

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031621\
 Data File : VX021252.D
 Acq On : 16 Mar 2021 18:20
 Operator : JC/MD
 Sample : M1666-02 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1858

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\82X031621W.M
 Title : SW846 8260

Signal : TIC: VX021252.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.475	62	66	78	rVB	23596	28284	1.46%	0.353%
2	2.093	165	171	181	rBV	94238	145791	7.53%	1.821%
3	3.917	469	481	492	rBV4	8924	25396	1.31%	0.317%
4	4.640	595	604	616	rBV2	10574	31929	1.65%	0.399%
5	5.464	732	744	756	rBV2	51996	154280	7.96%	1.928%
6	5.629	759	772	785	rBV	96932	267235	13.79%	3.339%
7	6.029	829	840	852	rBV	63685	166384	8.59%	2.079%
8	6.829	965	976	988	rBV	145943	338720	17.48%	4.232%
9	8.694	1286	1293	1300	rBV	297617	456962	23.59%	5.709%
10	10.094	1524	1531	1541	rBV	279746	380675	19.65%	4.756%
11	11.118	1700	1705	1718	rVB	224072	294791	15.22%	3.683%
12	11.965	1845	1849	1854	rVB	30610	36136	1.87%	0.451%
13	12.059	1860	1865	1873	rVB	281871	348337	17.98%	4.352%
14	12.141	1873	1879	1890	rBV	1539439	1937317	100.00%	24.204%
15	12.624	1947	1961	1973	rBV5	9692	22997	1.19%	0.287%
16	12.894	2002	2007	2012	rBV	68682	82280	4.25%	1.028%
17	13.006	2021	2026	2038	rBV	83010	140268	7.24%	1.752%
18	13.106	2038	2043	2045	rVV	110904	142973	7.38%	1.786%
19	13.136	2045	2048	2065	rVB	275740	431407	22.27%	5.390%
20	13.459	2098	2103	2114	rBV	1063219	1300224	67.11%	16.245%
21	13.547	2114	2118	2126	rVB	273071	385024	19.87%	4.810%
22	13.748	2146	2152	2154	rVV	43174	92506	4.77%	1.156%
23	13.789	2156	2159	2161	rVV	56127	82243	4.25%	1.028%
24	13.812	2161	2163	2171	rVV	53866	69330	3.58%	0.866%
25	13.900	2173	2178	2179	rVV	48176	59617	3.08%	0.745%
26	13.930	2179	2183	2195	rVB2	100053	177193	9.15%	2.214%
27	14.236	2229	2235	2255	rBV	176658	318624	16.45%	3.981%
28	14.442	2266	2270	2274	rBV	76929	87102	4.50%	1.088%

