

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062521\
 Data File : VX022963.D
 Acq On : 26 Jun 2021 08:08
 Operator : JC/MD
 Sample : M2832-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 56 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TP-3-WC

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\82X062321W.M
 Title : SW846 8260

Signal : TIC: VX022963.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.800	272	281	287	rBV	11768	22688	1.38%	0.339%
2	5.397	696	707	719	rBV2	42318	122554	7.45%	1.833%
3	5.562	722	734	745	rBV2	69145	193495	11.76%	2.895%
4	5.964	791	800	810	rBV	58910	152450	9.26%	2.281%
5	6.354	854	864	873	rBV3	8272	21350	1.30%	0.319%
6	6.769	923	932	944	rBV	124665	295517	17.96%	4.421%
7	7.805	1094	1102	1123	rBV	709153	1226500	74.53%	18.349%
8	8.555	1218	1225	1234	rBV	112489	177190	10.77%	2.651%
9	8.653	1234	1241	1261	rVB	271545	432958	26.31%	6.477%
10	8.958	1286	1291	1298	rBV	12627	18949	1.15%	0.283%
11	9.250	1332	1339	1345	rBV	31409	44650	2.71%	0.668%
12	9.348	1351	1355	1359	rBV	81480	99098	6.02%	1.483%
13	9.488	1372	1378	1389	rBV	1281669	1645619	100.00%	24.620%
14	9.586	1389	1394	1406	rVB	140084	188858	11.48%	2.825%
15	9.915	1443	1448	1459	rBV	773626	986696	59.96%	14.762%
16	10.055	1464	1471	1479	rBV	281447	382362	23.24%	5.720%
17	10.640	1563	1567	1580	rVB	26700	35018	2.13%	0.524%
18	11.085	1634	1640	1648	rVB	226683	277290	16.85%	4.148%
19	12.024	1789	1794	1801	rVB	296380	360920	21.93%	5.400%

