

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
 Data File : VU048010.D
 Acq On : 13 Apr 2022 17:44
 Operator : SY/MD
 Sample : N2316-09ME
 Misc : 6.57g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNQ8ME

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: VU048010.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	102	rBV	95974	177033	11.88%	1.299%
2	2.539	362	373	386	rBV	248270	419526	28.16%	3.077%
3	3.141	557	560	562	rBV2	393	265	0.02%	0.002%
4	3.433	647	651	653	rBV2	641	428	0.03%	0.003%
5	3.758	747	752	755	rBV3	252	293	0.02%	0.002%
6	3.845	776	779	780	rBV2	275	155	0.01%	0.001%
7	3.861	783	784	792	rVB3	525	341	0.02%	0.003%
8	3.893	792	794	796	rBV	218	114	0.01%	0.001%
9	3.912	796	800	802	rBV2	130	109	0.01%	0.001%
10	3.925	802	804	805	rBV	263	144	0.01%	0.001%
11	3.977	816	820	823	rBV2	260	138	0.01%	0.001%
12	3.993	823	825	826	rBV2	242	101	0.01%	0.001%
13	4.018	831	833	837	rVB2	313	183	0.01%	0.001%
14	4.057	842	845	848	rBV2	270	198	0.01%	0.001%
15	4.105	856	860	862	rBV2	304	253	0.02%	0.002%
16	4.173	878	881	882	rBV	230	142	0.01%	0.001%
17	4.221	894	896	899	rBV	165	131	0.01%	0.001%
18	4.276	910	913	915	rBV	300	176	0.01%	0.001%
19	4.343	932	934	939	rVB2	424	236	0.02%	0.002%
20	4.536	992	994	998	rVB3	176	115	0.01%	0.001%
21	4.559	998	1001	1002	rBV	287	180	0.01%	0.001%
22	4.633	1010	1024	1079	rBV	116295	370319	24.86%	2.716%
23	5.060	1140	1157	1183	rBV	236779	536224	35.99%	3.933%
24	5.427	1268	1271	1273	rBV2	305	173	0.01%	0.001%
25	5.552	1307	1310	1314	rBV2	314	278	0.02%	0.002%
26	5.597	1322	1324	1326	rBV	223	122	0.01%	0.001%
27	5.645	1337	1339	1341	rBV2	346	181	0.01%	0.001%
28	5.719	1341	1362	1375	rBV2	528853	1399349	93.93%	10.264%
29	5.877	1406	1411	1412	rBV3	765	654	0.04%	0.005%
30	5.951	1431	1434	1437	rVB2	441	244	0.02%	0.002%
31	5.977	1437	1442	1444	rBV2	651	542	0.04%	0.004%
32	6.015	1450	1454	1455	rBV2	268	173	0.01%	0.001%
33	6.076	1471	1473	1475	rBV	255	124	0.01%	0.001%
34	6.105	1479	1482	1485	rBV2	361	234	0.02%	0.002%
35	6.150	1493	1496	1499	rVB3	303	219	0.01%	0.002%
36	6.173	1499	1503	1505	rBV	240	152	0.01%	0.001%

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 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNQ8ME

