

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
 Data File : VU048001.D
 Acq On : 13 Apr 2022 14:16
 Operator : SY/MD
 Sample : N2293-22ME
 Misc : 6.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNQ5ME

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: VU048001.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.598	74	80	104	rVB	41918	79413	5.12%	0.850%
2	2.543	364	374	385	rBV	112674	189993	12.25%	2.035%
3	3.337	617	621	623	rBV2	400	309	0.02%	0.003%
4	3.424	645	648	653	rBV2	332	434	0.03%	0.005%
5	3.482	663	666	667	rBV	361	205	0.01%	0.002%
6	3.568	688	693	697	rBV2	545	563	0.04%	0.006%
7	3.604	702	704	707	rVB2	529	319	0.02%	0.003%
8	3.687	727	730	733	rBV	276	209	0.01%	0.002%
9	3.707	733	736	739	rVV2	212	159	0.01%	0.002%
10	3.777	755	758	763	rBV2	267	215	0.01%	0.002%
11	3.829	772	774	776	rBV	234	120	0.01%	0.001%
12	3.932	803	806	809	rBV2	233	202	0.01%	0.002%
13	3.983	819	822	829	rBV4	424	494	0.03%	0.005%
14	4.080	849	852	854	rBV	213	136	0.01%	0.001%
15	4.163	876	878	881	rBV2	300	147	0.01%	0.002%
16	4.202	888	890	892	rVB2	223	83	0.01%	0.001%
17	4.218	892	895	897	rBV2	255	140	0.01%	0.001%
18	4.295	916	919	923	rBV2	317	261	0.02%	0.003%
19	4.318	923	926	930	rVV3	316	253	0.02%	0.003%
20	4.353	934	937	939	rVB3	290	132	0.01%	0.001%
21	4.392	947	949	952	rBV3	247	154	0.01%	0.002%
22	4.559	998	1001	1003	rBV	369	284	0.02%	0.003%
23	4.633	1011	1024	1073	rBV	92654	295061	19.03%	3.160%
24	5.060	1140	1157	1186	rVB	154924	354690	22.88%	3.798%
25	5.202	1199	1201	1205	rVB2	269	157	0.01%	0.002%
26	5.221	1205	1207	1208	rBV	192	69	0.00%	0.001%
27	5.266	1215	1221	1222	rBV4	540	550	0.04%	0.006%
28	5.433	1272	1273	1276	rVB2	244	72	0.00%	0.001%
29	5.462	1276	1282	1284	rBV2	337	334	0.02%	0.004%
30	5.520	1297	1300	1302	rVB	200	119	0.01%	0.001%
31	5.546	1302	1308	1309	rBV2	224	194	0.01%	0.002%
32	5.581	1315	1319	1323	rBV3	400	373	0.02%	0.004%
33	5.604	1323	1326	1331	rVV3	281	257	0.02%	0.003%
34	5.626	1331	1333	1336	rVB2	162	110	0.01%	0.001%
35	5.720	1341	1362	1375	rBV2	322398	867325	55.94%	9.288%
36	6.166	1498	1501	1502	rBV2	172	101	0.01%	0.001%

