

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
 Data File : VX042408.D
 Acq On : 19 Jul 2024 17:42
 Operator : JC/MD
 Sample : P3215-13MERE
 Misc : 5.07g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4D26MERE

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\SFAMXML070324WMA.M

Title : VOC Analysis

Signal : TIC: VX042408.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	21	25	27	rBV	42755	50668	18.66%	2.301%
2	1.368	43	46	48	rBV	6182	7244	2.67%	0.329%
3	1.630	86	89	95	rBV3	6418	16366	6.03%	0.743%
4	2.276	189	195	204	rBV	20355	35567	13.10%	1.615%
5	2.398	211	215	225	rVB4	2516	6225	2.29%	0.283%
6	2.721	262	268	273	rBV	3686	8254	3.04%	0.375%
7	2.947	297	305	316	rBV	7748	20008	7.37%	0.909%
8	3.075	321	326	332	rVV3	1156	2060	0.76%	0.094%
9	4.282	518	524	531	rVB5	1087	2747	1.01%	0.125%
10	4.507	554	561	574	rBV	5882	21869	8.05%	0.993%
11	5.062	640	652	665	rVV	16637	53841	19.83%	2.445%
12	5.452	700	716	726	rBV6	5562	18985	6.99%	0.862%
13	5.818	767	776	782	rBV9	1294	3724	1.37%	0.169%
14	5.964	789	800	819	rBV3	50887	146149	53.82%	6.636%
15	6.336	855	861	868	rBV7	1137	3369	1.24%	0.153%
16	6.757	921	930	947	rBV	97780	238586	87.86%	10.833%
17	7.305	1014	1020	1025	rBV	26798	57444	21.15%	2.608%
18	7.373	1026	1031	1043	rVB2	24350	54643	20.12%	2.481%
19	7.763	1087	1095	1101	rBV7	1464	2968	1.09%	0.135%
20	7.952	1120	1126	1130	rVB3	1161	2124	0.78%	0.096%
21	8.269	1174	1178	1182	rBV2	1416	2282	0.84%	0.104%
22	8.330	1182	1188	1195	rBV	13405	23672	8.72%	1.075%
23	8.592	1226	1231	1235	rVV2	6519	12020	4.43%	0.546%
24	8.647	1235	1240	1248	rVV	72078	121756	44.84%	5.529%
25	8.720	1248	1252	1256	rVV	4315	7919	2.92%	0.360%
26	8.769	1256	1260	1267	rVV3	3774	7283	2.68%	0.331%
27	8.915	1279	1284	1287	rBV3	2450	3810	1.40%	0.173%
28	8.958	1287	1291	1305	rVB3	10960	24857	9.15%	1.129%
29	9.098	1310	1314	1318	rVB3	2294	3415	1.26%	0.155%
30	9.275	1339	1343	1351	rBV6	4150	6441	2.37%	0.292%
31	9.397	1357	1363	1376	rBV	23999	57861	21.31%	2.627%
32	9.500	1376	1380	1384	rBV5	1999	3419	1.26%	0.155%
33	9.561	1384	1390	1394	rVB	6921	10433	3.84%	0.474%
34	9.616	1394	1399	1403	rBV2	6021	8827	3.25%	0.401%
35	9.817	1427	1432	1437	rBV3	2820	4989	1.84%	0.227%
36	9.903	1443	1446	1451	rVB2	1876	2518	0.93%	0.114%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
 Title : VOC Analysis