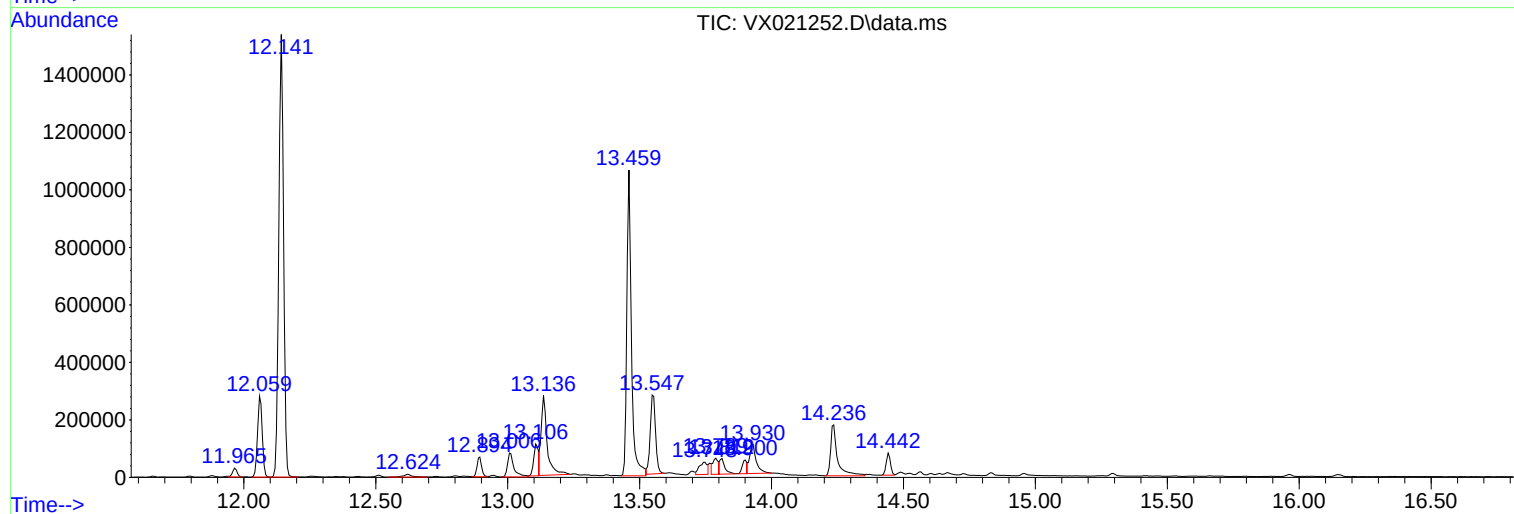
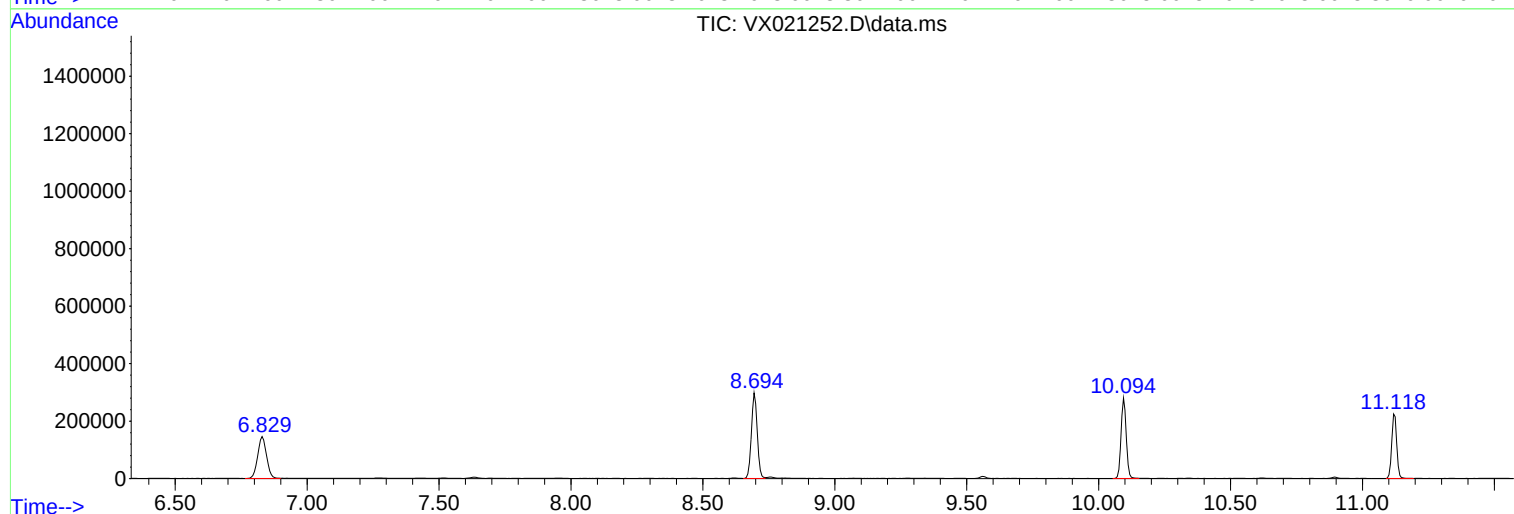
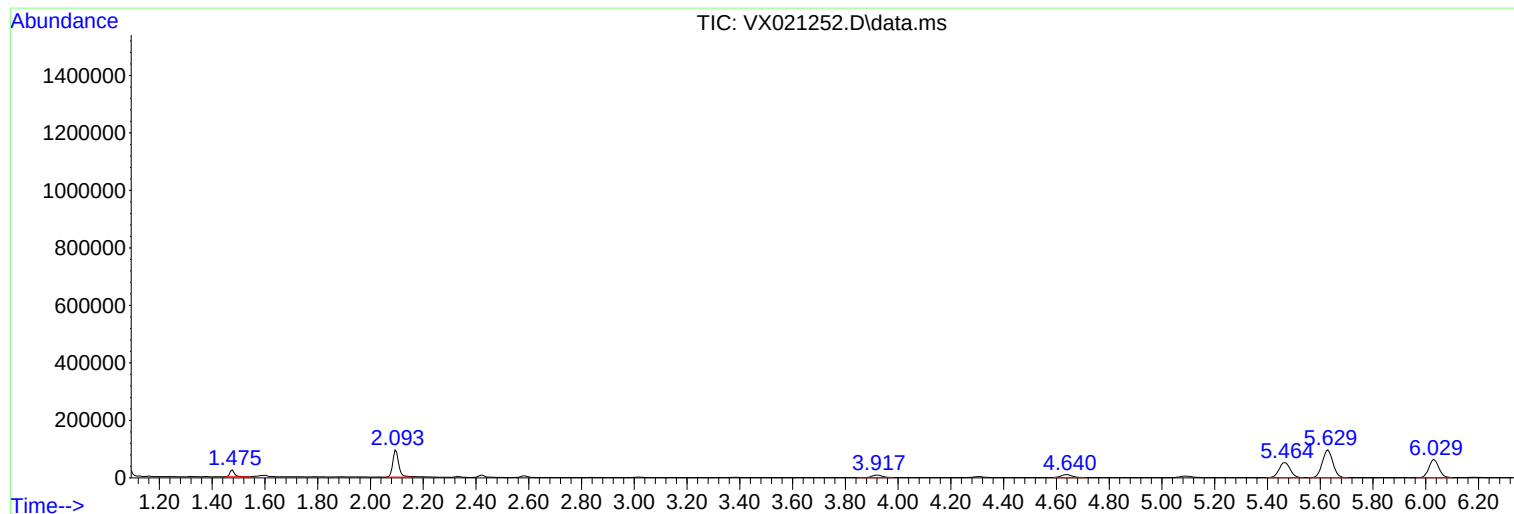
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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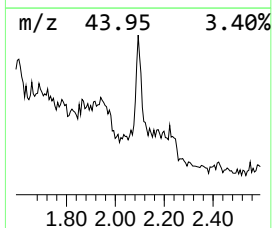
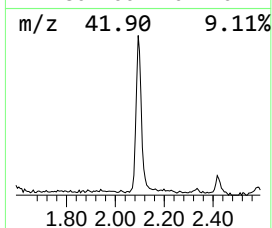
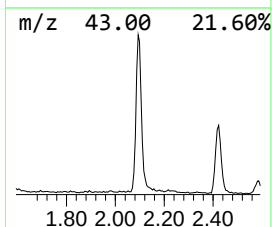
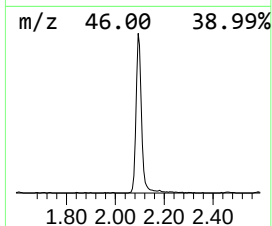
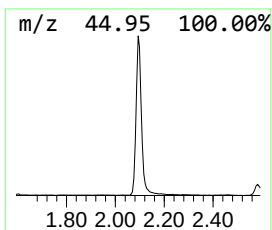
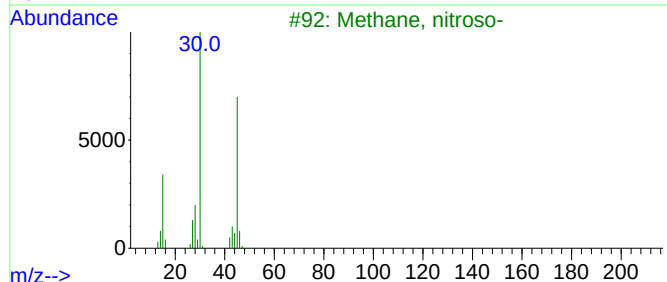
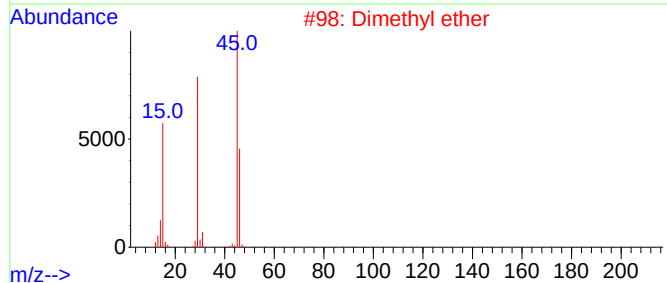
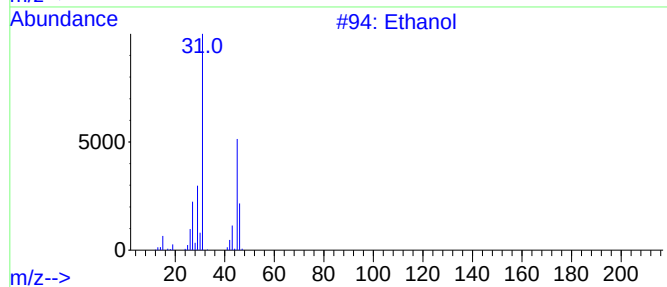
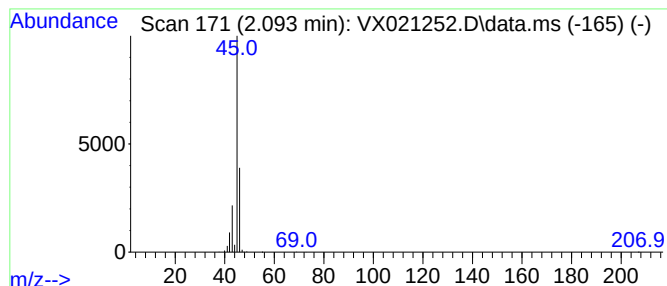
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Ethanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.093	27.28 ug/l	145791	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	64
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Formic acid	46	CH2O2	000064-18-6	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



