

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
 Data File : VU047967.D
 Acq On : 12 Apr 2022 19:37
 Operator : SY/MD
 Sample : N2290-01ME
 Misc : 3.15g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFFC8ME

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\SFAMULM032422WMA.M
 Title : VOC Analysis

Signal : TIC: VU047967.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	38	43	51	rBV4	2894	4497	0.29%	0.036%
2	1.598	73	80	104	rVB	97456	171534	10.97%	1.375%
3	1.813	122	147	148	rBV7	26873	76469	4.89%	0.613%
4	1.871	161	165	172	rBV	53848	63328	4.05%	0.507%
5	2.475	351	353	358	rBV2	413	311	0.02%	0.002%
6	2.546	362	375	416	rVB	257891	467011	29.86%	3.742%
7	2.868	470	475	477	rBV2	445	316	0.02%	0.003%
8	2.897	481	484	487	rVV3	484	265	0.02%	0.002%
9	2.987	509	512	518	rVB3	605	576	0.04%	0.005%
10	3.035	519	527	536	rBV6	1665	3120	0.20%	0.025%
11	3.173	565	570	574	rBV2	660	738	0.05%	0.006%
12	3.244	585	592	597	rVV2	471	627	0.04%	0.005%
13	3.279	601	603	609	rVV3	393	378	0.02%	0.003%
14	3.327	613	618	620	rVV3	375	325	0.02%	0.003%
15	3.704	730	735	738	rBV2	312	311	0.02%	0.002%
16	3.858	777	783	787	rVB2	303	318	0.02%	0.003%
17	4.228	895	898	902	rVB3	303	268	0.02%	0.002%
18	4.630	1008	1023	1073	rVV	164297	500221	31.98%	4.008%
19	4.852	1087	1092	1096	rVB2	492	485	0.03%	0.004%
20	4.970	1127	1129	1135	rBV3	246	284	0.02%	0.002%
21	5.061	1138	1157	1178	rBV	285472	635512	40.64%	5.093%
22	5.221	1205	1207	1217	rVB2	264	311	0.02%	0.002%
23	5.337	1231	1243	1251	rBV5	2108	4247	0.27%	0.034%
24	5.446	1270	1277	1281	rBV3	373	426	0.03%	0.003%
25	5.562	1310	1313	1317	rVV	397	331	0.02%	0.003%
26	5.720	1340	1362	1400	rBV2	589038	1563936	100.00%	12.532%
27	5.925	1423	1426	1429	rBV2	375	272	0.02%	0.002%
28	5.974	1429	1441	1459	rVV3	11367	26691	1.71%	0.214%
29	6.112	1478	1484	1486	rBV2	437	414	0.03%	0.003%
30	6.247	1512	1526	1551	rVV	283428	554416	35.45%	4.443%
31	6.520	1602	1611	1625	rBV6	4775	9865	0.63%	0.079%
32	6.601	1625	1636	1649	rBV3	5214	11566	0.74%	0.093%
33	6.691	1649	1664	1691	rBV	367983	733534	46.90%	5.878%
34	6.874	1716	1721	1725	rBV3	268	251	0.02%	0.002%
35	6.980	1751	1754	1757	rVB3	395	301	0.02%	0.002%
36	7.054	1769	1777	1786	rVB6	926	1872	0.12%	0.015%

