

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042522\
 Data File : VU048280.D
 Acq On : 25 Apr 2022 20:03
 Operator : SY/MD
 Sample : N2469-06ME
 Misc : 3.18g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFFG8ME

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: VU048280.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.482	39	44	49	rBV2	4455	5353	0.30%	0.037%
2	1.514	51	54	63	rVV3	3570	6035	0.34%	0.042%
3	1.597	73	80	87	rBV	80006	127539	7.20%	0.891%
4	2.530	357	370	388	rBV	285840	526269	29.69%	3.676%
5	2.899	480	485	487	rBV3	280	287	0.02%	0.002%
6	2.964	492	505	513	rBV2	3959	8440	0.48%	0.059%
7	3.182	558	573	587	rBV2	15040	41002	2.31%	0.286%
8	3.520	676	678	685	rVB2	318	291	0.02%	0.002%
9	3.571	690	694	695	rBV	257	176	0.01%	0.001%
10	3.594	697	701	704	rBV2	281	247	0.01%	0.002%
11	3.797	762	764	767	rVB	344	190	0.01%	0.001%
12	3.825	767	773	777	rVB2	239	289	0.02%	0.002%
13	3.893	789	794	798	rBV2	252	270	0.02%	0.002%
14	4.015	830	832	837	rVB2	253	176	0.01%	0.001%
15	4.141	868	871	879	rVV2	191	176	0.01%	0.001%
16	4.649	1014	1029	1086	rBV2	114790	528940	29.84%	3.695%
17	5.063	1140	1158	1186	rBV	270746	672788	37.96%	4.700%
18	5.472	1281	1285	1288	rBV2	246	222	0.01%	0.002%
19	5.719	1341	1362	1393	rBV2	709172	1772417	100.00%	12.381%
20	5.825	1393	1395	1403	rVB5	1351	1344	0.08%	0.009%
21	5.983	1431	1444	1467	rBV3	13757	37595	2.12%	0.263%
22	6.108	1479	1483	1485	rVV2	383	298	0.02%	0.002%
23	6.247	1511	1526	1567	rBV	502317	1062734	59.96%	7.424%
24	6.414	1576	1578	1582	rVB2	658	342	0.02%	0.002%
25	6.468	1593	1595	1599	rVB2	350	197	0.01%	0.001%
26	6.530	1599	1614	1622	rBV8	5696	11660	0.66%	0.081%
27	6.604	1628	1637	1648	rBV3	5486	11831	0.67%	0.083%
28	6.690	1650	1664	1692	rVB	370681	797934	45.02%	5.574%
29	6.787	1692	1694	1696	rBV2	660	338	0.02%	0.002%
30	6.973	1748	1752	1754	rBV2	349	307	0.02%	0.002%
31	7.054	1773	1777	1778	rBV	611	368	0.02%	0.003%
32	7.211	1811	1826	1829	rBV5	8610	17760	1.00%	0.124%
33	7.362	1870	1873	1878	rVB3	755	579	0.03%	0.004%
34	7.501	1911	1916	1921	rBV3	565	550	0.03%	0.004%
35	7.568	1922	1937	1967	rBV	179062	375855	21.21%	2.626%
36	7.697	1969	1977	1985	rBV5	1630	2717	0.15%	0.019%

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 Misc : 3.18g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFFG8ME

