

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
 Data File : VU050487.D
 Acq On : 29 Aug 2022 16:12
 Operator : SY/MD
 Sample : N4399-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBUZ1

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\SFAMULM082422WMA.M
 Title : VOC Analysis

Signal : TIC: VU050487.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.482	37	44	52	rBV	37838	44278	2.61%	0.233%
2	1.597	71	80	115	rBV2	277730	402082	23.66%	2.113%
3	1.867	160	164	168	rBV	28521	29539	1.74%	0.155%
4	1.896	168	173	197	rVB	138259	192972	11.35%	1.014%
5	2.559	366	379	392	rBV	317627	512661	30.16%	2.694%
6	2.639	392	404	431	rVV	771255	1307465	76.93%	6.870%
7	2.919	488	491	495	rBV2	638	516	0.03%	0.003%
8	3.041	515	529	555	rVB	192216	365374	21.50%	1.920%
9	3.166	564	568	570	rBV2	665	504	0.03%	0.003%
10	3.182	570	573	578	rVV2	573	586	0.03%	0.003%
11	3.346	610	624	649	rBV	262763	517041	30.42%	2.717%
12	3.433	649	651	654	rVB2	432	266	0.02%	0.001%
13	3.636	711	714	717	rBV	377	239	0.01%	0.001%
14	3.665	717	723	726	rVV2	233	252	0.01%	0.001%
15	3.729	739	743	748	rBV	294	350	0.02%	0.002%
16	3.793	757	763	766	rBV2	264	238	0.01%	0.001%
17	3.883	787	791	795	rBV	346	287	0.02%	0.002%
18	4.131	864	868	873	rBV2	270	279	0.02%	0.001%
19	4.334	925	931	934	rBV	187	261	0.02%	0.001%
