

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
 Data File : VX025587.D
 Acq On : 07 Dec 2021 18:36
 Operator : JC/MD
 Sample : M4883-08ME
 Misc : 5.06g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW9G4ME

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\SFAMXML112221WMA.M
 Title : VOC Analysis

Signal : TIC: VX025587.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	22	25	42	rVV2	4872	11702	3.95%	0.513%
2	1.368	43	46	53	rVB	29988	33966	11.45%	1.490%
3	1.648	88	92	99	rBV	20323	28408	9.58%	1.246%
4	2.282	189	196	206	rVB	46352	79841	26.92%	3.503%
5	2.374	206	211	214	rBV3	1090	1879	0.63%	0.082%
6	2.788	273	279	285	rVB5	1537	3065	1.03%	0.134%
7	2.886	292	295	297	rBV2	143	148	0.05%	0.006%
8	2.947	297	305	326	rBV	11300	33762	11.38%	1.481%
9	3.166	338	341	343	rBV2	99	102	0.03%	0.004%
10	3.300	360	363	367	rBV	135	203	0.07%	0.009%
11	3.739	431	435	438	rVB2	104	160	0.05%	0.007%
12	3.977	470	474	476	rBV2	90	149	0.05%	0.007%
13	4.489	548	558	581	rBV	14719	71303	24.04%	3.128%
14	4.940	629	632	633	rBV2	176	234	0.08%	0.010%
15	5.062	641	652	669	rBV	37501	121459	40.95%	5.328%
16	5.221	676	678	679	rBV	154	107	0.04%	0.005%
17	5.239	679	681	684	rBV	126	176	0.06%	0.008%
18	5.404	706	708	710	rBV2	119	138	0.05%	0.006%
19	5.428	710	712	715	rVB2	124	101	0.03%	0.004%
20	5.556	729	733	736	rBV2	183	236	0.08%	0.010%
21	5.757	765	766	769	rBV2	152	137	0.05%	0.006%
22	5.971	789	801	815	rBV2	102724	296611	100.00%	13.012%
23	6.373	859	867	872	rBV4	1952	5763	1.94%	0.253%
24	6.489	884	886	890	rBV2	96	136	0.05%	0.006%
25	6.574	897	900	902	rBV	108	140	0.05%	0.006%
26	6.763	921	931	951	rBV	63748	163161	55.01%	7.158%
27	6.940	958	960	962	rVB	180	104	0.04%	0.005%
28	7.123	983	990	1001	rBV	14806	34356	11.58%	1.507%
29	7.220	1001	1006	1011	rVV3	925	2190	0.74%	0.096%
30	7.312	1013	1021	1035	rVB	58752	136927	46.16%	6.007%
31	7.501	1050	1052	1053	rBV	117	98	0.03%	0.004%
32	7.824	1103	1105	1108	rVB2	129	100	0.03%	0.004%
33	7.958	1126	1127	1130	rBV2	280	315	0.11%	0.014%
34	8.165	1159	1161	1163	rBV2	89	117	0.04%	0.005%
35	8.330	1179	1188	1196	rBV2	29200	54180	18.27%	2.377%
36	8.519	1218	1219	1222	rBV2	139	101	0.03%	0.004%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

