

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
 Data File : VU054806.D
 Acq On : 18 Jul 2023 14:44
 Operator : MD/SY
 Sample : 03656-11
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH2Y4

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\SFAMULM071723WMA.M
 Title : VOC Analysis

Signal : TIC: VU054806.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.595	90	95	111	rVB	97579	117425	15.50%	1.579%
2	2.554	383	393	405	rBV	140749	225268	29.73%	3.029%
3	3.184	575	589	609	rBV3	69582	176425	23.28%	2.372%
4	3.512	688	691	695	rVB3	688	399	0.05%	0.005%
5	3.579	710	712	715	rBV2	667	465	0.06%	0.006%
6	3.837	789	792	794	rBV2	472	256	0.03%	0.003%
7	3.869	800	802	804	rBV	475	282	0.04%	0.004%
8	3.910	813	815	817	rBV	322	211	0.03%	0.003%
9	3.933	820	822	826	rBV3	522	471	0.06%	0.006%
10	4.004	842	844	845	rBV	415	150	0.02%	0.002%
11	4.046	855	857	859	rVB	347	158	0.02%	0.002%
12	4.087	868	870	873	rBV2	584	427	0.06%	0.006%
13	4.209	904	908	912	rBV5	900	1003	0.13%	0.013%
14	4.303	936	937	941	rVB2	553	163	0.02%	0.002%
15	4.370	955	958	960	rBV2	394	261	0.03%	0.004%
16	4.406	966	969	972	rBV3	446	364	0.05%	0.005%
17	4.428	972	976	979	rBV3	712	475	0.06%	0.006%
18	4.444	979	981	987	rBV3	656	579	0.08%	0.008%
19	4.618	1024	1035	1055	rBV	79035	192716	25.43%	2.591%
20	5.055	1155	1171	1192	rBV	144235	324272	42.80%	4.360%
21	5.242	1225	1229	1232	rBV4	662	627	0.08%	0.008%
22	5.274	1238	1239	1242	rBV	457	224	0.03%	0.003%
23	5.316	1250	1252	1253	rBV	451	153	0.02%	0.002%
24	5.470	1298	1300	1302	rBV2	653	412	0.05%	0.006%
25	5.496	1306	1308	1311	rVV3	606	359	0.05%	0.005%
26	5.515	1311	1314	1317	rVV	433	258	0.03%	0.003%
27	5.560	1323	1328	1333	rBV4	862	968	0.13%	0.013%
28	5.640	1349	1353	1356	rBV3	482	279	0.04%	0.004%
29	5.717	1357	1377	1396	rBV2	281126	757703	100.00%	10.188%
30	5.939	1444	1446	1448	rBV2	477	250	0.03%	0.003%
31	6.087	1490	1492	1495	rBV2	601	406	0.05%	0.005%
32	6.152	1509	1512	1513	rBV3	534	300	0.04%	0.004%
33	6.245	1528	1541	1561	rBV	239458	468134	61.78%	6.295%
34	6.451	1601	1605	1608	rBV4	823	723	0.10%	0.010%
35	6.518	1619	1626	1627	rBV3	1517	1420	0.19%	0.019%
36	6.685	1665	1678	1699	rBV2	176290	349882	46.18%	4.705%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
 Title : VOC Analysis

37	6.910	1746	1748	1750	rBV3	571	207	0.03%	0.003%
38	7.023	1780	1783	1784	rBV2	493	260	0.03%	0.003%
39	7.161	1813	1826	1847	rBV	98099	197892	26.12%	2.661%
40	7.328	1875	1878	1880	rVB2	779	364	0.05%	0.005%
41	7.344	1880	1883	1885	rBV3	779	478	0.06%	0.006%
42	7.377	1890	1893	1898	rBV5	941	747	0.10%	0.010%
43	7.463	1919	1920	1924	rBV	288	245	0.03%	0.003%
44	7.496	1928	1930	1931	rBV	597	220	0.03%	0.003%
45	7.560	1937	1950	1970	rBV	104194	189756	25.04%	2.552%
46	7.775	2015	2017	2021	rBV3	695	378	0.05%	0.005%
47	7.840	2035	2037	2038	rBV	544	217	0.03%	0.003%
48	7.894	2041	2054	2072	rBV	362906	623627	82.30%	8.386%
49	8.081	2108	2112	2114	rBV4	629	484	0.06%	0.007%
50	8.106	2118	2120	2123	rBV3	356	186	0.02%	0.003%
51	8.177	2130	2142	2165	rBV	72730	130493	17.22%	1.755%
52	8.428	2217	2220	2222	rBV3	487	292	0.04%	0.004%
53	8.631	2271	2283	2319	rBV2	230519	454669	60.01%	6.114%
54	8.840	2344	2348	2350	rBV3	712	653	0.09%	0.009%
55	8.897	2362	2366	2370	rBV4	618	584	0.08%	0.008%
56	8.946	2380	2381	2382	rBV	465	164	0.02%	0.002%
57	8.987	2387	2394	2398	rVB3	966	1099	0.15%	0.015%
58	9.007	2398	2400	2402	rBV3	535	254	0.03%	0.003%
59	9.135	2436	2440	2441	rBV2	678	478	0.06%	0.006%
60	9.254	2475	2477	2478	rBV	333	164	0.02%	0.002%
61	9.306	2491	2493	2495	rVB	568	212	0.03%	0.003%
62	9.322	2495	2498	2500	rBV2	548	331	0.04%	0.004%
63	9.354	2505	2508	2509	rBV	354	192	0.03%	0.003%
64	9.412	2514	2526	2546	rBV	357369	596043	78.66%	8.015%
65	9.534	2562	2564	2566	rBV2	427	187	0.02%	0.003%
66	9.550	2566	2569	2573	rBV3	1085	1051	0.14%	0.014%
67	9.791	2641	2644	2647	rVB2	646	434	0.06%	0.006%
68	9.878	2669	2671	2672	rBV	709	341	0.05%	0.005%
69	9.971	2696	2700	2701	rBV2	383	211	0.03%	0.003%
70	10.020	2712	2715	2716	rBV3	467	281	0.04%	0.004%
71	10.087	2726	2736	2737	rBV3	1051	936	0.12%	0.013%
72	10.103	2737	2741	2744	rBV5	1463	1643	0.22%	0.022%
73	10.193	2761	2769	2772	rBV7	733	1038	0.14%	0.014%
74	10.235	2780	2782	2784	rBV2	477	242	0.03%	0.003%
75	10.274	2792	2794	2798	rBV3	544	333	0.04%	0.004%
76	10.319	2800	2808	2817	rVB5	8336	12689	1.67%	0.171%

