

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
 Data File : VX035142.D
 Acq On : 18 Apr 2023 23:01
 Operator : JC/MD
 Sample : 02397-06
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COML8

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\SFAMXML041823WMA.M

Title : VOC Analysis

Signal : TIC: VX035142.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.282	25	32	42	rBV	36887	123378	0.05%	0.018%
2	1.368	42	46	57	rVB	258759	296042	0.13%	0.043%
3	1.673	92	96	106	rBV	184096	247385	0.11%	0.036%
4	2.307	194	200	211	rBV	446232	703561	0.31%	0.101%
5	2.386	211	213	221	rVB	3773	7093	0.00%	0.001%
6	2.508	228	233	240	rBV	8146	13603	0.01%	0.002%
7	2.617	249	251	254	rVB3	463	340	0.00%	0.000%
8	2.788	270	279	285	rVV2	9730	20334	0.01%	0.003%
9	2.861	286	291	302	rVV	22696	48986	0.02%	0.007%
10	2.953	304	306	308	rVV	549	440	0.00%	0.000%
11	3.105	325	331	339	rVB3	3957	9525	0.00%	0.001%
12	3.312	362	365	367	rBV3	322	393	0.00%	0.000%
13	3.453	379	388	392	rVV6	1352	3043	0.00%	0.000%
14	3.642	418	419	422	rBV3	361	344	0.00%	0.000%
15	3.672	422	424	427	rVB3	276	315	0.00%	0.000%
16	3.703	427	429	432	rBV2	306	367	0.00%	0.000%
17	3.739	432	435	438	rBV4	240	365	0.00%	0.000%
18	3.794	442	444	447	rVB2	314	375	0.00%	0.000%
19	3.837	450	451	455	rVB2	404	374	0.00%	0.000%
20	3.879	455	458	459	rBV2	296	323	0.00%	0.000%
21	3.928	464	466	470	rBV2	343	451	0.00%	0.000%
22	3.995	473	477	479	rVB3	467	516	0.00%	0.000%
23	4.099	490	494	495	rBV	325	437	0.00%	0.000%
24	4.306	514	528	541	rBV	65231	190660	0.08%	0.027%
25	4.465	543	554	574	rBV	123389	383734	0.17%	0.055%
26	4.611	577	578	581	rVB3	583	446	0.00%	0.000%
27	4.733	596	598	602	rBV2	438	532	0.00%	0.000%
28	5.068	636	653	674	rBV3	297288	1286326	0.56%	0.185%
29	5.257	683	684	690	rVB4	615	743	0.00%	0.000%
30	5.391	702	706	707	rBV2	516	570	0.00%	0.000%
31	5.477	710	720	731	rVV2	27925	87025	0.04%	0.013%
32	5.678	742	753	771	rBV2	135485	410341	0.18%	0.059%
33	5.849	775	781	789	rVB8	1683	4635	0.00%	0.001%
34	6.111	789	824	846	rBV2	47431350	230351622	100.00%	33.130%
35	6.763	922	931	948	rVB	486696	1145342	0.50%	0.165%
36	7.129	983	991	1003	rVV8	6498	16081	0.01%	0.002%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
 Title : VOC Analysis