20	4.629	1010	1023	1074	rBV	162310	471903	27.77%	2.480%
21	4.858	1091	1094	1096	rBV4	520	381	0.02%	0.002%
22	4.883	1100	1102	1105	rVB2	441	262	0.02%	0.001%
23	4.973	1128	1130	1141	rVB5	795	847	0.05%	0.004%
24	5.060	1141	1157	1179	rBV	308158	676639	39.81%	3.555%
25	5.240	1210	1213	1215	rBV3	389	294	0.02%	0.002%
26	5.314	1218	1236	1262	rVB2	121899	279607	16.45%	1.469%
27	5.414	1262	1267	1271	rBV	259	239	0.01%	0.001%
28	5.723	1338	1363	1400	rBV2	631081	1699565	100.00%	8.930%
29	5.973	1436	1441	1443	rBV3	287	264	0.02%	0.001%
30	6.079	1470	1474	1479	rVV3	837	806	0.05%	0.004%
31	6.166	1494	1501	1504	rBV3	491	592	0.03%	0.003%
32	6.247	1512	1526	1544	rBV	432906	818719	48.17%	4.302%
33	6.526	1607	1613	1615	rBV4	1655	1775	0.10%	0.009%
34	6.690	1650	1664	1686	rBV	400444	783308	46.09%	4.116%
35	6.903	1726	1730	1736	rBV2	206	263	0.02%	0.001%
36	6.944	1736	1743	1749	rVB2	488	720	0.04%	0.004%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
 Title : VOC Analysis

37	7.073	1780	1783	1789	rBV2	321	302	0.02%	0.002%
38	7.112	1793	1795	1803	rVB2	288	282	0.02%	0.001%
39	7.218	1810	1828	1847	rBV	32636	66383	3.91%	0.349%
40	7.327	1860	1862	1867	rVB	533	291	0.02%	0.002%
41	7.507	1916	1918	1923	rBV	269	234	0.01%	0.001%
42	7.565	1923	1936	1944	rBV	195760	347657	20.46%	1.827%
43	7.716	1972	1983	1995	rBV	34838	61100	3.60%	0.321%
