

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081722\
 Data File : VX030661.D
 Acq On : 17 Aug 2022 15:38
 Operator : JC/MD
 Sample : N4221-13
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0KN3

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: VX030661.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	15	rVB	85469	74465	0.18%	0.107%
2	1.264	23	29	37	rBV2	30541	52299	0.13%	0.075%
3	1.368	42	46	58	rVB2	384276	420668	1.04%	0.605%
4	1.666	91	95	103	rVB	141489	174379	0.43%	0.251%
5	1.746	105	108	114	rVB	7361	9455	0.02%	0.014%
6	1.904	131	134	138	rBV4	4225	6309	0.02%	0.009%
7	1.953	138	142	147	rBV2	6834	9690	0.02%	0.014%
8	2.319	194	202	218	rBV	4079870	6522376	16.09%	9.373%
9	2.605	247	249	251	rBV2	530	471	0.00%	0.001%
10	2.788	273	279	289	rBV3	7846	15877	0.04%	0.023%
11	2.934	300	303	304	rBV2	616	722	0.00%	0.001%
12	2.977	306	310	312	rBV5	1408	2279	0.01%	0.003%
13	3.099	324	330	338	rVV4	10572	20935	0.05%	0.030%
14	3.282	357	360	362	rBV	488	526	0.00%	0.001%
15	3.337	362	369	373	rBV3	1971	4068	0.01%	0.006%
16	3.447	378	387	393	rVB7	1774	4801	0.01%	0.007%
17	3.611	404	414	427	rBV	200050	478101	1.18%	0.687%
18	3.770	438	440	444	rVB	539	507	0.00%	0.001%
19	3.812	444	447	448	rBV2	539	463	0.00%	0.001%
20	4.038	483	484	489	rVB3	431	579	0.00%	0.001%
21	4.087	489	492	496	rVB2	459	726	0.00%	0.001%
22	4.209	511	512	514	rBV	483	438	0.00%	0.001%
23	4.263	517	521	522	rBV2	675	900	0.00%	0.001%
24	4.495	545	559	585	rBV2	990901	2883635	7.11%	4.144%
25	4.794	606	608	611	rBV3	452	482	0.00%	0.001%
26	5.068	640	653	668	rBV	183221	558296	1.38%	0.802%
27	5.190	671	673	678	rVV3	469	805	0.00%	0.001%
28	5.239	678	681	682	rVB2	858	744	0.00%	0.001%
29	5.391	696	706	718	rVB3	12421	39346	0.10%	0.057%
30	5.556	727	733	734	rBV3	1963	2713	0.01%	0.004%
31	5.818	773	776	778	rBV2	719	610	0.00%	0.001%
32	5.977	790	802	817	rBV2	472394	1400368	3.45%	2.012%
33	6.227	840	843	844	rBV2	795	807	0.00%	0.001%
34	6.391	861	870	879	rBV3	8879	23659	0.06%	0.034%
35	6.696	916	920	922	rBV3	486	561	0.00%	0.001%
36	6.763	922	931	943	rBV	163608	397333	0.98%	0.571%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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

