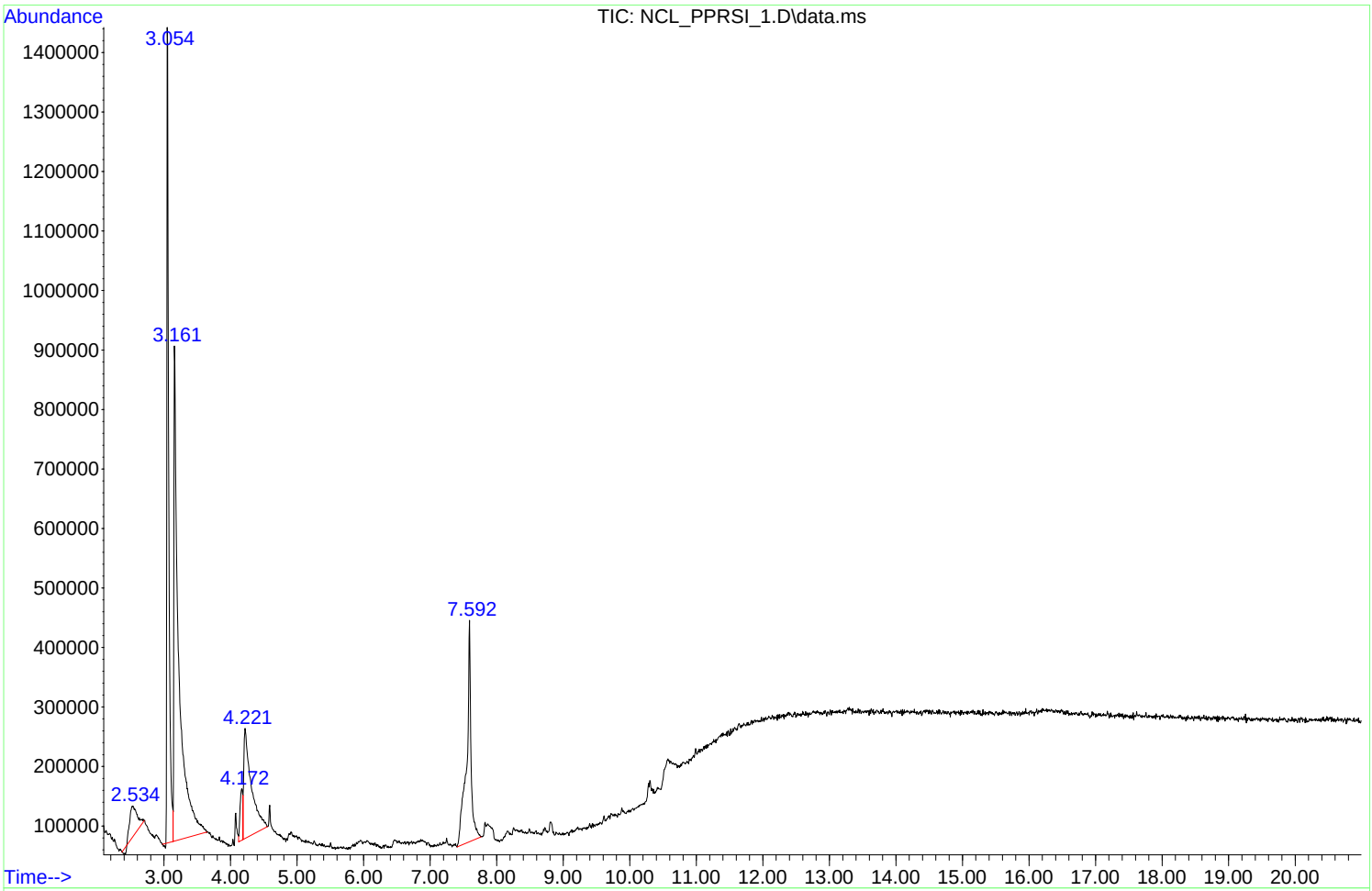
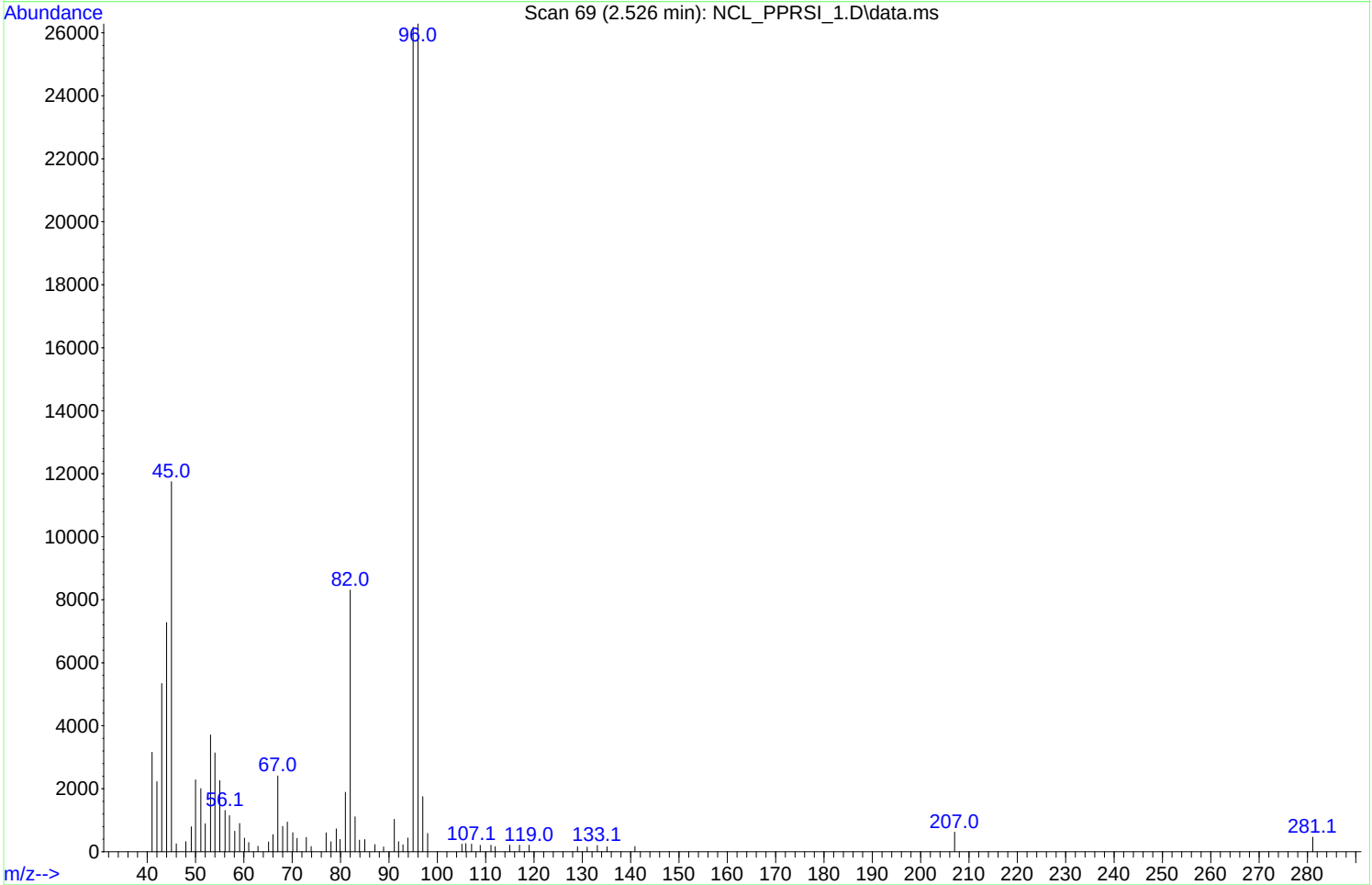
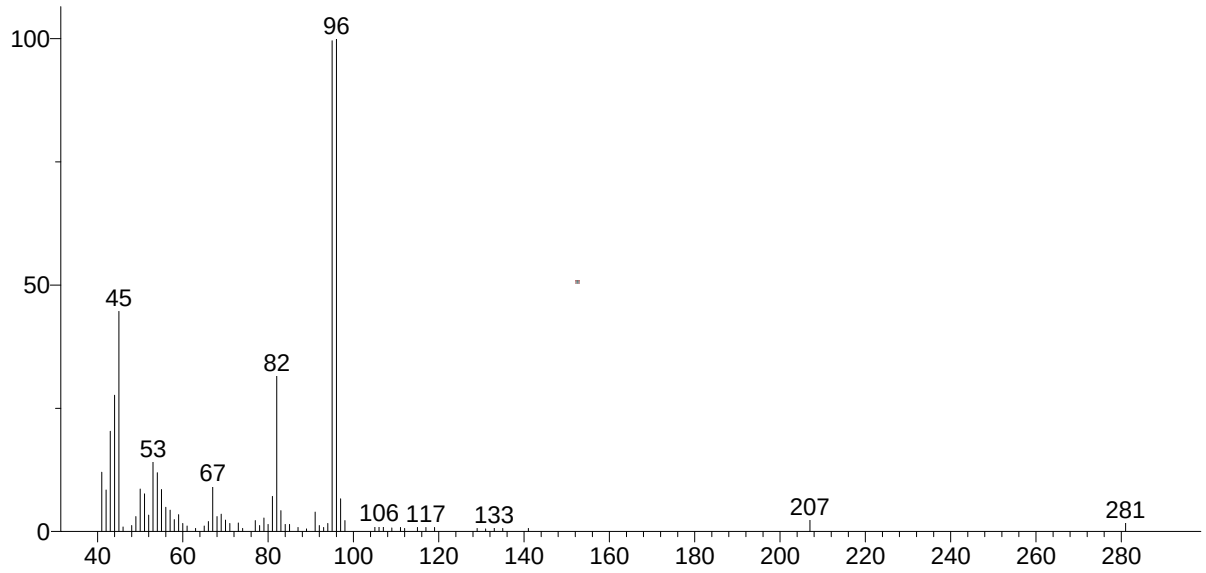
File :D:\NCL\DATA\OCD\Year_2023\NCL_PPRSI_1.D
Operator : Dr. Borikar
Acquired : 22 Jun 2023 00:40 using AcqMethod General_2022.M
Instrument : GC MSD
Sample Name: PPMI
Misc Info : PPMI
Vial Number: 1





Unknown; InLib=-799



(Text File) Scan 69 (2.526 min): NCL_PPRSI_1.D\data.ms

Name: Scan 69 (2.526 min): NCL_PPRSI_1.D\data.ms
MW: N/A ID#: 27024 DB: Text File
Comment: PPMI
10 largest peaks:

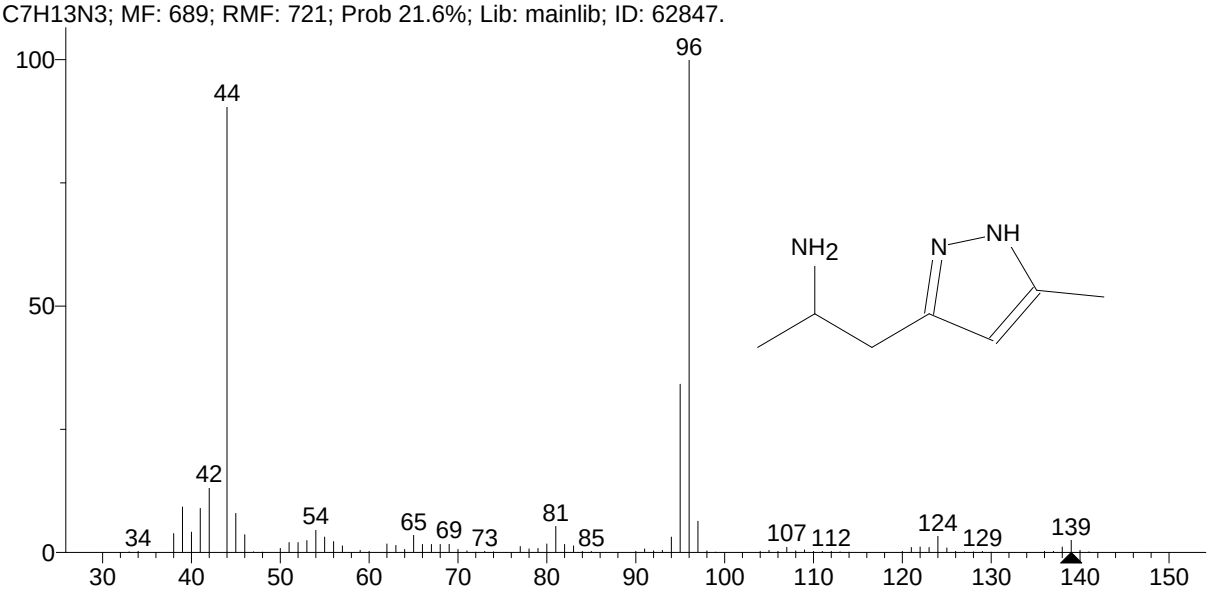
96 999	95 995	45 446	82 315	44 276	43 203	53 141	41 120	54 119	67 91

65 m/z Values and Intensities:

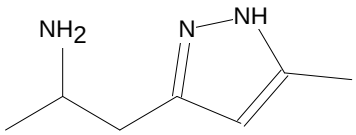
41 120	49 30	56 49	65 11	73 17	82 315	92 12	105 9	117 8	207 23
42 84	50 86	57 43	66 20	74 6	83 42	93 8	106 10	119 8	281 17
43 203	51 76	58 24	67 91	77 22	84 14	94 16	107 9	129 6	
44 276	52 33	59 34	68 30	78 12	85 14	95 995	109 7	131 5	
45 446	53 141	60 16	69 35	79 27	87 8	96 999	111 8	133 7	
46 9	54 119	61 11	70 23	80 14	89 5	97 66	112 6	135 6	
48 12	55 85	63 6	71 16	81 71	91 39	98 22	115 8	141 6	

Synonyms:
no synonyms.

Hit 1 : Ethylamine, 1-methyl-2-(5-methyl-1H-pyrazol-3-yl)-
C7H13N3; MF: 689; RMF: 721; Prob 21.6%; Lib: mainlib; ID: 62847.



