

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051023\
 Data File : VY013694.D
 Acq On : 10 May 2023 17:40
 Operator : KP/MD
 Sample : 02719-04
 Misc : 6.25g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SB-04_10-12_20230509

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042423S.M
 Title : SW846 8260

Signal : TIC: VY013694.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.857	3	6	12	rVB3	3783	5675	27.77%	3.280%
2	2.180	58	59	61	rBV	1133	910	4.45%	0.526%
3	2.290	75	77	80	rVB4	1273	1549	7.58%	0.895%
4	2.320	80	82	86	rVB3	1106	1240	6.07%	0.717%
5	2.351	86	87	89	rBV2	757	554	2.71%	0.320%
6	2.503	110	112	116	rVB5	977	1312	6.42%	0.758%
7	2.570	121	123	126	rBV3	385	421	2.06%	0.243%
8	2.662	134	138	141	rBV3	578	756	3.70%	0.437%
9	2.796	158	160	164	rVB2	613	611	2.99%	0.353%
10	2.851	166	169	171	rBV2	313	452	2.21%	0.261%
11	2.948	184	185	189	rBV3	293	429	2.10%	0.248%
12	3.156	217	219	223	rBV4	417	626	3.06%	0.362%
13	3.302	240	243	246	rVB2	318	398	1.95%	0.230%
14	3.540	281	282	285	rBV2	416	410	2.01%	0.237%
15	3.710	308	310	316	rVB2	372	525	2.57%	0.303%
16	4.247	397	398	401	rVB	577	415	2.03%	0.240%
17	4.399	420	423	426	rBV2	381	596	2.92%	0.344%
18	4.588	452	454	456	rBV2	369	415	2.03%	0.240%
19	4.698	467	472	473	rBV4	836	1032	5.05%	0.596%
20	4.722	473	476	479	rVB4	1099	1439	7.04%	0.832%
21	4.863	496	499	502	rBV2	328	375	1.84%	0.217%
22	5.058	528	531	535	rBV2	407	874	4.28%	0.505%
23	5.137	541	544	546	rBV	457	454	2.22%	0.262%
24	5.210	553	556	560	rBV	469	453	2.22%	0.262%
