

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
 Data File : VX028763.D
 Acq On : 17 May 2022 17:19
 Operator : JC/MD
 Sample : N2884-10
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 31803

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\82X051222W.M

Title : SW846 8260

Signal : TIC: VX028763.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.447	55	59	72	rBV	4493337	5767645	4.31%	1.289%
2	2.294	188	198	205	rBV	17708714	63127129	47.17%	14.103%
3	2.374	209	211	214	rVV	16851656	20107547	15.02%	4.492%
4	2.416	214	218	236	rVB	13148662	22379511	16.72%	5.000%
5	4.148	444	502	505	rBV	11838145	133827711	100.00%	29.898%
6	6.769	922	932	942	rBV	685648	1640895	1.23%	0.367%
7	8.653	1234	1241	1246	rBV	1391826	2280036	1.70%	0.509%
8	8.872	1270	1277	1291	rVB	2369760	3833065	2.86%	0.856%
9	9.025	1291	1302	1307	rBV	41337751	93182528	69.63%	20.817%
10	9.183	1319	1328	1333	rBV	35583898	67192501	50.21%	15.011%
11	9.330	1346	1352	1365	rVB	957641	1351538	1.01%	0.302%
12	10.079	1465	1475	1483	rBV2	5547109	9414370	7.03%	2.103%
13	10.159	1483	1488	1498	rBV	5409596	7381840	5.52%	1.649%
14	11.085	1634	1640	1645	rBV	1288382	1725699	1.29%	0.386%
15	11.658	1728	1734	1737	rBV	909966	1420029	1.06%	0.317%
16	11.957	1775	1783	1787	rBV	3045740	3864441	2.89%	0.863%
17	12.024	1790	1794	1797	rVV	1374728	1524124	1.14%	0.340%
18	12.219	1820	1826	1837	rBV	6287735	7596050	5.68%	1.697%

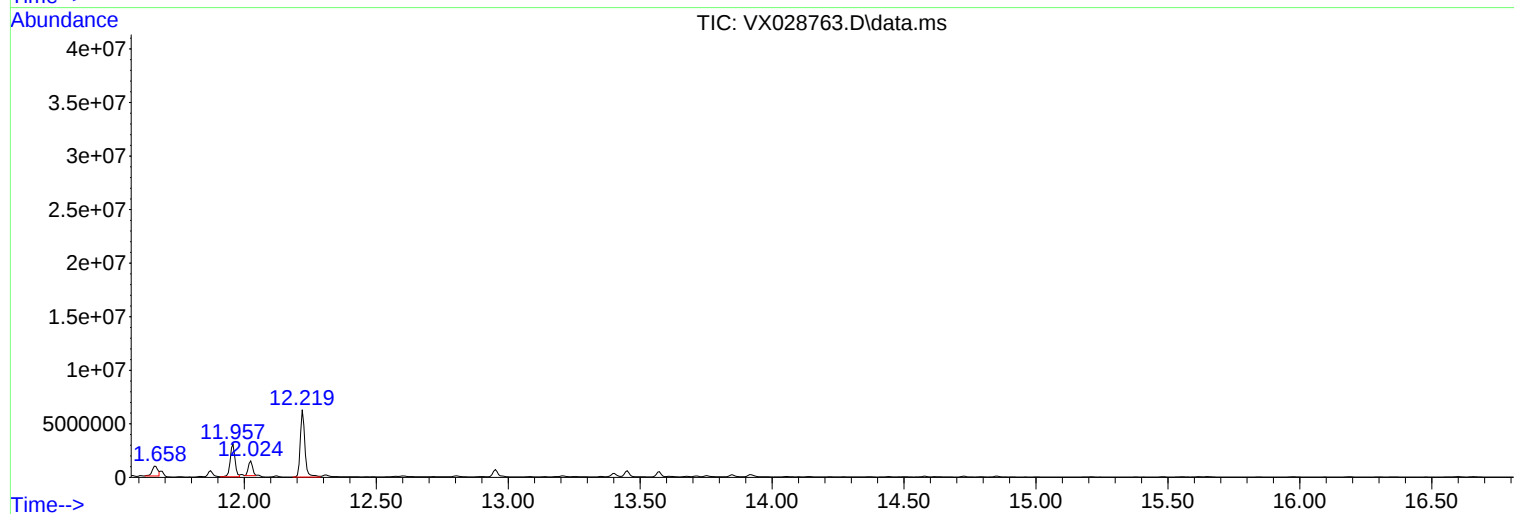
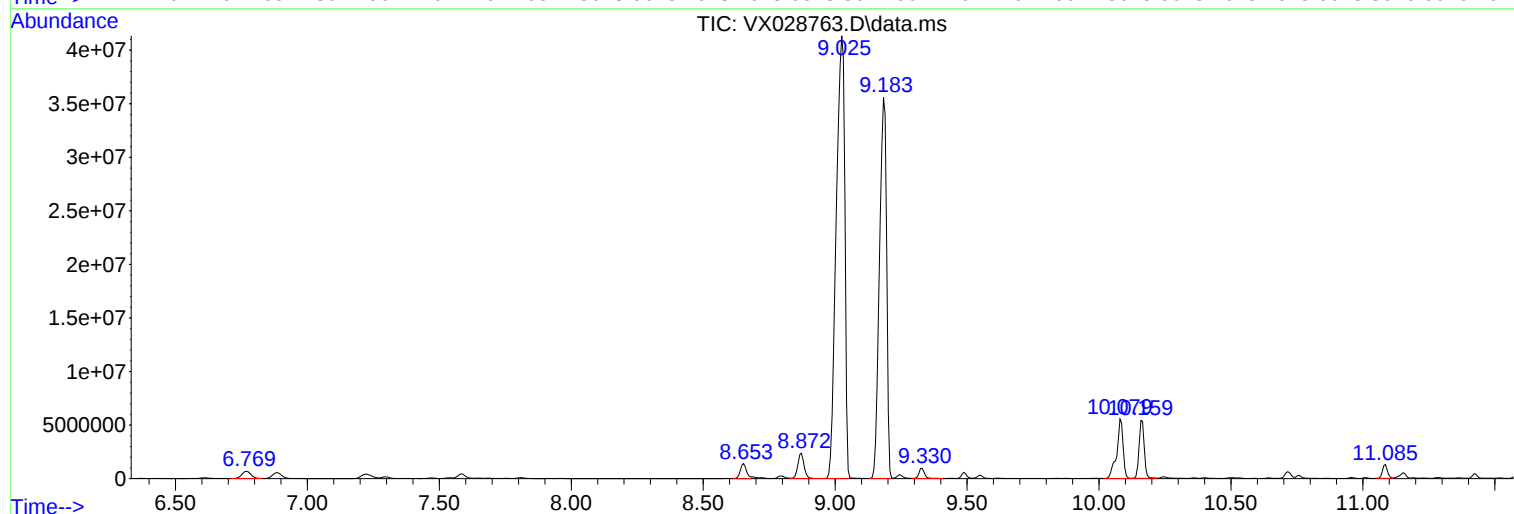
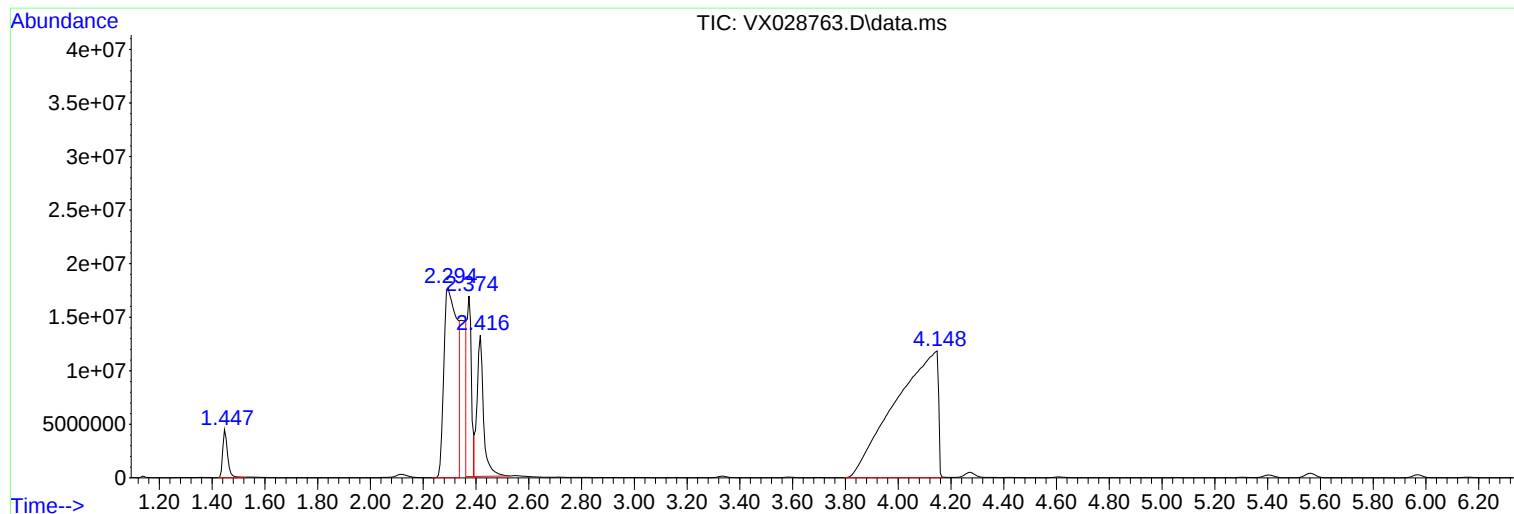
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Quant Title : SW846 8260

