

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092624\
 Data File : VX043179.D
 Acq On : 26 Sep 2024 15:34
 Operator : JC/MD
 Sample : P4202-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 50415

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\82X092324W.M
 Title : SW846 8260

Signal : TIC: VX043179.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.136	155	172	176	rBV	3658592	9724408	100.00%	61.134%
2	2.392	208	214	237	rVB	358542	670254	6.89%	4.214%
3	2.575	237	244	259	rVB	74827	153832	1.58%	0.967%
4	4.568	563	571	588	rBV	36035	111718	1.15%	0.702%
5	5.385	693	705	723	rBV2	56403	168773	1.74%	1.061%
6	5.550	723	732	750	rVB	81561	234551	2.41%	1.475%
7	5.952	789	798	805	rBV	64572	174685	1.80%	1.098%
8	6.031	805	811	823	rVB	106010	285037	2.93%	1.792%
9	6.757	922	930	944	rBV	144457	346446	3.56%	2.178%
10	7.226	1000	1007	1031	rBV	53150	134721	1.39%	0.847%
11	7.458	1039	1045	1065	rVB	61004	130688	1.34%	0.822%
12	8.647	1234	1240	1246	rBV	315445	483413	4.97%	3.039%
13	8.714	1246	1251	1260	rVB	586051	932557	9.59%	5.863%
14	10.055	1463	1471	1485	rBV	296260	415474	4.27%	2.612%
15	10.195	1489	1494	1502	rBV	97716	137386	1.41%	0.864%
16	10.299	1505	1511	1520	rVB	341546	460741	4.74%	2.897%
17	10.640	1562	1567	1572	rVB	234084	294388	3.03%	1.851%
18	11.079	1634	1639	1646	rBV	242436	311004	3.20%	1.955%
19	11.378	1681	1688	1695	rBV	58373	99984	1.03%	0.629%
20	11.750	1740	1749	1757	rVB	125325	158957	1.63%	0.999%
21	12.018	1788	1793	1800	rBV	283451	363032	3.73%	2.282%
22	13.774	2077	2081	2086	rVB	89574	114650	1.18%	0.721%

