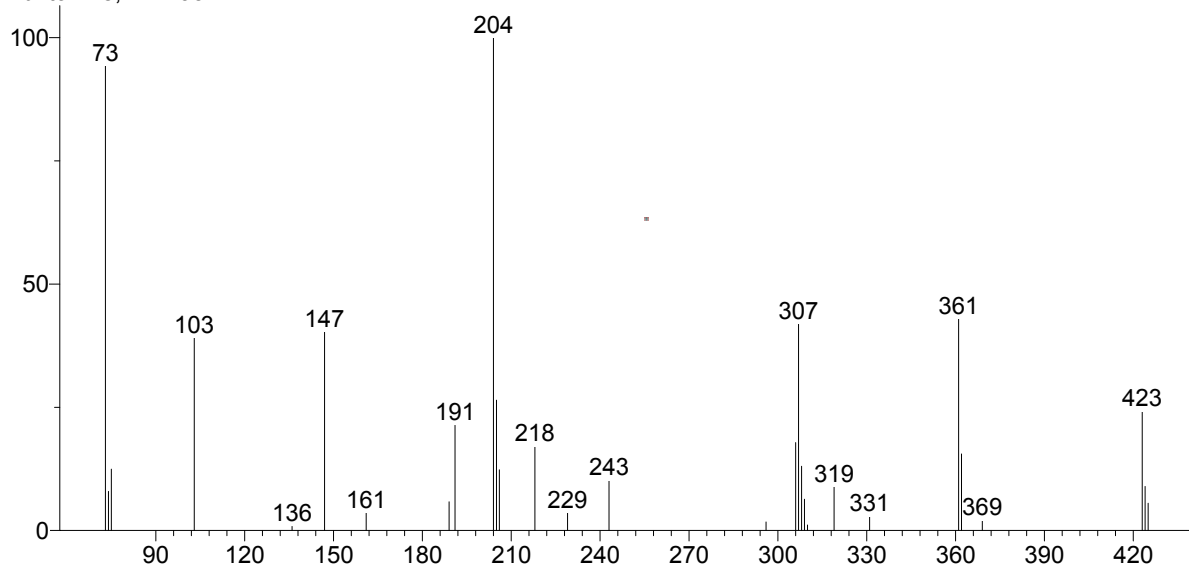
45	13	103	161	143	21	170	16	204	48	221	19	245	27	291	18	332	12	437	157
59	10	104	16	147	238	171	10	205	42	229	27	247	10	305	19	345	12	438	62
69	10	117	39	148	38	189	44	206	10	230	32	257	27	306	9	361	999	439	34
73	639	129	122	149	31	190	10	215	13	231	25	259	15	319	73	362	350	440	9
74	58	130	16	155	15	191	71	217	445	233	10	271	144	320	27	363	171	451	64
75	46	131	26	157	25	192	13	218	109	243	91	272	36	321	12	364	39	452	27
101	10	133	37	169	104	203	18	219	51	244	21	273	18	331	36	365	12	453	14

Synonyms:

1.SUCROSE-8T-CONF- [57-50-1];

Hit 193 : RH-T-2667.3-0.00%-[204,307,361,103,423]-RH03

Lib: tom18; ID: 193.



(tom18) RH-T-2667.3-0.00%-[204,307,361,103,423]-RH03 RI:2667.3,

Name: RH-T-2667.3-0.00%-[204,307,361,103,423]-RH03

MW: N/A ID#: 193 DB: tom18

RI: 2667.3,

Comment: RI=2667.3, 52.4202 min MG00244 [RI:2667.3]

10 largest peaks:

204 999 | 73 942 | 361 429 | 307 418 | 147 402 | 103 390 | 205 264 | 423 241 | 191 213 | 306 178 |

28 m/z Values and Intensities (1 low intensity peak is not shown):

73 942 | 103 390 | 189 58 | 205 264 | 229 35 | 306 178 | 309 63 | 331 28 | 369 20 | 425 55 |

74 79 | 147 402 | 191 213 | 206 123 | 243 101 | 307 418 | 310 11 | 361 429 | 423 241 |

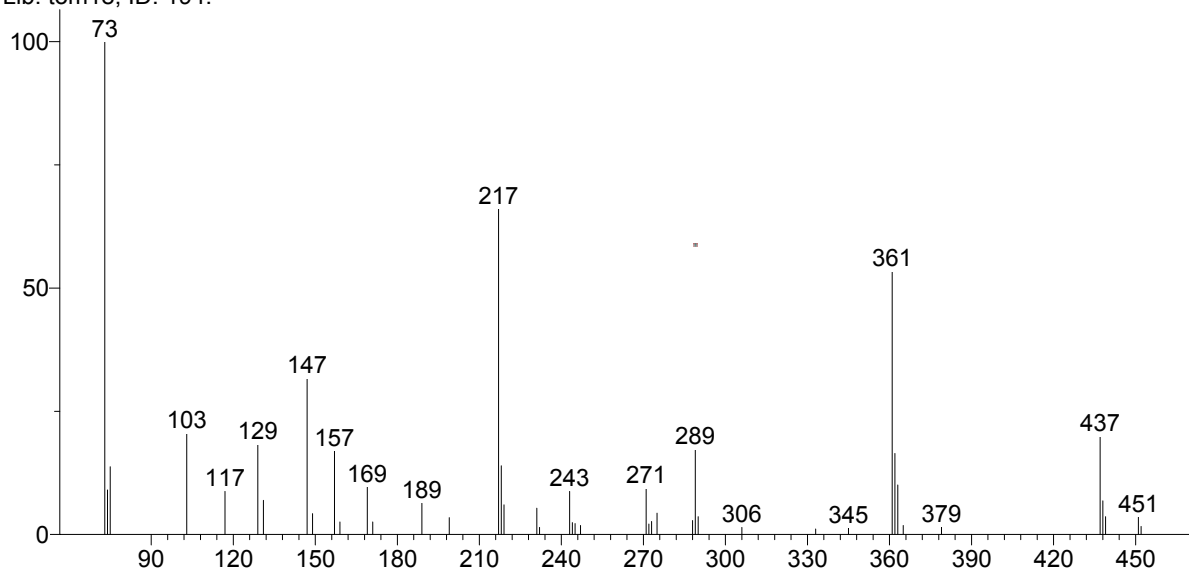
75 124 | 161 35 | 204 999 | 218 170 | 296 17 | 308 130 | 319 88 | 362 155 | 424 89 |

Synonyms:

1.m204,307,361,103,423;

Hit 194 : RH-T-2691.2-0.02%-[217,361,437,289,451,129,103]-RH01

Lib: tom18; ID: 194.



(tom18) RH-T-2691.2-0.02%-[217,361,437,289,451,129,103]-RH01 RI:2691.2,

Name: RH-T-2691.2-0.02%-[217,361,437,289,451,129,103]-RH01

MW: N/A ID#: 194 DB: tom18

RI: 2691.2,

Comment: RI=2691.2, 44.5835 min AB2129 |RI:2691.2|

10 largest peaks:

73 999 | 217 660 | 361 533 | 147 316 | 103 204 | 437 198 | 129 182 | 289 172 | 157 169 | 362 164 |

44 m/z Values and Intensities:

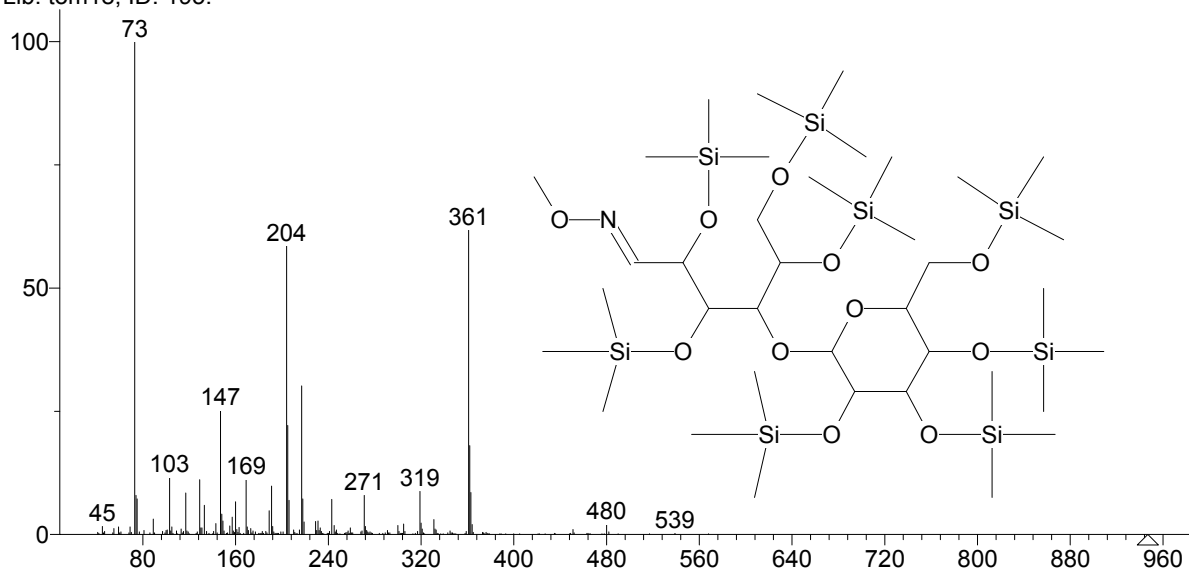
73 999	129 182	159 25	217 660	243 87	272 21	290 36	362 164	438 68
74 90	131 69	169 96	218 139	244 24	273 26	306 14	363 100	439 36
75 137	147 316	171 25	219 60	245 22	275 43	333 11	365 18	451 35
103 204	149 42	189 63	231 53	247 18	288 28	345 13	379 15	452 16
117 87	157 169	199 34	232 14	271 93	289 172	361 533	437 198	

Synonyms:

1.m217,361,437,289,451,129,103;

Hit 195 : RH-T-2729.5-0.00%-MALTOSE M8T PK1-TENT- 8135A18-G

Lib: tom18; ID: 195.



(tom18) RH-T-2729.5-0.00%-MALTOSE M8T PK1-TENT- 8135A18-G RI:2729.5,

Name: RH-T-2729.5-0.00%-MALTOSE M8T PK1-TENT- 8135A18-G

Formula: C₃₇H₈₉NO₁₁Si₈

MW: 947 ID#: 195 DB: tom18

RI: 2729.5,

Comment: RI=2729.5, 40.0559 min 8135A18 [RI:2729.5]

10 largest peaks:

73 999 | 361 617 | 204 585 | 217 301 | 147 251 | 205 221 | 362 180 | 103 115 | 129 111 | 169 111 |

63 m/z Values and Intensities (148 low intensity peaks are not shown):

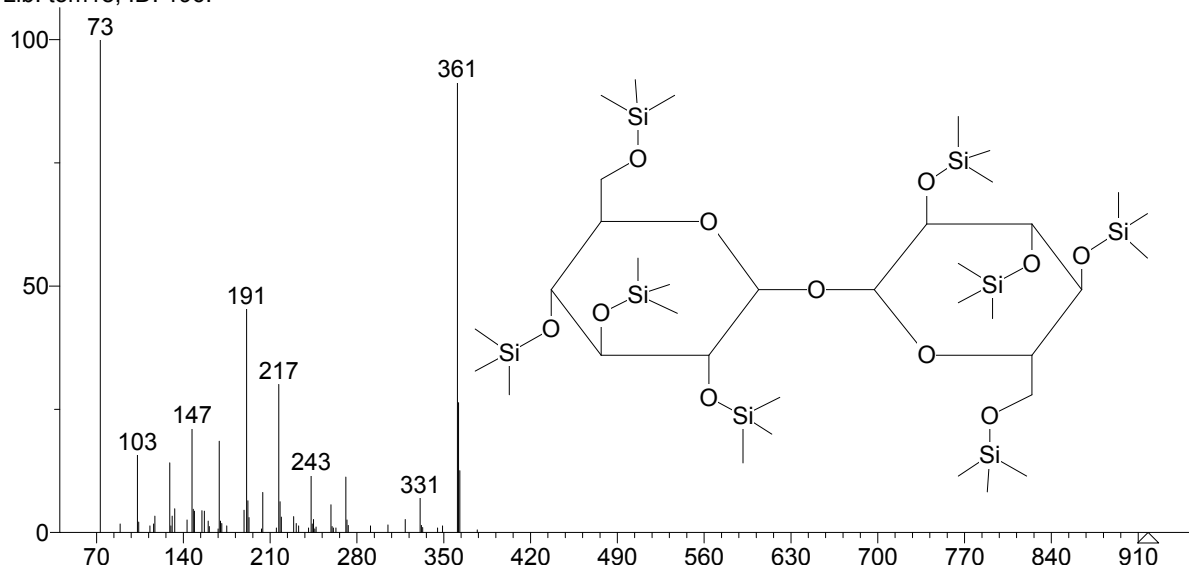
45	16	89	31	130	13	155	17	173	12	210	9	233	13	300	18	333	9
55	12	101	9	131	13	157	35	189	48	215	9	243	71	305	21	361	617
59	15	103	115	133	59	160	66	191	98	217	301	245	18	319	87	362	180
69	15	105	15	143	22	161	10	192	16	218	72	247	9	320	23	363	85
73	999	113	11	147	251	163	14	204	585	219	25	259	13	321	11	364	20
74	79	117	84	148	41	169	111	205	221	229	26	271	79	331	30	451	10
75	72	129	111	149	27	170	15	206	69	231	27	272	16	332	11	480	20

Synonyms:

1.MALTOSE M8T PK1-TENT;

Hit 196 : RH-T-2735.5-0.00%-TREHALOSE 8T-TENT-8135A18-G

Lib: tom18; ID: 196.



