

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111921\
 Data File : VX025242.D
 Acq On : 19 Nov 2021 18:39
 Operator : JC/MD
 Sample : M4779-12
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VHBLK002

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\SFAMXLM111121WMA.M
 Title : VOC Analysis

Signal : TIC: VX025242.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	33	rBV	40989	63753	11.16%	1.394%
2	1.368	42	46	54	rVB	94052	90613	15.86%	1.981%
3	1.666	90	95	104	rBV	66378	89466	15.66%	1.956%
4	2.306	193	200	209	rBV	125159	204148	35.73%	4.463%
5	2.526	231	236	237	rBV2	358	473	0.08%	0.010%
6	2.703	263	265	271	rBV2	312	424	0.07%	0.009%
7	2.788	275	279	286	rVB3	717	1296	0.23%	0.028%
8	2.940	297	304	314	rVB2	6610	15570	2.72%	0.340%
9	3.251	354	355	361	rBV	137	193	0.03%	0.004%
10	3.453	384	388	391	rVB2	157	189	0.03%	0.004%
11	3.812	444	447	451	rVB	183	199	0.03%	0.004%
12	4.458	543	553	565	rBV	45878	128967	22.57%	2.820%
13	5.062	640	652	669	rBV2	72365	227362	39.79%	4.971%
14	5.257	683	684	686	rBV	161	137	0.02%	0.003%
15	5.324	693	695	696	rBV2	187	158	0.03%	0.003%
16	5.562	731	734	736	rVV2	351	409	0.07%	0.009%
17	5.855	781	782	785	rVB	154	135	0.02%	0.003%
18	5.891	785	788	789	rBV	149	159	0.03%	0.003%
19	5.970	789	801	817	rVV2	191279	571423	100.00%	12.493%
20	6.415	873	874	877	rBV2	132	138	0.02%	0.003%
21	6.611	904	906	908	rBV2	144	154	0.03%	0.003%
22	6.763	920	931	946	rBV	145249	349754	61.21%	7.647%
23	7.043	973	977	980	rBV	117	207	0.04%	0.005%
24	7.117	983	989	997	rVB3	2070	4665	0.82%	0.102%
25	7.184	997	1000	1001	rBV	160	145	0.03%	0.003%
26	7.226	1005	1007	1009	rVB	147	123	0.02%	0.003%
27	7.312	1011	1021	1032	rBV	118158	256742	44.93%	5.613%
28	7.464	1045	1046	1047	rBV	257	153	0.03%	0.003%
29	7.562	1059	1062	1064	rBV2	129	143	0.03%	0.003%
30	7.805	1098	1102	1104	rBV3	321	436	0.08%	0.010%
31	7.927	1118	1122	1128	rVV4	791	1526	0.27%	0.033%
32	7.982	1128	1131	1132	rVB2	169	128	0.02%	0.003%
33	8.080	1143	1147	1149	rBV2	99	149	0.03%	0.003%
34	8.232	1170	1172	1176	rVB	181	176	0.03%	0.004%
35	8.269	1176	1178	1180	rBV2	160	167	0.03%	0.004%
36	8.324	1181	1187	1199	rVB	82829	138789	24.29%	3.034%