44	7.796	1996	2008	2027	rVV	262926	496788	29.23%	2.610%
45	7.899	2027	2040	2052	rVV	748932	1302575	76.64%	6.844%
46	7.970	2052	2062	2088	rVB	360409	629589	37.04%	3.308%
47	8.179	2116	2127	2133	rBV	139756	239322	14.08%	1.257%
48	8.356	2179	2182	2185	rBV3	467	280	0.02%	0.001%
49	8.404	2195	2197	2203	rVB2	760	534	0.03%	0.003%
50	8.433	2203	2206	2210	rBV3	328	227	0.01%	0.001%
51	8.552	2229	2243	2258	rBV	474523	796634	46.87%	4.186%
52	8.639	2258	2270	2304	rBV3	447330	965036	56.78%	5.071%
53	8.809	2312	2323	2342	rVB	186262	322691	18.99%	1.696%
54	8.944	2363	2365	2368	rVB2	478	269	0.02%	0.001%
55	8.967	2369	2372	2376	rBV3	401	301	0.02%	0.002%
56	9.105	2412	2415	2418	rVB	438	304	0.02%	0.002%
57	9.147	2422	2428	2432	rBV2	273	318	0.02%	0.002%
58	9.195	2439	2443	2445	rBV3	295	275	0.02%	0.001%
59	9.205	2445	2446	2453	rVB2	384	275	0.02%	0.001%
60	9.324	2482	2483	2488	rVB2	355	249	0.01%	0.001%
61	9.362	2488	2495	2496	rBV2	204	234	0.01%	0.001%
62	9.417	2496	2512	2519	rBV	620587	1114706	65.59%	5.857%
63	9.571	2547	2560	2590	rVB	455210	737156	43.37%	3.873%
64	9.697	2593	2599	2611	rVB3	2729	4565	0.27%	0.024%
65	9.774	2619	2623	2625	rVB3	385	290	0.02%	0.002%
66	9.822	2635	2638	2642	rVB2	390	282	0.02%	0.001%
67	9.928	2669	2671	2676	rVB2	608	383	0.02%	0.002%
68	9.980	2681	2687	2691	rVV2	315	372	0.02%	0.002%