(tom18) RH-T-2735.5-0.00%-TREHALOSE 8T-TENT-8135A18-G RI:2735.5,

Name: RH-T-2735.5-0.00%-TREHALOSE 8T-TENT-8135A18-G

Formula: C₃₆H₈₆O₁₁Si₈

MW: 918 ID#: 196 DB: tom18

RI: 2735.5,

Comment: RI=2735.5, 40.1459 min 8135A18 [RI:2735.5]

10 largest peaks:

73 999 | 361 912 | 191 453 | 217 300 | 362 263 | 147 210 | 169 185 | 103 157 | 129 141 | 363 125 |

58 m/z Values and Intensities (4 low intensity peaks are not shown):

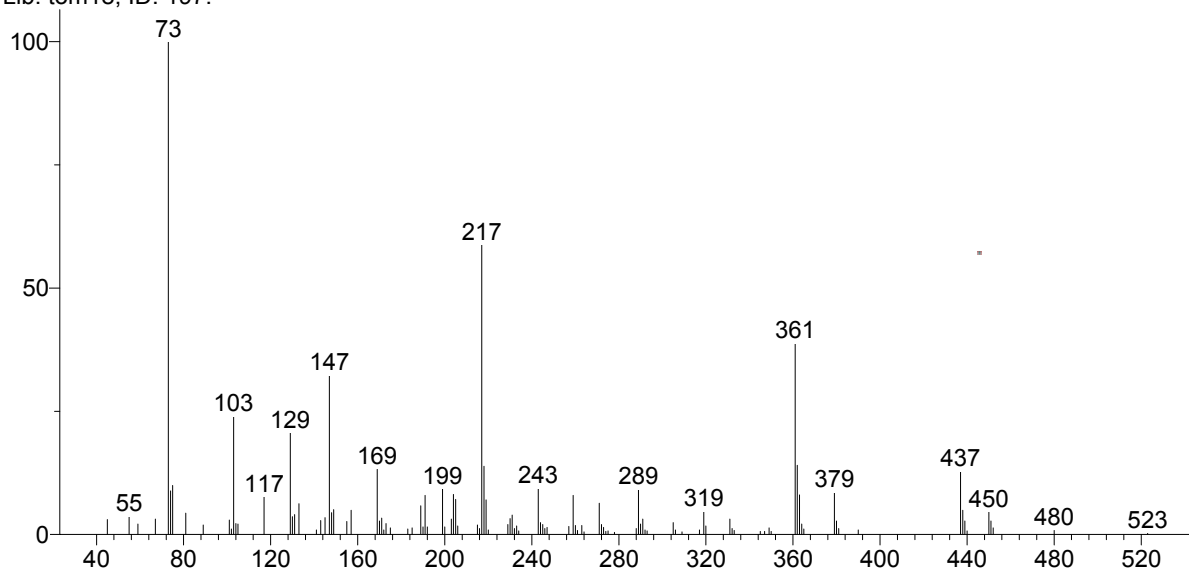
73 999	117 33	147 210	161 12	191 453	218 62	243 115	261 9	305 15	349 13
89 17	129 141	148 47	169 185	192 64	219 31	244 17	263 9	319 26	361 912
103 157	130 13	149 43	170 23	193 30	229 32	245 26	271 112	331 70	362 263
104 21	131 33	155 44	171 18	204 81	231 18	247 11	272 25	332 14	363 125
113 13	133 48	157 43	175 13	215 9	233 13	259 56	273 14	333 10	
116 17	143 25	160 23	189 45	217 300	241 9	260 12	291 13	345 9	

Synonyms:

1.TREHALOSE 8T-TENT;

Hit 197 : RH-T-2742.6-0.03%-[217,361,103,437]-RH03

Lib: tom18; ID: 197.



(tom18) RH-T-2742.6-0.03%-[217,361,103,437]-RH03

Name: RH-T-2742.6-0.03%-[217,361,103,437]-RH03

MW: N/A ID#: 197 DB: tom18

Comment: RI:MG00244 [RI:2742.6]

10 largest peaks:

73 999 | 217 587 | 361 387 | 147 322 | 103 239 | 129 206 | 362 140 | 218 138 | 169 132 | 437 127 |

96 m/z Values and Intensities (15 low intensity peaks are not shown):

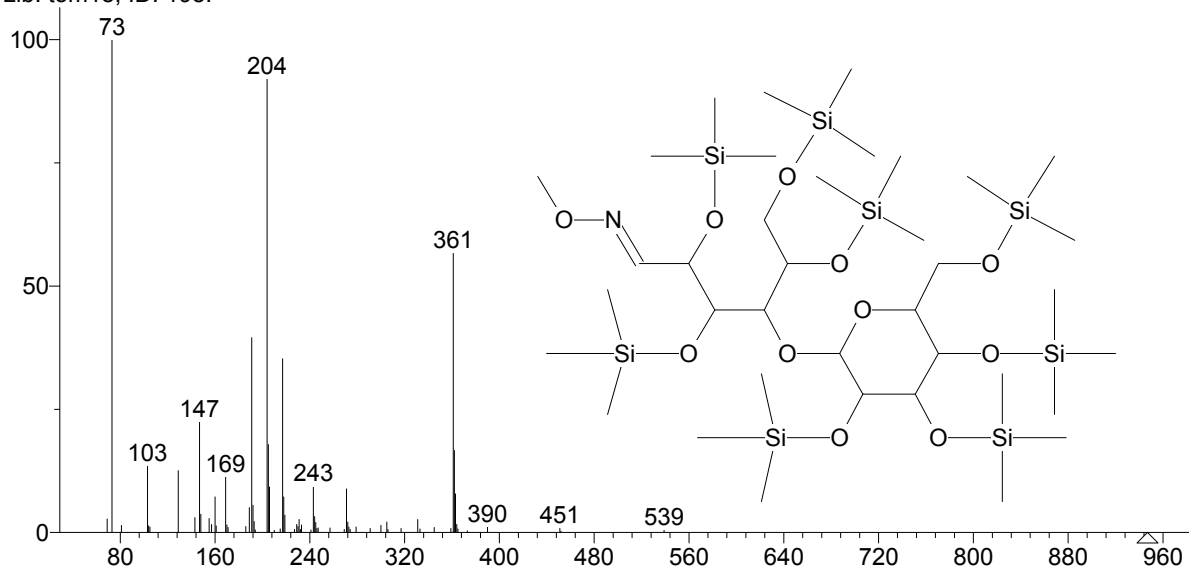
45	30	102	11	143	28	172	9	200	15	220	9	247	14	290	21	349	13	437	127
55	36	103	239	145	34	173	22	203	31	229	20	257	16	291	31	361	387	438	49
59	21	104	22	147	322	175	13	204	81	230	32	259	79	292	9	362	140	439	27
67	31	105	21	148	44	183	11	205	71	231	39	260	18	305	24	363	80	450	45
73	999	117	76	149	50	185	13	206	17	232	12	263	18	306	9	364	21	451	27
74	88	129	206	155	26	189	58	215	19	233	17	271	63	317	9	365	11	452	13
75	99	130	36	157	49	190	15	216	12	243	93	272	20	319	46	379	85		
81	43	131	40	169	132	191	79	217	587	244	24	273	14	320	17	380	27		
89	19	133	62	170	27	192	15	218	138	245	20	288	12	331	31	381	12		
101	29	141	9	171	33	199	92	219	70	246	12	289	91	332	12	390	9		

Synonyms:

1.m217,361,103,437;

Hit 198 : RH-T-2752.2-0.00%-MALTOSE M8T-PK2-TENT- 8135A18-G

Lib: tom18; ID: 198.



(tom18) RH-T-2752.2-0.00%-MALTOSE M8T-PK2-TENT- 8135A18-G RI:2752.2,

Name: RH-T-2752.2-0.00%-MALTOSE M8T-PK2-TENT- 8135A18-G

Formula: C₃₇H₈₉NO₁₁Si₈

MW: 947 ID#: 198 DB: tom18

RI: 2752.2,

Comment: RI=2752.2, 40.3964 min 8135A18 [RI:2752.2]

10 largest peaks:

73 999 | 204 919 | 361 566 | 191 395 | 217 352 | 147 224 | 205 178 | 362 166 | 103 134 | 129 125 |

50 m/z Values and Intensities (19 low intensity peaks are not shown):

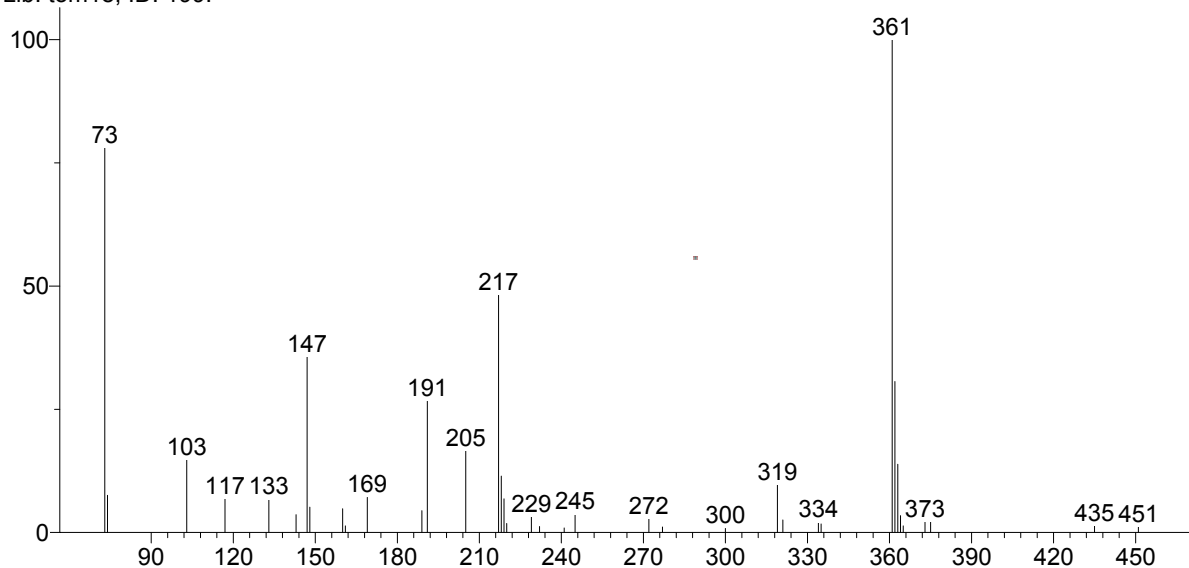
69	27	105	11	155	28	170	15	192	55	217	352	231	26	247	9	279	11	361	566
73	999	129	125	157	16	171	10	193	22	218	72	233	15	257	9	300	14	362	166
81	14	143	30	160	72	186	12	204	919	219	35	243	93	271	88	305	21	363	78
103	134	147	224	161	13	189	50	205	178	229	16	244	32	272	21	331	26	364	16
104	13	148	37	169	112	191	395	206	92	230	12	245	20	273	11	345	10	390	11

Synonyms:

1.MALTOSE M8T-PK2-TENT;

Hit 199 : RH-T-2757.4-0.00%-[361,217,191,319,103]-RH03

Lib: tom18; ID: 199.



(tom18) RH-T-2757.4-0.00%-[361,217,191,319,103]-RH03 RI:2757.4,

Name: RH-T-2757.4-0.00%-[361,217,191,319,103]-RH03

MW: N/A ID#: 199 DB: tom18

RI: 2757.4,

Comment: RI=2757.4, 54.0614 min MG00244 [RI:2757.4]

10 largest peaks:

361 999 | 73 779 | 217 481 | 147 356 | 362 306 | 191 266 | 205 165 | 103 147 | 363 138 | 218 114 |

37 m/z Values and Intensities (1 low intensity peak is not shown):

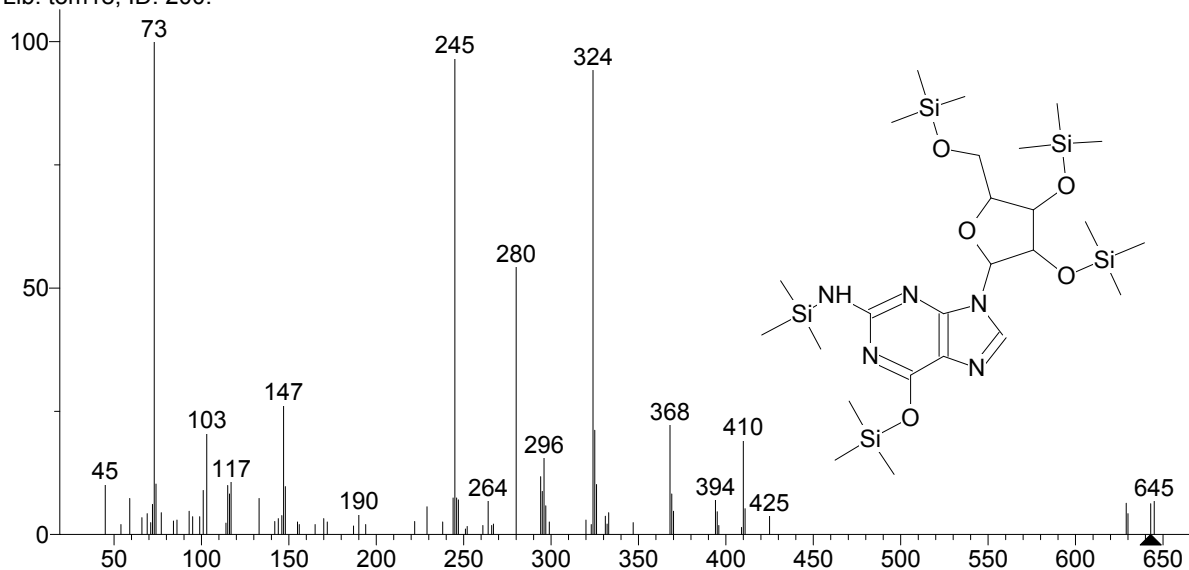
73 779	133 66	160 48	191 266	219 68	241 9	319 96	361 999	365 13	451 11
74 75	143 36	161 13	205 165	220 18	245 36	321 25	362 306	373 21	
103 147	147 356	169 71	217 481	229 31	272 27	334 20	363 138	375 21	
117 68	148 51	189 44	218 114	232 12	277 11	335 17	364 34	435 13	

Synonyms:

1.m361,217,191,319,103;

Hit 200 : RH-T-2774.1-0.01%-[N,G:Guanosine 5T]-TENT-RH03

Lib: tom18; ID: 200.