25	5.381	583	584	587	rVB2	420	426	2.08%	0.246%
26	5.405	587	588	591	rBV2	335	400	1.96%	0.231%
27	5.576	615	616	621	rVB2	298	454	2.22%	0.262%
28	5.655	626	629	630	rBV	420	413	2.02%	0.239%
29	5.722	636	640	641	rBV2	387	415	2.03%	0.240%
30	6.106	700	703	705	rVV	382	460	2.25%	0.266%
31	6.484	763	765	767	rBV2	436	456	2.23%	0.264%
32	6.631	788	789	794	rBV2	334	404	1.98%	0.233%
33	6.887	826	831	834	rBV2	403	764	3.74%	0.442%
34	7.021	851	853	856	rBV2	307	387	1.89%	0.224%
35	7.216	880	885	886	rBV2	388	468	2.29%	0.270%
36	7.411	915	917	920	rVB2	569	510	2.50%	0.295%

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37	7.533	934	937	939	rVB3	450	482	2.36%	0.279%
38	7.710	961	966	973	rBV5	3369	7690	37.63%	4.444%
39	7.789	973	979	988	rVB2	5050	11347	55.53%	6.558%
40	8.142	1028	1037	1044	rVV5	4529	10266	50.24%	5.933%
41	8.502	1093	1096	1099	rVB2	360	476	2.33%	0.275%
42	8.685	1121	1126	1134	rVB2	7610	14953	73.18%	8.642%
43	8.764	1134	1139	1141	rVB3	320	498	2.44%	0.288%
44	8.941	1162	1168	1177	rVB5	3991	8598	42.08%	4.969%
45	9.063	1187	1188	1192	rBV2	500	476	2.33%	0.275%
46	9.112	1192	1196	1197	rBV2	372	385	1.88%	0.223%
47	9.313	1228	1229	1233	rVB3	401	425	2.08%	0.246%
48	9.600	1275	1276	1281	rVB	377	481	2.35%	0.278%
49	9.923	1327	1329	1331	rBV	473	404	1.98%	0.233%
50	10.179	1365	1371	1379	rBV2	11538	20434	100.00%	11.810%
51	10.313	1389	1393	1396	rBV2	290	537	2.63%	0.310%
52	10.526	1426	1428	1430	rVV2	448	504	2.47%	0.291%
53	10.709	1455	1458	1459	rBV2	439	398	1.95%	0.230%
