

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046141.D
 Acq On : 07 Dec 2021 15:25
 Operator : SY/MD
 Sample : M4960-01 10X
 Misc : 6.06g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 15 Sample Multiplier: 1

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: VU046141.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	74	81	94	rVB	117224	129604	14.51%	1.724%
2	1.919	171	180	194	rVB	82277	107308	12.02%	1.428%
3	2.086	226	232	234	rBV3	646	762	0.09%	0.010%
4	2.314	301	303	306	rVB2	427	188	0.02%	0.003%
5	2.568	368	382	424	rBV	193962	328083	36.74%	4.365%
6	2.793	447	452	454	rBV2	269	243	0.03%	0.003%
7	2.954	499	502	509	rVB	223	265	0.03%	0.004%
8	3.047	525	531	532	rBV	1009	979	0.11%	0.013%
9	3.189	562	575	593	rBV	9267	22908	2.57%	0.305%
10	3.469	656	662	665	rBB	164	212	0.02%	0.003%
11	3.684	724	729	732	rBB	260	204	0.02%	0.003%
12	3.719	736	740	745	rBV	185	258	0.03%	0.003%
13	3.854	779	782	788	rBV	160	227	0.03%	0.003%
14	4.343	930	934	936	rBV2	228	190	0.02%	0.003%
15	4.398	946	951	954	rBV	172	195	0.02%	0.003%
16	4.639	1010	1026	1063	rBV2	70893	225850	25.29%	3.005%
17	5.067	1143	1159	1182	rBV	148672	338316	37.88%	4.501%
18	5.488	1283	1290	1293	rBB	161	226	0.03%	0.003%
19	5.726	1342	1364	1390	rBV2	332058	893025	100.00%	11.881%
20	5.973	1434	1441	1447	rVB4	903	1064	0.12%	0.014%
21	6.102	1478	1481	1486	rBV2	262	274	0.03%	0.004%
22	6.250	1512	1527	1549	rVV	290992	552163	61.83%	7.346%
23	6.404	1570	1575	1578	rBV2	214	218	0.02%	0.003%
24	6.533	1608	1615	1626	rBV2	1753	2856	0.32%	0.038%
25	6.694	1650	1665	1681	rBV	201095	386406	43.27%	5.141%
26	6.803	1695	1699	1701	rBV2	289	213	0.02%	0.003%
27	6.816	1701	1703	1709	rVB	315	184	0.02%	0.002%
28	7.038	1768	1772	1777	rBV2	211	239	0.03%	0.003%
29	7.189	1812	1819	1822	rVB2	269	325	0.04%	0.004%
30	7.362	1869	1873	1877	rBV	147	198	0.02%	0.003%
31	7.565	1921	1936	1956	rBV	119215	207781	23.27%	2.764%
32	7.681	1967	1972	1977	rBV2	349	401	0.04%	0.005%
33	7.700	1977	1978	1982	rVB	287	178	0.02%	0.002%
34	7.787	1995	2005	2014	rBB3	1177	2017	0.23%	0.027%
35	7.899	2025	2040	2055	rBV	442416	759607	85.06%	10.106%
36	7.970	2056	2062	2078	rVB	13027	21615	2.42%	0.288%

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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