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

37	6.247	1511	1526	1553	rBV	411764	804159	53.98%	5.898%
38	6.359	1559	1561	1564	rVB3	389	177	0.01%	0.001%
39	6.430	1579	1583	1584	rBV2	446	277	0.02%	0.002%
40	6.497	1599	1604	1605	rBV2	246	197	0.01%	0.001%
41	6.536	1605	1616	1626	rVB6	4166	8110	0.54%	0.059%
42	6.600	1630	1636	1640	rBV3	653	713	0.05%	0.005%
43	6.690	1649	1664	1684	rBV	306625	620268	41.63%	4.550%
44	6.797	1695	1697	1699	rBV2	574	308	0.02%	0.002%
45	6.909	1729	1732	1734	rVB2	198	123	0.01%	0.001%
46	6.938	1739	1741	1745	rVV2	321	208	0.01%	0.002%
47	6.993	1750	1758	1761	rBV5	1019	1340	0.09%	0.010%
48	7.047	1766	1775	1791	rVB4	1610	3685	0.25%	0.027%
49	7.115	1791	1796	1800	rBV4	416	453	0.03%	0.003%
50	7.186	1804	1818	1829	rBV3	10023	21315	1.43%	0.156%
51	7.321	1858	1860	1863	rVB2	347	190	0.01%	0.001%
52	7.343	1863	1867	1869	rBV2	325	222	0.01%	0.002%
53	7.366	1872	1874	1875	rVV	187	97	0.01%	0.001%
54	7.398	1881	1884	1886	rVV	176	99	0.01%	0.001%
55	7.411	1886	1888	1890	rVB2	215	102	0.01%	0.001%
56	7.443	1894	1898	1901	rVB	323	265	0.02%	0.002%
57	7.491	1906	1913	1924	rBV7	2812	5585	0.37%	0.041%
58	7.568	1924	1937	1960	rVV	156618	300540	20.17%	2.204%
59	7.768	1996	1999	2004	rBV3	192	161	0.01%	0.001%
60	7.838	2016	2021	2022	rBV	407	302	0.02%	0.002%
61	7.899	2026	2040	2055	rBV	628536	1127903	75.71%	8.273%
62	8.115	2105	2107	2109	rBV2	449	215	0.01%	0.002%
63	8.182	2115	2128	2145	rBV	106105	209350	14.05%	1.536%
64	8.436	2204	2207	2210	rBV3	524	400	0.03%	0.003%
65	8.578	2240	2251	2260	rBV	18702	35342	2.37%	0.259%
66	8.649	2261	2273	2302	rVB	468593	912522	61.25%	6.693%
67	8.909	2351	2354	2355	rBV2	422	211	0.01%	0.002%
68	9.102	2411	2414	2415	rBV	322	146	0.01%	0.001%
69	9.115	2416	2418	2420	rBV	142	87	0.01%	0.001%
70	9.176	2434	2437	2440	rVB4	743	431	0.03%	0.003%
71	9.227	2448	2453	2456	rBV3	440	463	0.03%	0.003%
72	9.311	2476	2479	2482	rBV3	241	219	0.01%	0.002%
73	9.420	2500	2513	2539	rBV2	616631	1274415	85.54%	9.348%
74	9.899	2658	2662	2669	rVB6	1254	1216	0.08%	0.009%
75	10.015	2695	2698	2699	rBV	407	264	0.02%	0.002%
76	10.044	2704	2707	2710	rVV3	541	392	0.03%	0.003%

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 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNQ8ME

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

77	10.099	2719	2724	2733	rBV8	2674	3552	0.24%	0.026%
78	10.218	2758	2761	2763	rBV3	1305	927	0.06%	0.007%
79	10.256	2771	2773	2774	rBV3	251	89	0.01%	0.001%
80	10.340	2794	2799	2808	rBV6	1013	1700	0.11%	0.012%
81	10.555	2862	2866	2875	rVB3	579	687	0.05%	0.005%
82	10.603	2878	2881	2884	rBV	258	174	0.01%	0.001%
83	10.668	2891	2901	2906	rBV7	3971	6376	0.43%	0.047%
84	10.764	2920	2931	2949	rVB	538381	876871	58.86%	6.432%
85	11.063	3021	3024	3026	rBV2	269	148	0.01%	0.001%
86	11.108	3029	3038	3039	rBV3	1390	1533	0.10%	0.011%
87	11.176	3057	3059	3062	rVB	318	158	0.01%	0.001%
88	11.195	3063	3065	3067	rBV2	278	93	0.01%	0.001%
89	11.246	3078	3081	3083	rBV2	334	191	0.01%	0.001%
90	11.288	3090	3094	3096	rBV2	256	226	0.02%	0.002%
91	11.337	3107	3109	3112	rBV	349	135	0.01%	0.001%
92	11.616	3193	3196	3197	rBV2	219	112	0.01%	0.001%
93	11.697	3215	3221	3228	rBV6	2353	3383	0.23%	0.025%
94	11.816	3246	3258	3276	rBV	820150	1301200	87.34%	9.544%
95	12.195	3364	3376	3398	rBV	752795	1243664	83.48%	9.122%
96	13.333	3723	3730	3737	rBV3	10858	17165	1.15%	0.126%
97	13.844	3882	3889	3898	rVB5	5114	8440	0.57%	0.062%
98	14.565	4110	4113	4114	rBV2	1501	928	0.06%	0.007%
99	15.545	4408	4418	4435	rVB2	274935	434395	29.16%	3.186%
100	16.388	4670	4680	4691	rBV	964469	1489785	100.00%	10.927%