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77	10.386	2827	2829	2832	rBV	642	415	0.05%	0.006%
78	10.486	2851	2860	2872	rBV3	30392	47580	6.28%	0.640%
79	10.753	2930	2943	2958	rBV	307955	491799	64.91%	6.613%
80	11.084	3043	3046	3049	rBV2	1050	711	0.09%	0.010%
81	11.158	3061	3069	3080	rVB5	8797	14350	1.89%	0.193%
82	11.286	3101	3109	3110	rBV6	3458	3058	0.40%	0.041%
83	11.444	3153	3158	3163	rBV4	3351	4596	0.61%	0.062%
84	11.505	3176	3177	3183	rVB3	829	513	0.07%	0.007%
85	11.547	3188	3190	3194	rVB4	1226	649	0.09%	0.009%
86	11.608	3201	3209	3225	rVB5	21246	39036	5.15%	0.525%
87	11.714	3231	3242	3244	rBV4	9799	12334	1.63%	0.166%
88	11.807	3259	3271	3289	rVB	398754	658890	86.96%	8.860%
89	11.991	3326	3328	3330	rBV3	743	377	0.05%	0.005%
90	12.039	3341	3343	3345	rBV2	842	447	0.06%	0.006%
91	12.190	3378	3390	3413	rVV	392574	632102	83.42%	8.500%
92	12.286	3417	3420	3423	rVB2	820	558	0.07%	0.008%
93	12.454	3463	3472	3481	rBV5	18086	29193	3.85%	0.393%
94	12.524	3485	3494	3509	rVB	176880	275672	36.38%	3.707%
95	12.839	3581	3592	3604	rBV4	44457	71167	9.39%	0.957%
96	13.608	3828	3831	3833	rBV2	1138	603	0.08%	0.008%
97	14.032	3954	3963	3973	rBV6	22767	38236	5.05%	0.514%
98	14.203	4014	4016	4020	rBV3	657	526	0.07%	0.007%
99	14.476	4094	4101	4120	rVB	166160	259411	34.24%	3.488%
100	15.691	4472	4479	4489	rBV9	6372	10751	1.42%	0.145%

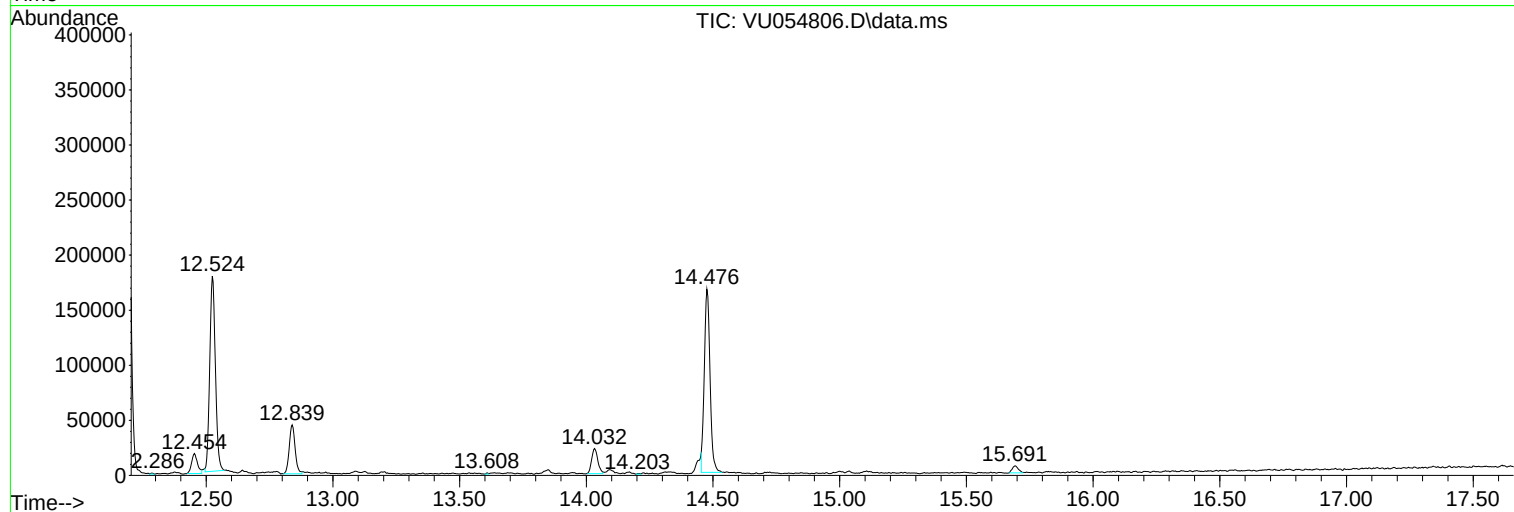
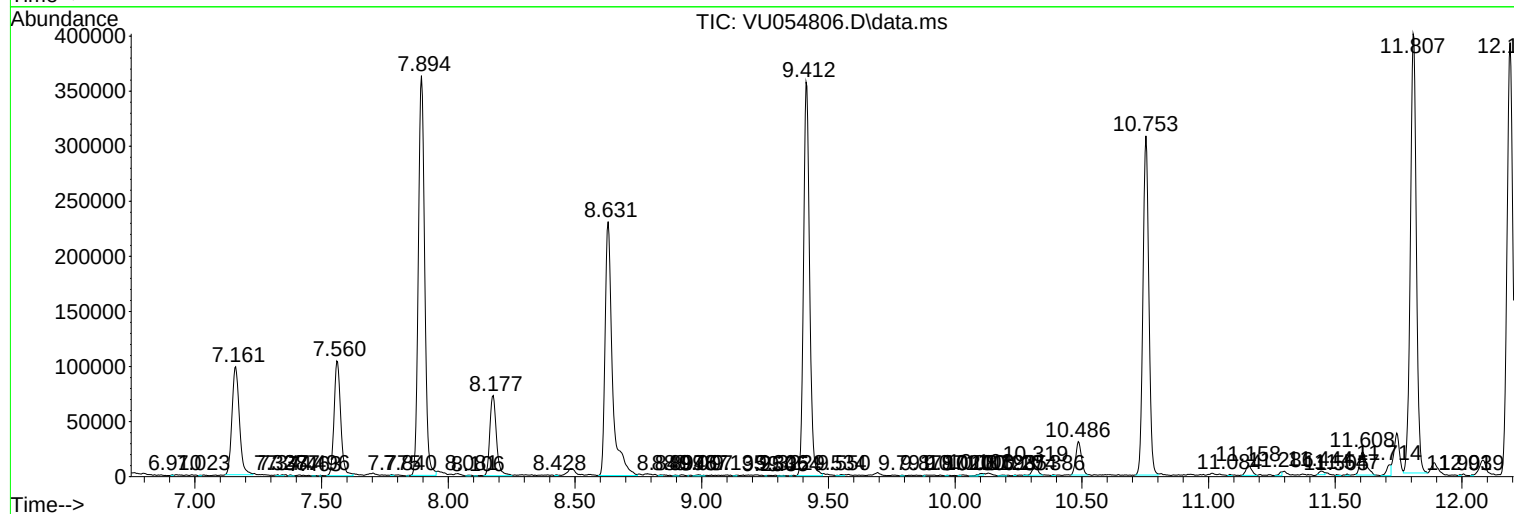
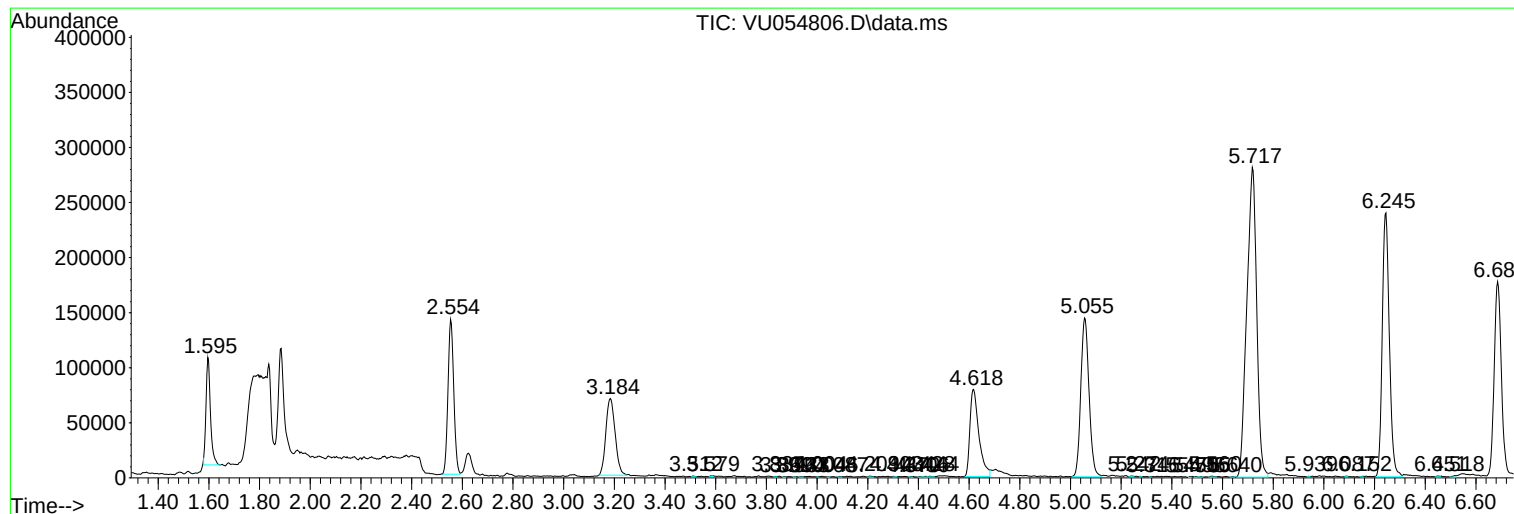
Sum of corrected areas: 7436917

