

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
 Data File : VU047934.D
 Acq On : 12 Apr 2022 02:28
 Operator : SY/MD
 Sample : N2293-18ME
 Misc : 6.14g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 42 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: VU047934.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.356	3	5	25	rVB	147287	155201	4.54%	1.042%
2	1.597	73	80	110	rVB	70032	145549	4.26%	0.977%
3	1.896	169	173	197	rVB	36004	65517	1.92%	0.440%
4	2.543	362	374	388	rBV	193486	335237	9.81%	2.251%
5	2.964	500	505	512	rVV4	1590	2592	0.08%	0.017%
6	3.224	582	586	595	rVB5	1066	1551	0.05%	0.010%
7	3.430	644	650	658	rVB4	935	1393	0.04%	0.009%
8	3.668	717	724	725	rBV2	901	895	0.03%	0.006%
9	4.514	981	987	993	rBV4	471	603	0.02%	0.004%
10	4.645	1013	1028	1083	rBV	80272	304608	8.92%	2.045%
11	5.063	1141	1158	1181	rVV	193089	440881	12.91%	2.960%
12	5.288	1221	1228	1237	rVB6	715	1213	0.04%	0.008%
13	5.369	1245	1253	1254	rBV5	1399	1552	0.05%	0.010%
14	5.584	1316	1320	1330	rVB6	949	1268	0.04%	0.009%
15	5.719	1338	1362	1374	rBV2	433617	1135210	33.23%	7.623%
16	5.886	1402	1414	1426	rVB9	2446	6169	0.18%	0.041%
17	5.980	1438	1443	1448	rVB6	970	1144	0.03%	0.008%
18	6.131	1479	1490	1496	rBV5	2614	4303	0.13%	0.029%
19	6.247	1511	1526	1555	rBV	574657	1150006	33.66%	7.722%
20	6.526	1606	1613	1624	rVB8	2144	4169	0.12%	0.028%
21	6.603	1632	1637	1640	rBV5	555	580	0.02%	0.004%
22	6.690	1647	1664	1693	rBV	246965	515805	15.10%	3.464%
23	7.208	1812	1825	1829	rBV3	5536	12312	0.36%	0.083%
24	7.497	1904	1915	1926	rBV4	15407	32844	0.96%	0.221%
25	7.568	1926	1937	1959	rVB	119129	235484	6.89%	1.581%
26	7.693	1972	1976	1977	rBV3	809	584	0.02%	0.004%
27	7.899	2009	2040	2054	rBV	490316	887737	25.99%	5.961%
28	7.973	2055	2063	2085	rVB3	27479	74171	2.17%	0.498%
29	8.124	2108	2110	2115	rBV3	830	574	0.02%	0.004%
30	8.182	2118	2128	2153	rVB	76282	158687	4.65%	1.066%
31	8.365	2174	2185	2186	rBV3	10878	13064	0.38%	0.088%
32	8.459	2208	2214	2215	rBV5	585	603	0.02%	0.004%
33	8.549	2237	2242	2245	rVB4	691	534	0.02%	0.004%
34	8.581	2245	2252	2260	rBV5	1405	2365	0.07%	0.016%
35	8.661	2260	2277	2305	rBV	321443	698347	20.44%	4.689%
36	8.867	2333	2341	2346	rVB5	1113	1791	0.05%	0.012%

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 Misc : 6.14g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
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 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

