

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050724\
 Data File : VX041409.D
 Acq On : 07 May 2024 16:13
 Operator : JC/MD
 Sample : P2389-02 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1401

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\82X043024W.M

Title : SW846 8260

Signal : TIC: VX041409.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	64	rBV	3317485	3935882	100.00%	37.358%
2	1.496	64	67	92	rVB	562308	1360086	34.56%	12.909%
3	2.093	158	165	181	rBV	215152	361276	9.18%	3.429%
4	4.233	507	516	536	rBV2	24319	93206	2.37%	0.885%
5	5.385	692	705	721	rBV2	96472	285897	7.26%	2.714%
6	5.544	721	731	755	rVB	176391	509722	12.95%	4.838%
7	5.952	789	798	811	rBV	101256	279531	7.10%	2.653%
8	6.757	920	930	942	rBV	257468	624309	15.86%	5.926%
9	6.873	942	949	974	rVB	76687	193545	4.92%	1.837%
10	7.208	996	1004	1028	rBV4	42168	123209	3.13%	1.169%
11	8.647	1233	1240	1248	rBV	436605	676391	17.19%	6.420%
12	10.055	1465	1471	1485	rBV	457319	644678	16.38%	6.119%
13	10.311	1503	1513	1524	rVB2	75253	108003	2.74%	1.025%
14	11.079	1634	1639	1655	rBV	410239	525390	13.35%	4.987%
15	12.018	1780	1793	1802	rBV	490250	644809	16.38%	6.120%
16	12.213	1819	1825	1837	rBV2	53736	100889	2.56%	0.958%
17	12.415	1853	1858	1864	rBV	52607	68760	1.75%	0.653%

