

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045234.D
 Acq On : 08 Oct 2021 01:51
 Operator : SY/MD
 Sample : M4138-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW7F2

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_U\Method\SFAMULM092321WMA.M
 Title : VOC Analysis

Signal : TIC: VU045234.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.465	31	39	54	rBV	160623	265294	20.67%	2.622%
2	1.597	75	80	103	rVB	176425	213990	16.67%	2.115%
3	1.896	166	173	192	rVB	131562	181022	14.11%	1.789%
4	2.562	368	380	396	rBV	244331	411870	32.09%	4.071%
5	2.697	416	422	430	rVB3	639	721	0.06%	0.007%
6	2.777	434	447	464	rBV2	11274	25907	2.02%	0.256%
7	2.870	472	476	478	rBV	331	210	0.02%	0.002%
8	2.903	482	486	490	rBV2	382	381	0.03%	0.004%
9	2.957	496	503	504	rBV2	563	619	0.05%	0.006%
10	3.047	527	531	539	rVB5	800	1065	0.08%	0.011%
11	3.192	563	576	588	rBV2	5101	10814	0.84%	0.107%
12	3.353	616	626	634	rBV3	1545	2523	0.20%	0.025%
13	3.440	648	653	656	rBV2	200	217	0.02%	0.002%
14	3.510	670	675	678	rBV	204	229	0.02%	0.002%
15	3.536	678	683	687	rVB	294	341	0.03%	0.003%
16	3.581	692	697	701	rBV3	628	649	0.05%	0.006%
17	3.816	765	770	773	rBV	193	203	0.02%	0.002%
18	3.835	773	776	780	rVV	210	190	0.01%	0.002%
19	3.893	791	794	803	rVB	258	280	0.02%	0.003%
20	4.079	847	852	861	rBV2	235	488	0.04%	0.005%
21	4.153	869	875	878	rBV2	194	240	0.02%	0.002%
22	4.304	919	922	926	rVB2	218	195	0.02%	0.002%
23	4.629	1008	1023	1045	rBV	148966	349773	27.26%	3.457%
24	5.067	1140	1159	1185	rVV	226282	492297	38.36%	4.866%
25	5.208	1197	1203	1205	rBV4	407	285	0.02%	0.003%
26	5.224	1205	1208	1213	rVB2	411	351	0.03%	0.003%
27	5.279	1222	1225	1226	rBV	354	191	0.01%	0.002%
28	5.385	1253	1258	1264	rVV5	703	801	0.06%	0.008%
29	5.729	1343	1365	1385	rBV2	472945	1283301	100.00%	12.685%
30	5.899	1414	1418	1424	rBV2	266	307	0.02%	0.003%
31	6.115	1482	1485	1489	rBV2	368	317	0.02%	0.003%
32	6.163	1494	1500	1505	rVV4	549	796	0.06%	0.008%
33	6.253	1513	1528	1550	rBV	367191	683924	53.29%	6.760%
34	6.330	1550	1552	1558	rBV3	249	220	0.02%	0.002%
35	6.539	1607	1617	1630	rVB8	2971	5621	0.44%	0.056%
36	6.693	1651	1665	1683	rBV	305835	593845	46.27%	5.870%