37	9.031	2380	2392	2403	rBV7	5175	12567	0.37%	0.084%
38	9.365	2487	2496	2500	rVV6	2717	3732	0.11%	0.025%
39	9.449	2500	2522	2553	rVV2	1096037	3416253	100.00%	22.940%
40	9.578	2555	2562	2571	rVB6	4101	6939	0.20%	0.047%
41	9.697	2588	2599	2607	rVV4	4179	7614	0.22%	0.051%
42	9.838	2636	2643	2645	rBV4	489	514	0.02%	0.003%
43	10.018	2695	2699	2704	rVB5	570	671	0.02%	0.005%
44	10.105	2716	2726	2738	rBV5	2881	5542	0.16%	0.037%
45	10.234	2763	2766	2771	rBV4	662	579	0.02%	0.004%
46	10.481	2840	2843	2851	rVB3	744	753	0.02%	0.005%
47	10.658	2889	2898	2909	rVV8	6403	10838	0.32%	0.073%
48	10.719	2909	2917	2919	rVV5	2194	3052	0.09%	0.020%
49	10.767	2919	2932	2950	rVB	405244	660804	19.34%	4.437%
50	10.893	2965	2971	2974	rBV2	1454	1639	0.05%	0.011%
51	10.986	2991	3000	3008	rBV7	3354	6812	0.20%	0.046%
52	11.105	3029	3037	3047	rVB8	1983	3120	0.09%	0.021%
53	11.295	3090	3096	3104	rVB6	1677	2327	0.07%	0.016%
54	11.475	3142	3152	3161	rBV5	3188	5802	0.17%	0.039%
55	11.516	3162	3165	3170	rVB3	1053	861	0.03%	0.006%
56	11.587	3182	3187	3189	rBV3	1097	955	0.03%	0.006%
57	11.754	3232	3239	3245	rBV5	2326	3065	0.09%	0.021%
58	11.815	3245	3258	3274	rVV	1044647	1662017	48.65%	11.160%
59	11.886	3274	3280	3290	rVV7	8712	16333	0.48%	0.110%
60	11.957	3293	3302	3312	rVV6	7951	14191	0.42%	0.095%
61	12.015	3315	3320	3326	rBV5	534	554	0.02%	0.004%
62	12.073	3334	3338	3341	rBV4	881	653	0.02%	0.004%
63	12.105	3341	3348	3353	rVV8	1633	2379	0.07%	0.016%
64	12.198	3363	3377	3400	rVV	568494	951144	27.84%	6.387%
65	12.375	3428	3432	3433	rBV3	1324	919	0.03%	0.006%
66	12.471	3457	3462	3463	rBV3	866	718	0.02%	0.005%
67	12.571	3489	3493	3503	rVB4	1067	1312	0.04%	0.009%
68	12.635	3505	3513	3517	rBV7	1227	1963	0.06%	0.013%
69	12.687	3524	3529	3530	rBV2	873	606	0.02%	0.004%
70	12.706	3533	3535	3540	rVB4	1127	869	0.03%	0.006%
71	12.770	3549	3555	3557	rBV2	1272	1335	0.04%	0.009%
72	12.838	3572	3576	3582	rBV5	1629	1910	0.06%	0.013%
73	12.880	3586	3589	3596	rVB6	1497	1602	0.05%	0.011%
74	12.973	3604	3618	3629	rBV4	27793	49397	1.45%	0.332%
75	13.031	3633	3636	3645	rVB7	2215	2560	0.07%	0.017%
76	13.079	3645	3651	3655	rBV5	881	1179	0.03%	0.008%

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 ALS Vial : 42 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

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Peak separation: 5

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

77	13.108	3655	3660	3666	rVV8	1051	1558	0.05%	0.010%
78	13.163	3670	3677	3685	rVB8	1925	3184	0.09%	0.021%
79	13.333	3720	3730	3736	rBV3	18240	29493	0.86%	0.198%
80	13.378	3736	3744	3754	rVB2	37916	59378	1.74%	0.399%
81	13.844	3881	3889	3900	rVB6	5079	9131	0.27%	0.061%
82	14.092	3960	3966	3973	rVB2	3551	4712	0.14%	0.032%
83	14.201	3990	4000	4009	rBV9	2126	3806	0.11%	0.026%
84	14.359	4040	4049	4063	rVB	19820	30613	0.90%	0.206%
85	14.436	4066	4073	4084	rVV9	6281	12048	0.35%	0.081%
86	14.494	4084	4091	4107	rVB6	11686	16730	0.49%	0.112%
87	14.812	4185	4190	4195	rVB7	1625	1861	0.05%	0.012%
88	14.883	4206	4212	4218	rVB8	2194	2863	0.08%	0.019%
89	15.024	4250	4256	4261	rVB7	1555	1890	0.06%	0.013%
90	15.073	4267	4271	4278	rBV4	1079	1157	0.03%	0.008%
91	15.121	4278	4286	4293	rBV8	4290	7740	0.23%	0.052%
92	15.227	4310	4319	4328	rVB7	3510	5340	0.16%	0.036%
93	15.314	4339	4346	4354	rVB3	11323	16581	0.49%	0.111%
94	15.410	4367	4376	4386	rVB5	8741	16667	0.49%	0.112%
95	15.545	4406	4418	4433	rBV2	189859	291842	8.54%	1.960%
96	15.796	4488	4496	4508	rBV5	16098	24341	0.71%	0.163%
97	15.889	4513	4525	4536	rVV3	42363	113308	3.32%	0.761%
98	15.954	4538	4545	4558	rVB	48787	79182	2.32%	0.532%
99	16.092	4578	4588	4601	rBV	84787	130709	3.83%	0.878%
100	16.388	4669	4680	4693	rBV	477532	767447	22.46%	5.153%

