

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042122\
 Data File : VX028248.D
 Acq On : 21 Apr 2022 17:56
 Operator : JC/MD
 Sample : N2459-18
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 4922A

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\82X041922W.M
 Title : SW846 8260

Signal : TIC: VX028248.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.069	152	161	179	rBV	3405560	6011209	49.90%	12.892%
2	2.380	205	212	230	rBV	412599	699196	5.80%	1.500%
3	2.538	230	238	248	rBV	80408	166314	1.38%	0.357%
4	5.391	693	706	721	rBV	292626	852039	7.07%	1.827%
5	5.556	721	733	748	rVB	384148	1104135	9.17%	2.368%
6	5.958	788	799	818	rBV	303190	795613	6.60%	1.706%
7	6.763	921	931	948	rBV	609278	1452359	12.06%	3.115%
8	8.653	1234	1241	1248	rVV	1524142	2379830	19.76%	5.104%
9	10.055	1465	1471	1481	rBV	1397537	1825658	15.16%	3.915%
10	11.079	1630	1639	1651	rBV	1277745	1727189	14.34%	3.704%
11	11.896	1765	1773	1780	rVV2	3006378	5169405	42.91%	11.087%
12	11.951	1780	1782	1789	rVV2	290500	533862	4.43%	1.145%
13	12.024	1789	1794	1802	rVB	1623182	2103404	17.46%	4.511%
14	12.103	1802	1807	1811	rBV2	411524	546066	4.53%	1.171%
15	12.152	1811	1815	1818	rVV	72207	133401	1.11%	0.286%
16	12.219	1822	1826	1831	rVV	1195314	1807440	15.00%	3.876%
17	12.286	1831	1837	1846	rVV3	4604920	12046323	100.00%	25.835%
18	12.359	1846	1849	1864	rVB	1599174	2797703	23.22%	6.000%
19	12.585	1881	1886	1897	rBV	573513	791620	6.57%	1.698%
20	12.774	1912	1917	1923	rBV2	372554	675548	5.61%	1.449%
21	12.835	1923	1927	1929	rVV2	182817	323077	2.68%	0.693%
22	12.859	1929	1931	1945	rVB2	236189	393232	3.26%	0.843%
23	12.969	1946	1949	1956	rBV4	81758	152128	1.26%	0.326%
24	13.103	1968	1971	1974	rBV3	133976	208562	1.73%	0.447%
25	13.219	1986	1990	1995	rBV	79035	123993	1.03%	0.266%
26	13.426	2020	2024	2034	rBV	263410	414446	3.44%	0.889%
27	13.774	2078	2081	2088	rVB	134339	190719	1.58%	0.409%
28	13.847	2088	2093	2098	rBV4	54744	125184	1.04%	0.268%
29	14.195	2146	2150	2166	rBV3	263202	605986	5.03%	1.300%
30	14.755	2239	2242	2245	rBV	135330	146700	1.22%	0.315%
31	15.493	2357	2363	2369	rBV2	105104	158274	1.31%	0.339%
32	15.560	2369	2374	2380	rBV2	107064	166814	1.38%	0.358%

