

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081722\
 Data File : VX030663.D
 Acq On : 17 Aug 2022 16:25
 Operator : JC/MD
 Sample : N4221-15
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0KN7

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: VX030663.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	17	rVB	95733	87392	0.38%	0.132%
2	1.264	24	29	42	rBV	37276	55112	0.24%	0.083%
3	1.374	42	47	54	rBV2	1078216	1226588	5.38%	1.847%
4	1.666	91	95	103	rVB	139343	168165	0.74%	0.253%
5	1.745	104	108	118	rVB	13572	21422	0.09%	0.032%
6	1.953	138	142	146	rBV	10809	12870	0.06%	0.019%
7	1.995	146	149	154	rVB	14397	18594	0.08%	0.028%
8	2.319	194	202	216	rBV	6978027	11047854	48.46%	16.636%
9	2.654	255	257	262	rBV3	639	783	0.00%	0.001%
10	2.788	274	279	284	rBV3	3522	6594	0.03%	0.010%
11	2.940	299	304	305	rBV3	1446	2365	0.01%	0.004%
12	3.099	321	330	338	rVB	18607	39368	0.17%	0.059%
13	3.270	355	358	367	rVB5	1048	1936	0.01%	0.003%
14	3.440	380	386	391	rBV5	2142	4286	0.02%	0.006%
15	3.520	397	399	402	rBV2	488	439	0.00%	0.001%
16	3.617	405	415	426	rBV	185285	434647	1.91%	0.655%
17	4.361	529	537	545	rBV2	11141	30715	0.13%	0.046%
18	4.495	545	559	577	rBV2	1905858	5318894	23.33%	8.009%
