

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
 Data File : VX042776.D
 Acq On : 31 Jul 2024 16:24
 Operator : JC/MD
 Sample : P3398-10
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E08L5

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: VX042776.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	22	25	34	rBV	14583	20399	4.71%	0.586%
2	1.367	43	46	56	rVB	36050	46366	10.71%	1.332%
3	1.648	89	92	101	rVB	27455	32674	7.55%	0.939%
4	1.770	111	112	113	rBV	387	177	0.04%	0.005%
5	2.294	192	198	210	rBV	85286	136727	31.59%	3.929%
6	2.623	249	252	254	rBV	158	220	0.05%	0.006%
7	2.934	297	303	305	rBV2	1444	2321	0.54%	0.067%
8	3.160	337	340	343	rBV	160	211	0.05%	0.006%
9	3.221	347	350	351	rBB	193	169	0.04%	0.005%
10	3.251	352	355	357	rBV	104	128	0.03%	0.004%
11	3.294	360	362	363	rBV	145	137	0.03%	0.004%
12	3.702	428	429	432	rBV	178	177	0.04%	0.005%
13	4.025	479	482	483	rVB	210	198	0.05%	0.006%
14	4.050	483	486	487	rBV2	157	160	0.04%	0.005%
15	4.141	494	501	504	rBB	214	366	0.08%	0.011%
16	4.196	508	510	513	rBB	178	120	0.03%	0.003%
17	4.269	521	522	527	rVB	199	238	0.05%	0.007%
18	4.348	533	535	536	rBB	211	132	0.03%	0.004%
