

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
 Data File : VX025382.D
 Acq On : 29 Nov 2021 20:05
 Operator : JC/MD
 Sample : M4837-18 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 20873

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\82X111721W.M
 Title : SW846 8260

Signal : TIC: VX025382.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.057	153	159	170	rBV	164908	242526	5.44%	2.089%
2	5.391	695	706	721	rBV	74795	219564	4.93%	1.891%
3	5.556	721	733	752	rVB	127968	366251	8.22%	3.154%
4	5.964	789	800	815	rBV	78122	208780	4.69%	1.798%
5	6.763	921	931	943	rBV	201795	476394	10.69%	4.103%
6	8.653	1234	1241	1249	rBV	404410	648040	14.54%	5.581%
7	9.567	1385	1391	1410	rBV	81152	198954	4.46%	1.713%
8	10.055	1465	1471	1490	rVB	440169	576847	12.94%	4.968%
9	11.079	1634	1639	1650	rBV	337367	442779	9.94%	3.813%
10	12.024	1789	1794	1801	rVB	464541	574332	12.89%	4.946%
11	12.104	1801	1807	1814	rVB	293375	369186	8.28%	3.179%
12	13.097	1967	1970	1985	rVB	112403	183424	4.12%	1.580%
13	13.427	2019	2024	2034	rBV	3927571	4456177	100.00%	38.376%
14	13.512	2034	2038	2049	rVB	75706	124381	2.79%	1.071%
15	13.707	2064	2070	2075	rBV	77122	113381	2.54%	0.976%
16	13.890	2097	2100	2113	rVB	74922	127229	2.86%	1.096%
17	14.195	2146	2150	2180	rBV	1779041	2066609	46.38%	17.797%
18	14.408	2180	2185	2189	rVV	58677	67425	1.51%	0.581%
19	14.920	2264	2269	2291	rBV	79972	149738	3.36%	1.290%

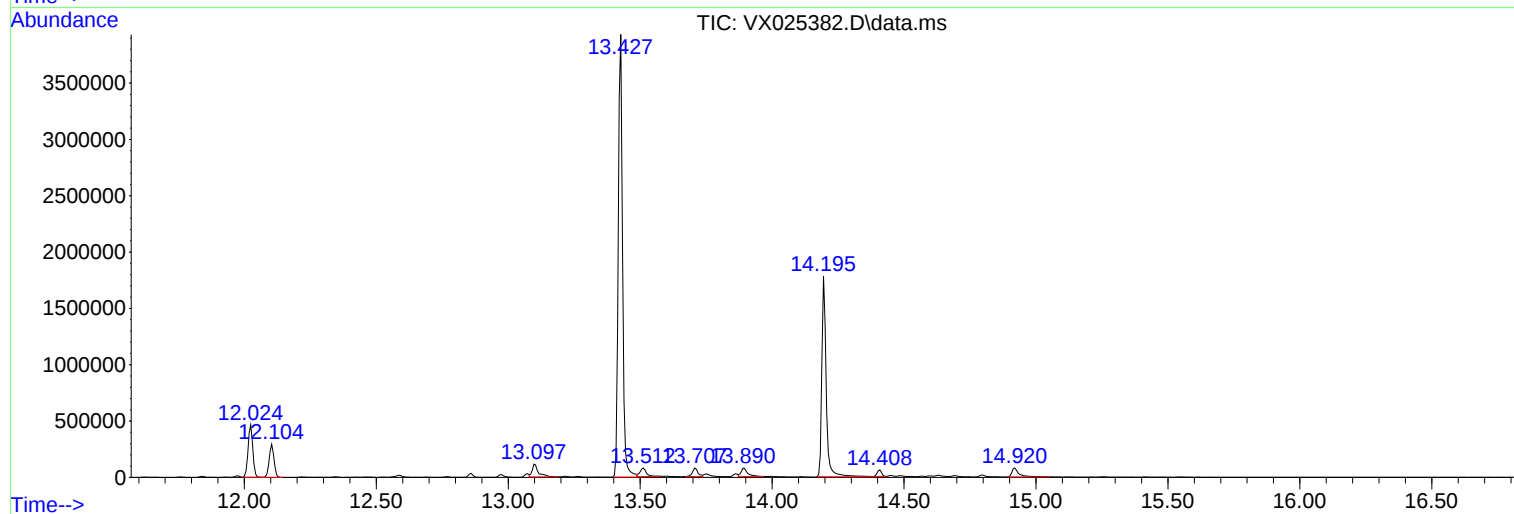
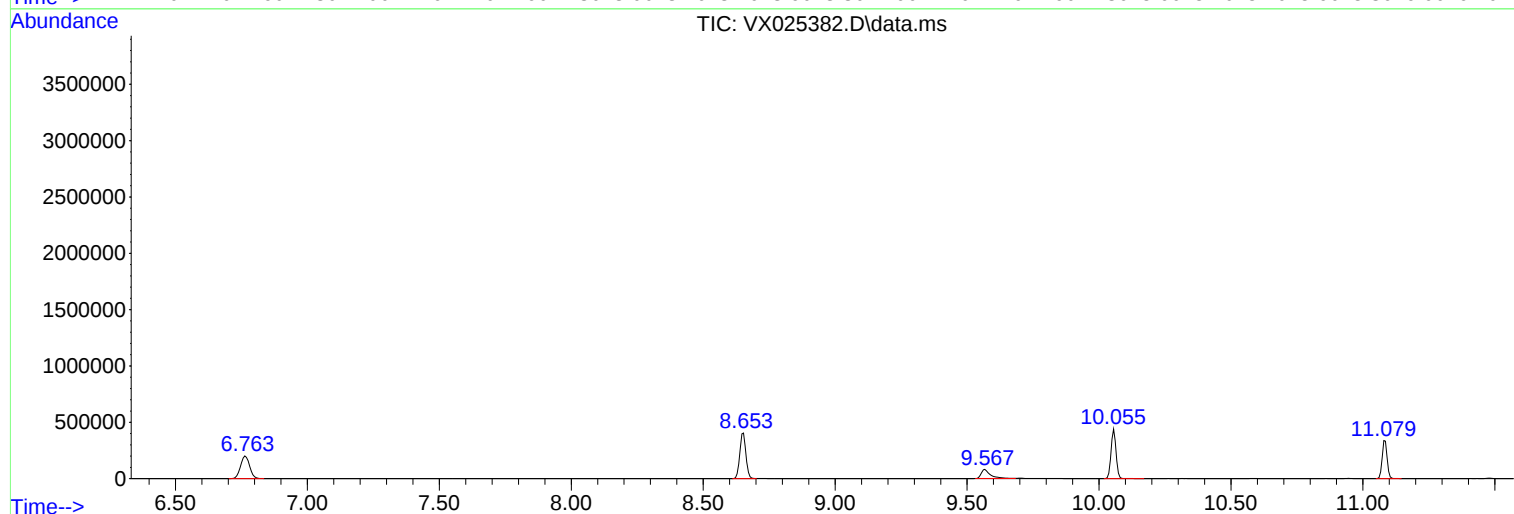
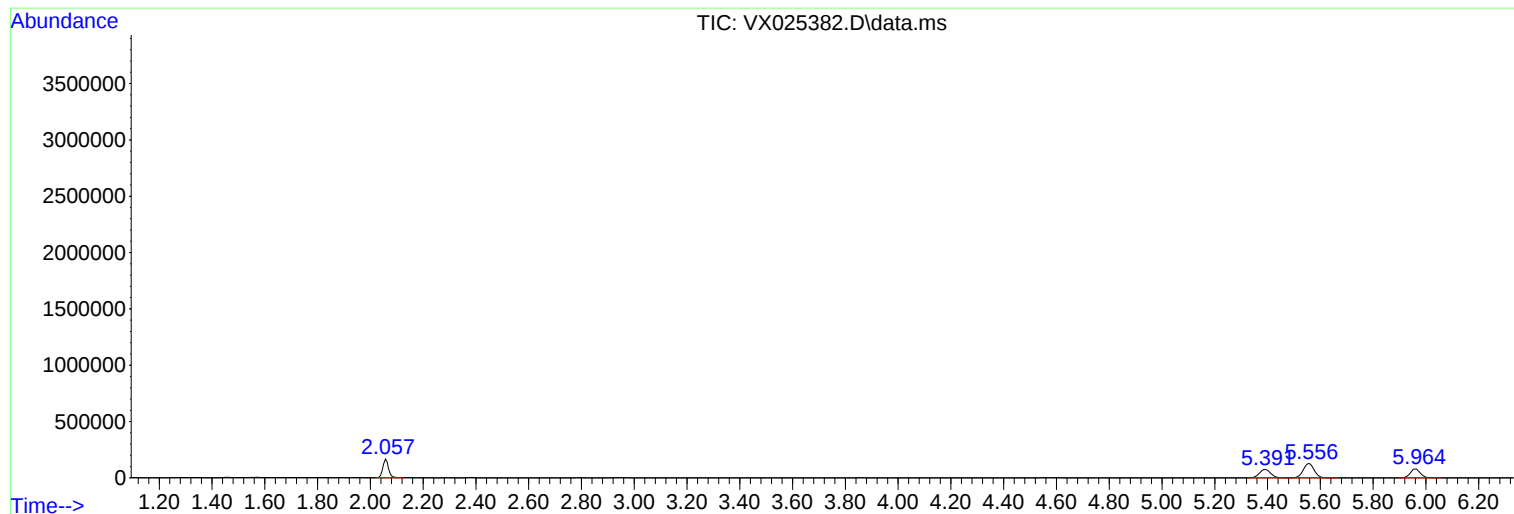
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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