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.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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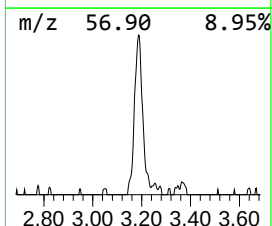
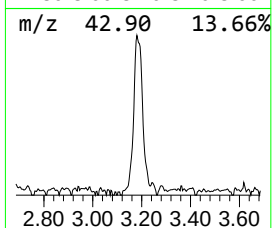
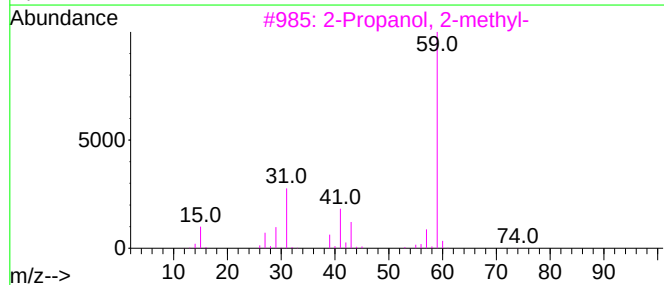
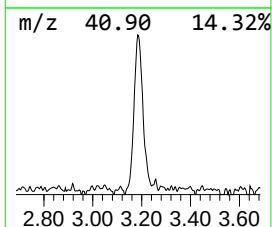
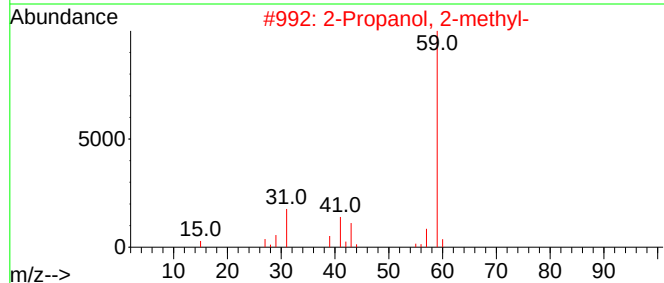
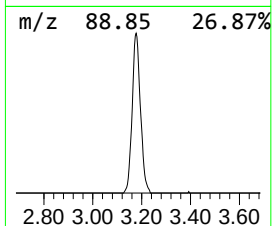
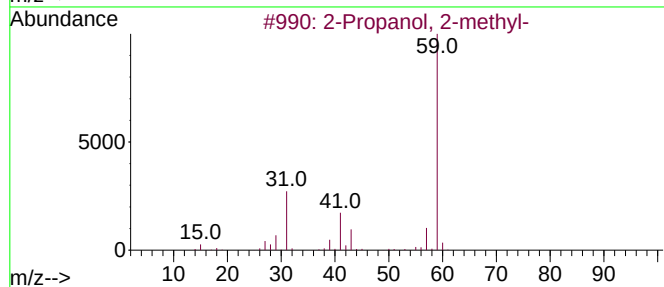
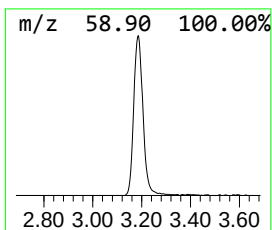
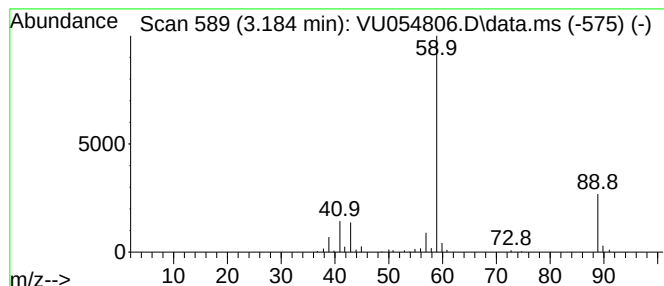
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 2-Propanol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.184	18.84 ug/L	176425	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	53
2	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	53
3	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	42
4	Butanoic acid, 2-hydroxy-, methy...			118	C5H10O3	029674-47-3	38
5	Propane, 2-methoxy-			74	C4H10O	000598-53-8	36



