

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
 Data File : VU048016.D
 Acq On : 13 Apr 2022 20:03
 Operator : SY/MD
 Sample : N2316-06ME
 Misc : 6.23g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNQ4ME

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: VU048016.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	72	80	116	rVB	131556	276301	6.62%	1.500%
2	1.768	120	133	134	rBV6	21322	29182	0.70%	0.158%
3	1.870	161	165	172	rBV	50365	58867	1.41%	0.320%
4	2.536	359	372	385	rBV	357448	624255	14.97%	3.390%
5	2.848	466	469	471	rBV3	533	336	0.01%	0.002%
6	3.025	520	524	525	rBV2	1166	861	0.02%	0.005%
7	3.092	540	545	547	rBV3	430	444	0.01%	0.002%
8	3.115	550	552	555	rVV3	496	295	0.01%	0.002%
9	3.169	562	569	572	rBV4	520	619	0.01%	0.003%
10	3.214	580	583	590	rVB3	362	418	0.01%	0.002%
11	3.440	651	653	659	rVV3	270	254	0.01%	0.001%
12	3.674	720	726	728	rBV2	507	550	0.01%	0.003%
13	3.745	743	748	750	rBV2	281	248	0.01%	0.001%
14	4.362	938	940	945	rVV2	246	272	0.01%	0.001%
15	4.420	952	958	963	rVB2	439	487	0.01%	0.003%
16	4.478	970	976	982	rBV2	208	261	0.01%	0.001%
17	4.632	1010	1024	1080	rBV	175486	562847	13.49%	3.057%
18	5.060	1137	1157	1181	rBV	348444	797809	19.13%	4.333%
19	5.224	1203	1208	1211	rVB3	395	352	0.01%	0.002%
20	5.288	1222	1228	1232	rBV3	776	1038	0.02%	0.006%
21	5.337	1236	1243	1252	rVB3	1466	2894	0.07%	0.016%
22	5.719	1341	1362	1394	rBV2	810317	2146170	51.45%	11.655%
23	5.890	1412	1415	1420	rVB3	519	389	0.01%	0.002%
24	5.976	1439	1442	1449	rVB5	888	936	0.02%	0.005%
25	6.038	1457	1461	1463	rBV2	391	258	0.01%	0.001%
26	6.176	1500	1504	1510	rBV2	296	366	0.01%	0.002%
27	6.247	1511	1526	1550	rBV	261352	519827	12.46%	2.823%
28	6.526	1604	1613	1624	rVB7	2744	5321	0.13%	0.029%
29	6.591	1630	1633	1635	rBV	529	396	0.01%	0.002%
30	6.603	1635	1637	1642	rVB3	498	451	0.01%	0.002%
31	6.690	1647	1664	1686	rBV	458676	940548	22.55%	5.108%
32	6.803	1693	1699	1706	rBV7	1291	1649	0.04%	0.009%
33	6.854	1711	1715	1718	rVB3	560	421	0.01%	0.002%
34	7.047	1765	1775	1785	rBV6	1667	3592	0.09%	0.020%
35	7.185	1807	1818	1838	rBV2	11082	24606	0.59%	0.134%
36	7.346	1863	1868	1873	rBV3	432	538	0.01%	0.003%