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37	8.403	1199	1200	1202	rBV	169	151	0.03%	0.003%
38	8.470	1207	1211	1216	rVB3	559	984	0.17%	0.022%
39	8.543	1219	1223	1224	rBV	138	161	0.03%	0.004%
40	8.586	1226	1230	1231	rBV2	164	187	0.03%	0.004%
41	8.653	1234	1241	1248	rBV	309389	482584	84.45%	10.551%
42	8.720	1248	1252	1260	rVB2	4809	7613	1.33%	0.166%
43	8.952	1285	1290	1300	rBV	62726	89506	15.66%	1.957%
44	9.281	1340	1344	1348	rBV3	367	531	0.09%	0.012%
45	9.384	1355	1361	1373	rBV	212389	292510	51.19%	6.395%
46	9.580	1390	1393	1398	rBV2	130	234	0.04%	0.005%
47	9.701	1409	1413	1418	rVB3	939	1402	0.25%	0.031%
48	9.951	1452	1454	1456	rBV	182	136	0.02%	0.003%
49	10.055	1465	1471	1488	rVB	313393	416585	72.90%	9.108%
50	10.165	1488	1489	1491	rBV2	137	141	0.02%	0.003%
51	10.195	1491	1494	1500	rVB2	637	809	0.14%	0.018%
52	10.305	1507	1512	1516	rVV	1309	1615	0.28%	0.035%
53	10.470	1536	1539	1541	rBV2	123	133	0.02%	0.003%
54	10.592	1557	1559	1562	rBV2	111	155	0.03%	0.003%
55	10.634	1565	1566	1567	rBV	342	226	0.04%	0.005%
56	10.787	1588	1591	1593	rBV2	126	170	0.03%	0.004%
57	10.970	1618	1621	1624	rBV2	256	363	0.06%	0.008%
58	11.079	1638	1639	1642	rBV	120	122	0.02%	0.003%
59	11.122	1642	1646	1650	rVB2	1742	2037	0.36%	0.045%
60	11.195	1652	1658	1668	rBV	222561	277652	48.59%	6.070%
61	11.280	1670	1672	1674	rBV2	198	161	0.03%	0.004%
62	11.384	1686	1689	1690	rBV2	211	218	0.04%	0.005%
63	11.457	1699	1701	1702	rBV	302	270	0.05%	0.006%
64	11.543	1714	1715	1719	rVB2	329	363	0.06%	0.008%
65	11.591	1719	1723	1725	rBV2	172	265	0.05%	0.006%
66	11.658	1733	1734	1738	rBV2	86	137	0.02%	0.003%
67	11.750	1744	1749	1754	rVB2	2215	2447	0.43%	0.053%
68	11.799	1754	1757	1759	rBV	126	167	0.03%	0.004%
69	11.841	1762	1764	1767	rVB	308	215	0.04%	0.005%
70	11.933	1775	1779	1782	rBV3	704	1004	0.18%	0.022%
71	12.024	1789	1794	1805	rBV	318101	393023	68.78%	8.592%
72	12.103	1805	1807	1809	rBV	185	189	0.03%	0.004%
73	12.128	1809	1811	1813	rBV2	403	470	0.08%	0.010%
74	12.244	1823	1830	1834	rBV	885	1170	0.20%	0.026%
75	12.323	1837	1843	1854	rVV	325534	413947	72.44%	9.050%
76	12.420	1855	1859	1865	rVB4	1396	2095	0.37%	0.046%

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77	12.658	1896	1898	1901	rBV2	178	199	0.03%	0.004%
78	12.762	1911	1915	1918	rBV2	225	255	0.04%	0.006%
79	12.853	1927	1930	1932	rBV2	372	478	0.08%	0.010%
80	13.061	1959	1964	1968	rBV3	268	409	0.07%	0.009%
81	13.506	2035	2037	2040	rVV	128	123	0.02%	0.003%
82	13.689	2065	2067	2072	rVB2	169	285	0.05%	0.006%
83	13.731	2072	2074	2075	rBV	222	216	0.04%	0.005%
84	13.780	2077	2082	2090	rVV	17467	24220	4.24%	0.530%
85	13.865	2094	2096	2101	rVV3	385	576	0.10%	0.013%
86	14.134	2136	2140	2144	rVB2	426	634	0.11%	0.014%
87	14.164	2144	2145	2148	rVB2	255	155	0.03%	0.003%
88	14.195	2148	2150	2152	rBV2	103	127	0.02%	0.003%
89	14.396	2180	2183	2185	rBV3	138	192	0.03%	0.004%
90	14.457	2191	2193	2195	rVB	251	159	0.03%	0.003%
91	14.487	2195	2198	2201	rBV2	193	303	0.05%	0.007%
92	14.591	2213	2215	2218	rBV	101	127	0.02%	0.003%
93	14.640	2220	2223	2228	rVB3	578	866	0.15%	0.019%
94	14.713	2234	2235	2238	rVB2	230	184	0.03%	0.004%
95	14.786	2244	2247	2250	rVB3	421	505	0.09%	0.011%
96	14.914	2265	2268	2269	rBV	165	141	0.02%	0.003%
97	15.511	2364	2366	2369	rVB	349	224	0.04%	0.005%
98	16.334	2497	2501	2507	rVB5	768	1276	0.22%	0.028%
99	16.493	2525	2527	2529	rBV	257	188	0.03%	0.004%
100	16.694	2556	2560	2565	rVB4	732	1375	0.24%	0.030%

