

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061424\
 Data File : VU059261.D
 Acq On : 14 Jun 2024 20:26
 Operator : MD/SY
 Sample : P2856-11ME
 Misc : 2.78g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0SH3ME

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: VU059261.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	1186	1460	0.14%	0.013%
2	1.592	86	94	115	rVB	48768	67035	6.30%	0.601%
3	1.872	133	181	200	rBV4	110274	507501	47.69%	4.550%
4	2.354	329	331	333	rBV2	812	459	0.04%	0.004%
5	2.547	379	391	405	rBV	112987	179876	16.90%	1.613%
6	2.631	409	417	423	rVB5	940	1401	0.13%	0.013%
7	2.763	455	458	461	rBV	557	408	0.04%	0.004%
8	2.933	505	511	516	rBV2	249	360	0.03%	0.003%
9	3.030	529	541	563	rVB2	16263	33509	3.15%	0.300%
10	3.171	572	585	608	rBV2	8625	22308	2.10%	0.200%
11	3.837	788	792	796	rBV2	373	329	0.03%	0.003%
12	4.197	901	904	910	rVV2	332	424	0.04%	0.004%
13	4.223	910	912	918	rVB2	351	310	0.03%	0.003%
14	4.612	1022	1033	1091	rBV	139886	399939	37.58%	3.586%
15	5.052	1154	1170	1198	rBV	168613	377869	35.51%	3.388%
16	5.277	1236	1240	1246	rVB2	401	424	0.04%	0.004%
17	5.547	1320	1324	1327	rBV2	346	320	0.03%	0.003%
18	5.714	1355	1376	1396	rBV2	287051	816071	76.68%	7.317%
19	5.972	1445	1456	1462	rBV5	1062	2067	0.19%	0.019%
20	6.129	1500	1505	1512	rBV2	303	354	0.03%	0.003%
21	6.239	1525	1539	1571	rBV	407017	781655	73.45%	7.009%
22	6.425	1593	1597	1600	rBV2	642	438	0.04%	0.004%
23	6.480	1611	1614	1618	rBV2	316	289	0.03%	0.003%
24	6.525	1618	1628	1643	rVV6	9799	21265	2.00%	0.191%
25	6.589	1645	1648	1652	rBV4	888	787	0.07%	0.007%
26	6.682	1663	1677	1702	rBV	218170	428317	40.25%	3.840%
27	6.811	1713	1717	1720	rBV2	320	320	0.03%	0.003%
28	6.956	1756	1762	1765	rBV	285	320	0.03%	0.003%
29	7.560	1938	1950	1972	rBV	97363	176448	16.58%	1.582%
30	7.702	1988	1994	1998	rBV4	1187	1404	0.13%	0.013%
31	7.801	2022	2025	2030	rVB2	314	257	0.02%	0.002%
32	7.891	2040	2053	2068	rVV	312020	527742	49.59%	4.732%
33	7.968	2070	2077	2093	rVB	11700	22566	2.12%	0.202%
34	8.094	2113	2116	2120	rVB2	368	297	0.03%	0.003%
35	8.174	2130	2141	2160	rBV2	69554	120566	11.33%	1.081%
36	8.255	2164	2166	2174	rVB3	420	390	0.04%	0.003%

