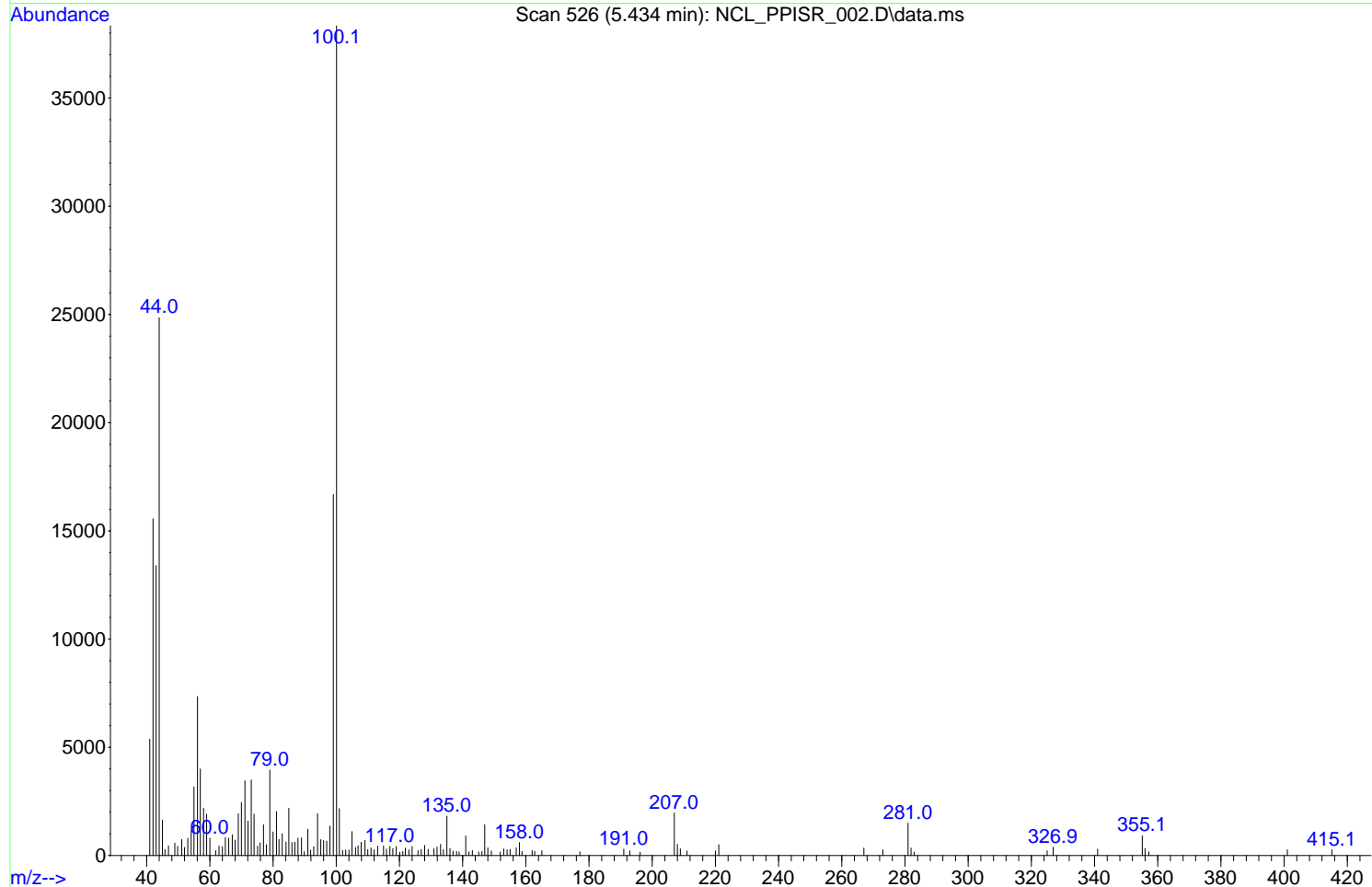
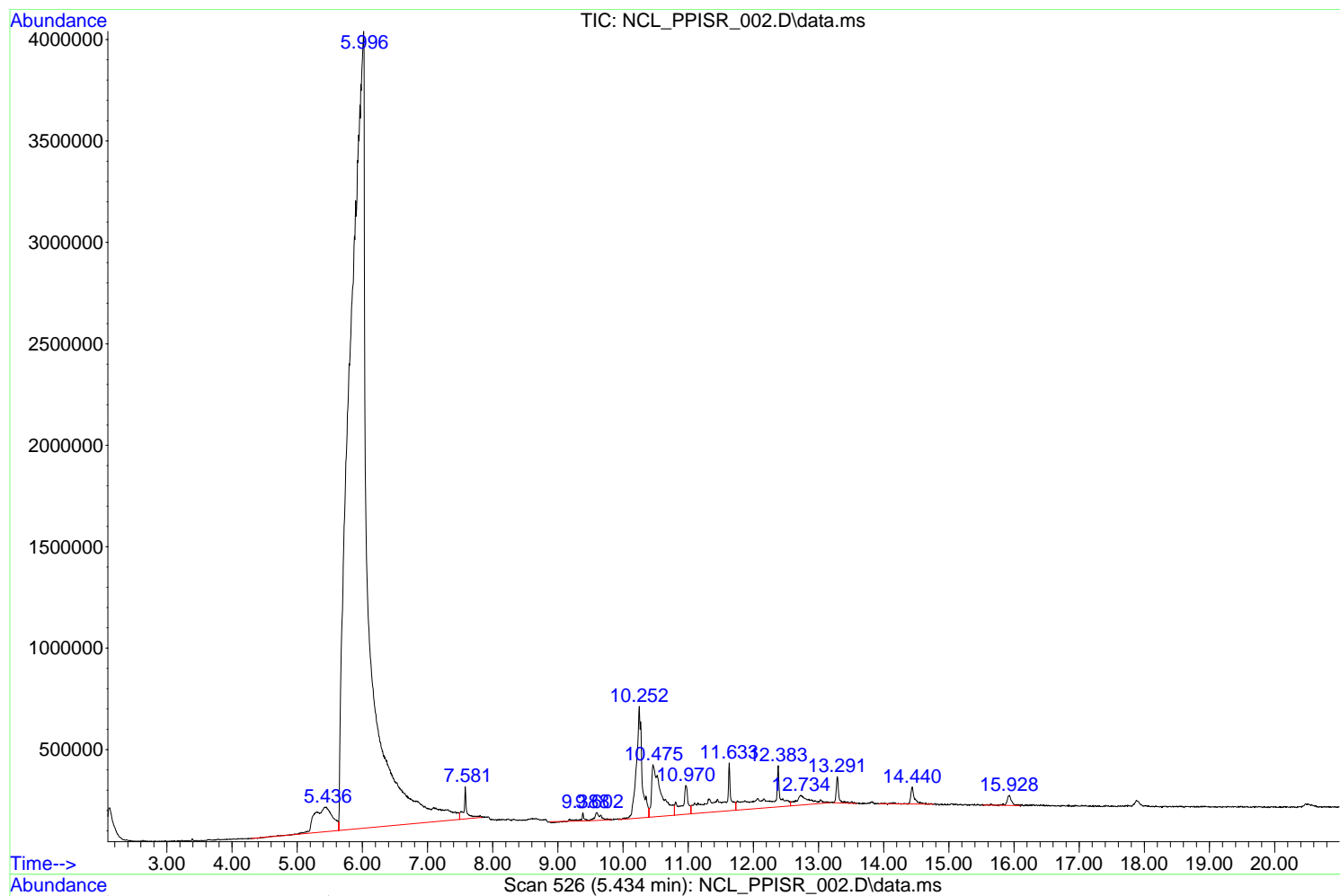
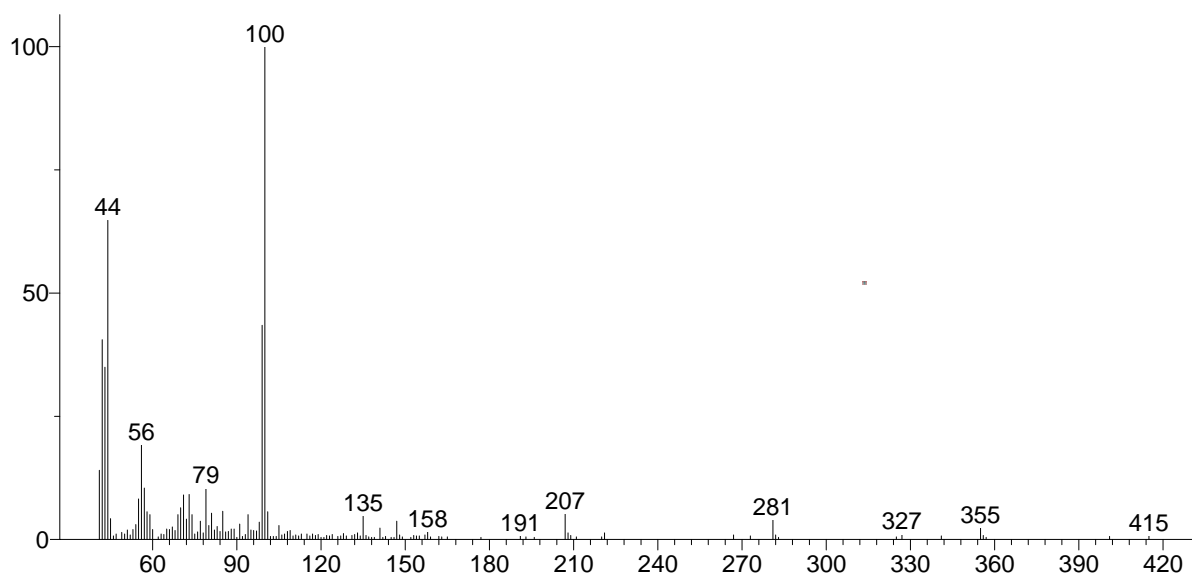