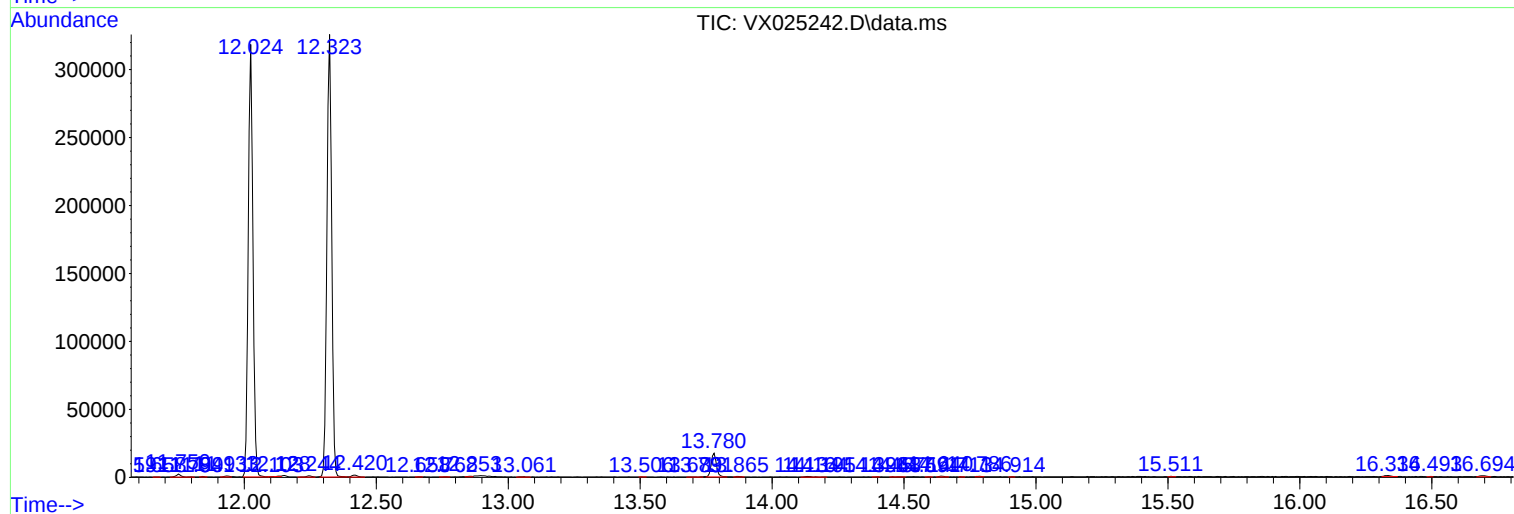
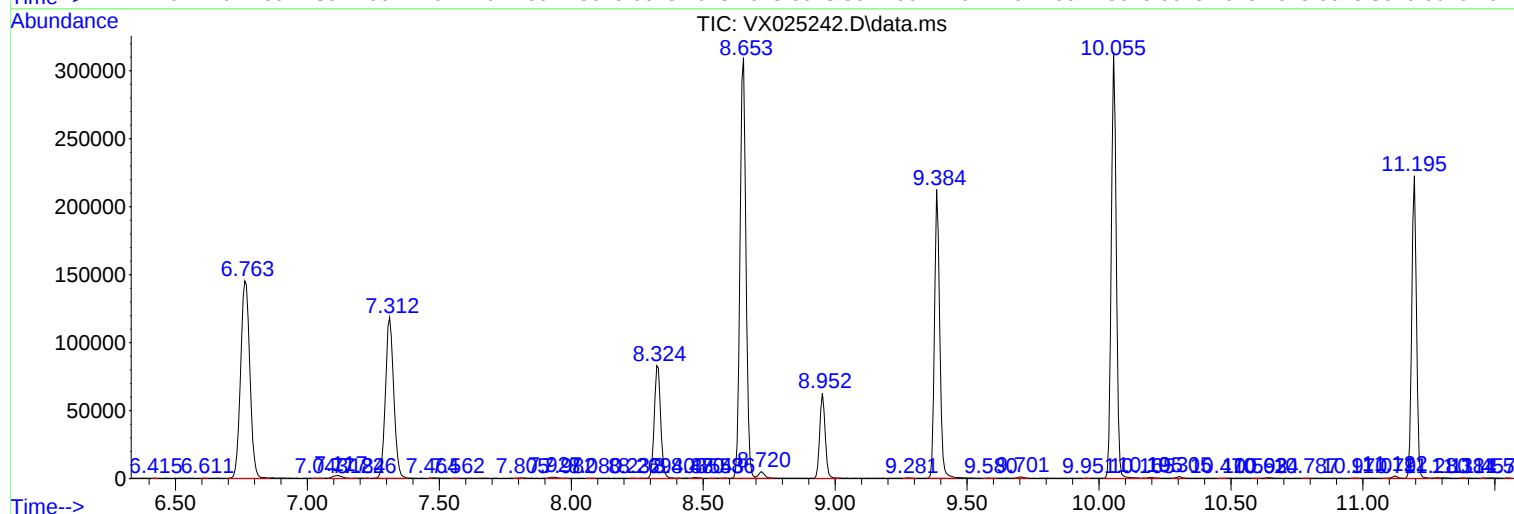
