

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120221\
 Data File : VU046053.D
 Acq On : 02 Dec 2021 15:34
 Operator : SY/MD
 Sample : M4868-02ME
 Misc : 6.84g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGKN9ME

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\SFAMULM112921WMA.M
 Title : VOC Analysis

Signal : TIC: VU046053.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	98	rVB	83609	110814	13.72%	1.488%
2	1.880	162	168	172	rBV	9961	13371	1.65%	0.180%
3	1.916	173	179	199	rVB	48226	81793	10.12%	1.099%
4	2.543	364	374	388	rBV	156188	256557	31.75%	3.446%
5	3.183	559	573	591	rBV	5698	15591	1.93%	0.209%
6	3.356	625	627	630	rBV	249	156	0.02%	0.002%
7	3.469	659	662	666	rBB	163	159	0.02%	0.002%
8	3.511	667	675	678	rBB	167	240	0.03%	0.003%
9	3.530	678	681	686	rBV	184	225	0.03%	0.003%
10	3.575	690	695	698	rBV	262	300	0.04%	0.004%
11	3.623	707	710	714	rBV	129	138	0.02%	0.002%
12	3.707	732	736	742	rBV	175	230	0.03%	0.003%
13	3.935	803	807	810	rBV	116	128	0.02%	0.002%
14	3.954	810	813	815	rBV	188	139	0.02%	0.002%
15	4.157	874	876	880	rBB	139	123	0.02%	0.002%
16	4.253	900	906	909	rBB	152	171	0.02%	0.002%
17	4.404	951	953	956	rBB	147	100	0.01%	0.001%
18	4.655	1013	1031	1066	rBV2	45303	191047	23.65%	2.566%
19	5.067	1143	1159	1186	rVB	128882	316098	39.12%	4.246%
20	5.166	1187	1190	1194	rBV	188	198	0.02%	0.003%
21	5.443	1272	1276	1279	rBB	144	144	0.02%	0.002%
22	5.462	1279	1282	1284	rBV	150	122	0.02%	0.002%
23	5.498	1290	1293	1296	rBB	139	119	0.01%	0.002%
24	5.723	1341	1363	1394	rBV2	316906	807975	100.00%	10.853%
25	5.842	1398	1400	1404	rBB	163	129	0.02%	0.002%
26	5.980	1433	1443	1468	rBB7	3739	9623	1.19%	0.129%
27	6.250	1511	1527	1549	rBV	269857	554393	68.62%	7.447%
28	6.533	1603	1615	1628	rBV7	5428	12633	1.56%	0.170%
29	6.690	1651	1664	1687	rBV	174302	361143	44.70%	4.851%
30	6.803	1696	1699	1706	rBV3	475	580	0.07%	0.008%
31	6.835	1707	1709	1713	rVB	256	142	0.02%	0.002%
32	6.880	1714	1723	1726	rBV	185	324	0.04%	0.004%
33	7.051	1771	1776	1778	rVB2	207	189	0.02%	0.003%
34	7.153	1802	1808	1811	rBV	178	265	0.03%	0.004%
35	7.192	1811	1820	1829	rVV2	1231	2208	0.27%	0.030%
36	7.305	1853	1855	1858	rBV	185	141	0.02%	0.002%

