

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
 Data File : VX030153.D
 Acq On : 20 Jul 2022 23:51
 Operator : JC/MD
 Sample : N3781-04 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 ORA-62322

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\82X071222W.M
 Title : SW846 8260

Signal : TIC: VX030153.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	69	rBV	199210	230370	1.11%	0.443%
2	2.300	192	199	235	rVB	11778311	20751525	100.00%	39.939%
3	3.873	446	457	478	rBV	698762	1849739	8.91%	3.560%
4	5.391	696	706	718	rBV	112224	325845	1.57%	0.627%
5	5.556	722	733	750	rVB	195295	559984	2.70%	1.078%
6	5.964	789	800	813	rBV	126221	350317	1.69%	0.674%
7	6.769	921	932	944	rBV	328597	777756	3.75%	1.497%
8	8.653	1233	1241	1254	rBV	654782	1058311	5.10%	2.037%
9	9.000	1291	1298	1318	rBV	8445034	12388985	59.70%	23.844%
10	9.165	1318	1325	1341	rVV	5677520	7840354	37.78%	15.090%
11	10.080	1465	1475	1484	rBV2	2056961	3493619	16.84%	6.724%
12	11.085	1634	1640	1646	rBV	489440	630067	3.04%	1.213%
13	11.665	1722	1735	1742	rBV	272294	435169	2.10%	0.838%
14	11.957	1775	1783	1788	rBV	372640	474804	2.29%	0.914%
15	12.024	1789	1794	1804	rVB	630818	791414	3.81%	1.523%

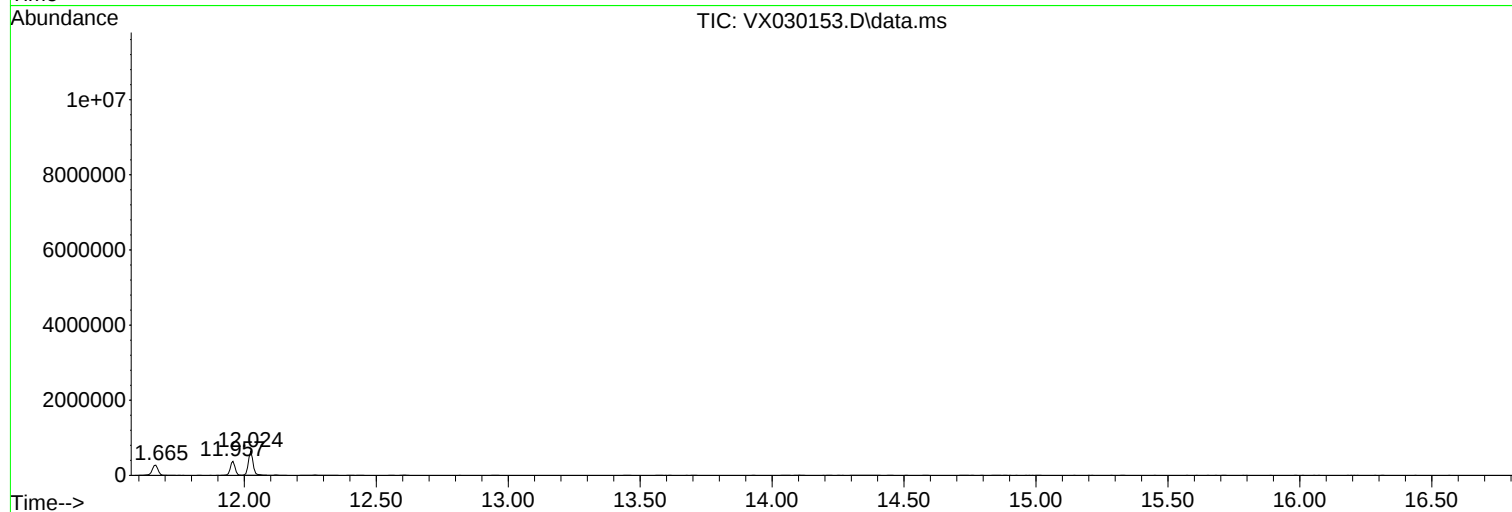
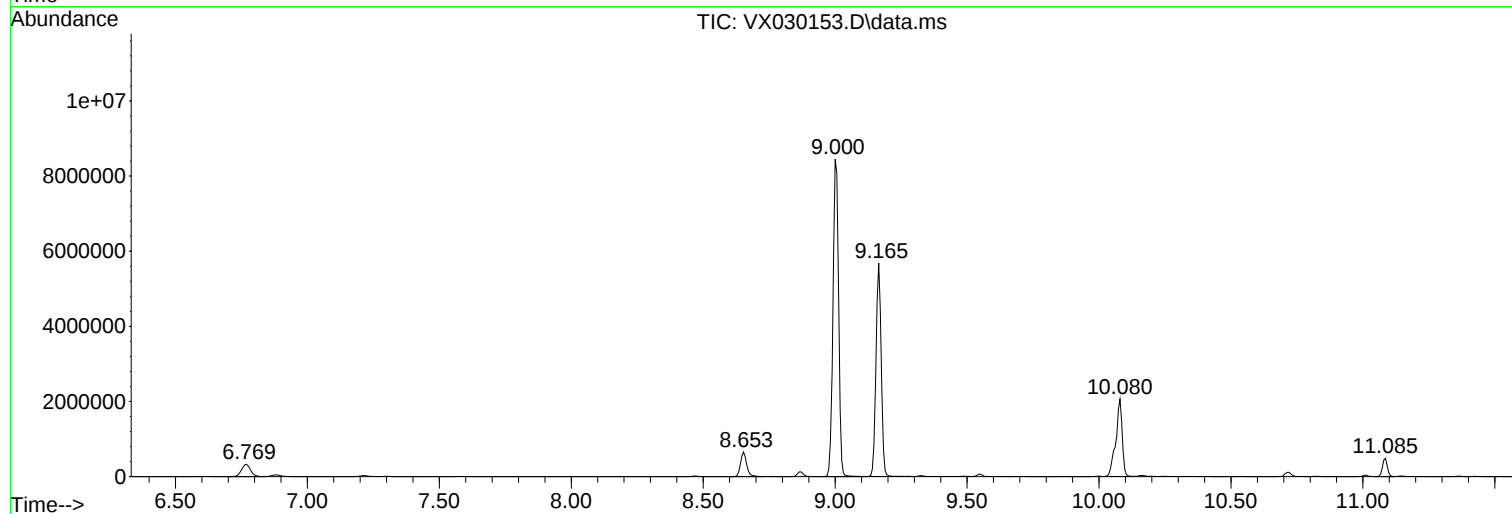
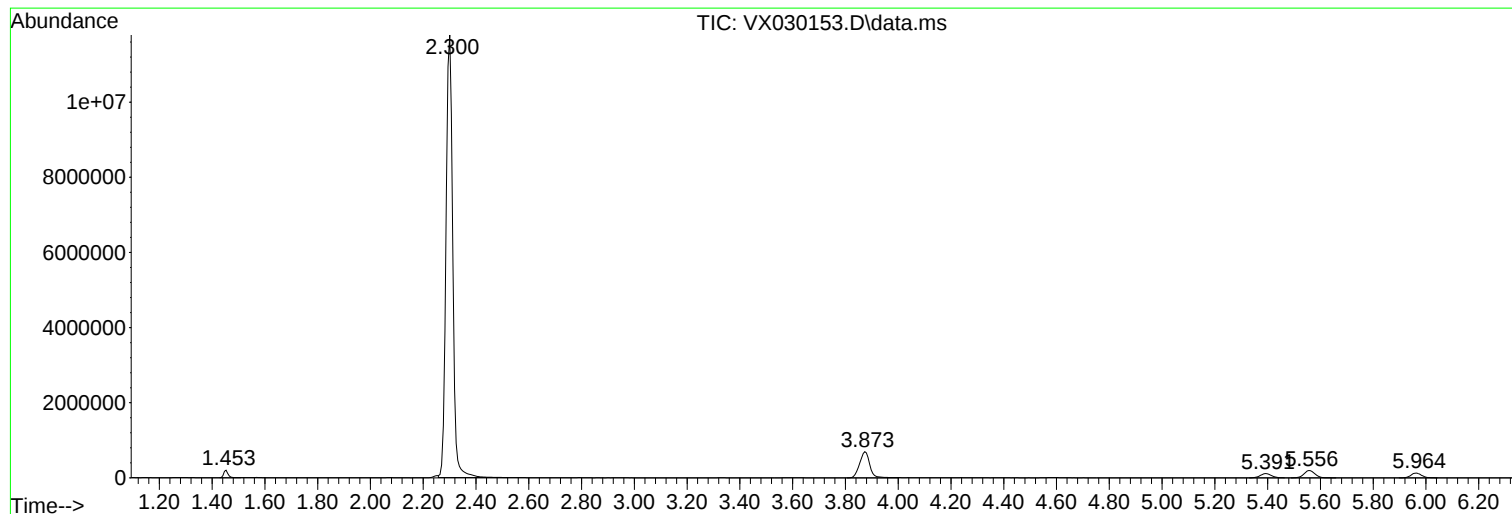
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

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



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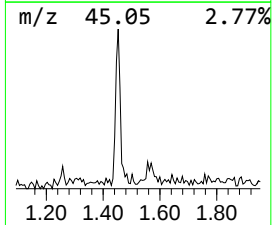
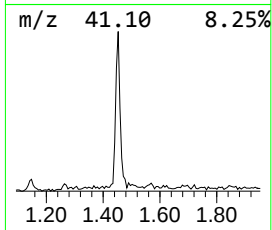
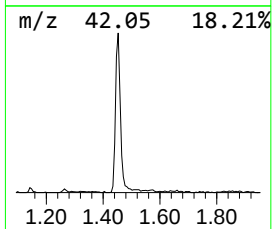
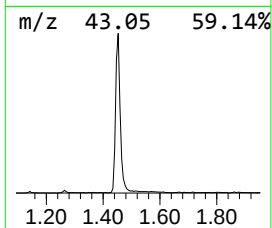
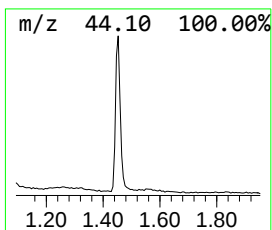
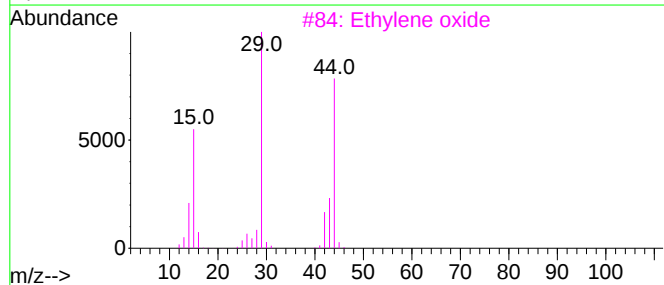
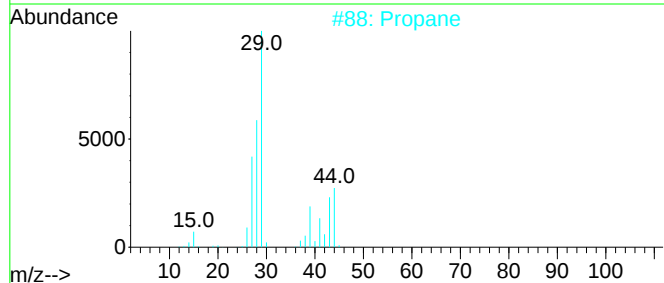
