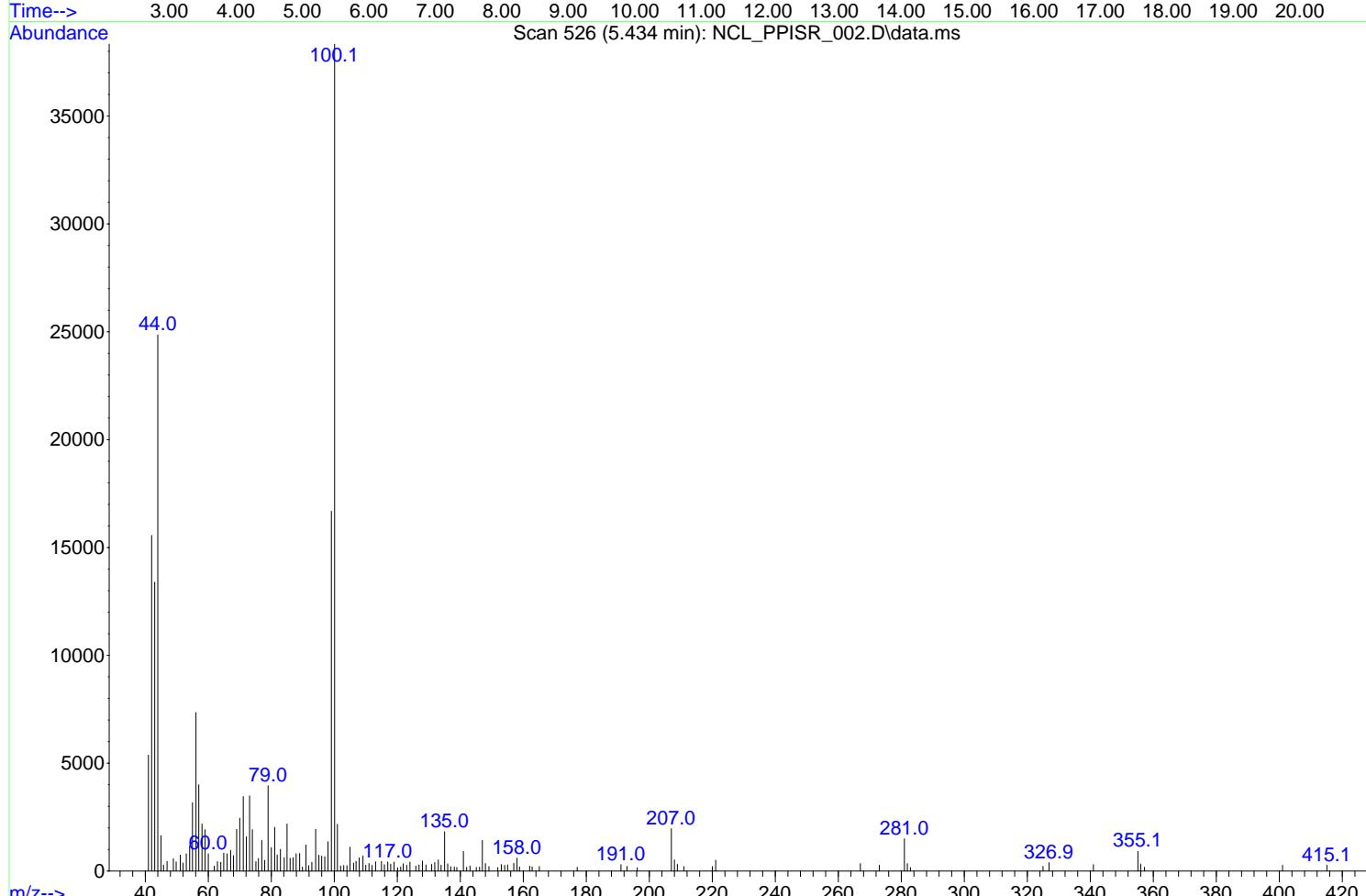
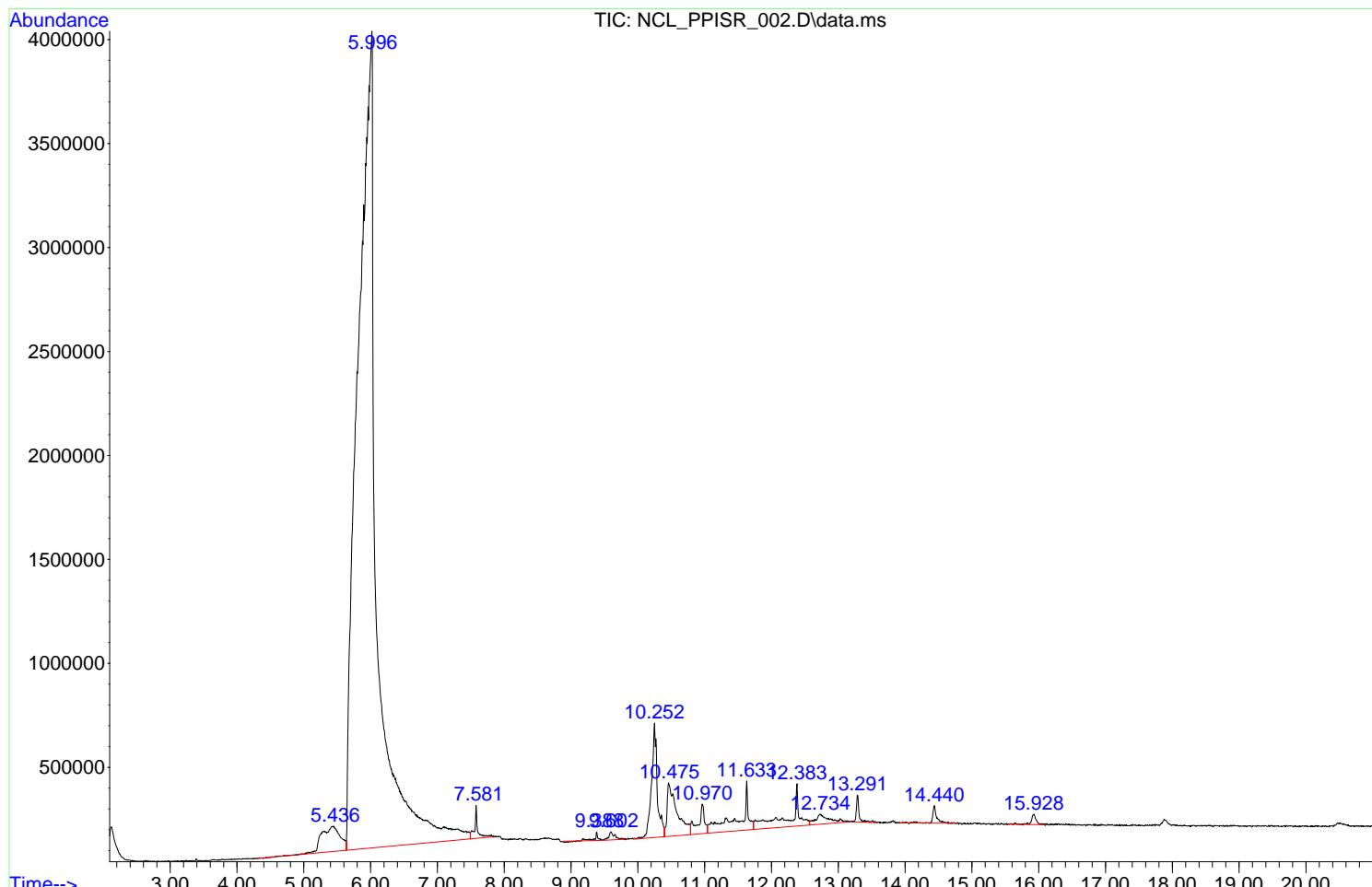
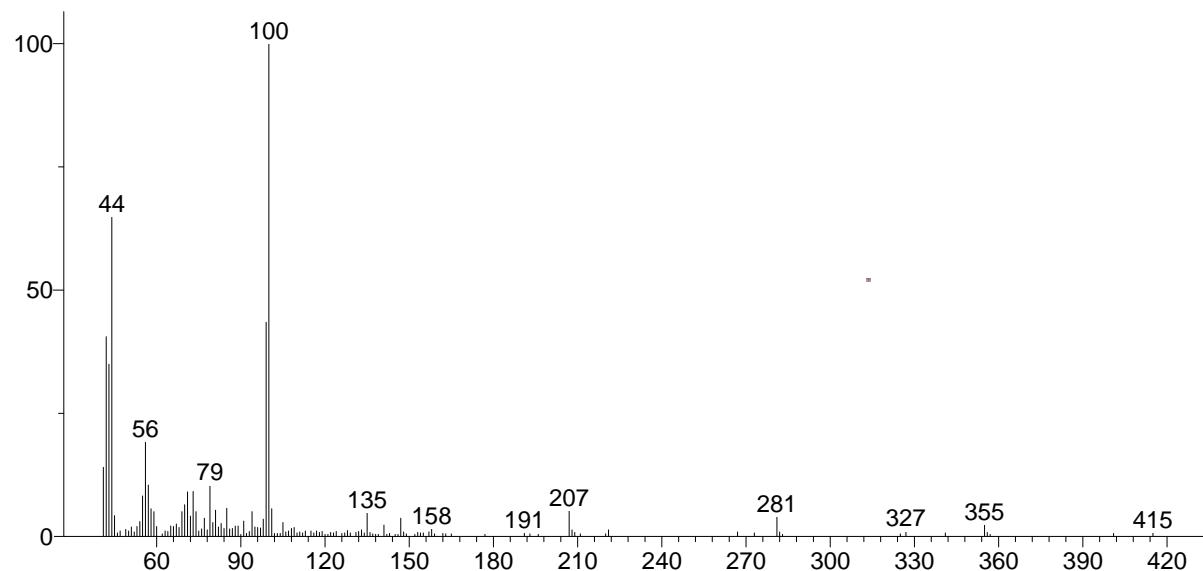


