

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041525\
 Data File : VX045792.D
 Acq On : 15 Apr 2025 12:26
 Operator : JC/MD
 Sample : Q1794-04 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 40325-A-B-COMP

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\82X040225W.M

Title : SW846 8260

Signal : TIC: VX045792.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.075	157	162	180	rBV	38219	76124	3.91%	1.352%
2	5.379	694	704	721	rBV2	60548	177805	9.13%	3.159%
3	5.544	721	731	747	rVV	88291	250411	12.85%	4.449%
4	5.952	788	798	815	rBV	73591	195873	10.05%	3.480%
5	6.757	921	930	948	rBV	151248	371520	19.07%	6.601%
6	7.226	999	1007	1024	rBV2	12535	41578	2.13%	0.739%
7	8.647	1234	1240	1256	rBV	318163	517266	26.55%	9.190%
8	10.049	1465	1470	1487	rBV	338918	471335	24.19%	8.374%
9	11.079	1634	1639	1651	rVB	284279	362175	18.59%	6.435%
10	12.018	1788	1793	1802	rBV	340858	428598	22.00%	7.615%
11	12.213	1821	1825	1838	rBV	71537	124144	6.37%	2.206%
12	12.585	1881	1886	1913	rBV	1445844	1948238	100.00%	34.613%
13	12.817	1920	1924	1928	rBV2	21228	25141	1.29%	0.447%
14	13.731	2069	2074	2079	rBV	49722	64917	3.33%	1.153%
15	14.195	2145	2150	2175	rBV	258403	496698	25.49%	8.825%
16	15.560	2368	2374	2381	rBV	53460	76794	3.94%	1.364%