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Instrument :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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	7.420	1886	1891	1893	rBV2	520	420	0.01%	0.002%
38	7.494	1903	1914	1923	rVV3	5748	11443	0.27%	0.062%
39	7.568	1924	1937	1957	rVV	235001	456968	10.96%	2.482%
40	7.655	1959	1964	1971	rVV5	4078	7018	0.17%	0.038%
41	7.693	1971	1976	1990	rVV4	4767	9181	0.22%	0.050%
42	7.899	2024	2040	2055	rBV	958354	1724513	41.34%	9.365%
43	7.970	2056	2062	2083	rVB2	27303	55365	1.33%	0.301%
44	8.131	2107	2112	2116	rVB4	1158	998	0.02%	0.005%
45	8.182	2116	2128	2149	rBV	153192	310497	7.44%	1.686%
46	8.372	2175	2187	2198	rVB9	2592	5921	0.14%	0.032%
47	8.578	2245	2251	2253	rBV3	572	569	0.01%	0.003%
48	8.648	2258	2273	2303	rBV	718209	1411367	33.84%	7.665%
49	9.021	2382	2389	2393	rBV4	1321	1925	0.05%	0.010%
50	9.118	2415	2419	2423	rBV	327	268	0.01%	0.001%
51	9.330	2481	2485	2491	rVB3	604	706	0.02%	0.004%
52	9.452	2499	2523	2545	rBV2	1928319	4171096	100.00%	22.652%
53	9.607	2566	2571	2574	rVB2	816	872	0.02%	0.005%
54	9.626	2574	2577	2579	rBV2	553	341	0.01%	0.002%
55	9.697	2592	2599	2611	rVB7	2771	4686	0.11%	0.025%
56	9.767	2617	2621	2624	rBV2	584	468	0.01%	0.003%
57	10.028	2697	2702	2703	rBV2	481	469	0.01%	0.003%
58	10.066	2711	2714	2717	rVB3	400	299	0.01%	0.002%
59	10.111	2718	2728	2734	rVV6	1418	2049	0.05%	0.011%
60	10.224	2758	2763	2765	rBV2	406	334	0.01%	0.002%
61	10.253	2766	2772	2776	rVB5	750	938	0.02%	0.005%
62	10.356	2801	2804	2806	rVV	397	260	0.01%	0.001%
63	10.388	2810	2814	2815	rBV	400	284	0.01%	0.002%
64	10.484	2841	2844	2846	rBV3	462	339	0.01%	0.002%
65	10.529	2853	2858	2862	rBV2	1008	1024	0.02%	0.006%
66	10.623	2880	2887	2891	rBV5	751	824	0.02%	0.004%
67	10.668	2891	2901	2912	rVB3	5454	9472	0.23%	0.051%
68	10.764	2912	2931	2949	rBV	812092	1309054	31.38%	7.109%
69	10.860	2957	2961	2963	rBV3	631	526	0.01%	0.003%
70	10.922	2978	2980	2983	rVB4	608	334	0.01%	0.002%
71	10.999	2999	3004	3007	rBV4	678	655	0.02%	0.004%
72	11.108	3032	3038	3042	rBV7	1968	2461	0.06%	0.013%
73	11.201	3064	3067	3073	rVB5	656	685	0.02%	0.004%
74	11.285	3087	3093	3094	rBV4	655	581	0.01%	0.003%
75	11.378	3115	3122	3124	rBV3	833	887	0.02%	0.005%
76	11.417	3128	3134	3140	rVV5	4502	5513	0.13%	0.030%

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Instrument :
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 ClientSampleId :
 ETNQ4ME

Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

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Stop Thrs : 0

Peak Location: TOP

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 Title : VOC Analysis

77	11.459	3140	3147	3160	rVV6	4626	8836	0.21%	0.048%
78	11.577	3177	3184	3189	rBV7	1843	2696	0.06%	0.015%
79	11.642	3198	3204	3209	rBV9	1601	2229	0.05%	0.012%
80	11.709	3215	3225	3233	rBV9	5070	10021	0.24%	0.054%
81	11.748	3233	3237	3245	rVB7	2589	3489	0.08%	0.019%
82	11.815	3245	3258	3273	rBV	518852	846165	20.29%	4.595%
83	12.086	3340	3342	3346	rVB4	895	611	0.01%	0.003%
84	12.195	3360	3376	3392	rBV	1110975	1831970	43.92%	9.949%
85	12.436	3449	3451	3455	rVB3	902	474	0.01%	0.003%
86	12.838	3570	3576	3585	rVB8	5688	7999	0.19%	0.043%
87	12.928	3598	3604	3612	rBV8	5514	10744	0.26%	0.058%
88	13.053	3636	3643	3652	rVB10	5358	8415	0.20%	0.046%
89	13.140	3663	3670	3678	rBV7	3055	4310	0.10%	0.023%
90	13.330	3726	3729	3731	rBV4	1660	1276	0.03%	0.007%
91	13.587	3803	3809	3816	rBV3	7831	10686	0.26%	0.058%
92	13.802	3873	3876	3878	rBV3	852	552	0.01%	0.003%
93	13.844	3884	3889	3896	rBV10	2267	3797	0.09%	0.021%
94	13.938	3916	3918	3919	rBV2	1096	471	0.01%	0.003%
95	14.192	3986	3997	4010	rVB7	6826	12469	0.30%	0.068%
96	14.491	4086	4090	4091	rBV3	3175	2045	0.05%	0.011%
97	14.568	4111	4114	4121	rBV9	3234	4090	0.10%	0.022%
98	15.208	4304	4313	4326	rBV9	5978	14169	0.34%	0.077%
99	15.545	4412	4418	4432	rVB3	29221	44029	1.06%	0.239%
100	16.391	4673	4681	4692	rBV3	39388	66798	1.60%	0.363%