File : D:\NCL\DATA\OCD\Year\_2023\NCL\_PPISR\_002.D  
Operator : Dr. Borikar  
Acquired : 22 Jun 2023 23:08 using AcqMethod General\_2022.M  
Instrument : GC MSD  
Sample Name: PPISRCI  
Misc Info : PPISRCI  
Vial Number: 1



Unknown; InLib=-988



(Text File) Scan 526 (5.434 min): NCL\_PPISR\_002.D\data.ms

Name: Scan 526 (5.434 min): NCL\_PPISR\_002.D\data.ms

MW: N/A ID#: 27031 DB: Text File

Comment: PPISRCI

10 largest peaks:

100 999 | 44 647 | 99 434 | 42 405 | 43 349 | 56 191 | 41 140 | 57 104 | 79 103 | 73 91 |

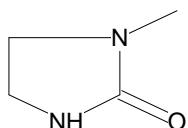
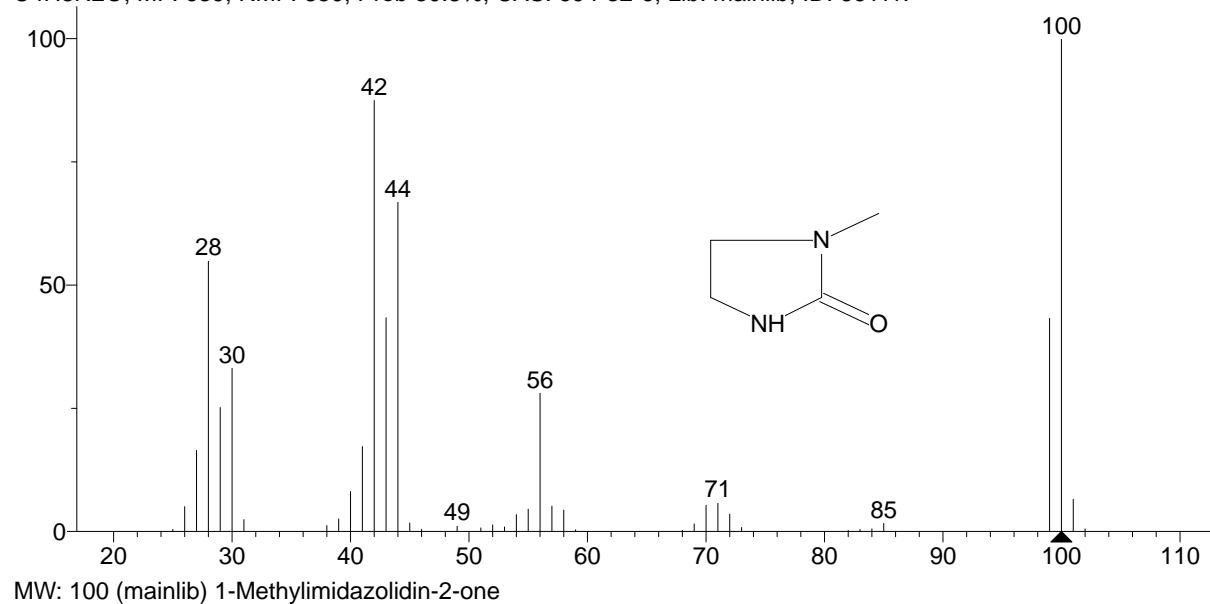
135 m/z Values and Intensities:

41 140	56 191	71 90	85 57	99 434	113 11	129 7	146 4	177 4	283 4
42 405	57 104	72 41	86 15	100 999	115 11	131 8	147 37	191 7	325 5
43 349	58 56	73 91	87 16	101 56	116 7	132 10	148 9	193 5	327 10
44 647	59 50	74 50	88 21	102 6	117 11	133 13	149 5	196 4	341 7
45 42	60 20	75 11	89 21	103 6	118 8	134 7	152 4	207 51	355 23
46 7	62 5	76 15	90 4	104 6	119 10	135 47	153 8	208 13	356 8
47 11	63 11	77 37	91 31	105 28	120 4	136 8	154 7	209 8	357 4
49 14	64 10	78 13	92 6	106 9	121 4	137 5	155 7	211 5	401 6
50 11	65 21	79 103	93 10	107 11	122 8	138 4	157 9	220 5	415 7
51 19	66 20	80 28	94 50	108 16	123 7	139 4	158 15	221 13	
52 9	67 25	81 53	95 19	109 18	124 10	141 23	159 5	267 9	
53 20	68 18	82 19	96 18	110 7	126 6	142 4	162 6	273 7	
54 30	69 50	83 26	97 17	111 9	127 7	143 6	163 5	281 39	
55 82	70 64	84 16	98 35	112 7	128 12	145 4	165 5	282 9	

Synonyms:

no synonyms.

Hit 1 : 1-Methylimidazolidin-2-one  
C4H8N2O; MF: 639; RMF: 850; Prob 30.8%; CAS: 694-32-6; Lib: mainlib; ID: 66111.



Name: 1-Methylimidazolidin-2-one

Formula: C<sub>4</sub>H<sub>8</sub>N<sub>2</sub>O

MW: 100 Exact Mass: 100.063663 CAS#: 694-32-6 NIST#: 196598 ID#: 66111 DB: mainlib

Other DBs: None

Contributor: Chemical Concepts

10 largest peaks:

