

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061021\
 Data File : VX022652.D
 Acq On : 10 Jun 2021 18:28
 Operator : JC/MD
 Sample : M2638-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 ND-1

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\82X061021W.M
 Title : SW846 8260

Signal : TIC: VX022652.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.794	274	280	288	rBV	13442	24590	1.80%	0.426%
2	5.397	695	707	721	rVB2	41799	119320	8.73%	2.069%
3	5.562	724	734	748	rBV2	70896	194931	14.27%	3.380%
4	5.964	789	800	814	rBV	57738	147403	10.79%	2.556%
5	6.355	855	864	872	rBV2	6958	17709	1.30%	0.307%
6	6.769	921	932	944	rBV	121934	292496	21.41%	5.072%
7	7.806	1094	1102	1122	rBV	559954	966554	70.74%	16.761%
8	8.555	1218	1225	1234	rBV	97086	157100	11.50%	2.724%
9	8.653	1234	1241	1261	rVB	268537	423289	30.98%	7.340%
10	8.958	1286	1291	1297	rBV	9598	14254	1.04%	0.247%
11	9.250	1332	1339	1345	rBV	28485	40174	2.94%	0.697%
12	9.348	1350	1355	1359	rBV	60146	78730	5.76%	1.365%
13	9.488	1372	1378	1389	rBV	1047680	1366417	100.00%	23.694%
14	9.586	1389	1394	1406	rVB	96073	131603	9.63%	2.282%
15	9.915	1443	1448	1462	rBV	673586	869284	63.62%	15.074%
16	10.055	1465	1471	1486	rVB	258453	364256	26.66%	6.316%
17	10.640	1563	1567	1573	rBV	18896	24457	1.79%	0.424%
18	11.085	1635	1640	1648	rBV	190076	240799	17.62%	4.176%
19	12.024	1789	1794	1800	rBV	244964	293453	21.48%	5.089%

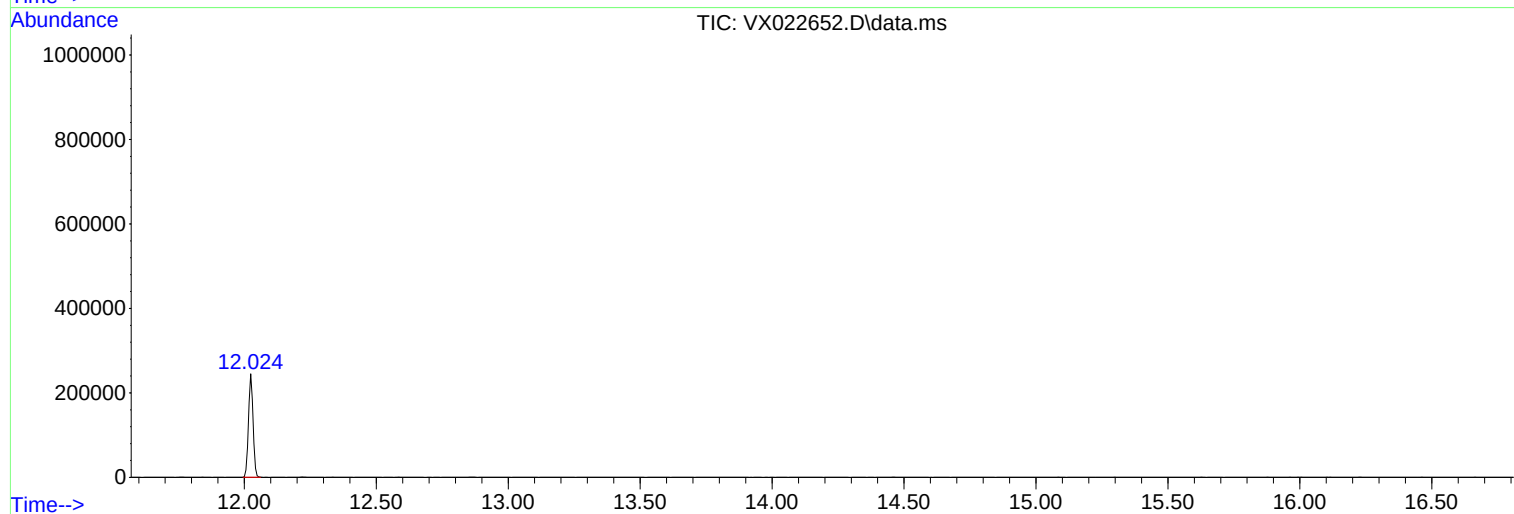
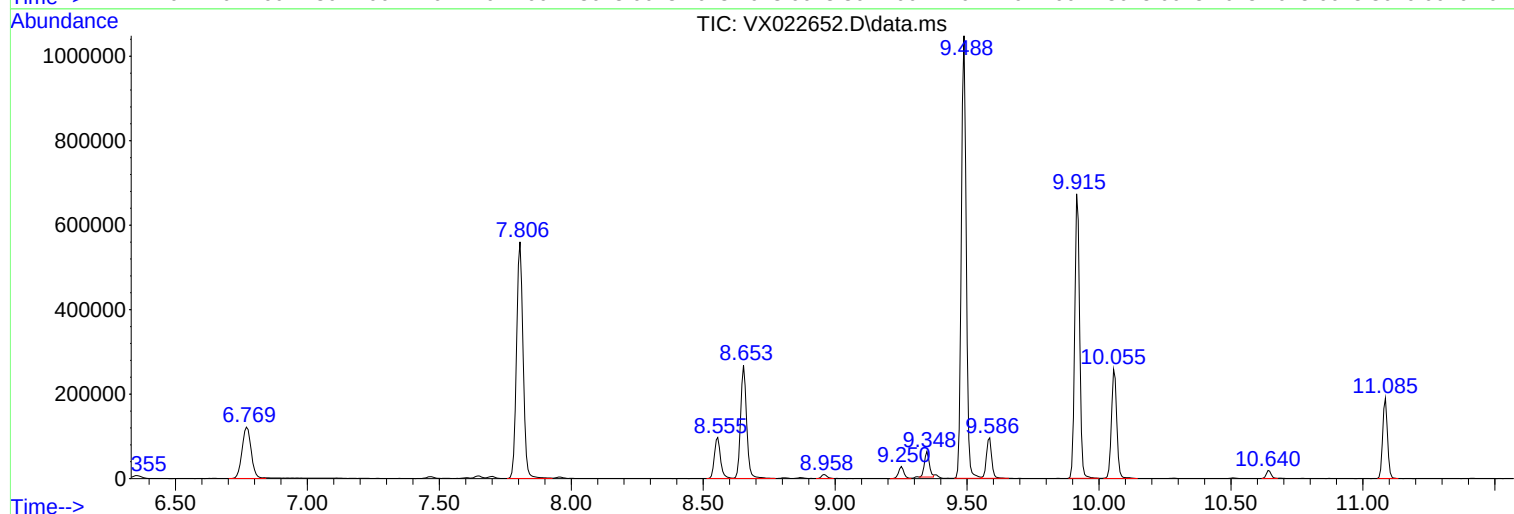
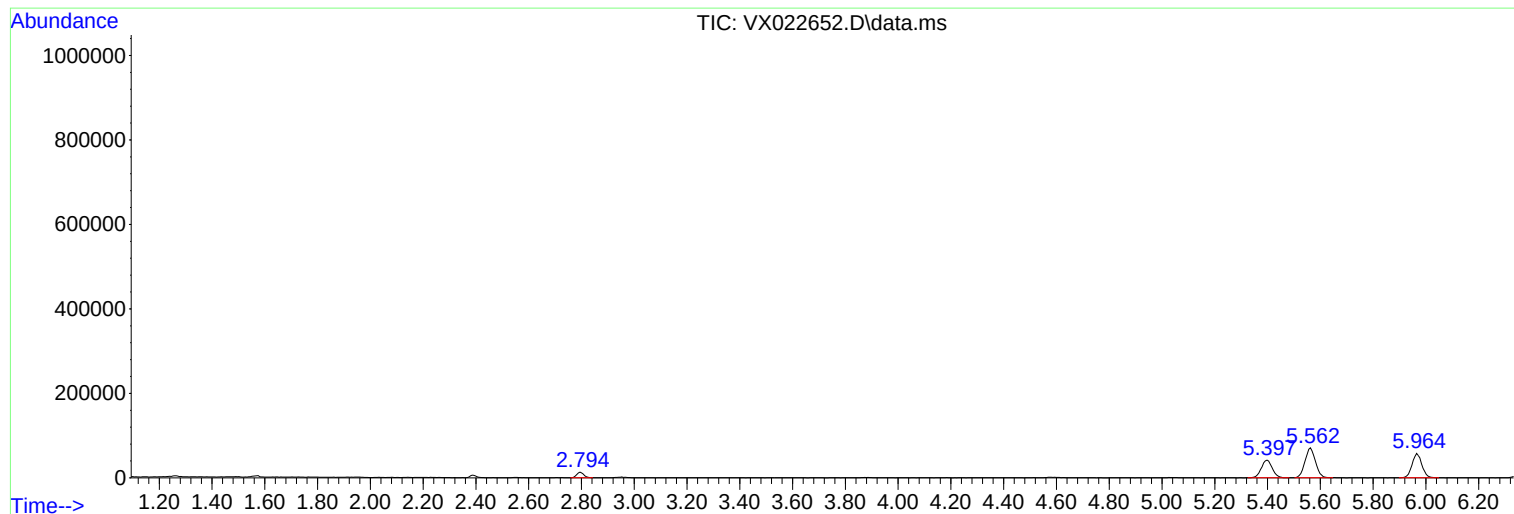
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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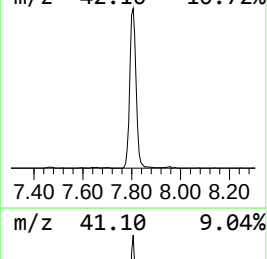
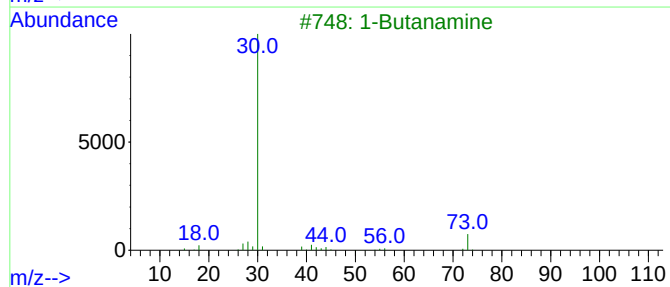
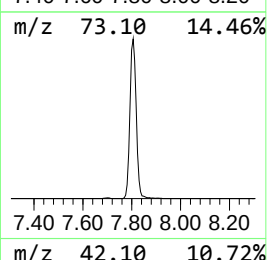
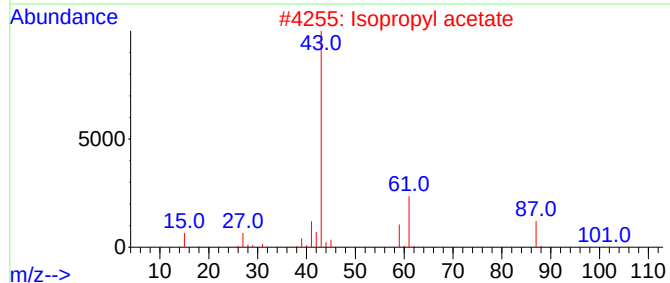
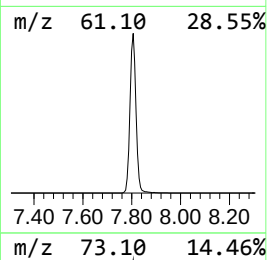
