

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081822\
 Data File : VX030688.D
 Acq On : 18 Aug 2022 16:24
 Operator : JC/MD
 Sample : N4231-07
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0KN5

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: VX030688.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	172659	148250	0.89%	0.287%
2	1.264	26	29	40	rVB2	24069	28157	0.17%	0.055%
3	1.368	41	46	53	rBV2	1628185	1889704	11.39%	3.661%
4	1.423	53	55	58	rVV	44293	40129	0.24%	0.078%
5	1.496	63	67	74	rVB	86258	88514	0.53%	0.171%
6	1.666	90	95	104	rVB	135715	172799	1.04%	0.335%
7	1.746	104	108	113	rVB4	8663	11638	0.07%	0.023%
8	1.904	131	134	138	rVB3	11173	13460	0.08%	0.026%
9	1.996	146	149	156	rVB	13297	16828	0.10%	0.033%
10	2.063	157	160	169	rVB	8114	13281	0.08%	0.026%
11	2.160	171	176	181	rVB2	15459	24247	0.15%	0.047%
12	2.319	193	202	216	rBV	6090111	9782955	58.96%	18.951%
13	2.654	252	257	262	rBV2	3491	6805	0.04%	0.013%
14	2.715	263	267	269	rBV4	1635	2546	0.02%	0.005%
15	2.794	275	280	288	rVB	5865	11556	0.07%	0.022%
16	2.874	288	293	296	rBV5	1096	1689	0.01%	0.003%
17	2.971	300	309	317	rVB3	4554	12722	0.08%	0.025%
18	3.093	321	329	340	rBB	31435	58831	0.35%	0.114%
19	3.282	356	360	363	rBV4	645	1126	0.01%	0.002%
20	3.319	363	366	367	rBV2	1354	1400	0.01%	0.003%
21	3.434	381	385	386	rBV2	810	888	0.01%	0.002%
22	3.617	405	415	427	rVV	196101	463005	2.79%	0.897%
23	3.849	451	453	456	rVB3	588	583	0.00%	0.001%
24	3.898	459	461	463	rVB	703	535	0.00%	0.001%
25	3.916	463	464	466	rBV	785	588	0.00%	0.001%
26	3.947	466	469	473	rVV5	808	1543	0.01%	0.003%
27	4.239	515	517	521	rVB3	1140	1177	0.01%	0.002%
28	4.355	529	536	537	rBV	12099	20015	0.12%	0.039%
29	4.495	545	559	582	rBV	2698660	7536748	45.43%	14.600%
30	5.068	640	653	669	rBV	175807	554323	3.34%	1.074%
31	5.391	695	706	717	rVB3	13629	43369	0.26%	0.084%
32	5.568	728	735	745	rVB6	2654	6783	0.04%	0.013%
33	5.977	789	802	818	rBV2	461587	1402957	8.46%	2.718%
34	6.245	842	846	858	rVB7	3921	10899	0.07%	0.021%
35	6.391	860	870	879	rVV2	20779	54279	0.33%	0.105%
36	6.611	902	906	910	rBV2	636	991	0.01%	0.002%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