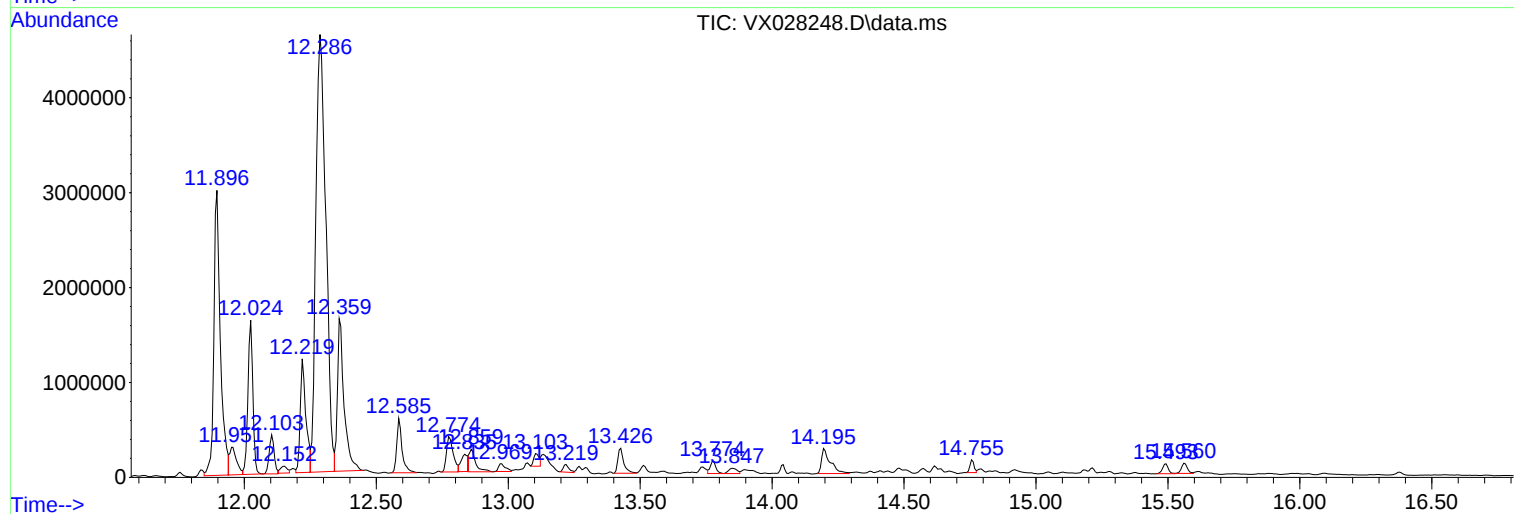
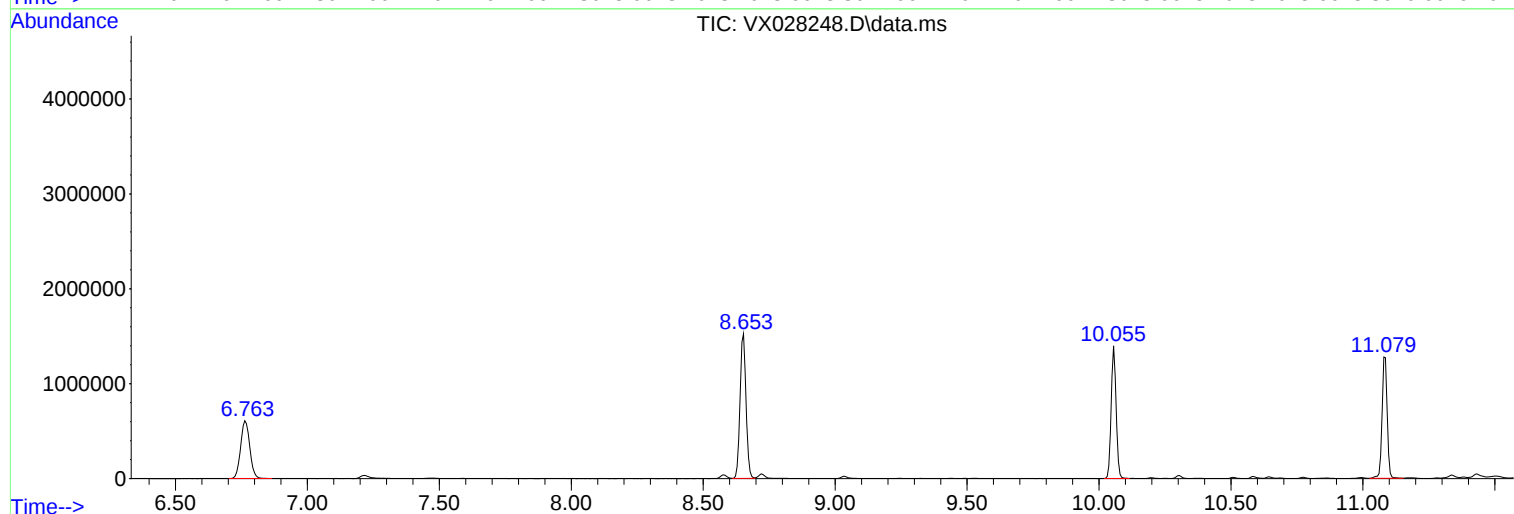
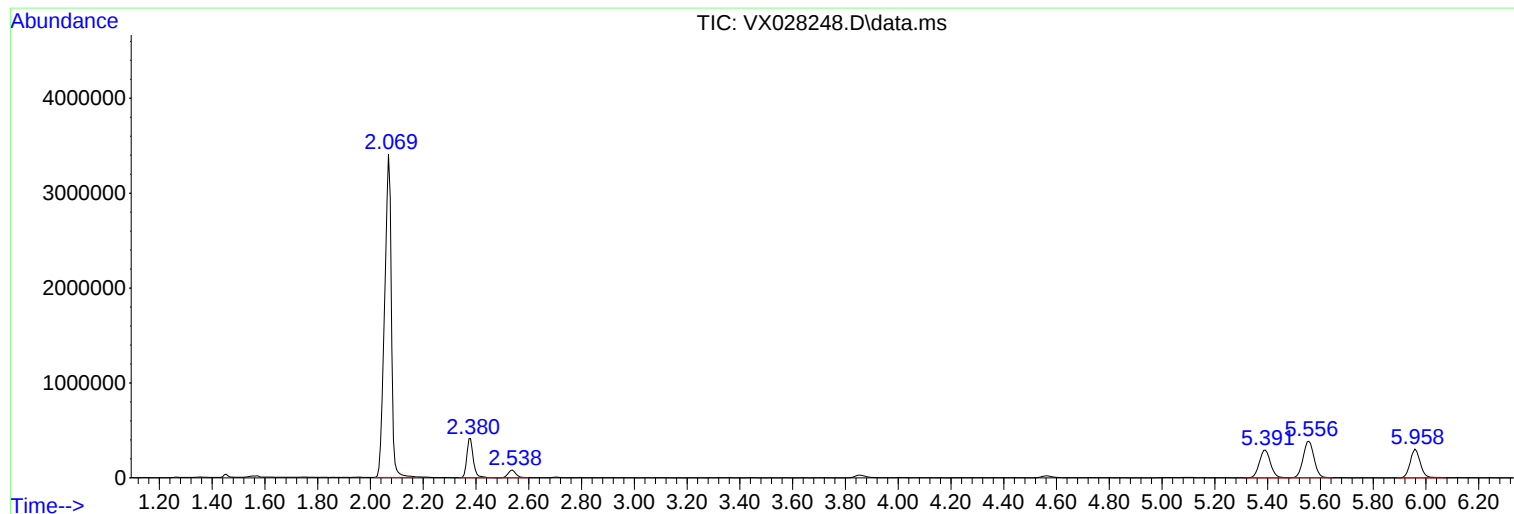
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Quant Title : SW846 8260

