

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042522\
 Data File : VU048279.D
 Acq On : 25 Apr 2022 19:39
 Operator : SY/MD
 Sample : N2469-05ME
 Misc : 3.27g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFFG7ME

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\SFAMULM042522WMA.M
 Title : VOC Analysis

Signal : TIC: VU048279.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.479	36	43	50	rBV2	7256	11317	0.57%	0.075%
2	1.598	72	80	112	rVB	117737	299688	15.14%	1.990%
3	1.871	162	165	172	rBV	30091	27465	1.39%	0.182%
4	2.479	352	354	358	rVB4	711	423	0.02%	0.003%
5	2.533	358	371	384	rBV	328972	584447	29.54%	3.882%
6	2.816	456	459	462	rBV2	394	236	0.01%	0.002%
7	2.887	478	481	483	rBV	440	296	0.01%	0.002%
8	2.958	493	503	516	rBV2	3452	7299	0.37%	0.048%
9	3.022	520	523	524	rBV2	761	469	0.02%	0.003%
10	3.099	545	547	552	rVB	380	290	0.01%	0.002%
11	3.180	552	572	588	rBV	29804	76881	3.89%	0.511%
12	3.488	660	668	670	rBV3	300	408	0.02%	0.003%
13	3.556	684	689	692	rVB2	410	341	0.02%	0.002%
14	3.591	692	700	707	rBV3	393	532	0.03%	0.004%
15	4.080	849	852	858	rVV2	197	233	0.01%	0.002%
16	4.636	1010	1025	1082	rBV	162197	576143	29.12%	3.826%
17	5.061	1140	1157	1190	rBV	314245	755797	38.19%	5.020%
18	5.192	1196	1198	1201	rVB3	491	234	0.01%	0.002%
19	5.279	1221	1225	1230	rBV3	506	651	0.03%	0.004%
20	5.716	1336	1361	1398	rBV2	766541	1978799	100.00%	13.142%
21	5.974	1430	1441	1468	rBV3	13439	33521	1.69%	0.223%
22	6.173	1499	1503	1509	rVB3	238	259	0.01%	0.002%
23	6.247	1509	1526	1556	rBV	445892	909823	45.98%	6.043%
24	6.520	1603	1611	1624	rBV9	5822	12599	0.64%	0.084%
25	6.597	1627	1635	1649	rVV3	6322	14009	0.71%	0.093%
26	6.691	1649	1664	1690	rVB	437627	914827	46.23%	6.076%
27	6.781	1690	1692	1694	rBV3	530	388	0.02%	0.003%
28	6.967	1747	1750	1759	rVB3	459	556	0.03%	0.004%
29	7.057	1766	1778	1781	rBV3	1188	1988	0.10%	0.013%
30	7.112	1791	1795	1798	rBV	277	241	0.01%	0.002%
31	7.192	1807	1820	1826	rBV3	9182	20630	1.04%	0.137%
32	7.298	1850	1853	1854	rBV2	462	255	0.01%	0.002%
33	7.504	1909	1917	1921	rBV3	643	834	0.04%	0.006%
34	7.565	1921	1936	1960	rBV	217128	432426	21.85%	2.872%
35	7.694	1966	1976	1979	rBV5	2329	3223	0.16%	0.021%
36	7.787	2002	2005	2011	rVB3	1351	1171	0.06%	0.008%

