

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
 Data File : VX042773.D
 Acq On : 31 Jul 2024 15:14
 Operator : JC/MD
 Sample : P3335-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 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: VX042773.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	rVV	15648	22220	5.47%	0.681%
2	1.368	43	46	58	rVB	31504	41492	10.21%	1.272%
3	1.648	89	92	100	rVB	27178	33456	8.23%	1.026%
4	2.294	192	198	211	rBV	81300	126828	31.21%	3.889%
5	2.526	235	236	240	rVB	172	201	0.05%	0.006%
6	2.788	274	279	287	rBB2	1433	2991	0.74%	0.092%
7	2.947	297	305	312	rBV2	5187	11377	2.80%	0.349%
8	3.099	327	330	332	rBB	183	216	0.05%	0.007%
9	3.349	368	371	373	rBB2	167	173	0.04%	0.005%
10	3.410	380	381	385	rBB	179	159	0.04%	0.005%
11	3.635	416	418	422	rBB	143	155	0.04%	0.005%
12	3.971	472	473	477	rBV	124	177	0.04%	0.005%
13	4.190	506	509	512	rBB	178	172	0.04%	0.005%
14	4.330	529	532	535	rBB	156	206	0.05%	0.006%
15	4.410	544	545	547	rBV	167	154	0.04%	0.005%
16	4.465	547	554	566	rBV2	25185	74801	18.41%	2.294%
17	4.715	593	595	598	rBV	267	238	0.06%	0.007%
18	4.775	602	605	607	rBB	208	196	0.05%	0.006%
19	4.855	615	618	621	rBB2	200	259	0.06%	0.008%