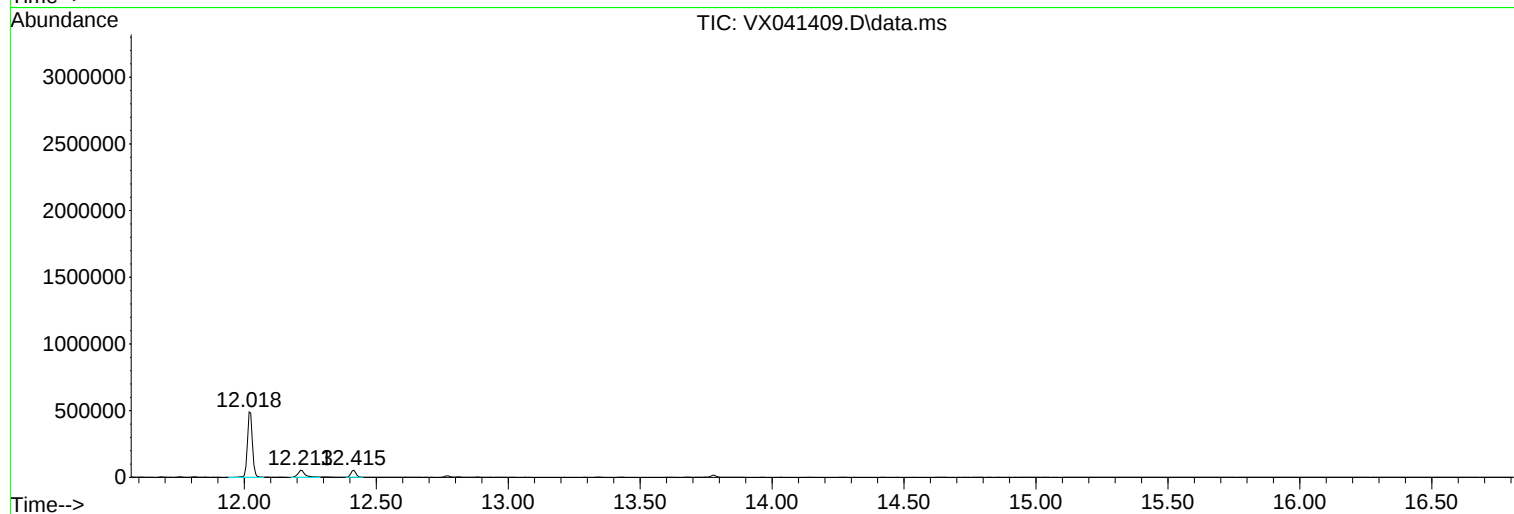
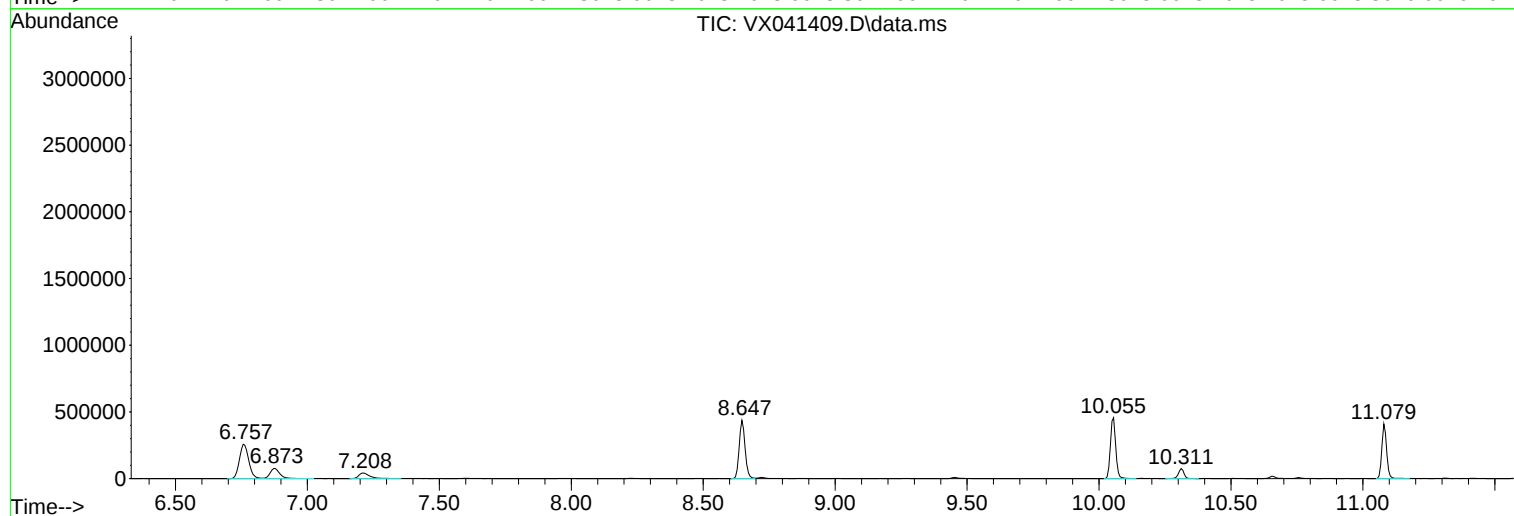
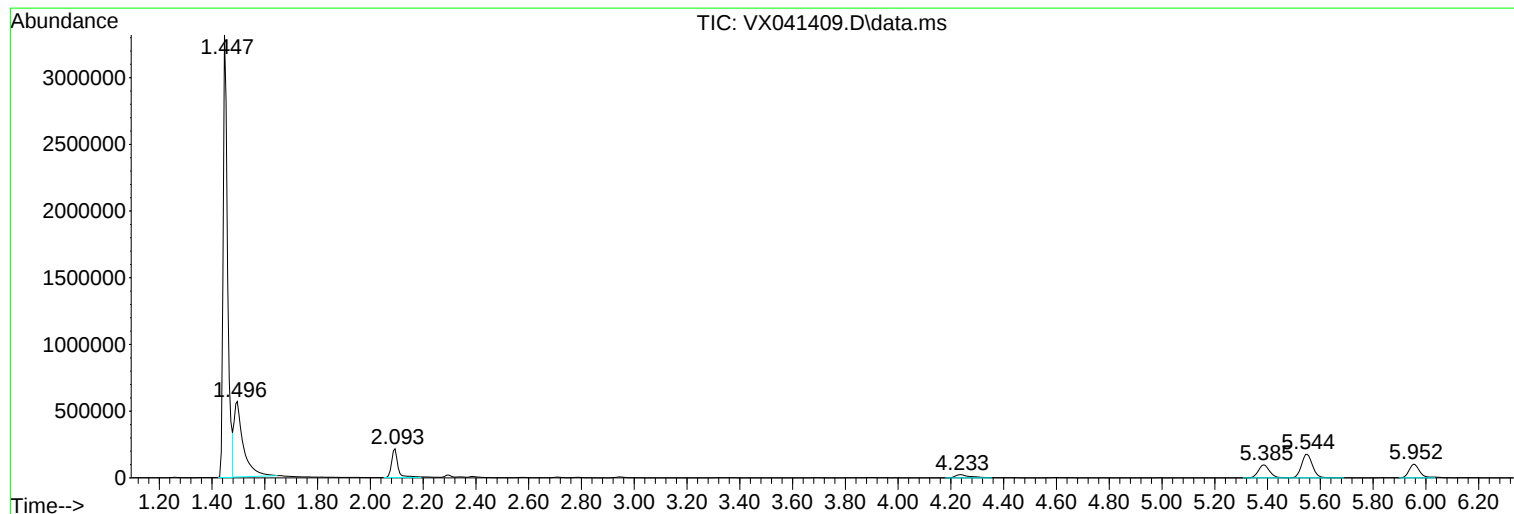
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

