

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
 Data File : VU047957.D
 Acq On : 12 Apr 2022 15:47
 Operator : SY/MD
 Sample : N2293-18ME
 Misc : 6.14g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNP6ME

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: VU047957.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	74	80	103	rVB	60845	107961	10.04%	1.128%
2	2.546	364	375	386	rBV	150951	252819	23.51%	2.642%
3	2.816	457	459	461	rBV3	378	185	0.02%	0.002%
4	3.369	629	631	633	rBV3	301	155	0.01%	0.002%
5	3.517	674	677	682	rVB2	553	423	0.04%	0.004%
6	3.588	697	699	702	rBV	223	163	0.02%	0.002%
7	3.636	711	714	716	rBV	258	167	0.02%	0.002%
8	3.700	731	734	738	rBV3	157	111	0.01%	0.001%
9	3.742	745	747	749	rBV2	293	185	0.02%	0.002%
10	3.854	780	782	783	rBV2	132	37	0.00%	0.000%
11	3.912	797	800	805	rVB2	457	389	0.04%	0.004%
12	3.944	805	810	813	rVB2	302	319	0.03%	0.003%
13	3.970	813	818	820	rBV2	410	407	0.04%	0.004%
14	4.205	888	891	896	rBV2	214	155	0.01%	0.002%
15	4.292	915	918	922	rBV	357	329	0.03%	0.003%
16	4.340	931	933	935	rVB	162	42	0.00%	0.000%
17	4.391	946	949	954	rBV2	314	222	0.02%	0.002%
18	4.433	959	962	964	rVB	262	145	0.01%	0.002%
19	4.478	973	976	977	rBV	270	179	0.02%	0.002%
20	4.555	997	1000	1001	rBV2	346	219	0.02%	0.002%
21	4.636	1011	1025	1079	rBV	96384	328777	30.57%	3.435%
22	5.063	1141	1158	1182	rBV	191422	429100	39.90%	4.484%
23	5.198	1198	1200	1202	rBV	144	64	0.01%	0.001%
24	5.462	1277	1282	1286	rBV2	343	373	0.03%	0.004%
25	5.510	1294	1297	1305	rVB2	216	174	0.02%	0.002%
26	5.616	1324	1330	1331	rBV2	280	276	0.03%	0.003%
27	5.719	1341	1362	1374	rBV2	402646	1075425	100.00%	11.237%
28	5.944	1429	1432	1435	rBV2	278	151	0.01%	0.002%
29	6.095	1474	1479	1480	rBV2	177	149	0.01%	0.002%
30	6.115	1480	1485	1487	rBV3	432	392	0.04%	0.004%
31	6.186	1503	1507	1511	rBV3	329	335	0.03%	0.004%
32	6.247	1511	1526	1557	rVV	387303	760233	70.69%	7.944%
33	6.452	1585	1590	1594	rBV3	316	396	0.04%	0.004%
34	6.497	1601	1604	1605	rBV2	191	86	0.01%	0.001%
35	6.571	1625	1627	1629	rBV	316	173	0.02%	0.002%
36	6.584	1629	1631	1632	rBV	359	152	0.01%	0.002%

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 ClientSampleId :
 ETNP6ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Peak separation: 5