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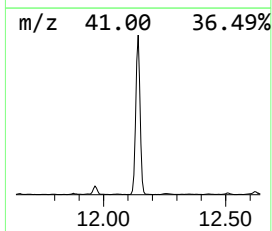
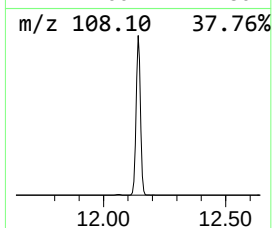
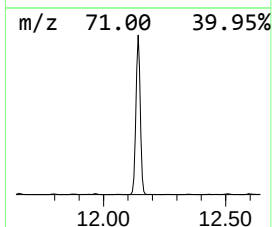
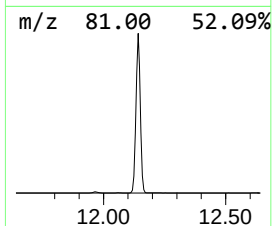
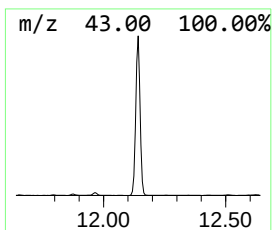
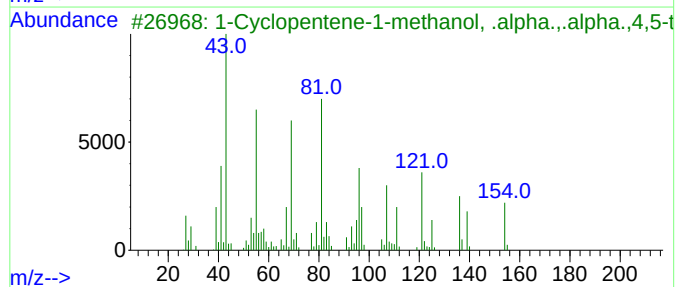
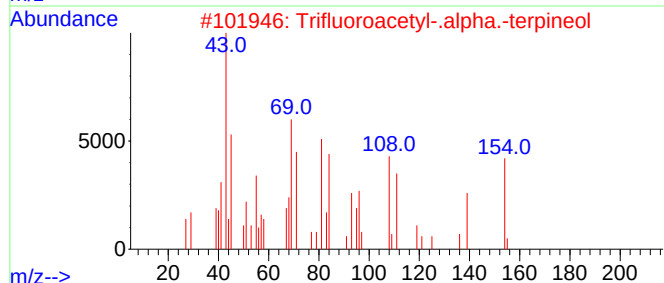
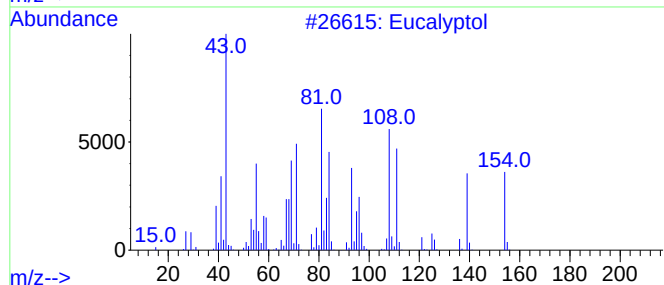
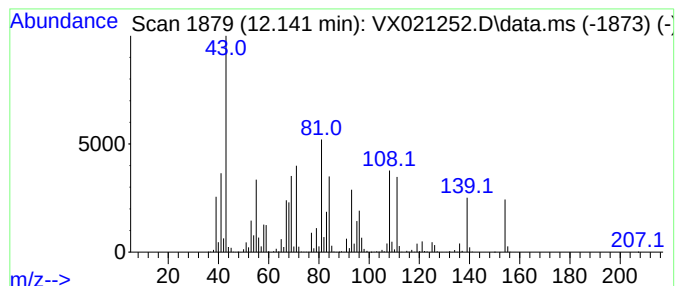
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Eucalyptol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.141	278.08 ug/l	1937320	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	98
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	64
3			1-Cyclopentene-1-methanol, .alph...	154	C10H18O	056666-68-3	22
4			2-Acetylcyclohexanone	154	C9H14O2	006126-53-0	14
5			Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	11



