

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
 Data File : VU046172.D
 Acq On : 08 Dec 2021 13:58
 Operator : SY/MD
 Sample : M4887-04ME
 Misc : 5.31g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX8A1ME

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: VU046172.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	73	81	98	rVB	119947	155012	13.44%	1.555%
2	1.919	170	180	199	rVB	74234	123027	10.67%	1.234%
3	2.121	237	243	244	rBV4	491	439	0.04%	0.004%
4	2.192	257	265	273	rBV7	1646	2776	0.24%	0.028%
5	2.340	307	311	312	rBV3	389	296	0.03%	0.003%
6	2.433	338	340	344	rBV4	571	463	0.04%	0.005%
7	2.488	353	357	361	rBV5	681	582	0.05%	0.006%
8	2.549	364	376	389	rBV	173576	289552	25.11%	2.905%
9	4.655	1016	1031	1080	rBV	60056	264664	22.95%	2.655%
10	5.067	1144	1159	1186	rVB3	175250	443928	38.50%	4.454%
11	5.723	1343	1363	1392	rBV2	446286	1152981	100.00%	11.568%
12	5.986	1437	1445	1461	rVB5	4199	9683	0.84%	0.097%
13	6.250	1513	1527	1547	rBV	260763	533158	46.24%	5.349%
14	6.539	1605	1617	1632	rBV	87242	170141	14.76%	1.707%
15	6.690	1650	1664	1691	rVB	248505	509906	44.23%	5.116%
16	6.944	1739	1743	1745	rBV2	540	504	0.04%	0.005%
17	7.038	1769	1772	1775	rBV	521	443	0.04%	0.004%
18	7.115	1793	1796	1800	rBV2	355	355	0.03%	0.004%
19	7.314	1853	1858	1860	rBV	360	374	0.03%	0.004%
20	7.346	1866	1868	1871	rBV	462	335	0.03%	0.003%
21	7.459	1897	1903	1907	rBV2	534	671	0.06%	0.007%
22	7.568	1924	1937	1961	rBV	138133	274004	23.76%	2.749%
23	7.690	1973	1975	1982	rBV4	384	324	0.03%	0.003%
24	7.793	1997	2007	2019	rVB5	2304	4857	0.42%	0.049%
25	7.899	2024	2040	2057	rBV	515499	974869	84.55%	9.781%
26	8.022	2076	2078	2084	rVB2	692	592	0.05%	0.006%
27	8.092	2098	2100	2106	rVB	525	465	0.04%	0.005%
28	8.182	2113	2128	2155	rVV	81308	185701	16.11%	1.863%
29	8.282	2155	2159	2164	rVB	563	491	0.04%	0.005%
30	8.308	2164	2167	2170	rVB	614	383	0.03%	0.004%
31	8.327	2170	2173	2176	rBV	444	408	0.04%	0.004%
32	8.362	2181	2184	2189	rBV2	546	525	0.05%	0.005%
33	8.555	2230	2244	2261	rBV	574323	1013924	87.94%	10.173%
34	8.684	2261	2284	2316	rVB	192205	606511	52.60%	6.085%
35	8.883	2341	2346	2349	rVB2	425	334	0.03%	0.003%
36	8.948	2361	2366	2367	rBV2	551	483	0.04%	0.005%