54	10.886	1486	1487	1490	rBV2	500	478	2.34%	0.276%
55	11.160	1531	1532	1537	rBV2	469	387	1.89%	0.224%
56	11.361	1562	1565	1566	rBV2	374	376	1.84%	0.217%
57	11.489	1580	1586	1594	rBV2	10956	18217	89.15%	10.528%
58	11.831	1640	1642	1647	rBV2	325	516	2.53%	0.298%
59	12.008	1668	1671	1672	rVB2	410	428	2.09%	0.247%
60	12.020	1672	1673	1675	rBV	726	583	2.85%	0.337%
61	12.093	1683	1685	1687	rVB2	503	379	1.85%	0.219%
62	12.148	1692	1694	1699	rBV3	495	409	2.00%	0.236%
63	12.312	1718	1721	1723	rVB2	350	398	1.95%	0.230%
64	12.392	1730	1734	1738	rBV3	464	833	4.08%	0.481%
65	12.483	1743	1749	1756	rBV3	7443	12170	59.56%	7.034%
66	12.605	1765	1769	1771	rBV2	432	569	2.78%	0.329%
67	12.636	1771	1774	1775	rBV2	290	388	1.90%	0.224%
68	12.678	1779	1781	1784	rBV	546	639	3.13%	0.369%
69	13.081	1843	1847	1850	rBV3	523	768	3.76%	0.444%
70	13.270	1876	1878	1882	rVB3	567	805	3.94%	0.465%
71	13.385	1894	1897	1898	rBV3	415	430	2.10%	0.249%
72	13.422	1898	1903	1910	rVB3	6071	9639	47.17%	5.571%
73	13.501	1913	1916	1922	rBV3	627	877	4.29%	0.507%
74	13.556	1924	1925	1929	rBV	395	466	2.28%	0.269%
75	13.727	1950	1953	1954	rBV2	447	500	2.45%	0.289%
76	13.745	1954	1956	1959	rVV3	474	564	2.76%	0.326%

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77	13.800	1962	1965	1968	rBV2	561	778	3.81%	0.450%
78	13.830	1968	1970	1973	rVB2	483	491	2.40%	0.284%
79	13.971	1989	1993	1994	rVB3	739	877	4.29%	0.507%
80	14.306	2045	2048	2050	rBV2	577	654	3.20%	0.378%
81	14.397	2061	2063	2064	rVB	878	505	2.47%	0.292%