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



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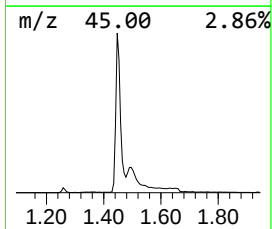
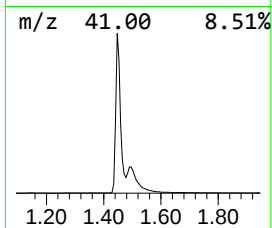
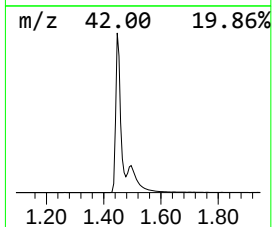
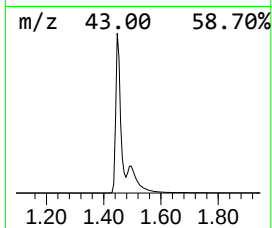
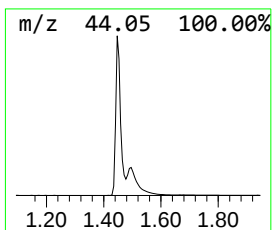
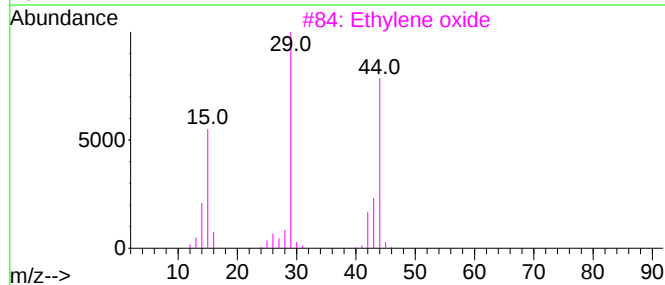
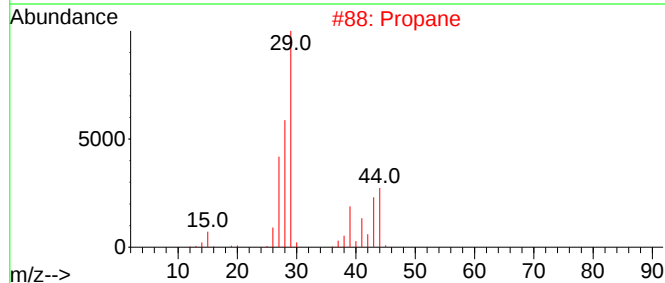
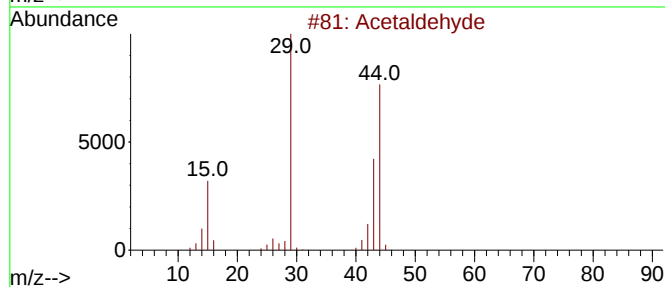
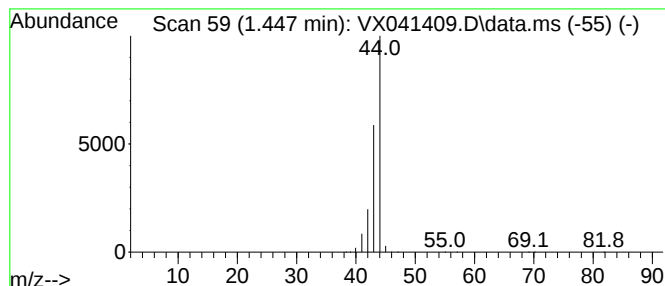
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Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.447	386.08 ug/l	3935880	Pentafluorobenzene	5.544