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



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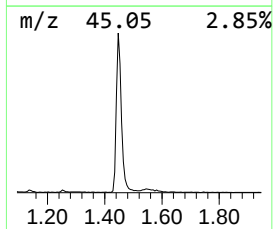
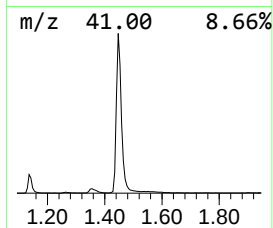
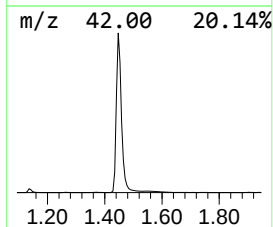
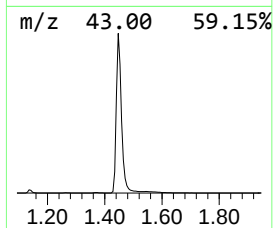
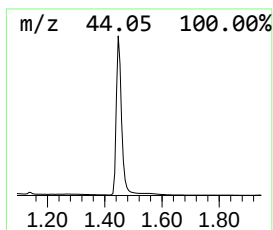
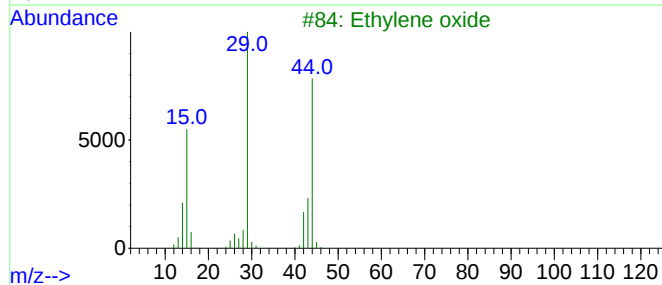
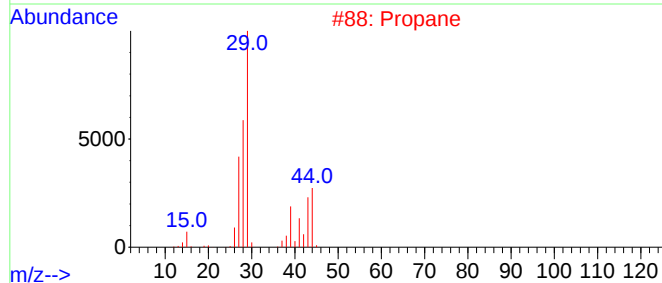
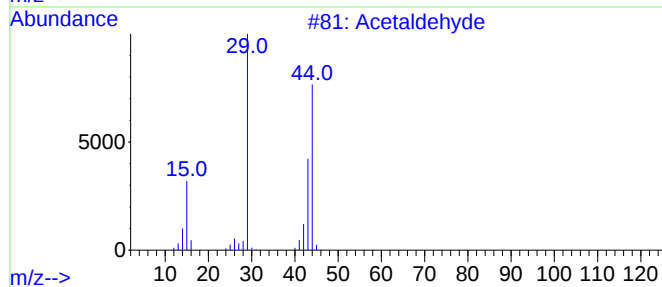
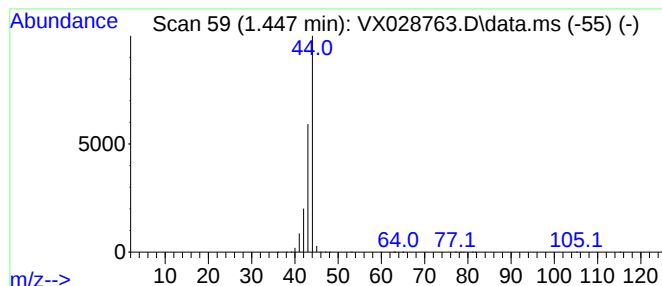
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Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.447	175.75 ug/l	5767650	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Alanine	89	C3H7NO2	000056-41-7	4
5			Hydrogen isocyanate	43	CHNO	000075-13-8	3