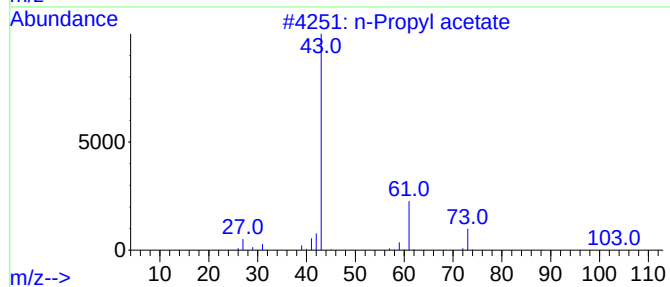
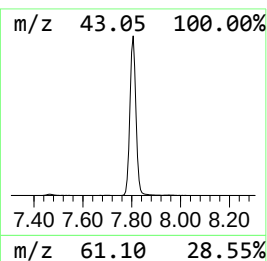
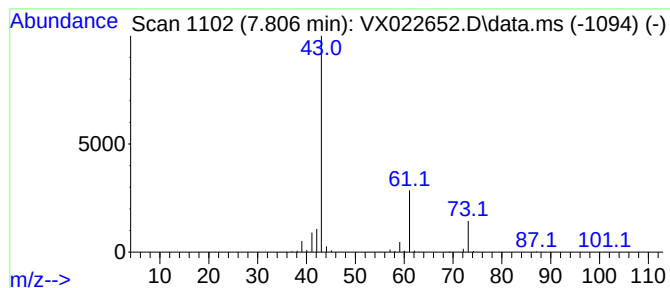
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.806	165.22 ug/l	966554	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Propyl acetate	102	C5H10O2	000109-60-4	83
2			Isopropyl acetate	102	C5H10O2	000108-21-4	36
3			1-Butanamine	73	C4H11N	000109-73-9	7
4			Isobutylamine	73	C4H11N	000078-81-9	7
5			Butane, 2-methyl-	72	C5H12	000078-78-4	4



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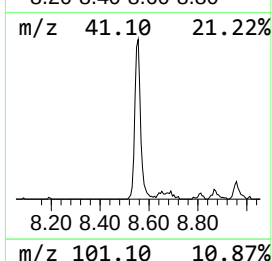
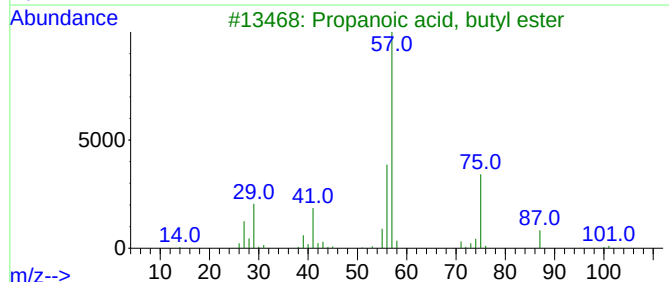
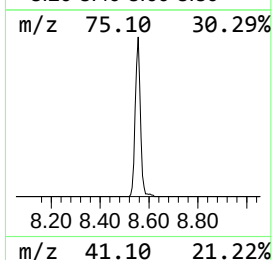
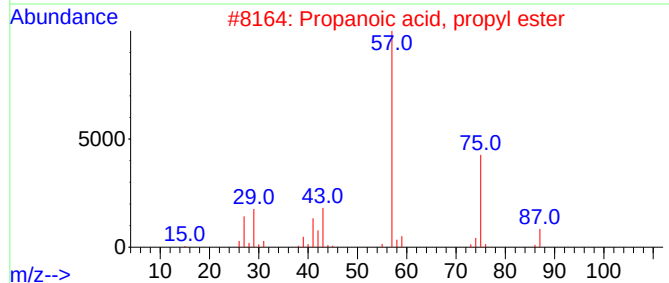
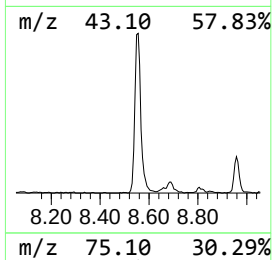
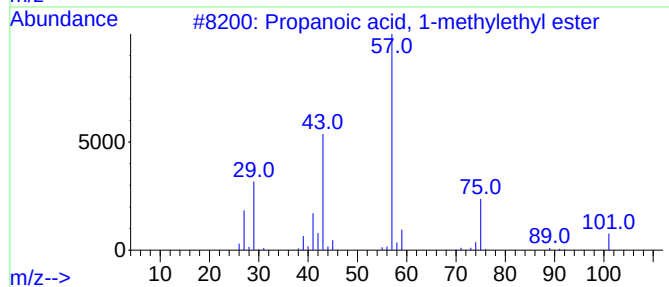
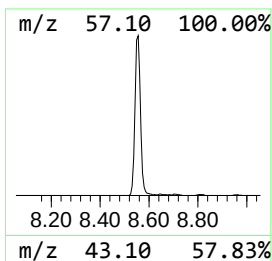
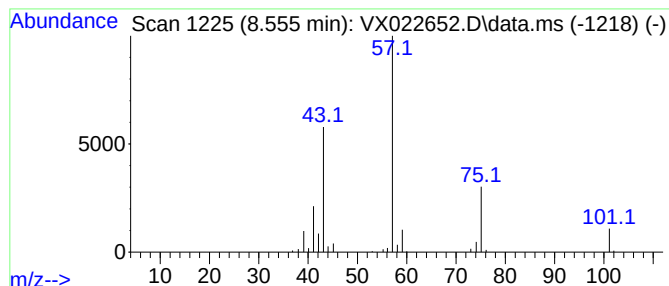
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.555	21.56 ug/l	157100	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