82	14.483	2075	2077	2080	rVB3	568	659	3.23%	0.381%
83	14.507	2080	2081	2086	rBV3	344	447	2.19%	0.258%
84	14.550	2086	2088	2089	rBV2	709	423	2.07%	0.244%
85	14.696	2110	2112	2113	rBV2	701	486	2.38%	0.281%
86	14.763	2121	2123	2125	rBV2	542	501	2.45%	0.290%
87	14.971	2155	2157	2160	rVB2	825	961	4.70%	0.555%
88	15.013	2162	2164	2166	rBV2	390	377	1.84%	0.218%
89	15.208	2193	2196	2197	rBV2	989	1009	4.94%	0.583%
90	15.318	2210	2214	2216	rBV4	1042	1496	7.32%	0.865%
91	15.452	2232	2236	2237	rBV2	653	798	3.91%	0.461%
92	15.537	2248	2250	2253	rVB3	966	1075	5.26%	0.621%
93	15.659	2268	2270	2273	rBV4	584	590	2.89%	0.341%
94	15.818	2295	2296	2302	rVB5	740	699	3.42%	0.404%
95	15.928	2312	2314	2316	rBV2	676	484	2.37%	0.280%
96	16.111	2342	2344	2348	rVB4	588	539	2.64%	0.312%
97	16.172	2352	2354	2356	rBV2	491	502	2.46%	0.290%
98	16.263	2367	2369	2370	rBV2	718	598	2.93%	0.346%
99	16.495	2405	2407	2411	rBV5	765	965	4.72%	0.558%
100	16.757	2448	2450	2451	rBV2	652	462	2.26%	0.267%

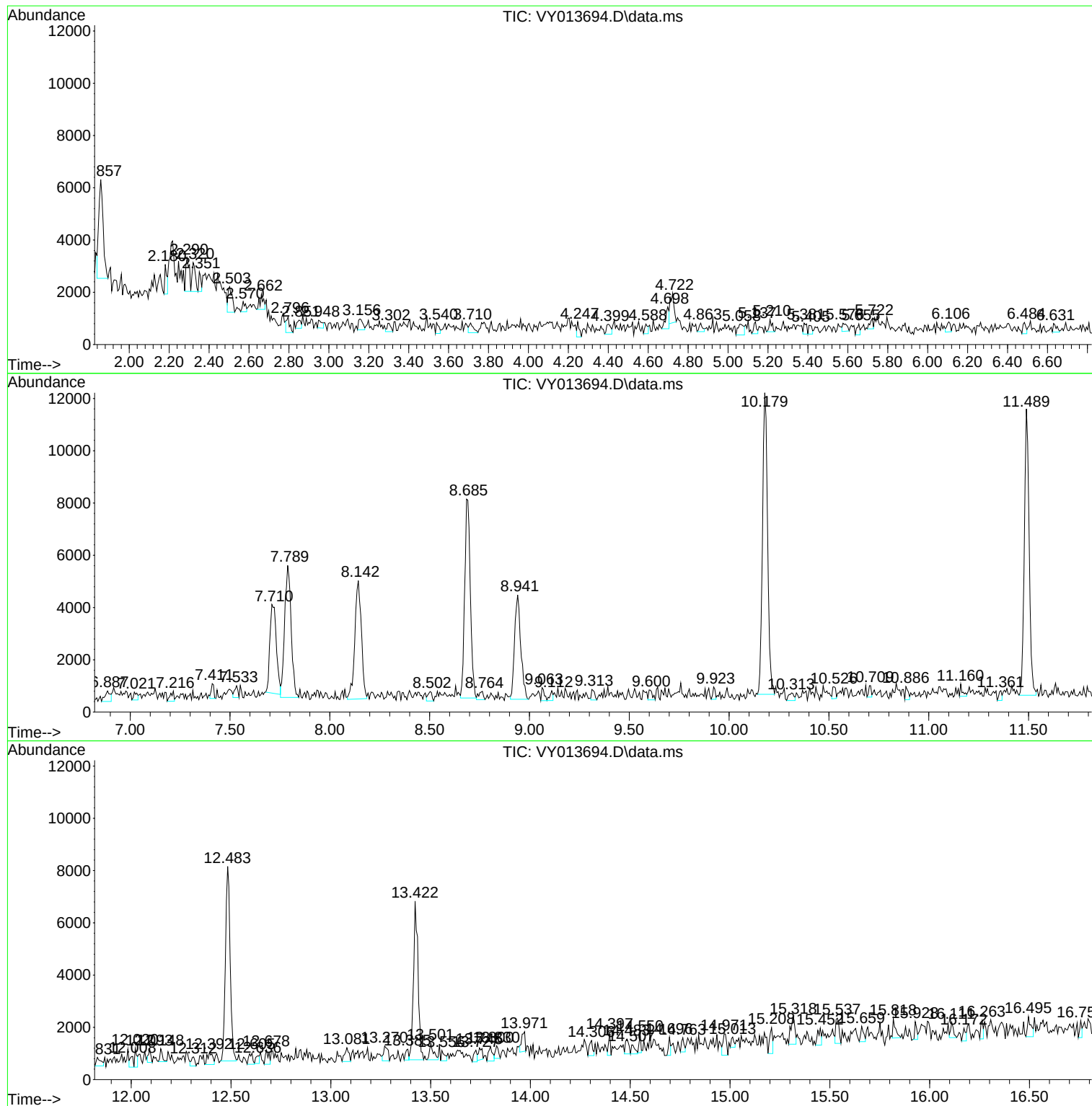
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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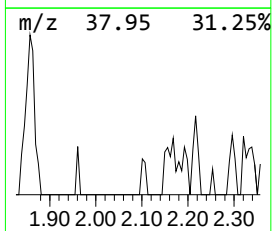
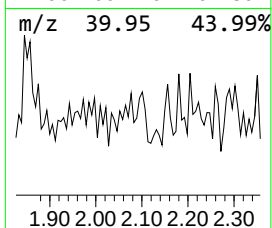
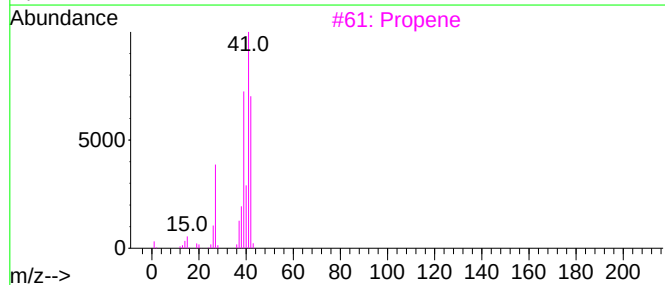
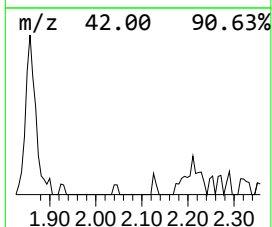
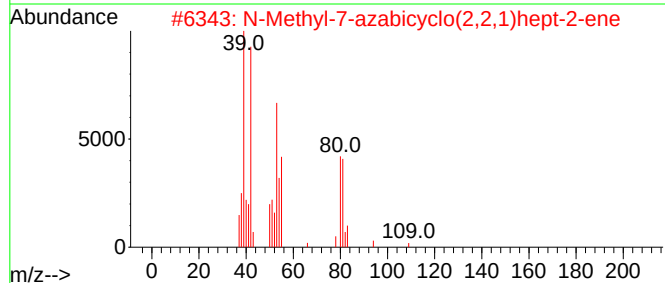
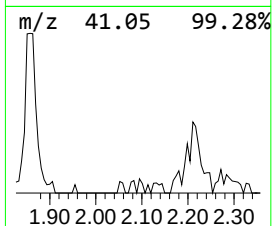
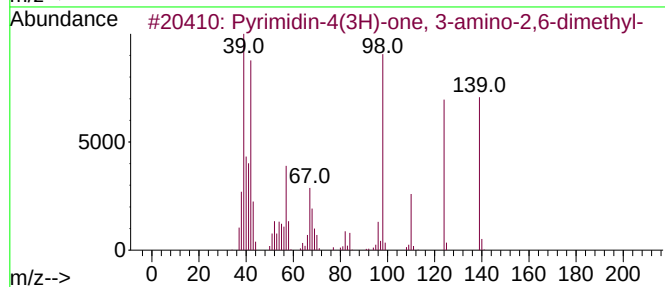
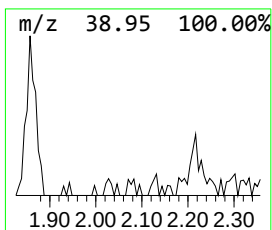
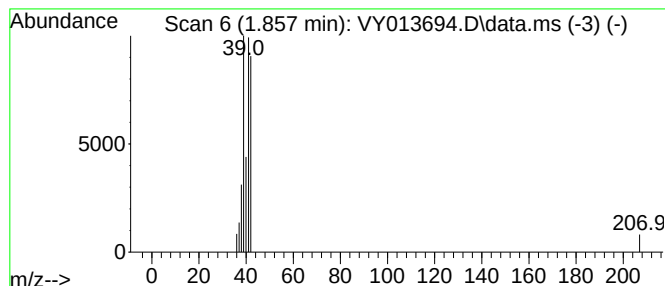
Instrument :