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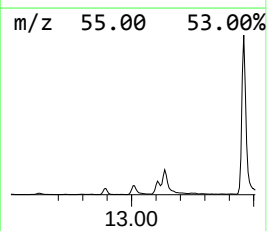
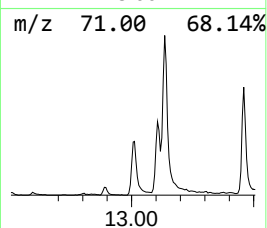
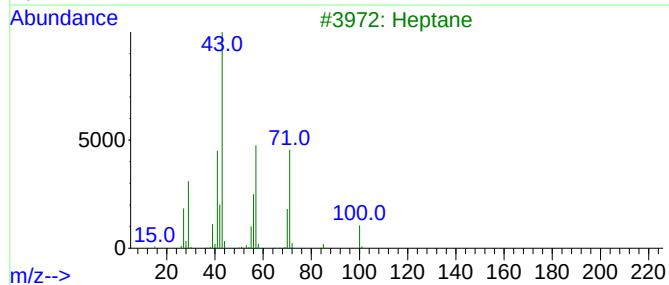
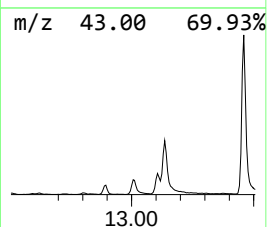
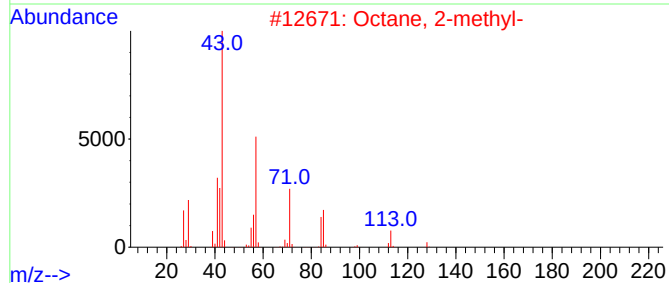
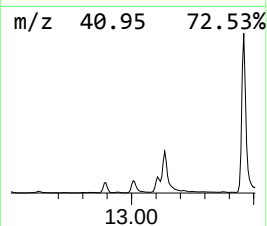
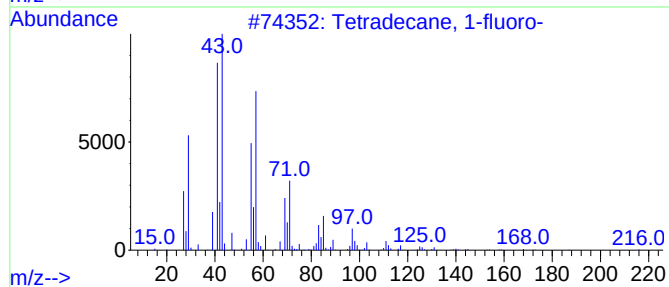
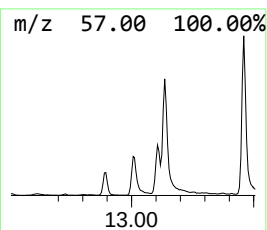
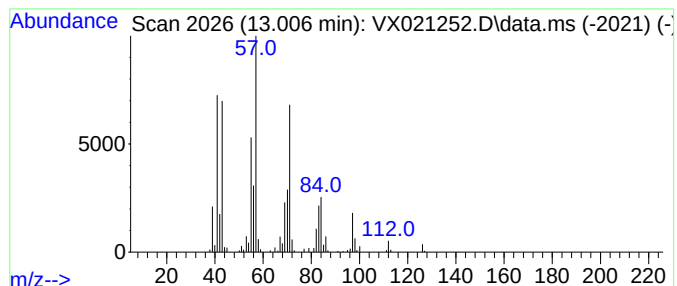
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Tetradecane, 1-fluoro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.006	20.13 ug/l	140268	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 1-fluoro-	216	C14H29F	000593-33-9	80
2			Octane, 2-methyl-	128	C9H20	003221-61-2	47
3			Heptane	100	C7H16	000142-82-5	46
4			Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	43
5			Cyclooctane, methyl-	126	C9H18	001502-38-1	38



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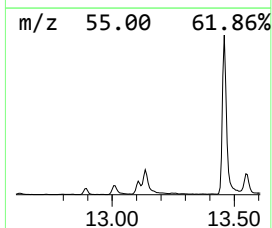
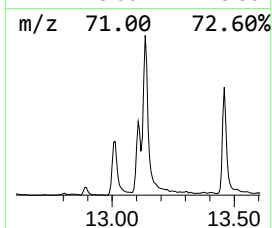
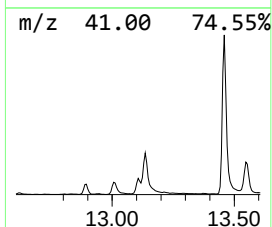
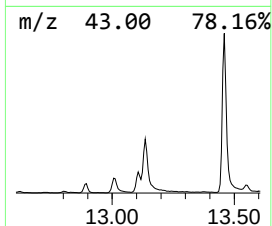
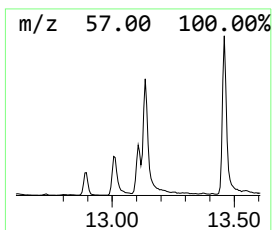
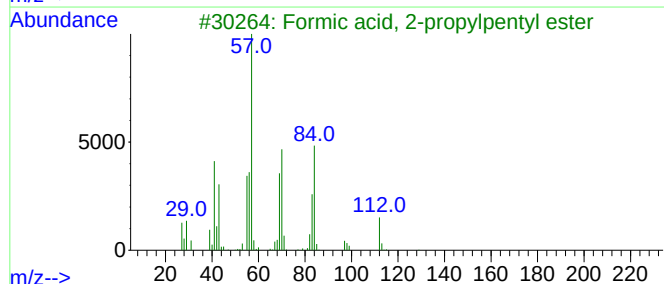
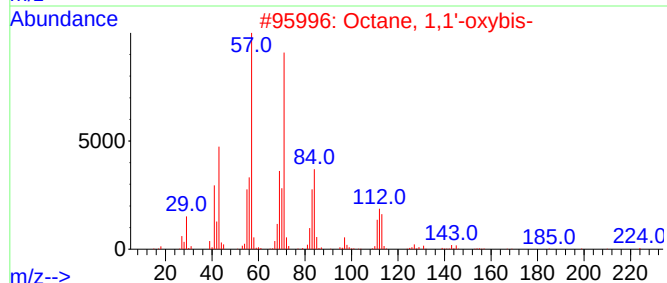
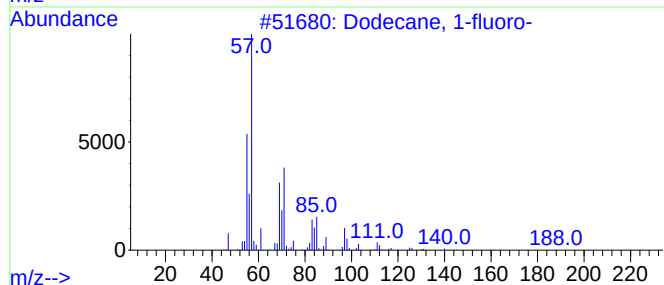
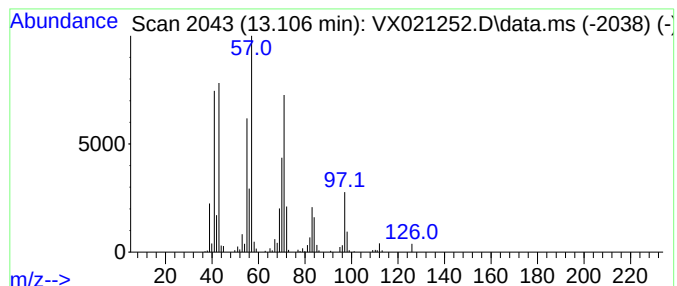
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Dodecane, 1-fluoro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.106	20.52 ug/l	142973	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-fluoro-	188	C12H25F	000334-68-9	53
2			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	47
3			Formic acid, 2-propylpentyl ester	158	C9H18O2	1000368-74-8	43
4			trans-1-Butyl-2-methylcyclopropane	112	C8H16	038851-70-6	38
5			cis-1-Butyl-2-methylcyclopropane	112	C8H16	038851-69-3	38