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 Title : VOC Analysis

37	8.335	2184	2191	2194	rBV2	394	476	0.04%	0.004%
38	8.464	2227	2231	2234	rBV2	613	504	0.05%	0.005%
39	8.547	2244	2257	2272	rBV	584954	997152	93.69%	8.941%
40	8.631	2272	2283	2317	rVV	408933	836710	78.62%	7.502%
41	9.004	2395	2399	2404	rBV3	348	307	0.03%	0.003%
42	9.110	2431	2432	2436	rVB2	666	307	0.03%	0.003%
43	9.213	2461	2464	2468	rVB2	886	546	0.05%	0.005%
44	9.328	2495	2500	2506	rBV2	890	939	0.09%	0.008%
45	9.412	2513	2526	2552	rBV	611983	1029083	96.69%	9.227%
46	9.566	2564	2574	2585	rBV2	28757	46538	4.37%	0.417%
47	9.692	2601	2613	2630	rVV2	27083	49001	4.60%	0.439%
48	9.753	2630	2632	2639	rVB3	661	539	0.05%	0.005%
49	9.836	2653	2658	2660	rBV2	323	269	0.03%	0.002%
50	9.952	2691	2694	2697	rVB2	428	284	0.03%	0.003%
51	10.010	2708	2712	2719	rVB5	1051	1412	0.13%	0.013%
52	10.097	2730	2739	2755	rBV3	13341	25316	2.38%	0.227%
53	10.251	2777	2787	2800	rVV6	5628	9303	0.87%	0.083%
54	10.312	2804	2806	2809	rVV	518	295	0.03%	0.003%
55	10.348	2809	2817	2824	rVV7	2567	5403	0.51%	0.048%
56	10.390	2825	2830	2840	rVB6	3426	5129	0.48%	0.046%
57	10.457	2845	2851	2853	rBV4	983	986	0.09%	0.009%
58	10.480	2855	2858	2866	rVB4	1595	1750	0.16%	0.016%
59	10.557	2869	2882	2883	rBV2	2502	3675	0.35%	0.033%
60	10.618	2891	2901	2908	rBV5	3623	6474	0.61%	0.058%
61	10.750	2929	2942	2971	rBV	502426	824978	77.52%	7.397%
62	10.856	2973	2975	2979	rVB	410	254	0.02%	0.002%
63	10.904	2979	2990	2997	rBV4	2044	3385	0.32%	0.030%
64	11.023	3010	3027	3033	rBV	11520	27307	2.57%	0.245%
65	11.200	3078	3082	3087	rVB2	497	374	0.04%	0.003%
66	11.299	3099	3113	3114	rBV5	2067	3320	0.31%	0.030%
67	11.370	3131	3135	3141	rBV5	1025	1329	0.12%	0.012%
68	11.412	3141	3148	3155	rVB4	7642	10287	0.97%	0.092%
69	11.467	3155	3165	3174	rBV	26567	40873	3.84%	0.366%
70	11.544	3181	3189	3197	rBV6	2799	5157	0.48%	0.046%
71	11.637	3211	3218	3221	rVV7	1269	1651	0.16%	0.015%
72	11.708	3230	3240	3247	rBV6	3524	5762	0.54%	0.052%
73	11.743	3247	3251	3252	rBV3	686	415	0.04%	0.004%
74	11.807	3259	3271	3289	rBV	656020	1064268	100.00%	9.543%
75	11.891	3293	3297	3309	rVB5	11305	18264	1.72%	0.164%
76	12.045	3342	3345	3349	rBB2	384	277	0.03%	0.002%

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C0SH3ME

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Integrator: RTE

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Title : VOC Analysis

77	12.097	3349	3361	3370	rVB2	4751	7286	0.68%	0.065%
78	12.187	3377	3389	3414	rBV	479536	785220	73.78%	7.041%
79	12.315	3419	3429	3441	rVV2	12018	21239	2.00%	0.190%
80	12.383	3448	3450	3457	rVB3	1261	946	0.09%	0.008%
81	12.682	3538	3543	3548	rBV3	536	561	0.05%	0.005%
82	12.762	3561	3568	3576	rVB3	1263	1973	0.19%	0.018%
83	13.100	3666	3673	3674	rBV	302	413	0.04%	0.004%
84	13.184	3694	3699	3701	rBV	296	277	0.03%	0.002%
85	13.229	3709	3713	3715	rBV2	425	352	0.03%	0.003%
86	13.293	3731	3733	3740	rVB	543	514	0.05%	0.005%
87	13.344	3746	3749	3752	rVV	355	275	0.03%	0.002%
88	13.367	3753	3756	3761	rVV	368	334	0.03%	0.003%
89	13.451	3776	3782	3783	rBV4	414	429	0.04%	0.004%
90	13.524	3799	3805	3815	rVB5	1375	2231	0.21%	0.020%
91	13.569	3815	3819	3823	rBV2	530	543	0.05%	0.005%
92	13.631	3830	3838	3849	rBV3	3071	5292	0.50%	0.047%
93	13.840	3901	3903	3908	rBV3	449	354	0.03%	0.003%
94	13.910	3922	3925	3932	rBV3	345	413	0.04%	0.004%
95	14.081	3965	3978	4005	rBV	463548	784414	73.70%	7.033%
96	14.209	4010	4018	4029	rVB2	7376	12168	1.14%	0.109%
97	14.463	4094	4097	4099	rBV2	461	337	0.03%	0.003%
98	14.569	4127	4130	4132	rBV	628	505	0.05%	0.005%
99	14.614	4139	4144	4149	rBV3	444	534	0.05%	0.005%
100	15.888	4537	4540	4544	rBV3	520	488	0.05%	0.004%

