

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
 Data File : VU048014.D
 Acq On : 13 Apr 2022 19:17
 Operator : SY/MD
 Sample : N2316-03ME
 Misc : 6.50g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNQ1ME

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: VU048014.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	114	rVB	83024	185064	4.56%	1.245%
2	1.771	119	134	135	rBV7	19447	32602	0.80%	0.219%
3	1.871	162	165	175	rVB	30272	24076	0.59%	0.162%
4	2.536	359	372	385	rBV	234670	410686	10.12%	2.763%
5	2.925	484	493	498	rBV3	2119	3695	0.09%	0.025%
6	3.022	519	523	524	rBV3	851	603	0.01%	0.004%
7	3.173	567	570	573	rBV2	540	442	0.01%	0.003%
8	3.462	656	660	663	rBV4	330	308	0.01%	0.002%
9	3.764	750	754	757	rBV2	406	401	0.01%	0.003%
10	3.964	813	816	820	rVB2	398	343	0.01%	0.002%
11	3.993	820	825	829	rVB2	344	350	0.01%	0.002%
12	4.311	920	924	930	rVB2	317	310	0.01%	0.002%
13	4.475	972	975	979	rBV2	343	345	0.01%	0.002%
14	4.636	1011	1025	1072	rBV	112611	370422	9.13%	2.492%
15	5.060	1139	1157	1182	rBV	231909	531371	13.10%	3.575%
16	5.182	1189	1195	1199	rBV3	471	440	0.01%	0.003%
17	5.333	1236	1242	1244	rBV	1166	1205	0.03%	0.008%
18	5.449	1275	1278	1286	rBV	381	427	0.01%	0.003%
19	5.719	1340	1362	1395	rBV2	537810	1456328	35.89%	9.798%
20	5.970	1438	1440	1442	rBV	490	317	0.01%	0.002%
21	6.121	1482	1487	1490	rVV5	533	604	0.01%	0.004%
22	6.247	1511	1526	1546	rBV	411278	817026	20.14%	5.497%
23	6.526	1606	1613	1621	rVB5	1899	3080	0.08%	0.021%
24	6.594	1629	1634	1637	rBV3	525	497	0.01%	0.003%
25	6.623	1641	1643	1649	rVB4	435	342	0.01%	0.002%
26	6.690	1649	1664	1685	rBV	302294	623128	15.36%	4.193%
27	6.793	1693	1696	1697	rBV2	851	501	0.01%	0.003%
28	7.050	1768	1776	1780	rBV5	1339	1941	0.05%	0.013%
29	7.186	1808	1818	1837	rVV4	8781	19386	0.48%	0.130%
30	7.494	1905	1914	1923	rBV5	4193	7896	0.19%	0.053%
31	7.568	1923	1937	1957	rVB	151158	295173	7.27%	1.986%
32	7.793	2001	2007	2009	rBV3	298	307	0.01%	0.002%
33	7.899	2020	2040	2055	rBV	622662	1127932	27.80%	7.589%
34	8.182	2116	2128	2154	rVB	101957	205209	5.06%	1.381%
35	8.366	2176	2185	2199	rVB7	3066	6688	0.16%	0.045%
36	8.478	2216	2220	2225	rVB3	728	749	0.02%	0.005%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Stop Thrs : 0

