

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
 Data File : VX042775.D
 Acq On : 31 Jul 2024 16:00
 Operator : JC/MD
 Sample : P3398-09
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E08L4

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: VX042775.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	37	rBV	15871	22421	5.15%	0.675%
2	1.368	43	46	57	rVB	36996	46618	10.70%	1.403%
3	1.648	89	92	100	rVB	27766	34251	7.86%	1.031%
4	2.294	192	198	207	rBV	84405	133803	30.71%	4.027%
5	2.502	228	232	233	rBV2	293	283	0.06%	0.009%
6	2.642	253	255	257	rBV	204	187	0.04%	0.006%
7	2.782	276	278	284	rVB2	907	1238	0.28%	0.037%
8	2.935	297	303	306	rBV2	2268	4048	0.93%	0.122%
9	3.337	367	369	372	rBB	212	191	0.04%	0.006%
10	3.514	397	398	401	rBB	166	144	0.03%	0.004%
11	3.611	410	414	415	rBB	155	161	0.04%	0.005%
12	3.965	469	472	474	rBB	167	153	0.04%	0.005%
13	4.075	486	490	493	rBB	315	294	0.07%	0.009%
14	4.117	494	497	498	rBV	142	176	0.04%	0.005%
15	4.264	518	521	523	rVB	166	162	0.04%	0.005%
16	4.386	539	541	546	rBB	120	185	0.04%	0.006%
17	4.465	546	554	568	rBV	29836	85563	19.64%	2.575%
18	4.751	599	601	605	rVB2	193	198	0.05%	0.006%
19	4.818	610	612	614	rVB	252	178	0.04%	0.005%