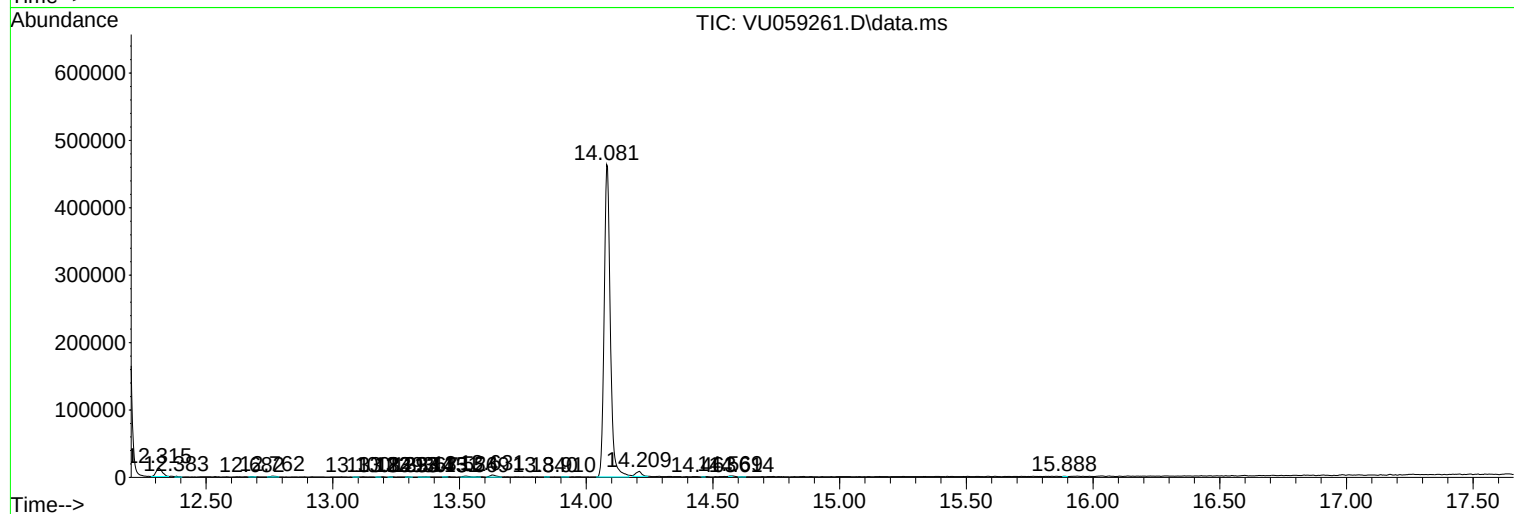
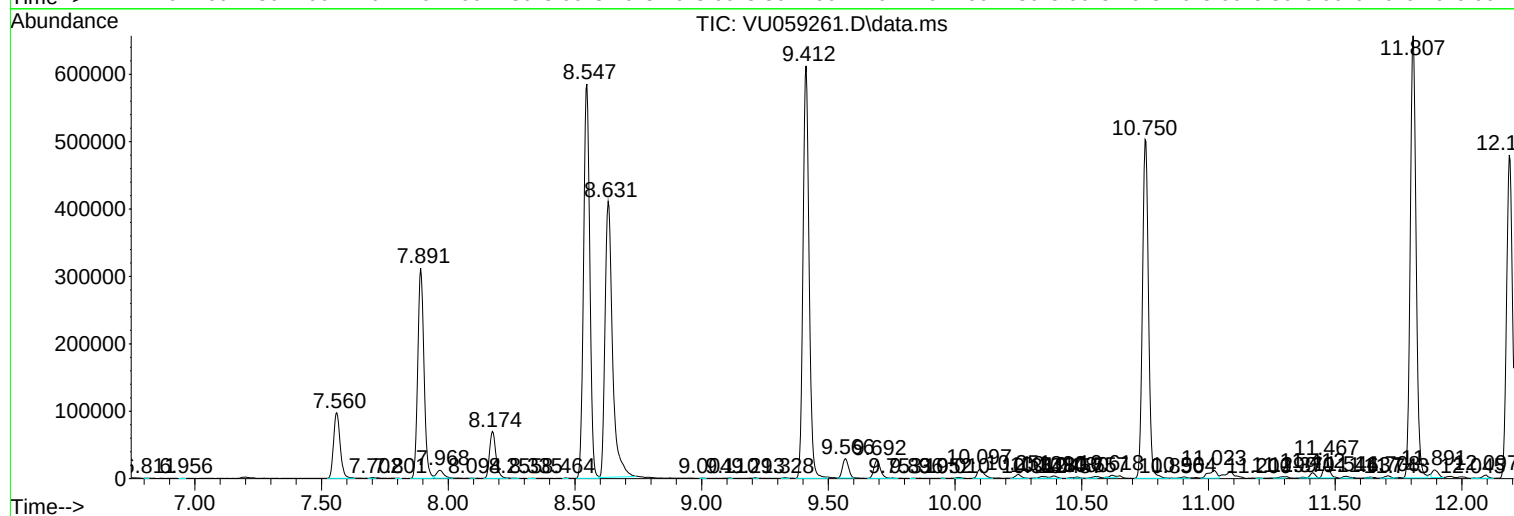