37	8.179	2115	2127	2148	rBV	81626	136954	15.34%	1.822%
38	8.472	2212	2218	2220	rBV	588	446	0.05%	0.006%
39	8.555	2235	2244	2251	rBV6	2302	3672	0.41%	0.049%
40	8.636	2257	2269	2302	rBV	257512	479066	53.65%	6.374%
41	8.755	2304	2306	2316	rVB2	467	426	0.05%	0.006%
42	8.912	2348	2355	2363	rBV2	1172	1910	0.21%	0.025%
43	9.417	2500	2512	2538	rBV	413683	701389	78.54%	9.332%
44	9.571	2551	2560	2575	rBB	3916	6255	0.70%	0.083%
45	9.693	2589	2598	2612	rVV2	10275	16300	1.83%	0.217%
46	10.105	2715	2726	2737	rVB5	4103	6732	0.75%	0.090%
47	10.488	2837	2845	2850	rBV2	657	940	0.11%	0.013%
48	10.568	2862	2870	2881	rVB4	5368	8231	0.92%	0.110%
49	10.674	2894	2903	2911	rBV3	2608	3926	0.44%	0.052%
50	10.758	2915	2929	2947	rBV	303979	478413	53.57%	6.365%
51	10.877	2957	2966	2967	rBV2	536	683	0.08%	0.009%
52	10.893	2967	2971	2980	rVB3	1099	1612	0.18%	0.021%
53	10.996	2995	3003	3020	rVB3	1130	2290	0.26%	0.030%
54	11.095	3026	3034	3038	rBV3	1010	1423	0.16%	0.019%
55	11.205	3064	3068	3074	rVB	259	239	0.03%	0.003%
56	11.291	3090	3095	3103	rVB2	572	782	0.09%	0.010%
57	11.465	3140	3149	3160	rVB5	5633	9464	1.06%	0.126%
58	11.581	3179	3185	3190	rVB3	845	970	0.11%	0.013%
59	11.697	3213	3221	3228	rVB3	1107	1644	0.18%	0.022%
60	11.812	3244	3257	3277	rBV	486822	771337	86.37%	10.262%
61	11.941	3293	3297	3301	rBV3	964	1133	0.13%	0.015%
62	11.970	3302	3306	3316	rVB3	2532	3316	0.37%	0.044%
63	12.060	3324	3334	3340	rBV6	1736	2755	0.31%	0.037%
64	12.121	3350	3353	3357	rBV3	213	195	0.02%	0.003%
65	12.192	3361	3375	3391	rVV	458249	735167	82.32%	9.781%
66	12.275	3397	3401	3407	rBV3	230	247	0.03%	0.003%
67	12.330	3412	3418	3424	rVB5	897	1232	0.14%	0.016%
68	12.398	3435	3439	3446	rVB3	779	757	0.08%	0.010%
69	12.465	3456	3460	3462	rBV	313	221	0.02%	0.003%
70	12.558	3486	3489	3493	rVV3	582	482	0.05%	0.006%
71	12.581	3493	3496	3499	rVB	280	215	0.02%	0.003%
72	12.635	3509	3513	3521	rBV2	492	563	0.06%	0.007%
73	12.774	3548	3556	3564	rBV3	840	1330	0.15%	0.018%
74	12.889	3588	3592	3597	rVB2	287	291	0.03%	0.004%
75	12.947	3605	3610	3617	rBV2	1005	1392	0.16%	0.019%
76	12.980	3617	3620	3621	rBV	441	213	0.02%	0.003%

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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