37	6.641	910	911	915	rBV2	736	807	0.00%	0.002%
38	6.769	922	932	949	rBV	313750	752652	4.54%	1.458%
39	7.001	967	970	975	rBV2	626	739	0.00%	0.001%
40	7.135	980	992	1012	rBV	7382717	16591623	100.00%	32.140%
41	7.312	1014	1021	1034	rVB	277035	619228	3.73%	1.200%
42	7.665	1072	1079	1095	rVB	95146	191425	1.15%	0.371%
43	7.891	1114	1116	1117	rBV	686	527	0.00%	0.001%
44	8.135	1150	1156	1158	rBV6	2512	4208	0.03%	0.008%
45	8.232	1171	1172	1174	rBV2	613	547	0.00%	0.001%
46	8.263	1175	1177	1181	rVV3	1345	2128	0.01%	0.004%
47	8.330	1181	1188	1201	rVB	182956	303617	1.83%	0.588%
48	8.586	1225	1230	1234	rBV4	2869	4971	0.03%	0.010%
49	8.653	1234	1241	1248	rVV	722154	1124049	6.77%	2.177%
50	8.720	1249	1252	1257	rVB	16965	26604	0.16%	0.052%
51	8.812	1263	1267	1268	rBV2	3405	4050	0.02%	0.008%
52	8.848	1269	1273	1282	rVB2	24779	40865	0.25%	0.079%
53	8.952	1284	1290	1297	rBV	133686	195245	1.18%	0.378%
54	9.013	1297	1300	1306	rVB	8550	12591	0.08%	0.024%
55	9.171	1319	1326	1331	rBV3	11284	19160	0.12%	0.037%
56	9.275	1331	1343	1354	rBV	3401699	5061435	30.51%	9.805%
57	9.385	1356	1361	1372	rVV	472308	695380	4.19%	1.347%
58	9.525	1381	1384	1387	rBV3	3577	5440	0.03%	0.011%
59	9.683	1405	1410	1414	rBV6	1620	2475	0.01%	0.005%
60	9.738	1414	1419	1423	rVB3	7608	10408	0.06%	0.020%
61	9.811	1427	1431	1433	rBV2	674	1107	0.01%	0.002%
62	10.000	1457	1462	1465	rBV5	2634	5475	0.03%	0.011%
63	10.055	1466	1471	1486	rVB	646886	885546	5.34%	1.715%
64	10.275	1504	1507	1516	rVB5	3675	6693	0.04%	0.013%
65	10.378	1519	1524	1529	rBV	35770	48726	0.29%	0.094%
66	10.604	1560	1561	1565	rVB3	1249	1117	0.01%	0.002%
67	10.689	1571	1575	1580	rVB2	5495	7484	0.05%	0.014%
68	10.775	1584	1589	1590	rBV5	809	1240	0.01%	0.002%
69	10.866	1599	1604	1607	rBV3	2112	3305	0.02%	0.006%
70	10.957	1616	1619	1620	rBV3	739	732	0.00%	0.001%
71	11.031	1625	1631	1635	rVV7	4857	8043	0.05%	0.016%
72	11.085	1638	1640	1644	rVB4	847	885	0.01%	0.002%
73	11.195	1652	1658	1667	rVB	527363	650619	3.92%	1.260%
74	11.317	1673	1678	1683	rBV3	8564	11324	0.07%	0.022%
75	11.427	1692	1696	1699	rBV4	1454	2012	0.01%	0.004%
76	11.573	1716	1720	1721	rBV2	910	723	0.00%	0.001%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

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Sampling : 1

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 Title : VOC Analysis

77	11.701	1739	1741	1748	rVB5	882	1398	0.01%	0.003%
78	11.890	1768	1772	1775	rBV4	1232	1612	0.01%	0.003%
79	11.933	1775	1779	1784	rBV3	5748	7440	0.04%	0.014%
80	12.024	1789	1794	1803	rVV	727457	857981	5.17%	1.662%
81	12.232	1823	1828	1834	rBV2	5784	11543	0.07%	0.022%
82	12.323	1837	1843	1850	rBV	774013	971009	5.85%	1.881%
83	12.482	1868	1869	1873	rBV2	467	564	0.00%	0.001%
84	12.524	1873	1876	1877	rVV2	882	873	0.01%	0.002%
85	12.573	1880	1884	1886	rVB2	612	777	0.00%	0.002%
86	12.604	1886	1889	1892	rBV3	847	1131	0.01%	0.002%
87	12.640	1892	1895	1897	rBV	506	641	0.00%	0.001%
88	12.701	1902	1905	1909	rVV4	1748	2872	0.02%	0.006%
89	12.768	1912	1916	1920	rVB2	4356	5803	0.03%	0.011%
90	12.860	1926	1931	1936	rBV	14712	18906	0.11%	0.037%
91	12.914	1938	1940	1942	rVB	1000	658	0.00%	0.001%
92	13.103	1969	1971	1975	rBV4	764	731	0.00%	0.001%
93	13.536	2040	2042	2044	rBV2	538	591	0.00%	0.001%
94	14.134	2136	2140	2143	rBV4	1342	2169	0.01%	0.004%
95	14.426	2185	2188	2193	rBV3	710	1413	0.01%	0.003%
96	14.530	2204	2205	2210	rVB3	522	614	0.00%	0.001%
97	14.658	2224	2226	2230	rBV4	1028	1321	0.01%	0.003%
98	15.316	2332	2334	2336	rBV2	887	687	0.00%	0.001%
99	15.493	2361	2363	2364	rBV2	823	586	0.00%	0.001%
100	16.158	2470	2472	2474	rBV3	867	789	0.00%	0.002%

