

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV092324\
 Data File : VV037490.D
 Acq On : 23 Sep 2024 18:04
 Operator : SY/MD
 Sample : P4106-03
 Misc : 5mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0SX8

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: VV037490.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.172	34	41	52	rBV	63196	98580	3.07%	0.407%
2	1.278	67	74	90	rVB	420177	452429	14.07%	1.867%
3	1.388	102	108	113	rBV	15740	17937	0.56%	0.074%
4	1.532	145	153	168	rBV	354122	420575	13.08%	1.735%
5	2.060	307	317	332	rBV	743292	1066831	33.18%	4.402%
6	2.220	358	367	389	rBV	155211	283388	8.81%	1.169%
7	3.320	706	709	712	rBV4	908	740	0.02%	0.003%
8	3.481	756	759	762	rVB4	999	679	0.02%	0.003%
9	3.638	794	808	814	rBV4	3395	8342	0.26%	0.034%
10	3.793	846	856	897	rBV2	162842	538407	16.75%	2.222%
11	4.121	955	958	963	rBV6	984	972	0.03%	0.004%
12	4.162	968	971	974	rBV4	660	525	0.02%	0.002%
13	4.243	977	996	1023	rBV	510394	1304384	40.57%	5.382%
14	4.455	1059	1062	1065	rVB4	1325	831	0.03%	0.003%
15	4.545	1087	1090	1093	rBV4	647	427	0.01%	0.002%
16	4.564	1093	1096	1099	rVV4	1073	658	0.02%	0.003%
17	4.587	1101	1103	1109	rVV4	1056	1046	0.03%	0.004%
