

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050522\
 Data File : VU048433.D
 Acq On : 05 May 2022 13:35
 Operator : SY/MD
 Sample : N2623-04ME
 Misc : 4.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFFJ5ME

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: VU048433.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	105	rVB	99170	216387	15.73%	1.925%
2	1.874	162	166	177	rVB	36133	37251	2.71%	0.331%
3	2.539	360	373	398	rBV	245080	451737	32.85%	4.018%
4	2.768	437	444	452	rVB3	852	1452	0.11%	0.013%
5	2.816	456	459	462	rBV3	215	180	0.01%	0.002%
6	2.851	468	470	474	rVB	502	232	0.02%	0.002%
7	2.877	474	478	480	rBV2	309	222	0.02%	0.002%
8	2.954	490	502	518	rVV2	9350	19820	1.44%	0.176%
9	3.038	518	528	543	rVV3	5108	10283	0.75%	0.091%
10	3.176	559	571	591	rVV	19224	45116	3.28%	0.401%
11	3.472	656	663	668	rBV2	143	197	0.01%	0.002%
12	3.501	668	672	675	rVB	246	209	0.02%	0.002%
13	3.668	721	724	726	rBV2	331	201	0.01%	0.002%
14	3.896	792	795	799	rVB	356	296	0.02%	0.003%
15	3.922	799	803	805	rBV	231	201	0.01%	0.002%
16	4.459	968	970	975	rVB	239	184	0.01%	0.002%
17	4.584	1005	1009	1011	rBV	336	251	0.02%	0.002%
18	4.632	1011	1024	1045	rBV2	107307	332743	24.19%	2.960%
19	4.960	1123	1126	1131	rBV2	265	246	0.02%	0.002%
20	4.986	1131	1134	1139	rBV2	306	259	0.02%	0.002%
21	5.063	1139	1158	1182	rBV	227546	519104	37.74%	4.617%
22	5.295	1223	1230	1232	rBV3	495	636	0.05%	0.006%
23	5.337	1235	1243	1245	rBV2	782	1049	0.08%	0.009%
24	5.719	1339	1362	1388	rBV2	547250	1375357	100.00%	12.233%
25	5.973	1430	1441	1457	rBV2	10673	25052	1.82%	0.223%
26	6.147	1491	1495	1496	rBV	586	400	0.03%	0.004%
27	6.166	1498	1501	1505	rVV3	429	474	0.03%	0.004%
28	6.247	1512	1526	1549	rBV	412451	821638	59.74%	7.308%
29	6.465	1589	1594	1601	rBV3	250	304	0.02%	0.003%
30	6.526	1601	1613	1625	rBV7	4932	9813	0.71%	0.087%
31	6.600	1626	1636	1647	rVV3	4179	9629	0.70%	0.086%
32	6.690	1650	1664	1688	rVB	300612	613493	44.61%	5.457%
33	6.774	1688	1690	1693	rBV2	361	191	0.01%	0.002%
34	6.793	1693	1696	1699	rBV4	386	392	0.03%	0.003%
35	6.922	1733	1736	1737	rBV	269	193	0.01%	0.002%
36	6.941	1739	1742	1743	rBV2	356	175	0.01%	0.002%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Peak Location: TOP