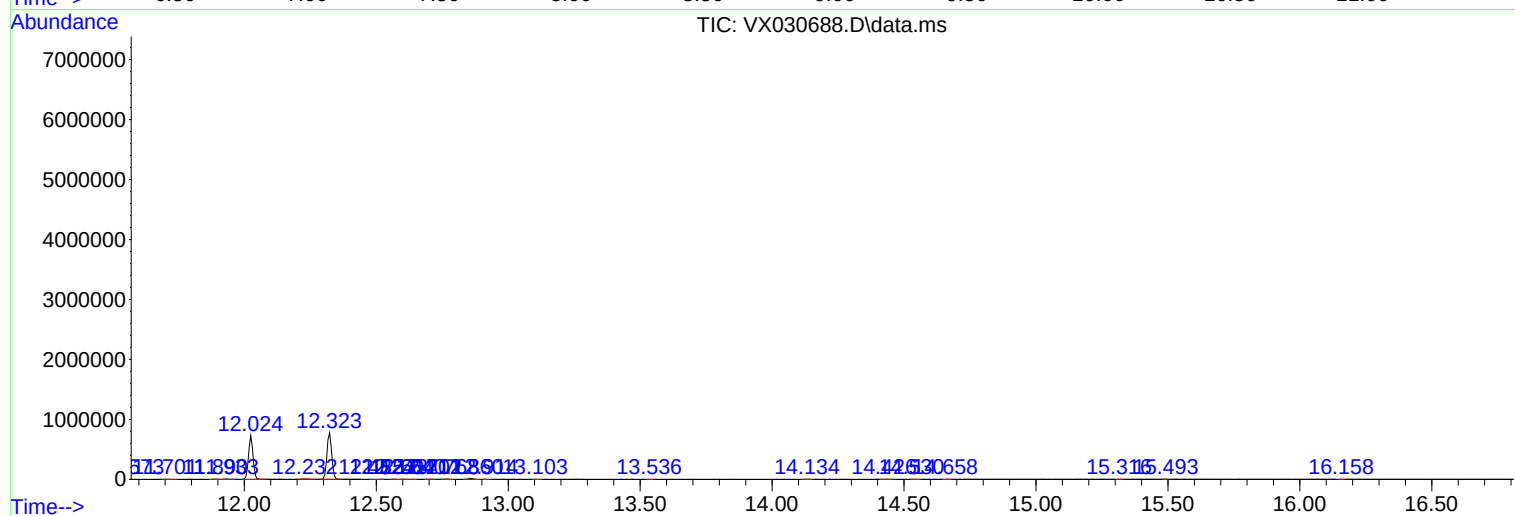
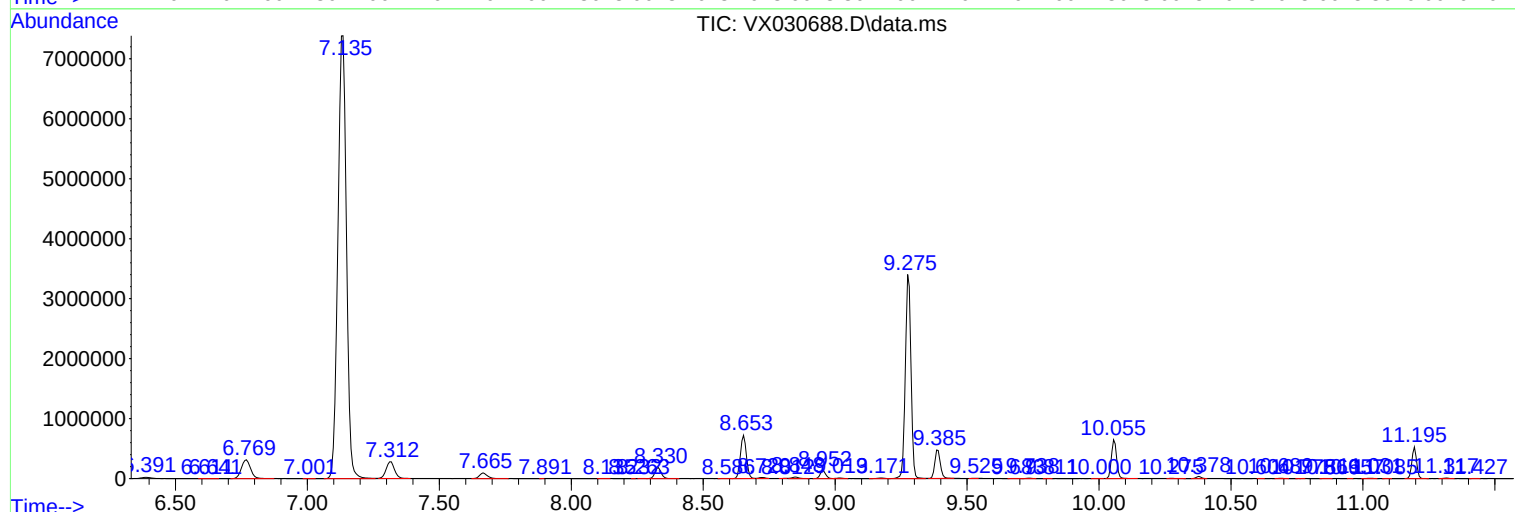