File :D:\NCL\DATA\OCD\Year_2023\NCL_PPISR_002.D
Operator : Dr. Borikar
Acquired : 22 Jun 2023 23:08 using AcqMethod General_2022.M
Instrument : GC MSD
Sample Name: PPISRCI
Misc Info : PPISRCI
Vial Number: 1



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
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135 m/z Values and Intensities:

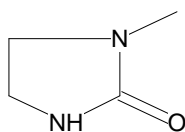
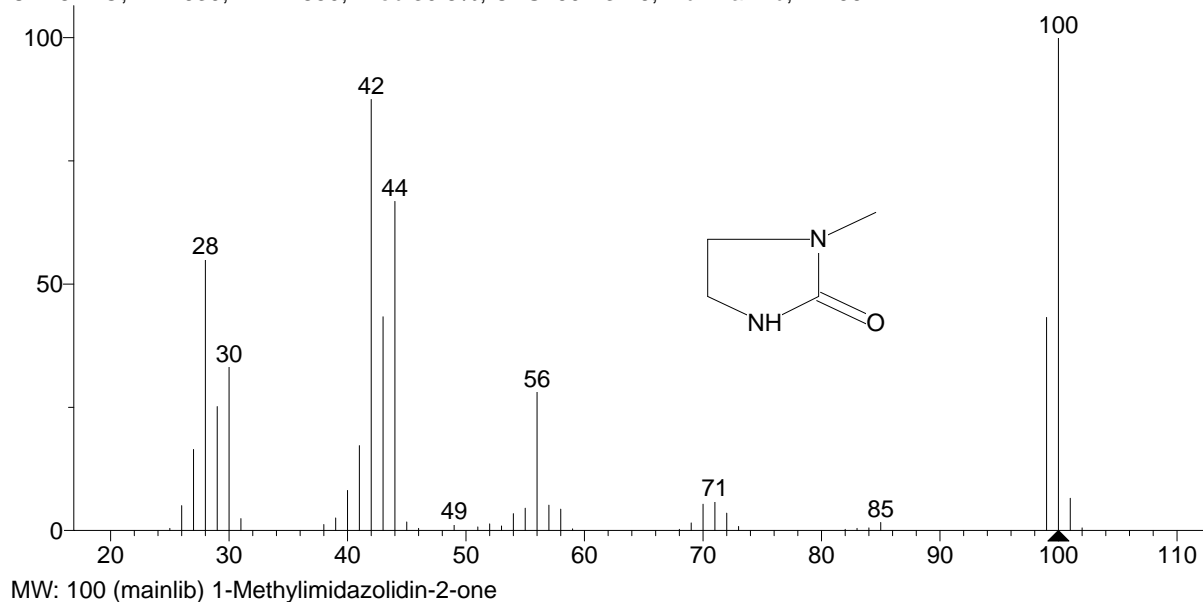
41 140	56 191	71 90	85 57	99 434	113 11	129 7	146 4	177 4	283 4
42 405	57 104	72 41	86 15	100 999	115 11	131 8	147 37	191 7	325 5
43 349	58 56	73 91	87 16	101 56	116 7	132 10	148 9	193 5	327 10
44 647	59 50	74 50	88 21	102 6	117 11	133 13	149 5	196 4	341 7
45 42	60 20	75 11	89 21	103 6	118 8	134 7	152 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: C₄H₈N₂O