20	4.940	630	632	635	rBB2	136	145	0.04%	0.004%
21	5.056	639	651	664	rBV2	53360	167414	41.20%	5.133%
22	5.312	689	693	694	rBB	133	164	0.04%	0.005%
23	5.379	702	704	706	rBV	309	228	0.06%	0.007%
24	5.464	716	718	722	rBV2	150	205	0.05%	0.006%
25	5.538	728	730	732	rBV2	205	189	0.05%	0.006%
26	5.562	732	734	736	rVV	194	164	0.04%	0.005%
27	5.611	739	742	747	rBB2	157	217	0.05%	0.007%
28	5.690	753	755	757	rBB2	176	140	0.03%	0.004%
29	5.812	773	775	777	rBB	194	153	0.04%	0.005%
30	5.970	788	801	818	rBV3	137460	406313	100.00%	12.459%
31	6.635	905	910	912	rBB	160	187	0.05%	0.006%
32	6.763	922	931	943	rBV	116177	281290	69.23%	8.625%
33	7.092	983	985	986	rBV	271	219	0.05%	0.007%
34	7.306	1013	1020	1034	rBV	80051	179442	44.16%	5.502%
35	7.482	1047	1049	1050	rBV	293	195	0.05%	0.006%
36	7.531	1053	1057	1061	rBV	232	356	0.09%	0.011%

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37	7.604	1065	1069	1070	rBB	203	201	0.05%	0.006%
38	7.629	1071	1073	1074	rBV	141	142	0.03%	0.004%
39	7.793	1098	1100	1102	rBB	197	153	0.04%	0.005%
40	8.037	1138	1140	1144	rBV	118	168	0.04%	0.005%
41	8.324	1182	1187	1201	rVV2	50664	86268	21.23%	2.645%
42	8.458	1207	1209	1213	rVB2	456	443	0.11%	0.014%
