

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
 Data File : VX042770.D
 Acq On : 31 Jul 2024 14:04
 Operator : JC/MD
 Sample : P3382-01ME
 Misc : 7.60g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20R1ME

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\SFAMXML072624WMA.M
 Title : VOC Analysis

Signal : TIC: VX042770.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	36	rBV2	13522	28800	6.81%	0.855%
2	1.380	43	48	49	rBV	10440	16465	3.89%	0.489%
3	2.276	189	195	208	rBV	58572	112354	26.55%	3.337%
4	2.672	258	260	263	rBV2	166	140	0.03%	0.004%
5	2.733	266	270	272	rVB	239	300	0.07%	0.009%
6	2.770	272	276	278	rBV	1903	2519	0.60%	0.075%
7	2.941	299	304	309	rBV3	1542	3312	0.78%	0.098%
8	3.075	321	326	335	rBV2	3410	6781	1.60%	0.201%
9	3.215	344	349	350	rBV2	136	212	0.05%	0.006%
10	3.282	358	360	363	rBB	159	197	0.05%	0.006%
11	3.422	381	383	387	rBB	195	222	0.05%	0.007%
12	3.495	394	395	399	rBV	139	174	0.04%	0.005%
13	3.727	431	433	435	rBV	214	183	0.04%	0.005%
14	3.849	449	453	455	rBV	94	165	0.04%	0.005%
15	3.892	458	460	463	rBB	120	134	0.03%	0.004%
16	3.977	473	474	476	rVB	230	141	0.03%	0.004%
17	4.020	480	481	484	rBB	181	167	0.04%	0.005%