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

37	9.076	2403	2406	2412	rVB	541	429	0.04%	0.004%
38	9.243	2453	2458	2461	rBV	543	409	0.04%	0.004%
39	9.298	2472	2475	2478	rBV	398	290	0.03%	0.003%
40	9.427	2499	2515	2542	rVV	295437	676195	58.65%	6.785%
41	9.571	2553	2560	2572	rBV3	2500	4648	0.40%	0.047%
42	9.700	2592	2600	2616	rVB3	7264	14058	1.22%	0.141%
43	9.796	2622	2630	2632	rBV	713	858	0.07%	0.009%
44	9.874	2647	2654	2657	rBV	741	956	0.08%	0.010%
45	10.057	2709	2711	2715	rVB	494	335	0.03%	0.003%
46	10.118	2715	2730	2743	rVB5	2718	5747	0.50%	0.058%
47	10.230	2761	2765	2768	rBV2	450	383	0.03%	0.004%
48	10.253	2768	2772	2776	rBV	632	627	0.05%	0.006%
49	10.324	2790	2794	2798	rVV2	378	315	0.03%	0.003%
50	10.443	2828	2831	2838	rVB2	564	632	0.05%	0.006%
51	10.494	2841	2847	2850	rBV	518	527	0.05%	0.005%
52	10.523	2853	2856	2858	rBV	431	291	0.03%	0.003%
53	10.581	2869	2874	2877	rBV	421	367	0.03%	0.004%
54	10.616	2882	2885	2888	rVV2	490	378	0.03%	0.004%
55	10.671	2891	2902	2913	rVV3	4193	7190	0.62%	0.072%
56	10.774	2920	2934	2951	rBV	364800	600257	52.06%	6.023%
57	10.989	2996	3001	3004	rBV	716	698	0.06%	0.007%
58	11.115	3025	3040	3050	rBV8	4141	8222	0.71%	0.082%
59	11.198	3063	3066	3071	rVV3	354	424	0.04%	0.004%
60	11.369	3117	3119	3124	rVB2	497	334	0.03%	0.003%
61	11.414	3130	3133	3139	rVV4	864	1073	0.09%	0.011%
62	11.468	3140	3150	3163	rVB5	5588	12203	1.06%	0.122%
63	11.546	3168	3174	3179	rBV4	1194	1673	0.15%	0.017%
64	11.648	3201	3206	3207	rBV	478	337	0.03%	0.003%
65	11.697	3213	3221	3229	rBV6	2225	3697	0.32%	0.037%
66	11.742	3229	3235	3246	rVB5	1779	2663	0.23%	0.027%
67	11.819	3246	3259	3272	rBV	447072	707369	61.35%	7.097%
68	11.941	3293	3297	3299	rBV5	1091	936	0.08%	0.009%
69	12.002	3314	3316	3322	rVB4	1324	1014	0.09%	0.010%
70	12.073	3330	3338	3344	rBV4	2709	4616	0.40%	0.046%
71	12.201	3364	3378	3392	rVB	559146	906058	78.58%	9.091%
72	12.272	3396	3400	3407	rVB5	886	1135	0.10%	0.011%
73	12.327	3407	3417	3428	rBV5	9615	15398	1.34%	0.154%
74	12.378	3431	3433	3435	rBV2	600	319	0.03%	0.003%
75	12.652	3516	3518	3520	rBV3	484	296	0.03%	0.003%
76	12.732	3540	3543	3545	rBV3	440	298	0.03%	0.003%

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 Title : VOC Analysis

77	13.047	3632	3641	3646	rBV7	2535	3958	0.34%	0.040%
78	13.137	3660	3669	3676	rBV5	2025	3643	0.32%	0.037%
79	13.195	3684	3687	3693	rBV4	401	464	0.04%	0.005%
80	13.227	3694	3697	3700	rVB2	707	386	0.03%	0.004%
81	13.430	3752	3760	3771	rBV3	11666	18378	1.59%	0.184%
82	13.523	3785	3789	3792	rVB3	913	636	0.06%	0.006%
83	13.587	3800	3809	3817	rBV3	6461	9634	0.84%	0.097%
84	13.626	3818	3821	3828	rVB4	1758	1992	0.17%	0.020%
85	13.661	3828	3832	3835	rBV4	858	713	0.06%	0.007%
86	13.709	3844	3847	3850	rVB4	534	308	0.03%	0.003%
87	13.803	3872	3876	3877	rBV3	572	378	0.03%	0.004%
88	13.877	3896	3899	3900	rBV2	797	532	0.05%	0.005%
89	13.967	3924	3927	3929	rBV4	1062	684	0.06%	0.007%
90	14.041	3946	3950	3951	rBV	1314	879	0.08%	0.009%
91	14.089	3956	3965	3981	rVB	36289	57784	5.01%	0.580%
92	14.192	3987	3997	4005	rBV6	9914	15833	1.37%	0.159%
93	14.449	4071	4077	4089	rVB2	22950	30874	2.68%	0.310%
94	15.217	4306	4316	4327	rVB3	10858	20606	1.79%	0.207%
95	15.375	4360	4365	4368	rBV4	9642	11394	0.99%	0.114%
96	15.745	4478	4480	4483	rBV3	1253	853	0.07%	0.009%
97	16.192	4613	4619	4630	rVB10	7028	10349	0.90%	0.104%
98	16.410	4681	4687	4693	rBV3	9535	12603	1.09%	0.126%
99	17.375	4982	4987	4996	rVB2	17236	23427	2.03%	0.235%
100	17.539	5030	5038	5050	rBV2	20378	33593	2.91%	0.337%