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 Title : VOC Analysis

37	7.186	1807	1818	1825	rBV5	7764	16223	1.04%	0.130%
38	7.488	1910	1912	1914	rBV2	517	283	0.02%	0.002%
39	7.568	1923	1937	1957	rBV	182028	348099	22.26%	2.789%
40	7.691	1965	1975	1980	rBV8	1999	3761	0.24%	0.030%
41	7.797	2004	2008	2011	rVB3	305	261	0.02%	0.002%
42	7.819	2011	2015	2017	rBV2	369	286	0.02%	0.002%
43	7.900	2026	2040	2055	rBV	688839	1216037	77.75%	9.744%
44	8.183	2115	2128	2145	rBV	128128	247068	15.80%	1.980%
45	8.343	2173	2178	2179	rBV3	787	636	0.04%	0.005%
46	8.356	2179	2182	2189	rVB7	1597	1816	0.12%	0.015%
47	8.646	2253	2272	2311	rBV	662069	1270817	81.26%	10.183%
48	8.797	2314	2319	2329	rVB6	4352	7045	0.45%	0.056%
49	8.932	2358	2361	2366	rVV4	584	544	0.03%	0.004%
50	8.967	2369	2372	2377	rVB3	434	375	0.02%	0.003%
51	9.160	2429	2432	2438	rVB3	506	484	0.03%	0.004%
52	9.273	2464	2467	2475	rVB	327	374	0.02%	0.003%
53	9.330	2483	2485	2492	rVB2	255	287	0.02%	0.002%
54	9.420	2500	2513	2539	rBV	439145	784259	50.15%	6.284%
55	9.578	2554	2562	2566	rBV4	1154	1026	0.07%	0.008%
56	9.697	2593	2599	2605	rVV4	1161	1318	0.08%	0.011%
57	9.768	2616	2621	2623	rBV2	280	258	0.02%	0.002%
58	9.784	2623	2626	2634	rVB	280	370	0.02%	0.003%
59	10.099	2718	2724	2729	rBV	472	530	0.03%	0.004%
60	10.359	2801	2805	2809	rBV2	437	293	0.02%	0.002%
61	10.398	2811	2817	2819	rBV	363	287	0.02%	0.002%
62	10.469	2833	2839	2844	rBV3	811	923	0.06%	0.007%
63	10.620	2882	2886	2892	rVV4	1090	987	0.06%	0.008%
64	10.665	2892	2900	2913	rVB7	3090	5721	0.37%	0.046%
65	10.761	2913	2930	2952	rBV	717884	1149278	73.49%	9.209%
66	10.871	2958	2964	2966	rBV4	774	647	0.04%	0.005%
67	10.896	2969	2972	2976	rVB2	766	563	0.04%	0.005%
68	11.002	3000	3005	3008	rBV	610	582	0.04%	0.005%
69	11.018	3008	3010	3013	rVB4	415	263	0.02%	0.002%
70	11.067	3021	3025	3031	rBV4	490	463	0.03%	0.004%
71	11.115	3033	3040	3048	rVV8	2551	3750	0.24%	0.030%
72	11.192	3059	3064	3066	rBV3	387	334	0.02%	0.003%
73	11.314	3100	3102	3109	rVB3	608	497	0.03%	0.004%
74	11.366	3114	3118	3120	rBV3	712	605	0.04%	0.005%
75	11.420	3132	3135	3141	rBV6	759	611	0.04%	0.005%
76	11.459	3141	3147	3148	rBV	1998	1853	0.12%	0.015%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
 Title : VOC Analysis

77	11.575	3174	3183	3184	rBV4	572	693	0.04%	0.006%
78	11.697	3213	3221	3229	rBV3	2882	4230	0.27%	0.034%
79	11.752	3233	3238	3245	rVB3	765	1039	0.07%	0.008%
80	11.816	3245	3258	3282	rBV	555709	873106	55.83%	6.996%
81	11.919	3282	3290	3300	rBV8	9853	17861	1.14%	0.143%
82	12.115	3347	3351	3354	rBV2	565	411	0.03%	0.003%
83	12.195	3358	3376	3396	rVV	856417	1396075	89.27%	11.187%
84	12.485	3462	3466	3469	rBV	447	375	0.02%	0.003%
85	12.732	3538	3543	3546	rBV2	375	372	0.02%	0.003%
86	12.774	3549	3556	3563	rVV3	882	1224	0.08%	0.010%
87	12.977	3612	3619	3630	rVB3	2600	4112	0.26%	0.033%
88	13.115	3659	3662	3667	rBV3	263	283	0.02%	0.002%
89	13.150	3669	3673	3677	rBV3	357	387	0.02%	0.003%
90	13.333	3724	3730	3734	rBV2	1723	2016	0.13%	0.016%
91	13.382	3738	3745	3754	rVB3	2861	4048	0.26%	0.032%
92	13.533	3788	3792	3795	rBV2	403	315	0.02%	0.003%
93	13.845	3886	3889	3890	rBV2	747	419	0.03%	0.003%
94	14.366	4047	4051	4058	rVB3	1863	2252	0.14%	0.018%
95	14.433	4069	4072	4074	rBV2	383	246	0.02%	0.002%
96	15.034	4254	4259	4261	rBV2	517	547	0.03%	0.004%
97	15.546	4413	4418	4426	rVB5	5382	7047	0.45%	0.056%
98	16.121	4587	4597	4610	rBV	139963	223584	14.30%	1.792%
99	16.391	4674	4681	4699	rVB	10533	19755	1.26%	0.158%
100	16.478	4702	4708	4717	rVB8	9963	13807	0.88%	0.111%