(tom18) RH-T-2774.1-0.01%-[N,G:Guanosine 5T]-TENT-RH03 RI:2774.1,

Name: RH-T-2774.1-0.01%-[N,G:Guanosine 5T]-TENT-RH03

Formula: C₂₅H₅₃N₅O₅Si₅

MW: 643 ID#: 200 DB: tom18

RI: 2774.1,

Comment: RI=2774.1, 54.3645 min MG00244 [RI:2774.1]

10 largest peaks:

73 999 | 245 965 | 324 941 | 280 542 | 147 261 | 368 222 | 325 211 | 103 204 | 410 190 | 296 155 |

77 m/z Values and Intensities:

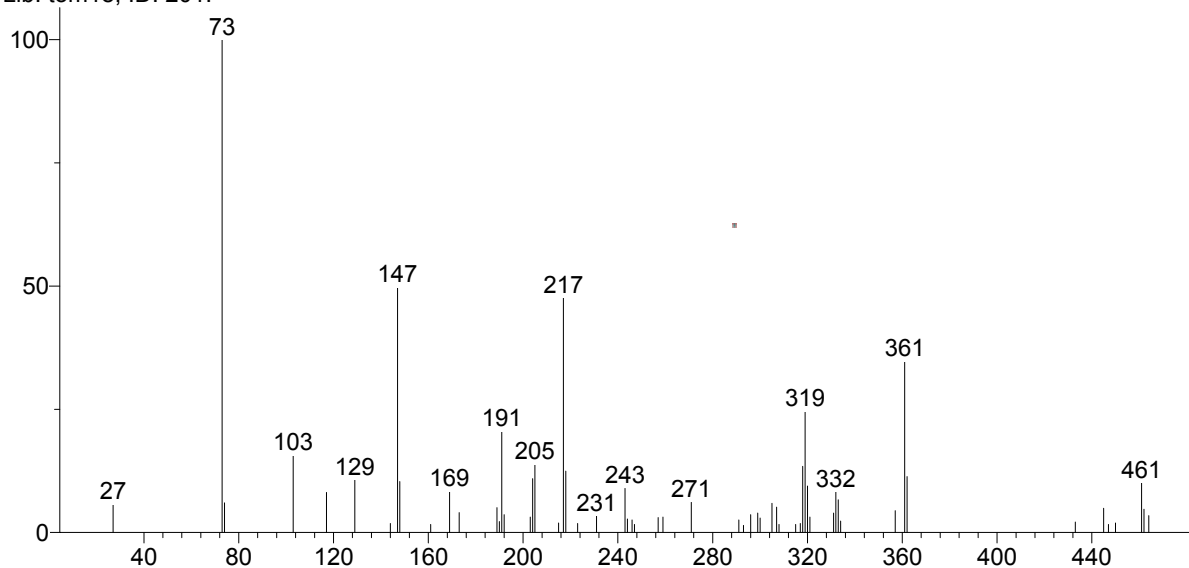
45 101	74 102	103 204	146 38	187 17	246 74	280 542	324 941	369 82	425 37
54 20	77 44	114 23	147 261	190 40	247 70	294 117	325 211	370 47	629 63
59 73	84 27	115 99	148 97	194 20	251 11	295 87	326 101	394 70	630 42
66 34	86 29	116 82	155 25	222 26	252 16	296 155	331 37	395 46	643 62
69 42	93 47	117 106	156 20	229 56	261 18	297 58	332 21	396 18	645 67
71 24	95 36	133 73	165 20	238 25	264 68	299 25	333 44	409 14	
72 61	99 36	142 26	170 32	244 74	266 18	320 29	347 24	410 190	
73 999	101 89	144 32	172 25	245 965	267 21	323 20	368 222	411 52	

Synonyms:

1.Guanosine 5T;

Hit 201 : RH-T-2811.8-0.00%-[217,361,319,191,461]-RH03

Lib: tom18; ID: 201.



(tom18) RH-T-2811.8-0.00%-[217,361,319,191,461]-RH03 RI:2811.8,

Name: RH-T-2811.8-0.00%-[217,361,319,191,461]-RH03

MW: N/A ID#: 201 DB: tom18

RI: 2811.8,

Comment: RI=2811.8, 55.0295 min MG00244 [RI:2811.8]

10 largest peaks:

73 999 | 147 496 | 217 475 | 361 346 | 319 245 | 191 204 | 103 156 | 205 137 | 318 134 | 218 124 |

59 m/z Values and Intensities:

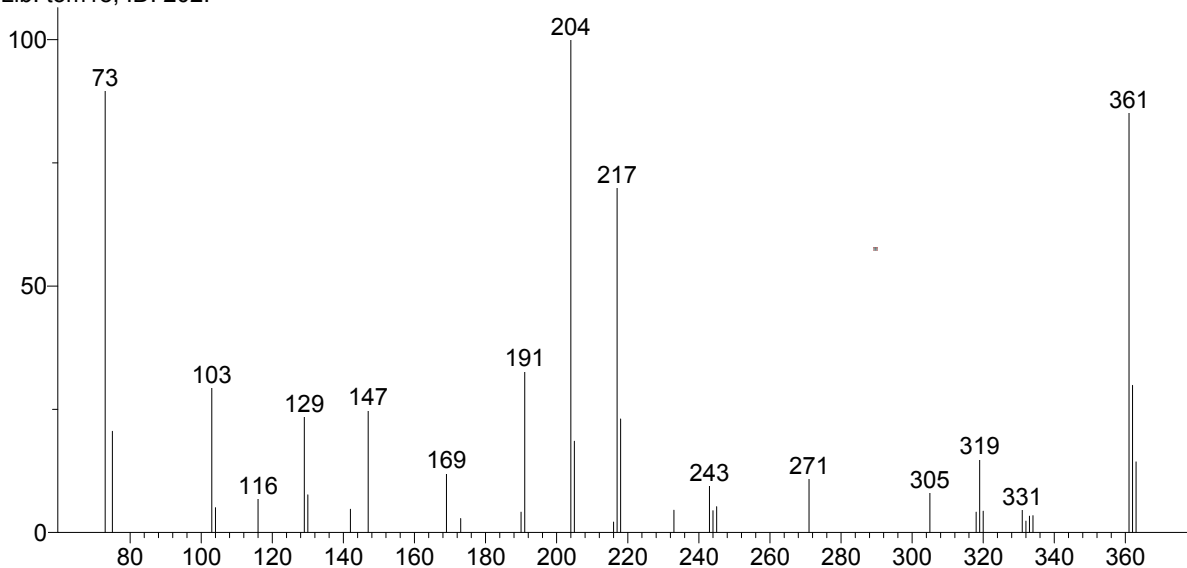
27	56	144	18	189	50	205	137	243	89	271	61	305	59	319	245	334	23	447	16
73	999	147	496	190	22	215	19	244	27	291	25	307	51	320	94	357	44	450	19
74	60	148	103	191	204	217	475	246	25	293	14	308	16	321	31	361	346	461	100
103	156	161	16	192	36	218	124	247	16	296	36	315	16	331	39	362	113	462	47
117	81	169	83	203	31	223	18	257	30	299	39	317	18	332	82	433	21	464	34
129	106	173	40	204	109	231	33	259	31	300	29	318	134	333	66	445	49		

Synonyms:

1.m217,361,319,191,461;

Hit 202 : RH-T-2822.4-0.06%-[204,361,217,191,103,129,319]-RH03-X

Lib: tom18; ID: 202.



(tom18) RH-T-2822.4-0.06%-[204,361,217,191,103,129,319]-RH03-X RI:2822.4,

Name: RH-T-2822.4-0.06%-[204,361,217,191,103,129,319]-RH03-X

MW: N/A ID#: 202 DB: tom18

RI: 2822.4,

Comment: RI=2822.4, 55.2039 min MG00244 |RI:2822.4|

10 largest peaks:

204 999 | 73 895 | 361 851 | 217 698 | 191 326 | 362 298 | 103 293 | 147 247 | 129 234 | 218 230 |

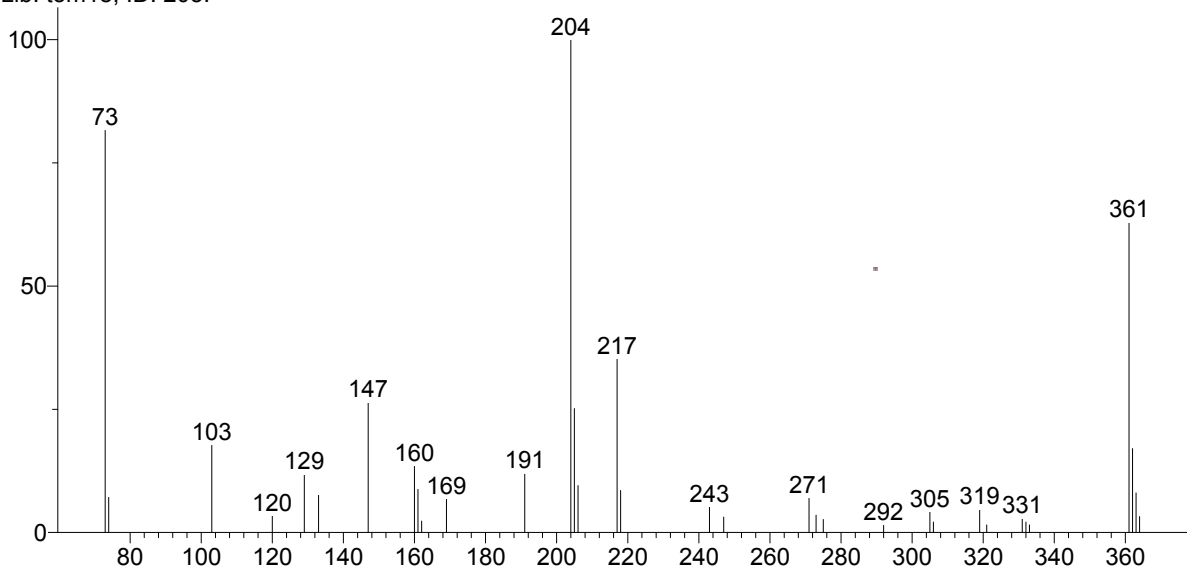
34 m/z Values and Intensities:

73 895 | 116 68 | 147 247 | 191 326 | 217 698 | 244 44 | 318 41 | 332 23 | 362 298 |
75 205 | 129 234 | 169 119 | 204 999 | 218 230 | 245 52 | 319 148 | 333 33 | 363 143 |
103 293 | 130 76 | 173 28 | 205 185 | 233 45 | 271 108 | 320 43 | 334 34 |
104 50 | 142 47 | 190 41 | 216 21 | 243 94 | 305 80 | 331 45 | 361 851 |

Synonyms:

1.m204,361,217,191,103,129,319;

Hit 203 : RH-T-2850.1-0.01%-[204,361,217,103, N: sim. isomaltose M8T]-RH03-X
Lib: tom18; ID: 203.



(tom18) RH-T-2850.1-0.01%-[204,361,217,103, N: sim. isomaltose M8T]-RH03-X

Name: RH-T-2850.1-0.01%-[204,361,217,103, N: sim. isomaltose M8T]-RH03-X

MW: N/A ID#: 203 DB: tom18

Comment: RI:MG00238 |RI:2850.1|

10 largest peaks:

204 999 | 73 815 | 361 628 | 217 351 | 147 263 | 205 251 | 103 177 | 362 170 | 160 134 | 191 119 |

34 m/z Values and Intensities:

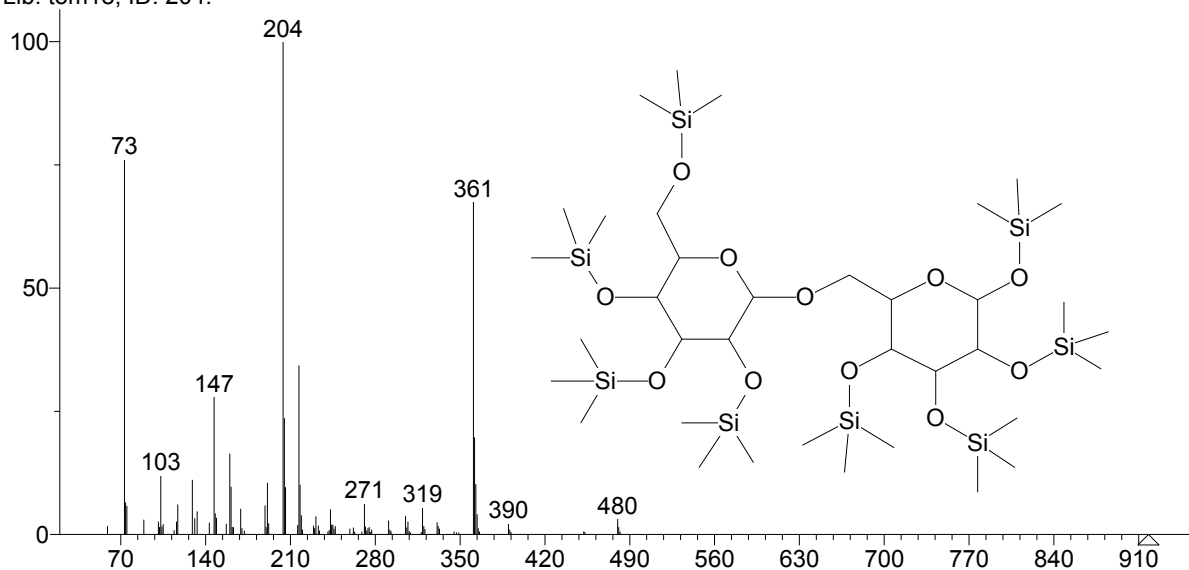
73 815 | 129 117 | 161 87 | 204 999 | 218 85 | 273 35 | 306 21 | 332 21 | 363 80 |
74 71 | 133 75 | 162 23 | 205 251 | 243 51 | 275 26 | 319 46 | 333 15 | 364 32 |
103 177 | 147 263 | 169 67 | 206 95 | 247 31 | 292 14 | 321 15 | 361 628 |
120 33 | 160 134 | 191 119 | 217 351 | 271 69 | 305 41 | 331 28 | 362 170 |

Synonyms:

1.m204,361,217,103, N: sim. isomaltose M8T;

Hit 204 : RH-T-2850.6-0.06%-GENTIOBIOSE-8T-TENT-[56-73-5]-RH03

Lib: tom18; ID: 204.



