

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050824\
 Data File : VX041417.D
 Acq On : 08 May 2024 13:43
 Operator : JC/MD
 Sample : P2389-01 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1400

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M

Title : SW846 8260

Signal : TIC: VX041417.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	56	60	78	rBV	1568499	2173525	70.32%	16.950%
2	2.069	153	161	171	rBV	58154	88252	2.86%	0.688%
3	2.294	192	198	207	rBV	33582	60500	1.96%	0.472%
4	2.380	207	212	222	rVB	72351	121487	3.93%	0.947%
5	4.373	529	539	555	rBV	73020	212083	6.86%	1.654%
6	5.385	693	705	721	rBV	93657	278914	9.02%	2.175%
7	5.550	721	732	747	rVV	166206	477074	15.44%	3.720%
8	5.952	788	798	810	rBV	97261	260873	8.44%	2.034%
9	6.757	921	930	940	rBV	246943	592097	19.16%	4.617%
10	6.867	940	948	965	rVB	1313165	3090822	100.00%	24.103%
11	7.202	995	1003	1015	rBV	209267	455234	14.73%	3.550%
12	8.647	1233	1240	1249	rBV	452704	716310	23.18%	5.586%
13	8.994	1291	1297	1309	rBV	89039	135115	4.37%	1.054%
14	10.055	1465	1471	1483	rBV	441002	629935	20.38%	4.912%
15	10.988	1616	1624	1633	rBV	42816	68189	2.21%	0.532%
16	11.079	1633	1639	1653	rVV2	519559	684916	22.16%	5.341%
17	11.195	1653	1658	1667	rVB	43660	60392	1.95%	0.471%
18	12.024	1789	1794	1804	rVB	512886	678299	21.95%	5.290%
19	12.219	1820	1826	1837	rBV	35249	58246	1.88%	0.454%
20	12.768	1911	1916	1928	rBV	1650125	1981184	64.10%	15.450%

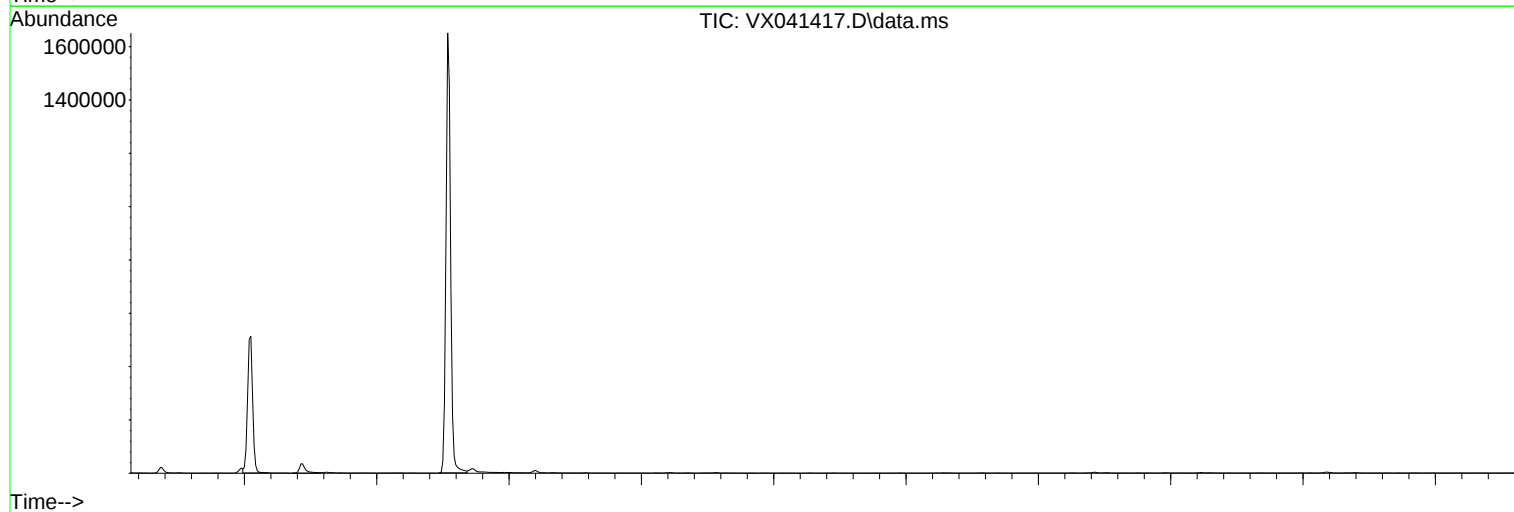
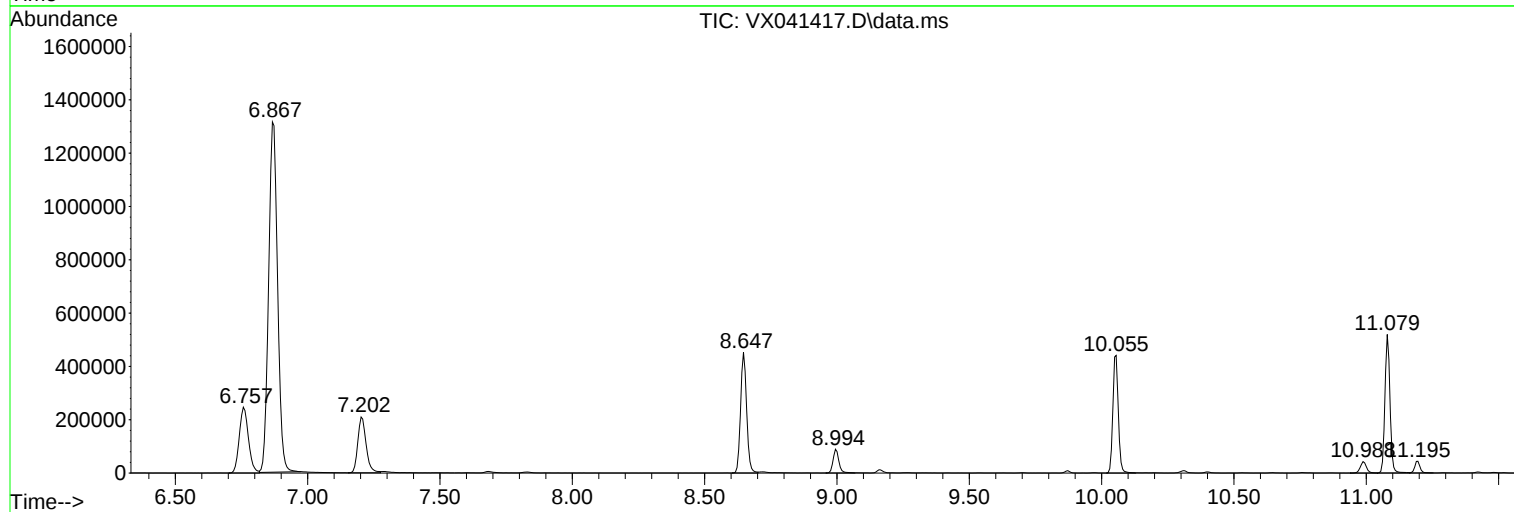
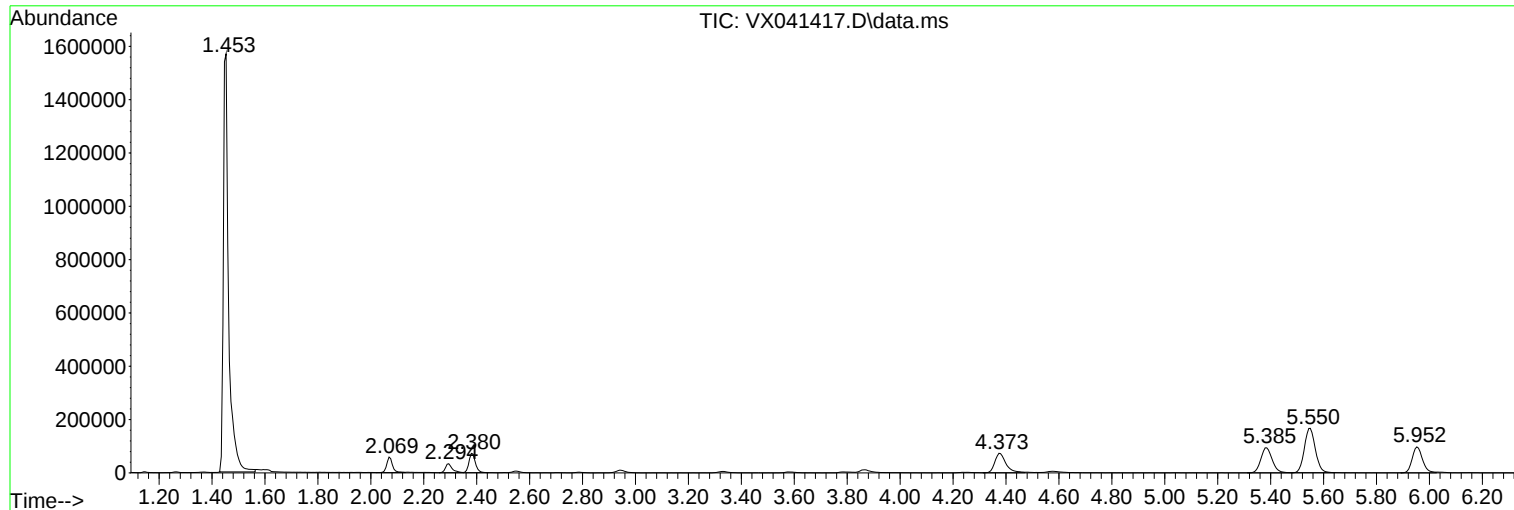
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Quant Title : SW846 8260