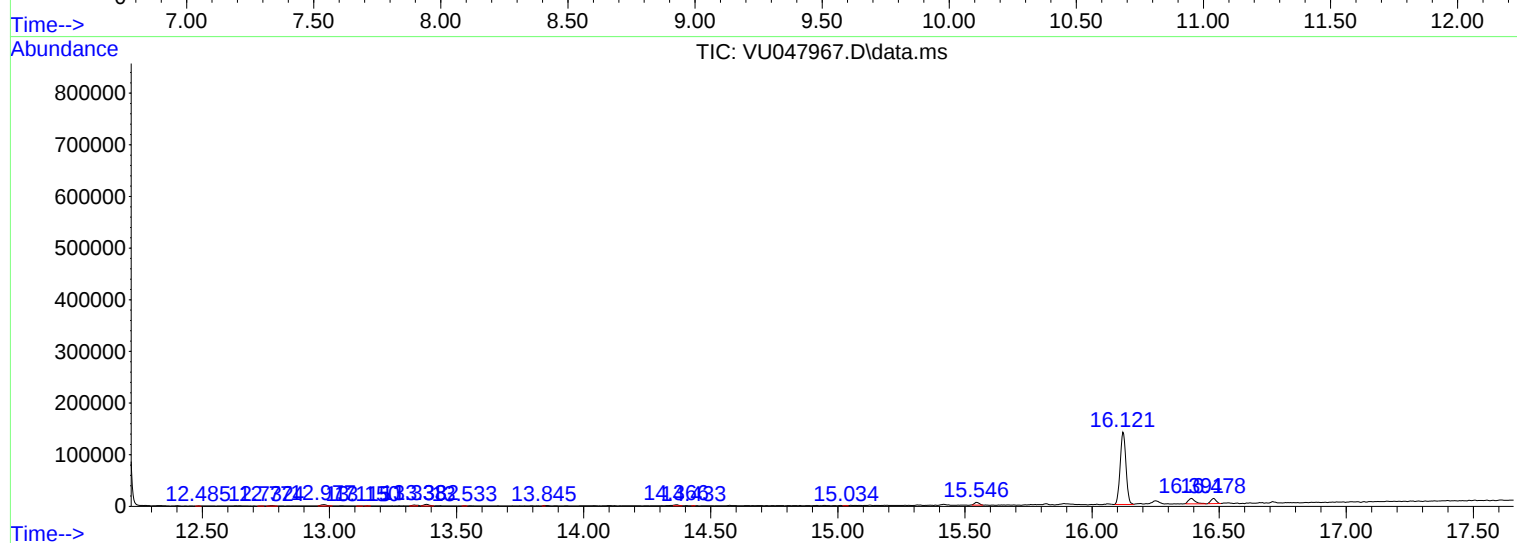
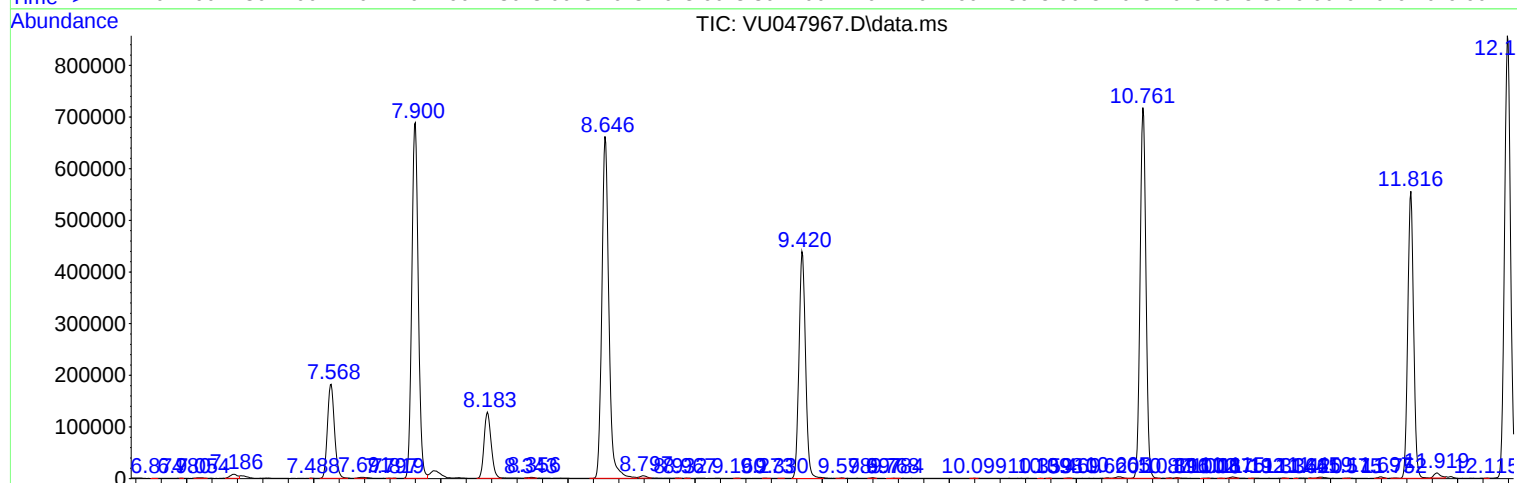