43	8.494	1214	1215	1220	rBB	281	357	0.09%	0.011%
44	8.555	1223	1225	1227	rBV	163	223	0.05%	0.007%
45	8.647	1234	1240	1255	rBV	207000	336158	82.73%	10.308%
46	8.878	1275	1278	1281	rBB	240	331	0.08%	0.010%
47	8.909	1281	1283	1285	rBV	263	253	0.06%	0.008%
48	8.952	1285	1290	1303	rVV	37091	55461	13.65%	1.701%
49	9.244	1334	1338	1339	rBB	214	185	0.05%	0.006%
50	9.275	1340	1343	1345	rBV	250	227	0.06%	0.007%
51	9.384	1356	1361	1378	rBV	117421	182153	44.83%	5.585%
52	9.640	1401	1403	1408	rBV2	386	605	0.15%	0.019%
53	9.750	1418	1421	1423	rVB	174	172	0.04%	0.005%
54	9.842	1434	1436	1440	rBV	368	383	0.09%	0.012%
55	9.982	1456	1459	1460	rBB	185	161	0.04%	0.005%
56	10.055	1466	1471	1489	rVB	238691	333903	82.18%	10.238%
57	10.403	1526	1528	1530	rBV	168	155	0.04%	0.005%
58	10.543	1548	1551	1554	rBB	136	151	0.04%	0.005%
59	10.598	1558	1560	1563	rVB	163	163	0.04%	0.005%
60	10.652	1564	1569	1572	rBV2	408	537	0.13%	0.016%
61	11.000	1624	1626	1629	rBV	137	237	0.06%	0.007%
62	11.067	1636	1637	1639	rBV	157	143	0.04%	0.004%
63	11.189	1652	1657	1667	rBV	156797	212862	52.39%	6.527%
64	11.354	1682	1684	1686	rBB	179	173	0.04%	0.005%
65	11.408	1690	1693	1694	rBV2	236	265	0.07%	0.008%
