

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
 Data File : VU047960.D
 Acq On : 12 Apr 2022 16:55
 Operator : SY/MD
 Sample : N2293-19ME
 Misc : 6.47g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNP7ME

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: VU047960.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.485	38	45	49	rBV6	2468	3340	0.13%	0.032%
2	1.597	73	80	104	rBV	50186	93472	3.60%	0.908%
3	1.854	120	160	161	rBV5	40685	174285	6.72%	1.693%
4	2.543	363	374	385	rBV	122872	210687	8.12%	2.047%
5	3.038	518	528	537	rBV5	1522	2780	0.11%	0.027%
6	3.118	551	553	561	rVB4	540	724	0.03%	0.007%
7	3.179	565	572	584	rVB6	1003	2224	0.09%	0.022%
8	3.305	601	611	618	rBV2	546	1095	0.04%	0.011%
9	4.633	1009	1024	1061	rBV	100812	317686	12.25%	3.086%
10	5.060	1141	1157	1185	rVV	168334	386441	14.90%	3.754%
11	5.282	1221	1226	1229	rBV3	349	359	0.01%	0.003%
12	5.340	1235	1244	1261	rVB2	2613	6199	0.24%	0.060%
13	5.616	1324	1330	1335	rBV3	292	327	0.01%	0.003%
14	5.719	1338	1362	1374	rBV2	351282	953460	36.77%	9.262%
15	5.886	1411	1414	1418	rVB3	468	415	0.02%	0.004%
16	5.977	1433	1442	1443	rBV4	606	590	0.02%	0.006%
17	6.247	1510	1526	1555	rBV	354941	694742	26.79%	6.749%
18	6.520	1606	1611	1612	rBV2	714	522	0.02%	0.005%
19	6.607	1631	1638	1644	rVB5	1013	1336	0.05%	0.013%
20	6.690	1650	1664	1690	rVB	222062	450253	17.36%	4.374%
21	6.800	1695	1698	1706	rVV3	711	758	0.03%	0.007%
22	6.883	1720	1724	1727	rBV2	299	310	0.01%	0.003%
23	7.031	1759	1770	1772	rBV3	420	650	0.03%	0.006%
24	7.050	1772	1776	1786	rVB4	905	1515	0.06%	0.015%
25	7.189	1807	1819	1835	rBV3	7627	17622	0.68%	0.171%
26	7.497	1907	1915	1925	rBV6	3941	7594	0.29%	0.074%
27	7.568	1925	1937	1956	rVB	98920	193812	7.47%	1.883%
28	7.697	1972	1977	1990	rVV6	1300	2257	0.09%	0.022%
29	7.812	2008	2013	2015	rBV2	563	469	0.02%	0.005%
30	7.899	2026	2040	2055	rBV	338821	613115	23.64%	5.956%
31	7.973	2055	2063	2083	rVB2	14276	33323	1.29%	0.324%
32	8.182	2115	2128	2147	rVV	69000	138970	5.36%	1.350%
33	8.365	2172	2185	2189	rBV4	2567	4267	0.16%	0.041%
34	8.475	2212	2219	2229	rVB2	2257	3638	0.14%	0.035%
35	8.571	2246	2249	2250	rVV2	720	404	0.02%	0.004%
36	8.581	2250	2252	2258	rVB5	1391	1033	0.04%	0.010%

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Instrument :
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 ETNP7ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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Max Peaks: 100