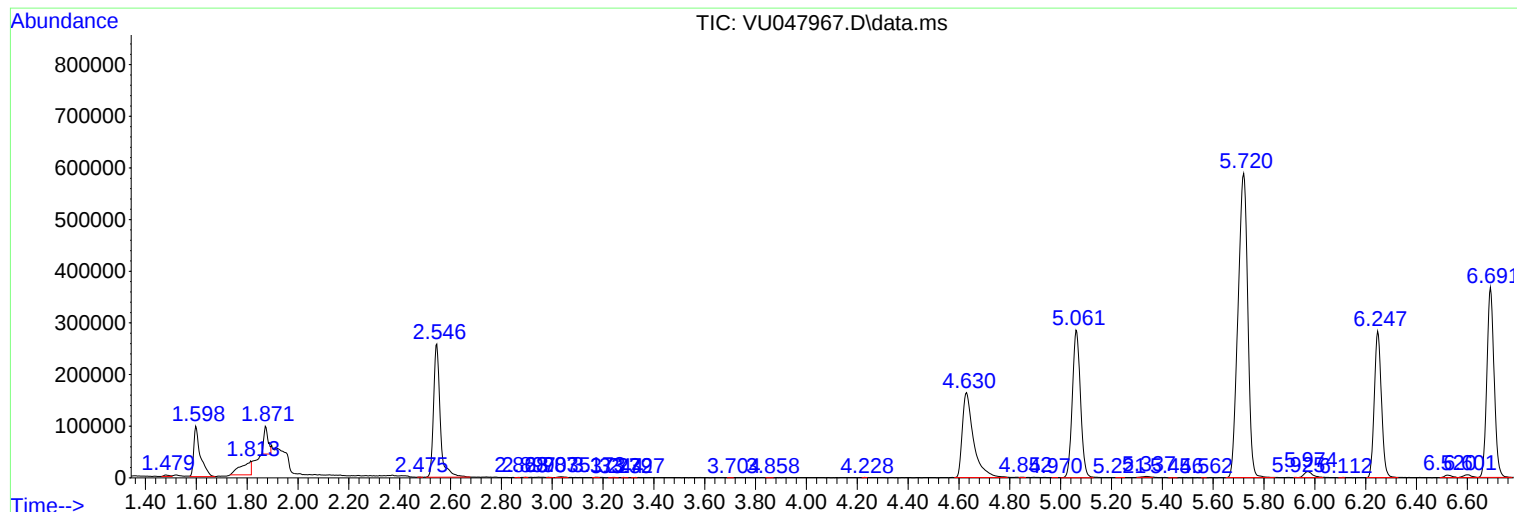
Sum of corrected areas: 12479345