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 Title : VOC Analysis

37	7.375	1872	1877	1881	rBV2	441	490	0.06%	0.007%
38	7.436	1893	1896	1898	rBV	149	123	0.02%	0.002%
39	7.568	1923	1937	1961	rVV	94678	184233	22.80%	2.475%
40	7.690	1966	1975	1982	rBV3	962	1653	0.20%	0.022%
41	7.800	1999	2009	2015	rBV3	810	1485	0.18%	0.020%
42	7.825	2015	2017	2024	rVB3	525	512	0.06%	0.007%
43	7.899	2026	2040	2056	rBV	355447	668572	82.75%	8.980%
44	8.054	2085	2088	2091	rBV2	169	169	0.02%	0.002%
45	8.128	2108	2111	2113	rBV	346	270	0.03%	0.004%
46	8.182	2117	2128	2154	rVB	58759	123793	15.32%	1.663%
47	8.465	2213	2216	2224	rVB2	291	443	0.05%	0.006%
48	8.523	2231	2234	2235	rBV	172	122	0.02%	0.002%
49	8.581	2248	2252	2258	rBV	163	257	0.03%	0.003%
50	8.678	2259	2282	2313	rVV2	134792	421842	52.21%	5.666%
51	8.803	2320	2321	2325	rBV2	335	259	0.03%	0.003%
52	8.941	2359	2364	2365	rBV2	586	468	0.06%	0.006%
53	9.012	2381	2386	2389	rBV	183	238	0.03%	0.003%
54	9.108	2411	2416	2418	rBV	189	220	0.03%	0.003%
55	9.163	2430	2433	2435	rVB2	190	100	0.01%	0.001%
56	9.214	2448	2449	2452	rBV	329	168	0.02%	0.002%
57	9.333	2482	2486	2487	rBV	263	175	0.02%	0.002%
58	9.427	2500	2515	2540	rBV	331560	693812	85.87%	9.319%
59	9.575	2550	2561	2578	rVB	27635	49974	6.19%	0.671%
60	9.697	2587	2599	2622	rBV	85877	166054	20.55%	2.230%
61	9.800	2626	2631	2632	rBV3	400	382	0.05%	0.005%
62	10.025	2696	2701	2702	rBV	365	253	0.03%	0.003%
63	10.108	2715	2727	2742	rBV	24309	44999	5.57%	0.604%
64	10.253	2768	2772	2776	rVV3	781	719	0.09%	0.010%
65	10.353	2799	2803	2809	rBV5	1458	2024	0.25%	0.027%
66	10.491	2839	2846	2858	rVB3	2268	3343	0.41%	0.045%
67	10.558	2864	2867	2872	rVB2	345	300	0.04%	0.004%
68	10.600	2876	2880	2882	rBV	309	198	0.02%	0.003%
69	10.620	2884	2886	2887	rBV	366	162	0.02%	0.002%
70	10.771	2919	2933	2949	rVB	237930	400976	49.63%	5.386%
71	10.864	2958	2962	2964	rBV2	355	286	0.04%	0.004%
72	11.002	2994	3005	3020	rBV2	10364	22973	2.84%	0.309%
73	11.298	3087	3097	3107	rBV	4398	7045	0.87%	0.095%
74	11.372	3116	3120	3121	rBV2	610	431	0.05%	0.006%
75	11.417	3128	3134	3140	rBV3	1477	2081	0.26%	0.028%
76	11.472	3140	3151	3165	rVB	29906	49146	6.08%	0.660%

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 Title : VOC Analysis

77	11.700	3214	3222	3228	rBV5	3945	5897	0.73%	0.079%
78	11.819	3246	3259	3272	rBV	454628	712514	88.19%	9.571%
79	12.063	3330	3335	3336	rBV2	218	197	0.02%	0.003%
80	12.102	3339	3347	3352	rBV2	4568	7513	0.93%	0.101%
81	12.198	3366	3377	3393	rVB	397047	636266	78.75%	8.546%
82	12.327	3406	3417	3426	rVB4	7487	12261	1.52%	0.165%
83	12.385	3428	3435	3445	rVB7	1802	3078	0.38%	0.041%
84	12.436	3449	3451	3453	rBV2	282	141	0.02%	0.002%
85	12.472	3456	3462	3465	rBV4	2420	2824	0.35%	0.038%
86	12.578	3489	3495	3503	rVB2	3968	4728	0.59%	0.064%
87	13.031	3631	3636	3647	rVB3	4592	6703	0.83%	0.090%
88	13.732	3851	3854	3856	rBV2	332	227	0.03%	0.003%
89	13.841	3879	3888	3901	rBV8	5662	9713	1.20%	0.130%
90	14.089	3954	3965	3978	rBV	129998	200538	24.82%	2.694%
91	14.291	4024	4028	4029	rBV3	833	600	0.07%	0.008%
92	14.484	4082	4088	4099	rBV6	1517	2522	0.31%	0.034%
93	14.571	4113	4115	4116	rBV2	653	270	0.03%	0.004%
94	15.002	4243	4249	4250	rBV3	1003	869	0.11%	0.012%
95	15.160	4295	4298	4299	rBV	432	241	0.03%	0.003%
96	15.224	4306	4318	4331	rBV	87010	136459	16.89%	1.833%
97	15.410	4367	4376	4386	rVB	37413	58006	7.18%	0.779%
98	16.150	4599	4606	4614	rBV2	5015	7438	0.92%	0.100%
99	16.262	4633	4641	4651	rBV	17972	28140	3.48%	0.378%
100	16.410	4680	4687	4693	rBV2	12782	19203	2.38%	0.258%