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Integrator: RTE

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 Title : VOC Analysis

37	7.896	2024	2039	2056	rBV	862577	1565401	79.11%	10.397%
38	8.183	2115	2128	2154	rVV	136248	289170	14.61%	1.921%
39	8.282	2157	2159	2163	rBV3	398	262	0.01%	0.002%
40	8.327	2168	2173	2174	rBV2	403	283	0.01%	0.002%
41	8.347	2175	2179	2181	rBV4	1496	1196	0.06%	0.008%
42	8.437	2205	2207	2210	rVV2	402	237	0.01%	0.002%
43	8.472	2213	2218	2226	rBV4	838	1126	0.06%	0.007%
44	8.655	2257	2275	2306	rBV	586930	1306060	66.00%	8.674%
45	8.890	2346	2348	2352	rVB3	414	243	0.01%	0.002%
46	8.999	2378	2382	2386	rVB2	439	409	0.02%	0.003%
47	9.070	2399	2404	2409	rVB3	398	401	0.02%	0.003%
48	9.298	2471	2475	2480	rVB3	267	282	0.01%	0.002%
49	9.420	2498	2513	2551	rVB	605532	1169438	59.10%	7.767%
50	9.568	2554	2559	2562	rBV3	862	869	0.04%	0.006%
51	9.629	2575	2578	2585	rVB2	242	244	0.01%	0.002%
52	9.684	2590	2595	2597	rBV2	874	798	0.04%	0.005%
53	9.703	2598	2601	2610	rVB3	1477	1499	0.08%	0.010%
54	10.138	2734	2736	2740	rVB3	468	289	0.01%	0.002%
55	10.192	2749	2753	2756	rBV	321	289	0.01%	0.002%
56	10.269	2771	2777	2781	rBV2	252	296	0.01%	0.002%
57	10.462	2834	2837	2838	rBV	462	339	0.02%	0.002%
58	10.530	2856	2858	2859	rBV2	654	243	0.01%	0.002%
59	10.601	2874	2880	2882	rBV2	456	443	0.02%	0.003%
60	10.623	2882	2887	2891	rVV5	653	661	0.03%	0.004%
61	10.671	2891	2902	2915	rVB3	6258	11126	0.56%	0.074%
62	10.764	2915	2931	2949	rBV	775630	1266911	64.02%	8.414%
63	10.867	2957	2963	2965	rBV3	1032	1084	0.05%	0.007%
64	10.896	2968	2972	2979	rVB6	2244	2673	0.14%	0.018%
65	10.954	2987	2990	2995	rBV2	264	281	0.01%	0.002%
66	11.002	3001	3005	3006	rBV2	374	232	0.01%	0.002%
67	11.118	3028	3041	3048	rBV8	4221	7673	0.39%	0.051%
68	11.202	3062	3067	3071	rBV4	695	818	0.04%	0.005%
69	11.253	3079	3083	3086	rBV2	374	270	0.01%	0.002%
70	11.308	3097	3100	3108	rVB2	994	1032	0.05%	0.007%
71	11.369	3116	3119	3126	rVB3	1125	977	0.05%	0.006%
72	11.417	3129	3134	3138	rBV4	1536	1303	0.07%	0.009%
73	11.459	3138	3147	3156	rBV7	3512	7014	0.35%	0.047%
74	11.578	3178	3184	3185	rBV3	1073	1070	0.05%	0.007%
75	11.697	3211	3221	3230	rVB5	3768	5523	0.28%	0.037%
76	11.745	3230	3236	3244	rBV5	1237	1588	0.08%	0.011%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
 Title : VOC Analysis

77	11.816	3244	3258	3281	rBV	716155	1149822	58.11%	7.637%
78	11.919	3281	3290	3300	rBV6	17001	28487	1.44%	0.189%
79	12.041	3326	3328	3333	rVB	358	287	0.01%	0.002%
80	12.108	3346	3349	3351	rBV4	371	278	0.01%	0.002%
81	12.195	3359	3376	3393	rBV	894833	1473894	74.48%	9.789%
82	12.334	3412	3419	3429	rVB5	2480	3658	0.18%	0.024%
83	12.398	3430	3439	3440	rBV6	1175	1438	0.07%	0.010%
84	12.472	3458	3462	3464	rBV	611	508	0.03%	0.003%
85	12.639	3510	3514	3519	rBV4	796	680	0.03%	0.005%
86	12.771	3550	3555	3563	rVB3	1457	1993	0.10%	0.013%
87	12.871	3580	3586	3590	rBV3	370	441	0.02%	0.003%
88	12.999	3622	3626	3630	rVB2	299	250	0.01%	0.002%
89	13.147	3669	3672	3674	rVV3	463	333	0.02%	0.002%
90	13.221	3692	3695	3700	rBV3	595	487	0.02%	0.003%
91	13.362	3736	3739	3742	rVB	443	284	0.01%	0.002%
92	13.716	3845	3849	3853	rBV3	622	532	0.03%	0.004%
93	13.790	3869	3872	3875	rBV2	431	250	0.01%	0.002%
94	13.851	3883	3891	3899	rBV4	1937	2668	0.13%	0.018%
95	14.096	3963	3967	3974	rBV4	1447	1818	0.09%	0.012%
96	14.208	3999	4002	4006	rBV2	528	355	0.02%	0.002%
97	14.234	4007	4010	4012	rBV2	454	324	0.02%	0.002%
98	14.337	4035	4042	4053	rVB4	1652	2378	0.12%	0.016%
99	15.211	4312	4314	4318	rBV2	602	532	0.03%	0.004%
100	16.121	4588	4597	4607	rVB2	43016	66465	3.36%	0.441%