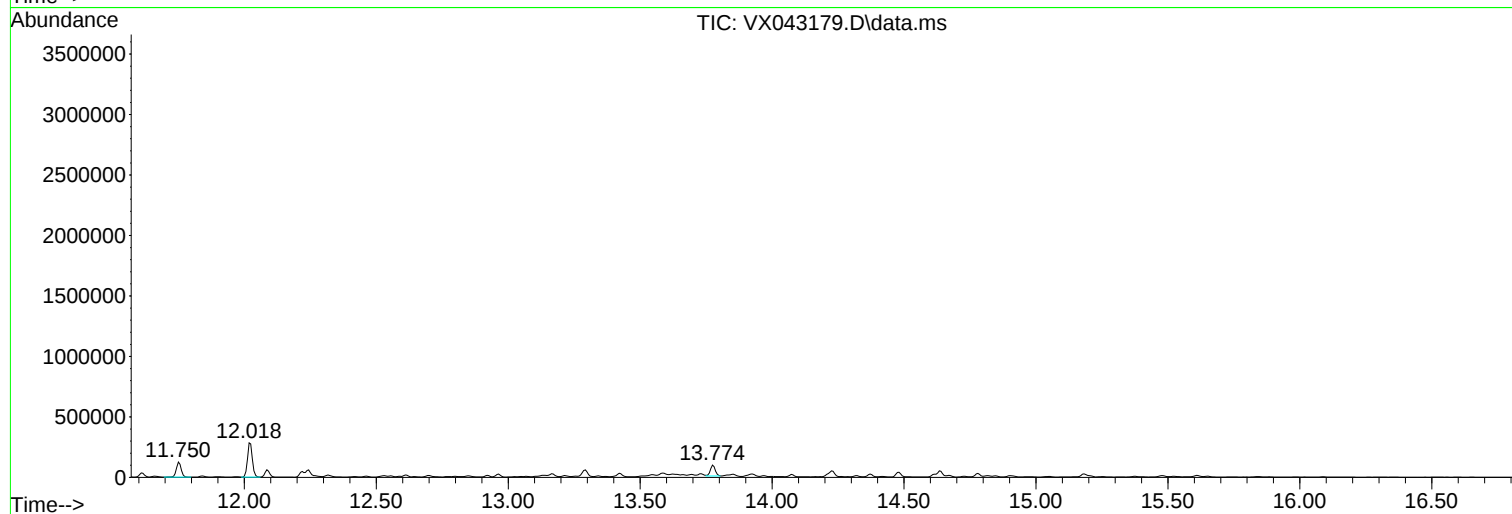
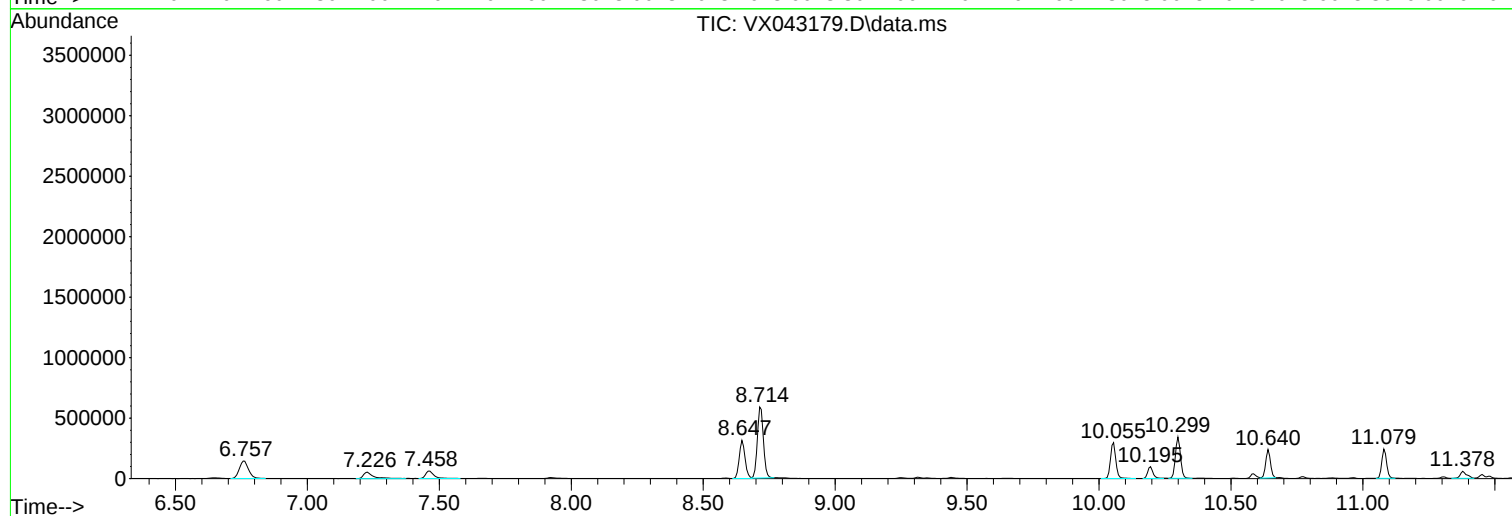