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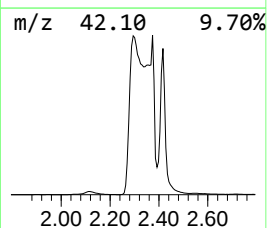
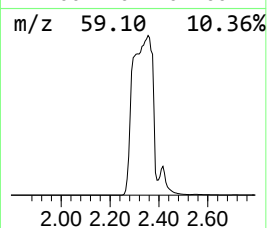
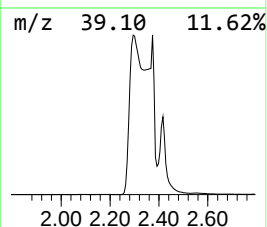
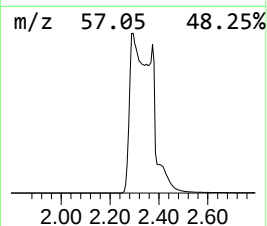
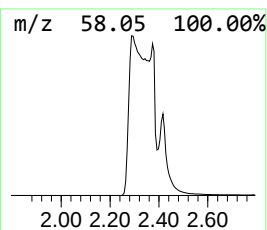
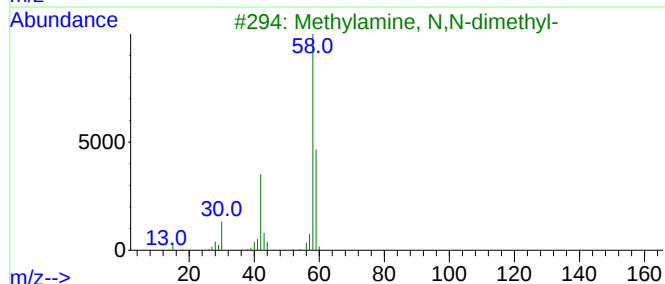
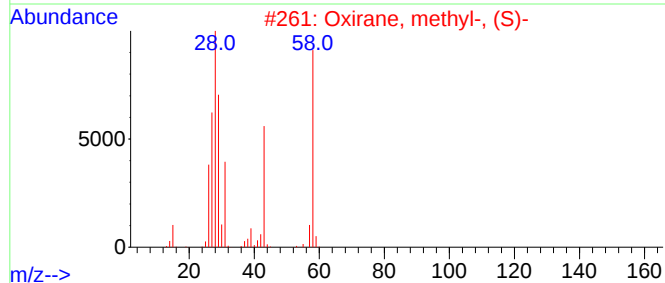
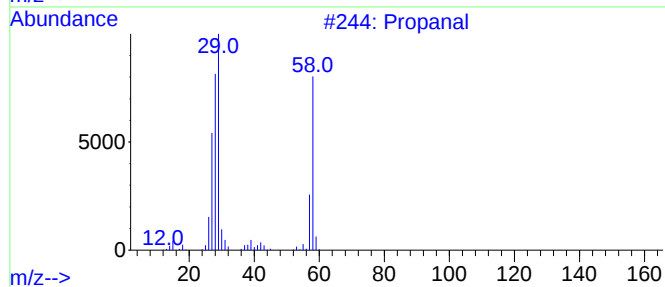
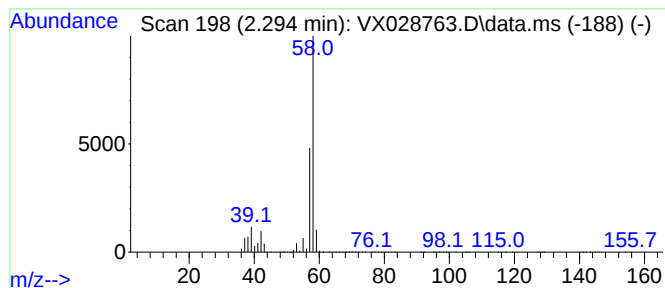
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 2 Propanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.294	1923.56 ug/l	63127100	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	56
2			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7
3			Methylamine, N,N-dimethyl-	59	C3H9N	000075-50-3	5
4			2-Propen-1-amine	57	C3H7N	000107-11-9	4
5			Decane, -1,10-diamino, -N,N,N',N'-...	228	C14H32N2	001938-62-1	4



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ALS Vial : 17 Sample Multiplier: 1