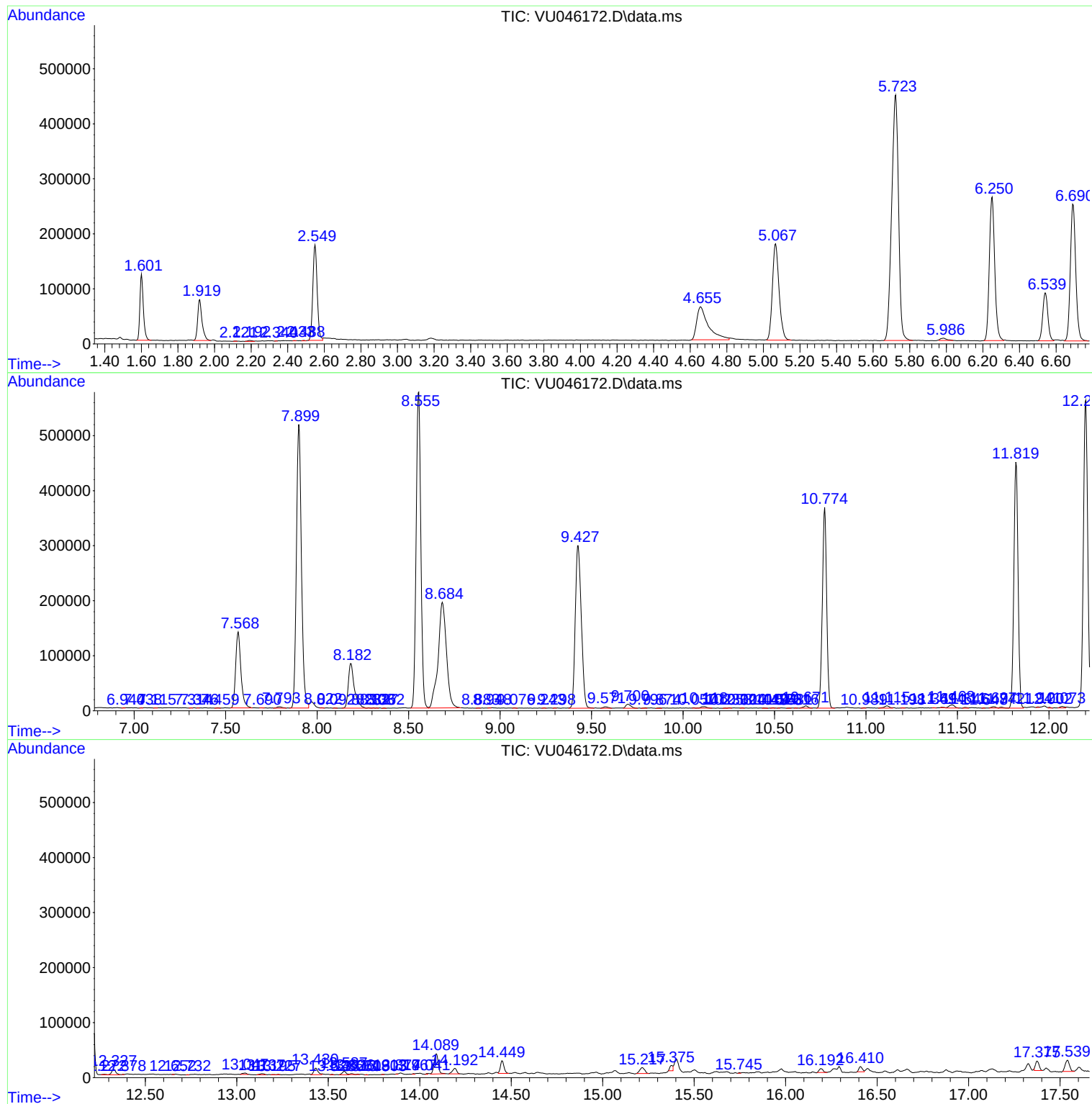
Sum of corrected areas: 9966717

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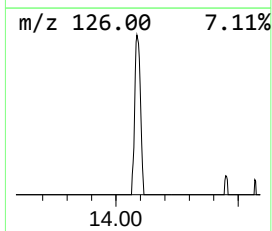
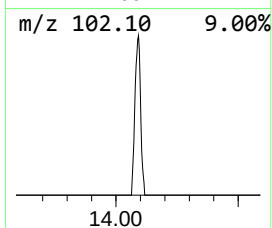
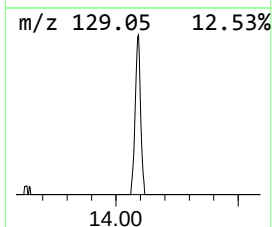
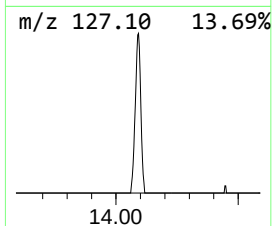
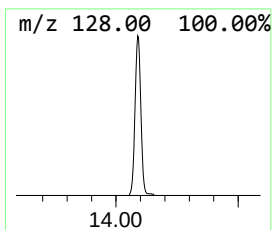
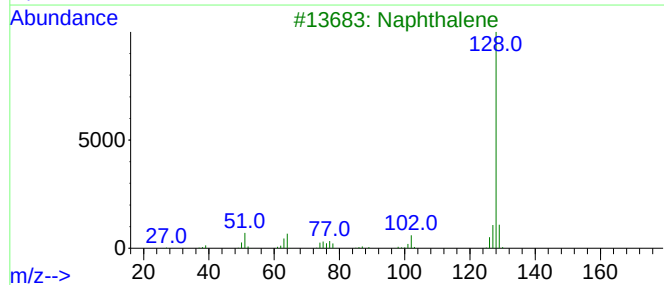