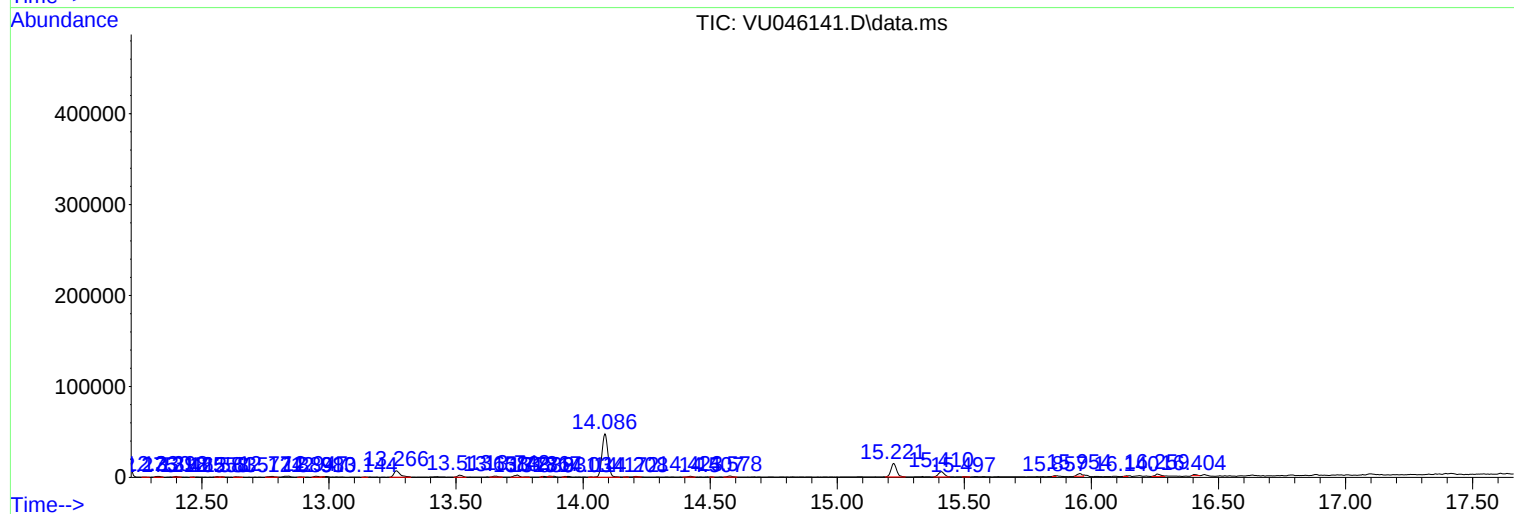
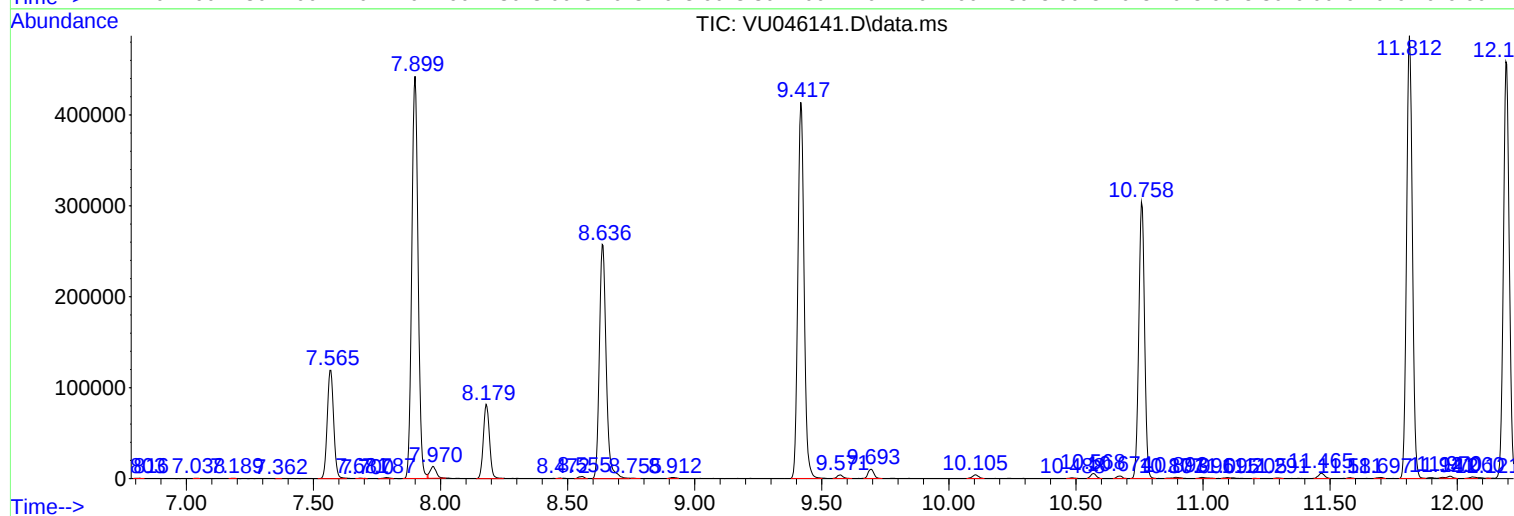
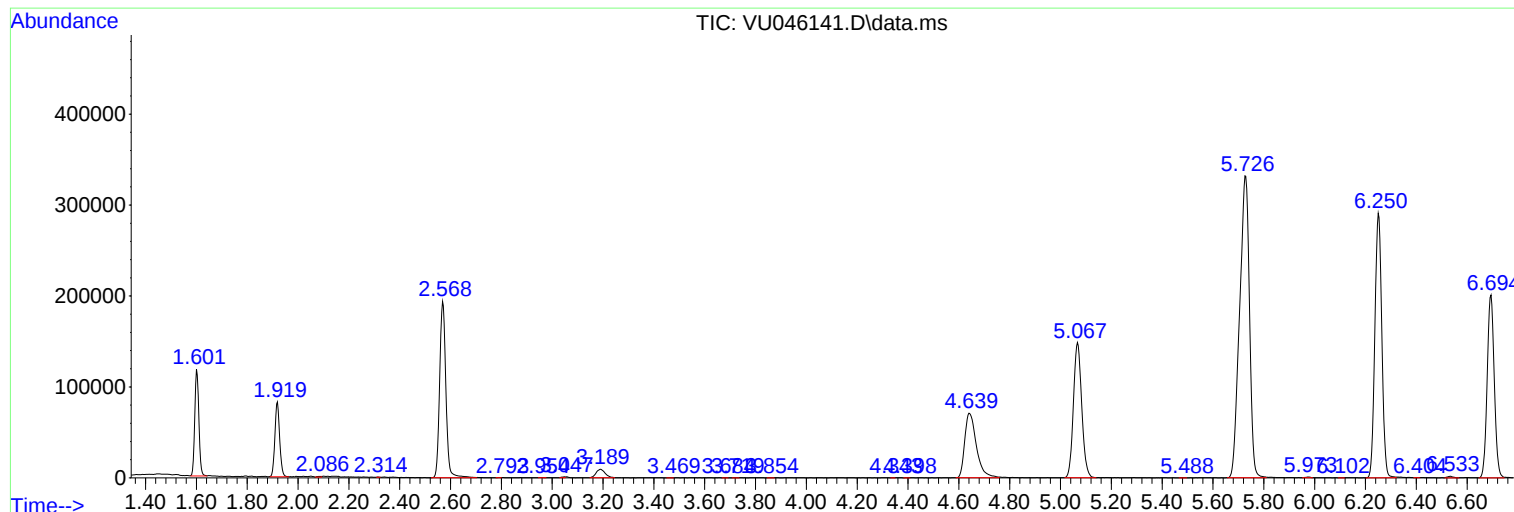
77	13.144	3666	3671	3674	rBV3	359	258	0.03%	0.003%
78	13.266	3701	3709	3727	rVB2	6999	12540	1.40%	0.167%
79	13.513	3779	3786	3794	rBV5	2170	3007	0.34%	0.040%
80	13.658	3823	3831	3839	rBV3	1080	1602	0.18%	0.021%
81	13.742	3849	3857	3863	rVB6	2330	3164	0.35%	0.042%
82	13.777	3863	3868	3872	rBV2	248	337	0.04%	0.004%
83	13.838	3884	3887	3888	rBV	772	369	0.04%	0.005%
84	13.867	3893	3896	3900	rVV3	716	636	0.07%	0.008%
85	13.931	3911	3916	3917	rBV2	665	529	0.06%	0.007%
86	14.034	3944	3948	3950	rVB2	331	190	0.02%	0.003%
87	14.086	3950	3964	3982	rBV	47658	76857	8.61%	1.023%
88	14.172	3986	3991	3993	rBV3	275	276	0.03%	0.004%
89	14.208	3999	4002	4009	rVB2	565	553	0.06%	0.007%
90	14.423	4059	4069	4075	rVB2	911	1136	0.13%	0.015%
91	14.507	4092	4095	4098	rVB2	388	234	0.03%	0.003%
92	14.578	4109	4117	4126	rBV2	1244	1689	0.19%	0.022%
93	15.221	4307	4317	4332	rVB	14843	22682	2.54%	0.302%
94	15.410	4366	4376	4386	rBV	5754	9171	1.03%	0.122%
95	15.497	4401	4403	4411	rBV2	331	363	0.04%	0.005%
96	15.857	4511	4515	4516	rBV3	1035	671	0.08%	0.009%
97	15.954	4538	4545	4550	rBV3	3006	4240	0.47%	0.056%
98	16.140	4598	4603	4604	rBV4	820	580	0.06%	0.008%
99	16.259	4633	4640	4649	rBV6	2715	4274	0.48%	0.057%
100	16.404	4682	4685	4692	rBV4	1346	1473	0.16%	0.020%