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



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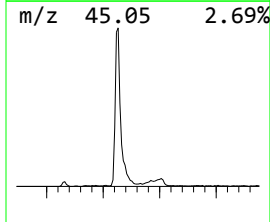
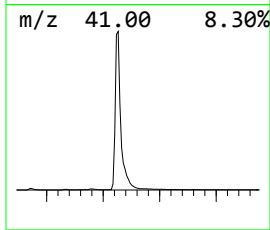
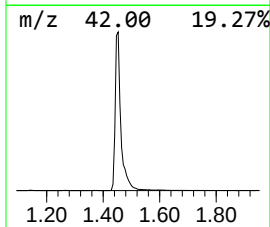
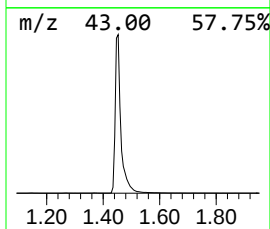
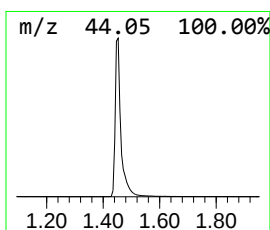
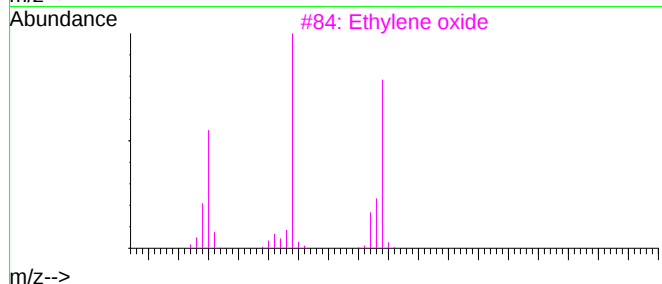
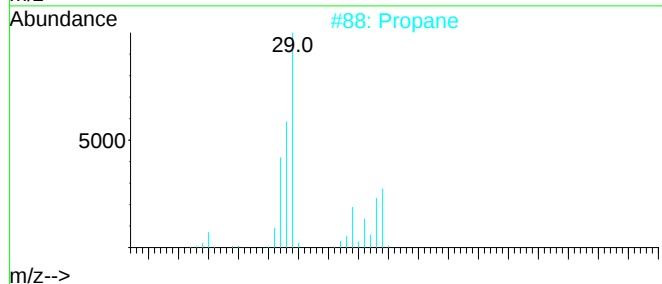
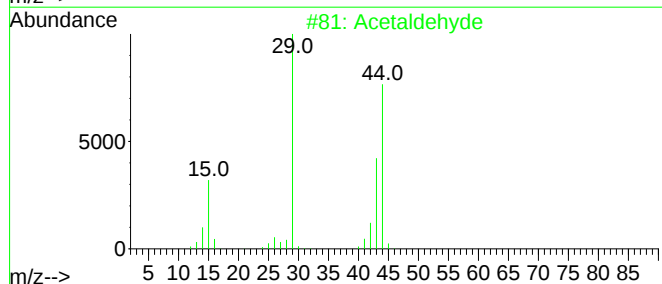
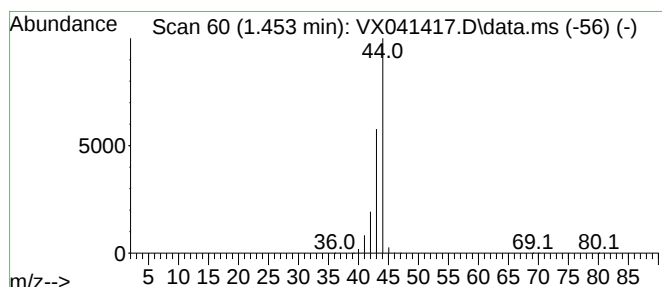
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	227.80 ug/l	2173530	Pentafluorobenzene	5.550

