

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081722\
 Data File : VX030662.D
 Acq On : 17 Aug 2022 16:02
 Operator : JC/MD
 Sample : N4221-14
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0KN6

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_X\Method\SFAMXML080422WMA.M
 Title : VOC Analysis

Signal : TIC: VX030662.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	16	rVB	92444	82793	0.37%	0.127%
2	1.264	24	29	41	rBV2	34186	52353	0.24%	0.080%
3	1.374	43	47	54	rVB2	1021921	1156209	5.23%	1.767%
4	1.666	91	95	104	rVB	130338	158954	0.72%	0.243%
5	1.746	104	108	114	rBV3	12244	18086	0.08%	0.028%
6	1.953	139	142	146	rVV2	10206	11995	0.05%	0.018%
7	1.996	146	149	155	rVB	13985	16815	0.08%	0.026%
8	2.319	194	202	216	rBV	6775556	10755415	48.63%	16.441%
9	2.502	231	232	233	rBV	1104	644	0.00%	0.001%
10	2.794	275	280	285	rVV5	2522	5643	0.03%	0.009%
11	2.940	303	304	307	rBV3	687	926	0.00%	0.001%
12	3.093	323	329	336	rBV3	17981	35690	0.16%	0.055%
13	3.264	354	357	358	rBV2	1021	891	0.00%	0.001%
14	3.343	367	370	373	rVB2	474	597	0.00%	0.001%
15	3.373	373	375	379	rVB2	580	479	0.00%	0.001%
16	3.446	382	387	393	rVV4	1926	3763	0.02%	0.006%
17	3.611	405	414	426	rBV	174568	414464	1.87%	0.634%
18	3.873	453	457	461	rVB2	435	665	0.00%	0.001%