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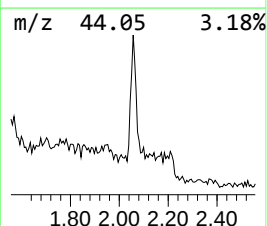
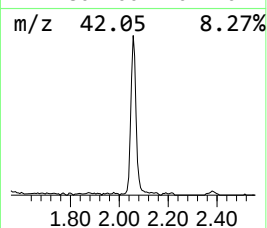
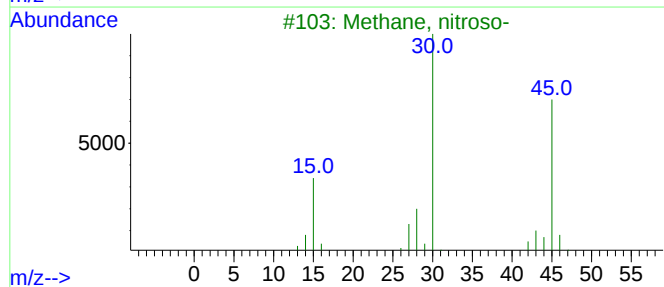
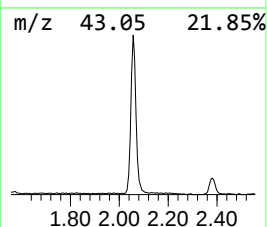
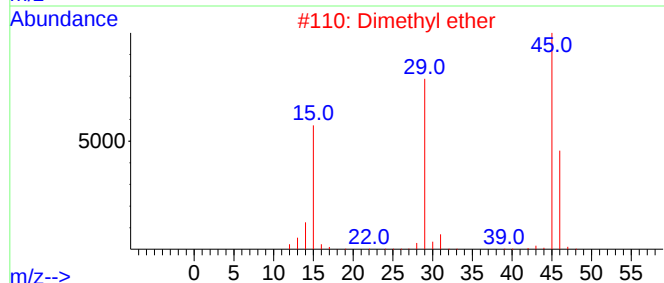
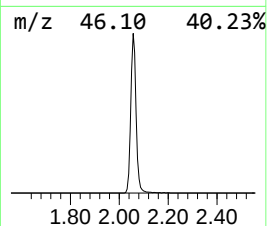
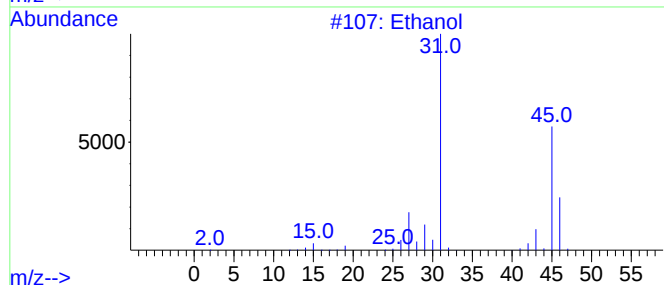
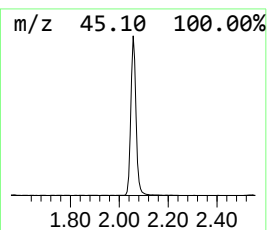
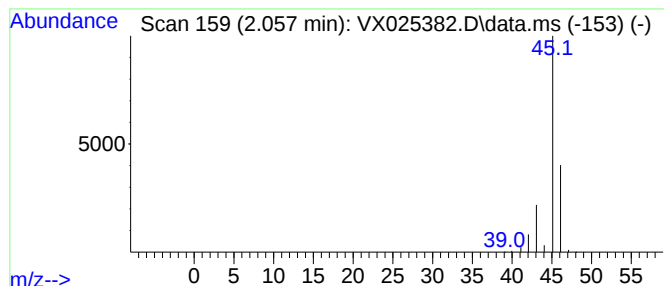
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.057	33.11 ug/l	242526	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	74
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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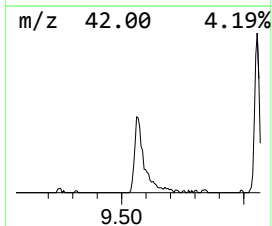
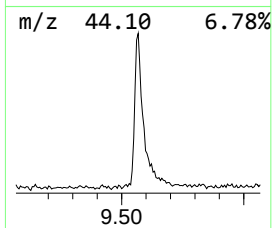
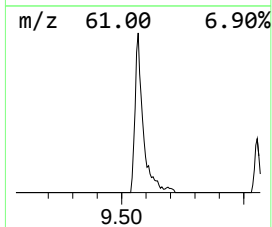
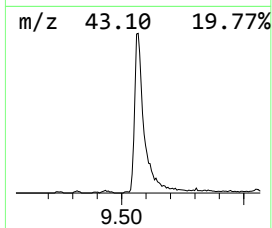
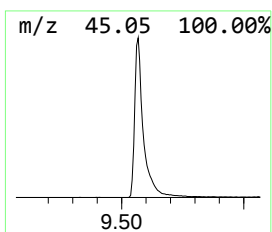
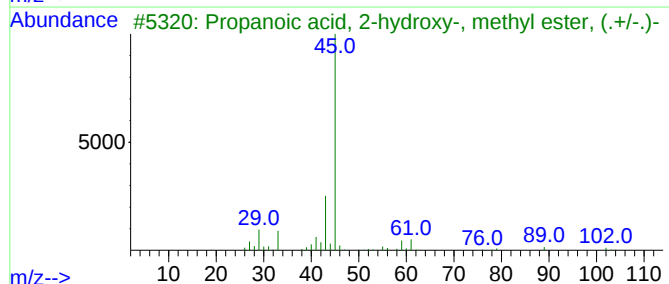
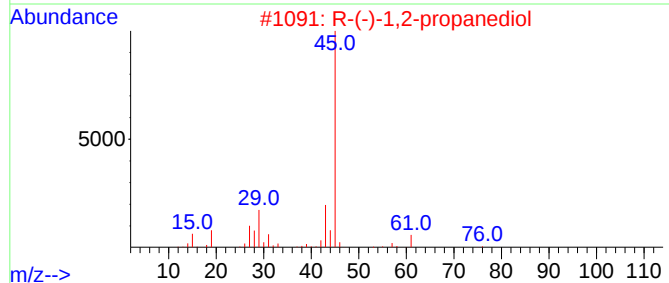
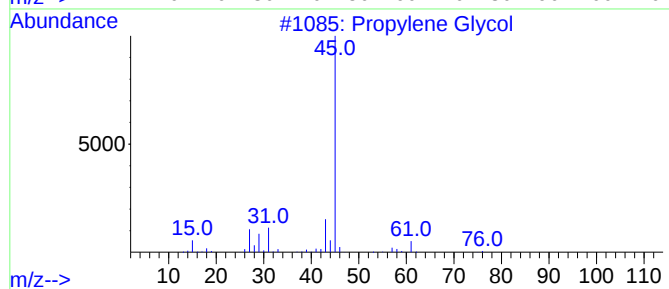
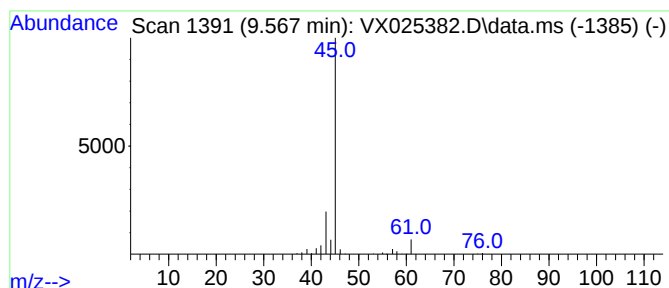
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
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Peak Number 2 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.567	17.25 ug/l	198954	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	78
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
5			(S)-(+)-2-Pentanol	88	C5H12O	026184-62-3	9