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

37	8.581	2245	2252	2259	rBV4	1260	1637	0.04%	0.011%
38	8.652	2259	2274	2302	rBV	462624	921961	22.72%	6.203%
39	8.854	2335	2337	2343	rVB3	1060	1093	0.03%	0.007%
40	9.025	2386	2390	2401	rVB5	1150	1796	0.04%	0.012%
41	9.185	2436	2440	2444	rBV2	361	325	0.01%	0.002%
42	9.330	2481	2485	2487	rVV2	604	464	0.01%	0.003%
43	9.359	2489	2494	2499	rVV3	1140	1540	0.04%	0.010%
44	9.449	2499	2522	2554	rVV2	1652839	4057596	100.00%	27.300%
45	9.574	2555	2561	2570	rVB6	2372	4172	0.10%	0.028%
46	9.697	2590	2599	2610	rVB3	2977	5663	0.14%	0.038%
47	9.742	2610	2613	2620	rVB3	618	516	0.01%	0.003%
48	9.857	2646	2649	2652	rVV3	468	368	0.01%	0.002%
49	9.902	2660	2663	2673	rVB2	438	554	0.01%	0.004%
50	10.105	2719	2726	2731	rBV3	1890	2684	0.07%	0.018%
51	10.668	2888	2901	2910	rBV7	3424	6404	0.16%	0.043%
52	10.716	2910	2916	2918	rBV2	859	857	0.02%	0.006%
53	10.764	2918	2931	2949	rVB	542197	868434	21.40%	5.843%
54	10.864	2958	2962	2965	rBV3	603	527	0.01%	0.004%
55	10.989	2991	3001	3003	rBV3	1770	2045	0.05%	0.014%
56	11.060	3019	3023	3027	rBV5	896	885	0.02%	0.006%
57	11.115	3038	3040	3044	rBV2	891	610	0.02%	0.004%
58	11.195	3062	3065	3068	rBV	505	348	0.01%	0.002%
59	11.295	3091	3096	3098	rBV3	625	572	0.01%	0.004%
60	11.330	3105	3107	3111	rVB2	585	380	0.01%	0.003%
61	11.420	3132	3135	3137	rBV2	742	336	0.01%	0.002%
62	11.465	3140	3149	3151	rBV5	3200	4156	0.10%	0.028%
63	11.613	3191	3195	3201	rVB3	535	466	0.01%	0.003%
64	11.648	3201	3206	3207	rBV	437	373	0.01%	0.003%
65	11.709	3216	3225	3232	rBV6	2758	4570	0.11%	0.031%
66	11.751	3232	3238	3245	rVB6	1679	2233	0.06%	0.015%
67	11.816	3245	3258	3274	rBV	819090	1310286	32.29%	8.816%
68	11.954	3291	3301	3303	rBV8	3895	5655	0.14%	0.038%
69	12.198	3355	3377	3393	rBV	739699	1237073	30.49%	8.323%
70	12.394	3429	3438	3439	rBV5	1039	1235	0.03%	0.008%
71	12.549	3484	3486	3491	rVB3	468	314	0.01%	0.002%
72	12.761	3549	3552	3553	rBV2	748	377	0.01%	0.003%
73	12.841	3573	3577	3584	rVB7	2109	2521	0.06%	0.017%
74	12.883	3584	3590	3593	rBV4	594	564	0.01%	0.004%
75	12.973	3609	3618	3630	rVB5	8022	14283	0.35%	0.096%
76	13.124	3661	3665	3667	rBV3	590	410	0.01%	0.003%

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 MSVOA_U
 ClientSampleId :
 ETNQ1ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Peak Location: TOP

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

77	13.224	3690	3696	3703	rVB4	2199	3096	0.08%	0.021%
78	13.272	3707	3711	3714	rBV4	911	948	0.02%	0.006%
79	13.336	3724	3731	3737	rBV6	2738	4059	0.10%	0.027%
80	13.378	3737	3744	3756	rVB7	5922	8677	0.21%	0.058%
81	13.494	3776	3780	3781	rBV4	583	313	0.01%	0.002%
82	13.533	3789	3792	3795	rBV3	695	504	0.01%	0.003%
83	13.844	3882	3889	3899	rVB6	2274	3663	0.09%	0.025%
84	14.092	3963	3966	3972	rBV3	1050	1144	0.03%	0.008%
85	14.163	3985	3988	3993	rBV3	833	753	0.02%	0.005%
86	14.362	4045	4050	4060	rBV6	2247	3237	0.08%	0.022%
87	14.497	4084	4092	4105	rVB10	8907	14137	0.35%	0.095%
88	14.574	4111	4116	4117	rBV	1823	1403	0.03%	0.009%
89	14.661	4135	4143	4155	rBV8	7756	11812	0.29%	0.079%
90	14.754	4170	4172	4174	rBV2	638	355	0.01%	0.002%
91	14.790	4181	4183	4186	rBV2	558	415	0.01%	0.003%
92	14.809	4186	4189	4192	rBV4	1609	1281	0.03%	0.009%
93	14.883	4209	4212	4217	rVB5	1931	1387	0.03%	0.009%
94	15.050	4262	4264	4271	rBV5	784	942	0.02%	0.006%
95	15.102	4271	4280	4281	rBV6	3851	4975	0.12%	0.033%
96	15.278	4328	4335	4339	rBV7	2045	2761	0.07%	0.019%
97	15.349	4352	4357	4370	rVB8	7749	11845	0.29%	0.080%
98	15.413	4371	4377	4385	rVB7	5981	9167	0.23%	0.062%
99	15.545	4408	4418	4429	rBV2	41678	66451	1.64%	0.447%
100	16.391	4672	4681	4699	rBV2	67496	113038	2.79%	0.761%