19	4.020	478	481	484	rBV2	394	556	0.00%	0.001%
20	4.257	516	520	523	rBV2	472	787	0.00%	0.001%
21	4.294	523	526	527	rBV2	424	499	0.00%	0.001%
22	4.361	530	537	545	rBV2	10107	25978	0.12%	0.040%
23	4.495	546	559	579	rBV	1815431	5075065	22.95%	7.758%
24	4.812	609	611	614	rVB2	796	790	0.00%	0.001%
25	4.843	614	616	617	rBV	705	464	0.00%	0.001%
26	4.928	627	630	631	rBV2	578	533	0.00%	0.001%
27	4.958	631	635	636	rVV3	415	430	0.00%	0.001%
28	5.062	638	652	670	rVV	158940	511865	2.31%	0.782%
29	5.391	694	706	720	rVB3	113421	353378	1.60%	0.540%
30	5.562	727	734	746	rVB6	2211	5476	0.02%	0.008%
31	5.708	756	758	761	rVB2	348	419	0.00%	0.001%
32	5.885	783	787	788	rVB3	483	529	0.00%	0.001%
33	5.977	788	802	817	rBV2	436487	1289045	5.83%	1.970%
34	6.202	836	839	840	rVB2	458	444	0.00%	0.001%
35	6.245	840	846	849	rBV7	1198	2509	0.01%	0.004%
36	6.391	863	870	880	rVB3	10747	28276	0.13%	0.043%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
 Title : VOC Analysis

37	6.665	910	915	916	rVB2	608	588	0.00%	0.001%
38	6.769	922	932	948	rBV	332402	789627	3.57%	1.207%
39	6.903	951	954	956	rVB4	833	1002	0.00%	0.002%
40	7.007	969	971	975	rVB2	577	617	0.00%	0.001%
41	7.135	979	992	1013	rBV	10154095	22117771	100.00%	33.809%
42	7.312	1014	1021	1033	rVB	262285	570241	2.58%	0.872%
43	7.488	1047	1050	1056	rBV6	1726	2771	0.01%	0.004%