Sum of corrected areas: 18414009

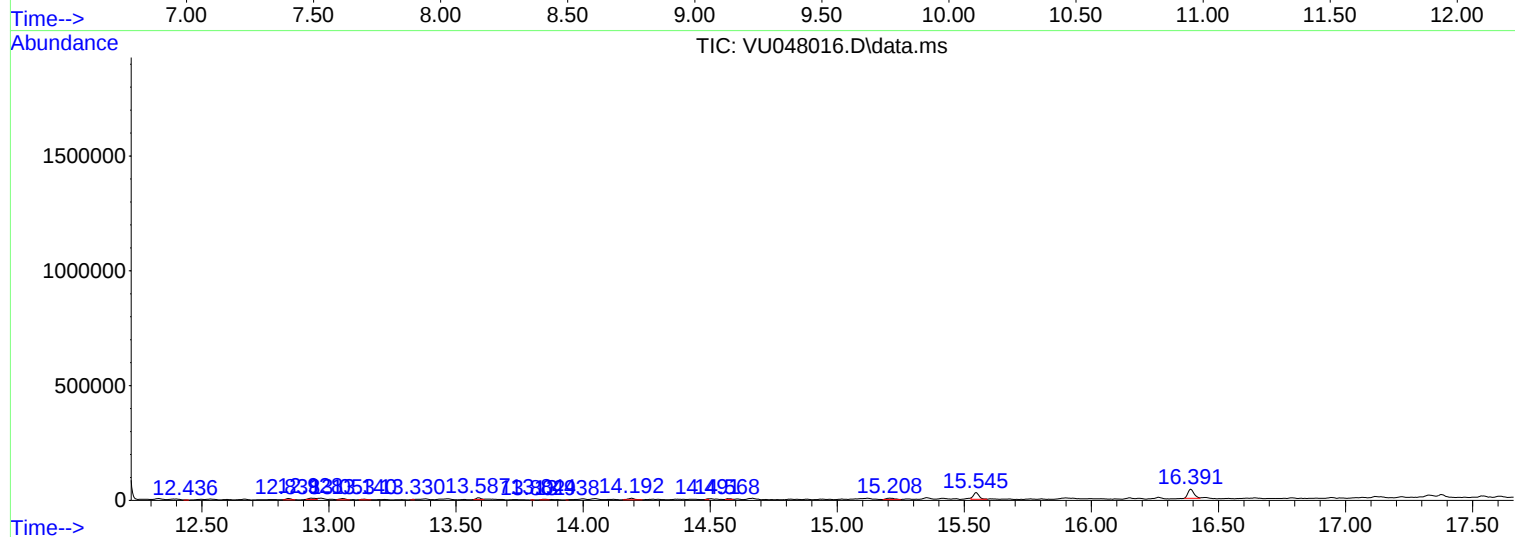
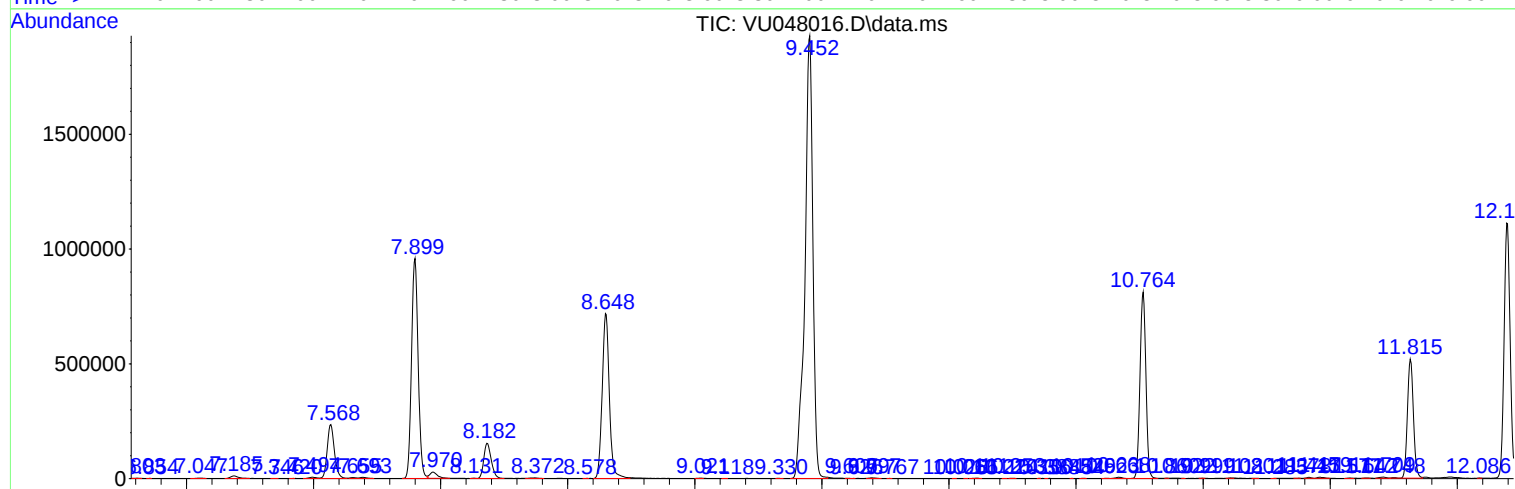
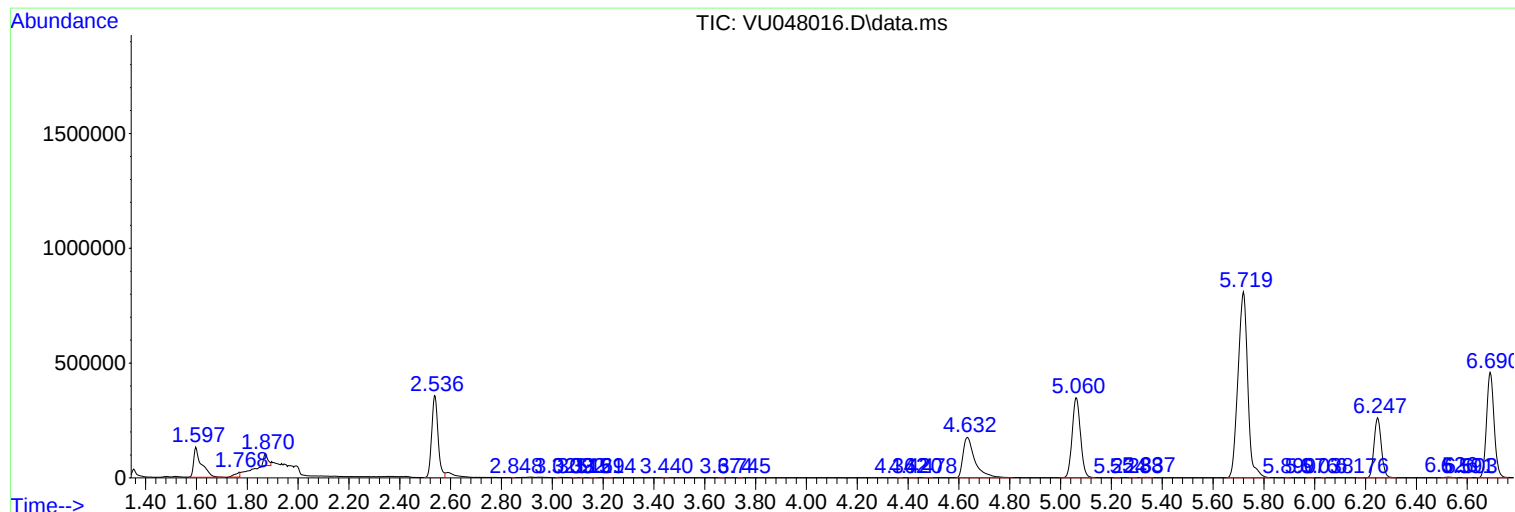
Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
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ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNQ4ME

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 : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNQ4ME