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

37	6.690	1650	1664	1681	rBV	247071	499020	46.40%	5.214%
38	6.941	1740	1742	1743	rBV	275	136	0.01%	0.001%
39	6.980	1752	1754	1758	rBV3	362	342	0.03%	0.004%
40	7.060	1767	1779	1783	rBV6	1315	2425	0.23%	0.025%
41	7.185	1809	1818	1835	rBV3	8512	17344	1.61%	0.181%
42	7.279	1845	1847	1853	rVB3	446	283	0.03%	0.003%
43	7.497	1903	1915	1925	rBV3	14054	30026	2.79%	0.314%
44	7.568	1927	1937	1956	rVB	114093	220467	20.50%	2.304%
45	7.899	2026	2040	2054	rBV	413408	738001	68.62%	7.711%
46	8.182	2114	2128	2149	rBV	77894	159365	14.82%	1.665%
47	8.369	2175	2186	2202	rVB7	12069	27672	2.57%	0.289%
48	8.652	2259	2274	2309	rBV	430139	828959	77.08%	8.662%
49	9.028	2384	2391	2402	rVB4	6471	12186	1.13%	0.127%
50	9.147	2423	2428	2432	rBV3	358	389	0.04%	0.004%
51	9.185	2432	2440	2446	rVV5	566	961	0.09%	0.010%
52	9.337	2484	2487	2488	rBV5	312	165	0.02%	0.002%
53	9.365	2493	2496	2499	rBV3	921	718	0.07%	0.008%
54	9.423	2500	2514	2516	rBV	607753	848100	78.86%	8.862%
55	9.851	2645	2647	2650	rVV3	358	194	0.02%	0.002%
56	9.870	2650	2653	2657	rVB	352	223	0.02%	0.002%
57	9.941	2674	2675	2678	rVB	204	70	0.01%	0.001%
58	9.980	2684	2687	2689	rBV	296	176	0.02%	0.002%
59	10.028	2698	2702	2704	rBV2	565	456	0.04%	0.005%
60	10.105	2718	2726	2738	rVB6	2274	3667	0.34%	0.038%
61	10.655	2890	2897	2908	rVB7	4766	7565	0.70%	0.079%
62	10.764	2919	2931	2955	rVB	474045	765794	71.21%	8.002%
63	10.976	2990	2997	3012	rBV8	2897	5888	0.55%	0.062%
64	11.098	3028	3035	3036	rBV2	959	895	0.08%	0.009%
65	11.160	3051	3054	3057	rBV2	230	145	0.01%	0.002%
66	11.172	3057	3058	3063	rVV	279	174	0.02%	0.002%
67	11.230	3074	3076	3081	rVB2	435	228	0.02%	0.002%
68	11.256	3081	3084	3086	rBV2	362	272	0.03%	0.003%
69	11.288	3091	3094	3095	rBV	747	405	0.04%	0.004%
70	11.587	3184	3187	3191	rBV2	808	653	0.06%	0.007%
71	11.751	3232	3238	3239	rBV4	1632	1628	0.15%	0.017%
72	11.816	3245	3258	3273	rBV	676500	1068205	99.33%	11.162%
73	12.098	3342	3346	3351	rVB4	1331	1032	0.10%	0.011%
74	12.198	3363	3377	3393	rBV	519824	876008	81.46%	9.153%
75	12.970	3609	3617	3630	rVB4	12169	20958	1.95%	0.219%
76	13.057	3642	3644	3648	rBV3	413	376	0.03%	0.004%

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 ClientSampleId :
 ETNP6ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Peak Location: TOP

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Title : VOC Analysis

77	13.275	3707	3712	3717	rBV3	911	1305	0.12%	0.014%
78	13.378	3738	3744	3757	rVB3	19597	29538	2.75%	0.309%
79	14.362	4043	4050	4059	rVB2	14824	21344	1.98%	0.223%
80	14.426	4066	4070	4083	rVV8	4096	6068	0.56%	0.063%
81	14.497	4085	4092	4103	rVB6	7512	11144	1.04%	0.116%
82	15.545	4408	4418	4438	rBV2	89732	138310	12.86%	1.445%
83	16.092	4581	4588	4601	rVB	37832	56552	5.26%	0.591%
84	16.388	4672	4680	4694	rVB	129563	203598	18.93%	2.127%