44	7.562	1060	1062	1067	rVB3	957	891	0.00%	0.001%
45	7.677	1074	1081	1097	rBV	52346	107557	0.49%	0.164%
46	7.848	1107	1109	1113	rBV2	355	592	0.00%	0.001%
47	7.891	1113	1116	1117	rVV	1063	1071	0.00%	0.002%
48	7.927	1120	1122	1124	rVV2	2207	2415	0.01%	0.004%
49	7.976	1126	1130	1138	rVV3	11387	19751	0.09%	0.030%
50	8.129	1152	1155	1160	rBV4	960	1678	0.01%	0.003%
51	8.330	1181	1188	1196	rBV	182914	292859	1.32%	0.448%
52	8.580	1227	1229	1231	rVB3	823	763	0.00%	0.001%
53	8.653	1234	1241	1249	rBV	676504	1031577	4.66%	1.577%
54	8.720	1249	1252	1258	rVB	10225	15725	0.07%	0.024%
55	8.848	1269	1273	1281	rVB2	13728	21390	0.10%	0.033%
56	8.952	1284	1290	1297	rBV	124793	189759	0.86%	0.290%
57	9.171	1319	1326	1333	rBV5	12712	26376	0.12%	0.040%
58	9.281	1333	1344	1356	rBV	10987553	16109386	72.83%	24.625%
59	9.384	1357	1361	1371	rVB	440558	638631	2.89%	0.976%
60	9.732	1414	1418	1424	rVB2	15877	23080	0.10%	0.035%
61	9.951	1450	1454	1458	rBV3	592	1052	0.00%	0.002%
62	9.994	1458	1461	1462	rBV2	3369	3982	0.02%	0.006%
63	10.055	1466	1471	1483	rVB	673197	920293	4.16%	1.407%
64	10.201	1492	1495	1497	rVB2	2202	2276	0.01%	0.003%
65	10.275	1504	1507	1511	rBV4	3327	3978	0.02%	0.006%
66	10.378	1518	1524	1533	rBV	71024	100089	0.45%	0.153%
67	10.445	1533	1535	1536	rBV2	756	539	0.00%	0.001%