19	4.873	618	621	624	rBV3	488	505	0.00%	0.001%
20	5.068	639	653	668	rBV	172350	543286	2.38%	0.818%
21	5.391	694	706	724	rVB2	101860	317496	1.39%	0.478%
22	5.556	727	733	735	rBV4	2538	4897	0.02%	0.007%
23	5.684	753	754	759	rBV2	522	719	0.00%	0.001%
24	5.739	761	763	767	rBV2	408	509	0.00%	0.001%
25	5.818	773	776	777	rVB3	555	474	0.00%	0.001%
26	5.836	777	779	783	rBV2	478	587	0.00%	0.001%
27	5.976	789	802	817	rBV2	462486	1364193	5.98%	2.054%
28	6.251	843	847	854	rVB8	1128	2642	0.01%	0.004%
29	6.299	854	855	859	rVB3	678	665	0.00%	0.001%
30	6.391	859	870	879	rBV3	13352	34590	0.15%	0.052%
31	6.470	882	883	887	rVB3	592	537	0.00%	0.001%
32	6.556	894	897	899	rBV3	577	600	0.00%	0.001%
33	6.769	921	932	948	rBV	315213	754482	3.31%	1.136%
34	7.135	979	992	1011	rBV	10483868	22799917	100.00%	34.333%
35	7.312	1014	1021	1038	rVB	272971	609118	2.67%	0.917%
36	7.677	1074	1081	1098	rVB2	51992	118390	0.52%	0.178%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Max Peaks: 100

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
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37	7.927	1115	1122	1126	rVV6	1882	5418	0.02%	0.008%
38	7.976	1126	1130	1137	rVB2	10243	19820	0.09%	0.030%