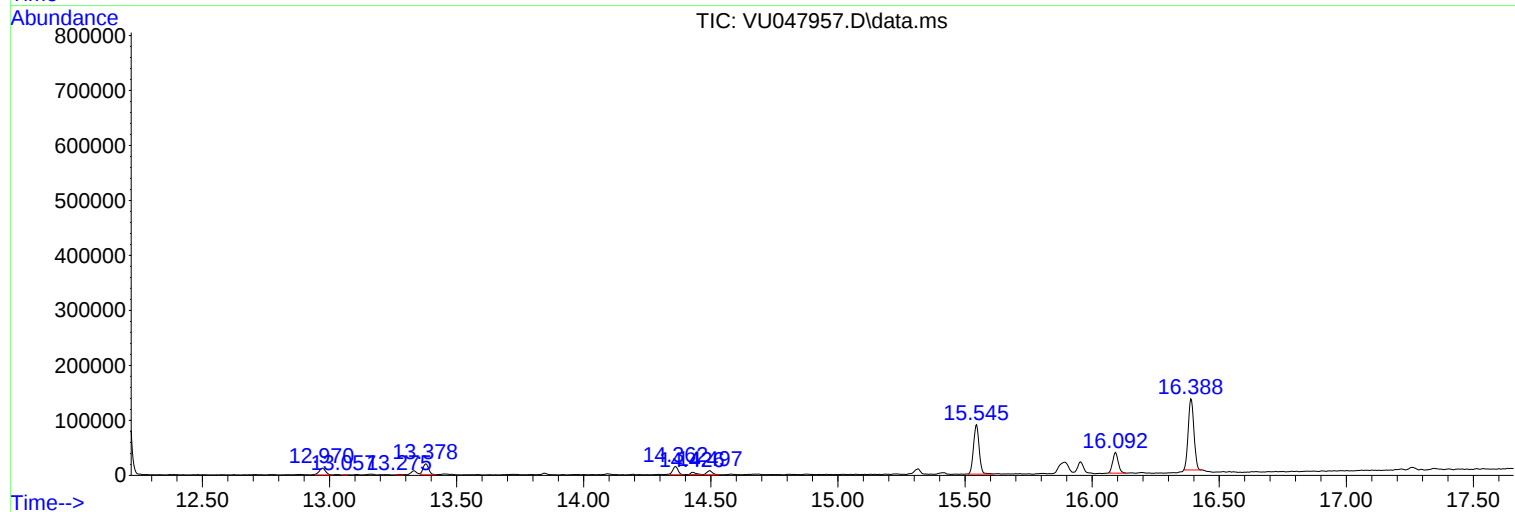
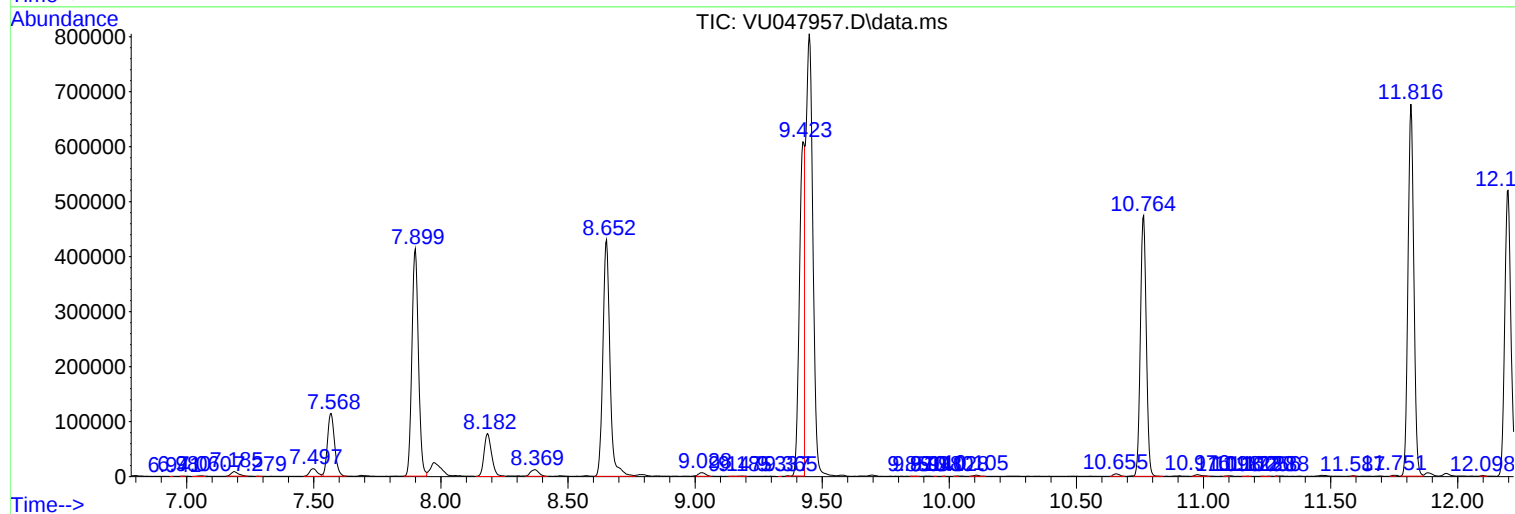