20	4.898	623	625	628	rBB	190	191	0.04%	0.006%
21	5.062	639	652	669	rBV2	57700	180712	41.47%	5.439%
22	5.391	703	706	708	rBV	328	395	0.09%	0.012%
23	5.684	752	754	757	rBB	180	187	0.04%	0.006%
24	5.971	789	801	817	rBV2	148135	435721	100.00%	13.115%
25	6.172	833	834	836	rVB	348	193	0.04%	0.006%
26	6.251	845	847	848	rBV	166	151	0.03%	0.005%
27	6.324	858	859	861	rBV	203	155	0.04%	0.005%
28	6.385	868	869	872	rBV	201	184	0.04%	0.006%
29	6.477	882	884	887	rBB	194	152	0.03%	0.005%
30	6.574	899	900	903	rVB	351	273	0.06%	0.008%
31	6.763	922	931	946	rBV	111854	275088	63.13%	8.280%
32	7.001	967	970	971	rBV	215	221	0.05%	0.007%
33	7.050	976	978	982	rBV	225	281	0.06%	0.008%
34	7.117	986	989	990	rBV2	741	688	0.16%	0.021%
35	7.306	1012	1020	1032	rBV2	87004	193756	44.47%	5.832%
36	7.489	1048	1050	1052	rBV	276	234	0.05%	0.007%

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37	7.641	1074	1075	1078	rBB	240	219	0.05%	0.007%
38	7.690	1079	1083	1085	rBV	182	204	0.05%	0.006%
39	7.824	1103	1105	1108	rBV2	265	338	0.08%	0.010%
40	7.903	1116	1118	1121	rVB2	203	161	0.04%	0.005%
41	7.958	1125	1127	1128	rBV	207	174	0.04%	0.005%
42	8.019	1133	1137	1140	rBV2	192	339	0.08%	0.010%
43	8.110	1149	1152	1154	rBV	196	274	0.06%	0.008%