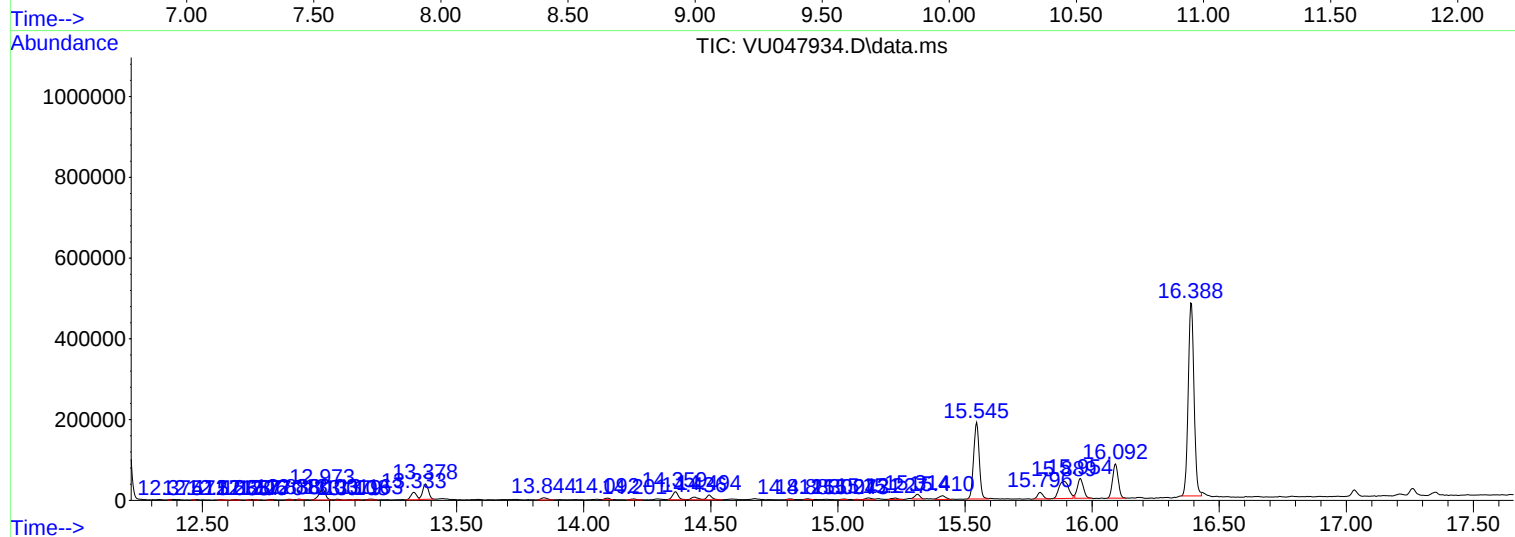
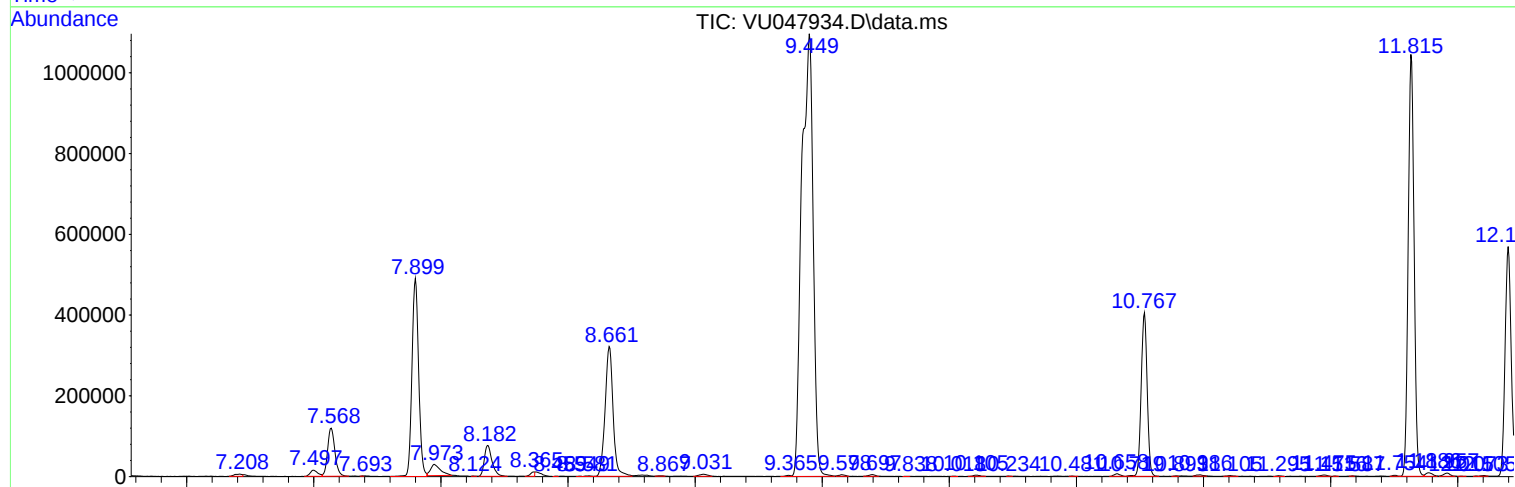
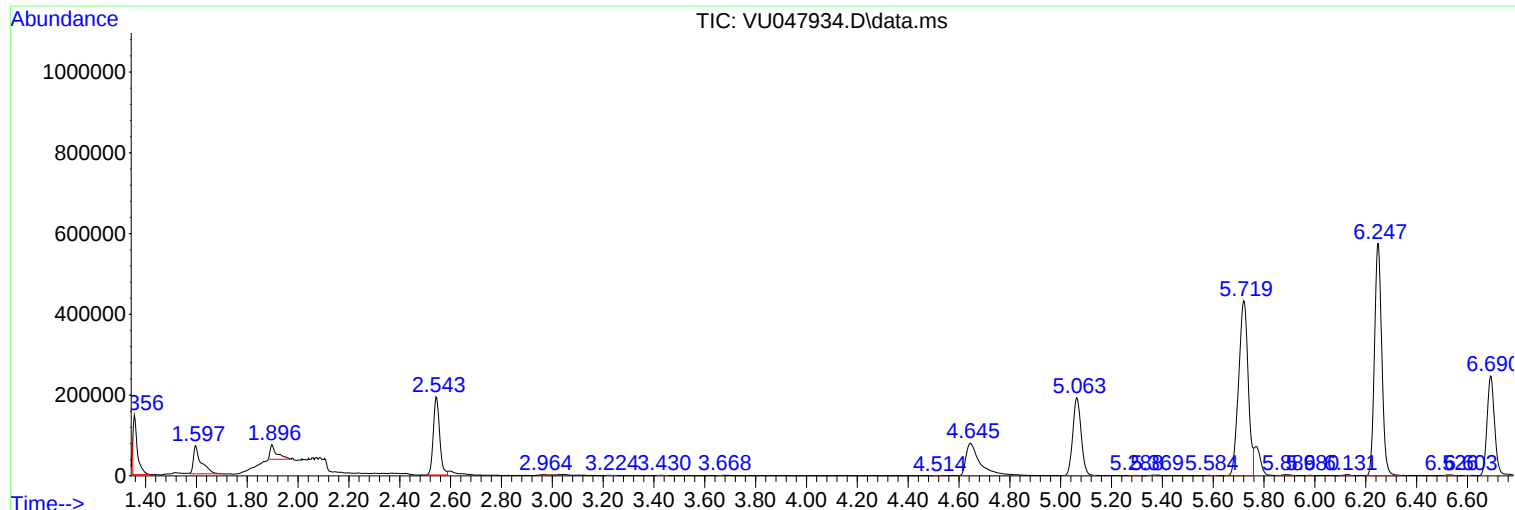
Sum of corrected areas: 14892204

