

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV092324\
 Data File : VV037489.D
 Acq On : 23 Sep 2024 17:42
 Operator : SY/MD
 Sample : P4106-02
 Misc : 5mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0SX7

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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_V\Method\SFAMVLM082624WMA.M

Title : VOC Analysis

Signal : TIC: VV037489.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.175	33	42	51	rBV	58825	89649	2.81%	0.363%
2	1.278	67	74	89	rBV	423113	450251	14.11%	1.822%
3	1.532	145	153	170	rVB	354472	422993	13.25%	1.712%
4	2.060	307	317	332	rBV	739654	1063318	33.31%	4.303%
5	2.220	357	367	389	rBV	306126	563159	17.64%	2.279%
6	3.288	697	699	706	rVB6	1425	1143	0.04%	0.005%
7	3.320	706	709	711	rBV2	1285	917	0.03%	0.004%
8	3.365	721	723	728	rVB5	1058	878	0.03%	0.004%
9	3.397	728	733	737	rBV5	723	728	0.02%	0.003%
10	3.458	750	752	758	rVB4	935	622	0.02%	0.003%
11	3.497	762	764	767	rVB3	1270	654	0.02%	0.003%
12	3.568	784	786	791	rVB5	968	582	0.02%	0.002%
13	3.596	791	795	797	rBV4	729	465	0.01%	0.002%
14	3.635	797	807	810	rBV9	5755	9793	0.31%	0.040%
15	3.703	826	828	833	rVB5	1106	637	0.02%	0.003%
16	3.793	847	856	900	rBV2	156613	516655	16.19%	2.091%
17	4.243	979	996	1031	rBV2	505134	1293921	40.54%	5.236%
18	4.513	1076	1080	1083	rBV6	1269	1037	0.03%	0.004%
19	4.564	1093	1096	1103	rVB6	1708	1787	0.06%	0.007%
20	4.613	1103	1111	1112	rBV4	1216	1470	0.05%	0.006%
21	4.677	1125	1131	1133	rBV4	1237	1151	0.04%	0.005%
22	4.712	1138	1142	1144	rVV2	1151	726	0.02%	0.003%
23	4.725	1144	1146	1148	rVV2	1294	631	0.02%	0.003%
24	4.751	1151	1154	1159	rVV7	744	591	0.02%	0.002%
25	4.850	1181	1185	1189	rBV5	1366	1408	0.04%	0.006%
26	4.950	1199	1216	1257	rVV2	1262654	3191803	100.00%	12.916%
27	5.227	1298	1302	1307	rVB6	1845	1577	0.05%	0.006%
28	5.368	1341	1346	1349	rVB6	1190	807	0.03%	0.003%
29	5.442	1364	1369	1370	rBV4	1040	975	0.03%	0.004%
30	5.529	1383	1396	1434	rBV	928948	1917154	60.06%	7.758%
31	5.760	1466	1468	1472	rVB5	1935	1221	0.04%	0.005%
32	5.786	1472	1476	1478	rBV5	1300	938	0.03%	0.004%
33	5.831	1478	1490	1494	rBV8	6465	11536	0.36%	0.047%
34	5.985	1519	1538	1562	rBV	690802	1430782	44.83%	5.790%
35	6.230	1611	1614	1616	rVB3	1621	959	0.03%	0.004%
36	6.249	1617	1620	1622	rBV4	1133	756	0.02%	0.003%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
 Title : VOC Analysis