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Instrument :
MSVOA_U
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BFFC8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_U
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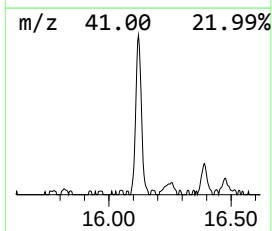
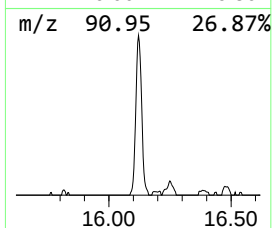
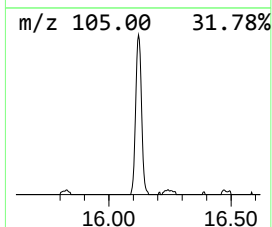
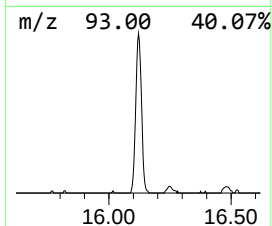
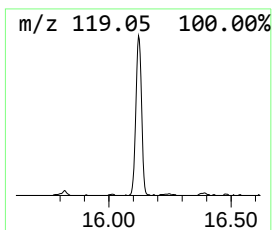
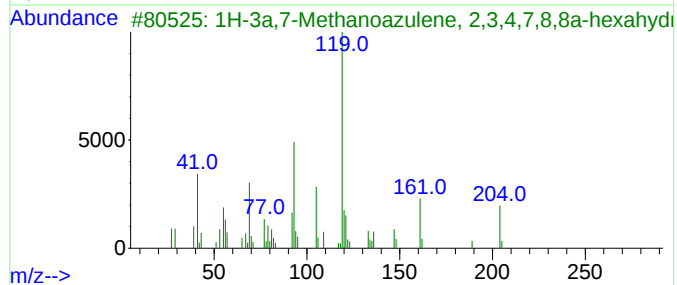
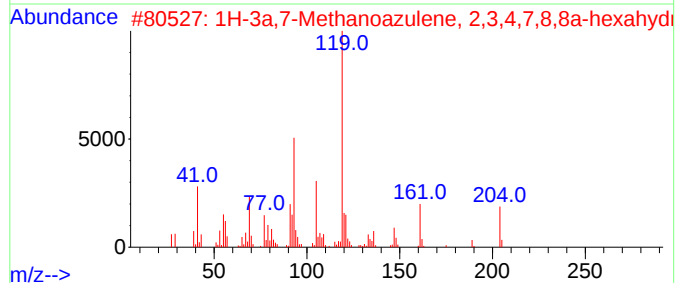
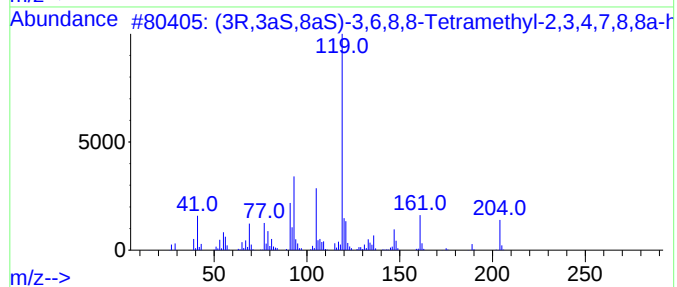
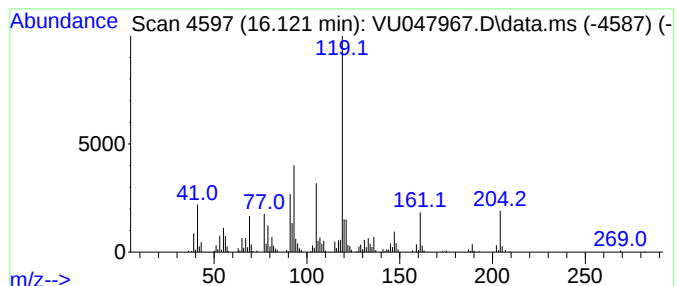
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (3R,3aS,8aS)-3,6,8,8-Tetram... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.121	12.80 ug/L	223584	1,4-Dichlorobenzene-d4	11.816

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



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(3R,3aS,8aS)-3,...	16.121	12.8	ug/L	223584	3	11.816	873106	50.0