

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
 Data File : VU059322.D
 Acq On : 18 Jun 2024 19:32
 Operator : MD/SY
 Sample : P2856-17 200X
 Misc : 2.15g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0SJ2

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\SFAMULM052924WMA.M

Title : VOC Analysis

Signal : TIC: VU059322.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	87	95	111	rBV	50428	59540	12.68%	1.546%
2	1.763	138	147	162	rBV	7184	11966	2.55%	0.311%
3	1.907	184	192	211	rVB	47440	64806	13.80%	1.683%
4	2.560	383	395	408	rBV	80552	131929	28.09%	3.425%
5	2.743	449	452	454	rVV3	294	201	0.04%	0.005%
6	2.760	454	457	460	rVV2	431	272	0.06%	0.007%
7	2.782	461	464	473	rVB3	340	499	0.11%	0.013%
8	3.039	532	544	565	rVB	30041	57297	12.20%	1.488%
9	3.184	585	589	593	rVB2	362	392	0.08%	0.010%
10	3.274	615	617	622	rVB2	256	223	0.05%	0.006%
11	3.313	622	629	635	rBV	395	489	0.10%	0.013%
12	3.576	708	711	714	rVV	315	190	0.04%	0.005%
13	3.805	779	782	786	rVB2	278	204	0.04%	0.005%
14	4.075	863	866	869	rBV2	216	215	0.05%	0.006%
15	4.145	882	888	892	rVB2	201	228	0.05%	0.006%
16	4.177	893	898	902	rBV2	171	189	0.04%	0.005%
17	4.309	933	939	946	rVB2	312	420	0.09%	0.011%
18	4.483	990	993	996	rVB	293	188	0.04%	0.005%
19	4.557	1014	1016	1023	rVB2	319	323	0.07%	0.008%
20	4.615	1023	1034	1064	rBV	47699	120408	25.64%	3.126%
21	4.821	1091	1098	1101	rBV	435	489	0.10%	0.013%
22	4.920	1125	1129	1133	rVB	479	416	0.09%	0.011%
23	4.943	1133	1136	1139	rBV2	313	222	0.05%	0.006%
24	4.962	1139	1142	1146	rVB2	340	280	0.06%	0.007%
25	5.055	1156	1171	1188	rBV2	82854	184157	39.21%	4.781%
26	5.206	1216	1218	1228	rVB3	531	563	0.12%	0.015%
27	5.377	1267	1271	1274	rBV2	249	223	0.05%	0.006%
28	5.515	1308	1314	1318	rVB2	264	324	0.07%	0.008%
29	5.570	1328	1331	1335	rVB2	245	247	0.05%	0.006%
30	5.640	1348	1353	1357	rBV2	206	277	0.06%	0.007%
31	5.721	1357	1378	1403	rVV2	164679	449058	95.62%	11.659%
32	5.917	1437	1439	1442	rVV2	286	190	0.04%	0.005%
33	6.071	1485	1487	1492	rVB	259	204	0.04%	0.005%
34	6.245	1527	1541	1569	rBV	189978	371485	79.10%	9.645%
35	6.444	1601	1603	1605	rBV	376	208	0.04%	0.005%
36	6.534	1621	1631	1643	rVB7	5203	11009	2.34%	0.286%