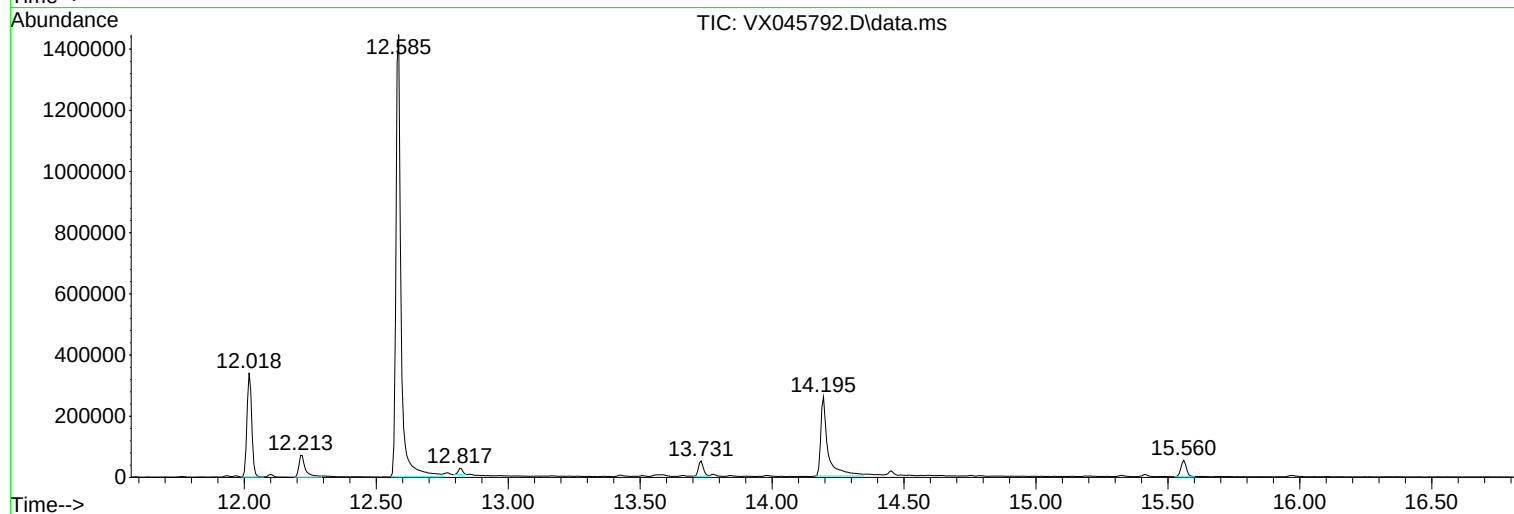
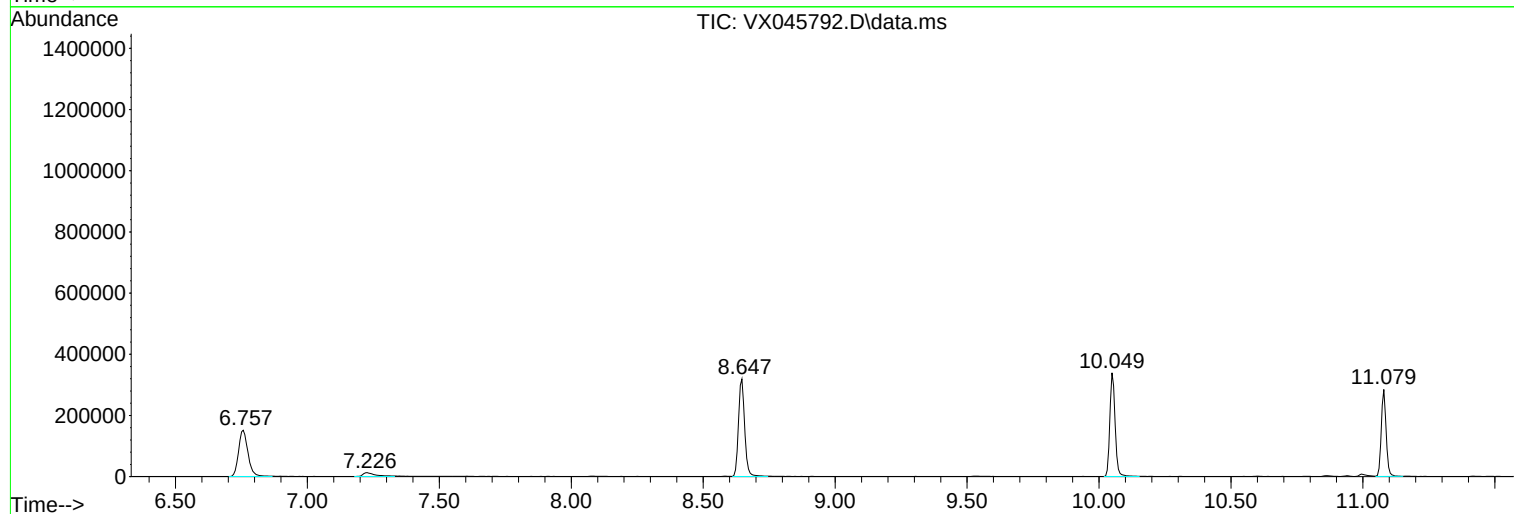
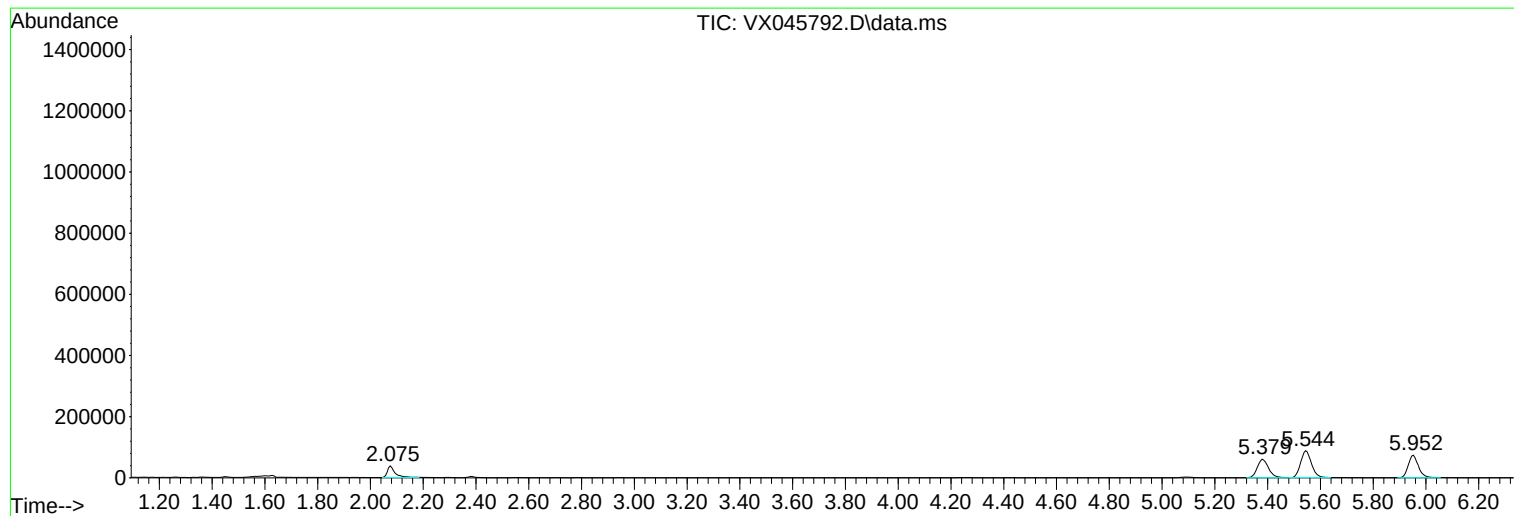
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

