

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
 Data File : VU047923.D
 Acq On : 11 Apr 2022 22:14
 Operator : SY/MD
 Sample : N2293-05ME
 Misc : 6.63g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNN5ME

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: VU047923.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	87	rBV	65267	93135	5.48%	0.779%
2	1.829	120	152	153	rBV7	35408	128796	7.58%	1.077%
3	2.536	360	372	385	rBV	197406	342529	20.16%	2.865%
4	2.768	437	444	453	rVB2	2138	3827	0.23%	0.032%
5	2.954	496	502	513	rVB6	3519	6822	0.40%	0.057%
6	3.038	521	528	534	rBV7	1033	1631	0.10%	0.014%
7	3.118	550	553	558	rVB2	315	254	0.01%	0.002%
8	3.170	562	569	572	rBV2	553	727	0.04%	0.006%
9	3.324	614	617	620	rBV2	367	301	0.02%	0.003%
10	3.343	621	623	628	rVB3	457	305	0.02%	0.003%
11	3.491	666	669	675	rVB3	347	371	0.02%	0.003%
12	3.597	698	702	711	rVB3	217	331	0.02%	0.003%
13	3.797	761	764	768	rVB2	277	257	0.02%	0.002%
14	3.880	786	790	792	rBV	365	253	0.01%	0.002%
15	3.945	808	810	816	rVV2	302	269	0.02%	0.002%
16	4.144	865	872	876	rBV2	281	369	0.02%	0.003%
17	4.195	884	888	891	rBV	322	258	0.02%	0.002%
18	4.218	891	895	898	rVV	376	284	0.02%	0.002%
19	4.266	905	910	915	rBV2	352	354	0.02%	0.003%
20	4.443	962	965	970	rBV3	302	271	0.02%	0.002%
21	4.636	1011	1025	1073	rBV	98318	331179	19.50%	2.770%
22	5.060	1140	1157	1179	rBV	199810	462034	27.20%	3.865%
23	5.276	1218	1224	1225	rBV2	351	288	0.02%	0.002%
24	5.292	1225	1229	1233	rBV2	409	384	0.02%	0.003%
25	5.337	1235	1243	1245	rBV5	1084	1573	0.09%	0.013%
26	5.469	1280	1284	1287	rBV2	231	232	0.01%	0.002%
27	5.642	1331	1338	1341	rBV3	284	264	0.02%	0.002%
28	5.719	1341	1362	1399	rBV2	451583	1238688	72.92%	10.361%
29	5.893	1414	1416	1423	rVV2	449	445	0.03%	0.004%
30	5.941	1427	1431	1433	rVB	370	273	0.02%	0.002%
31	5.970	1433	1440	1442	rBV4	569	435	0.03%	0.004%
32	5.983	1442	1444	1449	rVV2	406	327	0.02%	0.003%
33	6.247	1509	1526	1554	rBV	525150	1061806	62.51%	8.882%
34	6.526	1607	1613	1615	rBV4	1317	1613	0.09%	0.013%
35	6.597	1625	1635	1642	rBV4	830	1060	0.06%	0.009%
36	6.690	1648	1664	1693	rBV	262311	537926	31.67%	4.500%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Peak Location: TOP