39	8.080	1145	1147	1149	rBV2	793	564	0.00%	0.001%
40	8.141	1153	1157	1160	rVB3	1419	1848	0.01%	0.003%
41	8.183	1160	1164	1168	rVB3	551	811	0.00%	0.001%
42	8.330	1181	1188	1202	rVV	190984	313159	1.37%	0.472%
43	8.653	1233	1241	1249	rBV	718747	1105469	4.85%	1.665%
44	8.848	1269	1273	1280	rVB	13399	22447	0.10%	0.034%
45	8.897	1280	1281	1283	rBV2	595	385	0.00%	0.001%
46	8.951	1285	1290	1297	rBV	135489	203261	0.89%	0.306%
47	9.171	1319	1326	1333	rBV5	13097	26756	0.12%	0.040%
48	9.281	1333	1344	1357	rBV	10453275	15464046	67.83%	23.286%
49	9.390	1357	1362	1372	rVB	468171	691706	3.03%	1.042%
50	9.646	1401	1404	1405	rVB3	721	701	0.00%	0.001%
51	9.665	1405	1407	1409	rBV2	429	460	0.00%	0.001%
52	9.732	1413	1418	1423	rBV	16007	22870	0.10%	0.034%
53	9.805	1428	1430	1431	rBV	849	542	0.00%	0.001%
54	9.860	1437	1439	1441	rVB2	521	418	0.00%	0.001%
55	9.890	1441	1444	1446	rBV2	483	542	0.00%	0.001%
56	9.939	1449	1452	1454	rBV3	445	611	0.00%	0.001%
57	9.994	1457	1461	1466	rBV6	3814	8995	0.04%	0.014%
58	10.055	1466	1471	1481	rVB	666118	888862	3.90%	1.338%
59	10.280	1504	1508	1510	rBV3	3021	3280	0.01%	0.005%
60	10.305	1510	1512	1517	rVB3	1909	2388	0.01%	0.004%
61	10.378	1518	1524	1534	rBV	71768	98117	0.43%	0.148%