Sampling : 1

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
 Title : VOC Analysis

37	8.653	1233	1241	1249	rBV	123633	204741	69.03%	8.982%
38	8.720	1249	1252	1257	rVB2	1543	2177	0.73%	0.096%
39	8.891	1278	1280	1285	rBV2	97	147	0.05%	0.006%
40	8.958	1285	1291	1300	rBV	19928	34179	11.52%	1.499%
41	9.275	1339	1343	1348	rVB4	1136	1380	0.47%	0.061%
42	9.348	1353	1355	1357	rBV	125	129	0.04%	0.006%
43	9.403	1357	1364	1377	rVV	92505	155035	52.27%	6.801%
44	9.671	1405	1408	1410	rBV	139	169	0.06%	0.007%
45	9.714	1410	1415	1420	rVV	2261	3117	1.05%	0.137%
46	9.939	1450	1452	1453	rBV2	120	126	0.04%	0.006%
47	10.061	1466	1472	1482	rVB	120654	180640	60.90%	7.924%
48	10.305	1507	1512	1517	rVV3	522	838	0.28%	0.037%
49	10.476	1538	1540	1541	rVB	218	105	0.04%	0.005%
50	10.647	1565	1568	1573	rVB2	243	330	0.11%	0.014%
51	11.122	1642	1646	1651	rVB2	1182	1468	0.49%	0.064%
52	11.195	1653	1658	1669	rBV	118607	157720	53.17%	6.919%
53	11.275	1669	1671	1674	rVB	265	262	0.09%	0.011%
54	11.457	1698	1701	1702	rBV2	268	255	0.09%	0.011%
55	11.750	1745	1749	1754	rVV4	1371	2144	0.72%	0.094%
56	11.817	1758	1760	1761	rVV	206	135	0.05%	0.006%
57	11.841	1761	1764	1770	rVV3	268	403	0.14%	0.018%
58	11.933	1776	1779	1783	rVB2	655	678	0.23%	0.030%
59	12.024	1789	1794	1804	rBV	147507	178451	60.16%	7.828%
60	12.226	1824	1827	1828	rBV2	268	242	0.08%	0.011%
61	12.262	1832	1833	1835	rVB	187	115	0.04%	0.005%
62	12.323	1838	1843	1852	rVV	165639	202880	68.40%	8.900%
63	12.427	1856	1860	1863	rVB3	796	1034	0.35%	0.045%
64	12.482	1867	1869	1870	rVB2	232	116	0.04%	0.005%
65	12.658	1895	1898	1900	rBV3	326	450	0.15%	0.020%
66	12.878	1932	1934	1936	rVV	211	229	0.08%	0.010%
67	12.921	1940	1941	1945	rVB2	359	241	0.08%	0.011%
68	13.006	1954	1955	1957	rVB	208	112	0.04%	0.005%
69	13.049	1960	1962	1964	rVB	292	187	0.06%	0.008%
70	13.122	1970	1974	1976	rBV2	120	210	0.07%	0.009%
71	13.238	1991	1993	1995	rBV2	150	125	0.04%	0.005%
72	13.268	1995	1998	2003	rVB	674	765	0.26%	0.034%
73	13.384	2015	2017	2020	rVV2	466	521	0.18%	0.023%
74	13.414	2020	2022	2025	rVB2	112	100	0.03%	0.004%
75	13.488	2033	2034	2037	rVB	134	115	0.04%	0.005%
76	13.573	2044	2048	2051	rBV2	180	312	0.11%	0.014%

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Instrument :
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 ClientSampleId :
 EW9G4ME

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\SFAMXML112221WMA.M
 Title : VOC Analysis

77	13.677	2064	2065	2068	rBV2	236	234	0.08%	0.010%
78	13.780	2077	2082	2088	rVB	21454	27256	9.19%	1.196%
79	13.841	2089	2092	2095	rVB2	652	731	0.25%	0.032%
80	13.994	2115	2117	2119	rBV2	135	122	0.04%	0.005%
81	14.036	2121	2124	2128	rVB2	1380	1526	0.51%	0.067%
82	14.122	2136	2138	2145	rBV3	619	889	0.30%	0.039%
83	14.420	2185	2187	2188	rBV	188	102	0.03%	0.004%
84	14.439	2188	2190	2192	rBV2	133	146	0.05%	0.006%
85	14.554	2206	2209	2212	rVB2	132	147	0.05%	0.006%
86	14.640	2216	2223	2229	rBV	7231	9843	3.32%	0.432%
87	14.756	2236	2242	2244	rBV2	2116	3104	1.05%	0.136%
88	14.780	2244	2246	2251	rVB	5559	6430	2.17%	0.282%
89	14.847	2253	2257	2259	rBV3	767	763	0.26%	0.033%
90	14.890	2262	2264	2265	rBV	321	279	0.09%	0.012%
91	14.957	2274	2275	2276	rBV	257	126	0.04%	0.006%
92	15.213	2313	2317	2323	rVB2	1304	1798	0.61%	0.079%
93	15.481	2357	2361	2367	rVB5	1649	2974	1.00%	0.130%
94	15.615	2379	2383	2387	rBV3	2812	4024	1.36%	0.177%
95	15.688	2393	2395	2396	rBV	179	117	0.04%	0.005%
96	15.993	2441	2445	2446	rBV2	394	402	0.14%	0.018%
97	16.091	2459	2461	2464	rVB2	685	535	0.18%	0.023%
98	16.322	2495	2499	2501	rBV2	386	612	0.21%	0.027%
99	16.597	2539	2544	2549	rBV3	886	1390	0.47%	0.061%
100	16.658	2549	2554	2557	rBV2	1091	2006	0.68%	0.088%