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



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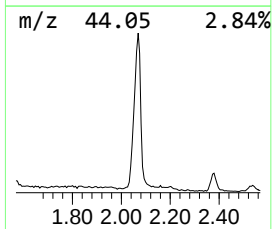
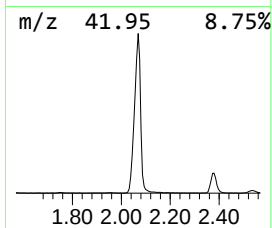
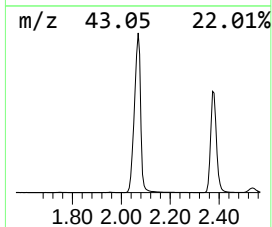
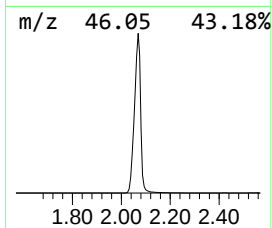
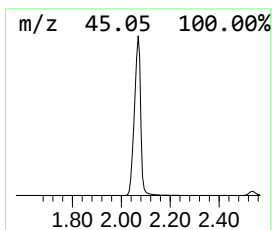
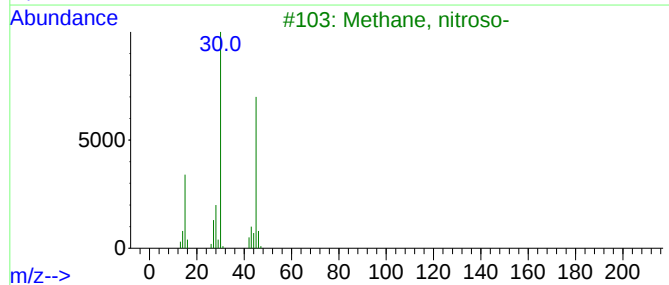
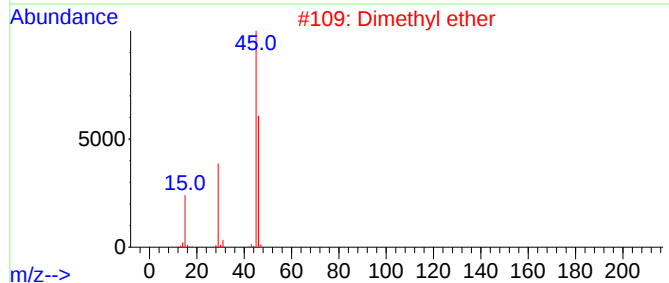
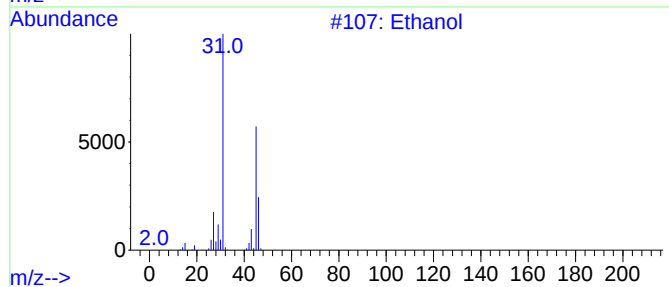
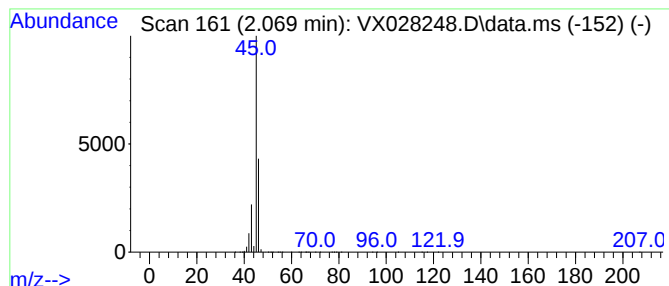
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.069	272.21 ug/l	6011210	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	83
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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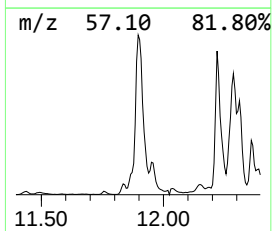
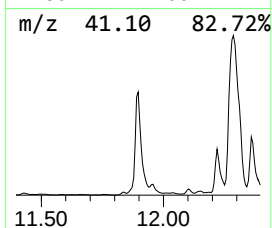
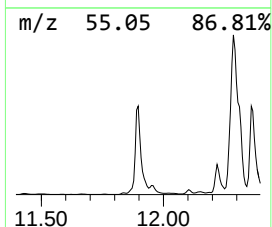
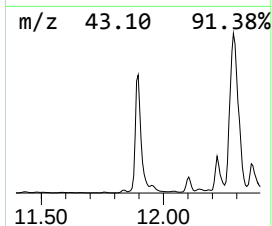
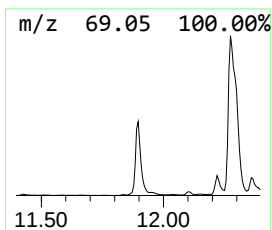
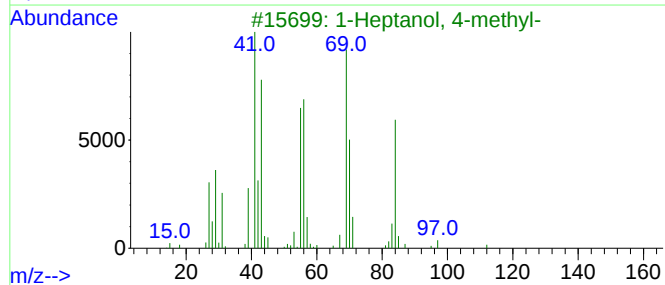
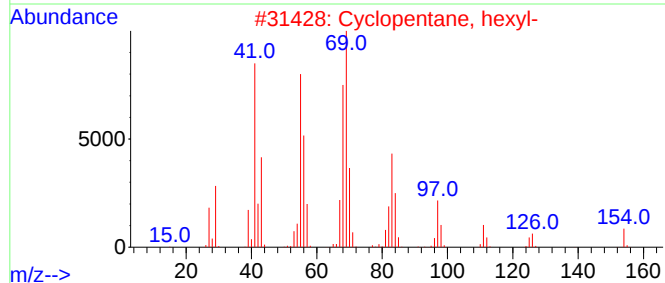
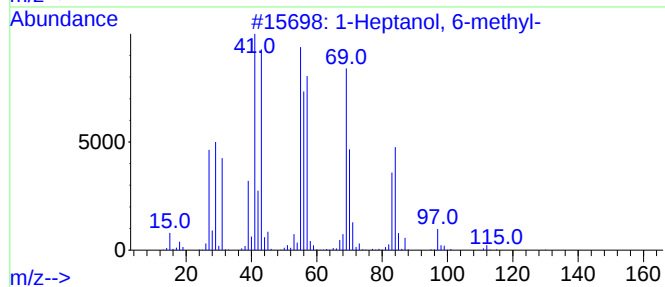
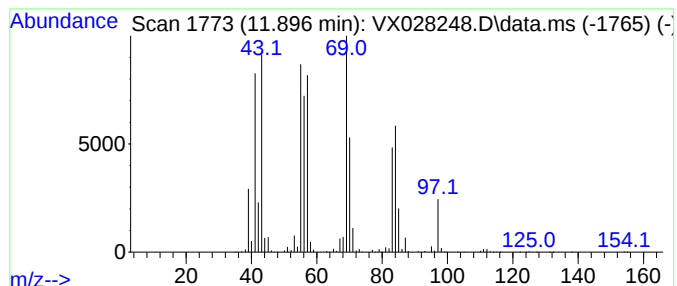
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Heptanol, 6-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.896	122.88 ug/l	5169410	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	80
2		Cyclopentane, hexyl-	154	C11H22	004457-00-5	64
3		1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	59
4		1-Undecanol	172	C11H24O	000112-42-5	47
5		3-Ethyl-4-methylpentan-1-ol	130	C8H18O	038514-13-5	43