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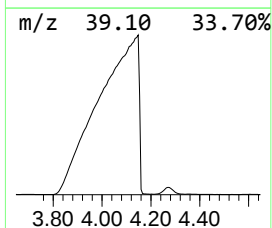
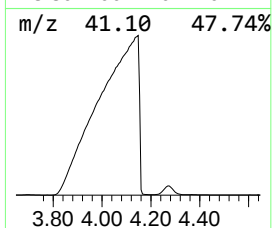
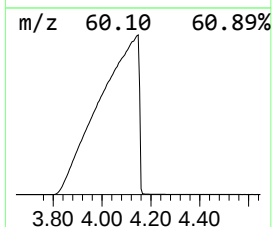
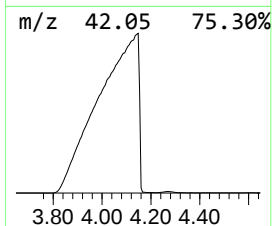
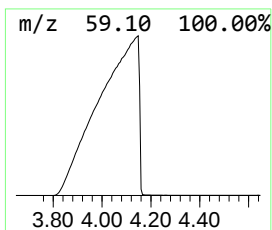
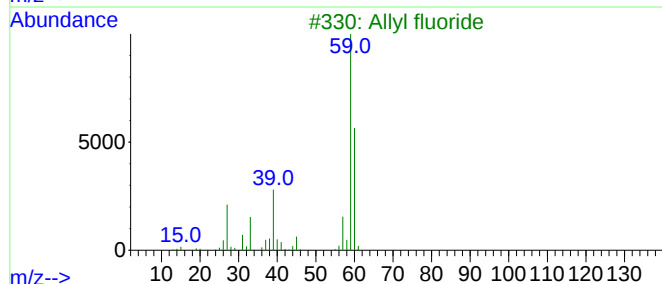
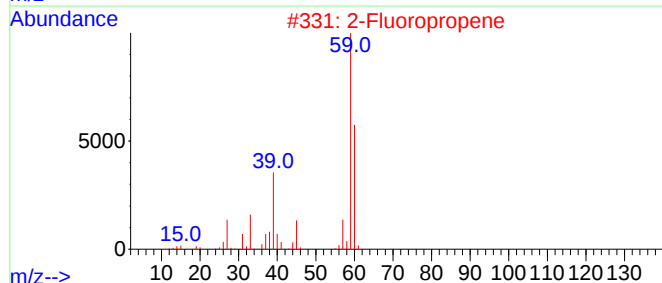
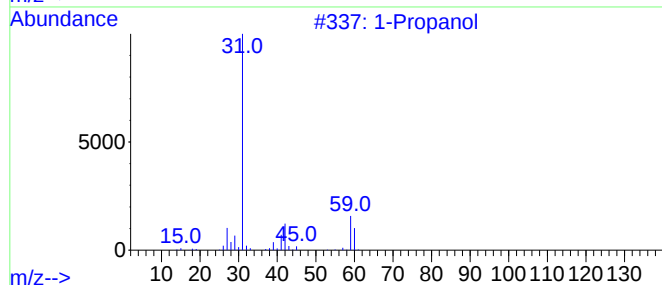
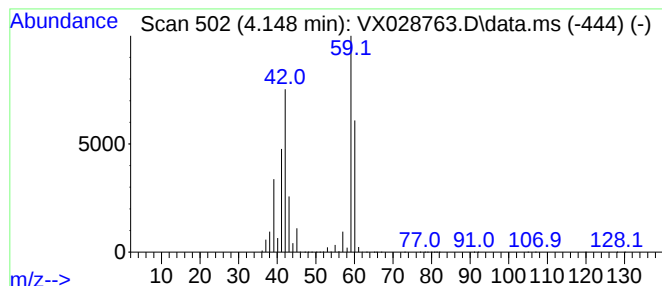
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.148	4077.89 ug/l	133828000	Pentafluorobenzene	5.562

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol	60	C3H8O	000071-23-8	78
2		2-Fluoropropene	60	C3H5F	001184-60-7	43
3		Allyl fluoride	60	C3H5F	000818-92-8	38
4		Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	9
5		Cyclopropane	42	C3H6	000075-19-4	9



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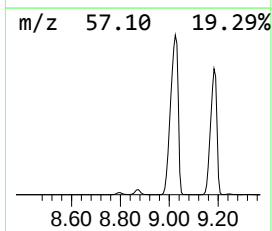
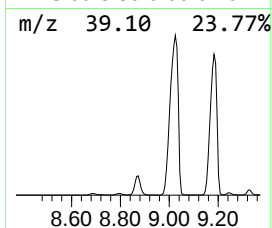
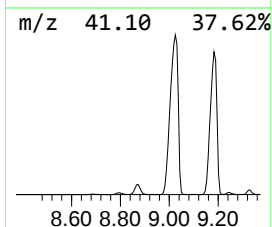
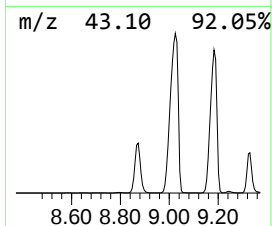
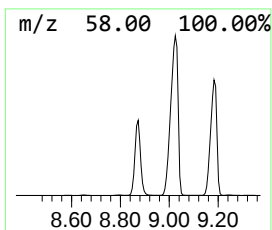
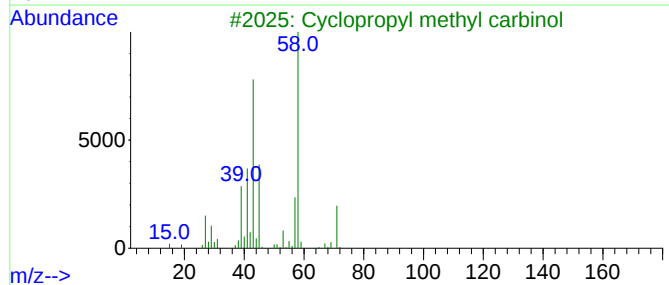
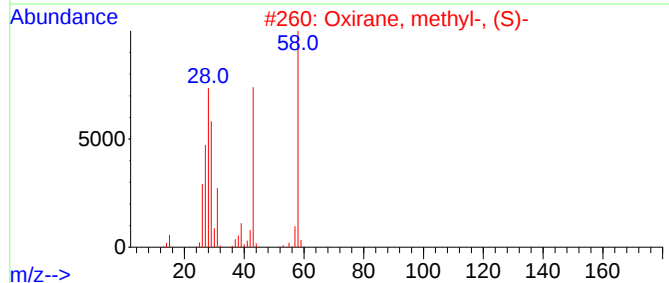
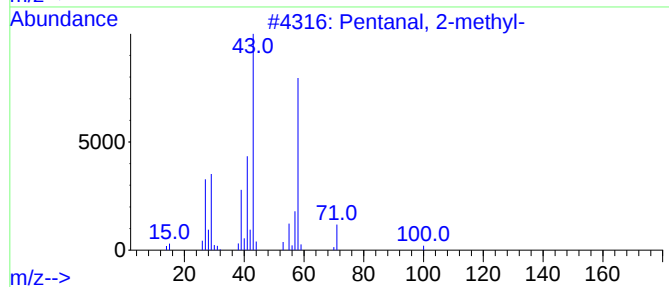
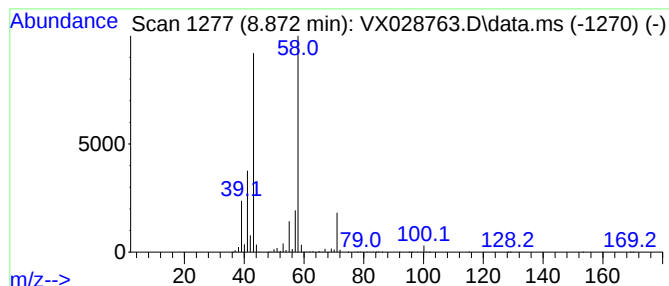
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentanal, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.872	20.36 ug/l	3833070	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal, 2-methyl-	100	C6H12O	000123-15-9	90
2			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	78
3			Cyclopropyl methyl carbinol	86	C5H10O	000765-42-4	72
4			Butanimidamide	86	C4H10N2	000107-90-4	50
5			Carbonic acid, 2-dimethylaminoet...	175	C8H17NO3	1000331-38-5	38