Stop Thrs : 0

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Peak separation: 5

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

37	8.648	2258	2273	2308	rBV	391248	787755	30.38%	7.653%
38	8.890	2345	2348	2354	rBV3	579	666	0.03%	0.006%
39	9.025	2380	2390	2397	rBV8	1317	2130	0.08%	0.021%
40	9.362	2490	2495	2498	rBV3	695	575	0.02%	0.006%
41	9.449	2498	2522	2558	rBV2	965816	2593223	100.00%	25.191%
42	9.693	2592	2598	2607	rBV5	1248	2194	0.08%	0.021%
43	10.108	2716	2727	2733	rBV5	972	1728	0.07%	0.017%
44	10.250	2766	2771	2783	rBV3	443	646	0.02%	0.006%
45	10.362	2801	2806	2809	rBV2	412	416	0.02%	0.004%
46	10.401	2815	2818	2822	rBV2	374	325	0.01%	0.003%
47	10.484	2838	2844	2849	rBV3	426	560	0.02%	0.005%
48	10.655	2890	2897	2908	rVB7	2207	4061	0.16%	0.039%
49	10.761	2917	2930	2949	rBV	439799	711918	27.45%	6.916%
50	10.893	2956	2971	2983	rBV4	3310	5788	0.22%	0.056%
51	10.976	2992	2997	3002	rBV3	739	692	0.03%	0.007%
52	11.098	3033	3035	3037	rVV2	495	310	0.01%	0.003%
53	11.115	3037	3040	3045	rVB3	549	481	0.02%	0.005%
54	11.301	3095	3098	3102	rVB3	534	401	0.02%	0.004%
55	11.381	3117	3123	3127	rVV3	346	416	0.02%	0.004%
56	11.414	3128	3133	3139	rVB5	1560	1872	0.07%	0.018%
57	11.452	3139	3145	3146	rBV2	1129	968	0.04%	0.009%
58	11.471	3146	3151	3156	rVB5	1504	1864	0.07%	0.018%
59	11.510	3161	3163	3168	rBV2	495	320	0.01%	0.003%
60	11.568	3178	3181	3184	rBV2	546	432	0.02%	0.004%
61	11.697	3214	3221	3224	rBV4	1353	1538	0.06%	0.015%
62	11.751	3232	3238	3245	rBV6	2803	3480	0.13%	0.034%
63	11.816	3245	3258	3273	rBV	569431	896782	34.58%	8.712%
64	11.999	3313	3315	3322	rVB4	1676	1640	0.06%	0.016%
65	12.070	3334	3337	3338	rBV2	757	452	0.02%	0.004%
66	12.195	3361	3376	3393	rBV	413130	690931	26.64%	6.712%
67	12.291	3404	3406	3410	rVB3	579	374	0.01%	0.004%
68	12.324	3411	3416	3419	rBV7	1663	1724	0.07%	0.017%
69	12.385	3426	3435	3438	rBV4	1249	1707	0.07%	0.017%
70	12.475	3459	3463	3465	rBV3	743	582	0.02%	0.006%
71	12.523	3476	3478	3479	rBV2	799	348	0.01%	0.003%
72	12.587	3493	3498	3499	rBV2	511	358	0.01%	0.003%
73	12.668	3518	3523	3531	rVB5	1920	2875	0.11%	0.028%
74	12.835	3570	3575	3576	rBV3	1471	1017	0.04%	0.010%
75	12.902	3588	3596	3599	rBV5	1608	2107	0.08%	0.020%
76	12.938	3601	3607	3608	rBV5	1635	1838	0.07%	0.018%

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Instrument :
 MSVOA_U
 ClientSampleId :
 ETNP7ME

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

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

77	13.047	3635	3641	3651	rVB8	2290	3567	0.14%	0.035%
78	13.134	3663	3668	3677	rVB5	1328	1704	0.07%	0.017%
79	13.221	3692	3695	3699	rVB3	605	440	0.02%	0.004%
80	13.272	3705	3711	3713	rBV3	799	852	0.03%	0.008%
81	13.304	3718	3721	3723	rBV2	488	346	0.01%	0.003%
82	13.333	3723	3730	3736	rBV5	4450	6932	0.27%	0.067%
83	13.378	3737	3744	3756	rVB3	10863	16407	0.63%	0.159%
84	13.433	3757	3761	3762	rBV4	1428	959	0.04%	0.009%
85	13.584	3799	3808	3818	rBV8	5017	9774	0.38%	0.095%
86	13.844	3882	3889	3893	rBV7	1411	1900	0.07%	0.018%
87	14.044	3947	3951	3960	rVB8	2819	3762	0.15%	0.037%
88	14.095	3961	3967	3972	rBV4	2866	3972	0.15%	0.039%
89	14.195	3987	3998	4003	rBV7	3189	5518	0.21%	0.054%
90	14.266	4017	4020	4024	rVB5	999	595	0.02%	0.006%
91	14.362	4041	4050	4062	rBV4	7994	12844	0.50%	0.125%
92	14.494	4084	4091	4106	rBV4	6458	12462	0.48%	0.121%
93	14.899	4214	4217	4220	rBV4	1009	843	0.03%	0.008%
94	15.182	4303	4305	4307	rBV3	816	488	0.02%	0.005%
95	15.211	4310	4314	4319	rVV7	2534	3260	0.13%	0.032%
96	15.314	4340	4346	4354	rVB7	3931	5488	0.21%	0.053%
97	15.545	4409	4418	4427	rVB3	32619	50813	1.96%	0.494%
98	15.889	4517	4525	4540	rVB9	7515	18225	0.70%	0.177%
99	15.954	4540	4545	4556	rBV7	3705	7347	0.28%	0.071%
100	16.388	4671	4680	4692	rBV3	47586	77418	2.99%	0.752%