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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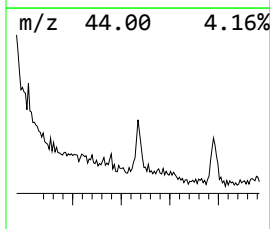
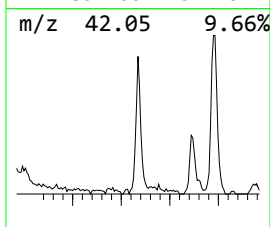
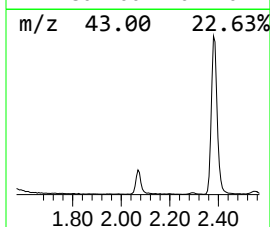
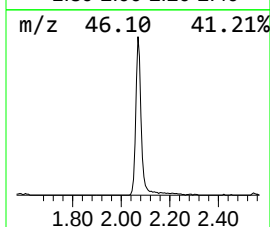
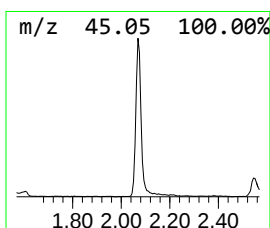
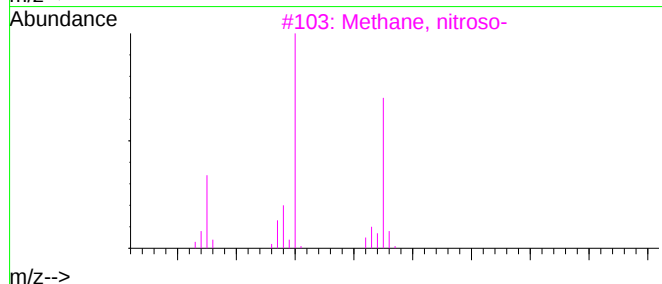
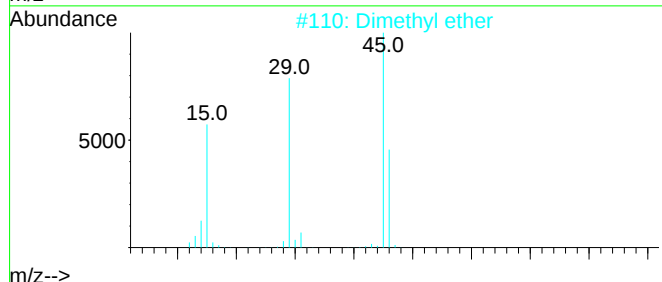
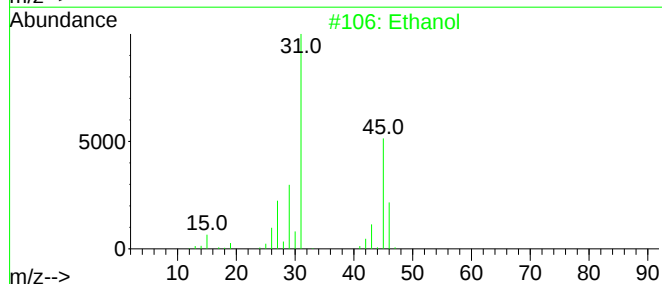
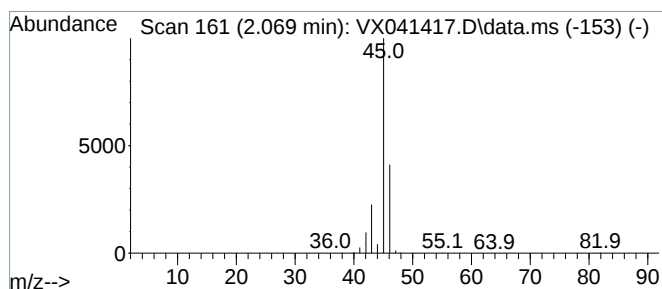
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.069	9.25 ug/l	88252	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	64
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	Propanedioic acid, dihydroxy-	136	C3H4O6	000560-27-0	4



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Instrument :
MSVOA_X
ClientSampleId :
1400