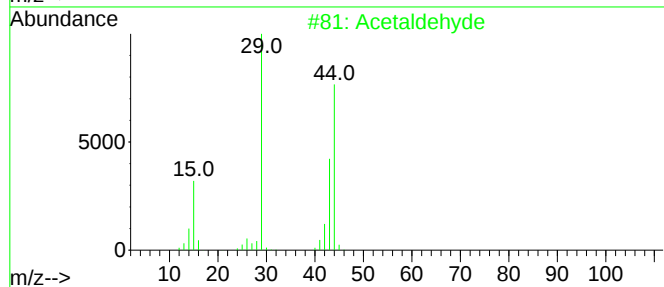
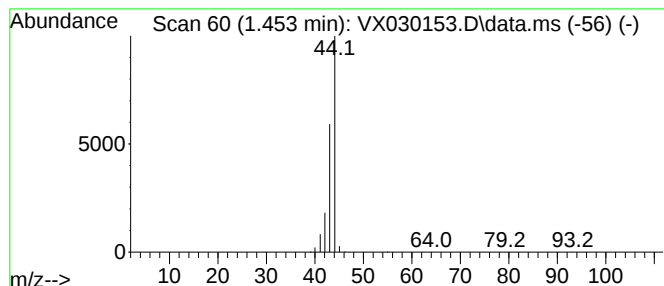
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Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	20.57 ug/l	230370	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	56
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			1,2-Propanediamine	74	C3H10N2	000078-90-0	4
5			Carbon dioxide	44	CO2	000124-38-9	3



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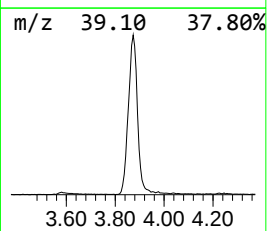
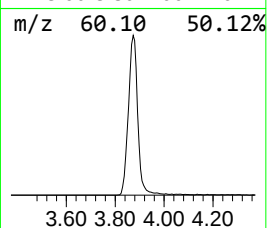
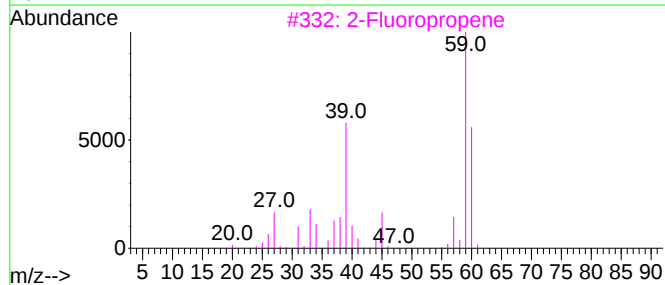
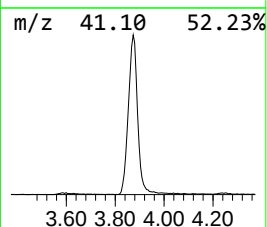
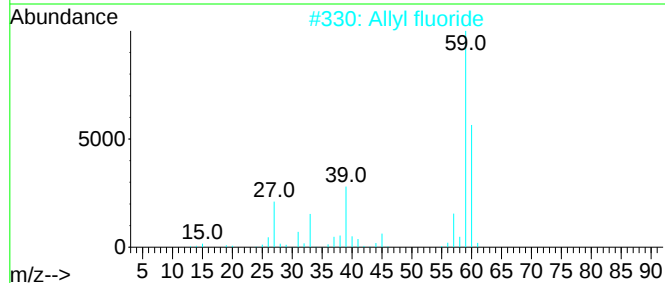
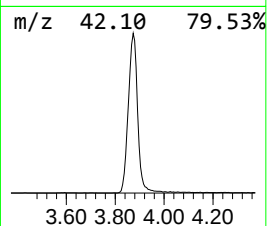
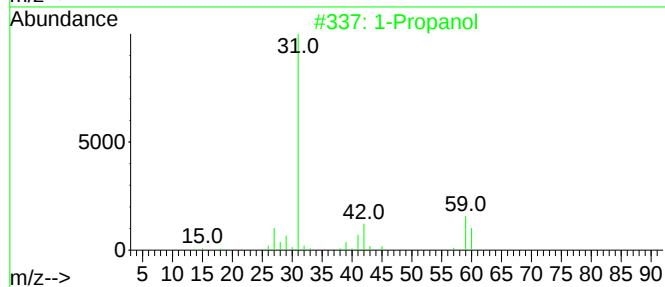
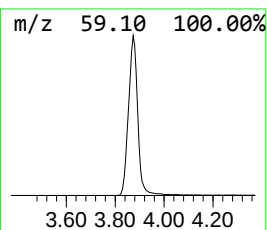
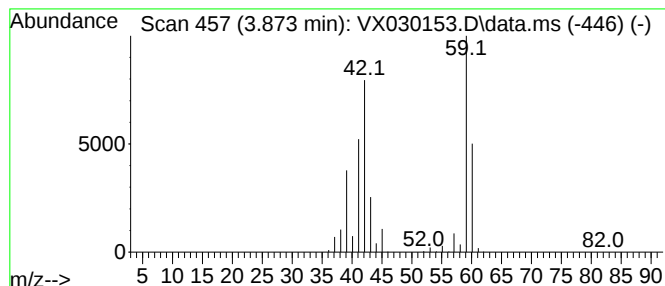