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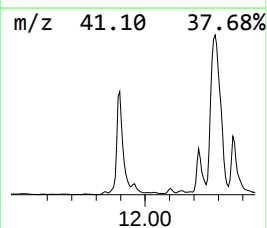
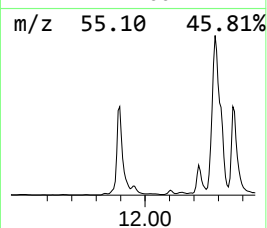
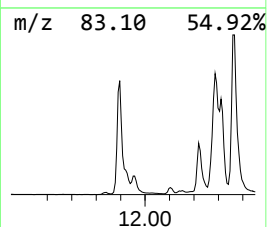
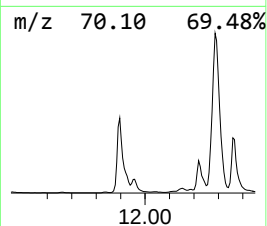
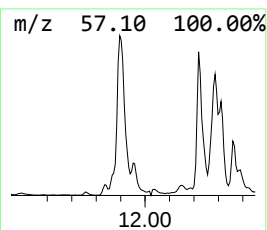
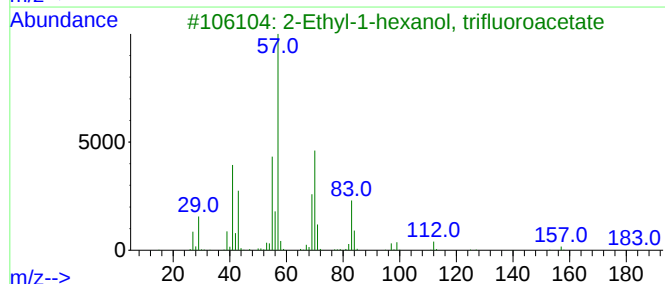
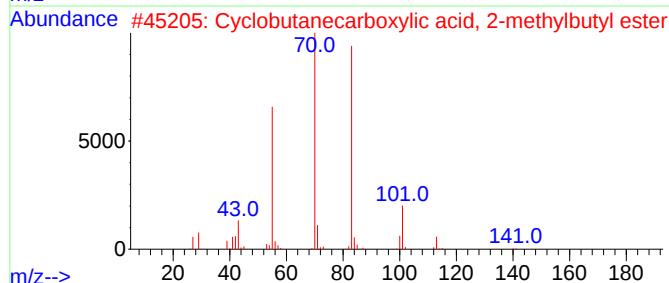
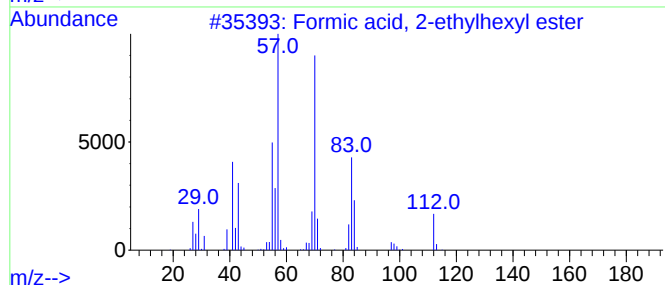
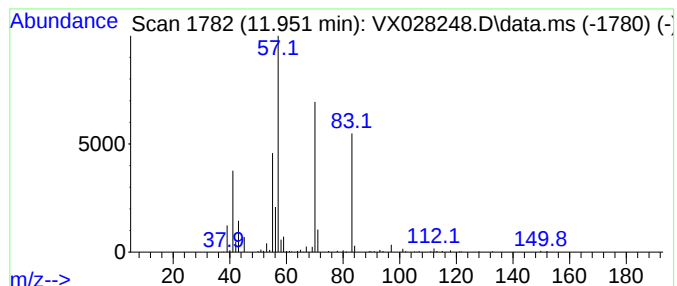
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Formic acid, 2-ethylhexyl e... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	12.69 ug/l	533862	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Formic acid, 2-ethylhexyl ester	158	C9H18O2	1000368-94-7	50
2			Cyclobutanecarboxylic acid, 2-me...	170	C10H18O2	1000331-08-4	40
3			2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	053800-08-1	38
4			1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	38
5			Propanoic acid, pentyl ester	144	C8H16O2	000624-54-4	37



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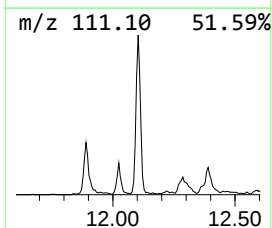
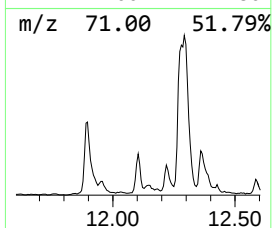
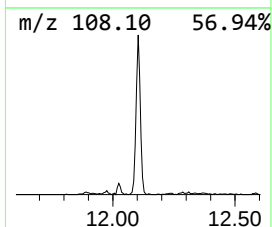
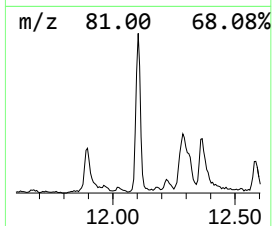
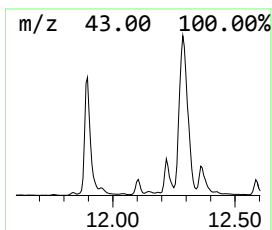
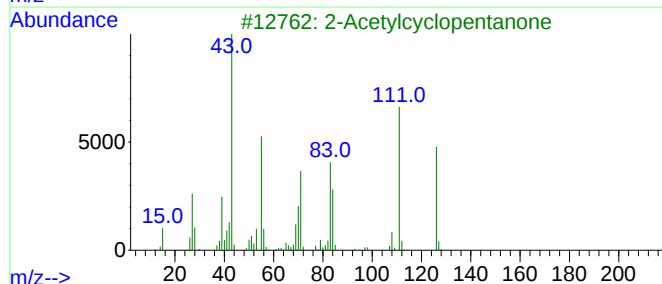
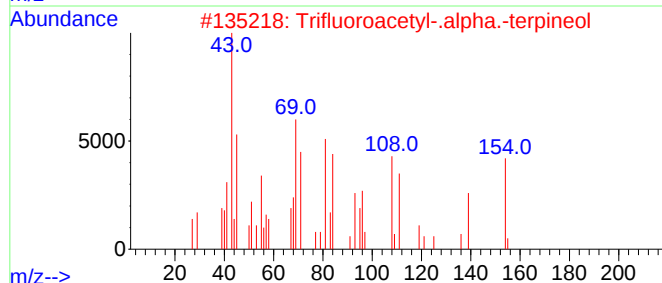
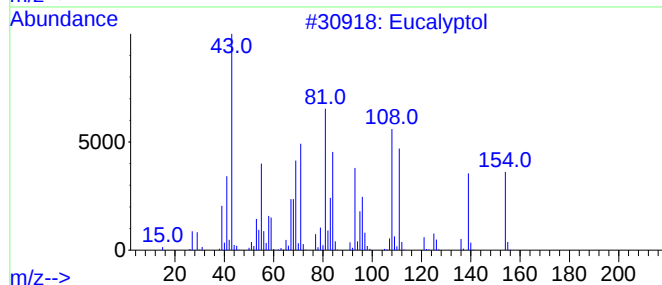
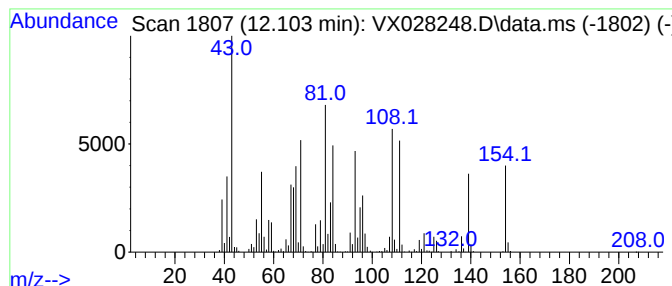
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Eucalyptol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.103	12.98 ug/l	546066	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	64
3			2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	27
4			2-Acetoncylclohexanone	154	C9H14O2	006126-53-0	27
5			3-Hepten-2-one, 3-propyl-	154	C10H18O	032064-69-0	15