(tom18) RH-T-2850.6-0.06%-GENTIOBIOSE-8T-TENT-[56-73-5]-RH03

Name: RH-T-2850.6-0.06%-GENTIOBIOSE-8T-TENT-[56-73-5]-RH03

Formula: C₃₆H₈₆O₁₁Si₈

MW: 918 ID#: 204 DB: tom18

Comment: RI:MG00238 [RI:2850.6]

10 largest peaks:

204 999 | 73 760 | 361 674 | 217 342 | 147 279 | 205 235 | 362 196 | 160 163 | 103 119 | 129 110 |

74 m/z Values and Intensities (21 low intensity peaks are not shown):

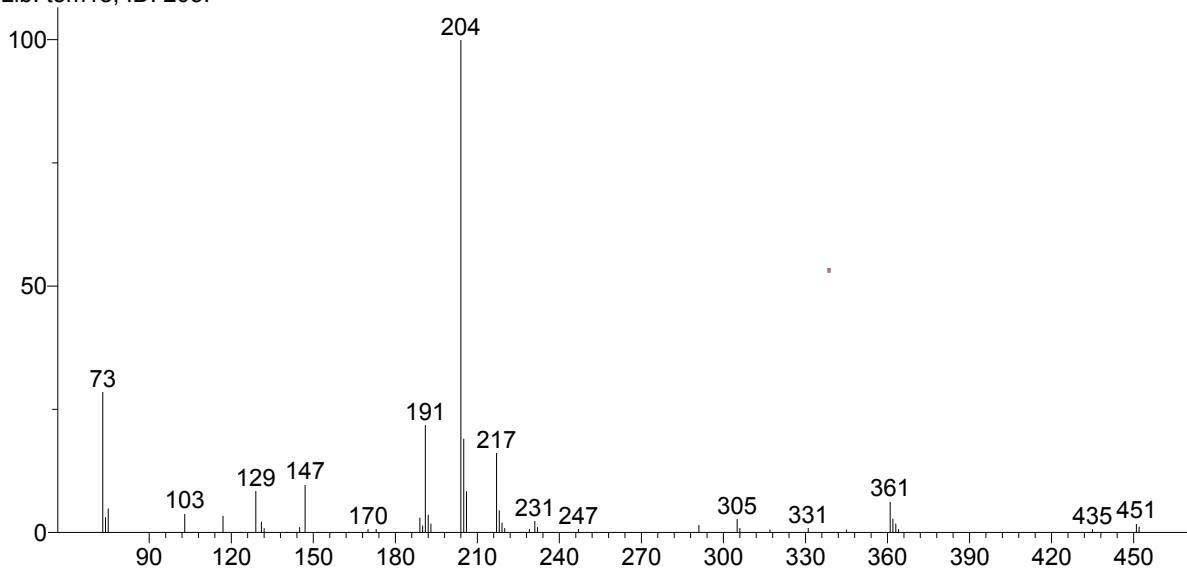
59 16	104 15	147 279	169 51	206 95	231 36	262 13	305 37	333 11	480 31
73 760	105 20	148 42	170 12	216 18	233 17	271 62	306 13	361 674	481 14
74 64	116 25	149 33	189 58	217 342	243 50	272 15	307 25	362 196	
75 57	117 60	157 21	190 14	218 100	244 19	274 12	319 54	363 101	
89 29	129 110	160 163	191 104	219 38	245 19	275 14	320 16	364 40	
101 25	131 32	161 96	192 22	220 9	246 11	277 9	321 10	365 12	
102 14	133 46	162 14	204 999	229 17	247 16	291 27	331 24	390 22	
103 119	143 23	163 14	205 235	230 12	259 11	292 9	332 16	391 9	

Synonyms:

1.GENTIOBIOSE-8T-TENT-[56-73-5];

Hit 205 : RH-T-2917.3-0.00%-[204,191,217,129,361,451]-RH03

Lib: tom18; ID: 205.



(tom18) RH-T-2917.3-0.00%-[204,191,217,129,361,451]-RH03 RI:2917.3,

Name: RH-T-2917.3-0.00%-[204,191,217,129,361,451]-RH03

MW: N/A ID#: 205 DB: tom18

RI: 2917.3,

Comment: RI=2917.3, 56.7671 min MG00244 [RI:2917.3]

10 largest peaks:

204 999 | 73 284 | 191 217 | 205 189 | 217 161 | 147 97 | 129 84 | 206 83 | 361 62 | 75 48 |

30 m/z Values and Intensities (11 low intensity peaks are not shown):

73 284 | 103 38 | 131 21 | 189 29 | 192 35 | 205 189 | 218 44 | 232 10 | 331 9 | 363 17 |

74 30 | 117 33 | 145 10 | 190 13 | 193 17 | 206 83 | 219 19 | 291 14 | 361 62 | 451 18 |

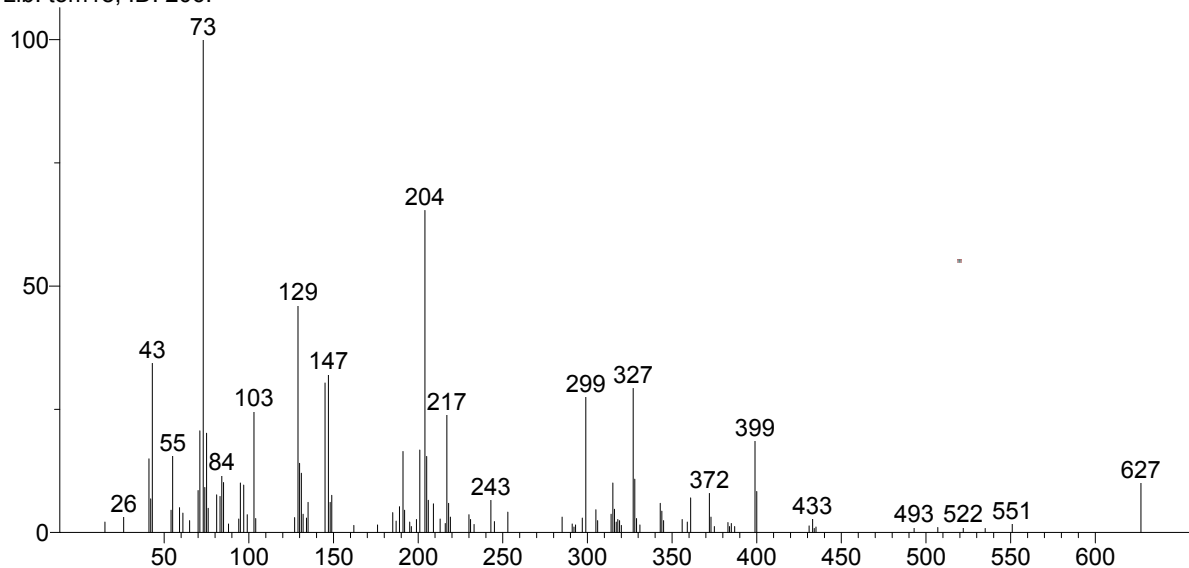
75 48 | 129 84 | 147 97 | 191 217 | 204 999 | 217 161 | 231 23 | 305 27 | 362 27 | 452 11 |

Synonyms:

1.m204,191,217,129,361,451;

Hit 206 : RH-T-2935.7-0.04%-[204,129,327,399,299,217,145]-RH01

Lib: tom18; ID: 206.



(tom18) RH-T-2935.7-0.04%-[204,129,327,399,299,217,145]-RH01 RI:2935.7,

Name: RH-T-2935.7-0.04%-[204,129,327,399,299,217,145]-RH01

MW: N/A ID#: 206 DB: tom18

RI: 2935.7,

Comment: RI=2935.7, 48.1629 min AB2129 [RI:2935.7]

10 largest peaks:

73 999 | 204 653 | 129 460 | 43 343 | 147 320 | 145 303 | 327 292 | 299 274 | 103 245 | 217 238 |

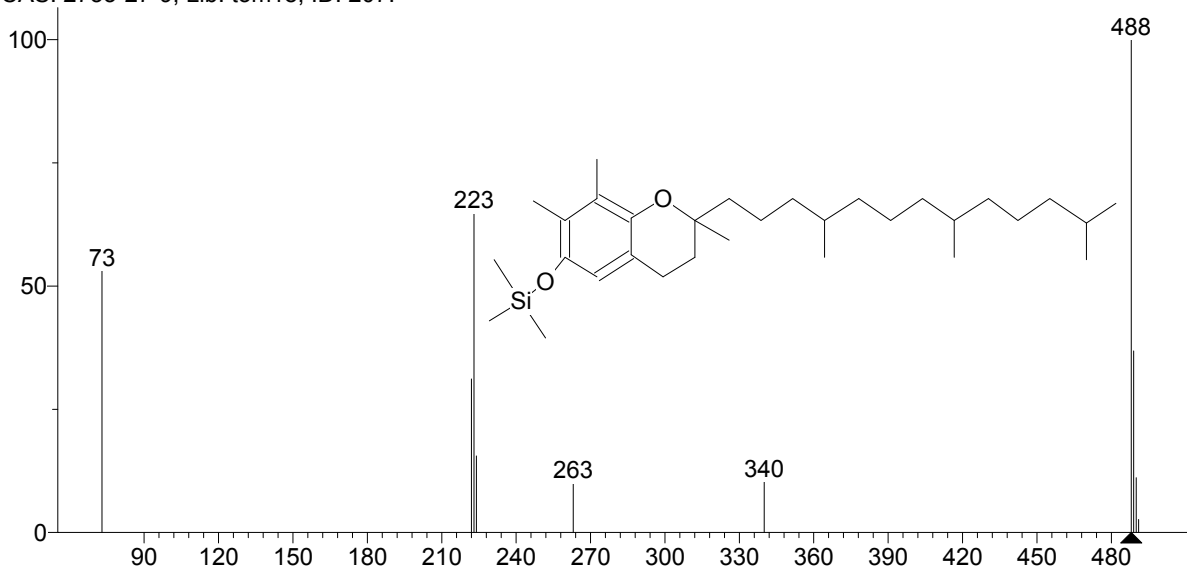
106 m/z Values and Intensities (2 low intensity peaks are not shown):

15	21	71	206	95	100	135	61	192	45	217	238	292	11	319	24	361	70	433	27
26	31	73	999	97	96	145	303	195	21	218	59	293	15	320	14	372	79	435	11
41	149	74	91	99	36	147	320	196	12	219	31	297	29	327	292	373	31	493	10
42	68	75	201	103	245	148	61	199	26	230	36	299	274	328	108	375	12	507	10
43	343	76	49	104	28	149	75	201	167	231	26	305	46	329	28	383	20	522	10
54	45	81	76	127	30	162	14	204	653	233	16	306	24	331	15	384	12	551	17
55	155	83	73	129	460	176	15	205	154	243	65	314	37	343	59	385	18	627	100
59	50	84	115	130	140	185	40	206	65	245	22	315	100	344	43	387	12		
61	39	85	101	131	120	187	23	209	58	253	41	316	47	345	24	399	185		
65	24	88	17	132	37	189	52	213	27	285	31	317	21	356	26	400	83		
70	85	94	27	134	29	191	164	216	18	291	17	318	26	359	21	431	13		

Synonyms:

1.m204,129,327,399,299,217,145;

Hit 207 : RH-T-2991.1-0.00%-GAMMA-TOCOPHEROL 1T-TENT-[54-28-4]-RH03-X
CAS: 2733-27-9; Lib: tom18; ID: 207.