37	7.312	1012	1021	1029	rBV	400243	898308	0.39%	0.129%
38	7.458	1043	1045	1046	rBV2	466	346	0.00%	0.000%
39	7.482	1046	1049	1054	rVV6	1228	2077	0.00%	0.000%
40	7.598	1067	1068	1072	rVB4	645	500	0.00%	0.000%
41	7.665	1072	1079	1082	rBV5	2991	6497	0.00%	0.001%
42	7.940	1120	1124	1132	rBV6	1806	4060	0.00%	0.001%
43	8.056	1141	1143	1146	rBV2	611	621	0.00%	0.000%
44	8.117	1148	1153	1159	rVB8	3054	5911	0.00%	0.001%
45	8.220	1169	1170	1172	rVB2	586	325	0.00%	0.000%
46	8.324	1181	1187	1197	rBV	258259	430756	0.19%	0.062%
47	8.647	1234	1240	1248	rBV	1039452	1656525	0.72%	0.238%
48	8.720	1248	1252	1260	rVV	14073	26737	0.01%	0.004%
49	8.805	1264	1266	1268	rBV2	522	411	0.00%	0.000%
50	8.952	1284	1290	1303	rBV	187495	278320	0.12%	0.040%
51	9.116	1315	1317	1322	rBV3	524	806	0.00%	0.000%
52	9.153	1322	1323	1326	rVB2	607	441	0.00%	0.000%
53	9.189	1326	1329	1330	rBV3	725	805	0.00%	0.000%
54	9.275	1337	1343	1351	rBV	19237	29404	0.01%	0.004%
55	9.391	1356	1362	1378	rBV	566697	857766	0.37%	0.123%
56	9.763	1421	1423	1430	rVB5	1568	2702	0.00%	0.000%
57	9.988	1458	1460	1463	rVB2	606	623	0.00%	0.000%
58	10.116	1465	1481	1487	rBV4	57163889	205286471	89.12%	29.525%
59	10.957	1618	1619	1622	rVB3	1130	773	0.00%	0.000%
60	11.195	1652	1658	1667	rBV2	713427	984242	0.43%	0.142%
61	11.366	1681	1686	1692	rVB	37144	46754	0.02%	0.007%
62	11.421	1692	1695	1697	rBV4	1535	1754	0.00%	0.000%
63	11.457	1697	1701	1707	rVB	18421	25399	0.01%	0.004%
64	11.683	1736	1738	1739	rBV2	743	534	0.00%	0.000%
65	11.713	1741	1743	1747	rVB5	1323	1557	0.00%	0.000%
66	11.762	1749	1751	1753	rVV2	906	618	0.00%	0.000%
67	11.976	1780	1786	1791	rBV	8629256	11690749	5.08%	1.681%
68	12.061	1791	1800	1805	rVV	58732266	117529455	51.02%	16.903%
69	12.354	1838	1848	1853	rBV	53554816	94546137	41.04%	13.598%
70	12.872	1931	1933	1937	rVV4	2125	1957	0.00%	0.000%
71	12.921	1937	1941	1946	rVB	66838	82396	0.04%	0.012%
72	13.061	1959	1964	1966	rBV3	20462	32019	0.01%	0.005%
73	13.103	1966	1971	1982	rVV	696211	915239	0.40%	0.132%
74	13.195	1983	1986	1994	rVB	34661	52777	0.02%	0.008%
75	13.384	2015	2017	2021	rVB5	5378	5971	0.00%	0.001%
76	13.591	2045	2051	2066	rVB	15873050	19893779	8.64%	2.861%

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Instrument :
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 ClientSampleId :
 COM18

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 >

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
 Title : VOC Analysis

77	13.780	2078	2082	2088	rVB	8965	12795	0.01%	0.002%
78	13.963	2106	2112	2123	rVB	2304568	2891701	1.26%	0.416%
79	14.164	2143	2145	2146	rBV2	1446	1561	0.00%	0.000%
80	14.262	2156	2161	2170	rBV2	72292	99885	0.04%	0.014%
81	14.506	2197	2201	2205	rBV3	10902	15897	0.01%	0.002%
82	14.628	2218	2221	2228	rVB6	3560	5276	0.00%	0.001%
83	14.725	2236	2237	2238	rBV	962	580	0.00%	0.000%
84	14.780	2239	2246	2254	rVB	325659	471615	0.20%	0.068%
85	15.249	2316	2323	2335	rVB	776138	1085905	0.47%	0.156%
86	15.493	2361	2363	2364	rBV2	862	782	0.00%	0.000%
87	15.512	2364	2366	2368	rVB3	999	688	0.00%	0.000%
88	15.615	2381	2383	2384	rBV2	722	577	0.00%	0.000%
89	15.658	2388	2390	2393	rVB3	1050	1030	0.00%	0.000%
90	15.688	2393	2395	2396	rBV2	886	604	0.00%	0.000%
91	15.707	2396	2398	2400	rBV3	736	509	0.00%	0.000%
92	16.024	2448	2450	2453	rBV3	827	852	0.00%	0.000%
93	16.164	2471	2473	2476	rVB3	790	622	0.00%	0.000%
94	16.255	2486	2488	2491	rBV3	701	680	0.00%	0.000%
95	16.377	2504	2508	2512	rBV6	888	1207	0.00%	0.000%
96	16.505	2524	2529	2538	rVB3	28357	51669	0.02%	0.007%
97	16.572	2538	2540	2542	rVB4	829	560	0.00%	0.000%
98	16.597	2542	2544	2545	rBV	596	523	0.00%	0.000%
99	16.761	2568	2571	2572	rBV3	943	728	0.00%	0.000%
100	16.780	2572	2574	2575	rBV	531	493	0.00%	0.000%

