

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
 Data File : VU047950.D
 Acq On : 12 Apr 2022 13:10
 Operator : SY/MD
 Sample : N2280-02ME
 Misc : 4.32g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFFC1ME

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: VU047950.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	102	rBV	69627	127479	10.01%	1.182%
2	1.874	162	166	170	rBV	35351	29459	2.31%	0.273%
3	2.543	362	374	401	rVV	189709	346632	27.22%	3.214%
4	2.710	423	426	429	rBV4	437	391	0.03%	0.004%
5	2.774	442	446	448	rVB4	407	309	0.02%	0.003%
6	2.842	461	467	468	rBV2	266	237	0.02%	0.002%
7	2.871	473	476	477	rBV3	414	252	0.02%	0.002%
8	2.954	494	502	516	rVB2	4776	9536	0.75%	0.088%
9	3.038	523	528	534	rBV5	1400	1677	0.13%	0.016%
10	3.108	544	550	554	rVB2	345	377	0.03%	0.003%
11	3.128	554	556	559	rBV	462	321	0.03%	0.003%
12	3.179	564	572	582	rVB4	1030	1625	0.13%	0.015%
13	3.308	607	612	615	rVB2	319	294	0.02%	0.003%
14	3.517	671	677	681	rBV3	309	292	0.02%	0.003%
15	3.591	692	700	701	rBV	333	307	0.02%	0.003%
16	3.684	723	729	731	rVV2	256	250	0.02%	0.002%
17	4.253	902	906	910	rBV2	209	231	0.02%	0.002%
18	4.494	975	981	984	rVV	405	387	0.03%	0.004%
19	4.552	996	999	1005	rBV2	486	532	0.04%	0.005%
20	4.629	1010	1023	1071	rBV	106313	340045	26.71%	3.153%
21	5.063	1141	1158	1181	rBV2	203337	459095	36.06%	4.257%
22	5.285	1223	1227	1228	rBV	333	254	0.02%	0.002%
23	5.317	1233	1237	1238	rBV2	747	451	0.04%	0.004%
24	5.330	1238	1241	1242	rBV	848	476	0.04%	0.004%
25	5.719	1341	1362	1386	rBV2	428457	1130470	88.79%	10.483%
26	5.841	1398	1400	1404	rVB2	431	228	0.02%	0.002%
27	5.973	1429	1441	1456	rBV3	12419	27534	2.16%	0.255%
28	6.105	1478	1482	1485	rBV3	529	418	0.03%	0.004%
29	6.247	1510	1526	1558	rBV	410452	813665	63.91%	7.545%
30	6.404	1571	1575	1580	rVB5	580	539	0.04%	0.005%
31	6.520	1602	1611	1624	rVV7	4013	9164	0.72%	0.085%
32	6.597	1626	1635	1649	rVV4	5763	11935	0.94%	0.111%
33	6.690	1649	1664	1690	rVB	258682	525320	41.26%	4.871%
34	6.784	1690	1693	1698	rBV4	719	636	0.05%	0.006%
35	6.864	1714	1718	1722	rBV	368	353	0.03%	0.003%
36	7.050	1765	1776	1778	rBV3	1092	1402	0.11%	0.013%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Sampling : 1

Min Area: 0 % of largest Peak

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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