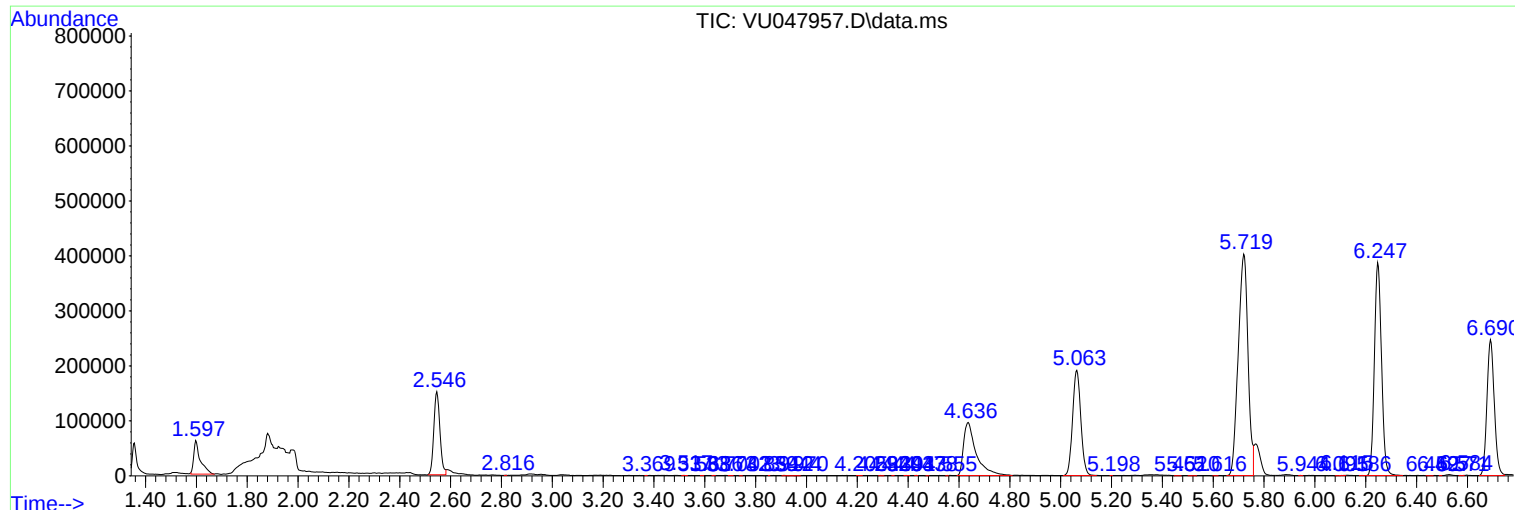
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP6ME