3			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	25
4			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
5			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10



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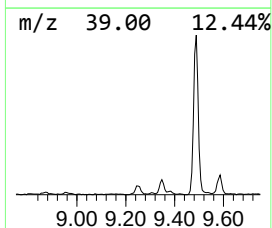
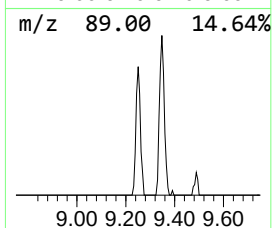
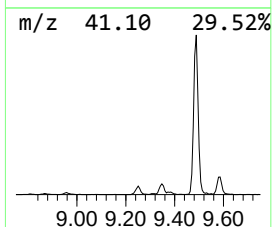
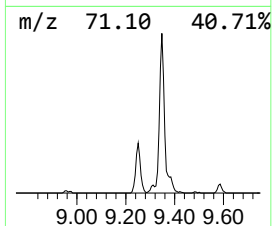
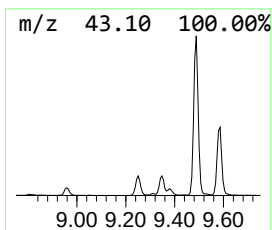
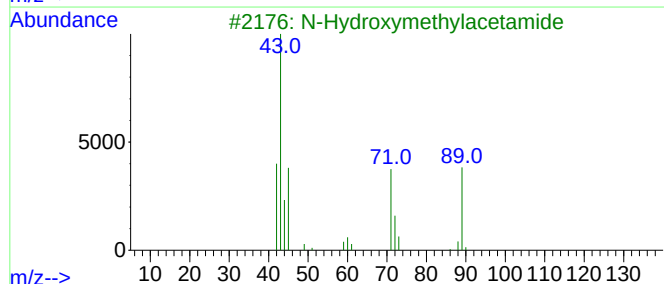
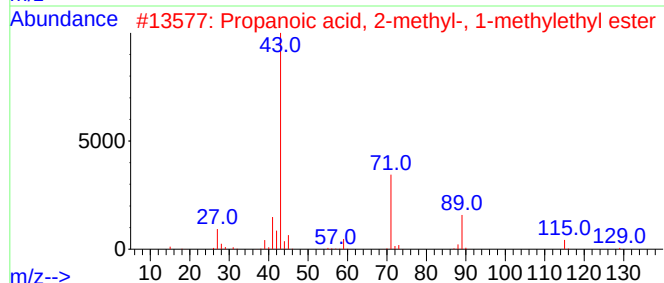
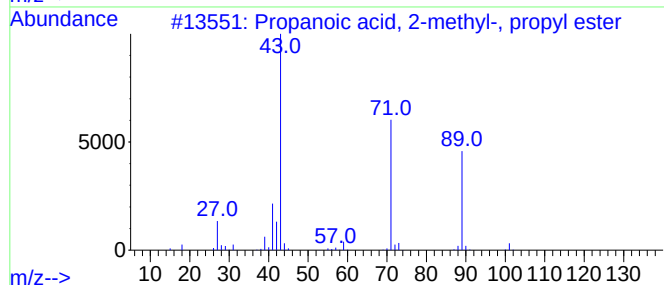
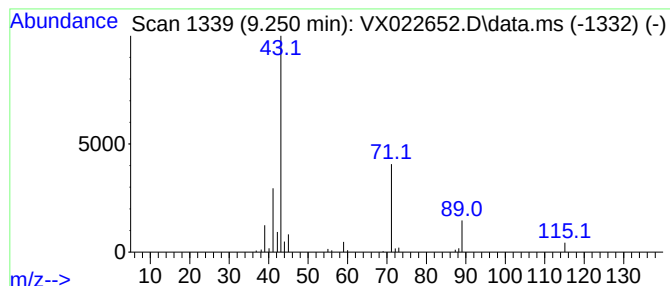
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Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.250	5.51 ug/l	40174	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
3			N-Hydroxymethylacetamide	89	C3H7NO2	000625-51-4	59