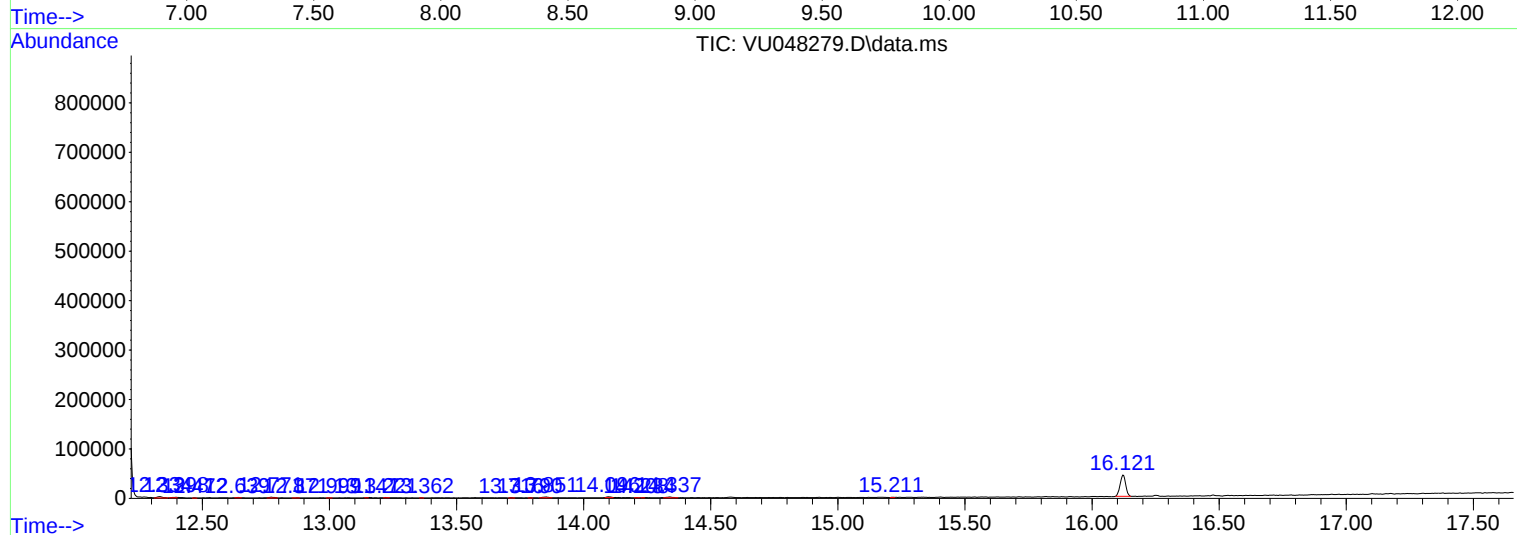
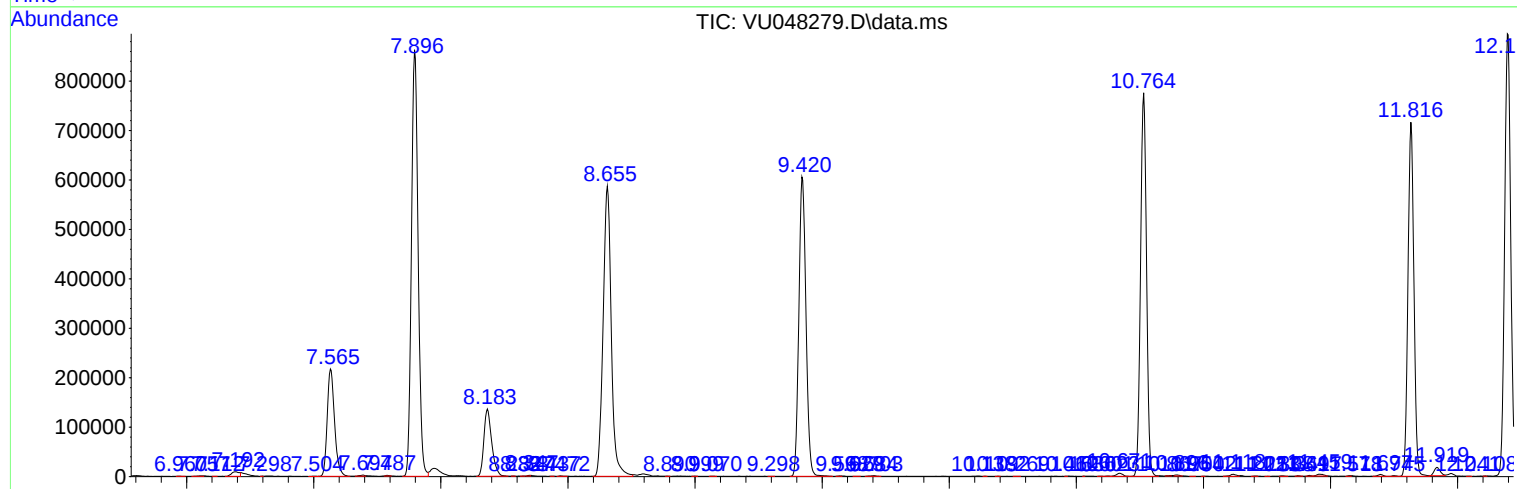
