

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041423\
 Data File : VX035063.D
 Acq On : 13 Apr 2023 14:50
 Operator : JC/MD
 Sample : 02257-03 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 ELI-WATER-0407

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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_X\Method\82X032923W.M
 Title : SW846 8260

Signal : TIC: VX035063.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.392	206	214	220	rBV	8160	14651	1.06%	0.141%
2	4.580	564	573	585	rBV4	7661	25334	1.83%	0.245%
3	5.385	694	705	720	rBV2	150268	443069	31.95%	4.278%
4	5.549	720	732	753	rVB	272870	784890	56.60%	7.579%
5	5.958	789	799	819	rBV	175807	471689	34.02%	4.555%
6	6.763	920	931	946	rBV	430090	1026320	74.01%	9.910%
7	8.646	1234	1240	1257	rBV	861387	1386648	100.00%	13.390%
8	10.055	1465	1471	1486	rBV	881849	1181298	85.19%	11.407%
9	11.079	1634	1639	1651	rBV	687791	906299	65.36%	8.751%
10	12.024	1788	1794	1801	rBV	871657	1110943	80.12%	10.728%
11	12.103	1801	1807	1817	rVB	1066658	1377229	99.32%	13.299%
12	12.219	1821	1826	1834	rVB4	7721	15182	1.09%	0.147%
13	12.768	1911	1916	1917	rBV	27763	33941	2.45%	0.328%
14	12.792	1917	1920	1926	rVB2	38722	60501	4.36%	0.584%
15	12.859	1926	1931	1937	rBV2	120934	206616	14.90%	1.995%
16	12.975	1945	1950	1952	rBV	55702	81653	5.89%	0.788%
17	13.073	1962	1966	1968	rBV2	52350	75181	5.42%	0.726%
18	13.103	1968	1971	1973	rBV2	100501	133755	9.65%	1.292%
19	13.219	1986	1990	1996	rBV	48499	71747	5.17%	0.693%
20	13.426	2020	2024	2033	rBV3	17252	31886	2.30%	0.308%
21	13.511	2033	2038	2049	rVB	138358	219647	15.84%	2.121%
22	13.707	2065	2070	2075	rBV	185735	235953	17.02%	2.278%
23	13.749	2075	2077	2092	rVB4	27057	56386	4.07%	0.544%
24	13.865	2092	2096	2097	rBV2	25658	33388	2.41%	0.322%
25	13.889	2097	2100	2119	rVB2	53536	137617	9.92%	1.329%
26	14.408	2180	2185	2189	rBV	124902	152982	11.03%	1.477%
27	14.450	2189	2192	2196	rVV5	15149	26336	1.90%	0.254%
28	14.481	2196	2197	2207	rVB7	8887	17221	1.24%	0.166%
29	14.597	2209	2216	2219	rBV7	8485	17667	1.27%	0.171%
30	14.633	2219	2222	2228	rVB5	11230	19927	1.44%	0.192%