69	10.108	2720	2727	2728	rBV4	764	821	0.05%	0.004%
70	10.121	2729	2731	2739	rVB3	1432	1700	0.10%	0.009%
71	10.362	2802	2806	2810	rVV2	259	274	0.02%	0.001%
72	10.433	2824	2828	2832	rBV2	291	235	0.01%	0.001%
73	10.462	2832	2837	2842	rBV2	413	454	0.03%	0.002%
74	10.591	2872	2877	2882	rVB2	383	367	0.02%	0.002%
75	10.616	2882	2885	2891	rBV3	314	322	0.02%	0.002%
76	10.645	2891	2894	2897	rBV3	306	242	0.01%	0.001%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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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\SFAMULM082422WMA.M
 Title : VOC Analysis

77	10.758	2915	2929	2946	rBV	578166	933721	54.94%	4.906%
78	10.906	2963	2975	2990	rBV	681258	1062089	62.49%	5.580%
79	10.976	2991	2997	3010	rVB2	21475	36322	2.14%	0.191%
80	11.047	3017	3019	3022	rBV3	410	222	0.01%	0.001%
81	11.211	3066	3070	3074	rBV3	697	668	0.04%	0.004%
82	11.336	3099	3109	3126	rVB2	13042	20588	1.21%	0.108%
83	11.610	3189	3194	3198	rBV3	354	350	0.02%	0.002%
84	11.645	3202	3205	3214	rVB3	863	934	0.05%	0.005%
85	11.690	3215	3219	3221	rBV4	371	261	0.02%	0.001%
86	11.812	3245	3257	3279	rBV	503472	792719	46.64%	4.165%
87	11.941	3294	3297	3302	rVB4	527	418	0.02%	0.002%
88	11.992	3311	3313	3316	rVB2	434	226	0.01%	0.001%
89	12.028	3316	3324	3333	rBV7	1776	3222	0.19%	0.017%