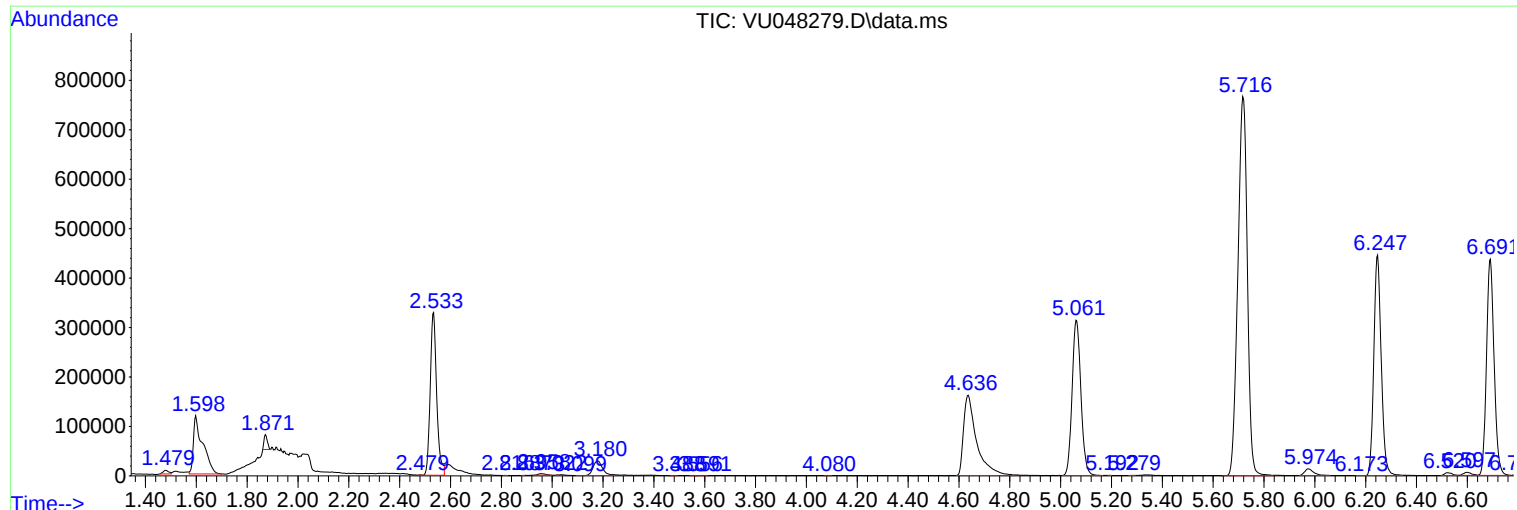
Sum of corrected areas: 15056914

