

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045239.D
 Acq On : 08 Oct 2021 10:19
 Operator : SY/MD
 Sample : VU1008MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK023

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: VU045239.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.475	36	42	54	rBV	8919	17670	1.30%	0.177%
2	1.600	74	81	93	rBV	216302	235028	17.34%	2.348%
3	1.916	170	179	192	rVB	151211	205156	15.14%	2.050%
4	2.488	353	357	362	rVB2	350	295	0.02%	0.003%
5	2.568	370	382	407	rBV	298828	495838	36.59%	4.954%
6	2.797	445	453	463	rVV2	930	1549	0.11%	0.015%
7	2.964	501	505	512	rVB2	384	392	0.03%	0.004%
8	3.051	525	532	539	rBV3	1309	2078	0.15%	0.021%
9	3.115	546	552	554	rBV2	227	243	0.02%	0.002%
10	3.189	566	575	576	rBV3	495	647	0.05%	0.006%
11	3.362	623	629	630	rBV2	503	448	0.03%	0.004%
12	3.420	644	647	651	rBV2	215	175	0.01%	0.002%
13	3.578	691	696	698	rBV2	196	194	0.01%	0.002%
14	3.594	698	701	707	rVB	246	265	0.02%	0.003%
15	3.639	713	715	720	rBV2	217	175	0.01%	0.002%
16	3.735	742	745	749	rBV2	211	218	0.02%	0.002%
17	3.925	801	804	810	rVB2	203	252	0.02%	0.003%
18	4.173	878	881	884	rBV2	208	192	0.01%	0.002%
19	4.552	994	999	1002	rBV2	189	194	0.01%	0.002%
20	4.626	1005	1022	1056	rBV	136602	330834	24.41%	3.306%
21	5.070	1139	1160	1186	rBV	237277	518340	38.25%	5.179%
22	5.218	1204	1206	1209	rVB3	539	311	0.02%	0.003%
23	5.231	1209	1210	1215	rBV3	228	174	0.01%	0.002%
24	5.292	1223	1229	1238	rVB2	646	1043	0.08%	0.010%
25	5.391	1257	1260	1268	rVB2	384	514	0.04%	0.005%
26	5.732	1343	1366	1395	rBV2	503574	1355182	100.00%	13.541%
27	6.041	1459	1462	1464	rBV2	356	226	0.02%	0.002%
28	6.253	1513	1528	1550	rBV	359409	678520	50.07%	6.780%
29	6.333	1551	1553	1556	rVB2	618	298	0.02%	0.003%
30	6.385	1566	1569	1571	rBV2	340	210	0.02%	0.002%
31	6.430	1579	1583	1585	rBV2	266	185	0.01%	0.002%
32	6.536	1605	1616	1625	rBV7	3546	6916	0.51%	0.069%
33	6.597	1632	1635	1639	rBV3	251	209	0.02%	0.002%
34	6.697	1652	1666	1694	rBV	313841	610701	45.06%	6.102%
35	6.845	1710	1712	1715	rBV3	333	186	0.01%	0.002%
36	6.893	1725	1727	1730	rVB3	411	219	0.02%	0.002%