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
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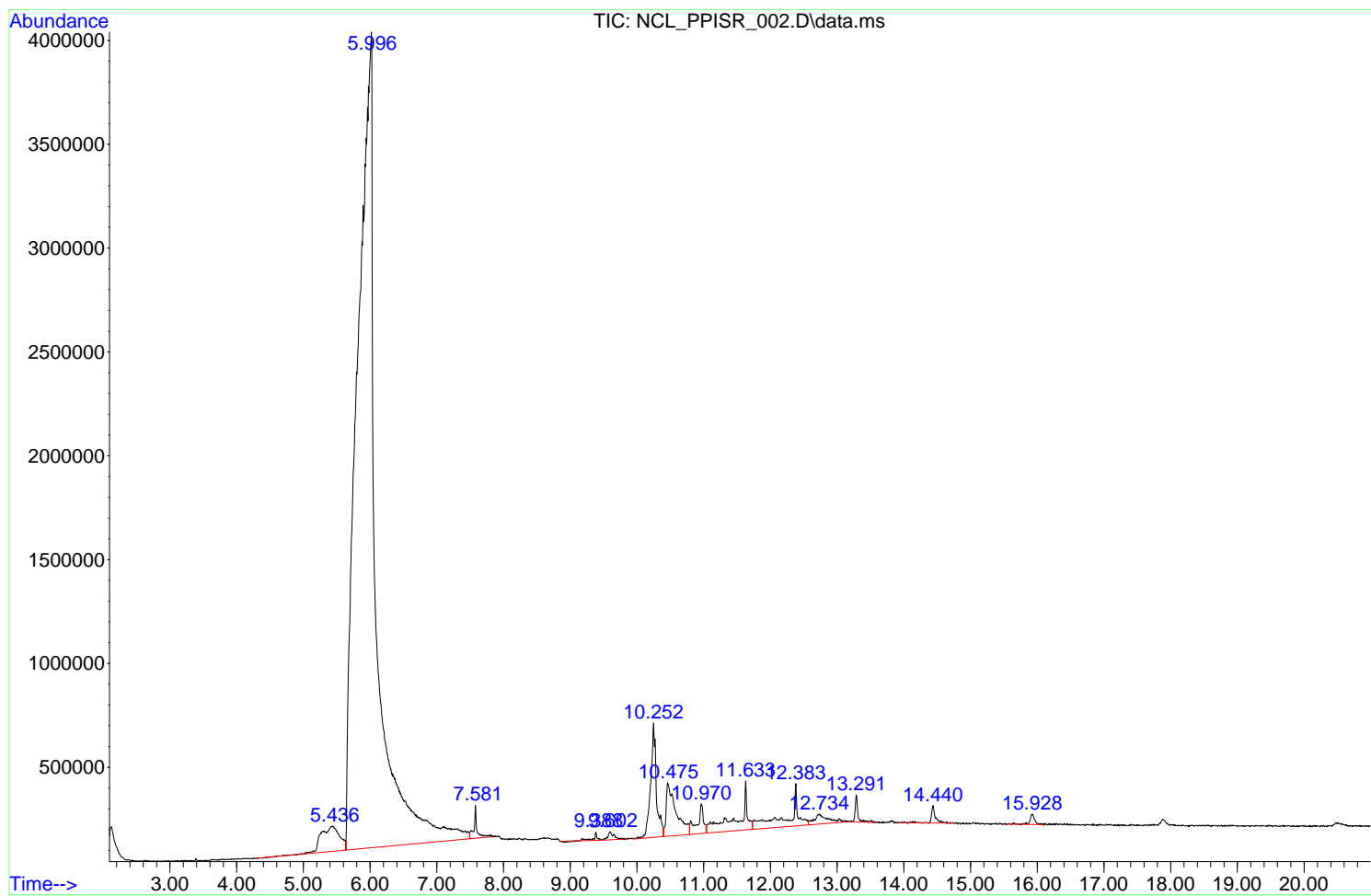
40 m/z Values and Intensities:

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

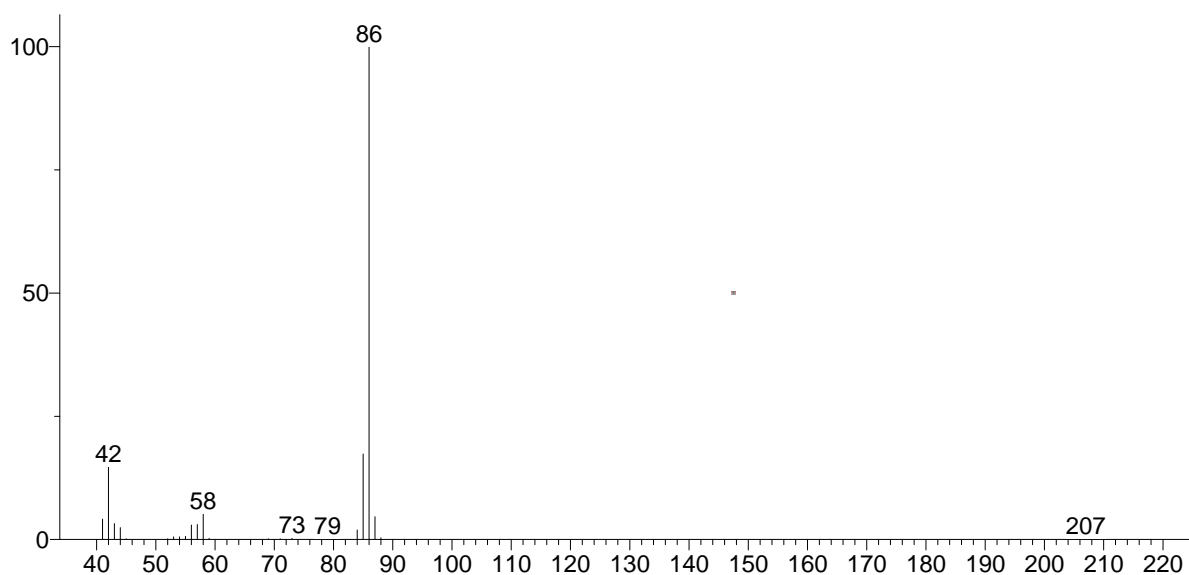
Synonyms:

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
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24 m/z Values and Intensities:

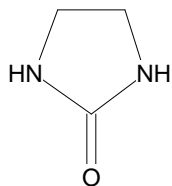
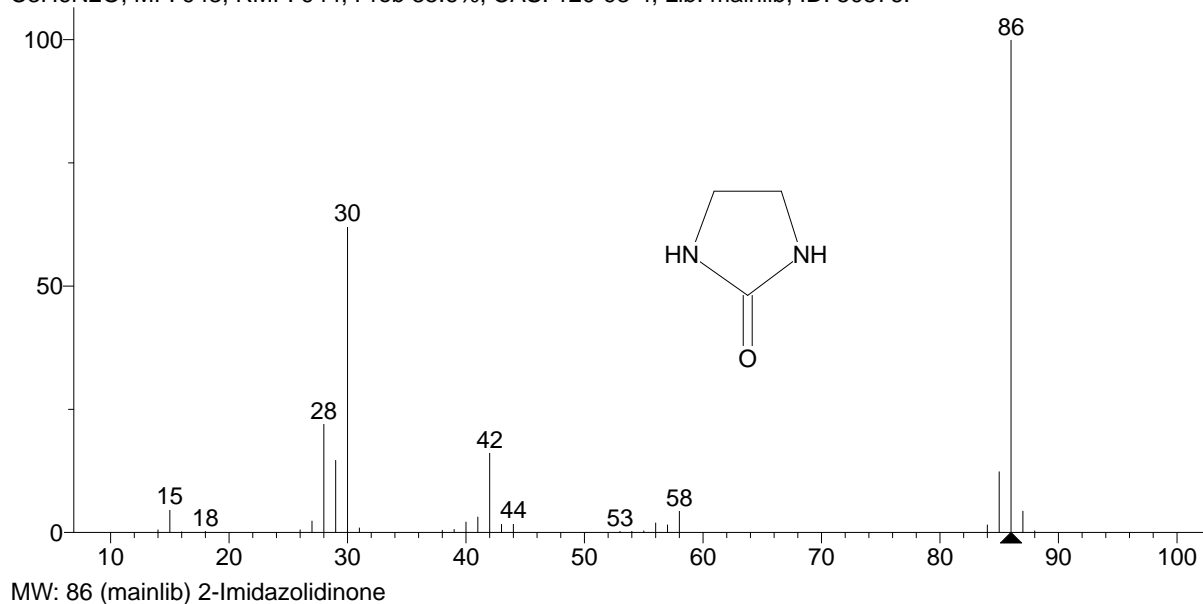
41	41	44	24	53	5	56	29	59	2	73	2	84	19	87	46
42	147	45	1	54	5	57	30	69	1	79	1	85	173	88	3
43	32	52	1	55	6	58	51	71	1	81	1	86	999	207	1

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: C₃H₆N₂O

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
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28 m/z Values and Intensities:

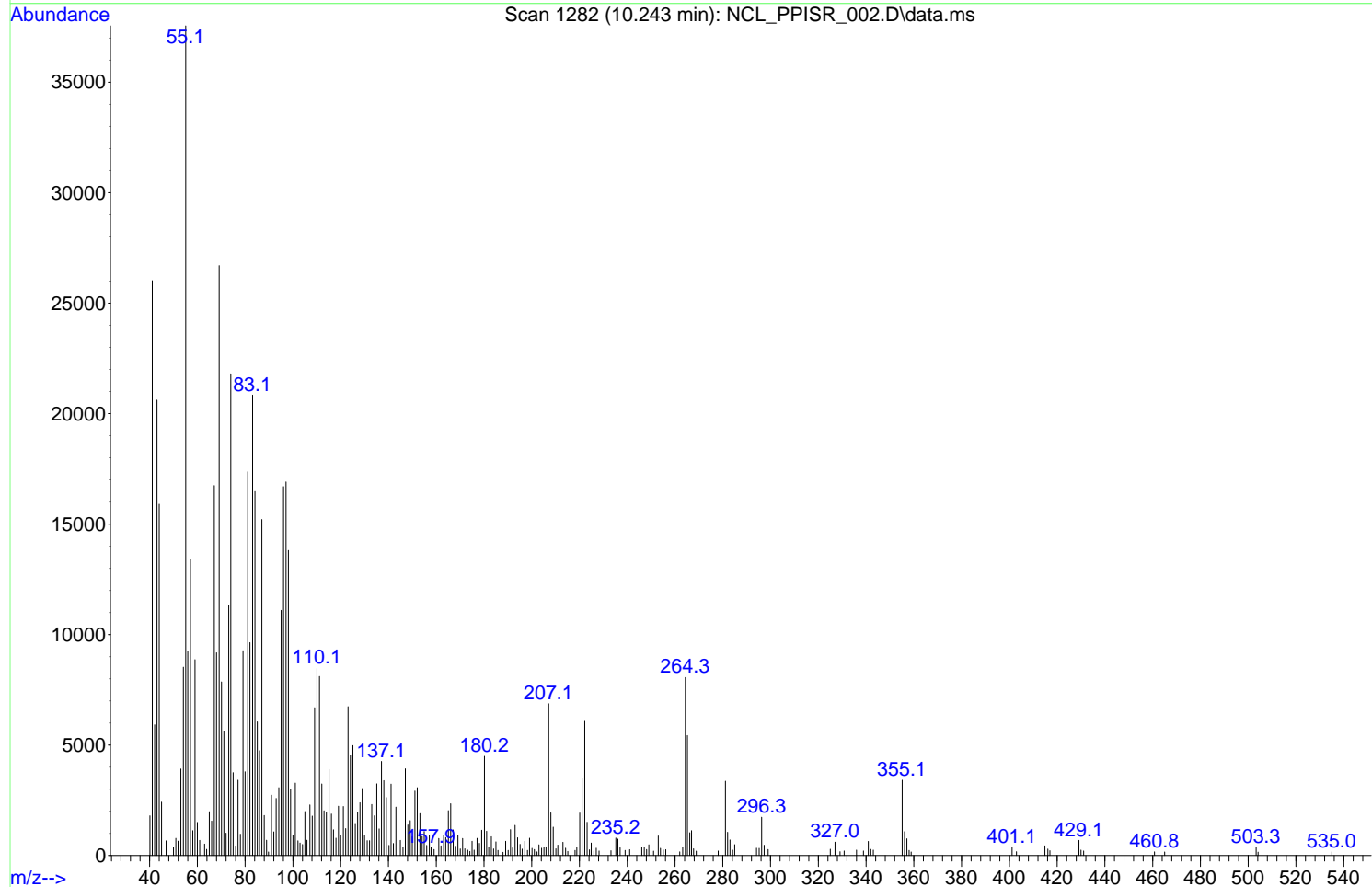
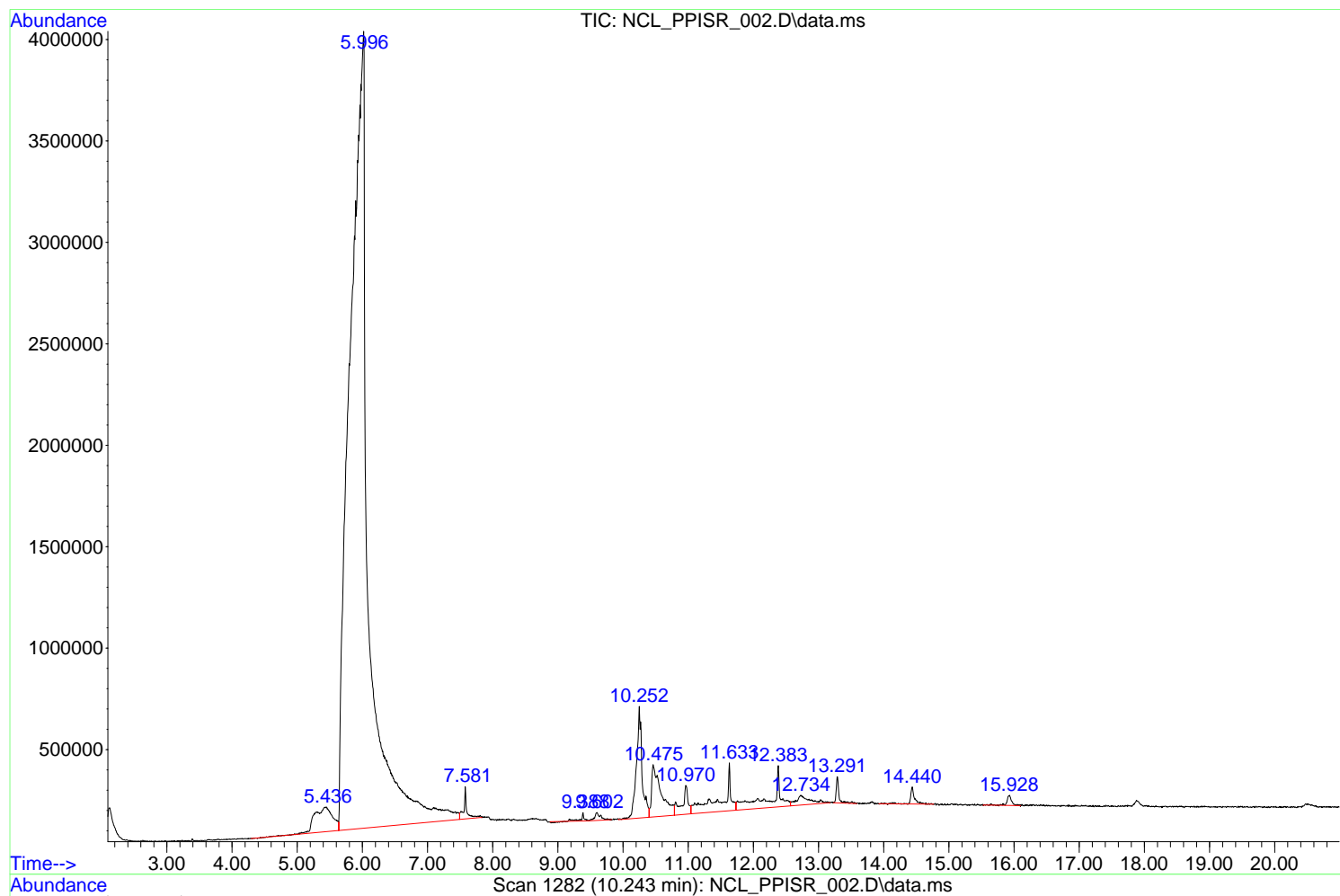
14	5	18	2	28	220	31	9	40	21	43	16	54	3	57	15	85	123	88	3
15	46	26	5	29	146	38	4	41	31	44	18	55	3	58	43	86	999		
16	1	27	23	30	620	39	6	42	161	53	3	56	19	84	15	87	43		

Synonyms:

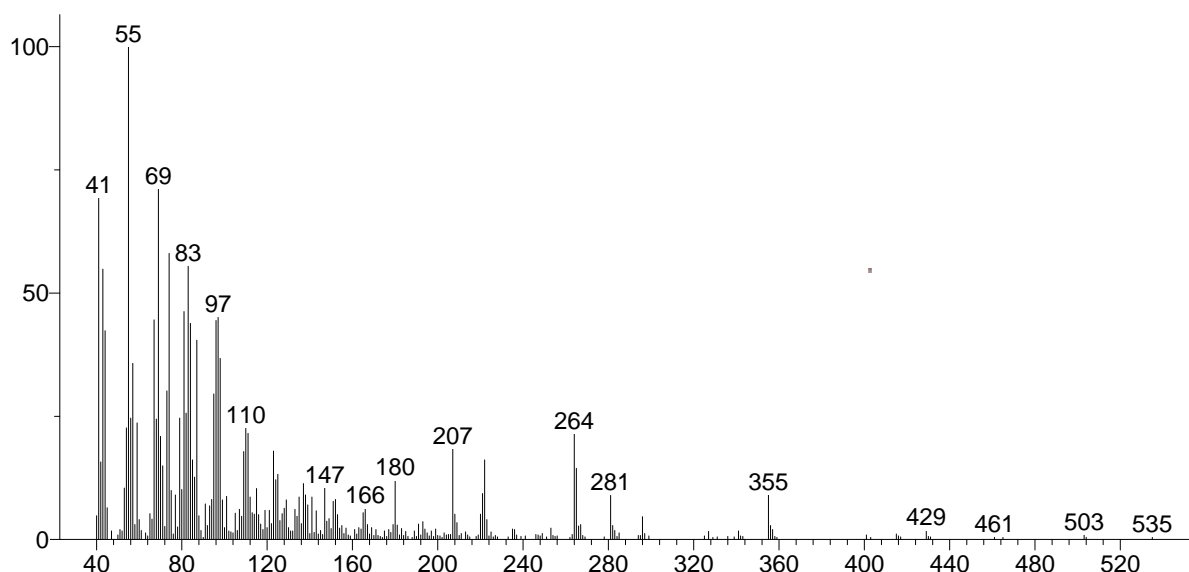
- 1.Ethyleneurea
- 2.Imidazolid-2-one
- 3.N,N'-Ethyleneurea
- 4.SD 6073