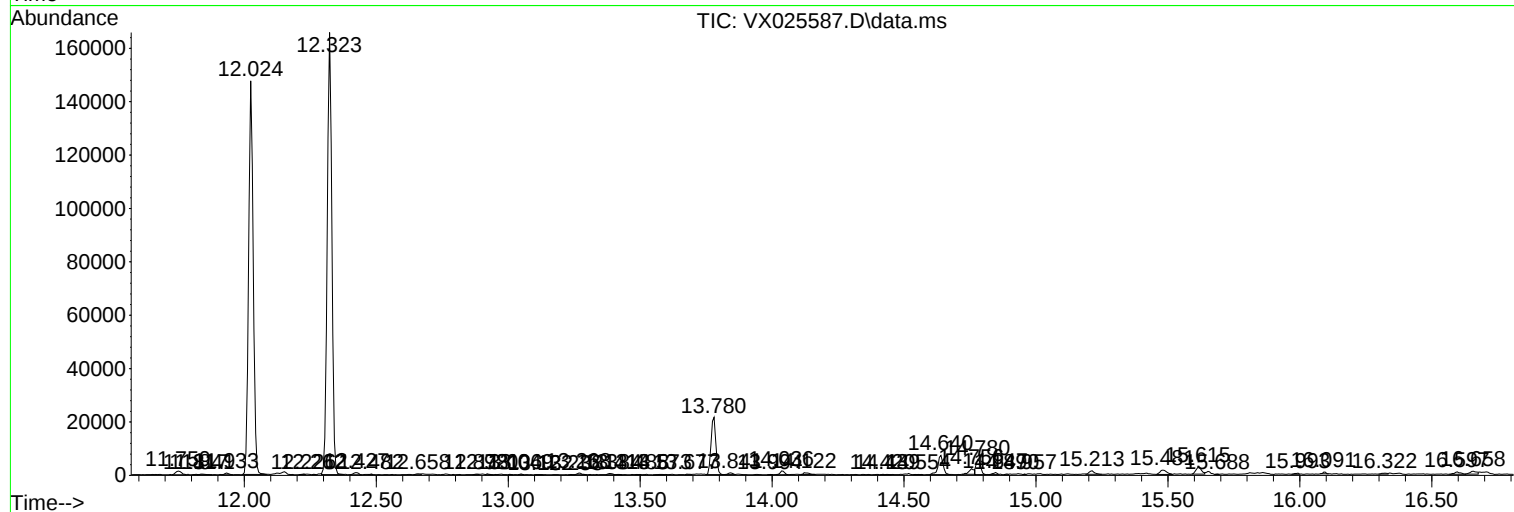
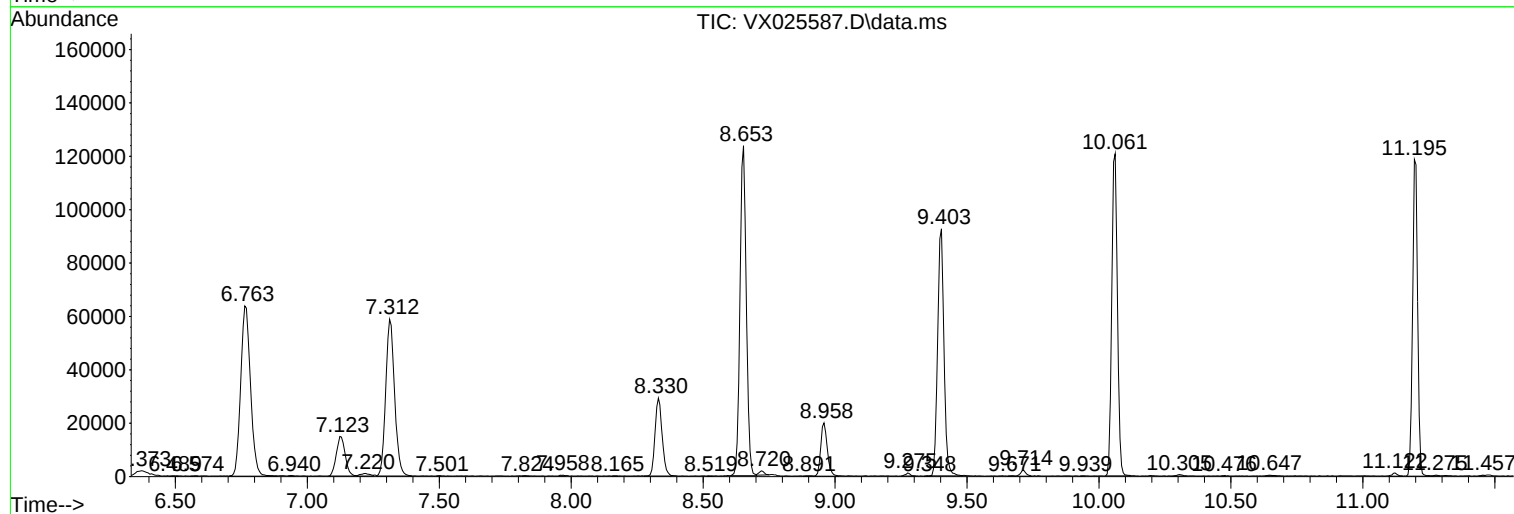