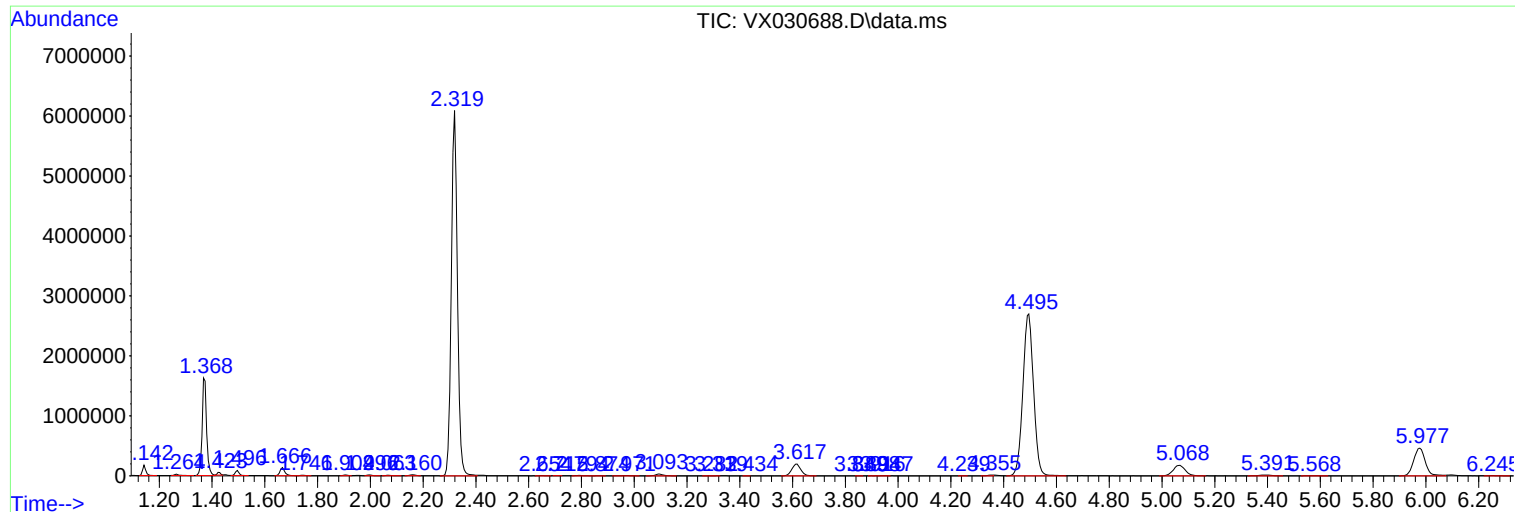
Sum of corrected areas: 51622634