44	8.165	1160	1161	1167	rBV2	225	405	0.09%	0.012%
45	8.214	1167	1169	1172	rVV2	225	220	0.05%	0.007%
46	8.324	1180	1187	1198	rBV2	52880	91548	21.01%	2.755%
47	8.647	1234	1240	1251	rBV	221144	352807	80.97%	10.619%
48	8.952	1285	1290	1299	rBV	39160	58745	13.48%	1.768%
49	9.080	1310	1311	1314	rBV	254	242	0.06%	0.007%
50	9.141	1319	1321	1322	rBV	241	173	0.04%	0.005%
51	9.159	1322	1324	1325	rVB	240	142	0.03%	0.004%
52	9.275	1339	1343	1350	rVB2	2274	3549	0.81%	0.107%
53	9.385	1356	1361	1381	rBV	134692	202312	46.43%	6.089%
54	9.665	1404	1407	1409	rVB2	369	423	0.10%	0.013%
55	9.793	1425	1428	1429	rBB	242	172	0.04%	0.005%
56	9.836	1433	1435	1437	rBV	164	164	0.04%	0.005%
57	9.854	1437	1438	1441	rVV	247	218	0.05%	0.007%
58	10.055	1466	1471	1488	rVB	234531	319695	73.37%	9.622%
59	10.269	1502	1506	1508	rBV	105	158	0.04%	0.005%
60	10.317	1508	1514	1517	rVB2	779	1429	0.33%	0.043%
61	10.348	1517	1519	1522	rBB2	199	228	0.05%	0.007%
62	10.500	1543	1544	1548	rBV	204	266	0.06%	0.008%
63	10.647	1565	1568	1572	rBV2	747	1001	0.23%	0.030%
64	10.714	1578	1579	1583	rBB2	187	194	0.04%	0.006%
65	10.775	1587	1589	1592	rBB2	181	159	0.04%	0.005%
66	10.811	1593	1595	1597	rBV	260	252	0.06%	0.008%
67	10.878	1604	1606	1607	rBV	212	169	0.04%	0.005%