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Peak separation: 5

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

37	7.060	1774	1779	1783	rBV4	529	590	0.04%	0.005%
38	7.134	1800	1802	1806	rVB	387	238	0.02%	0.002%
39	7.185	1806	1818	1845	rBV6	7468	25516	1.86%	0.227%
40	7.497	1912	1915	1920	rVB2	584	440	0.03%	0.004%
41	7.568	1924	1937	1956	rBV	153307	297235	21.61%	2.644%
42	7.697	1969	1977	1983	rBV4	1453	2526	0.18%	0.022%
43	7.793	1998	2007	2008	rBV4	1422	1843	0.13%	0.016%
44	7.899	2026	2040	2056	rBV	628815	1134268	82.47%	10.089%
45	8.185	2115	2129	2150	rBV	97622	201270	14.63%	1.790%
46	8.308	2164	2167	2171	rBV3	388	391	0.03%	0.003%
47	8.353	2176	2181	2188	rBV6	1061	1286	0.09%	0.011%
48	8.452	2209	2212	2213	rBV6	330	175	0.01%	0.002%
49	8.558	2243	2245	2250	rVB3	267	189	0.01%	0.002%
50	8.655	2253	2275	2311	rBV	377103	834642	60.69%	7.424%
51	8.864	2338	2340	2343	rVB2	376	199	0.01%	0.002%
52	8.951	2358	2367	2368	rBV3	421	379	0.03%	0.003%
53	8.970	2371	2373	2375	rBV2	331	205	0.01%	0.002%
54	9.028	2387	2391	2393	rBV2	289	181	0.01%	0.002%
55	9.243	2455	2458	2460	rBV	331	208	0.02%	0.002%
56	9.272	2463	2467	2471	rVV2	204	193	0.01%	0.002%
57	9.423	2500	2514	2544	rBV	572077	1084858	78.88%	9.649%
58	9.542	2549	2551	2555	rVB2	394	277	0.02%	0.002%
59	9.574	2556	2561	2562	rBV2	623	481	0.03%	0.004%
60	9.693	2593	2598	2599	rBV2	1118	662	0.05%	0.006%
61	9.957	2677	2680	2683	rBV	276	263	0.02%	0.002%
62	10.105	2720	2726	2727	rBV3	421	361	0.03%	0.003%
63	10.121	2729	2731	2735	rVB2	474	336	0.02%	0.003%
64	10.246	2765	2770	2773	rVB2	207	175	0.01%	0.002%
65	10.471	2833	2840	2850	rBV5	1833	2677	0.19%	0.024%
66	10.671	2896	2902	2916	rVB6	2929	4497	0.33%	0.040%
67	10.764	2916	2931	2950	rBV	514608	829289	60.30%	7.376%
68	10.873	2960	2965	2967	rBV	429	430	0.03%	0.004%
69	10.896	2967	2972	2982	rVB5	1233	1761	0.13%	0.016%
70	11.092	3029	3033	3034	rBV2	332	225	0.02%	0.002%
71	11.118	3034	3041	3049	rVV6	3613	5602	0.41%	0.050%
72	11.375	3119	3121	3126	rVB2	371	286	0.02%	0.003%
73	11.462	3141	3148	3160	rVV7	1758	3907	0.28%	0.035%
74	11.581	3180	3185	3188	rBV3	645	529	0.04%	0.005%
75	11.700	3214	3222	3229	rBV5	1510	2274	0.17%	0.020%
76	11.751	3234	3238	3245	rBV2	943	1057	0.08%	0.009%

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 MSVOA_U
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 BFFJ5ME

Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

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

77	11.819	3245	3259	3279	rBV	676046	1101372	80.08%	9.796%
78	11.918	3279	3290	3303	rBV2	64384	106541	7.75%	0.948%
79	12.024	3320	3323	3325	rBV2	302	196	0.01%	0.002%
80	12.044	3325	3329	3334	rVV3	535	494	0.04%	0.004%
81	12.124	3352	3354	3357	rBV	323	178	0.01%	0.002%
82	12.198	3361	3377	3399	rBV	663625	1070735	77.85%	9.524%
83	12.323	3413	3416	3418	rBV3	781	529	0.04%	0.005%
84	12.407	3438	3442	3445	rVB2	841	666	0.05%	0.006%
85	12.478	3461	3464	3467	rBV2	310	204	0.01%	0.002%
86	12.539	3481	3483	3486	rBV	317	182	0.01%	0.002%
87	12.558	3486	3489	3492	rVV	362	263	0.02%	0.002%
88	12.629	3509	3511	3515	rBV2	300	247	0.02%	0.002%
89	12.777	3547	3557	3564	rVB5	1433	2268	0.16%	0.020%
90	12.909	3594	3598	3600	rBV2	343	318	0.02%	0.003%
91	12.947	3606	3610	3615	rBV3	371	432	0.03%	0.004%
92	13.230	3695	3698	3704	rVB4	1045	872	0.06%	0.008%
93	13.558	3797	3800	3804	rBV2	349	365	0.03%	0.003%
94	13.594	3806	3811	3814	rVV3	366	350	0.03%	0.003%
95	13.854	3885	3892	3899	rBV3	1378	1827	0.13%	0.016%
96	14.095	3962	3967	3978	rVB3	1641	2001	0.15%	0.018%
97	14.333	4037	4041	4051	rBV3	1029	1614	0.12%	0.014%
98	14.452	4072	4078	4084	rVB3	1400	1467	0.11%	0.013%
99	14.963	4235	4237	4243	rVB3	585	527	0.04%	0.005%
100	16.121	4591	4597	4605	rVB6	8632	12020	0.87%	0.107%