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Integrator: RTE

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

37	6.247	1511	1526	1554	rBV	398229	783037	50.50%	8.385%
38	6.520	1602	1611	1615	rBV5	910	1234	0.08%	0.013%
39	6.604	1633	1637	1642	rBV3	569	527	0.03%	0.006%
40	6.691	1649	1664	1687	rBV	197869	409636	26.42%	4.387%
41	6.803	1698	1699	1700	rBV	504	174	0.01%	0.002%
42	6.842	1709	1711	1714	rBV2	410	229	0.01%	0.002%
43	6.858	1714	1716	1719	rVB2	280	94	0.01%	0.001%
44	6.912	1730	1733	1737	rVB2	262	206	0.01%	0.002%
45	6.964	1746	1749	1751	rBV2	267	156	0.01%	0.002%
46	7.028	1766	1769	1770	rBV	452	250	0.02%	0.003%
47	7.112	1790	1795	1799	rBV2	326	350	0.02%	0.004%
48	7.182	1805	1817	1833	rBV3	8779	19081	1.23%	0.204%
49	7.334	1862	1864	1866	rBV	191	104	0.01%	0.001%
50	7.498	1904	1915	1924	rBV6	3449	6626	0.43%	0.071%
51	7.568	1925	1937	1956	rVB	92120	178837	11.53%	1.915%
52	7.684	1970	1973	1974	rBV2	800	482	0.03%	0.005%
53	7.784	2002	2004	2007	rBV	290	198	0.01%	0.002%
54	7.900	2026	2040	2054	rBV	309821	563236	36.33%	6.031%
55	8.125	2106	2110	2111	rBV2	613	391	0.03%	0.004%
56	8.182	2117	2128	2146	rBV	61098	124357	8.02%	1.332%
57	8.649	2259	2273	2305	rBV	358247	719362	46.40%	7.703%
58	9.015	2384	2387	2389	rBV3	684	488	0.03%	0.005%
59	9.163	2430	2433	2436	rBV2	391	256	0.02%	0.003%
60	9.314	2478	2480	2482	rBB2	255	97	0.01%	0.001%
61	9.424	2499	2514	2549	rBV2	538223	1550444	100.00%	16.603%
62	9.642	2580	2582	2584	rBV2	222	145	0.01%	0.002%
63	9.652	2584	2585	2588	rVV2	395	199	0.01%	0.002%
64	9.694	2591	2598	2608	rVB4	2130	2978	0.19%	0.032%
65	9.774	2621	2623	2624	rBV4	186	68	0.00%	0.001%
66	9.848	2644	2646	2649	rBV	193	144	0.01%	0.002%
67	9.928	2668	2671	2673	rBV	315	206	0.01%	0.002%
68	9.996	2689	2692	2695	rBV2	268	170	0.01%	0.002%
69	10.015	2695	2698	2700	rBV3	369	265	0.02%	0.003%
70	10.102	2717	2725	2732	rBV3	2174	2841	0.18%	0.030%
71	10.150	2737	2740	2744	rBV2	376	281	0.02%	0.003%
72	10.205	2755	2757	2758	rBV	287	102	0.01%	0.001%
73	10.256	2771	2773	2777	rBV3	347	202	0.01%	0.002%
74	10.362	2803	2806	2812	rVB2	530	466	0.03%	0.005%
75	10.395	2813	2816	2818	rBV	282	179	0.01%	0.002%
76	10.417	2819	2823	2833	rVV3	694	859	0.06%	0.009%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Min Area: 0 % of largest Peak

Start Thrs: 0.2

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Stop Thrs : 0

Peak Location: TOP

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

77	10.523	2854	2856	2857	rBV2	321	156	0.01%	0.002%
78	10.658	2894	2898	2904	rBV6	748	639	0.04%	0.007%
79	10.713	2906	2915	2918	rBV5	2615	3978	0.26%	0.043%
80	10.761	2919	2930	2948	rVB	397757	647690	41.77%	6.936%
81	10.825	2948	2950	2952	rBV	540	227	0.01%	0.002%
82	10.890	2964	2970	2972	rBV2	1872	1632	0.11%	0.017%
83	10.989	2991	3001	3013	rBV	9171	14339	0.92%	0.154%
84	11.102	3028	3036	3046	rBV2	7136	10577	0.68%	0.113%
85	11.272	3086	3089	3092	rBV2	352	315	0.02%	0.003%
86	11.324	3103	3105	3107	rBV	203	108	0.01%	0.001%
87	11.391	3123	3126	3131	rBV2	290	286	0.02%	0.003%
88	11.462	3144	3148	3149	rBV	913	656	0.04%	0.007%
89	11.559	3174	3178	3180	rBV	290	225	0.01%	0.002%
90	11.751	3232	3238	3245	rVB5	1841	2654	0.17%	0.028%
91	11.816	3245	3258	3275	rBV	570344	914841	59.01%	9.797%
92	11.954	3293	3301	3314	rVB5	7896	12252	0.79%	0.131%
93	12.195	3364	3376	3394	rBV	381058	643835	41.53%	6.894%
94	12.841	3569	3577	3585	rBV7	1506	2520	0.16%	0.027%
95	12.973	3605	3618	3628	rBV3	17783	32634	2.10%	0.349%
96	13.330	3720	3729	3736	rBV2	11511	18741	1.21%	0.201%
97	14.491	4084	4090	4102	rVB5	15055	23866	1.54%	0.256%
98	15.121	4280	4286	4297	rVB8	4678	7273	0.47%	0.078%
99	15.546	4407	4418	4432	rBV	182724	287032	18.51%	3.074%
100	16.388	4670	4680	4707	rVB	336481	549352	35.43%	5.883%

Sum of corrected areas: 9338422

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Misc : 6.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNQ5ME