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



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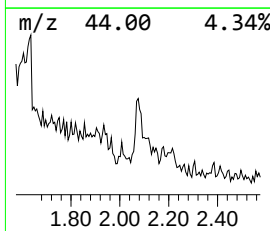
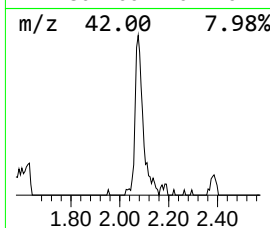
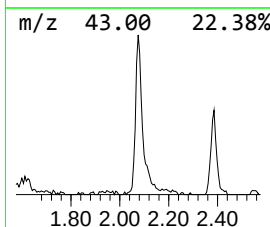
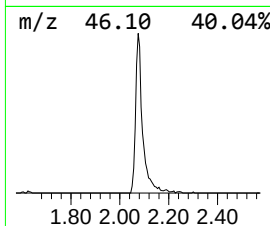
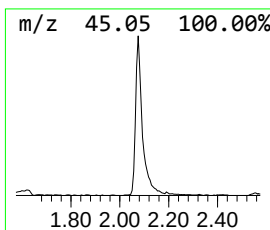
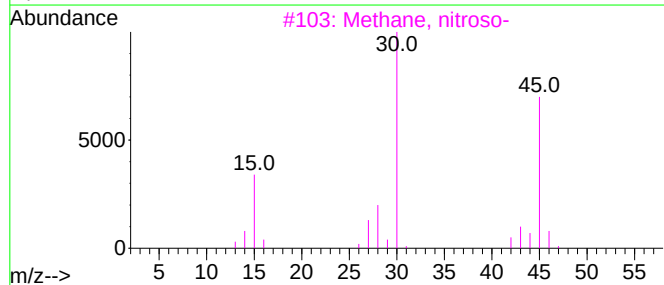
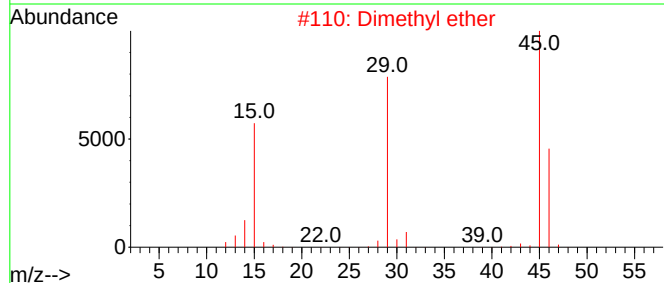
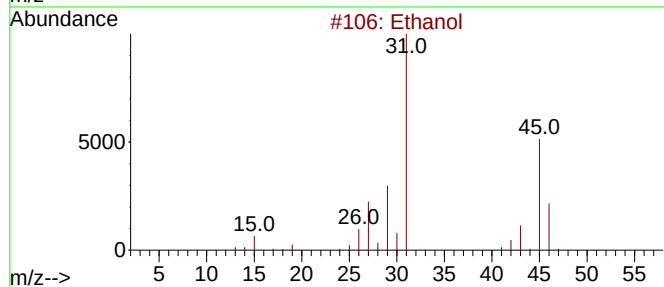
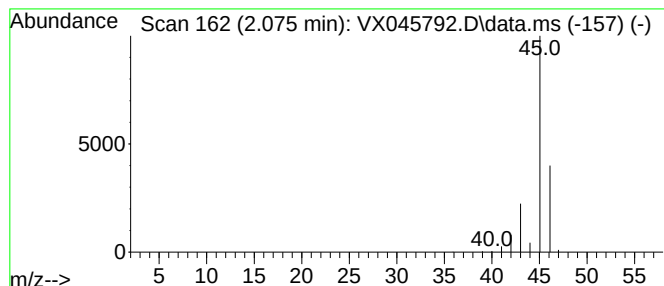
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Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.075	15.20 ug/l	76124	Pentafluorobenzene	5.544