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.873	165.16 ug/l	1849740	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	78
2	Allyl fluoride			60	C3H5F	000818-92-8	47
3	2-Fluoropropene			60	C3H5F	001184-60-7	37
4	Cyclopropane			42	C3H6	000075-19-4	16
5	Formamidoxime			60	CH4N2O	000624-82-8	7



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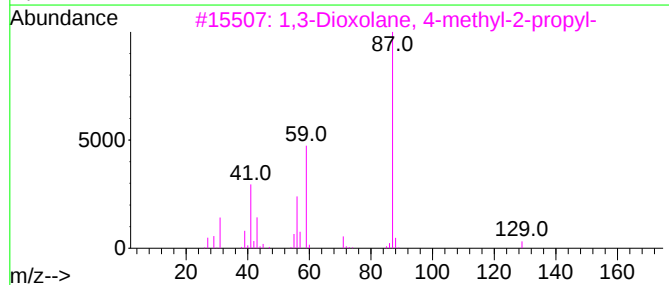
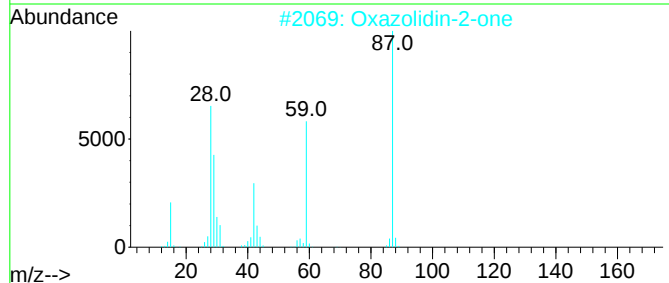
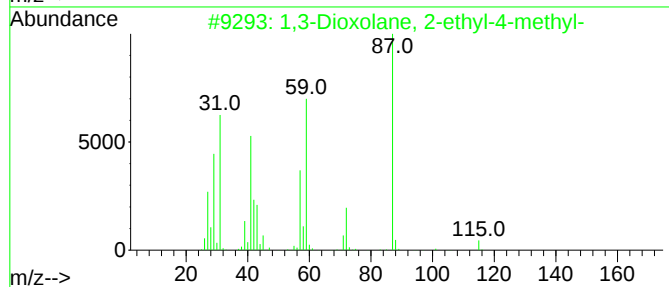
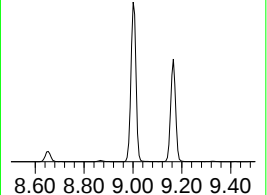
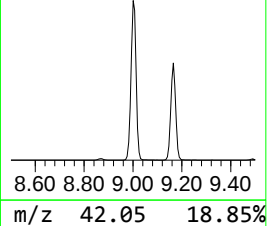
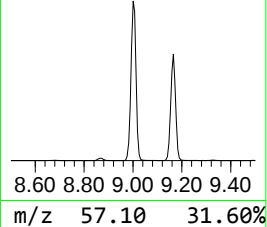
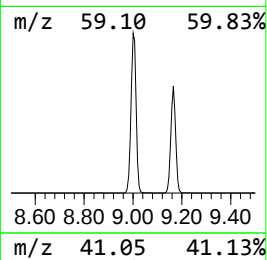
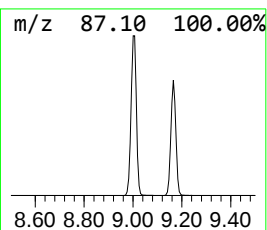
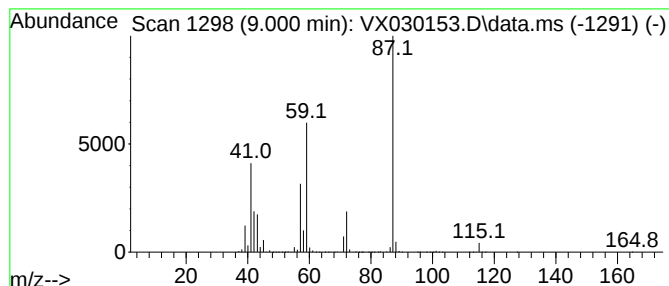
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Peak Number 3 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.000	177.31 ug/l	12389000	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	95