37	10.055	1465	1471	1480	rBV	190876	271553	100.00%	12.330%
38	10.305	1500	1512	1517	rBV2	12314	25135	9.26%	1.141%
39	10.360	1517	1521	1528	rVB2	4336	6995	2.58%	0.318%
40	10.585	1551	1558	1564	rBV6	3851	8938	3.29%	0.406%
41	10.646	1564	1568	1577	rVB2	7200	12619	4.65%	0.573%
42	10.756	1581	1586	1587	rBV3	2268	3209	1.18%	0.146%
43	10.780	1587	1590	1594	rVB2	5614	6835	2.52%	0.310%
44	10.854	1594	1602	1605	rBV4	5542	9532	3.51%	0.433%
45	10.890	1605	1608	1615	rVB5	4381	6904	2.54%	0.313%
46	10.963	1615	1620	1622	rBV3	1791	2092	0.77%	0.095%
47	11.030	1628	1631	1635	rVB2	1950	2297	0.85%	0.104%
48	11.195	1653	1658	1672	rVB	52884	78394	28.87%	3.560%
49	11.305	1672	1676	1679	rBV4	1583	2739	1.01%	0.124%
50	11.384	1685	1689	1694	rVB4	4852	6279	2.31%	0.285%
51	11.451	1694	1700	1702	rBV3	8404	13340	4.91%	0.606%
52	11.475	1702	1704	1709	rVB2	7654	8985	3.31%	0.408%
53	11.610	1721	1726	1733	rBV5	2401	5313	1.96%	0.241%
54	11.689	1733	1739	1740	rBV3	2050	3690	1.36%	0.168%
55	11.713	1740	1743	1744	rBV	7921	7751	2.85%	0.352%
56	11.853	1760	1766	1767	rBV4	1738	2873	1.06%	0.130%
57	11.890	1769	1772	1775	rVB4	2925	3513	1.29%	0.160%
58	11.939	1777	1780	1783	rBV4	2814	4106	1.51%	0.186%
59	12.024	1789	1794	1800	rBV	203116	270786	99.72%	12.296%
60	12.317	1837	1842	1850	rBV	83441	118952	43.80%	5.401%
61	12.420	1855	1859	1864	rVV	10193	13495	4.97%	0.613%
62	12.469	1864	1867	1872	rVB5	2722	4208	1.55%	0.191%
63	12.530	1872	1877	1879	rBV4	1770	2813	1.04%	0.128%
64	12.579	1883	1885	1889	rVB4	3187	3867	1.42%	0.176%
65	12.683	1899	1902	1905	rBV3	1761	2232	0.82%	0.101%
66	12.719	1905	1908	1913	rVB6	1741	2893	1.07%	0.131%
67	12.817	1921	1924	1928	rVB6	2280	3240	1.19%	0.147%
68	12.890	1933	1936	1945	rVV8	3594	8801	3.24%	0.400%
69	12.975	1946	1950	1956	rVB4	4501	6285	2.31%	0.285%
70	13.036	1956	1960	1964	rBV5	2333	3016	1.11%	0.137%
71	13.085	1964	1968	1974	rVB6	1557	2557	0.94%	0.116%
72	13.268	1993	1998	2001	rBV	10323	13275	4.89%	0.603%
73	13.384	2013	2017	2020	rBV	7548	11190	4.12%	0.508%
74	13.621	2053	2056	2062	rVV7	2618	4113	1.51%	0.187%
75	13.688	2062	2067	2071	rVV7	2218	3830	1.41%	0.174%
76	13.737	2071	2075	2078	rVV6	2493	3709	1.37%	0.168%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
 Title : VOC Analysis

77	13.774	2078	2081	2088	rVB	9269	15439	5.69%	0.701%
78	13.841	2088	2092	2096	rBV	10105	11906	4.38%	0.541%
79	13.987	2114	2116	2120	rBV5	1909	2893	1.07%	0.131%
80	14.036	2120	2124	2129	rVV	9602	11521	4.24%	0.523%
81	14.438	2187	2190	2194	rVB4	1746	2195	0.81%	0.100%
82	14.518	2198	2203	2206	rVB5	2522	4623	1.70%	0.210%
83	14.615	2215	2219	2220	rBV2	4008	4560	1.68%	0.207%
84	14.640	2220	2223	2226	rVV	8942	11283	4.15%	0.512%
85	14.670	2226	2228	2235	rVB6	3697	4358	1.60%	0.198%
86	14.755	2238	2242	2243	rVV	7634	8036	2.96%	0.365%
87	14.780	2243	2246	2252	rVV2	13936	20240	7.45%	0.919%
88	14.841	2253	2256	2261	rVB7	2399	3625	1.33%	0.165%
89	15.103	2293	2299	2307	rBV9	2631	7226	2.66%	0.328%
90	15.176	2307	2311	2313	rVV4	1685	2914	1.07%	0.132%
91	15.213	2313	2317	2322	rVV5	5731	7932	2.92%	0.360%
92	15.267	2322	2326	2330	rVB4	2017	3295	1.21%	0.150%
93	15.377	2340	2344	2347	rBV5	4235	5514	2.03%	0.250%
94	15.414	2347	2350	2354	rVV5	3670	5967	2.20%	0.271%
95	15.487	2357	2362	2370	rVB4	7410	14329	5.28%	0.651%
96	15.615	2378	2383	2386	rBV3	8662	14498	5.34%	0.658%
97	15.737	2398	2403	2409	rVB7	2539	4887	1.80%	0.222%
98	15.987	2441	2444	2450	rVB7	1391	2234	0.82%	0.101%
99	16.084	2456	2460	2468	rBV5	1873	3259	1.20%	0.148%
100	16.596	2541	2544	2550	rVB6	1695	2873	1.06%	0.130%