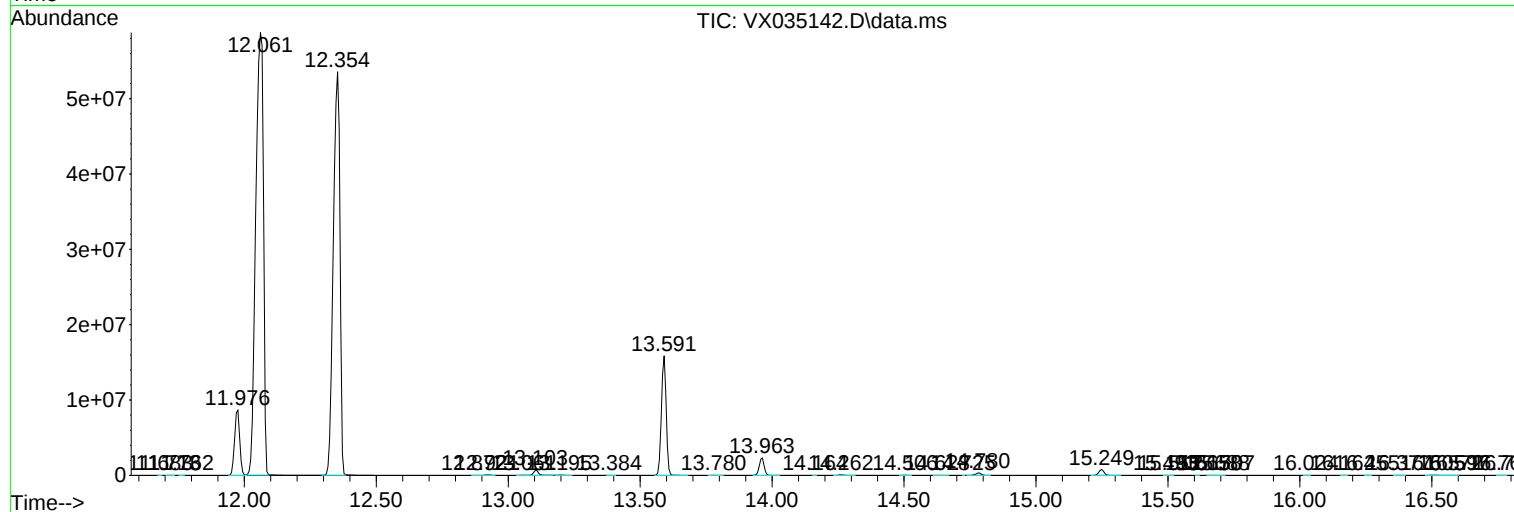
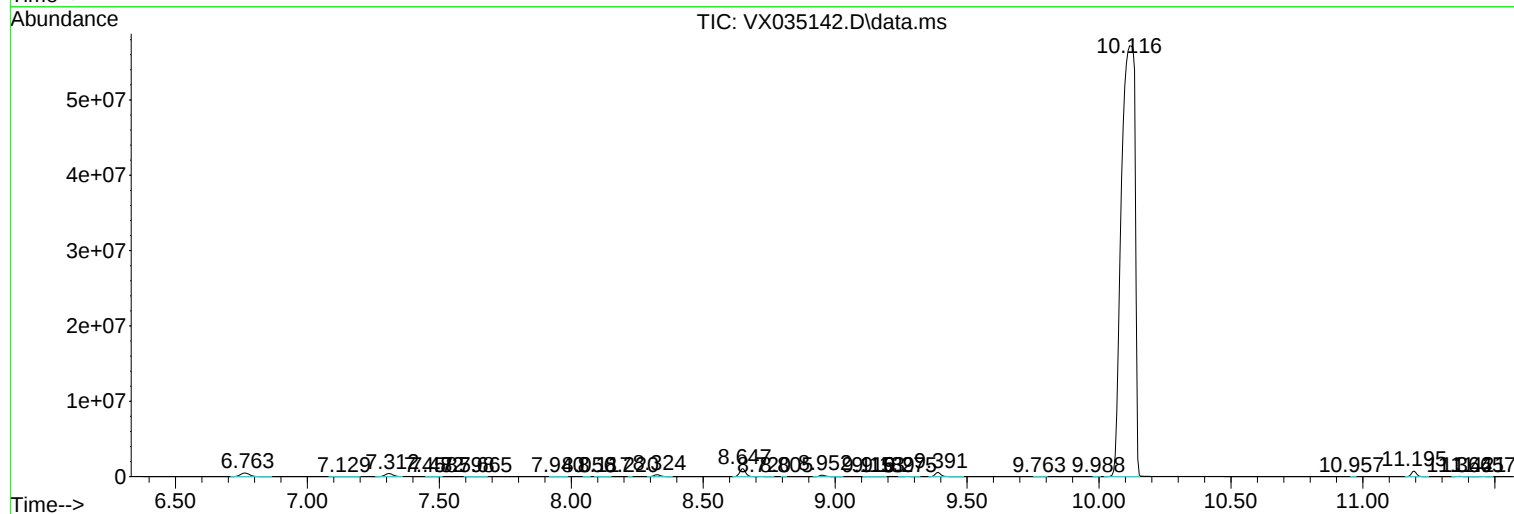