5.Urea, N,N'-(1,2-Ethanediy)-
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
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241 m/z Values and Intensities:

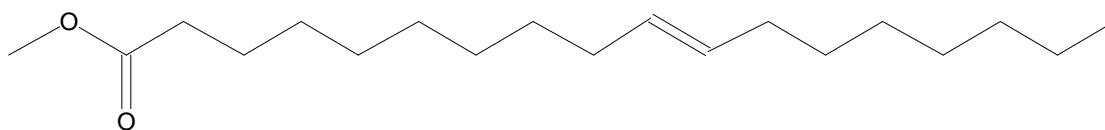
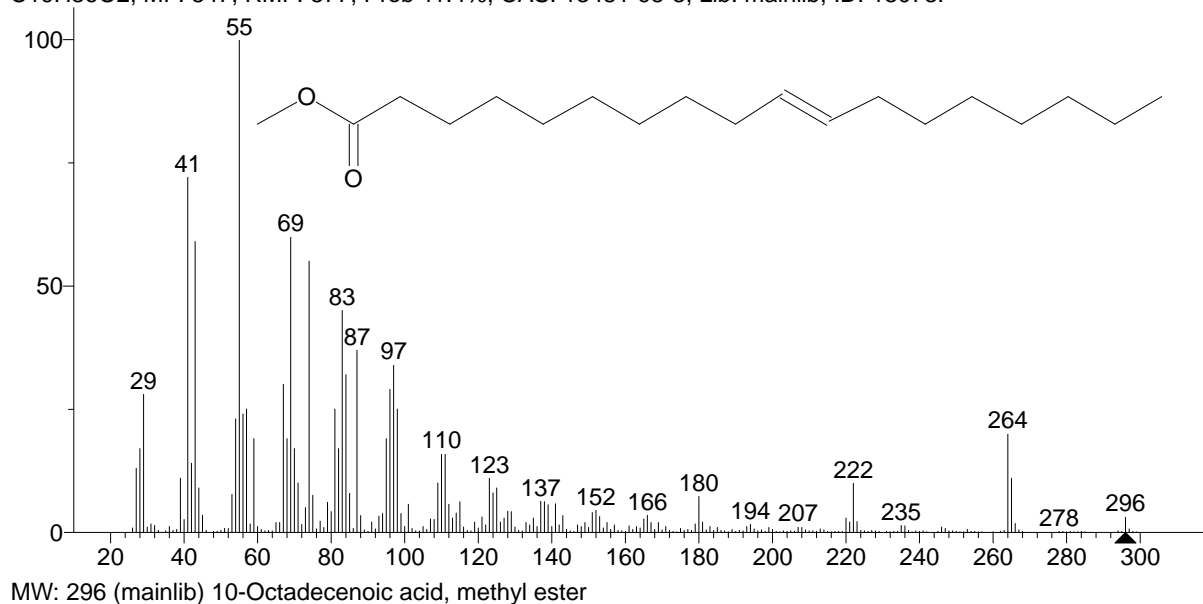
40 48	69 710	94 81	119 59	144 11	170 8	196 7	224 7	267 30	357 20
41 692	70 209	95 295	120 24	145 18	171 20	197 17	225 15	268 8	358 6
42 157	71 149	96 444	121 59	146 10	172 8	198 6	226 5	269 5	359 4
43 548	72 26	97 450	122 32	147 104	173 6	199 21	227 8	278 5	401 9
44 423	73 301	98 367	123 179	148 37	174 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: C₁₉H₃₆O₂

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
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249 m/z Values and Intensities:

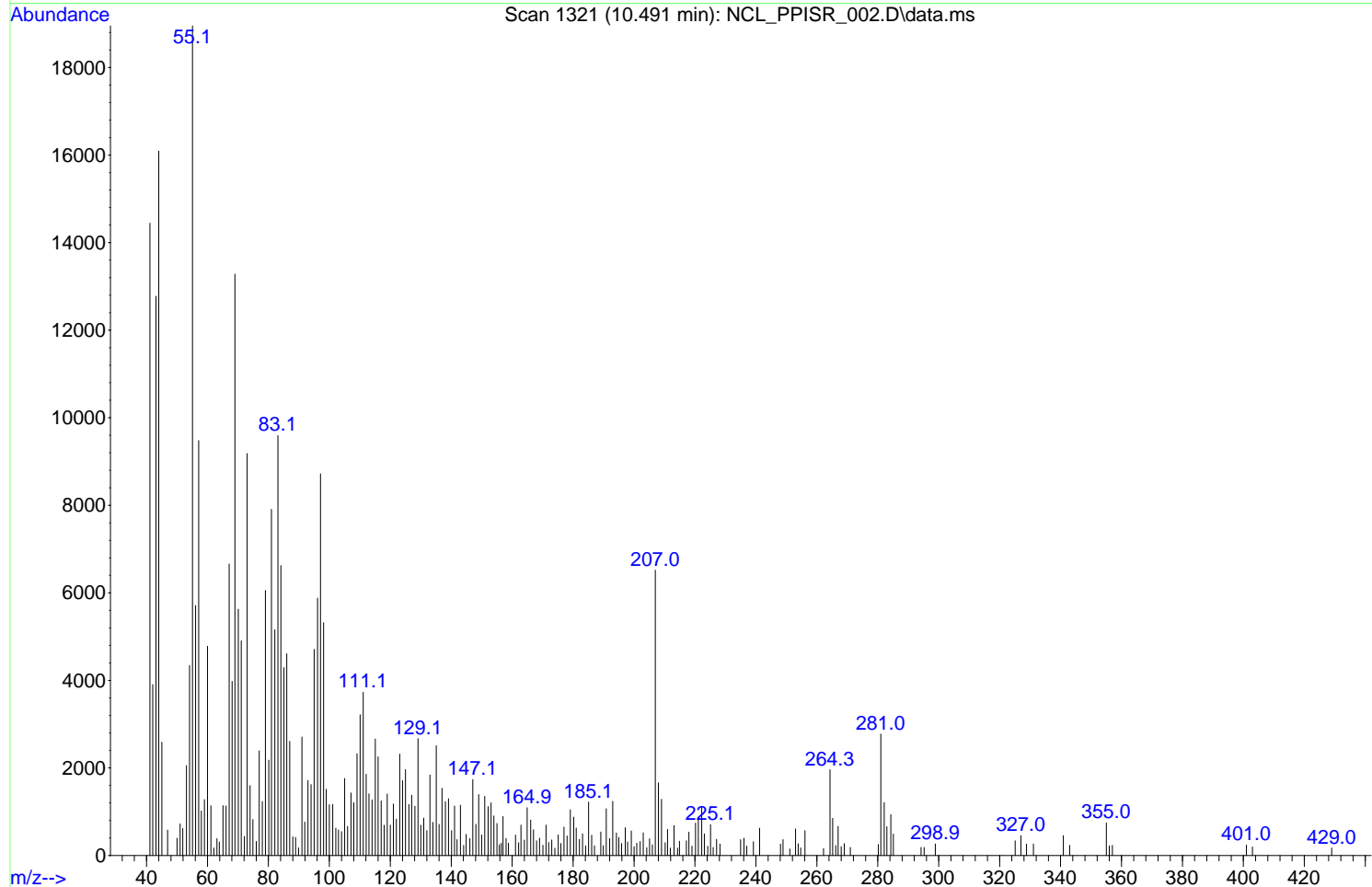
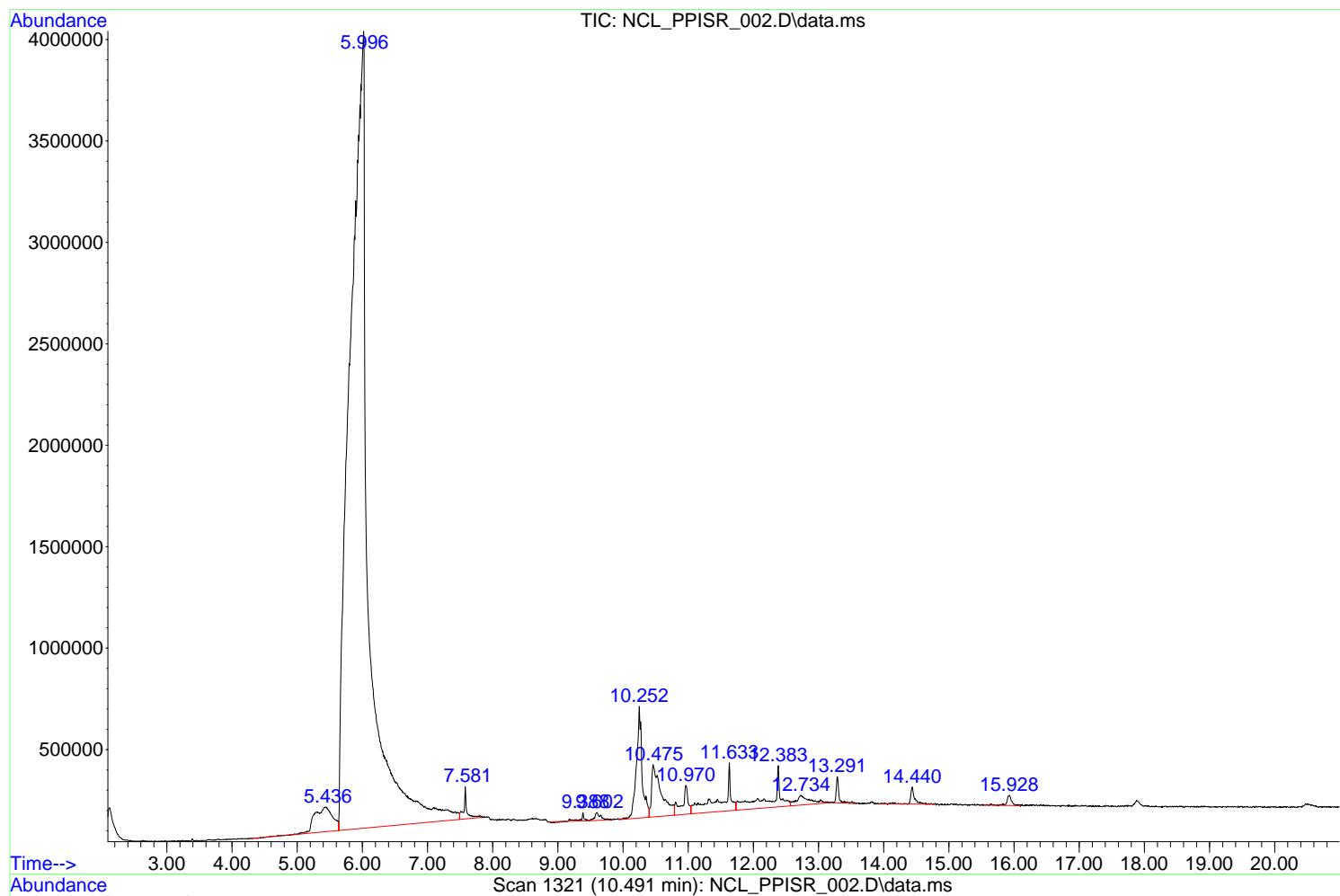
26	9	53	77	78	10	103	3	128	43	153	32	178	4	203	3	228	3	256	1
27	130	54	230	79	61	104	3	129	42	154	9	179	17	204	2	229	2	257	1
28	170	55	999	80	42	105	12	130	11	155	20	180	73	205	3	231	2	260	1
29	280	56	240	81	250	106	6	131	4	156	6	181	21	206	2	232	1	262	2
30	11	57	250	82	170	107	27	132	3	157	15	182	5	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				