MW: 139 (mainlib) Ethylamine, 1-methyl-2-(5-methyl-1H-pyrazol-3-yl)-



Name: Ethylamine, 1-methyl-2-(5-methyl-1H-pyrazol-3-yl)-
Formula: $C_7H_{13}N_3$
MW: 139 Exact Mass: 139.110948 NIST#: 316413 ID#: 62847 DB: mainlib
Contributor: A.A.Kutin, Moscow, Russia
10 largest peaks:

96	999	44	904	95	341	42	131	39	92	41	89	45	79	97	63	81	53	54	46

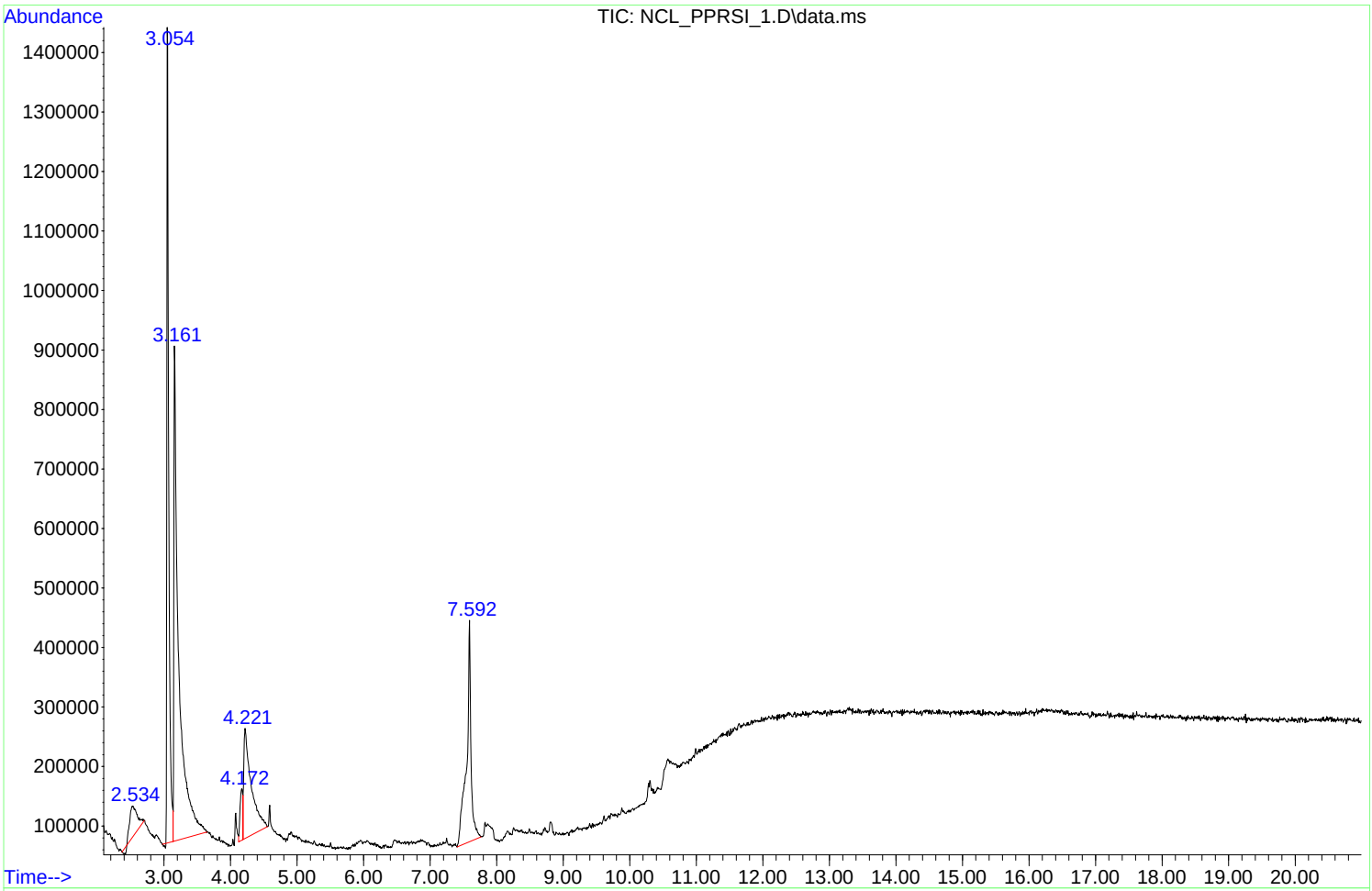
82 m/z Values and Intensities:

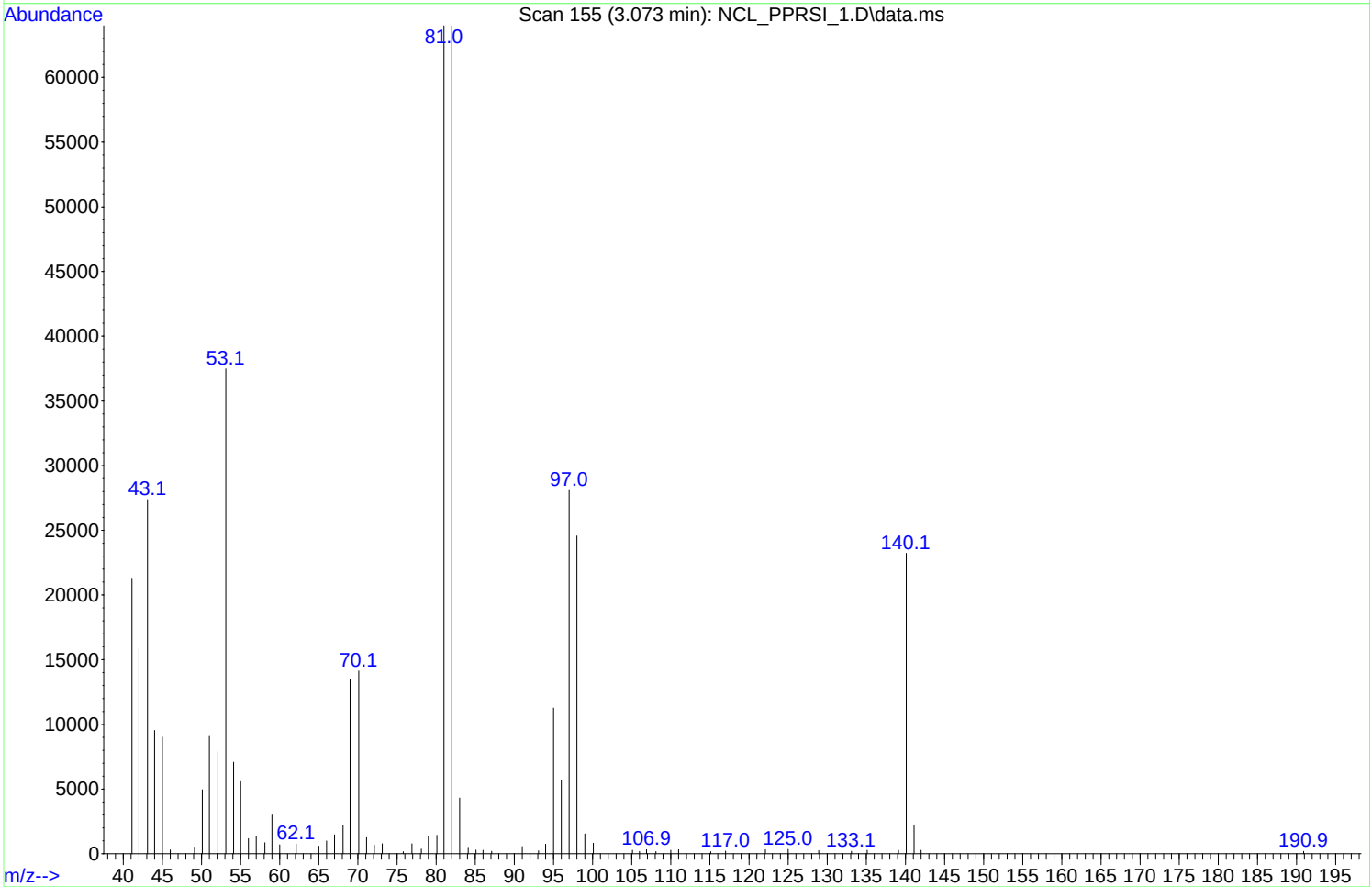
33	1	46	36	56	22	67	16	78	7	91	7	104	2	113	1	127	1	141	1
34	3	47	1	57	13	68	16	79	8	92	3	105	4	114	Tr	128	1		
38	38	48	Tr	59	4	69	18	80	17	93	4	106	2	120	2	129	2		
39	92	50	8	60	2	70	6	81	53	94	31	107	12	121	10	130	Tr		
40	41	51	20	62	17	71	3	82	16	95	341	108	3	122	11	136	2		
41	89	52	20	63	14	72	Tr	83	13	96	999	109	5	123	10	137	2		
42	131	53	24	64	6	73	3	84	2	97	63	110	2	124	33	138	11		
44	904	54	46	65	35	74	1	85	2	98	3	111	2	125	9	139	25		
45	79	55	31	66	16	77	12	90	2	99	Tr	112	2	126	2	140	4		

Synonyms:

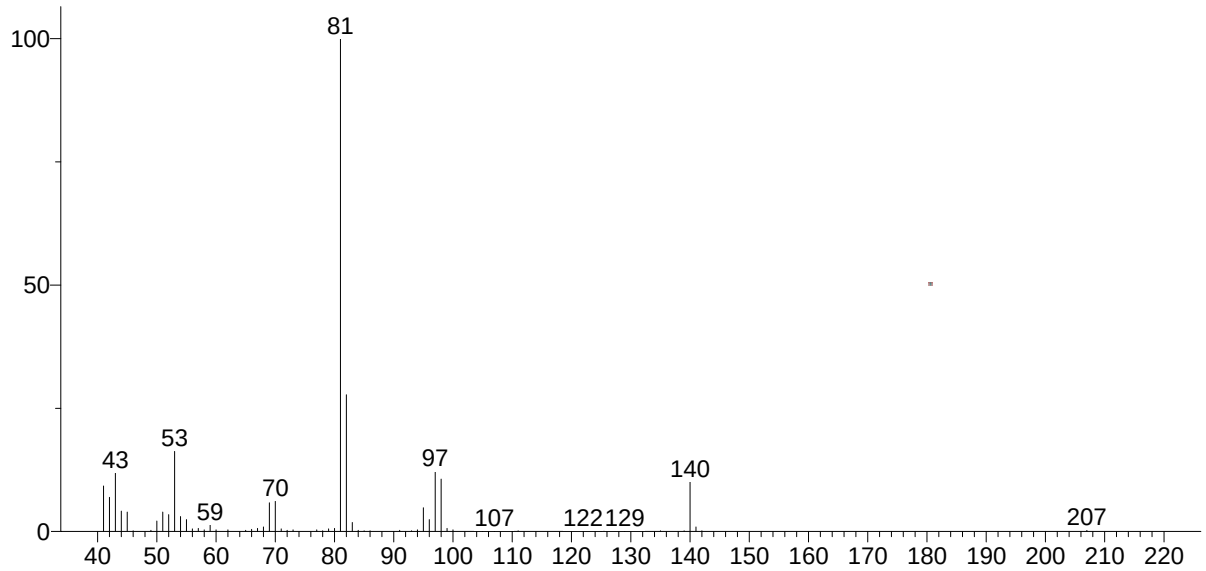
no synonyms.

File :D:\NCL\DATA\OCD\Year_2023\NCL_PPRSI_1.D
Operator : Dr. Borikar
Acquired : 22 Jun 2023 00:40 using AcqMethod General_2022.M
Instrument : GC MSD
Sample Name: PPMI
Misc Info : PPMI
Vial Number: 1





Unknown; InLib=-496



(Text File) Scan 155 (3.073 min): NCL_PPRSI_1.D\data.ms

Name: Scan 155 (3.073 min): NCL_PPRSI_1.D\data.ms
MW: N/A ID#: 27025 DB: Text File
Comment: PPMI
10 largest peaks:

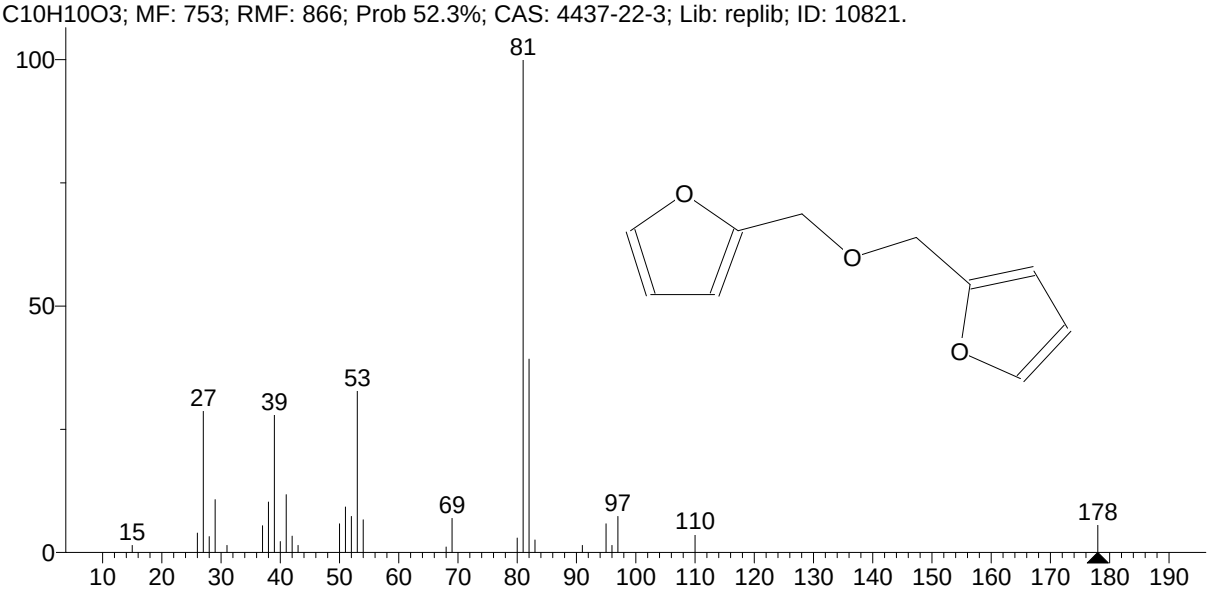
81 999	82 277	53 162	97 121	43 118	98 106	140 100	41 92	42 69	70 61

60 m/z Values and Intensities:

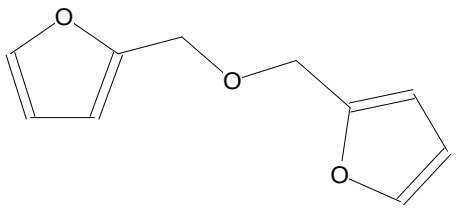
41	92	49	2	55	24	62	3	70	61	79	5	85	1	96	24	107	1	135	1
42	69	50	21	56	5	65	2	71	5	80	6	86	1	97	121	110	1	139	1
43	118	51	39	57	6	66	4	72	2	81	999	91	2	98	106	111	1	140	100
44	41	52	34	58	3	67	6	73	3	82	277	93	1	99	6	122	1	141	9
45	39	53	162	59	13	68	9	77	3	83	18	94	3	100	3	125	1	142	1
46	1	54	30	60	3	69	58	78	1	84	2	95	48	105	1	129	1	207	2

Synonyms:
no synonyms.