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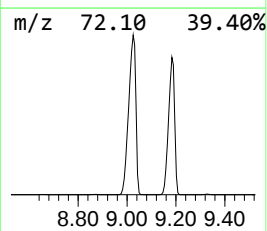
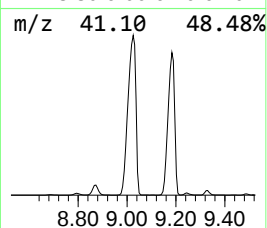
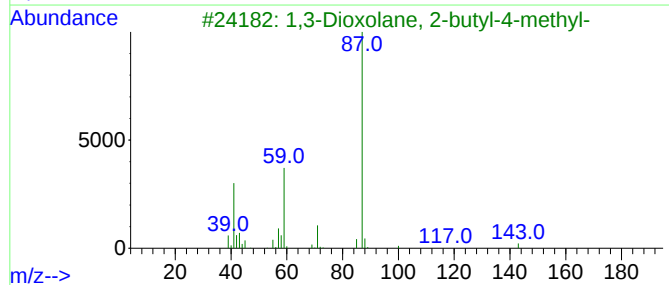
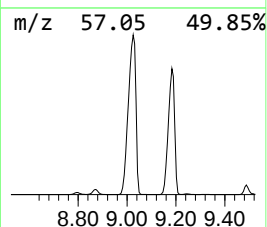
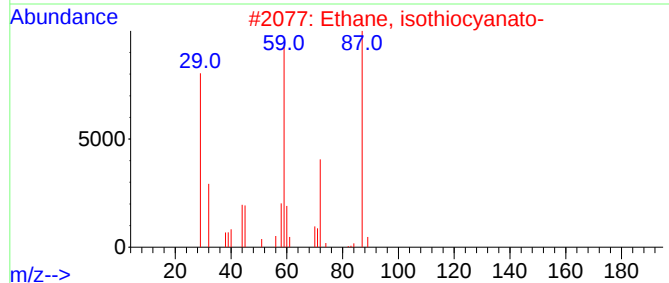
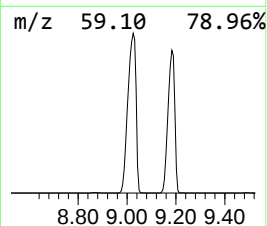
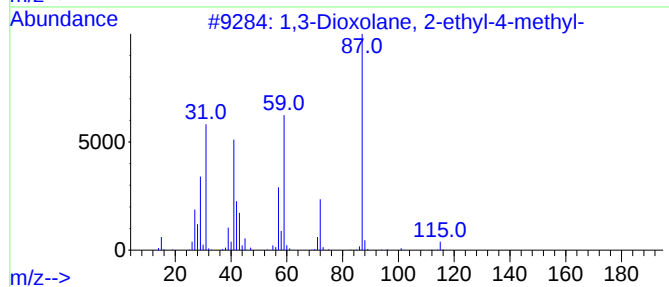
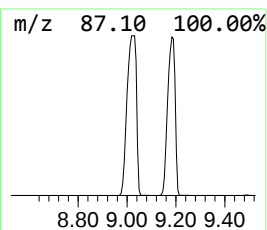
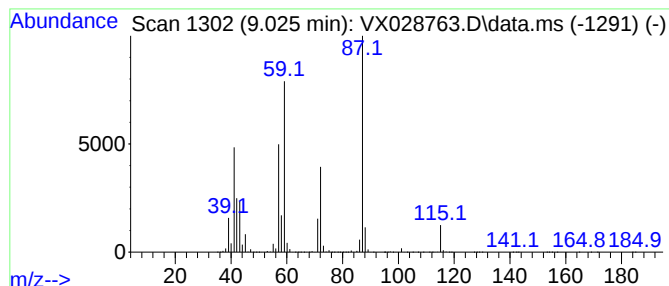
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Quant Title : SW846 8260

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

Peak Number 5 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.025	494.89 ug/l	93182500	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	72
2			Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	64
3			1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	59
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	47
5			DL-Lactamide, N,O-dimethyl-	117	C5H11NO2	1000452-56-3	42



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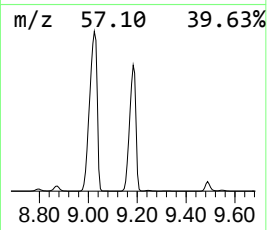
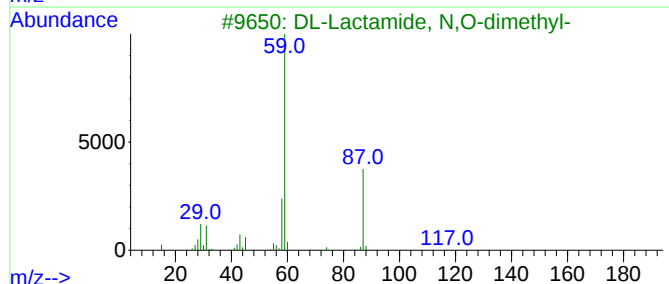
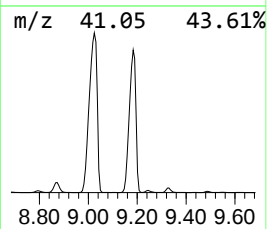
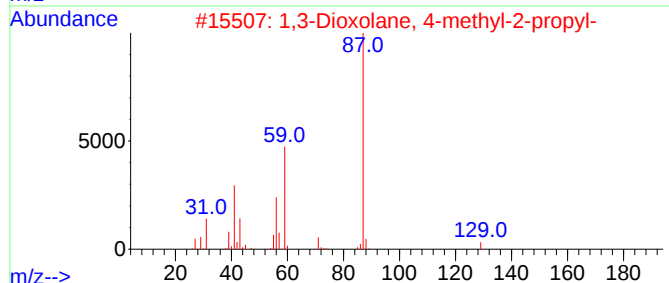
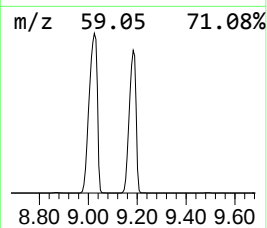
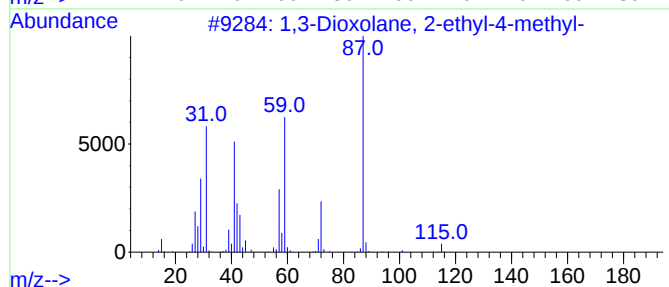
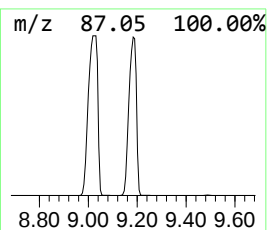
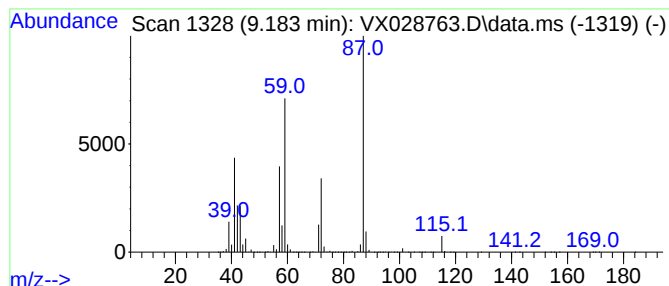
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Quant Title : SW846 8260