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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Operator : SY/MD
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP6ME

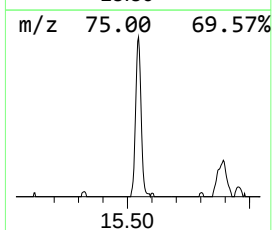
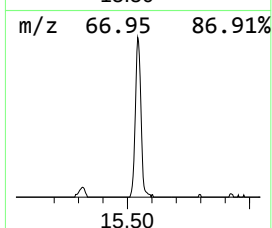
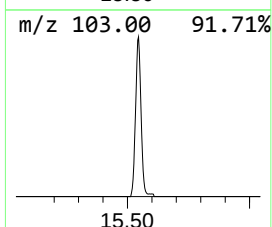
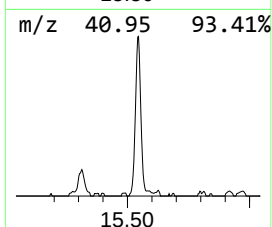
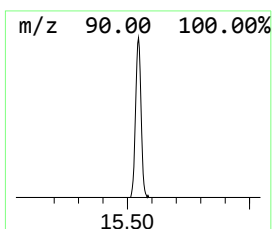
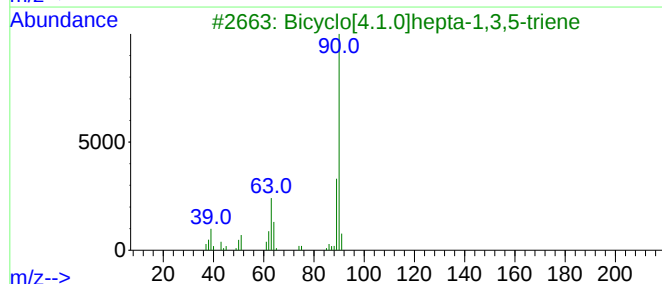
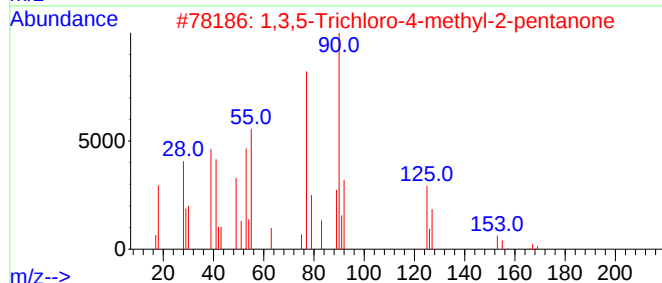
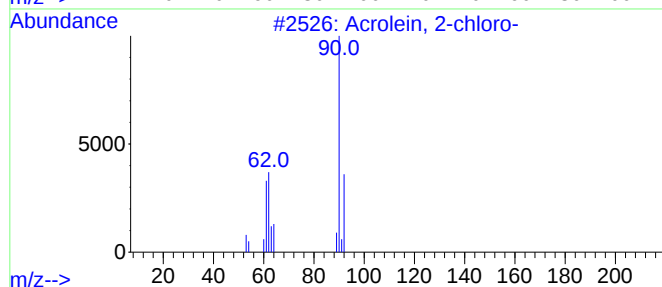
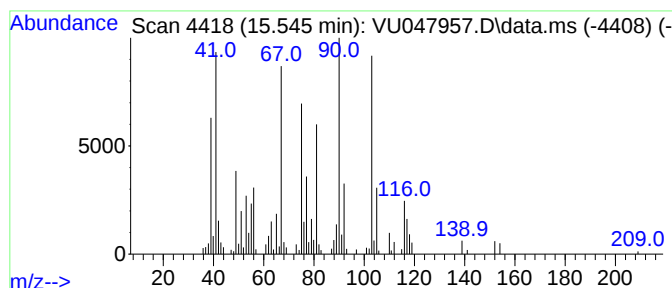
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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	6.47 ug/L	138310	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	37
2			1,3,5-Trichloro-4-methyl-2-penta...	202	C6H9Cl3O	1000140-03-8	30
3			Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	27
4			1-Pentene, 5-chloro-4-(chloromet...	152	C6H10Cl2	027990-74-5	20
5			2,2-Bis(chloromethyl)-1-propanol	156	C5H10Cl2O	005355-54-4	17



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Misc : 6.14g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP6ME