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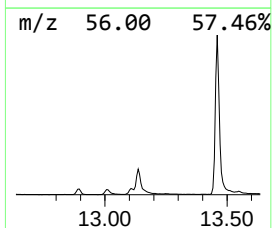
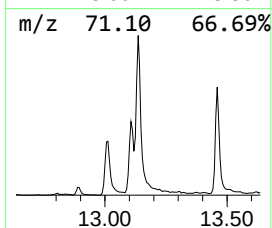
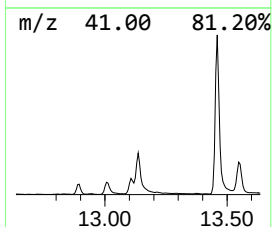
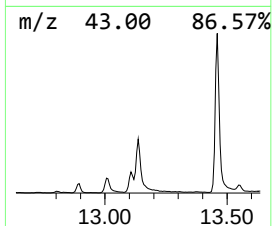
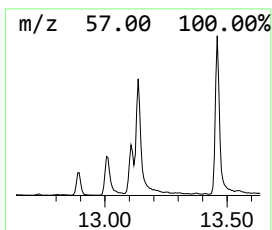
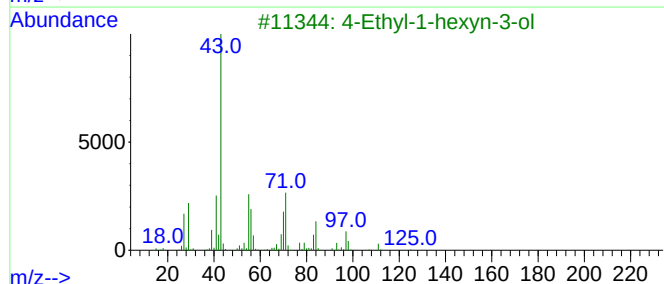
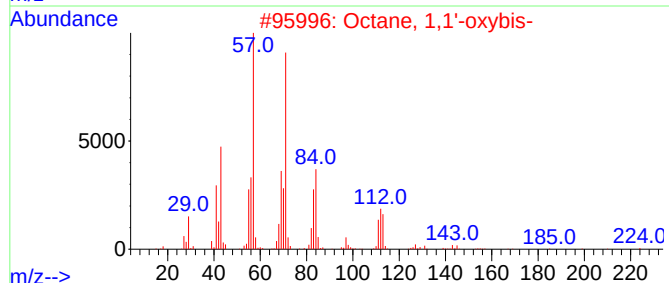
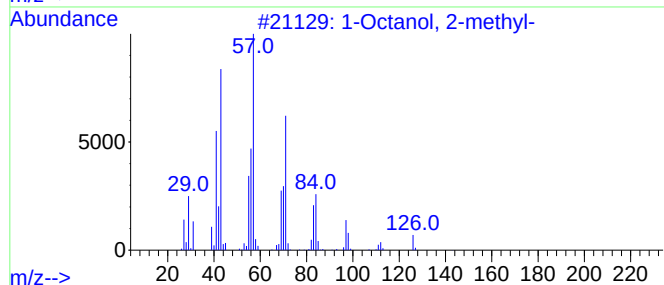
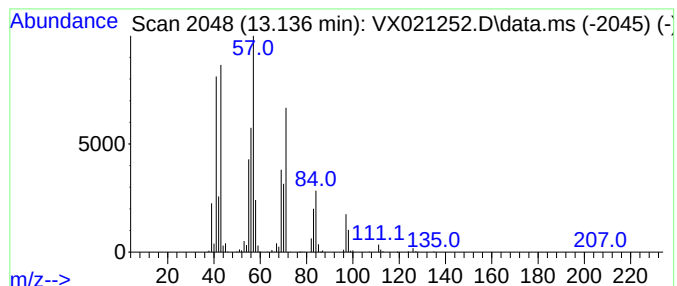
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Octanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.136	61.92 ug/l	431407	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	86
2			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	53
3			4-Ethyl-1-hexyn-3-ol	126	C8H14O	051277-03-3	47
4			1-Octanol	130	C8H18O	000111-87-5	47
5			Cyclobutane, 1,2-diethyl-, cis-	112	C8H16	061141-50-2	43



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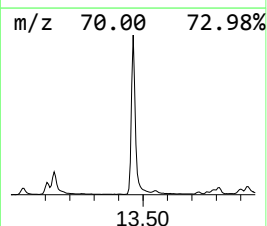
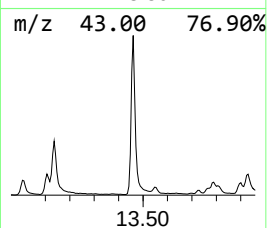
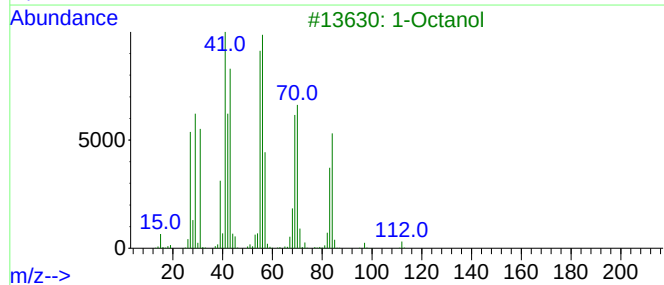
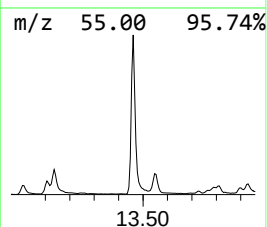
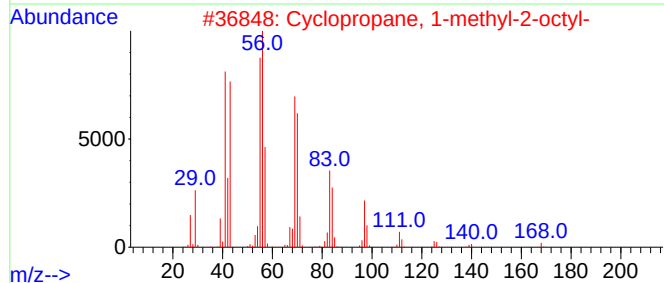
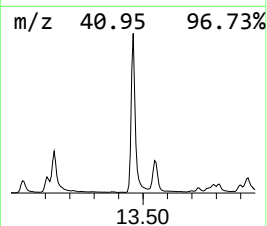
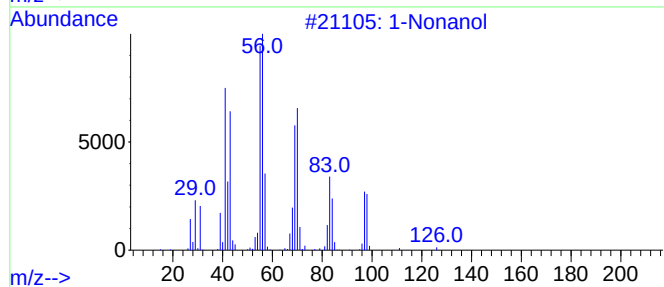
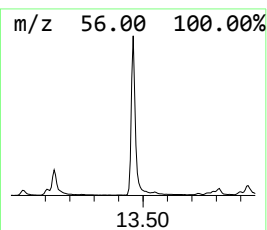
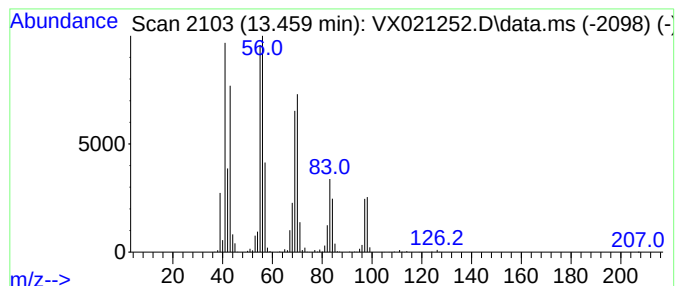
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Nonanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.459	186.63 ug/l	1300220	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonanol	144	C9H20O	000143-08-8	91
2			Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	80
3			1-Octanol	130	C8H18O	000111-87-5	72
4			Isopropylcyclobutane	98	C7H14	000872-56-0	68
5			Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031621\
Data File : VX021252.D
Acq On : 16 Mar 2021 18:20
Operator : JC/MD
Sample : M1666-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1858