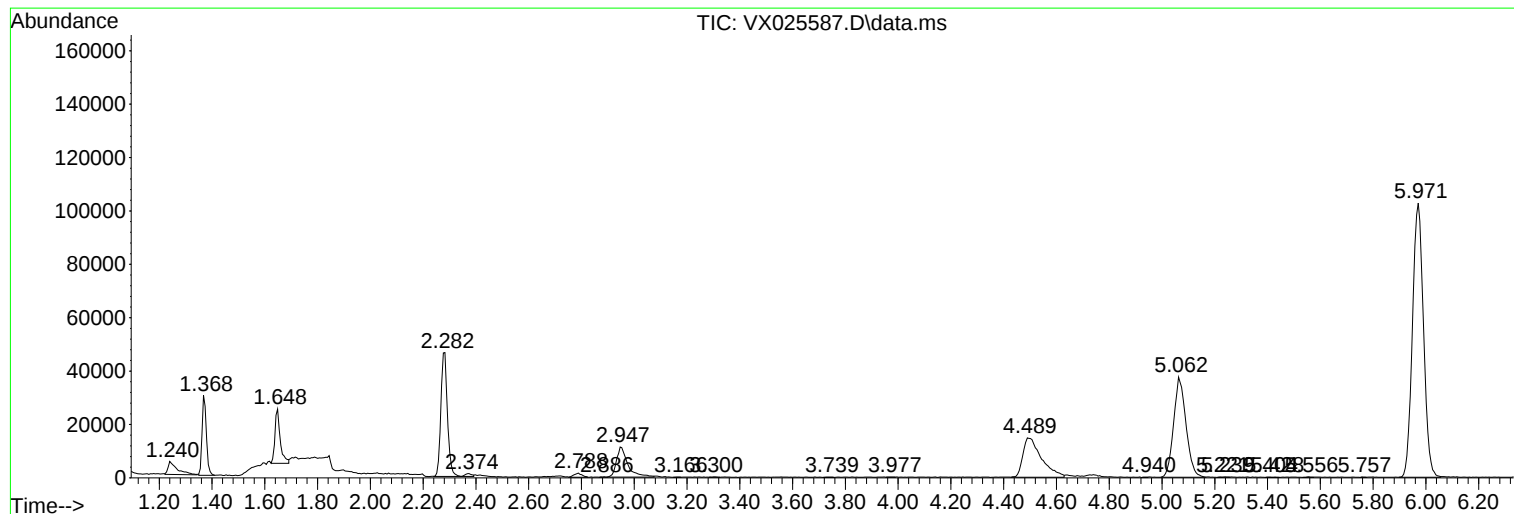
Sum of corrected areas: 2279514