2			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	64
3			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	64
4			2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	50



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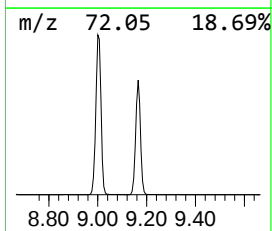
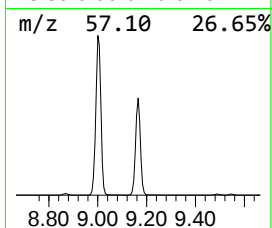
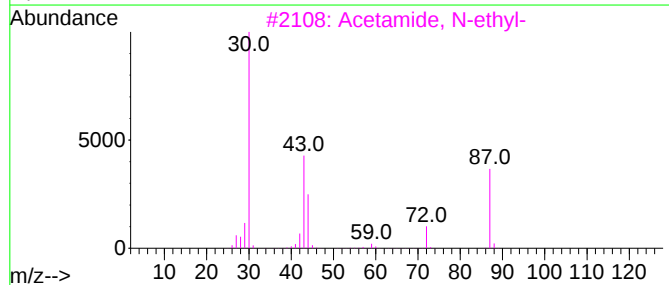
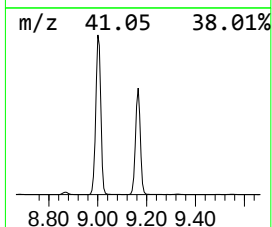
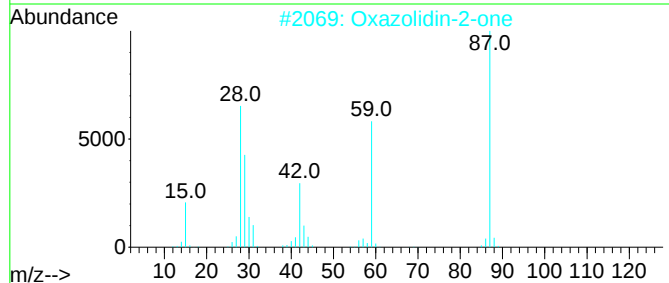
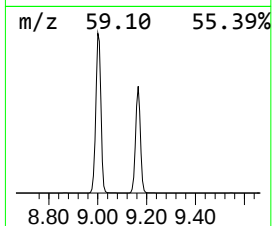
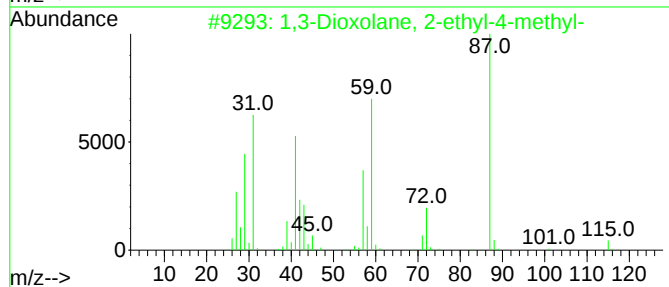
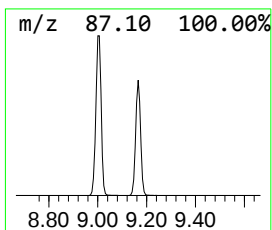
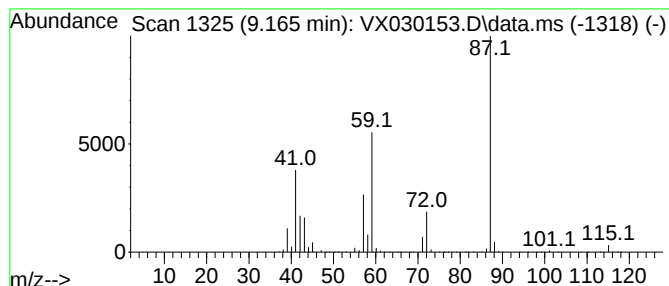
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Peak Number 4 Oxazolidin-2-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.165	112.21 ug/l	7840350	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	95
2			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	80