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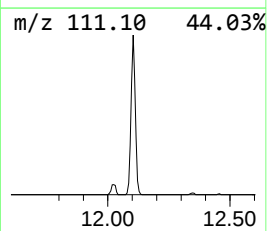
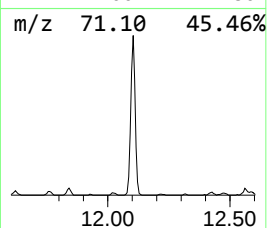
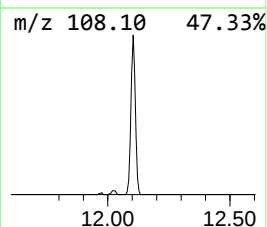
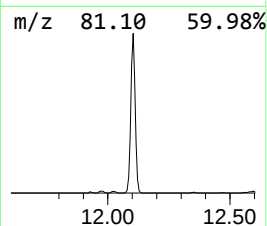
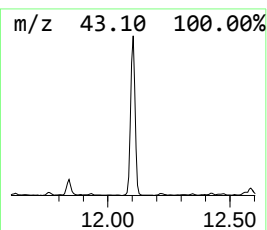
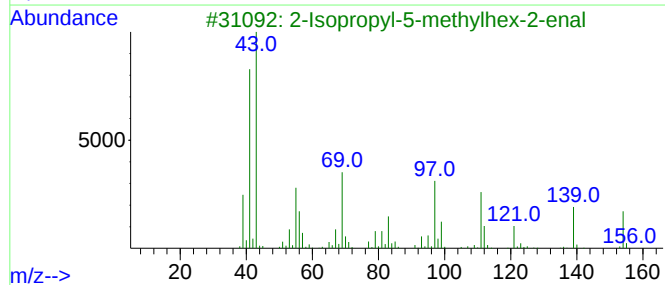
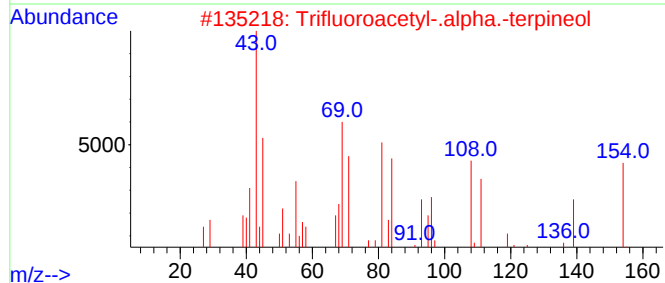
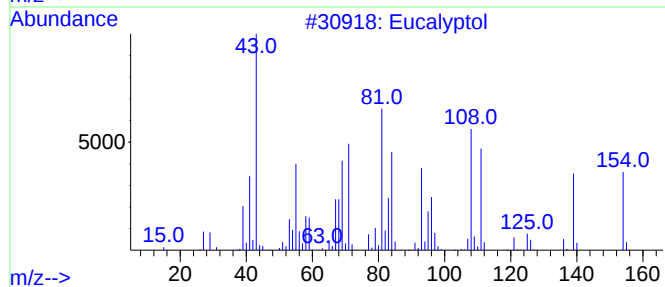
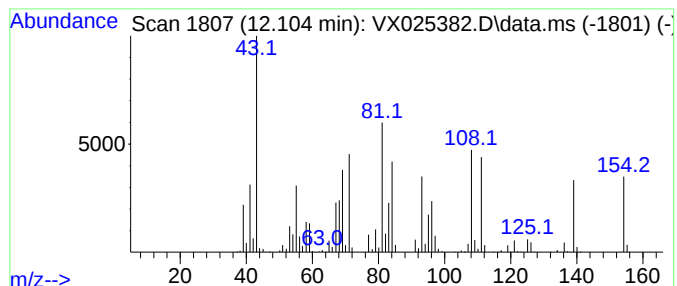
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Peak Number 3 Eucalyptol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.104	32.14 ug/l	369186	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	47
3			2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	27
4			3-Hepten-2-one, 3-propyl-	154	C10H18O	032064-69-0	25
5			2-Acetylcyclohexanone	154	C9H14O2	006126-53-0	22