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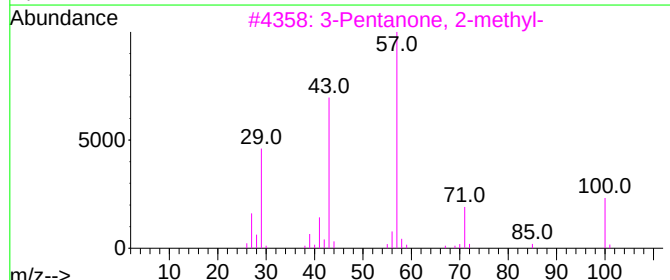
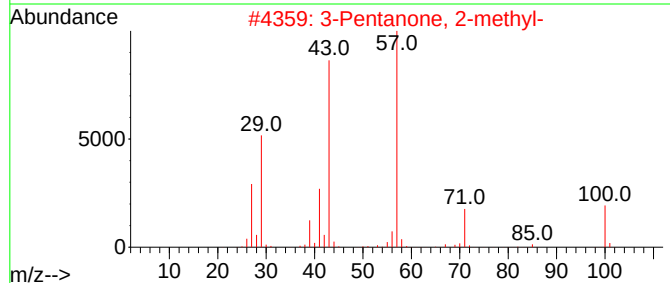
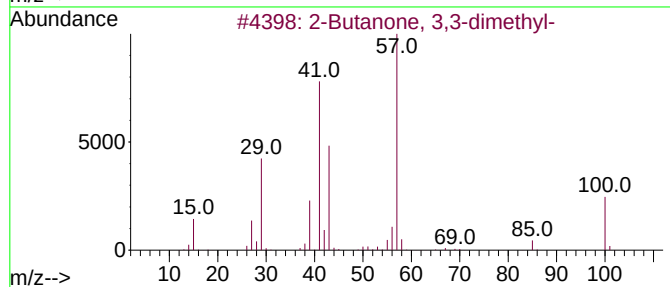
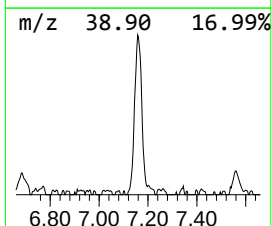
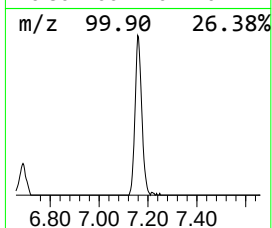
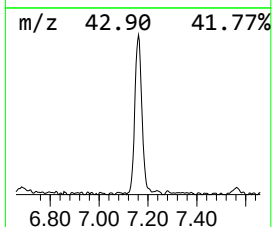
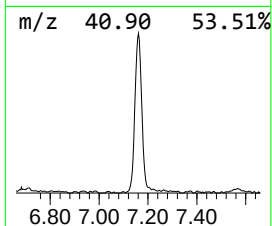
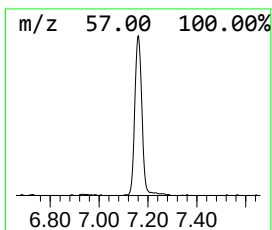
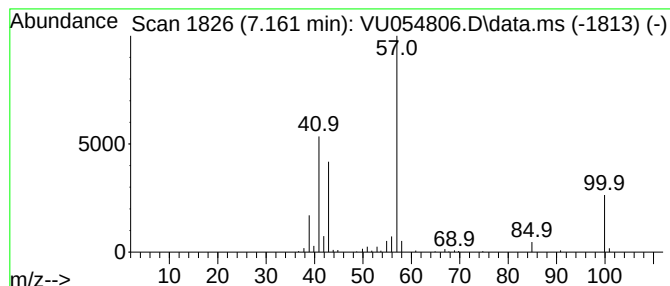
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 2-Butanone, 3,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.161	21.14 ug/L	197892	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	78
2	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	59
3	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	59
4	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	50
5	trans-1-Ethoxy-1-butene			100	C6H12O	1000139-43-9	50