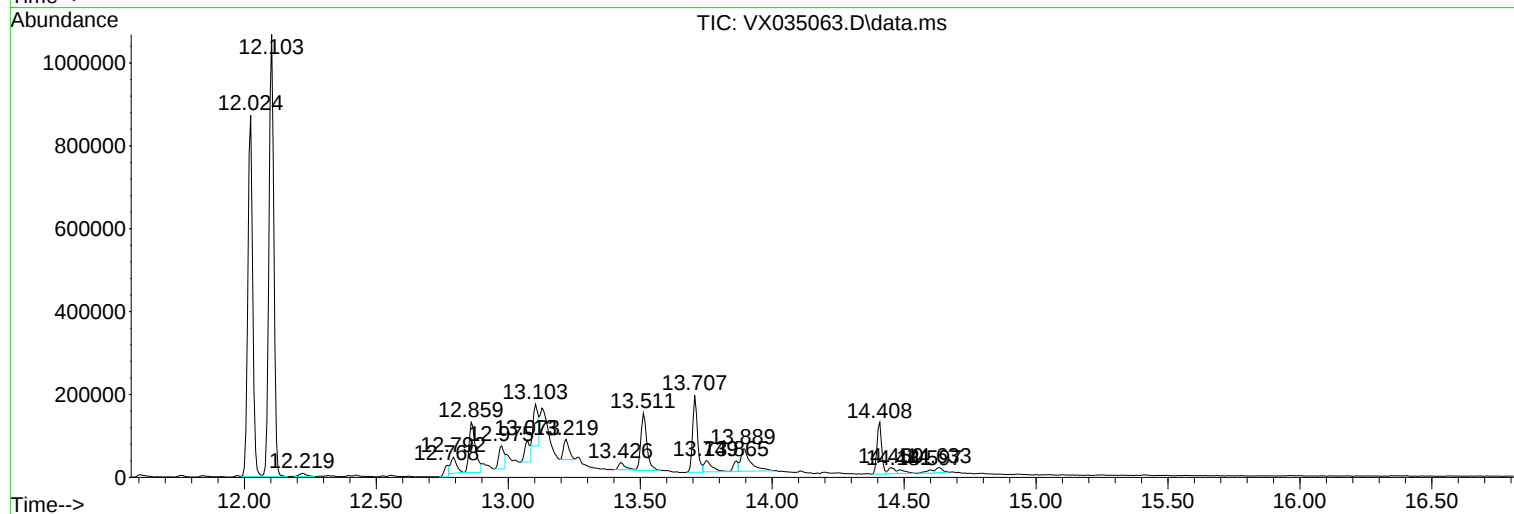
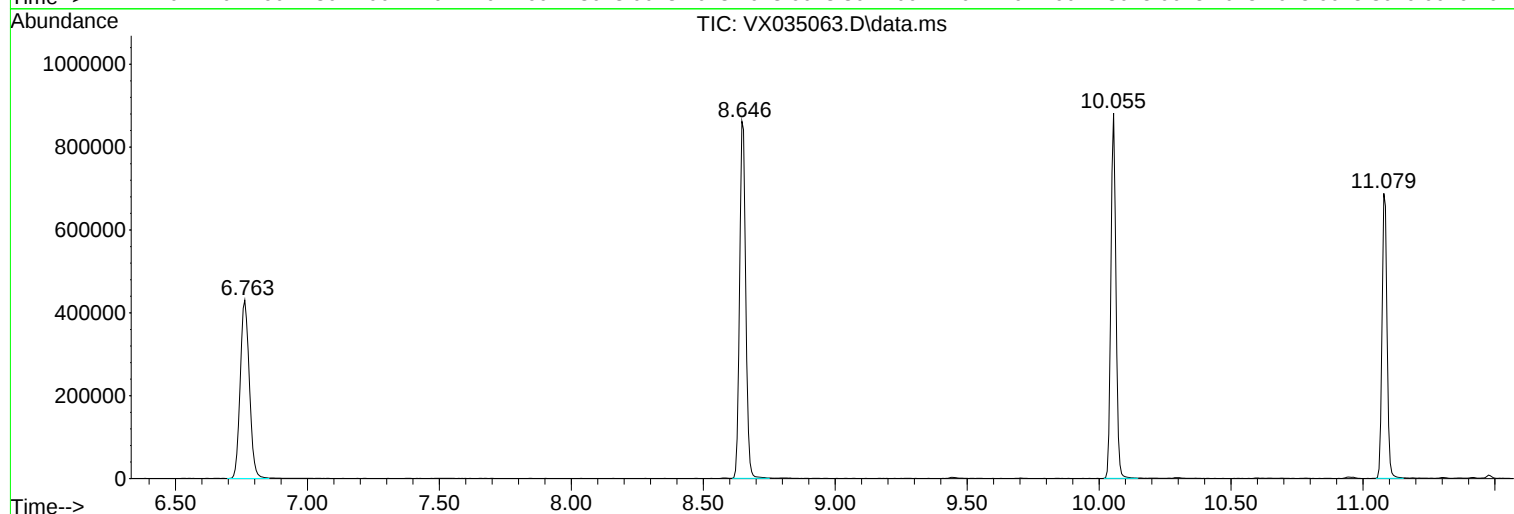
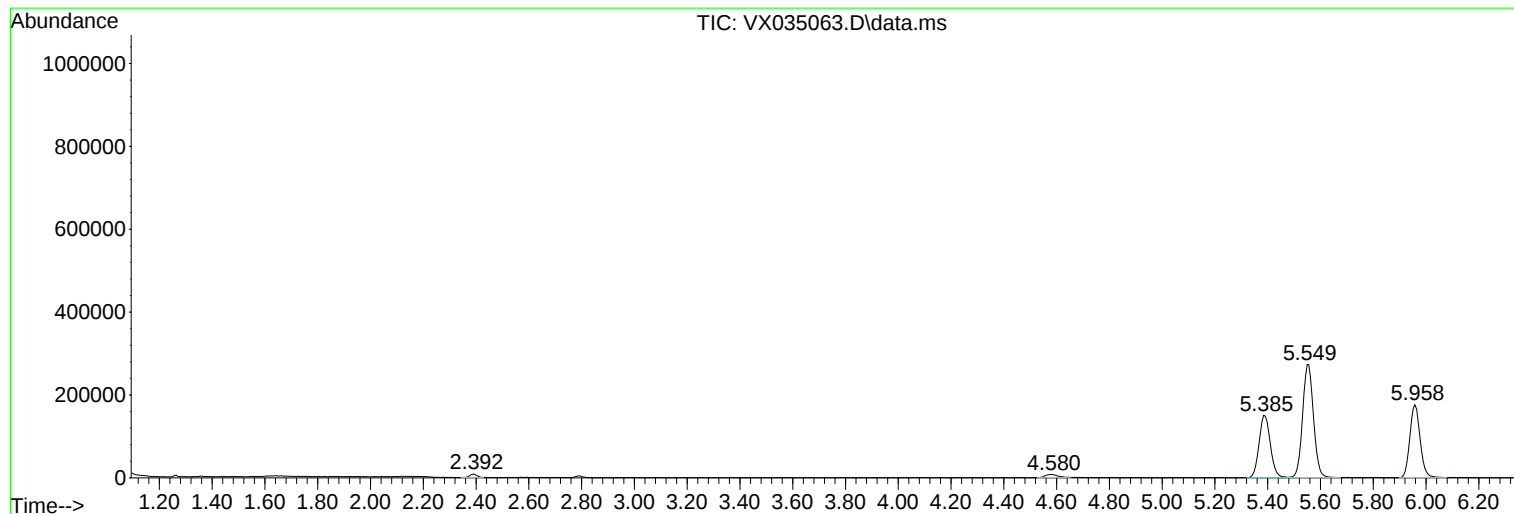
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ELI-WATER-0407

