

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
 Data File : VX042774.D
 Acq On : 31 Jul 2024 15:37
 Operator : JC/MD
 Sample : P3373-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VHBLK001

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: VX042774.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	15667	20390	4.78%	0.613%
2	1.368	43	46	60	rVB	37296	46371	10.86%	1.394%
3	1.648	89	92	101	rVB	28121	35009	8.20%	1.053%
4	2.294	192	198	211	rBV	84497	135143	31.65%	4.064%
5	2.495	229	231	234	rBV	257	329	0.08%	0.010%
6	2.788	274	279	286	rBV3	1591	3410	0.80%	0.103%
7	2.947	297	305	313	rBV2	4942	11881	2.78%	0.357%
8	3.142	334	337	341	rBB2	176	306	0.07%	0.009%
9	3.227	347	351	353	rBB	175	186	0.04%	0.006%
10	3.471	389	391	394	rBB	138	160	0.04%	0.005%
11	3.526	397	400	403	rBB	112	146	0.03%	0.004%
12	4.330	528	532	533	rBV2	167	191	0.04%	0.006%
13	4.391	539	542	544	rBB2	205	169	0.04%	0.005%
14	4.410	544	545	547	rBV2	297	194	0.05%	0.006%
15	4.471	547	555	569	rBV	28702	83092	19.46%	2.499%
16	4.708	592	594	597	rBV	249	199	0.05%	0.006%
17	4.782	602	606	609	rVV2	214	190	0.04%	0.006%
18	4.897	623	625	628	rBV	201	278	0.07%	0.008%
19	5.056	639	651	668	rBV	56591	177169	41.49%	5.328%
20	5.397	703	707	709	rBB3	405	522	0.12%	0.016%
21	5.483	717	721	722	rBB3	207	204	0.05%	0.006%
22	5.531	726	729	730	rBV	230	187	0.04%	0.006%
23	5.586	736	738	740	rVB	295	202	0.05%	0.006%
24	5.666	749	751	754	rBB	258	213	0.05%	0.006%
25	5.855	779	782	784	rBB	192	180	0.04%	0.005%
26	5.964	789	800	815	rBV3	148056	427011	100.00%	12.841%
27	6.196	835	838	841	rVB	226	269	0.06%	0.008%
28	6.385	867	869	872	rBB	215	198	0.05%	0.006%
29	6.556	894	897	900	rBB	141	198	0.05%	0.006%
30	6.610	904	906	912	rBB2	188	343	0.08%	0.010%
31	6.665	912	915	918	rBB	179	265	0.06%	0.008%
32	6.763	922	931	945	rBV	115750	272757	63.88%	8.202%
33	7.001	965	970	973	rBV	251	360	0.08%	0.011%
34	7.074	980	982	983	rBB	239	169	0.04%	0.005%
35	7.117	983	989	993	rBV3	969	2064	0.48%	0.062%
36	7.305	1012	1020	1039	rBV2	86618	196885	46.11%	5.921%