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

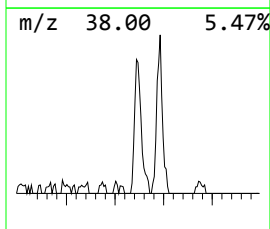
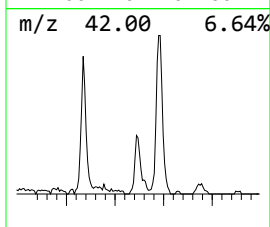
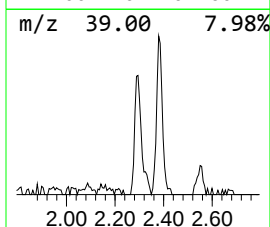
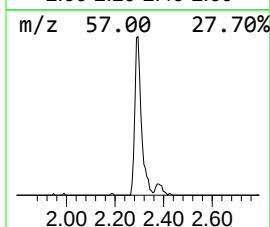
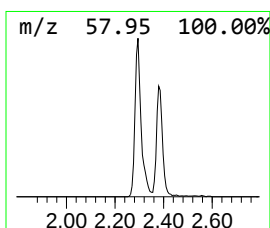
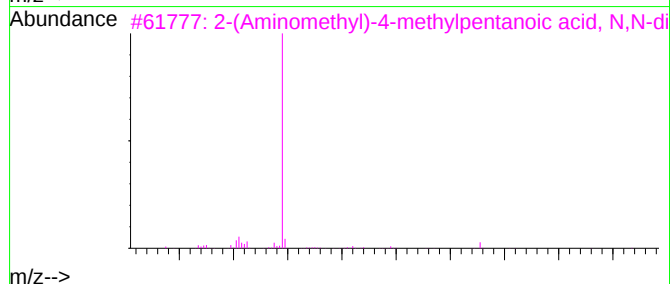
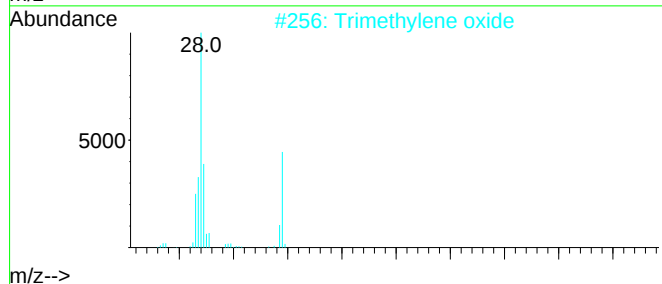
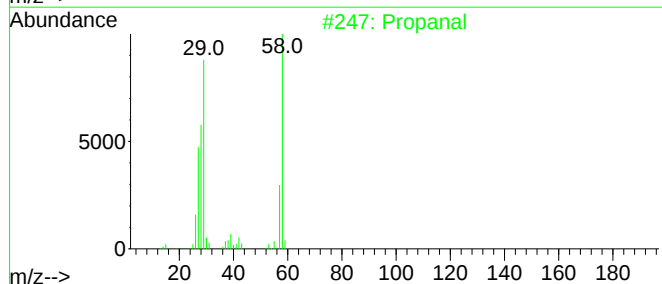
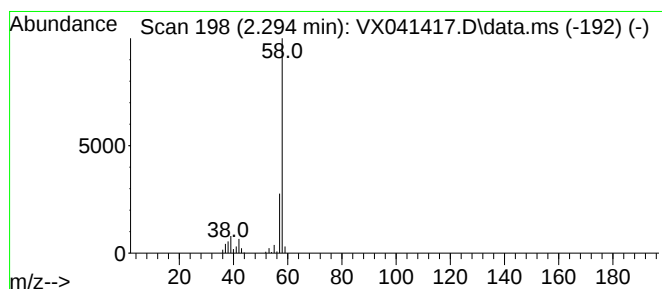
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.294	6.34 ug/l	60500	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	78
2	Trimethylene oxide	58	C3H6O	000503-30-0	9
3	2-(Aminomethyl)-4-methylpentanoic...	187	C10H21NO2	1891211-54-3	9
4	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7
5	Propylene oxide	58	C3H6O	000075-56-9	7



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Instrument :
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ClientSampleId :
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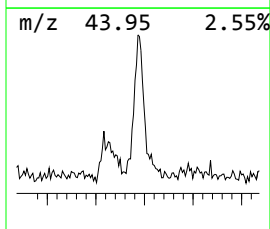
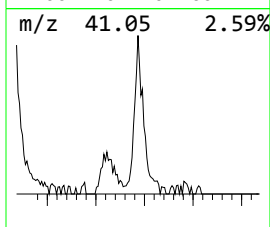
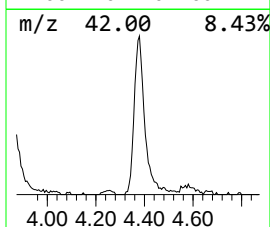
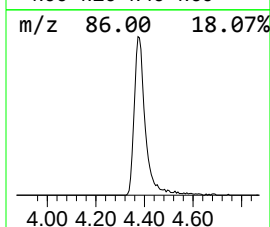
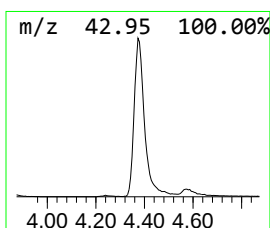
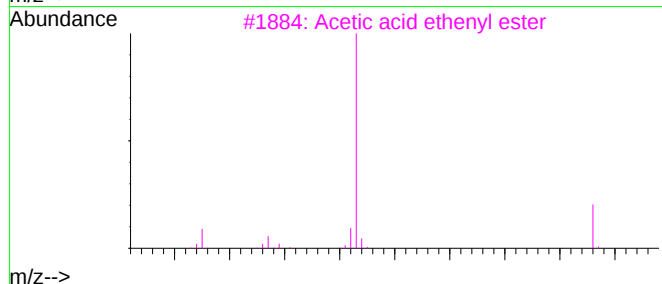
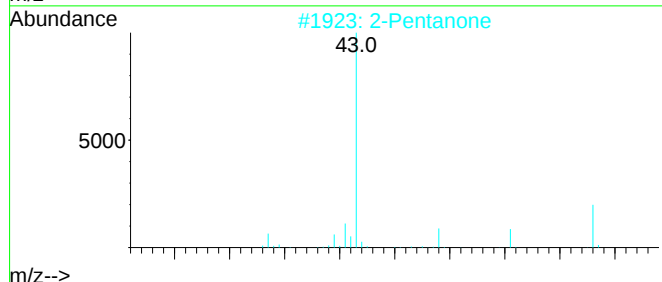
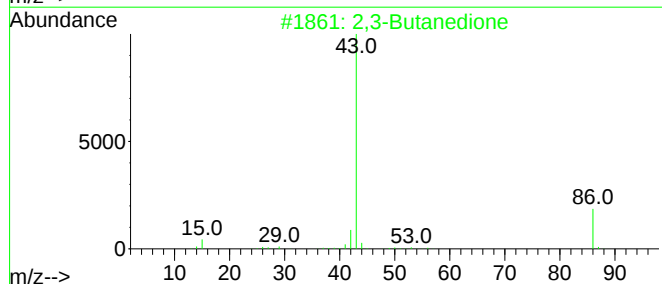
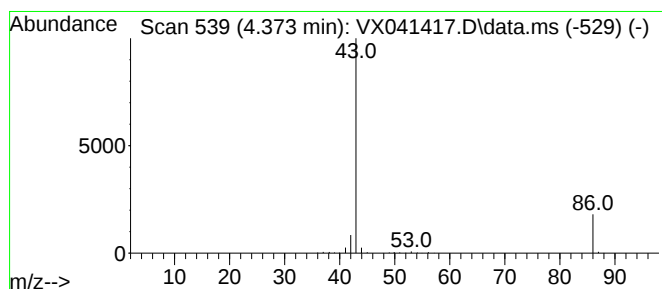
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