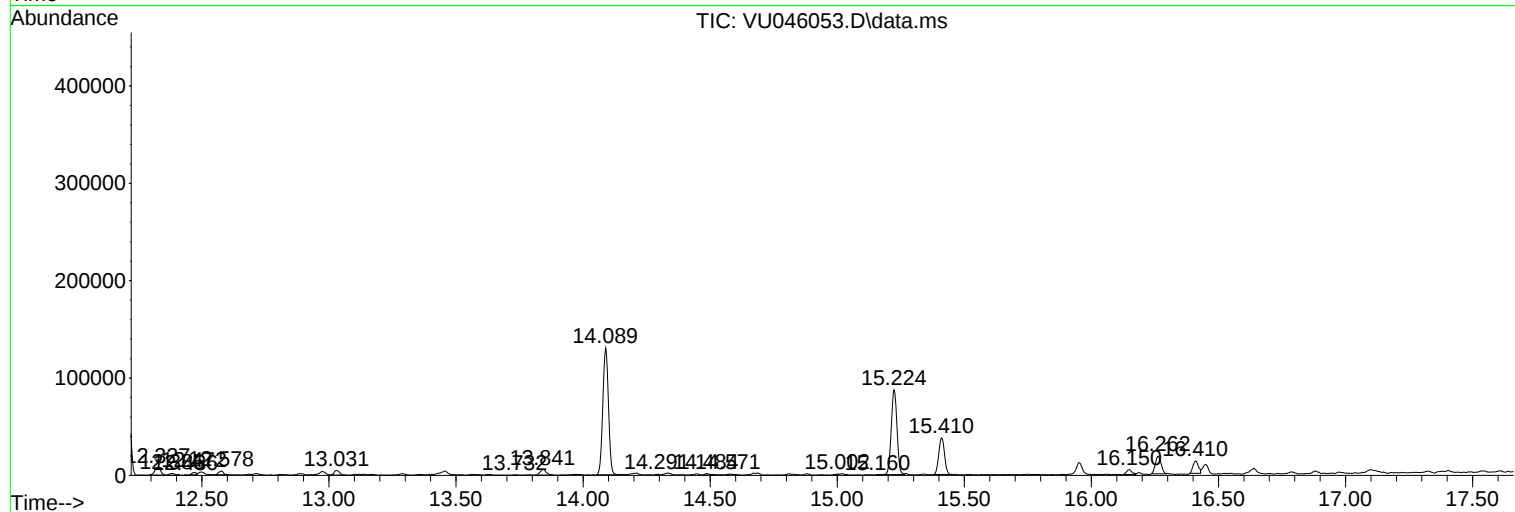
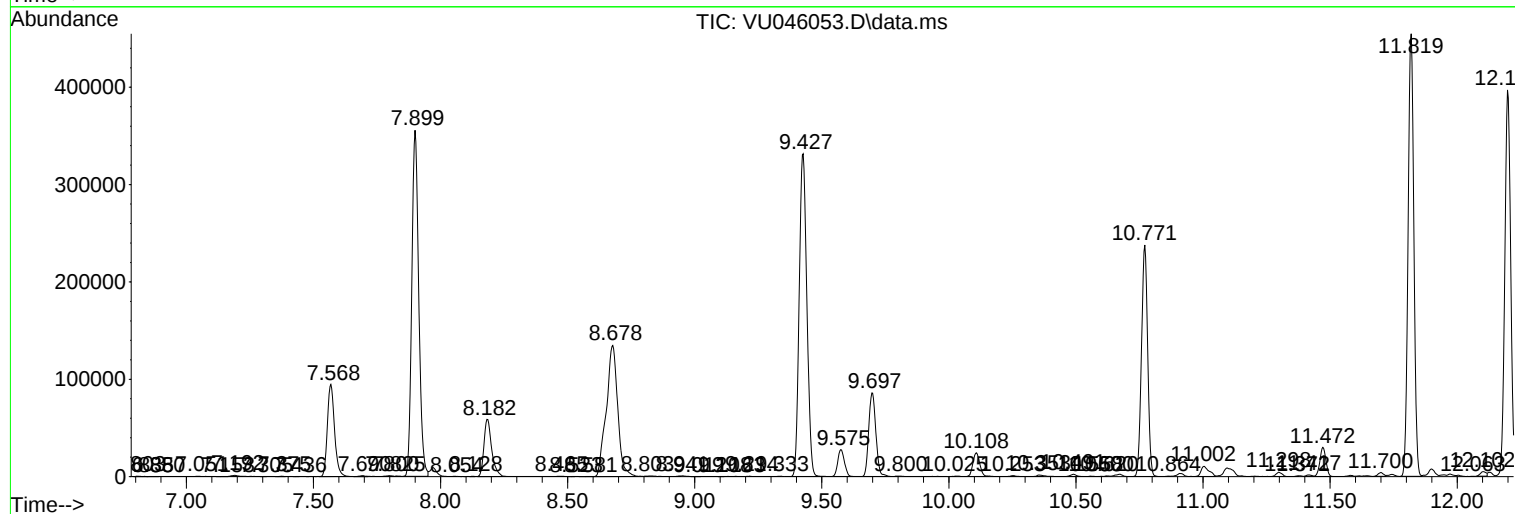
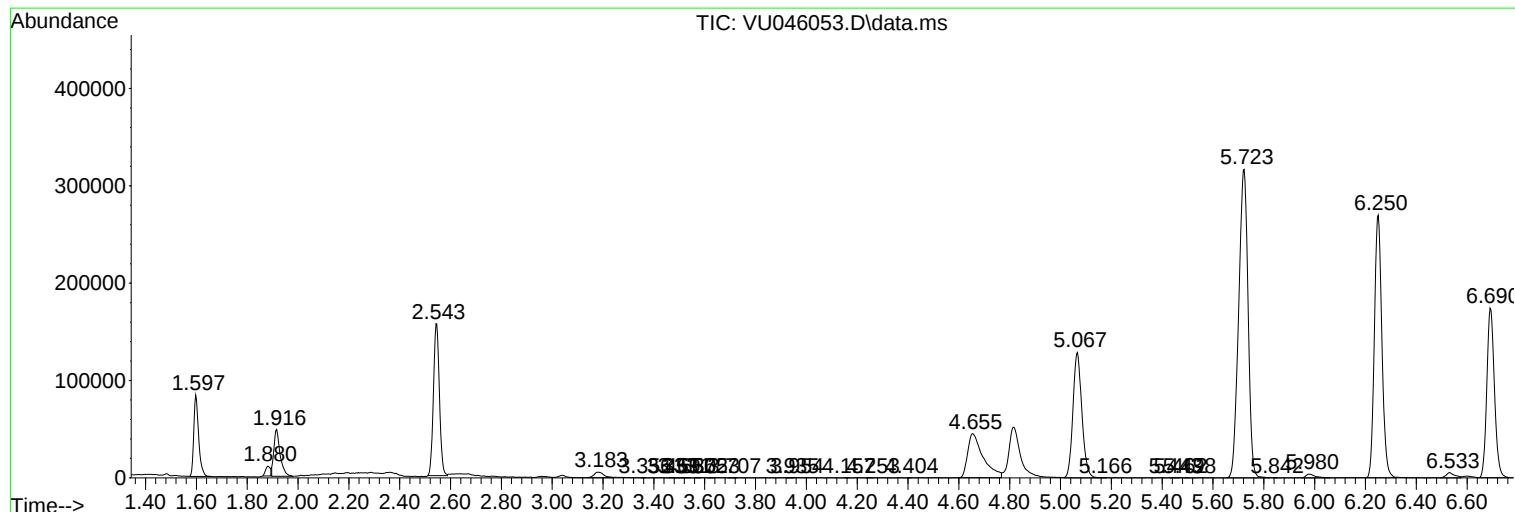
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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