62	10.579	1554	1557	1565	rVB5	3808	6430	0.03%	0.010%
63	10.646	1566	1568	1571	rVB3	976	708	0.00%	0.001%
64	10.750	1583	1585	1587	rVB2	681	471	0.00%	0.001%
65	10.786	1587	1591	1593	rBV3	680	781	0.00%	0.001%
66	10.841	1598	1600	1603	rBV4	619	942	0.00%	0.001%
67	10.902	1609	1610	1614	rVB3	670	716	0.00%	0.001%
68	10.957	1617	1619	1621	rVV2	676	587	0.00%	0.001%
69	11.018	1624	1629	1633	rBV4	2335	3119	0.01%	0.005%
70	11.091	1638	1641	1646	rVB5	1291	1684	0.01%	0.003%
71	11.195	1652	1658	1669	rVB	489080	613912	2.69%	0.924%
72	11.317	1674	1678	1684	rVB3	3094	4496	0.02%	0.007%
73	11.427	1693	1696	1697	rBV3	607	507	0.00%	0.001%
74	11.701	1738	1741	1746	rVB4	2993	3935	0.02%	0.006%
75	11.756	1746	1750	1752	rBV3	856	1156	0.01%	0.002%
76	11.792	1753	1756	1763	rVB2	5231	6355	0.03%	0.010%

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77	11.896	1766	1773	1778	rBV6	1708	2920	0.01%	0.004%
78	11.963	1782	1784	1788	rBV3	631	1064	0.00%	0.002%
79	12.024	1788	1794	1804	rBV	704629	860451	3.77%	1.296%
80	12.219	1822	1826	1837	rBV	24373	40286	0.18%	0.061%
81	12.323	1837	1843	1850	rVB	733150	927808	4.07%	1.397%
82	12.524	1872	1876	1879	rVB5	670	1028	0.00%	0.002%
83	12.554	1879	1881	1882	rBV2	396	391	0.00%	0.001%