19	4.403	542	544	547	rBV	209	224	0.05%	0.006%
20	4.470	547	555	570	rBV2	27957	87079	20.12%	2.502%
21	4.940	630	632	633	rBV	215	138	0.03%	0.004%
22	5.062	637	652	675	rBV2	61254	226791	52.40%	6.517%
23	5.232	677	680	682	rBB	187	170	0.04%	0.005%
24	5.269	685	686	688	rBB	221	121	0.03%	0.003%
25	5.385	703	705	706	rBV	184	154	0.04%	0.004%
26	5.501	720	724	726	rBV	285	296	0.07%	0.009%
27	5.543	729	731	732	rBV	251	192	0.04%	0.006%
28	5.647	744	748	751	rBB	195	289	0.07%	0.008%
29	5.708	756	758	762	rVV	206	207	0.05%	0.006%
30	5.970	790	801	815	rBV2	148505	432778	100.00%	12.435%
31	6.232	842	844	847	rVB2	215	223	0.05%	0.006%
32	6.281	848	852	855	rBV2	129	218	0.05%	0.006%
33	6.519	888	891	895	rBB	157	211	0.05%	0.006%
34	6.561	895	898	900	rBV	259	266	0.06%	0.008%
35	6.671	912	916	920	rBB2	180	315	0.07%	0.009%
36	6.763	922	931	944	rBV	118582	289741	66.95%	8.325%

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 Title : VOC Analysis

37	7.116	986	989	992	rBV3	835	1381	0.32%	0.040%
38	7.214	1002	1005	1008	rBV2	367	480	0.11%	0.014%
39	7.311	1011	1021	1032	rBV	87969	193594	44.73%	5.563%
40	7.445	1041	1043	1044	rBV	257	192	0.04%	0.006%
41	7.494	1048	1051	1053	rBV2	336	358	0.08%	0.010%