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	53
4			2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
5			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	50



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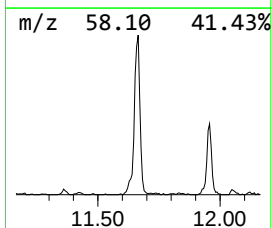
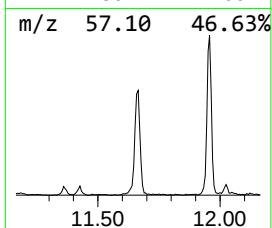
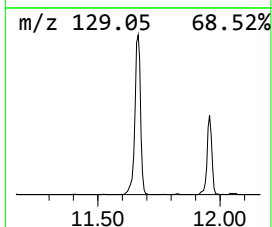
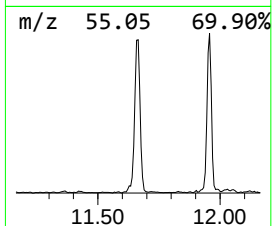
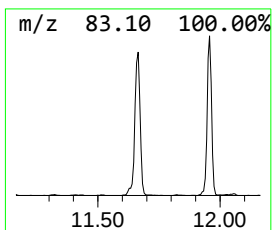
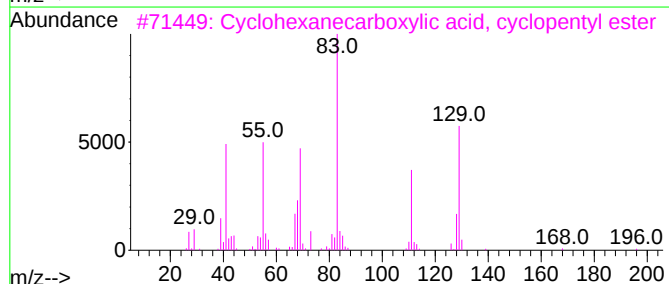
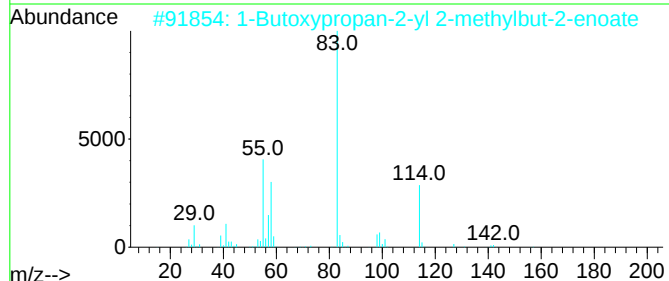
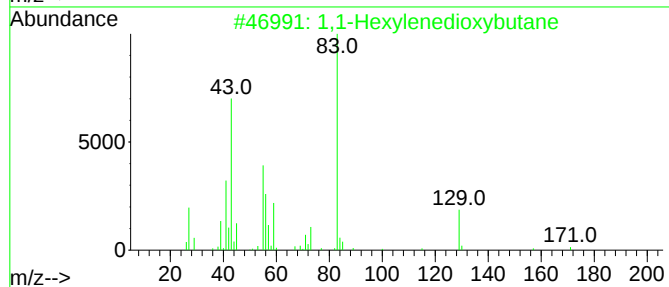
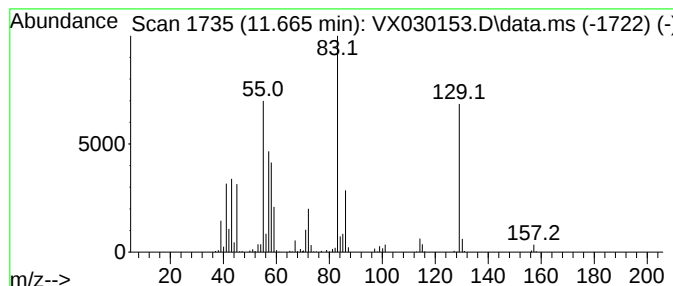
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown11.665 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.665	27.49 ug/l	435169	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	38
2			1-Butoxypropan-2-yl 2-methylbut-...	214	C12H22O3	1000367-09-3	32