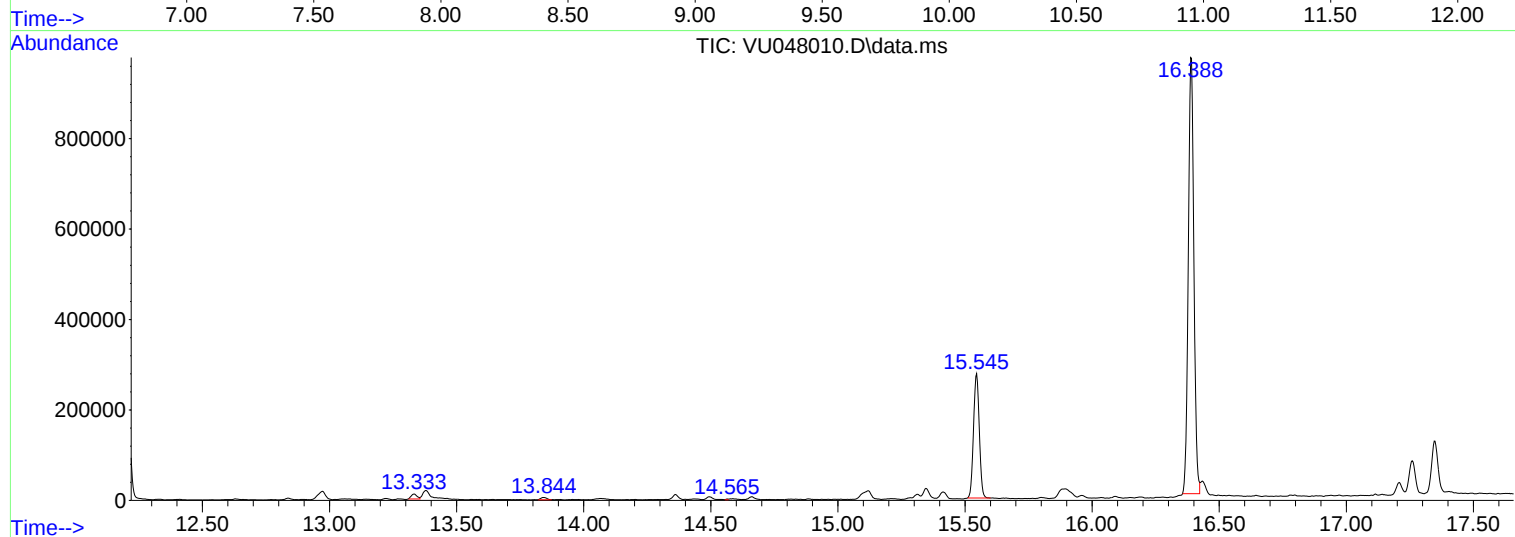
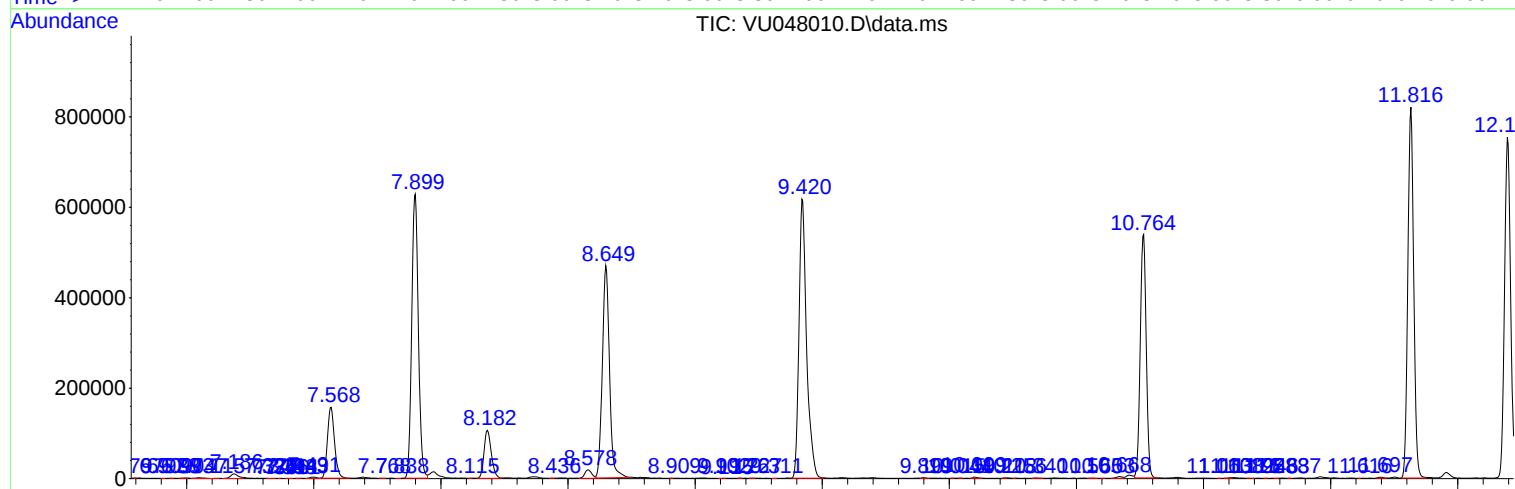