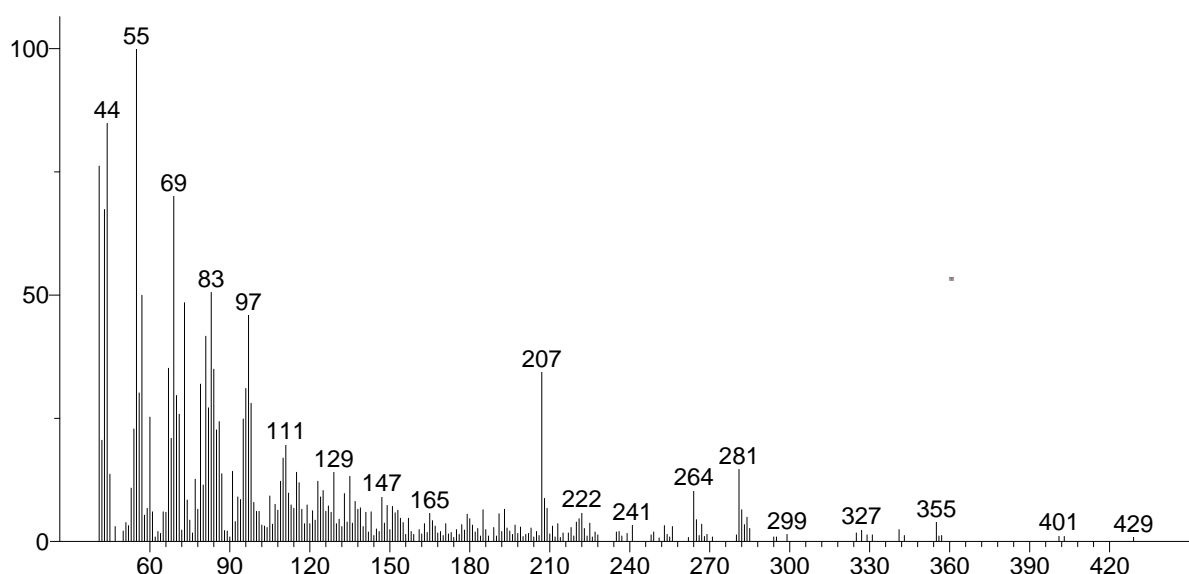
Synonyms:

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
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223 m/z Values and Intensities:

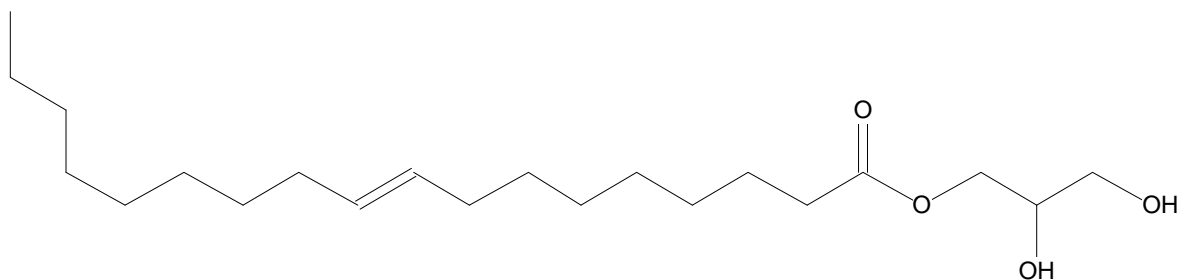
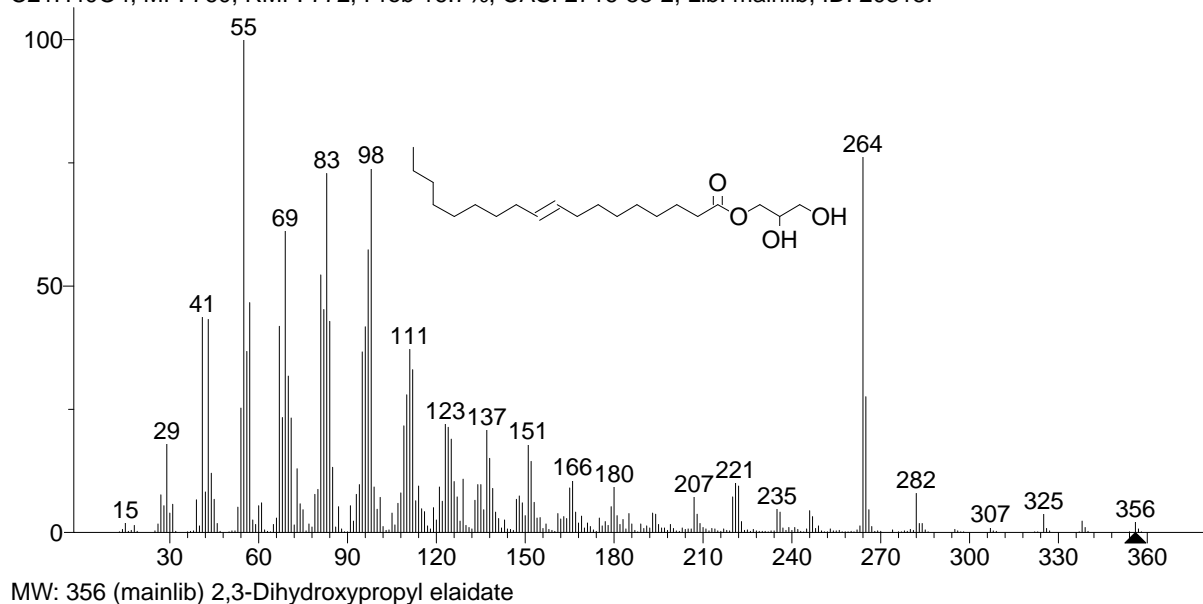
41 761	67 351	90 9	113 74	136 37	159 14	183 26	207 343	237 11	285 26
42 205	68 209	91 142	114 67	137 81	161 24	184 11	208 87	239 16	294 9
43 673	69 700	92 40	115 140	138 65	162 15	185 64	209 67	241 33	295 9
44 848	70 296	93 90	116 119	139 68	163 36	186 24	210 15	248 13	299 14
45 136	71 258	94 85	117 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

C₂₁H₄₀O₄; MF: 760; RMF: 772; Prob 16.7%; CAS: 2716-53-2; Lib: mainlib; ID: 20315.



Name: 2,3-Dihydroxypropyl elaidate

Formula: C₂₁H₄₀O₄

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
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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 #