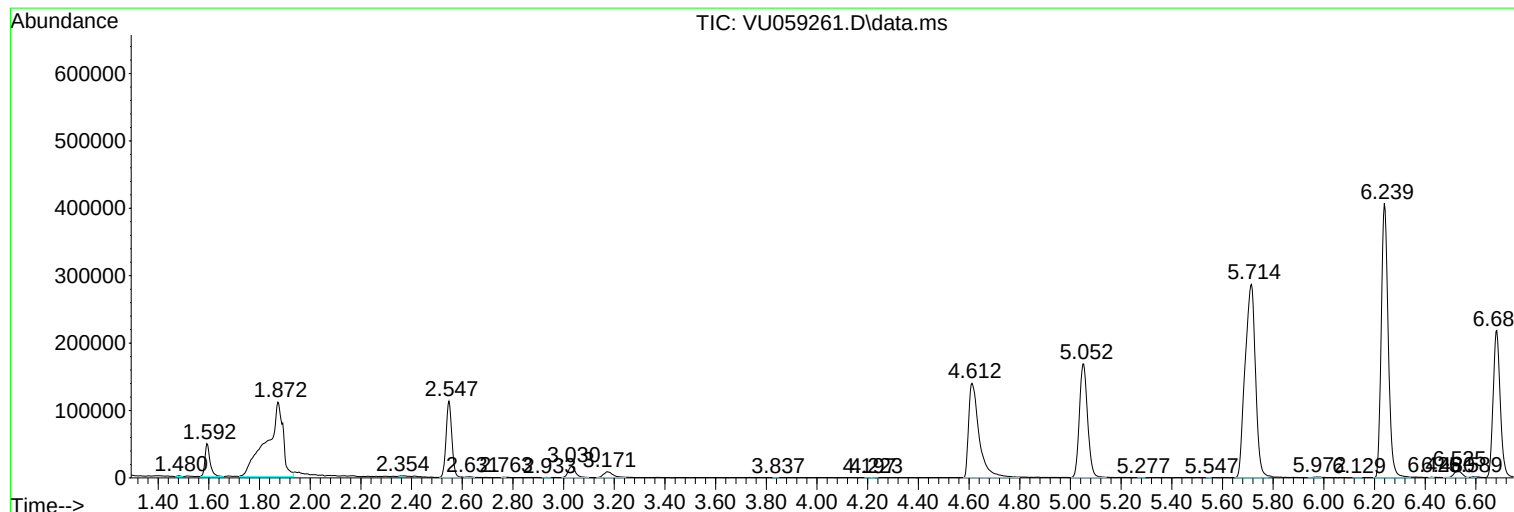
Sum of corrected areas: 11152882