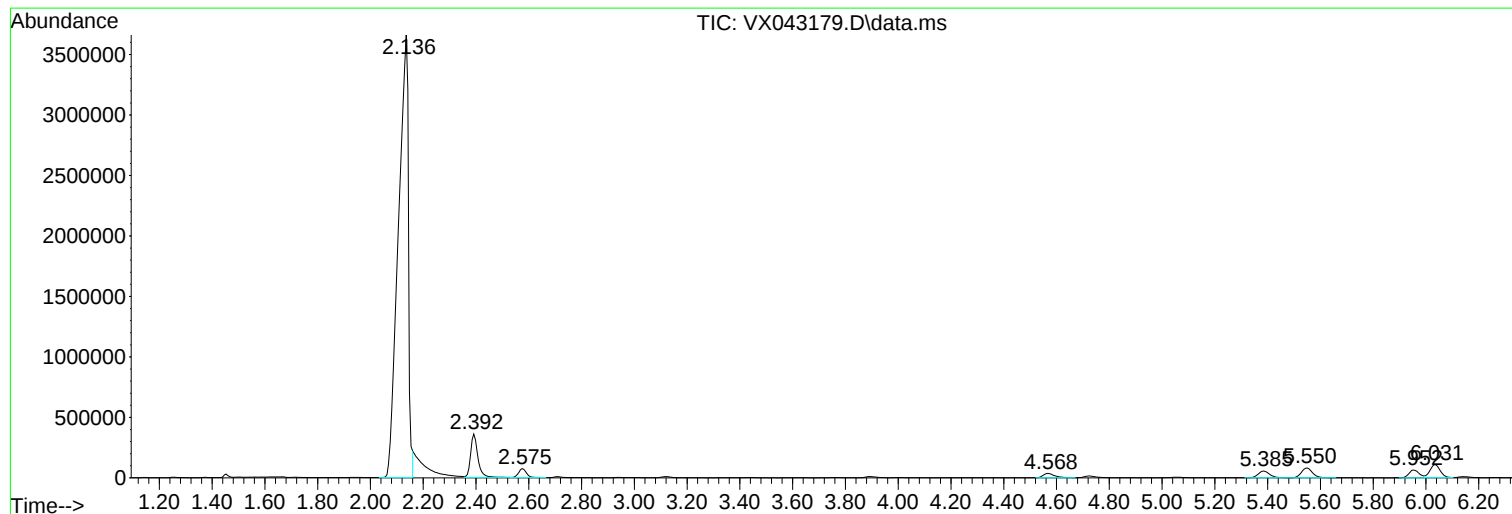
Sum of corrected areas: 15906699