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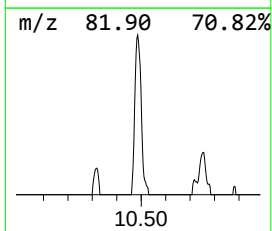
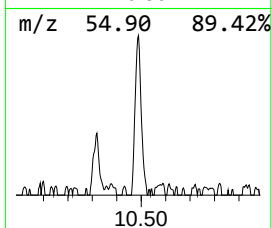
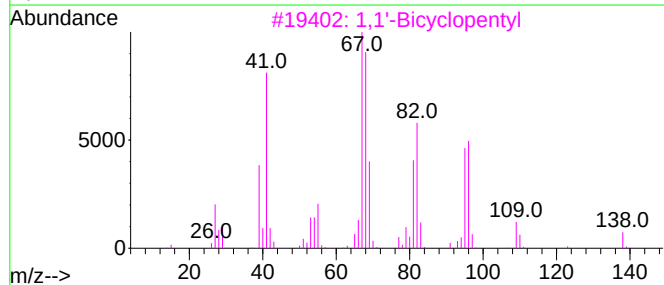
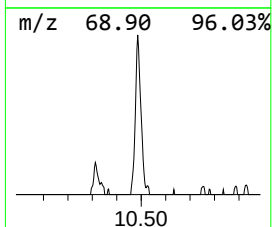
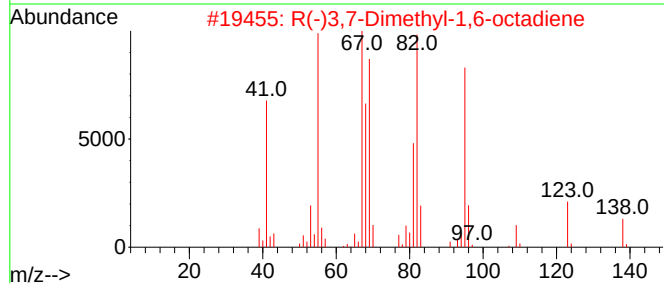
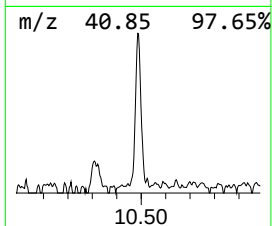
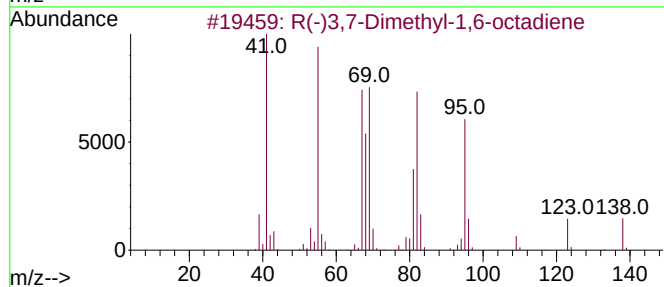
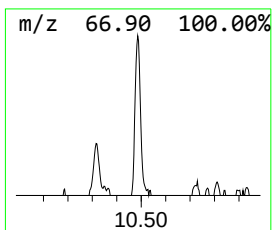
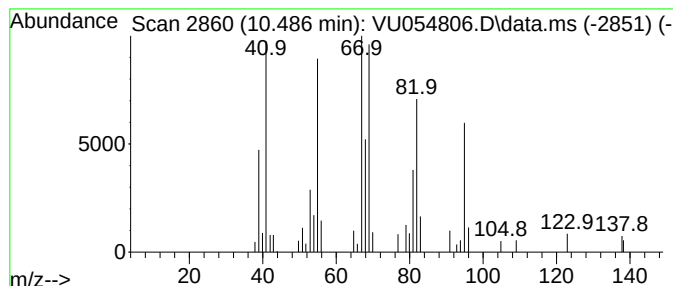
Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 R(-)3,7-Dimethyl-1,6-octadiene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.486	3.99 ug/L	47580	Chlorobenzene-d5	9.412	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R(-)3,7-Dimethyl-1,6-octadiene	138	C10H18	010281-56-8	86
2	R(-)3,7-Dimethyl-1,6-octadiene	138	C10H18	010281-56-8	64
3	1,1'-Bicyclopentyl	138	C10H18	001636-39-1	46
4	trans-1,4-Hexadiene	82	C6H10	007319-00-8	38
5	1,3-Butadiene, 2,3-dimethyl-	82	C6H10	000513-81-5	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054806.D
Acq On : 18 Jul 2023 14:44
Operator : MD/SY
Sample : 03656-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2Y4

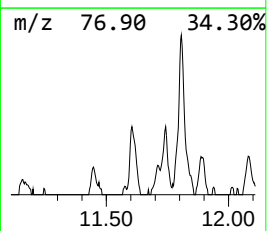
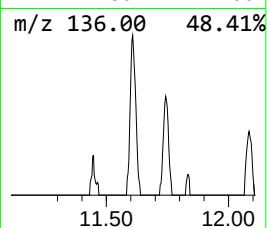
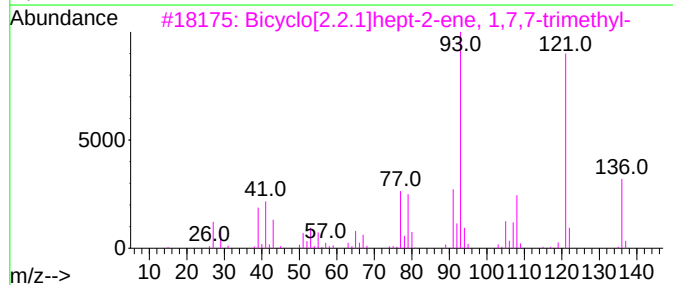
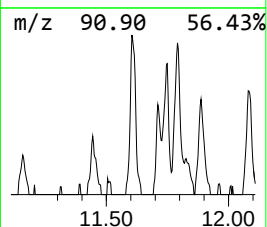
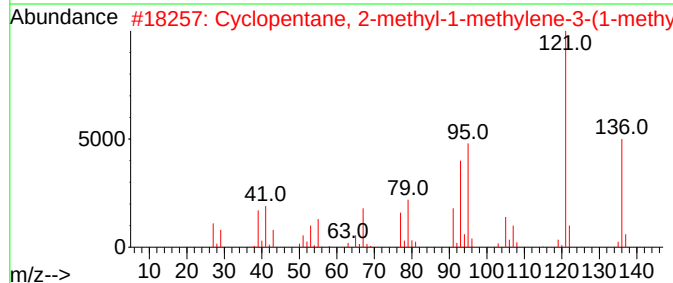
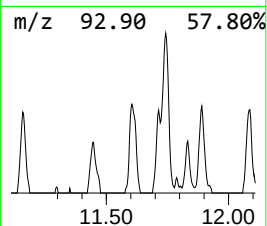
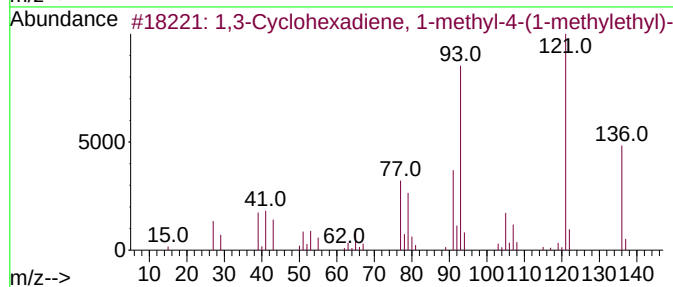
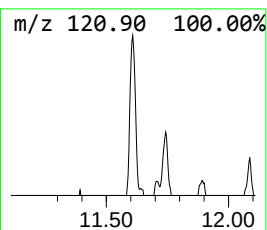
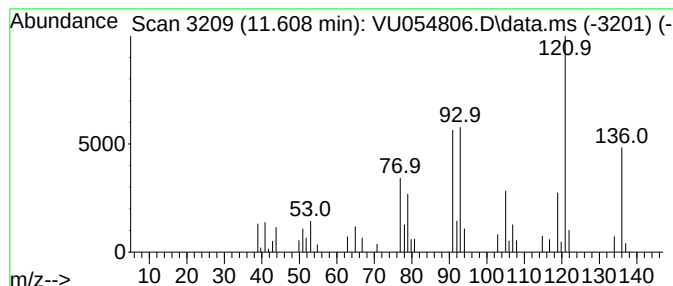
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Quant Title : VOC Analysis