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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



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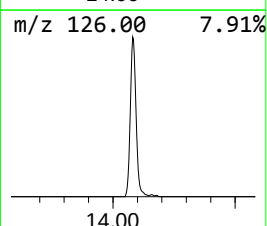
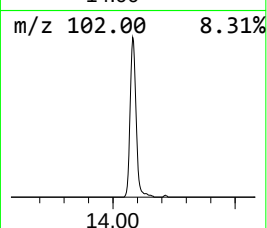
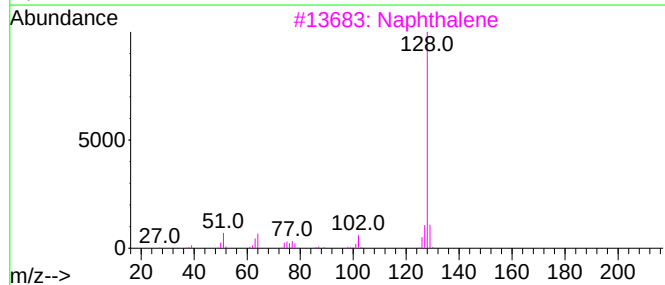
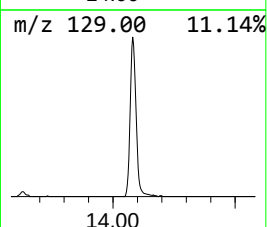
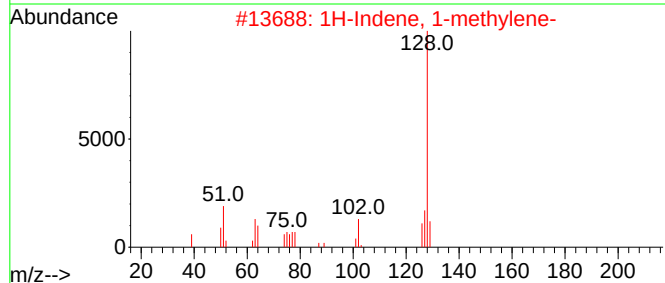
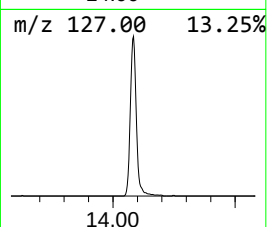
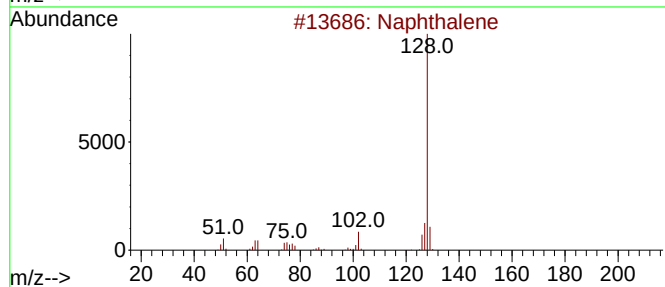
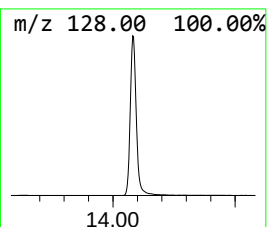
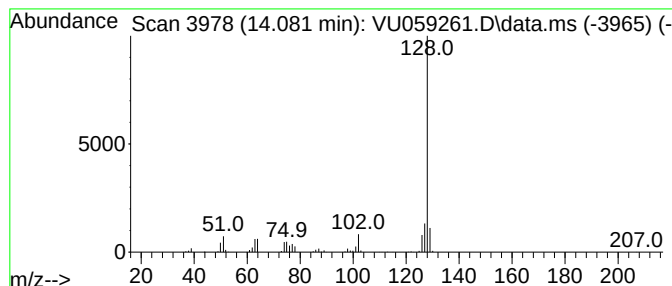
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.081	36.85 ug/L	784414	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	95
3			Naphthalene	128	C10H8	000091-20-3	94
4			Azulene	128	C10H8	000275-51-4	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	14.081	36.9	ug/L	784414	3	11.807	1064270	50.0