90	12.092	3341	3344	3347	rBV3	612	466	0.03%	0.002%
91	12.195	3359	3376	3399	rBV	588414	970949	57.13%	5.102%
92	12.513	3471	3475	3478	rBV	406	292	0.02%	0.002%
93	12.709	3533	3536	3540	rBV3	282	273	0.02%	0.001%
94	12.861	3579	3583	3590	rVB2	501	617	0.04%	0.003%
95	13.188	3680	3685	3688	rBV3	453	474	0.03%	0.002%
96	13.208	3688	3691	3693	rBV2	447	334	0.02%	0.002%
97	13.645	3825	3827	3831	rBV	312	240	0.01%	0.001%
98	13.777	3863	3868	3870	rBV2	317	321	0.02%	0.002%
99	13.960	3922	3925	3929	rBV2	531	401	0.02%	0.002%
100	15.430	4380	4382	4385	rVB3	632	355	0.02%	0.002%

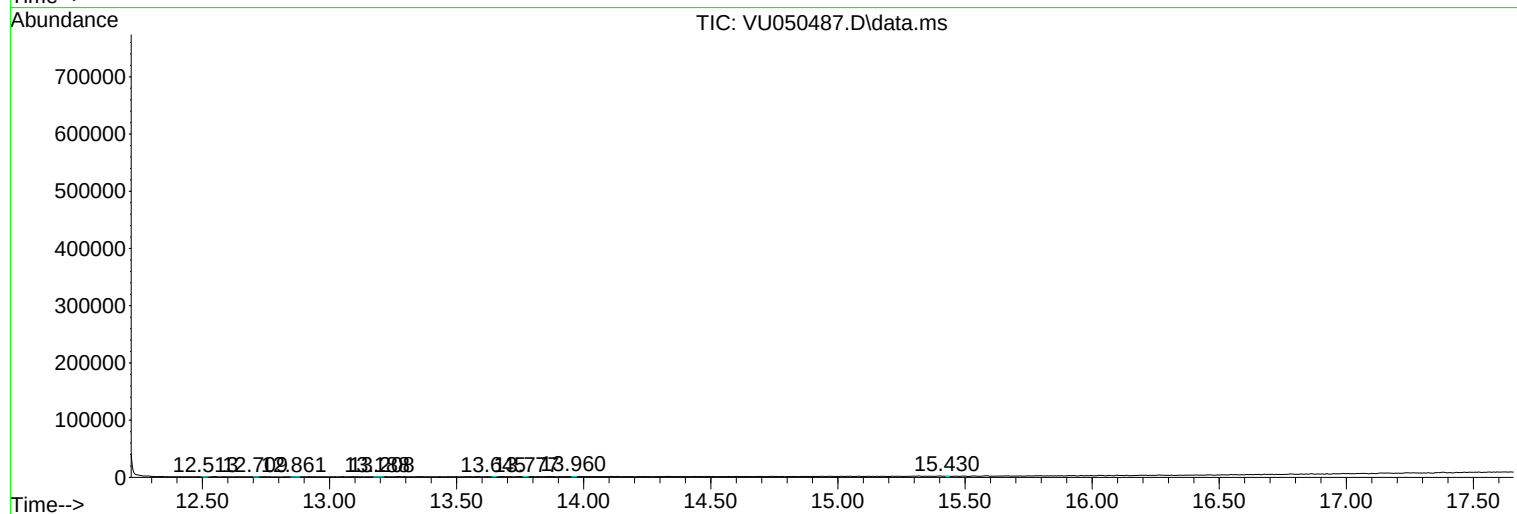
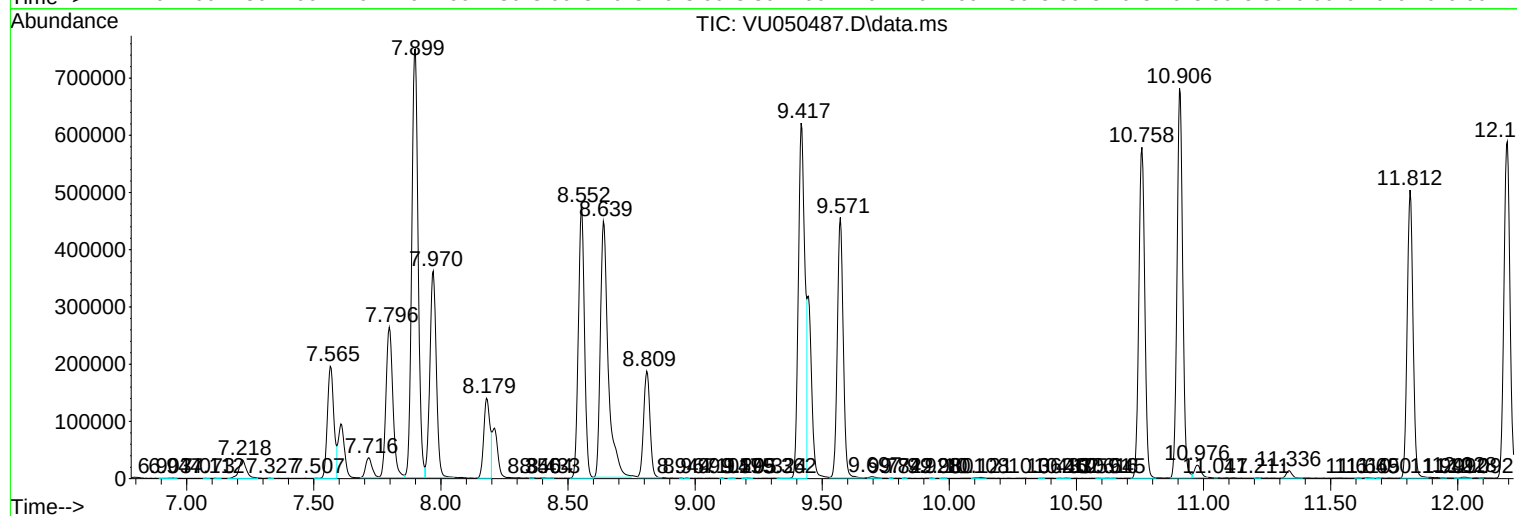
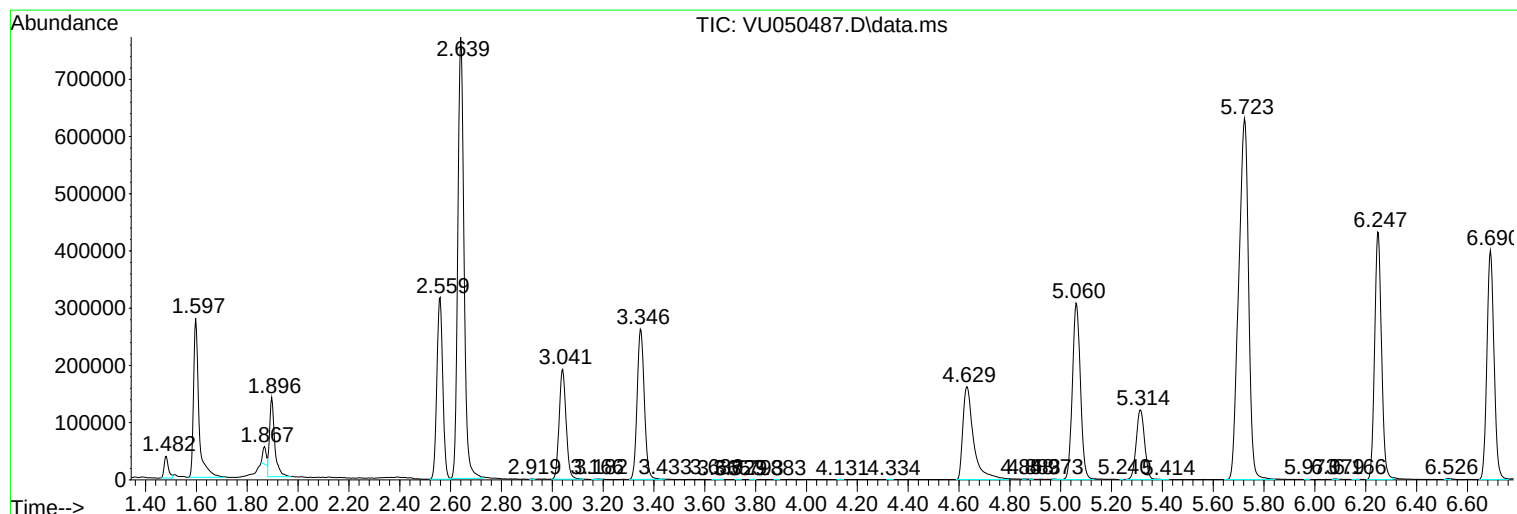
Sum of corrected areas: 19032155

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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DBUZ1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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ClientSampleId :
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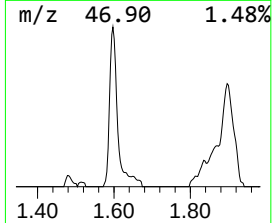
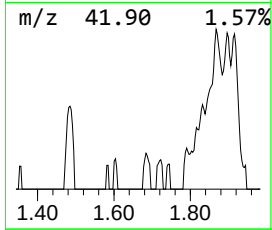
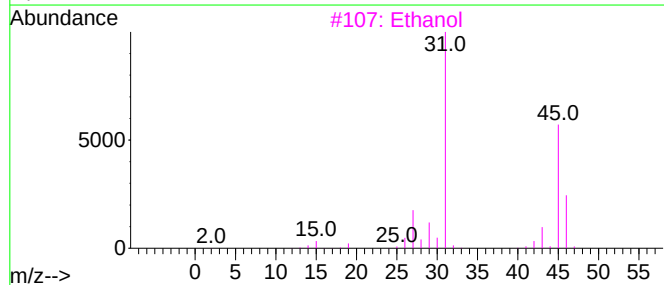
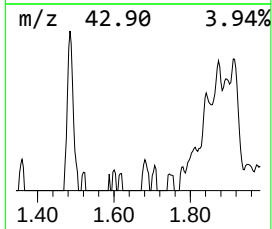
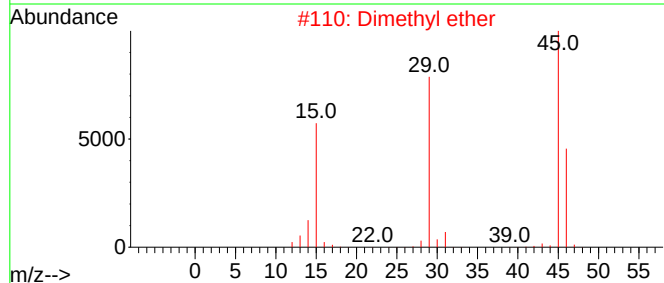
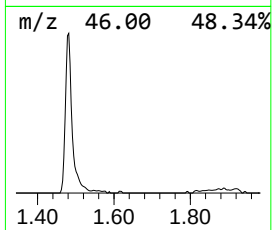
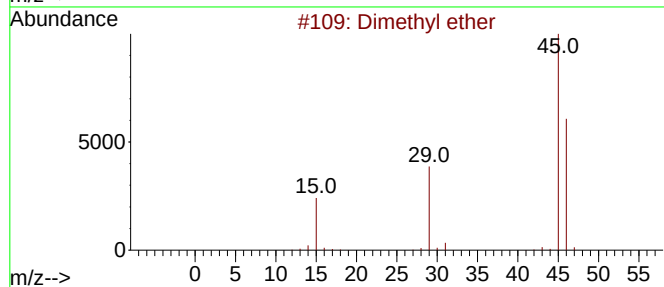
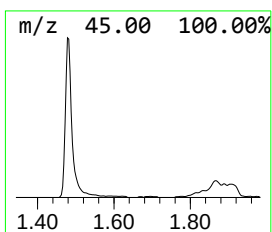