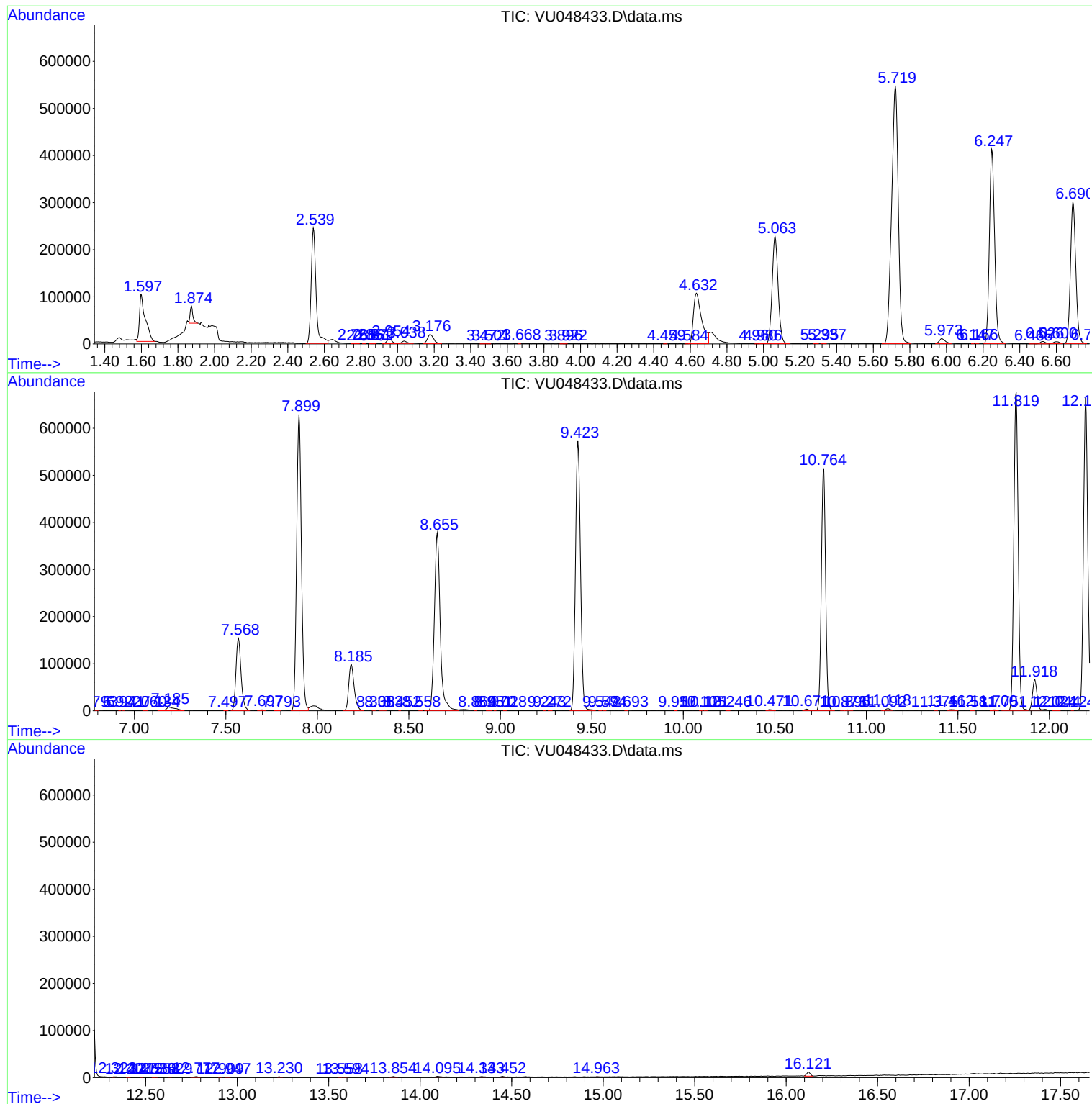
Sum of corrected areas: 11242956

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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFFJ5ME