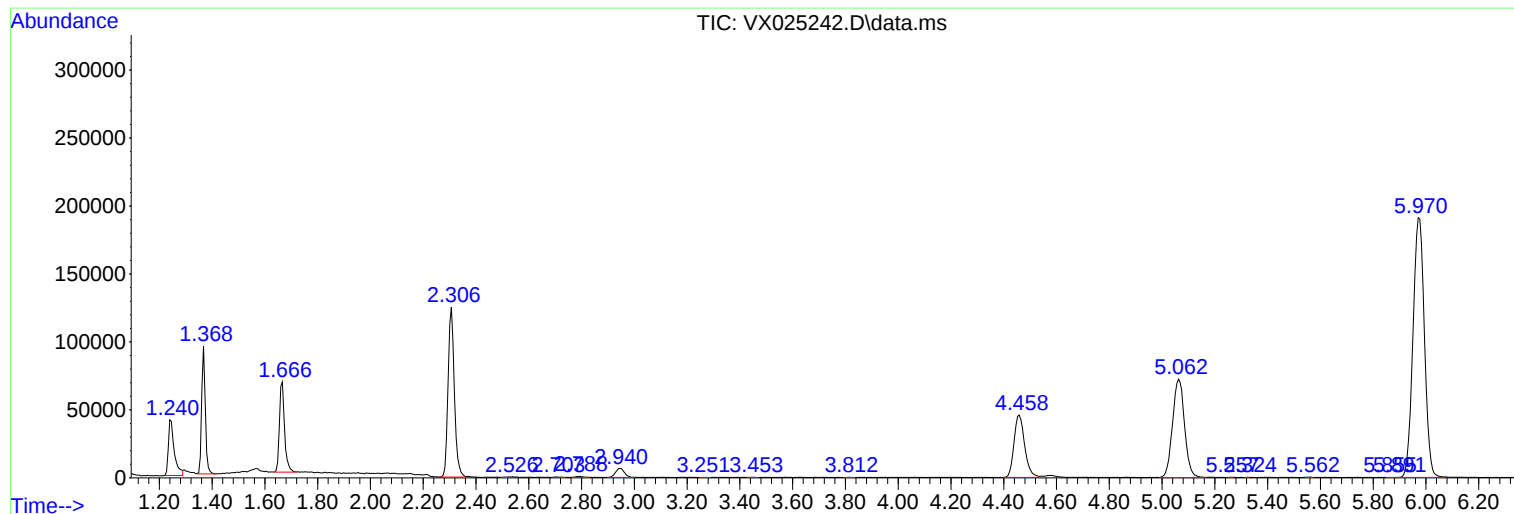
Sum of corrected areas: 4574034