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 Title : VOC Analysis

37	6.803	1696	1699	1708	rVB7	948	1474	0.11%	0.015%
38	6.886	1720	1725	1730	rBV	170	260	0.02%	0.003%
39	7.050	1773	1776	1779	rVB	327	273	0.02%	0.003%
40	7.111	1791	1795	1800	rVB2	260	192	0.01%	0.002%
41	7.185	1805	1818	1827	rBV5	1820	3275	0.26%	0.032%
42	7.362	1868	1873	1877	rBV2	195	198	0.02%	0.002%
43	7.410	1881	1888	1890	rBV	196	216	0.02%	0.002%
44	7.568	1924	1937	1961	rBV	160622	283098	22.06%	2.798%
45	7.690	1969	1975	1976	rBV2	888	818	0.06%	0.008%
46	7.719	1977	1984	1995	rVB3	4190	7304	0.57%	0.072%
47	7.800	2000	2009	2023	rVB3	3679	6491	0.51%	0.064%
48	7.902	2027	2041	2055	rBV	571086	982268	76.54%	9.709%
49	7.973	2056	2063	2079	rVB	12910	21909	1.71%	0.217%
50	8.102	2099	2103	2110	rVB3	304	351	0.03%	0.003%
51	8.140	2110	2115	2116	rBV2	201	206	0.02%	0.002%
52	8.182	2116	2128	2149	rVV	114983	191411	14.92%	1.892%
53	8.336	2171	2176	2180	rBV2	202	197	0.02%	0.002%
54	8.369	2183	2186	2190	rVB	228	190	0.01%	0.002%
55	8.407	2195	2198	2201	rVB	440	278	0.02%	0.003%
56	8.475	2212	2219	2229	rVB2	696	1201	0.09%	0.012%
57	8.558	2238	2245	2249	rVV3	937	1117	0.09%	0.011%
58	8.636	2256	2269	2306	rBV	439710	780885	60.85%	7.719%
59	8.783	2313	2315	2317	rBV2	352	190	0.01%	0.002%
60	8.928	2356	2360	2365	rVV2	606	721	0.06%	0.007%
61	9.098	2410	2413	2419	rBV2	180	205	0.02%	0.002%
62	9.211	2445	2448	2455	rBV2	181	248	0.02%	0.002%
63	9.259	2457	2463	2466	rVB2	278	299	0.02%	0.003%
64	9.279	2466	2469	2478	rBV2	222	352	0.03%	0.003%
65	9.420	2499	2513	2535	rBV	506144	832860	64.90%	8.233%
66	9.574	2551	2561	2572	rBV	14617	21824	1.70%	0.216%
67	9.697	2586	2599	2614	rBV	39731	66978	5.22%	0.662%
68	10.105	2717	2726	2740	rVB3	12008	21017	1.64%	0.208%
69	10.298	2779	2786	2790	rBV3	319	350	0.03%	0.003%
70	10.320	2790	2793	2797	rVB2	221	188	0.01%	0.002%
71	10.491	2834	2846	2856	rBV3	2991	4514	0.35%	0.045%
72	10.674	2896	2903	2910	rBV3	1760	2205	0.17%	0.022%
73	10.761	2916	2930	2945	rBV	432477	698150	54.40%	6.901%
74	10.825	2945	2950	2960	rVB3	2522	3652	0.28%	0.036%
75	10.896	2966	2972	2977	rBV4	330	481	0.04%	0.005%
76	11.002	2995	3005	3009	rBV3	610	1071	0.08%	0.011%

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77	11.053	3018	3021	3024	rBV	248	199	0.02%	0.002%
78	11.092	3025	3033	3041	rVV2	2711	3669	0.29%	0.036%
79	11.288	3088	3094	3096	rBV	280	255	0.02%	0.003%
80	11.320	3101	3104	3113	rBV2	172	325	0.03%	0.003%
81	11.407	3125	3131	3136	rVB2	195	300	0.02%	0.003%
82	11.471	3141	3151	3164	rVB3	5382	9036	0.70%	0.089%
83	11.578	3179	3184	3187	rBV2	384	430	0.03%	0.004%
84	11.700	3219	3222	3227	rVB3	561	511	0.04%	0.005%
85	11.751	3229	3238	3245	rBV2	4087	5632	0.44%	0.056%
86	11.815	3245	3258	3275	rVV	449937	707853	55.16%	6.997%
87	11.899	3280	3284	3289	rVB4	489	582	0.05%	0.006%
88	11.934	3289	3295	3296	rBV2	485	505	0.04%	0.005%
89	11.976	3305	3308	3316	rVB3	1134	1143	0.09%	0.011%
90	12.069	3328	3337	3346	rBV3	3794	6340	0.49%	0.063%
91	12.195	3363	3376	3397	rVB	498857	813675	63.40%	8.043%
92	12.487	3462	3467	3470	rBV2	209	200	0.02%	0.002%
93	12.635	3507	3513	3515	rBV3	271	294	0.02%	0.003%
94	12.729	3539	3542	3545	rBV	214	194	0.02%	0.002%
95	12.777	3554	3557	3562	rVB2	417	356	0.03%	0.004%
96	13.002	3620	3627	3636	rVB6	1994	2629	0.20%	0.026%
97	13.224	3687	3696	3704	rBV3	5786	7849	0.61%	0.078%
98	13.844	3880	3889	3899	rVB3	10065	15029	1.17%	0.149%
99	14.092	3953	3966	3980	rBV	31746	51881	4.04%	0.513%
100	14.336	4031	4042	4052	rVB3	12528	19352	1.51%	0.191%