18	4.667	1127	1128	1131	rBV3	820	454	0.01%	0.002%
19	4.693	1133	1136	1137	rBV2	957	439	0.01%	0.002%
20	4.732	1146	1148	1151	rBV2	951	731	0.02%	0.003%
21	4.760	1155	1157	1161	rBV4	680	535	0.02%	0.002%
22	4.802	1165	1170	1175	rVB4	1821	1495	0.05%	0.006%
23	4.831	1175	1179	1182	rBV3	625	624	0.02%	0.003%
24	4.950	1198	1216	1251	rBV2	1262042	3214925	100.00%	13.266%
25	5.304	1320	1326	1328	rBV5	1742	1893	0.06%	0.008%
26	5.410	1356	1359	1363	rVB5	926	610	0.02%	0.003%
27	5.465	1374	1376	1379	rBV2	1401	692	0.02%	0.003%
28	5.529	1384	1396	1435	rBV	916496	1893378	58.89%	7.813%
29	5.715	1452	1454	1458	rVB5	1965	1309	0.04%	0.005%
30	5.760	1465	1468	1473	rBV6	1401	894	0.03%	0.004%
31	5.828	1479	1489	1496	rBV10	7139	14358	0.45%	0.059%
32	5.889	1506	1508	1515	rVB5	1618	1122	0.03%	0.005%
33	5.928	1515	1520	1523	rBV5	1669	1600	0.05%	0.007%
34	5.982	1524	1537	1575	rVV	687203	1439795	44.78%	5.941%
35	6.313	1634	1640	1647	rVB10	1160	1641	0.05%	0.007%
36	6.349	1647	1651	1654	rBV4	1190	939	0.03%	0.004%

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 Title : VOC Analysis

37	6.410	1665	1670	1675	rBV5	1067	1329	0.04%	0.005%
38	6.452	1680	1683	1685	rBV2	620	430	0.01%	0.002%
39	6.577	1719	1722	1724	rVV3	824	572	0.02%	0.002%