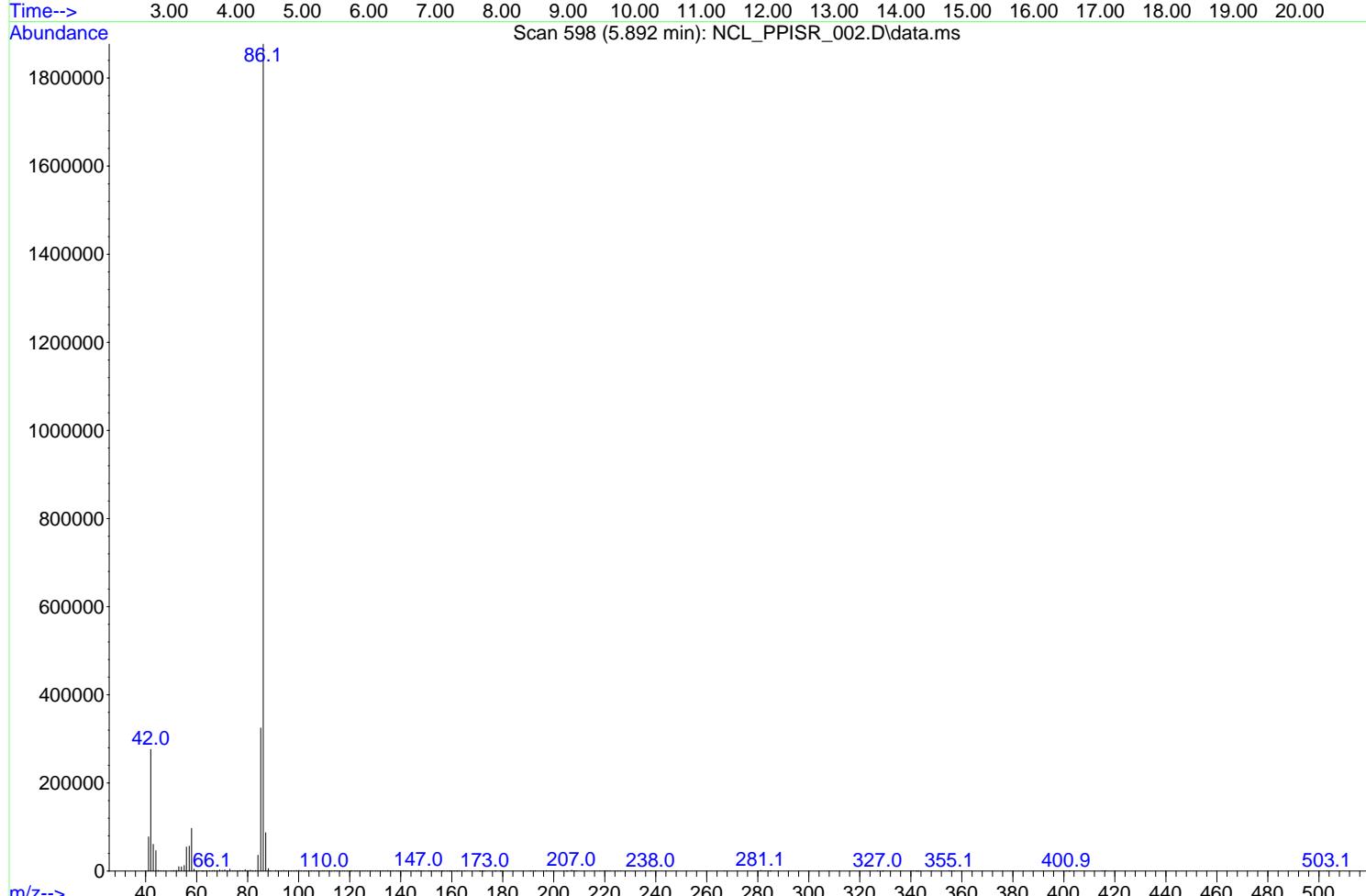
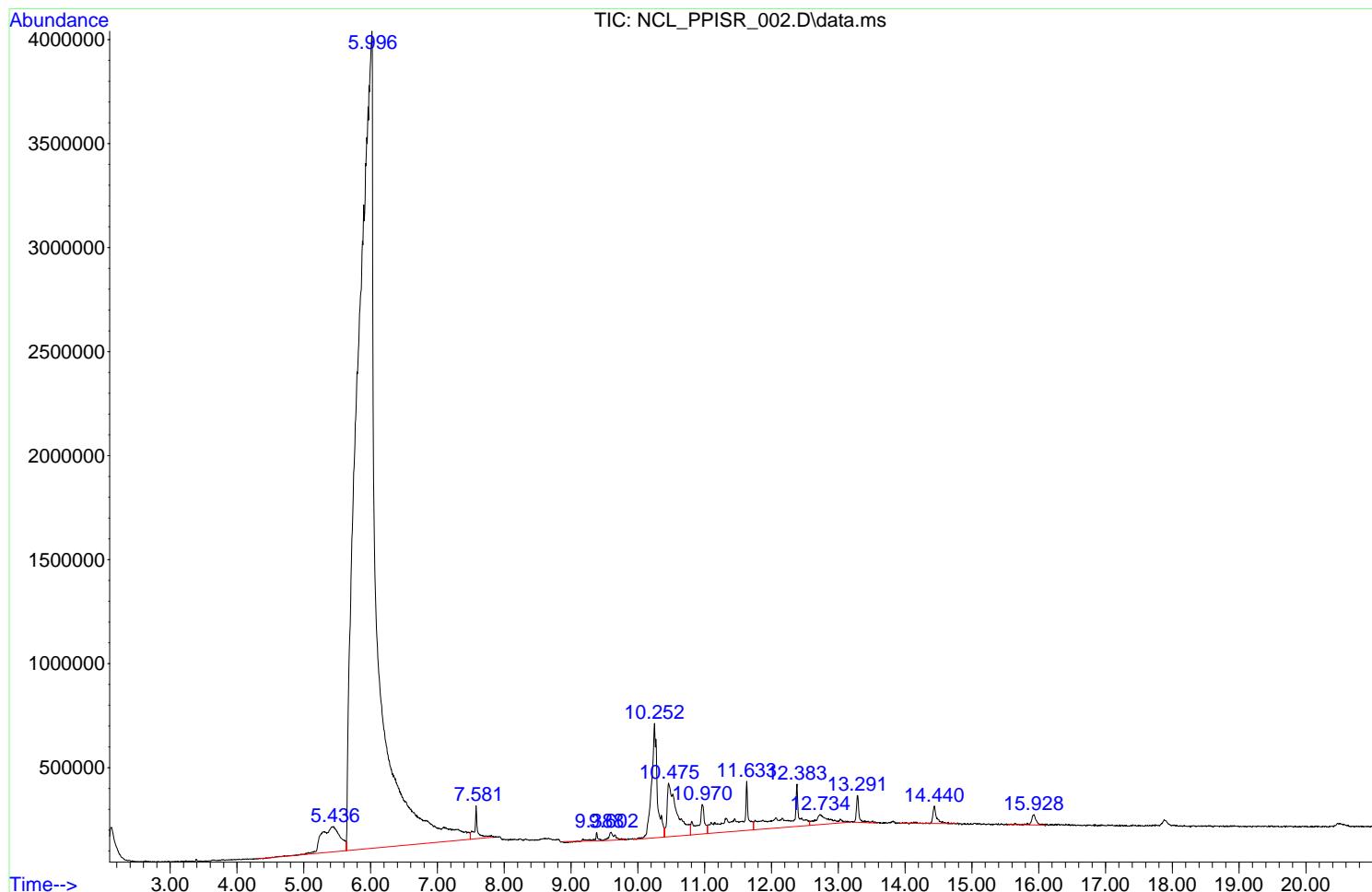
100 999 | 42 874 | 44 667 | 28 549 | 43 433 | 99 432 | 30 331 | 56 281 | 29 251 | 41 172 |  
40 m/z Values and Intensities:

25	4		29	251		39	25		43	433		49	12		54	34		58	43		70	53		82	2		99	432	
26	50		30	331		40	81		44	667		51	7		55	45		59	3		71	58		83	4		100	999	
27	164		31	24		41	172		45	17		52	13		56	281		68	2		72	35		84	5		101	65	
28	549		38	12		42	874		46	4		53	9		57	51		69	15		73	8		85	16		102	5	

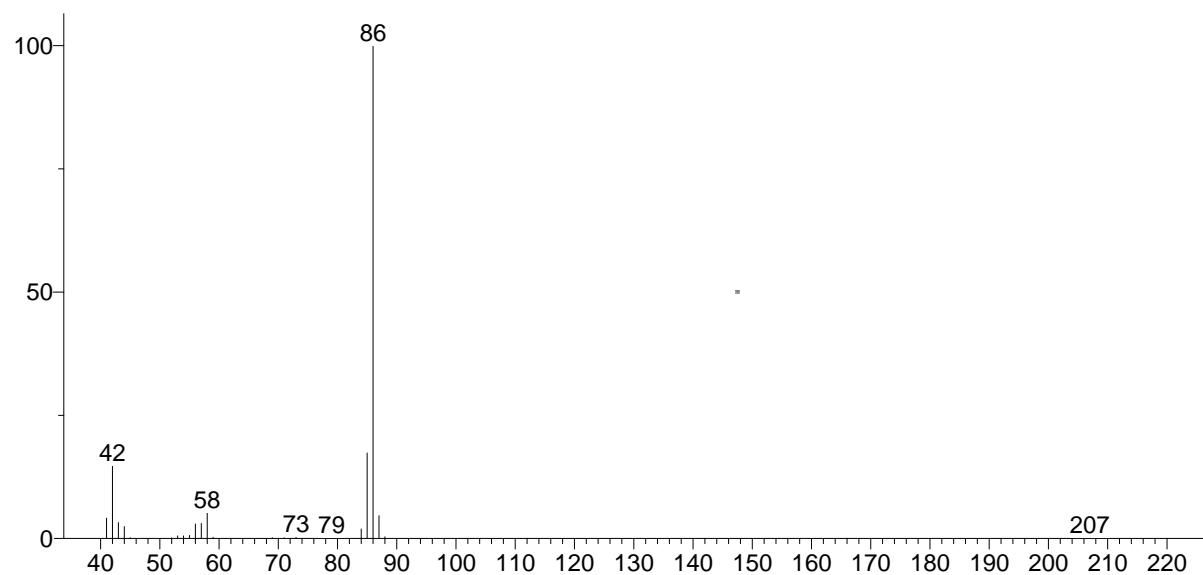
Synonyms:

1.1-Methyl-2-imidazolidinone #

File : D:\NCL\DATA\OCD\Year\_2023\NCL\_PPISR\_002.D  
Operator : Dr. Borikar  
Acquired : 22 Jun 2023 23:08 using AcqMethod General\_2022.M  
Instrument : GC MSD  
Sample Name: PPISRCI  
Misc Info : PPISRCI  
Vial Number: 1



Unknown; InLib=466



(Text File) Scan 598 (5.892 min): NCL\_PPISR\_002.D\data.ms

Name: Scan 598 (5.892 min): NCL\_PPISR\_002.D\data.ms

MW: N/A ID#: 27032 DB: Text File

Comment: PPISRCI

10 largest peaks:

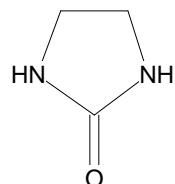
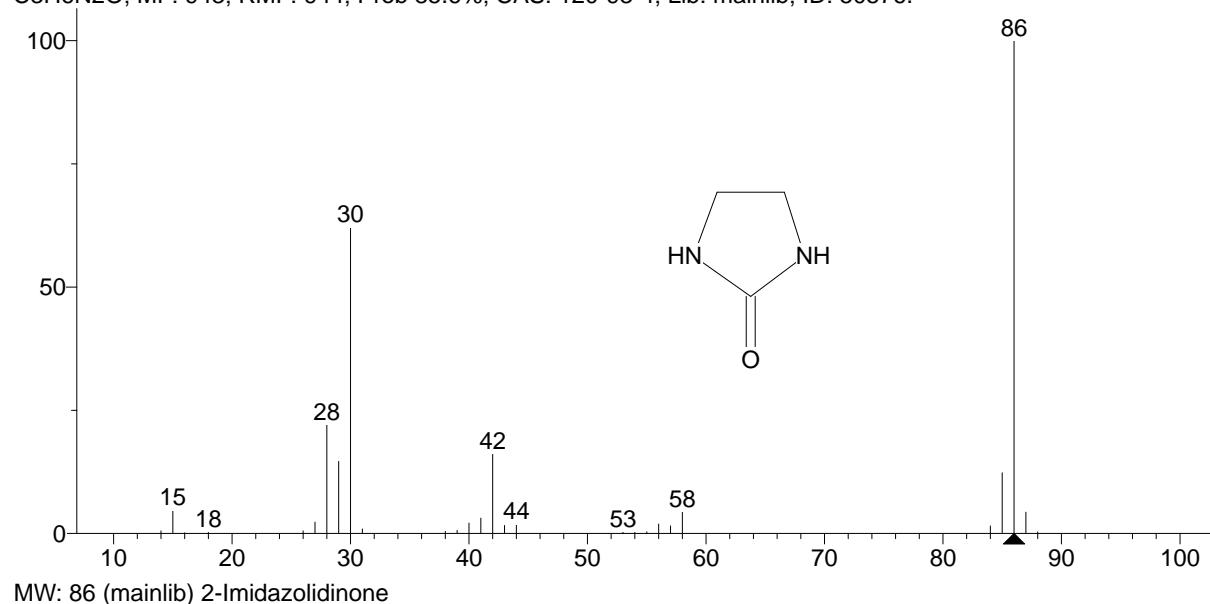
86 999 | 85 173 | 42 147 | 58 51 | 87 46 | 41 41 | 43 32 | 57 30 | 56 29 | 44 24 |  
24  $m/z$  Values and Intensities:

41	41		44	24		53	5		56	29		59	2		73	2		84	19		87	46	
42	147		45	1		54	5		57	30		69	1		79	1		85	173		88	3	
43	32		52	1		55	6		58	51		71	1		81	1		86	999		207	1	

Synonyms:

no synonyms.

Hit 1 : 2-Imidazolidinone  
C3H6N2O; MF: 943; RMF: 944; Prob 85.6%; CAS: 120-93-4; Lib: mainlib; ID: 50576.



Name: 2-Imidazolidinone

Formula: C<sub>3</sub>H<sub>6</sub>N<sub>2</sub>O

MW: 86 Exact Mass: 86.0480127 CAS#: 120-93-4 NIST#: 229112 ID#: 50576 DB: mainlib

Other DBs: Fine, TSCA, RTECS, HODOC, NIH, EINECS

Contributor: Japan AIST/NIMC Database- Spectrum MS-NW- 489

Related CAS#: 76895-63-1

10 largest peaks:

86 999 | 30 620 | 28 220 | 42 161 | 29 146 | 85 123 | 15 46 | 58 43 | 87 43 | 41 31 |

28 m/z Values and Intensities:

14 5	18 2	28 220	31 9	40 21	43 16	54 3	57 15	85 123	88 3
15 46	26 5	29 146	38 4	41 31	44 18	55 3	58 43	86 999	
16 1	27 23	30 620	39 6	42 161	53 3	56 19	84 15	87 43	

Synonyms:

1.Ethyleneurea

2.Imidazolid-2-one

3.N,N'-Ethyleneurea

4.SD 6073

5.Urea, N,N'-(1,2-Ethanediyl)-

6.2-Imidazolidone

7.2-Oxoimidazolidine

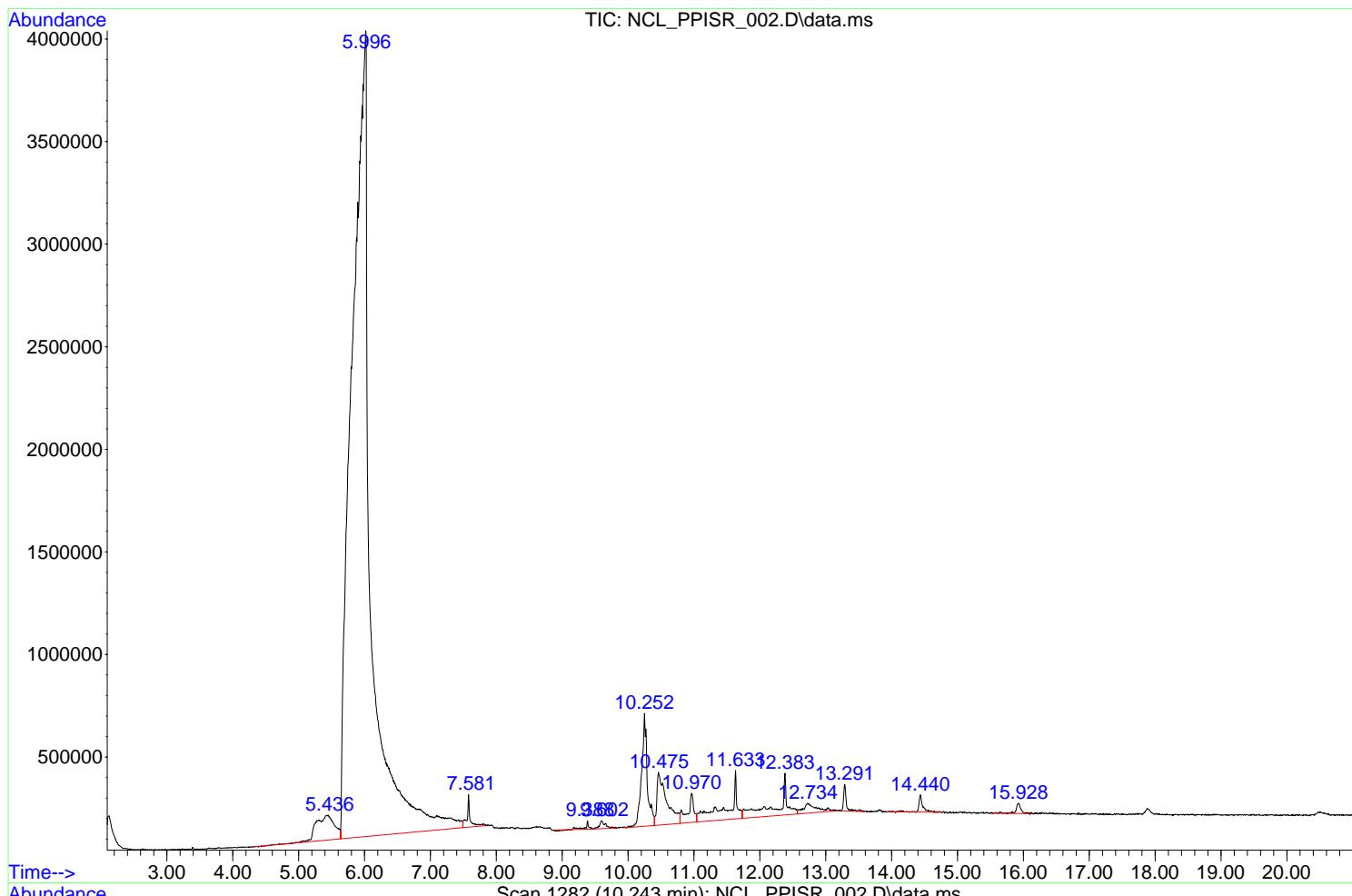
8.Urea, 1,3-ethylene-

9.1,3-Ethyleneurea

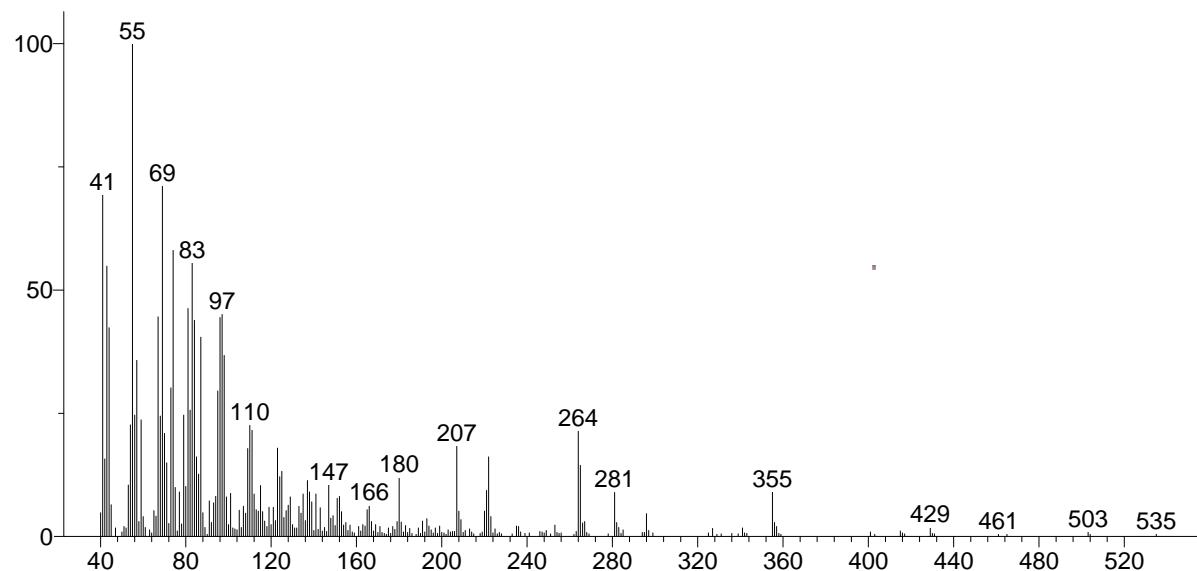
10.Imidazoliden-2-one

11.NSC 21314

File : D:\NCL\DATA\OCD\Year\_2023\NCL\_PPISR\_002.D  
Operator : Dr. Borikar  
Acquired : 22 Jun 2023 23:08 using AcqMethod General\_2022.M  
Instrument : GC MSD  
Sample Name: PPISRCI  
Misc Info : PPISRCI  
Vial Number: 1



Unknown; InLib=-181



(Text File) Scan 1282 (10.243 min): NCL\_PPISR\_002.D\data.ms

Name: Scan 1282 (10.243 min): NCL\_PPISR\_002.D\data.ms

MW: N/A ID#: 27034 DB: Text File

Comment: PPISRCI

10 largest peaks:

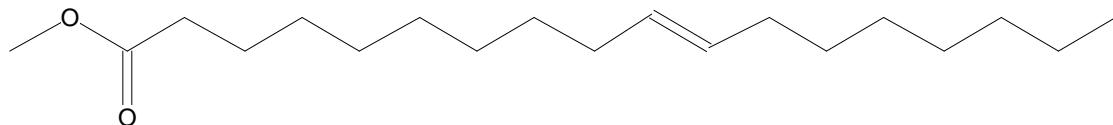
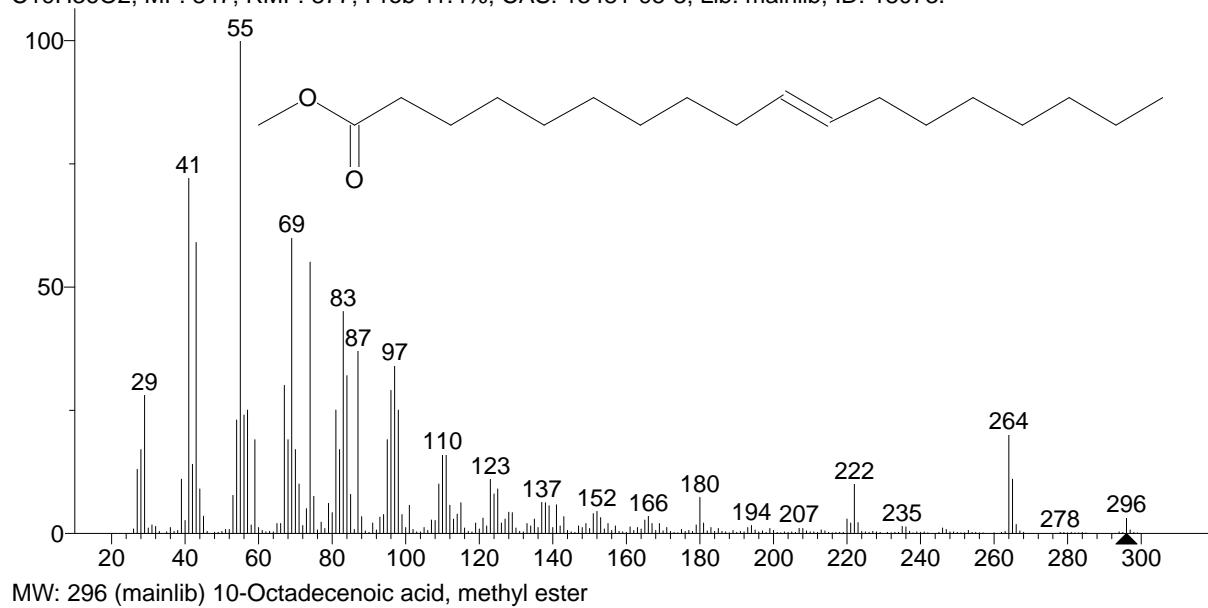
55 999		69 710		41 692		74 580		83 554		43 548		81 462		97 450		67 445		96 444	
241 m/z Values and Intensities:																			