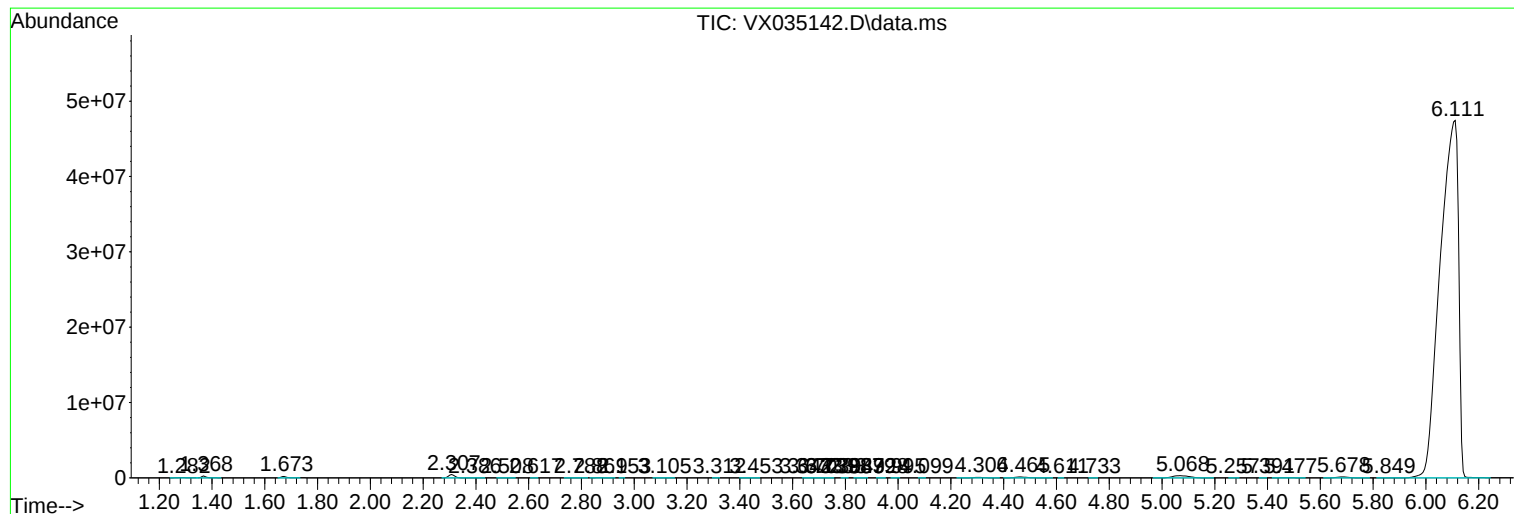
Sum of corrected areas: 695305308