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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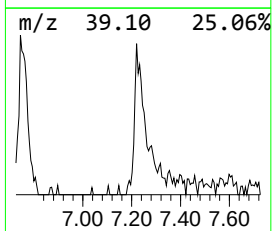
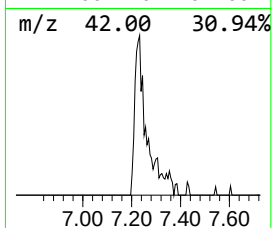
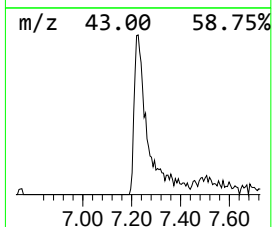
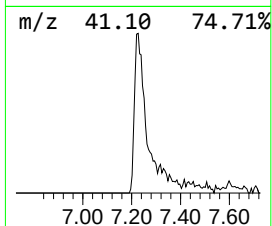
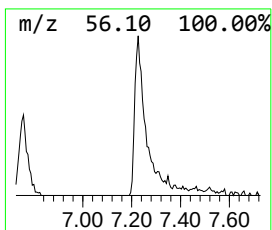
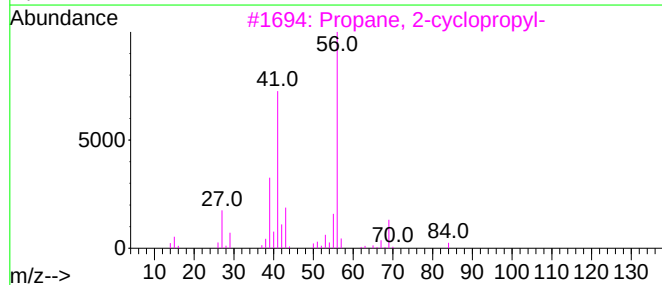
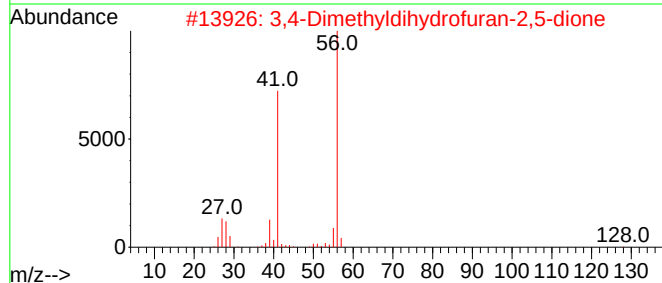
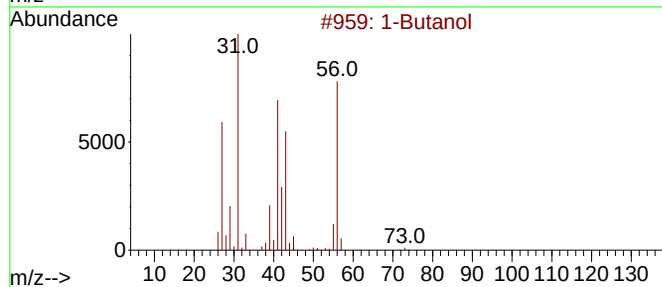
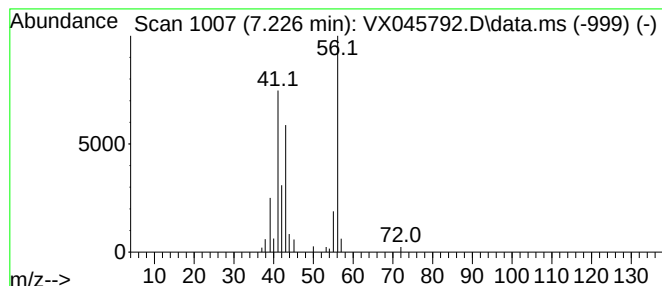
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.226	5.60 ug/l	41578	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol			74	C4H10O	000071-36-3	83
2	3,4-Dimethyldihydrofuran-2,5-dione			128	C6H8O3	007475-92-5	42
3	Propane, 2-cyclopropyl-			84	C6H12	003638-35-5	39
4	Cyclobutane, ethyl-			84	C6H12	004806-61-5	9
5	Butane, 1-chloro-			92	C4H9Cl	000109-69-3	9