37	6.281	1628	1630	1634	rBV4	869	721	0.02%	0.003%
38	6.484	1688	1693	1695	rBV4	935	744	0.02%	0.003%
39	6.622	1730	1736	1739	rVV7	595	503	0.02%	0.002%
40	6.645	1739	1743	1750	rVV7	1013	1409	0.04%	0.006%
41	6.680	1750	1754	1757	rVB5	837	632	0.02%	0.003%
42	6.706	1759	1762	1765	rVB5	581	460	0.01%	0.002%
43	6.815	1793	1796	1804	rVV7	810	905	0.03%	0.004%
44	6.908	1815	1825	1857	rBV	382129	730977	22.90%	2.958%
45	7.153	1897	1901	1907	rBV5	942	1072	0.03%	0.004%
46	7.236	1915	1927	1957	rBV	1453621	2575866	80.70%	10.424%
47	7.497	2005	2008	2012	rBV6	1566	1211	0.04%	0.005%
48	7.551	2015	2025	2050	rVV	245693	458268	14.36%	1.854%
49	7.863	2118	2122	2124	rBV4	1552	1161	0.04%	0.005%
50	7.931	2140	2143	2146	rBV3	695	536	0.02%	0.002%
51	7.973	2152	2156	2157	rBV4	684	471	0.01%	0.002%
52	8.024	2162	2172	2210	rBV	509634	1020113	31.96%	4.128%
53	8.349	2271	2273	2281	rVB9	1598	1361	0.04%	0.006%
54	8.413	2291	2293	2296	rBV2	1021	483	0.02%	0.002%
55	8.551	2334	2336	2342	rVV5	1865	1911	0.06%	0.008%
56	8.577	2342	2344	2347	rVV4	1050	753	0.02%	0.003%
57	8.600	2349	2351	2358	rVB4	2440	2339	0.07%	0.009%
58	8.635	2358	2362	2365	rBV5	1344	1178	0.04%	0.005%
59	8.722	2384	2389	2394	rVB6	1758	1939	0.06%	0.008%
60	8.780	2394	2407	2432	rBV	1416644	2318655	72.64%	9.383%
61	9.069	2495	2497	2501	rBV4	967	837	0.03%	0.003%
62	9.198	2534	2537	2540	rBV4	609	483	0.02%	0.002%
63	9.278	2560	2562	2565	rVB4	1232	655	0.02%	0.003%
64	9.304	2565	2570	2571	rBV5	1380	1006	0.03%	0.004%
65	9.400	2596	2600	2603	rBV4	1805	1197	0.04%	0.005%
66	9.452	2613	2616	2622	rVB4	742	805	0.03%	0.003%
67	9.497	2626	2630	2633	rBV5	1394	1290	0.04%	0.005%
68	9.728	2700	2702	2707	rBV4	1338	1223	0.04%	0.005%
69	9.783	2715	2719	2721	rBV4	1235	936	0.03%	0.004%
70	9.866	2741	2745	2748	rBV5	908	827	0.03%	0.003%
71	9.956	2763	2773	2780	rBV8	3266	4360	0.14%	0.018%
72	10.021	2780	2793	2797	rVV8	4397	6544	0.21%	0.026%
73	10.046	2798	2801	2809	rVB7	4328	5231	0.16%	0.021%
74	10.146	2816	2832	2852	rBV	828008	1315730	41.22%	5.324%
75	10.516	2941	2947	2963	rVB2	19757	33361	1.05%	0.135%
76	10.580	2963	2967	2969	rBV4	1333	994	0.03%	0.004%

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 Title : VOC Analysis

77	10.702	3001	3005	3006	rBV3	1422	998	0.03%	0.004%
78	10.712	3006	3008	3016	rVB7	2515	2153	0.07%	0.009%
79	10.779	3023	3029	3031	rBV6	1872	2004	0.06%	0.008%
80	10.812	3035	3039	3046	rVB7	5839	7357	0.23%	0.030%
81	10.860	3048	3054	3063	rBV10	2893	5096	0.16%	0.021%
82	10.940	3075	3079	3080	rBV2	1083	745	0.02%	0.003%
83	10.969	3082	3088	3096	rVV7	3210	5788	0.18%	0.023%
84	11.127	3133	3137	3142	rVB7	3077	3207	0.10%	0.013%
85	11.178	3142	3153	3178	rBV	1521371	2374340	74.39%	9.608%
86	11.403	3218	3223	3233	rVB7	8035	11201	0.35%	0.045%
87	11.490	3241	3250	3259	rBV6	17147	39726	1.24%	0.161%
88	11.554	3259	3270	3293	rVB	1471099	2377095	74.47%	9.619%
89	11.725	3316	3323	3335	rVB	34019	50299	1.58%	0.204%
90	12.230	3477	3480	3481	rBV3	2226	1158	0.04%	0.005%
91	12.255	3486	3488	3491	rVB4	1744	935	0.03%	0.004%
92	12.345	3512	3516	3523	rBV9	3804	4912	0.15%	0.020%
93	12.397	3528	3532	3538	rBV8	5394	6088	0.19%	0.025%
94	12.821	3659	3664	3674	rVB3	24150	31978	1.00%	0.129%
95	12.979	3706	3713	3722	rBV9	6770	10490	0.33%	0.042%
96	13.143	3761	3764	3767	rBV5	2408	2109	0.07%	0.009%
97	13.197	3773	3781	3795	rBV6	23077	43700	1.37%	0.177%
98	13.323	3813	3820	3826	rBV6	12300	18954	0.59%	0.077%
99	13.837	3973	3980	3988	rBV4	22081	30697	0.96%	0.124%
100	15.779	4577	4584	4597	rVB	130454	198237	6.21%	0.802%