3			Cyclohexanecarboxylic acid, cycl...	196	C12H20O2	005420-91-7	32
4			1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	18
5			2-(2-(2-Methoxyethoxy)ethoxy)eth...	248	C12H24O5	1000366-97-4	16



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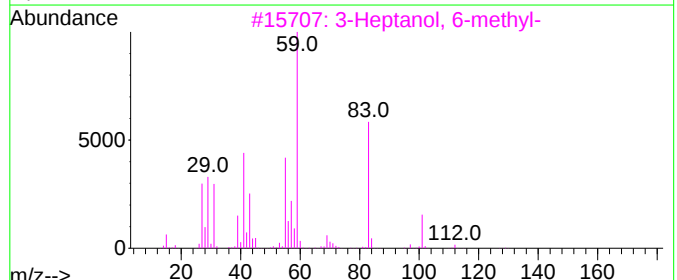
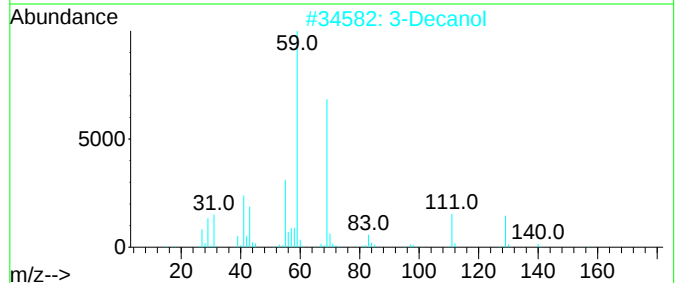
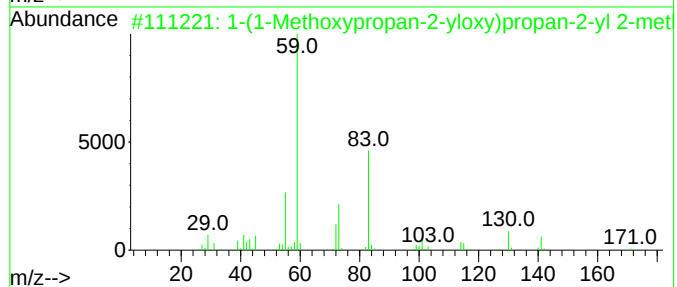
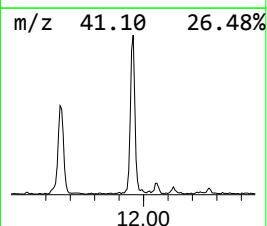
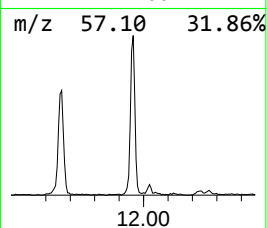
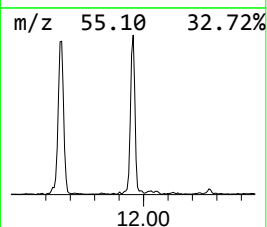
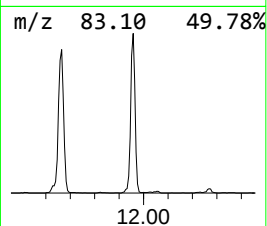
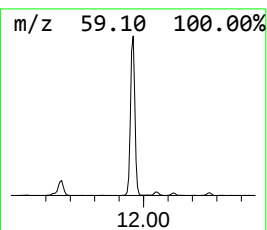
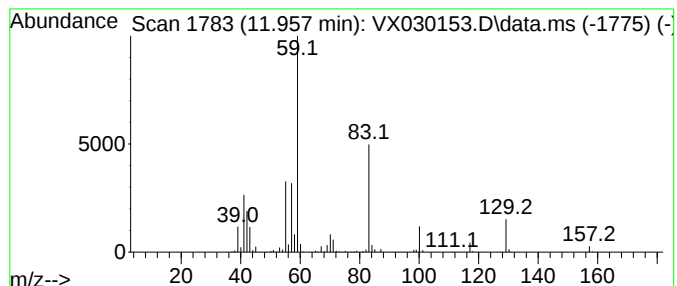
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

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

Peak Number 6 1-(1-Methoxypropan-2-yloxy)... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	30.00 ug/l	474804	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	50
2			3-Decanol	158	C10H22O	001565-81-7	47
3			3-Heptanol, 6-methyl-	130	C8H18O	018720-66-6	45
4			3-Octanol	130	C8H18O	000589-98-0	45
5			Butyl aldoxime, 3-methyl-, anti	101	C5H11NO	005775-74-6	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
Data File : VX030153.D
Acq On : 20 Jul 2022 23:51
Operator : JC/MD
Sample : N3781-04 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-62322

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.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	1.453	20.6	ug/l	230370	1	5.556	559984	50.0
1-Propanol	3.873	165.2	ug/l	1849740	1	5.556	559984	50.0
1,3-Dioxolane, ...	9.000	177.3	ug/l	12389000	3	10.055	3493620	50.0
Oxazolidin-2-one	9.165	112.2	ug/l	7840350	3	10.055	3493620	50.0
unknown11.665	11.665	27.5	ug/l	435169	4	12.024	791414	50.0
1-(1-Methoxypro...	11.957	30.0	ug/l	474804	4	12.024	791414	50.0