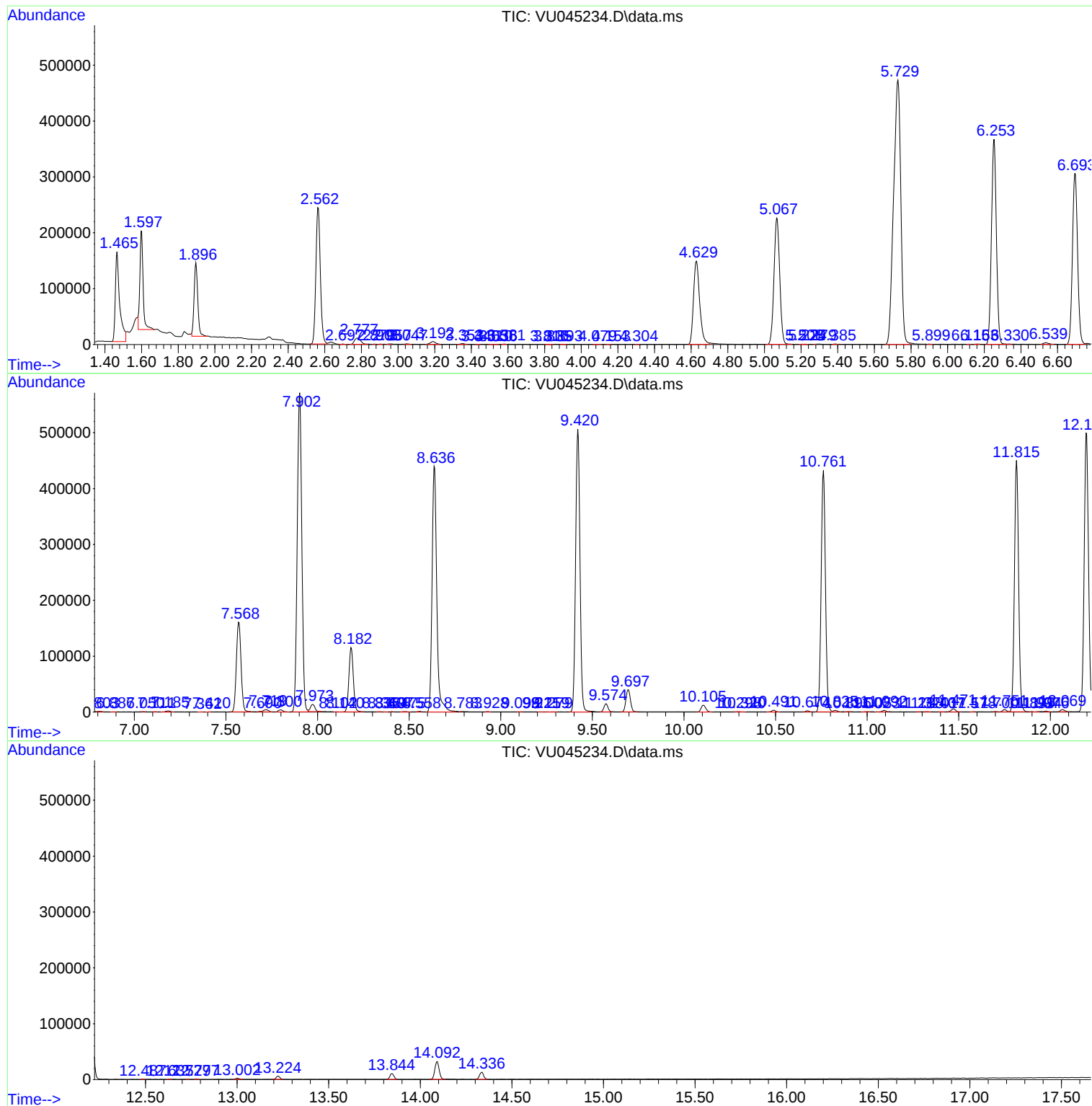
Sum of corrected areas: 10116633

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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