37	7.182	1804	1817	1825	rBV3	8257	17060	1.34%	0.158%
38	7.314	1852	1858	1869	rVB6	693	1488	0.12%	0.014%
39	7.484	1907	1911	1914	rBV3	358	337	0.03%	0.003%
40	7.568	1923	1937	1959	rBV	131627	249064	19.56%	2.310%
41	7.693	1968	1976	1978	rBV4	1418	1623	0.13%	0.015%
42	7.809	2008	2012	2015	rBV2	326	274	0.02%	0.003%
43	7.899	2026	2040	2056	rBV	490766	878740	69.02%	8.148%
44	7.976	2057	2064	2086	rVB5	12142	33843	2.66%	0.314%
45	8.182	2114	2128	2149	rBV	88880	174665	13.72%	1.620%
46	8.346	2176	2179	2180	rBV3	649	405	0.03%	0.004%
47	8.472	2215	2218	2222	rVB2	768	616	0.05%	0.006%
48	8.648	2258	2273	2303	rBV	433717	854918	67.15%	7.927%
49	8.800	2313	2320	2336	rVB5	4665	9516	0.75%	0.088%
50	8.935	2358	2362	2365	rVV4	607	432	0.03%	0.004%
51	9.031	2388	2392	2395	rBV2	444	286	0.02%	0.003%
52	9.082	2404	2408	2412	rVB2	387	331	0.03%	0.003%
53	9.111	2413	2417	2421	rBV3	335	407	0.03%	0.004%
54	9.230	2446	2454	2457	rVB2	323	375	0.03%	0.003%
55	9.269	2464	2466	2472	rVB2	354	243	0.02%	0.002%
56	9.301	2472	2476	2478	rBV2	259	247	0.02%	0.002%
57	9.420	2498	2513	2547	rBV	642033	1148652	90.21%	10.651%
58	9.574	2559	2561	2562	rVV	661	312	0.02%	0.003%
59	9.697	2593	2599	2610	rBB4	832	1446	0.11%	0.013%
60	9.976	2683	2686	2690	rVB2	425	331	0.03%	0.003%
61	10.230	2757	2765	2769	rBV	334	348	0.03%	0.003%
62	10.324	2790	2794	2801	rVB3	320	432	0.03%	0.004%
63	10.475	2833	2841	2843	rBV4	426	412	0.03%	0.004%
64	10.552	2861	2865	2867	rVV2	459	363	0.03%	0.003%
65	10.565	2867	2869	2873	rVB3	478	319	0.03%	0.003%
66	10.594	2874	2878	2881	rBV2	203	217	0.02%	0.002%
67	10.623	2881	2887	2890	rVV6	740	849	0.07%	0.008%
68	10.668	2890	2901	2908	rVB5	2496	4203	0.33%	0.039%
69	10.761	2917	2930	2947	rBV	488047	795425	62.47%	7.376%
70	10.864	2958	2962	2964	rBV3	644	592	0.05%	0.005%
71	10.893	2967	2971	2976	rVV5	1261	1266	0.10%	0.012%
72	11.002	2998	3005	3010	rBV4	710	823	0.06%	0.008%
73	11.118	3033	3041	3048	rVV7	3572	5650	0.44%	0.052%
74	11.150	3048	3051	3057	rVV3	776	669	0.05%	0.006%
75	11.320	3097	3104	3109	rVB2	975	1007	0.08%	0.009%
76	11.369	3116	3119	3120	rBV2	485	275	0.02%	0.003%

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Integration Parameters: LSCINT.P

Integrator: RTE

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

77	11.417	3130	3134	3139	rVB3	755	762	0.06%	0.007%
78	11.459	3139	3147	3152	rBV6	1609	2784	0.22%	0.026%
79	11.574	3179	3183	3189	rVV4	634	811	0.06%	0.008%
80	11.700	3213	3222	3230	rBV5	1861	2890	0.23%	0.027%
81	11.745	3232	3236	3238	rBV	863	498	0.04%	0.005%
82	11.816	3243	3258	3274	rBV	805091	1273239	100.00%	11.806%
83	11.918	3279	3290	3303	rBV2	107025	177615	13.95%	1.647%
84	12.108	3347	3349	3354	rVB2	364	322	0.03%	0.003%
85	12.147	3355	3361	3362	rBV4	640	545	0.04%	0.005%
86	12.195	3362	3376	3400	rVV	608321	998179	78.40%	9.256%
87	12.330	3414	3418	3419	rBV2	1050	689	0.05%	0.006%
88	12.407	3434	3442	3447	rBV5	848	1248	0.10%	0.012%
89	12.590	3496	3499	3503	rBV3	289	268	0.02%	0.002%
90	12.774	3548	3556	3561	rBV2	836	1170	0.09%	0.011%
91	12.844	3575	3578	3582	rBV3	292	294	0.02%	0.003%
92	12.912	3594	3599	3600	rBV2	319	303	0.02%	0.003%
93	13.224	3692	3696	3699	rBV2	554	483	0.04%	0.004%
94	13.844	3885	3889	3890	rBV3	947	601	0.05%	0.006%
95	14.105	3962	3970	3976	rBV4	768	1427	0.11%	0.013%
96	14.169	3988	3990	3993	rBV2	492	296	0.02%	0.003%
97	14.764	4172	4175	4178	rBV2	409	347	0.03%	0.003%
98	14.973	4237	4240	4245	rBV3	622	548	0.04%	0.005%
99	16.124	4586	4598	4610	rBV	174974	277030	21.76%	2.569%
100	16.474	4701	4707	4716	rBV7	7872	10936	0.86%	0.101%