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 Title : VOC Analysis

37	6.685	1665	1678	1702	rVV	104482	206071	43.88%	5.350%
38	6.894	1739	1743	1745	rBV2	214	201	0.04%	0.005%
39	7.193	1829	1836	1841	rBV4	881	1167	0.25%	0.030%
40	7.309	1868	1872	1875	rBV	223	206	0.04%	0.005%
41	7.386	1893	1896	1899	rVB	361	258	0.05%	0.007%
42	7.563	1940	1951	1968	rBV	47123	83829	17.85%	2.176%
43	7.711	1991	1997	2003	rVV5	766	1262	0.27%	0.033%
44	7.785	2013	2020	2024	rBV	263	308	0.07%	0.008%
45	7.894	2039	2054	2074	rBV	175681	312877	66.62%	8.123%
46	8.177	2132	2142	2167	rBV	33086	56614	12.06%	1.470%
47	8.373	2201	2203	2207	rVB	329	210	0.04%	0.005%
48	8.418	2210	2217	2221	rBV2	327	547	0.12%	0.014%
49	8.550	2248	2258	2270	rBV3	13700	23061	4.91%	0.599%
50	8.627	2273	2282	2313	rBV	110942	226680	48.27%	5.885%
51	8.904	2365	2368	2372	rVB	248	206	0.04%	0.005%
52	9.158	2441	2447	2452	rBV2	324	390	0.08%	0.010%
53	9.235	2466	2471	2475	rBV2	153	192	0.04%	0.005%
54	9.415	2510	2527	2542	rBV	276115	469618	100.00%	12.193%
55	9.576	2573	2577	2581	rVB3	771	523	0.11%	0.014%
56	9.698	2610	2615	2618	rBV4	470	490	0.10%	0.013%
57	10.058	2722	2727	2729	rBV	220	248	0.05%	0.006%
58	10.100	2736	2740	2742	rBV2	353	256	0.05%	0.007%
59	10.254	2783	2788	2790	rBV2	266	238	0.05%	0.006%
60	10.299	2798	2802	2806	rVV2	288	246	0.05%	0.006%
61	10.750	2930	2942	2968	rVV	158158	256067	54.53%	6.648%
62	10.984	3010	3015	3021	rVB2	316	400	0.09%	0.010%
63	11.023	3021	3027	3030	rVB2	320	385	0.08%	0.010%
64	11.319	3115	3119	3121	rVV2	242	204	0.04%	0.005%
65	11.348	3124	3128	3132	rVV2	367	356	0.08%	0.009%
66	11.438	3151	3156	3158	rBV	240	200	0.04%	0.005%
67	11.476	3164	3168	3169	rBV2	395	302	0.06%	0.008%
68	11.521	3178	3182	3185	rBV	340	296	0.06%	0.008%
69	11.541	3185	3188	3190	rBV2	304	228	0.05%	0.006%
70	11.701	3233	3238	3244	rBV2	270	351	0.07%	0.009%
71	11.740	3248	3250	3252	rBV	319	188	0.04%	0.005%
72	11.811	3260	3272	3296	rBV	250572	419506	89.33%	10.892%
73	11.981	3321	3325	3329	rVB3	335	282	0.06%	0.007%
74	12.190	3378	3390	3415	rBV	165950	282885	60.24%	7.345%
75	12.386	3447	3451	3455	rBV2	219	201	0.04%	0.005%
76	12.611	3519	3521	3532	rVB2	305	403	0.09%	0.010%

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 Title : VOC Analysis

77	12.666	3535	3538	3542	rVB	289	241	0.05%	0.006%
78	12.692	3542	3546	3551	rBV	235	268	0.06%	0.007%
79	12.762	3564	3568	3571	rBV2	504	448	0.10%	0.012%
80	12.987	3636	3638	3643	rBV2	339	325	0.07%	0.008%
81	13.267	3721	3725	3733	rBV2	287	373	0.08%	0.010%
82	13.405	3765	3768	3770	rBV	334	259	0.06%	0.007%
83	13.483	3788	3792	3795	rBV2	237	211	0.04%	0.005%
84	13.711	3859	3863	3868	rBV3	327	331	0.07%	0.009%
85	13.830	3896	3900	3903	rBV3	214	216	0.05%	0.006%
86	14.090	3972	3981	4004	rBV	12843	26734	5.69%	0.694%
87	14.450	4091	4093	4097	rVV	403	229	0.05%	0.006%
88	14.483	4101	4103	4110	rVB3	435	355	0.08%	0.009%
89	14.550	4120	4124	4126	rBV3	384	287	0.06%	0.007%
90	14.968	4251	4254	4256	rBV3	308	222	0.05%	0.006%
91	15.036	4273	4275	4277	rBV	368	200	0.04%	0.005%
92	15.052	4277	4280	4281	rVV	306	193	0.04%	0.005%
93	15.219	4329	4332	4335	rBV3	260	239	0.05%	0.006%
94	15.804	4510	4514	4517	rBV2	370	327	0.07%	0.008%
95	15.897	4540	4543	4546	rBV2	456	438	0.09%	0.011%
96	16.074	4596	4598	4602	rBV2	442	338	0.07%	0.009%
97	16.135	4615	4617	4620	rVB	633	228	0.05%	0.006%
98	16.203	4635	4638	4639	rBV	359	203	0.04%	0.005%
99	16.280	4657	4662	4667	rBV5	744	1161	0.25%	0.030%
100	16.392	4694	4697	4700	rBV4	520	444	0.09%	0.012%