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML111121WMA.M
Quant Title : VOC Analysis

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



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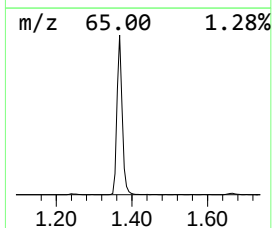
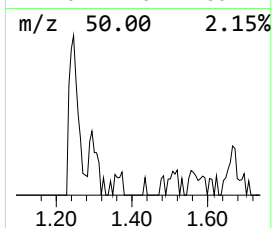
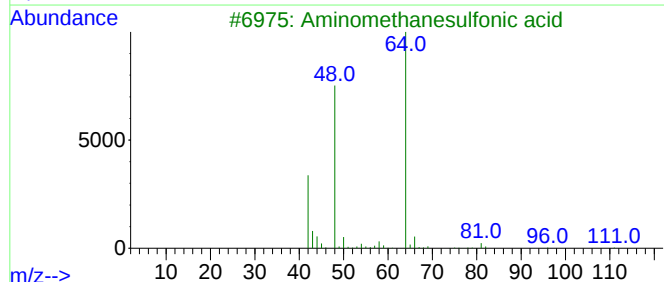
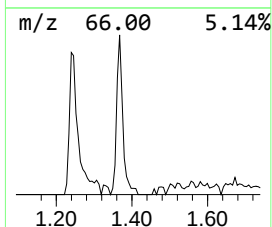
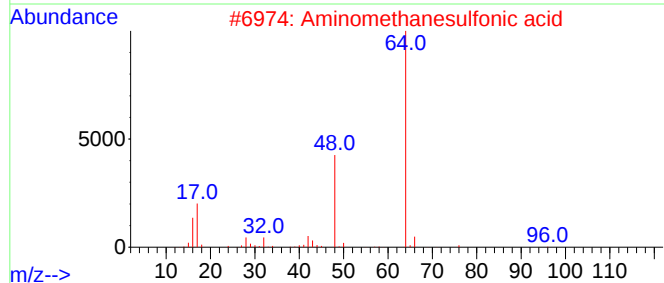
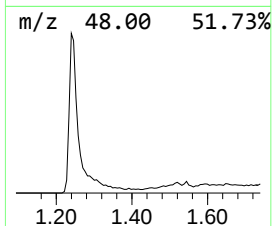
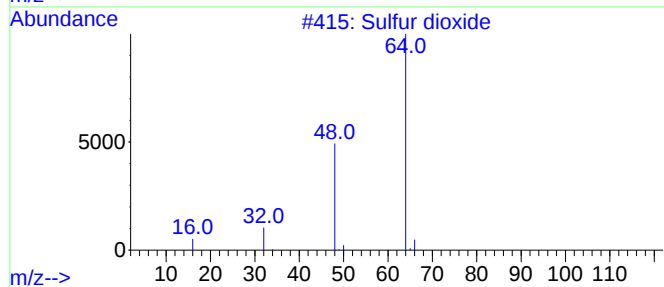
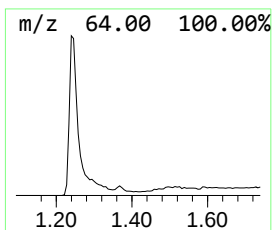
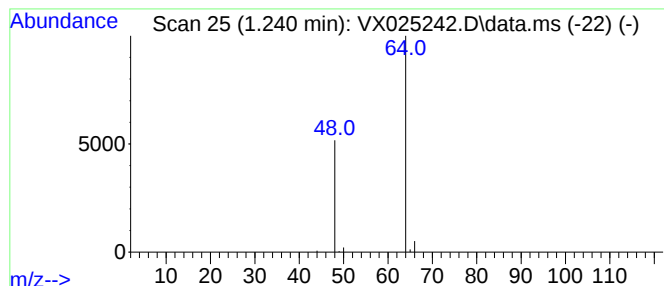
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM111121WMA.M
Quant Title : VOC Analysis