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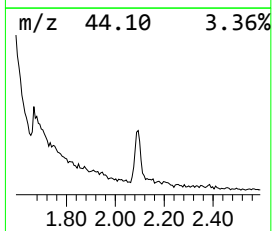
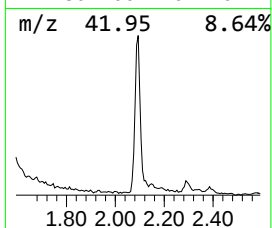
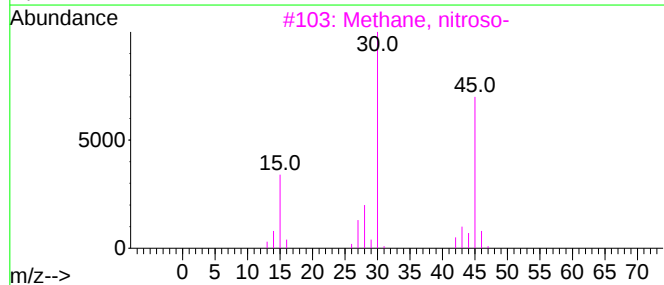
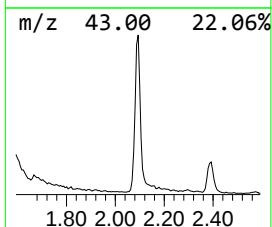
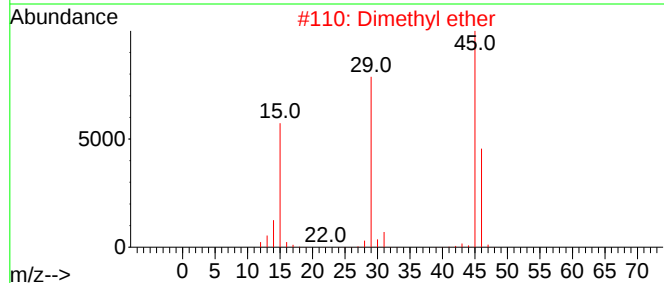
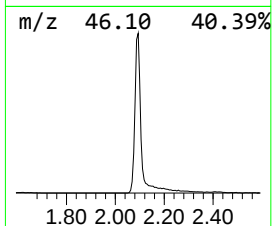
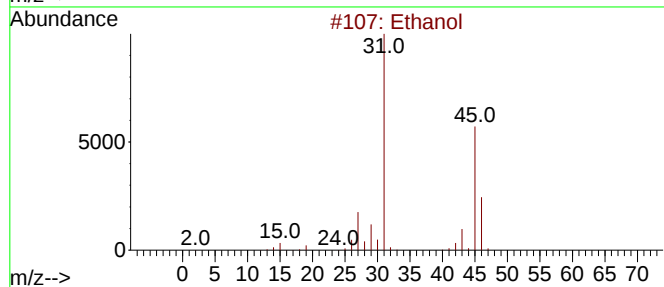
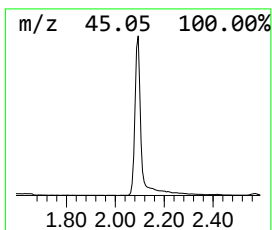
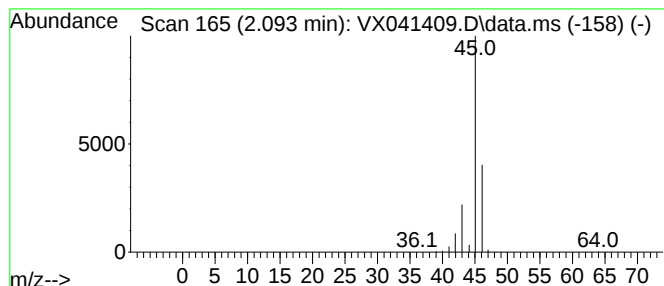
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

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

Peak Number 3 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.093	35.44 ug/l	361276	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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Instrument :
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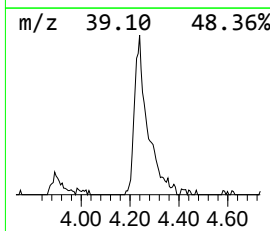
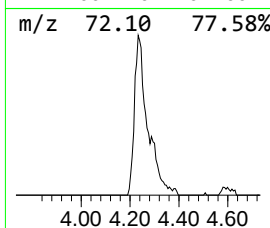
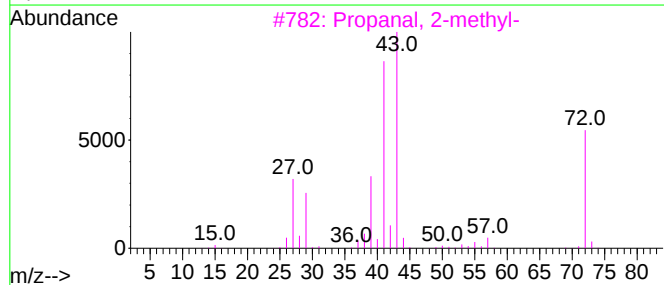
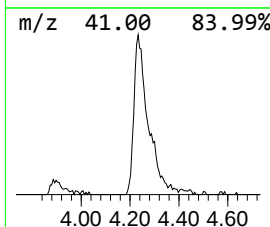
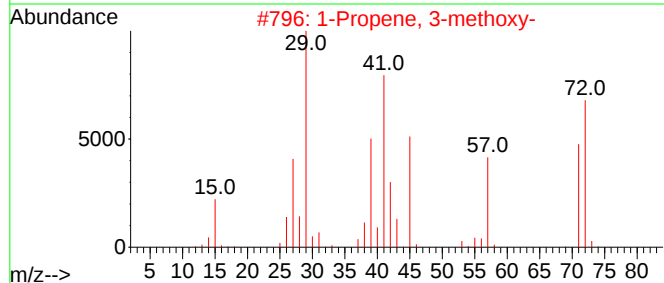
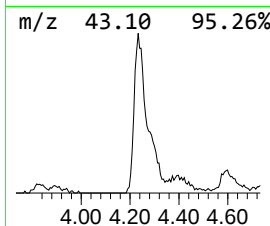
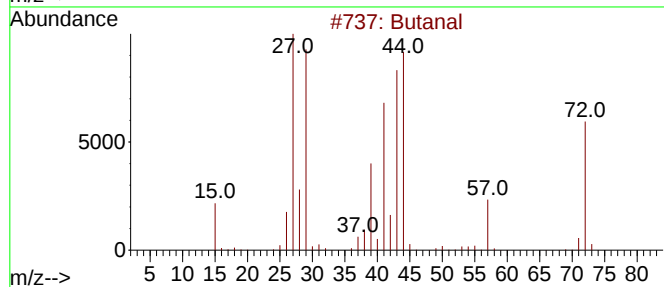
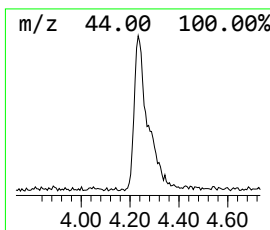
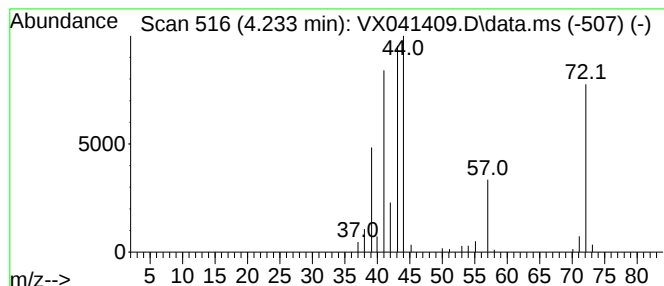
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