42	7.537	1057	1058	1062	rBB2	152	162	0.04%	0.005%
43	7.580	1062	1065	1069	rBB2	214	253	0.06%	0.007%
44	7.744	1091	1092	1094	rBV2	233	134	0.03%	0.004%
45	7.823	1099	1105	1115	rBB2	4066	8268	1.91%	0.238%
46	7.909	1116	1119	1123	rBV2	565	799	0.18%	0.023%
47	7.964	1127	1128	1129	rBV2	243	143	0.03%	0.004%
48	8.329	1179	1188	1200	rBV	53239	92604	21.40%	2.661%
49	8.598	1229	1232	1234	rBV	206	230	0.05%	0.007%
50	8.652	1234	1241	1250	rBV	212626	353237	81.62%	10.150%
51	8.951	1285	1290	1301	rBV	40072	59901	13.84%	1.721%
52	9.091	1311	1313	1314	rBV	198	140	0.03%	0.004%
53	9.244	1334	1338	1339	rBV	154	227	0.05%	0.007%
54	9.280	1339	1344	1350	rVB2	2848	4686	1.08%	0.135%
55	9.390	1357	1362	1380	rBV	128263	201868	46.64%	5.800%
56	9.695	1411	1412	1415	rVV	316	262	0.06%	0.008%
57	9.750	1419	1421	1423	rVB	314	248	0.06%	0.007%
58	9.811	1429	1431	1433	rVB	299	191	0.04%	0.005%
59	9.860	1438	1439	1441	rBV	183	149	0.03%	0.004%
60	9.982	1458	1459	1462	rBB	189	137	0.03%	0.004%
61	10.012	1462	1464	1465	rBV	181	139	0.03%	0.004%
62	10.055	1466	1471	1489	rVB	246204	341821	78.98%	9.822%
63	10.286	1505	1509	1510	rVB	264	288	0.07%	0.008%
64	10.305	1510	1512	1514	rBV2	547	643	0.15%	0.018%