Sum of corrected areas: 10294084

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Misc : 6.47g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP7ME

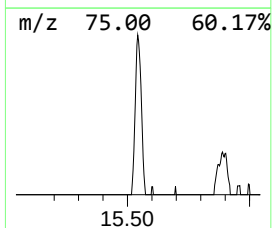
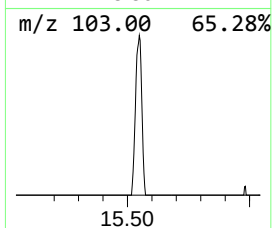
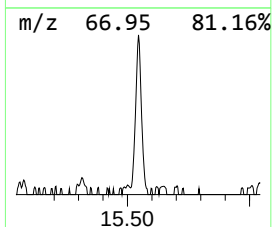
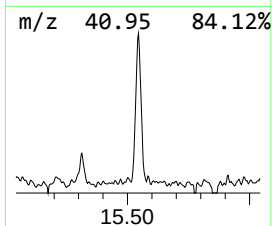
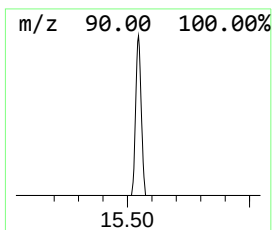
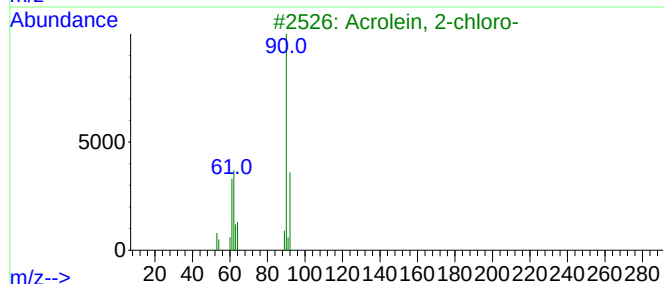
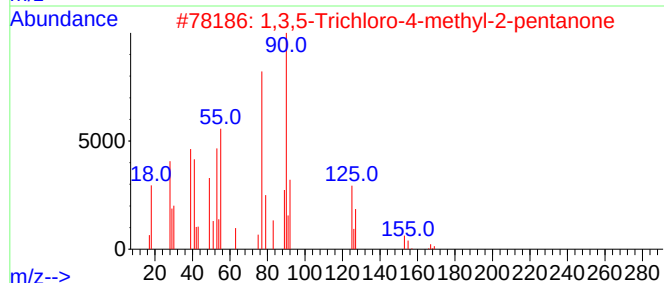
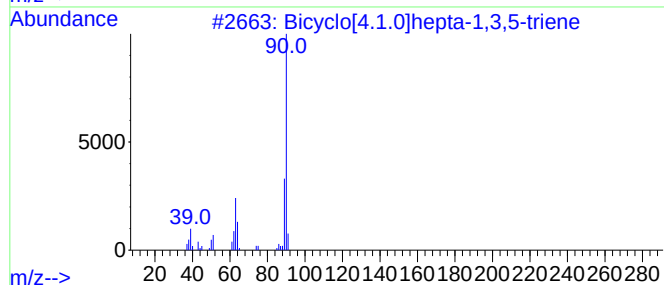
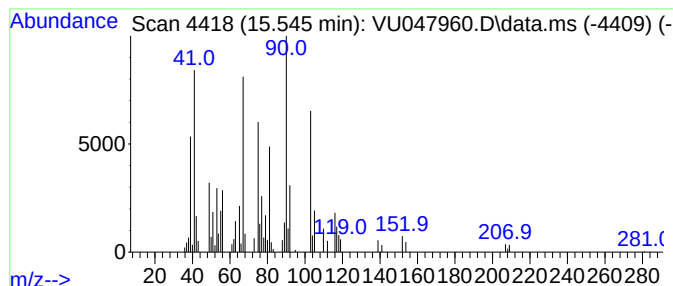
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	2.83 ug/L	50813	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			1,3,5-Trichloro-4-methyl-2-penta...	202	C6H9Cl3O	1000140-03-8	30
3			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	28
4			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	25
5			1H-1,2,4-Triazole,3-chloro-1,5-d...	131	C4H6ClN3	056616-94-5	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
Data File : VU047960.D
Acq On : 12 Apr 2022 16:55
Operator : SY/MD
Sample : N2293-19ME
Misc : 6.47g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP7ME