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ALS Vial : 42 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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ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP6ME

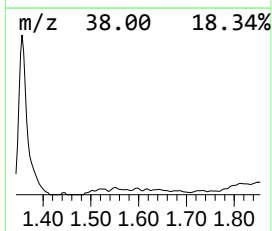
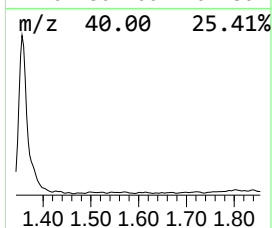
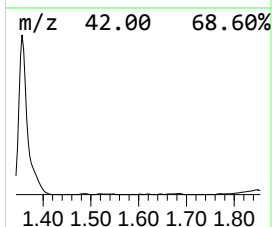
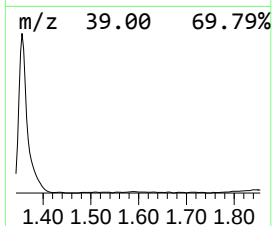
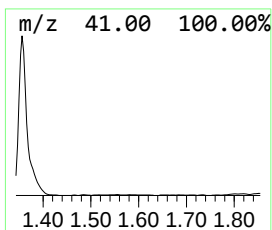
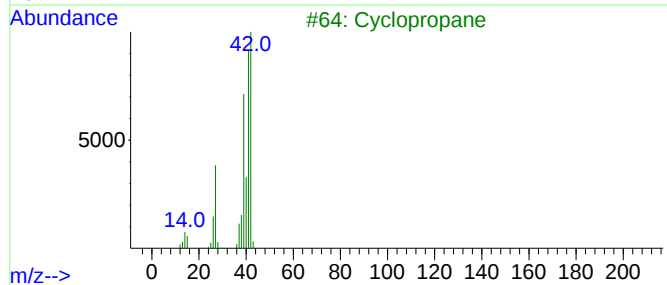
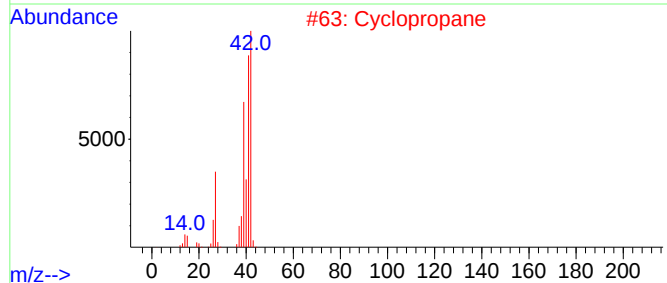
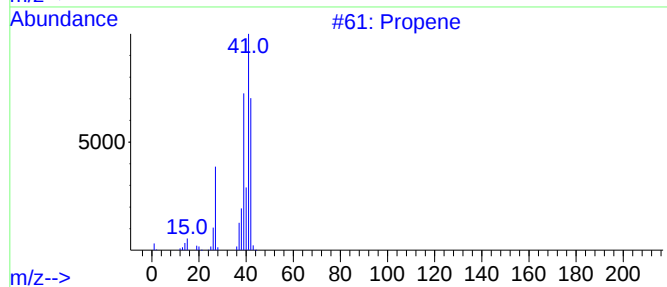
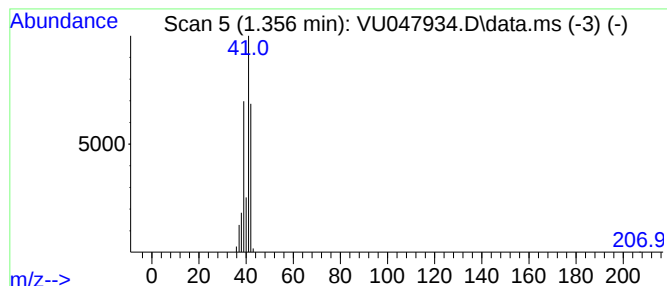
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.356	6.75 ug/L	155201	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Cyclopropane	42	C3H6	000075-19-4	86
3			Cyclopropane	42	C3H6	000075-19-4	78
4			Propene	42	C3H6	000115-07-1	50
5			Cyclopropene	40	C3H4	002781-85-3	16