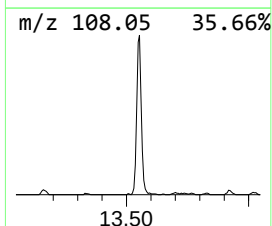
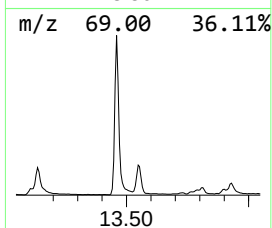
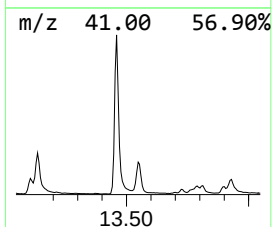
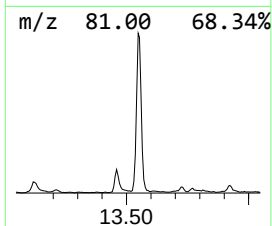
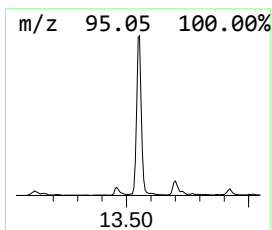
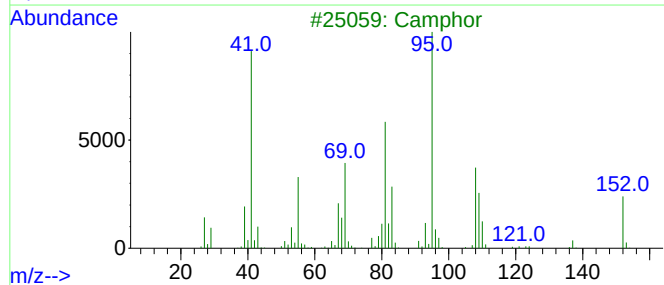
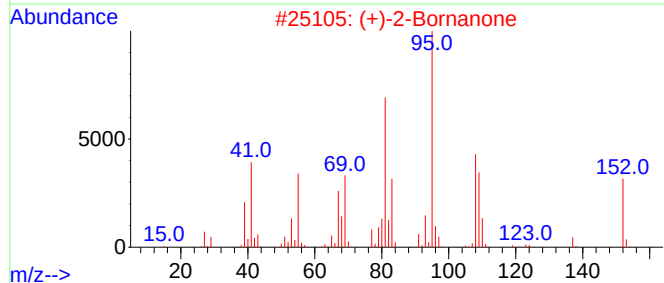
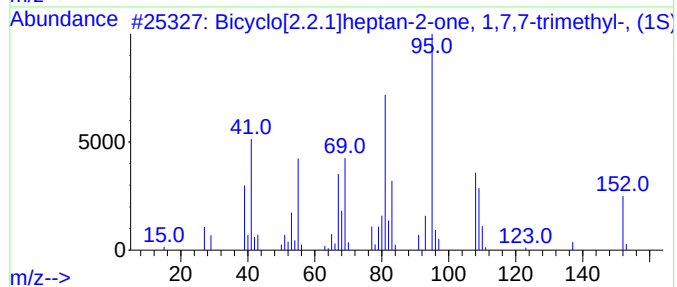
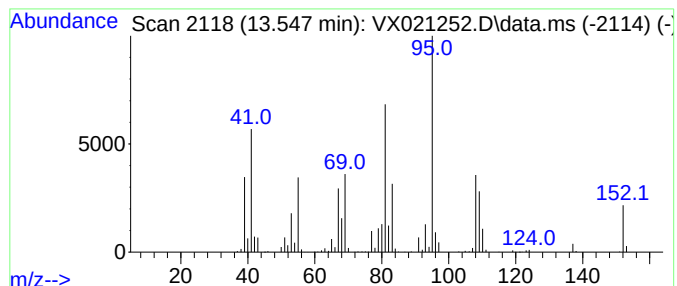
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.547	55.27 ug/l	385024	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	98
2			(+)-2-Bornanone	152	C10H16O	000464-49-3	97
3			Camphor	152	C10H16O	000076-22-2	97
4			5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	58
5			1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031621\
Data File : VX021252.D
Acq On : 16 Mar 2021 18:20
Operator : JC/MD
Sample : M1666-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1858