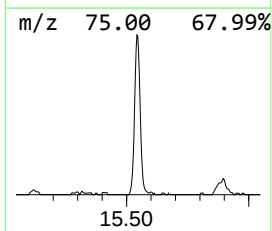
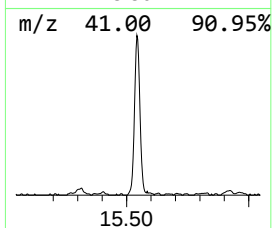
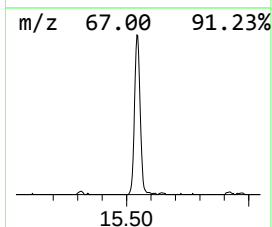
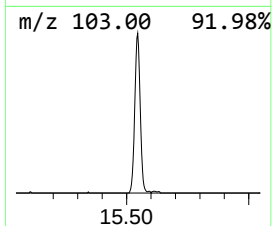
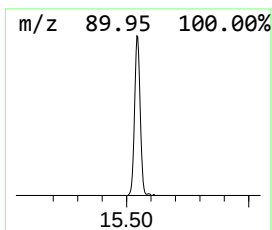
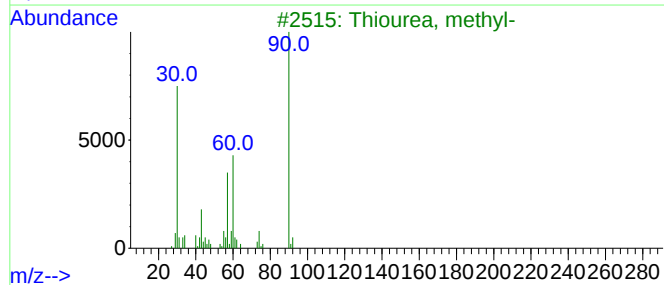
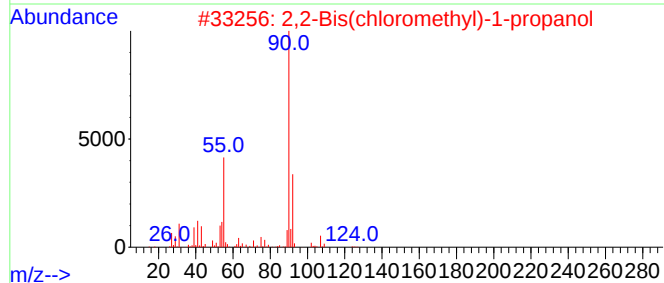
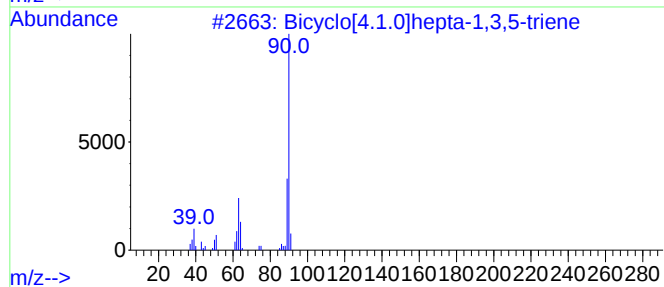
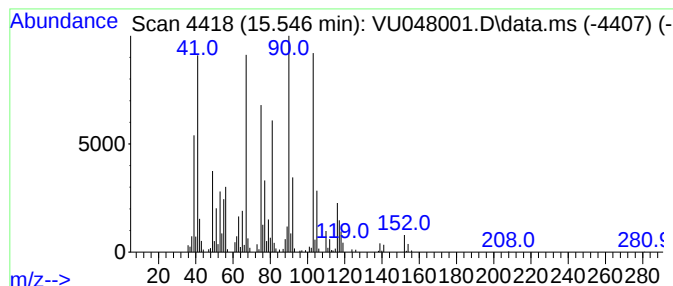
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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.
15.546	15.69 ug/L	287032	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			2,2-Bis(chloromethyl)-1-propanol	156	C5H10Cl2O	005355-54-4	38
3			Thiourea, methyl-	90	C2H6N2S	000598-52-7	35
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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Sample : N2293-22ME
Misc : 6.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNQ5ME