37	6.946	959	961	963	rBV2	504	435	0.00%	0.001%
38	7.141	979	993	1013	rBV	17581353	40535729	100.00%	58.255%
39	7.312	1014	1021	1037	rVB	280679	637048	1.57%	0.916%
40	7.671	1073	1080	1091	rVB	42670	88246	0.22%	0.127%
41	7.836	1106	1107	1110	rVB2	539	441	0.00%	0.001%
42	7.976	1126	1130	1136	rVB4	5366	10019	0.02%	0.014%
43	8.269	1176	1178	1181	rBV2	528	542	0.00%	0.001%
44	8.330	1181	1188	1198	rVV	199578	319668	0.79%	0.459%
45	8.653	1234	1241	1249	rBV	729961	1129526	2.79%	1.623%
46	8.842	1269	1272	1277	rVB4	5374	8823	0.02%	0.013%
47	8.952	1284	1290	1297	rBV	146145	205580	0.51%	0.295%
48	9.159	1318	1324	1331	rBV6	6447	12643	0.03%	0.018%
49	9.281	1332	1344	1356	rBV	6761253	10248543	25.28%	14.728%
50	9.384	1356	1361	1371	rVB	472875	671951	1.66%	0.966%
51	9.732	1414	1418	1423	rVB3	9519	12984	0.03%	0.019%
52	10.012	1457	1464	1466	rBV5	2117	4632	0.01%	0.007%
53	10.055	1466	1471	1483	rVV	346908	476092	1.17%	0.684%
54	10.147	1484	1486	1491	rVB4	1575	1951	0.00%	0.003%
55	10.201	1491	1495	1499	rBV5	2773	4060	0.01%	0.006%
56	10.305	1509	1512	1516	rVB4	2518	3389	0.01%	0.005%
57	10.378	1518	1524	1530	rBV	23037	31395	0.08%	0.045%
58	10.653	1565	1569	1571	rVB4	1416	1958	0.00%	0.003%
59	10.854	1601	1602	1604	rBV2	776	481	0.00%	0.001%
60	11.018	1625	1629	1634	rVB4	2004	3051	0.01%	0.004%
61	11.092	1634	1641	1646	rBV6	1714	3260	0.01%	0.005%
62	11.195	1652	1658	1669	rVV	485318	614109	1.51%	0.883%
63	11.317	1673	1678	1684	rVB	31169	41574	0.10%	0.060%
64	11.415	1693	1694	1696	rBV	590	547	0.00%	0.001%
65	11.701	1736	1741	1745	rBV5	1456	2107	0.01%	0.003%
66	11.799	1754	1757	1763	rBV3	937	1244	0.00%	0.002%
67	11.896	1768	1773	1774	rBV4	832	825	0.00%	0.001%
68	11.933	1776	1779	1782	rBV2	1523	1700	0.00%	0.002%
69	12.024	1789	1794	1803	rBV	362396	438493	1.08%	0.630%
70	12.219	1822	1826	1832	rBV3	2736	5037	0.01%	0.007%
71	12.323	1837	1843	1856	rVV	736164	912769	2.25%	1.312%
72	12.421	1858	1859	1862	rVB2	1703	1343	0.00%	0.002%
73	12.762	1909	1915	1920	rVB	10921	15462	0.04%	0.022%
74	12.823	1923	1925	1927	rVV2	559	481	0.00%	0.001%
75	12.853	1927	1930	1935	rVV2	4162	5584	0.01%	0.008%
76	12.914	1939	1940	1944	rVV2	728	583	0.00%	0.001%

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Integration Parameters: LSCINT.P

Integrator: RTE

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 Title : VOC Analysis

77	13.152	1977	1979	1984	rVB3	596	833	0.00%	0.001%
78	13.231	1989	1992	1994	rBV2	597	758	0.00%	0.001%
79	13.469	2028	2031	2033	rBV2	607	584	0.00%	0.001%
80	13.573	2045	2048	2049	rVV	640	524	0.00%	0.001%
81	13.652	2057	2061	2062	rVV2	447	535	0.00%	0.001%
82	13.683	2062	2066	2070	rVV3	590	992	0.00%	0.001%
83	13.731	2072	2074	2077	rBV2	589	701	0.00%	0.001%
84	13.786	2080	2083	2090	rVV4	803	1354	0.00%	0.002%
85	13.878	2096	2098	2099	rVV	830	442	0.00%	0.001%
86	13.975	2111	2114	2117	rVV3	345	506	0.00%	0.001%
87	14.134	2135	2140	2144	rBV3	2006	2754	0.01%	0.004%
88	14.298	2165	2167	2170	rVB2	611	572	0.00%	0.001%
89	14.323	2170	2171	2173	rBV2	581	465	0.00%	0.001%
90	14.420	2185	2187	2191	rVB2	864	908	0.00%	0.001%
91	14.451	2191	2192	2196	rBV3	493	477	0.00%	0.001%
92	14.652	2221	2225	2228	rBV3	889	1758	0.00%	0.003%
93	15.054	2289	2291	2292	rBV2	684	462	0.00%	0.001%
94	15.133	2302	2304	2308	rVB2	799	708	0.00%	0.001%
95	15.201	2313	2315	2316	rBV	565	435	0.00%	0.001%
96	15.682	2392	2394	2399	rVB4	780	1034	0.00%	0.001%
97	15.737	2402	2403	2405	rBV2	852	446	0.00%	0.001%
98	16.225	2481	2483	2486	rBV4	915	774	0.00%	0.001%
99	16.456	2519	2521	2522	rBV2	613	545	0.00%	0.001%
100	16.731	2564	2566	2568	rBV	807	499	0.00%	0.001%