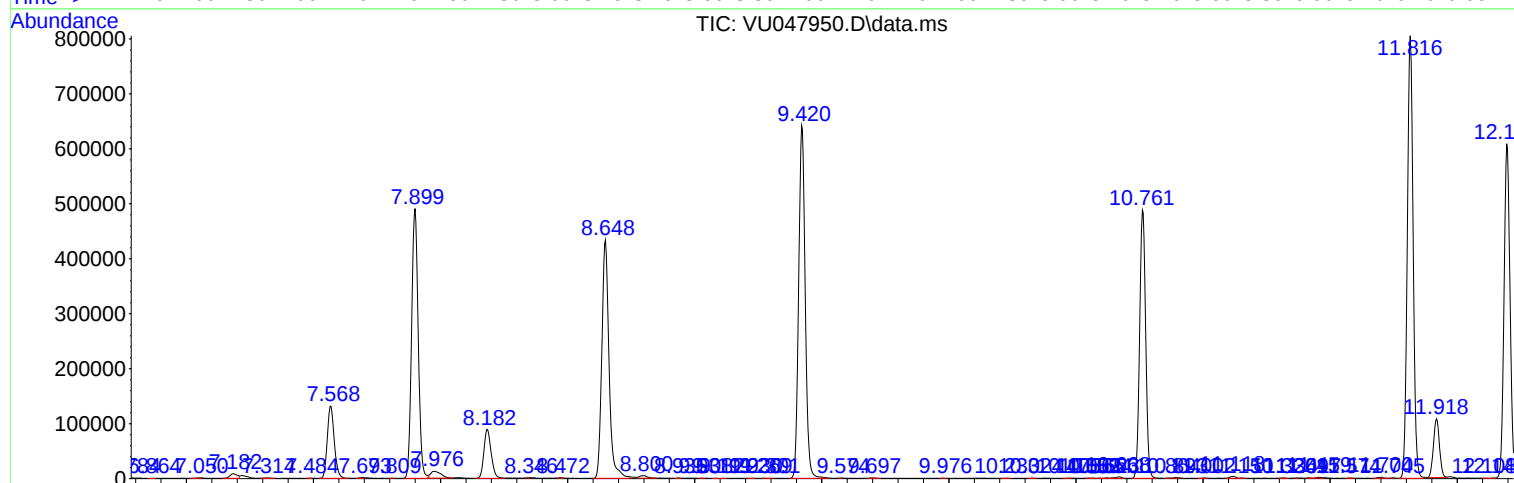
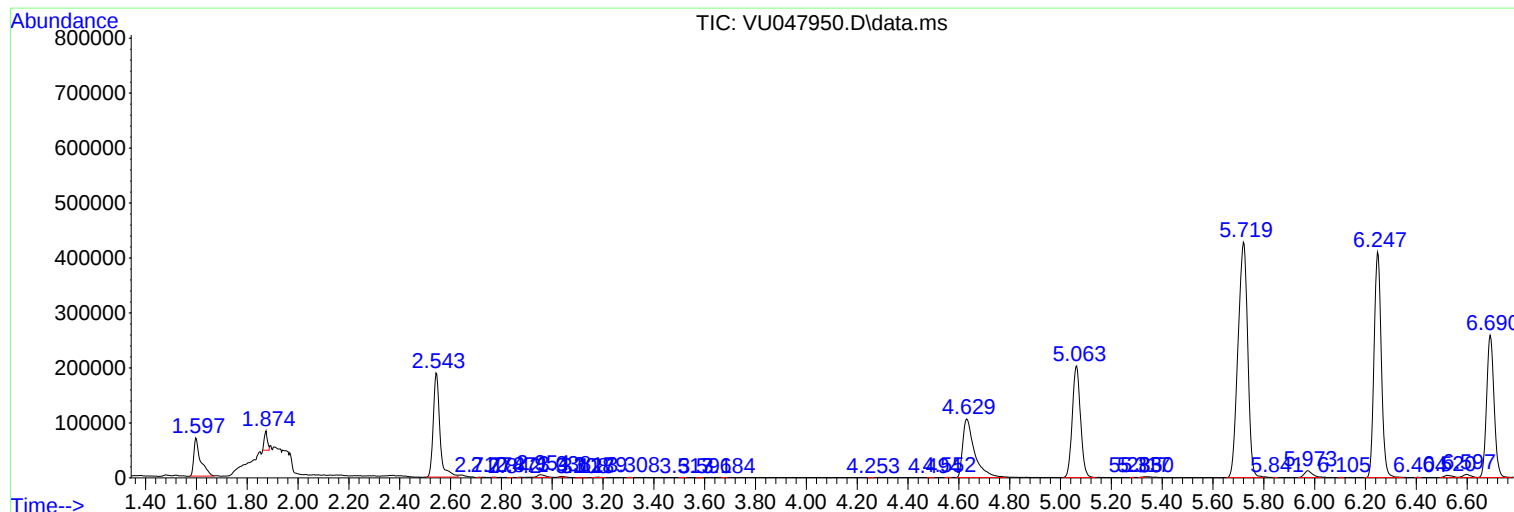
Sum of corrected areas: 10784319