40	6.596	1726	1728	1734	rVB5	925	891	0.03%	0.004%
41	6.629	1734	1738	1740	rBV4	585	455	0.01%	0.002%
42	6.674	1748	1752	1756	rVB5	1200	1036	0.03%	0.004%
43	6.706	1756	1762	1765	rBV7	873	1136	0.04%	0.005%
44	6.754	1774	1777	1779	rVB3	1063	561	0.02%	0.002%
45	6.773	1779	1783	1786	rBV4	1253	1096	0.03%	0.005%
46	6.838	1798	1803	1805	rBV4	1116	919	0.03%	0.004%
47	6.908	1815	1825	1852	rBV	383028	723592	22.51%	2.986%
48	7.182	1908	1910	1914	rVB5	1285	671	0.02%	0.003%
49	7.236	1916	1927	1956	rBV	1450636	2564487	79.77%	10.582%
50	7.548	2015	2024	2053	rBV	250335	464890	14.46%	1.918%
51	7.857	2118	2120	2122	rBV3	1009	567	0.02%	0.002%
52	7.944	2144	2147	2149	rBV2	1274	716	0.02%	0.003%
53	8.024	2163	2172	2199	rBV	509012	1006248	31.30%	4.152%
54	8.410	2287	2292	2297	rBV8	1094	1199	0.04%	0.005%
55	8.538	2329	2332	2333	rBV3	788	432	0.01%	0.002%
56	8.571	2340	2342	2345	rVV3	989	479	0.01%	0.002%
57	8.596	2348	2350	2354	rBV4	812	485	0.02%	0.002%
58	8.683	2374	2377	2383	rVB6	1246	1160	0.04%	0.005%
59	8.725	2387	2390	2392	rBV4	973	631	0.02%	0.003%
60	8.780	2395	2407	2437	rBV	1379814	2289102	71.20%	9.445%
61	9.140	2514	2519	2528	rVB9	2107	3035	0.09%	0.013%
62	9.210	2538	2541	2542	rBV3	976	489	0.02%	0.002%