(tom18) RH-T-2991.1-0.00%-GAMMA-TOCOPHEROL 1T-TENT-[54-28-4]-RH03-X

Name: RH-T-2991.1-0.00%-GAMMA-TOCOPHEROL 1T-TENT-[54-28-4]-RH03-X

Formula: C₃₁H₅₆O₂Si

MW: 488 CAS#: 2733-27-9 ID#: 207 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:2991.1|

10 largest peaks:

488 999 | 223 646 | 73 530 | 489 368 | 222 311 | 224 155 | 490 111 | 340 102 | 263 99 | 491 26 |

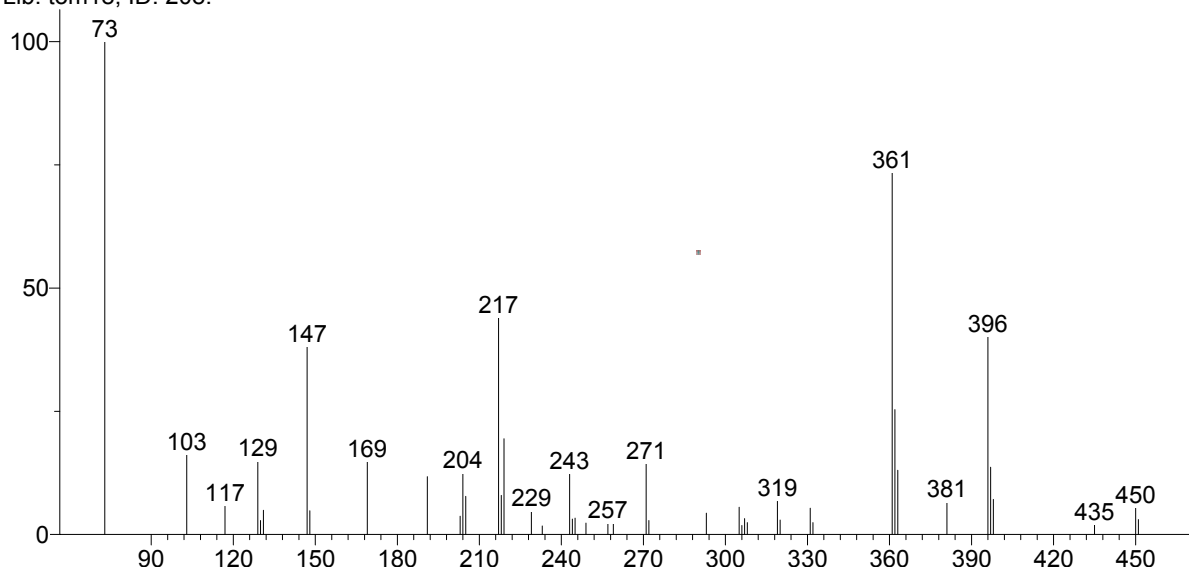
10 m/z Values and Intensities:

73 530 | 222 311 | 223 646 | 224 155 | 263 99 | 340 102 | 488 999 | 489 368 | 490 111 | 491 26 |

Synonyms:

1.GAMMA-TOCOPHEROL 1T-TENT-[54-28-4];

Hit 208 : RH-T-2994.6-0.00%-[361,396,217,450, N: sim. D-Glucopyranoside-fructofuranosyl]-RH03
Lib: tom18; ID: 208.



(tom18) RH-T-2994.6-0.00%-[361,396,217,450, N: sim. D-Glucopyranoside-fructofuranosyl]-RH03 RI:2994.6,

Name: RH-T-2994.6-0.00%-[361,396,217,450, N: sim. D-Glucopyranoside-fructofuranosyl]-RH03

MW: N/A ID#: 208 DB: tom18

RI: 2994.6,

Comment: RI=2994.6, 58.0384 min MG00244 [RI:2994.6]

10 largest peaks:

73 999 | 361 733 | 217 439 | 396 400 | 147 380 | 362 253 | 219 194 | 103 161 | 129 148 | 169 147 |

45 m/z Values and Intensities:

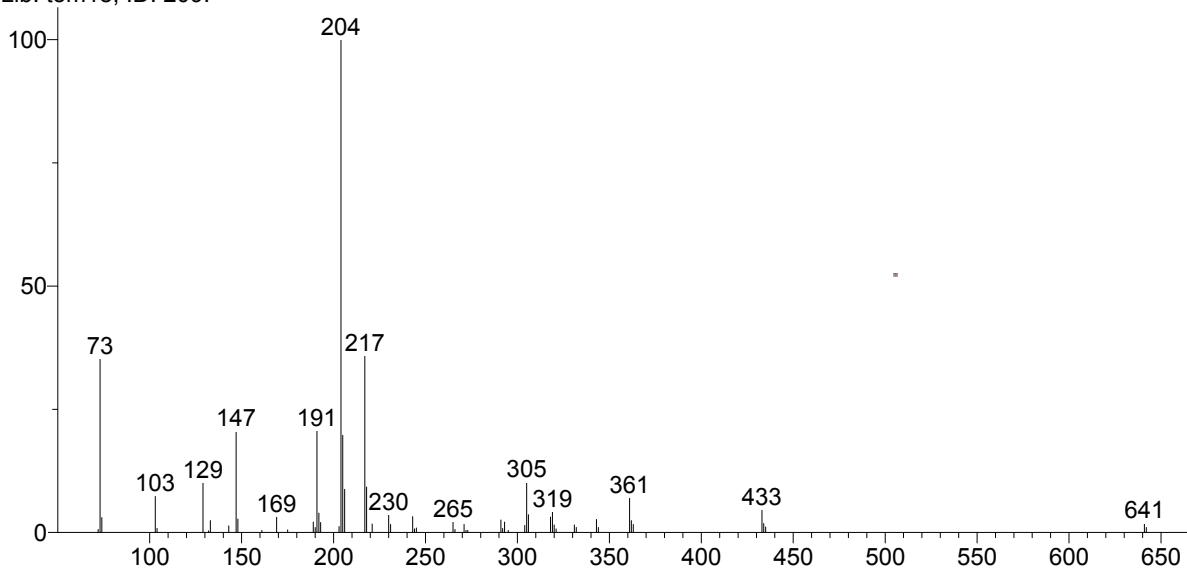
73	999	131	49	203	37	219	194	245	33	272	28	308	24	361	733	397	136
103	161	147	380	204	123	229	46	249	23	293	43	319	67	362	253	398	71
117	57	148	48	205	77	233	17	257	22	305	55	320	29	363	130	435	19
129	148	169	147	217	439	243	122	259	22	306	18	331	53	381	64	450	53
130	28	191	117	218	79	244	31	271	143	307	32	332	24	396	400	451	30

Synonyms:

1.m361,396,217,450, N: sim. D-Glucopyranoside-fructofuranosyl;

Hit 209 : RH-T-3006.0-0.00%-[204,217,191,305,361,433,641]-RH03

Lib: tom18; ID: 209.



(tom18) RH-T-3006.0-0.00%-[204,217,191,305,361,433,641]-RH03 RI:3006.6,

Name: RH-T-3006.0-0.00%-[204,217,191,305,361,433,641]-RH03

MW: N/A ID#: 209 DB: tom18

RI: 3006.6,

Comment: RI=3006.6, 58.2363 min MG00238 [RI:3006.6]

10 largest peaks:

204 999 | 217 357 | 73 351 | 191 206 | 147 204 | 205 197 | 305 101 | 129 100 | 218 92 | 206 87 |

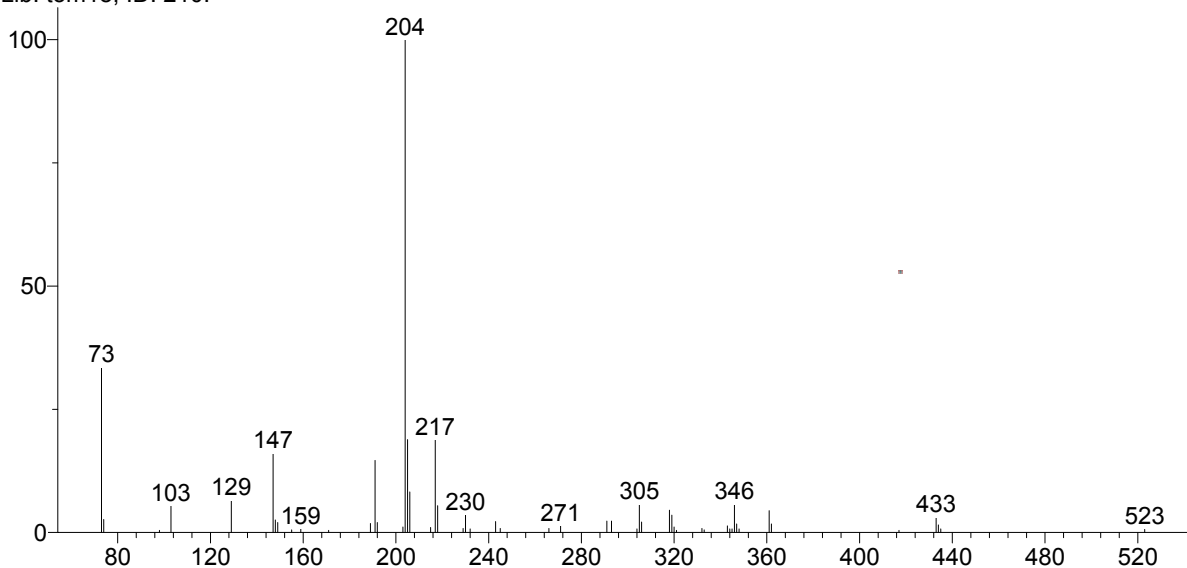
47 m/z Values and Intensities (12 low intensity peaks are not shown):

73 351	143 13	190 10	204 999	221 17	265 21	305 101	331 15	362 24	641 18
74 30	147 204	191 206	205 197	230 35	271 16	306 36	332 10	363 16	642 10
103 73	148 27	192 39	206 87	231 16	291 25	318 31	343 26	433 45	
129 100	169 31	193 20	217 357	243 32	293 21	319 41	344 10	434 18	
133 24	189 21	203 12	218 92	245 9	304 14	320 15	361 69	435 11	

Synonyms:

1.m204,217,191,305,361,433,641;

Hit 210 : RH-T-3030.2-0.01%-[204,217,191,433,346,305, N: sim. D-Glucose,4-galactopyranosyl]-RH03
Lib: tom18; ID: 210.



(tom18) RH-T-3030.2-0.01%-[204,217,191,433,346,305, N: sim. D-Glucose,4-galactopyranosyl]-RH03 RI:3030.2,

Name: RH-T-3030.2-0.01%-[204,217,191,433,346,305, N: sim. D-Glucose,4-galactopyranosyl]-RH03

MW: N/A ID#: 210 DB: tom18

RI: 3030.2,

Comment: RI=3030.2, 58.6237 min MG00244 [RI:3030.2]

10 largest peaks:

204 999 | 73 334 | 205 188 | 217 187 | 147 160 | 191 146 | 206 82 | 129 64 | 305 56 | 346 56 |

34 m/z Values and Intensities (18 low intensity peaks are not shown):

73 334 | 147 160 | 191 146 | 205 188 | 218 54 | 291 23 | 318 45 | 346 56 | 433 30 |

74 26 | 148 25 | 192 20 | 206 82 | 230 35 | 293 23 | 319 35 | 347 17 | 434 15 |

103 53 | 149 20 | 203 11 | 215 10 | 243 22 | 305 56 | 320 11 | 361 44 |

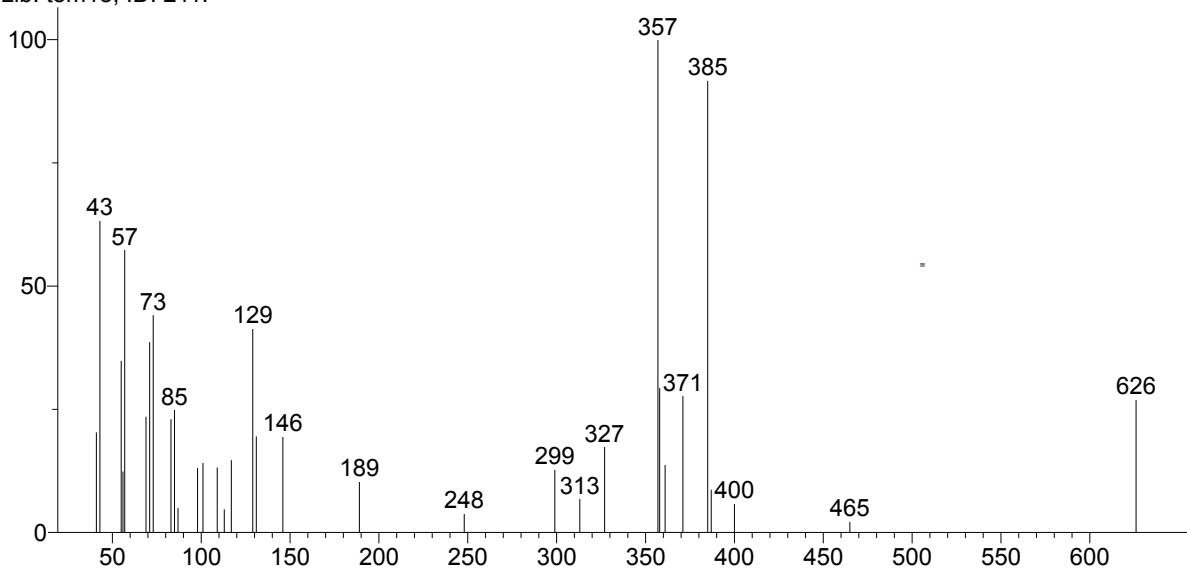
129 64 | 189 18 | 204 999 | 217 187 | 271 13 | 306 21 | 343 13 | 362 17 |

Synonyms:

1.m204,217,191,433,346,305, N: sim. D-Glucose,4-galactopyranosy;

Hit 211 : RH-T-3041.3-0.08%-[357,385,626,129,371]-RH01-X

Lib: tom18; ID: 211.