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092624\
Data File : VX043179.D
Acq On : 26 Sep 2024 15:34
Operator : JC/MD
Sample : P4202-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50415

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092324W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092624\
Data File : VX043179.D
Acq On : 26 Sep 2024 15:34
Operator : JC/MD
Sample : P4202-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50415

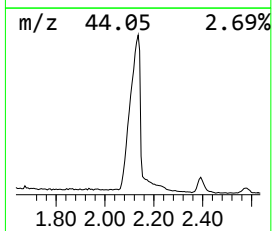
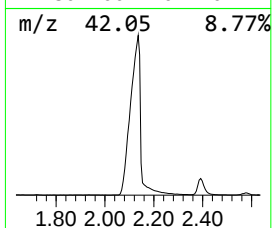
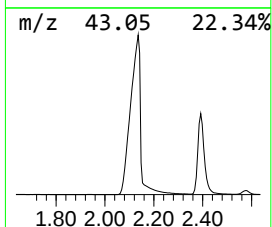
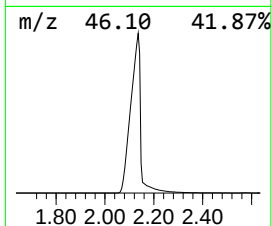
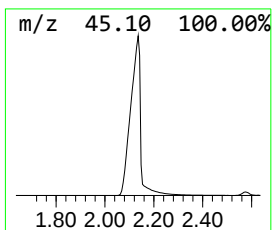
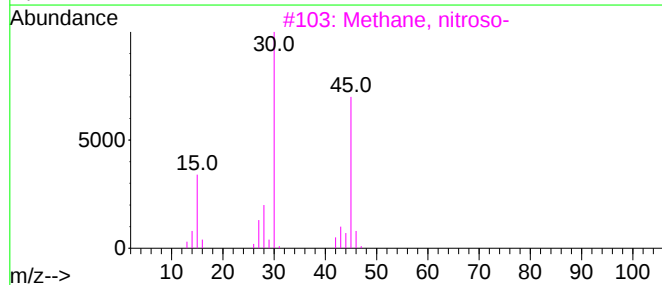
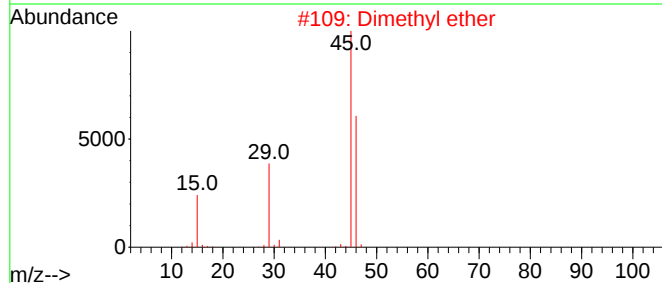
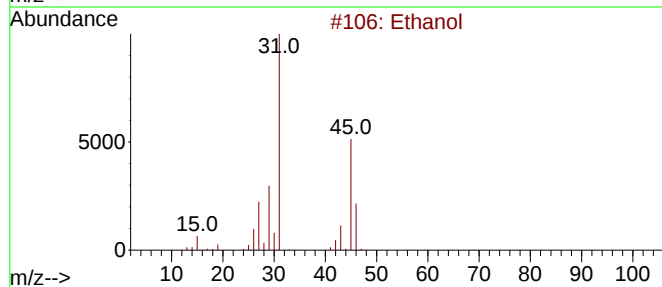
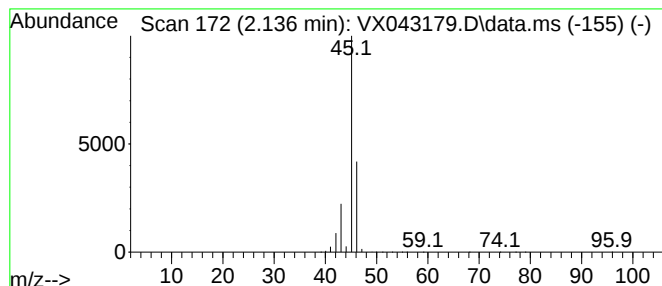
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092324W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.136	2072.98 ug/l	9724410	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	86
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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092624\
Data File : VX043179.D
Acq On : 26 Sep 2024 15:34
Operator : JC/MD
Sample : P4202-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50415