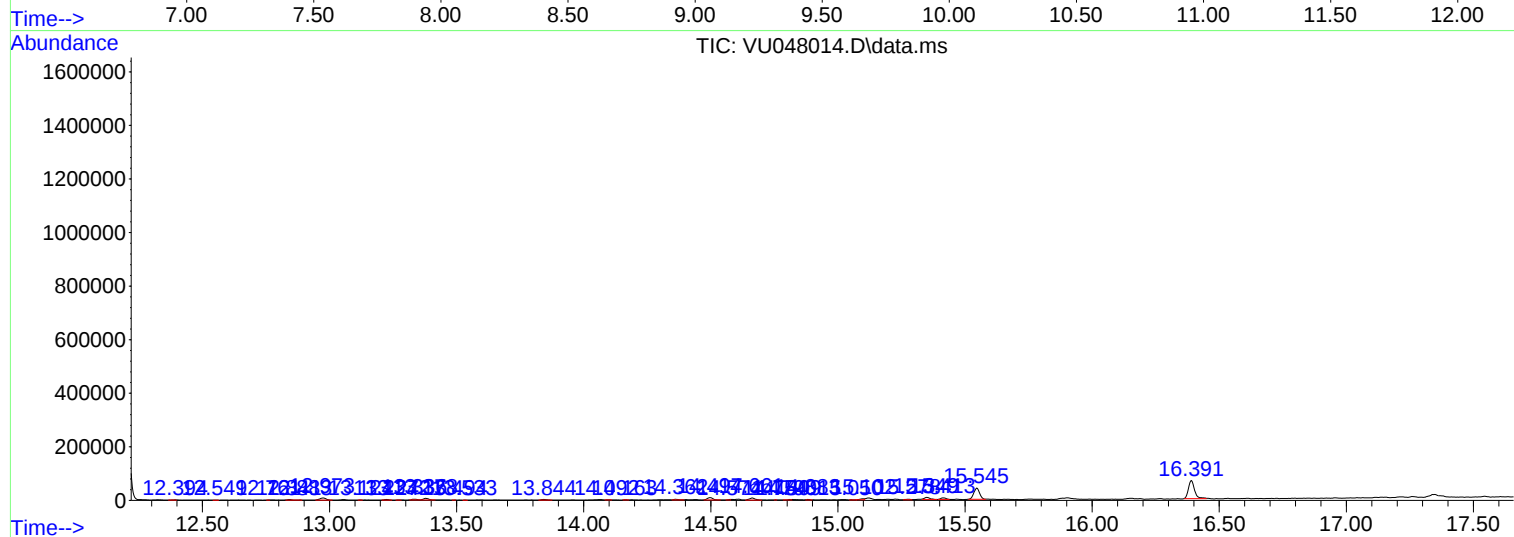
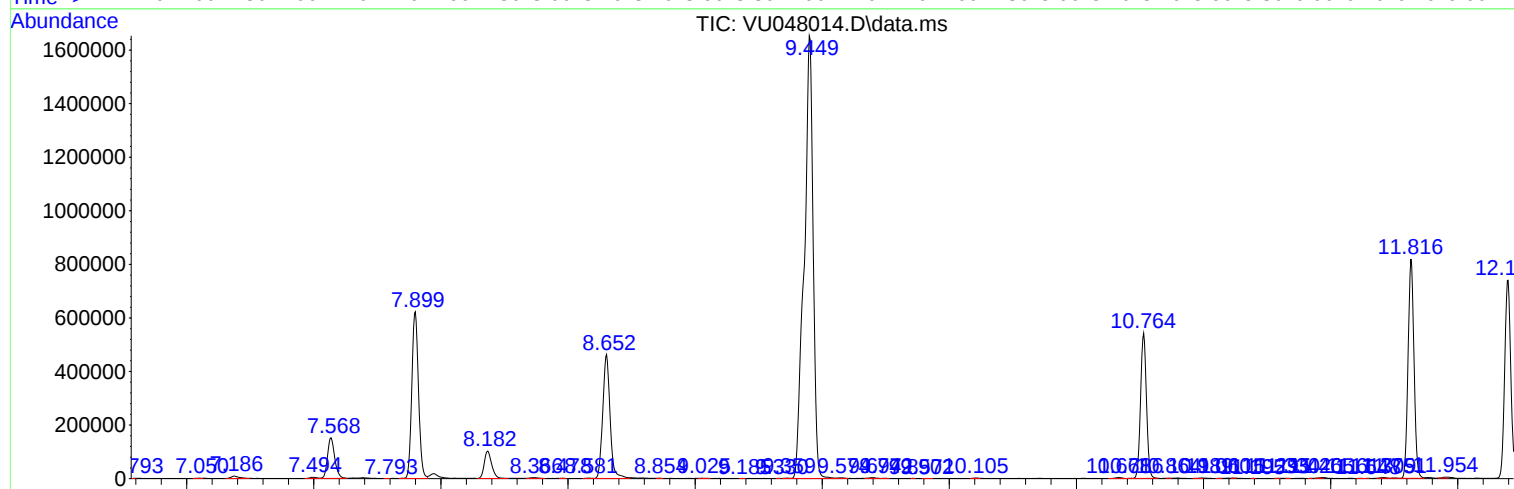