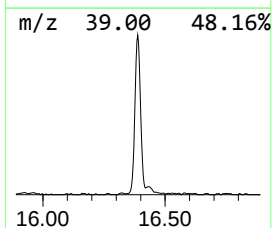
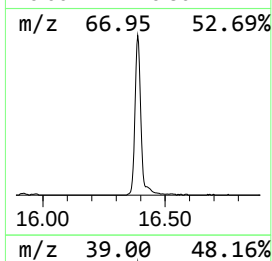
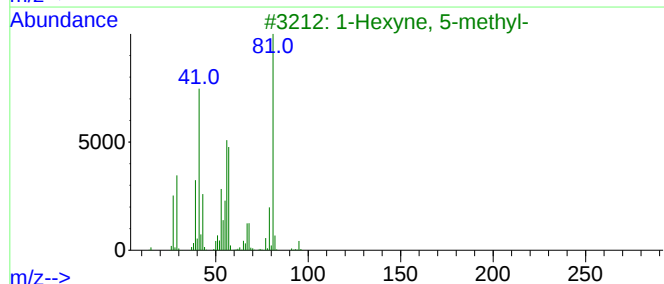
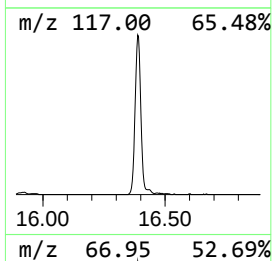
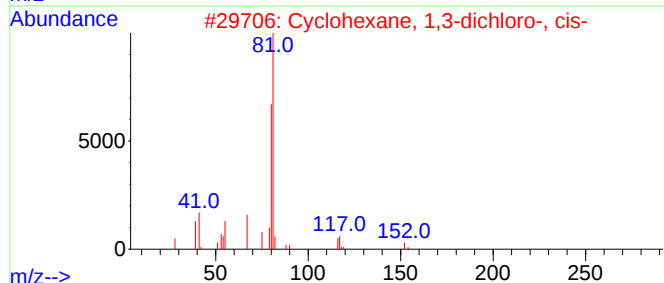
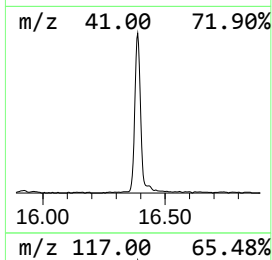
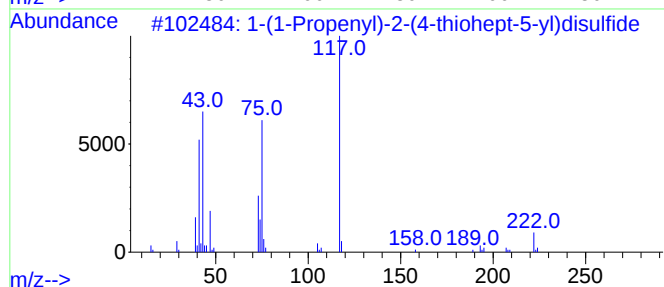
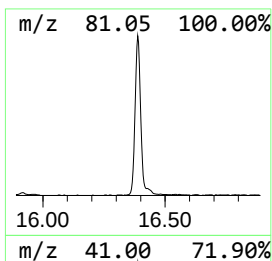
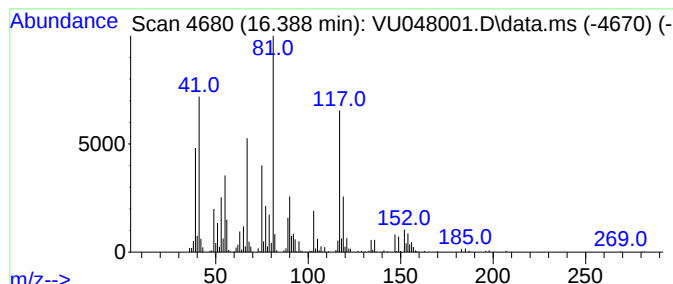
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.388	30.02 ug/L	549352	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(1-Propenyl)-2-(4-thiohept-5-y...	222	C9H18S3	1000322-30-9	10		
2	Cyclohexane, 1,3-dichloro-, cis-	152	C6H10Cl2	024955-63-3	10		
3	1-Hexyne, 5-methyl-	96	C7H12	002203-80-7	10		
4	Cyclopentene, 4,4-dimethyl-	96	C7H12	019037-72-0	10		
5	2-Furanacetaldehyde, .alpha.-pro...	152	C9H12O2	031681-26-2	10		



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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	15.546	15.7	ug/L	287032	3	11.816	914841	50.0
unknown-02	16.388	30.0	ug/L	549352	3	11.816	914841	50.0