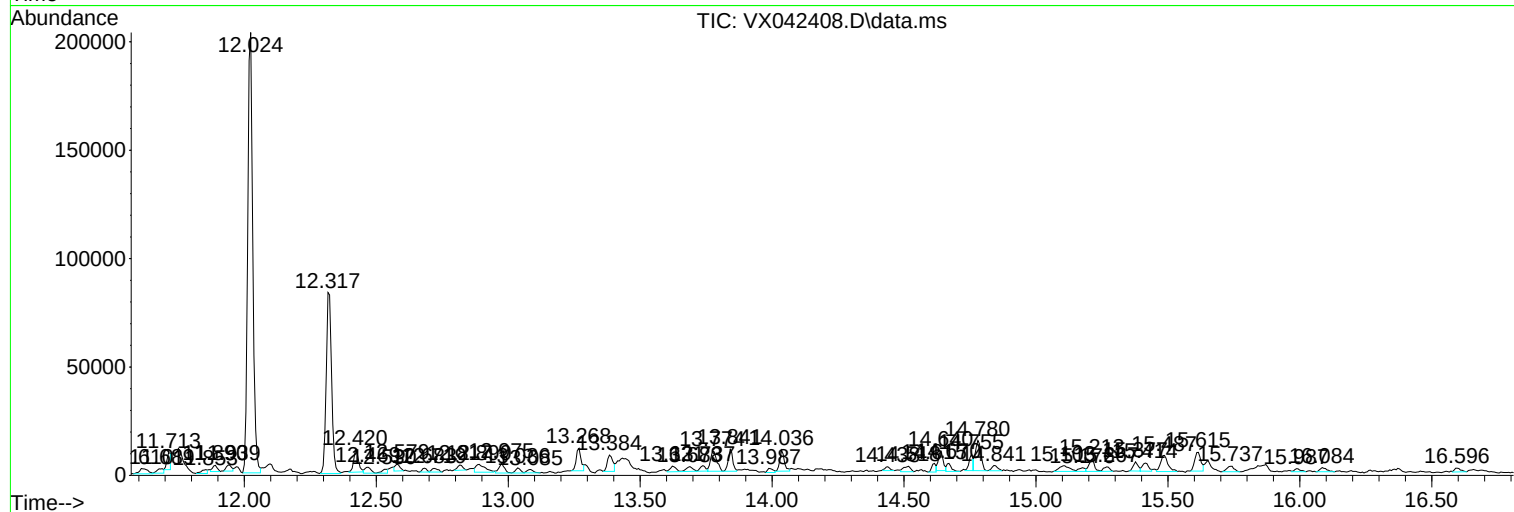
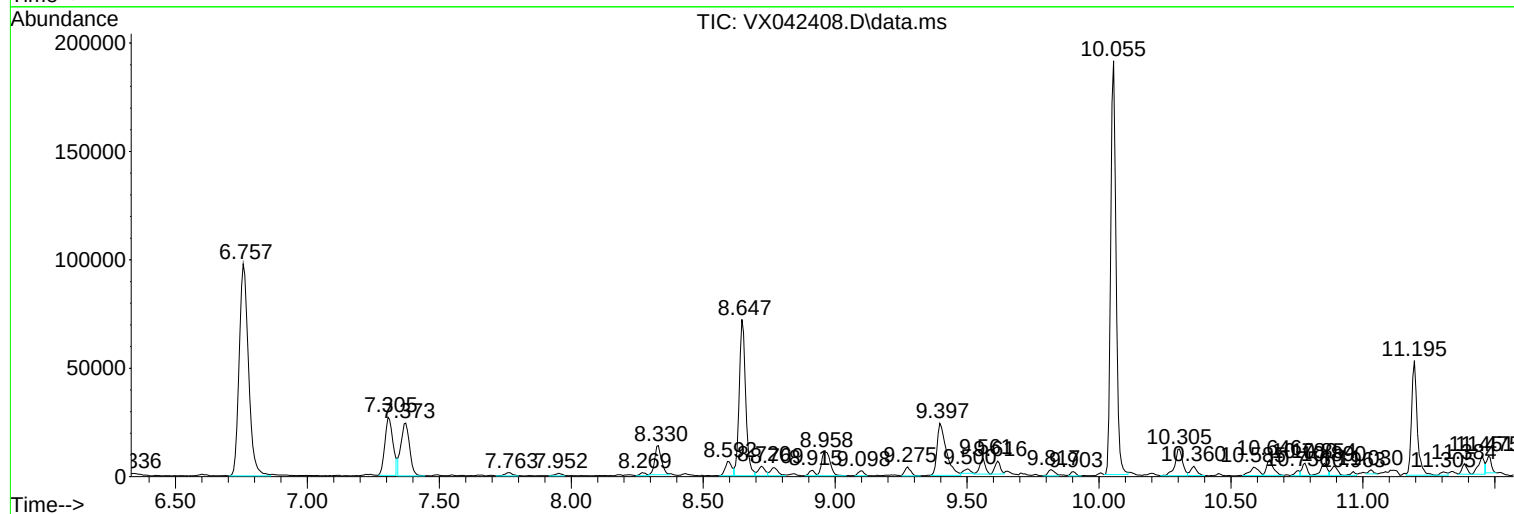