63	9.278	2560	2562	2563	rBV	957	472	0.01%	0.002%
64	9.326	2573	2577	2585	rBV	669	882	0.03%	0.004%
65	9.397	2596	2599	2600	rBV2	1089	498	0.02%	0.002%
66	9.503	2629	2632	2635	rVB3	1052	748	0.02%	0.003%
67	9.551	2644	2647	2651	rVB4	678	447	0.01%	0.002%
68	9.638	2670	2674	2677	rBV5	1218	1070	0.03%	0.004%
69	9.673	2684	2685	2690	rVB4	1128	641	0.02%	0.003%
70	9.699	2690	2693	2696	rBV3	1024	711	0.02%	0.003%
71	9.783	2714	2719	2720	rBV5	1266	1180	0.04%	0.005%
72	9.873	2743	2747	2752	rVB6	1171	1333	0.04%	0.006%
73	9.960	2772	2774	2778	rVB5	1231	752	0.02%	0.003%
74	9.995	2782	2785	2786	rBV3	911	522	0.02%	0.002%
75	10.021	2790	2793	2795	rBV2	1298	693	0.02%	0.003%
76	10.046	2799	2801	2811	rVB8	2991	3537	0.11%	0.015%

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77	10.146	2820	2832	2857	rBV	843152	1315527	40.92%	5.428%
78	10.442	2921	2924	2926	rBV4	1296	998	0.03%	0.004%
79	10.516	2942	2947	2958	rVB5	12332	17724	0.55%	0.073%
80	10.667	2992	2994	2998	rVB5	938	428	0.01%	0.002%
81	10.706	3002	3006	3013	rVB9	2086	2486	0.08%	0.010%
82	10.754	3018	3021	3023	rBV4	1458	756	0.02%	0.003%
83	10.815	3034	3040	3045	rVB9	3532	4440	0.14%	0.018%
84	10.972	3081	3089	3094	rBV8	2585	4000	0.12%	0.017%