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

Peak Number 4 Butanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	9.14 ug/l	93206	Pentafluorobenzene	5.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	49
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
4			Ethene, ethoxy-	72	C4H8O	000109-92-2	40
5			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

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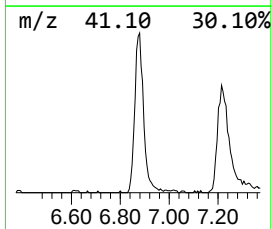
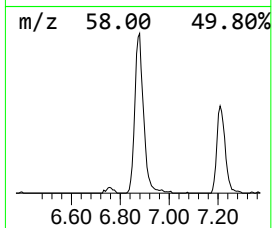
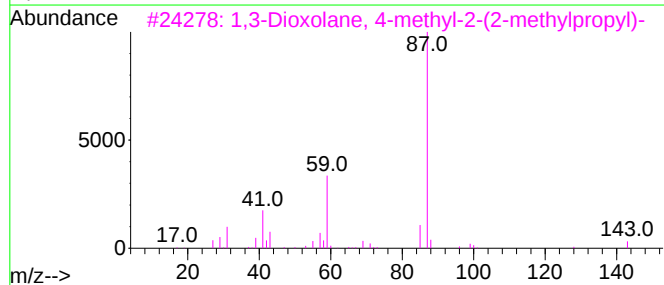
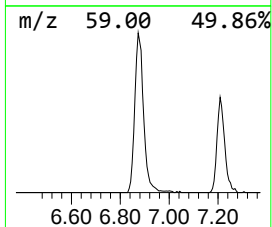
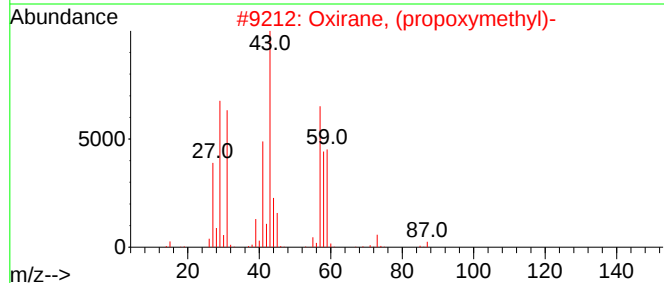
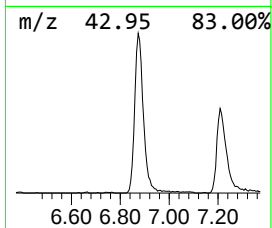
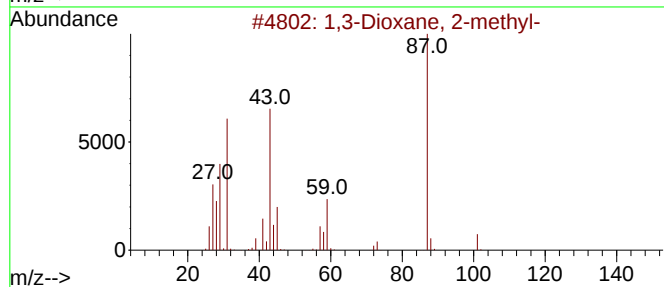
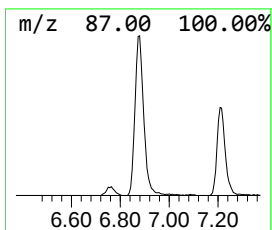
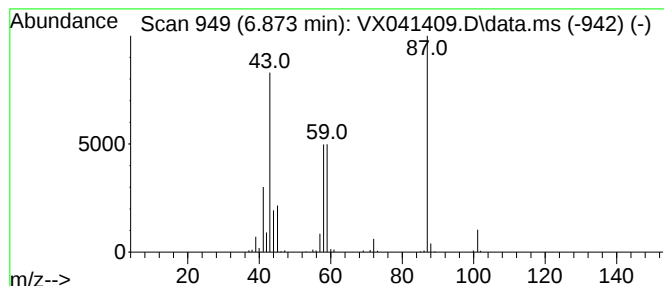
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

