

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
 Data File : VU059327.D
 Acq On : 18 Jun 2024 21:28
 Operator : MD/SY
 Sample : P2873-15
 Misc : 5.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0SK3

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: VU059327.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.480	55	59	65	rBV3	2151	2047	0.33%	0.041%
2	1.592	87	94	115	rVB	27907	54076	8.68%	1.083%
3	1.872	134	181	200	rBV7	64260	483568	77.61%	9.685%
4	2.239	293	295	299	rBV4	767	412	0.07%	0.008%
5	2.531	374	386	406	rBV	83849	136645	21.93%	2.737%
6	2.631	411	417	420	rBV5	1185	1653	0.27%	0.033%
7	2.711	438	442	448	rBV6	428	523	0.08%	0.010%
8	2.801	466	470	475	rBV3	364	368	0.06%	0.007%
9	2.840	480	482	484	rVB2	466	204	0.03%	0.004%
10	3.026	529	540	553	rBV3	6652	14584	2.34%	0.292%
11	3.171	575	585	595	rBV3	1244	3144	0.50%	0.063%
12	3.264	612	614	618	rVB	477	330	0.05%	0.007%
13	3.290	618	622	624	rBV2	263	232	0.04%	0.005%
14	3.612	718	722	724	rBV	245	203	0.03%	0.004%
15	3.670	737	740	747	rVB2	521	497	0.08%	0.010%
16	3.776	769	773	776	rBV2	262	236	0.04%	0.005%
17	3.866	796	801	805	rBV2	235	296	0.05%	0.006%
18	4.168	891	895	899	rBV	271	242	0.04%	0.005%
19	4.190	899	902	906	rVB2	274	234	0.04%	0.005%
20	4.216	906	910	913	rBV2	319	305	0.05%	0.006%
21	4.309	933	939	941	rBV2	170	204	0.03%	0.004%
22	4.345	947	950	954	rBV2	238	222	0.04%	0.004%
23	4.628	1028	1038	1078	rBV	41953	132792	21.31%	2.660%
24	4.952	1136	1139	1143	rVB2	298	256	0.04%	0.005%
25	5.052	1153	1170	1189	rBV2	83521	191473	30.73%	3.835%
26	5.229	1220	1225	1228	rBV2	253	257	0.04%	0.005%
27	5.345	1256	1261	1264	rVB2	304	288	0.05%	0.006%
28	5.364	1264	1267	1271	rBV	208	216	0.03%	0.004%
29	5.393	1273	1276	1283	rVB	220	230	0.04%	0.005%
30	5.621	1340	1347	1348	rBV2	209	212	0.03%	0.004%
31	5.711	1357	1375	1404	rBV2	179353	479556	76.96%	9.605%
32	5.975	1450	1457	1458	rBV3	1572	1507	0.24%	0.030%
33	6.123	1500	1503	1507	rBV2	272	208	0.03%	0.004%
34	6.242	1527	1540	1574	rBV	249233	490838	78.77%	9.831%
35	6.357	1574	1576	1583	rVB	734	599	0.10%	0.012%
36	6.393	1583	1587	1590	rBV2	308	261	0.04%	0.005%