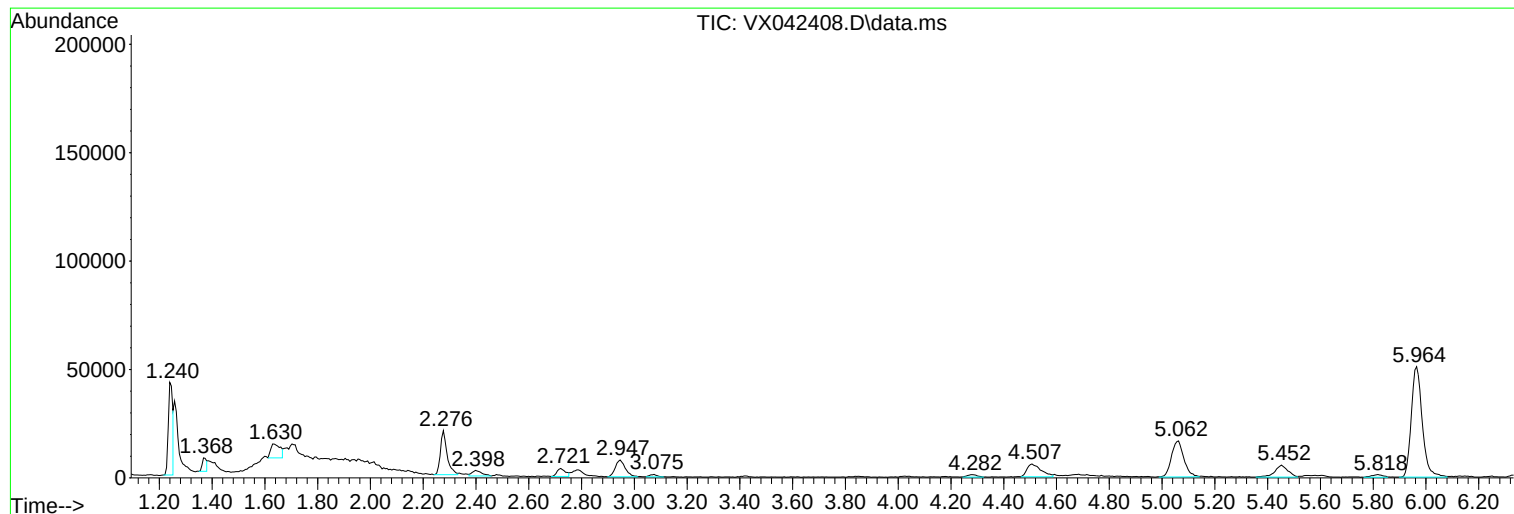
Sum of corrected areas: 2202304