65	10.420	1529	1531	1533	rVB	191	150	0.03%	0.004%
66	10.475	1538	1540	1542	rVB	238	182	0.04%	0.005%
67	10.506	1542	1545	1548	rBB2	190	252	0.06%	0.007%
68	10.555	1549	1553	1557	rBB	187	249	0.06%	0.007%
69	10.597	1557	1560	1561	rBB	205	199	0.05%	0.006%
70	10.646	1565	1568	1569	rBV	491	478	0.11%	0.014%
71	10.737	1579	1583	1584	rBV	117	138	0.03%	0.004%
72	10.768	1587	1588	1591	rBV2	144	124	0.03%	0.004%
73	10.835	1596	1599	1600	rBV	115	135	0.03%	0.004%
74	10.884	1605	1607	1608	rBV	224	130	0.03%	0.004%
75	11.030	1629	1631	1634	rBV	180	233	0.05%	0.007%
76	11.073	1634	1638	1640	rBV2	173	277	0.06%	0.008%

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77	11.195	1652	1658	1667	rBV	180196	242024	55.92%	6.954%
78	11.311	1673	1677	1683	rBV4	2692	4146	0.96%	0.119%
79	11.353	1683	1684	1686	rBV	235	175	0.04%	0.005%
80	11.414	1693	1694	1698	rVB2	186	149	0.03%	0.004%
81	11.652	1730	1733	1734	rBV	148	185	0.04%	0.005%
82	11.719	1743	1744	1746	rBV	183	122	0.03%	0.004%
83	11.756	1748	1750	1752	rVB	514	398	0.09%	0.011%
84	11.902	1772	1774	1777	rBV	174	211	0.05%	0.006%
85	12.024	1789	1794	1801	rBV	255687	323414	74.73%	9.293%