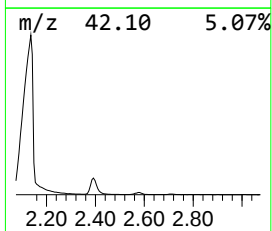
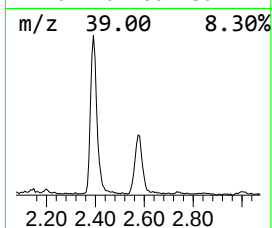
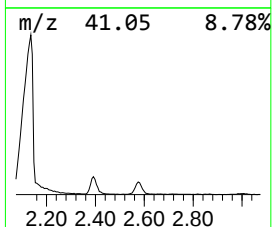
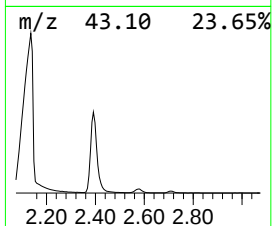
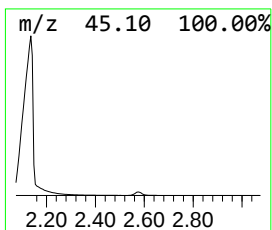
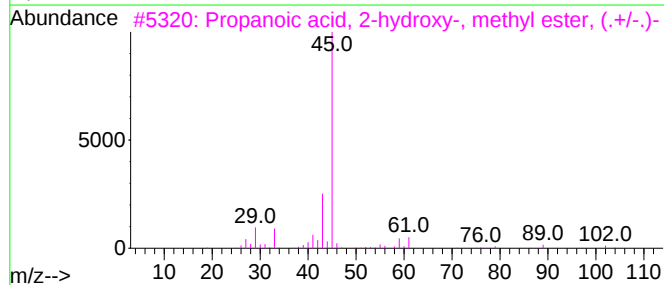
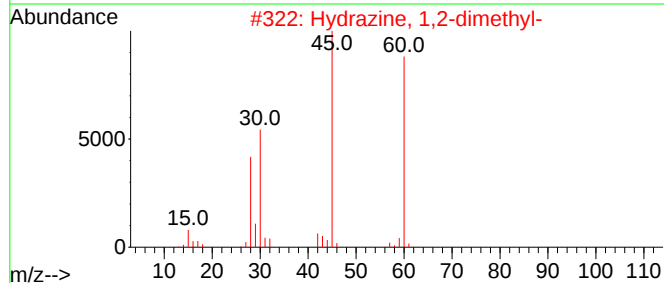
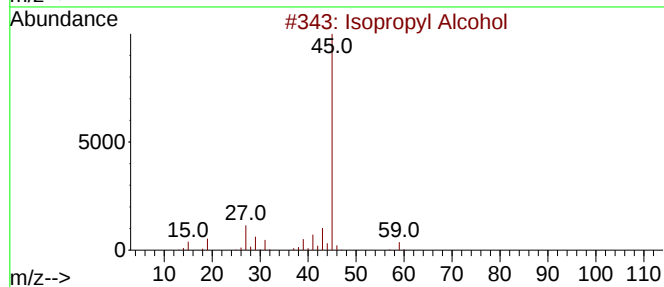
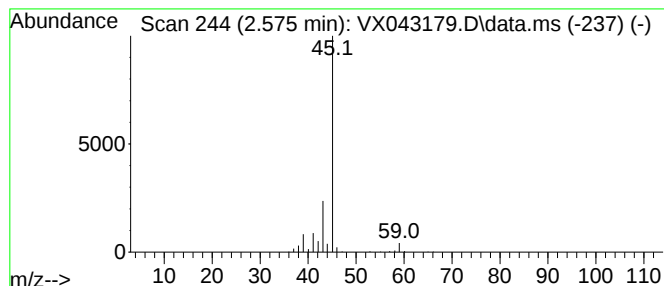
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092324W.M
Quant Title : SW846 8260

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.575	32.79 ug/l	153832	Pentafluorobenzene	5.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2		Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
4		Ethylamine	45	C2H7N	000075-04-7	5
5		Formamide	45	CH3NO	000075-12-7	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092624\
Data File : VX043179.D
Acq On : 26 Sep 2024 15:34
Operator : JC/MD
Sample : P4202-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50415