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

37	6.845	1708	1712	1721	rVB3	375	424	0.02%	0.004%
38	6.973	1749	1752	1755	rVB2	393	265	0.02%	0.002%
39	6.993	1755	1758	1764	rBV3	418	534	0.03%	0.004%
40	7.060	1767	1779	1780	rBV4	836	1271	0.07%	0.011%
41	7.192	1805	1820	1838	rBV2	8048	19994	1.18%	0.167%
42	7.414	1887	1889	1892	rBV	465	265	0.02%	0.002%
43	7.568	1924	1937	1959	rBV	126360	248110	14.61%	2.075%
44	7.697	1970	1977	1979	rBV6	1165	1359	0.08%	0.011%
45	7.806	2008	2011	2013	rBV2	388	285	0.02%	0.002%
46	7.899	2025	2040	2055	rBV	507044	927139	54.58%	7.755%
47	7.970	2057	2062	2082	rVB	15523	28875	1.70%	0.242%
48	8.182	2116	2128	2148	rBV	82693	170161	10.02%	1.423%
49	8.263	2152	2153	2161	rVB3	401	291	0.02%	0.002%
50	8.652	2259	2274	2308	rBV	374525	794185	46.75%	6.643%
51	9.047	2394	2397	2400	rVB3	392	287	0.02%	0.002%
52	9.070	2400	2404	2406	rBV2	393	309	0.02%	0.003%
53	9.185	2434	2440	2446	rBV3	299	400	0.02%	0.003%
54	9.317	2478	2481	2486	rVB2	370	337	0.02%	0.003%
55	9.423	2499	2514	2552	rBV2	777121	1698650	100.00%	14.209%
56	9.575	2554	2561	2567	rVV7	1599	2044	0.12%	0.017%
57	9.616	2572	2574	2581	rVB2	251	246	0.01%	0.002%
58	9.697	2589	2599	2608	rVB5	2746	4607	0.27%	0.039%
59	9.806	2629	2633	2635	rBV	293	236	0.01%	0.002%
60	10.054	2705	2710	2713	rBV	308	269	0.02%	0.002%
61	10.111	2718	2728	2738	rBV7	1690	3212	0.19%	0.027%
62	10.205	2753	2757	2760	rBV	271	272	0.02%	0.002%
63	10.275	2776	2779	2783	rVB2	316	280	0.02%	0.002%
64	10.298	2783	2786	2788	rBV	319	230	0.01%	0.002%
65	10.436	2825	2829	2833	rVB2	354	351	0.02%	0.003%
66	10.475	2837	2841	2842	rBV	433	276	0.02%	0.002%
67	10.674	2894	2903	2910	rVB4	1591	2462	0.14%	0.021%
68	10.764	2918	2931	2952	rVV	466356	771006	45.39%	6.449%
69	10.861	2958	2961	2963	rBV3	349	251	0.01%	0.002%
70	10.883	2963	2968	2970	rBV2	535	522	0.03%	0.004%
71	10.973	2992	2996	2998	rBV3	438	409	0.02%	0.003%
72	11.038	3013	3016	3020	rBV2	460	421	0.02%	0.004%
73	11.086	3027	3031	3032	rBV3	480	352	0.02%	0.003%
74	11.121	3039	3042	3046	rVB3	791	638	0.04%	0.005%
75	11.150	3046	3051	3054	rBV	439	445	0.03%	0.004%
76	11.269	3084	3088	3091	rBV2	360	281	0.02%	0.002%

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Instrument :
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 ClientSampleId :
 ETNN5ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

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Peak Location: TOP

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Peak separation: 5

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

77	11.292	3091	3095	3100	rBV4	449	575	0.03%	0.005%
78	11.423	3132	3136	3139	rVV3	375	372	0.02%	0.003%
79	11.472	3142	3151	3160	rVB6	2925	5150	0.30%	0.043%
80	11.607	3186	3193	3196	rBV2	401	398	0.02%	0.003%
81	11.693	3217	3220	3226	rBV3	639	664	0.04%	0.006%
82	11.755	3230	3239	3246	rBV5	4696	7445	0.44%	0.062%
83	11.816	3246	3258	3277	rBV	1025773	1612352	94.92%	13.487%
84	11.957	3295	3302	3314	rVB9	5007	8413	0.50%	0.070%
85	12.037	3325	3327	3331	rVB	487	323	0.02%	0.003%
86	12.060	3331	3334	3340	rBV4	602	689	0.04%	0.006%
87	12.198	3363	3377	3396	rBV	609004	1002034	58.99%	8.382%
88	12.375	3429	3432	3434	rBV2	455	349	0.02%	0.003%
89	12.684	3525	3528	3533	rBV4	312	254	0.01%	0.002%
90	12.771	3551	3555	3567	rVB4	1139	1612	0.09%	0.013%
91	12.973	3608	3618	3634	rBV3	35476	57140	3.36%	0.478%
92	13.333	3720	3730	3738	rVV2	16662	26243	1.54%	0.220%
93	13.381	3738	3745	3754	rVB4	9027	13691	0.81%	0.115%
94	13.700	3841	3844	3848	rBV3	320	233	0.01%	0.002%
95	13.848	3885	3890	3898	rVB3	2633	3778	0.22%	0.032%
96	14.095	3959	3967	3976	rBV2	3501	5444	0.32%	0.046%
97	14.336	4036	4042	4050	rVB5	1856	2557	0.15%	0.021%
98	14.497	4087	4092	4097	rBV5	1454	1391	0.08%	0.012%
99	15.545	4407	4418	4432	rBV2	178992	283610	16.70%	2.372%
100	16.388	4674	4680	4690	rBV4	12800	18179	1.07%	0.152%