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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0KN5

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081822\
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Operator : JC/MD
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Instrument :
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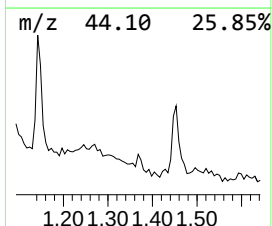
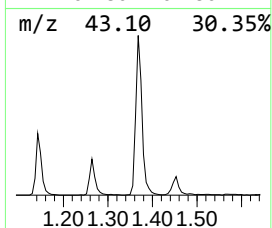
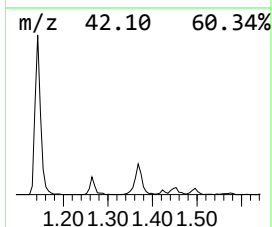
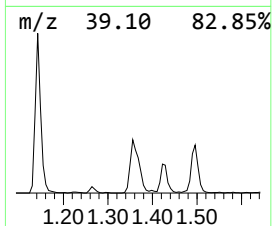
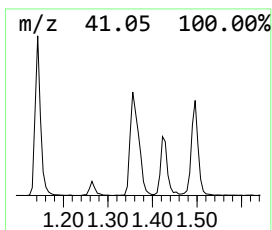
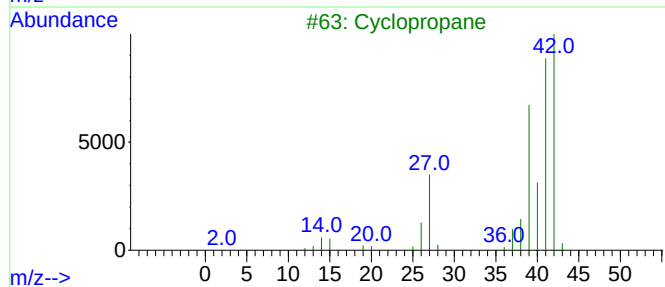
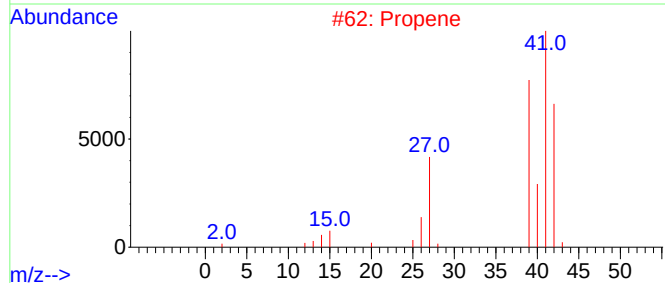
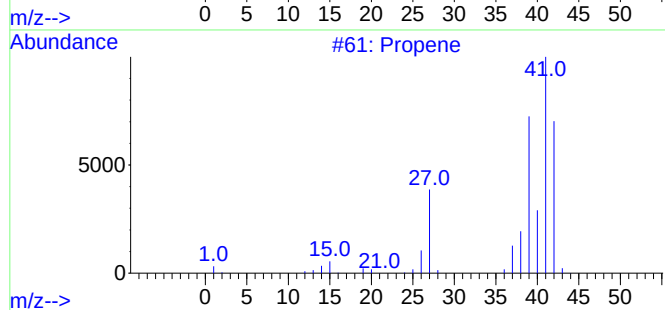
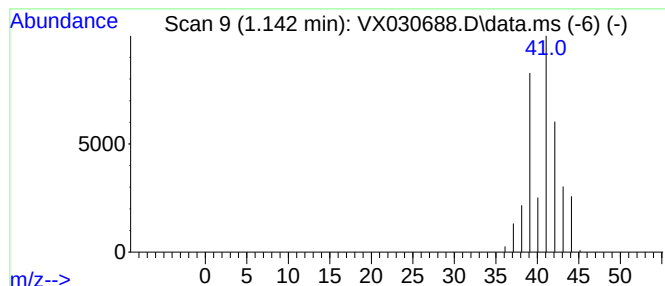
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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	9.85 ug/L	148250	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Propene	42	C3H6	000115-07-1	42
3			Cyclopropane	42	C3H6	000075-19-4	40
4			Cyclopropane	42	C3H6	000075-19-4	9
5			Cyclopropene	40	C3H4	002781-85-3	9