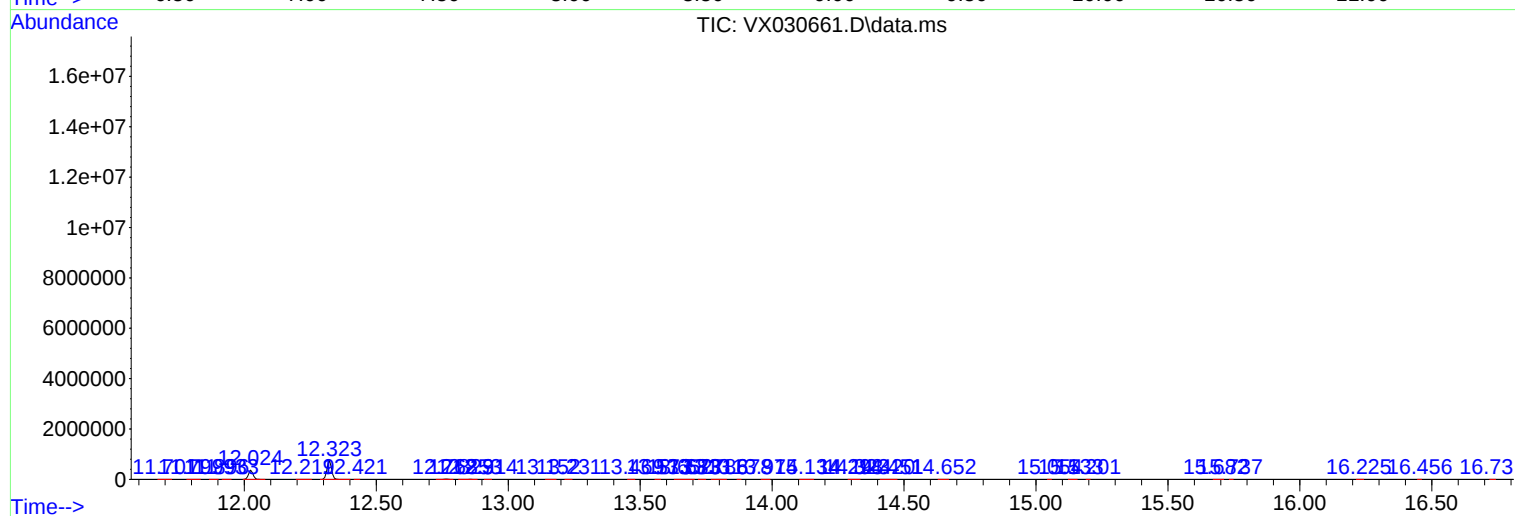
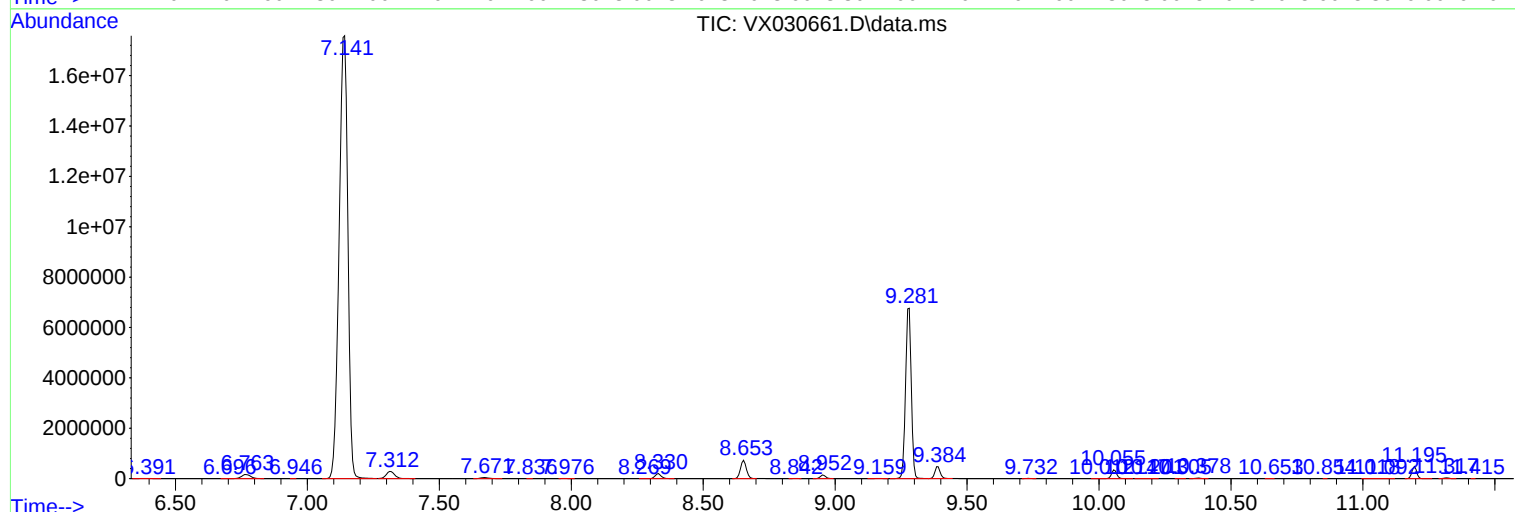