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.
1.240	9.11 ug/L	63753	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	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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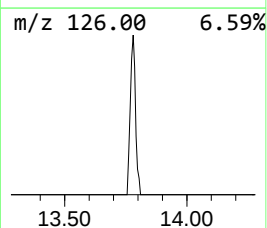
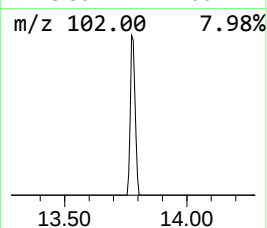
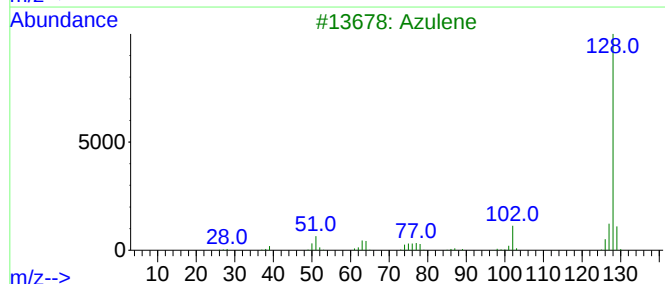
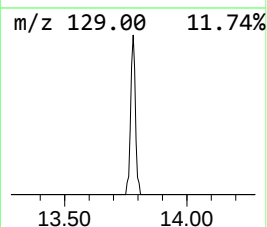
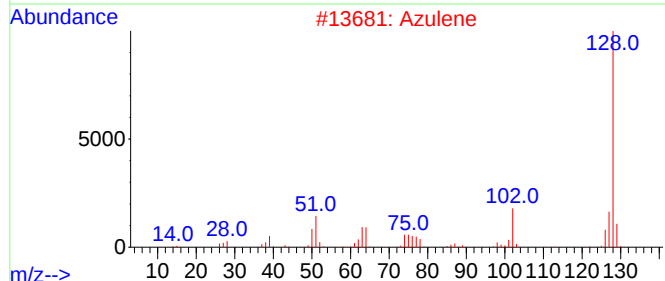
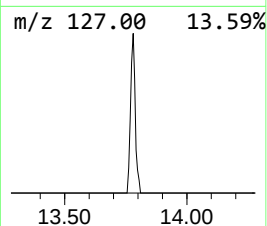
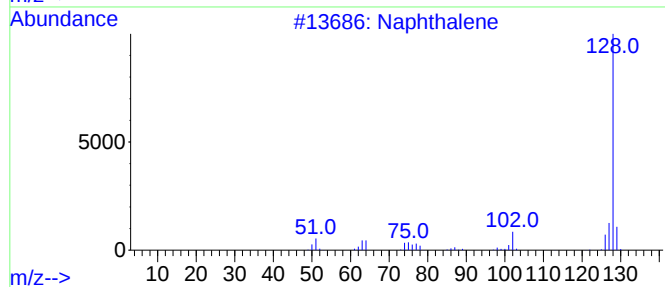
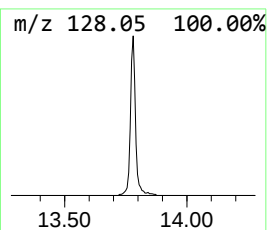
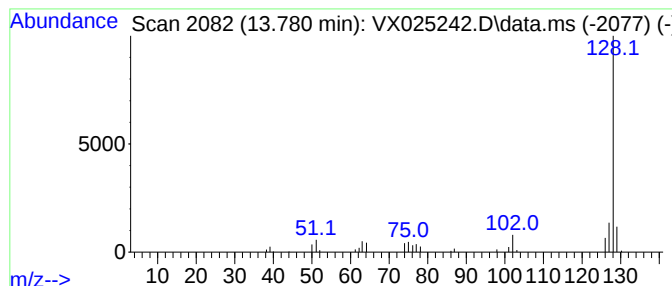
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Quant Title : VOC Analysis

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	3.08 ug/L	24220	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	91
3			Azulene	128	C10H8	000275-51-4	90
4			Naphthalene	128	C10H8	000091-20-3	90
5			Naphthalene	128	C10H8	000091-20-3	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	9.1	ug/L	63753	1	6.763	349754	50.0
Azulene	13.780	3.1	ug/L	24220	3	12.024	393023	50.0