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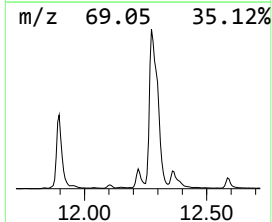
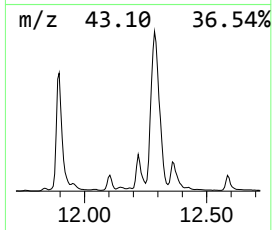
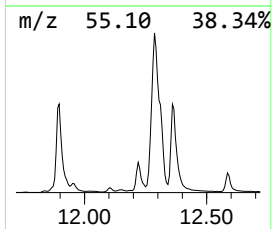
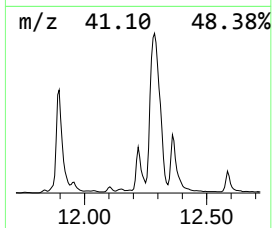
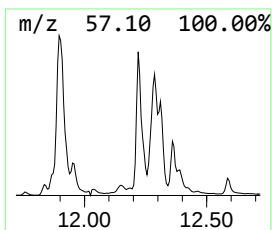
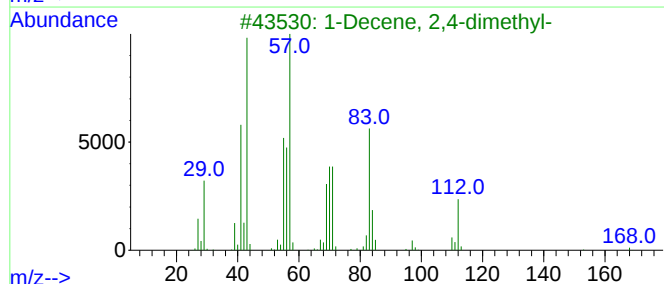
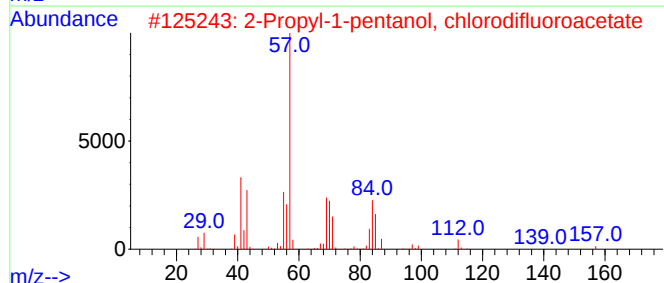
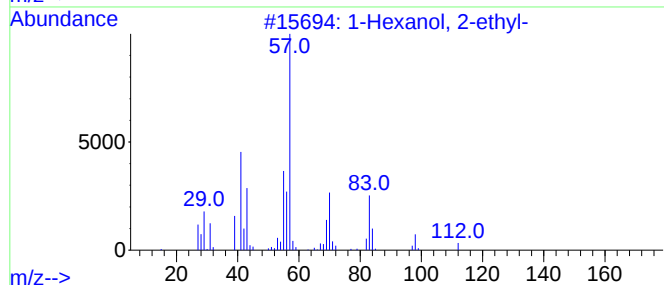
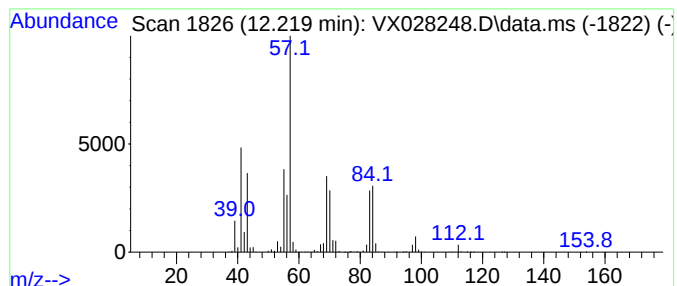
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	42.96 ug/l	1807440	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2			2-Propyl-1-pentanol, chlorodiflu...	242	C10H17ClF2O2	1000447-27-3	64
3			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	59
4			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	50
5			Formic acid, 2-propylpentyl ester	158	C9H18O2	1000368-74-8	50



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ALS Vial : 19 Sample Multiplier: 1

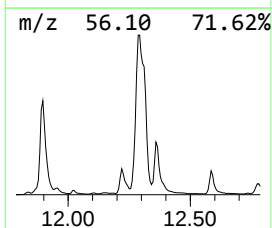
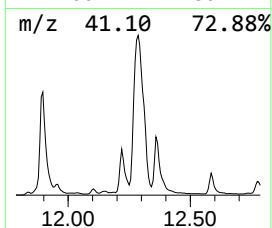
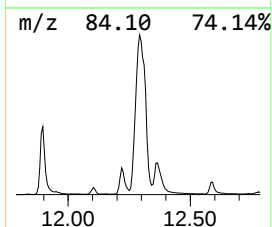
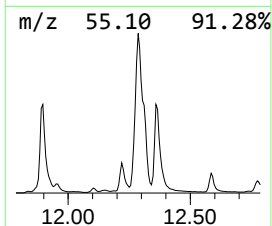
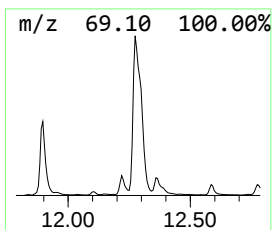
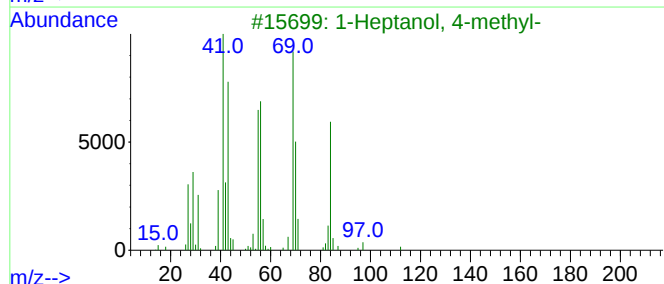
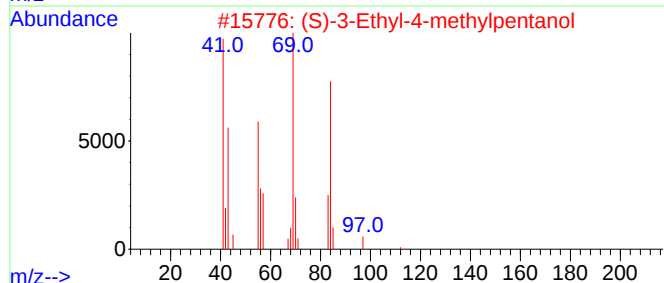
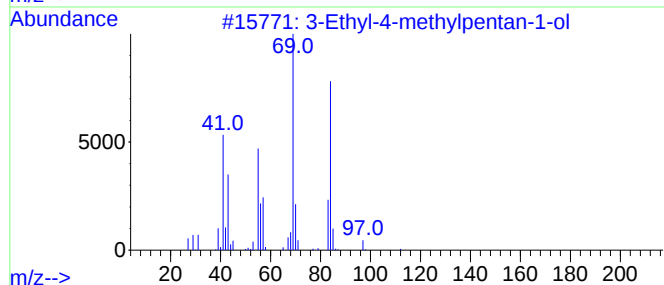
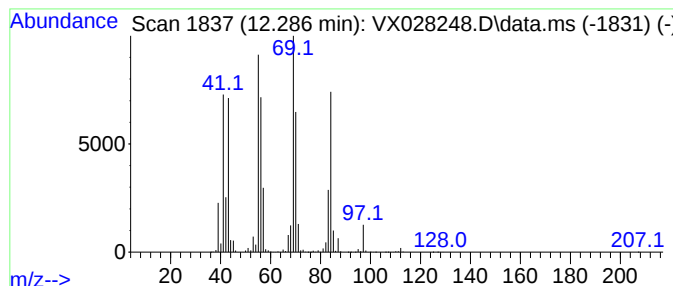
Instrument :
MSVOA_X
ClientSampleId :
4922A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 6 3-Ethyl-4-methylpentan-1-ol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.286	286.35 ug/l	12046300	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Ethyl-4-methylpentan-1-ol	130	C8H18O	038514-13-5	59
2	(S)-3-Ethyl-4-methylpentanol	130	C8H18O	1000144-07-1	59
3	1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	59
4	Formic acid, 3-methylpentyl ester	130	C7H14O2	1000368-21-3	53
5	(S)-(+)-3-Methyl-1-pentanol	102	C6H14O	042072-39-9	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042122\
Data File : VX028248.D
Acq On : 21 Apr 2022 17:56
Operator : JC/MD
Sample : N2459-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