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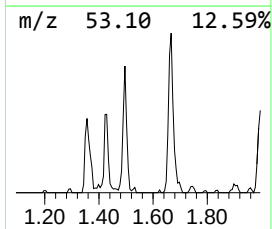
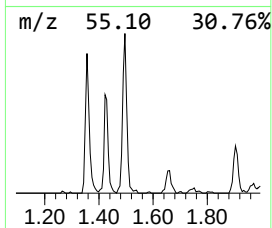
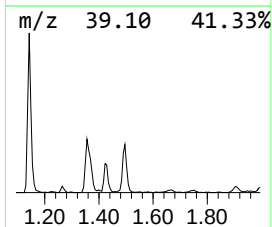
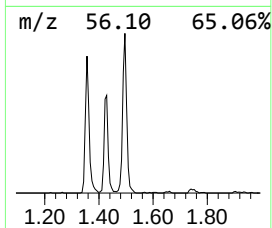
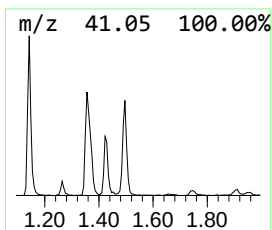
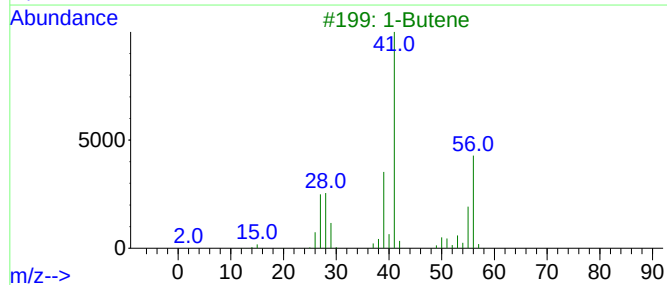
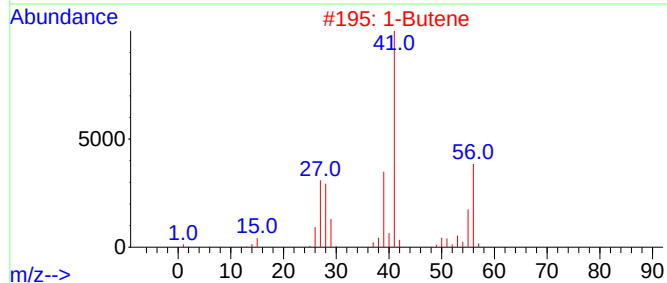
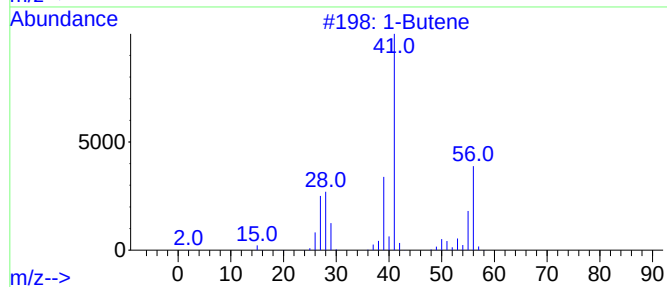
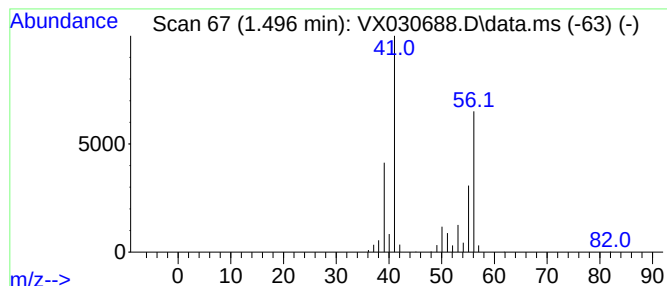
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.496	5.88 ug/L	88514	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene			56	C4H8	000106-98-9	87
2	1-Butene			56	C4H8	000106-98-9	87
3	1-Butene			56	C4H8	000106-98-9	87
4	1-Propene, 2-methyl-			56	C4H8	000115-11-7	83
5	1-Propene, 2-methyl-			56	C4H8	000115-11-7	80



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ALS Vial : 14 Sample Multiplier: 1