68	10.585	1554	1558	1564	rBV6	3981	6163	0.03%	0.009%
69	10.762	1585	1587	1589	rBV2	764	779	0.00%	0.001%
70	10.799	1591	1593	1596	rVV2	676	624	0.00%	0.001%
71	10.854	1596	1602	1606	rVV4	1325	1841	0.01%	0.003%
72	10.902	1608	1610	1614	rVB4	768	1084	0.00%	0.002%
73	11.018	1625	1629	1635	rVB5	2478	3754	0.02%	0.006%
74	11.091	1639	1641	1647	rVB5	1510	2053	0.01%	0.003%
75	11.195	1652	1658	1666	rBV	442722	569214	2.57%	0.870%
76	11.317	1674	1678	1684	rVB2	4664	6525	0.03%	0.010%

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 Title : VOC Analysis

77	11.482	1702	1705	1706	rBV2	513	454	0.00%	0.001%
78	11.701	1737	1741	1745	rVB5	3106	4652	0.02%	0.007%
79	11.768	1745	1752	1753	rBV3	698	1569	0.01%	0.002%
80	11.793	1753	1756	1762	rVB3	5500	7629	0.03%	0.012%
81	11.866	1766	1768	1769	rBV	558	476	0.00%	0.001%
82	11.975	1783	1786	1788	rBV2	742	742	0.00%	0.001%
83	12.024	1789	1794	1803	rVV	720555	881022	3.98%	1.347%
84	12.219	1821	1826	1835	rBV2	12558	21412	0.10%	0.033%
85	12.323	1837	1843	1851	rBV	721399	881739	3.99%	1.348%
86	12.420	1856	1859	1864	rVB3	2736	3623	0.02%	0.006%
87	12.768	1912	1916	1919	rVB2	1587	2234	0.01%	0.003%
88	12.878	1933	1934	1937	rVB2	1005	473	0.00%	0.001%
89	12.914	1937	1940	1942	rBV	557	668	0.00%	0.001%