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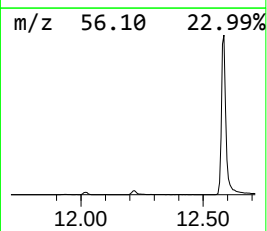
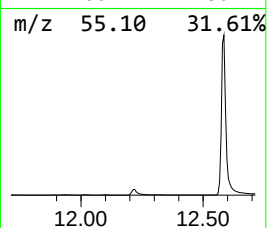
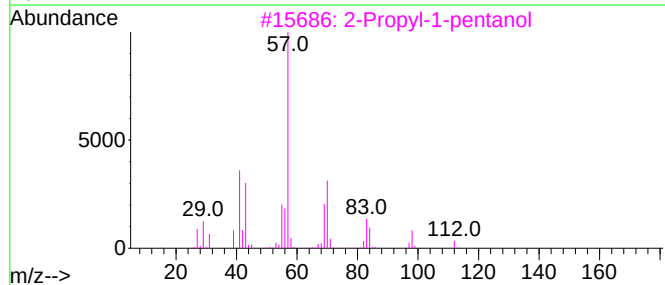
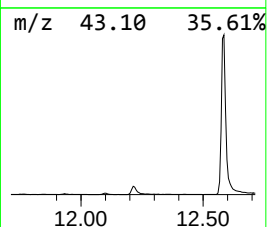
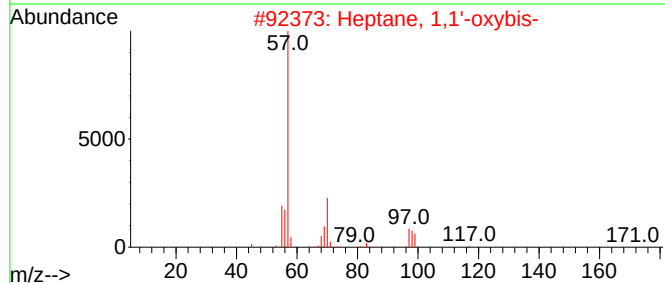
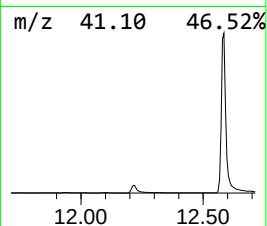
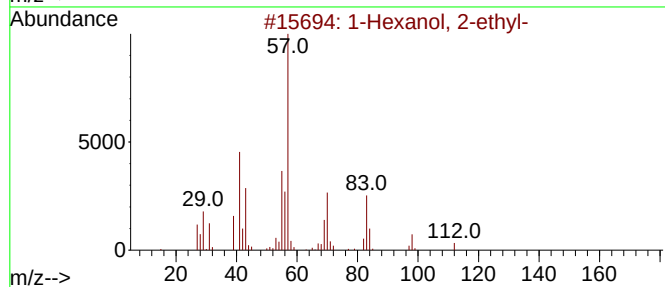
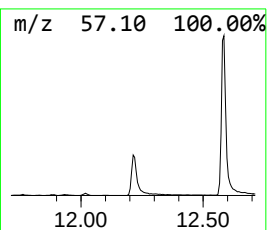
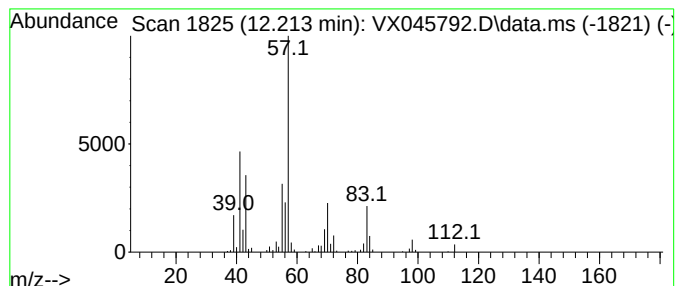
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Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.213	14.48 ug/l	124144	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
5			Heptane, 3-ethyl-	128	C9H20	015869-80-4	50



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Instrument :
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ClientSampleId :
40325-A-B-COMP