Sum of corrected areas: 11954718

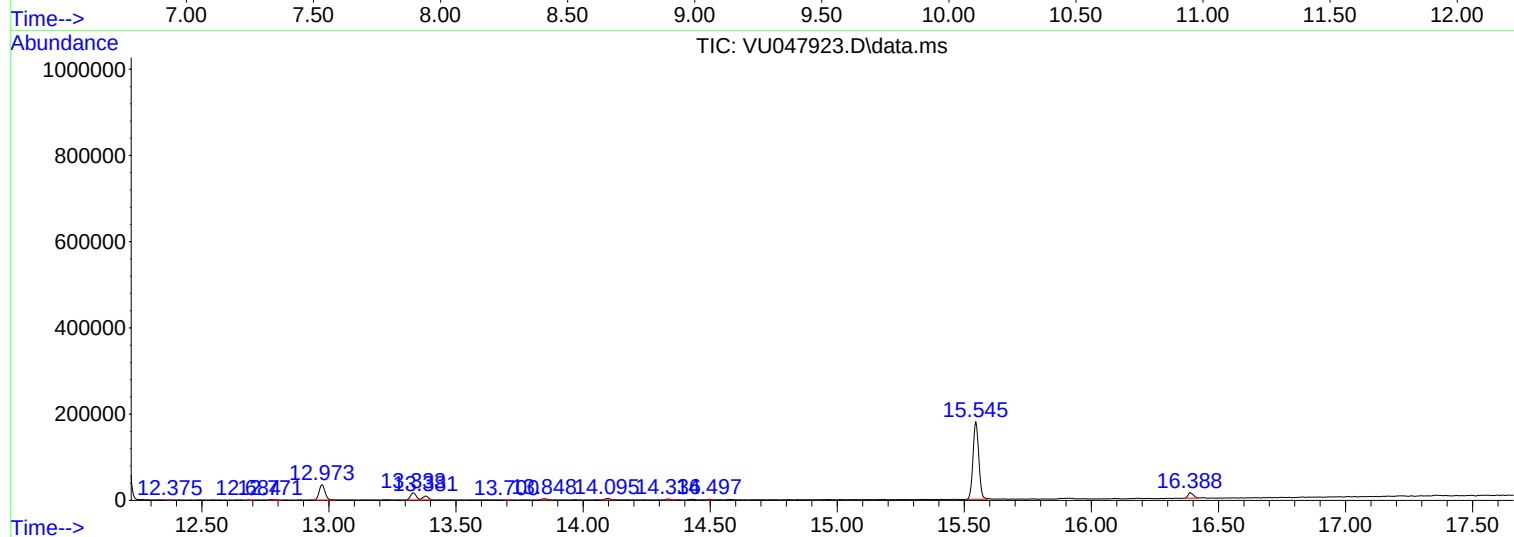
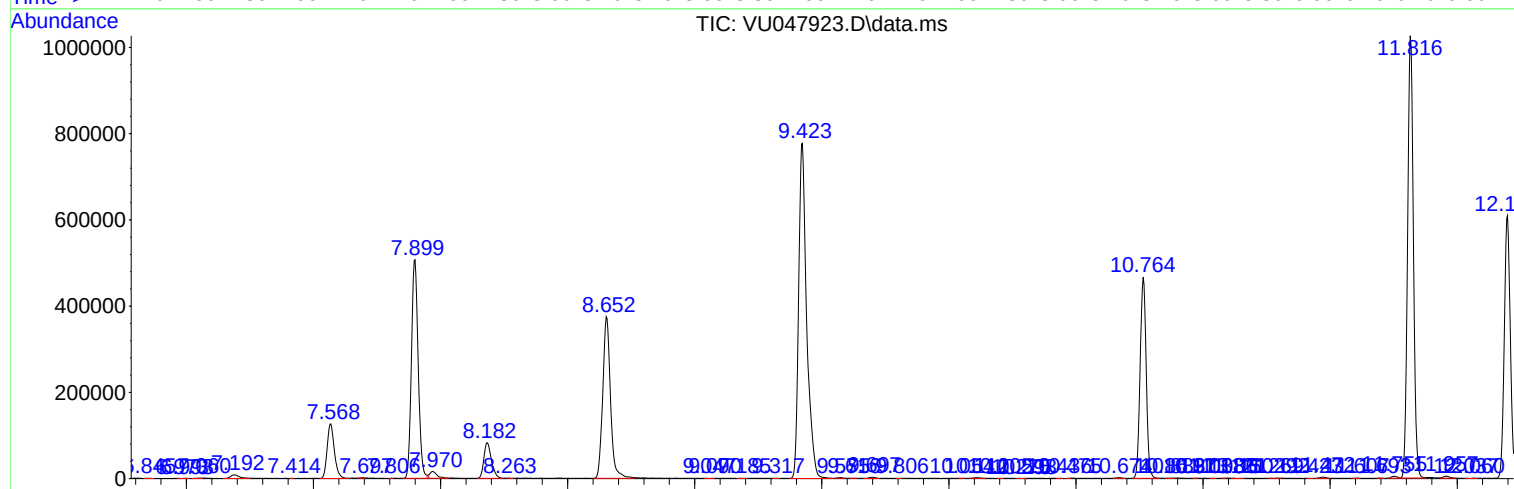
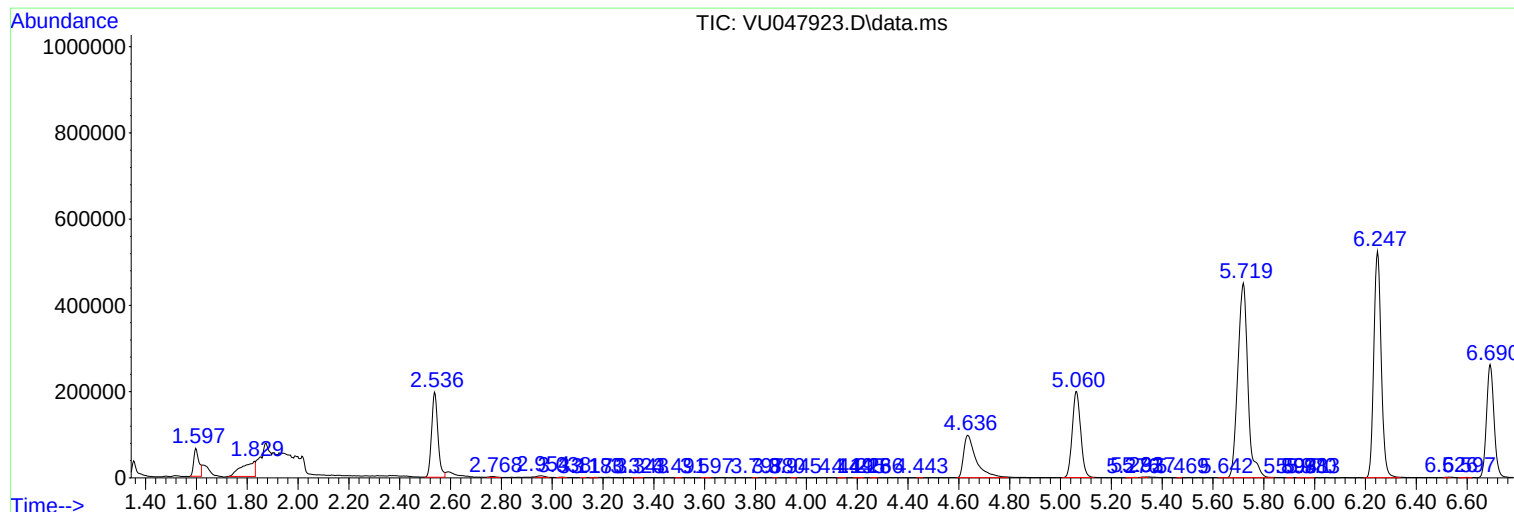
Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047923.D
Acq On : 11 Apr 2022 22:14
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ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN5ME

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 : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN5ME