90	13.262	1995	1997	1999	rBV	861	514	0.00%	0.001%
91	13.591	2049	2051	2053	rBV3	928	799	0.00%	0.001%
92	13.786	2080	2083	2085	rBV	602	469	0.00%	0.001%
93	14.127	2134	2139	2143	rBV4	1731	2855	0.01%	0.004%
94	14.304	2166	2168	2172	rVB2	898	650	0.00%	0.001%
95	14.341	2172	2174	2176	rBV3	450	424	0.00%	0.001%
96	14.463	2192	2194	2197	rBV3	599	622	0.00%	0.001%
97	14.694	2230	2232	2233	rBV2	949	571	0.00%	0.001%
98	15.859	2421	2423	2427	rBV4	873	1091	0.00%	0.002%
99	16.499	2527	2528	2530	rBV2	923	699	0.00%	0.001%
100	16.523	2530	2532	2535	rVV3	1020	880	0.00%	0.001%

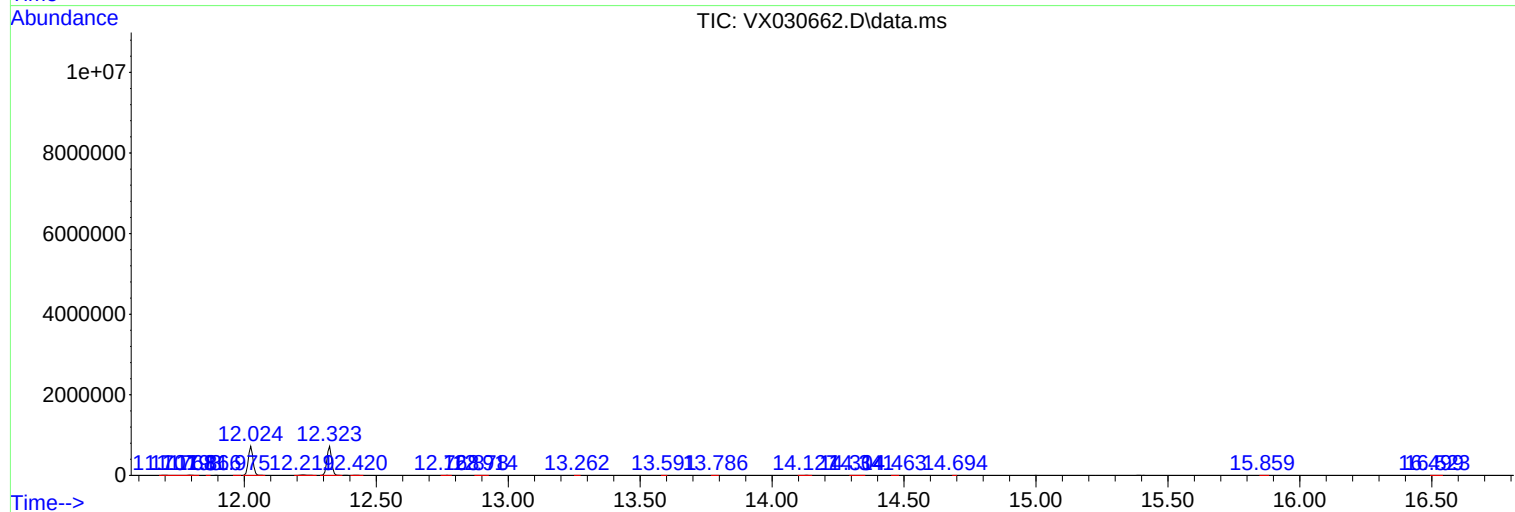
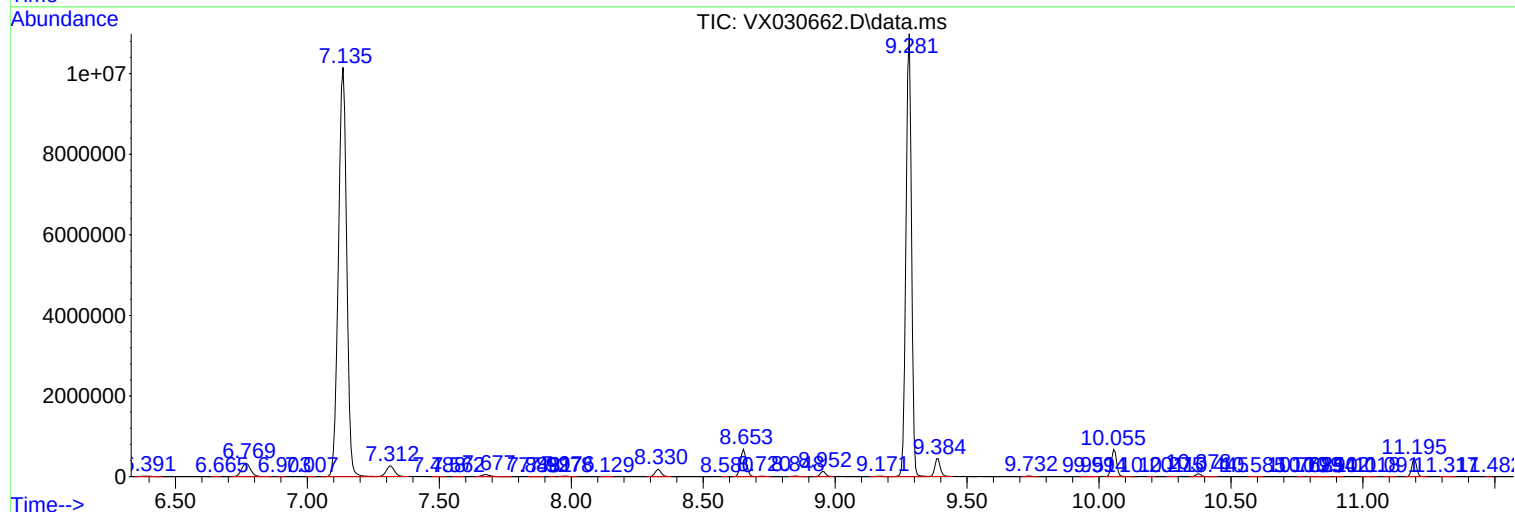
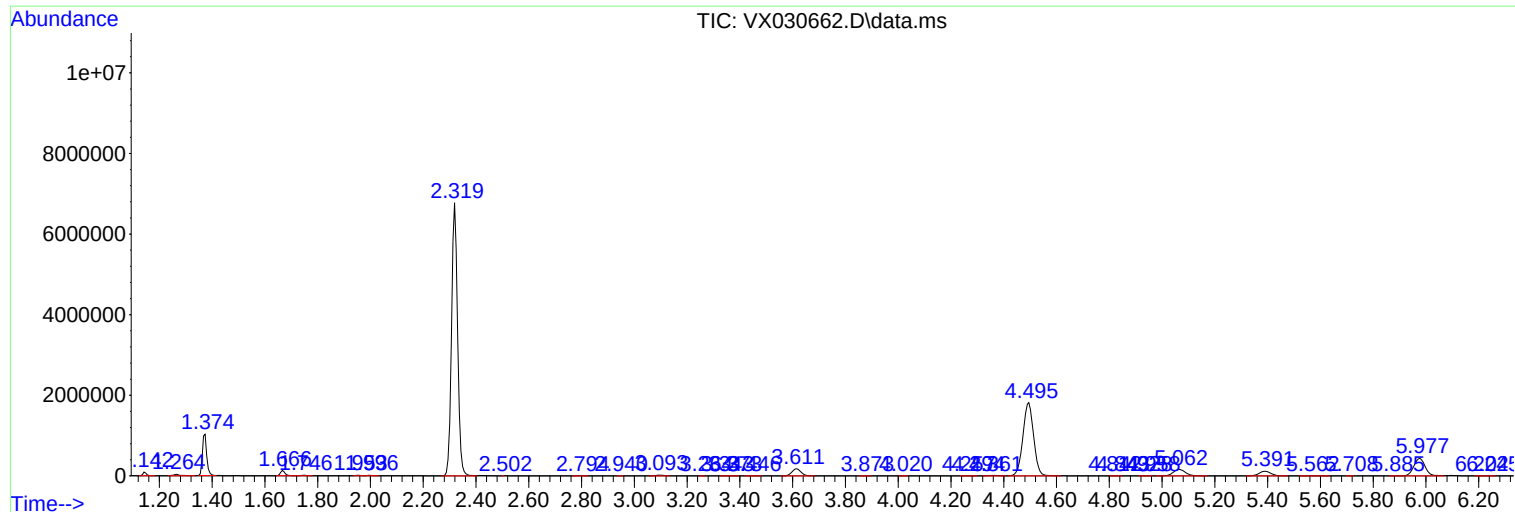
Sum of corrected areas: 65420056

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Instrument :
MSVOA_X
ClientSampleId :
C0KN6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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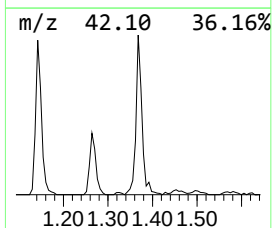
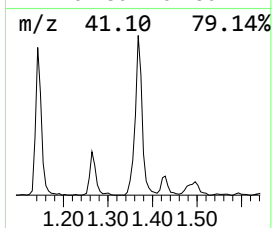
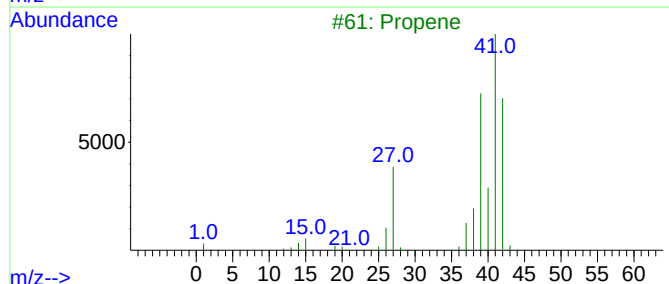
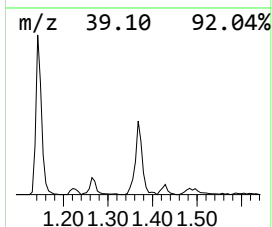
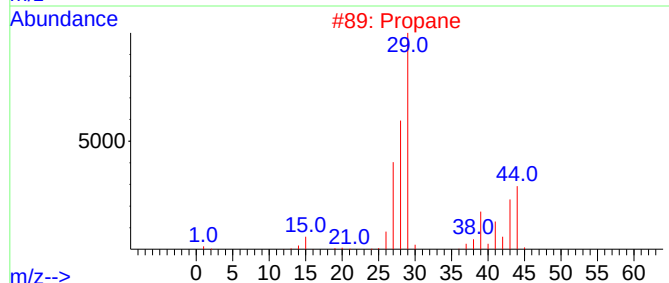
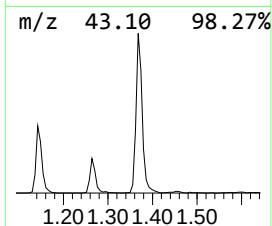
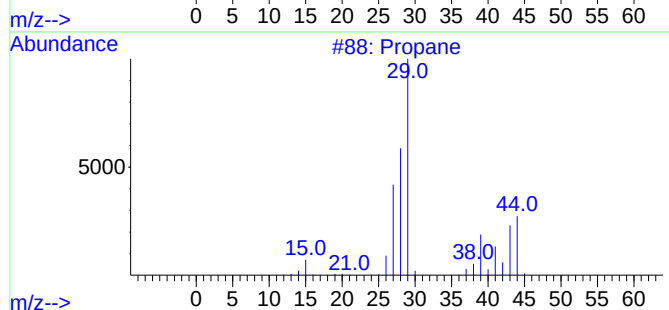
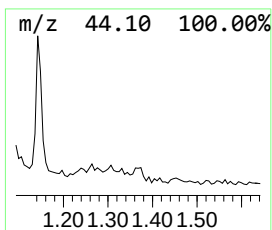
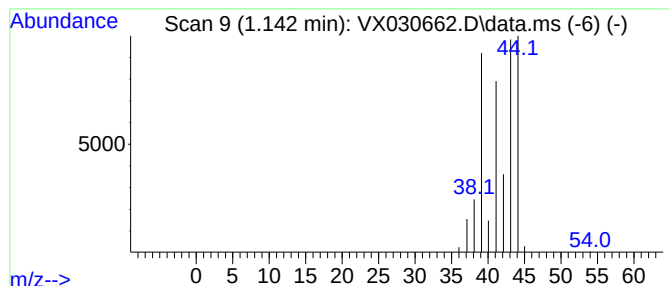