(tom18) RH-T-3041.3-0.08%-[357,385,626,129,371]-RH01-X RI:3041.3,

Name: RH-T-3041.3-0.08%-[357,385,626,129,371]-RH01-X

MW: N/A ID#: 211 DB: tom18

RI: 3041.3,

Comment: RI=3041.3, 49.7096 min AB2129 |RI:3041.3|

10 largest peaks:

357 999 | 385 916 | 43 632 | 57 573 | 73 440 | 129 413 | 71 385 | 55 347 | 358 292 | 371 276 |

33 m/z Values and Intensities:

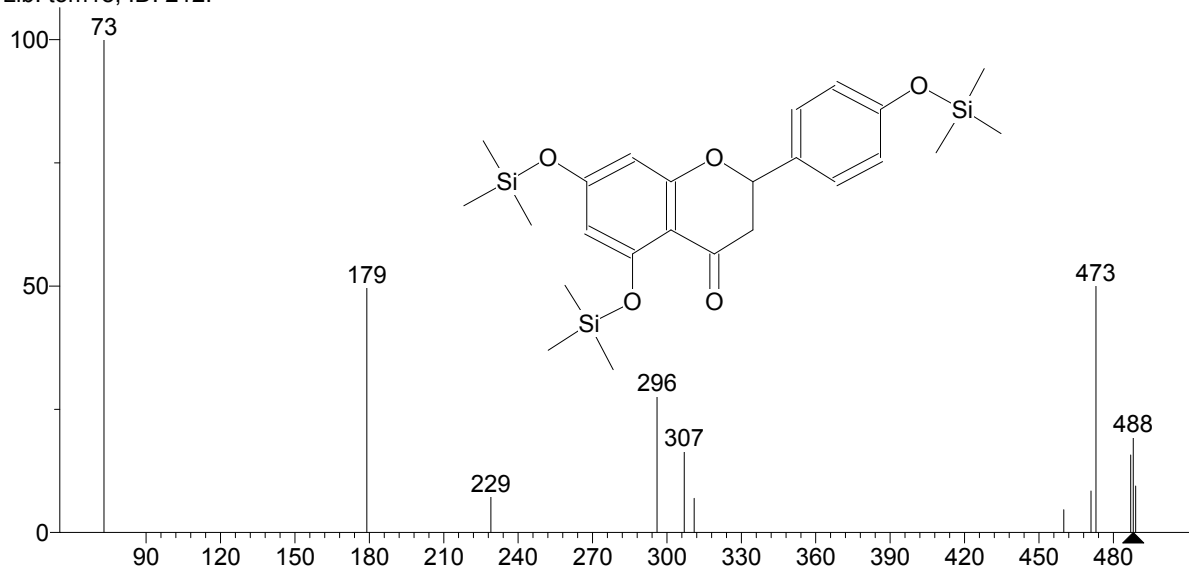
41 202	57 573	83 229	101 140	129 413	248 38	357 999	385 916	626 269
43 632	69 234	85 248	109 131	131 194	299 127	358 292	387 86	
55 347	71 385	87 49	113 46	146 194	313 67	361 136	400 58	
56 123	73 440	98 130	117 146	189 103	327 173	371 276	465 22	

Synonyms:

1.m357,385,626,129,371;

Hit 212 : RH-T-3047.7-0.00%-[G: sim. NARINGENIN-3T-TENT]-G-X

Lib: tom18; ID: 212.



(tom18) RH-T-3047.7-0.00%-[G: sim. NARINGENIN-3T-TENT]-G-X RI:3047.7,

Name: RH-T-3047.7-0.00%-[G: sim. NARINGENIN-3T-TENT]-G-X

Formula: C₂₄H₃₆O₅Si₃

MW: 488 ID#: 212 DB: tom18

RI: 3047.7,

Comment: RI=3047.7, 43.8388 min 8135A18 [RI:3047.7]

10 largest peaks:

73 999 | 473 499 | 179 495 | 296 275 | 488 192 | 307 164 | 487 157 | 489 94 | 471 84 | 229 72 |

12 m/z Values and Intensities:

73 999 | 229 72 | 307 164 | 460 46 | 473 499 | 488 192 |

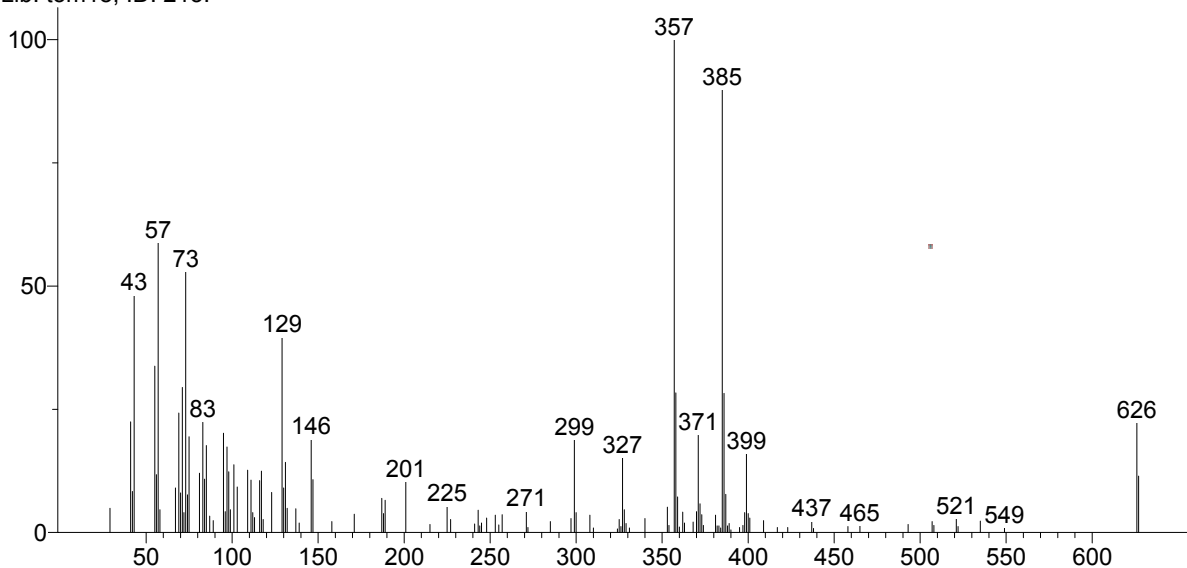
179 495 | 296 275 | 311 69 | 471 84 | 487 157 | 489 94 |

Synonyms:

1.NARINGENIN-3T-TENT;

Hit 213 : RH-T-3085.8-0.09%-[357,385,129,626,299]-RH01-X

Lib: tom18; ID: 213.



(tom18) RH-T-3085.8-0.09%-[357,385,129,626,299]-RH01-X RI:3085.8,

Name: RH-T-3085.8-0.09%-[357,385,129,626,299]-RH01-X

MW: N/A ID#: 213 DB: tom18

RI: 3085.8,

Comment: RI=3085.8, 50.3613 min AB2129 |RI:3085.8|

10 largest peaks:

357 999 | 385 897 | 57 587 | 73 528 | 43 480 | 129 395 | 55 337 | 71 294 | 358 283 | 386 282 |

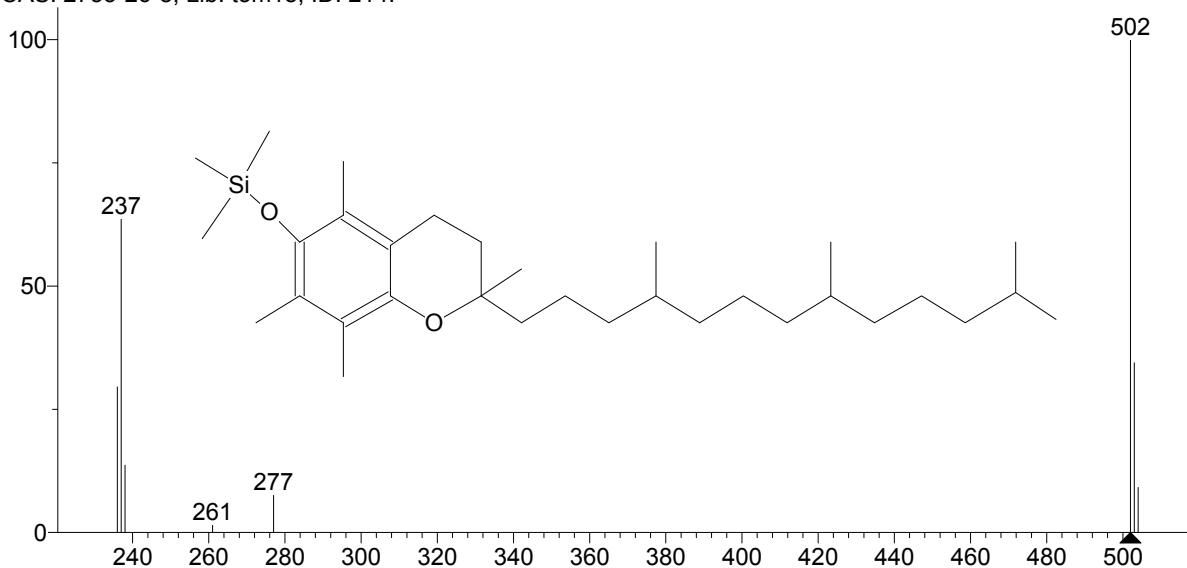
121 m/z Values and Intensities (3 low intensity peaks are not shown):

29 49	73 528	99 46	131 142	225 52	297 28	354 14	381 35	400 38	535 23
41 224	74 76	101 137	132 49	227 26	299 187	357 999	382 13	401 29	549 9
42 83	75 194	103 92	137 48	241 17	300 40	358 283	383 13	409 24	626 222
43 480	81 120	109 126	139 19	243 45	308 35	359 72	384 9	417 10	627 114
55 337	83 223	111 106	146 188	244 13	310 9	360 11	385 897	423 10	
56 117	84 108	112 40	147 107	245 19	325 26	362 41	386 282	437 22	
57 587	85 176	113 30	158 22	248 29	326 12	363 19	387 77	458 12	
58 46	87 33	116 105	171 37	253 35	327 151	368 21	388 13	465 13	
67 90	89 24	117 124	187 69	255 15	328 46	370 42	389 18	493 16	
69 242	95 201	118 26	188 38	257 36	329 18	371 197	395 10	507 22	
70 80	96 42	123 81	189 65	271 42	331 9	372 58	397 14	508 14	
71 294	97 173	129 395	201 102	272 10	340 28	373 36	398 40	521 27	
72 40	98 123	130 90	215 16	285 22	353 51	374 14	399 159	522 12	

Synonyms:

1.m357,385,129,626,299;

Hit 214 : RH-T-3126.9-0.00%-ALPHA-TOCOPHEROL 1T-TENT-[59-02-9]-RH03-X
CAS: 2733-26-8; Lib: tom18; ID: 214.



(tom18) RH-T-3126.9-0.00%-ALPHA-TOCOPHEROL 1T-TENT-[59-02-9]-RH03-X

Name: RH-T-3126.9-0.00%-ALPHA-TOCOPHEROL 1T-TENT-[59-02-9]-RH03-X

Formula: C₃₂H₅₈O₂Si

MW: 502 CAS#: 2733-26-8 ID#: 214 DB: tom18

Other DBs: None

Comment: RI:MG00238 |RI:3126.9|

8 largest peaks:

502 999 | 237 635 | 503 344 | 236 295 | 238 136 | 504 91 | 277 75 | 261 15 |

8 m/z Values and Intensities:

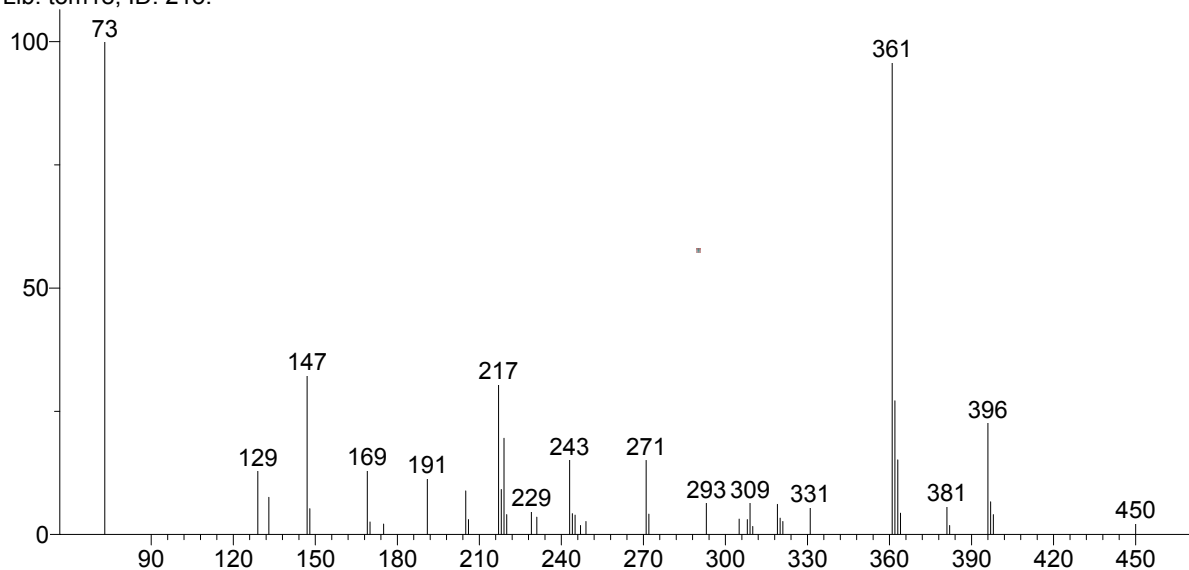
236 295 | 237 635 | 238 136 | 261 15 | 277 75 | 502 999 | 503 344 | 504 91 |

Synonyms:

1.ALPHA-TOCOPHEROL 1T-TENT-[59-02-9];

Hit 215 : RH-T-3147.8-0.00%-[361,217,396,219,271,243]-RH03

Lib: tom18; ID: 215.