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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFFC1ME

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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ALS Vial : 11 Sample Multiplier: 1

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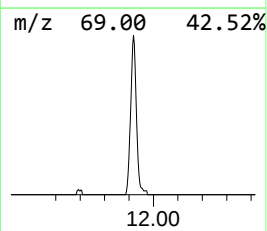
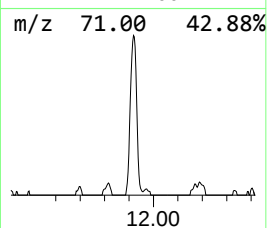
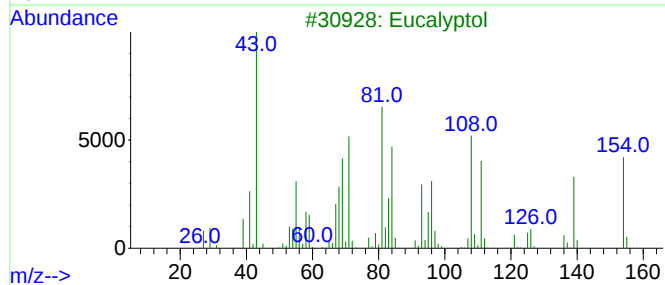
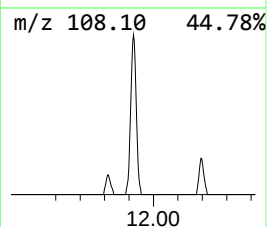
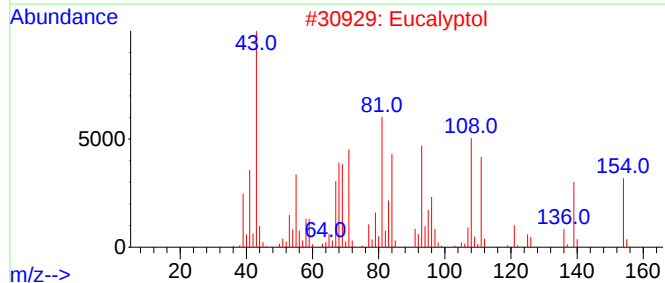
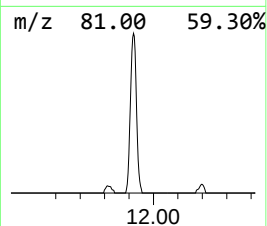
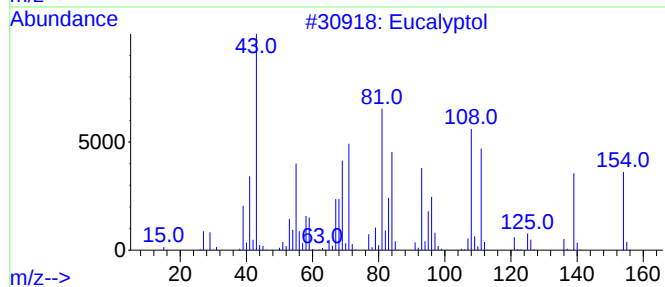
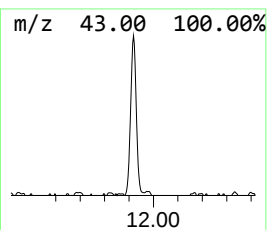
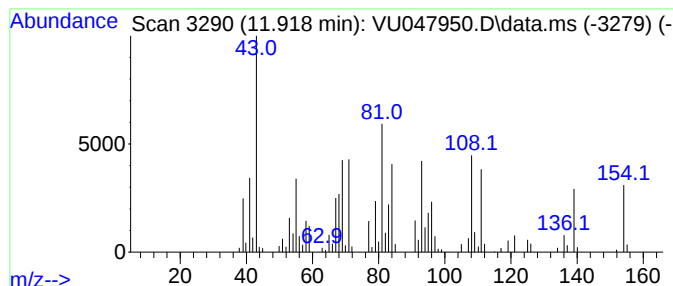
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Eucalyptol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.918	6.97 ug/L	177615	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	99
2			Eucalyptol	154	C10H18O	000470-82-6	98
3			Eucalyptol	154	C10H18O	000470-82-6	96
4			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	87
5			Eucalyptol	154	C10H18O	000470-82-6	81