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	5.24 ug/L	82793	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane	44	C3H8	000074-98-6	74
2			Propane	44	C3H8	000074-98-6	9
3			Propene	42	C3H6	000115-07-1	9
4			Propane	44	C3H8	000074-98-6	5
5			Cyclopropene	40	C3H4	002781-85-3	4



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Instrument :
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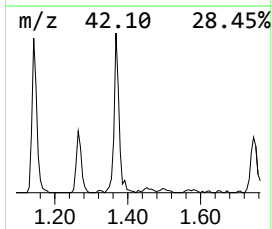
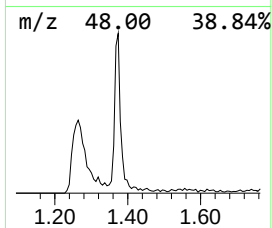
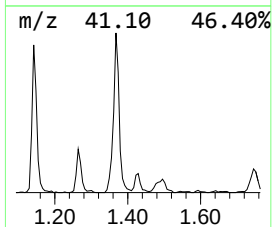
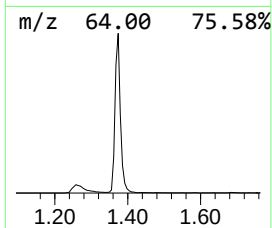
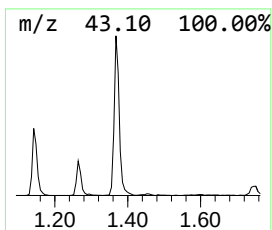
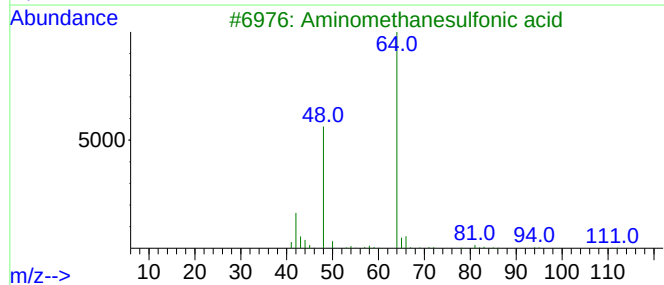
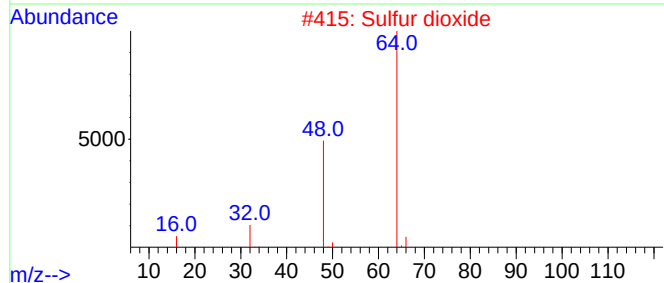
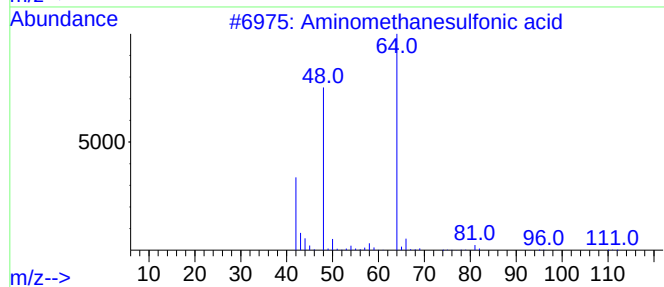
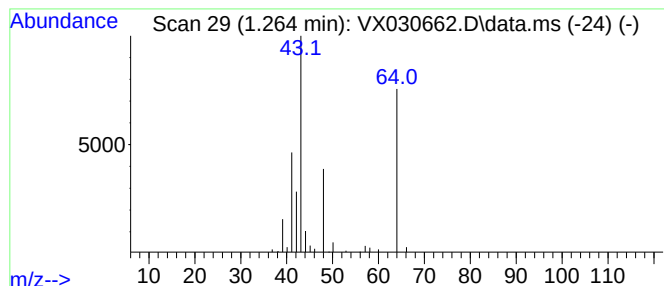
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Aminomethanesulfonic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	3.32 ug/L	52353	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	72
2			Sulfur dioxide	64	O2S	007446-09-5	56
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Ethyl Chloride	64	C2H5Cl	000075-00-3	7
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5



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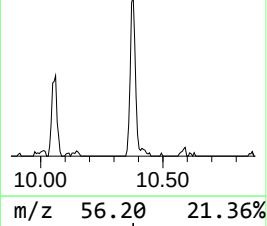
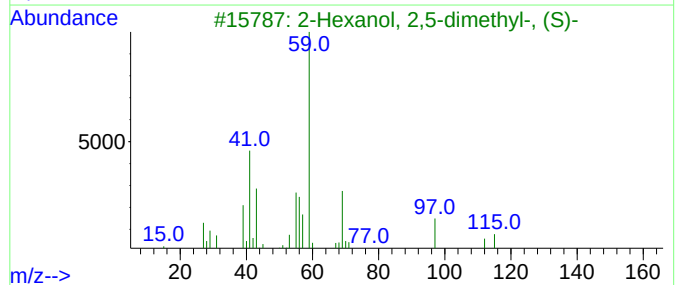
