

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
 Data File : VX025381.D
 Acq On : 29 Nov 2021 19:42
 Operator : JC/MD
 Sample : M4837-20 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 20937

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\82X111721W.M
 Title : SW846 8260

Signal : TIC: VX025381.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	70	rBV	98144	110814	3.90%	1.244%
2	2.294	192	198	207	rBV	345435	555463	19.53%	6.236%
3	2.380	207	212	222	rVB	32644	55021	1.93%	0.618%
4	2.538	230	238	245	rBV	16082	30593	1.08%	0.343%
5	3.861	444	455	476	rBV	241817	618606	21.75%	6.945%
6	4.379	532	540	553	rBV	13347	37853	1.33%	0.425%
7	5.391	691	706	721	rBV	75669	219699	7.72%	2.467%
8	5.556	721	733	748	rVB	127266	362953	12.76%	4.075%
9	5.958	789	799	812	rBV	82988	210274	7.39%	2.361%
10	6.763	919	931	941	rBV	197754	471994	16.59%	5.299%
11	6.873	941	949	960	rVB	106477	251520	8.84%	2.824%
12	7.208	997	1004	1013	rBV	18650	40562	1.43%	0.455%
13	8.653	1233	1241	1250	rBV	401401	645833	22.70%	7.251%
14	9.000	1290	1298	1310	rBV	1976089	2844719	100.00%	31.939%
15	9.159	1318	1324	1333	rBV	338768	474407	16.68%	5.326%
16	9.567	1384	1391	1410	rBV	118935	316660	11.13%	3.555%
17	10.055	1465	1471	1482	rBV	451336	607372	21.35%	6.819%
18	10.153	1482	1487	1499	rVB	36060	50545	1.78%	0.567%
19	11.085	1634	1640	1647	rBV	336866	442285	15.55%	4.966%
20	12.024	1788	1794	1805	rVB	443498	559481	19.67%	6.282%

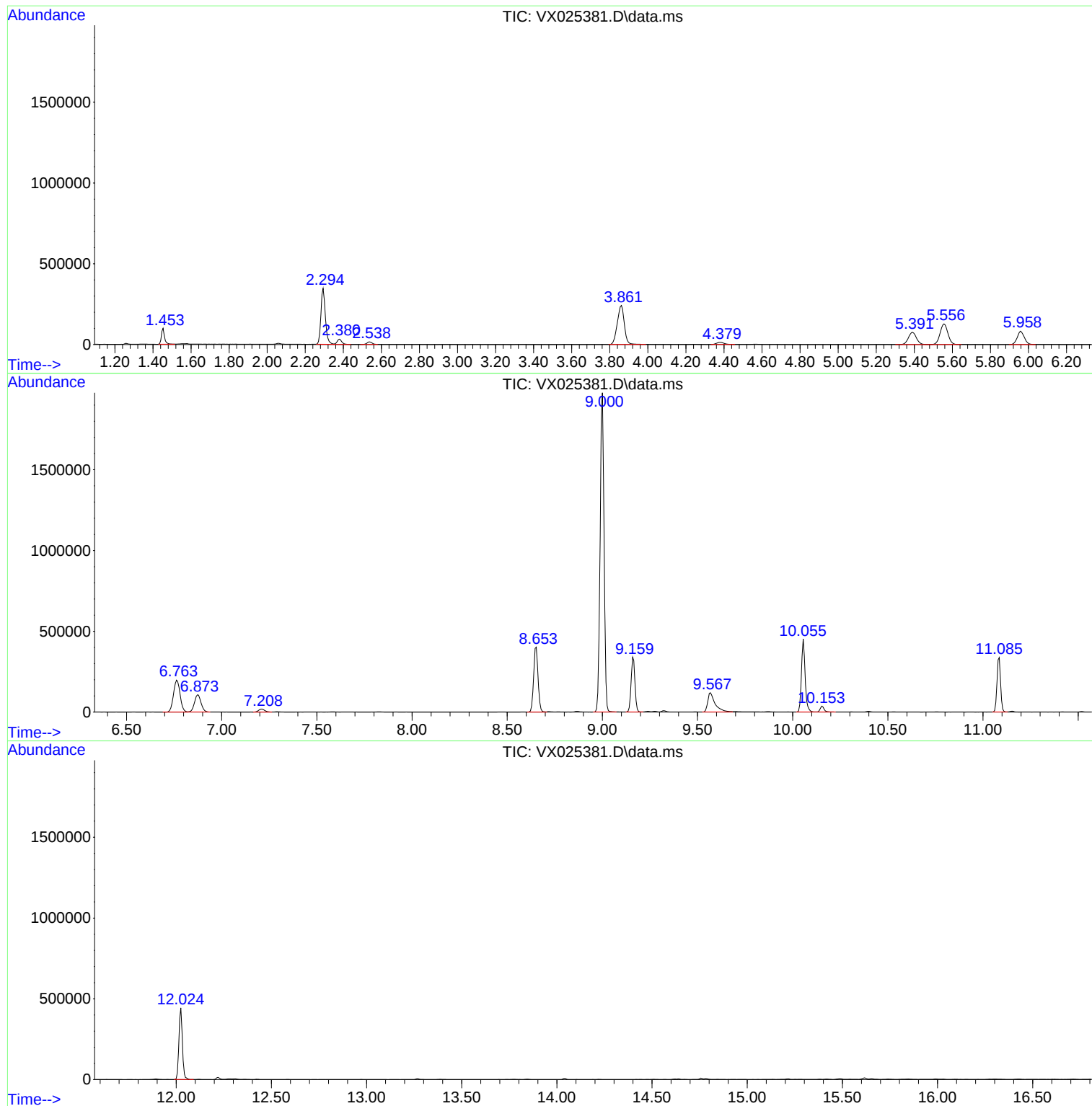
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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



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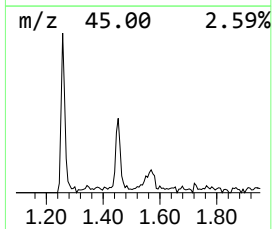
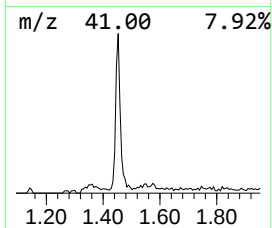
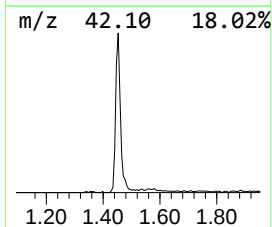
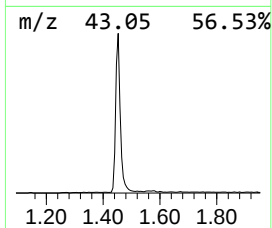
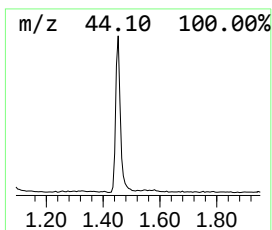
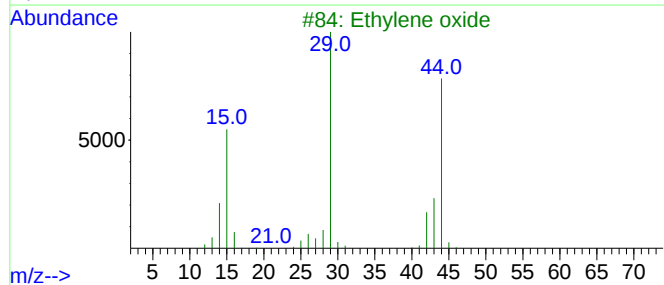
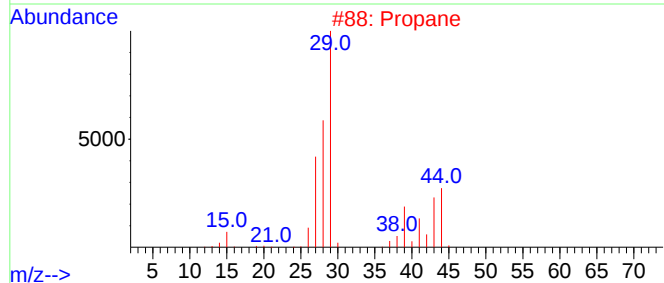