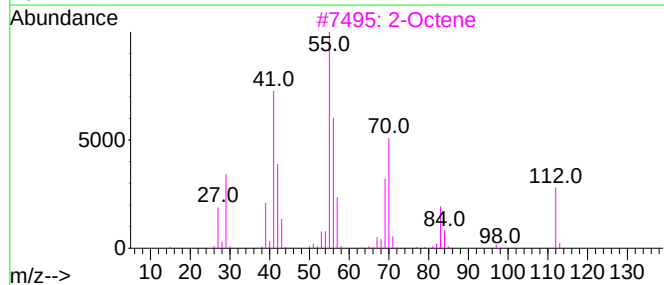
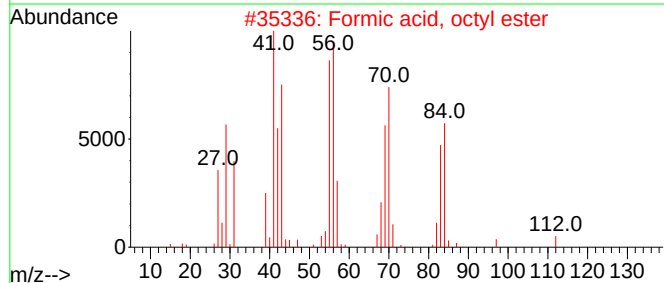
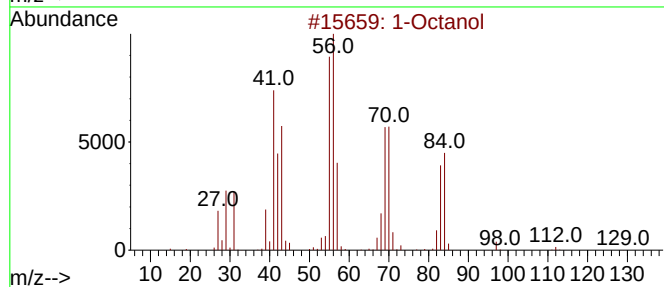
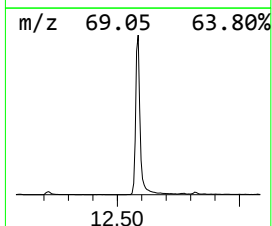
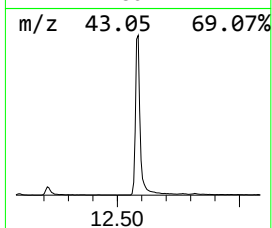
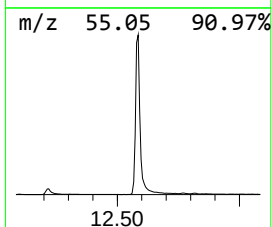
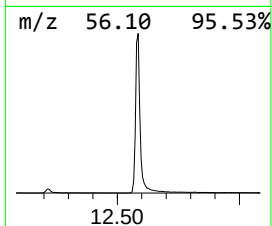
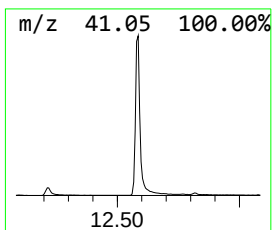
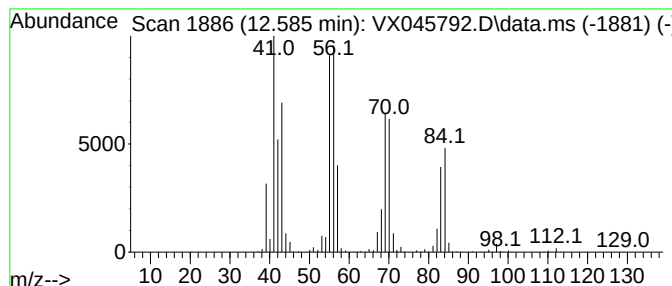
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Quant Title : SW846 8260

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

Peak Number 4 1-Octanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.585	227.28 ug/l	1948240	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol	130	C8H18O	000111-87-5	91
2			Formic acid, octyl ester	158	C9H18O2	000112-32-3	90
3			2-Octene	112	C8H16	000111-67-1	47
4			Formic acid, heptyl ester	144	C8H16O2	000112-23-2	47
5			1-Pentene, 3-methyl-	84	C6H12	000760-20-3	46