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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



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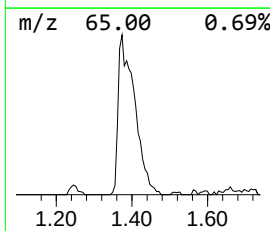
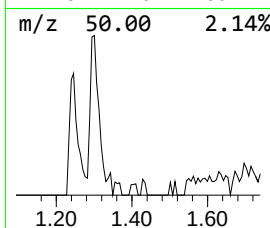
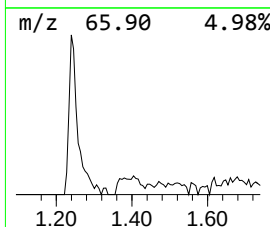
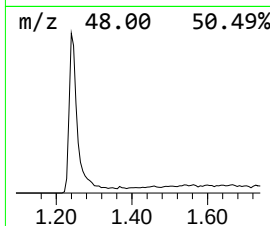
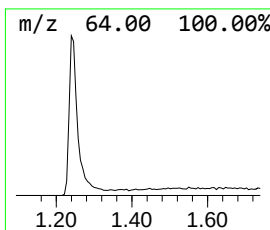
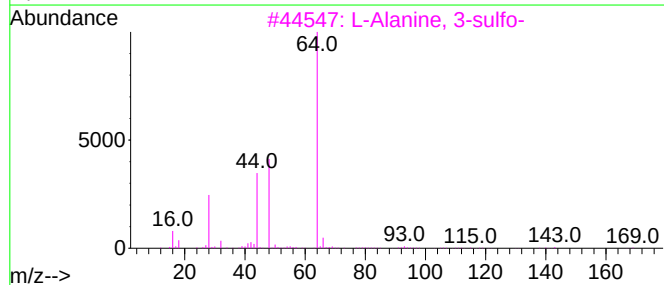
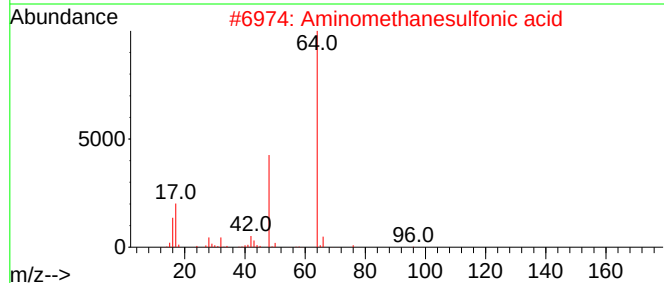
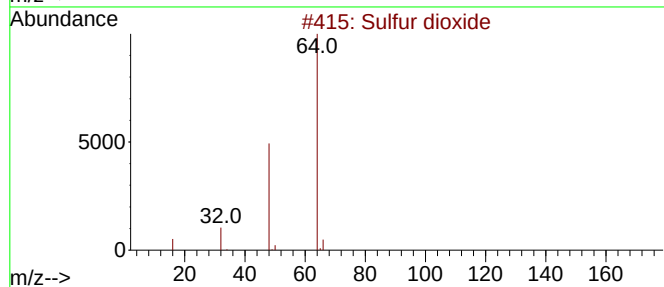
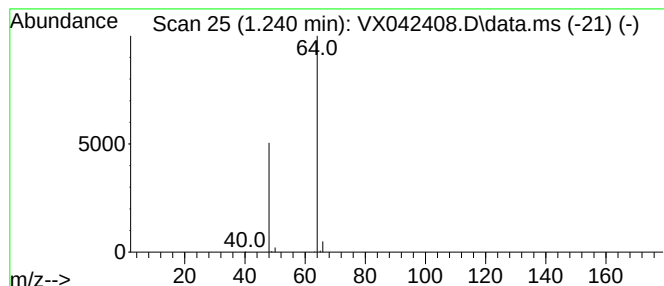
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	10.62 ug/L	50668	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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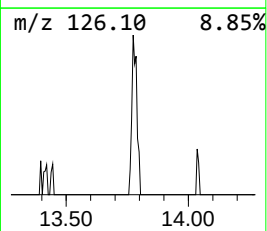