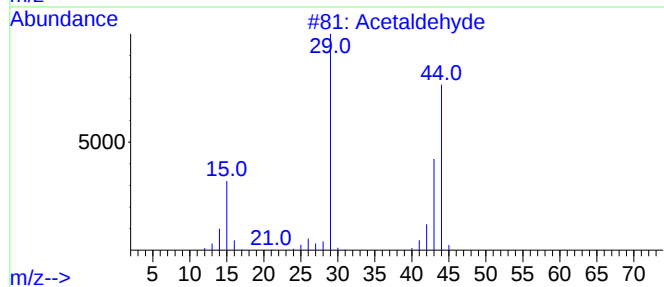
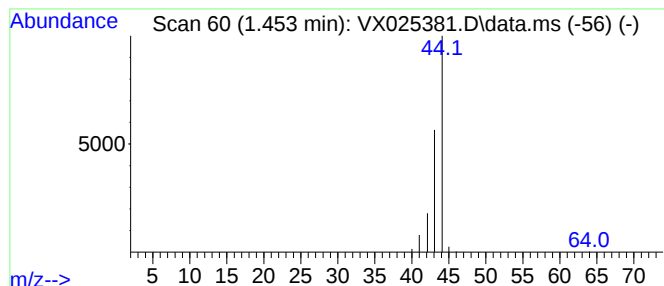
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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	15.27 ug/l	110814	Pentafluorobenzene	5.556

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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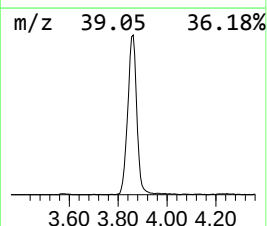
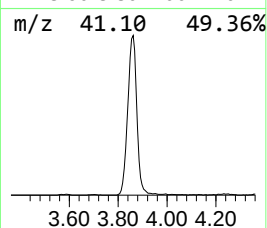
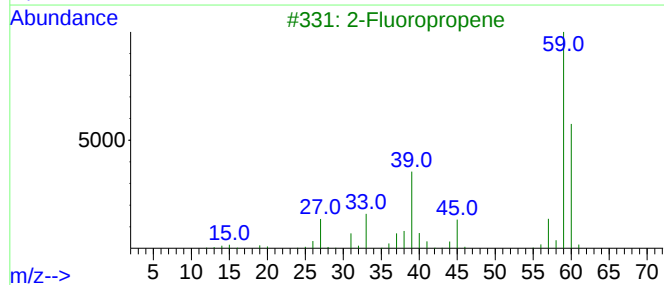
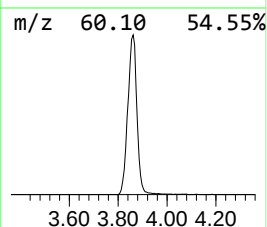
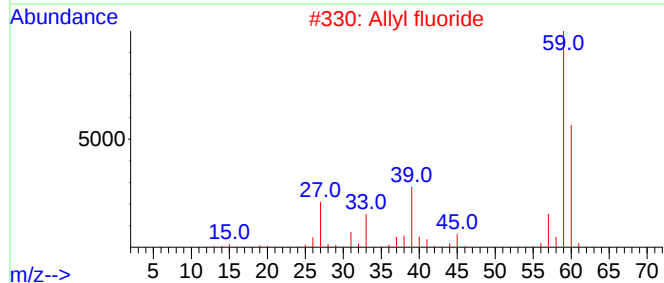
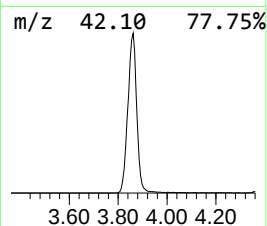
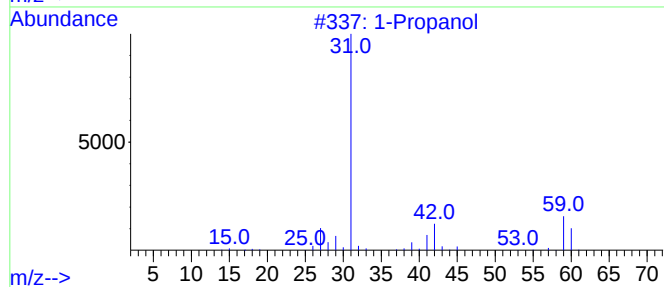
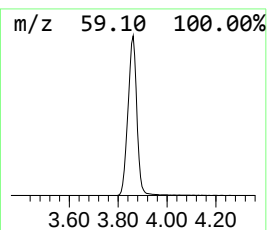
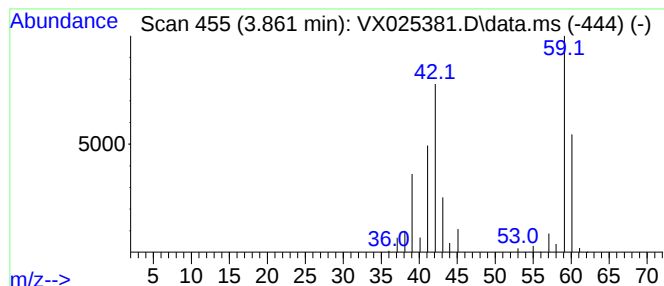
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.861	85.22 ug/l	618606	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	43
4	Cyclopropane			42	C3H6	000075-19-4	16
5	Methanamine, N-hydroxy-N-methyl-			61	C2H7NO	005725-96-2	9