40 48		69 710		94 81		119 59		144 11		170 8		196 7		224 7		267 30		357 20	
41 692		70 209		95 295		120 24		145 18		171 20		197 17		225 15		268 8		358 6	
42 157		71 149		96 444		121 59		146 10		172 8		198 6		226 5		269 5		359 4	
43 548		72 26		97 450		122 32		147 104		173 6		199 21		227 8		278 5		401 9	
44 423		73 301		98 367		123 179		148 37		174 4		200 8		228 5		281 89		403 4	
45 64		74 580		99 80		124 121		149 42		175 17		201 7		233 5		282 28		415 11	
47 17		75 99		100 24		125 132		150 22		176 6		202 4		235 21		283 18		416 7	
50 9		76 11		101 87		126 38		151 77		177 20		203 13		236 20		284 6		417 5	
51 20		77 90		102 17		127 52		152 81		178 14		204 9		237 9		285 13		429 18	
52 17		78 25		103 15		128 63		153 50		179 30		205 10		239 6		294 8		430 6	
53 104		79 246		104 13		129 80		154 23		180 119		206 10		241 7		295 8		431 5	
54 226		80 101		105 53		130 24		155 28		181 29		207 183		246 10		296 46		461 4	
55 999		81 462		106 18		131 17		156 12		182 9		208 51		247 9		297 12		465 4	
56 246		82 256		107 61		132 17		157 23		183 22		209 34		248 7		299 7		503 9	
57 357		83 554		108 47		133 61		158 9		184 8		210 8		249 12		325 7		504 4	
58 30		84 438		109 178		134 47		159 7		185 16		211 12		251 5		327 16		535 4	
59 236		85 161		110 225		135 86		161 20		186 6		213 15		253 23		329 4			
60 40		86 126		111 215		136 32		162 11		188 4		214 9		254 8		331 5			
61 18		87 404		112 86		137 113		163 24		189 17		215 5		255 6		336 6			
63 13		88 48		113 54		138 90		164 21		190 6		218 6		256 7		339 5			
64 7		89 18		114 51		139 70		165 54		191 31		219 9		262 4		341 17			
65 52		90 4		115 103		140 12		166 62		192 9		220 51		263 10		342 7			
66 41		91 72		116 50		141 86		167 30		193 36		221 93		264 214		343 6			
67 445		92 28		117 31		142 14		168 11		194 21		222 161		265 144		355 90			
68 244		93 68		118 20		143 58		169 24		195 13		223 40		266 27		356 28			

Synonyms:

no synonyms.

Hit 1 : 10-Octadecenoic acid, methyl ester  
C19H36O2; MF: 847; RMF: 877; Prob 11.4%; CAS: 13481-95-3; Lib: mainlib; ID: 18073.



Name: 10-Octadecenoic acid, methyl ester

Formula: C<sub>19</sub>H<sub>36</sub>O<sub>2</sub>

MW: 296 Exact Mass: 296.27153 CAS#: 13481-95-3 NIST#: 36207 ID#: 18073 DB: mainlib

Other DBs: None

Contributor: R.T.HOLMAN,UNIVERSITY OF MINNESOTA

10 largest peaks:

55 999 | 41 720 | 69 600 | 43 590 | 74 550 | 83 450 | 87 370 | 97 340 | 84 320 | 67 300 |

249 m/z Values and Intensities:

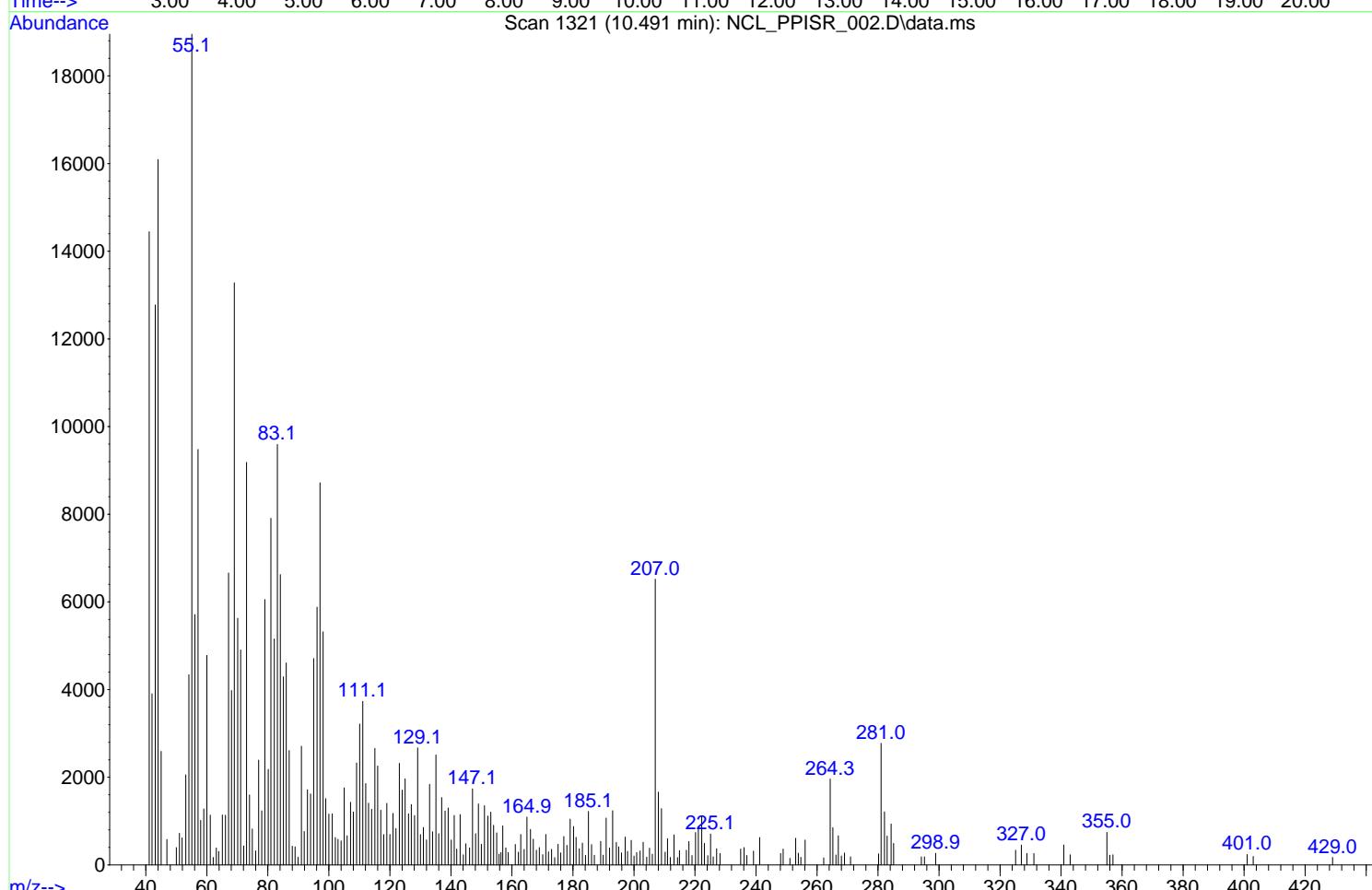
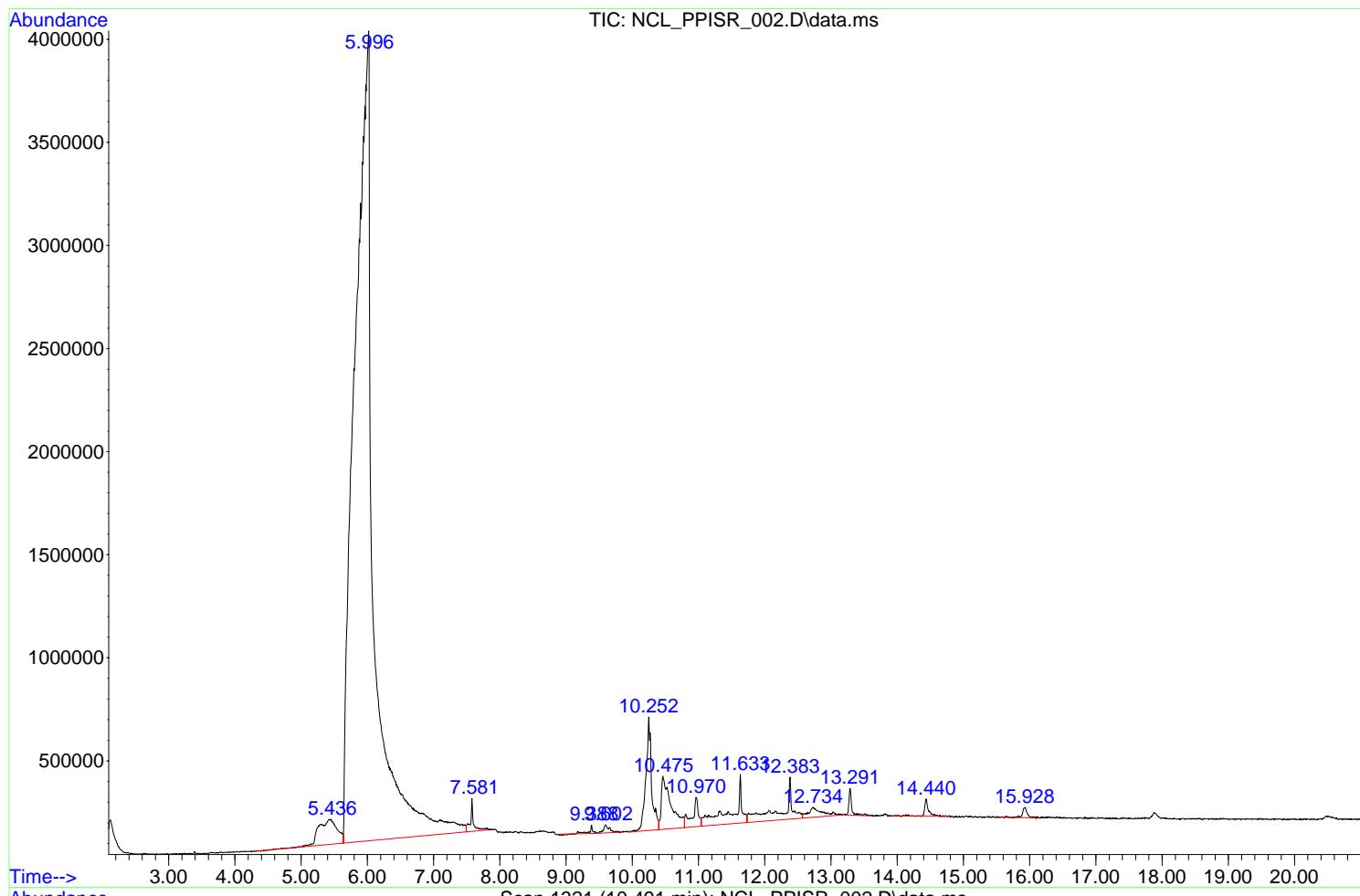
26	9		53	77		78	10		103	3		128	43		153	32		178	4		203	3		228	3		256	1	
27	130		54	230		79	61		104	3		129	42		154	9		179	17		204	2		229	2		257	1	
28	170		55	999		80	42		105	12		130	11		155	20		180	73		205	3		231	2		260	1	
29	280		56	240		81	250		106	6		131	4		156	6		181	21		206	2		232	1		262	2	
30	11		57	250		82	170		107	27		132	3		157	15		182	5		207	12		233	2		263	4	
31	17		58	17		83	450		108	26		133	20		158	4		183	12		208	10		234	2		264	200	
32	14		59	190		84	320		109	100		134	15		159	3		184	4		209	5		235	14		265	110	
33	4		60	12		85	79		110	160		135	29		160	2		185	10		210	3		236	13		266	18	
35	3		61	6		86	8		111	160		136	12		161	13		186	4		211	3		237	4		267	5	