Hit 1 : Furan, 2,2'-[oxybis(methylene)]bis-
C10H10O3; MF: 753; RMF: 866; Prob 52.3%; CAS: 4437-22-3; Lib: replib; ID: 10821.



MW: 178 (replib) Furan, 2,2'-[oxybis(methylene)]bis-



Name: Furan, 2,2'-[oxybis(methylene)]bis-
Formula: $C_{10}H_{10}O_3$
MW: 178 Exact Mass: 178.062994 CAS#: 4437-22-3 NIST#: 33095 ID#: 10821 DB: replib
Other DBs: TSCA, RTECS, HODOC, NIH
10 largest peaks:

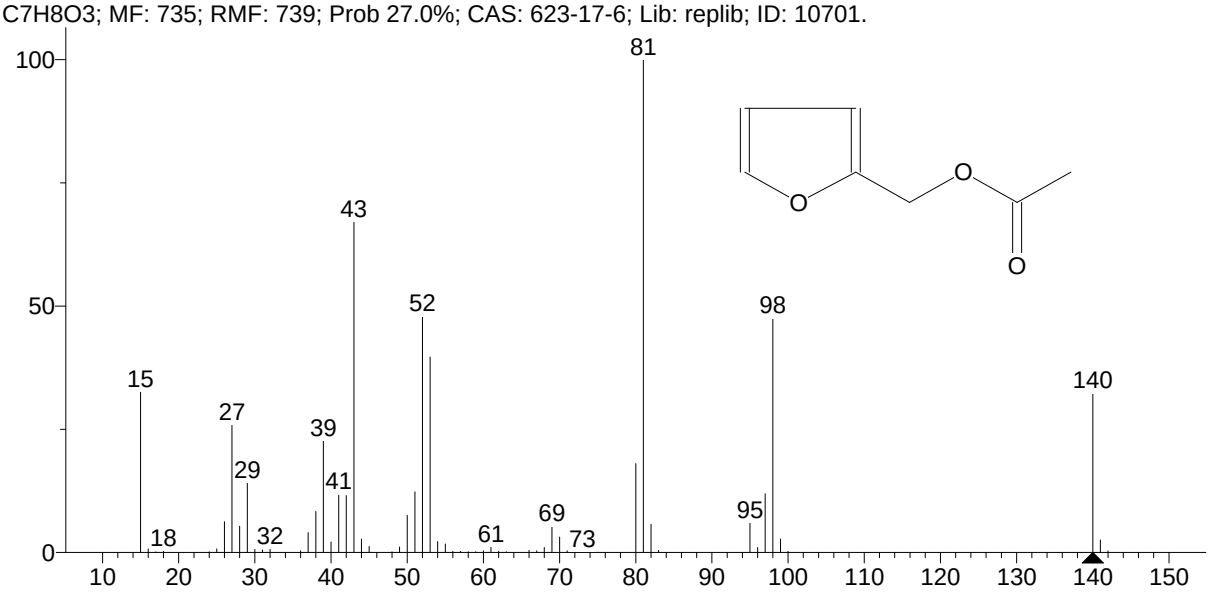
81 999 |	82 392 |	53 327 |	27 286 |	39 279 |	41 117 |	29 107 |	38 102 |	51 92 |	52 73 |

30 m/z Values and Intensities:

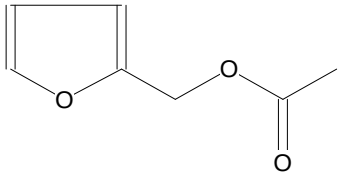
15 14 |	28 32 |	37 54 |	40 22 |	43 14 |	52 73 |	68 11 |	81 999 |	91 14 |	97 73 |
26 39 |	29 107 |	38 102 |	41 117 |	50 58 |	53 327 |	69 69 |	82 392 |	95 58 |	110 36 |
27 286 |	31 14 |	39 279 |	42 33 |	51 92 |	54 66 |	80 29 |	83 25 |	96 14 |	178 55 |

Synonyms:
1.Furan, 2,2'-(oxydimethylene)di-
2.Difurfuryl ether
3.Furfuryl ether
4.2,2'-[Oxybis(methylene)]bisfuran
5.2-[(2-Furylmethoxy)methyl]furan #

Hit 2 : 2-Furanmethanol, acetate
C7H8O3; MF: 735; RMF: 739; Prob 27.0%; CAS: 623-17-6; Lib: replib; ID: 10701.



MW: 140 (replib) 2-Furanmethanol, acetate



Name: 2-Furanmethanol, acetate
Formula: $C_7H_8O_3$
MW: 140 Exact Mass: 140.047344 CAS#: 623-17-6 NIST#: 21168 ID#: 10701 DB: replib
Other DBs: Fine, TSCA, RTECS, HODOC, NIH, EINECS, IRDB
10 largest peaks:

81 999	43 670	52 478	98 474	53 396	15 325	140 322	27 258	39 226	80 180

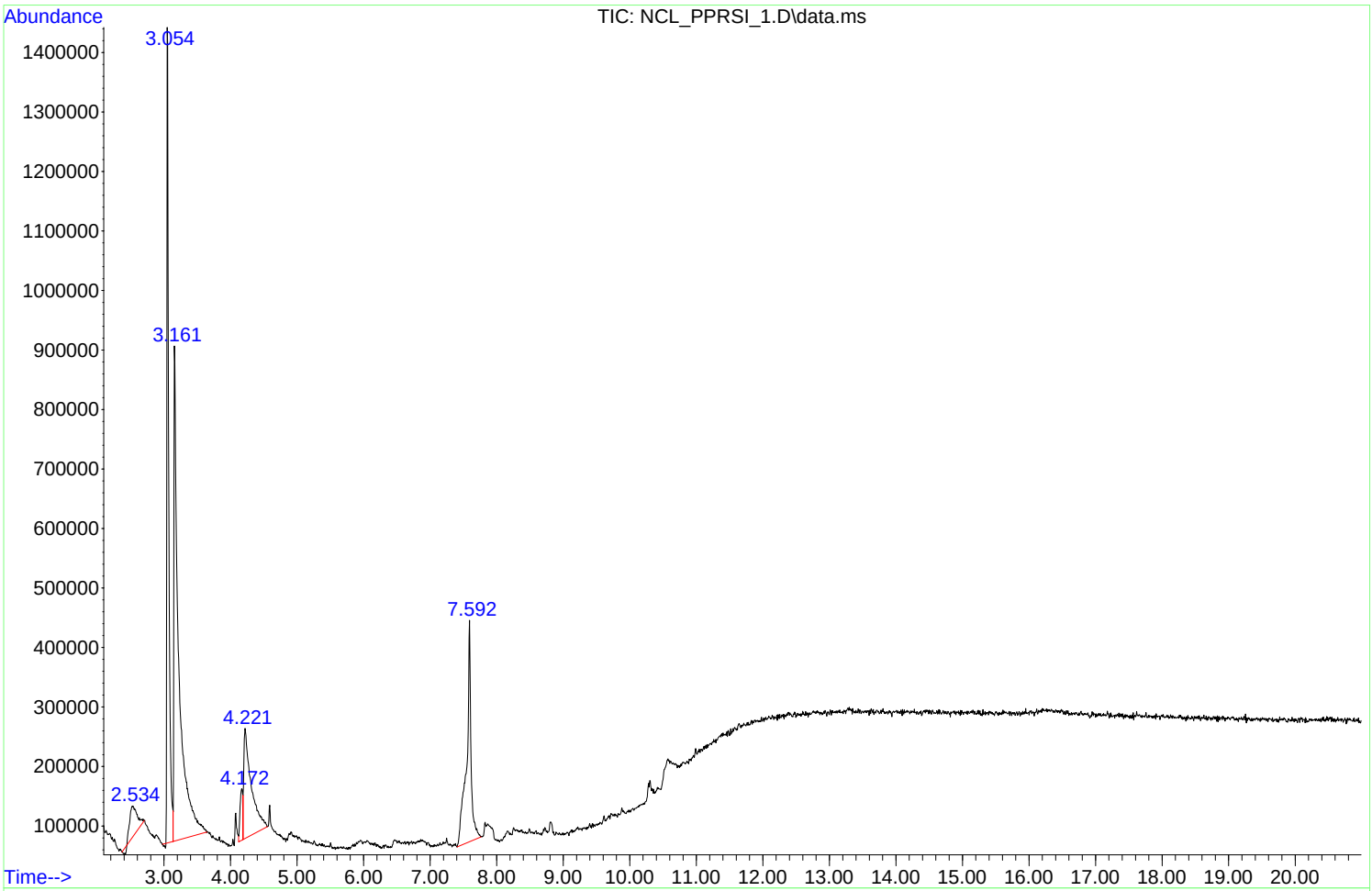
59 m/z Values and Intensities:

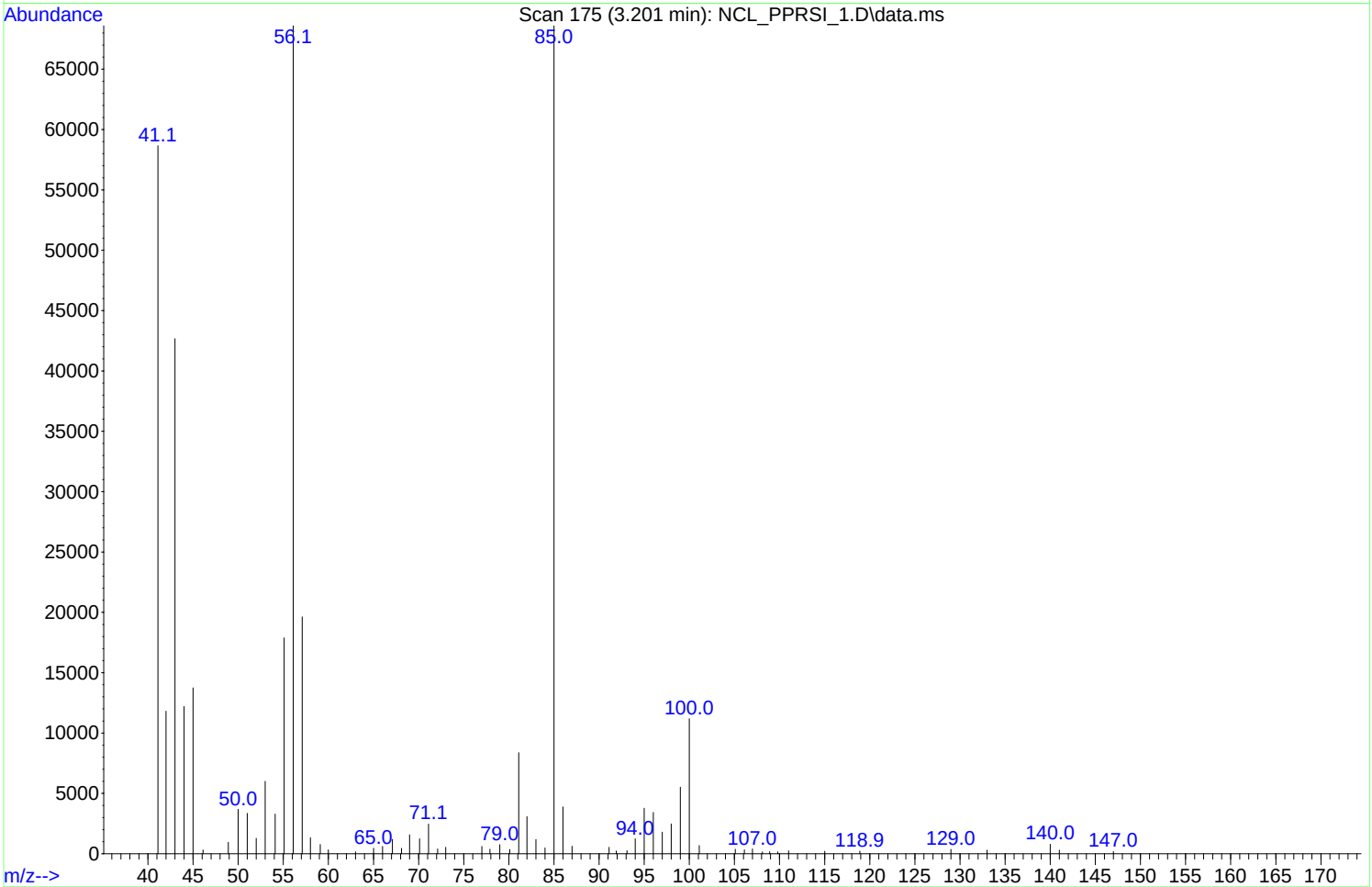
15	325	26	62	32	7	41	117	49	11	55	17	61	11	69	52	82	57	99	27
16	7	27	258	36	3	42	115	50	75	56	2	62	2	70	31	83	4	100	2
17	1	28	53	37	40	43	670	51	123	57	2	63	1	71	3	95	59	140	322
18	2	29	140	38	83	44	27	52	478	58	1	66	4	73	1	96	10	141	25
24	1	30	6	39	226	45	12	53	396	59	1	67	3	80	180	97	119	142	3
25	7	31	5	40	21	48	1	54	22	60	3	68	10	81	999	98	474		

Synonyms:
1.Furfuryl alcohol, acetate
2.Acetic acid furfurylester
3.Furfuryl acetate