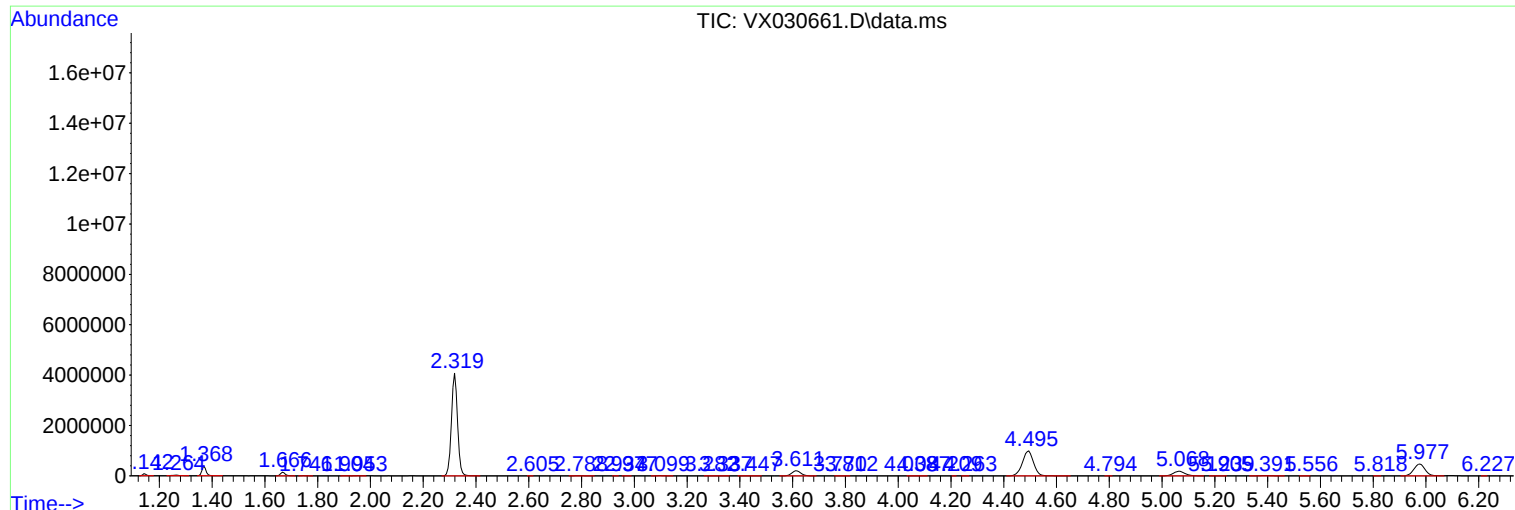
Sum of corrected areas: 69583764