MSVOA_Y
ClientSampleId :
SB-04_10-12_20230509

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042423S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Pyrimidin-4(3H)-one, 3-amin... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.857	25.01 ug/l	5675	Pentafluorobenzene	7.789	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrimidin-4(3H)-one, 3-amino-2,6...	139	C6H9N3O	093098-74-9	83
2	N-Methyl-7-azabicyclo(2,2,1)hept...	109	C7H11N	055590-26-6	74
3	Propene	42	C3H6	000115-07-1	74
4	Cyclopropane	42	C3H6	000075-19-4	72
5	5-Pyrimidinecarboxylic acid, hex...	214	C8H10N2O5	072088-02-9	64



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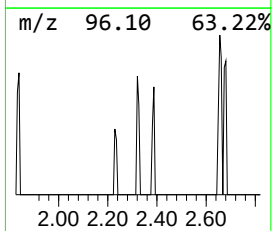
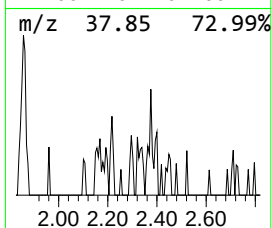
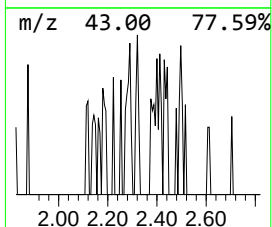
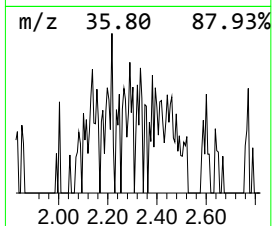
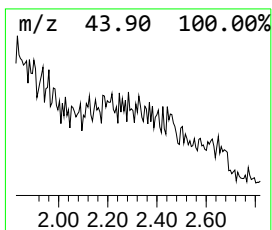
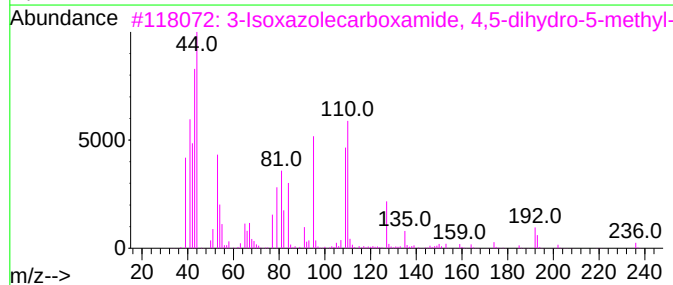
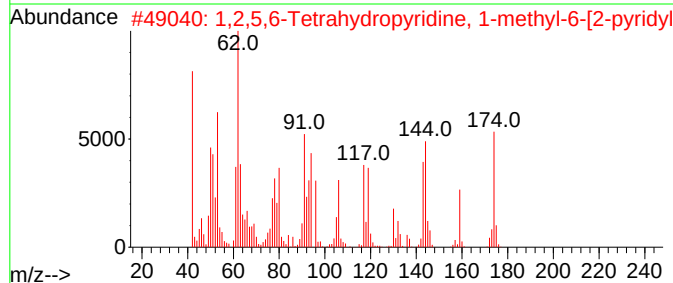
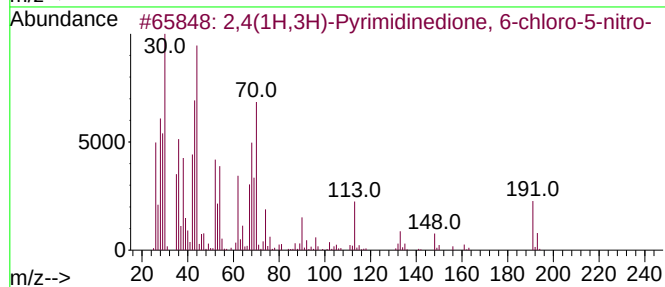
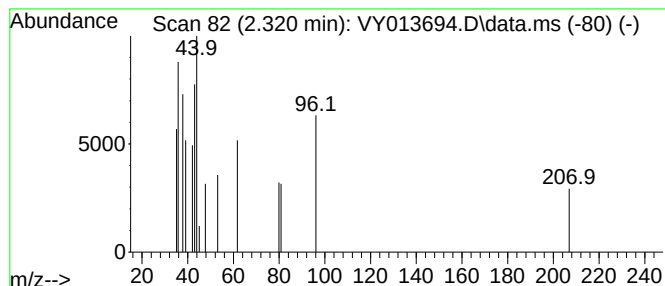
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown2.320 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.320	5.46 ug/l	1240	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4(1H,3H)-Pyrimidinedione, 6-ch...	191	C4H2ClN3O4	006630-30-4	36		
2	1,2,5,6-Tetrahydropyridine, 1-me...	174	C11H14N2	1000132-27-6	9		
3	3-Isoxazolecarboxamide, 4,5-dihy...	236	C12H16N2O3	1000362-31-0	7		
4	2-Chloroethanol	80	C2H5ClO	000107-07-3	5		
5	Ethanethiol	62	C2H6S	000075-08-1	5		