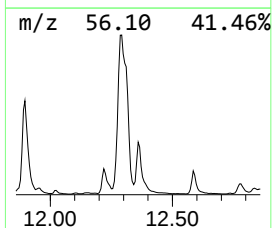
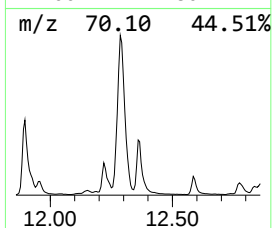
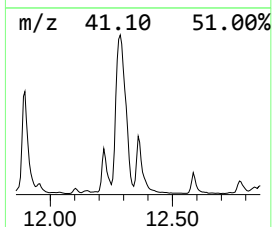
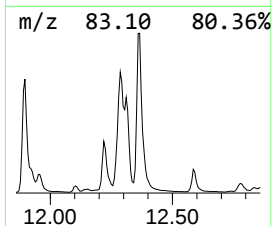
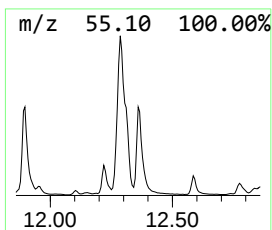
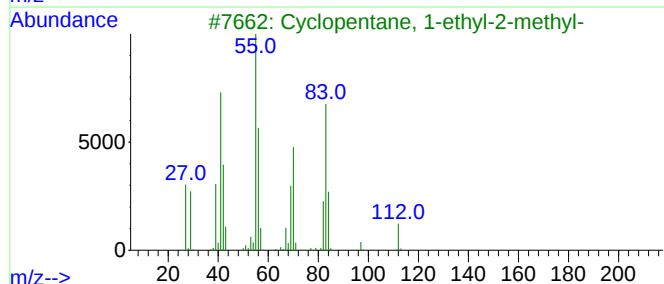
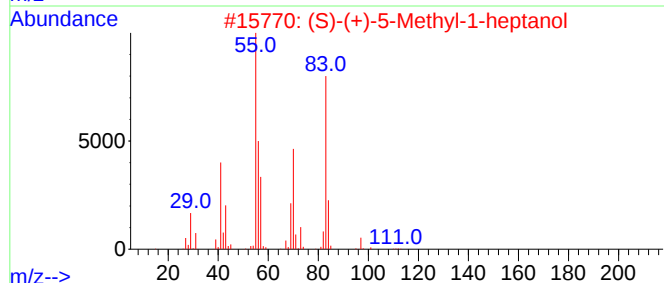
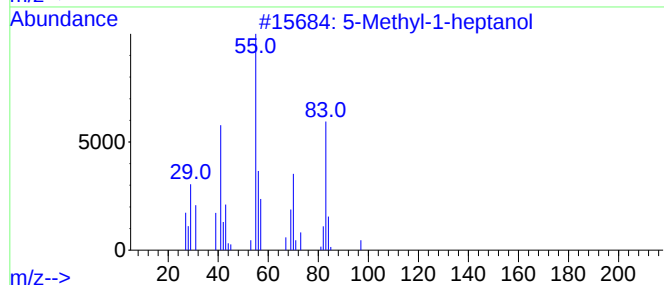
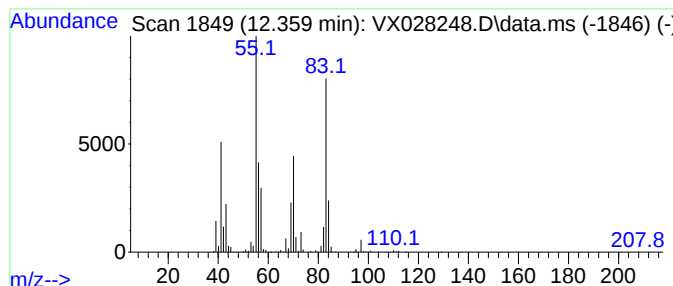
Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 7 5-Methyl-1-heptanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.360	66.50 ug/l	2797700	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Methyl-1-heptanol	130	C8H18O	007212-53-5	90
2	(S)-(+)-5-Methyl-1-heptanol	130	C8H18O	057803-73-3	90
3	Cyclopentane, 1-ethyl-2-methyl-	112	C8H16	003726-46-3	56
4	Cyclopentane, 1-ethyl-3-methyl-	112	C8H16	003726-47-4	45
5	Cyclobut-1-enylmethanol	84	C5H8O	089182-08-1	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042122\
Data File : VX028248.D
Acq On : 21 Apr 2022 17:56
Operator : JC/MD
Sample : N2459-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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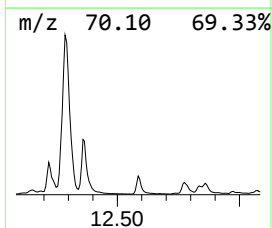
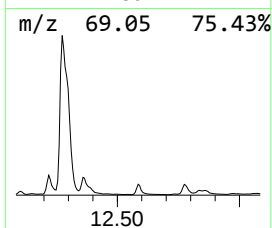
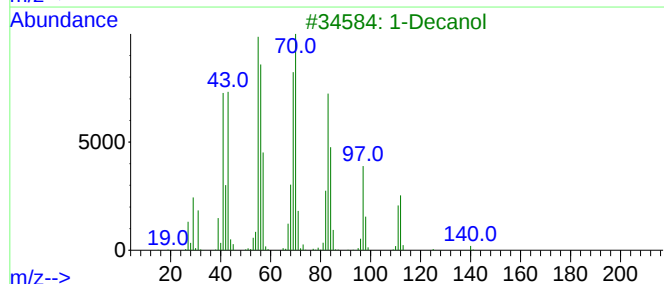
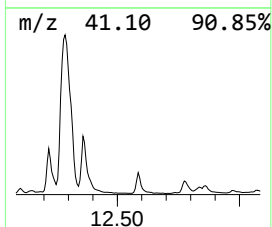
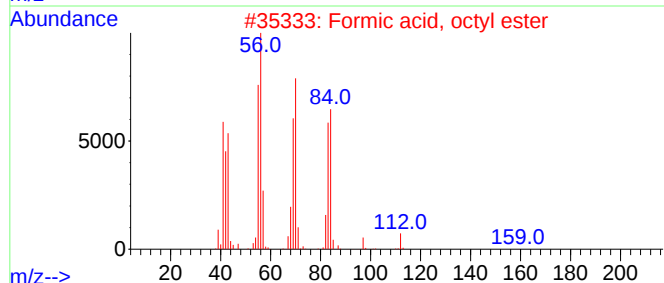
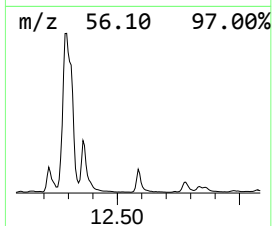
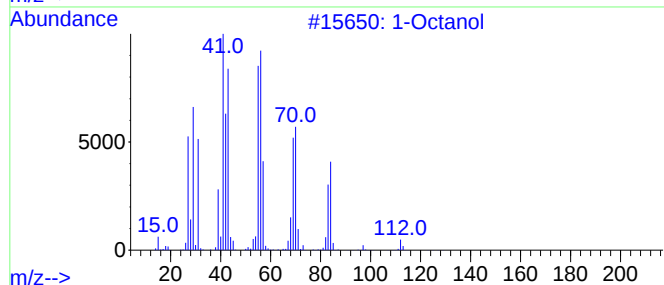
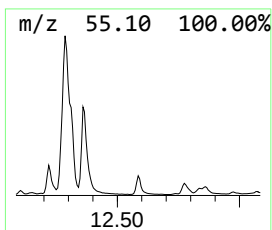
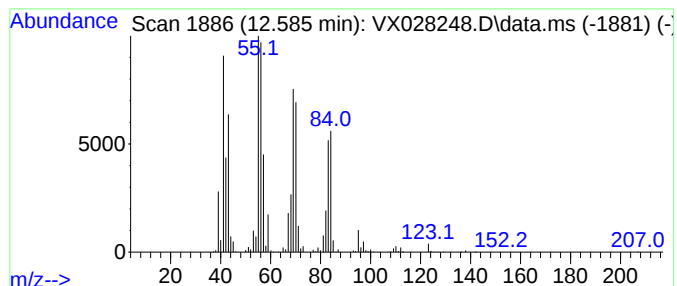
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Quant Title : SW846 8260