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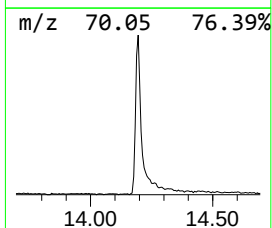
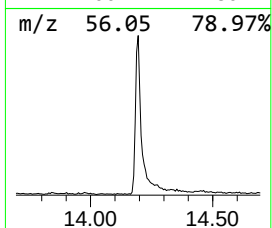
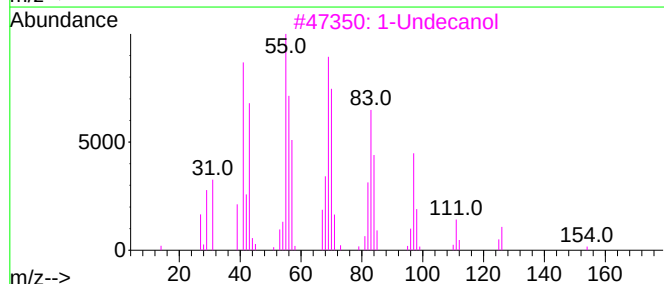
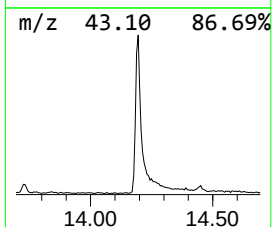
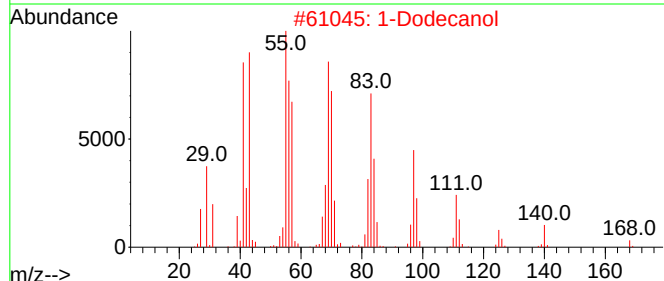
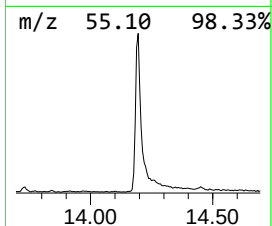
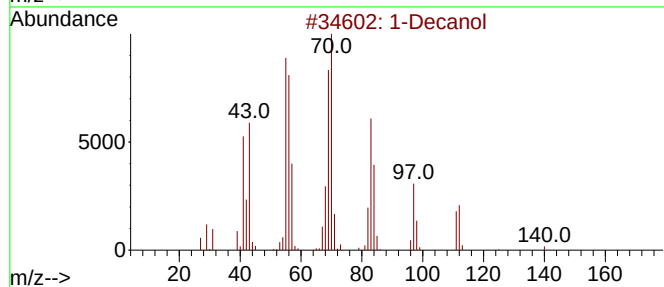
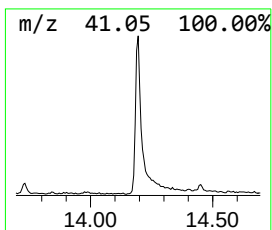
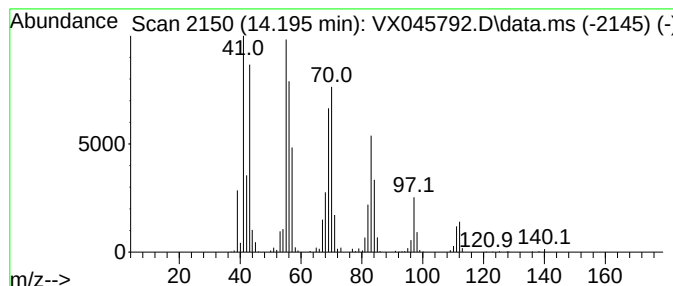
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Quant Title : SW846 8260

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

Peak Number 5 1-Decanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.195	57.94 ug/l	496698	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Decanol	158	C10H22O	000112-30-1	91
2			1-Dodecanol	186	C12H26O	000112-53-8	90
3			1-Undecanol	172	C11H24O	000112-42-5	90
4			Dichloroacetic acid, decyl ester	268	C12H22Cl2O2	083005-00-9	87
5			Formic acid, decyl ester	186	C11H22O2	005451-52-5	86