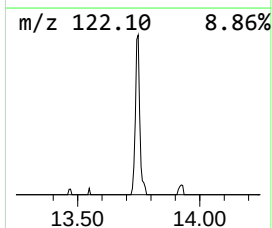
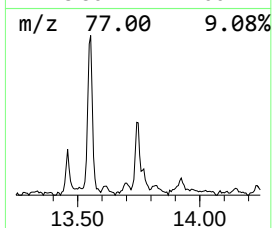
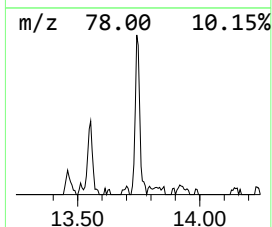
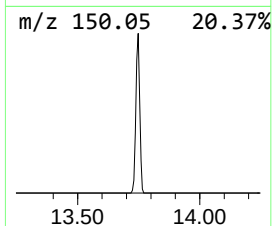
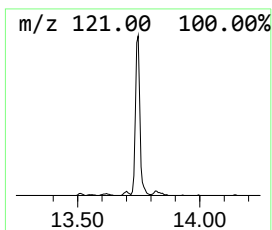
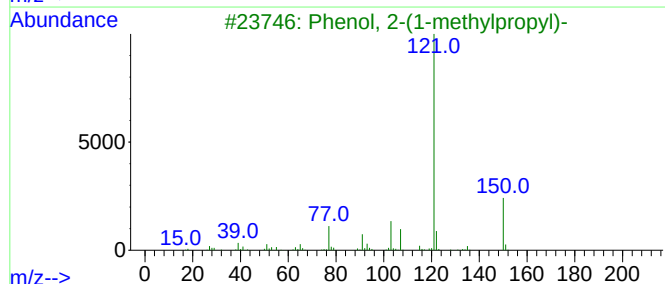
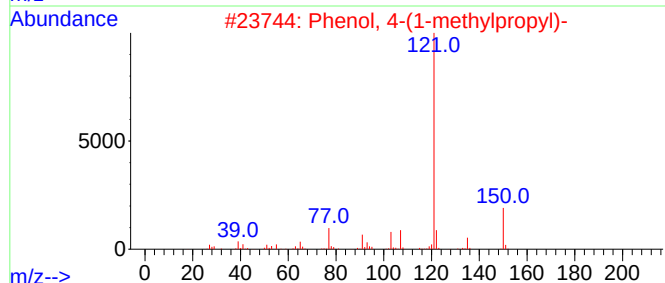
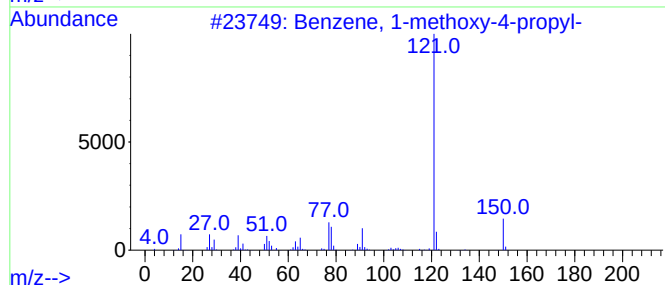
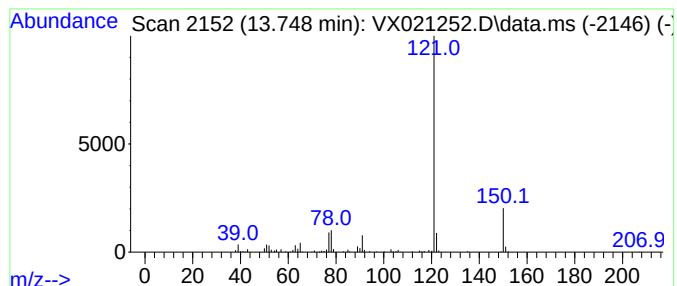
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzene, 1-methoxy-4-propyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.748	13.28 ug/l	92506	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methoxy-4-propyl-	150	C10H14O	000104-45-0	91
2			Phenol, 4-(1-methylpropyl)-	150	C10H14O	000099-71-8	80
3			Phenol, 2-(1-methylpropyl)-	150	C10H14O	000089-72-5	78
4			[2-(3,4-Dimethoxyphenyl)ethyl](4...	301	C18H23NO3	1000302-74-5	74
5			2-(4-Methoxyphenyl)ethanol	152	C9H12O2	000702-23-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031621\
Data File : VX021252.D
Acq On : 16 Mar 2021 18:20
Operator : JC/MD
Sample : M1666-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1858

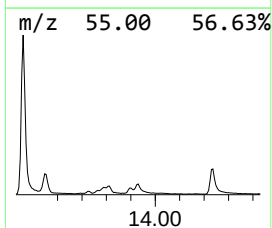
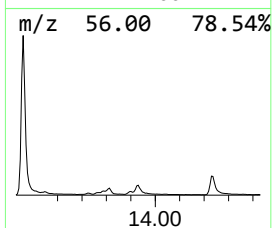
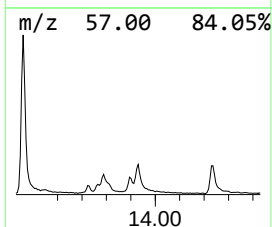
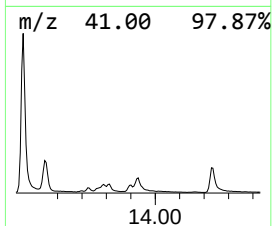
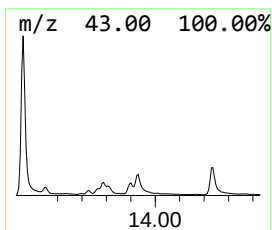
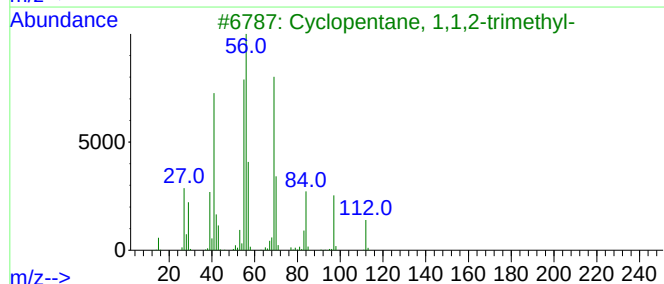
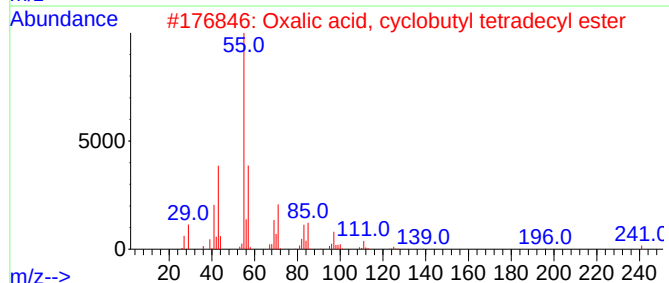
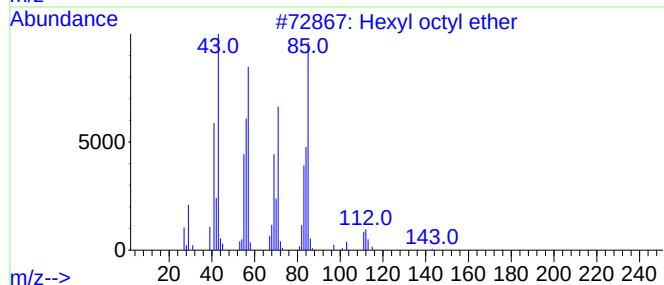
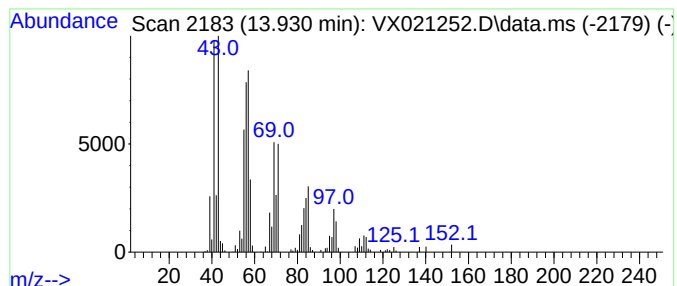
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown13.930 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.930	25.43 ug/l	177193	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexyl octyl ether	214	C14H30O	017071-54-4	47
2			Oxalic acid, cyclobutyl tetradec...	340	C20H36O4	1000309-70-9	47
3			Cyclopentane, 1,1,2-trimethyl-	112	C8H16	004259-00-1	46
4			1-Methylpentyl cyclopropane	126	C9H18	006976-28-9	43
5			Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031621\
Data File : VX021252.D
Acq On : 16 Mar 2021 18:20
Operator : JC/MD
Sample : M1666-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1858