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\WX041423\
Data File : VX035063.D
Acq On : 13 Apr 2023 14:50
Operator : JC/MD
Sample : 02257-03 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ELI-WATER-0407

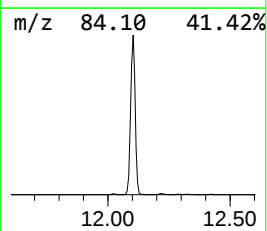
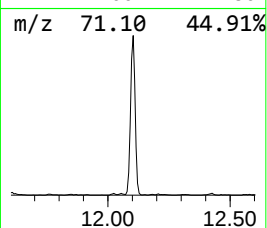
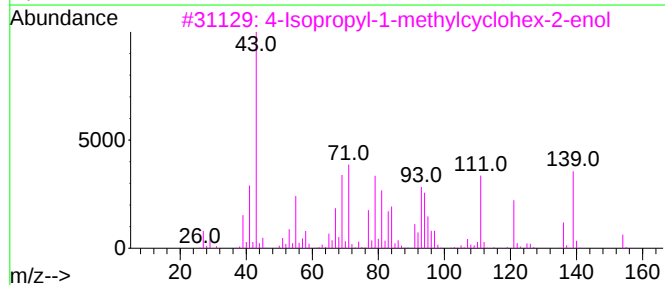
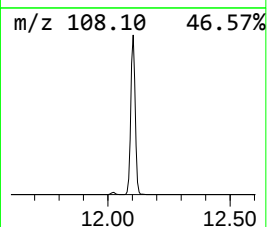
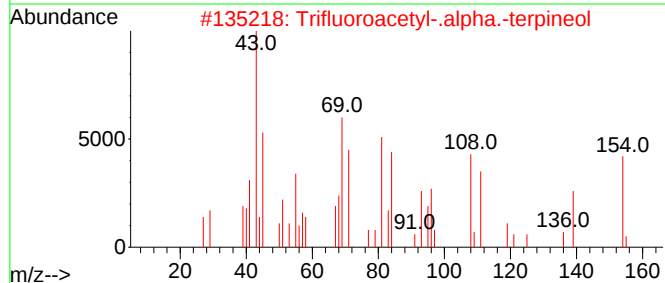
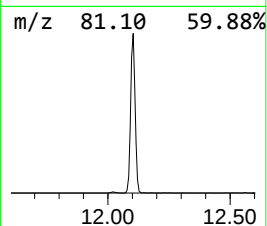
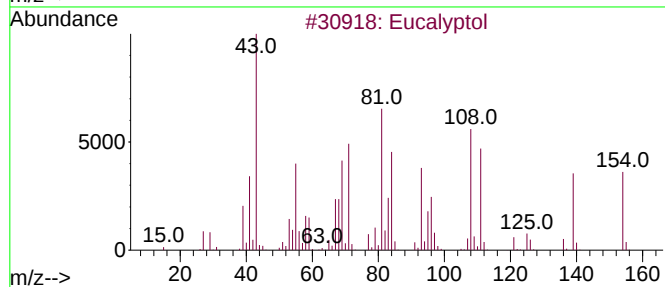
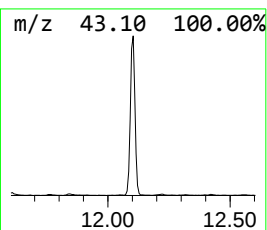
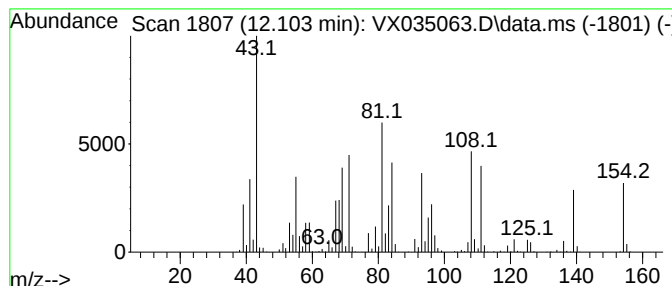
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

Peak Number 1 Eucalyptol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.103	61.98 ug/l	1377230	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	99
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	83
3			4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	38
4			2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	27
5			3-Hepten-2-one, 3-propyl-	154	C10H18O	032064-69-0	25



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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ELI-WATER-0407