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Instrument :
MSVOA_U
ClientSampleId :
ETNP6ME

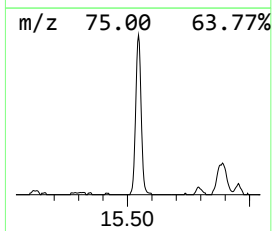
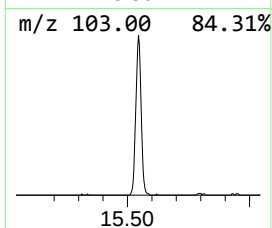
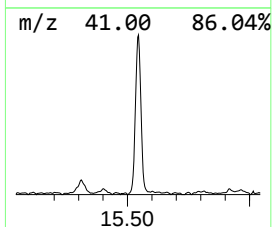
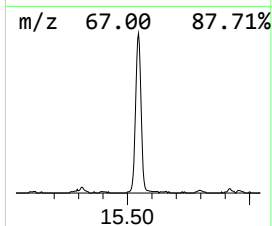
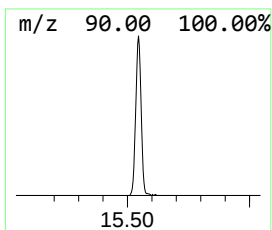
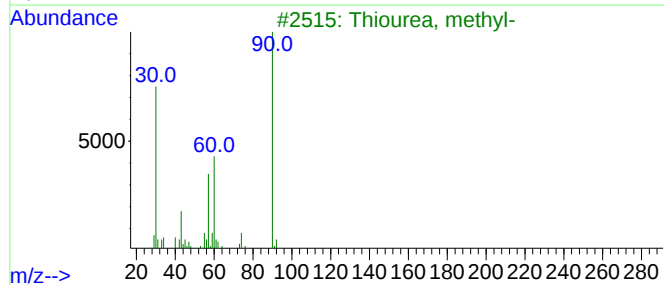
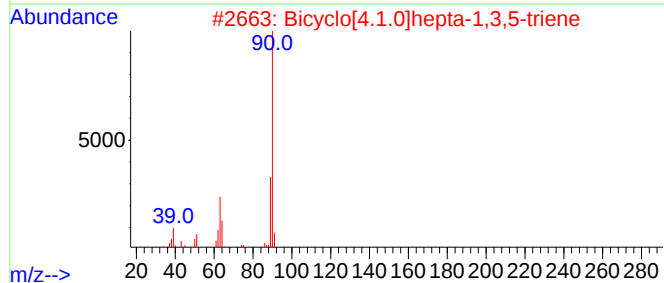
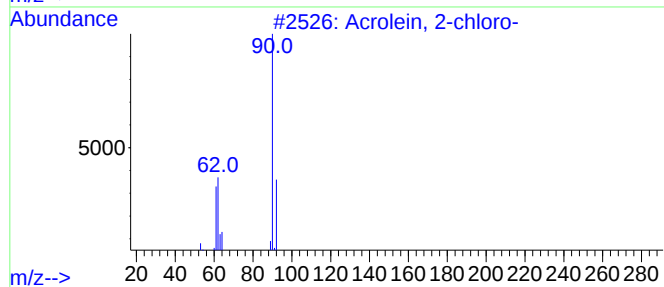
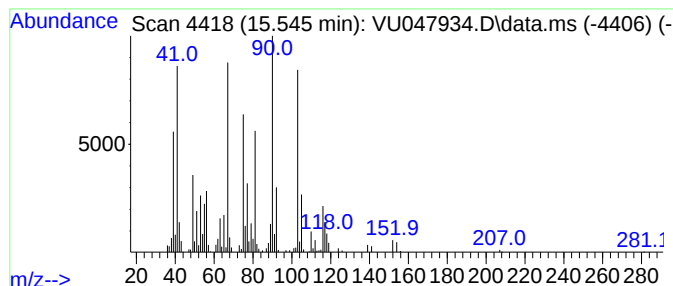
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	8.78 ug/L	291842	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	38
2			Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	35
3			Thiourea, methyl-	90	C2H6N2S	000598-52-7	35
4			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	25
5			1,3,5-Trichloro-4-methyl-2-penta...	202	C6H9Cl3O	1000140-03-8	25