(tom18) RH-T-3147.8-0.00%-[361,217,396,219,271,243]-RH03 RI:3147.8,

Name: RH-T-3147.8-0.00%-[361,217,396,219,271,243]-RH03

MW: N/A ID#: 215 DB: tom18

RI: 3147.8,

Comment: RI=3147.8, 60.5601 min MG00244 [RI:3147.8]

10 largest peaks:

73 999 | 361 957 | 147 322 | 217 304 | 362 271 | 396 226 | 219 195 | 243 151 | 363 151 | 271 150 |

43 m/z Values and Intensities:

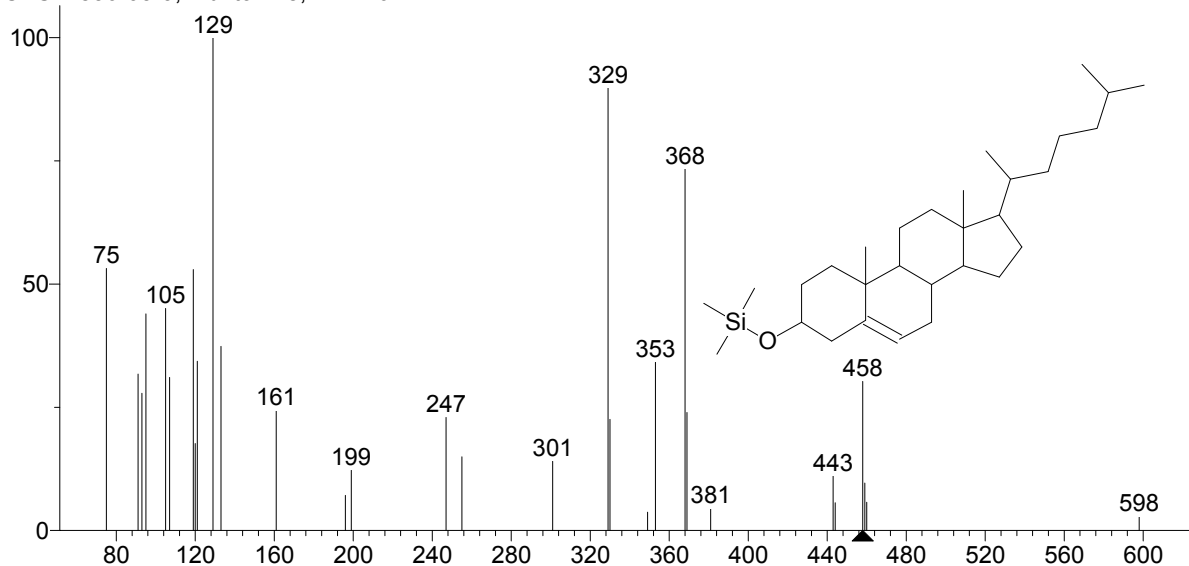
73 999	169 129	206 30	229 46	247 18	305 31	320 33	363 151	397 66
129 128	170 25	217 304	231 35	249 26	308 30	321 26	364 43	398 40
133 75	175 21	218 91	243 151	271 150	309 63	331 54	381 56	450 22
147 322	191 113	219 195	244 42	272 41	310 16	361 957	382 18	
148 52	205 88	220 40	245 39	293 63	319 61	362 271	396 226	

Synonyms:

1.m361,217,396,219,271,243;

Hit 216 : RH-T-3150.0-0.00%-CHOLESTEROL 1T-CONF-[57-88-5]-RH01-X

CAS: 1856-05-9; Lib: tom18; ID: 216.



(tom18) RH-T-3150.0-0.00%-CHOLESTEROL 1T-CONF-[57-88-5]-RH01-X RI:3102.0,

Name: RH-T-3150.0-0.00%-CHOLESTEROL 1T-CONF-[57-88-5]-RH01-X

Formula: C₃₀H₅₄OSi

MW: 458 CAS#: 1856-05-9 ID#: 216 DB: tom18

Other DBs: None

RI: 3102.0,

Comment: RI=3102.0, 50.5983 min AB2129 |RI:3150|

10 largest peaks:

129 999 | 329 897 | 368 733 | 75 531 | 119 529 | 105 450 | 95 439 | 133 373 | 121 343 | 353 341 |

30 m/z Values and Intensities:

75 531 | 95 439 | 119 529 | 129 999 | 196 71 | 255 149 | 330 225 | 368 733 | 443 110 | 459 96 |

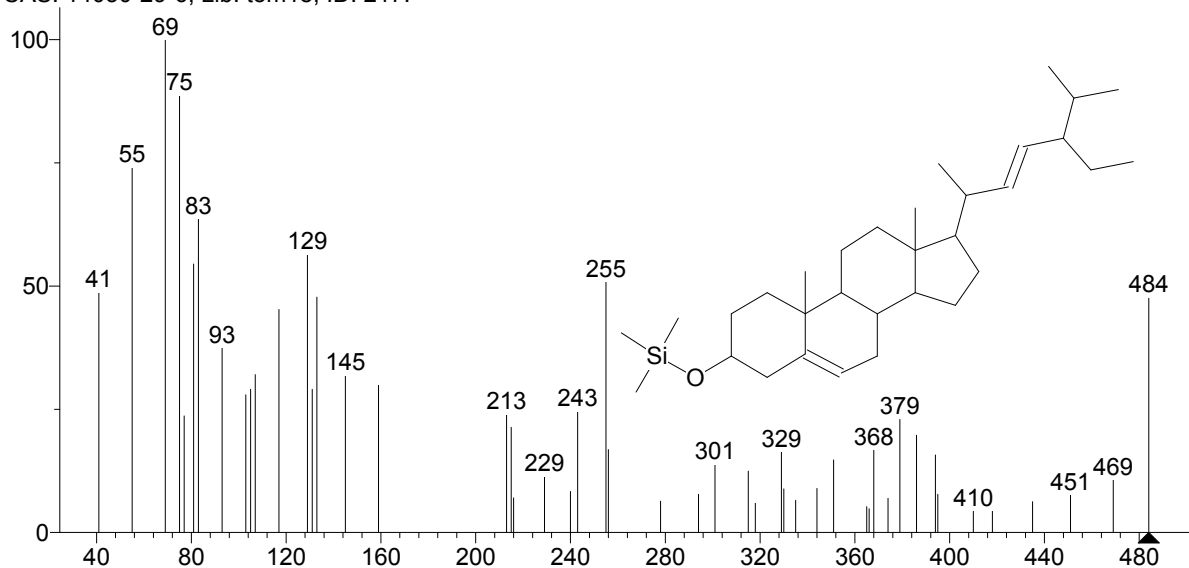
91 317 | 105 450 | 120 176 | 133 373 | 199 122 | 301 140 | 349 37 | 369 239 | 444 56 | 460 57 |

93 278 | 107 310 | 121 343 | 161 243 | 247 229 | 329 897 | 353 341 | 381 44 | 458 302 | 598 28 |

Synonyms:

1.CHOLESTEROL 1T-CONF-[57-88-5];

Hit 217 : RH-T-3288.0-0.00%-STIGMASTEROL 1T-CONF-[83-48-7]-RH01-X
CAS: 14030-29-6; Lib: tom18; ID: 217.



(tom18) RH-T-3288.0-0.00%-STIGMASTEROL 1T-CONF-[83-48-7]-RH01-X RI:3256.4,

Name: RH-T-3288.0-0.00%-STIGMASTEROL 1T-CONF-[83-48-7]-RH01-X

Formula: C₃₂H₅₆OSi

MW: 484 CAS#: 14030-29-6 ID#: 217 DB: tom18

Other DBs: None

RI: 3256.4,

Comment: RI=3256.4, 52.2198 min AB2129 [RI:3288]

10 largest peaks:

69 999 | 75 886 | 55 740 | 83 635 | 129 563 | 81 544 | 255 508 | 41 486 | 133 477 | 484 476 |

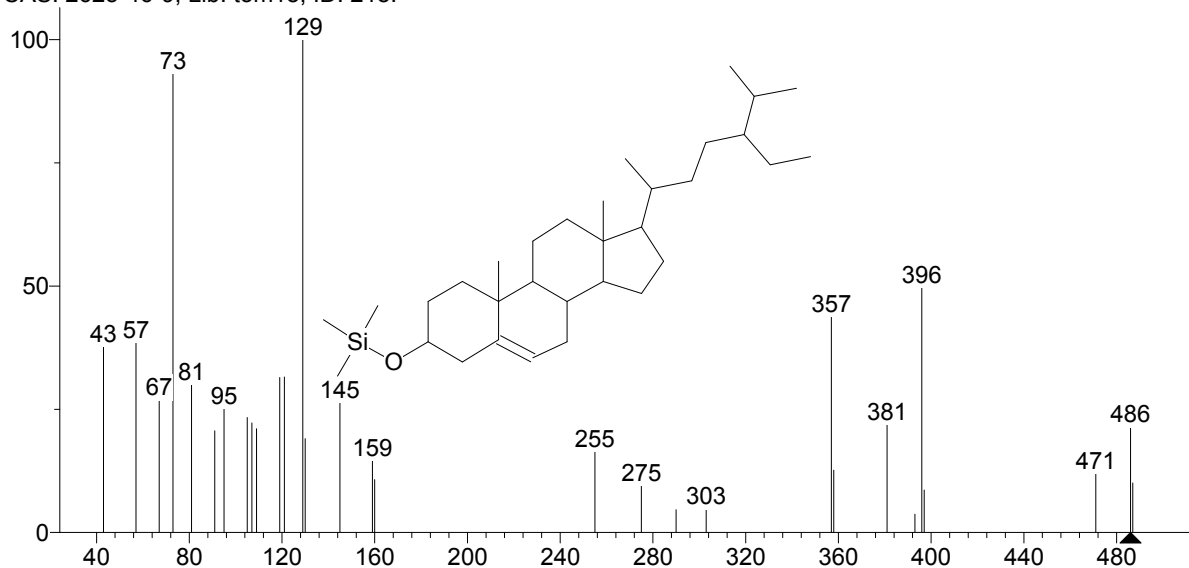
49 m/z Values and Intensities:

41 486	81 544	107 320	145 318	229 113	278 63	329 163	365 52	386 197	435 62
55 740	83 635	117 452	159 298	240 83	294 77	330 88	366 48	394 157	451 76
69 999	93 374	129 563	213 239	243 245	301 137	335 65	368 167	395 77	469 106
75 886	103 279	131 290	215 213	255 508	315 124	344 89	374 69	410 43	484 476
77 236	105 290	133 477	216 70	256 168	318 59	351 147	379 229	418 43	

Synonyms:

1.STIGMASTEROL 1T-CONF-[83-48-7];

Hit 218 : RH-T-3346.0-0.00%-BETA-SITOSTEROL 1T-CONF-[83-46-5]-JH03-X
CAS: 2625-46-9; Lib: tom18; ID: 218.



(tom18) RH-T-3346.0-0.00%-BETA-SITOSTEROL 1T-CONF-[83-46-5]-JH03-X

Name: RH-T-3346.0-0.00%-BETA-SITOSTEROL 1T-CONF-[83-46-5]-JH03-X

Formula: C₃₂H₅₈OSi

MW: 486 CAS#: 2625-46-9 ID#: 218 DB: tom18

Other DBs: None

Comment: RI:JH3446 |RI:3346.2|

10 largest peaks:

129 999 | 73 929 | 396 495 | 357 436 | 57 384 | 43 376 | 121 315 | 119 314 | 81 299 | 67 267 |

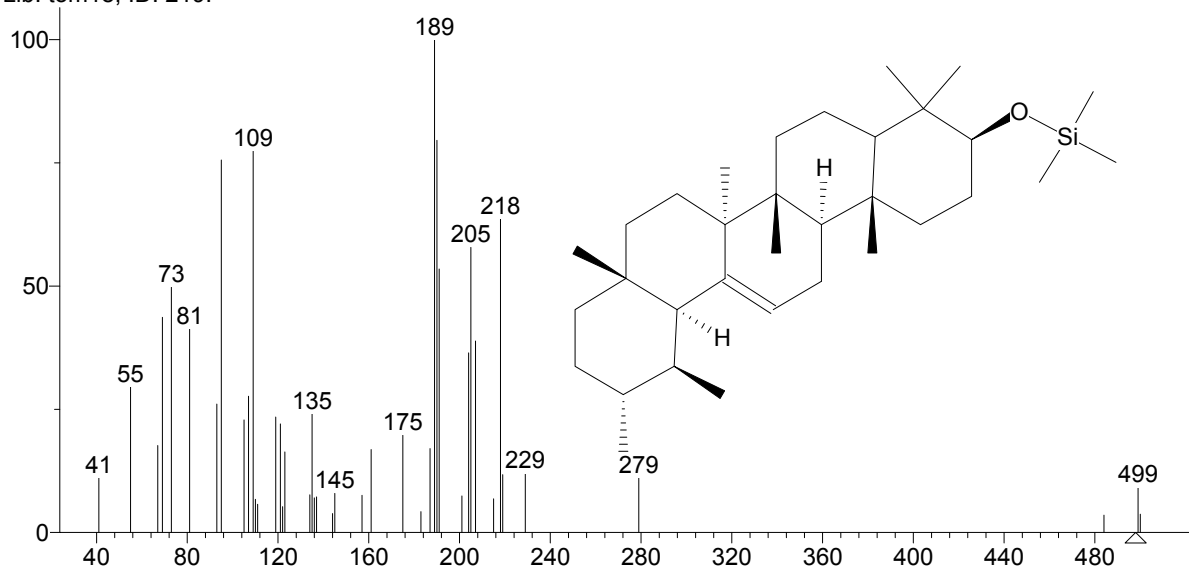
30 m/z Values and Intensities:

43 376 | 73 929 | 95 250 | 109 210 | 129 999 | 159 145 | 275 94 | 357 436 | 393 37 | 471 118 |
57 384 | 81 299 | 105 233 | 119 314 | 130 190 | 160 107 | 290 46 | 358 126 | 396 495 | 486 212 |
67 267 | 91 206 | 107 222 | 121 315 | 145 262 | 255 163 | 303 46 | 381 218 | 397 86 | 487 100 |

Synonyms:

1.BETA-SITOSTEROL 1T-CONF-[83-46-5];

Hit 219 : RH-T-3367.2-0.00%-[G:DELTA-AMYRIN-T]-8135A18-G-X
Lib: tom18; ID: 219.