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

Peak Number 6 1,3-Dioxolane, 4-methyl-2-p... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.183	356.86 ug/l	67192500	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	90
2			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	59
3			DL-Lactamide, N,O-dimethyl-	117	C5H11NO2	1000452-56-3	53
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	50
5			Ethanol, 2-[2-(2-methoxyethoxy)e...	206	C9H18O5	003610-27-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028763.D
Acq On : 17 May 2022 17:19
Operator : JC/MD
Sample : N2884-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31803

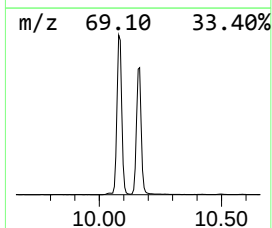
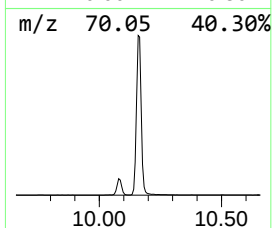
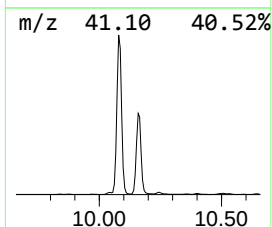
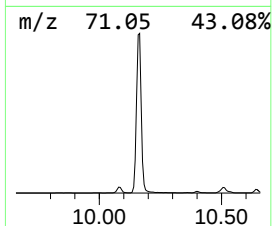
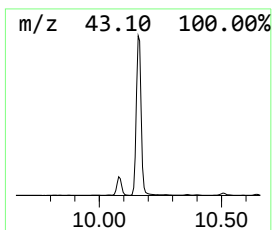
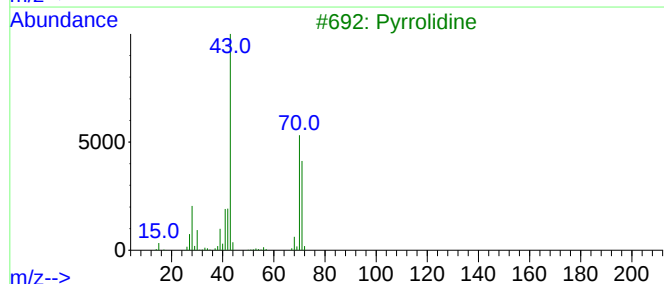
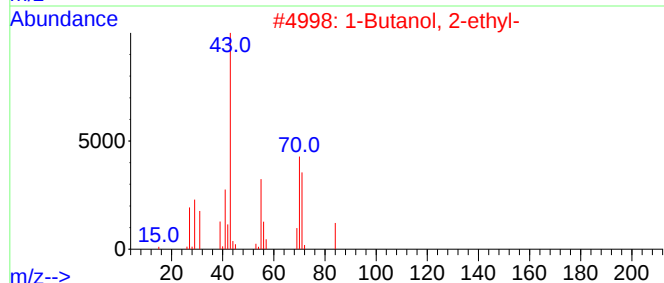
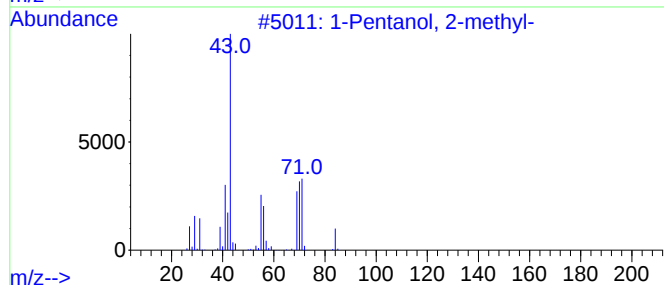
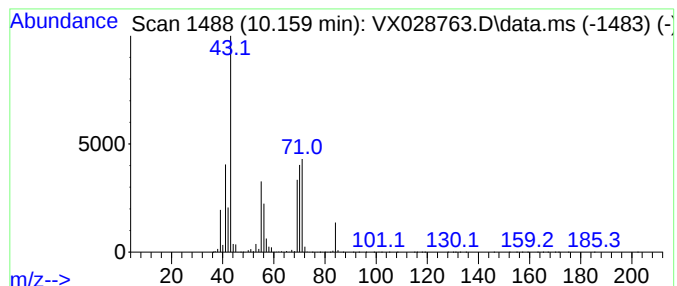
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Quant Title : SW846 8260

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

Peak Number 7 1-Pentanol, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.159	39.21 ug/l	7381840	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	90
2			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	78
3			Pyrrolidine	71	C4H9N	000123-75-1	64
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	50
5			Butane, 1-bromo-3-methyl-	150	C5H11Br	000107-82-4	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028763.D
Acq On : 17 May 2022 17:19
Operator : JC/MD
Sample : N2884-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31803