4			Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	42
5			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	40



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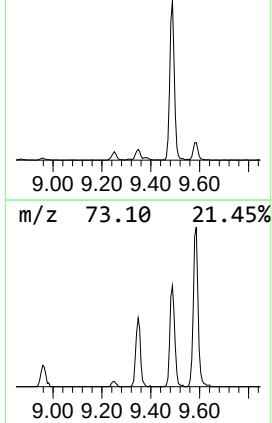
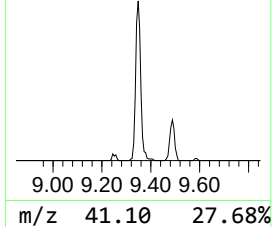
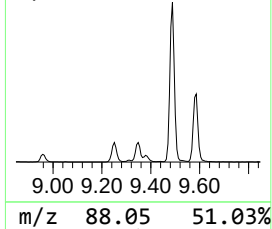
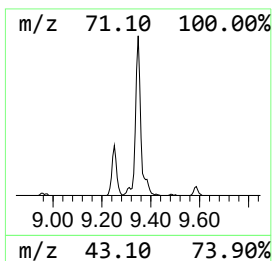
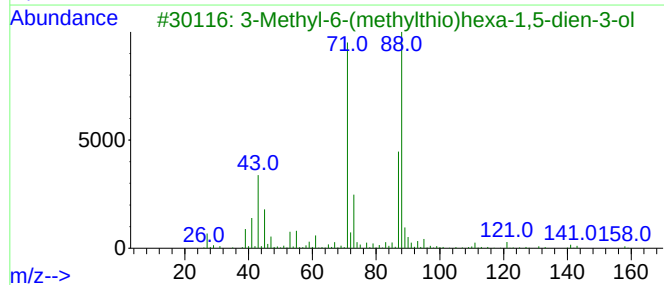
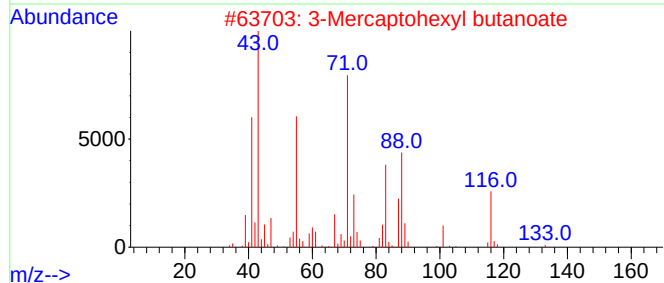
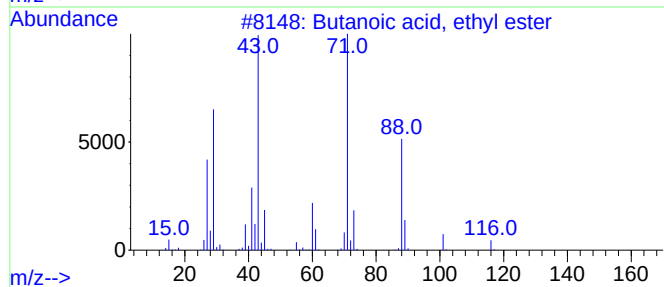
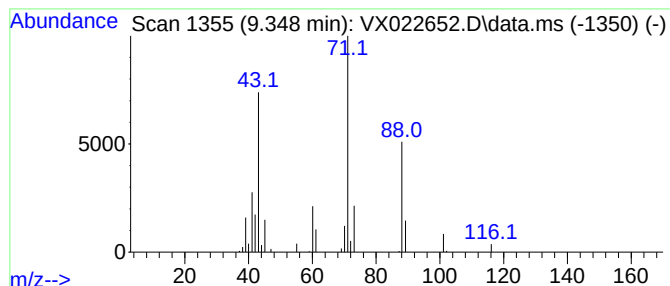
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.348	10.81 ug/l	78730	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	97
2			3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	45
3			3-Methyl-6-(methylthio)hexa-1,5-...	158	C8H14OS	1000191-74-2	45
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	40
5			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	40



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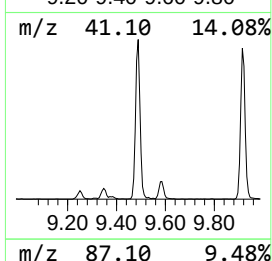