18	4.111	493	496	498	rBV	152	170	0.04%	0.005%
19	4.172	504	506	508	rBV	230	174	0.04%	0.005%
20	4.483	546	557	574	rBV4	46827	151984	35.92%	4.514%
21	4.867	618	620	621	rBV	253	181	0.04%	0.005%
22	5.050	640	650	667	rVB2	53905	167895	39.68%	4.987%
23	5.160	667	668	671	rBV3	366	271	0.06%	0.008%
24	5.379	701	704	705	rBV2	341	314	0.07%	0.009%
25	5.471	717	719	721	rBB2	139	132	0.03%	0.004%
26	5.556	729	733	736	rBV2	392	550	0.13%	0.016%
27	5.678	751	753	756	rBV	108	159	0.04%	0.005%
28	5.964	789	800	816	rBV2	146664	423146	100.00%	12.568%
29	6.239	843	845	848	rVB	222	195	0.05%	0.006%
30	6.288	848	853	856	rBB	226	356	0.08%	0.011%
31	6.324	857	859	862	rBB	171	155	0.04%	0.005%
32	6.379	862	868	869	rBV2	752	1171	0.28%	0.035%
33	6.440	877	878	881	rVB2	280	167	0.04%	0.005%
34	6.470	881	883	885	rBV	222	167	0.04%	0.005%
35	6.538	891	894	895	rBB	198	188	0.04%	0.006%
36	6.757	921	930	949	rBV	114655	282505	66.76%	8.391%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
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37	7.013	970	972	975	rBB	248	185	0.04%	0.005%
38	7.129	985	991	1001	rVB5	10207	22674	5.36%	0.673%
39	7.306	1013	1020	1037	rVB	87154	191835	45.34%	5.698%