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ClientSampleId :
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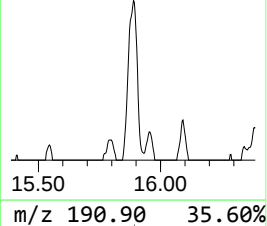
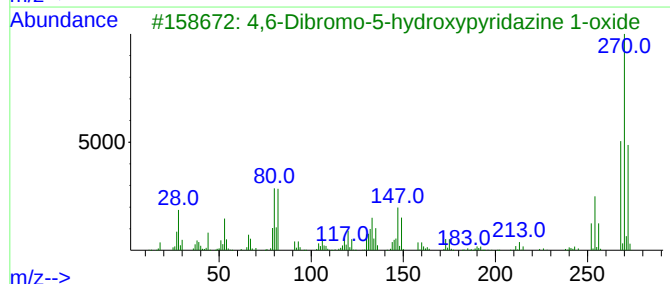
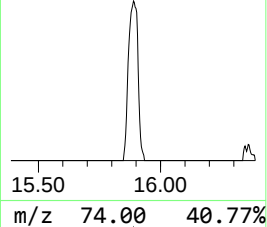
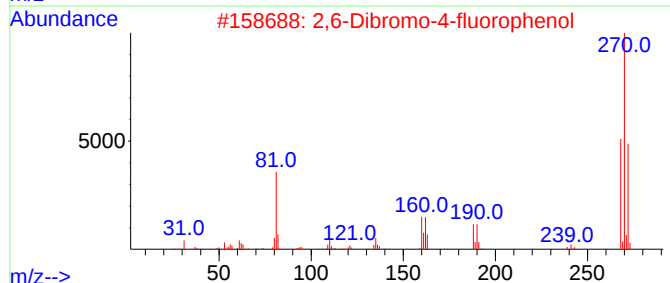
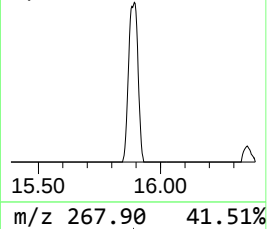
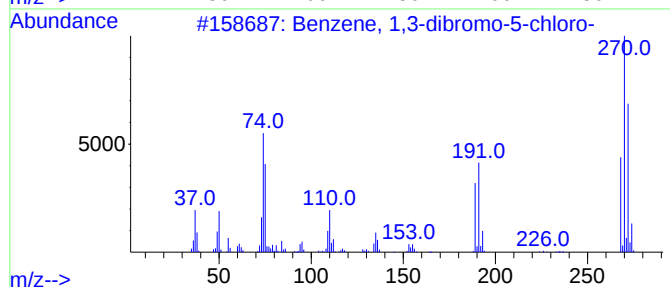
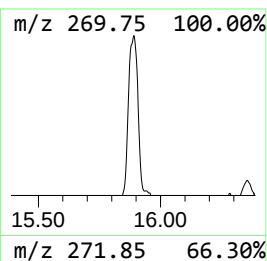
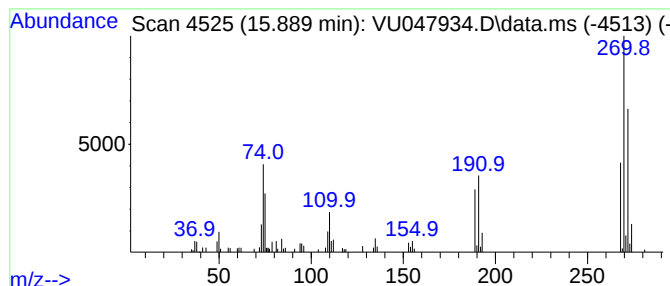
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Quant Title : VOC Analysis

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

Peak Number 4 Benzene, 1,3-dibromo-5-chloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.889	3.41 ug/L	113308	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-dibromo-5-chloro-	268	C6H3Br2Cl	014862-52-3	95
2			2,6-Dibromo-4-fluorophenol	268	C6H3Br2FO	000344-20-7	38
3			4,6-Dibromo-5-hydroxypyridazine ...	268	C4H2Br2N2O2	019971-61-0	25
4			Pyrimidine, 4,6-dichloro-2-(meth...	270	C11H8Cl2N2S	064415-11-8	23
5			4-(4-Bromophenyl)-2-chloropyrimi...	268	C10H6BrClN2	932162-80-6	17