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EW9G4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML112221WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P



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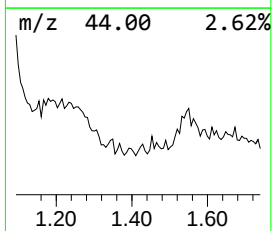
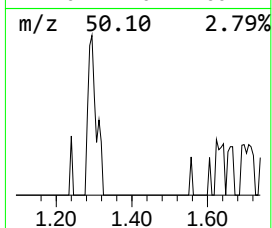
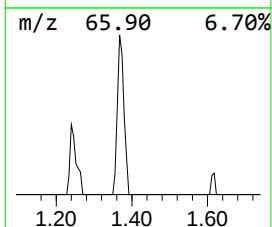
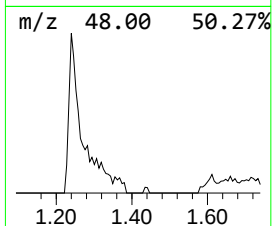
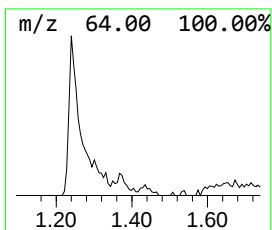
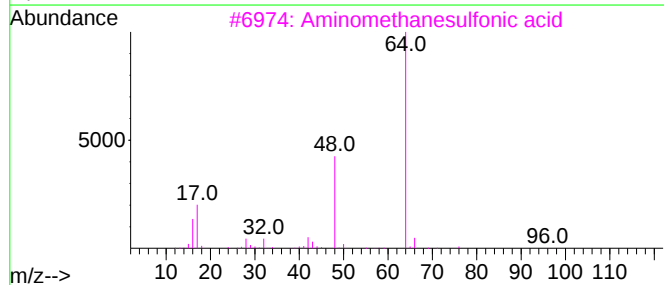
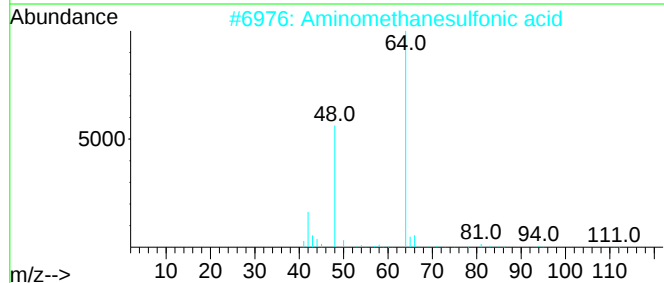
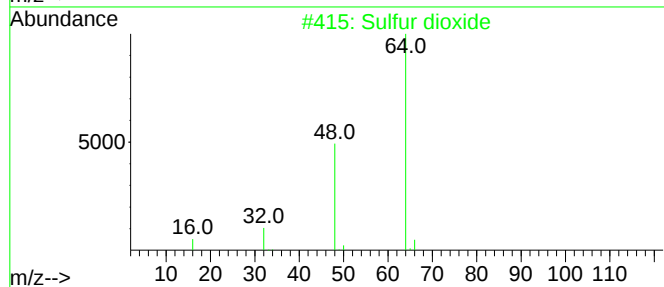
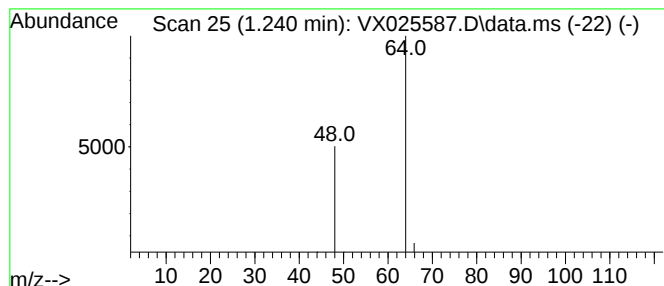
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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.
1.240	3.59 ug/L	11702	1,4-Difluorobenzene	6.763