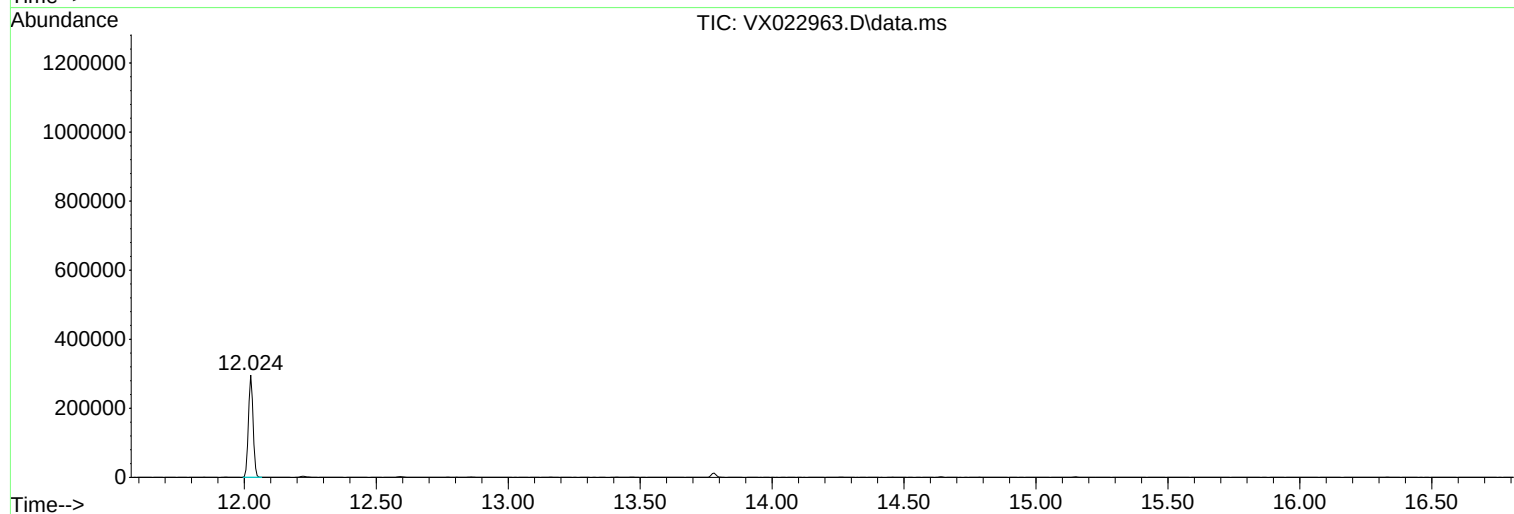
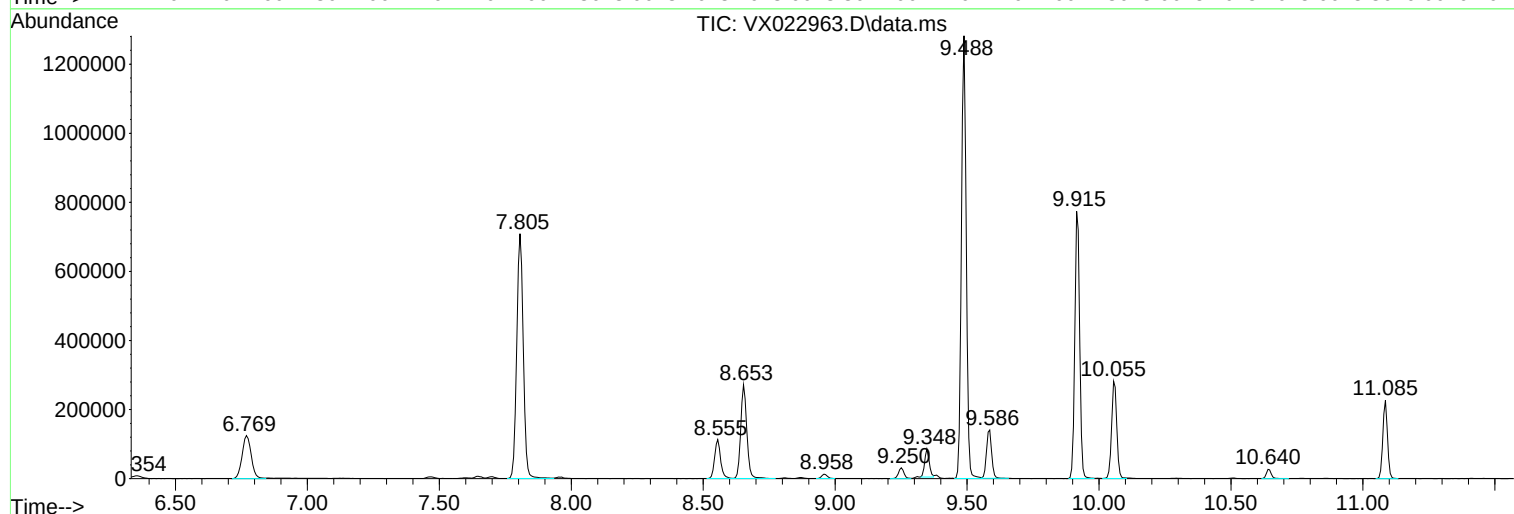
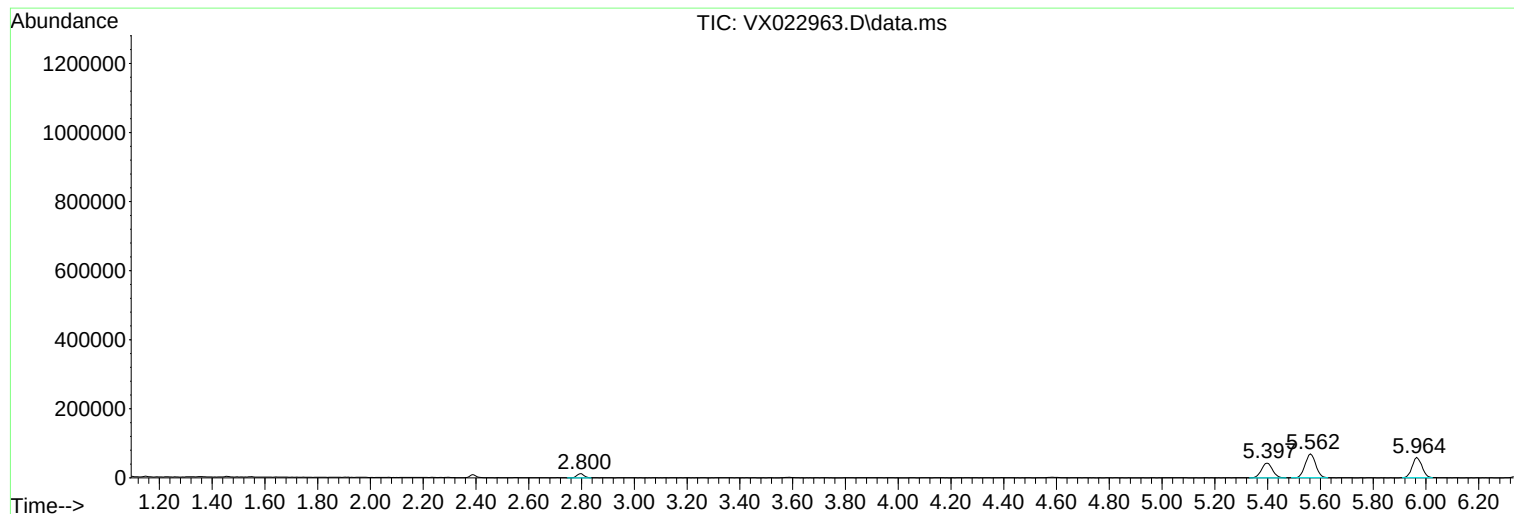
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Quant Title : SW846 8260