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

Peak Number 8 1-Octanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.585	18.82 ug/l	791620	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Octanol	130	C8H18O	000111-87-5	86
2		Formic acid, octyl ester	158	C9H18O2	000112-32-3	78
3		1-Decanol	158	C10H22O	000112-30-1	78
4		Cyclooctane	112	C8H16	000292-64-8	53
5		1-Undecanol	172	C11H24O	000112-42-5	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\WX042122\
Data File : VX028248.D
Acq On : 21 Apr 2022 17:56
Operator : JC/MD
Sample : N2459-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4922A

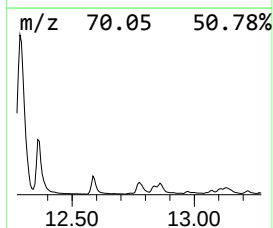
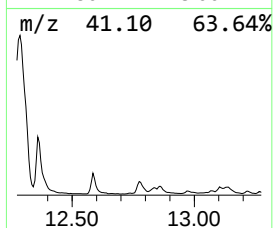
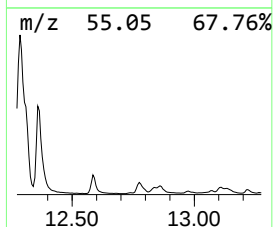
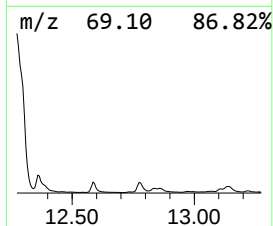
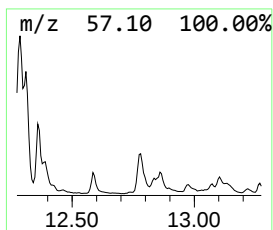
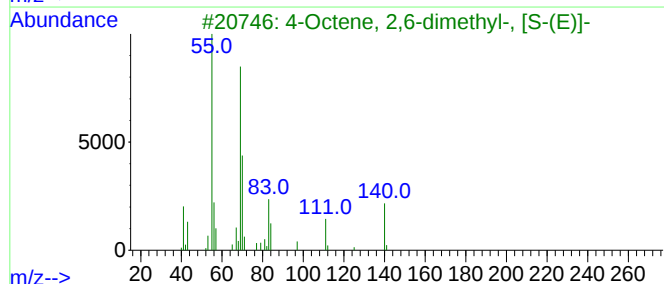
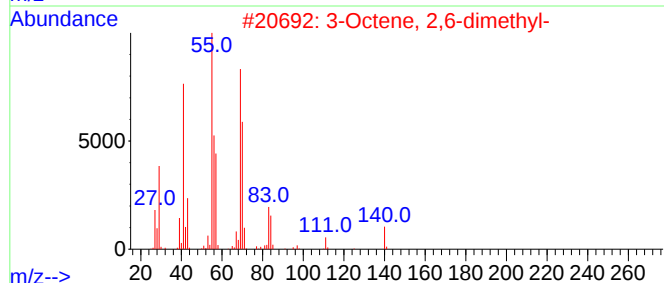
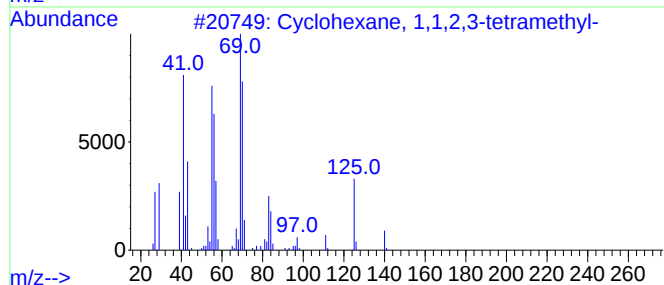
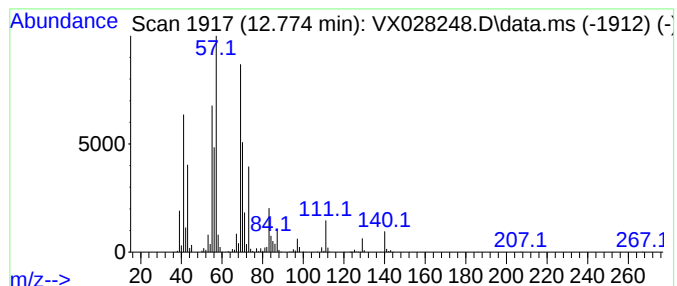
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 9 Cyclohexane, 1,1,2,3-tetram... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.774	16.06 ug/l	675548	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	81
2			3-Octene, 2,6-dimethyl-	140	C10H20	006874-28-8	74
3			4-Octene, 2,6-dimethyl-, [S-(E)]-	140	C10H20	062960-76-3	62
4			3-Octene, 4-ethyl-	140	C10H20	053966-51-1	58
5			2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042122\
Data File : VX028248.D
Acq On : 21 Apr 2022 17:56
Operator : JC/MD
Sample : N2459-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