(tom18) RH-T-3367.2-0.00%-[G:DELTA-AMYRIN-T]-8135A18-G-X RI:3367.2,

Name: RH-T-3367.2-0.00%-[G:DELTA-AMYRIN-T]-8135A18-G-X

Formula: C₃₃H₅₈OSi

MW: 498 ID#: 219 DB: tom18

RI: 3367.2,

Comment: RI=3367.2, 47.1508 min 8135A18 [RI:3367.2]

10 largest peaks:

189 999 | 190 795 | 109 773 | 95 755 | 218 635 | 205 578 | 191 534 | 73 497 | 69 436 | 81 412 |

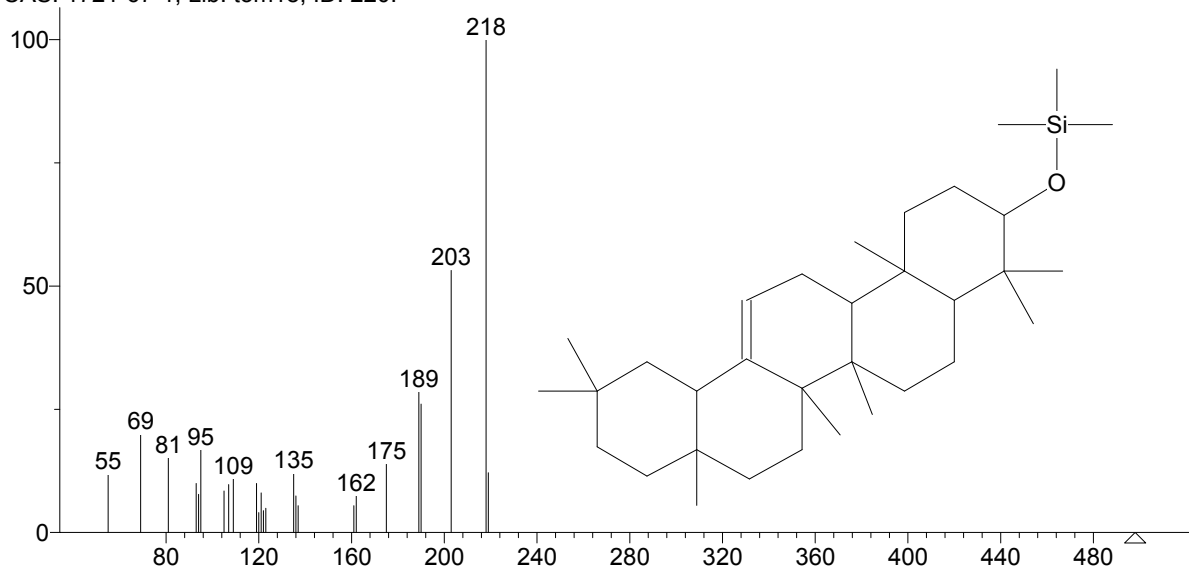
43 m/z Values and Intensities:

41 110	81 412	109 773	122 52	137 72	175 197	191 534	215 68	484 35
55 295	93 260	110 67	123 163	144 38	183 42	201 74	218 635	499 91
67 176	95 755	111 57	134 76	145 79	187 170	204 364	219 117	500 37
69 436	105 228	119 234	135 240	157 75	189 999	205 578	229 119	
73 497	107 276	121 220	136 70	161 168	190 795	207 388	279 110	

Synonyms:

1.DELTA-AMYRIN-T;

Hit 220 : RH-T-3377.4-0.00%-[G:BETA-AMYRIN-T]-G-X
CAS: 1721-67-1; Lib: tom18; ID: 220.



(tom18) RH-T-3377.4-0.00%-[G:BETA-AMYRIN-T]-G-X RI:3377.4,

Name: RH-T-3377.4-0.00%-[G:BETA-AMYRIN-T]-G-X

Formula: C₃₃H₅₈OSi

MW: 498 CAS#: 1721-67-1 ID#: 220 DB: tom18

Other DBs: None

RI: 3377.4,

Comment: RI=3377.4, 47.2513 min 8135A18 |RI:3377.4|

10 largest peaks:

218 999 | 203 531 | 189 284 | 190 260 | 69 198 | 95 167 | 81 151 | 175 138 | 219 121 | 135 119 |

25 m/z Values and Intensities:

55 117 | 93 99 | 105 84 | 119 99 | 122 44 | 136 74 | 162 74 | 190 260 | 219 121 |

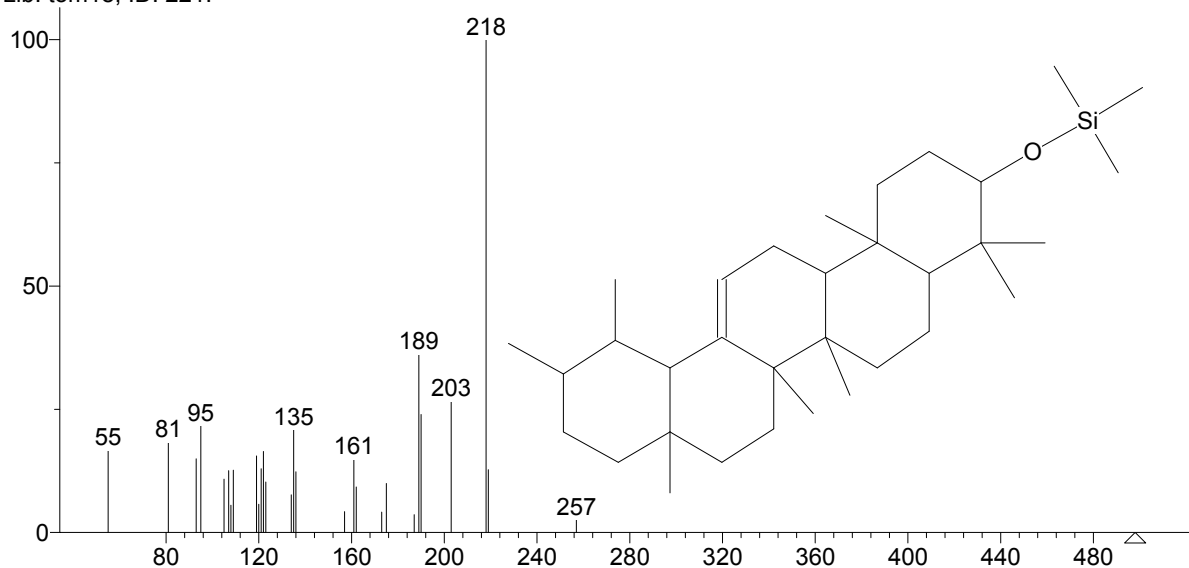
69 198 | 94 77 | 107 97 | 120 40 | 123 49 | 137 54 | 175 138 | 203 531 |

81 151 | 95 167 | 109 108 | 121 80 | 135 119 | 161 54 | 189 284 | 218 999 |

Synonyms:

1.BETA-AMYRIN-T;

Hit 221 : RH-T-3420.9-0.00%-[G: ALPHA-AMYRIN-T]-TENT-[638-95-9]-G-X
Lib: tom18; ID: 221.



(tom18) RH-T-3420.9-0.00%-[G: ALPHA-AMYRIN-T]-TENT-[638-95-9]-G-X RI:3420.9,

Name: RH-T-3420.9-0.00%-[G: ALPHA-AMYRIN-T]-TENT-[638-95-9]-G-X

Formula: C₃₃H₅₈OSi

MW: 498 ID#: 221 DB: tom18

RI: 3420.9,

Comment: RI=3420.9, 47.6762 min 8135A18 [RI:3420.9]

10 largest peaks:

218 999 | 189 360 | 203 265 | 190 239 | 95 216 | 135 208 | 81 182 | 55 166 | 122 164 | 119 155 |

28 m/z Values and Intensities:

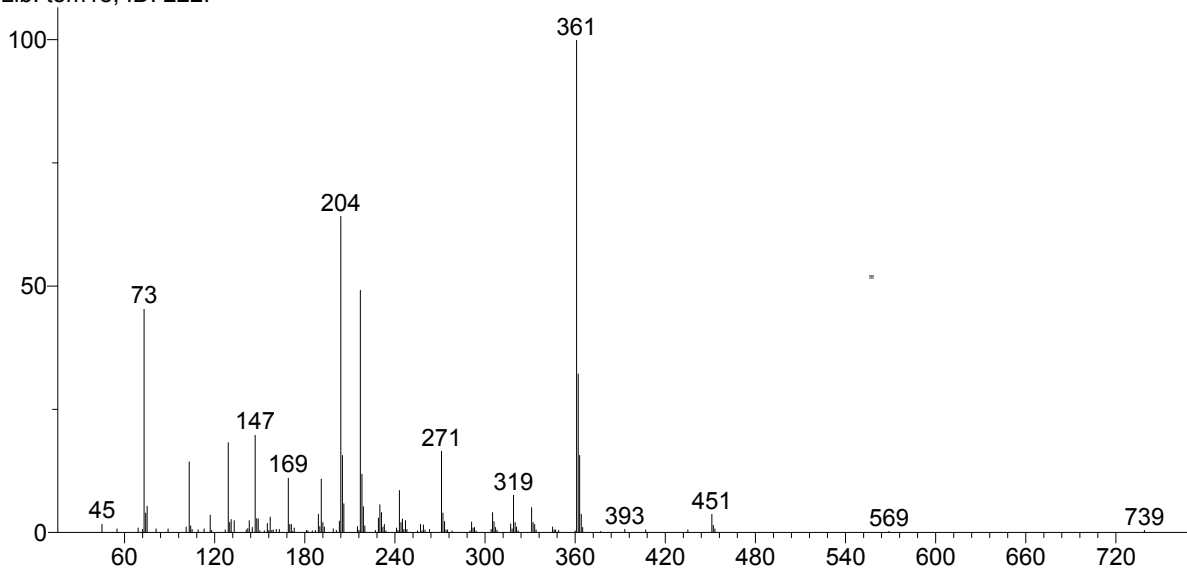
55 166 | 95 216 | 108 55 | 120 57 | 123 102 | 136 123 | 162 92 | 187 36 | 203 265 | 257 25 |
81 182 | 105 108 | 109 126 | 121 129 | 134 76 | 157 42 | 173 41 | 189 360 | 218 999 |
93 149 | 107 125 | 119 155 | 122 164 | 135 208 | 161 148 | 175 99 | 190 239 | 219 127 |

Synonyms:

1.ALPHA-AMYRIN-T;

Hit 222 : RH-T-3471.5-0.06%-[361,204,217,271,451,739]-RH03

Lib: tom18; ID: 222.



(tom18) RH-T-3471.5-0.06%-[361,204,217,271,451,739]-RH03 RI:3471.5,

Name: RH-T-3471.5-0.06%-[361,204,217,271,451,739]-RH03

MW: N/A ID#: 222 DB: tom18

RI: 3471.5,

Comment: RI=3471.5, 65.8865 min MG00244 [RI:3471.5]

10 largest peaks:

361 999 | 204 641 | 217 491 | 73 454 | 362 321 | 147 198 | 129 182 | 271 165 | 205 156 | 363 156 |

74 m/z Values and Intensities (56 low intensity peaks are not shown):

45	18	117	35	148	28	189	37	206	58	231	40	257	16	305	40	332	20	451	37
69	9	129	182	149	27	190	12	215	12	232	11	259	15	306	22	333	16	452	14
73	454	130	20	155	18	191	108	217	491	233	16	271	165	307	10	345	11		
74	39	131	26	157	31	192	20	218	118	241	9	272	39	317	17	361	999		
75	53	133	24	169	111	193	11	219	52	243	85	273	22	319	76	362	321		
101	11	143	24	170	16	203	23	220	13	244	20	291	21	320	20	363	156		
103	143	145	10	171	16	204	641	229	29	245	27	292	9	321	11	364	37		
104	13	147	198	173	9	205	156	230	56	247	24	293	10	331	50	365	10		

Synonyms:

1.m361,204,217,271,451,739;

Tomato sample	Lutein µg/g	Zeaxanthin µg/g	Canthaxanthin µg/g	β-carotene µg/g	Lycopene µg/g	Total µg/g
Ailsa Craig	15.223	1.942	0.104	84.443	749.375	851.092
M-82	13.354	0.541	0.055	382.000	374.3	770.250
PG-Antisense	12.275	2.152	0.102	63.584	94.878	172.990
PG-Sense	12.635	1.734	0.063	72.963	183.325	270.718
Kumato	27.573	0.315	0.282	56.286	61.585	146.040
Moneymaker	13.211	0.884	0.045	37.981	50.875	102.994