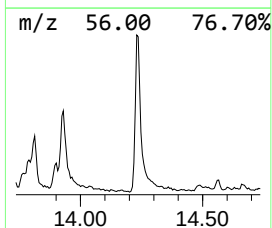
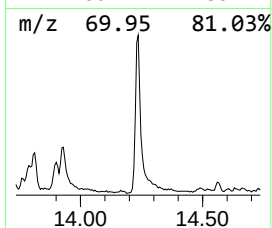
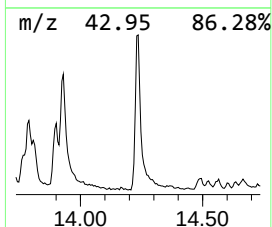
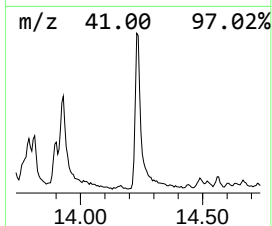
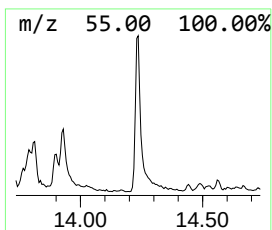
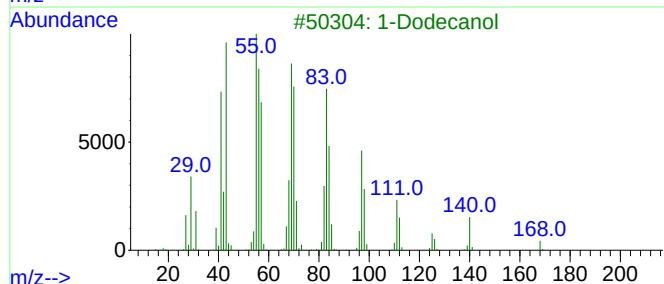
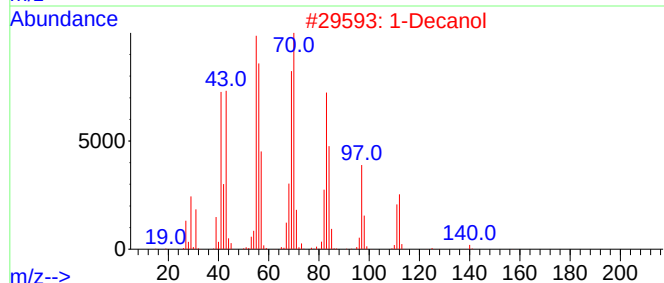
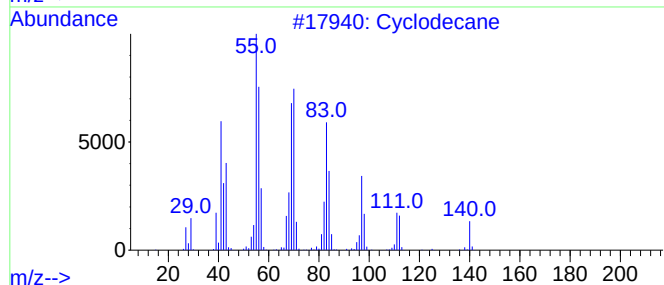
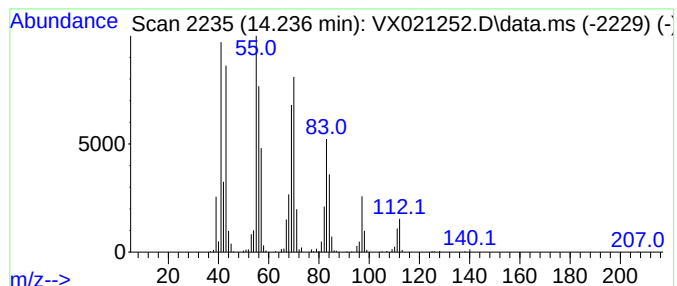
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Cyclodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.236	45.73 ug/l	318624	1,4-Dichlorobenzene-d4	12.059

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclodecane	140	C10H20	000293-96-9	96
2		1-Decanol	158	C10H22O	000112-30-1	90
3		1-Dodecanol	186	C12H26O	000112-53-8	90
4		2-Dodecene, (Z)-	168	C12H24	007206-26-0	87
5		2-Dodecene, (E)-	168	C12H24	007206-13-5	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031621\
Data File : VX021252.D
Acq On : 16 Mar 2021 18:20
Operator : JC/MD
Sample : M1666-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1858

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	2.093	27.3	ug/l	145791	1	5.629	267235	50.0
Eucalyptol	12.141	278.1	ug/l	1937320	4	12.059	348337	50.0
Tetradecane, 1-...	13.006	20.1	ug/l	140268	4	12.059	348337	50.0
Dodecane, 1-flu...	13.106	20.5	ug/l	142973	4	12.059	348337	50.0
1-Octanol, 2-me...	13.136	61.9	ug/l	431407	4	12.059	348337	50.0
1-Nonanol	13.459	186.6	ug/l	1300220	4	12.059	348337	50.0
Bicyclo[2.2.1]h...	13.547	55.3	ug/l	385024	4	12.059	348337	50.0
Benzene, 1-meth...	13.748	13.3	ug/l	92506	4	12.059	348337	50.0
unknown13.930	13.930	25.4	ug/l	177193	4	12.059	348337	50.0
Cyclodecane	14.236	45.7	ug/l	318624	4	12.059	348337	50.0