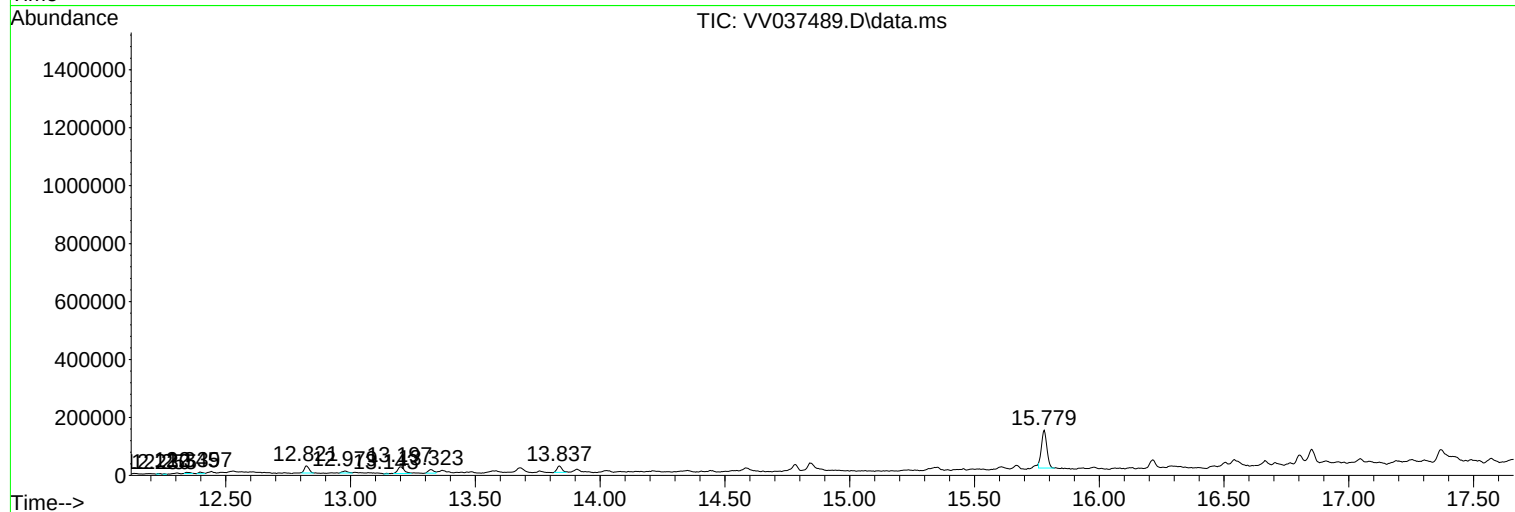
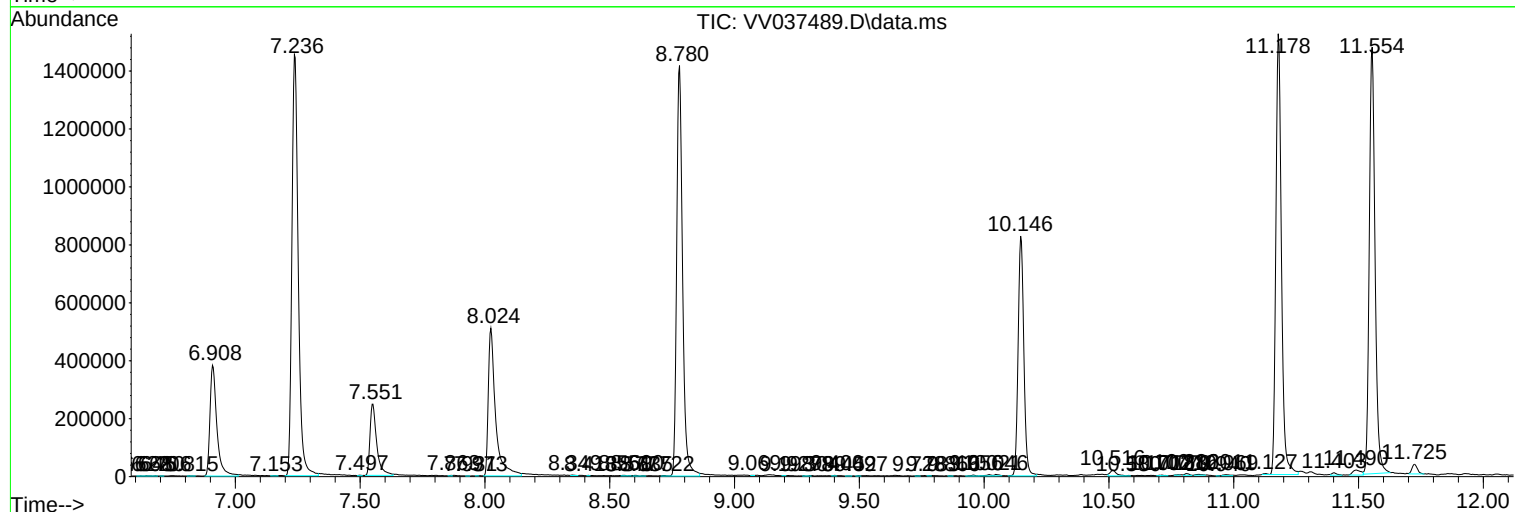
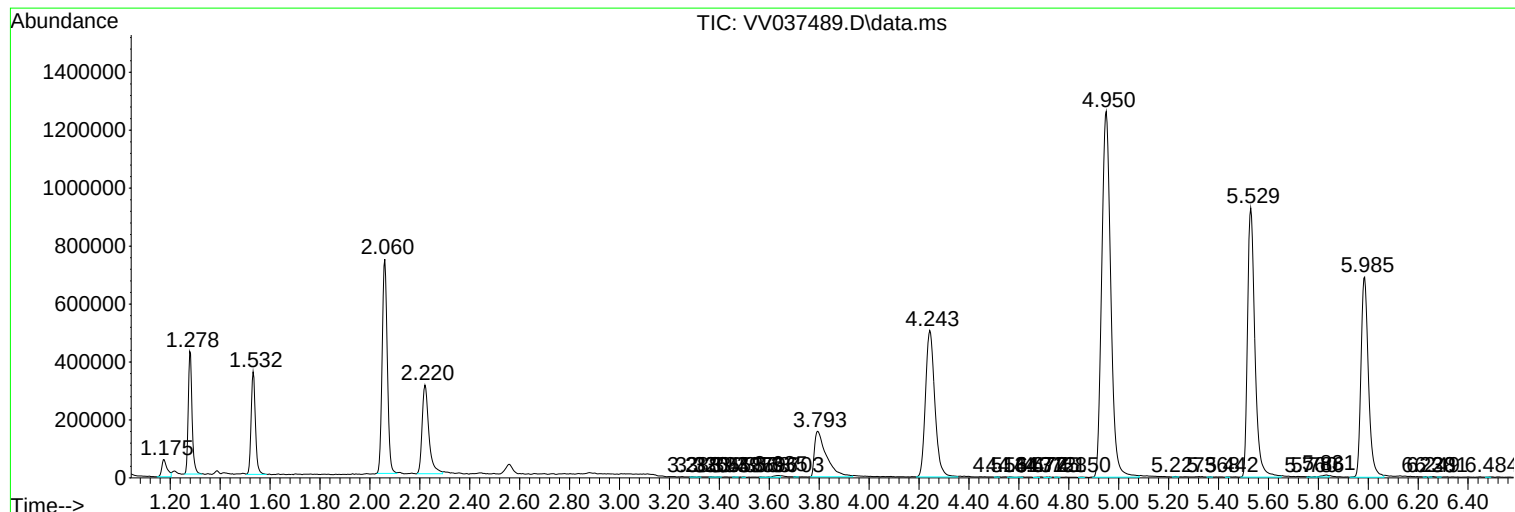
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ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0SX7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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