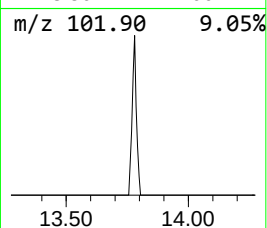
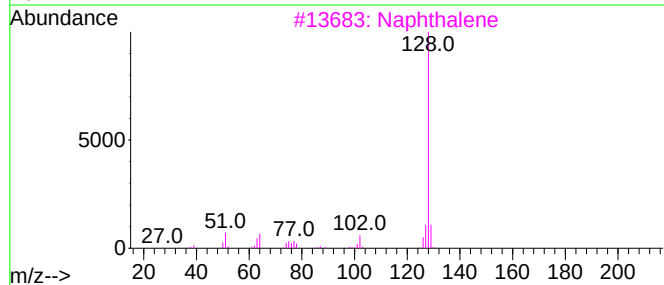
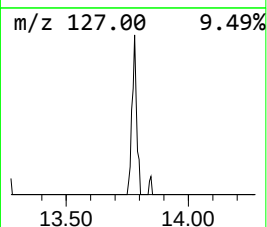
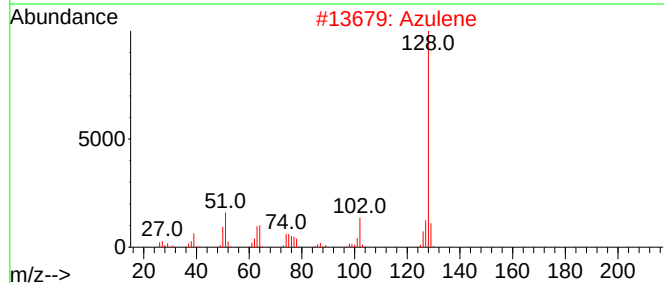
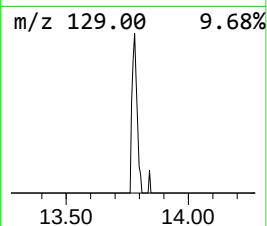
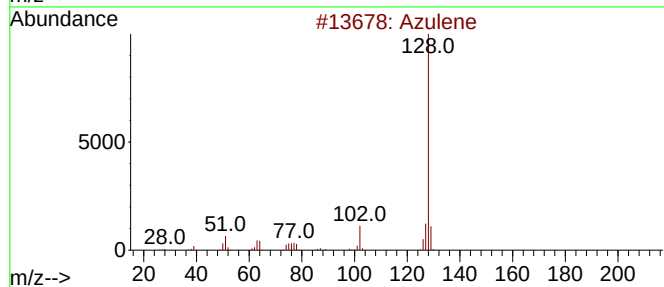
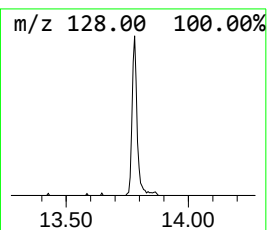
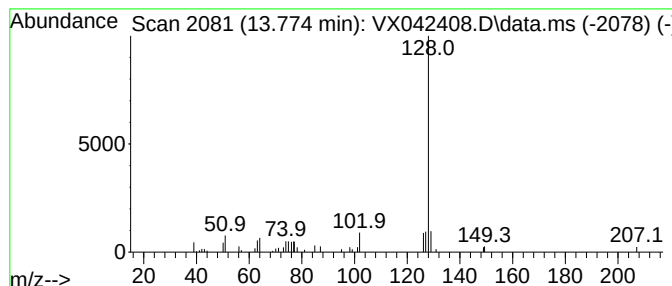
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Azulene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	2.85 ug/L	15439	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azulene	128	C10H8	000275-51-4	90
2			Azulene	128	C10H8	000275-51-4	87
3			Naphthalene	128	C10H8	000091-20-3	87
4			Naphthalene	128	C10H8	000091-20-3	87
5			Naphthalene	128	C10H8	000091-20-3	87