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

37	7.848	2020	2024	2025	rBV2	484	296	0.02%	0.002%
38	7.899	2026	2040	2056	rBV	746083	1386825	78.24%	9.688%
39	8.121	2107	2109	2114	rVB3	480	326	0.02%	0.002%
40	8.185	2115	2129	2158	rBV	115940	265346	14.97%	1.854%
41	8.349	2174	2180	2185	rBV4	1368	1771	0.10%	0.012%
42	8.427	2202	2204	2208	rBV3	315	216	0.01%	0.002%
43	8.520	2229	2233	2237	rVB3	366	316	0.02%	0.002%
44	8.671	2256	2280	2313	rBV	490552	1135095	64.04%	7.929%
45	8.857	2336	2338	2343	rVB4	747	532	0.03%	0.004%
46	8.941	2360	2364	2368	rVV4	584	483	0.03%	0.003%
47	9.041	2392	2395	2400	rBV2	351	331	0.02%	0.002%
48	9.147	2425	2428	2431	rBV2	238	190	0.01%	0.001%
49	9.282	2468	2470	2479	rVB4	440	423	0.02%	0.003%
50	9.423	2499	2514	2550	rBV	636806	1340535	75.63%	9.364%
51	9.574	2553	2561	2569	rVB5	1124	1551	0.09%	0.011%
52	9.661	2584	2588	2591	rBV2	303	268	0.02%	0.002%
53	9.700	2593	2600	2605	rBV4	1252	1645	0.09%	0.011%
54	9.761	2615	2619	2622	rBV2	255	218	0.01%	0.002%
55	9.806	2627	2633	2635	rVV3	179	196	0.01%	0.001%
56	9.935	2670	2673	2676	rVV	325	268	0.02%	0.002%
57	10.105	2722	2726	2728	rBV2	575	537	0.03%	0.004%
58	10.173	2745	2747	2753	rVB	284	181	0.01%	0.001%
59	10.208	2753	2758	2761	rBV2	390	395	0.02%	0.003%
60	10.314	2787	2791	2792	rBV3	430	329	0.02%	0.002%
61	10.468	2828	2839	2854	rVB4	7803	13026	0.73%	0.091%
62	10.555	2861	2866	2870	rBV4	612	659	0.04%	0.005%
63	10.600	2876	2880	2881	rBV2	429	266	0.02%	0.002%
64	10.626	2882	2888	2892	rVV4	982	906	0.05%	0.006%
65	10.671	2892	2902	2911	rVB2	5947	9739	0.55%	0.068%
66	10.767	2918	2932	2948	rBV	641055	1051905	59.35%	7.348%
67	10.867	2958	2963	2964	rBV2	862	621	0.04%	0.004%
68	10.970	2993	2995	2998	rVB3	454	234	0.01%	0.002%
69	11.012	3003	3008	3014	rBV5	609	702	0.04%	0.005%
70	11.115	3031	3040	3050	rBV6	4750	8465	0.48%	0.059%
71	11.211	3062	3070	3080	rBV4	673	1091	0.06%	0.008%
72	11.314	3096	3102	3106	rBV2	1610	1684	0.10%	0.012%
73	11.381	3114	3123	3127	rBV5	774	1129	0.06%	0.008%
74	11.417	3131	3134	3135	rBV3	792	460	0.03%	0.003%
75	11.455	3139	3146	3153	rBV6	2991	4853	0.27%	0.034%
76	11.574	3178	3183	3190	rBV4	1503	1811	0.10%	0.013%

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 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFFG8ME

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

77	11.697	3214	3221	3230	rVB5	3350	4631	0.26%	0.032%
78	11.748	3233	3237	3238	rBV3	1083	760	0.04%	0.005%
79	11.819	3245	3259	3280	rBV	819971	1317593	74.34%	9.204%
80	11.922	3281	3291	3302	rBV4	35606	57889	3.27%	0.404%
81	12.044	3327	3329	3332	rVB2	433	181	0.01%	0.001%
82	12.095	3341	3345	3347	rBV3	554	406	0.02%	0.003%
83	12.198	3359	3377	3395	rBV	812741	1310591	73.94%	9.155%
84	12.327	3413	3417	3418	rBV3	1259	903	0.05%	0.006%
85	12.369	3428	3430	3433	rBV3	357	216	0.01%	0.002%
86	12.401	3436	3440	3441	rBV3	936	598	0.03%	0.004%
87	12.568	3489	3492	3497	rBV3	250	223	0.01%	0.002%
88	12.590	3497	3499	3501	rBV	382	192	0.01%	0.001%
89	12.639	3506	3514	3517	rBV5	947	1161	0.07%	0.008%
90	12.770	3549	3555	3565	rVB5	1748	2543	0.14%	0.018%
91	12.838	3573	3576	3580	rBV3	379	307	0.02%	0.002%
92	13.140	3666	3670	3673	rBV3	564	541	0.03%	0.004%
93	13.262	3705	3708	3709	rBV	336	199	0.01%	0.001%
94	13.854	3885	3892	3897	rVB5	1387	1744	0.10%	0.012%
95	14.340	4040	4043	4053	rVB4	1816	1999	0.11%	0.014%
96	15.815	4499	4502	4510	rVB6	4010	4199	0.24%	0.029%
97	15.918	4528	4534	4544	rVB4	9852	13635	0.77%	0.095%
98	16.121	4586	4597	4613	rBV	154965	253085	14.28%	1.768%
99	16.478	4698	4708	4718	rBV4	43644	73595	4.15%	0.514%
100	16.712	4775	4781	4792	rVB9	11182	18802	1.06%	0.131%