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Instrument :
MSVOA_X
ClientSampleId :
COML8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.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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COML8

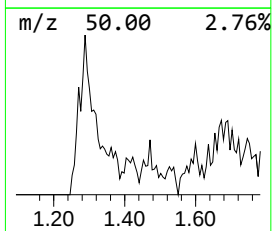
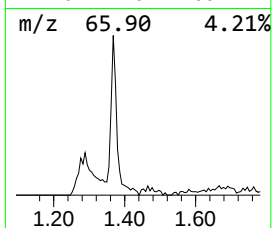
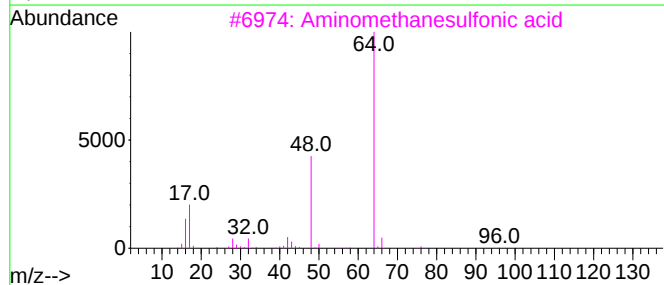
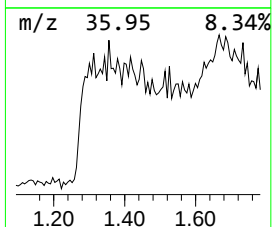
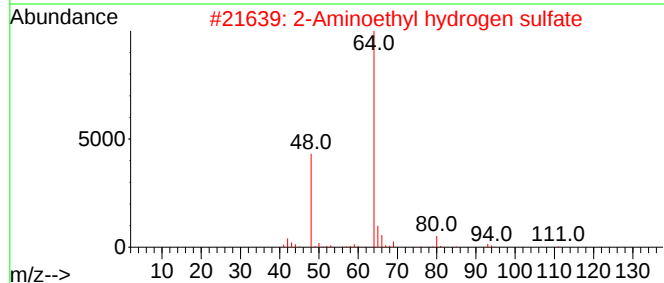
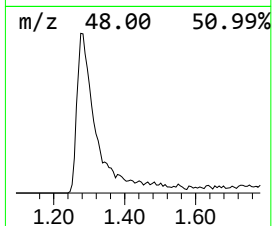
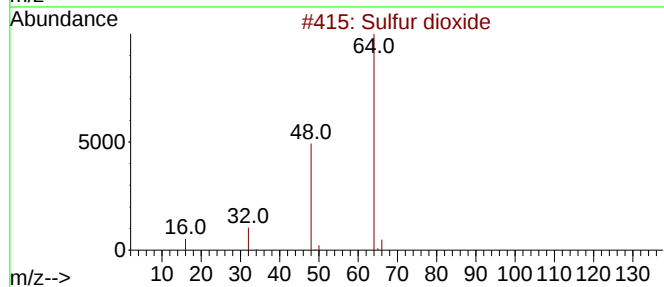
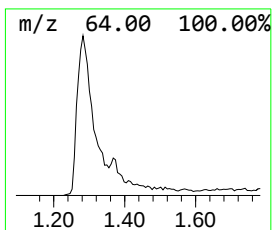
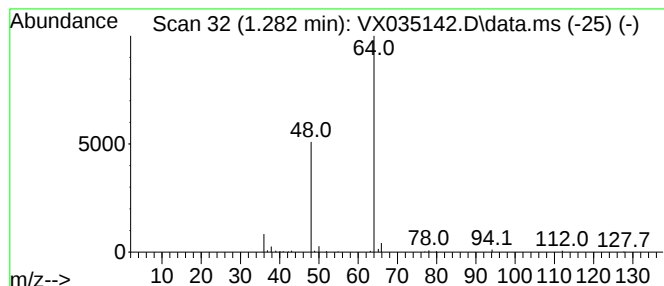
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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.
1.282	5.39 ug/L	123378	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	9