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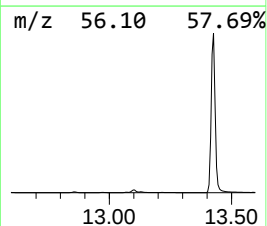
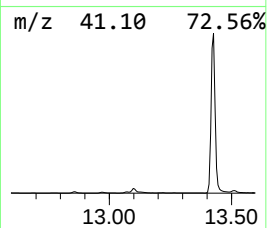
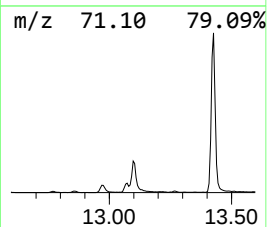
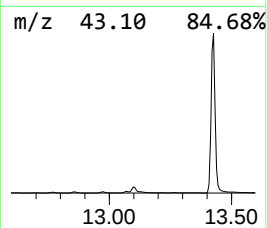
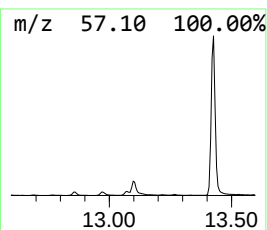
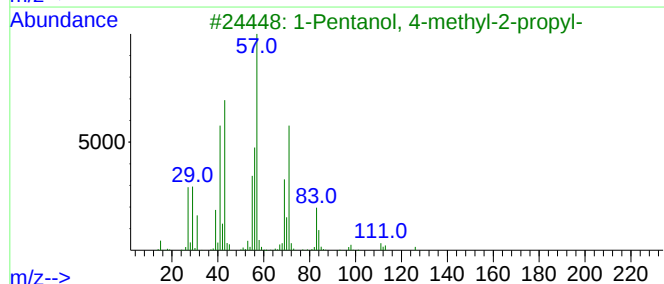
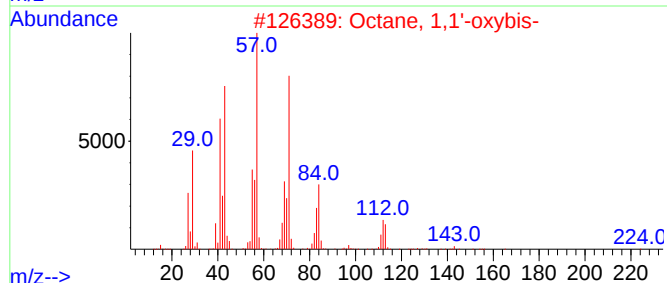
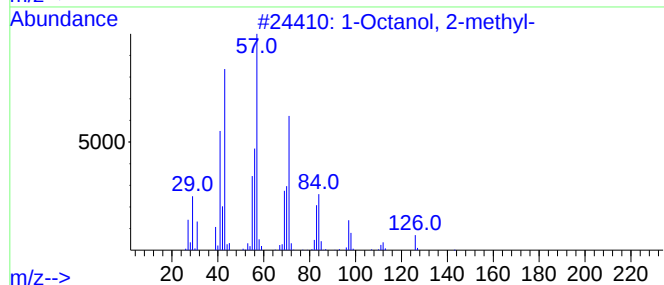
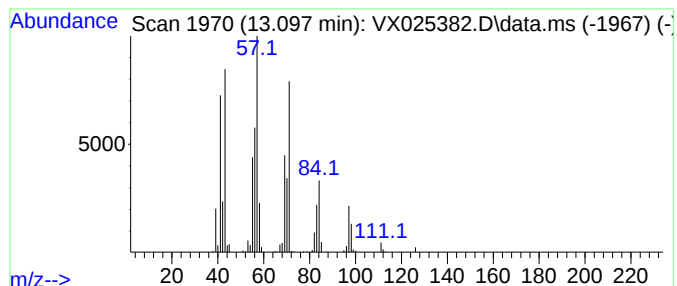
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Octanol, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.097	15.97 ug/l	183424	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	72
2			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	59
3			1-Pentanol, 4-methyl-2-propyl-	144	C9H20O	054004-41-0	53
4			Isobutyl pentyl carbonate	188	C10H20O3	178442-32-5	50
5			Decane, 1-fluoro-	160	C10H21F	000334-56-5	43