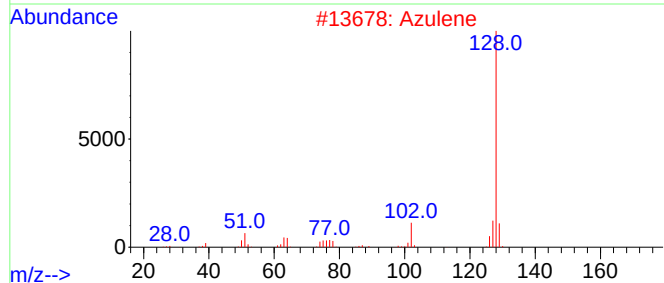
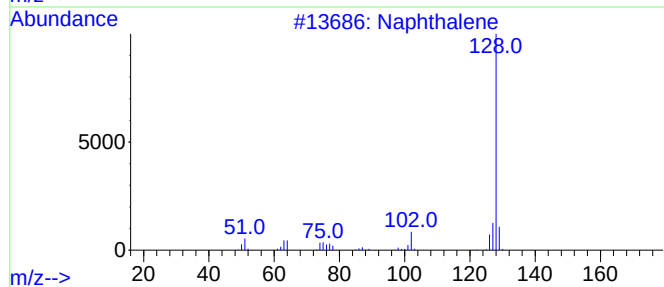
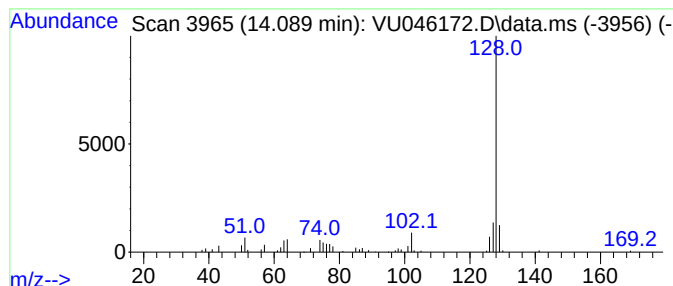
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.089	4.08 ug/L	57784	1,4-Dichlorobenzene-d4	11.822

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	94
4			Naphthalene	128	C10H8	000091-20-3	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	4.1	ug/L	57784	3	11.822	707369	50.0