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

Peak Number 5 1,3-Dioxane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.873	15.50 ug/l	193545	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			Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	37
3			1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	37
4			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	32
5			2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	28



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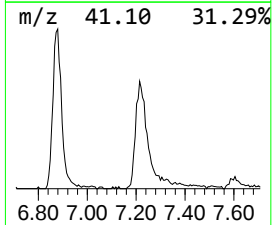
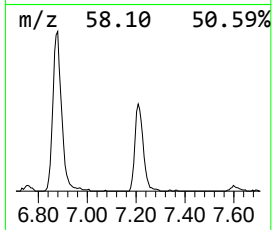
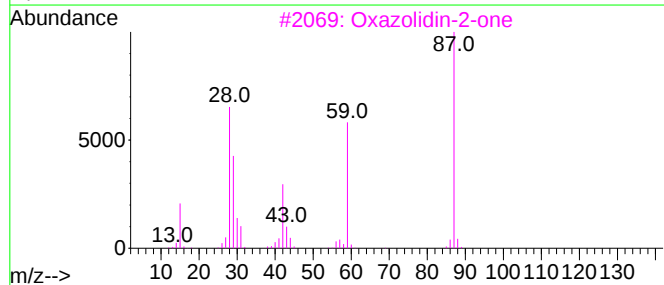
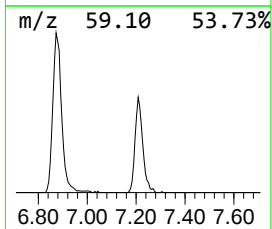
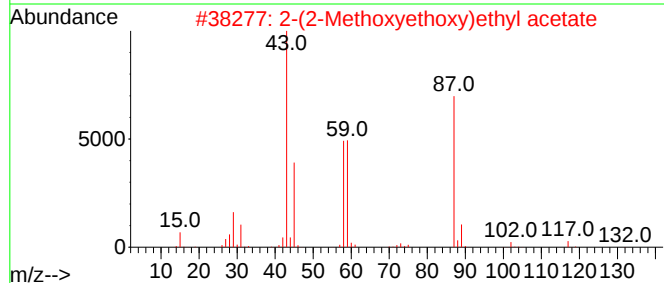
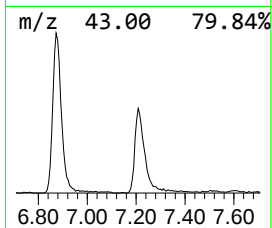
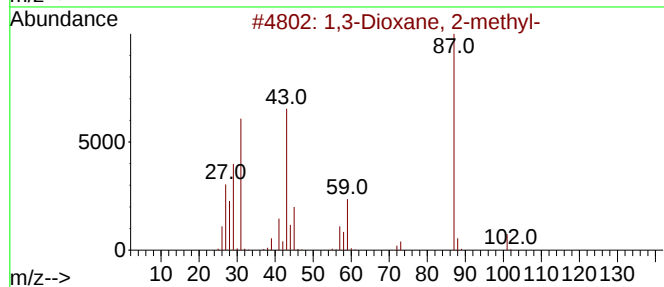
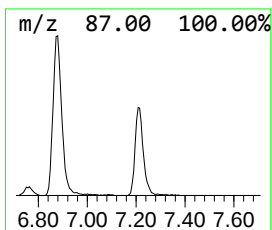
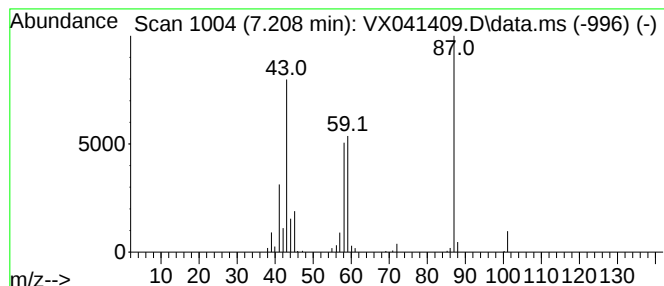
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