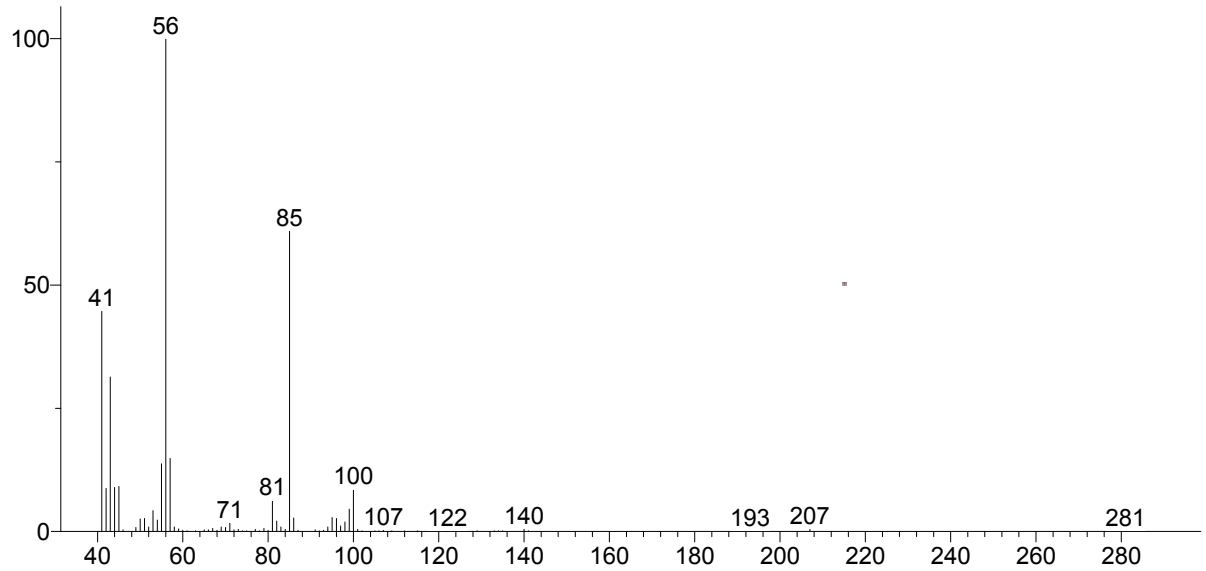
4.2-Acetoxymethylfuran
5.2-Furanmethyl acetate
6.2-Furfuryl-acetate
7.2-Furylmethyl acetate #
8.Furfuryl ethanoate

File :D:\NCL\DATA\OCD\Year_2023\NCL_PPRSI_1.D
Operator : Dr. Borikar
Acquired : 22 Jun 2023 00:40 using AcqMethod General_2022.M
Instrument : GC MSD
Sample Name: PPMI
Misc Info : PPMI
Vial Number: 1





Unknown; InLib=-103



(Text File) Scan 174 (3.194 min): NCL_PPRSI_1.D\data.ms

Name: Scan 174 (3.194 min): NCL_PPRSI_1.D\data.ms
MW: N/A ID#: 27027 DB: Text File
Comment: PPMI
10 largest peaks:

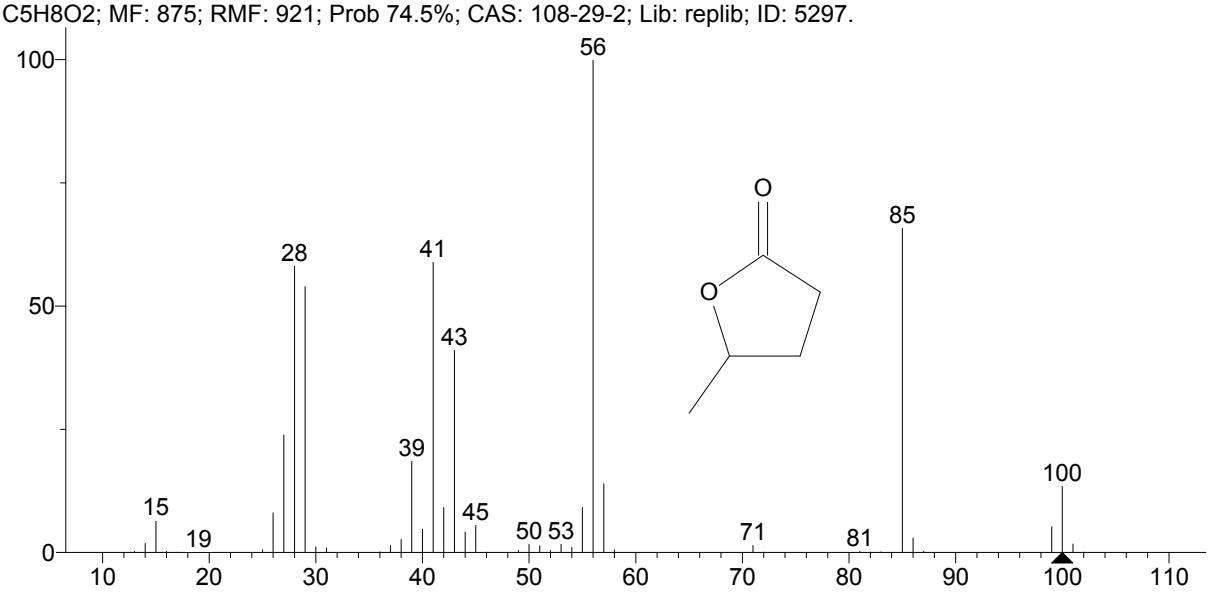
56 999	85 609	41 446	43 313	57 148	55 137	45 91	44 89	42 87	100 85

70 m/z Values and Intensities:

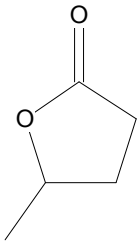
41	446	50	25	57	148	66	3	73	4	81	62	91	3	98	19	107	2	134	1
42	87	51	26	58	9	67	6	74	1	82	21	92	1	99	45	109	1	135	1
43	313	52	9	59	5	68	2	75	1	83	9	93	2	100	85	112	1	140	5
44	89	53	42	60	2	69	9	77	4	84	4	94	9	101	4	115	1	141	1
45	91	54	23	61	1	70	8	78	1	85	609	95	28	102	1	122	1	193	1
46	3	55	137	63	1	71	17	79	6	86	27	96	26	105	1	129	1	207	4
49	8	56	999	65	3	72	3	80	2	87	2	97	11	106	1	133	1	281	1

Synonyms:
no synonyms.

Hit 1 : 2(3H)-Furanone, dihydro-5-methyl-
C5H8O2; MF: 875; RMF: 921; Prob 74.5%; CAS: 108-29-2; Lib: replib; ID: 5297.



MW: 100 (replib) 2(3H)-Furanone, dihydro-5-methyl-



Name: 2(3H)-Furanone, dihydro-5-methyl-
Formula: $C_5H_8O_2$
MW: 100 Exact Mass: 100.0524297 CAS#: 108-29-2 NIST#: 107777 ID#: 5297 DB: replib
Other DBs: Fine, TSCA, RTECS, HODOC, NIH, EINECS
Contributor: Chuck Anderson, Aldrich Chemical Co.
Related CAS#: 57129-69-8
10 largest peaks:

56 999 |	85 657 |	41 589 |	28 581 |	29 539 |	43 410 |	27 238 |	39 185 |	57 139 |	100 134 |

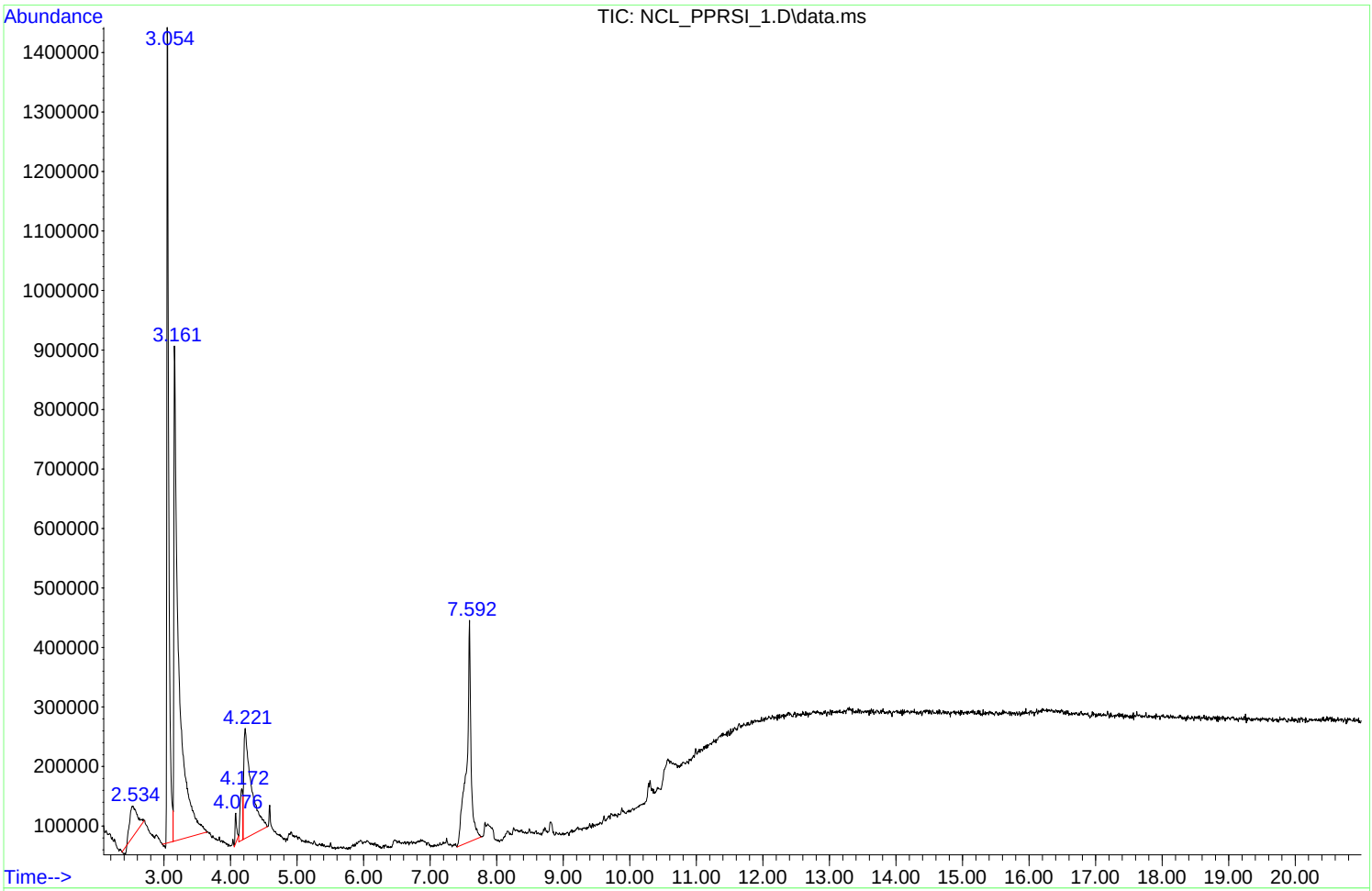
47 m/z Values and Intensities:

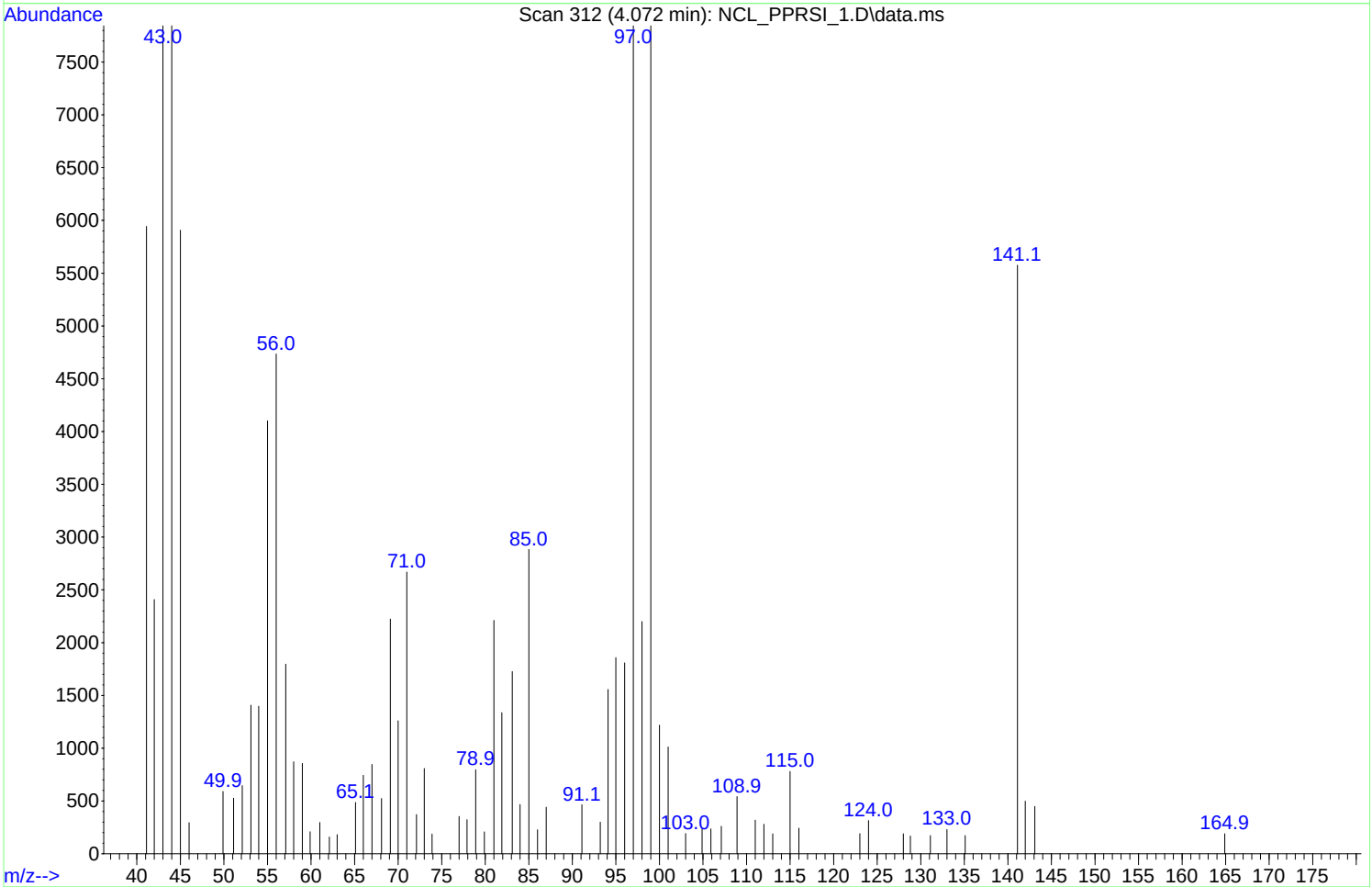
13	2 |	18	Tr |	28	581 |	37	14 |	42	91 |	49	4 |	54	10 |	71	14 |	85	657 |	101	17 |
14	18 |	19	1 |	29	539 |	38	26 |	43	410 |	50	16 |	55	91 |	72	Tr |	86	29 |	102	Tr |
15	64 |	25	5 |	30	11 |	39	185 |	44	41 |	51	13 |	56	999 |	81	2 |	87	2 |		
16	2 |	26	80 |	31	9 |	40	47 |	45	55 |	52	4 |	57	139 |	82	Tr |	99	52 |		
17	Tr |	27	238 |	36	1 |	41	589 |	46	Tr |	53	17 |	58	5 |	83	1 |	100	134 |		