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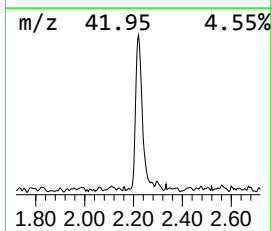
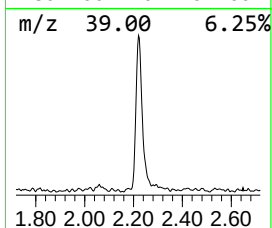
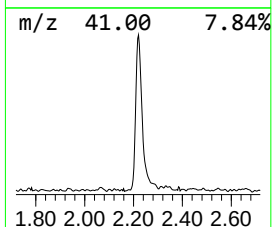
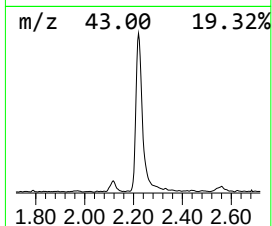
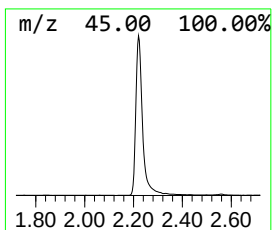
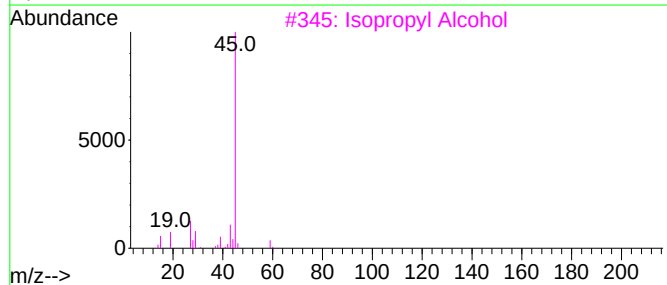
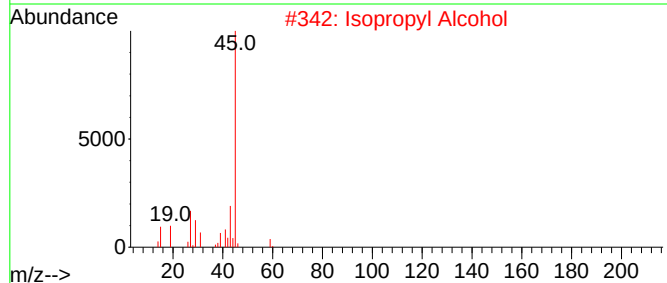
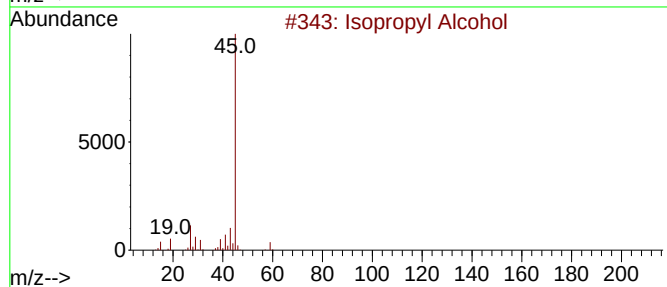
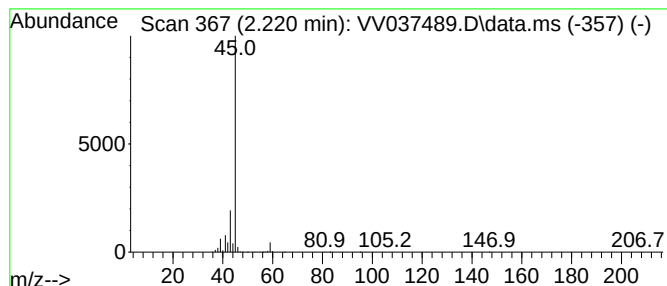
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.220	14.69 ug/L	563159	1,4-Difluorobenzene	5.529