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

Peak Number 5 1,3-Cyclohexadiene, 1-methyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.608	2.96 ug/L	39036	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	93
2			Cyclopentane, 2-methyl-1-methyle...	136	C10H16	056710-83-9	87
3			Bicyclo[2.2.1]hept-2-ene, 1,7,7-...	136	C10H16	000464-17-5	86
4			1,5,5-Trimethyl-6-methylene-cycl...	136	C10H16	000514-95-4	76
5			Cyclohexene, 3-methyl-6-(1-methy...	136	C10H16	000586-63-0	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054806.D
Acq On : 18 Jul 2023 14:44
Operator : MD/SY
Sample : 03656-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2Y4

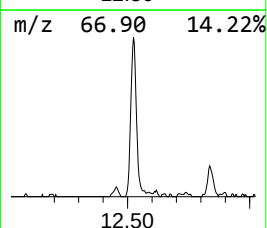
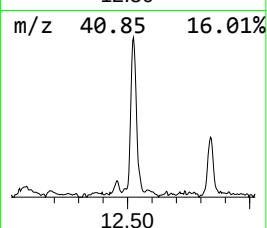
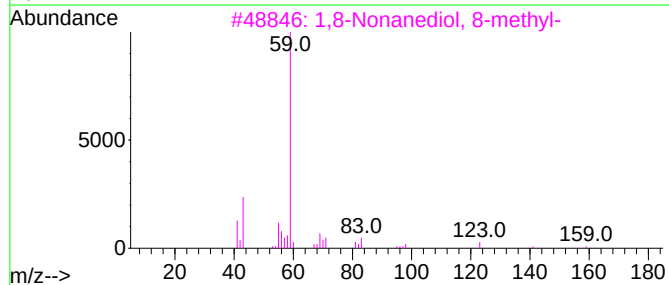
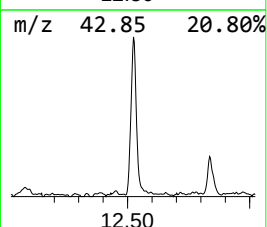
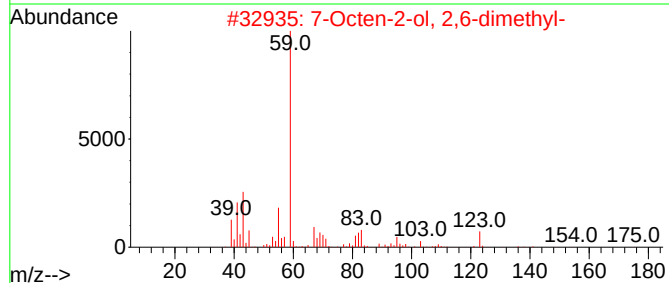
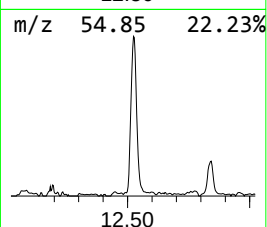
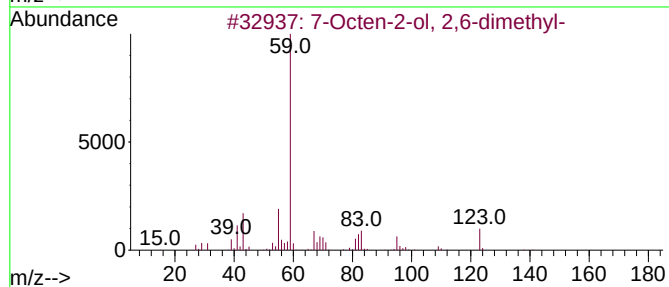
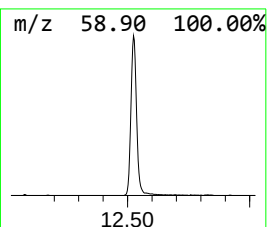
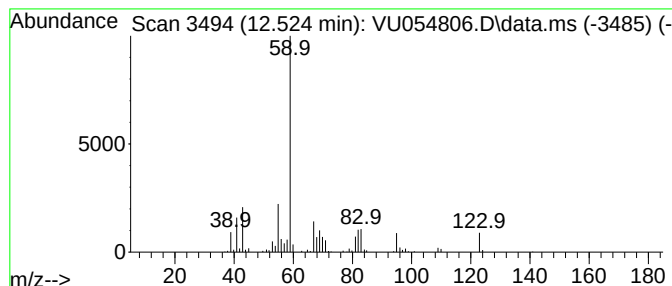
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Quant Title : VOC Analysis

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

Peak Number 6 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.524	20.92 ug/L	275672	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	90
2			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	72
3			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	59
4			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	58
5			3-Hexene, 1-(1-methoxyethoxy)-, ...	158	C9H18O2	054340-96-4	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054806.D
Acq On : 18 Jul 2023 14:44
Operator : MD/SY
Sample : 03656-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2Y4