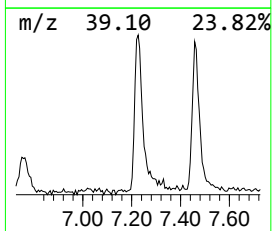
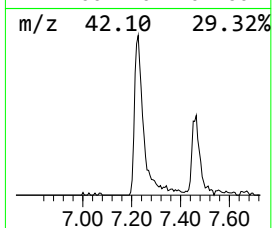
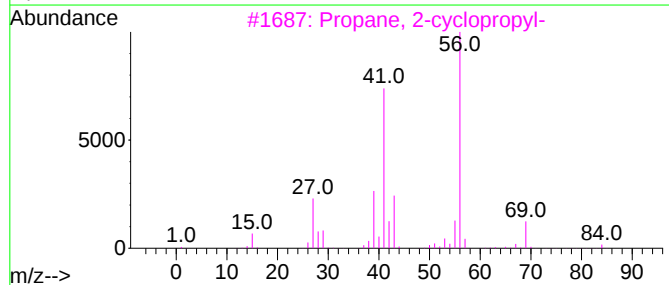
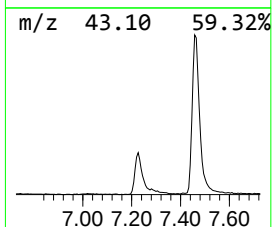
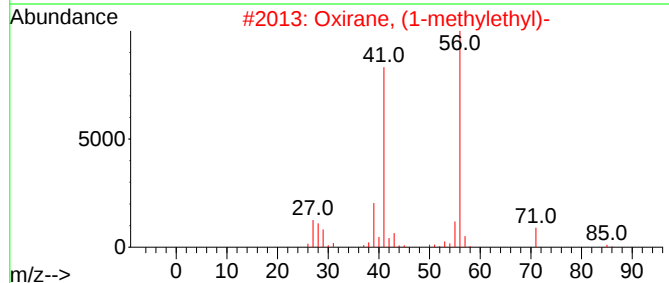
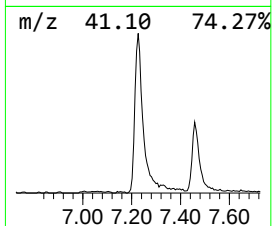
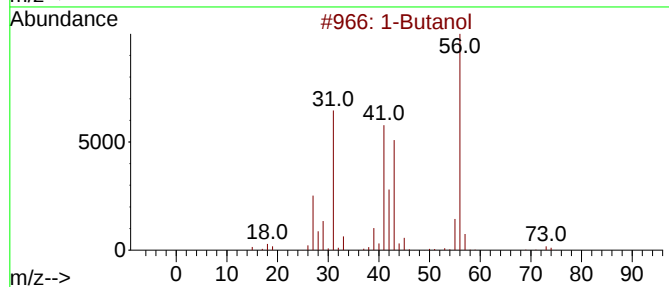
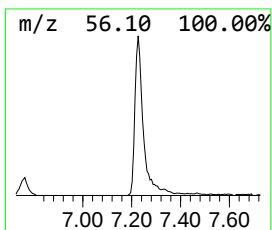
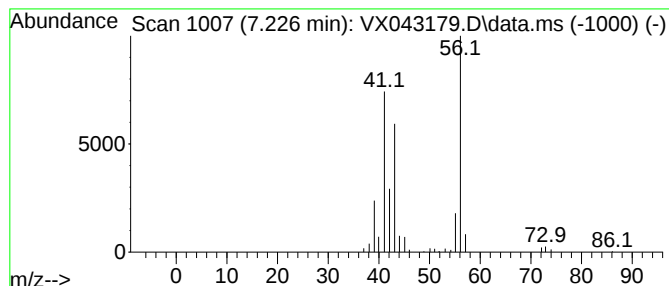
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092324W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.226	19.44 ug/l	134721	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol		74	C4H10O	000071-36-3	86
2	Oxirane, (1-methylethyl)-		86	C5H10O	001438-14-8	59
3	Propane, 2-cyclopropyl-		84	C6H12	003638-35-5	39
4	1-Hexanol		102	C6H14O	000111-27-3	38
5	2H-Pyran-2-one, tetrahydro-5,6-d...		128	C7H12O2	024405-16-1	33



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092624\
Data File : VX043179.D
Acq On : 26 Sep 2024 15:34
Operator : JC/MD
Sample : P4202-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50415