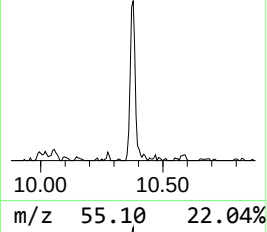
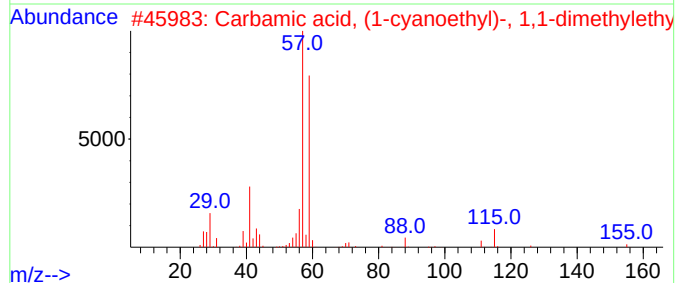
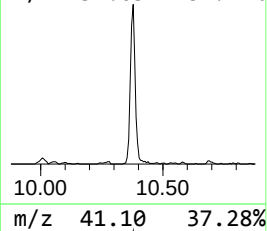
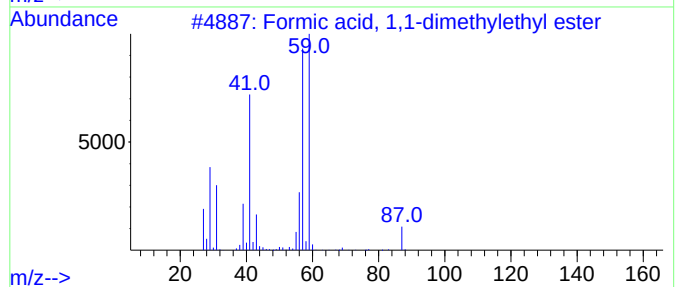
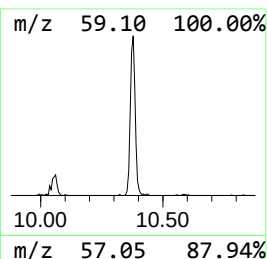
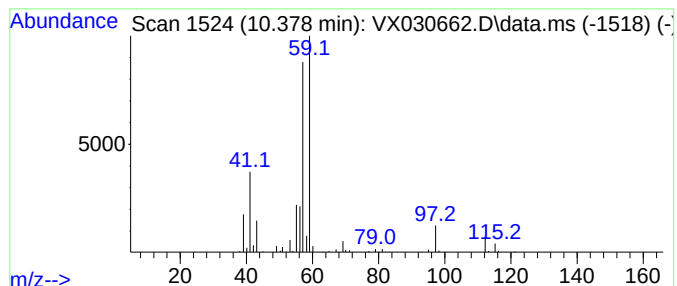
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Formic acid, 1,1-dimethylet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.378	5.44 ug/L	100089	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Formic acid, 1,1-dimethylethyl e...	102	C5H10O2	000762-75-4	50
2			Carbamic acid, (1-cyanoethyl)-, ...	170	C8H14N2O2	100927-09-1	50
3			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	50
4			Butanoic acid, 3,3-dimethyl-	116	C6H12O2	001070-83-3	40
5			Carbamic acid, (cyanomethyl)-, 1...	156	C7H12N2O2	085363-04-8	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081722\
Data File : VX030662.D
Acq On : 17 Aug 2022 16:02
Operator : JC/MD
Sample : N4221-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0KN6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.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
(DEL) Alkane: S...	1.142	5.2	ug/L	82793	1	6.769	789627	50.0
Aminomethanesul...	1.264	3.3	ug/L	52353	1	6.769	789627	50.0
Formic acid, 1,...	10.378	5.4	ug/L	100089	2	10.055	920293	50.0