84	12.762	1911	1915	1921	rBV3	1253	1844	0.01%	0.003%
85	13.000	1952	1954	1956	rBV2	426	495	0.00%	0.001%
86	13.176	1981	1983	1986	rBV3	423	392	0.00%	0.001%
87	13.225	1989	1991	1993	rBV2	598	453	0.00%	0.001%
88	13.286	1998	2001	2002	rBV2	575	542	0.00%	0.001%
89	13.408	2020	2021	2024	rBV	845	934	0.00%	0.001%
90	13.688	2064	2067	2068	rBV	648	579	0.00%	0.001%
91	13.737	2073	2075	2076	rBV	723	474	0.00%	0.001%
92	13.774	2079	2081	2084	rBV3	606	679	0.00%	0.001%
93	13.853	2092	2094	2098	rBV2	567	706	0.00%	0.001%
94	13.902	2101	2102	2104	rVV2	629	469	0.00%	0.001%
95	13.920	2104	2105	2108	rVB2	769	543	0.00%	0.001%
96	14.133	2136	2140	2144	rVB4	1862	2487	0.01%	0.004%
97	14.438	2188	2190	2193	rVB2	622	661	0.00%	0.001%
98	14.578	2211	2213	2214	rBV2	532	375	0.00%	0.001%
99	14.627	2219	2221	2224	rBV	809	987	0.00%	0.001%
100	15.072	2292	2294	2297	rBV2	861	734	0.00%	0.001%

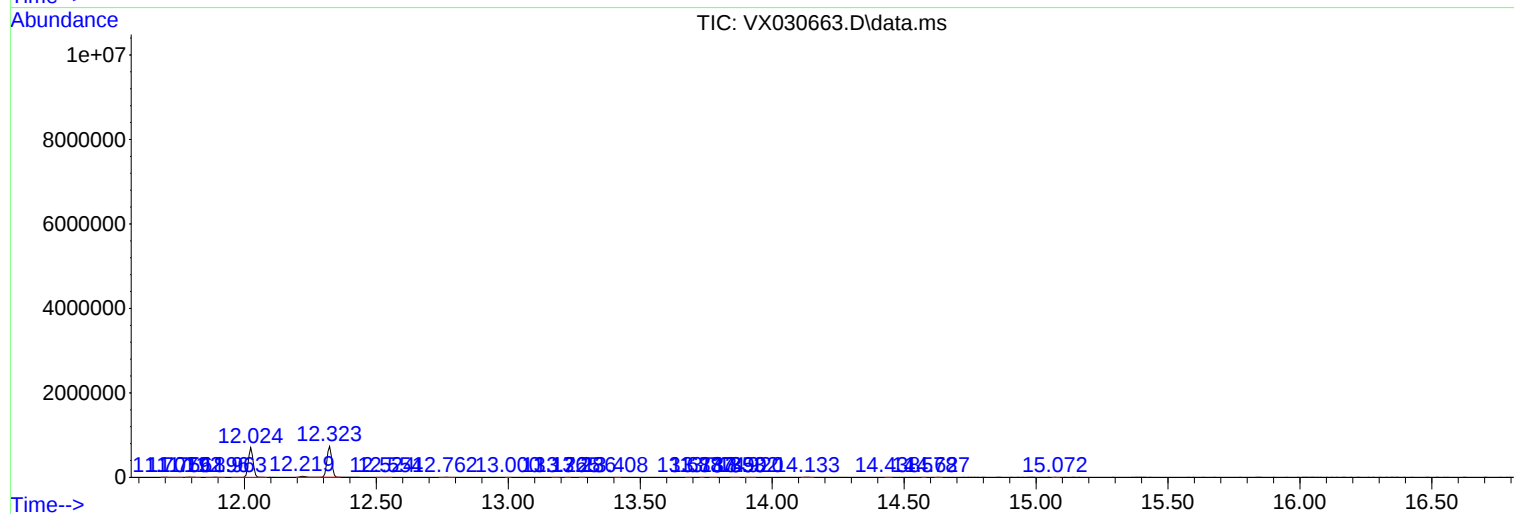
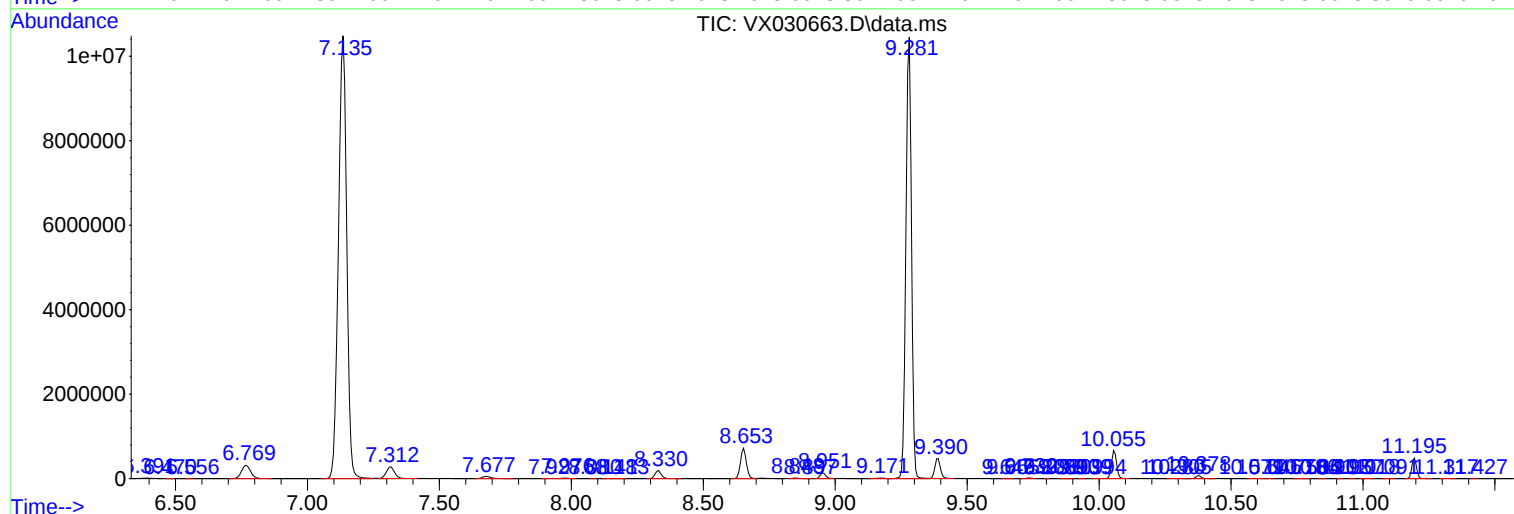
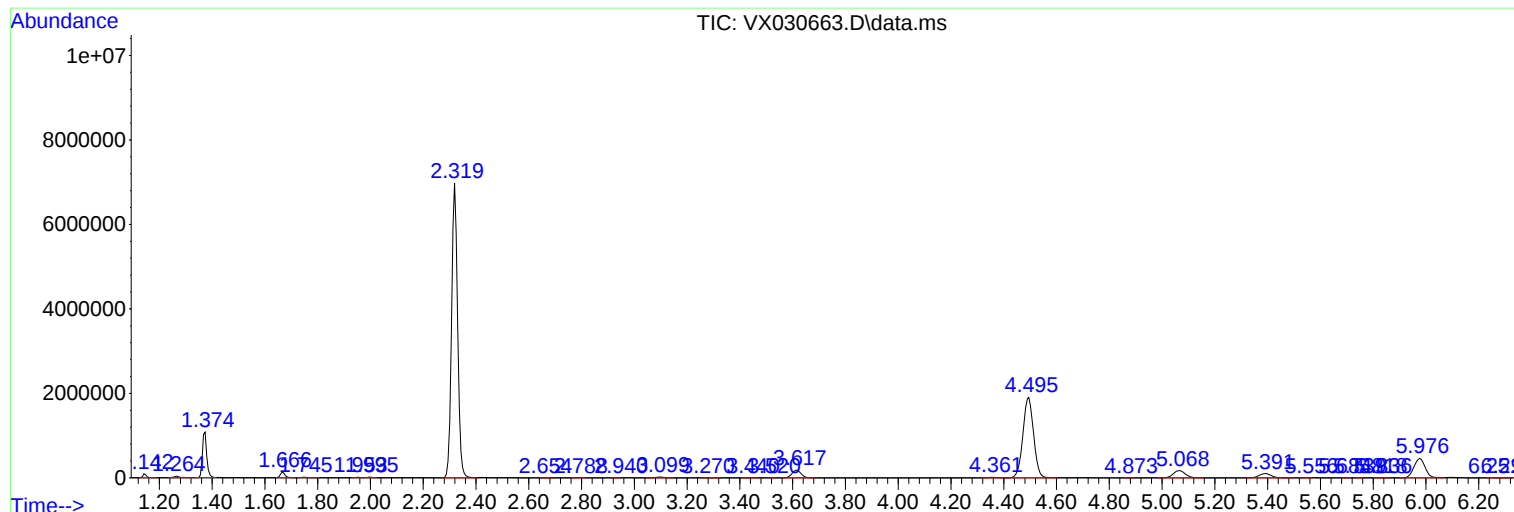
Sum of corrected areas: 66408208

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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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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