86	12.201	1821	1823	1824	rBV	203	138	0.03%	0.004%
87	12.219	1824	1826	1828	rBV2	1378	1397	0.32%	0.040%
88	12.323	1837	1843	1855	rBV	247477	336449	77.74%	9.668%
89	12.463	1864	1866	1867	rBV	275	127	0.03%	0.004%
90	12.554	1880	1881	1883	rBV	292	272	0.06%	0.008%
91	12.591	1886	1887	1889	rBV2	226	171	0.04%	0.005%
92	12.768	1909	1916	1918	rBV4	921	1646	0.38%	0.047%
93	12.822	1923	1925	1926	rBV2	412	408	0.09%	0.012%
94	12.908	1937	1939	1940	rBV2	223	147	0.03%	0.004%
95	13.578	2046	2049	2050	rBV2	288	255	0.06%	0.007%
96	13.731	2072	2074	2076	rBV	249	267	0.06%	0.008%
97	13.780	2077	2082	2090	rVV	12404	18222	4.21%	0.524%
98	14.133	2136	2140	2145	rVB3	2038	2852	0.66%	0.082%
99	14.786	2244	2247	2252	rBV2	924	1144	0.26%	0.033%
100	15.035	2286	2288	2291	rBV2	394	456	0.11%	0.013%

Sum of corrected areas: 3480190

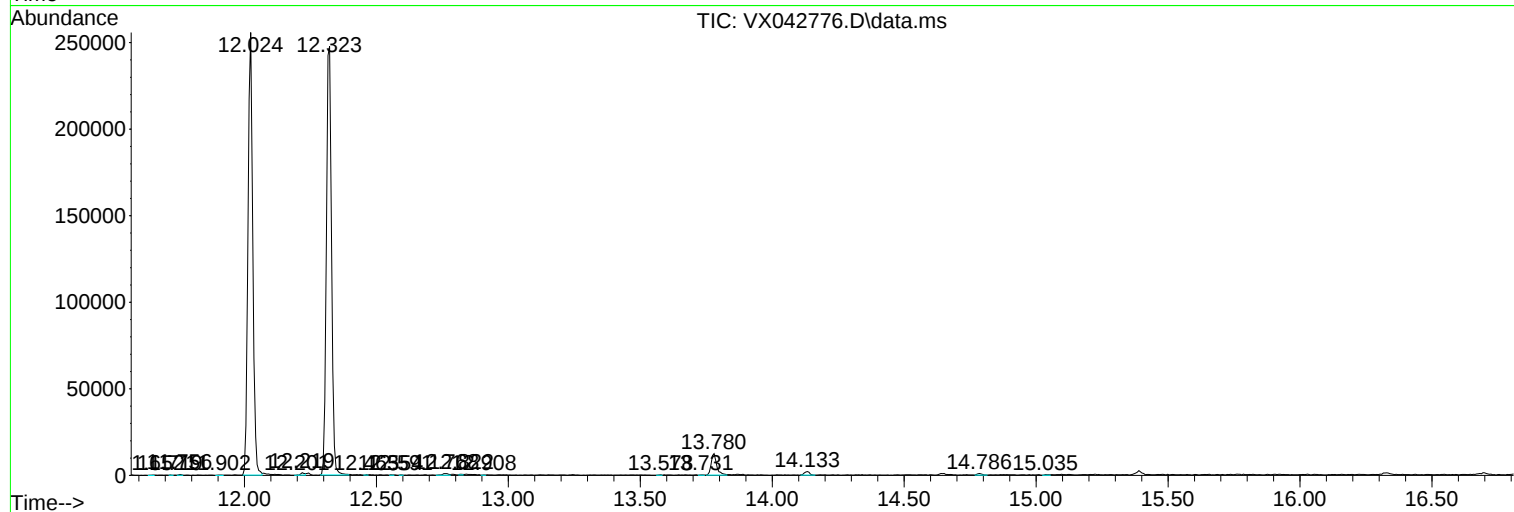
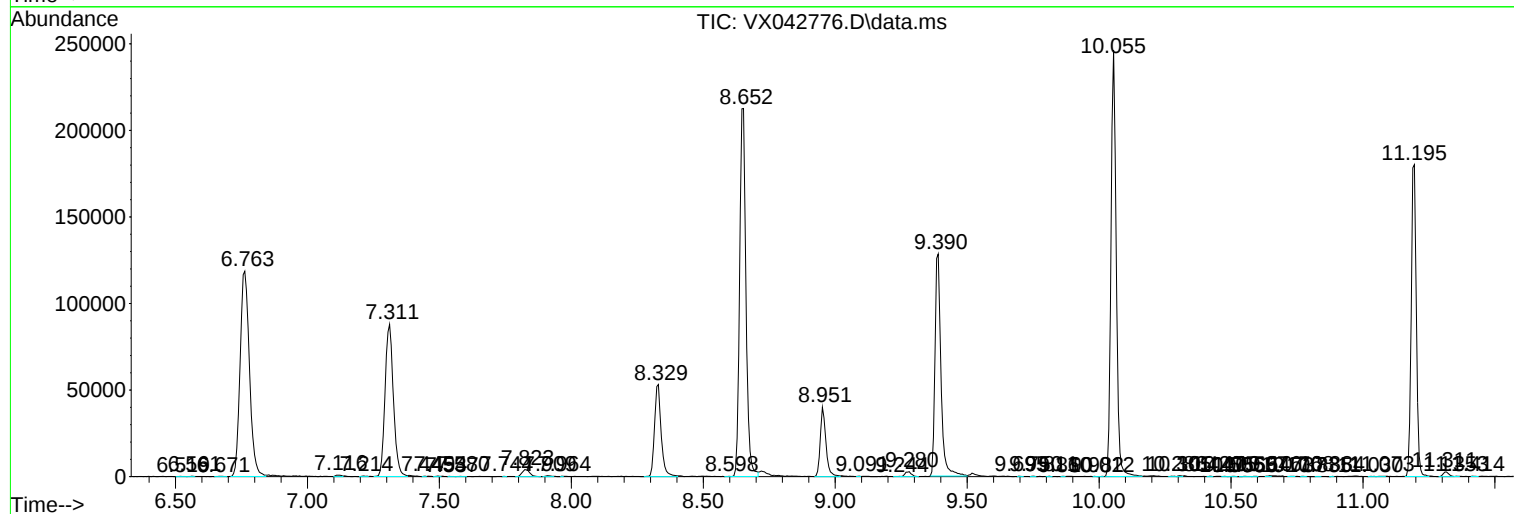
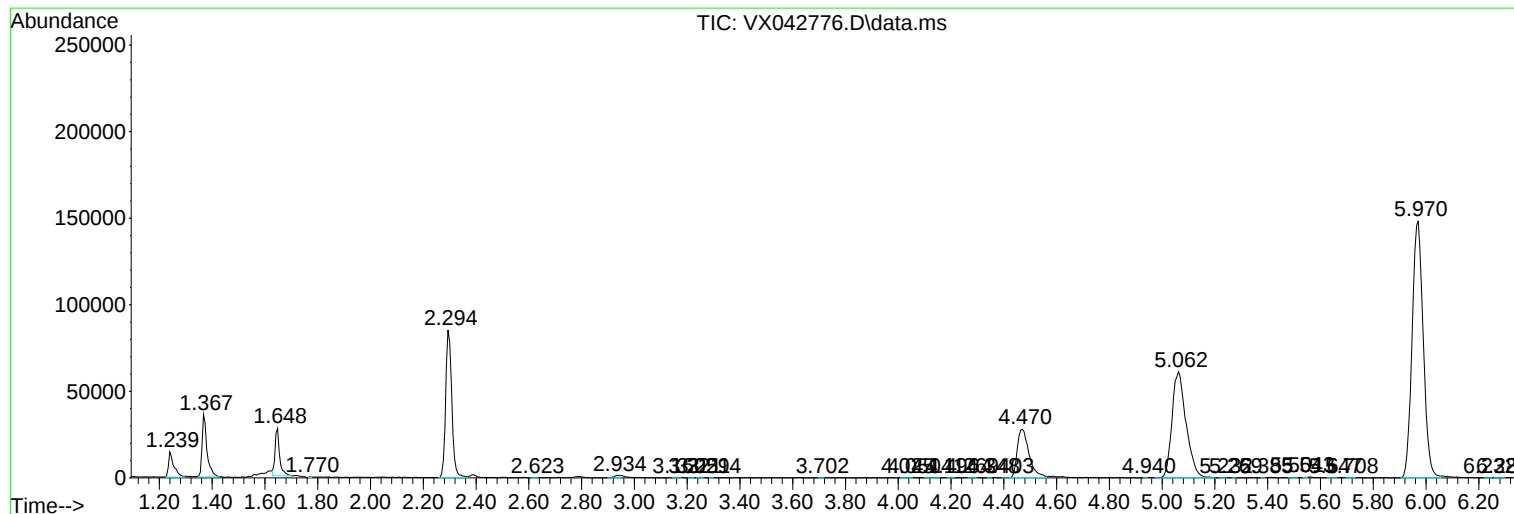
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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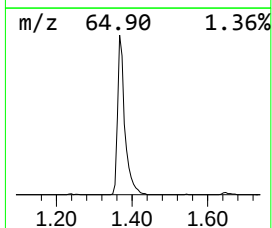
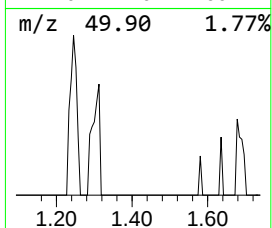
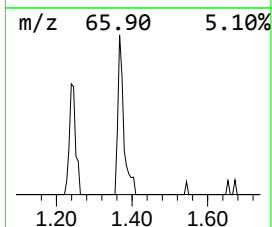