68	10.970	1618	1621	1623	rVB3	216	287	0.07%	0.009%
69	11.043	1628	1633	1635	rVV2	451	470	0.11%	0.014%
70	11.189	1652	1657	1669	rBV	171606	230185	52.83%	6.928%
71	11.317	1672	1678	1682	rVV2	1802	2660	0.61%	0.080%
72	11.384	1685	1689	1693	rBB	278	387	0.09%	0.012%
73	11.457	1697	1701	1704	rBV	288	546	0.13%	0.016%
74	11.707	1739	1742	1746	rBB	259	307	0.07%	0.009%
75	11.750	1747	1749	1754	rBB	641	916	0.21%	0.028%
76	11.866	1766	1768	1770	rBV	128	146	0.03%	0.004%

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77	11.951	1779	1782	1783	rBV	187	157	0.04%	0.005%
78	12.024	1788	1794	1803	rBV	215355	285671	65.56%	8.598%
79	12.244	1824	1830	1834	rBV3	942	1964	0.45%	0.059%
80	12.317	1837	1842	1850	rBV	234717	310848	71.34%	9.356%
81	12.543	1876	1879	1881	rBV	214	208	0.05%	0.006%
82	12.610	1887	1890	1891	rBV2	139	144	0.03%	0.004%
83	12.677	1900	1901	1903	rBV2	204	149	0.03%	0.004%
84	12.768	1911	1916	1917	rBV2	899	1198	0.27%	0.036%
85	12.957	1944	1947	1951	rBV2	237	428	0.10%	0.013%
86	13.012	1954	1956	1958	rVB	244	164	0.04%	0.005%
87	13.128	1974	1975	1977	rBV	175	152	0.03%	0.005%
88	13.195	1983	1986	1987	rBV	249	199	0.05%	0.006%
89	13.372	2014	2015	2017	rBV	280	174	0.04%	0.005%