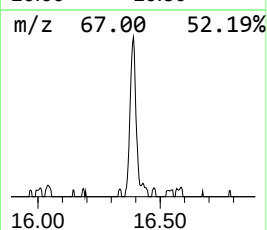
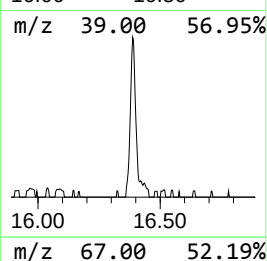
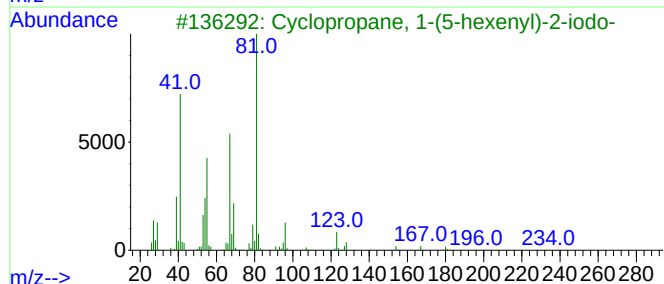
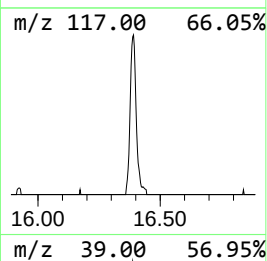
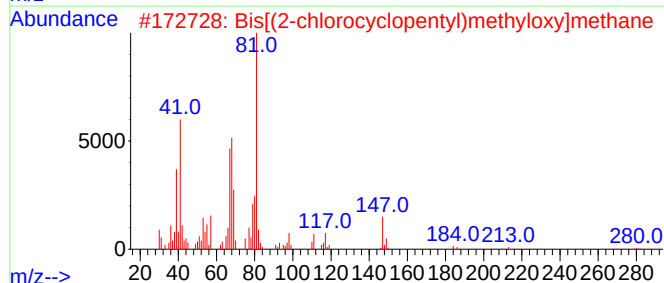
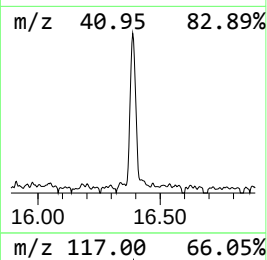
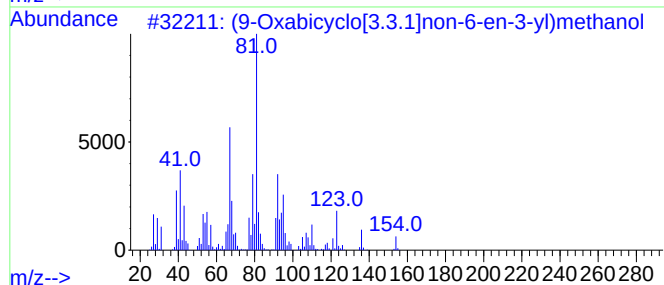
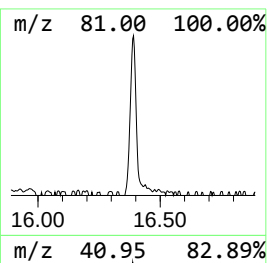
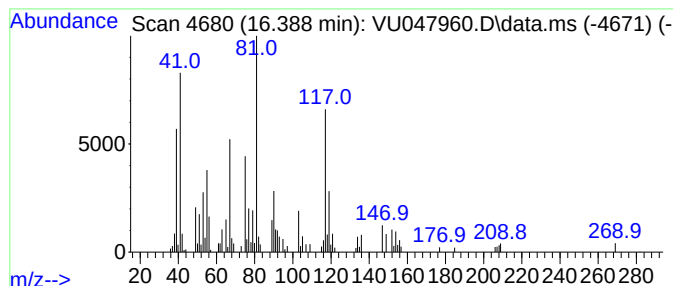
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.388	4.32 ug/L	77418	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(9-Oxabicyclo[3.3.1]non-6-en-3-y...	154	C9H14O2	1000191-02-8	22
2			Bis[(2-chlorocyclopentyl)methylo...	280	C13H22Cl2O2	1000216-83-2	12
3			Cyclopropane, 1-(5-hexenyl)-2-iodo-	250	C9H15I	074685-40-8	12
4			Cyclohexene, 3-(2-propynyl)-	120	C9H12	055956-43-9	11
5			1-Pentene, 5-chloro-4-(chloromet...	152	C6H10Cl2	027990-74-5	10



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ALS Vial : 21 Sample Multiplier: 1

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ClientSampleId :
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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
unknown-01	15.545	2.8	ug/L	50813	3	11.816	896782	50.0
unknown-02	16.388	4.3	ug/L	77418	3	11.816	896782	50.0