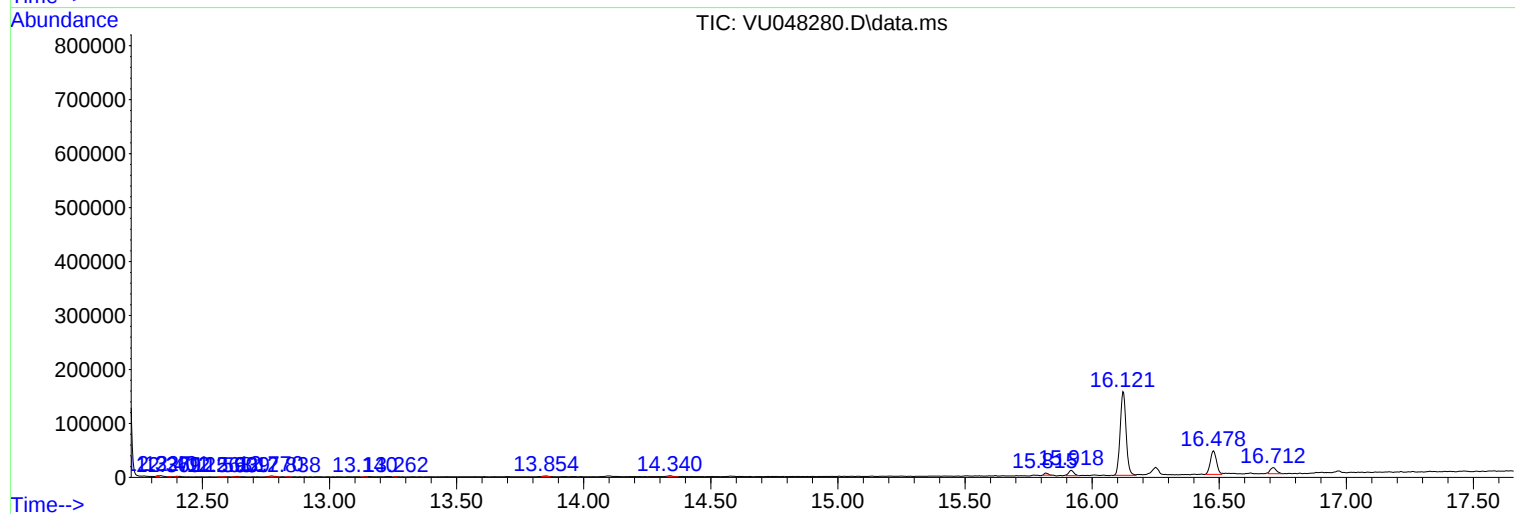
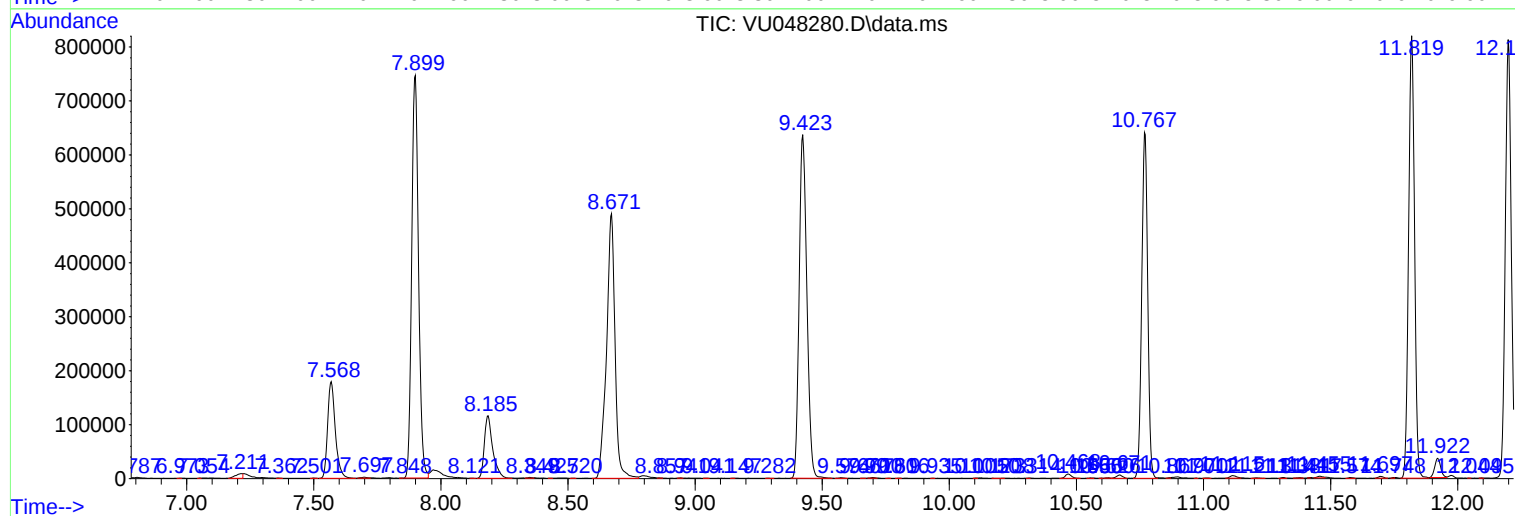