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



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ClientSampleId :
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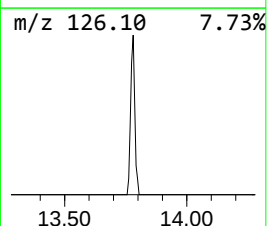
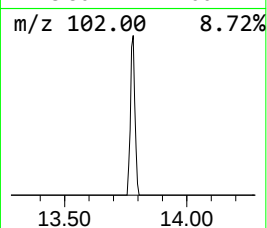
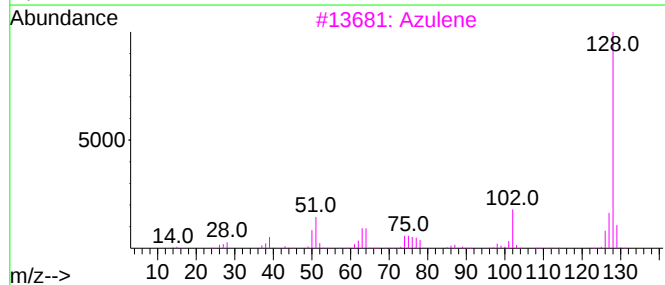
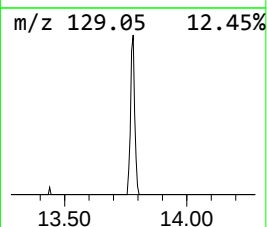
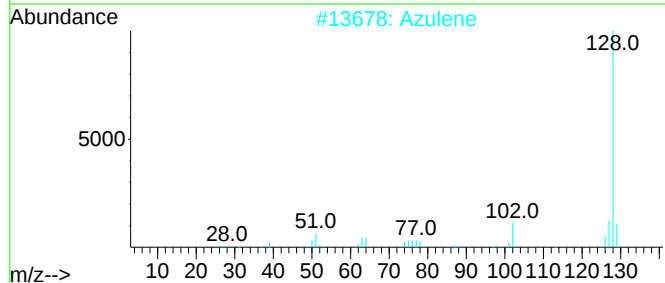
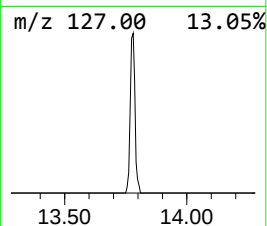
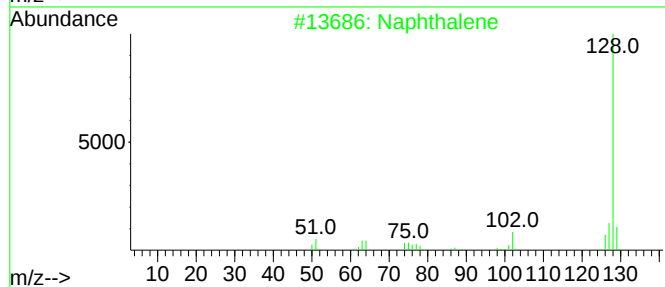
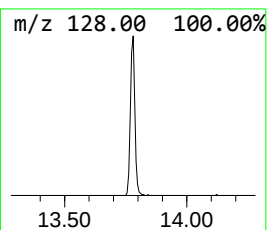
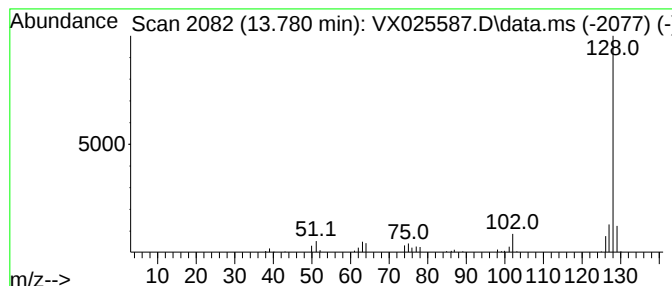
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	7.64 ug/L	27256	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	94
3			Azulene	128	C10H8	000275-51-4	94
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	91



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Instrument :
MSVOA_X
ClientSampleId :
EW9G4ME