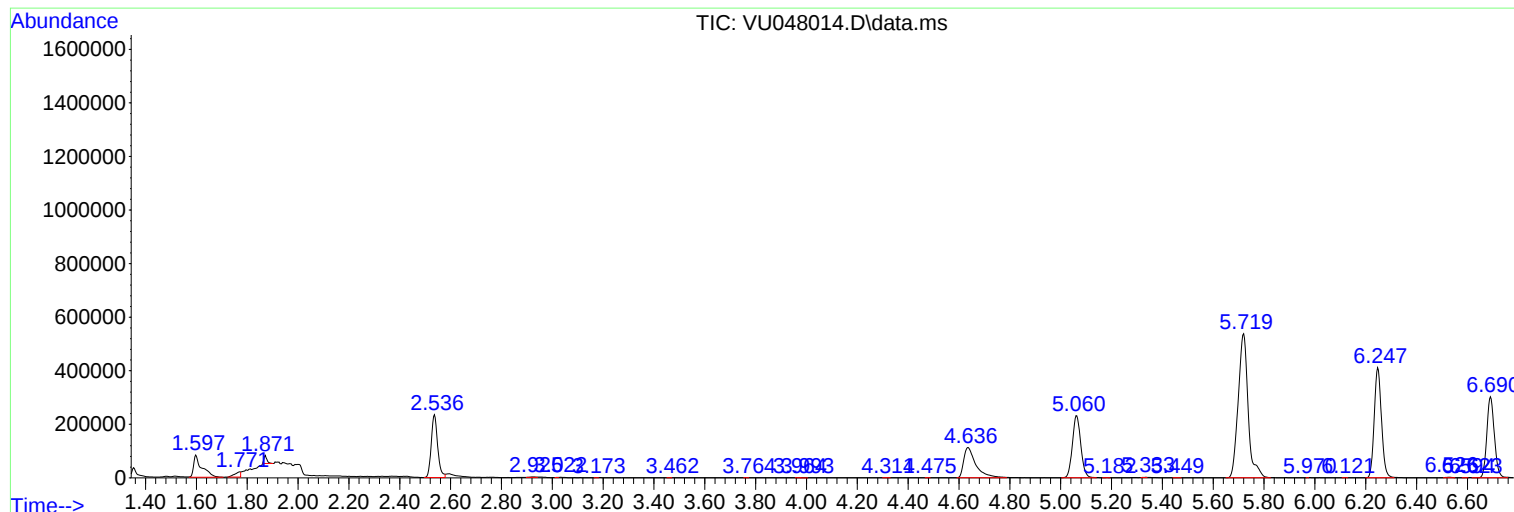
Sum of corrected areas: 14862840