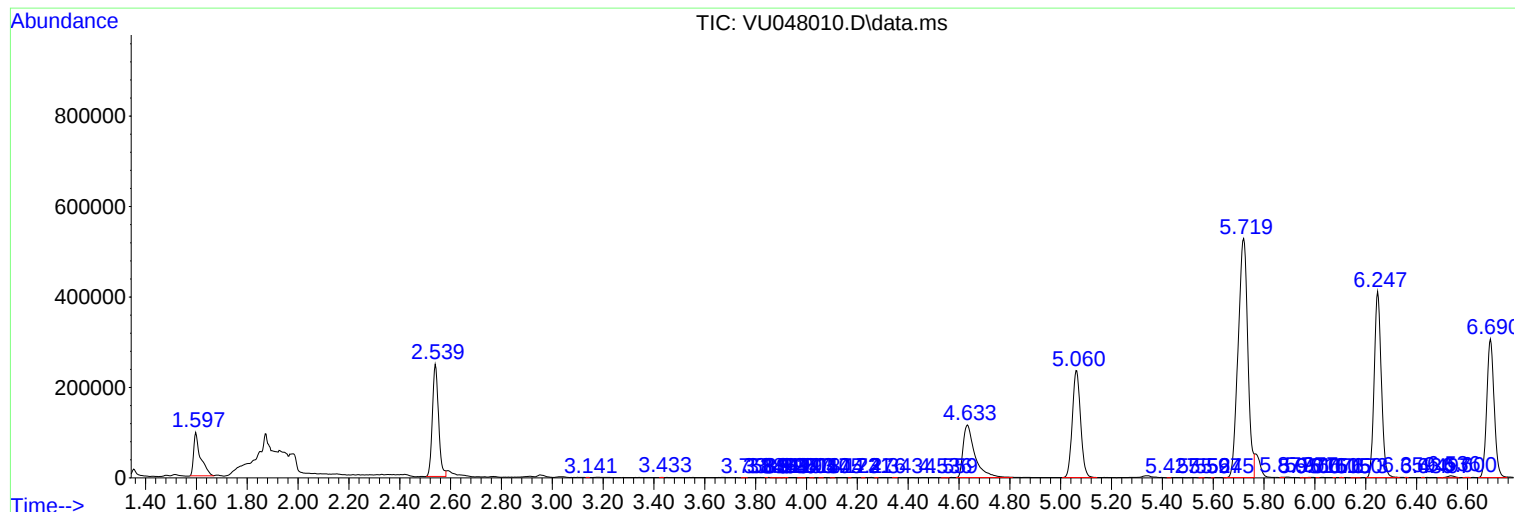
Sum of corrected areas: 13633653