85	11.037	3105	3109	3114	rVB6	3503	3637	0.11%	0.015%
86	11.082	3121	3123	3126	rBV3	912	577	0.02%	0.002%
87	11.107	3129	3131	3132	rBV2	1432	674	0.02%	0.003%
88	11.124	3132	3136	3142	rBV6	3691	4896	0.15%	0.020%
89	11.178	3143	3153	3178	rBV	1472096	2315880	72.04%	9.556%
90	11.484	3239	3248	3259	rBV2	23625	57302	1.78%	0.236%
91	11.554	3259	3270	3296	rVB	1463310	2356715	73.31%	9.724%
92	11.725	3316	3323	3337	rVB3	26544	41307	1.28%	0.170%
93	12.352	3513	3518	3526	rVB3	3769	4806	0.15%	0.020%
94	12.442	3541	3546	3552	rBV9	4692	6019	0.19%	0.025%
95	12.824	3658	3665	3672	rBV4	16527	21586	0.67%	0.089%
96	13.204	3772	3783	3796	rBV5	15672	32130	1.00%	0.133%
97	13.320	3813	3819	3825	rBV9	8830	13239	0.41%	0.055%
98	13.834	3973	3979	3988	rBV2	17353	24210	0.75%	0.100%
99	14.783	4269	4274	4284	rVB3	16316	20954	0.65%	0.086%
100	15.779	4577	4584	4600	rVB2	81710	130395	4.06%	0.538%

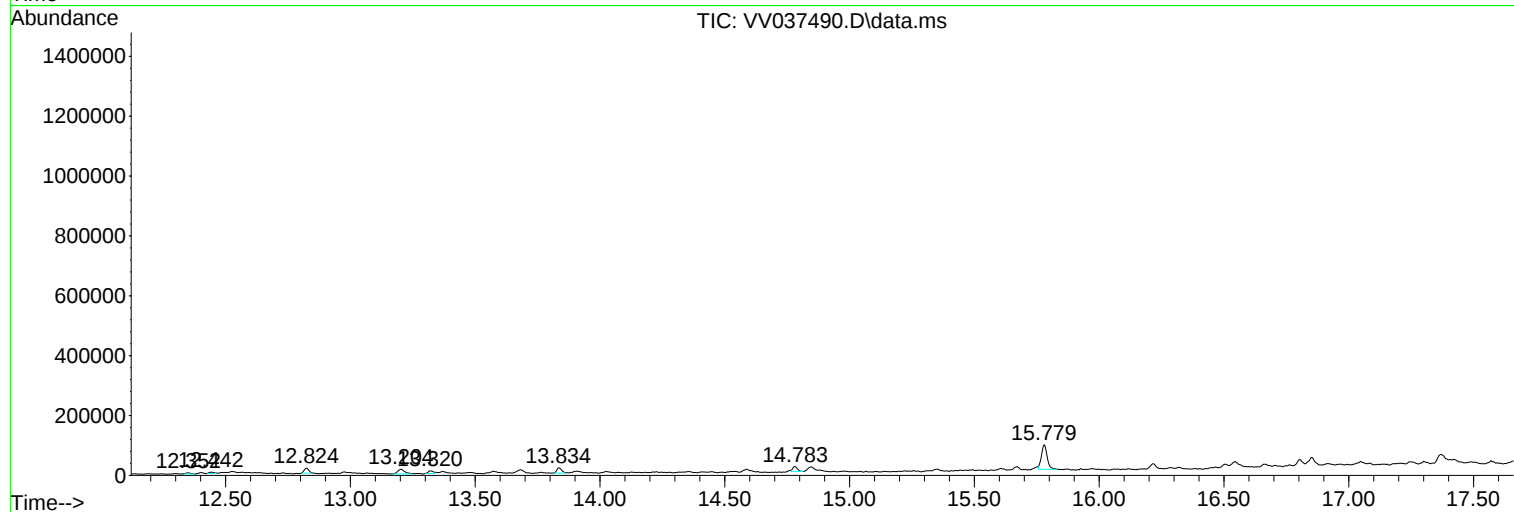
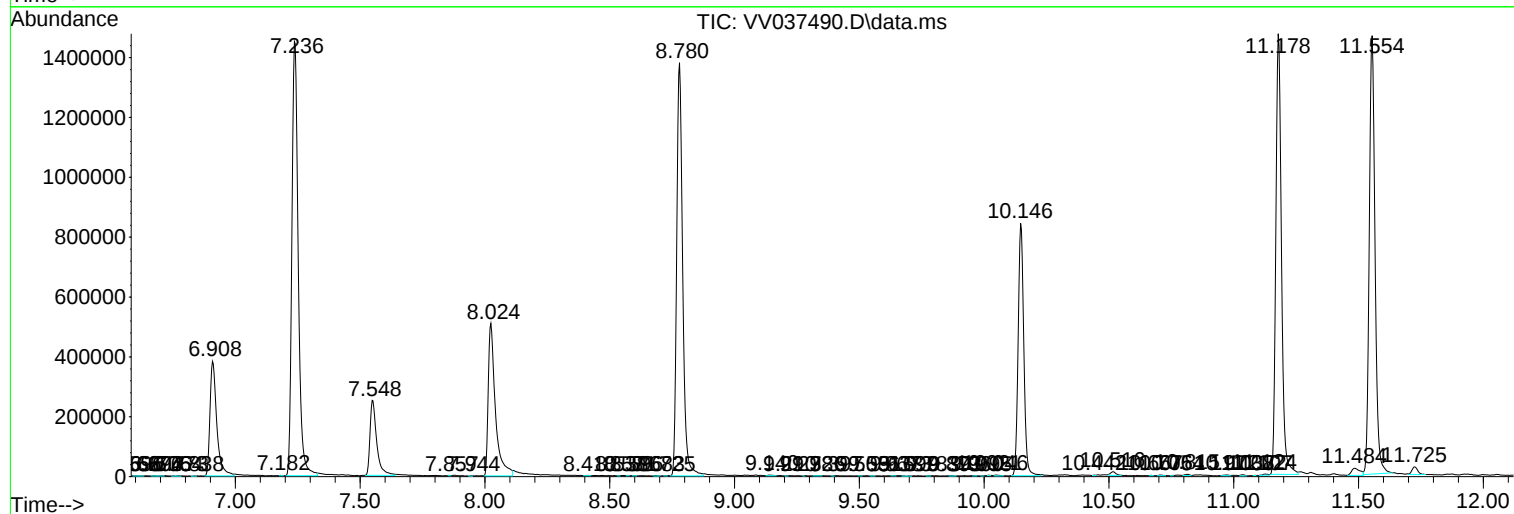
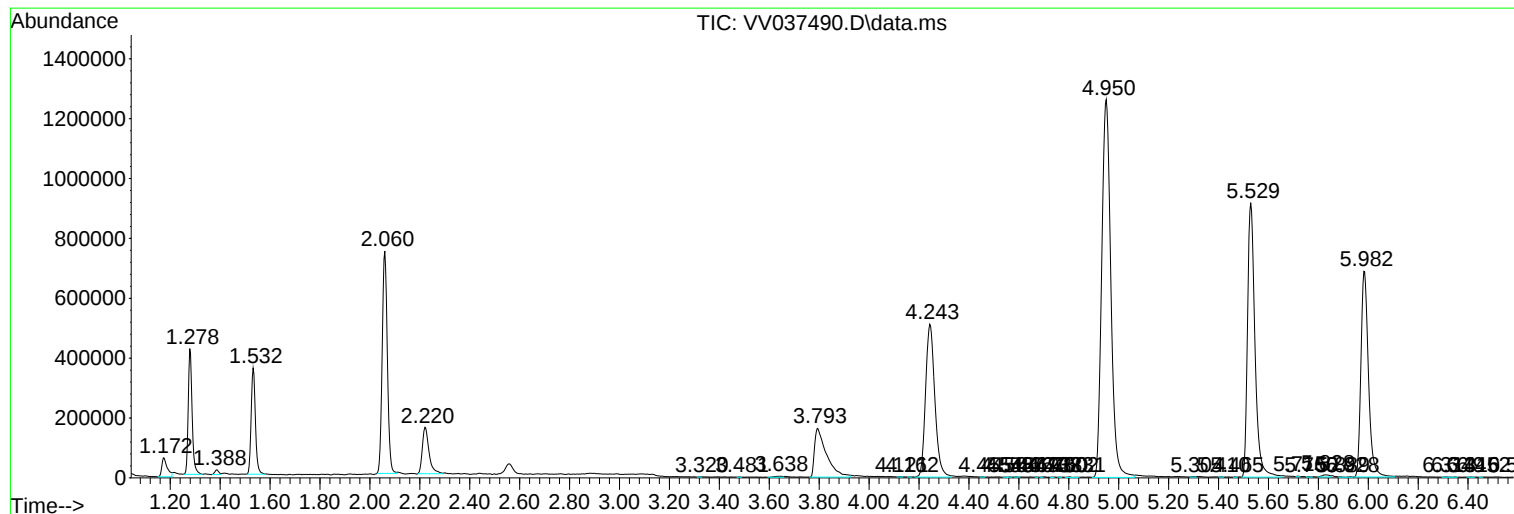
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ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0SX8

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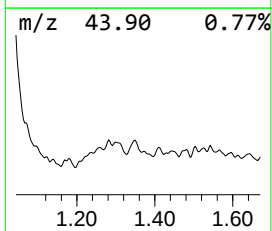