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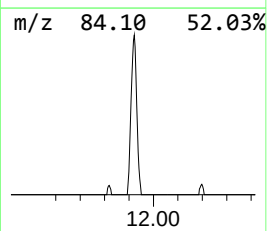
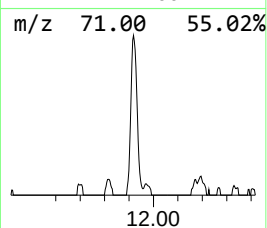
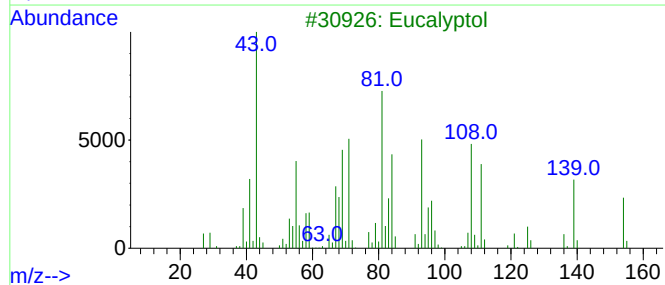
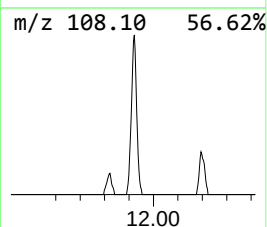
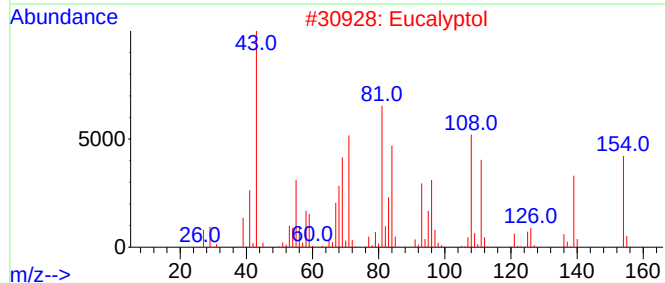
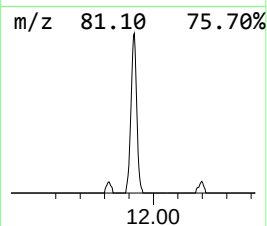
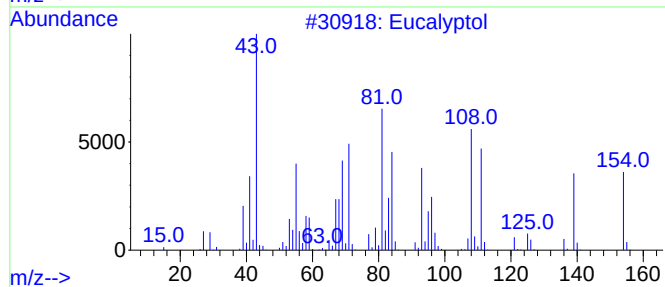
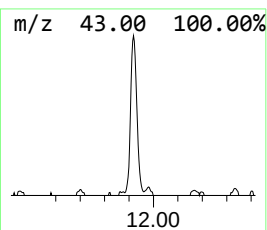
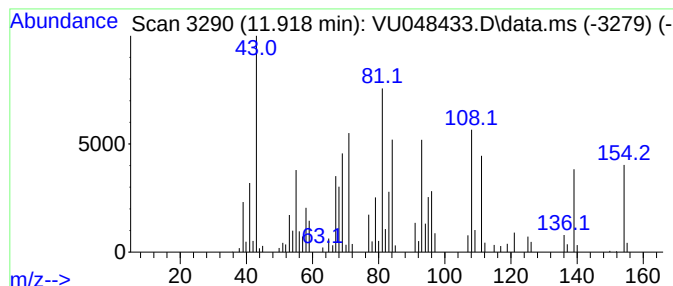
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Eucalyptol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.918	4.84 ug/L	106541	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	98
2			Eucalyptol	154	C10H18O	000470-82-6	96
3			Eucalyptol	154	C10H18O	000470-82-6	93
4			Eucalyptol	154	C10H18O	000470-82-6	90
5			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	53



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Eucalyptol	11.918	4.8	ug/L	106541	3	11.819	1101370	50.0