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 Title : VOC Analysis

37	7.470	1045	1047	1053	rVB2	268	431	0.10%	0.013%
38	7.702	1081	1085	1087	rBB2	203	252	0.06%	0.008%
39	7.805	1099	1102	1103	rBB2	172	158	0.04%	0.005%
40	7.836	1106	1107	1110	rBV2	184	161	0.04%	0.005%
41	7.940	1121	1124	1126	rBV	131	147	0.03%	0.004%
42	7.976	1128	1130	1133	rVB	190	181	0.04%	0.005%
43	8.098	1147	1150	1152	rBV	116	181	0.04%	0.005%
44	8.122	1152	1154	1158	rVB	282	251	0.06%	0.008%
45	8.232	1171	1172	1177	rBB	199	255	0.06%	0.008%
46	8.324	1182	1187	1200	rBV	52000	91578	21.45%	2.754%
47	8.452	1206	1208	1209	rBV	311	237	0.06%	0.007%
48	8.586	1228	1230	1233	rVB	287	214	0.05%	0.006%
49	8.647	1233	1240	1260	rBV	218390	358794	84.02%	10.789%
50	8.897	1280	1281	1285	rVB2	230	207	0.05%	0.006%
51	8.952	1285	1290	1306	rBV	38268	60075	14.07%	1.807%
52	9.141	1318	1321	1323	rBB	141	149	0.03%	0.004%
53	9.232	1335	1336	1338	rBV	257	234	0.05%	0.007%
54	9.384	1357	1361	1371	rBV	127884	194794	45.62%	5.858%
55	9.616	1397	1399	1403	rVB2	270	241	0.06%	0.007%
56	9.701	1410	1413	1419	rBB2	1061	1720	0.40%	0.052%
57	9.750	1419	1421	1425	rBV	147	188	0.04%	0.006%
58	9.799	1427	1429	1431	rVB	152	154	0.04%	0.005%
59	10.012	1461	1464	1465	rBV	177	161	0.04%	0.005%
60	10.055	1465	1471	1483	rBV	227777	319789	74.89%	9.616%
61	10.238	1499	1501	1503	rBB	167	147	0.03%	0.004%
62	10.299	1507	1511	1512	rBV	432	507	0.12%	0.015%
63	10.616	1560	1563	1566	rBV	184	256	0.06%	0.008%
64	10.646	1566	1568	1573	rVB	367	413	0.10%	0.012%
65	10.799	1591	1593	1595	rBV	274	226	0.05%	0.007%
66	10.872	1603	1605	1608	rBB	226	234	0.05%	0.007%
67	11.140	1647	1649	1652	rBV	175	190	0.04%	0.006%
68	11.195	1652	1658	1669	rVB	168361	228267	53.46%	6.864%
69	11.268	1669	1670	1672	rBV	372	216	0.05%	0.006%
70	11.506	1706	1709	1710	rBV	216	175	0.04%	0.005%
71	11.628	1727	1729	1732	rVB	294	289	0.07%	0.009%
72	11.707	1739	1742	1744	rBB	260	210	0.05%	0.006%
73	11.756	1747	1750	1751	rBB	271	204	0.05%	0.006%
74	11.774	1751	1753	1756	rBB	193	200	0.05%	0.006%
75	11.805	1756	1758	1760	rBV	171	190	0.04%	0.006%
76	11.969	1784	1785	1787	rBV	267	193	0.05%	0.006%

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77	12.024	1789	1794	1802	rBV	218636	286349	67.06%	8.611%
78	12.244	1827	1830	1834	rBV3	841	1195	0.28%	0.036%
79	12.317	1837	1842	1853	rBV	238609	318894	74.68%	9.589%
80	12.481	1867	1869	1870	rBV	248	189	0.04%	0.006%
81	12.573	1881	1884	1886	rVB2	276	313	0.07%	0.009%
82	12.603	1886	1889	1893	rBV	140	223	0.05%	0.007%
83	12.768	1911	1916	1918	rBV2	730	994	0.23%	0.030%
84	12.975	1948	1950	1951	rVV2	448	214	0.05%	0.006%
85	13.054	1961	1963	1965	rBV2	315	242	0.06%	0.007%
86	13.134	1974	1976	1978	rBV	236	199	0.05%	0.006%
87	13.195	1985	1986	1990	rBV	317	319	0.07%	0.010%
88	13.353	2010	2012	2013	rBV	195	162	0.04%	0.005%
89	13.506	2035	2037	2038	rBV	297	240	0.06%	0.007%
90	13.713	2070	2071	2073	rBV	219	208	0.05%	0.006%
91	13.780	2077	2082	2094	rVV	17990	26692	6.25%	0.803%
92	13.945	2106	2109	2113	rBV2	275	456	0.11%	0.014%
93	13.975	2113	2114	2117	rBV2	208	189	0.04%	0.006%
94	14.134	2135	2140	2148	rVB	3070	4921	1.15%	0.148%
95	14.195	2148	2150	2152	rBV	261	219	0.05%	0.007%
96	14.243	2155	2158	2159	rBV	234	257	0.06%	0.008%
97	14.390	2178	2182	2186	rBV3	297	412	0.10%	0.012%
98	14.566	2210	2211	2212	rBV	277	164	0.04%	0.005%
99	14.786	2242	2247	2253	rBV2	1644	2712	0.64%	0.082%
100	16.444	2518	2519	2522	rBV2	399	402	0.09%	0.012%