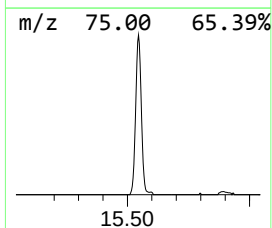
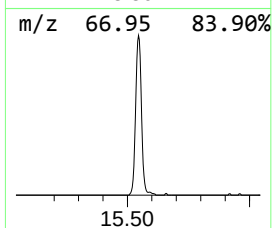
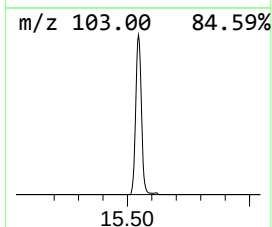
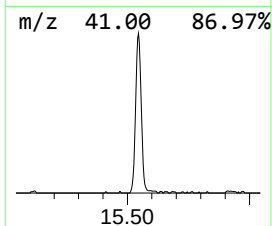
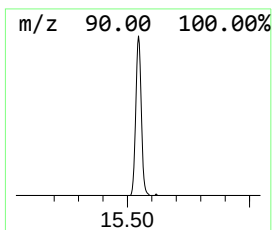
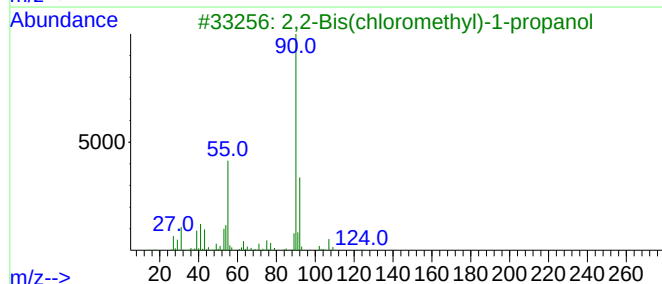
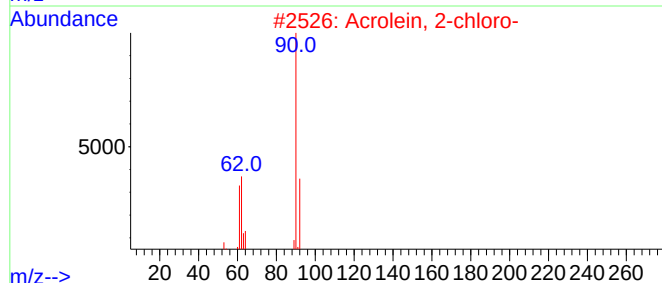
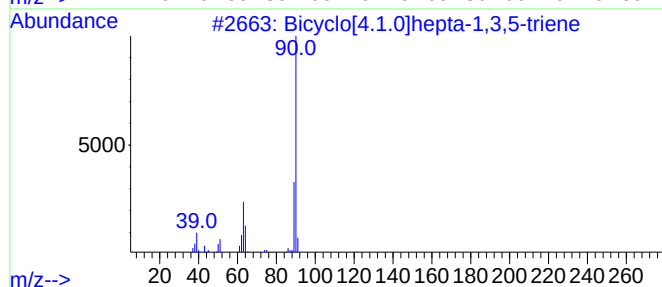
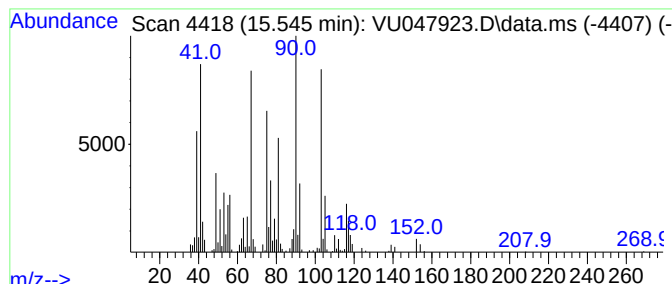
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	8.79 ug/L	283610	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	38
2			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	37
3			2,2-Bis(chloromethyl)-1-propanol	156	C5H10Cl2O	005355-54-4	32
4			1,3,5-Trichloro-4-methyl-2-penta...	202	C6H9Cl3O	1000140-03-8	28
5			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	28



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	15.545	8.8	ug/L	283610	3	11.816	1612350	50.0