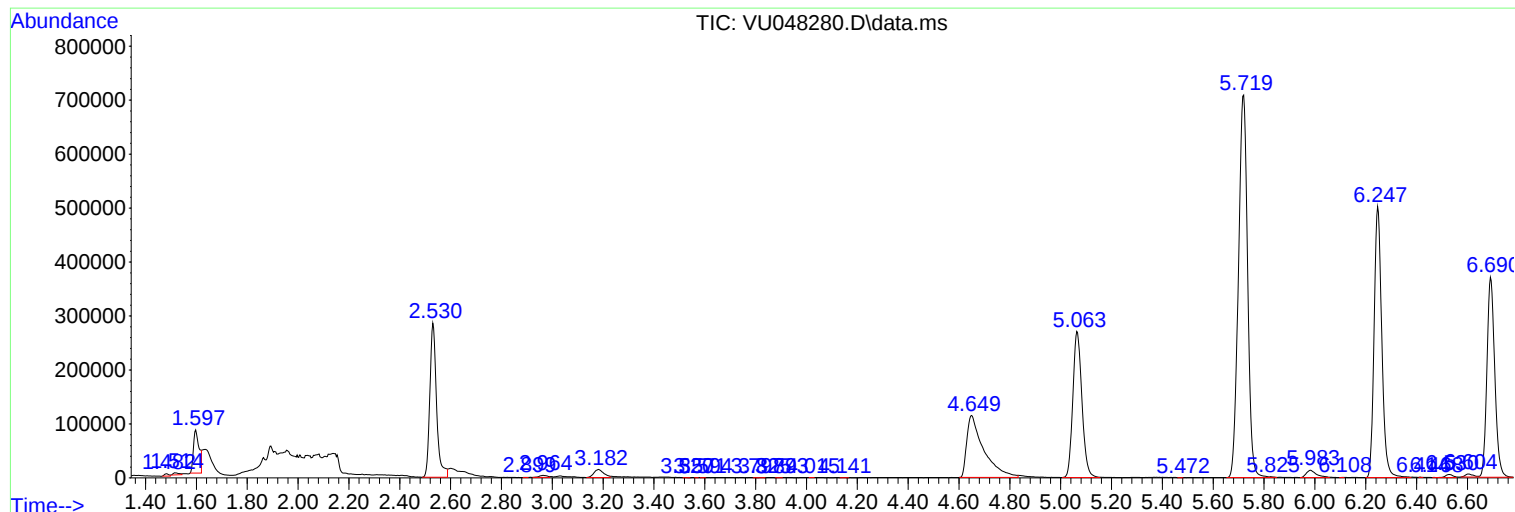
Sum of corrected areas: 14315333