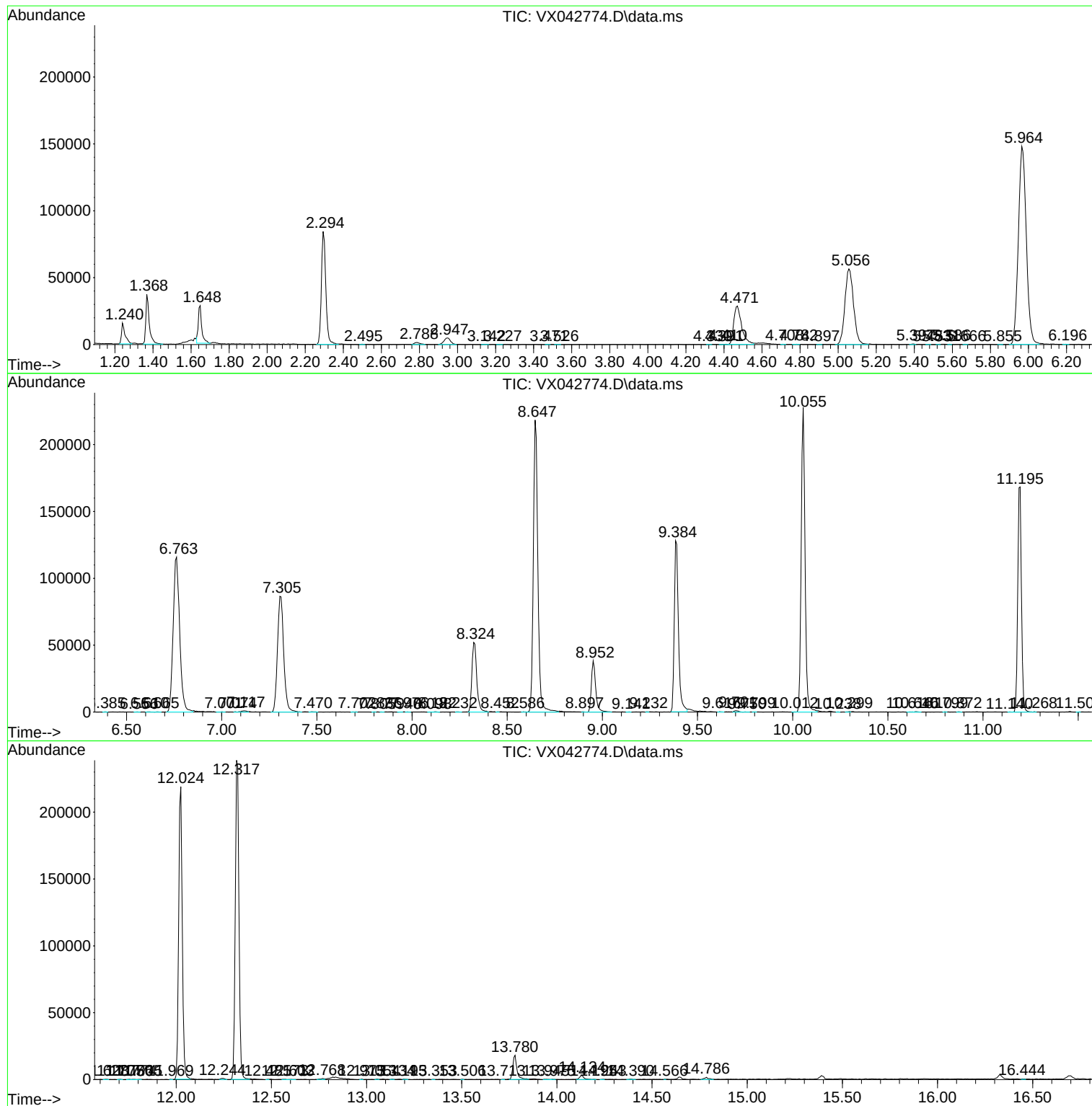
Sum of corrected areas: 3325474

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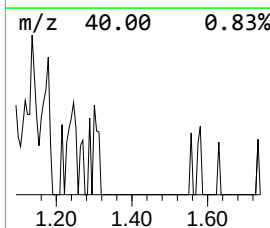
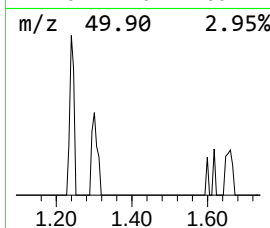
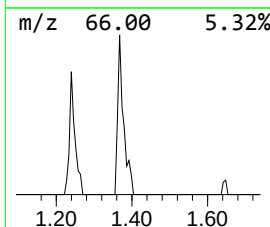
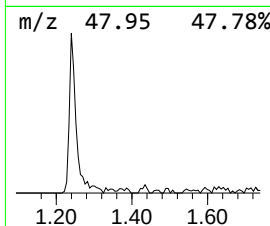
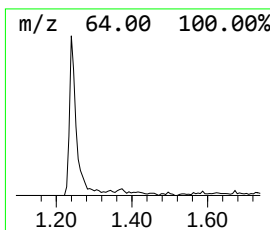
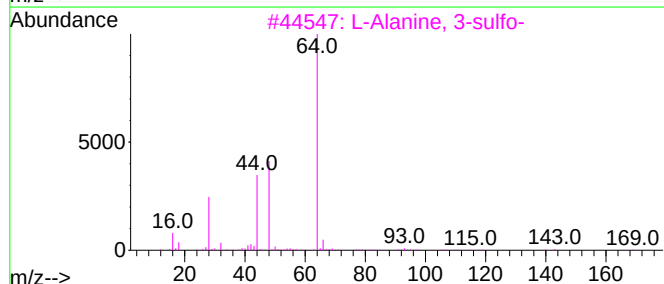