Synonyms:
1.γ-Methyl-γ-butyrolactone
2.γ-Pentalactone

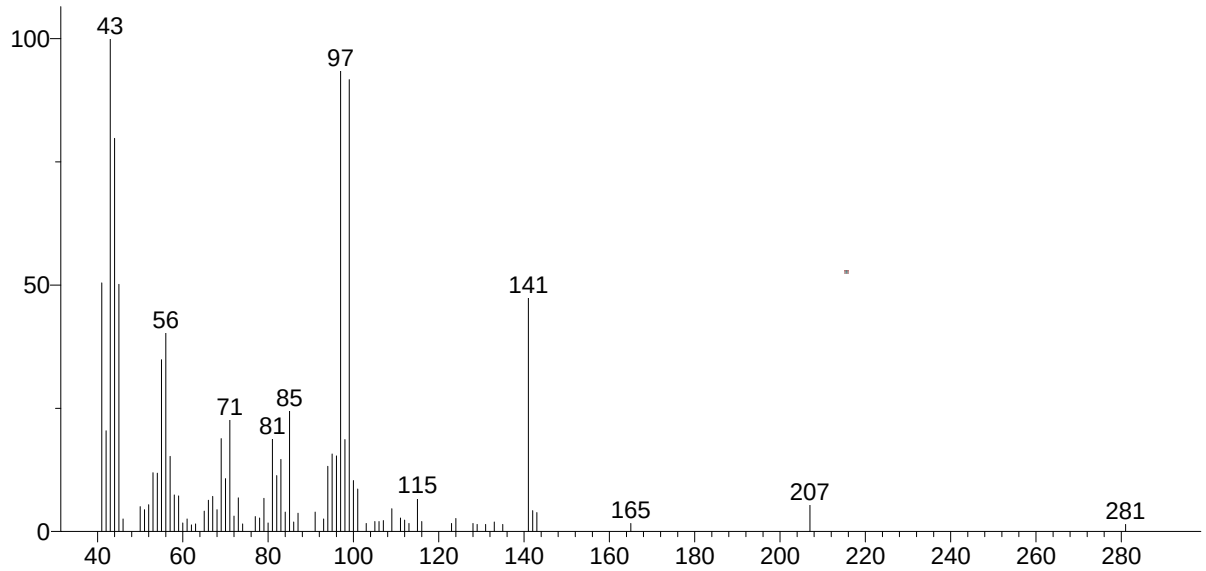
3.γ-Valerolactone
4.Pentanoic acid, 4-hydroxy-, γ-lactone
5.4-Hydroxypentanoic acid lactone
6.4-Hydroxyvaleric acid lactone
7.4-Methyl-γ-butyrolactone
8.4-Pentanolide
9.4-Valerolactone
10.γ-Pentanolactone
11.γ-Valerolakton
12.Dihydro-5-methyl-2(3H)-furanone
13.5-Methyldihydro-2(3H)-furanone #
14.Valeric acid, 4-hydroxy-, gamma-lactone
15.gamma-Valerolactone
16.5-Methyldihydrofuran-2(3H)-one
17.5-methyltetrahydrofuran-2-one
18.Dihydro-5-methyl-2-furanone
19.(±)-γ-Valerolactone
20.(±)-4-Methylbutyrolactone
21.5-Methyltetrahydro-2-furanone
22.NSC 33700
23.Valeric acid, 4-hydroxy-, γ-lactone

File :D:\NCL\DATA\OCD\Year_2023\NCL_PPRSI_1.D
Operator : Dr. Borikar
Acquired : 22 Jun 2023 00:40 using AcqMethod General_2022.M
Instrument : GC MSD
Sample Name: PPMI
Misc Info : PPMI
Vial Number: 1





Unknown; InLib=-1679



(Text File) Scan 312 (4.072 min): NCL_PPRSI_1.D\data.ms

Name: Scan 312 (4.072 min): NCL_PPRSI_1.D\data.ms
MW: N/A ID#: 27026 DB: Text File
Comment: PPMI
10 largest peaks:

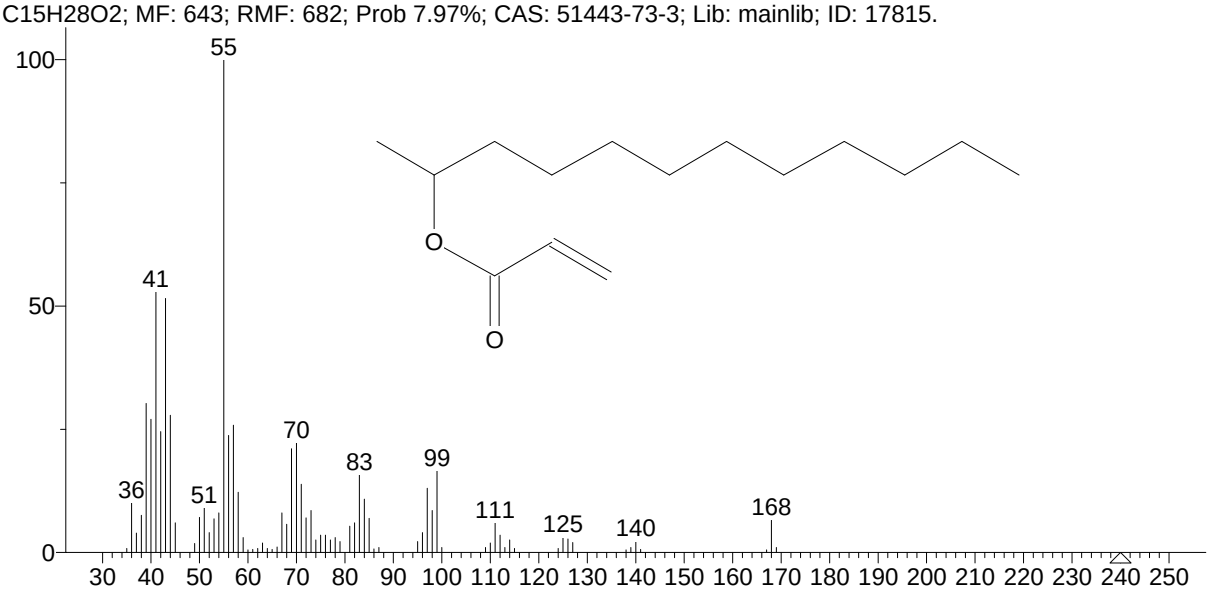
43 999	97 934	99 916	44 797	41 504	45 501	141 473	56 402	55 348	85 244

74 m/z Values and Intensities:

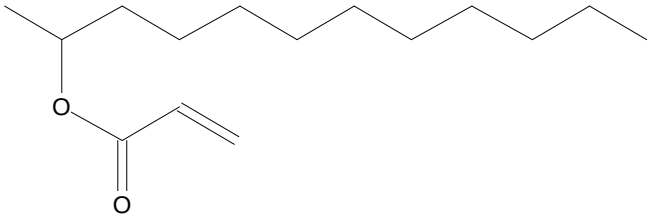
41	504	52	54	60	17	69	188	79	67	87	37	99	916	111	27	129	14	207	53
42	204	53	119	61	25	70	107	80	17	91	39	100	103	112	23	131	14	281	14
43	999	54	118	62	13	71	226	81	187	93	25	101	86	113	16	133	19		
44	797	55	348	63	15	72	31	82	113	94	132	103	16	115	66	135	14		
45	501	56	402	65	41	73	68	83	146	95	157	105	20	116	20	141	473		
46	25	57	152	66	63	74	15	84	39	96	153	106	20	123	16	142	42		
50	50	58	74	67	71	77	30	85	244	97	934	107	22	124	26	143	38		
51	44	59	72	68	44	78	27	86	19	98	186	109	46	128	16	165	16		

Synonyms:
no synonyms.

Hit 1 : 2-Propenoic acid, 1-methylundecyl ester
C15H28O2; MF: 643; RMF: 682; Prob 7.97%; CAS: 51443-73-3; Lib: mainlib; ID: 17815.



MW: 240 (mainlib) 2-Propenoic acid, 1-methylundecyl ester



Name: 2-Propenoic acid, 1-methylundecyl ester
Formula: $C_{15}H_{28}O_2$
MW: 240 Exact Mass: 240.20893 CAS#: 51443-73-3 NIST#: 245665 ID#: 17815 DB: mainlib
Other DBs: EINECS
Contributor: Vladimir Zaikin,TIPS RAS, Moscow, Russia
10 largest peaks:

55 999	41 528	43 515	39 302	44 278	40 270	57 258	42 245	56 237	70 222

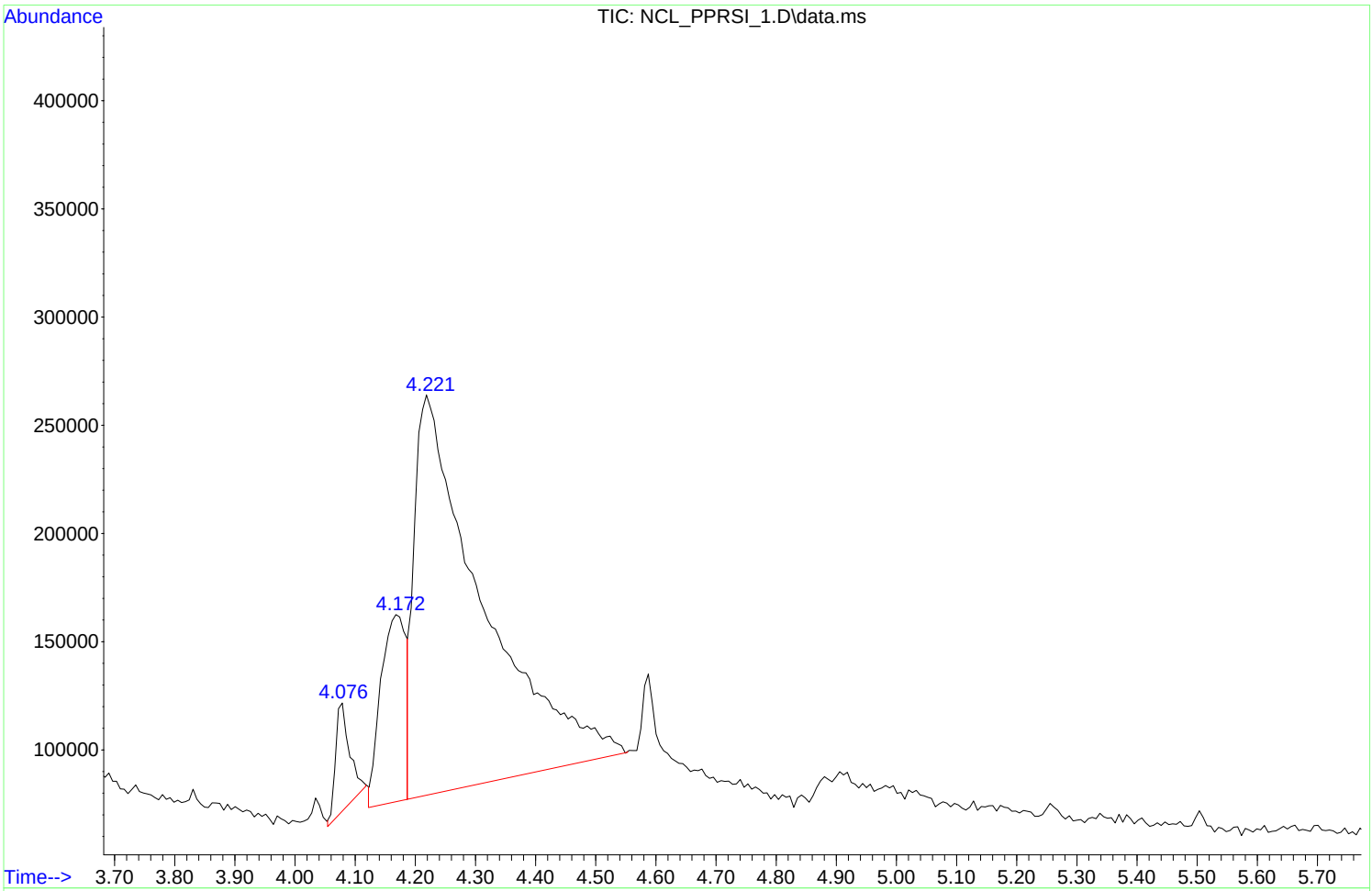
73 m/z Values and Intensities:

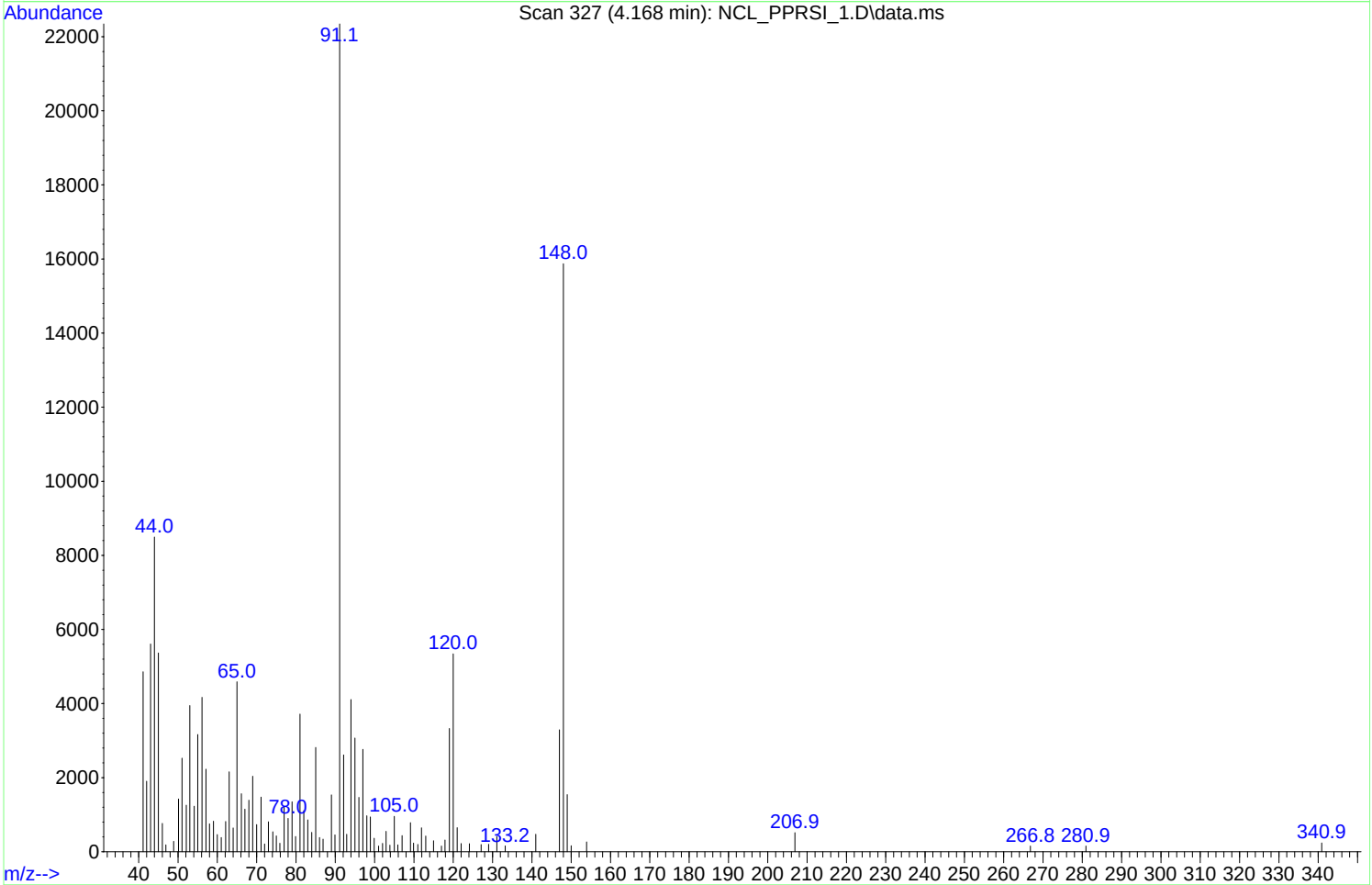
35	8	43	515	54	80	62	8	70	222	78	30	87	10	110	19	126	27	169	10
36	100	44	278	55	999	63	19	71	138	79	22	95	22	111	60	127	20		
37	39	45	60	56	237	64	8	72	70	81	53	96	40	112	35	138	5		
38	75	49	18	57	258	65	6	73	85	82	60	97	130	113	10	139	10		
39	302	50	71	58	122	66	11	74	25	83	157	98	85	114	25	140	22		
40	270	51	90	59	30	67	80	75	35	84	108	99	165	115	8	141	6		
41	528	52	40	60	5	68	57	76	35	85	69	100	10	124	8	167	5		
42	245	53	68	61	6	69	210	77	25	86	7	109	10	125	30	168	65		

Synonyms:

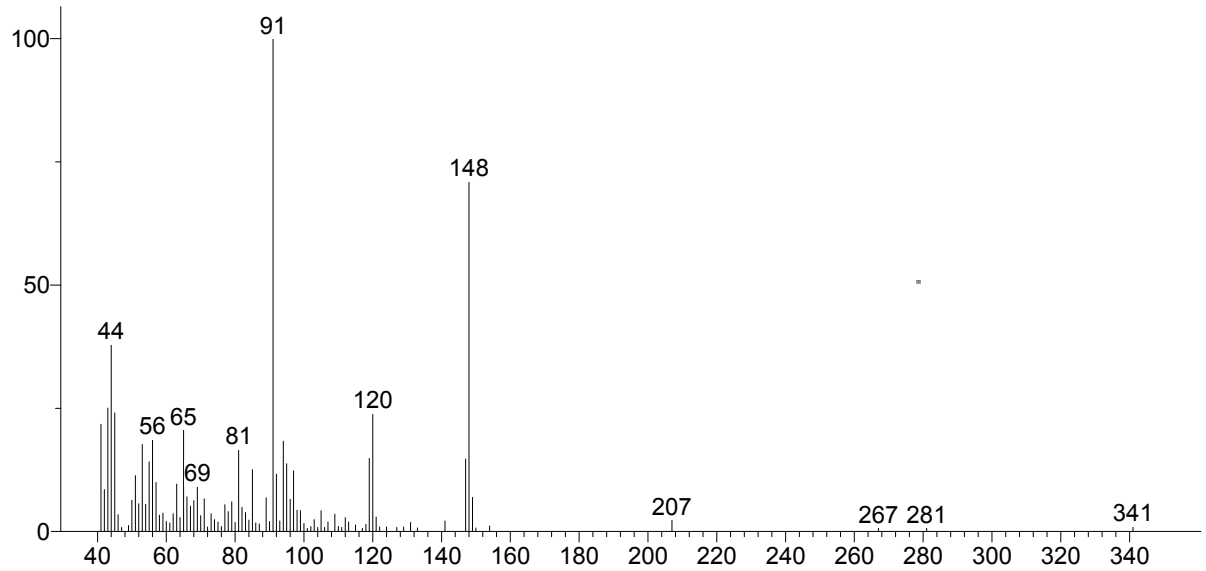
1.2-(Prop-2-enoyloxy)dodecane
2.1-Methylundecyl acrylate #

File :D:\NCL\DATA\OCD\Year_2023\NCL_PPRSI_1.D
Operator : Dr. Borikar
Acquired : 22 Jun 2023 00:40 using AcqMethod General_2022.M
Instrument : GC MSD
Sample Name: PPMI
Misc Info : PPMI
Vial Number: 1





Unknown; InLib=-733



(Text File) Scan 327 (4.168 min): NCL_PPRSI_1.D\data.ms

Name: Scan 327 (4.168 min): NCL_PPRSI_1.D\data.ms
MW: N/A ID#: 27028 DB: Text File
Comment: PPMI
10 largest peaks:

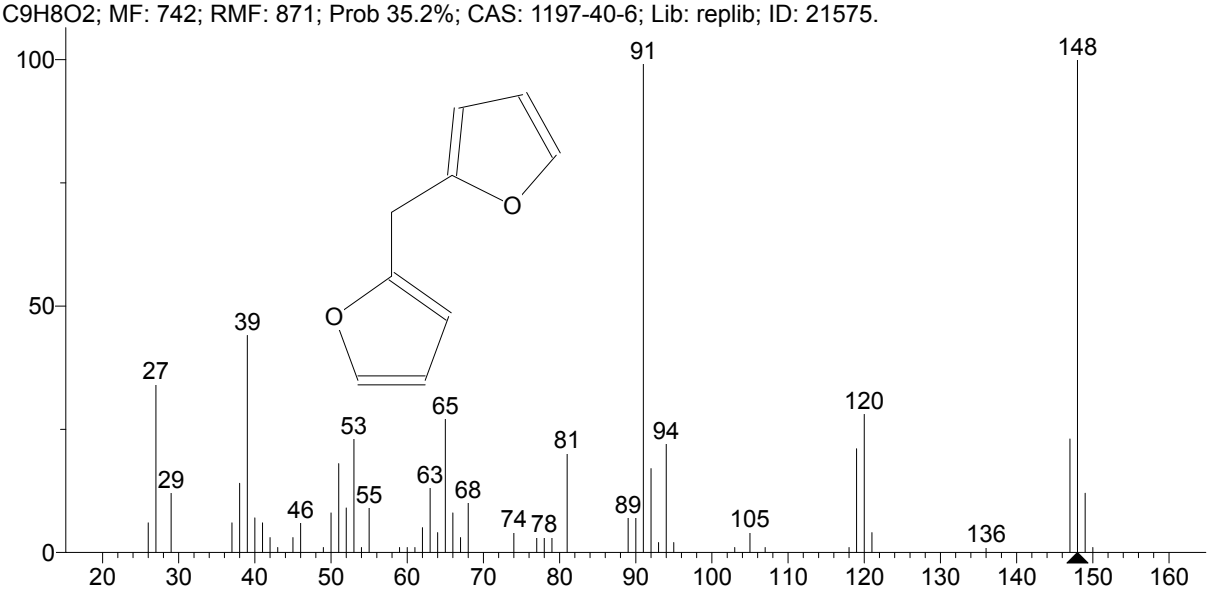
91 999	148 709	44 379	43 250	45 240	120 239	41 217	65 205	56 186	94 183

92 m/z Values and Intensities:

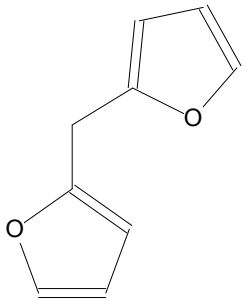
41	217	52	56	62	36	72	9	82	49	93	21	103	24	115	13	131	18	281	7
42	85	53	176	63	96	73	36	83	38	94	183	104	8	117	6	133	7	341	10
43	250	54	55	64	28	74	24	84	23	95	137	105	42	118	14	141	21		
44	379	55	141	65	205	75	19	85	125	96	65	106	8	119	148	147	147		
45	240	56	186	66	70	76	10	86	17	97	123	107	19	120	239	148	709		
46	34	57	99	67	51	77	54	87	15	98	43	109	35	121	29	149	69		
47	8	58	33	68	62	78	40	89	68	99	42	110	10	122	9	150	7		
49	12	59	37	69	91	79	60	90	20	100	16	111	8	124	9	154	11		
50	63	60	20	70	32	80	18	91	999	101	6	112	28	127	8	207	23		
51	113	61	17	71	66	81	166	92	116	102	10	113	19	129	9	267	7		

Synonyms:
no synonyms.

Hit 1 : Furan, 2,2'-methylenebis-
C9H8O2; MF: 742; RMF: 871; Prob 35.2%; CAS: 1197-40-6; Lib: replib; ID: 21575.



MW: 148 (replib) Furan, 2,2'-methylenebis-



Name: Furan, 2,2'-methylenebis-
Formula: $C_9H_8O_2$
MW: 148 Exact Mass: 148.052429 CAS#: 1197-40-6 NIST#: 57706 ID#: 21575 DB: replib
Other DBs: RTECS, HODOC, EINECS
Contributor: MASS SPECTRA OF ORGANIC COMPOUNDS, V. 5, B. H. KENNETT ET AL, DIV. OF FOOD RESEARCH, CSIRO, AUSTRALIA
10 largest peaks:

148 999	91 990	39 440	27 340	120 280	65 270	53 230	147 230	94 220	119 210

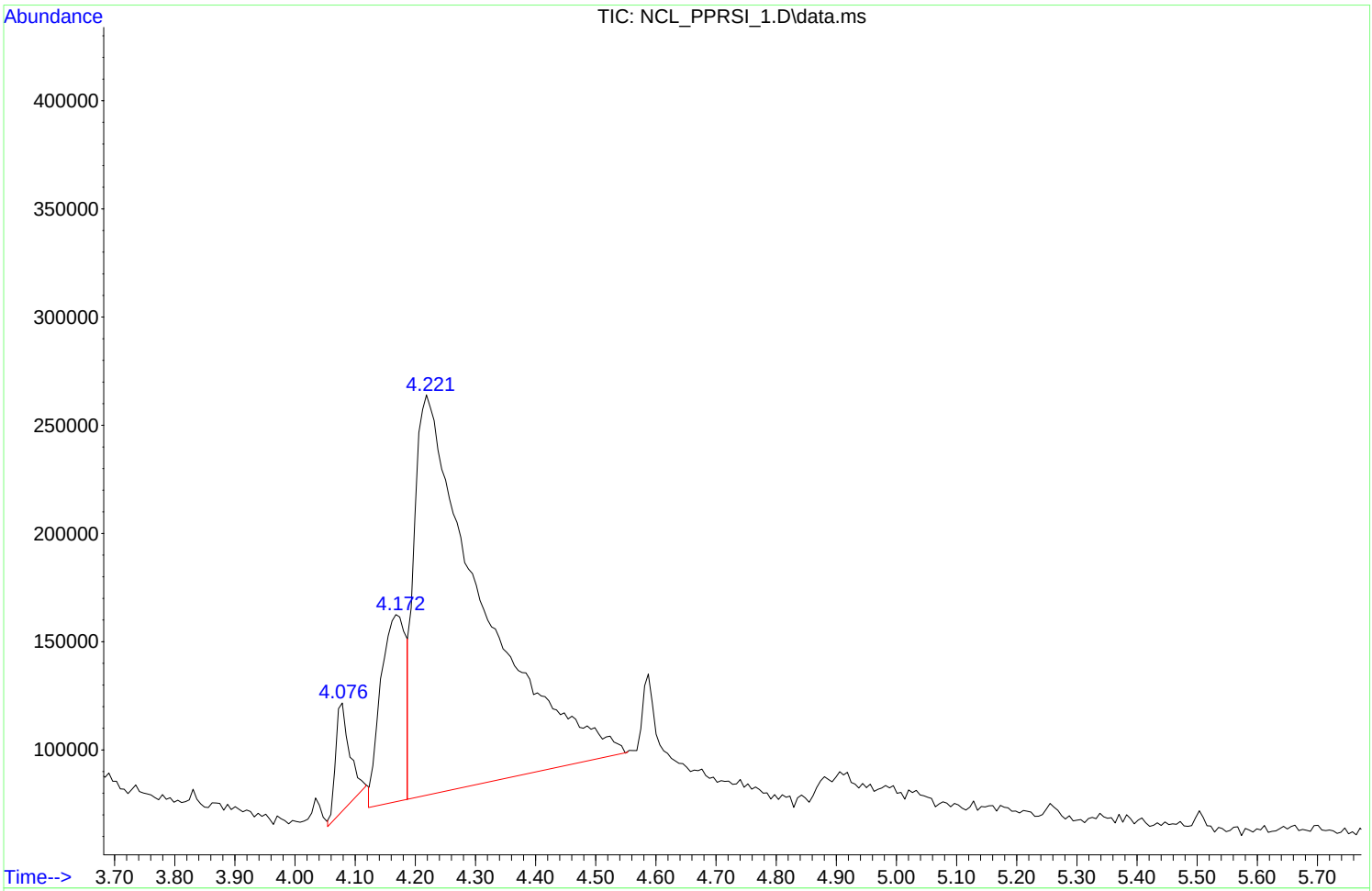
53 m/z Values and Intensities:

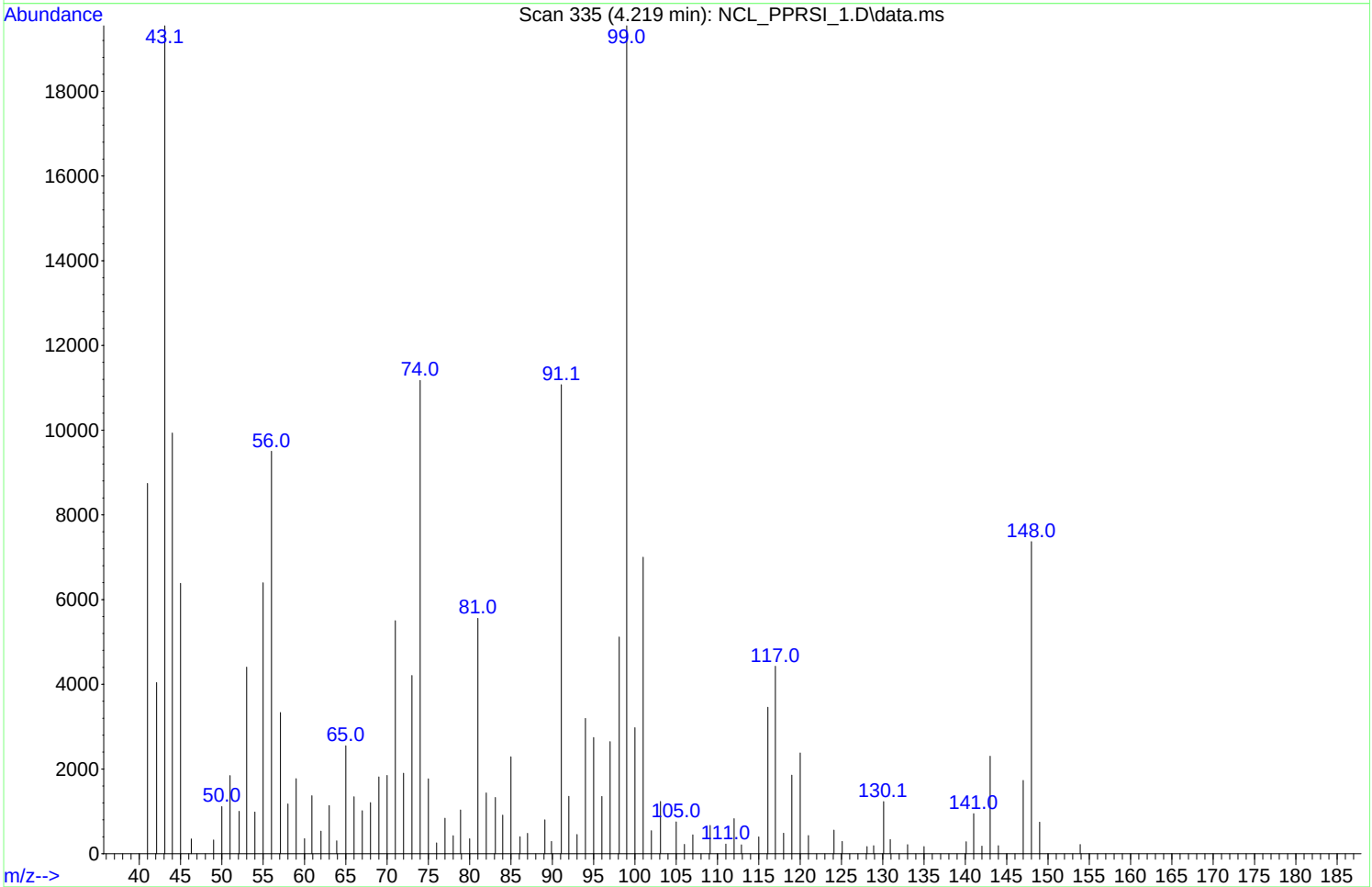
26	60	40	70	49	10	55	90	64	40	77	30	91	990	105	40	136	10
27	340	41	60	50	80	59	10	65	270	78	30	92	170	107	10	147	230
29	120	42	30	51	180	60	10	66	80	79	30	93	20	118	10	148	999
37	60	43	10	52	90	61	10	67	30	81	200	94	220	119	210	149	120
38	140	45	30	53	230	62	50	68	100	89	70	95	20	120	280	150	10
39	440	46	60	54	10	63	130	74	40	90	70	103	10	121	40		

Synonyms:
1.Furan, 2,2'-methylenedi-

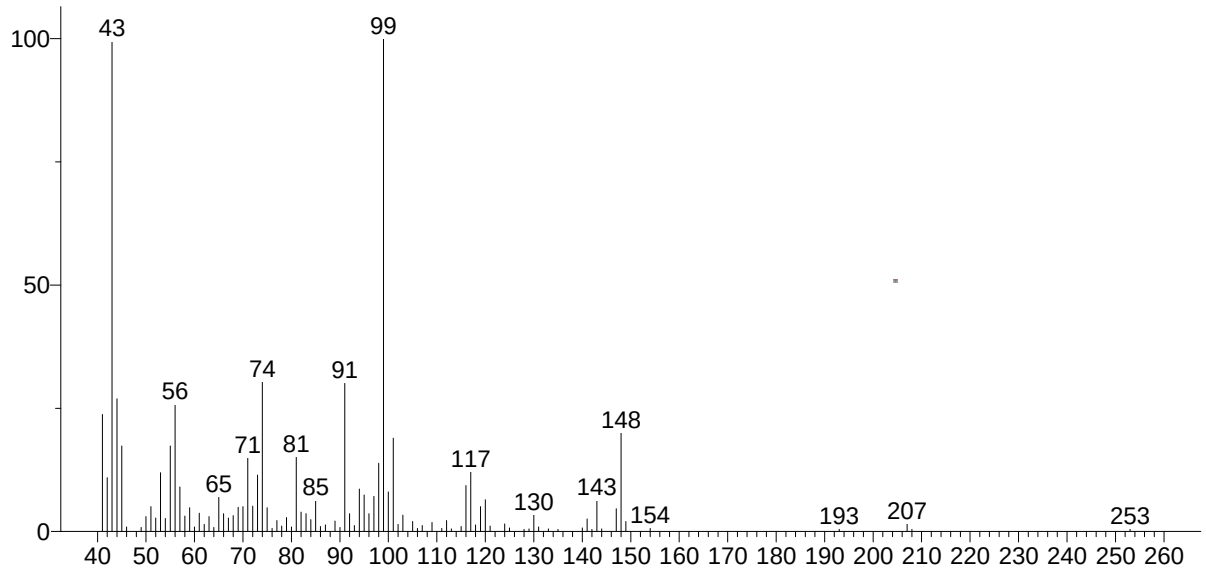
2.Di-α-furylmethane
3.2-Furfurylfuran
4.2,2'-Difurylmethane
5.2-(2-Furylmethyl)furan #
6.2,2'-Methylenebisfuran
7.2,2'-Methylene difuran

File :D:\NCL\DATA\OCD\Year_2023\NCL_PPRSI_1.D
Operator : Dr. Borikar
Acquired : 22 Jun 2023 00:40 using AcqMethod General_2022.M
Instrument : GC MSD
Sample Name: PPMI
Misc Info : PPMI
Vial Number: 1





Unknown; InLib=-988



(Text File) Scan 335 (4.219 min): NCL_PPRSI_1.D\data.ms

Name: Scan 335 (4.219 min): NCL_PPRSI_1.D\data.ms
MW: N/A ID#: 27029 DB: Text File
Comment: PPMI
10 largest peaks:

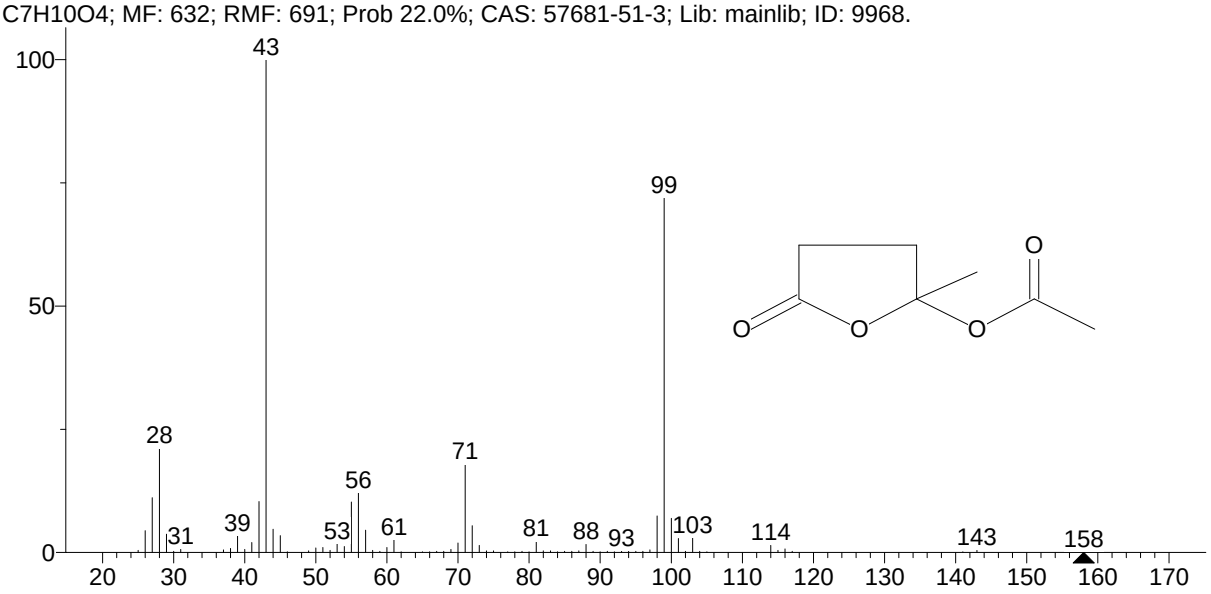
99 999	43 993	74 303	91 300	44 269	56 257	41 237	148 199	101 189	45 173

95 m/z Values and Intensities:

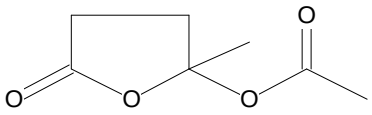
41	237	53	119	63	30	73	114	83	36	94	86	105	20	118	13	133	5	154	6
42	109	54	26	64	8	74	303	84	24	95	74	106	6	119	50	135	4	193	5
43	993	55	173	65	69	75	48	85	62	96	36	107	12	120	64	140	7	207	15
44	269	56	257	66	36	76	6	86	10	97	71	109	18	121	11	141	25	208	4
45	173	57	90	67	27	77	22	87	13	98	138	111	6	124	15	142	4	253	4
46	9	58	31	68	32	78	11	89	21	99	999	112	22	125	7	143	62		
49	8	59	48	69	49	79	28	90	8	100	80	113	5	128	4	144	5		
50	30	60	9	70	50	80	9	91	300	101	189	115	10	129	5	147	46		
51	50	61	37	71	149	81	150	92	36	102	14	116	93	130	33	148	199		
52	27	62	14	72	51	82	39	93	12	103	33	117	120	131	9	149	20		

Synonyms:
no synonyms.

Hit 1 : 2(3H)-Furanone, 5-(acetyloxy)dihydro-5-methyl-
C7H10O4; MF: 632; RMF: 691; Prob 22.0%; CAS: 57681-51-3; Lib: mainlib; ID: 9968.



MW: 158 (mainlib) 2(3H)-Furanone, 5-(acetyloxy)dihydro-5-methyl-



Name: 2(3H)-Furanone, 5-(acetyloxy)dihydro-5-methyl-
Formula: $C_7H_{10}O_4$
MW: 158 Exact Mass: 158.057909 CAS#: 57681-51-3 NIST#: 189398 ID#: 9968 DB: mainlib
Other DBs: None
Contributor: Chemical Concepts
10 largest peaks:

43	999	99	718	28	210	71	178	56	120	27	111	42	103	55	102	98	74	100	69

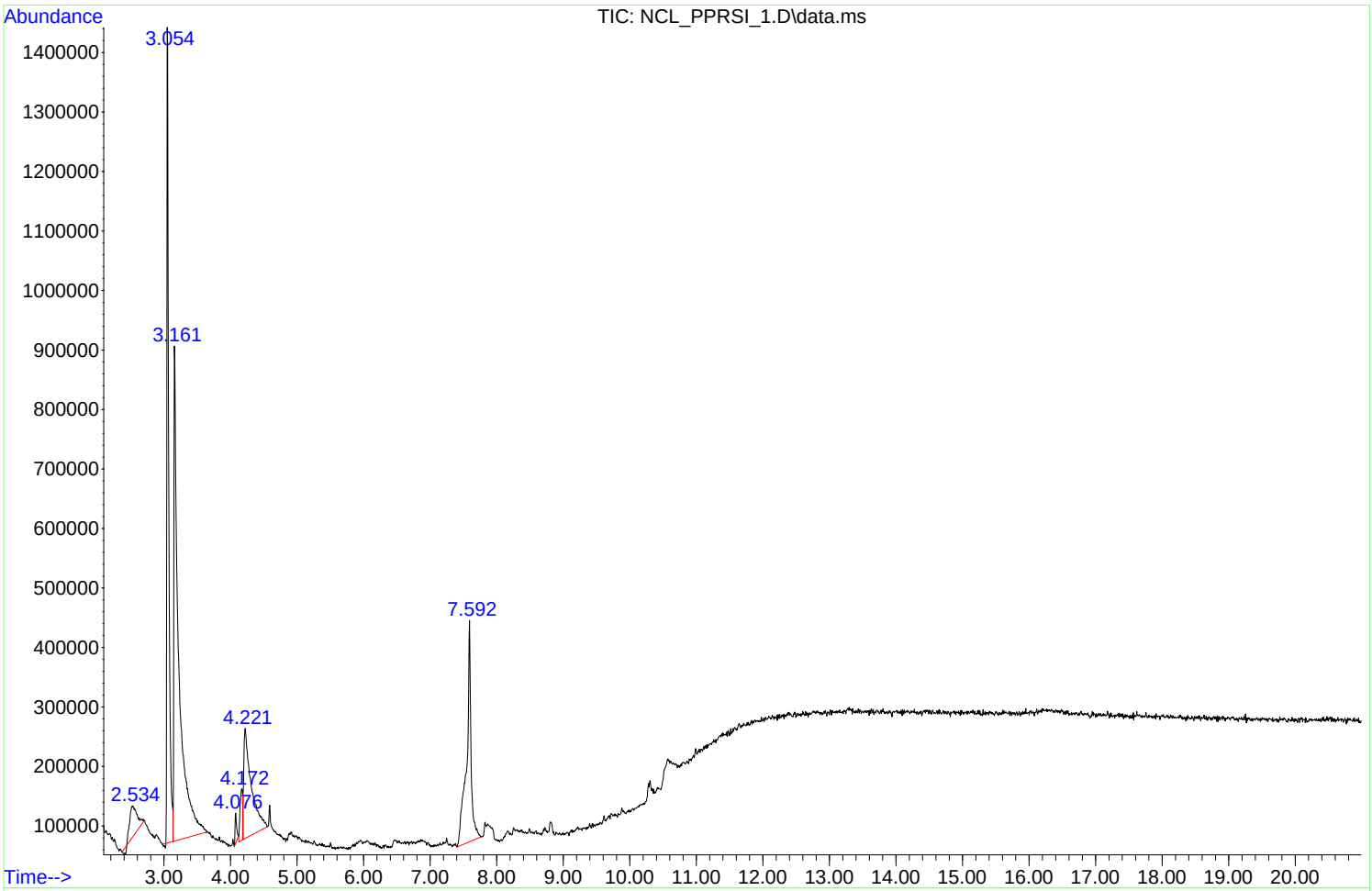
78 m/z Values and Intensities:

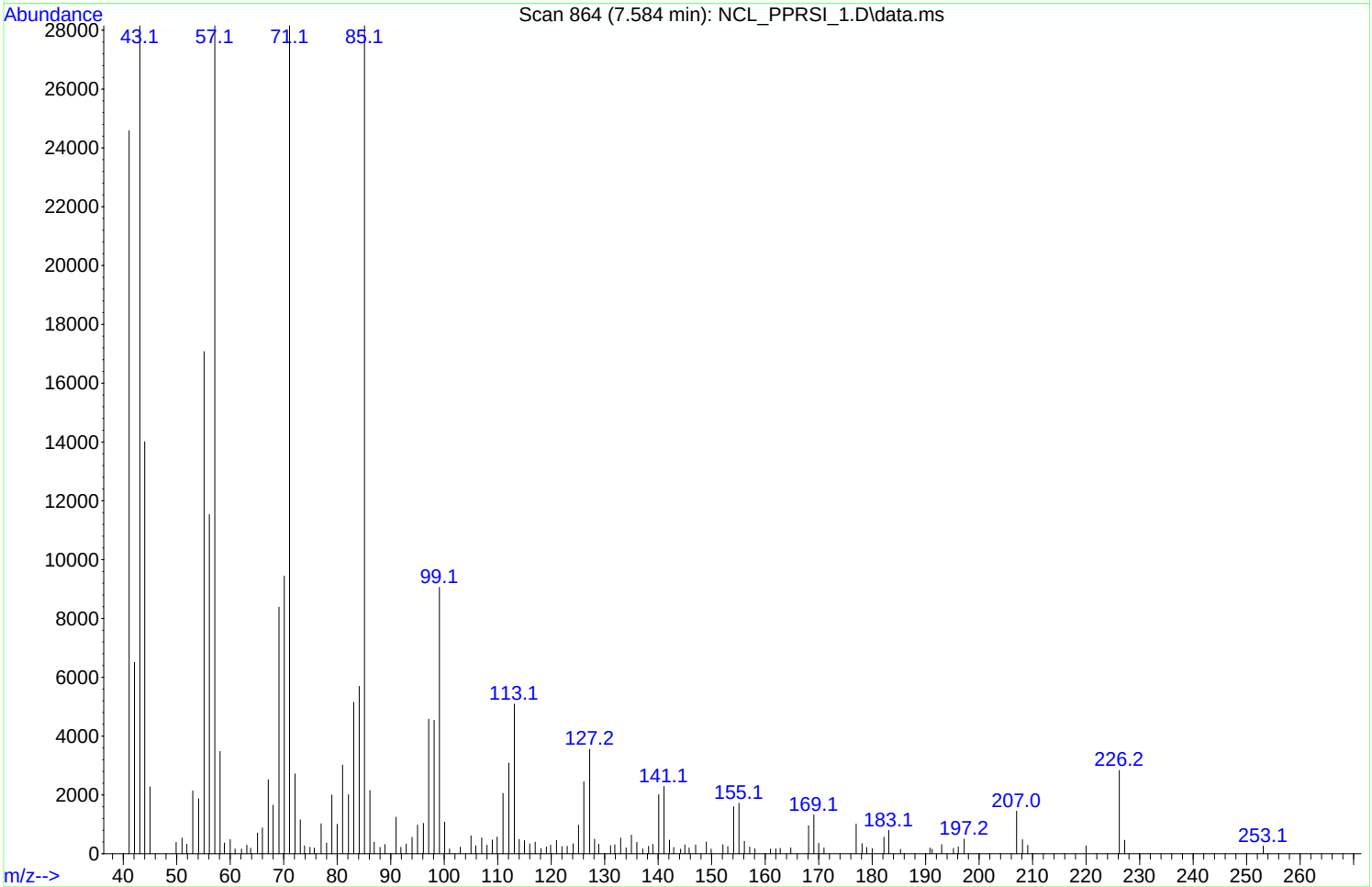
25	4	38	8	46	1	56	120	66	1	74	3	83	3	91	2	99	718	115	4
26	44	39	33	49	3	57	45	67	2	75	3	84	1	92	1	100	69	116	7
27	111	40	6	50	9	58	4	68	2	77	1	85	2	93	2	101	28	117	2
28	210	41	20	51	10	59	2	69	6	78	1	86	2	94	2	102	2	141	1
29	37	42	103	52	4	60	10	70	19	79	2	87	3	95	2	103	29	143	4
30	2	43	999	53	17	61	25	71	178	80	1	88	16	96	2	104	2	158	1
31	6	44	47	54	12	62	1	72	54	81	22	89	2	97	5	105	1		
37	5	45	34	55	102	65	1	73	14	82	3	90	1	98	74	114	14		

Synonyms:

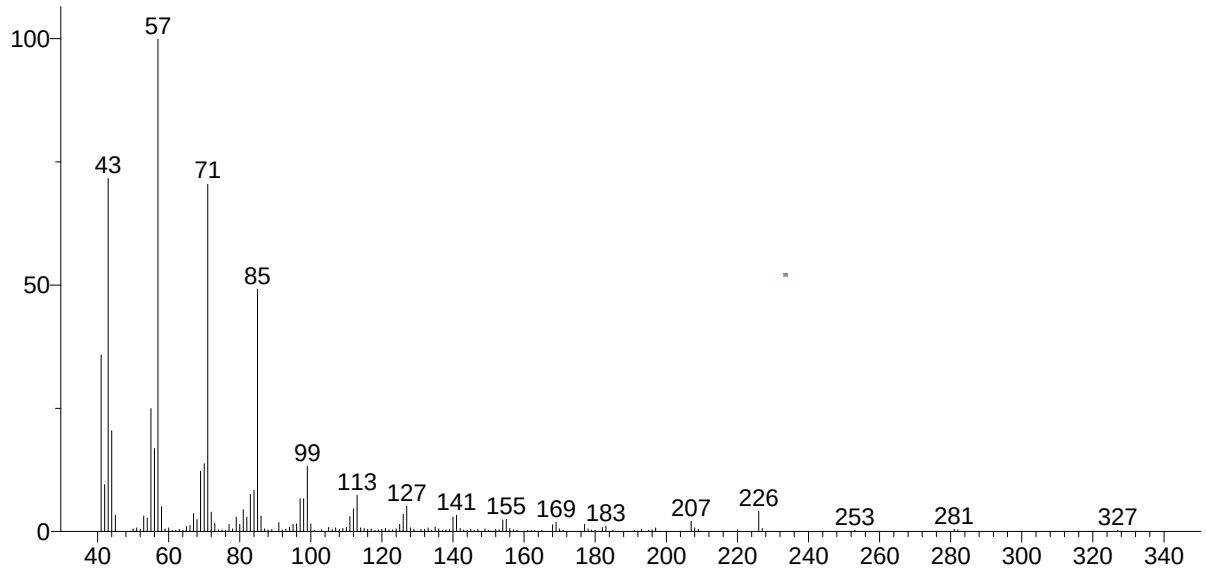
1.2-Methyl-5-oxotetrahydro-2-furanyl acetate #

File :D:\NCL\DATA\OCD\Year_2023\NCL_PPRSI_1.D
Operator : Dr. Borikar
Acquired : 22 Jun 2023 00:40 using AcqMethod General_2022.M
Instrument : GC MSD
Sample Name: PPMI
Misc Info : PPMI
Vial Number: 1





Unknown; InLib=-224



(Text File) Scan 864 (7.584 min): NCL_PPRSI_1.D\data.ms

Name: Scan 864 (7.584 min): NCL_PPRSI_1.D\data.ms
MW: N/A ID#: 27030 DB: Text File
Comment: PPMI
10 largest peaks:

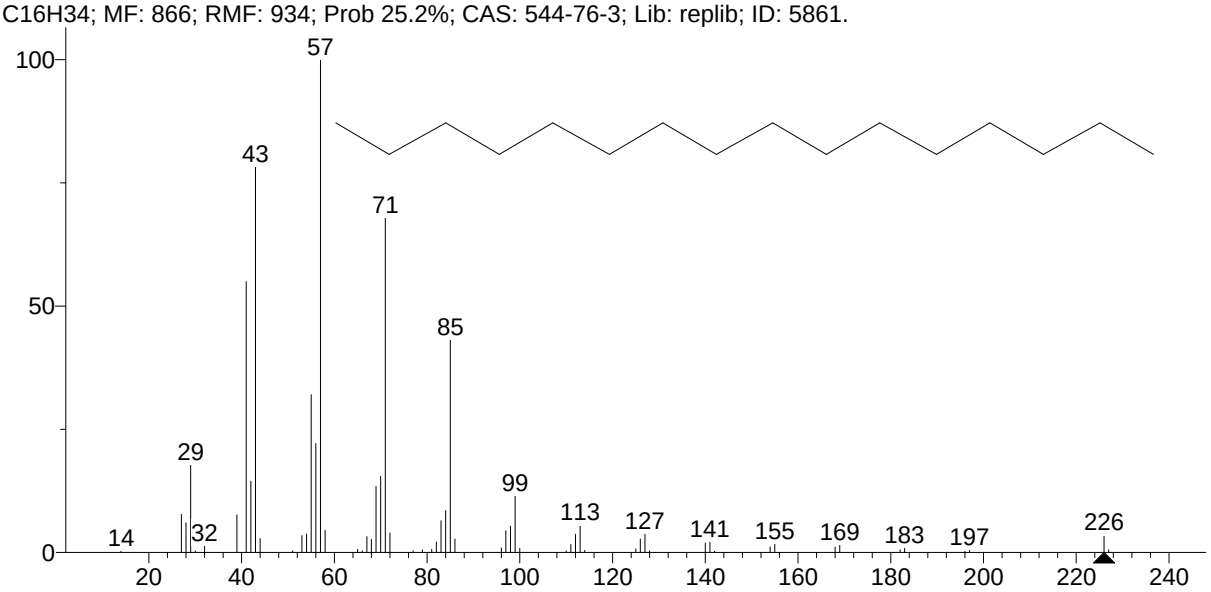
57 999	43 716	71 705	85 492	41 358	55 249	44 204	56 168	70 137	99 132

138 m/z Values and Intensities:

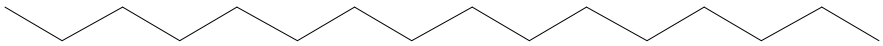
41	358	59	5	73	16	87	5	103	3	118	2	133	7	147	4	168	13	196	3
42	95	60	7	74	3	88	3	105	8	119	3	134	2	149	5	169	19	197	7
43	716	61	2	75	3	89	4	106	4	120	4	135	9	150	2	170	5	207	21
44	204	62	2	76	2	91	18	107	7	121	6	136	5	152	4	171	2	208	7
45	33	63	4	77	14	92	3	108	4	122	3	137	2	153	3	177	14	209	4
50	5	64	2	78	5	93	4	109	6	123	3	138	3	154	23	178	5	220	3
51	7	65	10	79	29	94	8	110	8	124	5	139	4	155	25	179	3	226	41
52	4	66	12	80	14	95	14	111	30	125	14	140	29	156	6	180	2	227	6
53	31	67	36	81	44	96	15	112	45	126	35	141	33	157	3	182	8	253	3
54	27	68	24	82	29	97	66	113	74	127	51	142	6	158	2	183	11	281	5
55	249	69	122	83	75	98	66	114	7	128	7	143	3	161	2	185	2	282	3
56	168	70	137	84	83	99	132	115	6	129	4	144	2	162	2	191	2	327	2
57	999	71	705	85	492	100	15	116	4	131	4	145	4	163	2	193	4		
58	50	72	39	86	31	101	2	117	5	132	4	146	2	165	2	195	2		

Synonyms:
no synonyms.

Hit 1 : Hexadecane
C16H34; MF: 866; RMF: 934; Prob 25.2%; CAS: 544-76-3; Lib: replib; ID: 5861.



MW: 226 (replib) Hexadecane



Name: Hexadecane
Formula: $C_{16}H_{34}$
MW: 226 Exact Mass: 226.266051 CAS#: 544-76-3 NIST#: 114191 ID#: 5861 DB: replib
Other DBs: Fine, TSCA, RTECS, EPA, HODOC, NIH, EINECS, IRDB
Contributor: NIST Mass Spectrometry Data Center, 1990.
10 largest peaks:

57 999	43 781	71 678	41 549	85 431	55 320	56 221	29 177	70 154	42 144

61 m/z Values and Intensities:

14	3	41	549	55	320	68	26	81	6	97	44	113	54	141	21	183	8
27	77	42	144	56	221	69	134	82	21	98	53	114	4	142	2	196	2
28	60	43	781	57	999	70	154	83	64	99	114	125	7	154	11	197	4
29	177	44	28	58	45	71	678	84	85	100	8	126	27	155	17	226	34
30	3	51	3	65	6	72	39	85	431	110	3	127	37	168	11	227	5
32	13	53	34	66	3	77	3	86	27	111	16	128	3	169	15		
39	76	54	37	67	32	79	5	96	9	112	37	140	19	182	5		

Synonyms:
1.n-Cetane

2.n-Hexadecane
3.Cetane