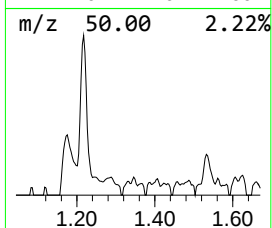
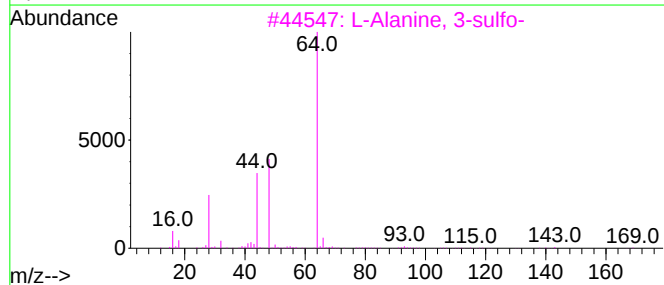
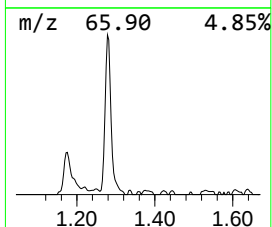
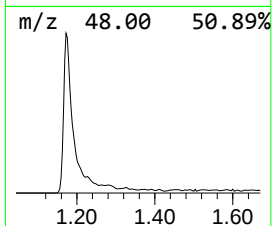
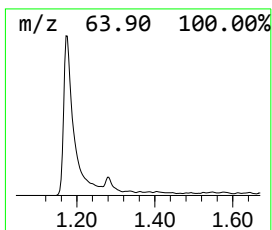
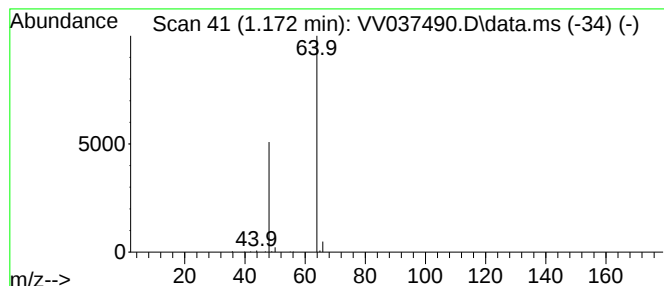
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.172	2.60 ug/L	98580	1,4-Difluorobenzene	5.529

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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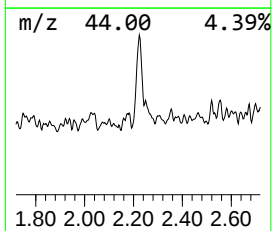
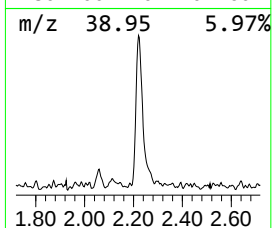
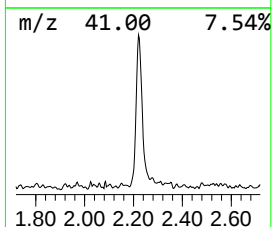
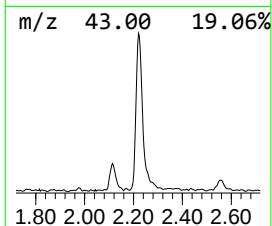
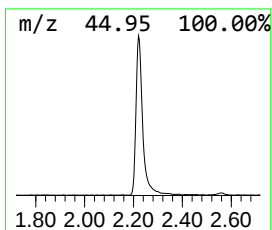
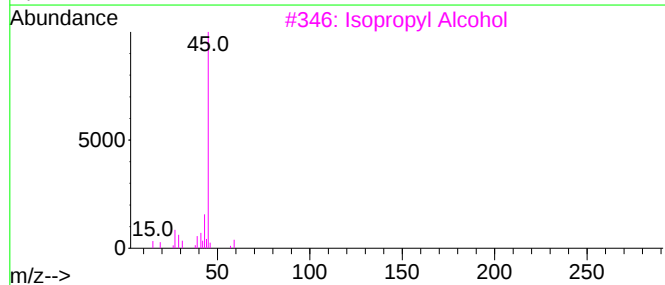
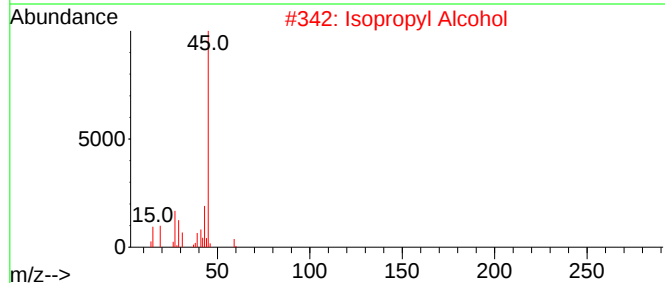
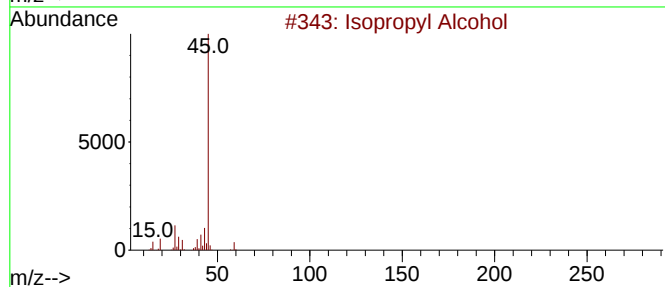
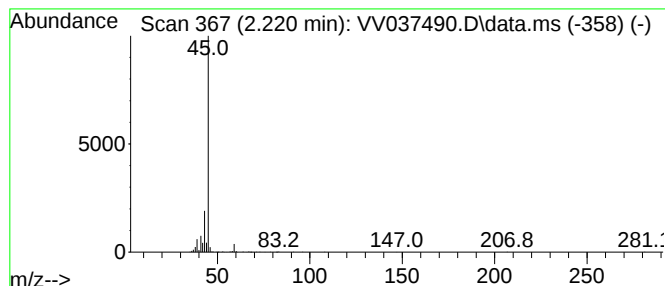
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.220	7.48 ug/L	283388	1,4-Difluorobenzene	5.529

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	83
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	83
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
5			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9