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	90
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	83
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
5			Isopropyl Alcohol	60	C3H8O	000067-63-0	9



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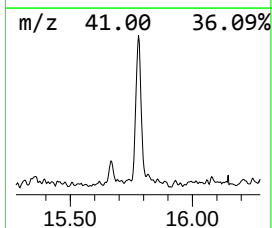
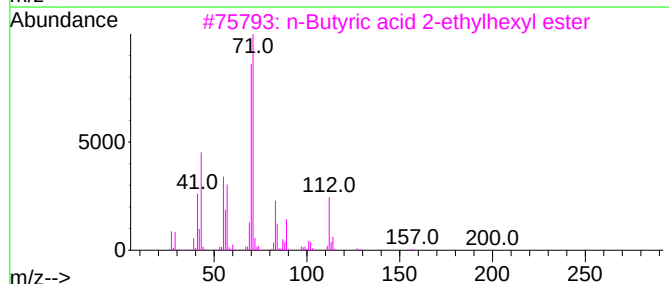
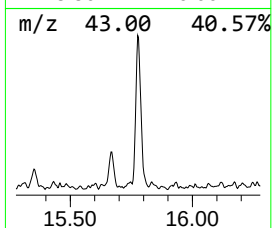
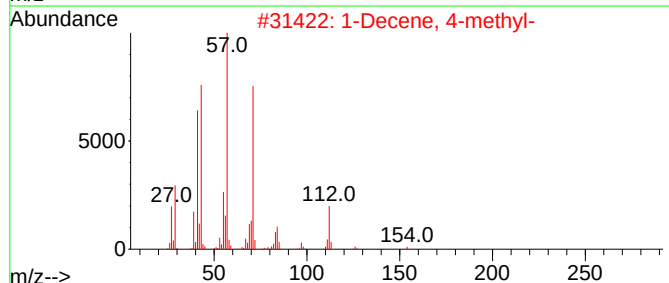
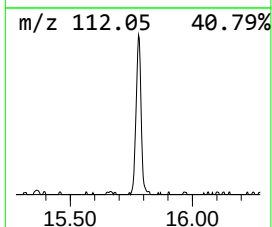
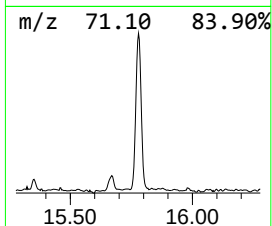
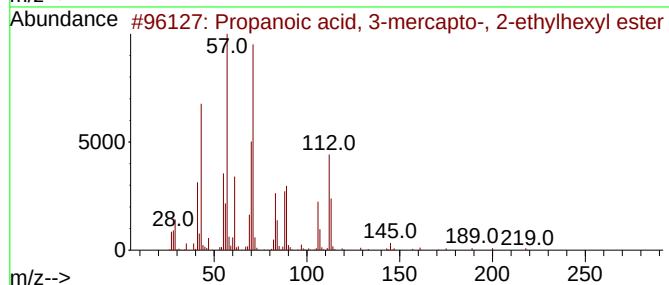
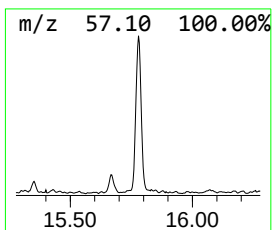
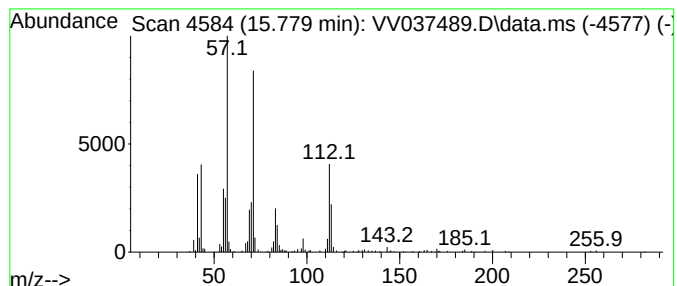
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 3-mercapto-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.779	4.17 ug/L	198237	1,4-Dichlorobenzene-d4	11.178

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 3-mercapto-, 2-e...	218	C11H22O2S	050448-95-8	72
2			1-Decene, 4-methyl-	154	C11H22	013151-29-6	59
3			n-Butyric acid 2-ethylhexyl ester	200	C12H24O2	025415-84-3	59
4			Carbonic acid, octyl vinyl ester	200	C11H20O3	1000383-25-5	59
5			Oxalic acid, 2-ethylhexyl octyl ...	314	C18H34O4	1000309-39-1	53



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Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	2.220	14.7	ug/L	563159	1	5.529	1917150	50.0
Propanoic acid,...	15.779	4.2	ug/L	198237	3	11.178	2374340	50.0