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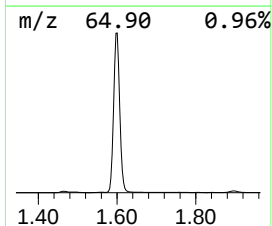
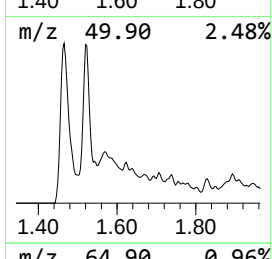
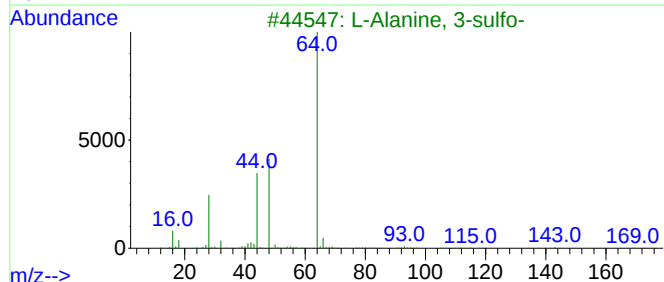
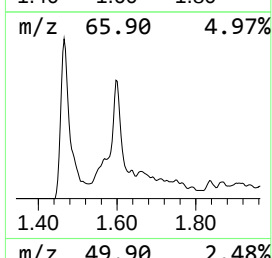
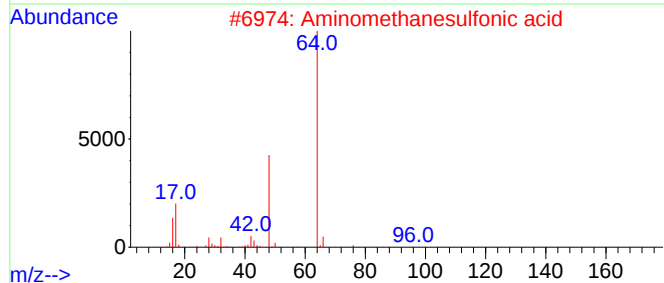
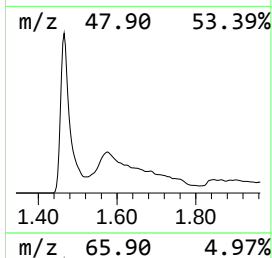
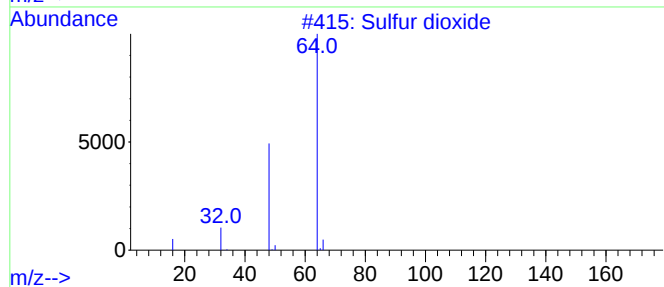
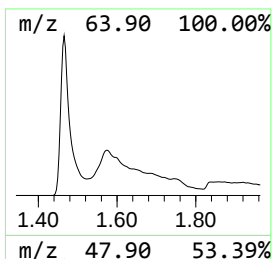
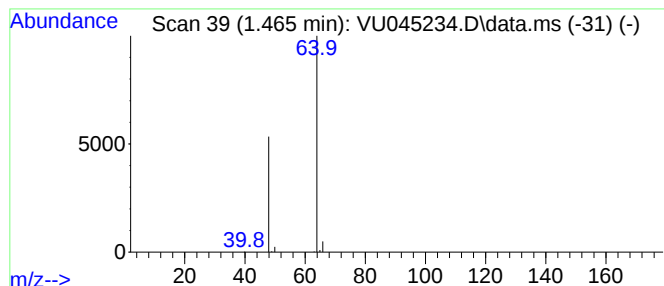
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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.
1.465	19.40 ug/L	265294	1,4-Difluorobenzene	6.253