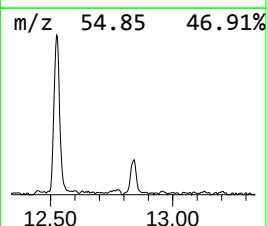
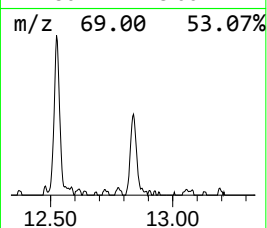
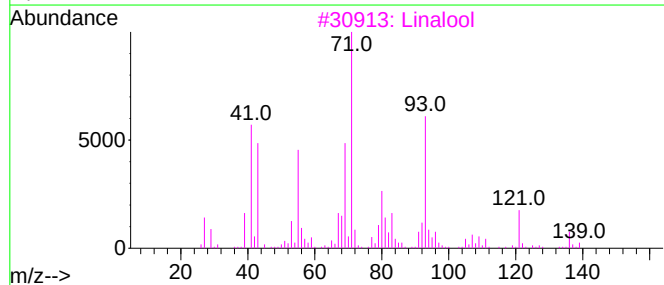
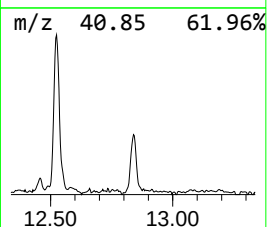
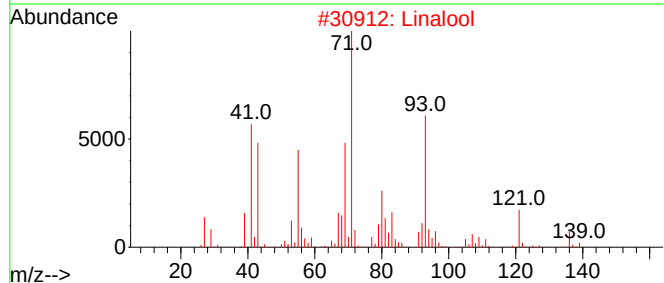
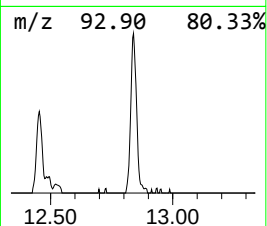
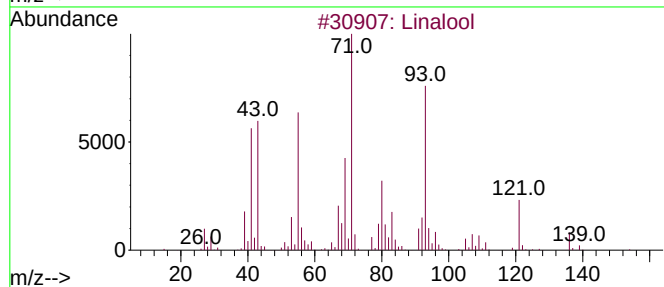
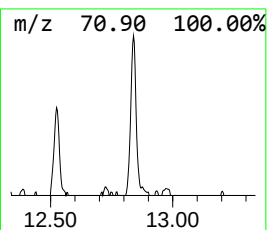
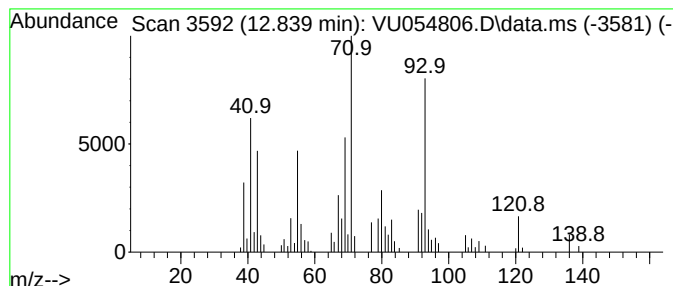
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Quant Title : VOC Analysis

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

Peak Number 7 Linalool Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.839	5.40 ug/L	71167	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Linalool	154	C10H18O	000078-70-6	90
2			Linalool	154	C10H18O	000078-70-6	68
3			Linalool	154	C10H18O	000078-70-6	58
4			(+)-3-Carene	136	C10H16	000498-15-7	50
5			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054806.D
Acq On : 18 Jul 2023 14:44
Operator : MD/SY
Sample : 03656-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2Y4

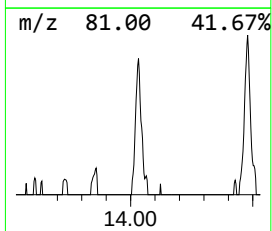
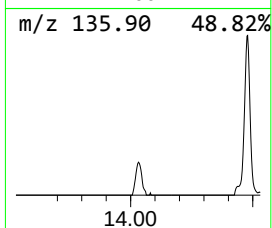
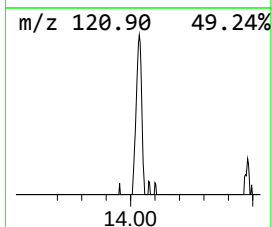
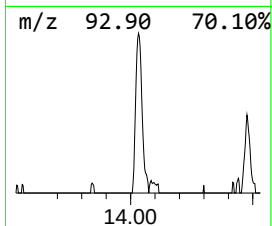
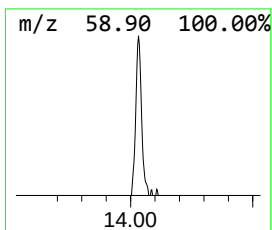
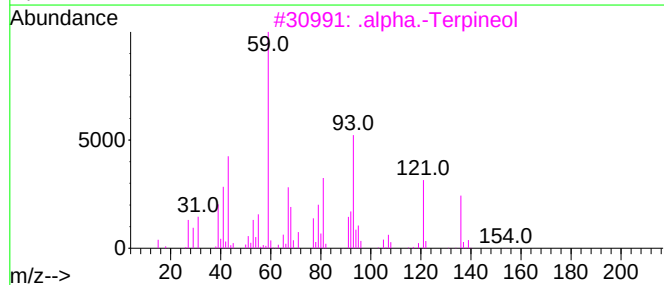
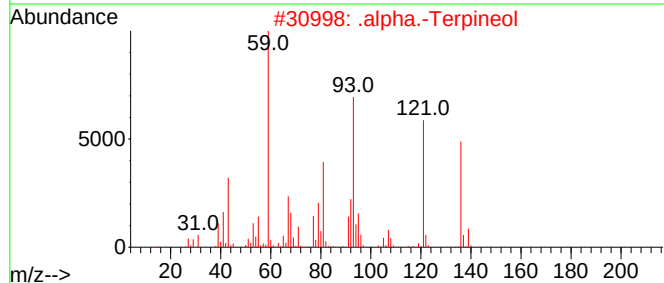
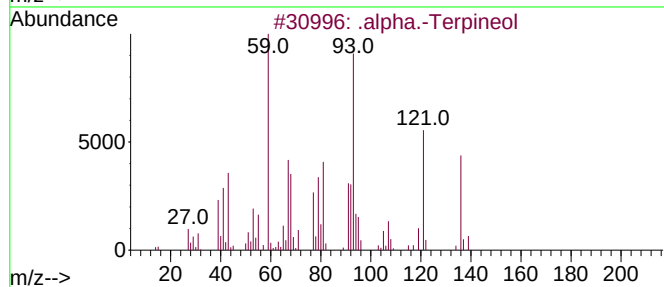
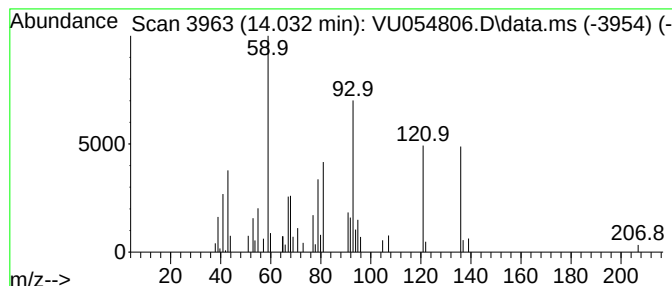
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Quant Title : VOC Analysis