40	7.428	1037	1040	1042	rBV	411	366	0.09%	0.011%
41	7.495	1049	1051	1055	rVB	365	382	0.09%	0.011%
42	7.525	1055	1056	1060	rBV	206	237	0.06%	0.007%
43	7.665	1076	1079	1082	rBB	147	141	0.03%	0.004%
44	7.867	1109	1112	1116	rVB	164	254	0.06%	0.008%
45	7.928	1119	1122	1123	rBV	227	158	0.04%	0.005%
46	8.086	1146	1148	1152	rBB	233	271	0.06%	0.008%
47	8.220	1169	1170	1172	rBV	249	193	0.05%	0.006%
48	8.324	1181	1187	1199	rBV	50564	86641	20.48%	2.573%
49	8.647	1234	1240	1251	rBV	222334	355593	84.04%	10.562%
50	8.903	1278	1282	1285	rBV	149	231	0.05%	0.007%
51	8.952	1285	1290	1301	rBV	35254	56304	13.31%	1.672%
52	9.244	1336	1338	1340	rBV2	249	288	0.07%	0.009%
53	9.269	1340	1342	1347	rVB	755	1086	0.26%	0.032%
54	9.342	1351	1354	1356	rBV	247	206	0.05%	0.006%
55	9.397	1357	1363	1381	rBV	89400	187435	44.30%	5.567%
56	9.714	1411	1415	1420	rVB3	794	1392	0.33%	0.041%
57	9.805	1427	1430	1431	rBB3	183	176	0.04%	0.005%
58	9.884	1439	1443	1445	rBV2	187	217	0.05%	0.006%
59	9.958	1452	1455	1457	rBV	225	274	0.06%	0.008%
60	10.055	1465	1471	1480	rBV	239804	332432	78.56%	9.874%
61	10.208	1492	1496	1499	rVB	371	523	0.12%	0.016%
62	10.232	1499	1500	1503	rVB	209	162	0.04%	0.005%
63	10.311	1509	1513	1517	rBV2	544	888	0.21%	0.026%