90	13.512	2036	2038	2039	rBV	218	203	0.05%	0.006%
91	13.670	2062	2064	2066	rVB	315	260	0.06%	0.008%
92	13.774	2076	2081	2090	rBV	14431	22253	5.11%	0.670%
93	14.073	2127	2130	2131	rVB	288	221	0.05%	0.007%
94	14.134	2136	2140	2147	rVV	1723	2546	0.58%	0.077%
95	14.225	2152	2155	2157	rBV	250	356	0.08%	0.011%
96	14.274	2162	2163	2167	rVB	323	274	0.06%	0.008%
97	14.372	2175	2179	2182	rBV	177	205	0.05%	0.006%
98	14.493	2197	2199	2202	rBV	154	144	0.03%	0.004%
99	14.640	2220	2223	2228	rBV3	867	1392	0.32%	0.042%
100	14.786	2242	2247	2251	rBV3	1078	1983	0.46%	0.060%

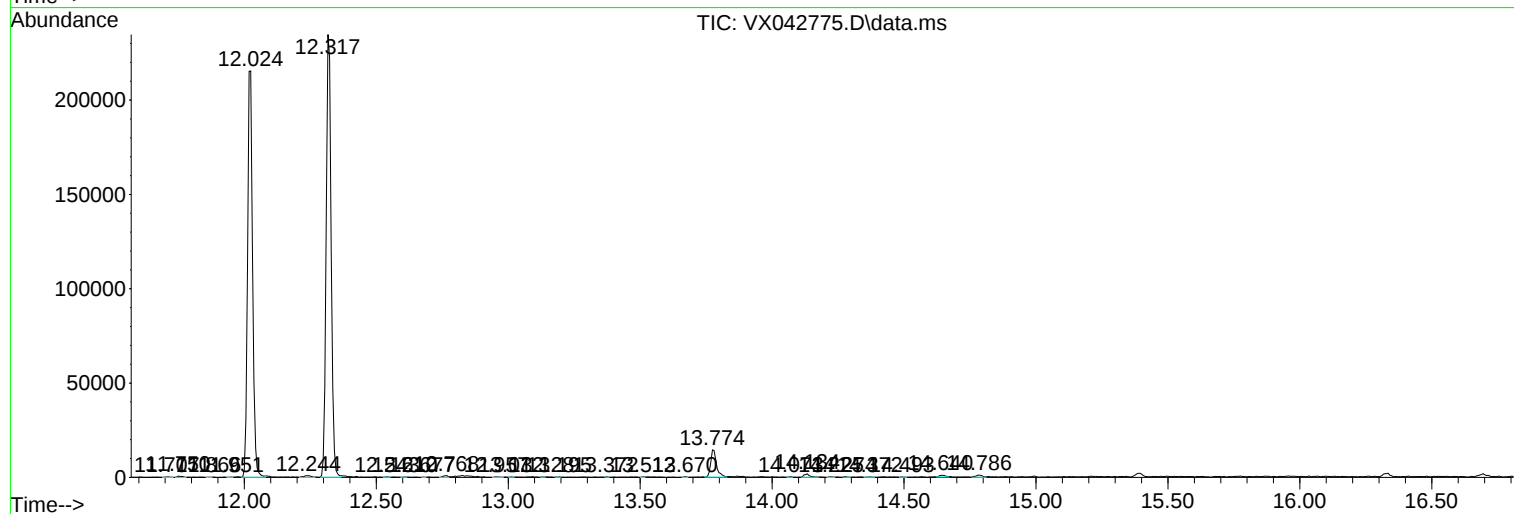
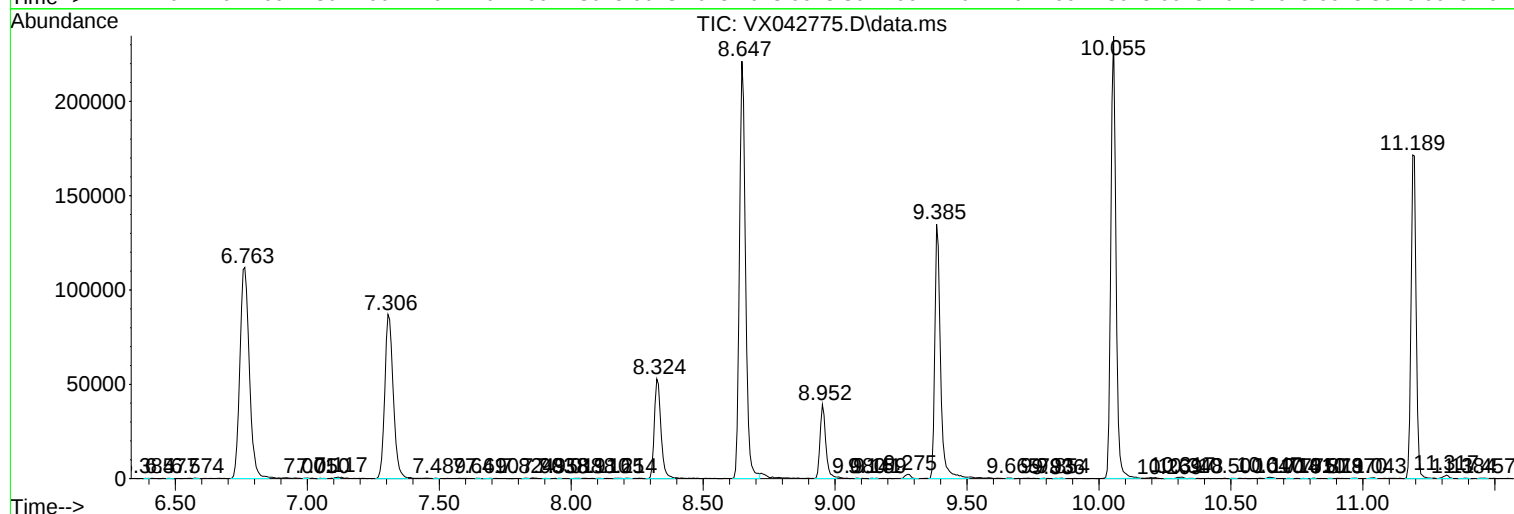
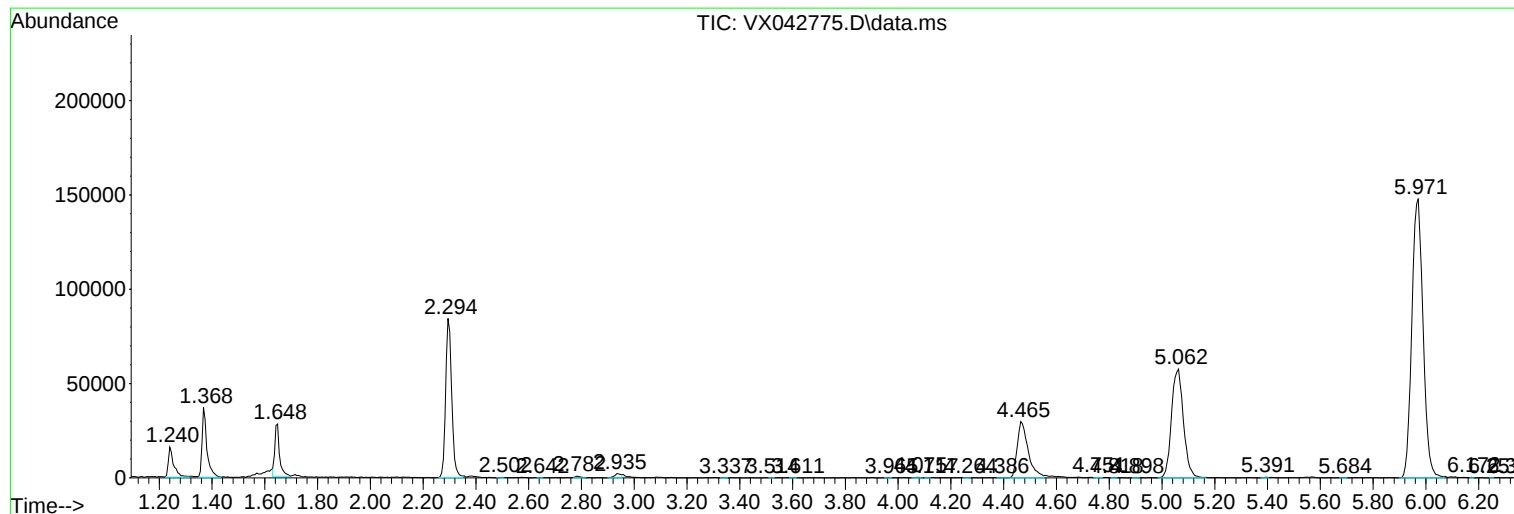
Sum of corrected areas: 3322413

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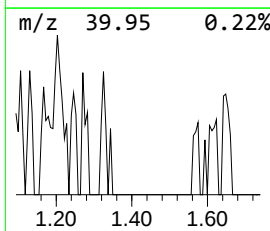
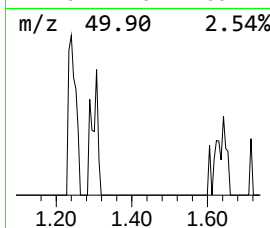
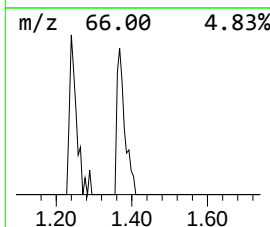
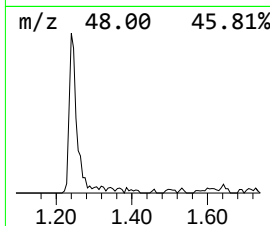
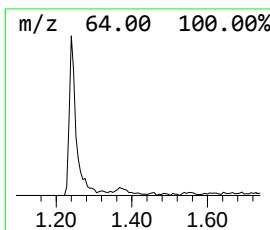
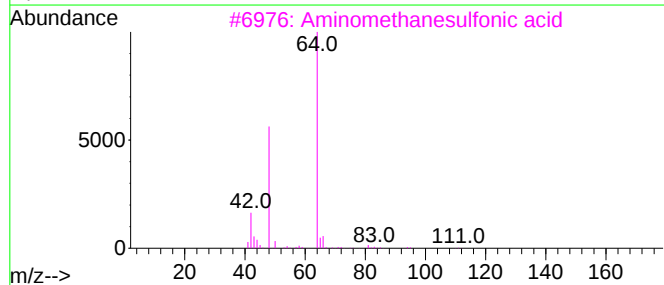
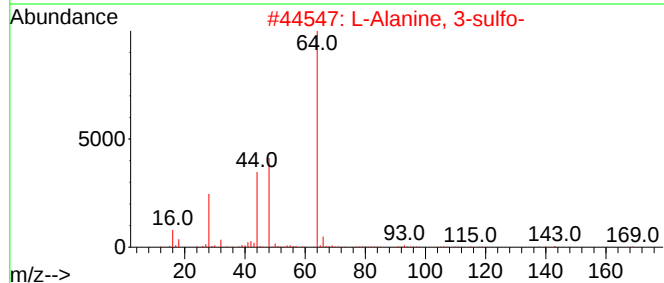
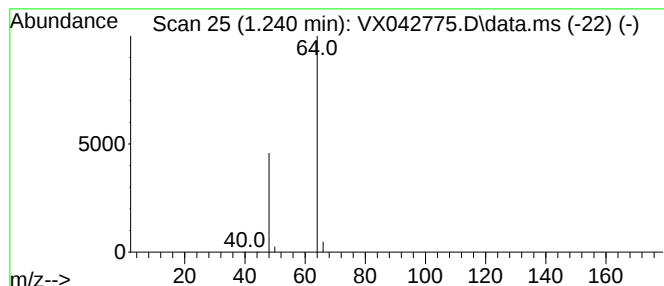
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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.