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 Title : VOC Analysis

37	7.047	1769	1775	1777	rBV	443	441	0.03%	0.004%
38	7.092	1786	1789	1794	rVB2	220	202	0.01%	0.002%
39	7.189	1813	1819	1825	rVB2	710	940	0.07%	0.009%
40	7.285	1844	1849	1851	rBV2	223	208	0.02%	0.002%
41	7.443	1894	1898	1903	rVB2	249	244	0.02%	0.002%
42	7.472	1903	1907	1910	rBV2	190	173	0.01%	0.002%
43	7.571	1925	1938	1961	rBV	172049	302581	22.33%	3.023%
44	7.671	1965	1969	1970	rBV3	336	230	0.02%	0.002%
45	7.796	1999	2008	2018	rVB4	1649	2562	0.19%	0.026%
46	7.902	2027	2041	2056	rBV	607803	1048042	77.34%	10.472%
47	8.185	2116	2129	2155	rBV	120542	202881	14.97%	2.027%
48	8.430	2203	2205	2210	rVB	262	194	0.01%	0.002%
49	8.484	2219	2222	2226	rVB2	261	195	0.01%	0.002%
50	8.517	2226	2232	2234	rBV2	266	280	0.02%	0.003%
51	8.636	2256	2269	2305	rBV	366828	699217	51.60%	6.987%
52	8.835	2329	2331	2337	rVB	294	196	0.01%	0.002%
53	8.928	2355	2360	2362	rBV2	410	346	0.03%	0.003%
54	8.980	2372	2376	2378	rBV2	191	183	0.01%	0.002%
55	9.288	2462	2472	2475	rVB2	180	295	0.02%	0.003%
56	9.423	2500	2514	2550	rVV	513407	853161	62.96%	8.525%
57	9.574	2555	2561	2569	rVB2	1203	1612	0.12%	0.016%
58	9.703	2592	2601	2612	rVB3	2834	4461	0.33%	0.045%
59	9.809	2627	2634	2637	rBV2	227	313	0.02%	0.003%
60	10.111	2717	2728	2737	rVV6	2014	3839	0.28%	0.038%
61	10.166	2742	2745	2750	rVB2	196	175	0.01%	0.002%
62	10.201	2750	2756	2764	rBV2	260	479	0.04%	0.005%
63	10.353	2800	2803	2808	rVB2	169	186	0.01%	0.002%
64	10.488	2837	2845	2850	rBV3	1284	1720	0.13%	0.017%
65	10.587	2873	2876	2879	rBV2	269	221	0.02%	0.002%
66	10.677	2895	2904	2912	rBV2	4281	5850	0.43%	0.058%
67	10.761	2917	2930	2947	rBV	405475	661837	48.84%	6.613%
68	10.870	2959	2964	2967	rBV3	523	513	0.04%	0.005%
69	11.031	3011	3014	3018	rVV2	279	210	0.02%	0.002%
70	11.092	3026	3033	3039	rBV2	913	1411	0.10%	0.014%
71	11.153	3047	3052	3055	rBV2	345	290	0.02%	0.003%
72	11.208	3065	3069	3072	rBV	209	241	0.02%	0.002%
73	11.324	3098	3105	3112	rBV2	226	441	0.03%	0.004%
74	11.468	3138	3150	3160	rBV6	3676	6828	0.50%	0.068%
75	11.584	3182	3186	3192	rVB2	423	489	0.04%	0.005%
76	11.700	3213	3222	3229	rBV4	1542	2090	0.15%	0.021%

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

77	11.751	3231	3238	3245	rVB4	2185	2886	0.21%	0.029%
78	11.816	3246	3258	3282	rBV	484051	764750	56.43%	7.641%
79	11.947	3292	3299	3302	rBV4	1156	1433	0.11%	0.014%
80	11.979	3303	3309	3318	rVB4	2929	4085	0.30%	0.041%
81	12.047	3326	3330	3332	rBV2	227	181	0.01%	0.002%
82	12.198	3362	3377	3396	rVV	551650	886520	65.42%	8.858%
83	12.336	3415	3420	3426	rBV2	711	775	0.06%	0.008%
84	12.372	3426	3431	3436	rVB2	165	195	0.01%	0.002%
85	12.439	3450	3452	3456	rBV2	203	186	0.01%	0.002%
86	12.545	3479	3485	3487	rBV	292	271	0.02%	0.003%
87	12.825	3568	3572	3575	rBV2	191	222	0.02%	0.002%
88	13.002	3621	3627	3637	rBV5	1088	1585	0.12%	0.016%
89	13.153	3670	3674	3678	rVV2	372	329	0.02%	0.003%
90	13.224	3689	3696	3702	rBV3	3547	4975	0.37%	0.050%
91	13.378	3741	3744	3749	rBV2	179	218	0.02%	0.002%
92	13.603	3811	3814	3821	rVB2	224	193	0.01%	0.002%
93	13.844	3881	3889	3899	rVV3	7770	11455	0.85%	0.114%
94	14.092	3956	3966	3985	rVB	24354	38638	2.85%	0.386%
95	14.333	4032	4041	4055	rBV2	10498	16555	1.22%	0.165%
96	14.504	4090	4094	4098	rVB2	313	291	0.02%	0.003%
97	14.584	4116	4119	4122	rBV	317	205	0.02%	0.002%
98	14.970	4234	4239	4241	rBV3	355	375	0.03%	0.004%
99	15.147	4287	4294	4298	rVB3	359	500	0.04%	0.005%
100	15.253	4324	4327	4332	rBV2	304	358	0.03%	0.004%