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042522\
Data File : VU048280.D
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Sample : N2469-06ME
Misc : 3.18g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFFG8ME

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042522\
Data File : VU048280.D
Acq On : 25 Apr 2022 20:03
Operator : SY/MD
Sample : N2469-06ME
Misc : 3.18g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFFG8ME

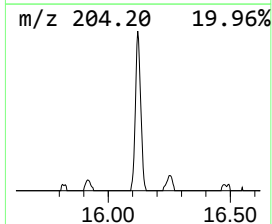
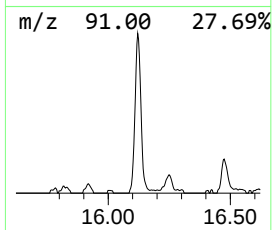
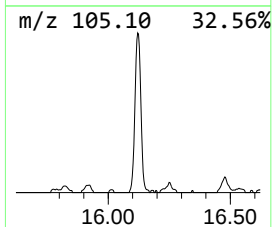
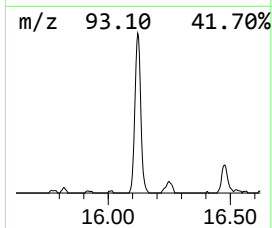
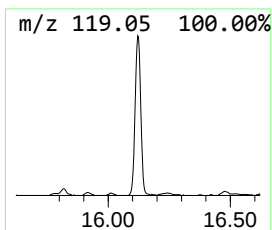
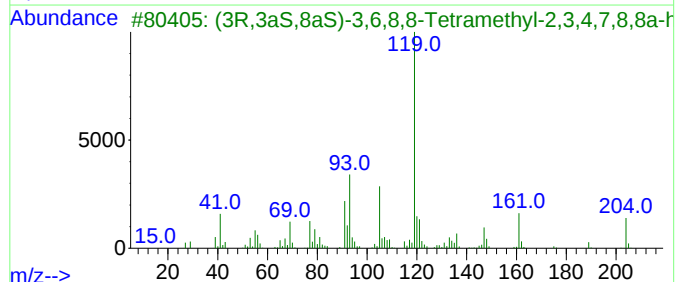
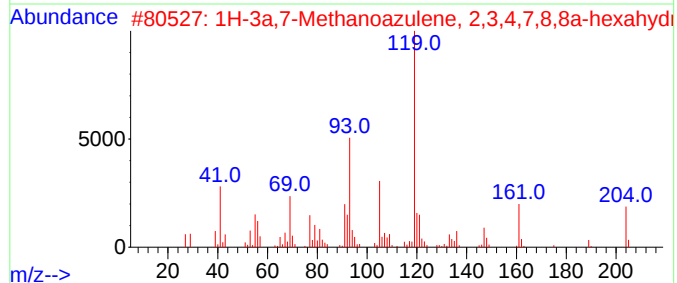
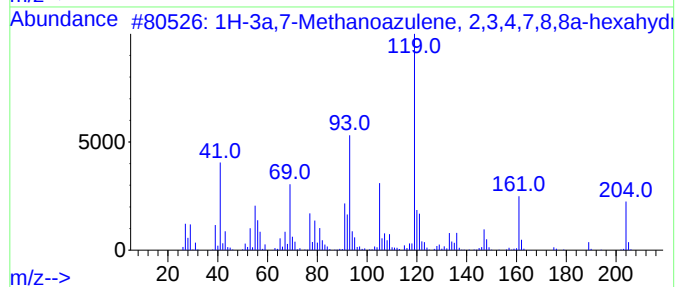
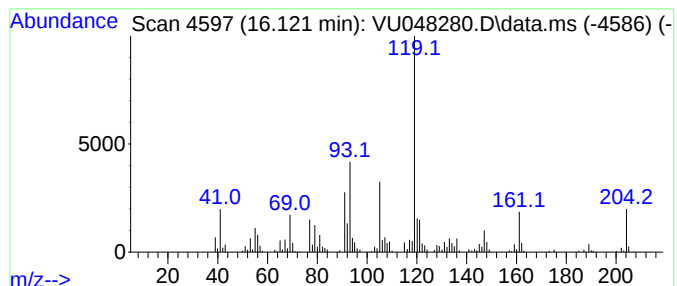
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.121	9.60 ug/L	253085	1,4-Dichlorobenzene-d4	11.819

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			1H-3a,7-Methanoazulene, 2,3,4,7,...	204	C15H24	000469-61-4	99
3			(3R,3aS,8aS)-3,6,8,8-Tetramethyl...	204	C15H24	022567-43-7	97
4			2-Epi-.alpha.-funebrene	204	C15H24	065354-33-8	95
5			1H-3a,7-Methanoazulene, 2,3,4,7,...	204	C15H24	000469-61-4	95



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Sample : N2469-06ME
Misc : 3.18g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFFG8ME