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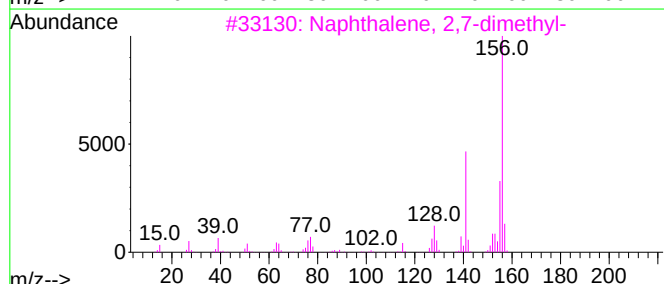
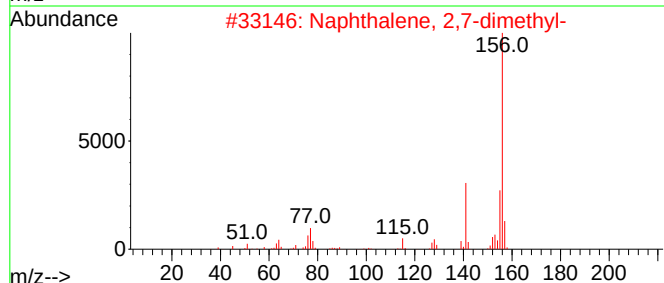
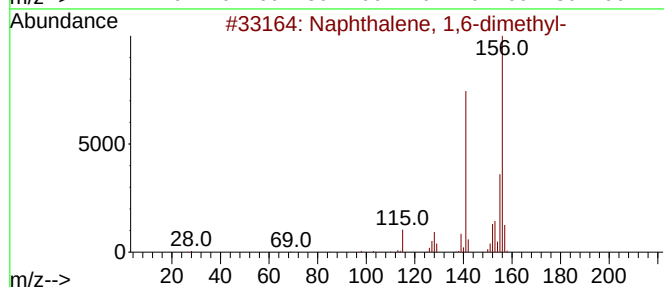
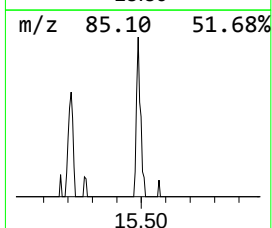
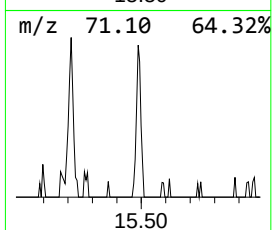
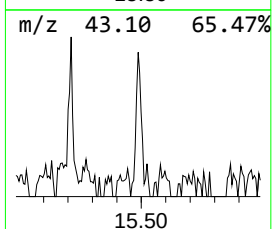
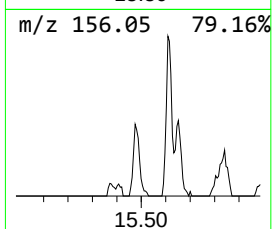
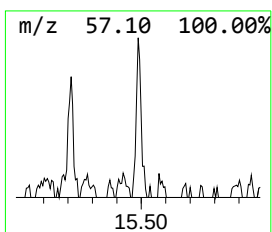
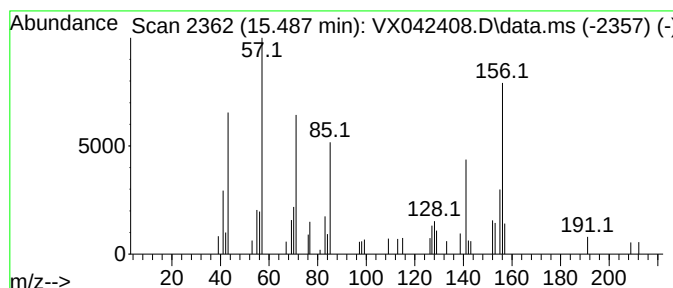
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Quant Title : VOC Analysis