1.240	4.08 ug/L	22421	1,4-Difluorobenzene	6.757

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



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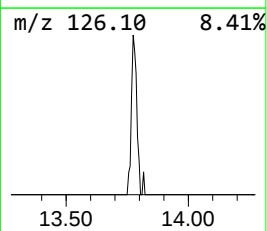
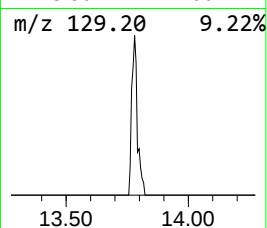
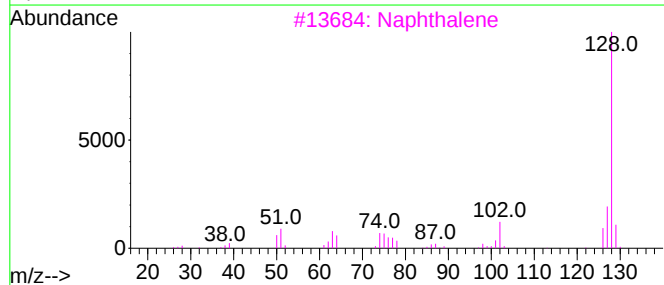
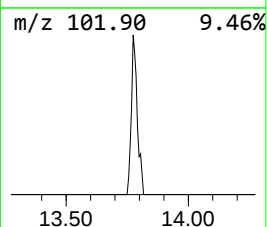
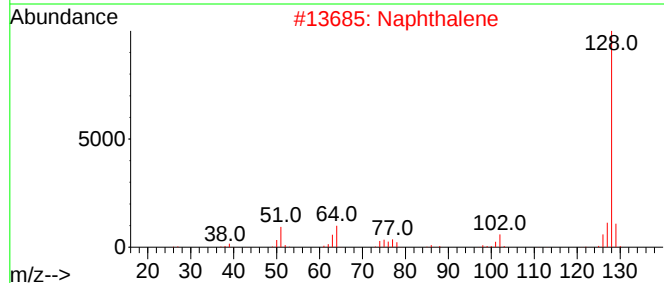
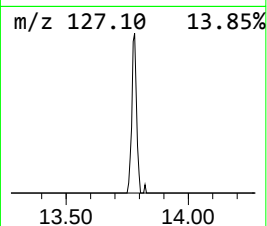
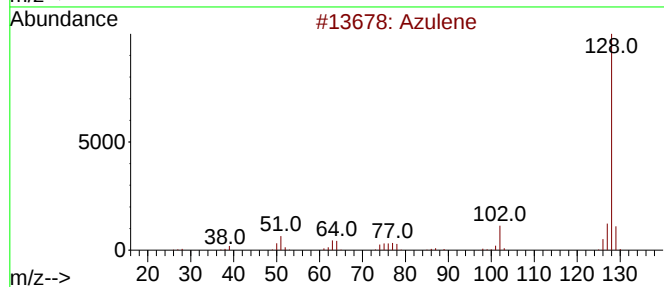
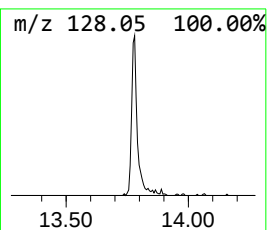
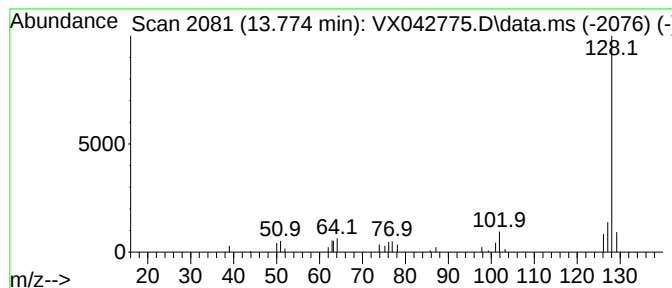
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

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.
13.774	3.89 ug/L	22253	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azulene	128	C10H8	000275-51-4	90
2			Naphthalene	128	C10H8	000091-20-3	90
3			Naphthalene	128	C10H8	000091-20-3	90
4			Naphthalene	128	C10H8	000091-20-3	87
5			Naphthalene	128	C10H8	000091-20-3	83



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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	4.1	ug/L	22421	1	6.757	275088	50.0
Azulene	13.774	3.9	ug/L	22253	3	12.024	285671	50.0