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

Peak Number 4 2,3-Butanedione Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.373	22.23 ug/l	212083	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione	86	C4H6O2	000431-03-8	78
2	2-Pentanone	86	C5H10O	000107-87-9	45
3	Acetic acid ethenyl ester	86	C4H6O2	000108-05-4	7
4	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	7
5	Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	7



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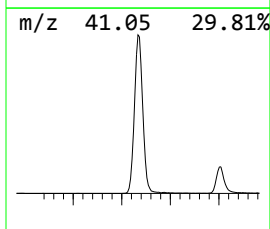
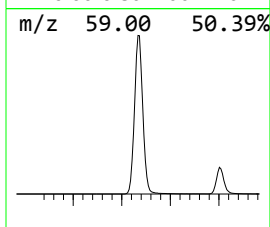
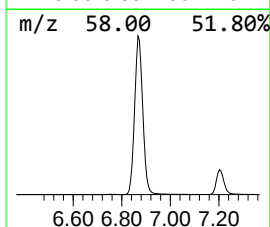
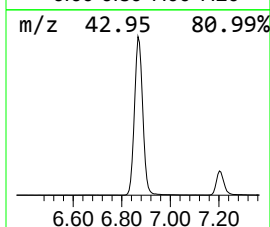
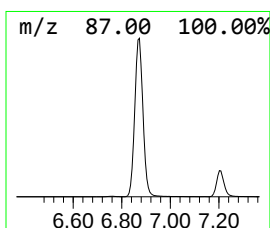
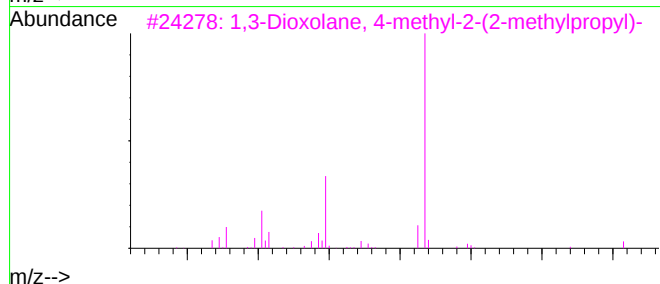
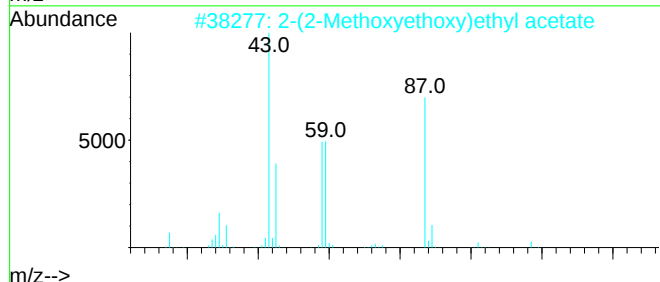
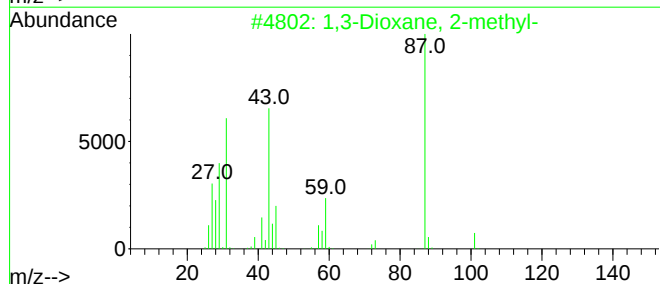
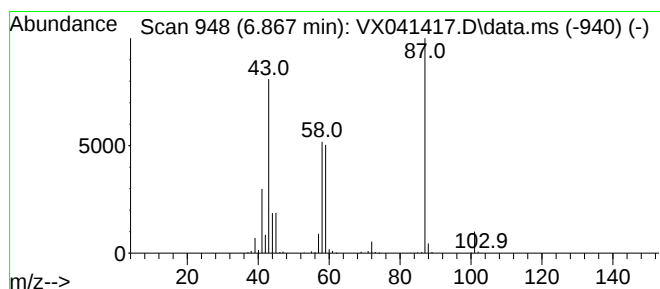
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.867	261.01 ug/l	3090820	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	59
2	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	40
3	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	37
4	Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	37
5	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	37