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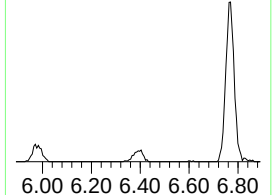
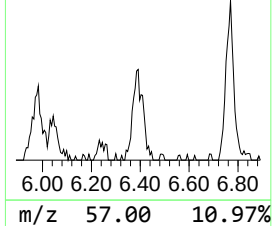
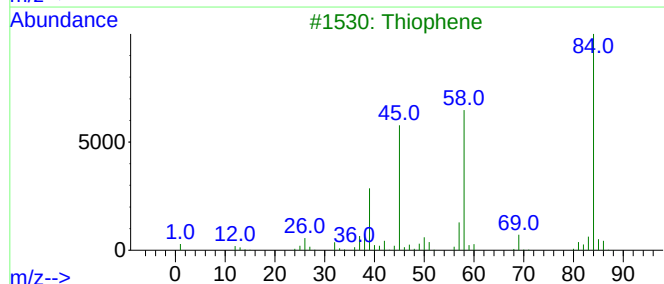
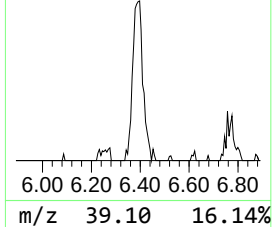
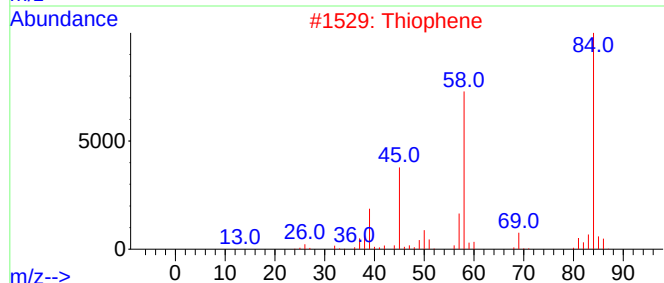
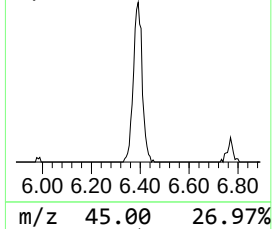
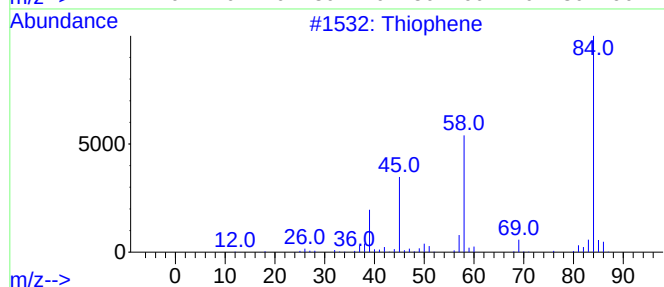
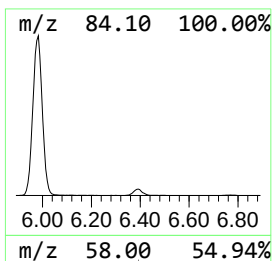
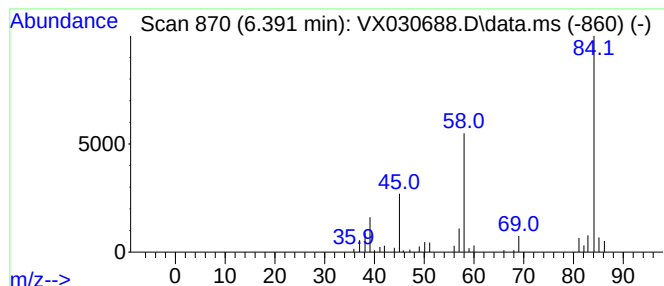
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Thiophene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.391	3.61 ug/L	54279	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene	84	C4H4S	000110-02-1	91
2			Thiophene	84	C4H4S	000110-02-1	91
3			Thiophene	84	C4H4S	000110-02-1	91
4			Thiophene	84	C4H4S	000110-02-1	90
5			4H-1,2,4-Triazol-4-amine	84	C2H4N4	000584-13-4	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081822\
Data File : VX030688.D
Acq On : 18 Aug 2022 16:24
Operator : JC/MD
Sample : N4231-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0KN5