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

Peak Number 8 .alpha.-Terpineol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.032	2.90 ug/L	38236	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.		.alpha.-Terpineol	154	C10H18O	000098-55-5	90
2	.		.alpha.-Terpineol	154	C10H18O	000098-55-5	80
3	.		.alpha.-Terpineol	154	C10H18O	000098-55-5	80
4	.		.alpha.-Terpineol	154	C10H18O	000098-55-5	74
5	.		.alpha.-Terpineol	154	C10H18O	000098-55-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054806.D
Acq On : 18 Jul 2023 14:44
Operator : MD/SY
Sample : 03656-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2Y4

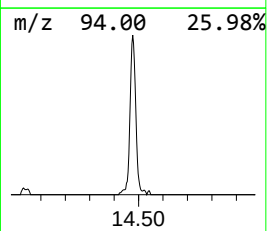
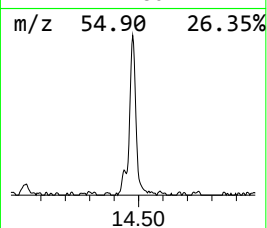
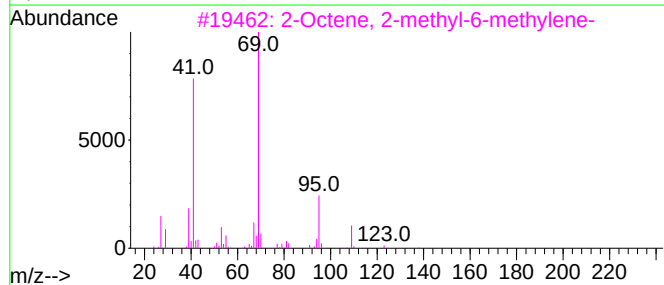
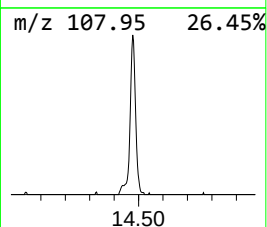
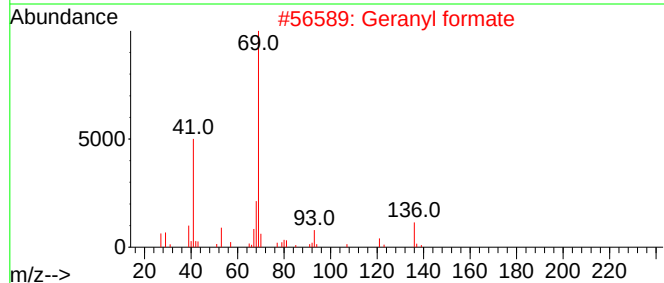
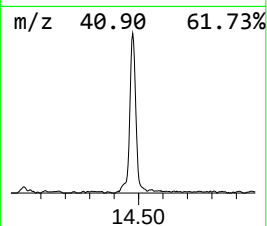
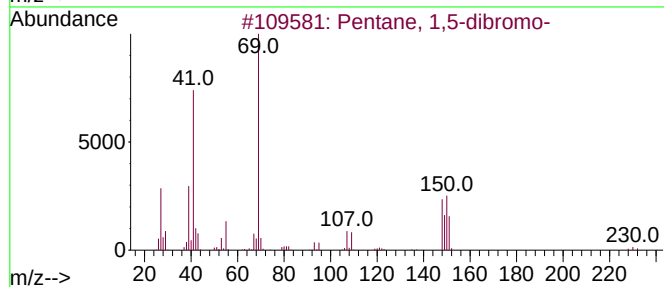
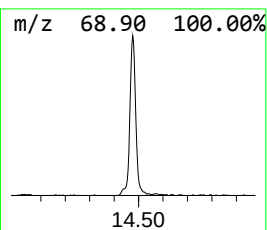
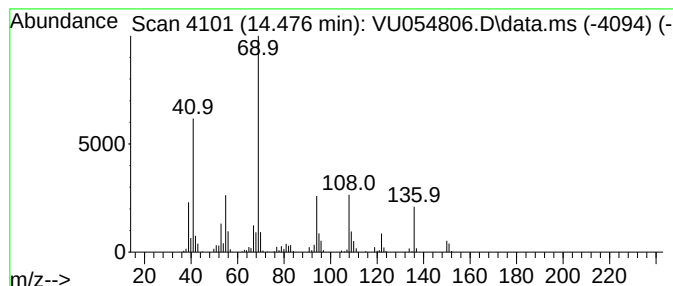
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Quant Title : VOC Analysis

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

Peak Number 9 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.476	19.69 ug/L	259411	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 1,5-dibromo-	228	C5H10Br2	000111-24-0	37
2			Geranyl formate	182	C11H18O2	000105-86-2	37
3			2-Octene, 2-methyl-6-methylene-	138	C10H18	010054-09-8	37
4			1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	35
5			4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071823\
Data File : VU054806.D
Acq On : 18 Jul 2023 14:44
Operator : MD/SY
Sample : 03656-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH2Y4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071723WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Propanol, 2-m...	3.184	18.8	ug/L	176425	1	6.245	468134	50.0
2-Butanone, 3,3...	7.161	21.1	ug/L	197892	1	6.245	468134	50.0
R(-)3,7-Dimethy...	10.486	4.0	ug/L	47580	2	9.412	596043	50.0
1,3-Cyclohexadi...	11.608	3.0	ug/L	39036	3	11.807	658890	50.0
7-Octen-2-ol, 2...	12.524	20.9	ug/L	275672	3	11.807	658890	50.0
Linalool	12.839	5.4	ug/L	71167	3	11.807	658890	50.0
.alpha.-Terpineol	14.032	2.9	ug/L	38236	3	11.807	658890	50.0
unknown-01	14.476	19.7	ug/L	259411	3	11.807	658890	50.0