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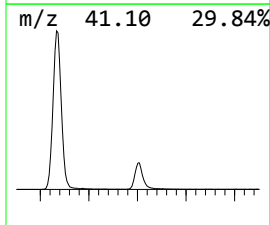
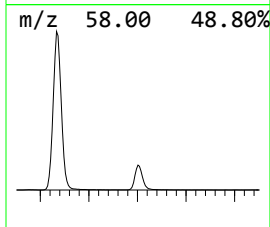
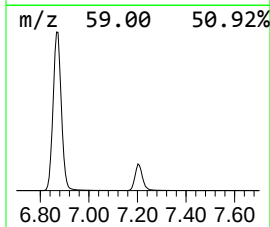
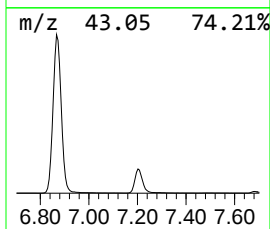
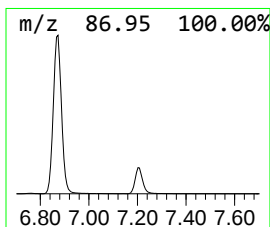
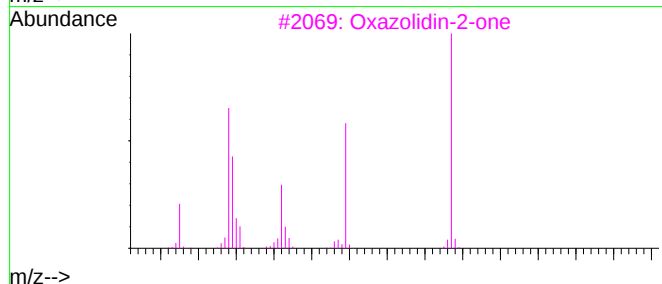
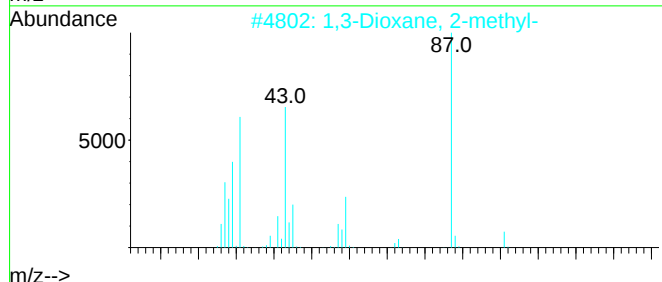
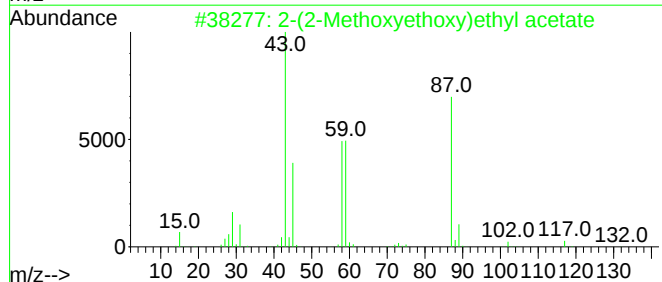
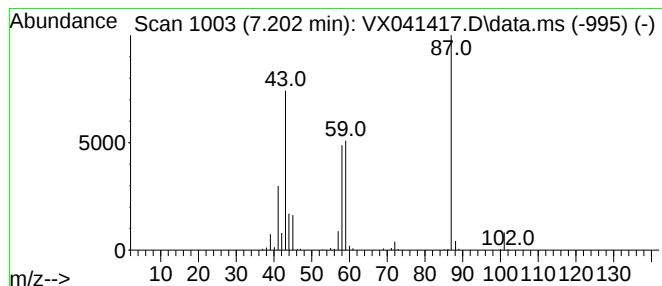
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 2-(2-Methoxyethoxy)ethyl ac... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.202	38.44 ug/l	455234	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	56
2	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	50
3	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	38
4	Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	37
5	1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	33



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050824\
Data File : VX041417.D
Acq On : 08 May 2024 13:43
Operator : JC/MD
Sample : P2389-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1400