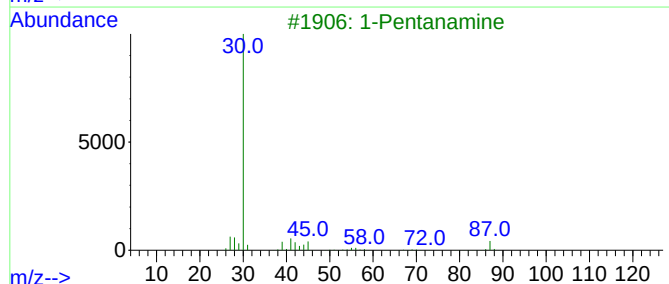
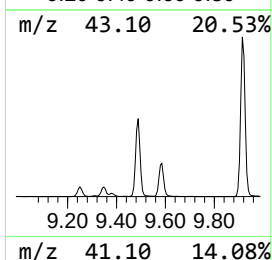
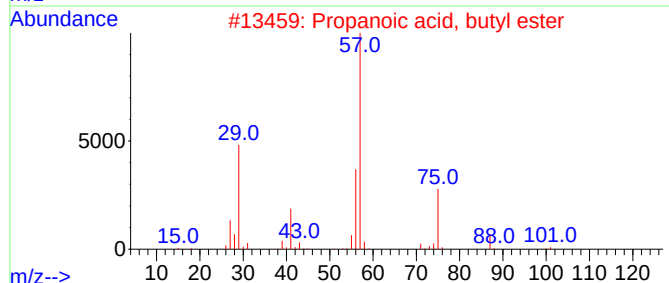
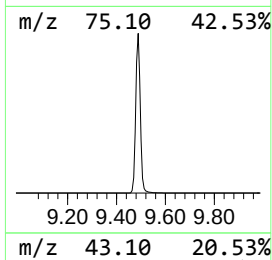
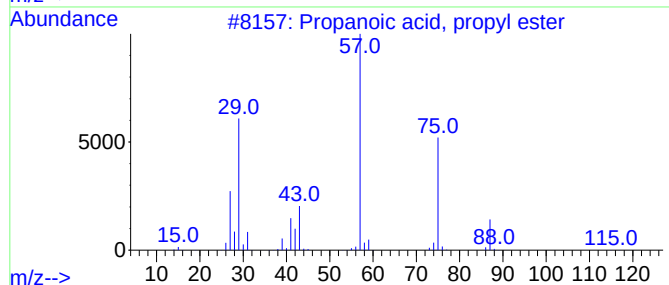
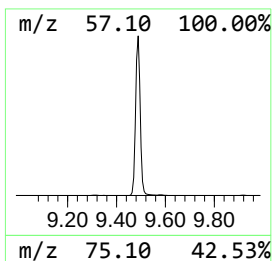
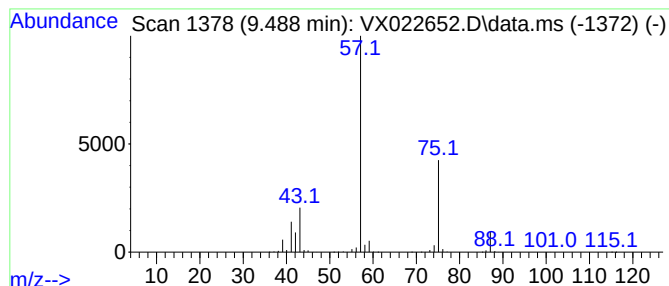
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.488	187.56 ug/l	1366420	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	25
3			1-Pentanamine	87	C5H13N	000110-58-7	10
4			Azetidine	57	C3H7N	000503-29-7	9
5			Isobutyl ether	130	C8H18O	000628-55-7	9



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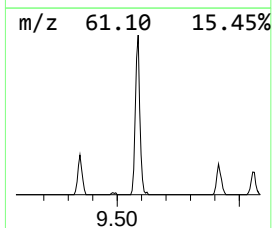
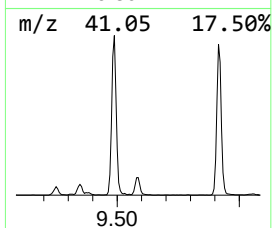
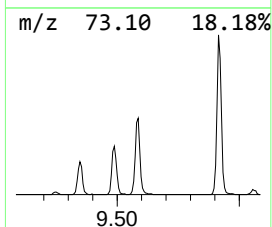
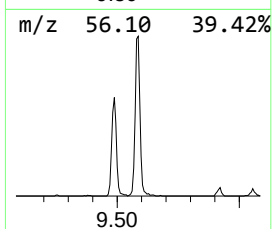
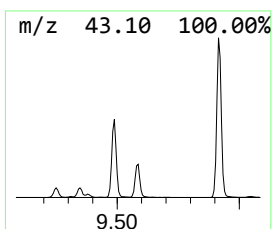
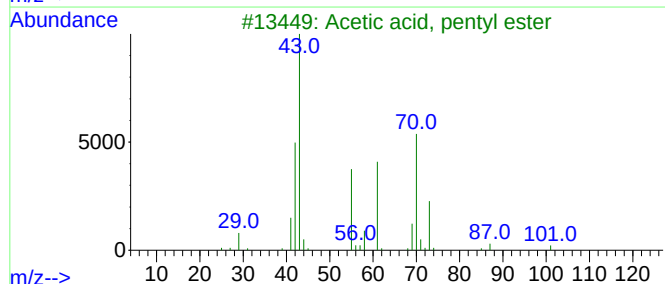
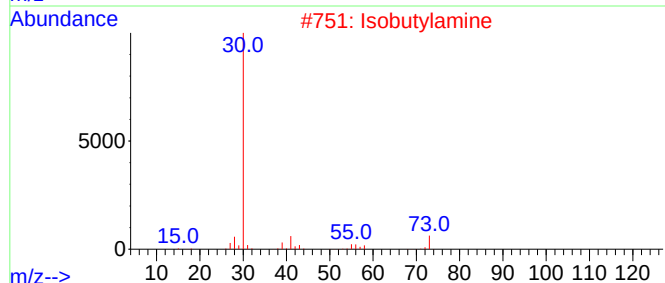