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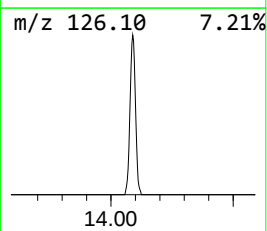
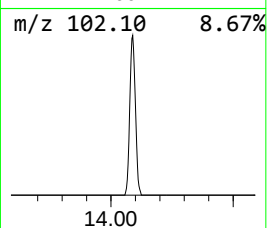
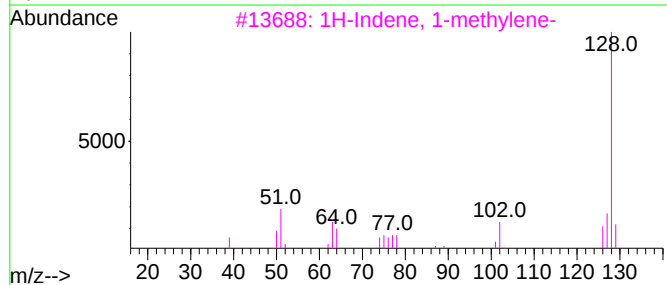
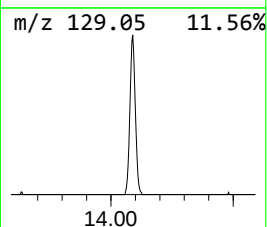
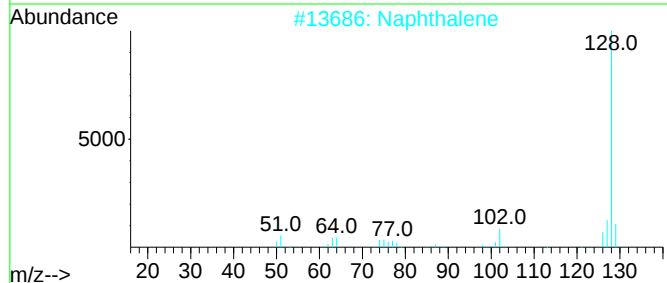
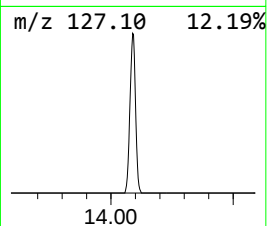
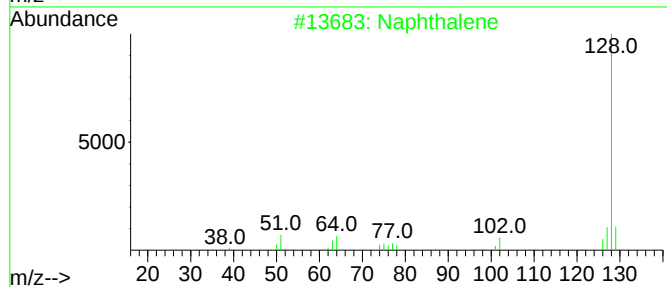
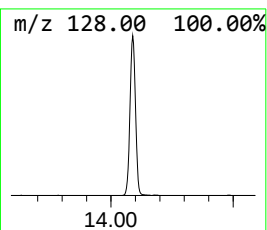
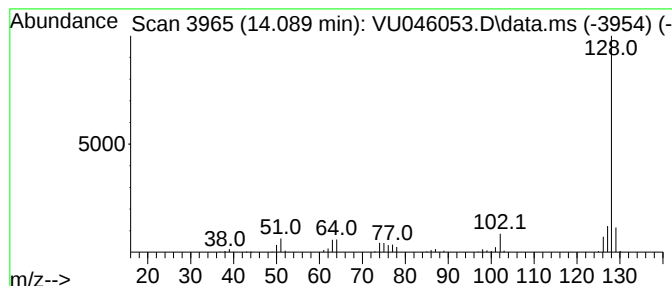
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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.
14.089	14.07 ug/L	200538	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Naphthalene	128	C10H8	000091-20-3	95
3			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	95
4			Azulene	128	C10H8	000275-51-4	94
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	14.089	14.1	ug/L	200538	3	11.819	712514	50.0