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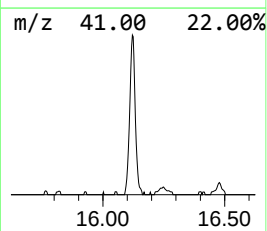
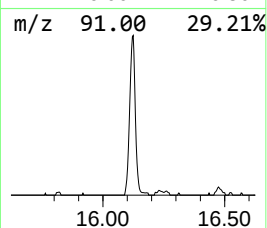
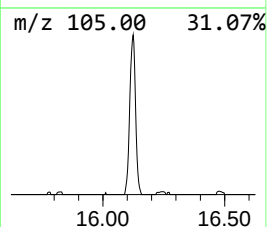
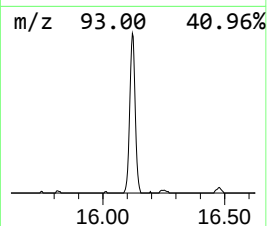
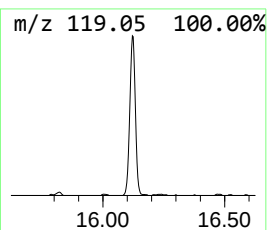
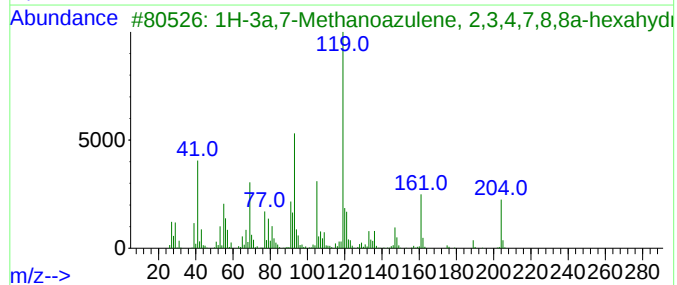
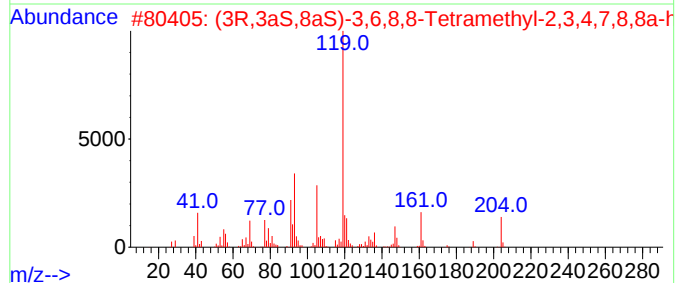
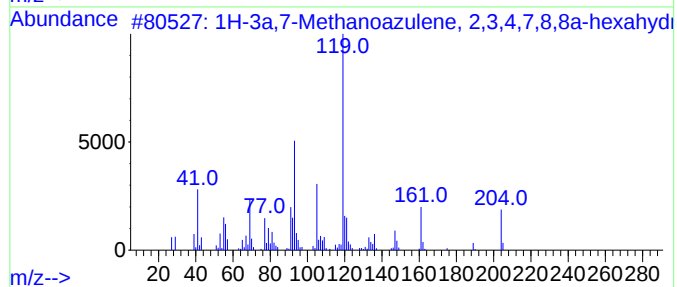
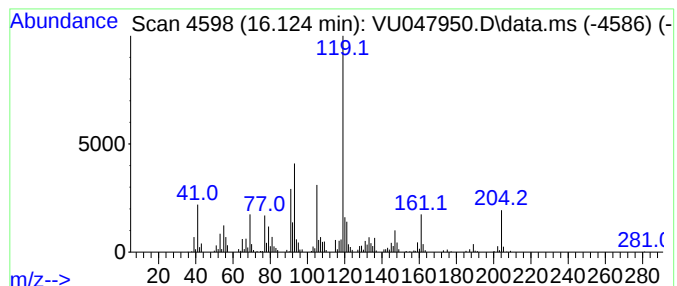
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.124	10.88 ug/L	277030	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	95
5			1H-3a,7-Methanoazulene, 2,3,4,7,...	204	C15H24	000469-61-4	94



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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
Eucalyptol	11.918	7.0	ug/L	177615	3	11.816	1273240	50.0
1H-3a,7-Methano...	16.124	10.9	ug/L	277030	3	11.816	1273240	50.0