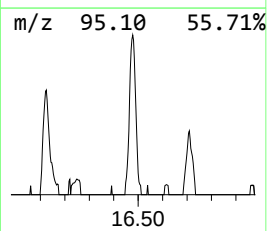
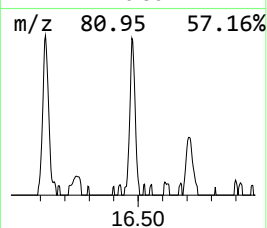
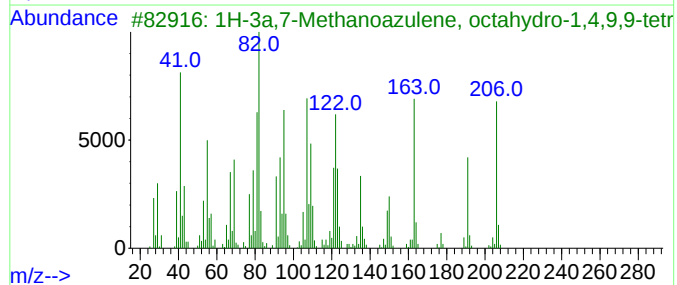
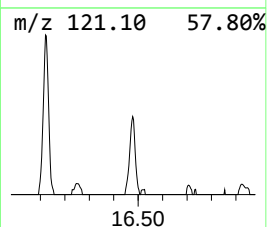
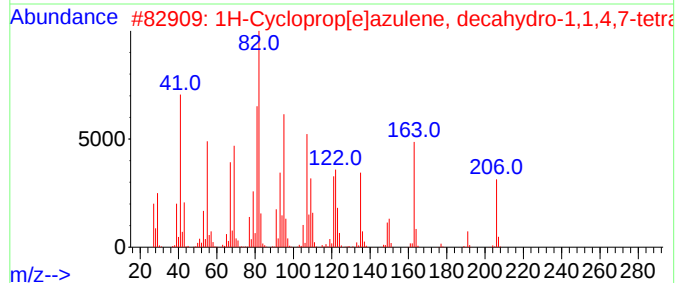
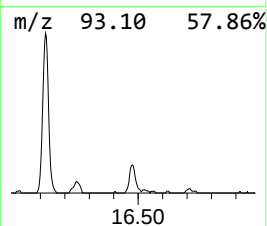
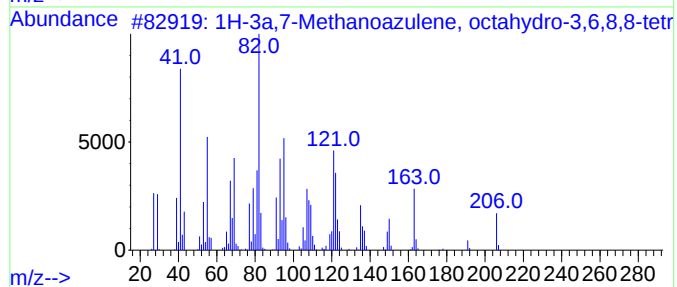
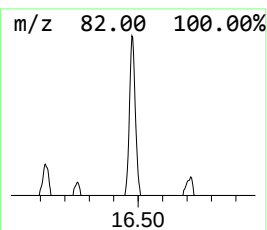
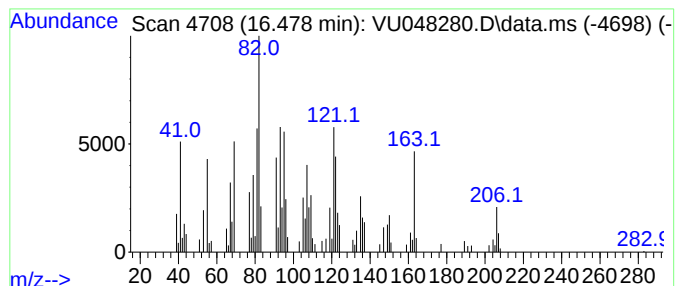
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.478	2.79 ug/L	73595	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-3a,7-Methanoazulene, octahydr...	206	C15H26	013567-54-9	96
2			1H-Cycloprop[e]azulene, decahydr...	206	C15H26	006790-78-9	86
3			1H-3a,7-Methanoazulene, octahydr...	206	C15H26	003724-42-3	81
4			4,7-Methanoazulene, decahydro-1,...	206	C15H26	020478-88-0	68
5			Aromadendran ('2')	206	C15H26	110769-62-5	45



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Misc : 3.18g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BFFG8ME

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1H-3a,7-Methano...	16.121	9.6	ug/L	253085	3	11.819	1317590	50.0
1H-3a,7-Methano...	16.478	2.8	ug/L	73595	3	11.819	1317590	50.0