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

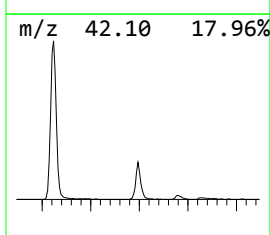
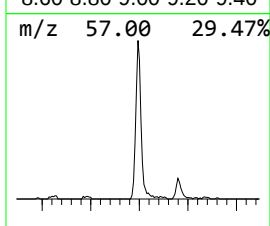
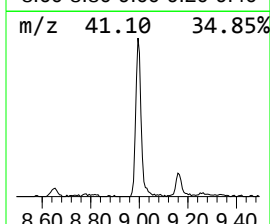
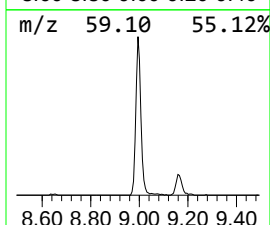
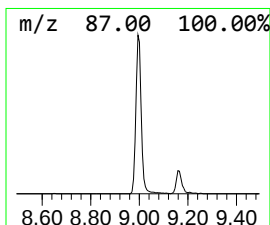
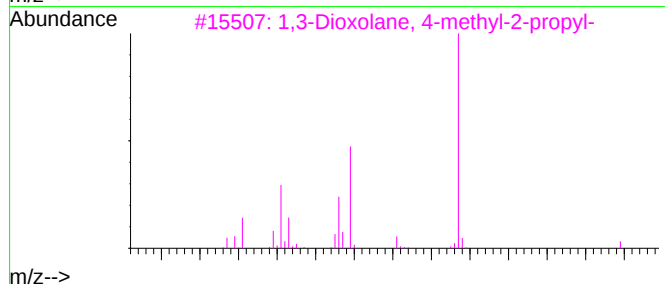
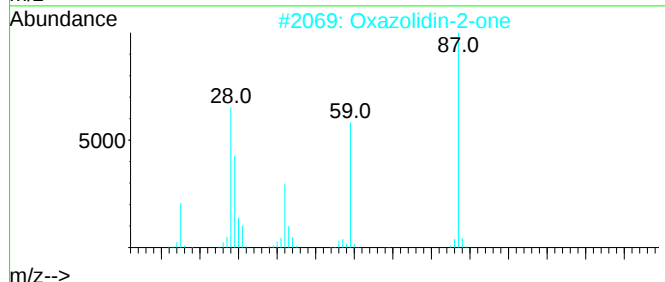
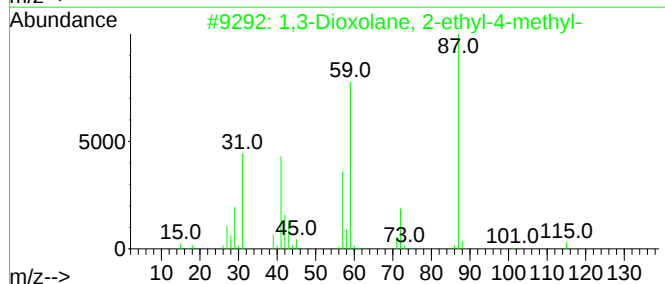
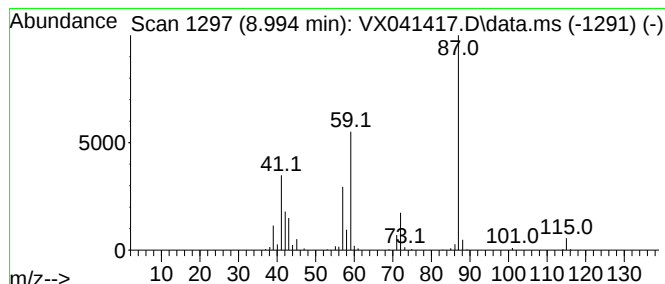
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.994	10.72 ug/l	135115	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	83
2	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	64
3	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	59
4	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050824\
Data File : VX041417.D
Acq On : 08 May 2024 13:43
Operator : JC/MD
Sample : P2389-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1400

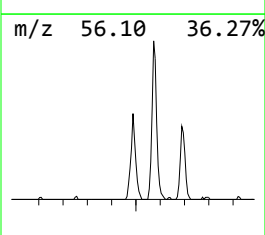
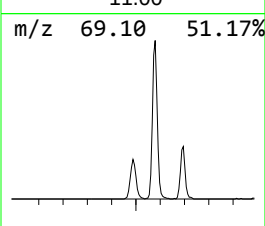
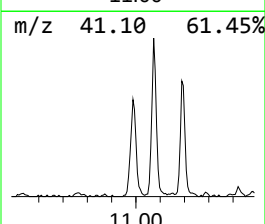
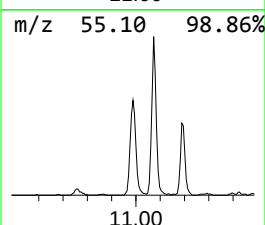
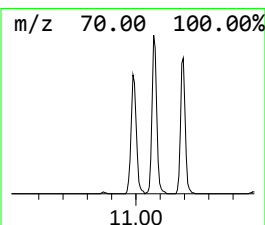
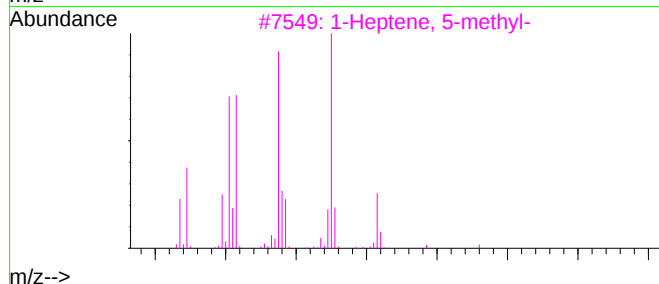
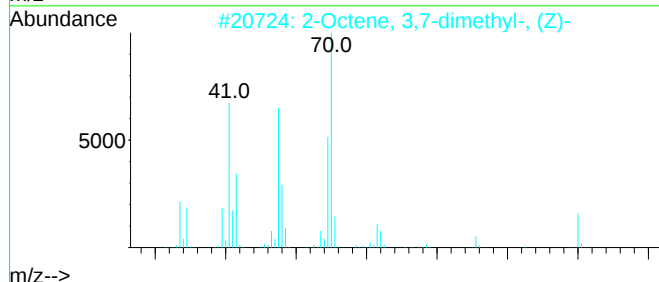
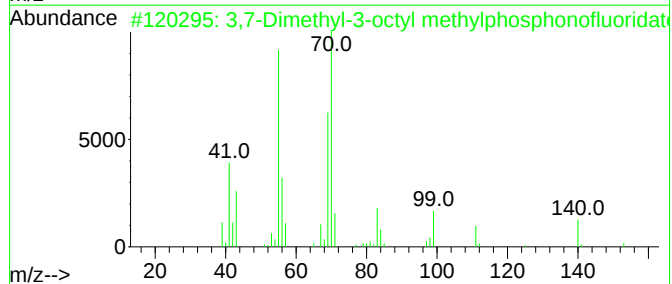
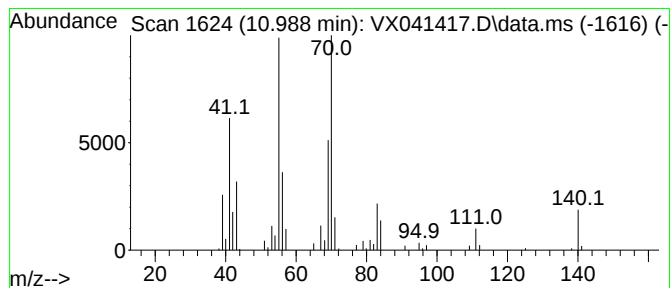
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Quant Title : SW846 8260