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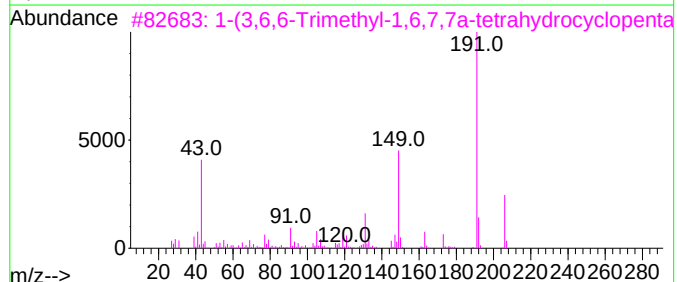
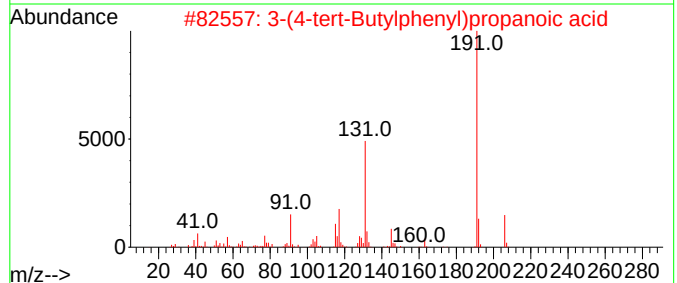
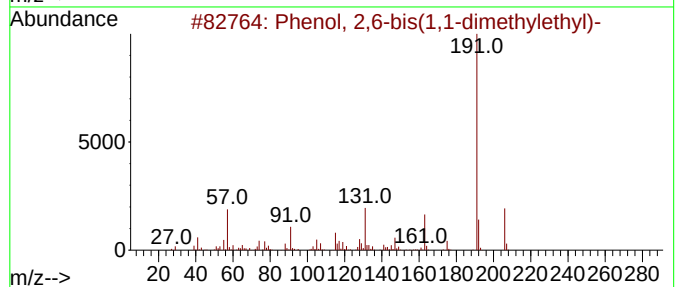
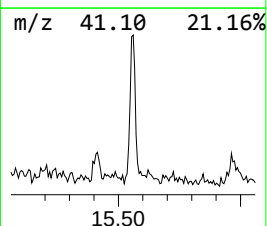
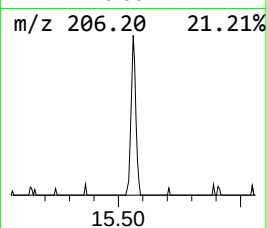
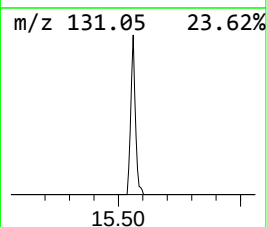
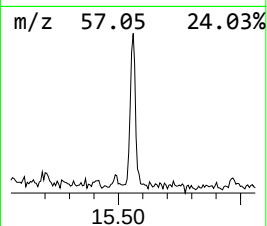
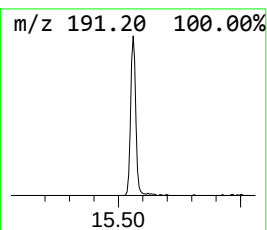
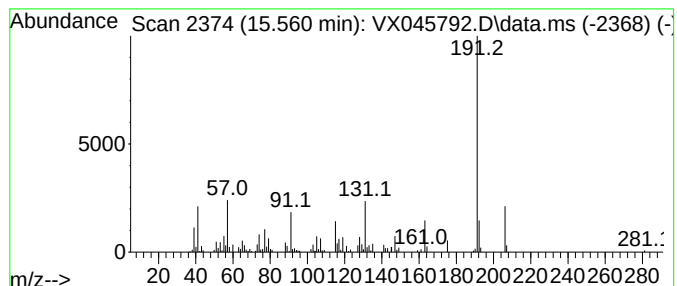
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

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

Peak Number 6 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.560	8.96 ug/l	76794	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	97
2			3-(4-tert-Butylphenyl)propanoic ...	206	C13H18O2	001208-64-6	83
3			1-(3,6,6-Trimethyl-1,6,7,7a-tetr...	206	C13H18O2	1000194-97-2	81
4			3-(4-(tert-Butyl)phenyl)-2-methy...	206	C14H22O	056107-04-1	81
5			Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041525\
Data File : VX045792.D
Acq On : 15 Apr 2025 12:26
Operator : JC/MD
Sample : Q1794-04 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
40325-A-B-COMP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.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	2.075	15.2	ug/l	76124	1	5.544	250411	50.0
1-Butanol	7.226	5.6	ug/l	41578	2	6.757	371520	50.0
1-Hexanol, 2-et...	12.213	14.5	ug/l	124144	4	12.018	428598	50.0
1-Octanol	12.585	227.3	ug/l	1948240	4	12.018	428598	50.0
1-Decanol	14.195	57.9	ug/l	496698	4	12.018	428598	50.0
Phenol, 2,6-bis...	15.560	9.0	ug/l	76794	4	12.018	428598	50.0