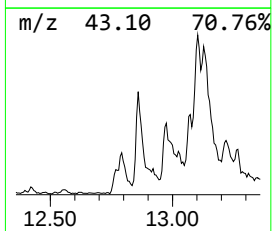
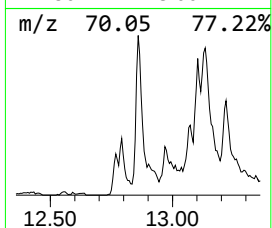
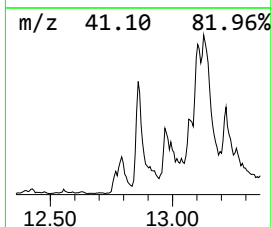
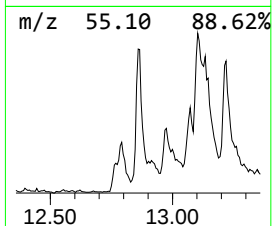
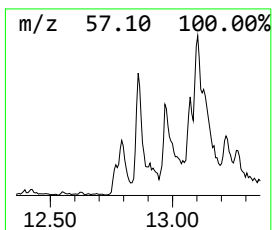
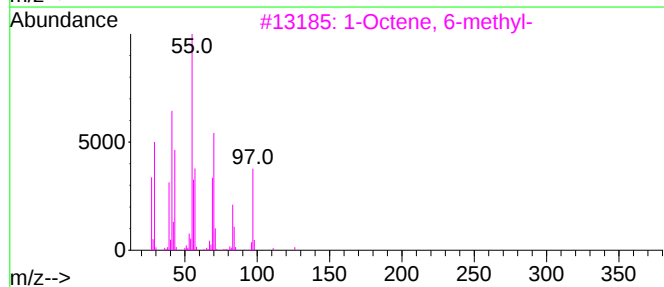
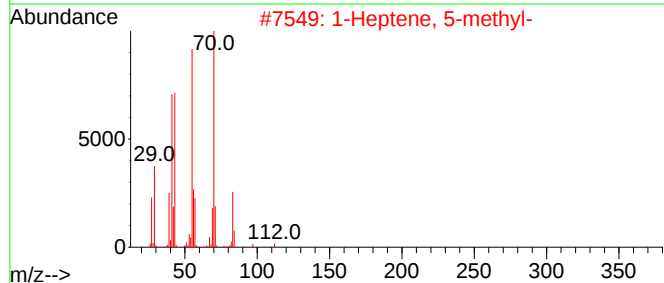
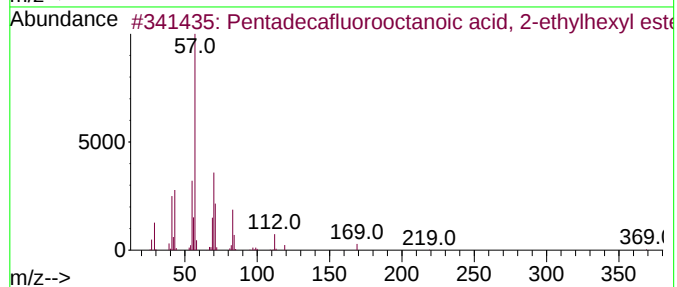
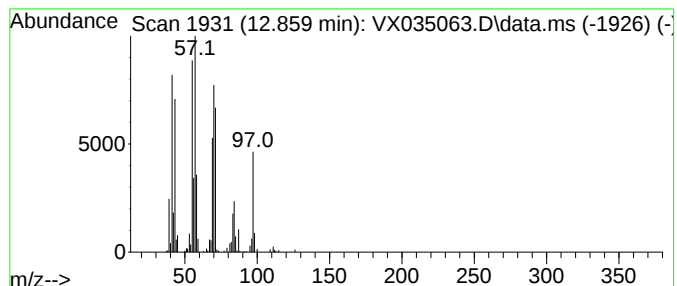
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.859	9.30 ug/l	206616	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	50
2			1-Heptene, 5-methyl-	112	C8H16	013151-04-7	43
3			1-Octene, 6-methyl-	126	C9H18	013151-10-5	43
4			1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	38
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	27



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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ELI-WATER-0407