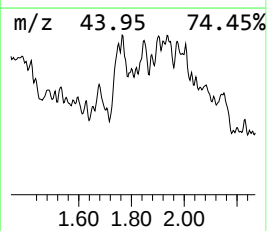
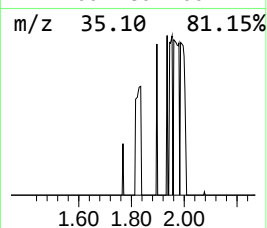
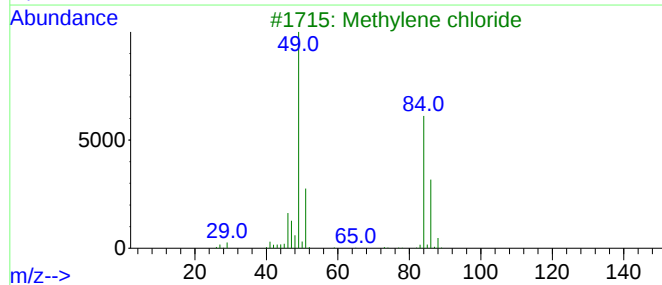
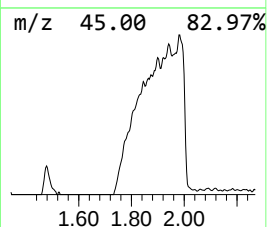
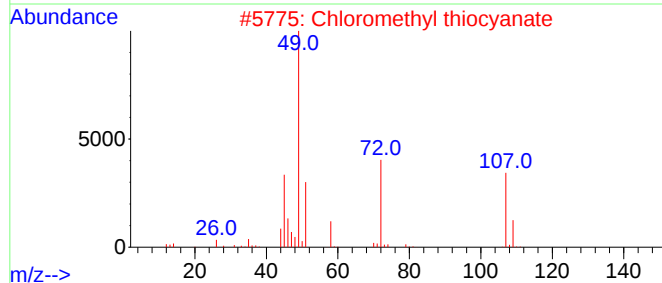
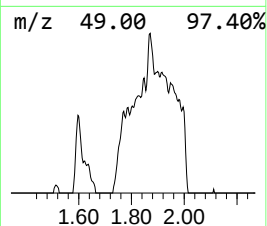
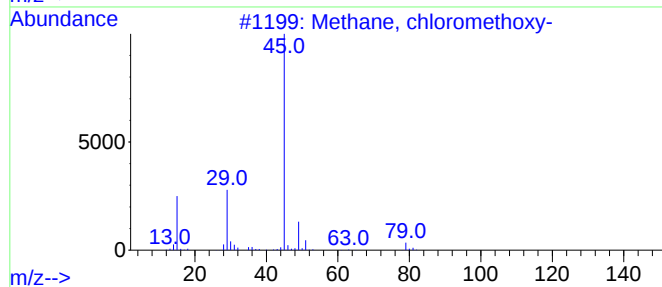
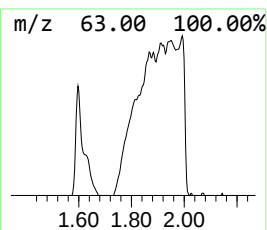
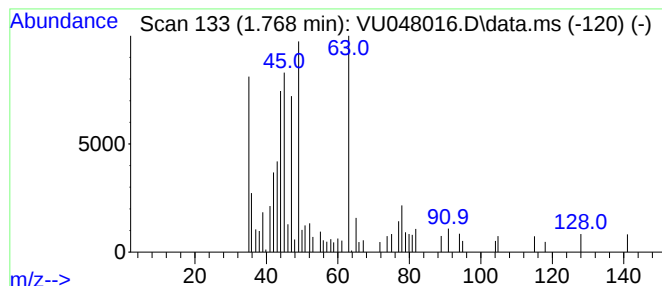
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.768	2.81 ug/L	29182	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, chloromethoxy-	80	C2H5ClO	000107-30-2	9
2			Chloromethyl thiocyanate	107	C2H2ClNS	003268-79-9	9
3			Methylene chloride	84	CH2Cl2	000075-09-2	9
4			bis(chloromethyl) carbonate	158	C3H4Cl2O3	1000404-37-0	6
5			3,4-Dichlorobutane nitrile	137	C4H5Cl2N	034362-21-5	4



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Instrument :
MSVOA_U
ClientSampleId :
ETNQ4ME