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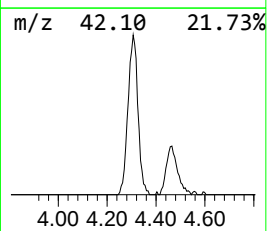
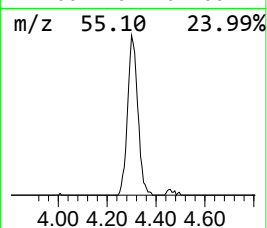
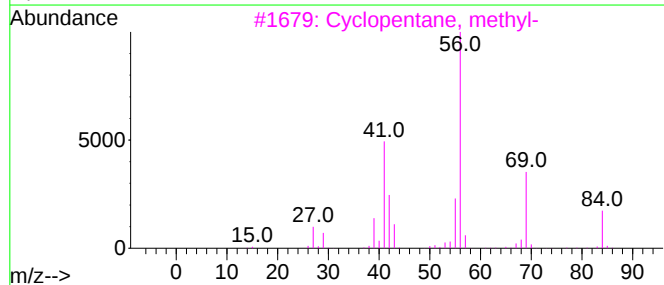
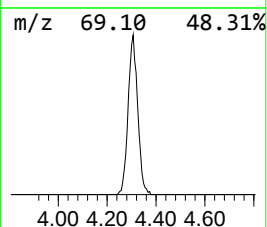
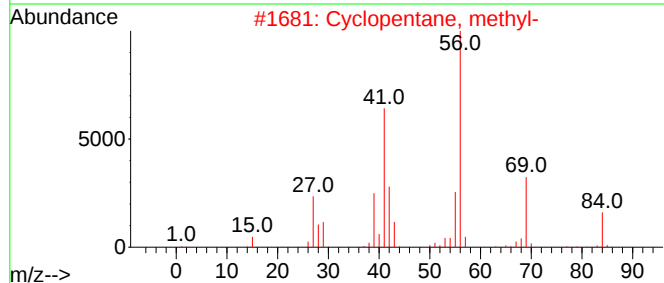
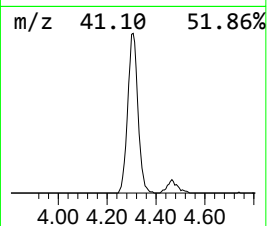
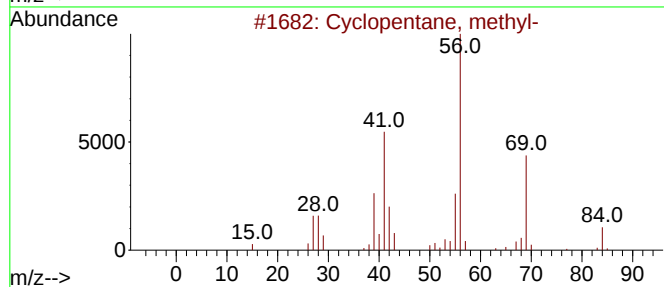
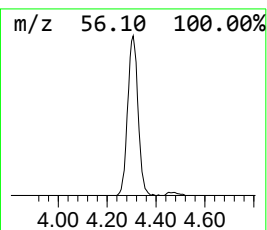
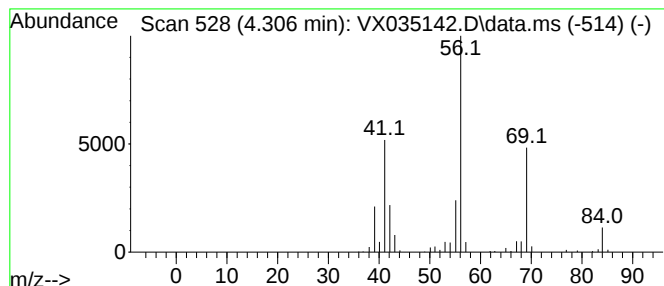
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Cyclic4.306 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	8.32 ug/L	190660	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	90
3			Cyclopentane, methyl-	84	C6H12	000096-37-7	83
4			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
5			Cyclohexane	84	C6H12	000110-82-7	78