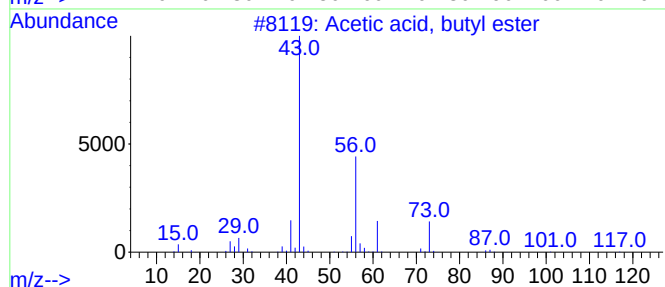
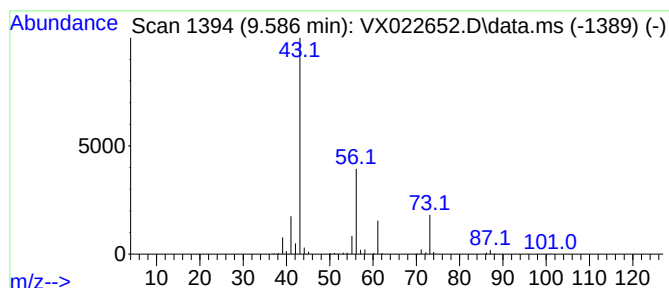
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 6 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.586	18.06 ug/l	131603	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2			Isobutylamine	73	C4H11N	000078-81-9	9
3			Acetic acid, pentyl ester	130	C7H14O2	000628-63-7	9
4			2-Pentanone	86	C5H10O	000107-87-9	9
5			Isobutyl acetate	116	C6H12O2	000110-19-0	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061021\
Data File : VX022652.D
Acq On : 10 Jun 2021 18:28
Operator : JC/MD
Sample : M2638-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ND-1

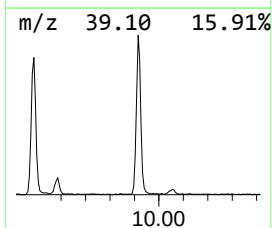
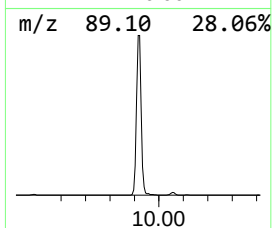
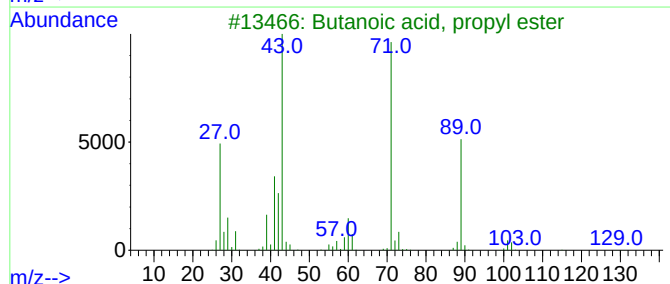
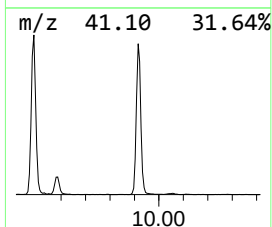
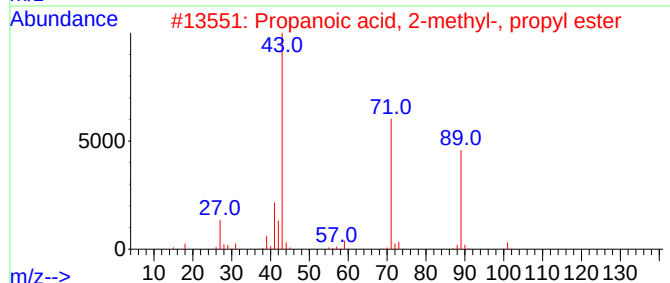
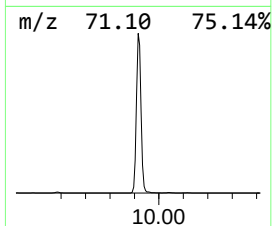