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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



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C0KN3

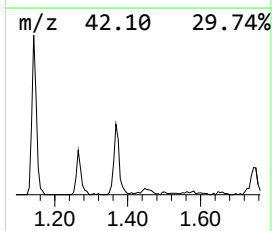
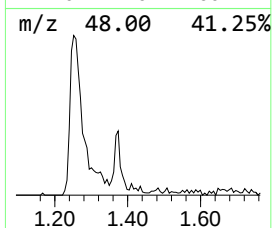
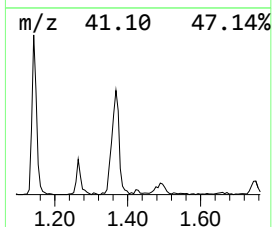
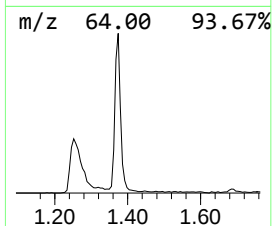
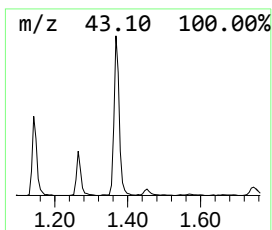
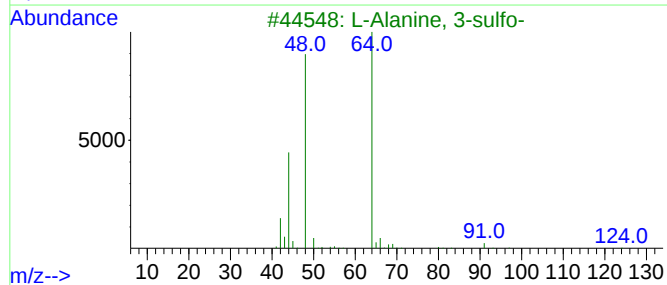
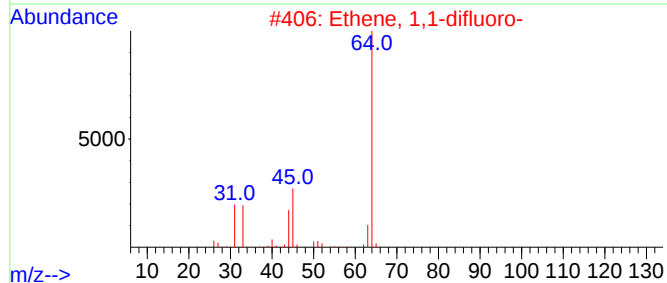
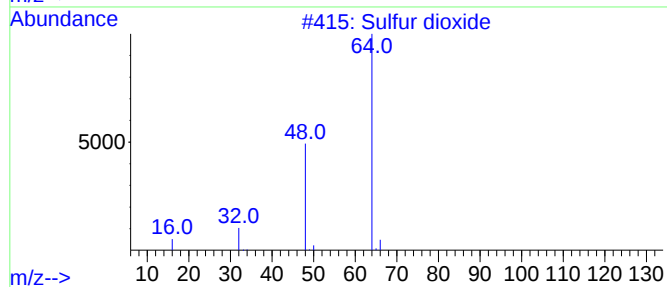
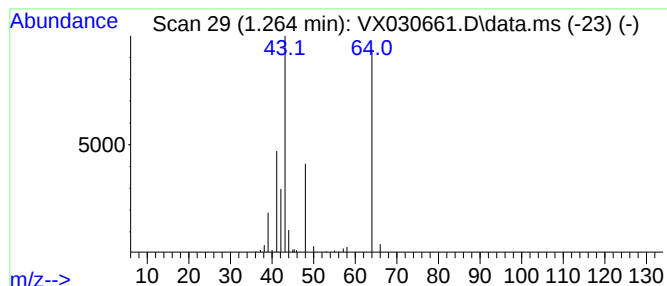
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	6.58 ug/L	52299	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	50
2			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	9