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047934.D
Acq On : 12 Apr 2022 02:28
Operator : SY/MD
Sample : N2293-18ME
Misc : 6.14g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP6ME

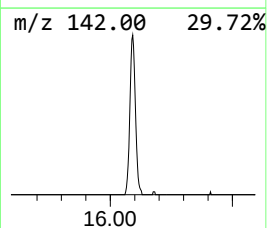
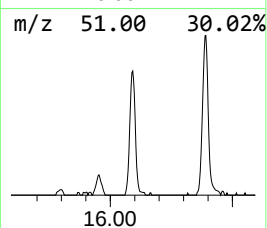
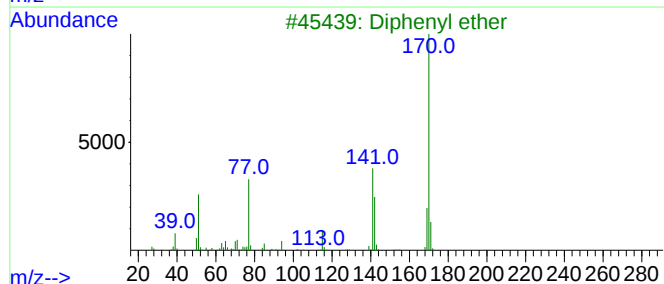
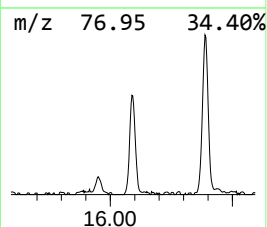
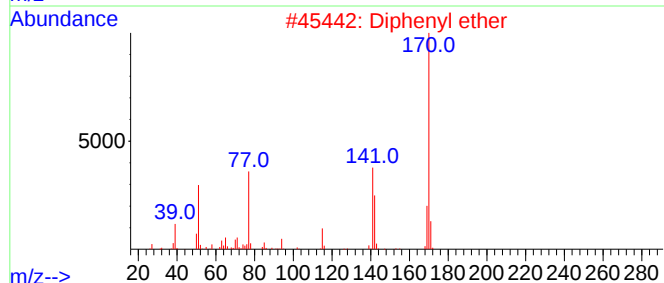
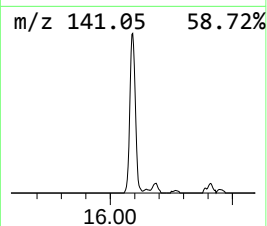
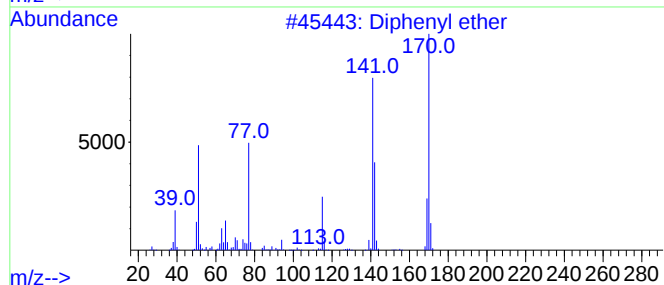
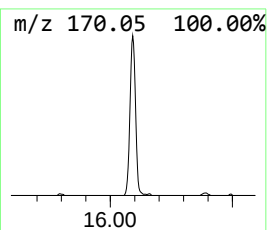
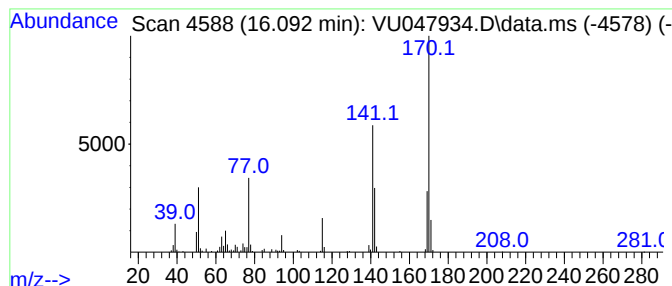
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Quant Title : VOC Analysis

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

Peak Number 5 Diphenyl ether Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.092	3.93 ug/L	130709	1,4-Dichlorobenzene-d4	11.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diphenyl ether	170	C12H10O	000101-84-8	93
2	Diphenyl ether	170	C12H10O	000101-84-8	93
3	Diphenyl ether	170	C12H10O	000101-84-8	93
4	Diphenyl ether	170	C12H10O	000101-84-8	91
5	Diphenyl ether	170	C12H10O	000101-84-8	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047934.D
Acq On : 12 Apr 2022 02:28
Operator : SY/MD
Sample : N2293-18ME
Misc : 6.14g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP6ME