66	11.457	1699	1701	1703	rVB2	210	210	0.05%	0.006%
67	11.689	1737	1739	1742	rBB2	125	153	0.04%	0.005%
68	11.732	1743	1746	1749	rBB	191	260	0.06%	0.008%
69	11.762	1749	1751	1753	rBV	164	188	0.05%	0.006%
70	11.890	1771	1772	1775	rBB	143	143	0.04%	0.004%
71	12.024	1788	1794	1807	rBV	228595	303376	74.67%	9.302%
72	12.244	1827	1830	1834	rVB2	1098	1391	0.34%	0.043%
73	12.317	1837	1842	1855	rVB	231950	299561	73.73%	9.185%
74	12.408	1855	1857	1862	rVB	359	335	0.08%	0.010%
75	12.451	1862	1864	1865	rBV	242	174	0.04%	0.005%
76	12.506	1870	1873	1875	rBV	211	268	0.07%	0.008%

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77	12.646	1894	1896	1899	rBB	145	176	0.04%	0.005%
78	12.677	1899	1901	1902	rBV	250	170	0.04%	0.005%
79	12.780	1908	1918	1919	rBV3	1589	3574	0.88%	0.110%
80	13.012	1953	1956	1958	rVB3	334	279	0.07%	0.009%
81	13.036	1958	1960	1961	rBV	281	269	0.07%	0.008%
82	13.396	2014	2019	2023	rVB2	176	362	0.09%	0.011%
83	13.530	2038	2041	2044	rBV	433	526	0.13%	0.016%
84	13.579	2047	2049	2051	rVB	250	185	0.05%	0.006%
85	13.676	2062	2065	2071	rBV	374	620	0.15%	0.019%
86	13.719	2071	2072	2074	rVB	213	150	0.04%	0.005%
87	13.780	2077	2082	2089	rVV	24402	37417	9.21%	1.147%