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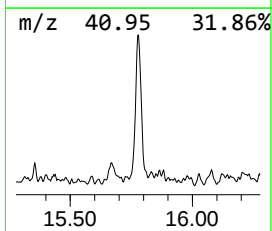
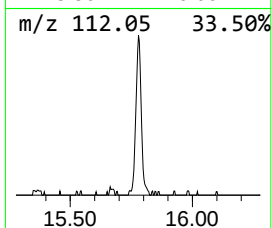
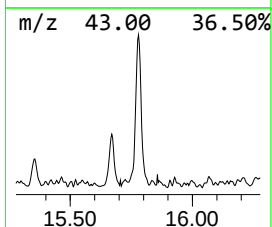
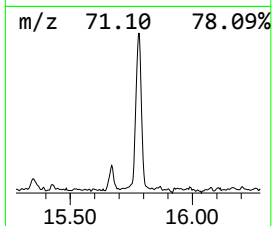
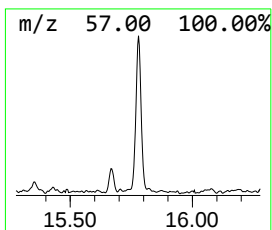
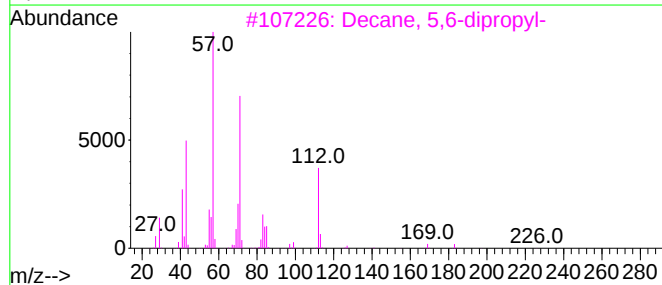
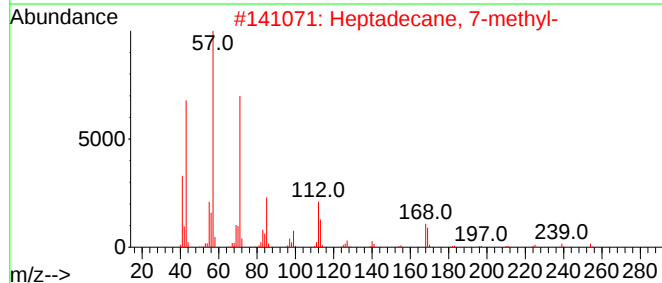
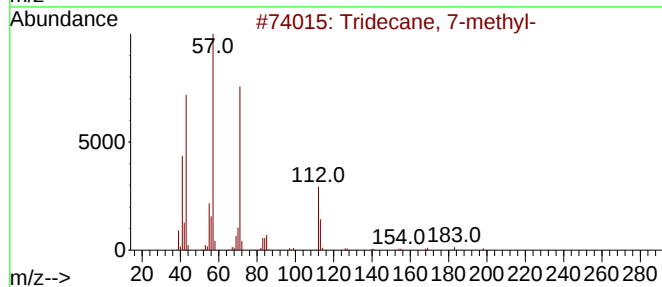
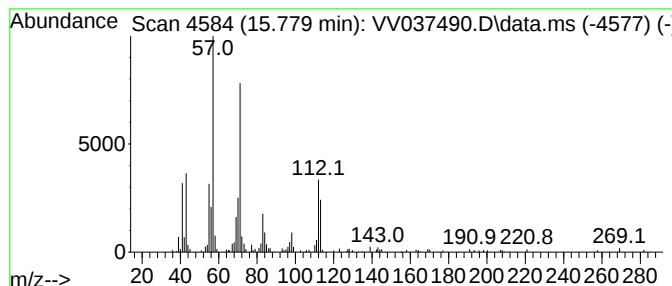
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.779	2.82 ug/L	130395	1,4-Dichlorobenzene-d4	11.178

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 7-methyl-	198	C14H30	026730-14-3	83
2			Heptadecane, 7-methyl-	254	C18H38	020959-33-5	72
3			Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	64
4			Oxalic acid, 2-ethylhexyl pentad...	412	C25H48O4	1000309-39-8	64
5			Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV092324\
Data File : VV037490.D
Acq On : 23 Sep 2024 18:04
Operator : SY/MD
Sample : P4106-03
Misc : 5mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0SX8

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.172	2.6	ug/L	98580	1	5.529	1893380	50.0
Isopropyl Alcohol	2.220	7.5	ug/L	283388	1	5.529	1893380	50.0
(DEL) Alkane: S...	15.779	2.8	ug/L	130395	3	11.178	2315880	50.0