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Instrument :
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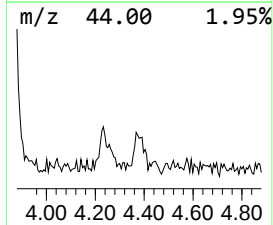
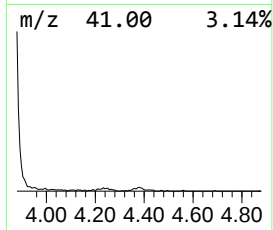
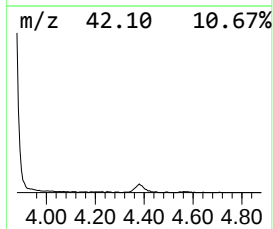
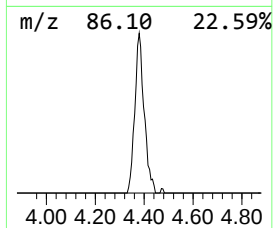
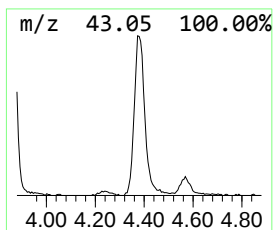
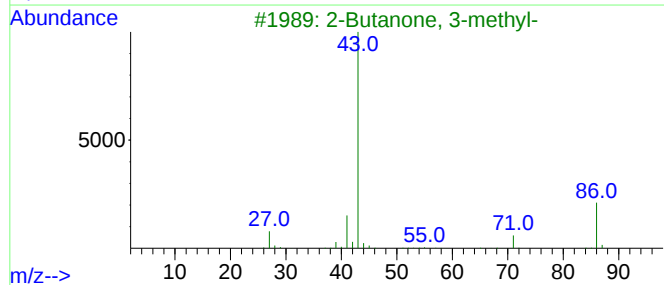
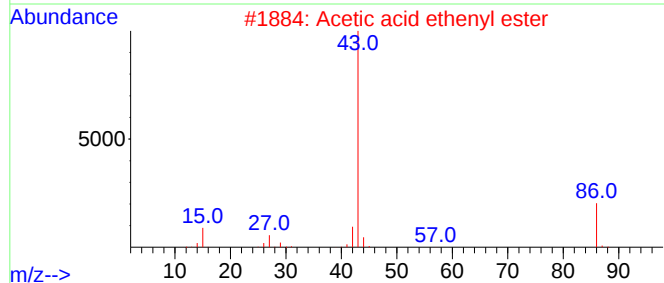
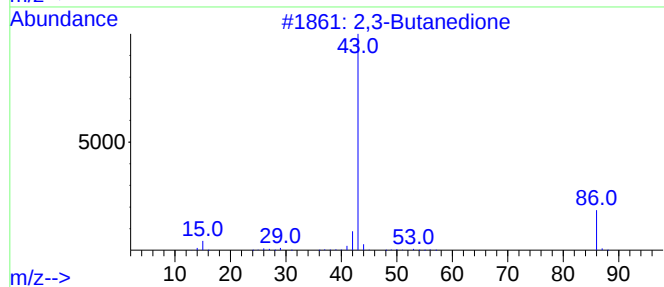
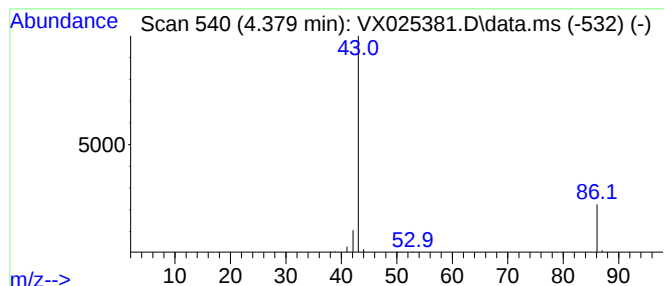
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2,3-Butanedione Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.379	5.21 ug/l	37853	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione		86	C4H6O2	000431-03-8	90
2	Acetic acid ethenyl ester		86	C4H6O2	000108-05-4	9
3	2-Butanone, 3-methyl-		86	C5H10O	000563-80-4	9
4	2-Pentanone		86	C5H10O	000107-87-9	9
5	2-Propanone, methylhydrazone		86	C4H10N2	005771-02-8	5



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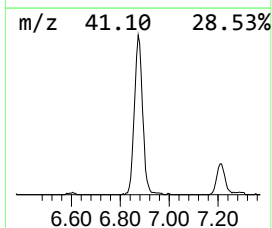