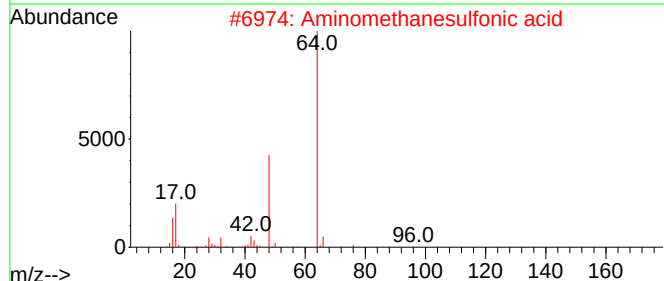
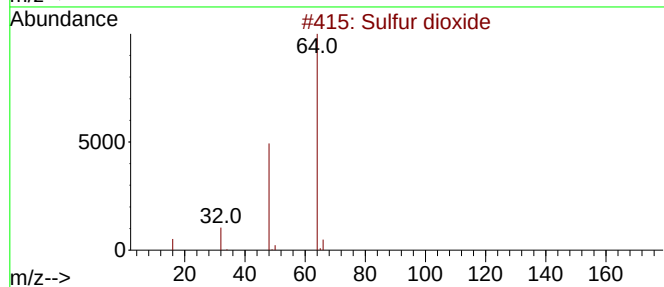
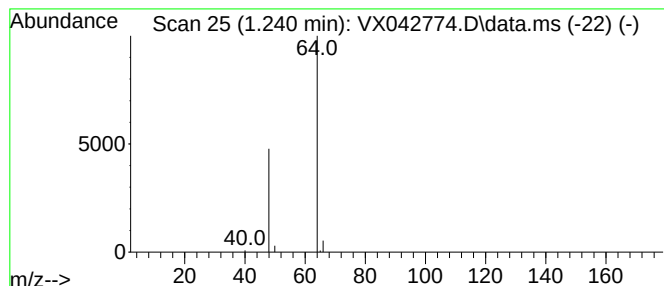
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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.
1.240	3.74 ug/L	20390	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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Sulfur dioxide	64	O2S	007446-09-5	4