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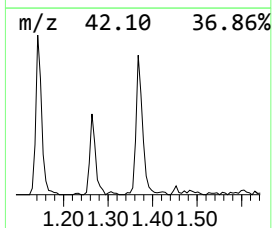
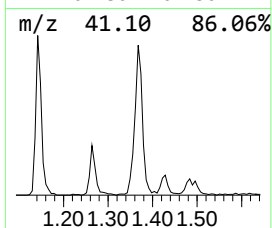
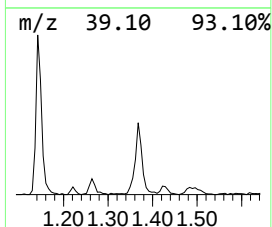
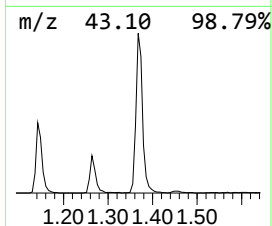
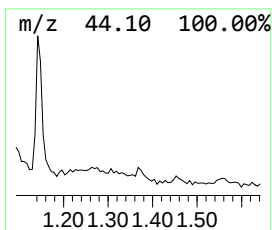
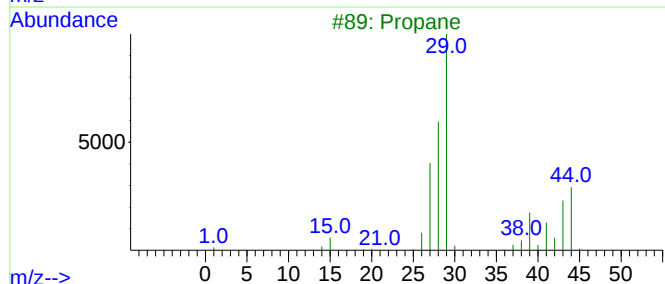
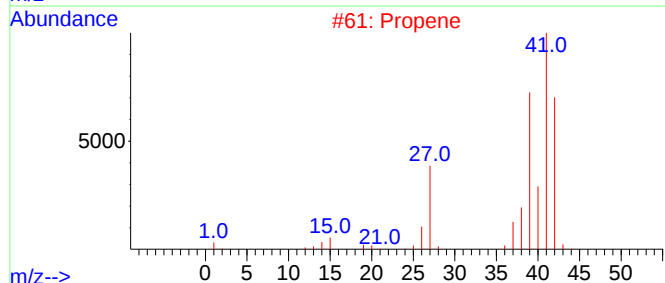
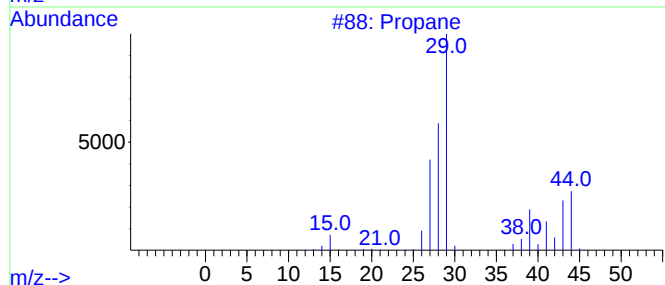
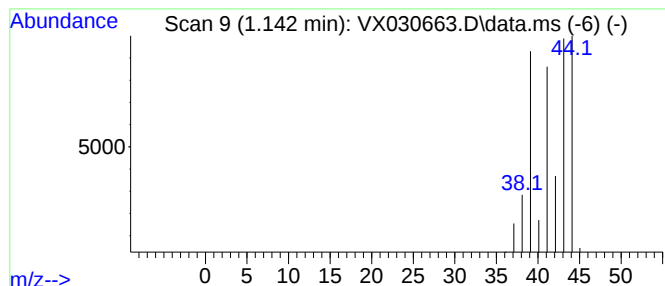
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	5.79 ug/L	87392	1,4-Difluorobenzene	6.769

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



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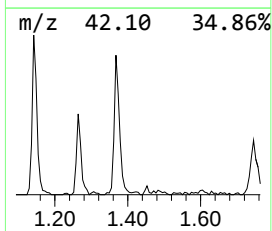
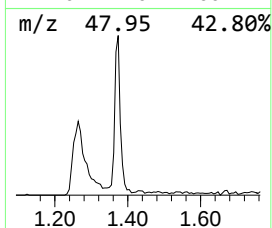
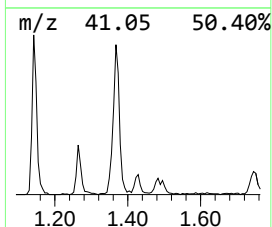
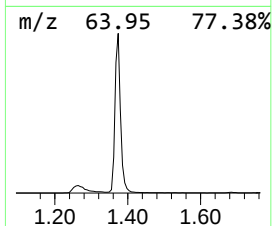
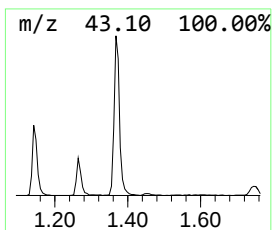
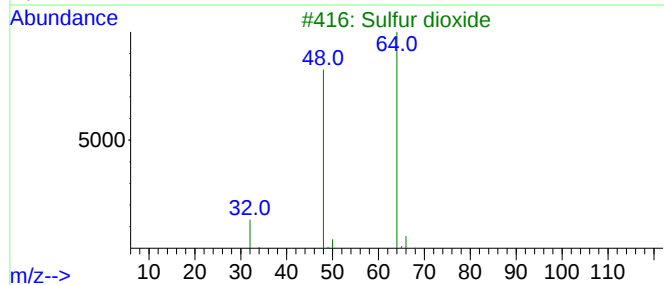
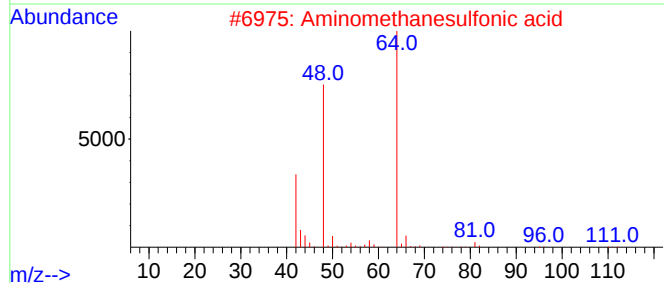
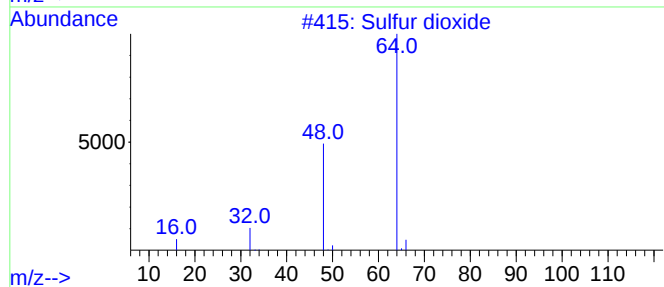
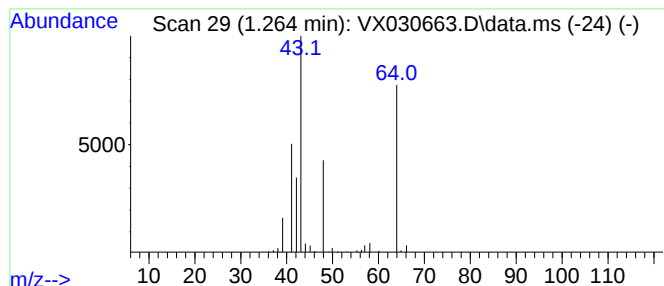
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	3.65 ug/L	55112	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	80
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	78