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
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Acq On : 13 Apr 2022 17:44
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Misc : 6.57g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNQ8ME

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 : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNQ8ME

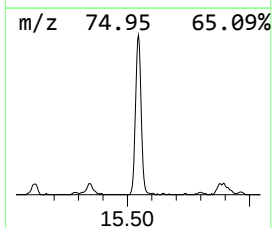
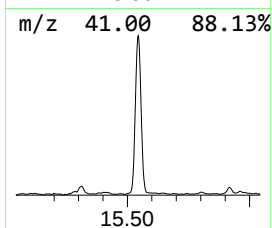
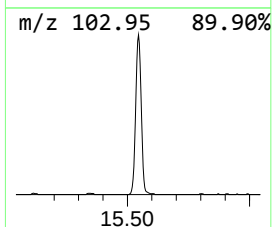
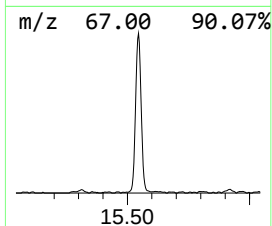
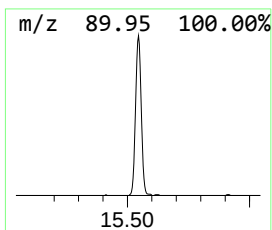
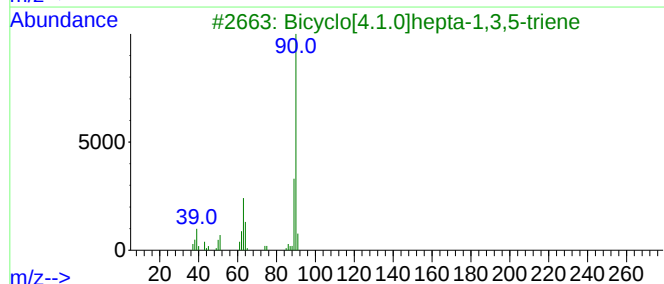
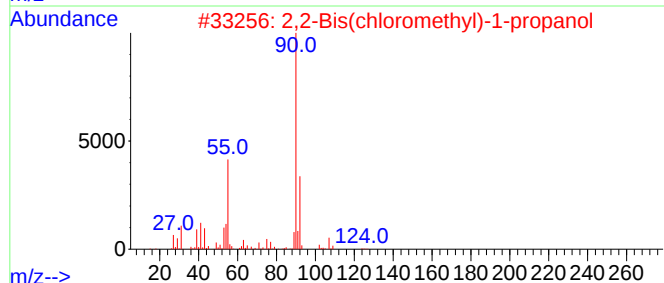
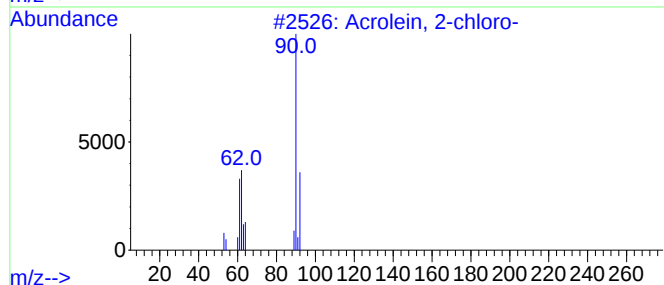
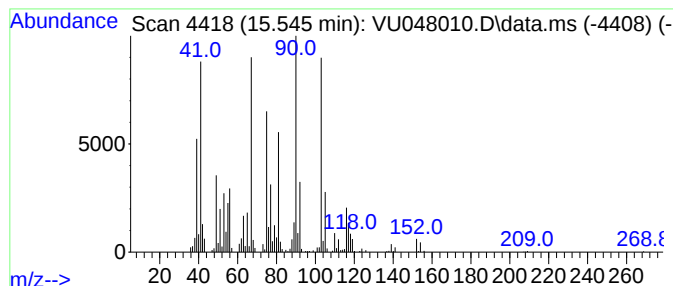
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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	16.69 ug/L	434395	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			2,2-Bis(chloromethyl)-1-propanol	156	C5H10Cl2O	005355-54-4	38
3			Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	38
4			Thiourea, methyl-	90	C2H6N2S	000598-52-7	35
5			2,2-Bis(chloromethyl)-1-propanol	156	C5H10Cl2O	005355-54-4	32



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Instrument :
MSVOA_U
ClientSampleId :
ETNQ8ME