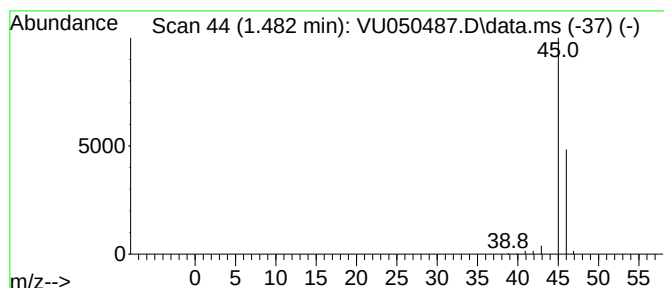
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.482	2.70 ug/L	44278	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	9
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Ethanol	46	C2H6O	000064-17-5	9
4			Ethanol	46	C2H6O	000064-17-5	7
5			Dimethyl ether	46	C2H6O	000115-10-6	7



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Instrument :
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ClientSampleId :
DBUZ1

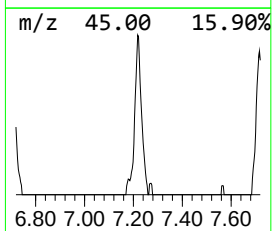
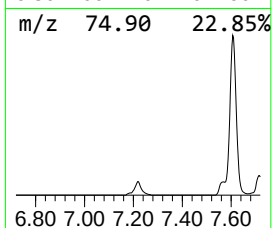
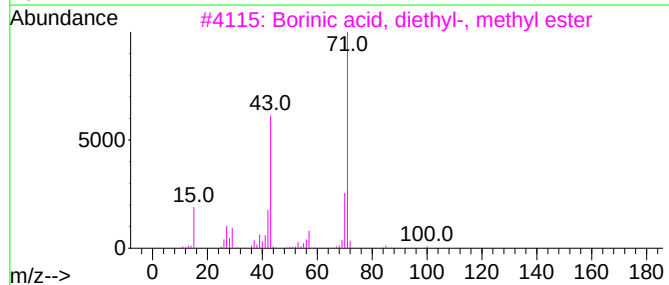
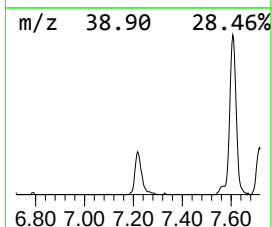
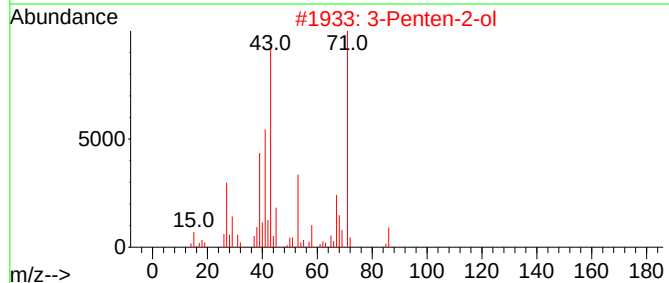
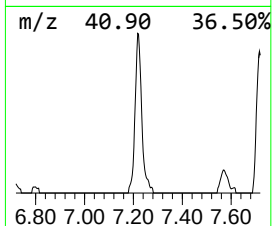
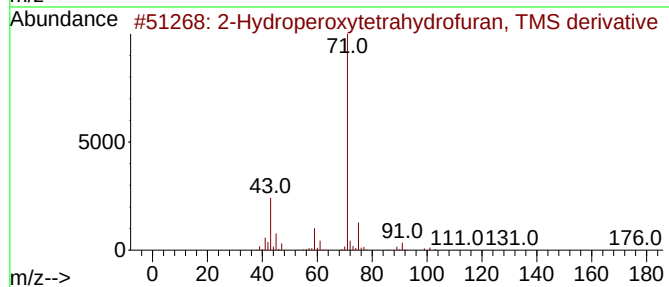
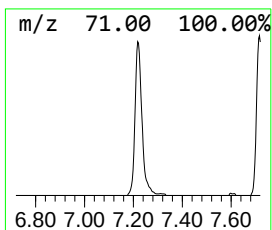
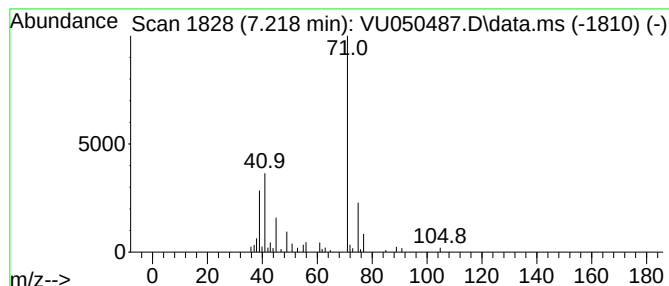
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.218	4.05 ug/L	66383	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroperoxytetrahydrofuran, TM...	176	C7H16O3Si	1000368-50-8	38		
2	3-Penten-2-ol	86	C5H10O	001569-50-2	10		
3	Borinic acid, diethyl-, methyl e...	100	C5H13BO	007397-46-8	9		
4	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	9		
5	Butanoic acid, 2-propenyl ester	128	C7H12O2	002051-78-7	9		