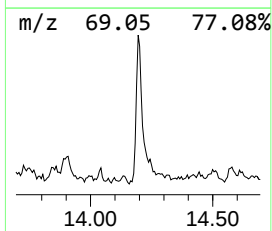
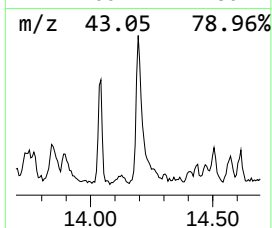
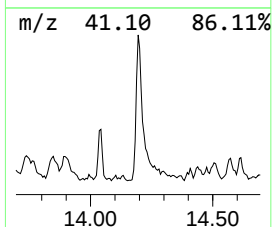
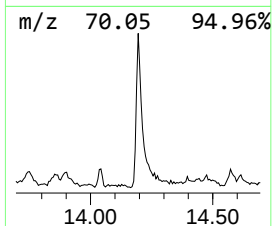
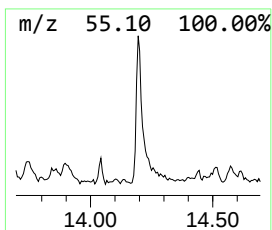
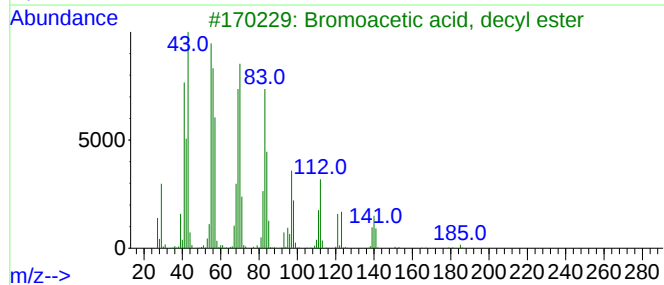
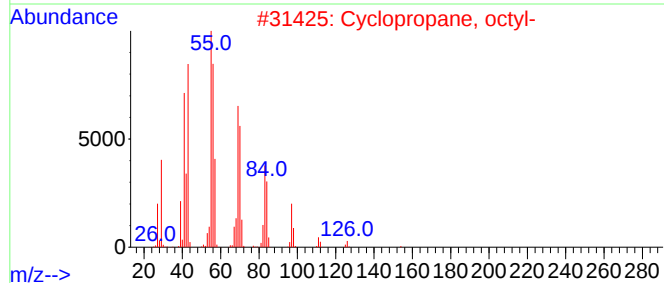
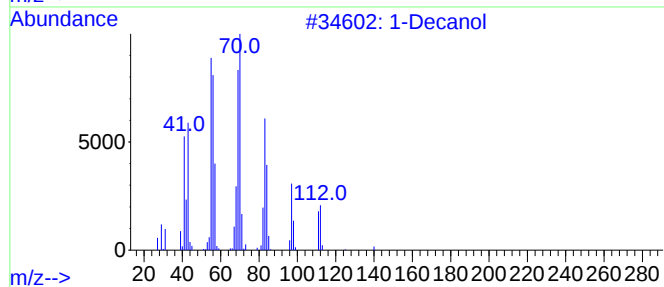
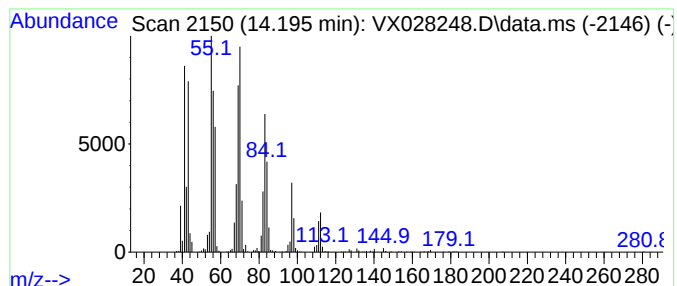
Instrument :
MSVOA_X
ClientSampleId :
4922A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

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

Peak Number 10 1-Decanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD			R.T.
14.195	14.40 ug/l	605986	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	Cyclopropane, octyl-		154	C11H22	001472-09-9	91
3	Bromoacetic acid, decyl ester		278	C12H23BrO2	005436-93-1	91
4	1-Dodecanol		186	C12H26O	000112-53-8	90
5	Cyclopropane, 1-ethyl-2-heptyl-		168	C12H24	074663-86-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042122\
 Data File : VX028248.D
 Acq On : 21 Apr 2022 17:56
 Operator : JC/MD
 Sample : N2459-18
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 4922A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.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	2.069	272.2	ug/l	6011210	1	5.556	1104140	50.0
1-Heptanol, 6-m...	11.896	122.9	ug/l	5169410	4	12.024	2103400	50.0
Formic acid, 2-...	11.951	12.7	ug/l	533862	4	12.024	2103400	50.0
Eucalyptol	12.103	13.0	ug/l	546066	4	12.024	2103400	50.0
1-Hexanol, 2-et...	12.219	43.0	ug/l	1807440	4	12.024	2103400	50.0
3-Ethyl-4-methy...	12.286	286.4	ug/l	12046300	4	12.024	2103400	50.0
5-Methyl-1-hept...	12.360	66.5	ug/l	2797700	4	12.024	2103400	50.0
1-Octanol	12.585	18.8	ug/l	791620	4	12.024	2103400	50.0
Cyclohexane, 1,...	12.774	16.1	ug/l	675548	4	12.024	2103400	50.0
1-Decanol	14.195	14.4	ug/l	605986	4	12.024	2103400	50.0