Sum of corrected areas: 7516226

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ALS Vial : 15 Sample Multiplier: 1

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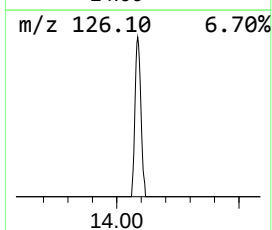
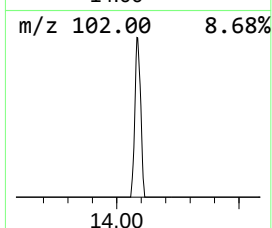
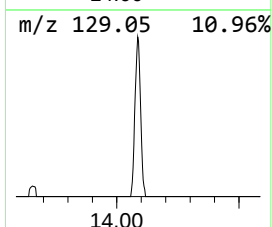
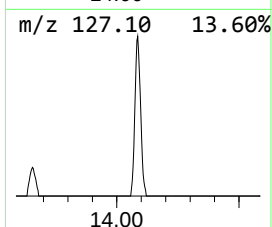
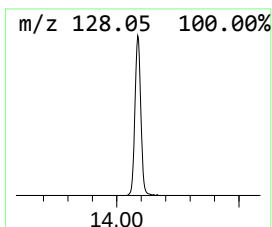
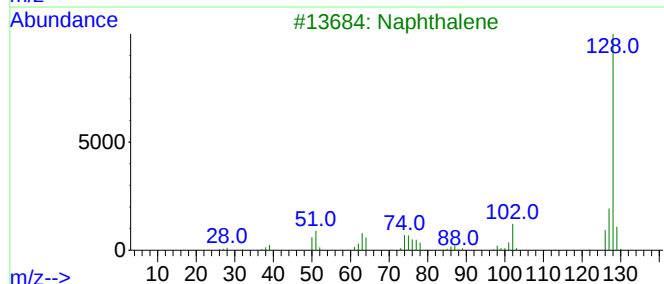
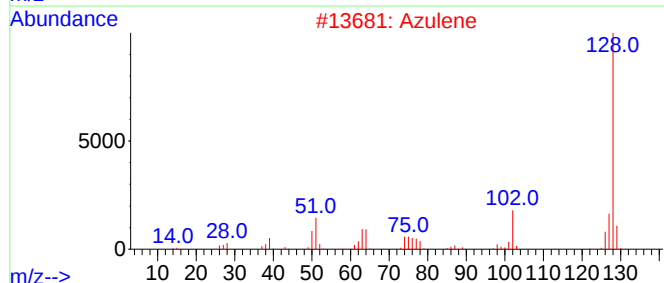
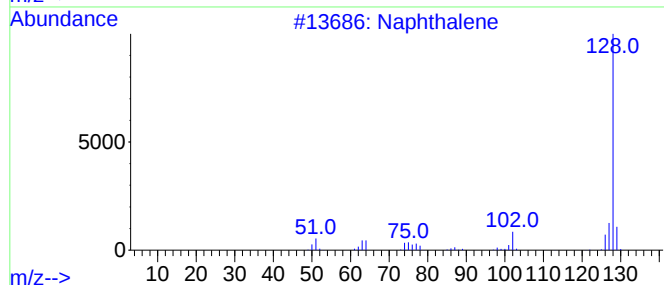
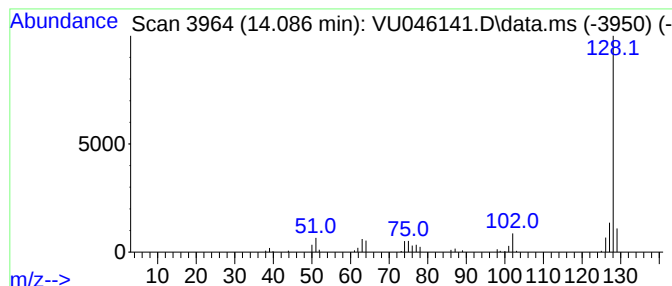
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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.
14.086	4.98 ug/L	76857	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	91
3			Naphthalene	128	C10H8	000091-20-3	91
4			Azulene	128	C10H8	000275-51-4	90
5			Naphthalene	128	C10H8	000091-20-3	90



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Azulene	14.086	5.0	ug/L	76857	3	11.812	771337	50.0