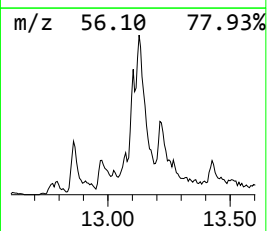
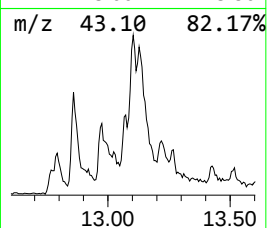
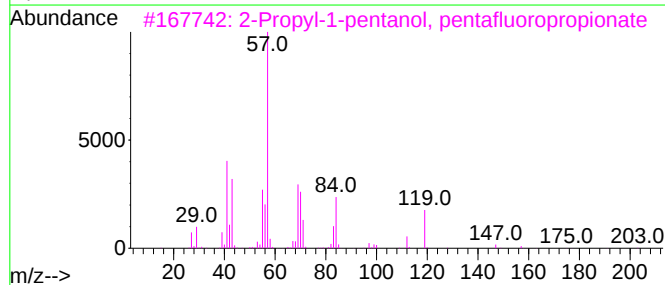
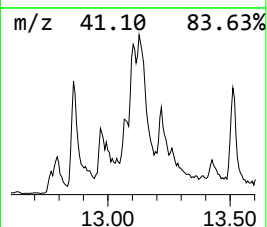
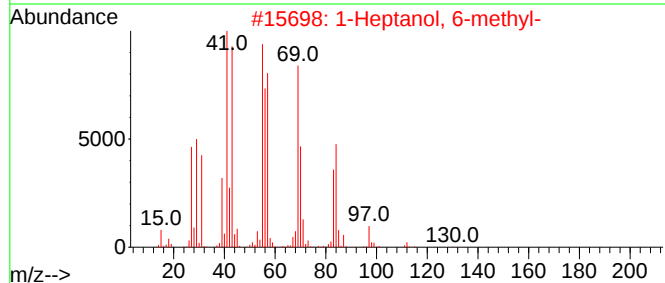
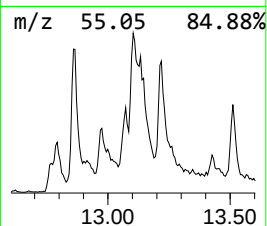
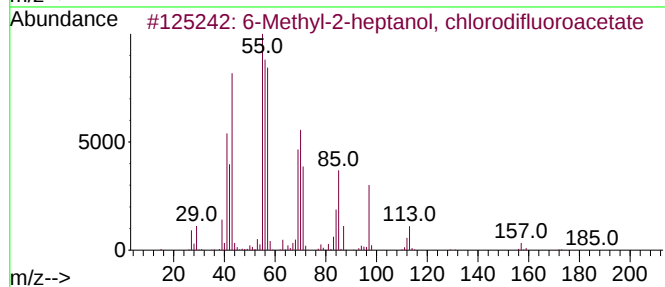
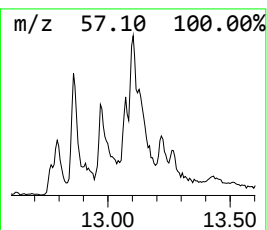
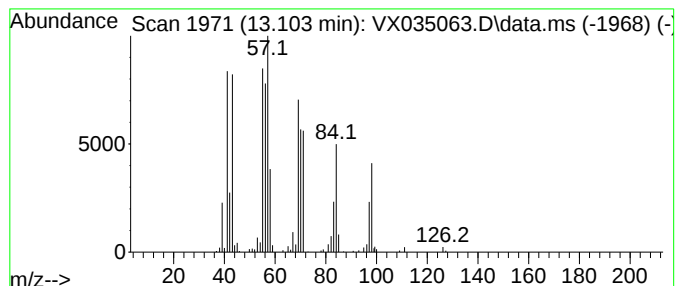
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

Peak Number 3 unknown13.103 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.103	6.02 ug/l	133755	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Methyl-2-heptanol, chlorodiflu...	242	C10H17ClF2O2	1000447-27-5	47
2			1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	46
3			2-Propyl-1-pentanol, pentafluoro...	276	C11H17F5O2	1000365-51-2	43
4			(Z)-2-Heptene	98	C7H14	006443-92-1	38
5			Heptane, 2-chloro-	134	C7H15Cl	001001-89-4	38



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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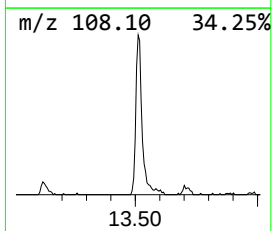
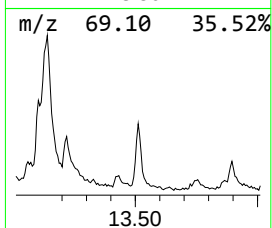
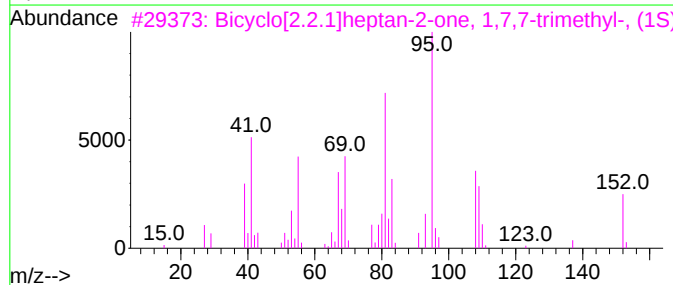
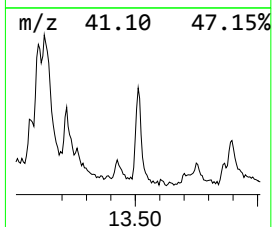
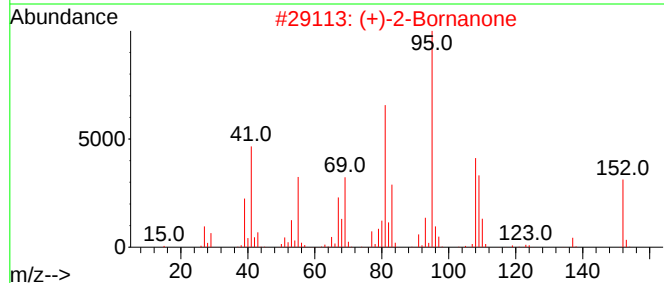
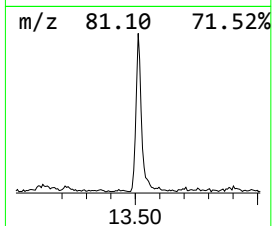
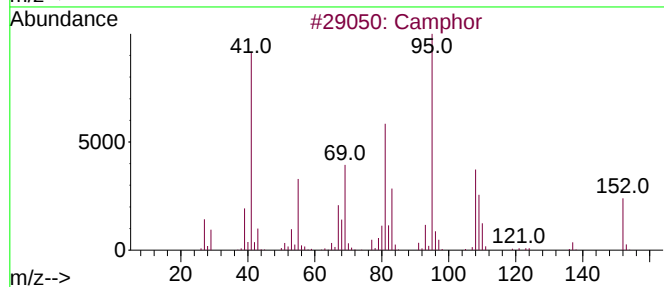
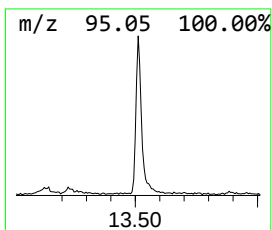
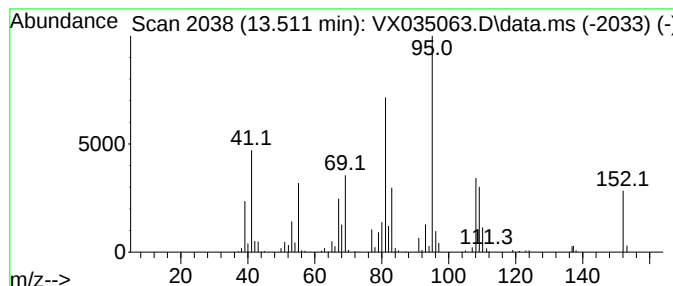
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Camphor Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.512	9.89 ug/l	219647	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Camphor	152	C10H16O	000076-22-2	98
2			(+)-2-Bornanone	152	C10H16O	000464-49-3	98
3			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	96
4			2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	49
5			3-Hydroxypyridine monoacetate	137	C7H7NO2	017747-43-2	43