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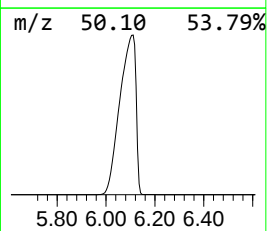
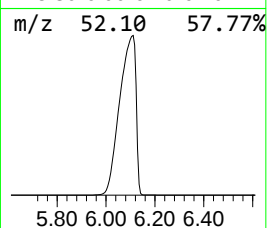
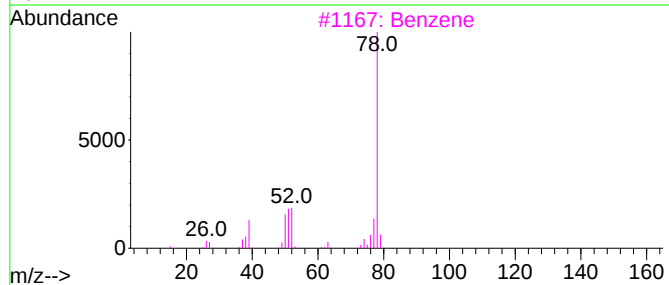
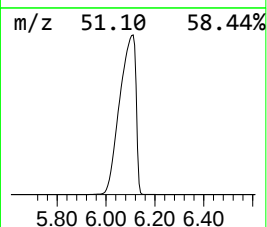
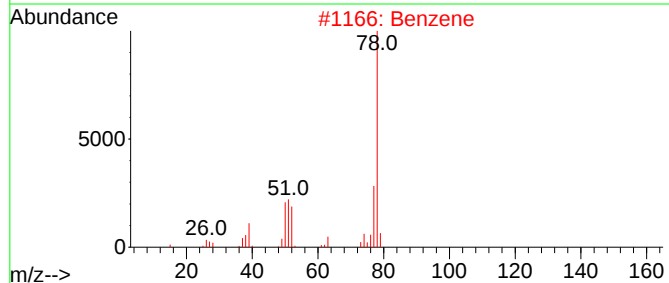
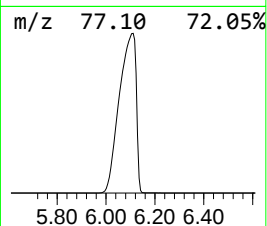
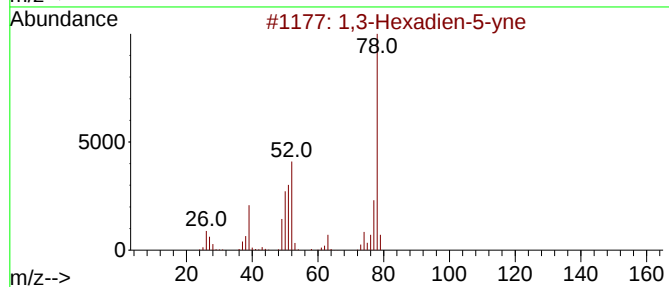
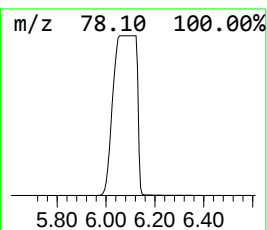
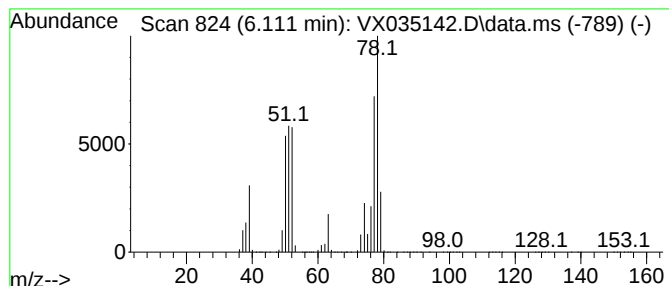
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 1,3-Hexadien-5-yne Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.111	10056.00 ug/L	230352000	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Hexadien-5-yne			78	C6H6	010420-90-3	90
2	Benzene			78	C6H6	000071-43-2	87
3	Benzene			78	C6H6	000071-43-2	87
4	2,4-Hexadiyne			78	C6H6	002809-69-0	83
5	Benzene			78	C6H6	000071-43-2	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
Data File : VX035142.D
Acq On : 18 Apr 2023 23:01
Operator : JC/MD
Sample : 02397-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COML8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.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	1.282	5.4	ug/L	123378	1	6.763	1145340	50.0
(DEL) Alkane: C...	4.306	8.3	ug/L	190660	1	6.763	1145340	50.0
1,3-Hexadien-5-yne	6.111	10056.0	ug/L	230352000	1	6.763	1145340	50.0