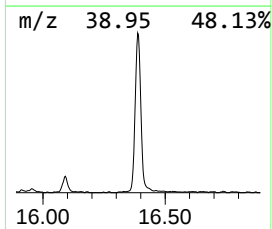
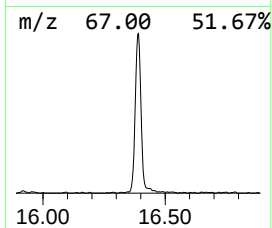
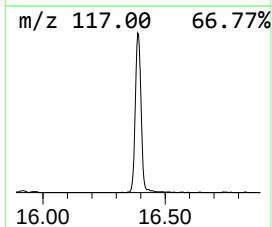
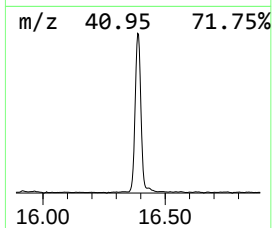
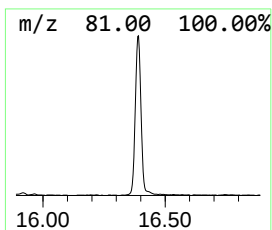
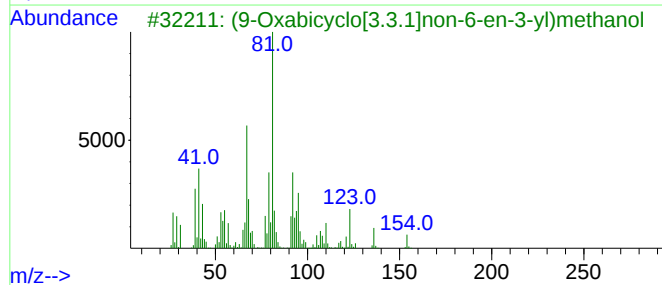
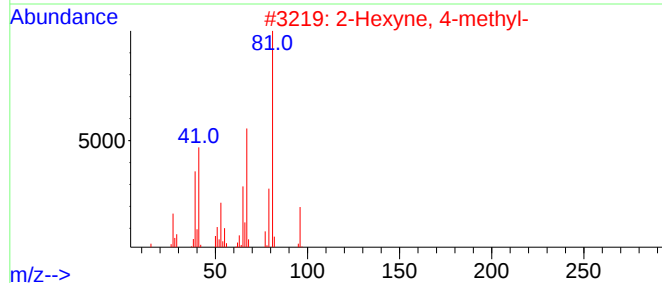
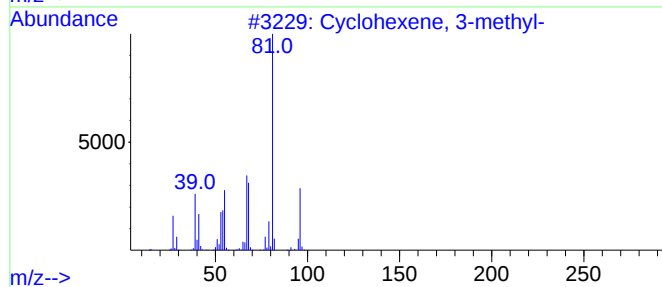
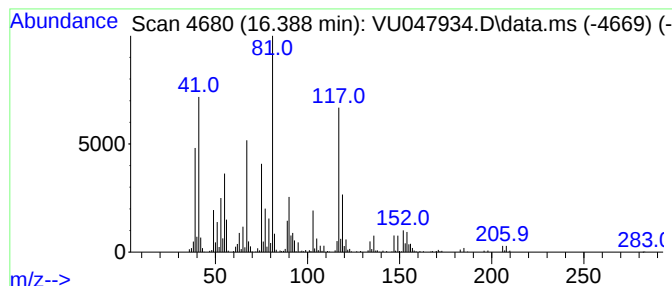
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Quant Title : VOC Analysis

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

Peak Number 6 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.388	23.09 ug/L	767447	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 3-methyl-	96	C7H12	000591-48-0	14
2			2-Hexyne, 4-methyl-	96	C7H12	020198-49-6	14
3			(9-Oxabicyclo[3.3.1]non-6-en-3-yl)...	154	C9H14O2	1000191-02-8	12
4			Cyclopropane, 1-(5-hexenyl)-2-iodo-	250	C9H15I	074685-40-8	12
5			Furan, 2-propyl-	110	C7H10O	004229-91-8	11



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047934.D
Acq On : 12 Apr 2022 02:28
Operator : SY/MD
Sample : N2293-18ME
Misc : 6.14g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 42 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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.356	6.8	ug/L	155201	1	6.250	1150010	50.0
unknown-01	15.545	8.8	ug/L	291842	3	11.816	1662020	50.0
Benzene, 1,3-di...	15.889	3.4	ug/L	113308	3	11.816	1662020	50.0
Diphenyl ether	16.092	3.9	ug/L	130709	3	11.816	1662020	50.0
unknown-02	16.388	23.1	ug/L	767447	3	11.816	1662020	50.0