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

Peak Number 6 Naphthalene, 1,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.487	2.65 ug/L	14329	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	80
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	64
3			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	64
4			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	64
5			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042408.D
Acq On : 19 Jul 2024 17:42
Operator : JC/MD
Sample : P3215-13MERE
Misc : 5.07g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D26MERE

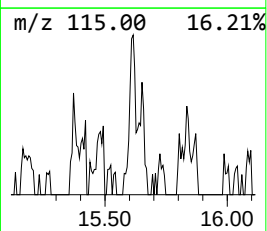
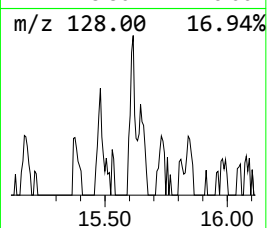
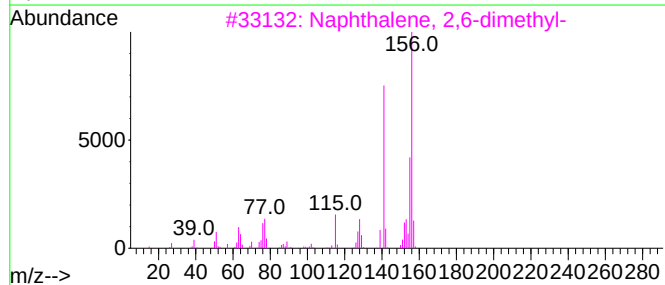
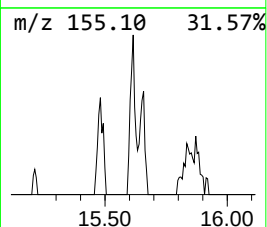
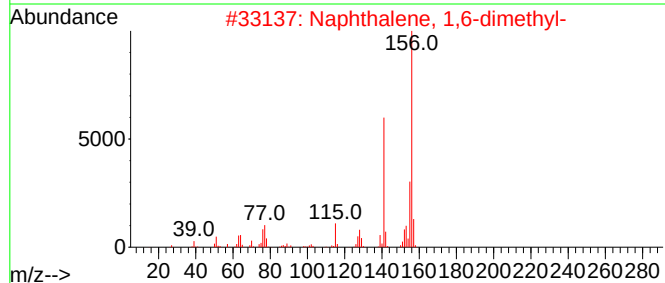
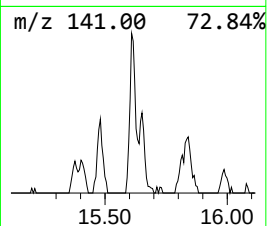
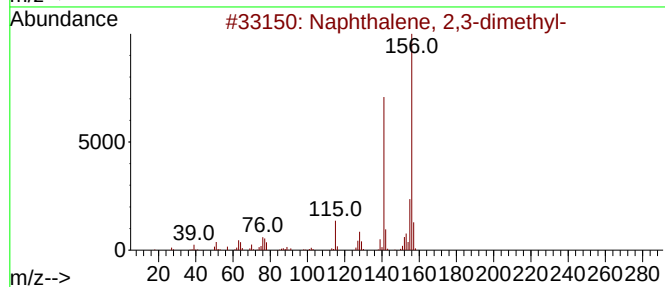
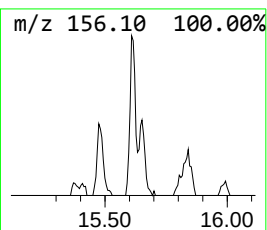
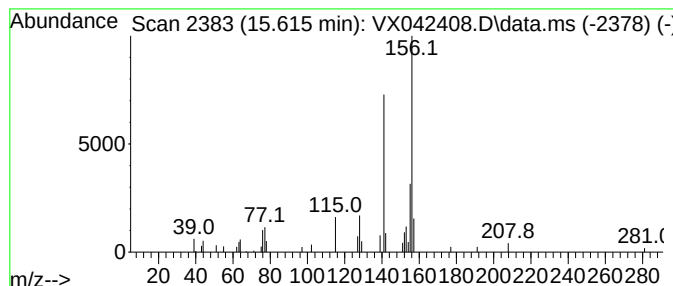
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Quant Title : VOC Analysis

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

Peak Number 7 Naphthalene, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	2.68 ug/L	14498	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
2			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
3			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042408.D
Acq On : 19 Jul 2024 17:42
Operator : JC/MD
Sample : P3215-13MERE
Misc : 5.07g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D26MERE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.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	1.240	10.6	ug/L	50668	1	6.757	238586	50.0
Azulene	13.774	2.9	ug/L	15439	3	12.024	270786	50.0
Naphthalene, 1,...	15.487	2.6	ug/L	14329	3	12.024	270786	50.0
Naphthalene, 2,...	15.615	2.7	ug/L	14498	3	12.024	270786	50.0