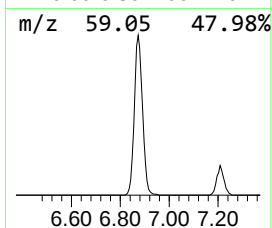
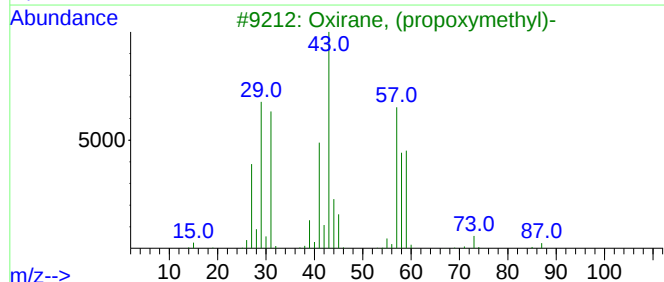
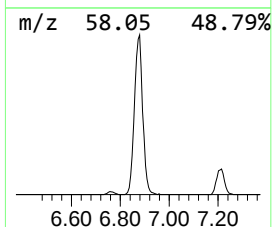
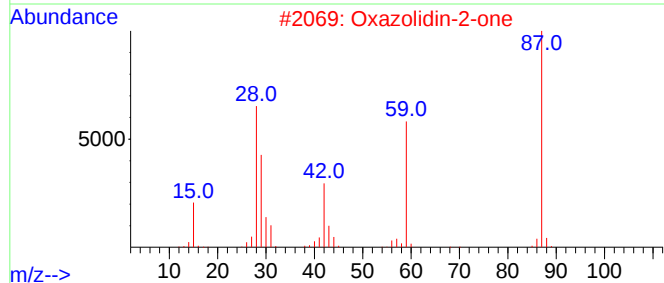
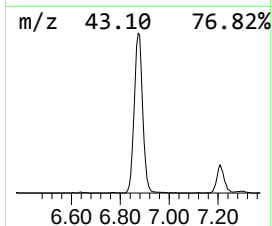
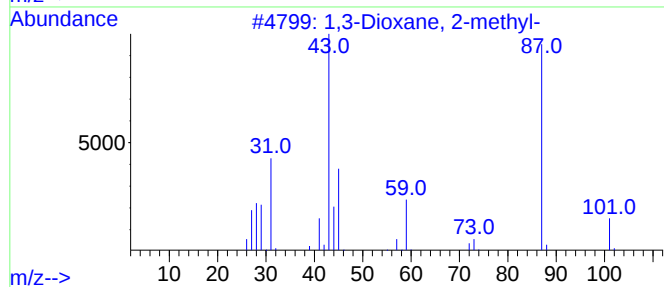
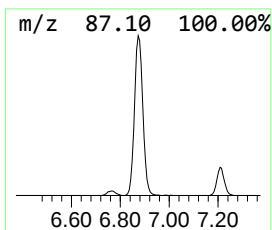
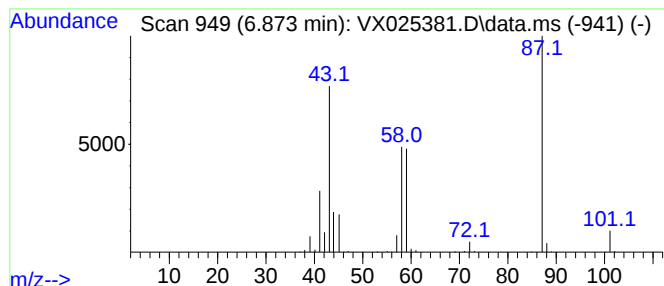
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.873 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.873	26.64 ug/l	251520	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	37
2			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	37
3			Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	37
4			1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	37
5			1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	33



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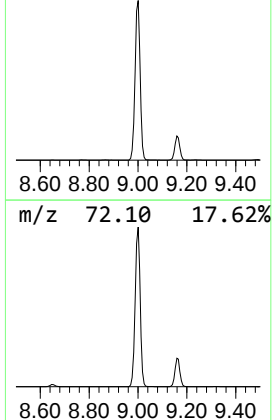
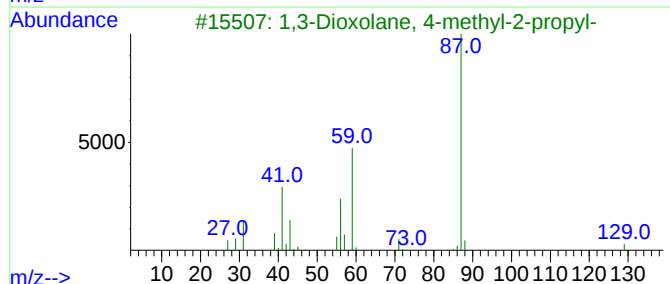
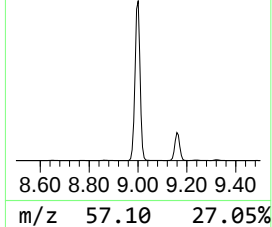