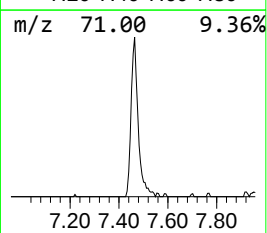
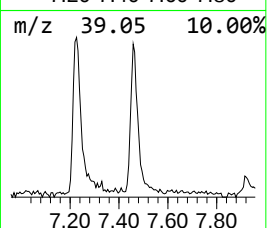
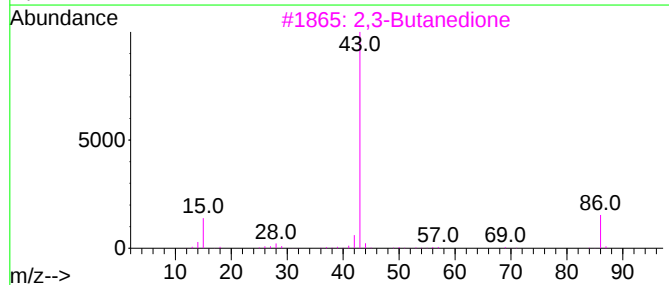
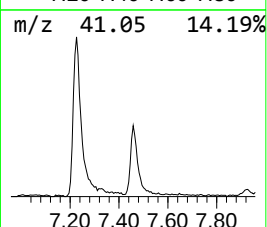
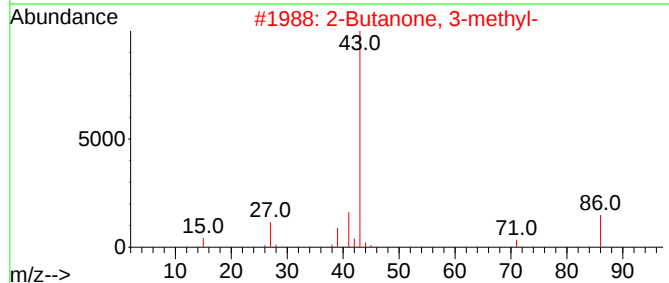
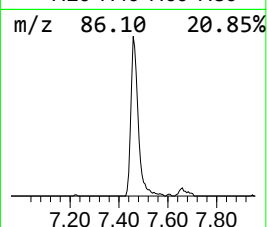
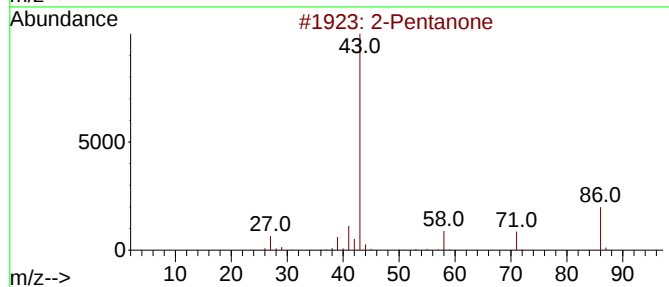
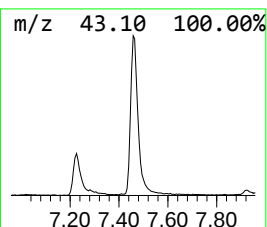
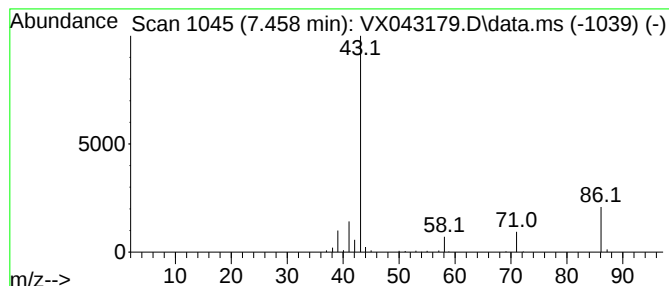
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092324W.M
Quant Title : SW846 8260

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

Peak Number 4 2-Pentanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.458	18.86 ug/l	130688	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone	86	C5H10O	000107-87-9	86
2			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	64
3			2,3-Butanedione	86	C4H6O2	000431-03-8	47
4			3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	36
5			Isobutane	58	C4H10	000075-28-5	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092624\
Data File : VX043179.D
Acq On : 26 Sep 2024 15:34
Operator : JC/MD
Sample : P4202-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50415