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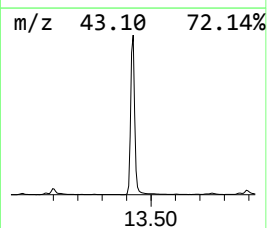
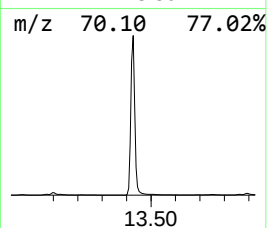
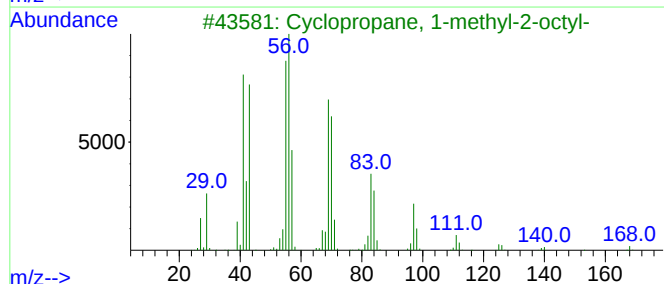
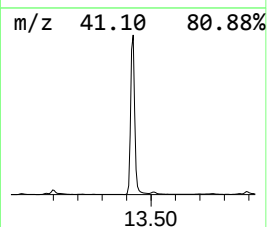
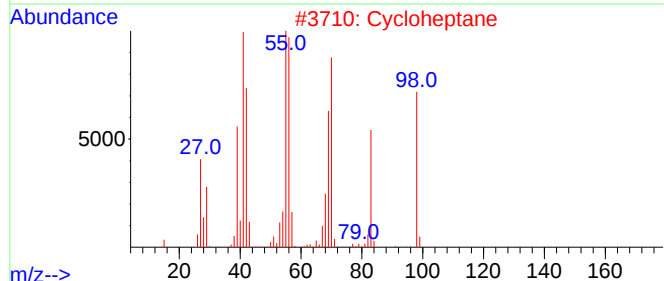
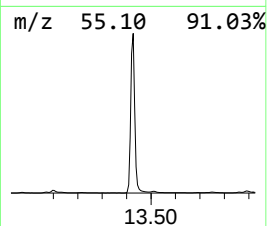
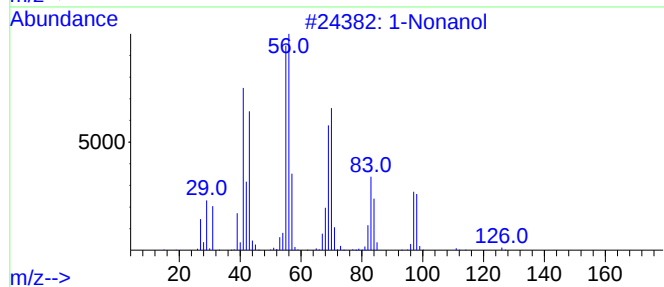
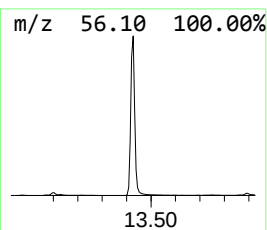
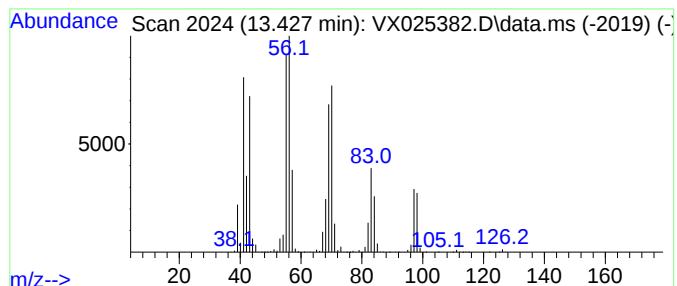
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Nonanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.427	387.94 ug/l	4456180	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonanol	144	C9H20O	000143-08-8	91
2			Cycloheptane	98	C7H14	000291-64-5	87
3			Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	72
4			Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	70
5			Isopropylcyclobutane	98	C7H14	000872-56-0	62



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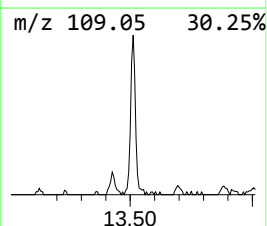
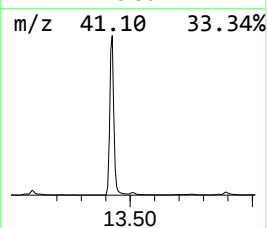
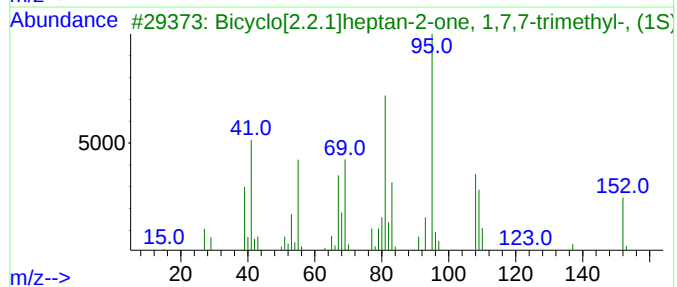
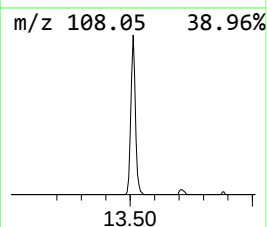
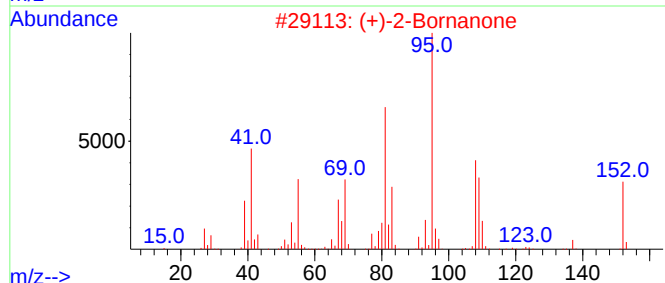
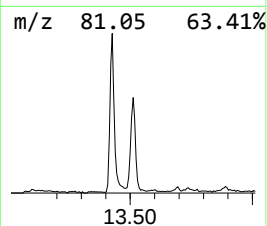
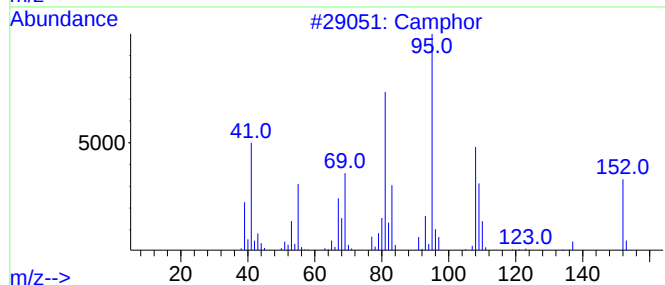
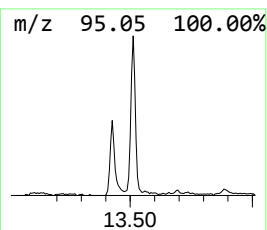
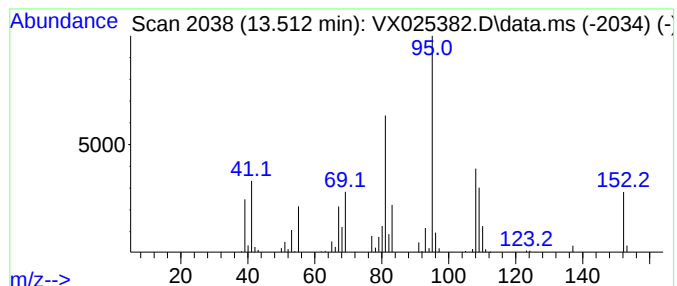
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Quant Title : SW846 8260