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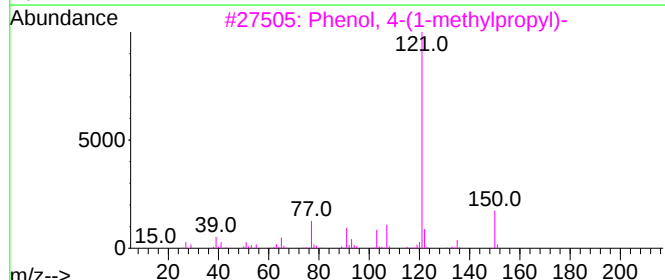
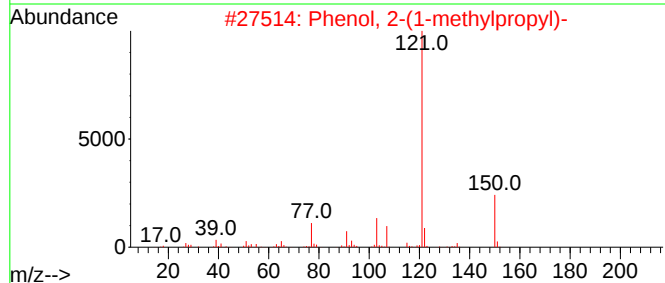
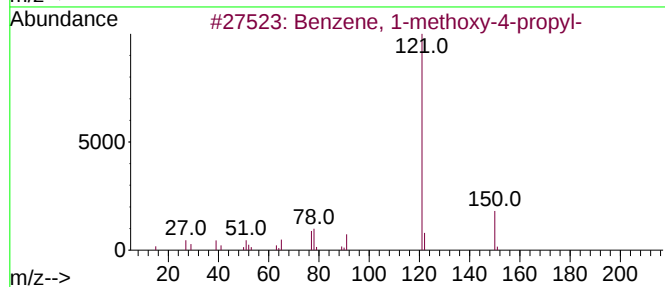
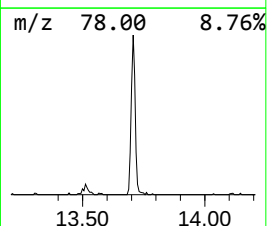
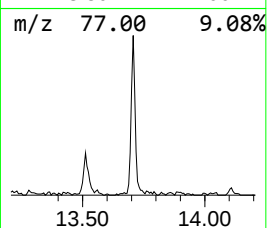
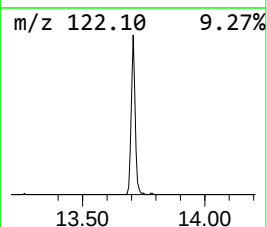
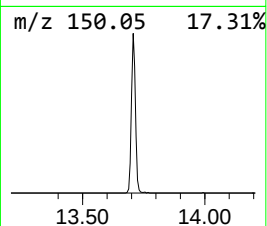
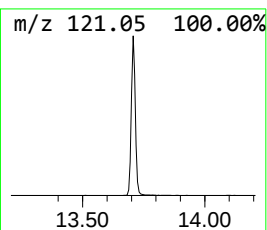
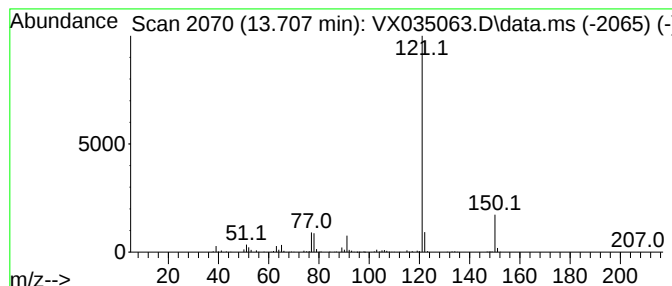
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 1-methoxy-4-propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.707	10.62 ug/l	235953	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methoxy-4-propyl-	150	C10H14O	000104-45-0	91
2			Phenol, 2-(1-methylpropyl)-	150	C10H14O	000089-72-5	86
3			Phenol, 4-(1-methylpropyl)-	150	C10H14O	000099-71-8	83
4			2-Methyl-6-propylphenol	150	C10H14O	003520-52-3	74
5			Benzene, 1-ethyl-4-methoxy-	136	C9H12O	001515-95-3	72