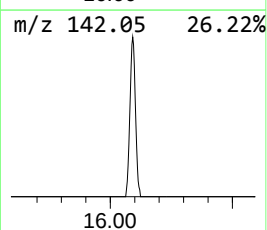
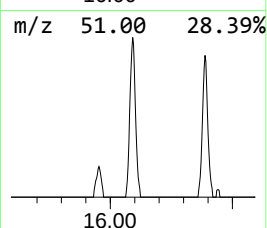
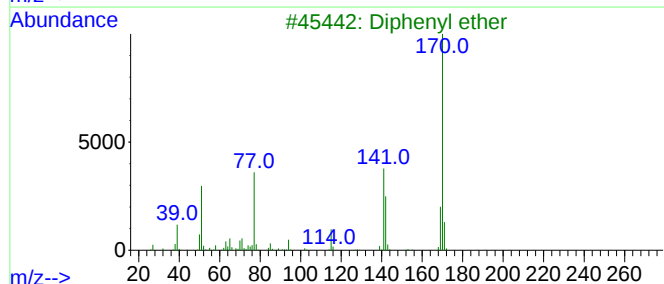
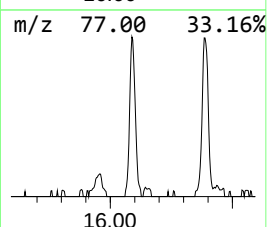
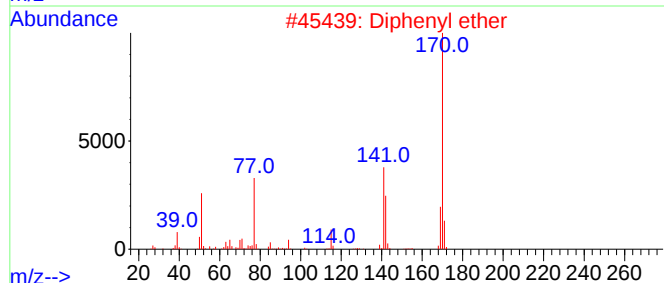
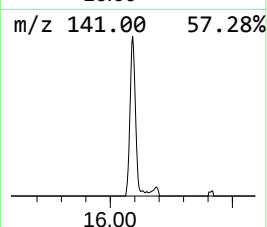
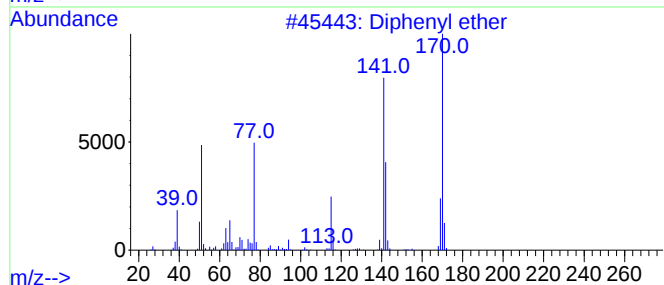
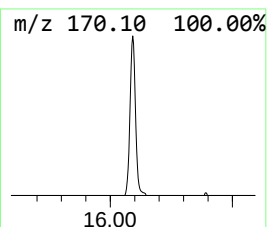
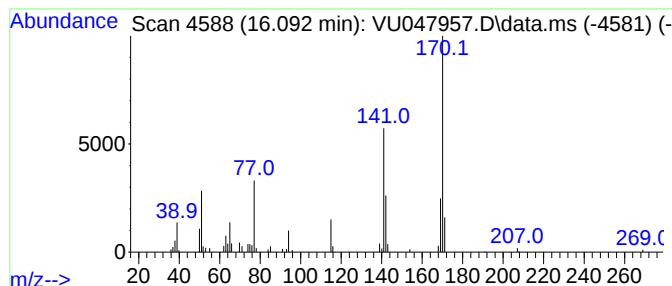
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Diphenyl ether Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.092	2.65 ug/L	56552	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diphenyl ether	170	C12H10O	000101-84-8	96
2			Diphenyl ether	170	C12H10O	000101-84-8	90
3			Diphenyl ether	170	C12H10O	000101-84-8	87
4			Diphenyl ether	170	C12H10O	000101-84-8	87
5			Diphenyl ether	170	C12H10O	000101-84-8	81



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ALS Vial : 18 Sample Multiplier: 1