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

Peak Number 6 Camphor Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.512	10.83 ug/l	124381	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Camphor	152	C10H16O	000076-22-2	95
2			(+)-2-Bornanone	152	C10H16O	000464-49-3	95
3			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	94
4			2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46
5			4-Pyridinol	95	C5H5NO	000626-64-2	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
Data File : VX025382.D
Acq On : 29 Nov 2021 20:05
Operator : JC/MD
Sample : M4837-18 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20873

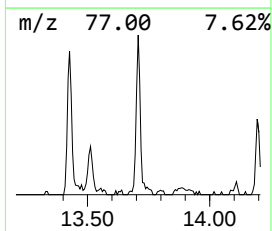
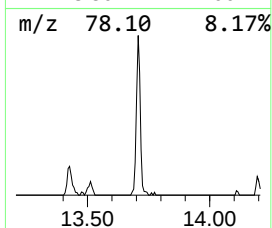
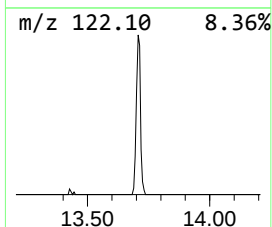
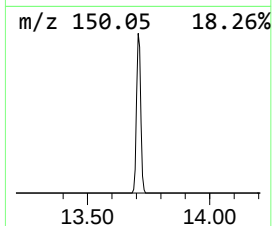
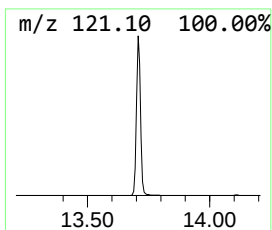
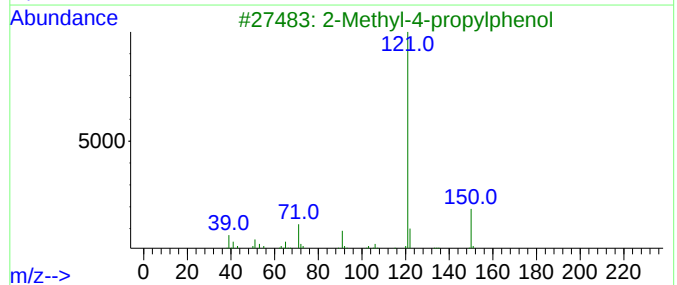
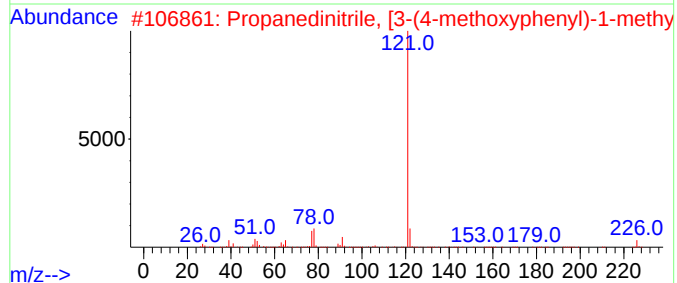
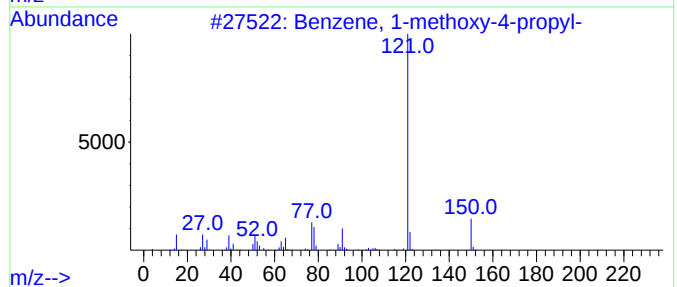
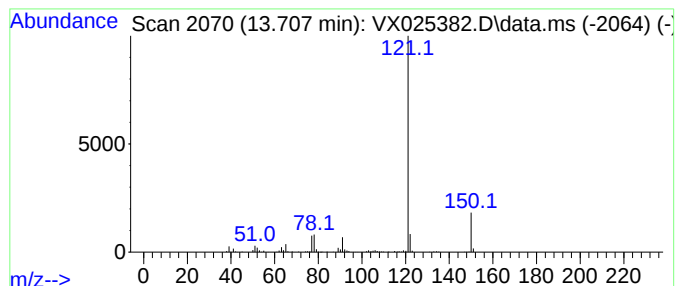
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-methoxy-4-propyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.707	9.87 ug/l	113381	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			Propanedinitrile, [3-(4-methoxyp...	226	C14H14N2O	069244-84-4	72
3			2-Methyl-4-propylphenol	150	C10H14O	018441-56-0	72
4			6-[4-Methoxybenzyloxy]-8-nitrole...	324	C18H16N2O4	1000213-39-1	72
5			4-Methoxybenzyl mercaptan, S-pen...	300	C11H9F5O2S	1000469-98-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
Data File : VX025382.D
Acq On : 29 Nov 2021 20:05
Operator : JC/MD
Sample : M4837-18 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20873