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

Peak Number 6 2-(2-Methoxyethoxy)ethyl ac... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	9.87 ug/l	123209	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	53
2		2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	50
3		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	43
4		Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	38
5		1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	38



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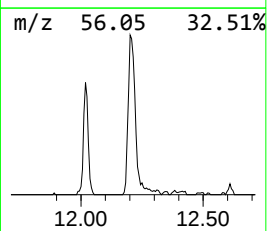
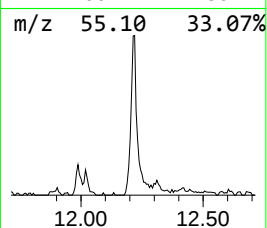
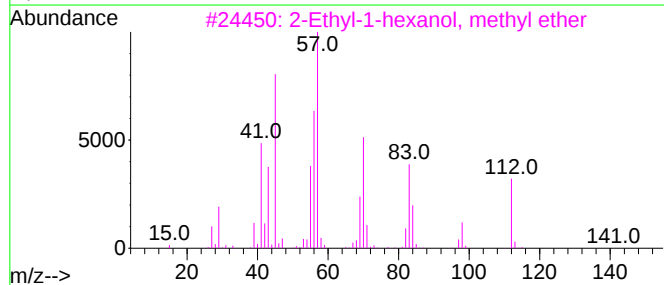
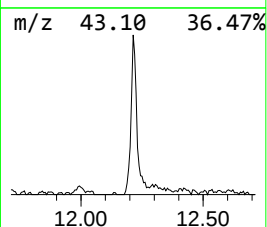
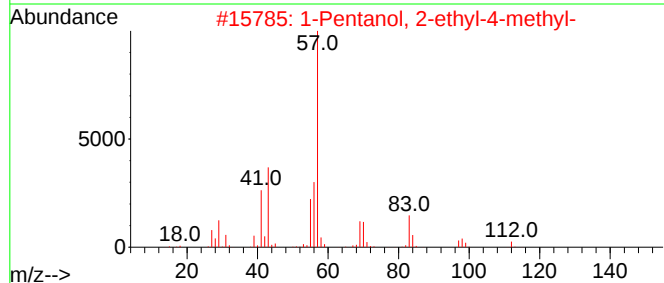
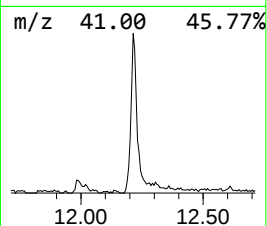
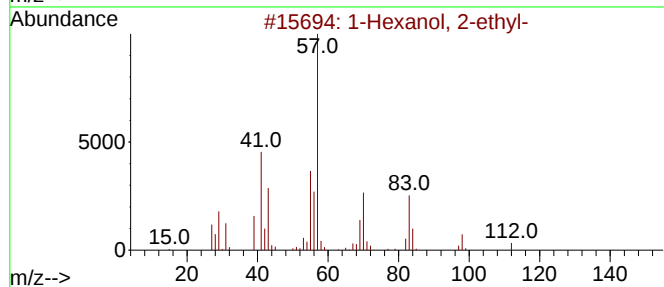
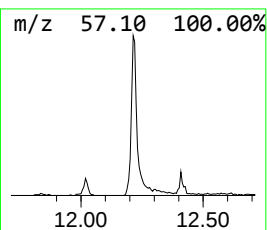
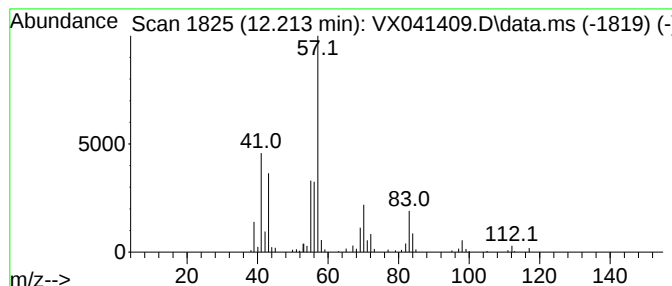
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Quant Title : SW846 8260

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.213	7.82 ug/l	100889	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	83
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	72
3			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	59
4			Oxirane, [[(2-ethylhexyl)oxy]met...	186	C11H22O2	002461-15-6	50
5			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050724\
Data File : VX041409.D
Acq On : 07 May 2024 16:13
Operator : JC/MD
Sample : P2389-02 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1401