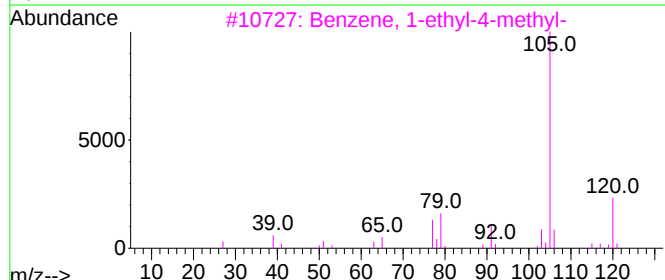
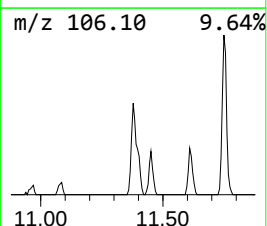
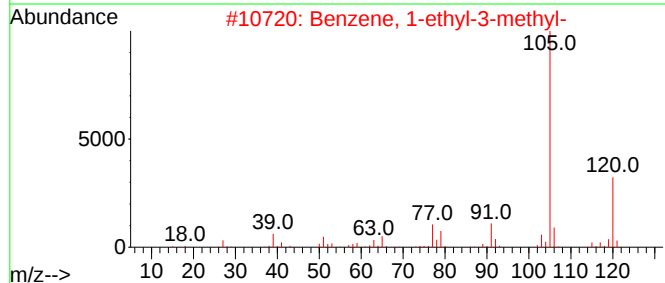
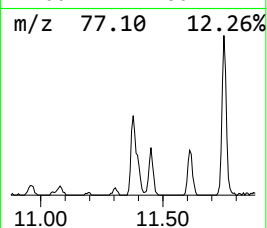
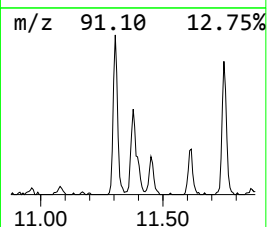
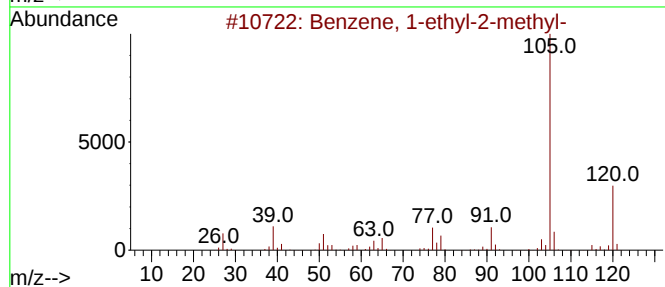
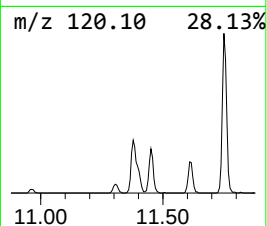
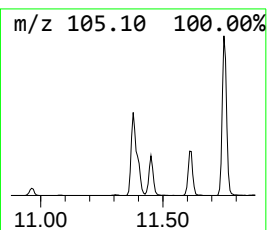
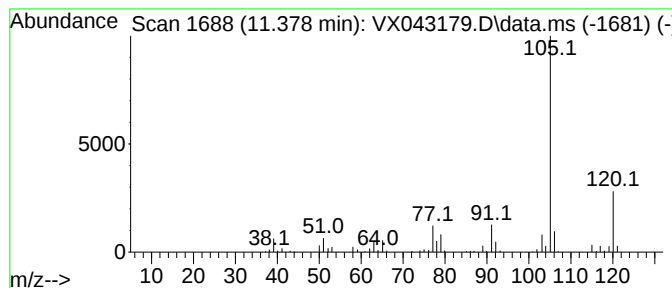
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092324W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	13.77 ug/l	99984	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092624\
Data File : VX043179.D
Acq On : 26 Sep 2024 15:34
Operator : JC/MD
Sample : P4202-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
50415

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X092324W.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
Ethanol	2.136	2073.0	ug/l	9724410	1	5.550	234551	50.0
Isopropyl Alcohol	2.575	32.8	ug/l	153832	1	5.550	234551	50.0
1-Butanol	7.226	19.4	ug/l	134721	2	6.763	346446	50.0
2-Pentanone	7.458	18.9	ug/l	130688	2	6.763	346446	50.0
Benzene, 1-ethy...	11.378	13.8	ug/l	99984	4	12.024	363032	50.0