36	12		62	3		87	370		112	57		137	63		162	6		187	3		212	2		238	1		268	2	
37	4		63	4		88	34		113	29		138	62		163	12		188	1		213	7		239	3		278	3	
38	6		64	3		89	5		114	39		139	56		164	9		189	6		214	5		240	2		279	2	
39	110		65	20		90	2		115	62		140	12		165	27		190	2		215	2		241	3		280	1	
40	26		66	20		91	21		116	11		141	58		166	35		191	4		216	1		242	1		281	2	
41	720		67	300		92	7		117	4		142	15		167	20		192	3		217	2		245	2		282	1	
42	140		68	190		93	33		118	3		143	34		168	6		193	12		218	2		246	11		283	1	
43	590		69	600		94	38		119	21		144	6		169	20		194	16		219	2		247	8		284	2	
44	90		70	170		95	190		120	9		145	3		170	5		195	7		220	29		248	3		285	1	
45	35		71	100		96	290		121	31		146	2		171	12		196	3		221	21		249	3		294	3	
46	4		72	16		97	340		122	15		147	15		172	4		197	5		222	100		250	2		295	2	
48	2		73	50		98	250		123	110		148	12		173	2		198	2		223	22		251	1		296	32	
49	2		74	550		99	38		124	80		149	20		174	1		199	10		224	4		252	1		297	7	
50	4		75	75		100	12		125	90		150	10		175	8		200	6		225	3		253	6		298	2	
51	8		76	7		101	57		126	21		151	40		176	4		201	2		226	2		254	2		299	1	
52	8		77	23		102	8		127	29		152	45		177	6		202	1		227	4		255	2				

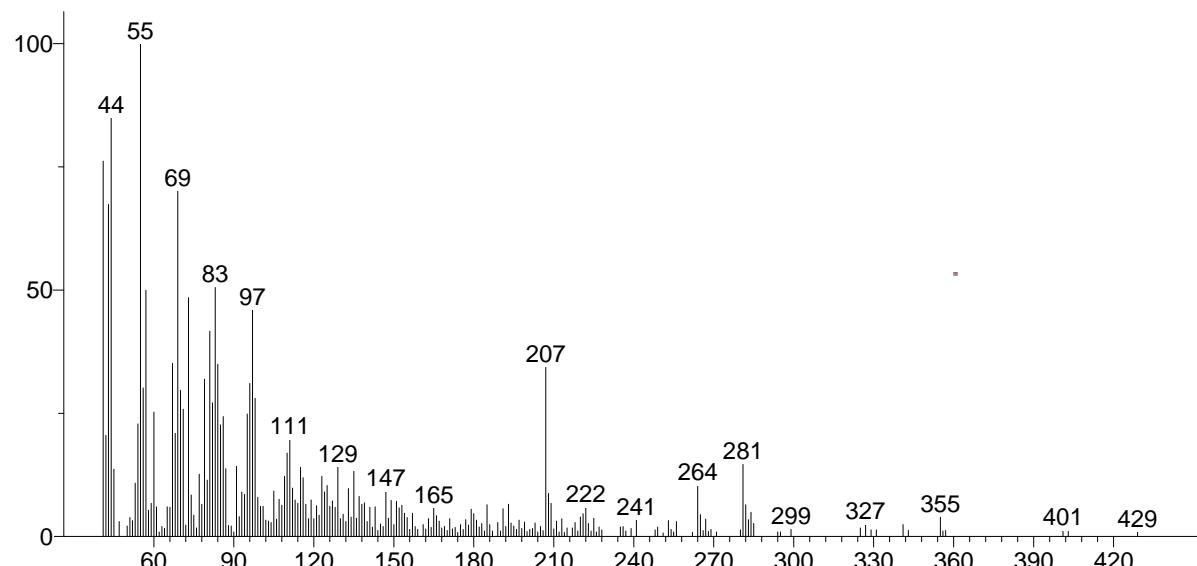
Synonyms:

1.Methyl 10-octadecenoate

File : D:\NCL\DATA\OCD\Year\_2023\NCL\_PPISR\_002.D  
Operator : Dr. Borikar  
Acquired : 22 Jun 2023 23:08 using AcqMethod General\_2022.M  
Instrument : GC MSD  
Sample Name: PPISRCI  
Misc Info : PPISRCI  
Vial Number: 1



Unknown; InLib=-778



(Text File) Scan 1321 (10.491 min): NCL\_PPISR\_002.D\data.ms

Name: Scan 1321 (10.491 min): NCL\_PPISR\_002.D\data.ms

MW: N/A ID#: 27035 DB: Text File

Comment: PPISRCI

10 largest peaks:

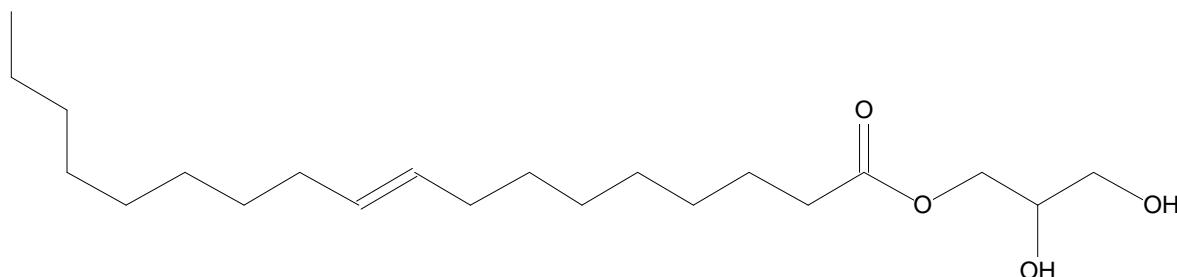
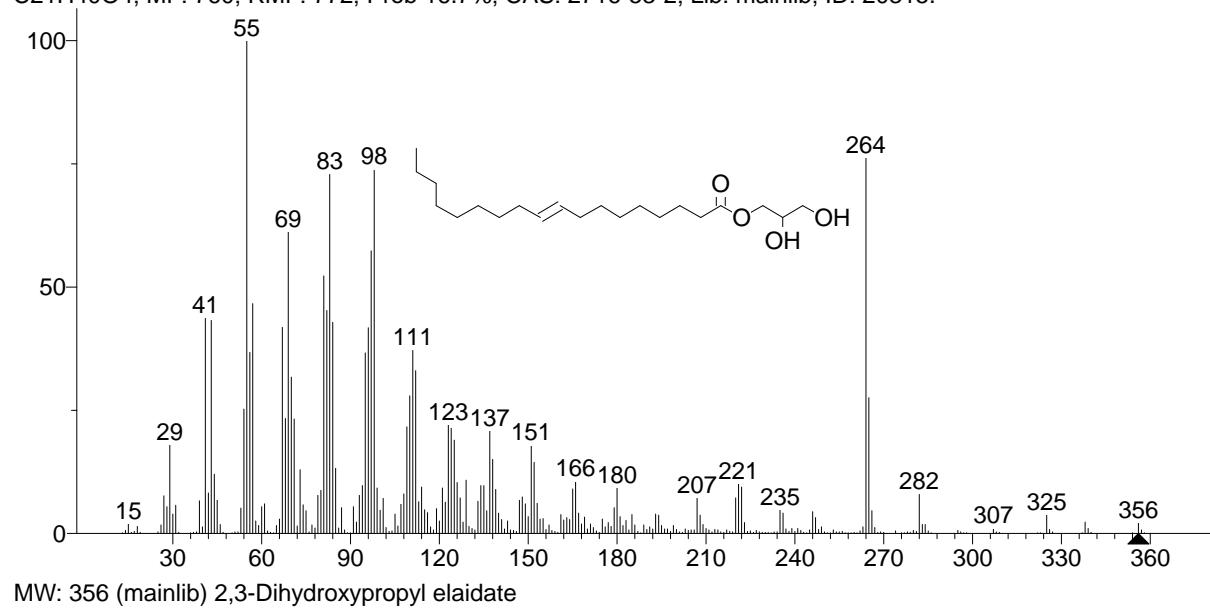
55 999		44 848		41 761		69 700		43 673		83 505		57 499		73 484		97 459		81 416	
223 m/z Values and Intensities:																			

41 761		67 351		90 9		113 74		136 37		159 14		183 26		207 343		237 11		285 26	
42 205		68 209		91 142		114 67		137 81		161 24		184 11		208 87		239 16		294 9	
43 673		69 700		92 40		115 140		138 65		162 15		185 64		209 67		241 33		295 9	
44 848		70 296		93 90		116 119		139 68		163 36		186 24		210 15		248 13		299 14	
45 136		71 258		94 85		117 65		140 30		164 18		187 11		211 31		249 19		325 17	
47 30		72 23		95 248		118 36		141 59		165 57		189 28		212 9		251 7		327 24	
50 21		73 484		96 310		119 74		142 19		166 42		190 11		213 36		253 32		329 13	
51 38		74 84		97 459		120 36		143 60		167 31		191 56		214 8		254 14		331 13	
52 32		75 43		98 280		121 62		144 12		168 17		192 20		215 17		255 9		341 24	
53 108		76 17		99 79		122 43		145 25		169 20		193 65		217 17		256 30		343 12	
54 228		77 126		100 61		123 122		146 20		170 12		194 27		218 28		262 8		355 39	
55 999		78 65		101 61		124 90		147 91		171 36		195 21		219 11		264 103		356 11	
56 301		79 319		102 33		125 103		148 37		172 15		196 14		220 39		265 44		357 12	
57 499		80 114		103 31		126 61		149 73		173 18		197 33		221 46		266 12		401 12	
58 53		81 416		104 28		127 72		150 24		174 8		198 16		222 58		267 35		403 10	
59 67		82 271		105 92		128 59		151 71		175 24		199 29		223 26		268 10		429 9	
60 252		83 505		106 35		129 140		152 58		176 14		200 10		224 11		269 14			
61 60		84 349		107 75		130 36		153 63		177 34		201 14		225 37		271 9			
62 9		85 226		108 63		131 45		154 47		178 23		202 16		226 9		280 13			
63 20		86 243		109 122		132 30		155 38		179 55		203 27		227 19		281 146			
64 16		87 137		110 169		133 97		156 14		180 46		204 9		228 13		282 64			
65 60		88 22		111 196		134 39		157 47		181 33		205 20		235 19		283 34			
66 59		89 21		112 98		135 132		158 20		182 19		206 12		236 20		284 49			

Synonyms:

no synonyms.

Hit 1 : 2,3-Dihydroxypropyl elaidate  
 C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>; MF: 760; RMF: 772; Prob 16.7%; CAS: 2716-53-2; Lib: mainlib; ID: 20315.



Name: 2,3-Dihydroxypropyl elaidate

Formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>

MW: 356 Exact Mass: 356.29266 CAS#: 2716-53-2 NIST#: 237266 ID#: 20315 DB: mainlib

Other DBs: None

Contributor: Japan AIST/NIMC Database- Spectrum MS-IW-4086

10 largest peaks:

55 999 | 264 761 | 98 738 | 83 728 | 69 611 | 97 573 | 81 522 | 57 466 | 82 452 | 41 436 |

280 m/z Values and Intensities:

13	1		51	3		79	77		107	59		135	97		163	32		191	13		219	3		247	32		279	2	
14	6		52	3		80	87		108	80		136	46		164	28		192	9		220	72		248	8		280	6	
15	19		53	51		81	522		109	216		137	208		165	90		193	39		221	100		249	13		281	4	
16	2		54	252		82	452		110	279		138	150		166	105		194	37		222	94		250	3		282	79	
17	4		55	999		83	728		111	371		139	89		167	41		195	16		223	22		251	1		283	18	
18	14		56	367		84	428		112	330		140	41		168	19		196	9		224	4		252	1		284	18	
19	2		57	466		85	132		113	64		141	28		169	33		197	9		225	5		253	7		285	5	
25	3		58	25		86	11		114	94		142	9		170	9		198	4		226	2		254	3		286	1	
26	17		59	16		87	52		115	48		143	25		171	19		199	16		227	6		255	3		295	6	

27	76		60	54		88	7		116	42		144	7		172	12		200	8		228	3		256	4		296	3	
28	54		61	60		89	1		117	13		145	6		173	5		201	3		229	2		257	1		297	1	
29	179		62	5		90	1		118	7		146	4		174	2		202	2		230	2		258	1		298	1	
30	39		63	2		91	54		119	50		147	67		175	29		203	9		231	2		259	1		307	10	
31	57		64	1		92	23		120	25		148	74		176	13		204	6		232	1		260	2		308	3	
32	2		65	16		93	77		121	92		149	60		177	22		205	7		233	3		261	1		309	2	
36	1		66	29		94	97		122	63		150	34		178	14		206	7		234	3		262	5		322	1	
37	2		67	418		95	366		123	220		151	178		179	52		207	72		235	47		263	13		323	1	
38	3		68	233		96	417		124	213		152	144		180	92		208	37		236	41		264	761		325	37	
39	66		69	611		97	573		125	189		153	61		181	34		209	18		237	9		265	275		326	8	
40	13		70	317		98	738		126	103		154	29		182	16		210	10		238	4		266	46		327	3	
41	436		71	232		99	92		127	72		155	30		183	26		211	7		239	10		267	12		337	1	
42	82		72	15		100	47		128	23		156	8		184	7		212	3		240	4		268	2		338	23	
43	432		73	129		101	71		129	108		157	17		185	38		213	8		241	10		269	3		339	10	
44	120		74	58		102	12		130	14		158	6		186	17		214	7		242	6		270	2		340	2	
45	67		75	46		103	4		131	10		159	4		187	4		215	3		243	2		274	5		354	1	
46	18		76	3		104	5		132	7		160	2		188	1		216	2		244	1		276	1		356	21	
47	2		77	17		105	39		133	65		161	38		189	17		217	7		245	7		277	1		357	7	
50	1		78	11		106	15		134	97		162	27		190	8		218	4		246	44		278	3		358	1	

Synonyms:

1,2,3-Dihydroxypropyl (9E)-9-octadecenoate #