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Instrument :
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ClientSampleId :
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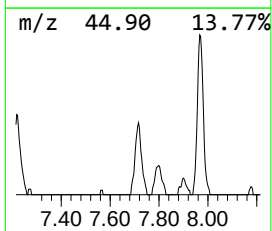
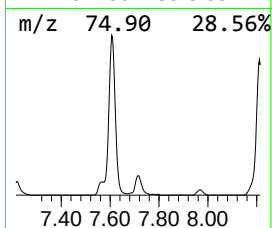
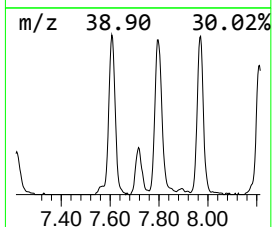
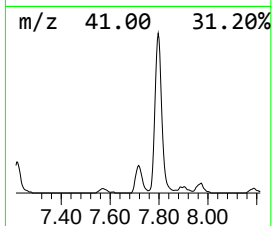
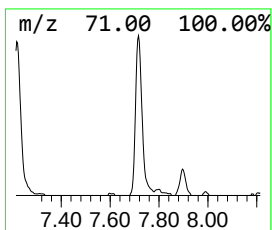
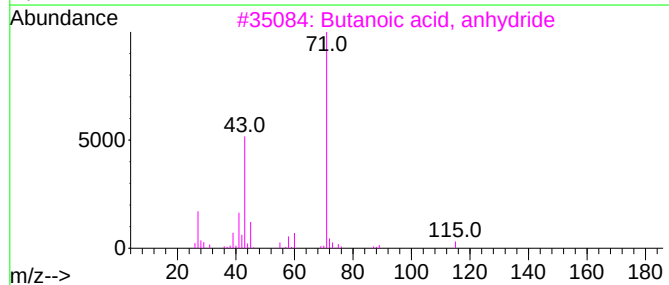
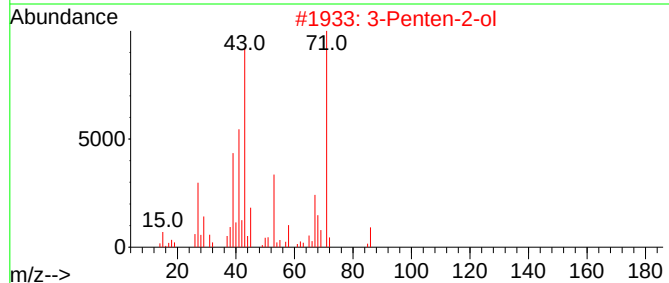
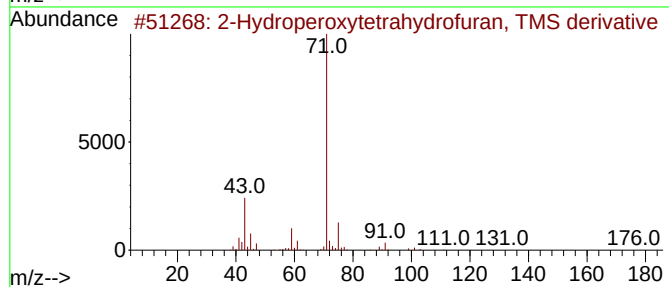
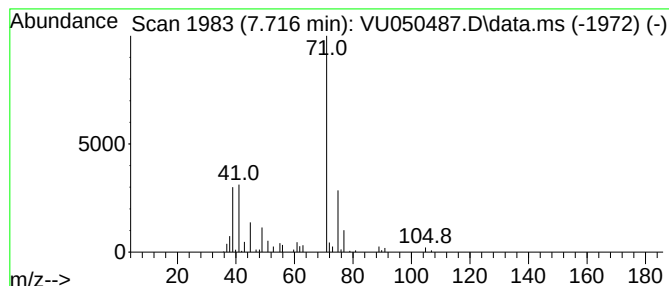
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 unknown-03 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.716	3.73 ug/L	61100	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroperoxytetrahydrofuran, TM...	176	C7H16O3Si	1000368-50-8	45		
2	3-Penten-2-ol	86	C5H10O	001569-50-2	40		
3	Butanoic acid, anhydride	158	C8H14O3	000106-31-0	33		
4	Sulfurous acid, 2-pentyl pentyl ...	222	C10H22O3S	1000309-15-4	33		
5	Isobutyric acid, 2,2,2-trichloro...	218	C6H9Cl3O2	1000354-63-4	28		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
Data File : VU050487.D
Acq On : 29 Aug 2022 16:12
Operator : SY/MD
Sample : N4399-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBUZ1

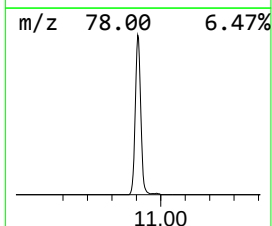
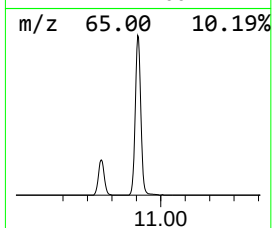