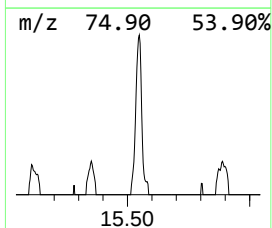
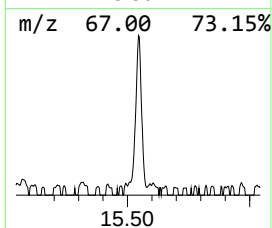
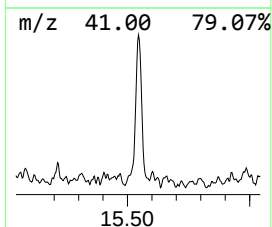
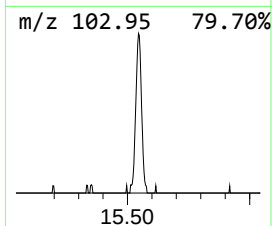
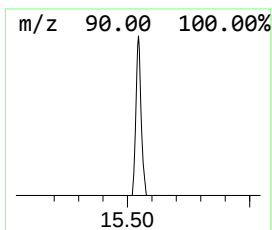
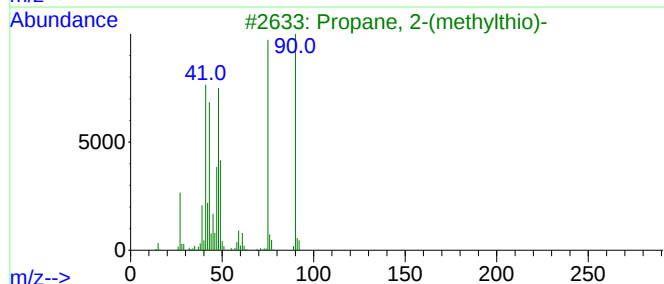
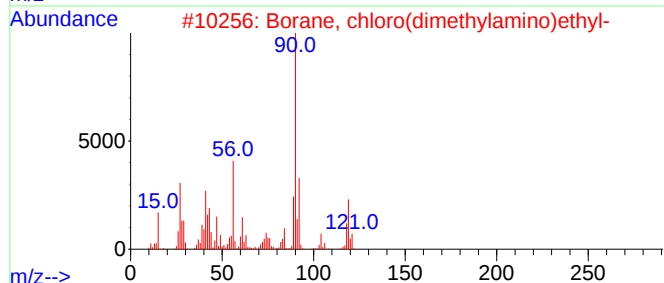
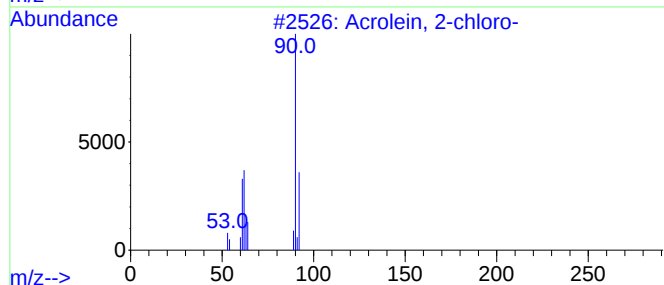
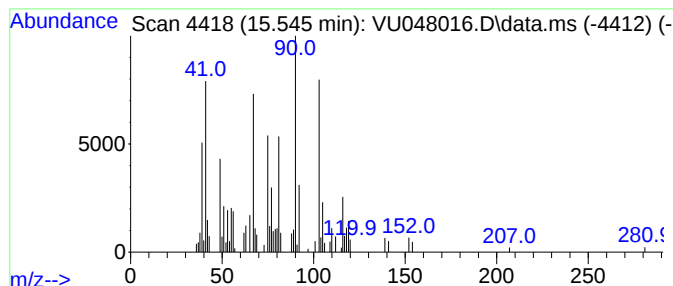
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	2.60 ug/L	44029	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	43
2			Borane, chloro(dimethylamino)ethyl-	119	C4H11BClN	001739-26-0	35
3			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	33
4			1,3,5-Trichloro-4-methyl-2-penta...	202	C6H9Cl3O	1000140-03-8	30
5			1H-Indole-2,3-dione, 1-(pentaflu...	293	C11H4F5NO3	1000143-04-0	17