Sum of corrected areas: 3851553

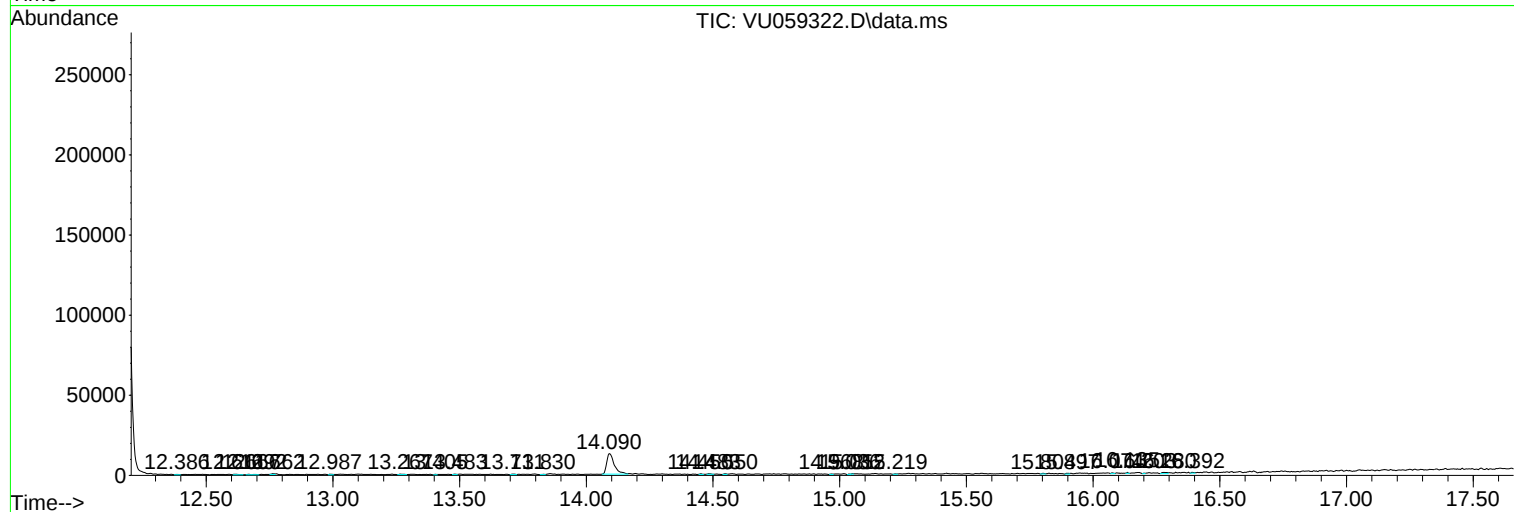
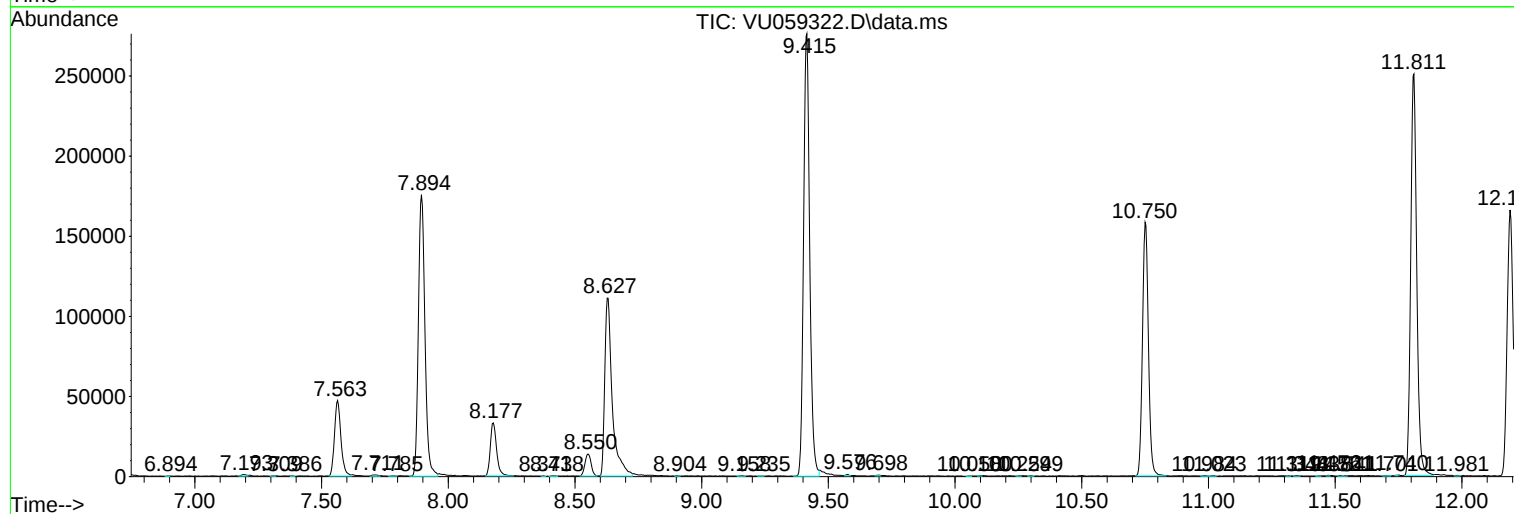
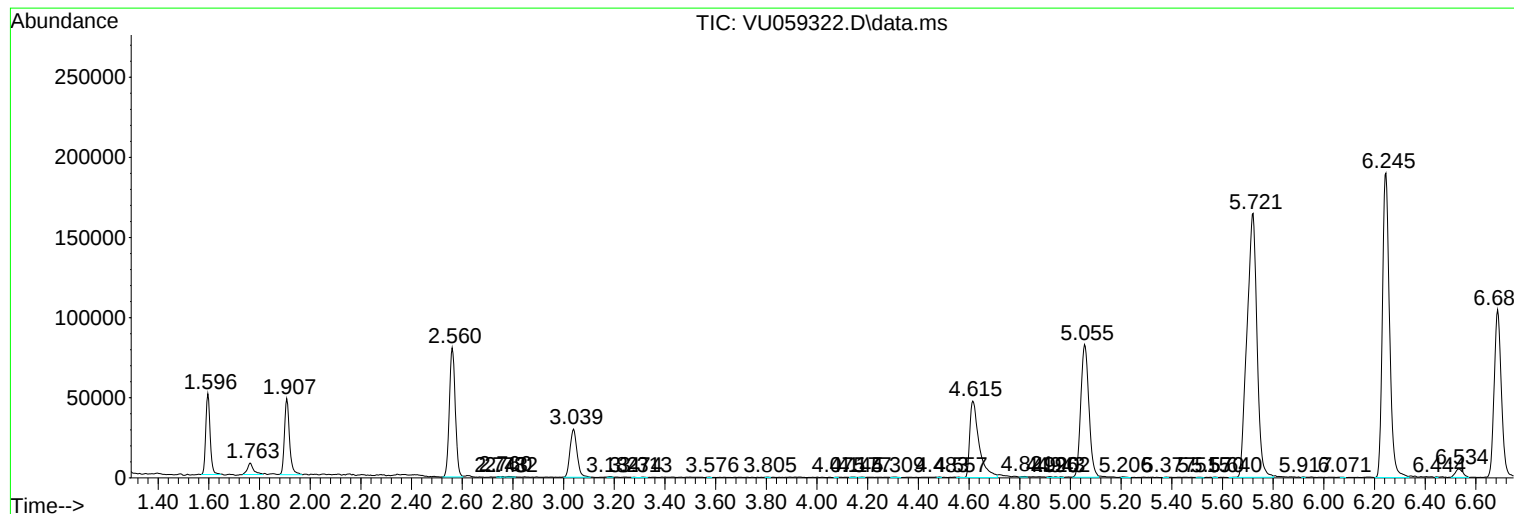
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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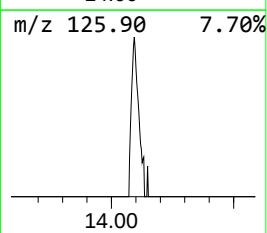
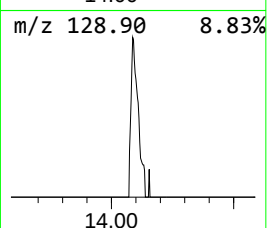