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

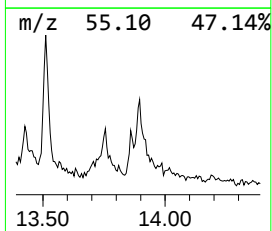
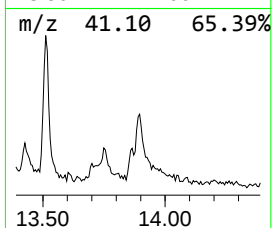
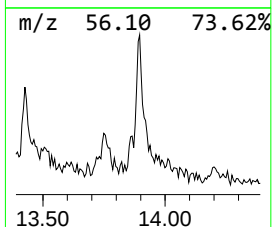
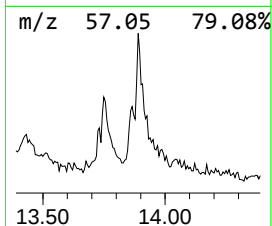
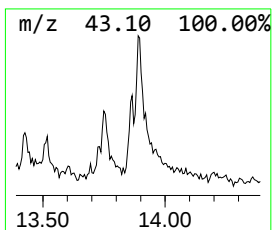
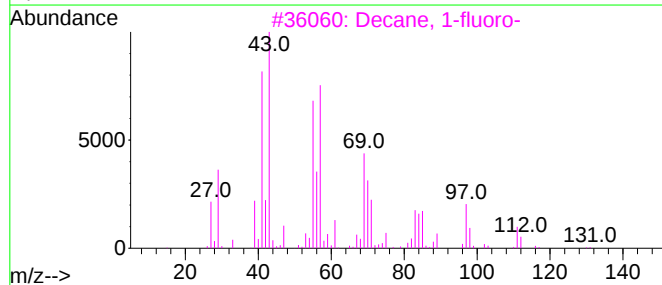
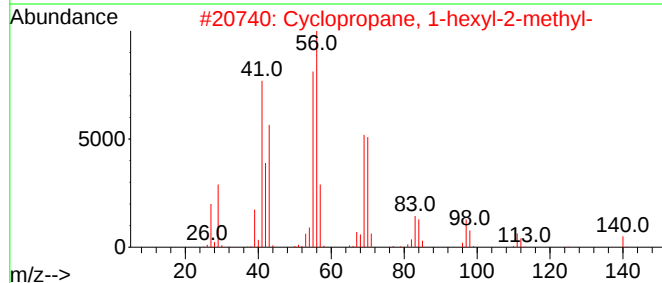
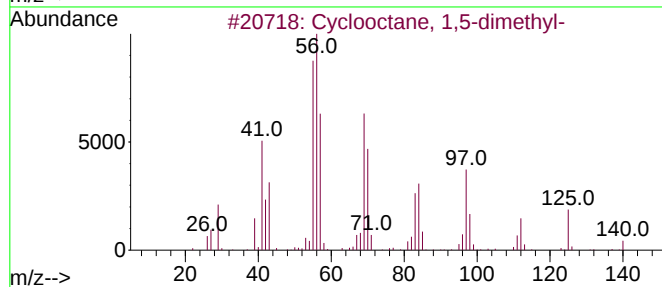
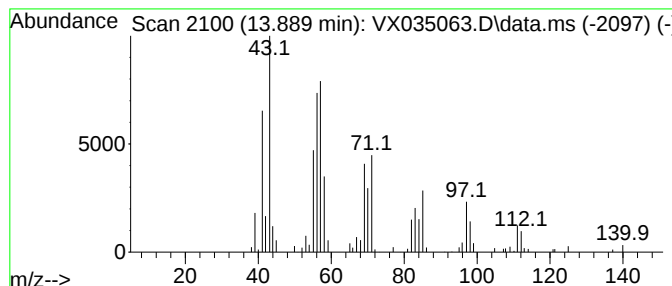
Instrument :
MSVOA_X
ClientSampleId :
ELI-WATER-0407

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

Peak Number 6 Cyclooctane, 1,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.890	6.19 ug/l	137617	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclooctane, 1,5-dimethyl-	140	C10H20	021328-57-4	70
2	Cyclopropane, 1-hexyl-2-methyl-	140	C10H20	062238-09-9	46
3	Decane, 1-fluoro-	160	C10H21F	000334-56-5	43
4	Cyclopentane, 1,1,2-trimethyl-	112	C8H16	004259-00-1	43
5	1-Heptene, 6-methyl-	112	C8H16	005026-76-6	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041423\
Data File : VX035063.D
Acq On : 13 Apr 2023 14:50
Operator : JC/MD
Sample : 02257-03 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ELI-WATER-0407