64	10.384	1522	1525	1526	rBB2	184	155	0.04%	0.005%
65	10.409	1526	1529	1530	rBV2	155	155	0.04%	0.005%
66	10.494	1540	1543	1547	rBB2	287	392	0.09%	0.012%
67	10.525	1547	1548	1549	rBV2	233	132	0.03%	0.004%
68	10.647	1565	1568	1572	rBV	386	573	0.14%	0.017%
69	10.750	1582	1585	1588	rBB2	210	187	0.04%	0.006%
70	10.896	1605	1609	1611	rBV2	181	322	0.08%	0.010%
71	10.964	1618	1620	1623	rBB2	483	458	0.11%	0.014%
72	11.116	1643	1645	1649	rBV	166	268	0.06%	0.008%
73	11.195	1652	1658	1671	rBV	168445	222026	52.47%	6.595%
74	11.323	1673	1679	1682	rBV	263	416	0.10%	0.012%
75	11.396	1688	1691	1693	rBV	264	222	0.05%	0.007%
76	11.451	1696	1700	1703	rBV	205	303	0.07%	0.009%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

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77	11.482	1703	1705	1708	rVB2	387	339	0.08%	0.010%
78	11.531	1708	1713	1714	rBB	146	184	0.04%	0.005%
79	11.549	1714	1716	1719	rBB	233	183	0.04%	0.005%
80	11.622	1726	1728	1731	rBV	271	309	0.07%	0.009%
81	11.762	1749	1751	1753	rBV	368	277	0.07%	0.008%
82	11.860	1766	1767	1769	rBB	229	136	0.03%	0.004%
83	11.884	1769	1771	1774	rBV	135	172	0.04%	0.005%
84	12.024	1789	1794	1803	rBV	250376	315819	74.64%	9.381%