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



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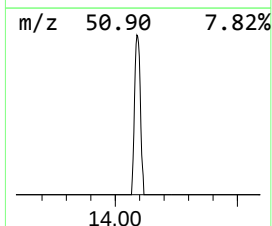
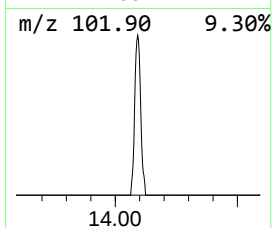
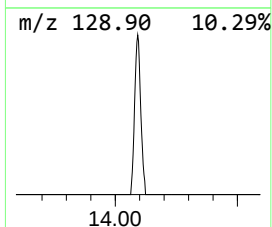
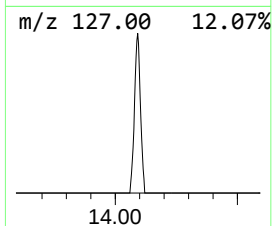
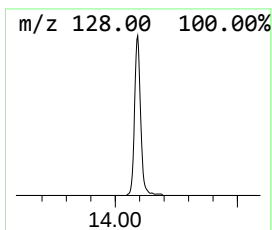
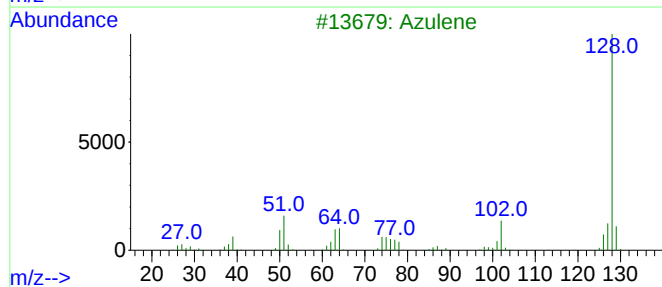
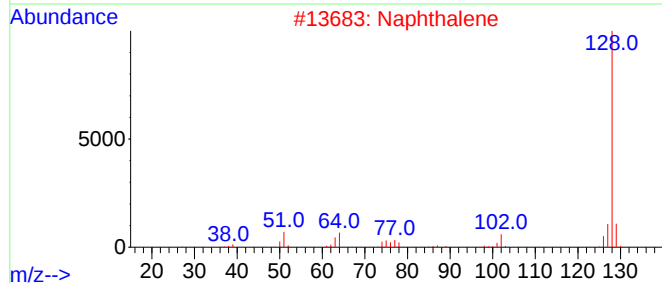
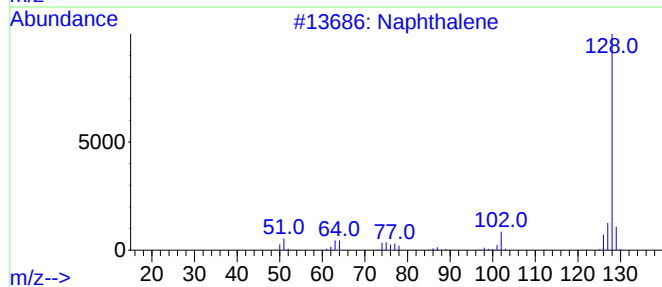
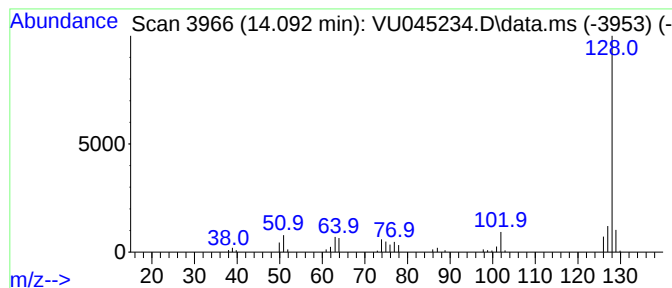
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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.
14.092	3.66 ug/L	51881	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Naphthalene	128	C10H8	000091-20-3	94
3			Azulene	128	C10H8	000275-51-4	94
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	91



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.465	19.4	ug/L	265294	1	6.253	683924	50.0
Azulene	14.092	3.7	ug/L	51881	3	11.815	707853	50.0