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 Title : VOC Analysis

37	6.460	1603	1608	1612	rBV2	312	339	0.05%	0.007%
38	6.531	1620	1630	1642	rVV10	5769	12262	1.97%	0.246%
39	6.599	1642	1651	1665	rVV6	2491	6002	0.96%	0.120%
40	6.682	1665	1677	1698	rVV2	109166	218307	35.04%	4.372%
41	6.769	1700	1704	1707	rVB3	499	306	0.05%	0.006%
42	6.853	1726	1730	1735	rVB2	188	208	0.03%	0.004%
43	7.087	1800	1803	1808	rVB2	261	228	0.04%	0.005%
44	7.113	1808	1811	1814	rBV2	227	203	0.03%	0.004%
45	7.193	1828	1836	1842	rVV3	1143	1746	0.28%	0.035%
46	7.219	1842	1844	1850	rVB3	1211	1118	0.18%	0.022%
47	7.560	1936	1950	1967	rBV2	49872	94454	15.16%	1.892%
48	7.705	1989	1995	1998	rBV3	648	782	0.13%	0.016%
49	7.824	2029	2032	2036	rBV3	374	245	0.04%	0.005%
50	7.891	2040	2053	2072	rBV	193327	341199	54.76%	6.834%
51	8.036	2096	2098	2105	rVB3	360	324	0.05%	0.006%
52	8.177	2131	2142	2161	rBV	34317	62586	10.04%	1.253%
53	8.550	2247	2258	2270	rBV2	47613	81399	13.06%	1.630%
54	8.644	2274	2287	2323	rBV	109724	272033	43.66%	5.448%
55	8.808	2334	2338	2345	rVB4	549	584	0.09%	0.012%
56	8.888	2359	2363	2367	rVB3	318	233	0.04%	0.005%
57	9.287	2483	2487	2491	rBV	313	306	0.05%	0.006%
58	9.361	2505	2510	2513	rBV2	273	234	0.04%	0.005%
59	9.415	2513	2527	2553	rBV	346268	623098	100.00%	12.479%
60	9.570	2568	2575	2576	rBV3	1109	879	0.14%	0.018%
61	9.698	2604	2615	2624	rBV4	4369	7143	1.15%	0.143%
62	9.917	2676	2683	2686	rBV2	232	288	0.05%	0.006%
63	10.107	2735	2742	2748	rBV3	1303	1759	0.28%	0.035%
64	10.155	2753	2757	2762	rBV3	320	374	0.06%	0.007%
65	10.316	2803	2807	2812	rBV2	189	202	0.03%	0.004%
66	10.534	2871	2875	2878	rVB2	376	259	0.04%	0.005%
67	10.611	2895	2899	2902	rBV2	223	200	0.03%	0.004%
68	10.756	2931	2944	2962	rBV	177022	296827	47.64%	5.945%
69	10.988	3012	3016	3020	rBV2	232	206	0.03%	0.004%
70	11.103	3049	3052	3057	rVV2	437	406	0.07%	0.008%
71	11.245	3089	3096	3103	rBV2	357	629	0.10%	0.013%
72	11.467	3162	3165	3170	rVB2	416	389	0.06%	0.008%
73	11.512	3175	3179	3181	rBV	337	269	0.04%	0.005%
74	11.598	3203	3206	3210	rVB2	319	219	0.04%	0.004%
75	11.811	3260	3272	3298	rBV	366426	586768	94.17%	11.752%
76	11.955	3315	3317	3321	rVV2	500	297	0.05%	0.006%

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 Title : VOC Analysis

77	12.193	3376	3391	3409	rBV	192965	328407	52.71%	6.577%
78	12.737	3551	3560	3562	rBV2	340	512	0.08%	0.010%
79	12.942	3621	3624	3627	rBV	346	289	0.05%	0.006%
80	13.248	3717	3719	3724	rVB3	490	430	0.07%	0.009%
81	13.364	3751	3755	3757	rBV	207	204	0.03%	0.004%
82	13.454	3780	3783	3788	rVB	358	304	0.05%	0.006%
83	13.560	3810	3816	3819	rBV2	346	366	0.06%	0.007%
84	13.666	3846	3849	3855	rBV2	371	425	0.07%	0.009%
85	14.094	3972	3982	3998	rBV2	16782	32868	5.27%	0.658%
86	14.254	4030	4032	4040	rVB	277	212	0.03%	0.004%
87	14.386	4070	4073	4076	rBV2	312	245	0.04%	0.005%
88	14.402	4076	4078	4081	rVB	403	216	0.03%	0.004%
89	14.483	4101	4103	4107	rVB3	444	281	0.05%	0.006%
90	14.573	4123	4131	4144	rVB3	1530	2563	0.41%	0.051%
91	14.627	4144	4148	4152	rBV2	410	417	0.07%	0.008%
92	14.675	4160	4163	4167	rBV2	496	368	0.06%	0.007%
93	14.698	4167	4170	4174	rBV3	314	276	0.04%	0.006%
94	14.888	4224	4229	4231	rBV2	299	313	0.05%	0.006%
95	15.020	4267	4270	4274	rBV2	318	243	0.04%	0.005%
96	15.235	4330	4337	4348	rBV3	2929	5566	0.89%	0.111%
97	15.421	4387	4395	4401	rBV3	1582	2400	0.39%	0.048%
98	15.791	4507	4510	4511	rBV	500	217	0.03%	0.004%
99	15.978	4565	4568	4575	rVB5	828	732	0.12%	0.015%
100	16.418	4702	4705	4709	rBV3	904	906	0.15%	0.018%