85	12.152	1814	1815	1817	rBV	254	176	0.04%	0.005%
86	12.244	1826	1830	1834	rVB3	1161	1582	0.37%	0.047%
87	12.323	1837	1843	1852	rBV	237750	323062	76.35%	9.596%
88	12.512	1872	1874	1878	rBB	178	215	0.05%	0.006%
89	12.543	1878	1879	1881	rBV	190	164	0.04%	0.005%
90	12.988	1951	1952	1953	rBV	357	183	0.04%	0.005%
91	13.311	2001	2005	2006	rBV2	176	215	0.05%	0.006%
92	13.451	2024	2028	2030	rBV2	176	275	0.06%	0.008%
93	13.597	2049	2052	2055	rVB2	409	394	0.09%	0.012%
94	13.689	2065	2067	2068	rBV	385	288	0.07%	0.009%
95	13.719	2071	2072	2073	rBV	309	176	0.04%	0.005%
96	13.780	2077	2082	2091	rVB	28708	42914	10.14%	1.275%
97	14.128	2136	2139	2144	rVB2	3666	4976	1.18%	0.148%
98	14.250	2158	2159	2162	rBV	424	440	0.10%	0.013%
99	14.609	2216	2218	2220	rBV2	1362	1232	0.29%	0.037%
100	14.640	2220	2223	2226	rVV2	3235	4739	1.12%	0.141%

Sum of corrected areas: 3366749

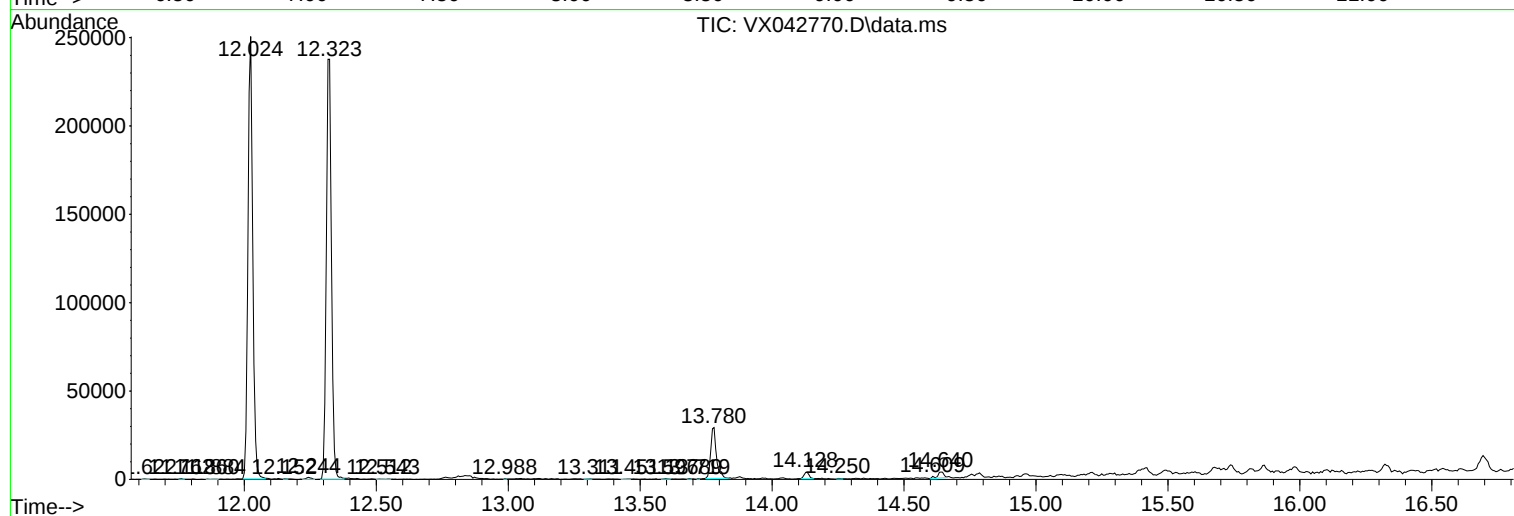
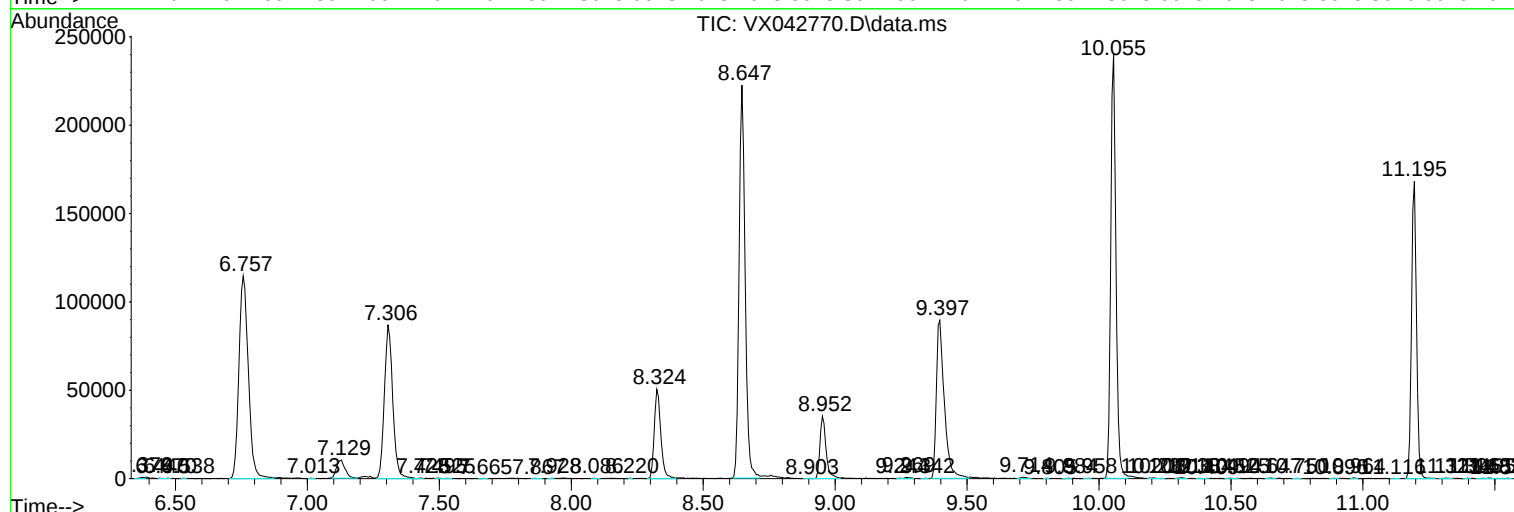
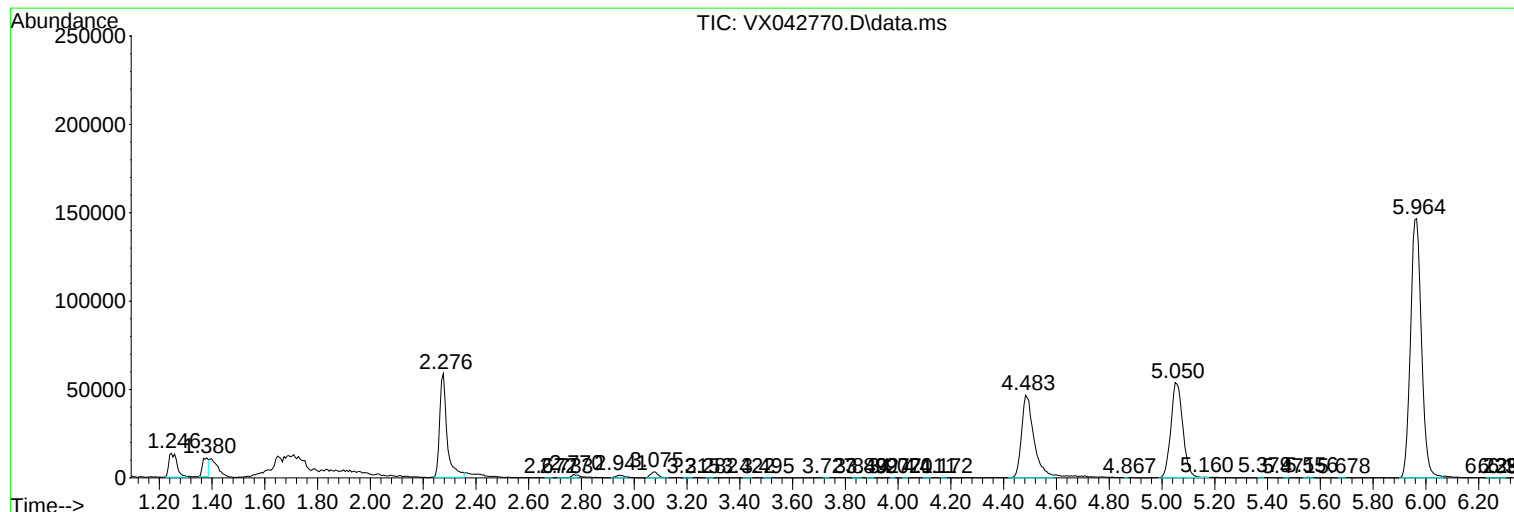
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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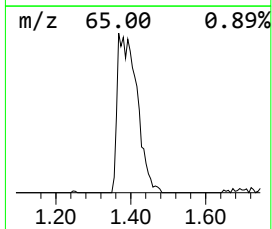
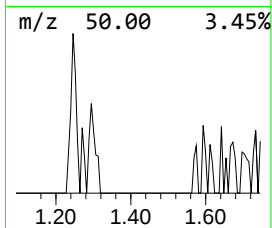