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNQ1ME

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 : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNQ1ME

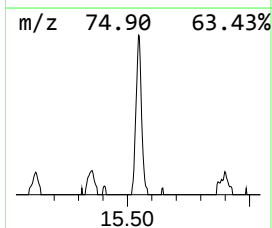
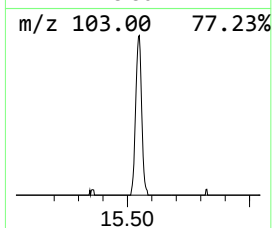
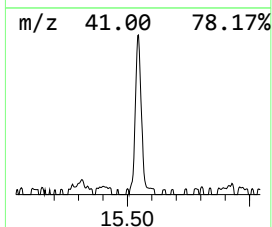
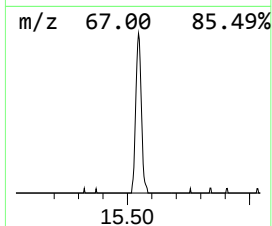
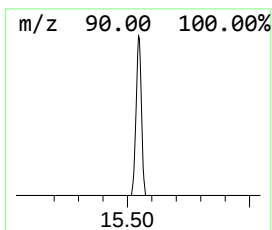
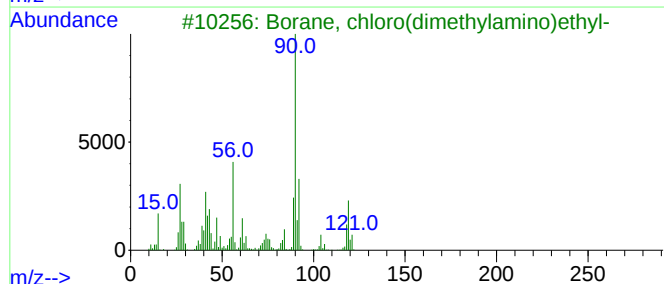
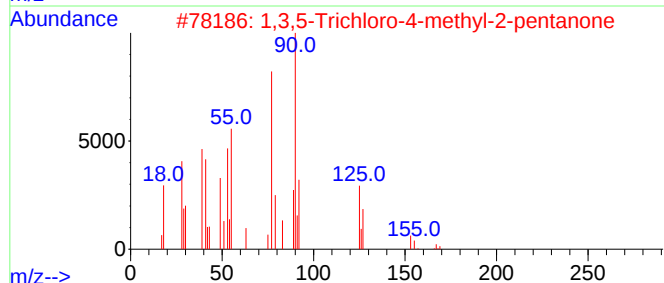
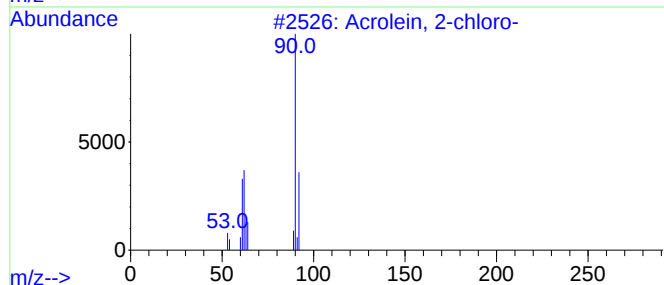
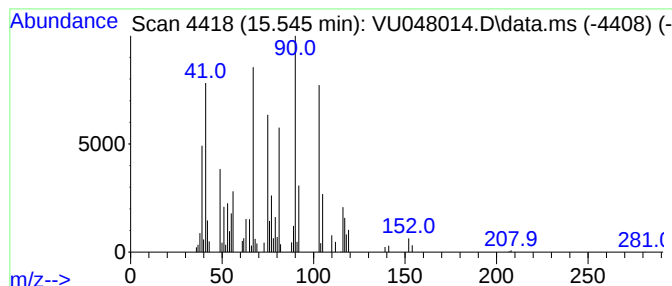
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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	2.54 ug/L	66451	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	43
2			1,3,5-Trichloro-4-methyl-2-penta...	202	C6H9Cl3O	1000140-03-8	33
3			Borane, chloro(dimethylamino)ethyl-	119	C4H11BClN	001739-26-0	17
4			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	17
5			1H-Benzotriazole, 1-chloro-	153	C6H4ClN3	021050-95-3	12