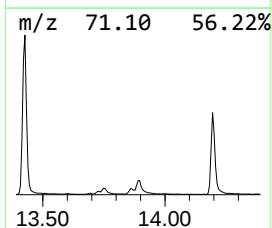
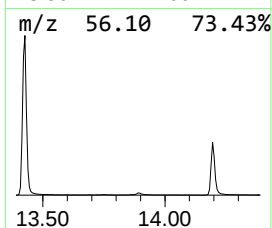
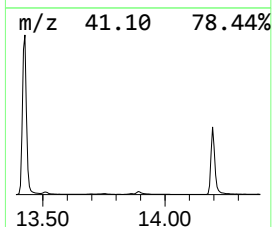
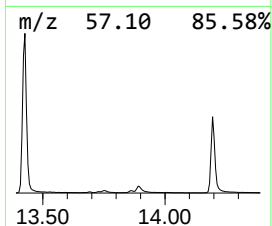
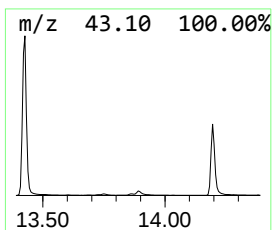
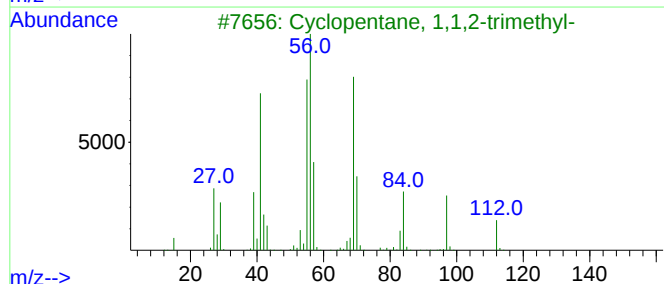
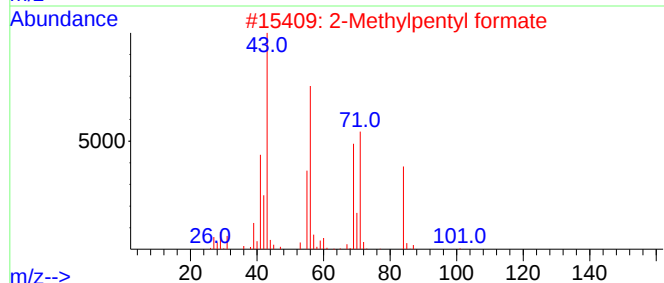
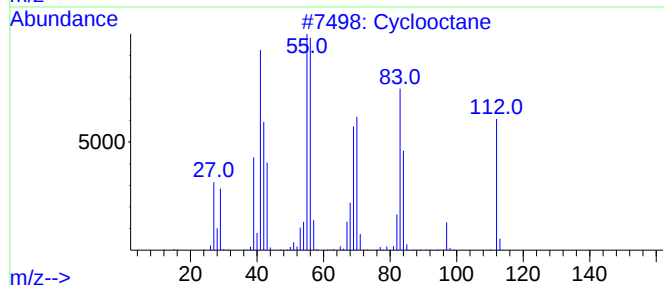
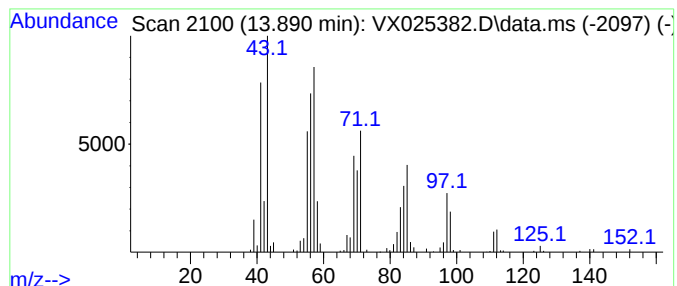
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Quant Title : SW846 8260

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

Peak Number 8 unknown13.890 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.890	11.08 ug/l	127229	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclooctane	112	C8H16	000292-64-8	45
2			2-Methylpentyl formate	130	C7H14O2	381670-34-4	43
3			Cyclopentane, 1,1,2-trimethyl-	112	C8H16	004259-00-1	38
4			3,3-Dimethyl-1,5-diazabicyclo[3....	112	C6H12N2	104518-71-0	38
5			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
Data File : VX025382.D
Acq On : 29 Nov 2021 20:05
Operator : JC/MD
Sample : M4837-18 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20873

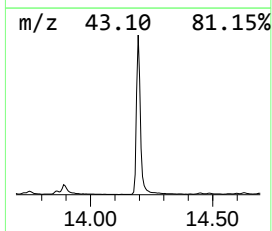
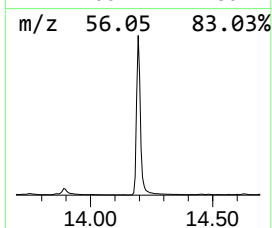
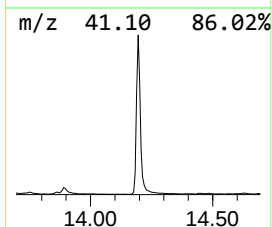
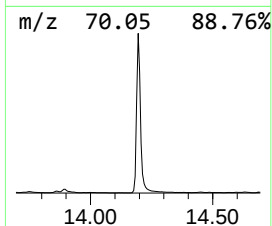
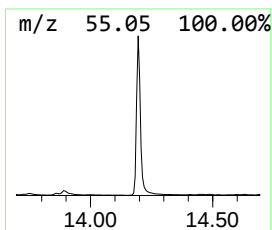
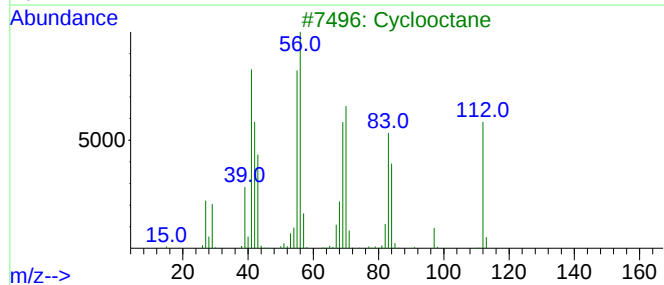
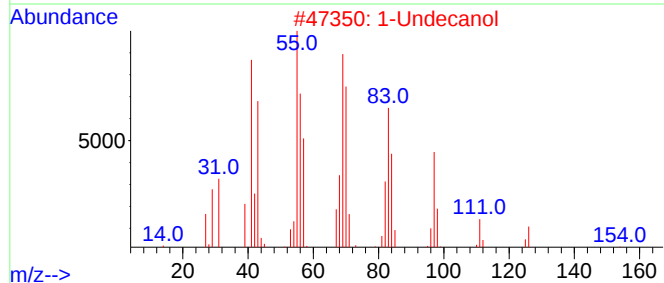
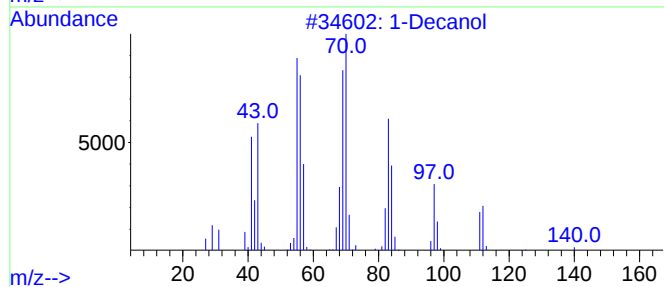
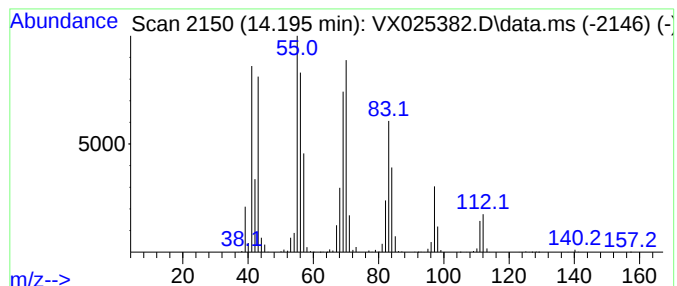
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Quant Title : SW846 8260