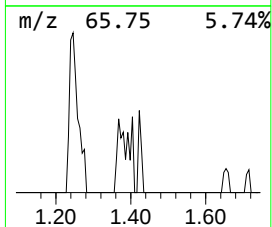
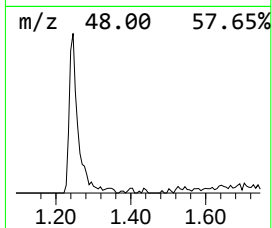
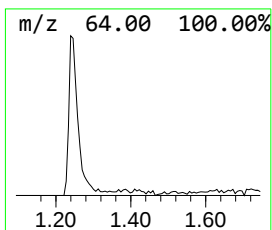
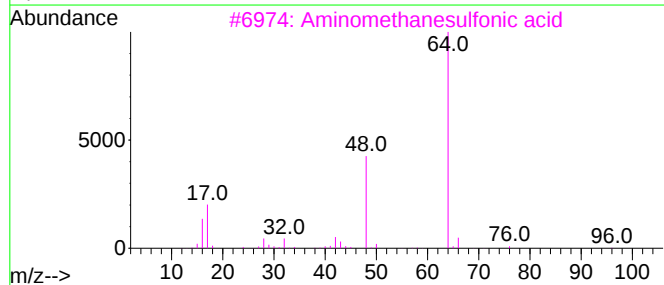
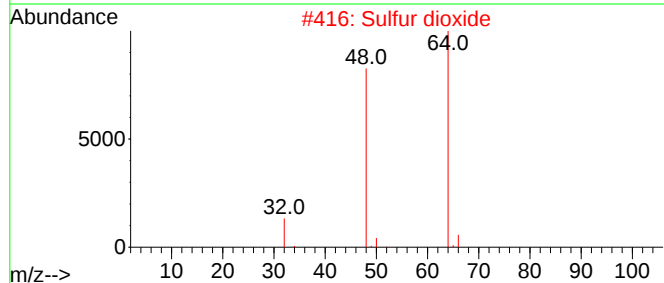
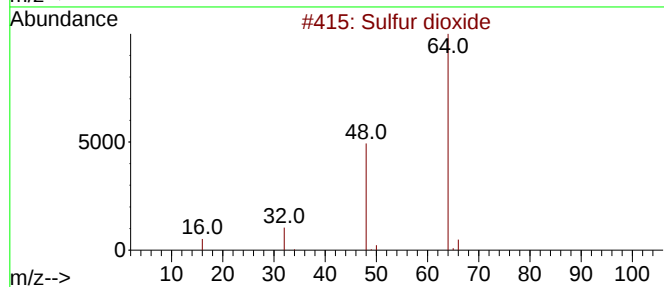
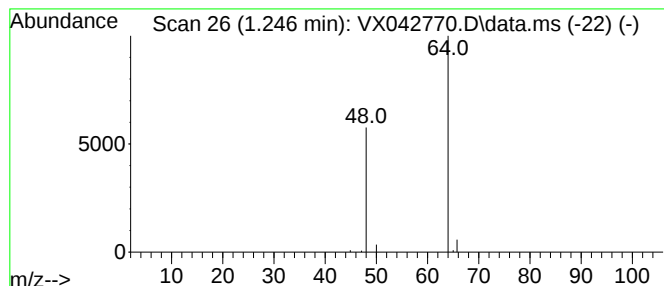
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	5.10 ug/L	28800	1,4-Difluorobenzene	6.757

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



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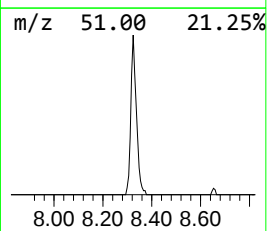
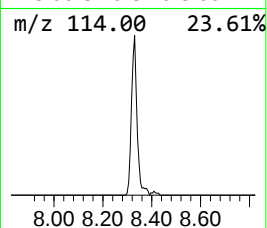
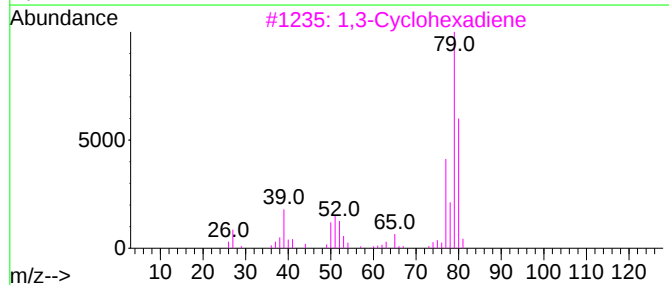
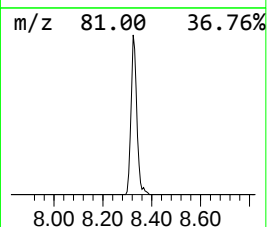
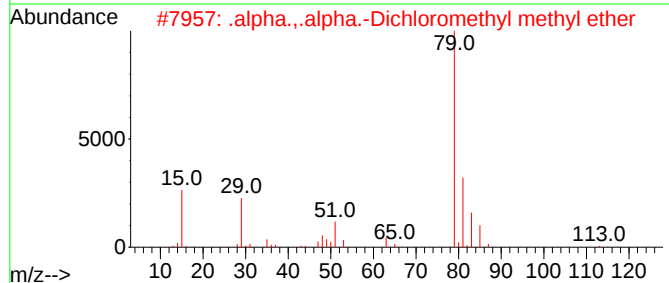
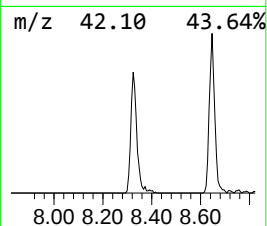
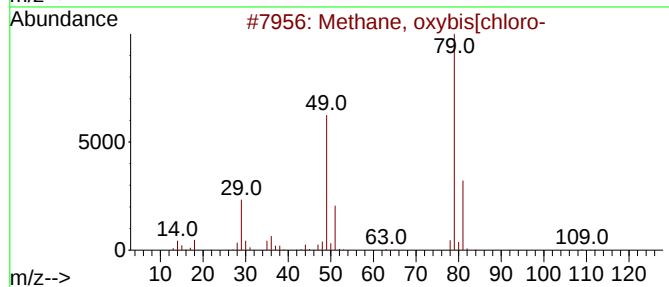
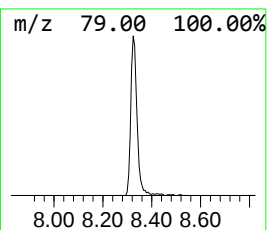
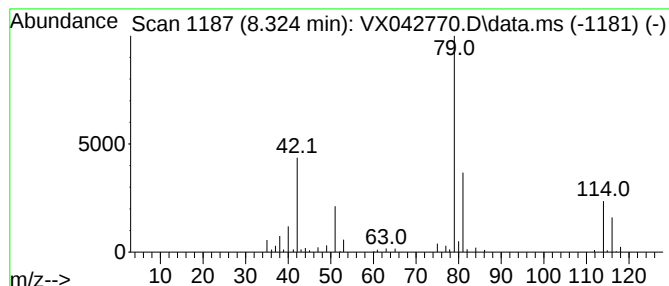
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.324	15.33 ug/L	86641	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	38
2			.alpha.,.alpha.-Dichloromethyl m...	114	C2H4Cl2O	004885-02-3	37
3			1,3-Cyclohexadiene	80	C6H8	000592-57-4	32
4			Thiophosgene	114	CCl2S	000463-71-8	28