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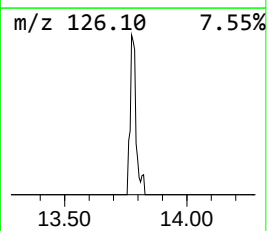
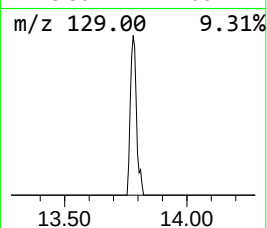
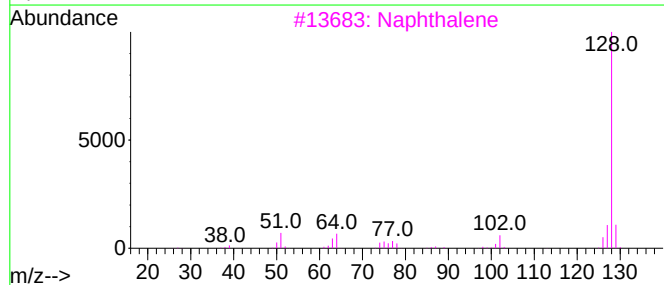
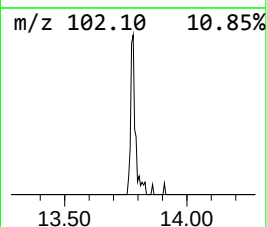
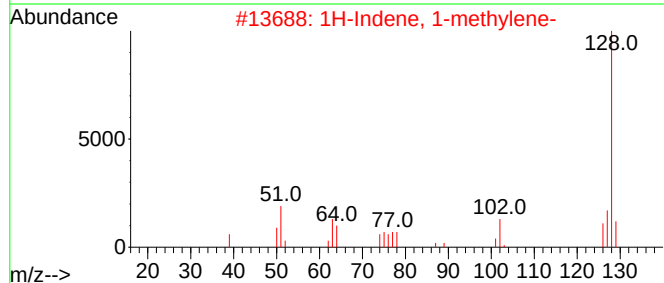
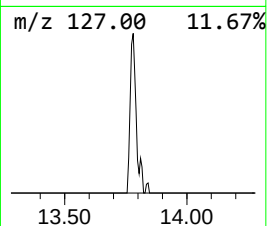
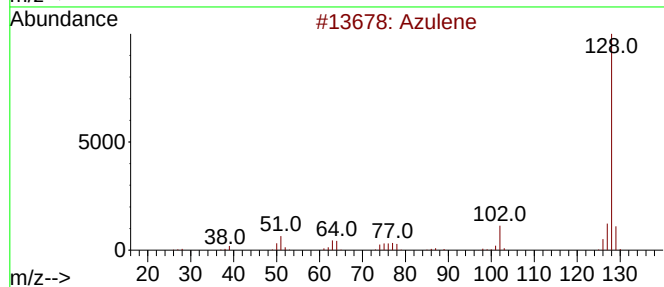
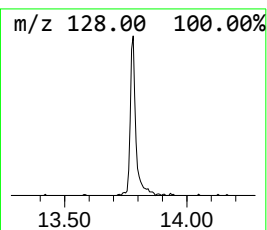
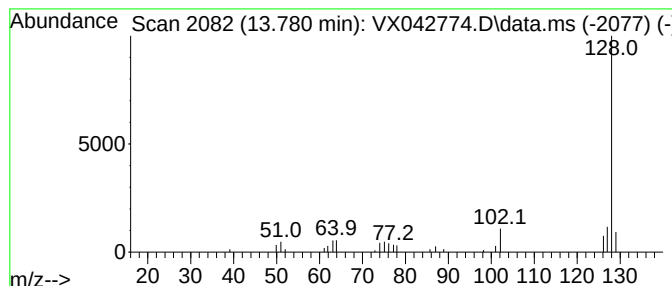
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	4.66 ug/L	26692	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azulene	128	C10H8	000275-51-4	91
2			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	91
3			Naphthalene	128	C10H8	000091-20-3	91
4			Naphthalene	128	C10H8	000091-20-3	91
5			Azulene	128	C10H8	000275-51-4	91



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	3.7	ug/L	20390	1	6.763	272757	50.0
Azulene	13.780	4.7	ug/L	26692	3	12.024	286349	50.0