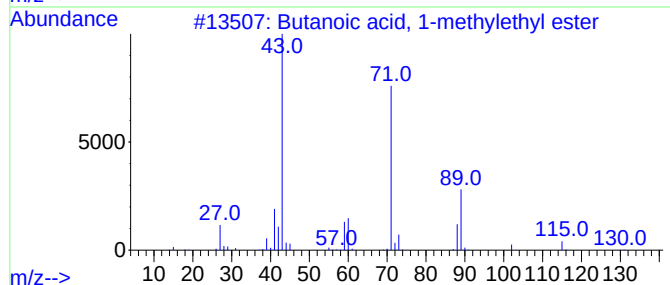
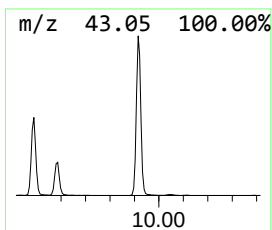
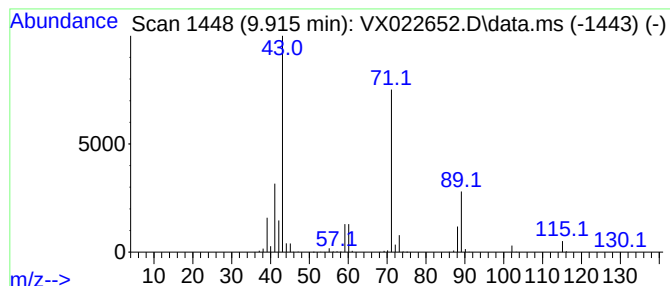
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	119.32 ug/l	869284	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
2			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
5			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061021\
Data File : VX022652.D
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ND-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	7.806	165.2	ug/l	966554	2	6.769	292496	50.0
Propanoic acid,...	8.555	21.6	ug/l	157100	3	10.055	364256	50.0
Propanoic acid,...	9.250	5.5	ug/l	40174	3	10.055	364256	50.0
Butanoic acid, ...	9.348	10.8	ug/l	78730	3	10.055	364256	50.0
Propanoic acid,...	9.488	187.6	ug/l	1366420	3	10.055	364256	50.0
Acetic acid, bu...	9.586	18.1	ug/l	131603	3	10.055	364256	50.0
Butanoic acid, ...	9.915	119.3	ug/l	869284	3	10.055	364256	50.0