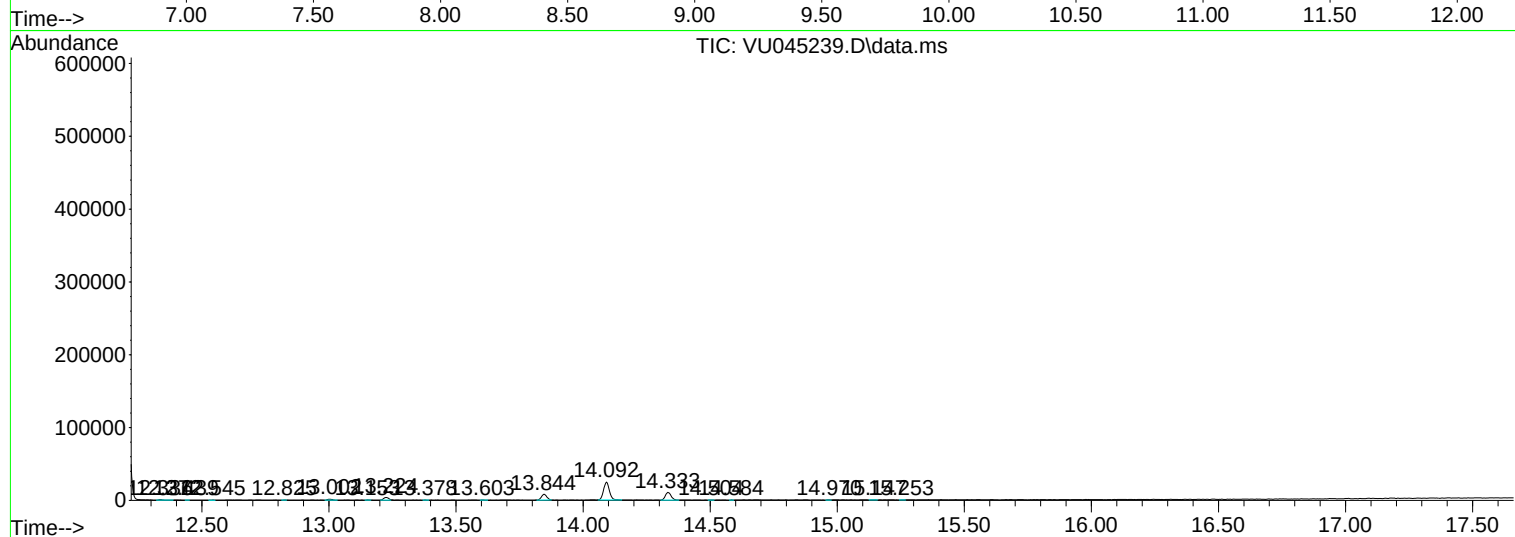
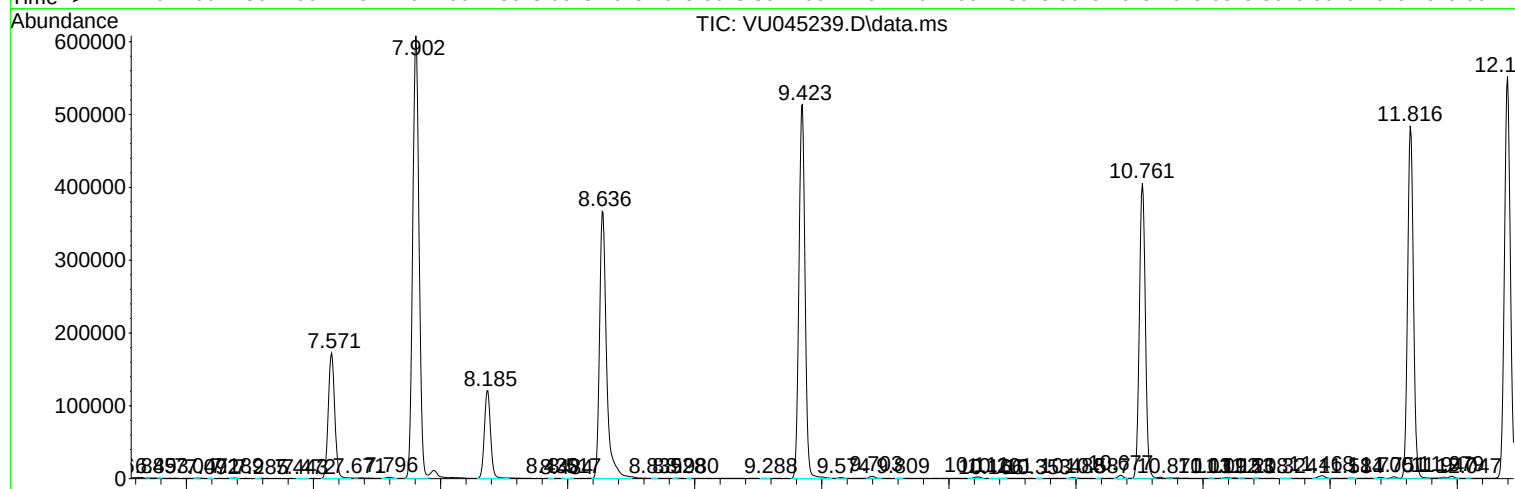
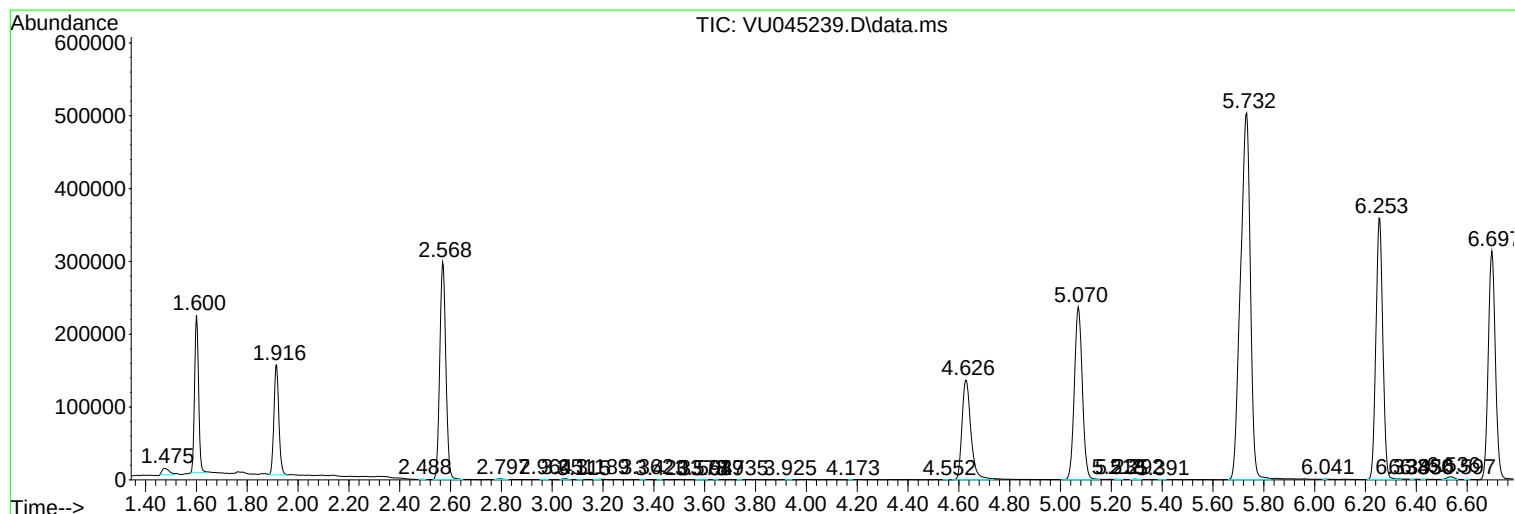
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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