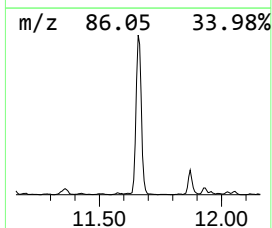
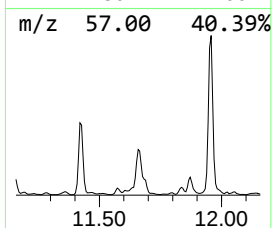
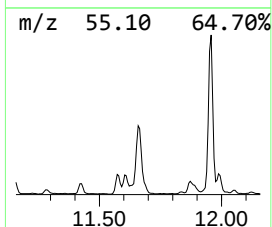
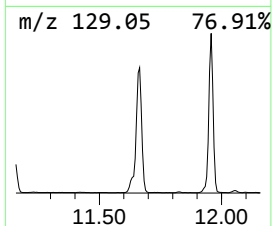
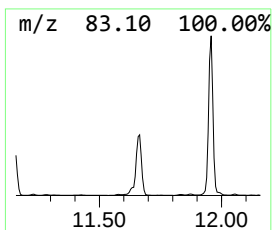
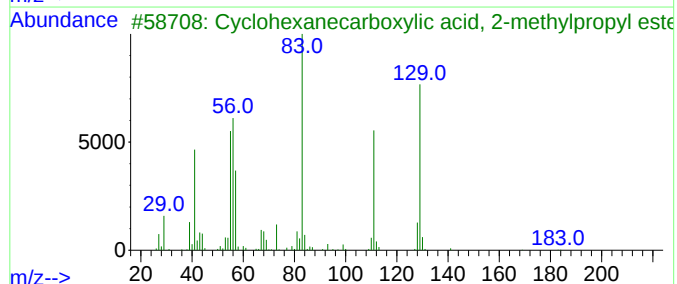
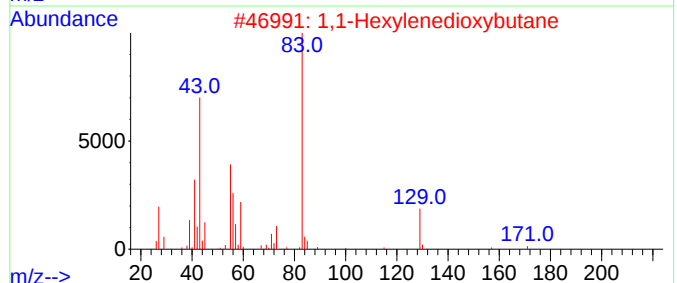
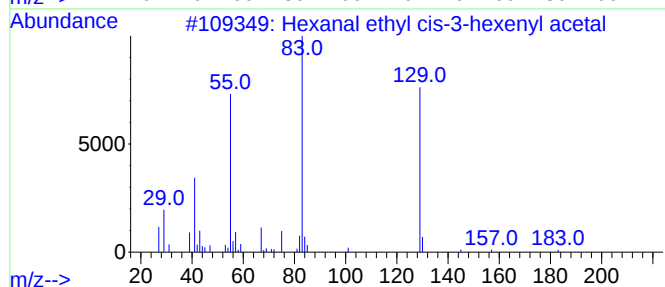
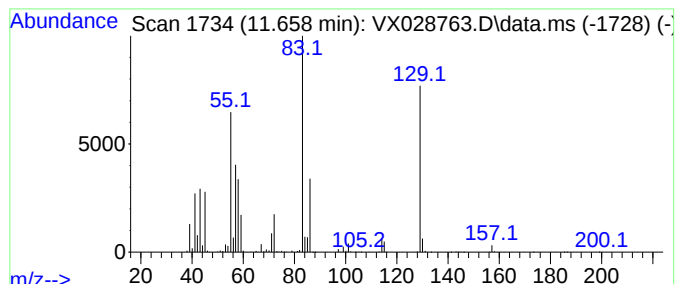
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Quant Title : SW846 8260

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

Peak Number 8 Hexanal ethyl cis-3-hexenyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.658	46.59 ug/l	1420030	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal ethyl cis-3-hexenyl acetal	228	C14H28O2	1000431-42-9	50
2			1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	43
3			Cyclohexanecarboxylic acid, 2-me...	184	C11H20O2	037139-85-8	40
4			2-(2-(2-Ethoxyethoxy)ethoxy)ethy...	262	C13H26O5	1010366-97-1	32
5			Goitrin	129	C5H7NO5	000500-12-9	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028763.D
Acq On : 17 May 2022 17:19
Operator : JC/MD
Sample : N2884-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31803

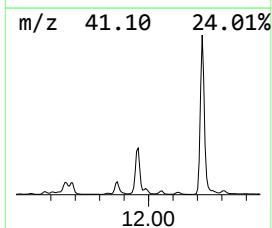
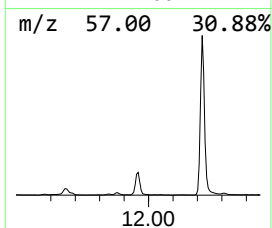
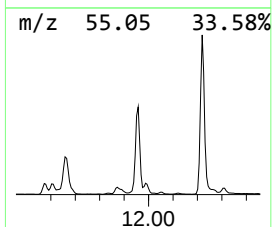
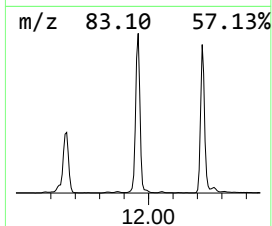
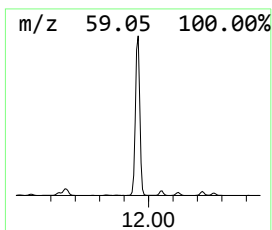
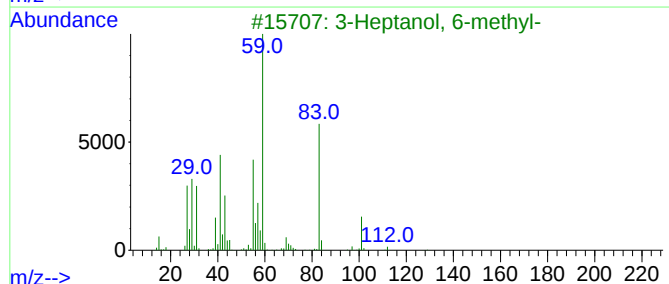
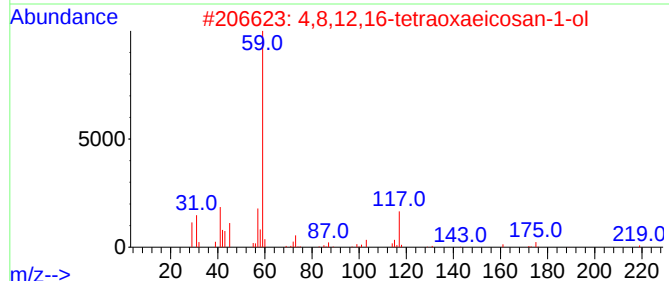
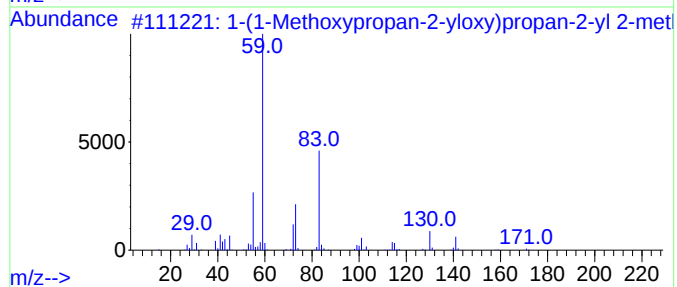
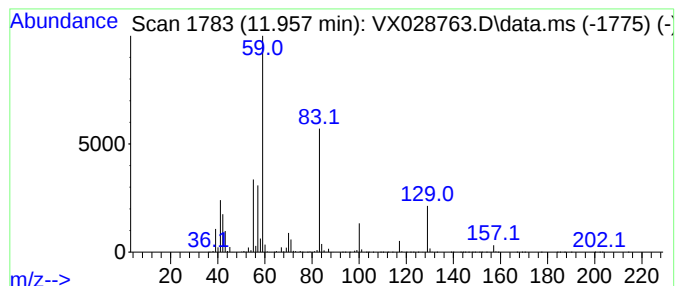
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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