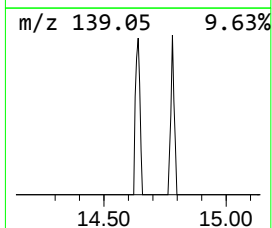
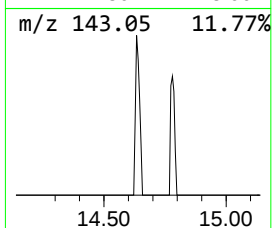
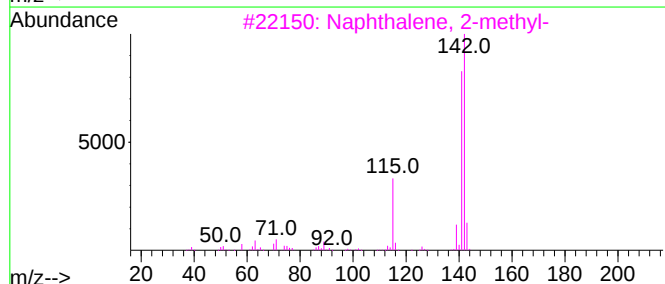
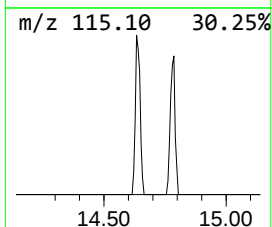
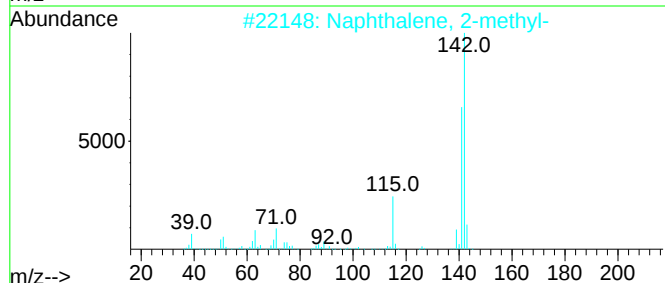
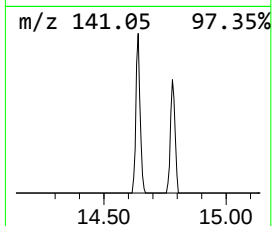
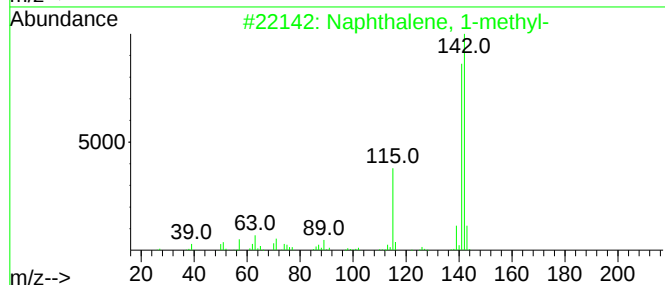
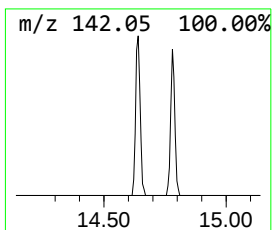
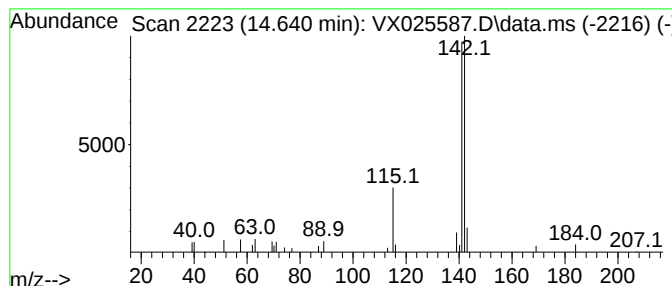
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Naphthalene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	2.76 ug/L	9843	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	91
3			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	91
4			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
5			Benzocycloheptatriene	142	C11H10	000264-09-5	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025587.D
Acq On : 07 Dec 2021 18:36
Operator : JC/MD
Sample : M4883-08ME
Misc : 5.06g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9G4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML112221WMA.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	3.6	ug/L	11702	1	6.763	163161	50.0
Azulene	13.780	7.6	ug/L	27256	3	12.024	178451	50.0
Naphthalene, 1-...	14.640	2.8	ug/L	9843	3	12.024	178451	50.0