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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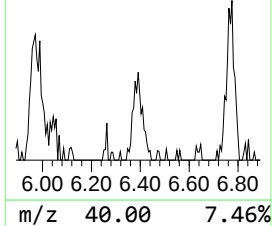
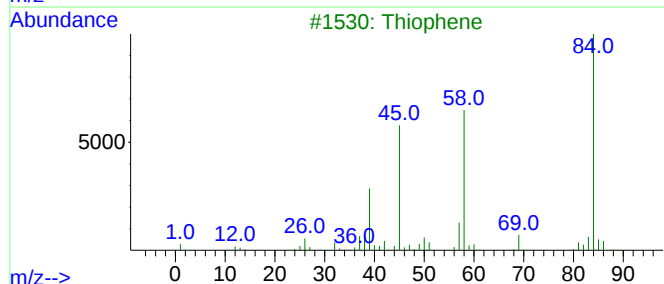
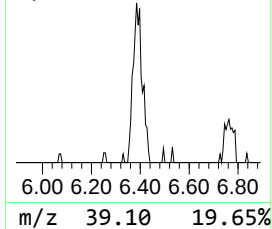
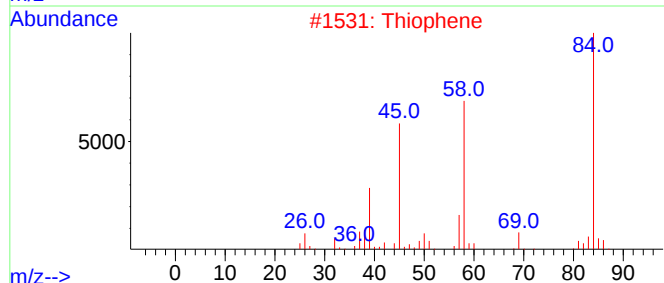
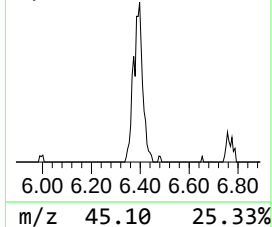
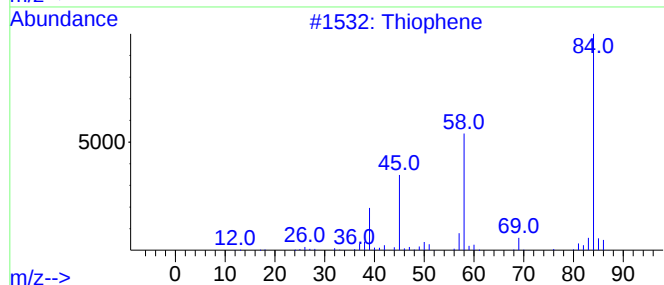
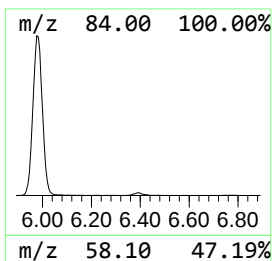
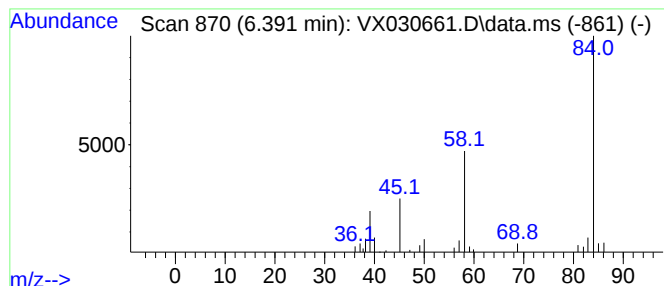
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Thiophene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.391	2.98 ug/L	23659	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	78
3			Thiophene	84	C4H4S	000110-02-1	72
4			Thiophene	84	C4H4S	000110-02-1	42
5			4H-1,2,4-Triazol-4-amine	84	C2H4N4	000584-13-4	9