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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFFG7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.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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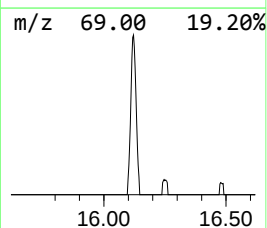
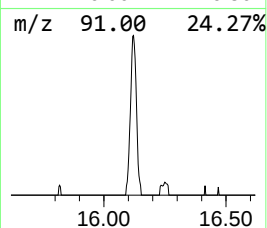
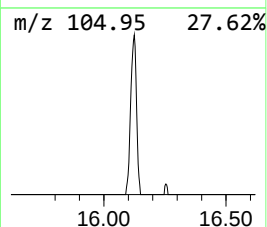
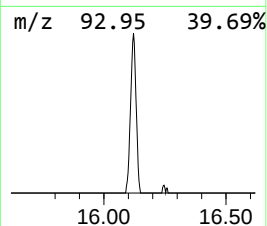
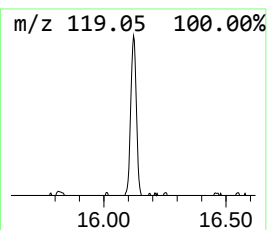
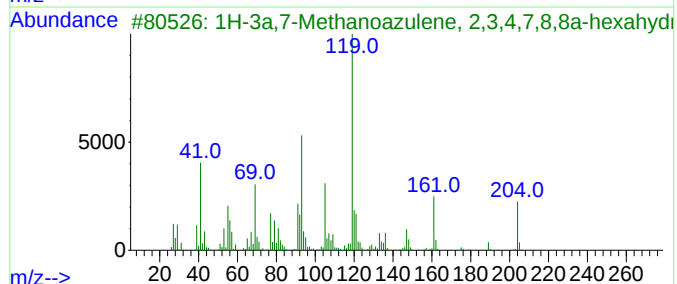
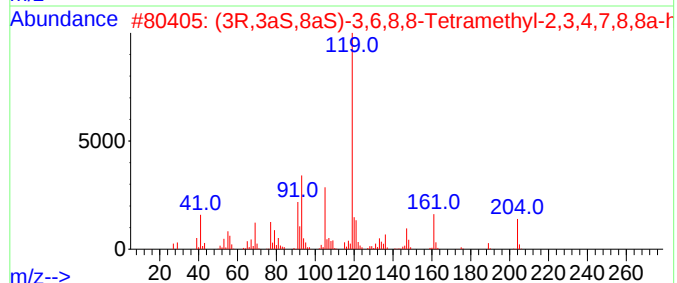
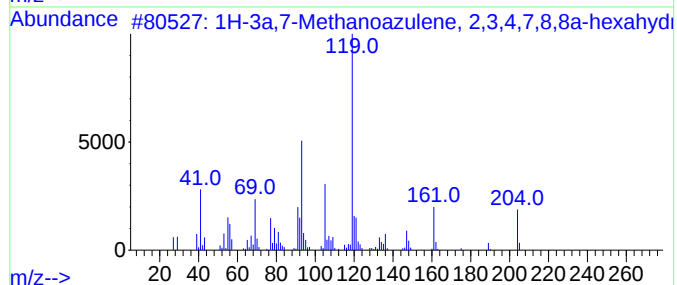
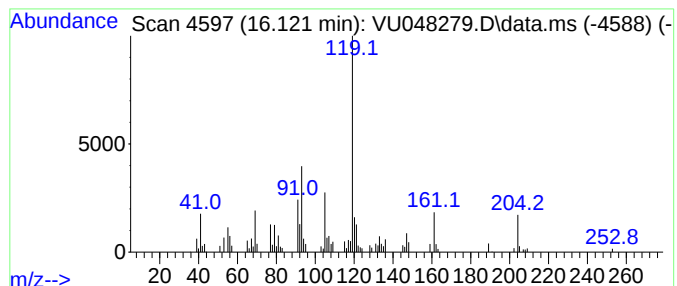
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 1H-3a,7-Methanoazulene, 2,3... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.121	2.89 ug/L	66465	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-3a,7-Methanoazulene, 2,3,4,7,...	204	C15H24	000469-61-4	99
2			(3R,3aS,8aS)-3,6,8,8-Tetramethyl...	204	C15H24	022567-43-7	99
3			1H-3a,7-Methanoazulene, 2,3,4,7,...	204	C15H24	000469-61-4	98
4			1H-3a,7-Methanoazulene, 2,3,4,7,...	204	C15H24	000469-61-4	98
5			1H-3a,7-Methanoazulene, 2,3,4,7,...	204	C15H24	000469-61-4	97



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1H-3a,7-Methano...	16.121	2.9	ug/L	66465	3	11.816	1149820	50.0