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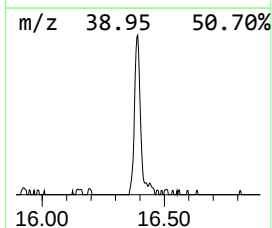
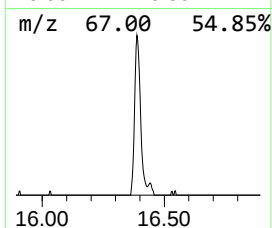
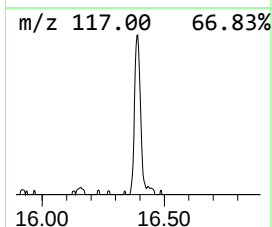
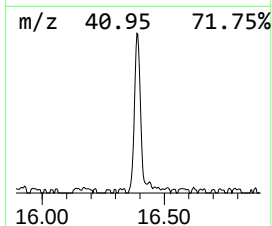
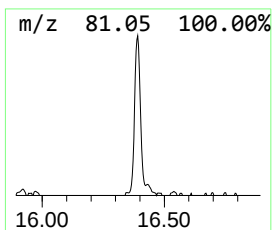
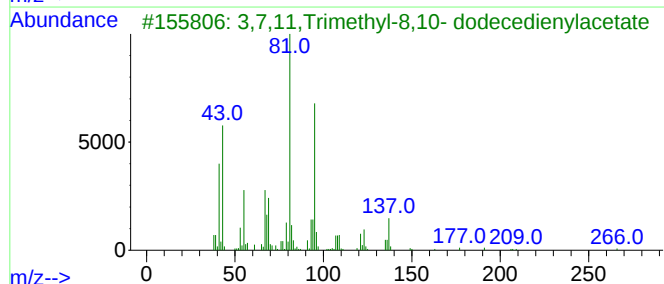
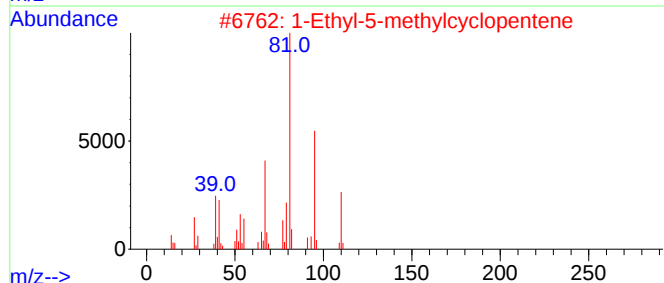
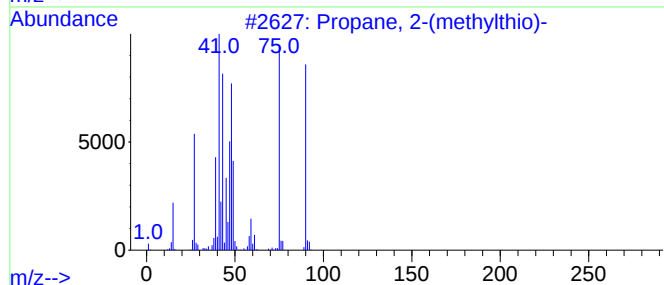
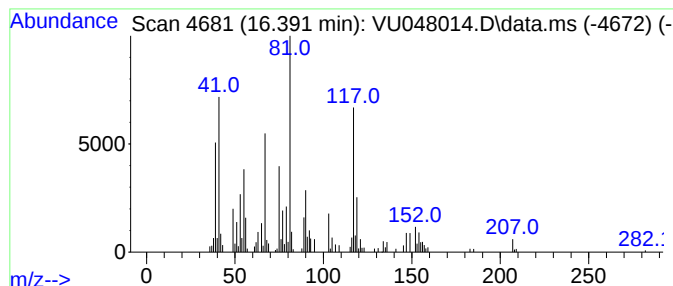
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.391	4.31 ug/L	113038	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	27
2			1-Ethyl-5-methylcyclopentene	110	C8H14	097797-57-4	22
3			3,7,11,Trimethyl-8,10- dodecedie...	266	C17H30O2	1000374-10-3	12
4			Methyl ethyl cyclopentene	110	C8H14	019780-56-4	12
5			2-Hexyne, 4-methyl-	96	C7H12	020198-49-6	12



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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	2.5	ug/L	66451	3	11.816	1310290	50.0
unknown-02	16.391	4.3	ug/L	113038	3	11.816	1310290	50.0