88	14.097	2132	2134	2136	rBV	327	372	0.09%	0.011%
89	14.127	2136	2139	2149	rVB	3927	5806	1.43%	0.178%
90	14.323	2169	2171	2174	rBV	246	309	0.08%	0.009%
91	14.396	2181	2183	2184	rBV	272	249	0.06%	0.008%
92	14.432	2187	2189	2190	rBV	197	176	0.04%	0.005%
93	14.603	2214	2217	2218	rVB2	288	251	0.06%	0.008%
94	14.640	2219	2223	2229	rBV2	3300	4143	1.02%	0.127%
95	14.786	2242	2247	2251	rBV	3433	4653	1.15%	0.143%
96	15.389	2340	2346	2353	rVB2	3190	5707	1.40%	0.175%
97	15.615	2379	2383	2384	rBV2	776	1165	0.29%	0.036%
98	15.950	2437	2438	2442	rBV2	438	439	0.11%	0.013%
99	16.328	2494	2500	2508	rBV3	7266	12557	3.09%	0.385%
100	16.688	2554	2559	2567	rBV	6532	10528	2.59%	0.323%

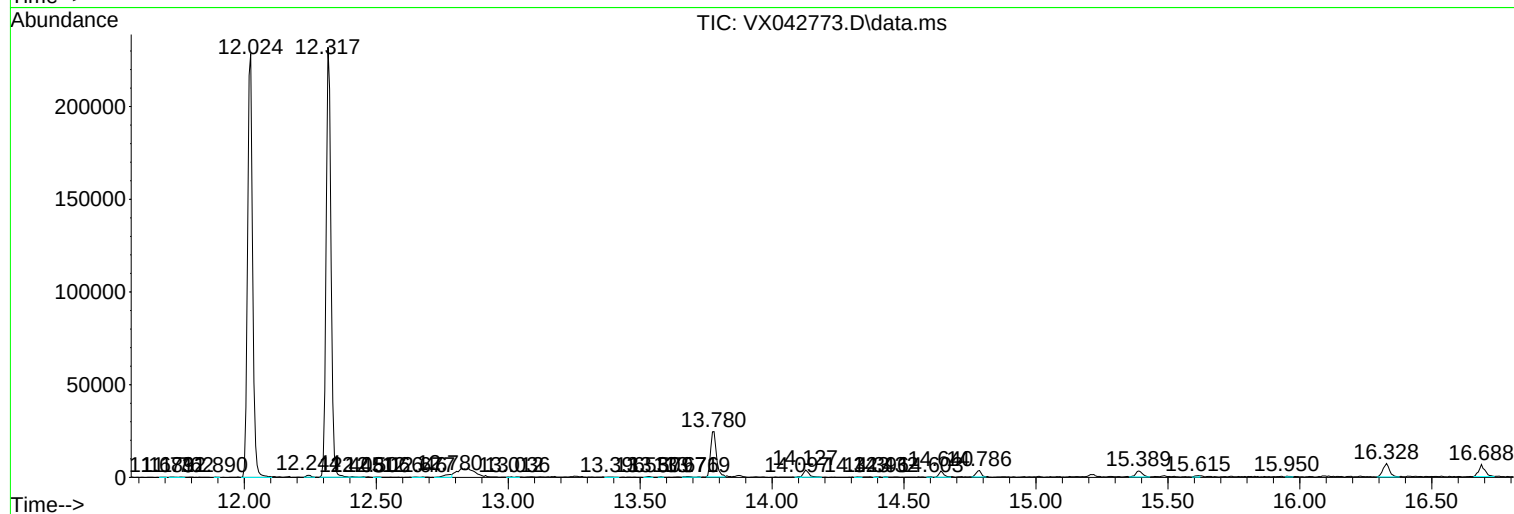
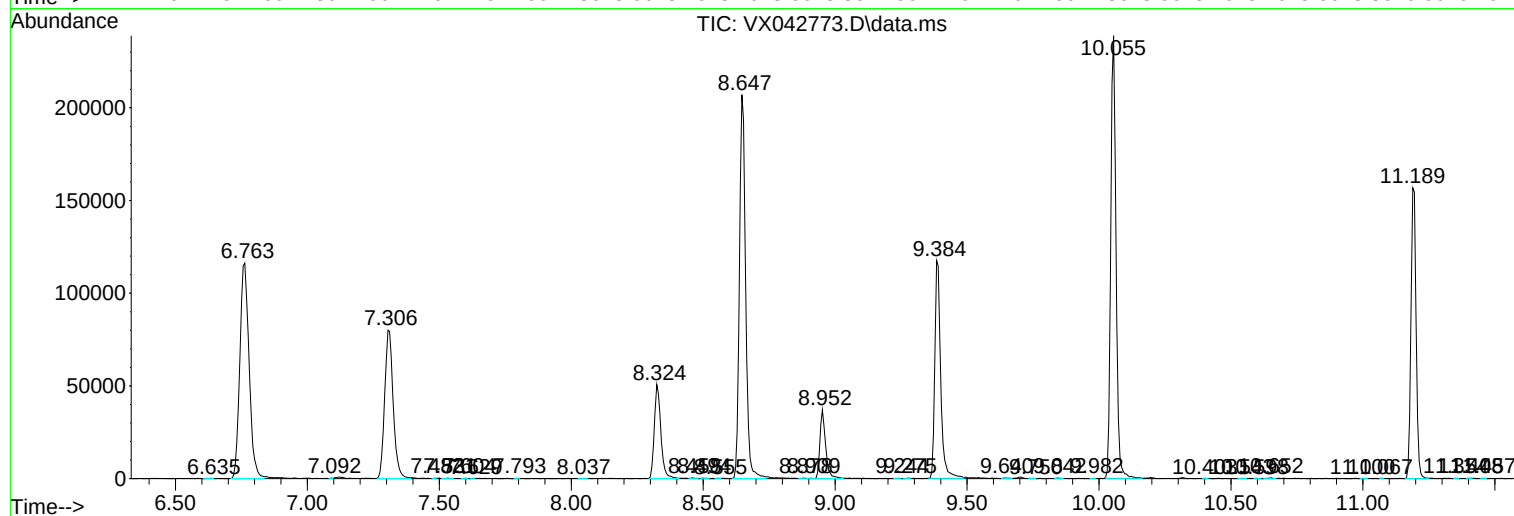
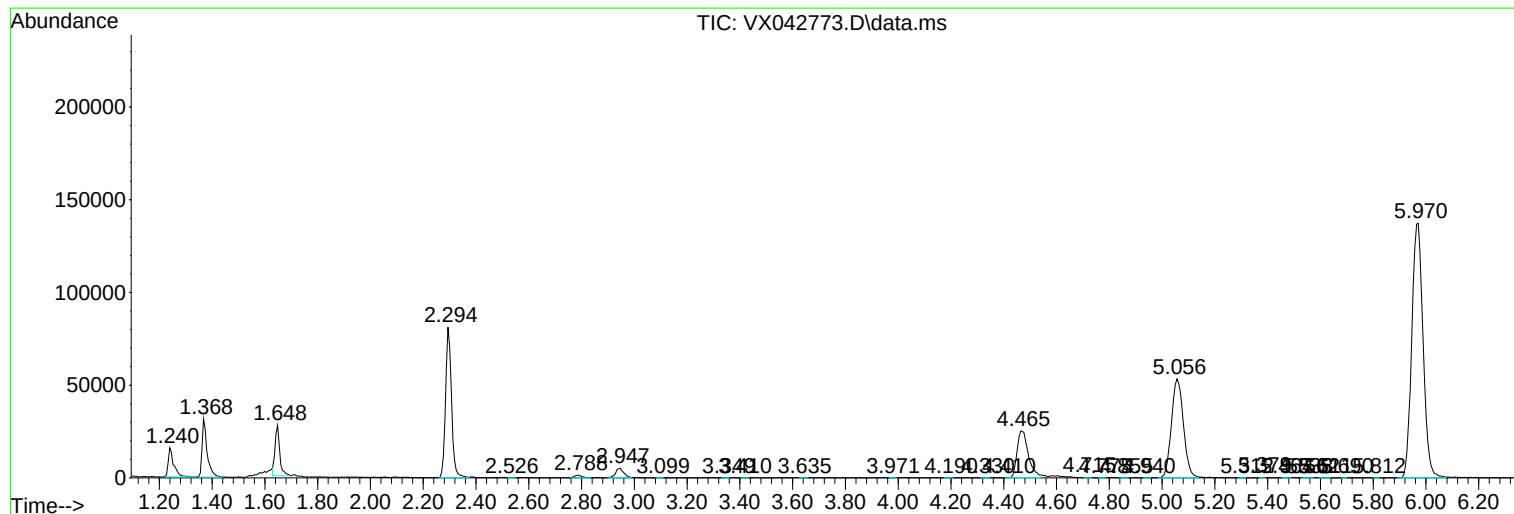
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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



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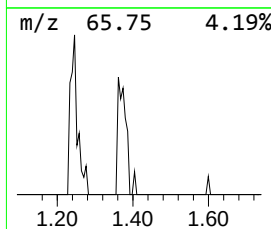
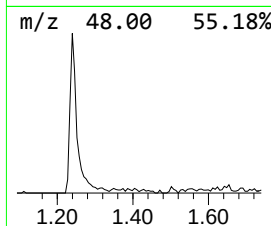
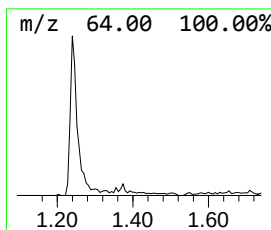
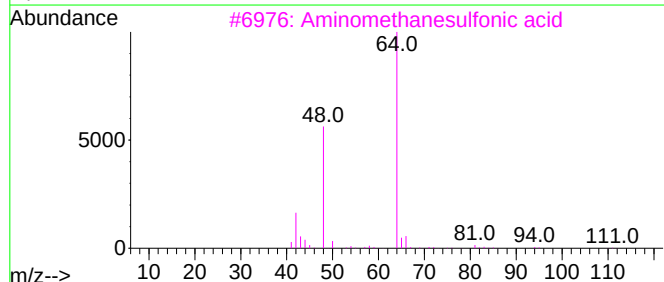
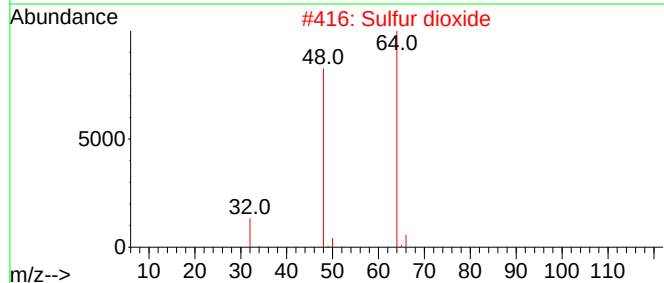
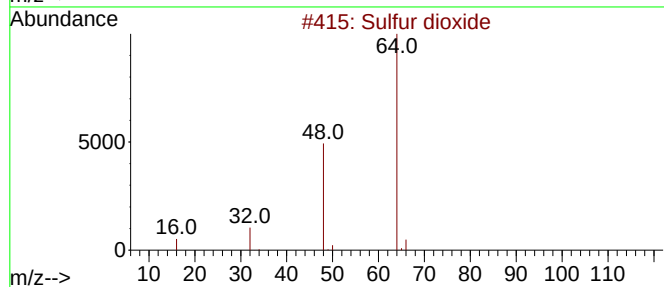