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

Peak Number 9 1-Decanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.195	179.91 ug/l	2066610	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol			158	C10H22O	000112-30-1	91
2	1-Undecanol			172	C11H24O	000112-42-5	91
3	Cyclooctane			112	C8H16	000292-64-8	87
4	Cyclopropane, 1-ethyl-2-heptyl-			168	C12H24	074663-86-8	86
5	Cyclopropane, 1-heptyl-2-methyl-			154	C11H22	074663-91-5	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
Data File : VX025382.D
Acq On : 29 Nov 2021 20:05
Operator : JC/MD
Sample : M4837-18 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20873

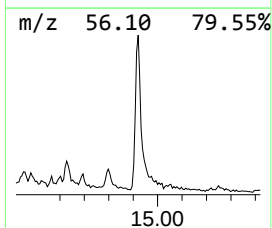
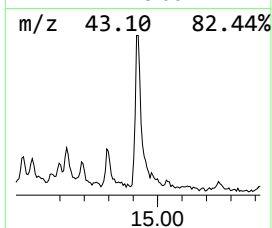
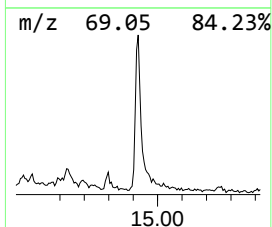
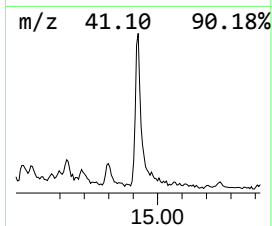
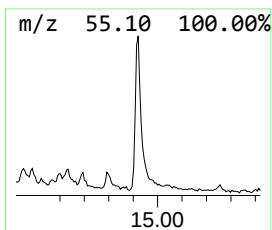
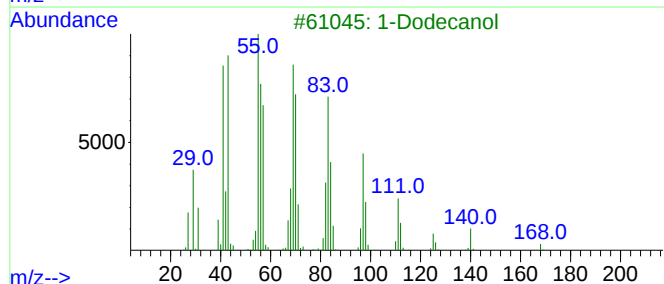
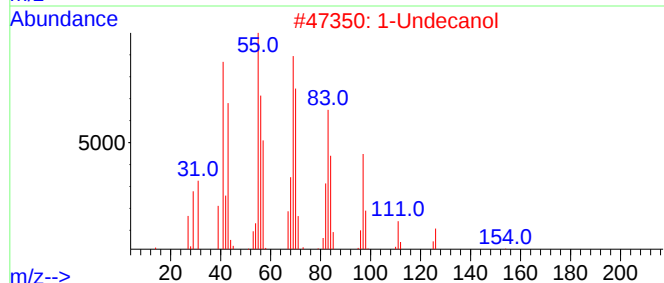
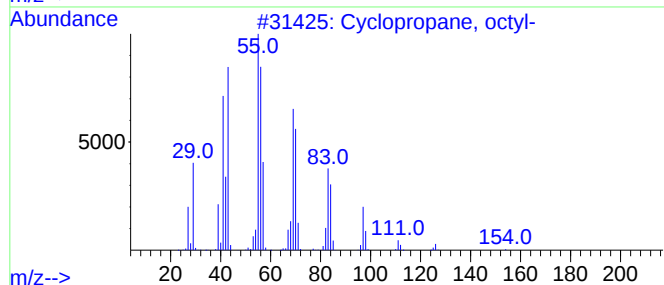
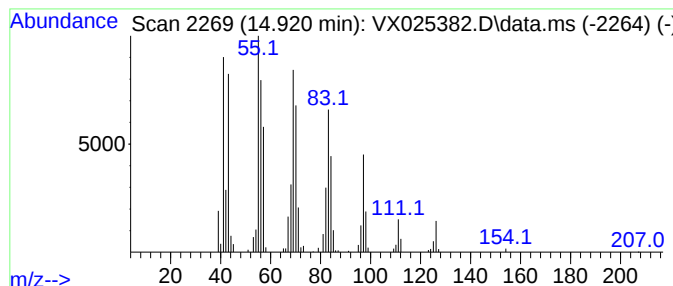
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Quant Title : SW846 8260

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

Peak Number 10 Cyclopropane, octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.920	13.04 ug/l	149738	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, octyl-	154	C11H22	001472-09-9	95
2			1-Undecanol	172	C11H24O	000112-42-5	91
3			1-Dodecanol	186	C12H26O	000112-53-8	90
4			n-Tridecan-1-ol	200	C13H28O	000112-70-9	87
5			Cyclodecane, methyl-	154	C11H22	013151-43-4	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
Data File : VX025382.D
Acq On : 29 Nov 2021 20:05
Operator : JC/MD
Sample : M4837-18 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20873

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.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
Ethanol	2.057	33.1	ug/l	242526	1	5.556	366251	50.0
Propylene Glycol	9.567	17.3	ug/l	198954	3	10.055	576847	50.0
Eucalyptol	12.104	32.1	ug/l	369186	4	12.024	574332	50.0
1-Octanol, 2-me...	13.097	16.0	ug/l	183424	4	12.024	574332	50.0
1-Nonanol	13.427	387.9	ug/l	4456180	4	12.024	574332	50.0
Camphor	13.512	10.8	ug/l	124381	4	12.024	574332	50.0
Benzene, 1-meth...	13.707	9.9	ug/l	113381	4	12.024	574332	50.0
unknown13.890	13.890	11.1	ug/l	127229	4	12.024	574332	50.0
1-Decanol	14.195	179.9	ug/l	2066610	4	12.024	574332	50.0
Cyclopropane, o...	14.920	13.0	ug/l	149738	4	12.024	574332	50.0