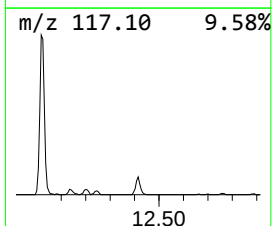
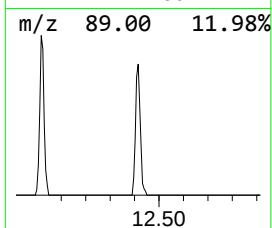
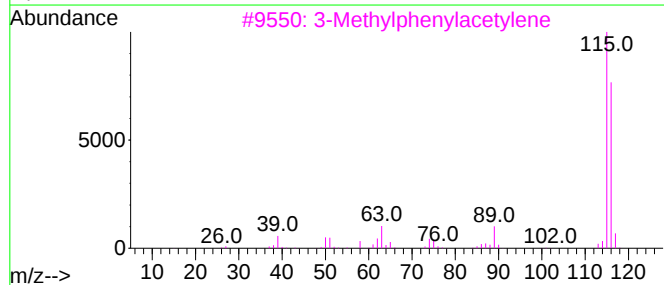
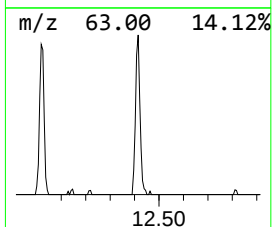
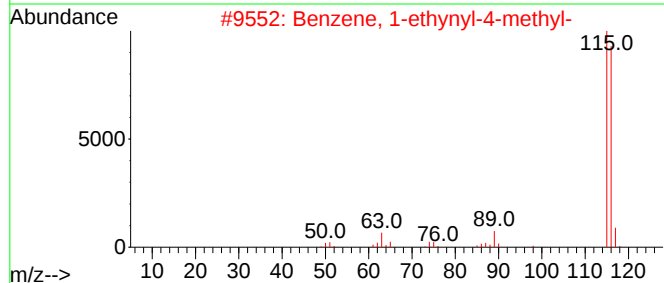
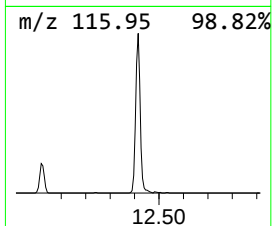
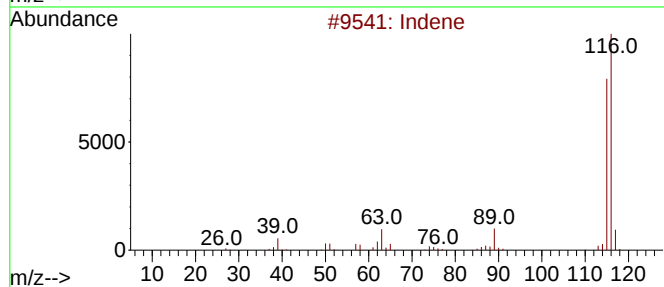
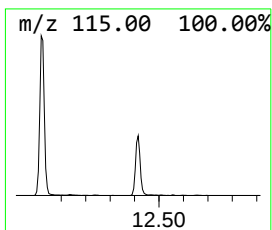
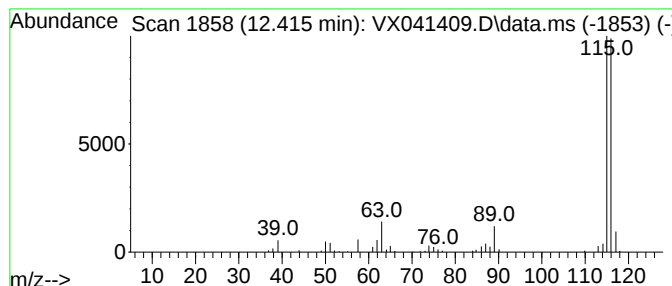
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Quant Title : SW846 8260

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

Peak Number 8 Indene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.415	5.33 ug/l	68760	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Indene	116	C9H8	000095-13-6	97
2		Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
3		3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4		Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	90
5		Benzene, 1-propynyl-	116	C9H8	000673-32-5	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050724\
Data File : VX041409.D
Acq On : 07 May 2024 16:13
Operator : JC/MD
Sample : P2389-02 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1401

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.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	386.1	ug/l	3935880	1	5.544	509722	50.0
Ethanol	2.093	35.4	ug/l	361276	1	5.544	509722	50.0
Butanal	4.233	9.1	ug/l	93206	1	5.544	509722	50.0
1,3-Dioxane, 2-...	6.873	15.5	ug/l	193545	2	6.757	624309	50.0
2-(2-Methoxyeth...	7.208	9.9	ug/l	123209	2	6.757	624309	50.0
1-Hexanol, 2-et...	12.213	7.8	ug/l	100889	4	12.024	644809	50.0
Indene	12.415	5.3	ug/l	68760	4	12.024	644809	50.0