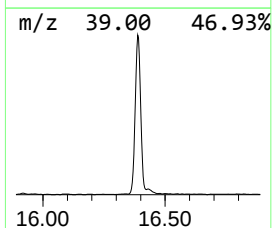
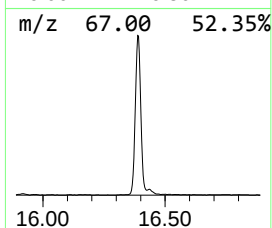
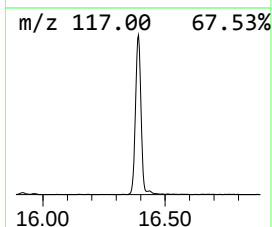
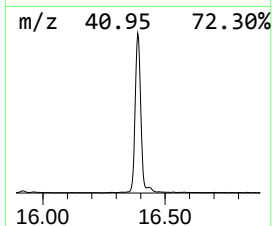
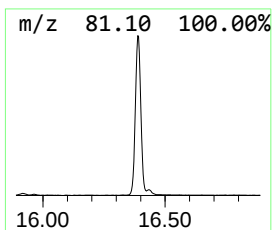
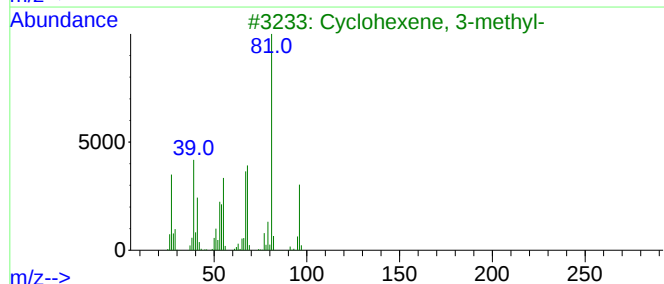
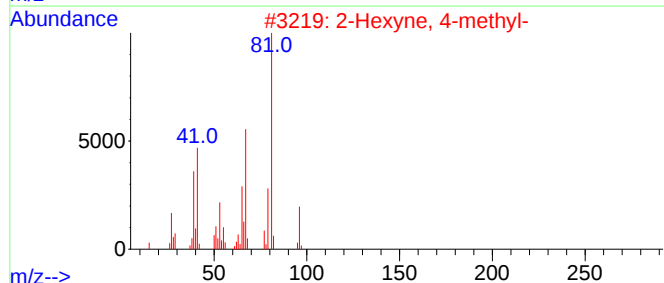
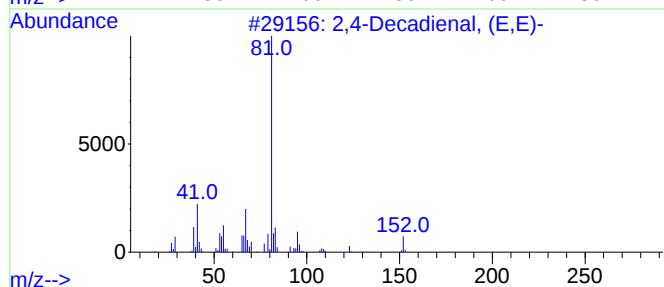
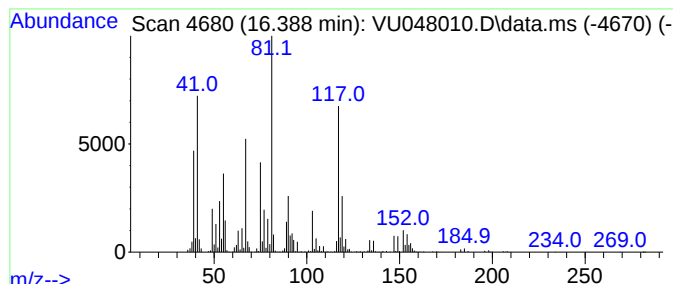
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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	57.25 ug/L	1489790	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	22
2			2-Hexyne, 4-methyl-	96	C7H12	020198-49-6	14
3			Cyclohexene, 3-methyl-	96	C7H12	000591-48-0	14
4			Cyclohexene, 3-(2-propynyl)-	120	C9H12	055956-43-9	10
5			4-(1H-Pyrazol-1-yl)butanoic acid	154	C7H10N2O2	1010468-88-1	10



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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNQ8ME

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	15.545	16.7	ug/L	434395	3	11.816	1301200	50.0
unknown-02	16.388	57.3	ug/L	1489790	3	11.816	1301200	50.0