3			Sulfur dioxide	64	O2S	007446-09-5	56
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	43
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	40



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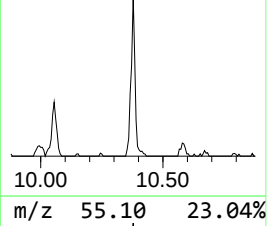
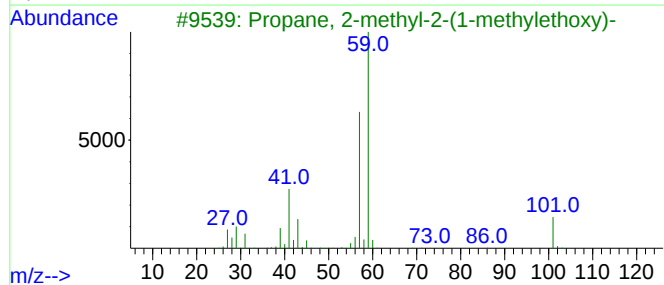
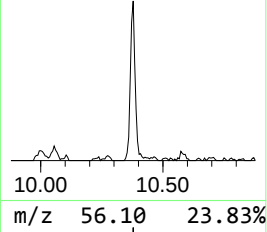
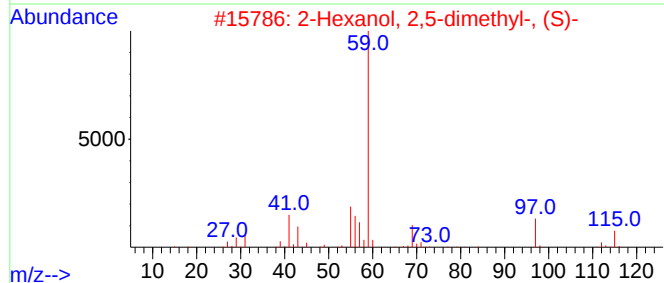
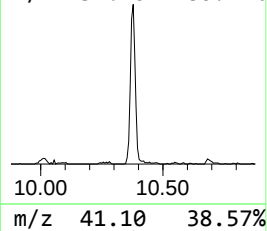
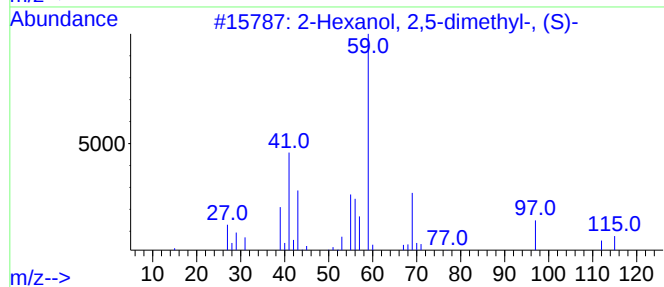
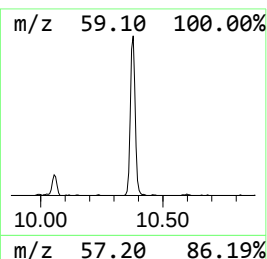
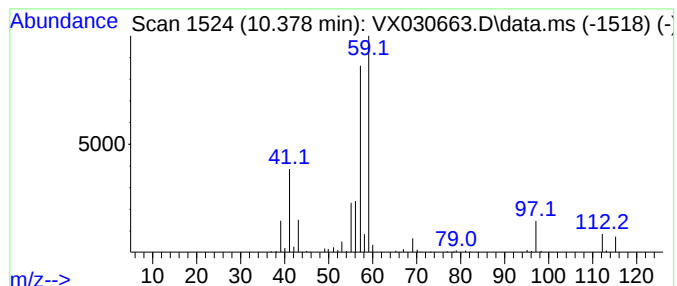
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.378	5.52 ug/L	98117	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	56
2			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	45
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
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 : VX030663.D
Acq On : 17 Aug 2022 16:25
Operator : JC/MD
Sample : N4221-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0KN7

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	5.8	ug/L	87392	1	6.769	754482	50.0
Sulfur dioxide	1.264	3.6	ug/L	55112	1	6.769	754482	50.0
2-Hexanol, 2,5-...	10.378	5.5	ug/L	98117	2	10.055	888862	50.0