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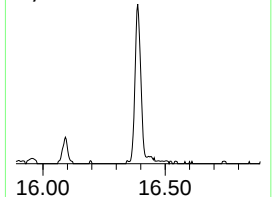
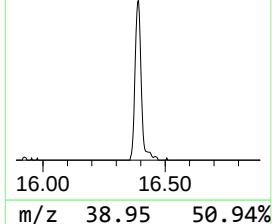
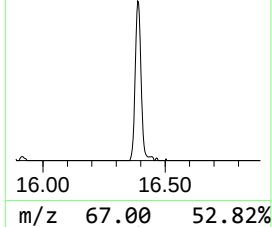
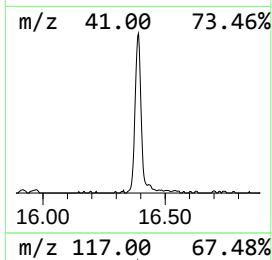
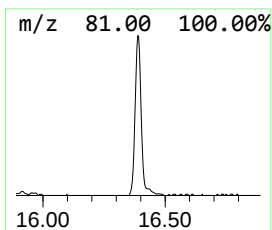
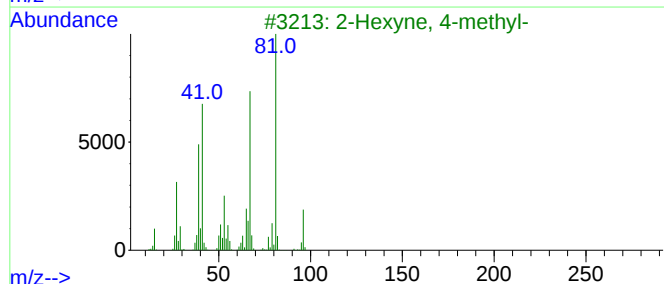
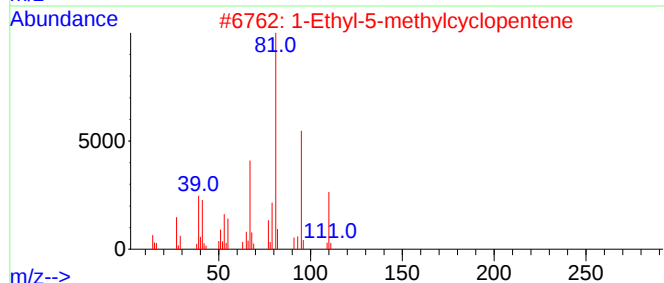
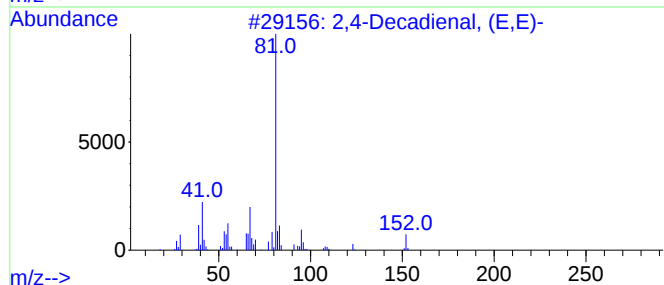
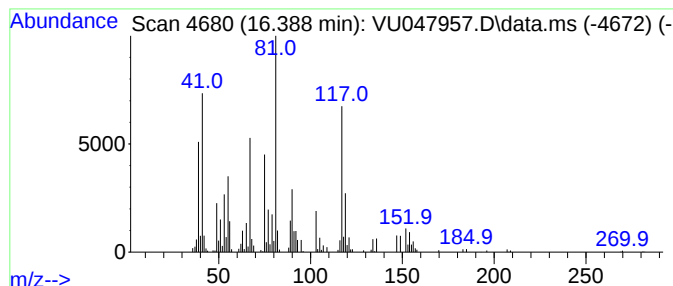
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.388	9.53 ug/L	203598	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	12
2			1-Ethyl-5-methylcyclopentene	110	C8H14	097797-57-4	12
3			2-Hexyne, 4-methyl-	96	C7H12	020198-49-6	12
4			2-Hexyne, 4-methyl-	96	C7H12	020198-49-6	12
5			Cyclopropane, 1-(5-hexenyl)-2-iodo-	250	C9H15I	074685-40-8	12



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Instrument :
MSVOA_U
ClientSampleId :
ETNP6ME

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	6.5	ug/L	138310	3	11.816	1068210	50.0
Diphenyl ether	16.092	2.6	ug/L	56552	3	11.816	1068210	50.0
unknown-02	16.388	9.5	ug/L	203598	3	11.816	1068210	50.0