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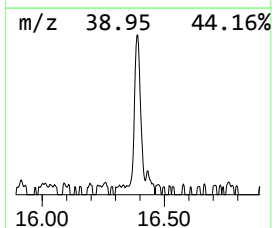
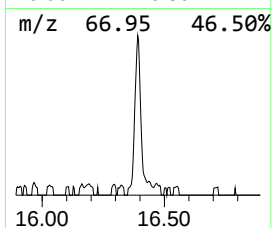
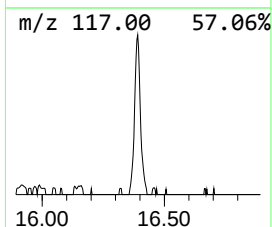
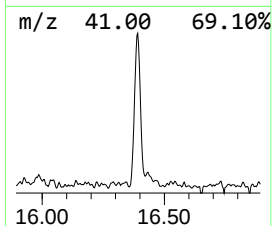
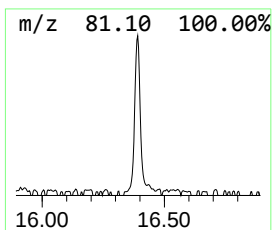
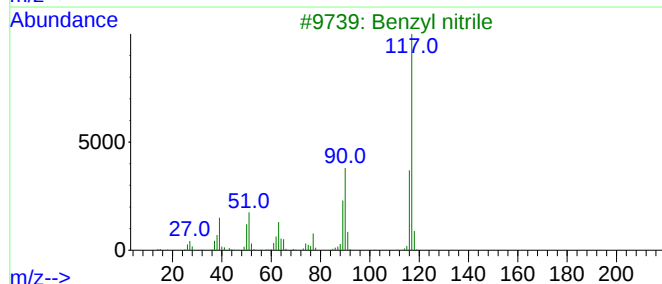
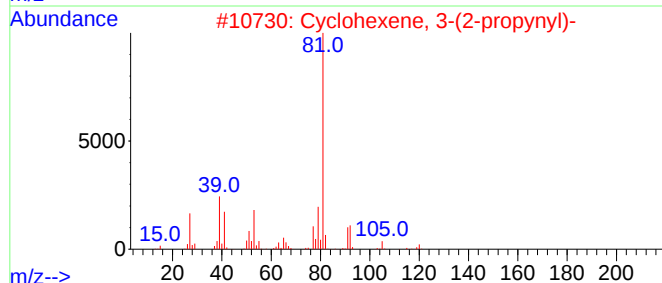
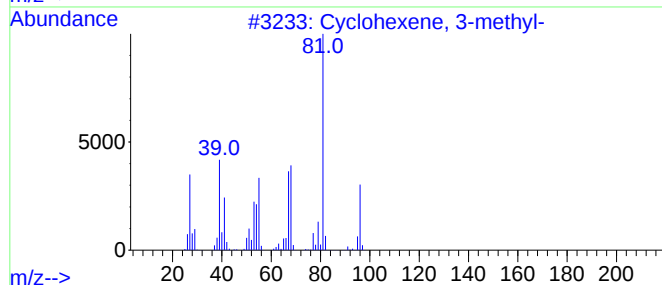
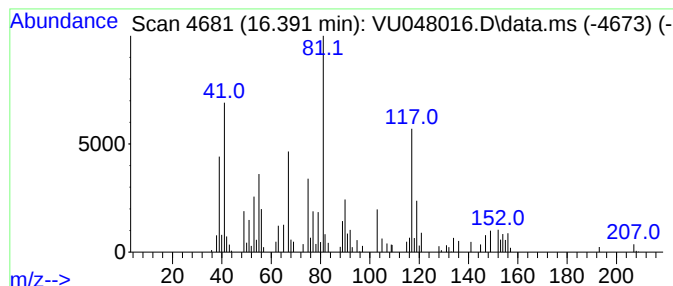
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 unknown-03 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.391	3.95 ug/L	66798	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 3-methyl-	96	C7H12	000591-48-0	35
2			Cyclohexene, 3-(2-propynyl)-	120	C9H12	055956-43-9	18
3			Benzyl nitrile	117	C8H7N	000140-29-4	15
4			Cyclopentene, 4,4-dimethyl-	96	C7H12	019037-72-0	14
5			Indole	117	C8H7N	000120-72-9	11



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU048016.D
Acq On : 13 Apr 2022 20:03
Operator : SY/MD
Sample : N2316-06ME
Misc : 6.23g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNQ4ME

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.768	2.8	ug/L	29182	1	6.247	519827	50.0
unknown-02	15.545	2.6	ug/L	44029	3	11.815	846165	50.0
unknown-03	16.391	4.0	ug/L	66798	3	11.815	846165	50.0