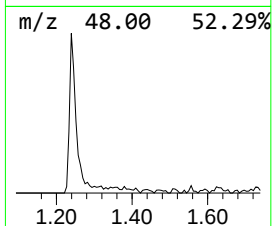
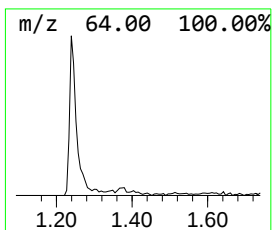
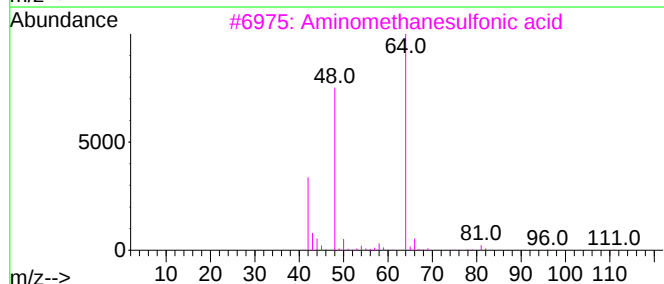
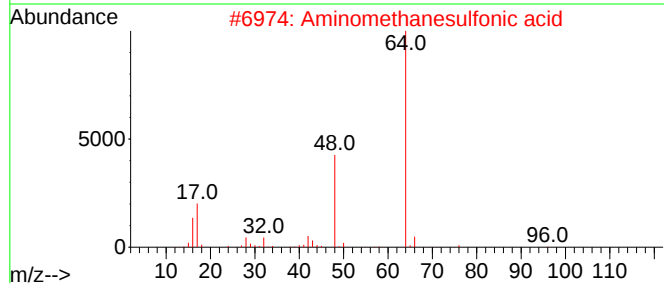
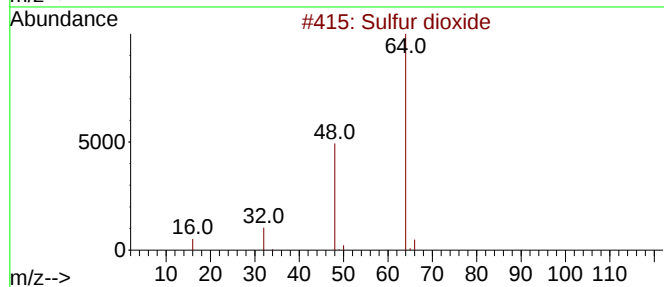
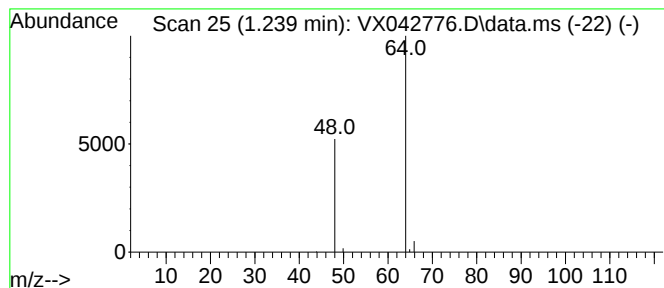
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.239	3.52 ug/L	20399	1,4-Difluorobenzene	6.763

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	64
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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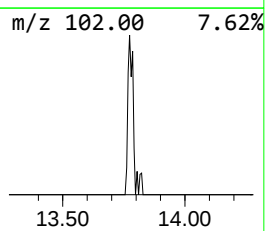
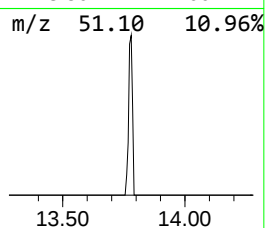
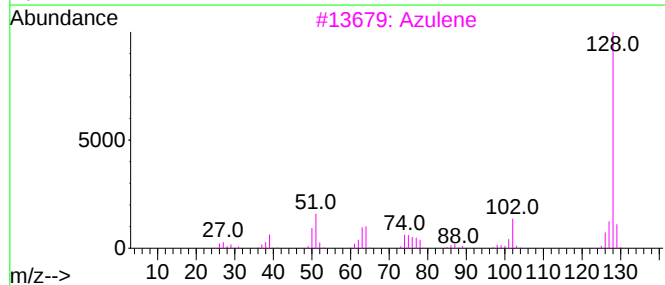
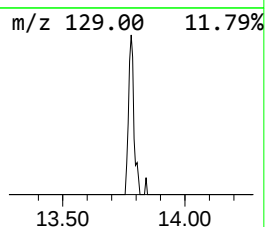
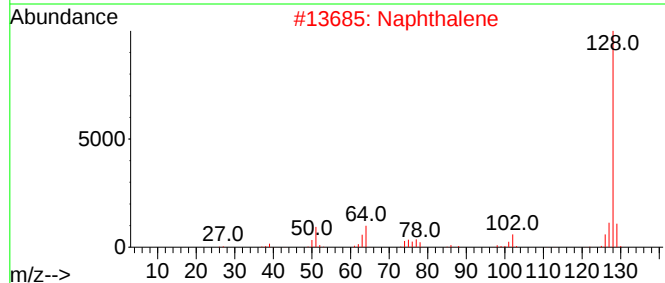
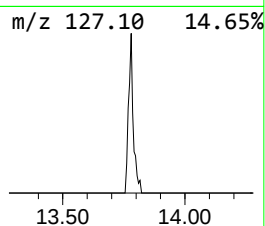
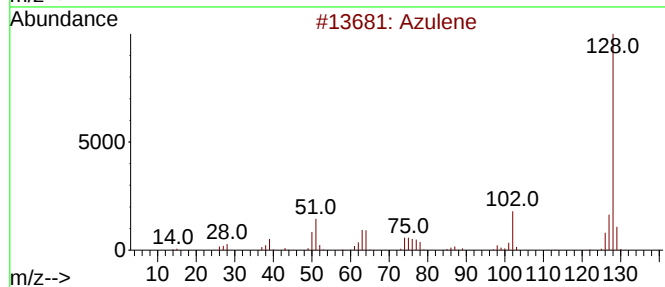
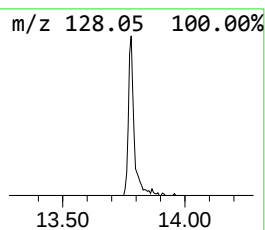
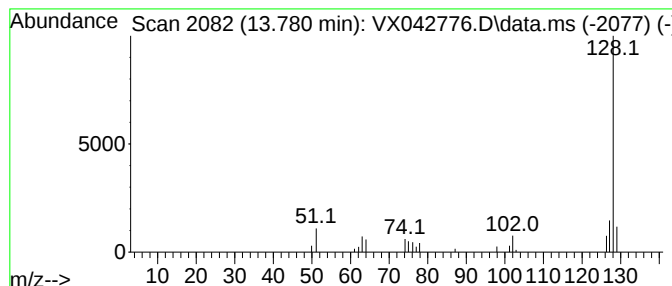
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	2.82 ug/L	18222	1,4-Dichlorobenzene-d4	12.024

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



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.239	3.5	ug/L	20399	1	6.763	289741	50.0
Azulene	13.780	2.8	ug/L	18222	3	12.024	323414	50.0