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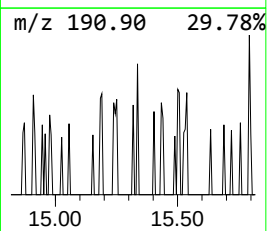
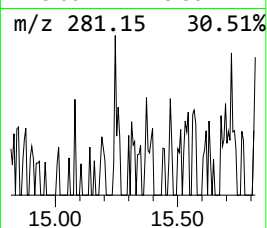
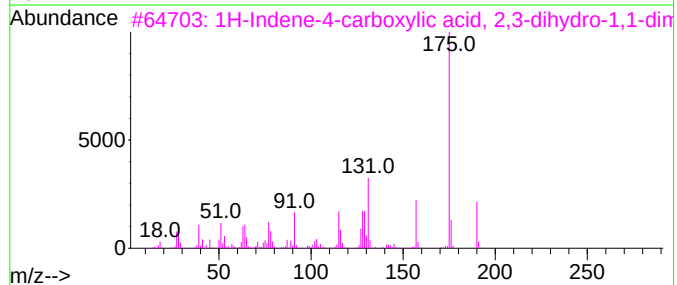
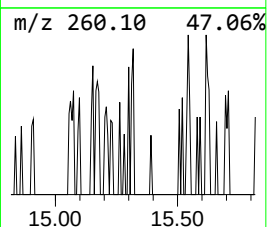
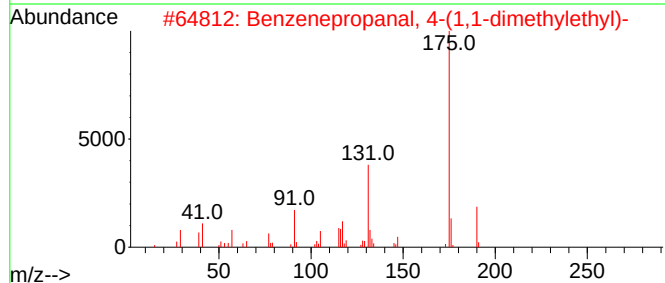
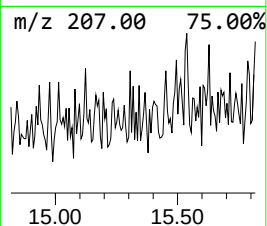
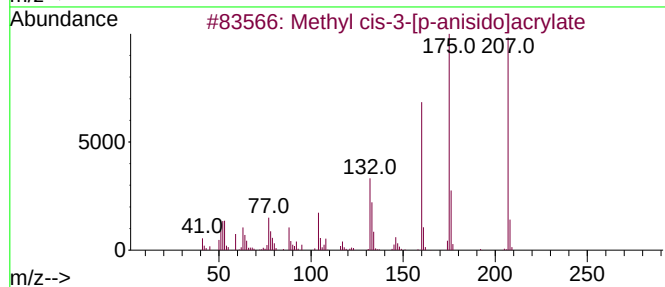
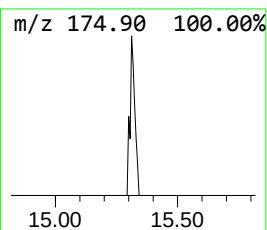
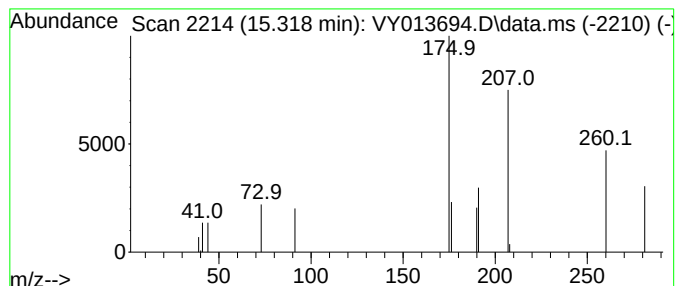
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Peak Number 8 unknown15.318 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.318	7.76 ug/l	1496	1,4-Dichlorobenzene-d4	13.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl cis-3-[p-anisido]acrylate	207	C11H13NO3	007542-88-3	28
2			Benzenepropanal, 4-(1,1-dimethyl...	190	C13H18O	018127-01-0	9
3			1H-Indene-4-carboxylic acid, 2,3...	190	C12H14O2	055712-38-4	9
4			Benzene, 1,3-bis(1,1-dimethyleth...	190	C14H22	001014-60-4	9
5			2H-1-Benzopyran-2-one, 7-amino-4...	175	C10H9NO2	026093-31-2	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051023\
Data File : VY013694.D
Acq On : 10 May 2023 17:40
Operator : KP/MD
Sample : 02719-04
Misc : 6.25g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-04_10-12_20230509

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042423S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pyrimidin-4(3H)...	1.857	25.0	ug/l	5675	1	7.789	11347	50.0
unknown2.320	2.320	5.5	ug/l	1240	1	7.789	11347	50.0
unknown15.318	15.318	7.8	ug/l	1496	4	13.434	9639	50.0