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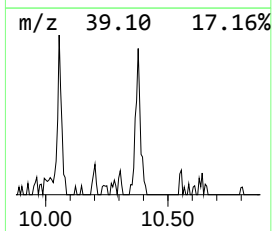
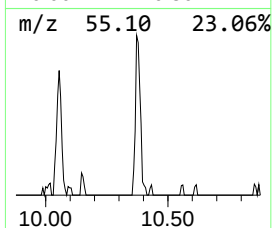
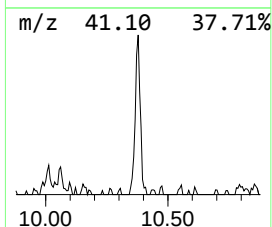
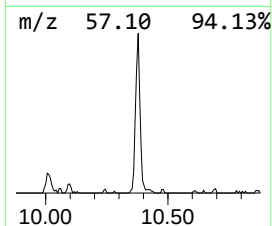
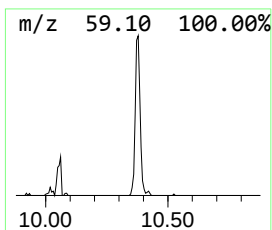
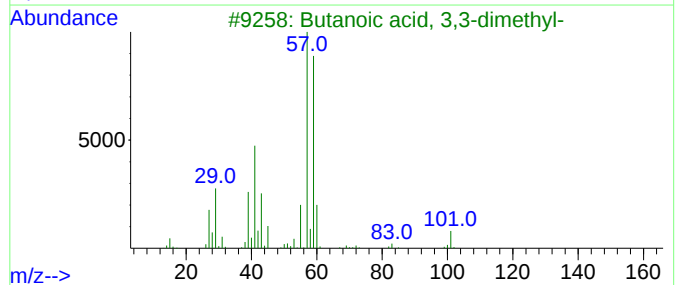
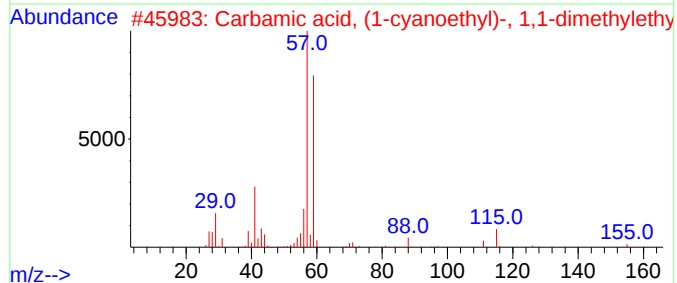
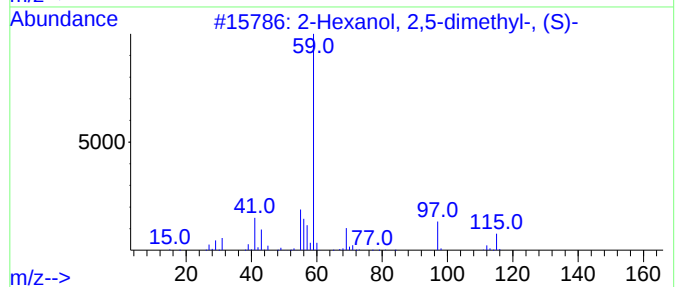
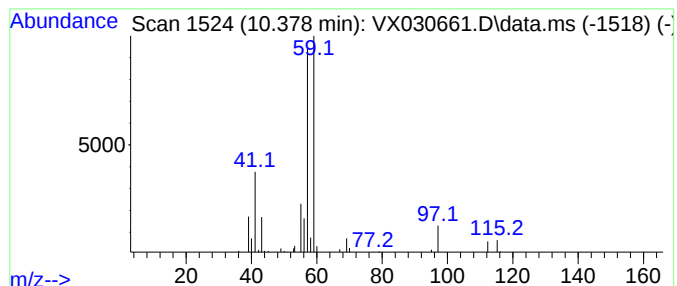
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.378	3.30 ug/L	31395	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	72
2			Carbamic acid, (1-cyanoethyl)-, ...	170	C8H14N2O2	100927-09-1	72
3			Butanoic acid, 3,3-dimethyl-	116	C6H12O2	001070-83-3	42
4			Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	40
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081722\
Data File : VX030661.D
Acq On : 17 Aug 2022 15:38
Operator : JC/MD
Sample : N4221-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0KN3

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
Sulfur dioxide	1.264	6.6	ug/L	52299	1	6.769	397333	50.0
Thiophene	6.391	3.0	ug/L	23659	1	6.769	397333	50.0
2-Hexanol, 2,5-...	10.378	3.3	ug/L	31395	2	10.055	476092	50.0