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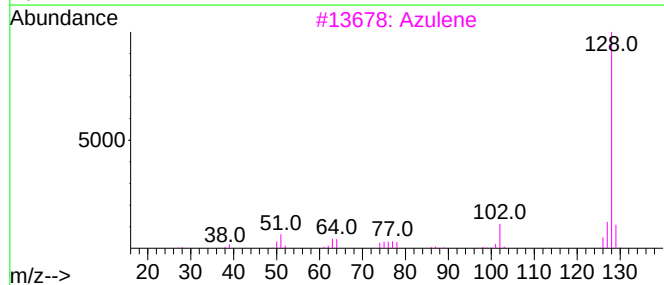
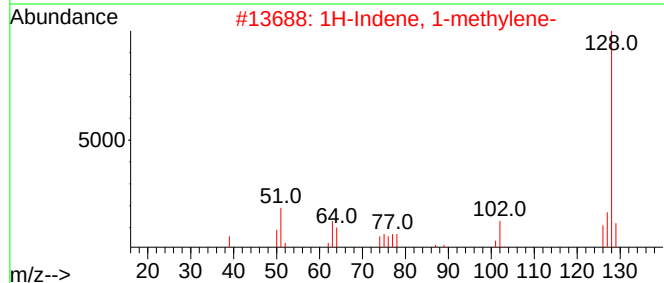
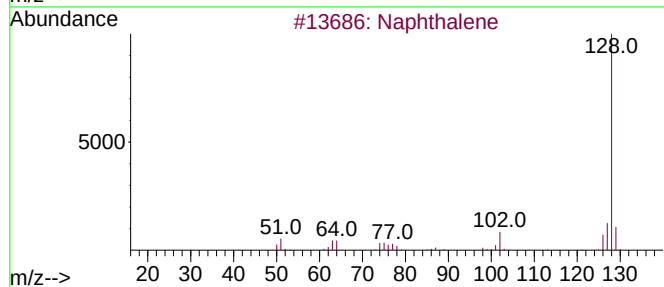
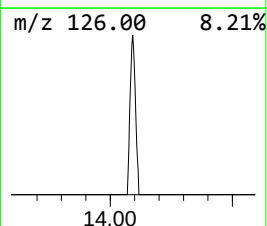
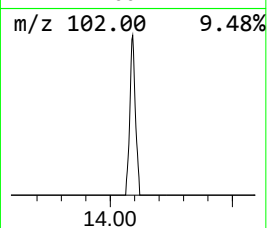
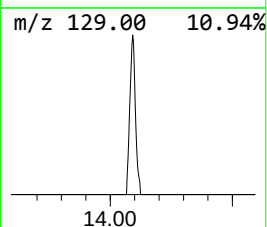
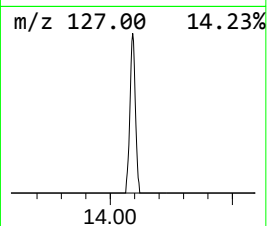
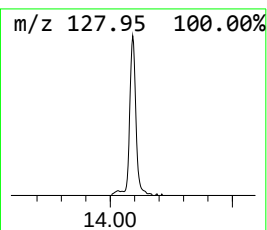
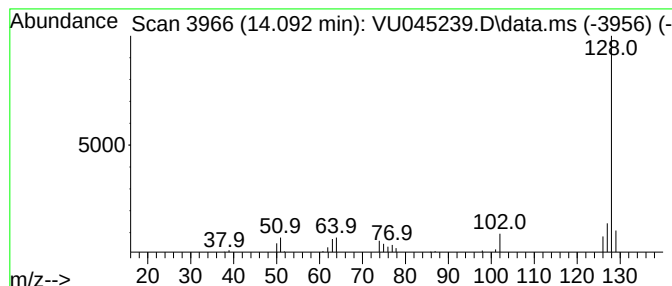
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.092	2.53 ug/L	38638	1,4-Dichlorobenzene-d4	11.816

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	94
3			Azulene	128	C10H8	000275-51-4	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	14.092	2.5	ug/L	38638	3	11.816	764750	50.0