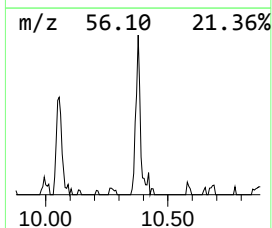
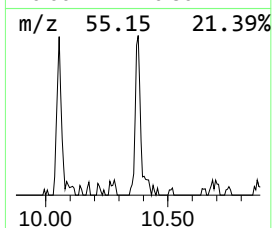
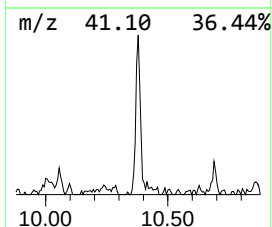
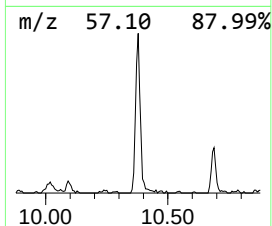
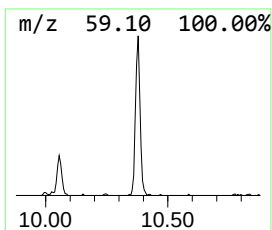
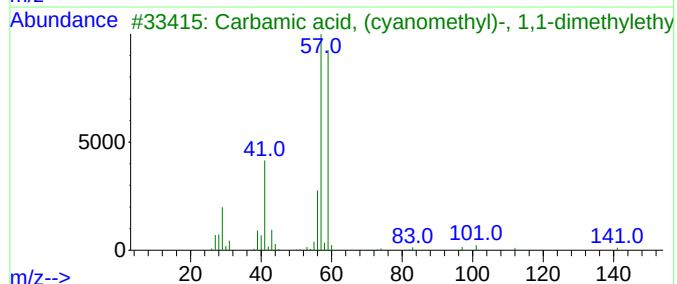
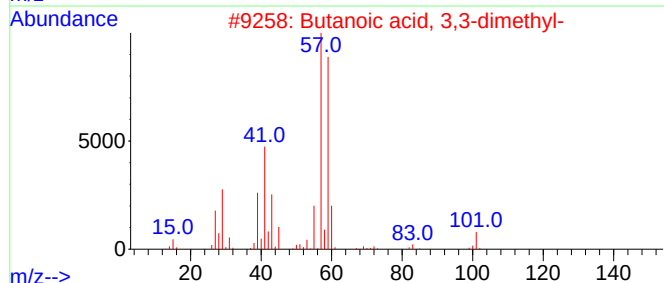
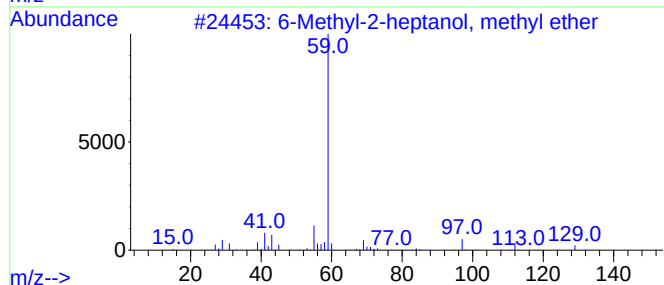
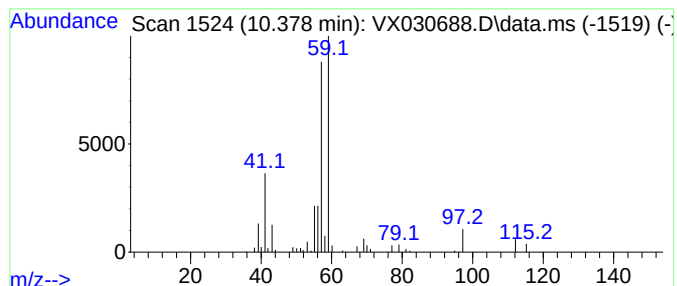
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Quant Title : VOC Analysis

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

Peak Number 6 6-Methyl-2-heptanol, methyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.378	2.75 ug/L	48726	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Methyl-2-heptanol, methyl ether	144	C9H20O	1000365-52-0	53
2			Butanoic acid, 3,3-dimethyl-	116	C6H12O2	001070-83-3	40
3			Carbamic acid, (cyanomethyl)-, 1...	156	C7H12N2O2	085363-04-8	39
4			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	38
5			Carbamic acid, (1-cyanoethyl)-, ...	170	C8H14N2O2	100927-09-1	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081822\
Data File : VX030688.D
Acq On : 18 Aug 2022 16:24
Operator : JC/MD
Sample : N4231-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0KN5

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	9.8	ug/L	148250	1	6.769	752652	50.0
(DEL) Alkane: S...	1.496	5.9	ug/L	88514	1	6.769	752652	50.0
Thiophene	6.391	3.6	ug/L	54279	1	6.769	752652	50.0
6-Methyl-2-hept...	10.378	2.8	ug/L	48726	2	10.055	885546	50.0