5			1,3-Cyclohexadiene	80	C6H8	000592-57-4	25



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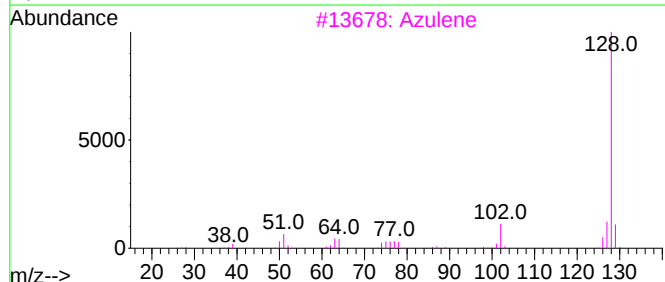
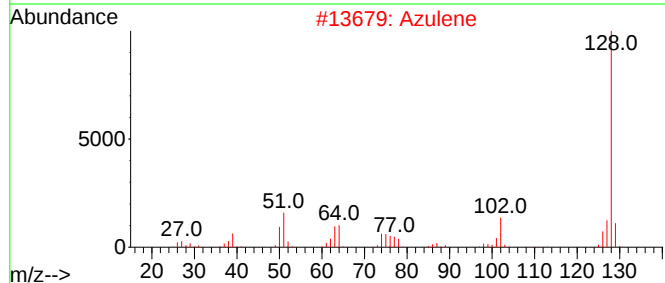
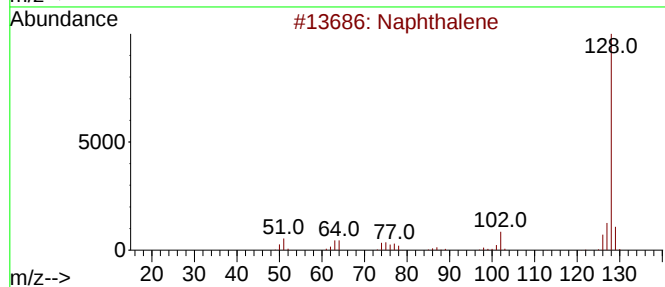
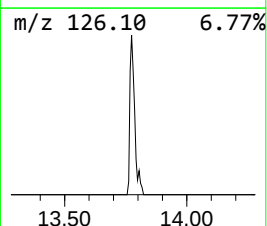
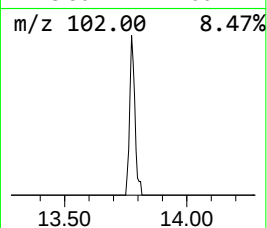
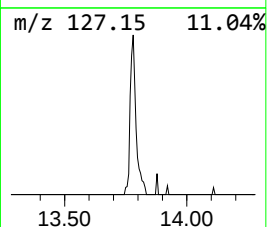
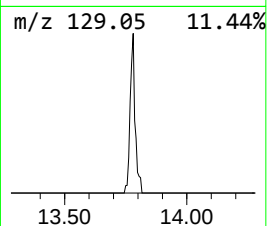
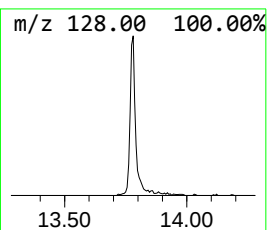
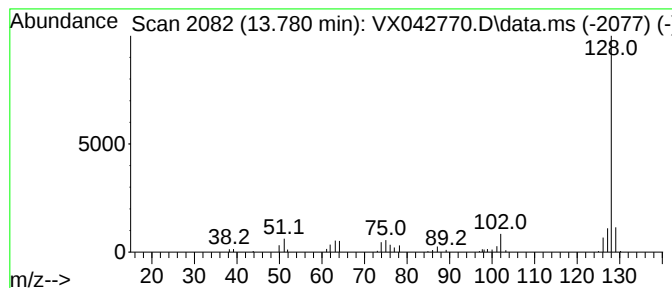
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	6.79 ug/L	42914	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	94
2			Azulene	128	C10H8	000275-51-4	91
3			Azulene	128	C10H8	000275-51-4	90
4			Naphthalene	128	C10H8	000091-20-3	90
5			Azulene	128	C10H8	000275-51-4	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042770.D
Acq On : 31 Jul 2024 14:04
Operator : JC/MD
Sample : P3382-01ME
Misc : 7.60g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20R1ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.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	1.246	5.1	ug/L	28800	1	6.757	282505	50.0
unknown-01	8.324	15.3	ug/L	86641	1	6.757	282505	50.0
Azulene	13.780	6.8	ug/L	42914	3	12.024	315819	50.0