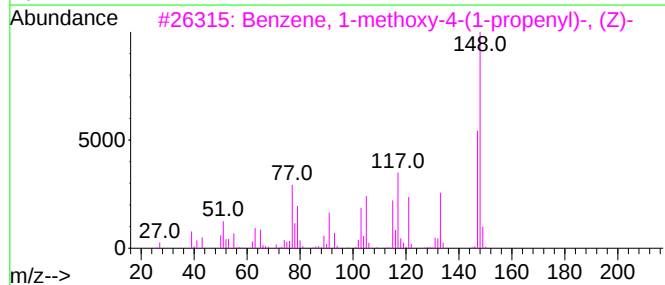
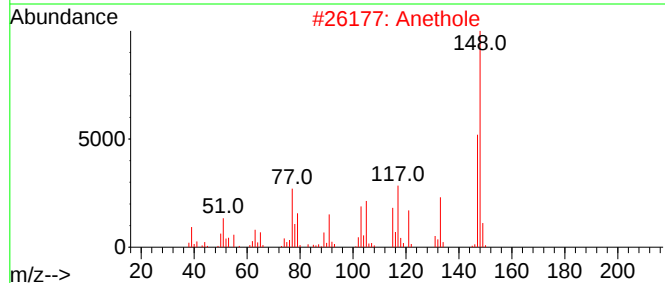
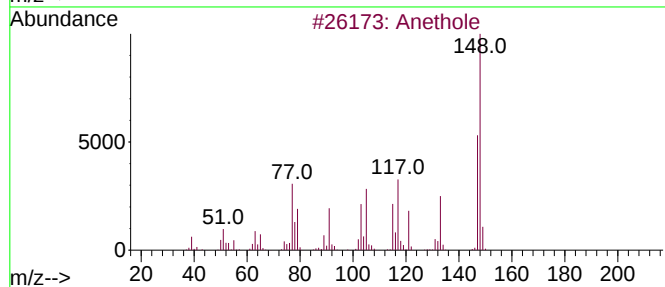
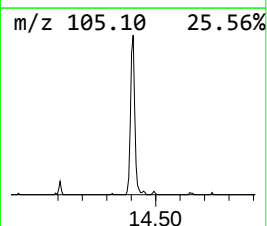
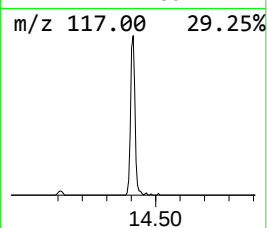
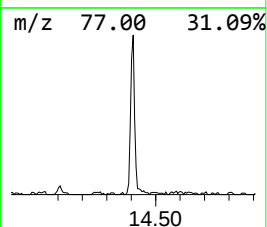
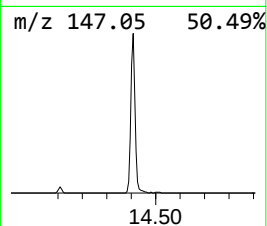
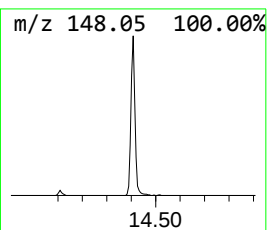
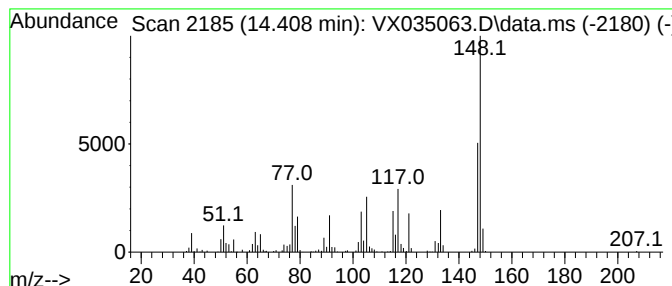
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

Peak Number 7 Anethole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.408	6.89 ug/l	152982	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anethole			148	C10H12O	004180-23-8	98
2	Anethole			148	C10H12O	000104-46-1	98
3	Benzene, 1-methoxy-4-(1-propenyl)-			148	C10H12O	025679-28-1	98
4	Estragole			148	C10H12O	000140-67-0	94
5	Methanimidamide, N,N-dimethyl-N'-			148	C9H12N2	001783-25-1	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041423\
Data File : VX035063.D
Acq On : 13 Apr 2023 14:50
Operator : JC/MD
Sample : 02257-03 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ELI-WATER-0407

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Eucalyptol	12.103	62.0	ug/l	1377230	4	12.024	1110940	50.0
Pentadecafluoro...	12.859	9.3	ug/l	206616	4	12.024	1110940	50.0
unknown13.103	13.103	6.0	ug/l	133755	4	12.024	1110940	50.0
Camphor	13.512	9.9	ug/l	219647	4	12.024	1110940	50.0
Benzene, 1-meth...	13.707	10.6	ug/l	235953	4	12.024	1110940	50.0
Cyclooctane, 1,...	13.890	6.2	ug/l	137617	4	12.024	1110940	50.0
Anethole	14.408	6.9	ug/l	152982	4	12.024	1110940	50.0