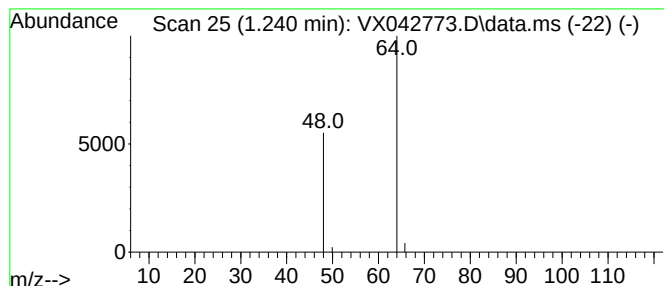
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	3.95 ug/L	22220	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			Sulfur dioxide	64	O2S	007446-09-5	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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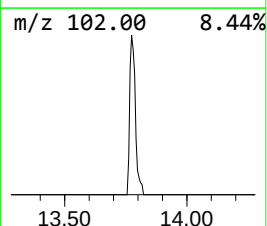
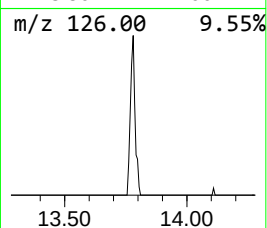
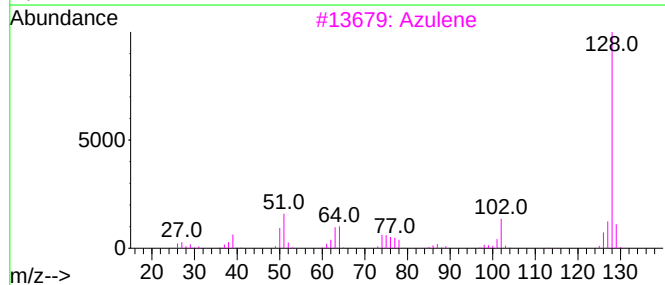
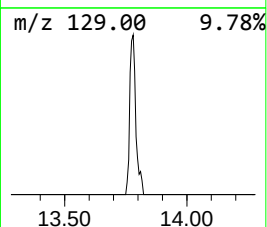
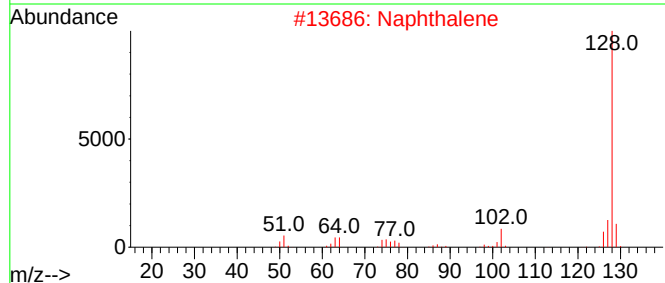
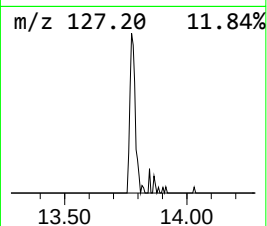
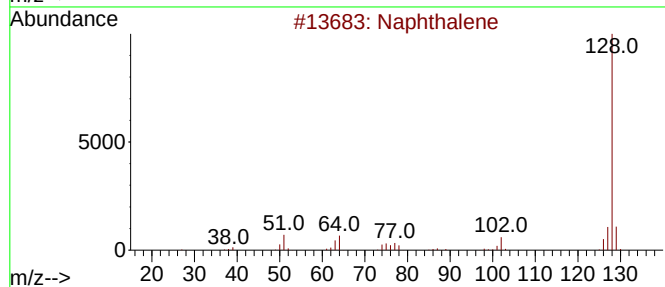
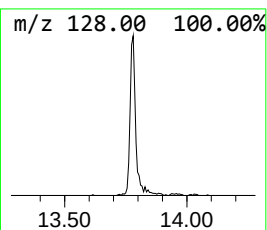
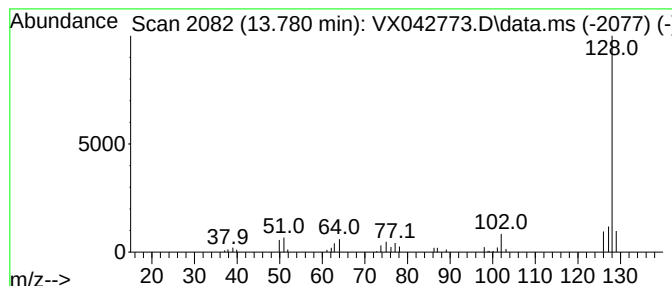
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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	6.17 ug/L	37417	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Naphthalene	128	C10H8	000091-20-3	95
3			Azulene	128	C10H8	000275-51-4	91
4			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	91
5			Azulene	128	C10H8	000275-51-4	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	1.240	4.0	ug/L	22220	1	6.763	281290	50.0
Azulene	13.780	6.2	ug/L	37417	3	12.024	303376	50.0