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

Peak Number 8 3,7-Dimethyl-3-octyl methyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.988	5.41 ug/l	68189	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,7-Dimethyl-3-octyl methylphosp...	238	C11H24F02P	159395-79-6	90
2	2-Octene, 3,7-dimethyl-, (Z)-	140	C10H20	006874-32-4	87
3	1-Heptene, 5-methyl-	112	C8H16	013151-04-7	80
4	4-Octene, 2,6-dimethyl-, [S-(Z)]-	140	C10H20	062960-77-4	68
5	2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050824\
Data File : VX041417.D
Acq On : 08 May 2024 13:43
Operator : JC/MD
Sample : P2389-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 6 Sample Multiplier: 1

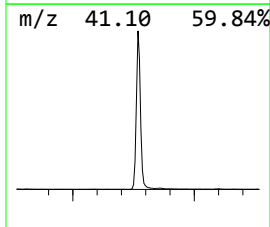
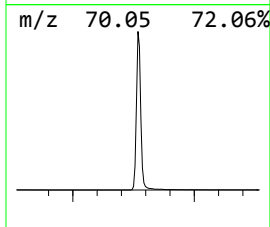
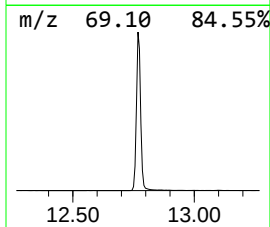
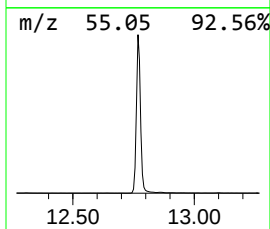
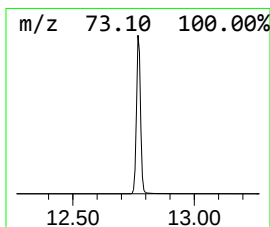
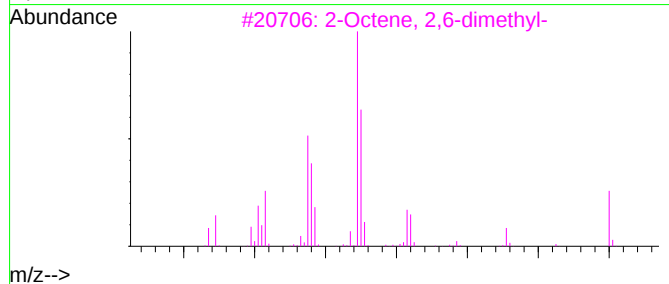
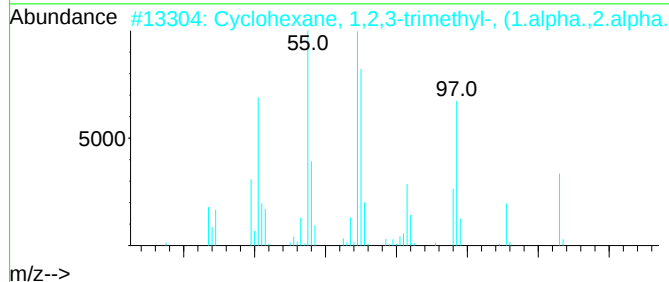
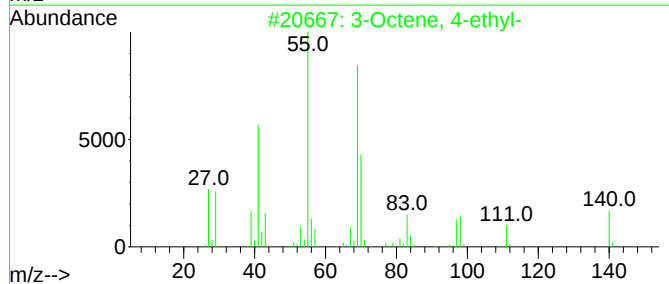
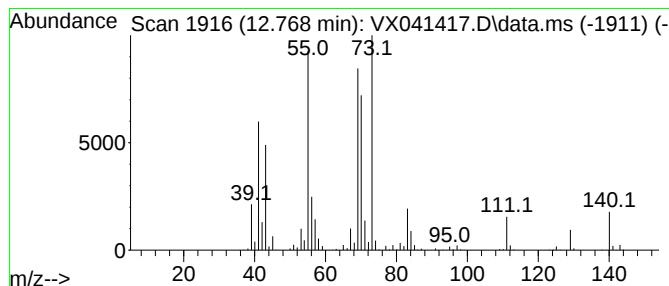
Instrument :
MSVOA_X
ClientSampleId :
1400

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

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

Peak Number 9 3-Octene, 4-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.768	146.04 ug/l	1981180	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octene, 4-ethyl-	140	C10H20	053966-51-1	74
2	Cyclohexane, 1,2,3-trimethyl-, (...)	126	C9H18	001839-88-9	72
3	2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	68
4	4-Octene, 2,6-dimethyl-, [S-(Z)]-	140	C10H20	062960-77-4	68
5	4-Octene, 2,6-dimethyl-, [S-(E)]-	140	C10H20	062960-76-3	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050824\
Data File : VX041417.D
Acq On : 08 May 2024 13:43
Operator : JC/MD
Sample : P2389-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1400

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.453	227.8	ug/l	2173530	1	5.550	477074	50.0
Ethanol	2.069	9.3	ug/l	88252	1	5.550	477074	50.0
Propanal	2.294	6.3	ug/l	60500	1	5.550	477074	50.0
2,3-Butanedione	4.373	22.2	ug/l	212083	1	5.550	477074	50.0
1,3-Dioxane, 2-...	6.867	261.0	ug/l	3090820	2	6.757	592097	50.0
2-(2-Methoxyeth...	7.202	38.4	ug/l	455234	2	6.757	592097	50.0
1,3-Dioxolane, ...	8.994	10.7	ug/l	135115	3	10.055	629935	50.0
3,7-Dimethyl-3-...	10.988	5.4	ug/l	68189	3	10.055	629935	50.0
3-Octene, 4-ethyl-	12.768	146.0	ug/l	1981180	4	12.024	678299	50.0