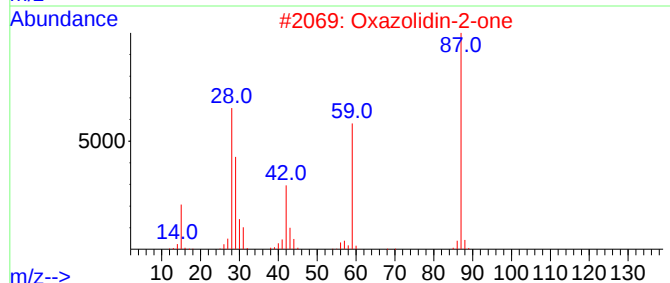
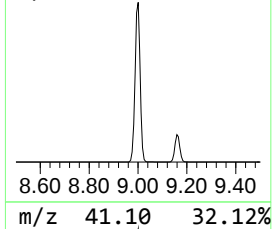
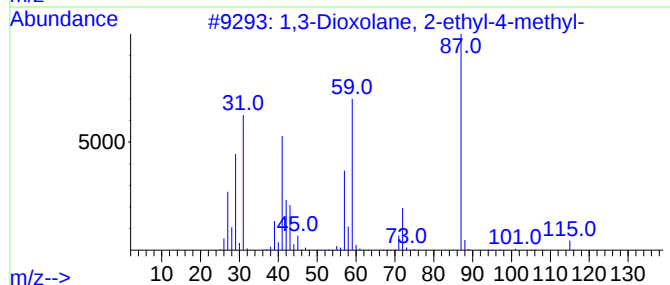
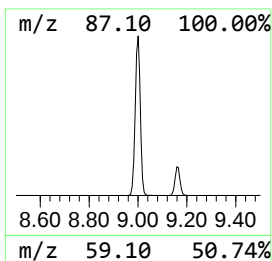
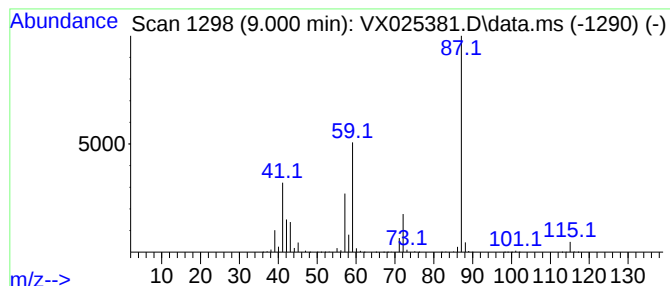
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.000	234.18 ug/l	2844720	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	91
2			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	72
3			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	72
4			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	64
5			2-Propanone, 0-methyloxime	87	C4H9NO	003376-35-0	52



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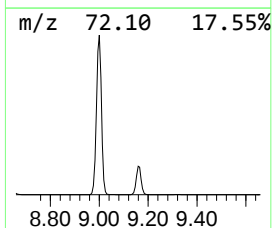
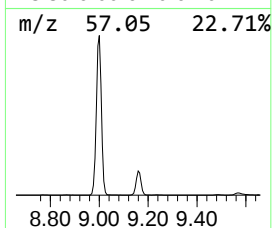
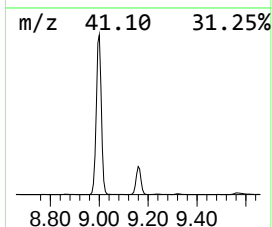
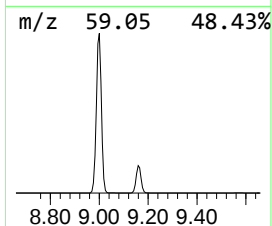
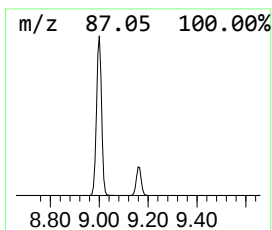
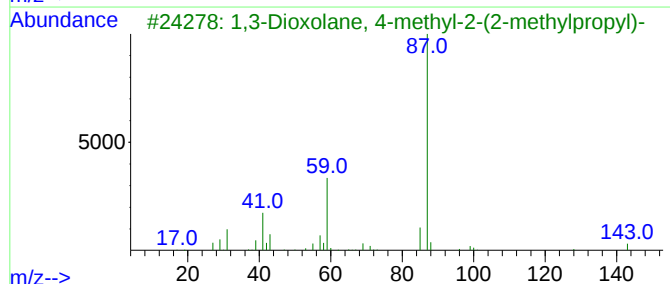
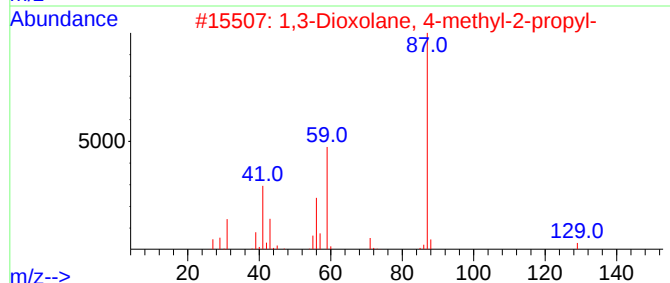
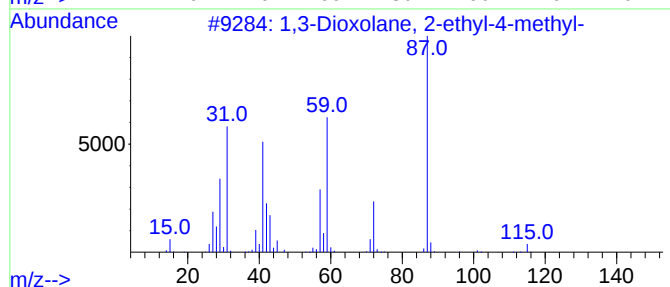