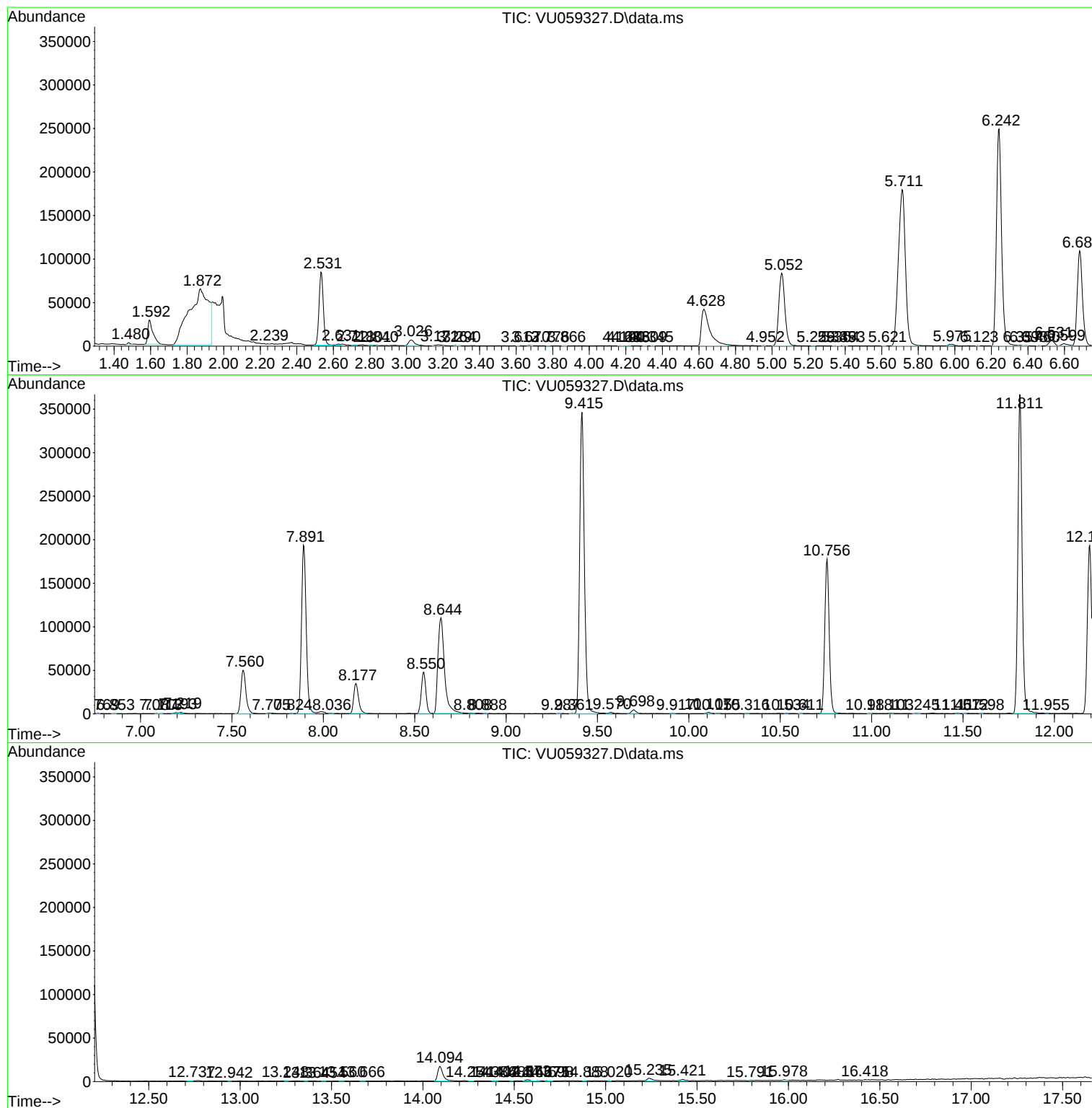
Sum of corrected areas: 4992988

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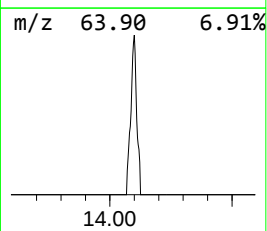
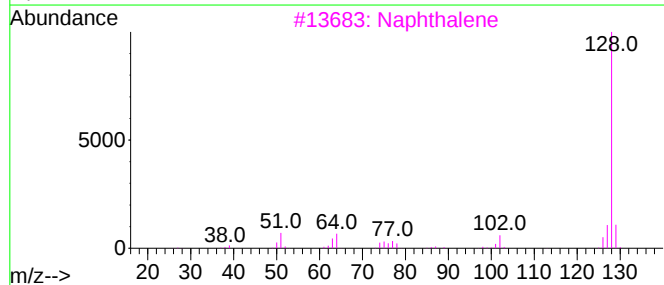
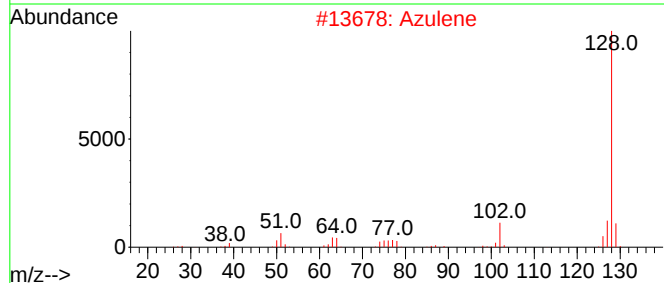
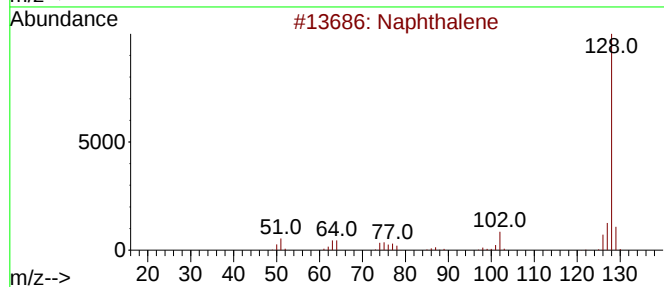
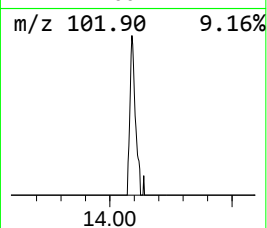
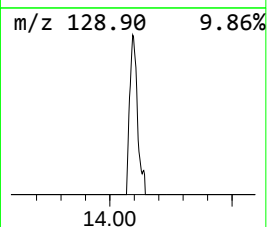
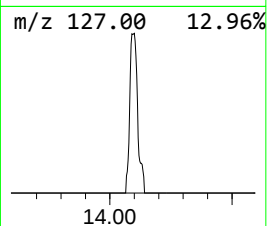
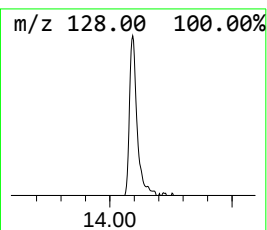
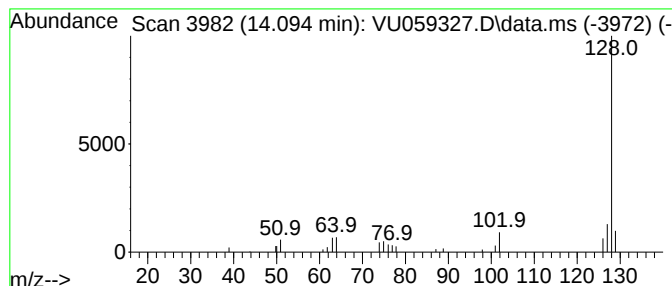
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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.
14.094	2.80 ug/L	32868	1,4-Dichlorobenzene-d4	11.811

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	94
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 Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Azulene	14.094	2.8	ug/L	32868	3	11.811	586768	50.0