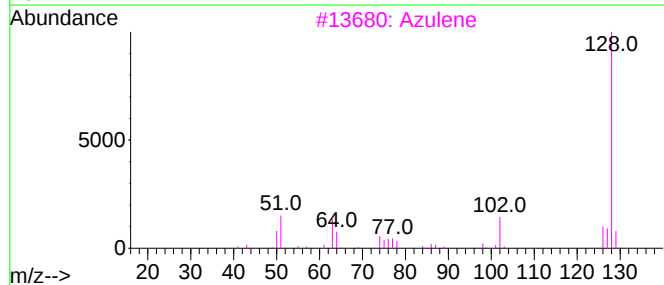
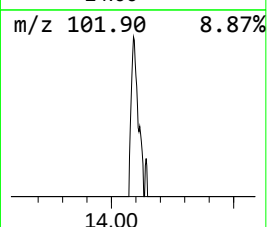
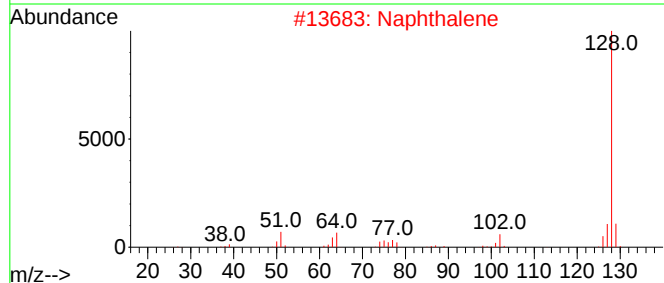
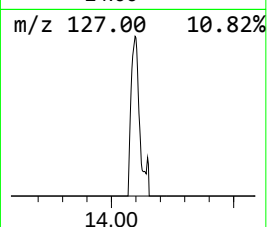
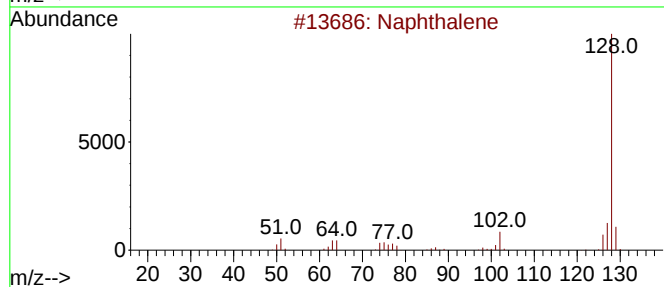
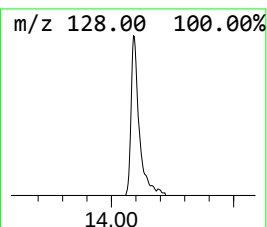
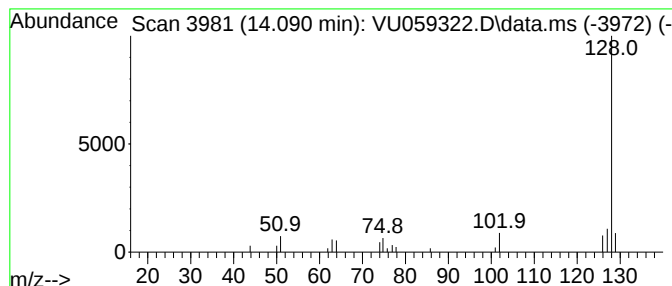
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.090	3.19 ug/L	26734	1,4-Dichlorobenzene-d4	11.811

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	91
2			Naphthalene	128	C10H8	000091-20-3	91
3			Azulene	128	C10H8	000275-51-4	90
4			Azulene	128	C10H8	000275-51-4	87
5			Azulene	128	C10H8	000275-51-4	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Azulene	14.090	3.2	ug/L	26734	3	11.811	419506	50.0