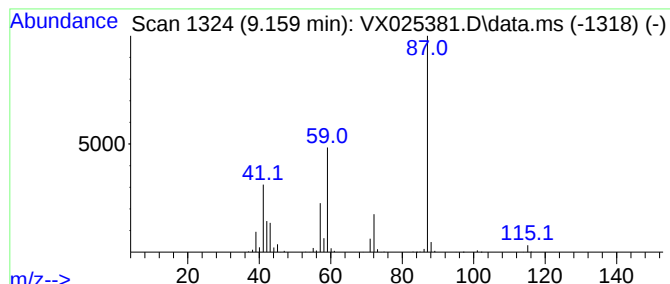
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.159	39.05 ug/l	474407	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	76
2			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	64
3			1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	56
4			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	56
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
Data File : VX025381.D
Acq On : 29 Nov 2021 19:42
Operator : JC/MD
Sample : M4837-20 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20937

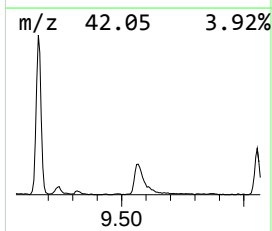
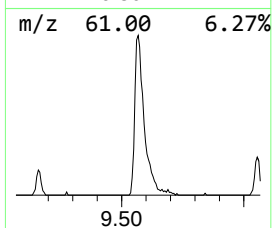
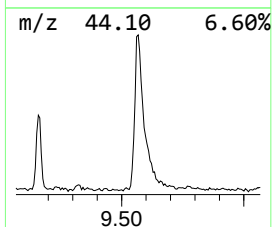
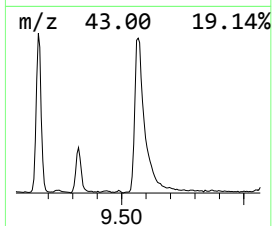
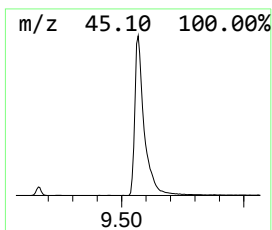
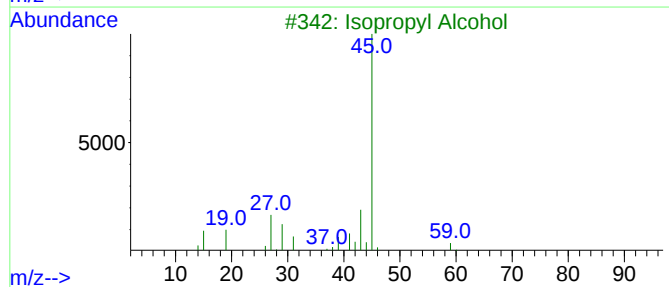
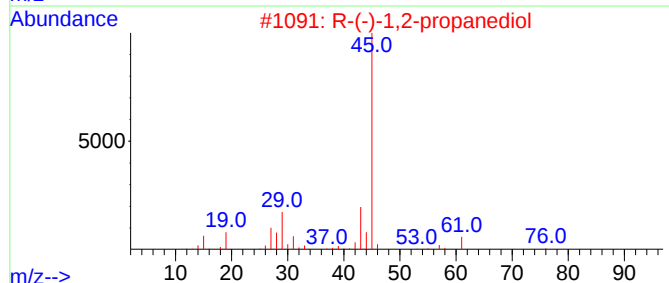
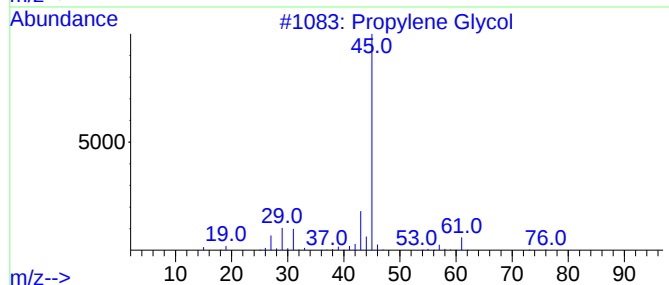
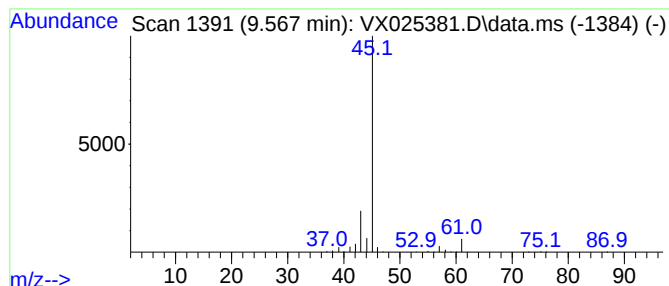
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Quant Title : SW846 8260

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

Peak Number 7 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.567	26.07 ug/l	316660	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	90
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
Data File : VX025381.D
Acq On : 29 Nov 2021 19:42
Operator : JC/MD
Sample : M4837-20 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20937

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.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	15.3	ug/l	110814	1	5.556	362953	50.0
1-Propanol	3.861	85.2	ug/l	618606	1	5.556	362953	50.0
2,3-Butanedione	4.379	5.2	ug/l	37853	1	5.556	362953	50.0
unknown6.873	6.873	26.6	ug/l	251520	2	6.763	471994	50.0
1,3-Dioxolane, ...	9.000	234.2	ug/l	2844720	3	10.055	607372	50.0
1,3-Dioxolane, ...	9.159	39.0	ug/l	474407	3	10.055	607372	50.0
Propylene Glycol	9.567	26.1	ug/l	316660	3	10.055	607372	50.0