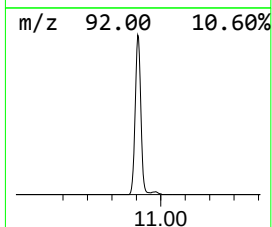
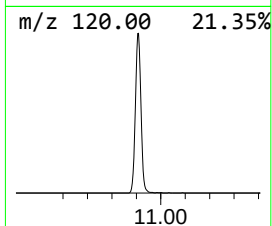
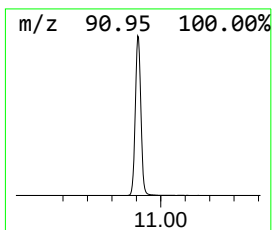
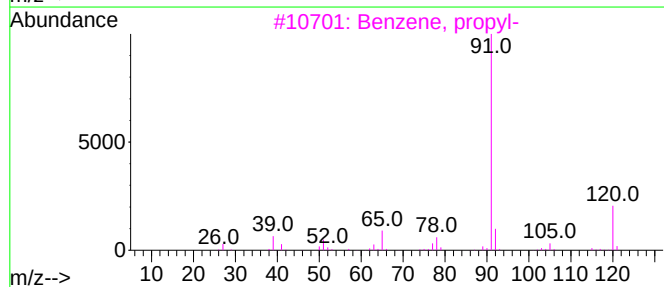
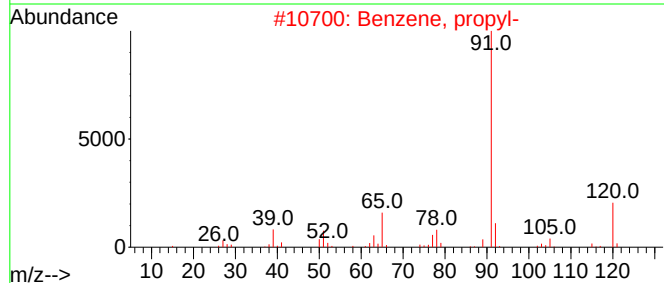
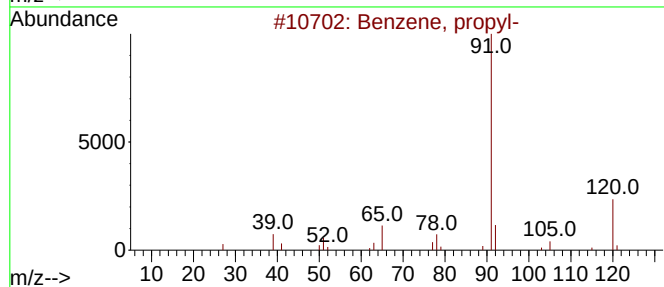
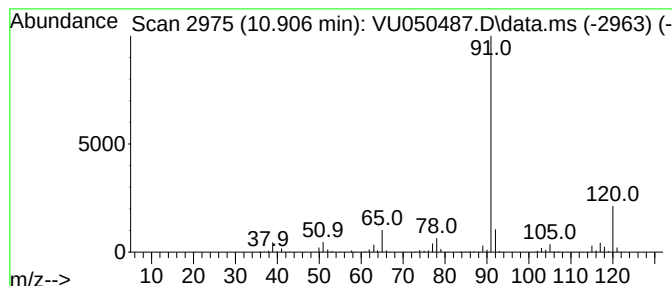
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Quant Title : VOC Analysis

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

Peak Number 4 Benzene, propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.906	66.99 ug/L	1062090	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, propyl-	120	C9H12	000103-65-1	93
2			Benzene, propyl-	120	C9H12	000103-65-1	87
3			Benzene, propyl-	120	C9H12	000103-65-1	87
4			Benzene, propyl-	120	C9H12	000103-65-1	83
5			N-Butylbenzylamine	163	C11H17N	002403-22-7	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
Data File : VU050487.D
Acq On : 29 Aug 2022 16:12
Operator : SY/MD
Sample : N4399-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBUZ1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.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	1.482	2.7	ug/L	44278	1	6.247	818719	50.0
unknown-02	7.218	4.0	ug/L	66383	1	6.247	818719	50.0
unknown-03	7.716	3.7	ug/L	61100	1	6.247	818719	50.0
Benzene, propyl-	10.906	67.0	ug/L	1062090	3	11.812	792719	50.0