Peak Number 9 unknown11.957 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	126.78 ug/l	3864440	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(1-Methoxypropan-2-yloxy)propa...	230	C12H22O4	1000367-11-3	45		
2	4,8,12,16-tetraoxaeicosan-1-ol	306	C16H34O5	1010397-63-6	38		
3	3-Heptanol, 6-methyl-	130	C8H18O	018720-66-6	36		
4	Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	33		
5	Acetaldoxime	59	C2H5NO	000107-29-9	32		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028763.D
Acq On : 17 May 2022 17:19
Operator : JC/MD
Sample : N2884-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31803

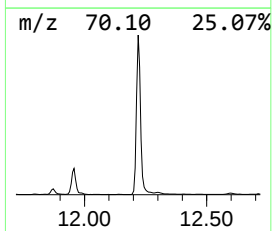
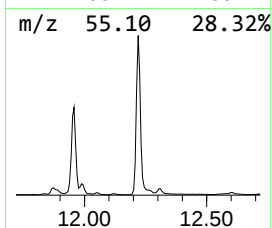
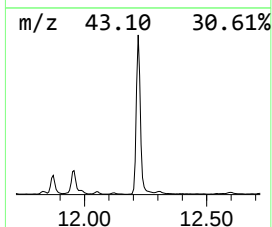
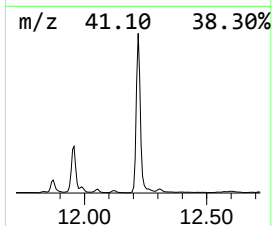
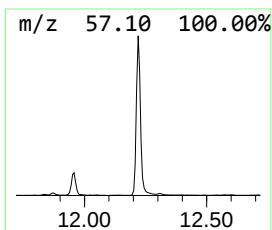
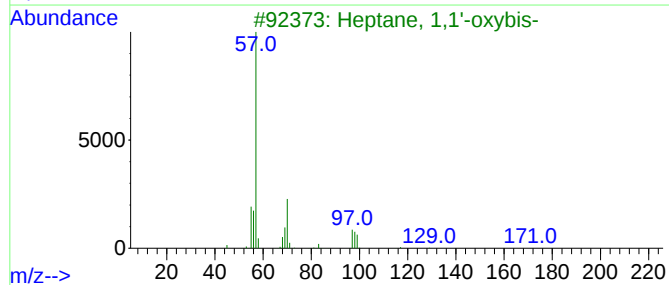
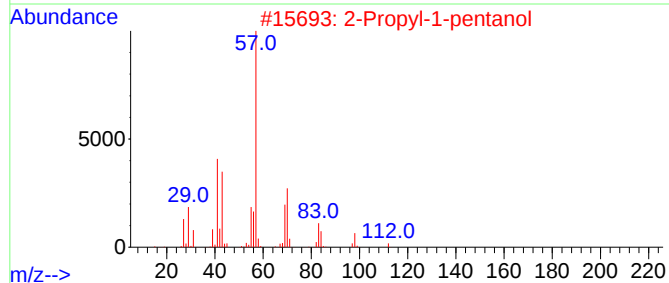
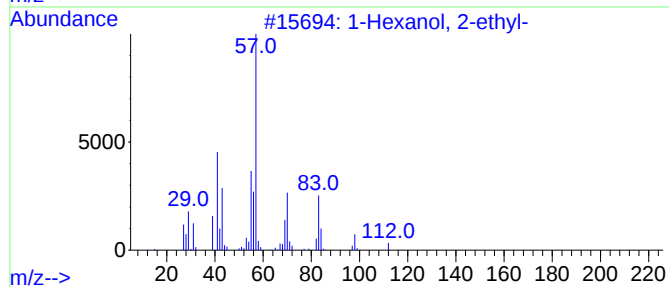
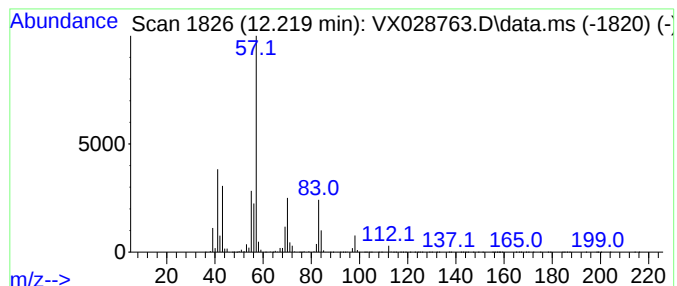
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Quant Title : SW846 8260

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

Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	249.19 ug/l	7596050	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	90
2		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
3		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4		2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
5		Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028763.D
Acq On : 17 May 2022 17:19
Operator : JC/MD
Sample : N2884-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31803

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.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
Acetaldehyde	1.447	175.8	ug/l	5767650	1	5.562	1640900	50.0
Propanal	2.294	1923.6	ug/l	63127100	1	5.562	1640900	50.0
1-Propanol	4.148	4077.9	ug/l	133828000	1	5.562	1640900	50.0
Pentanal, 2-met...	8.872	20.4	ug/l	3833070	3	10.055	9414370	50.0
1,3-Dioxolane, ...	9.025	494.9	ug/l	93182500	3	10.055	9414370	50.0
1,3-Dioxolane, ...	9.183	356.9	ug/l	67192500	3	10.055	9414370	50.0
1-Pentanol, 2-m...	10.159	39.2	ug/l	7381840	3	10.055	9414370	50.0
Hexanal ethyl c...	11.658	46.6	ug/l	1420030	4	12.024	1524120	50.0
unknown11.957	11.957	126.8	ug/l	3864440	4	12.024	1524120	50.0
1-Hexanol, 2-et...	12.219	249.2	ug/l	7596050	4	12.024	1524120	50.0