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



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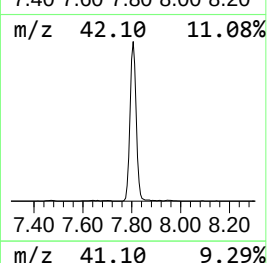
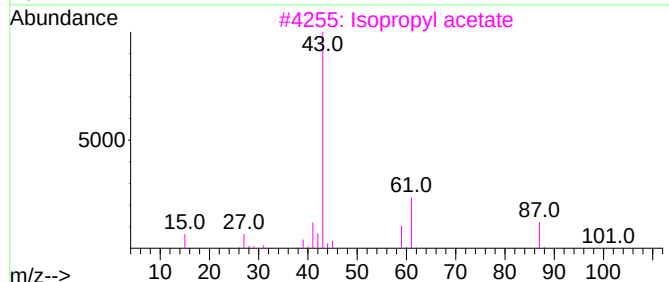
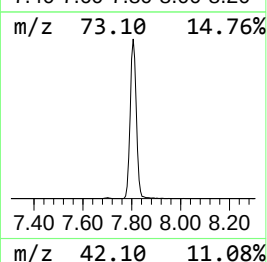
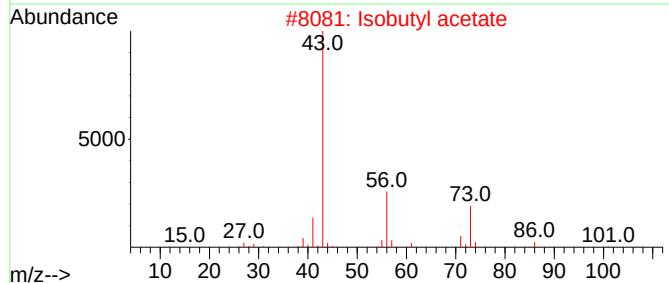
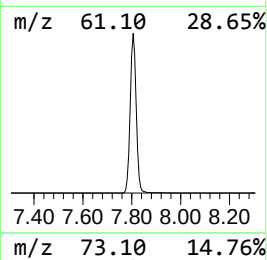
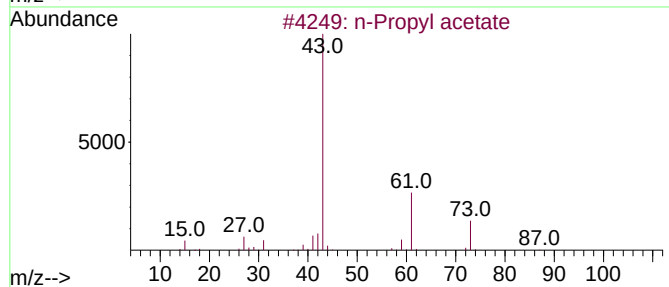
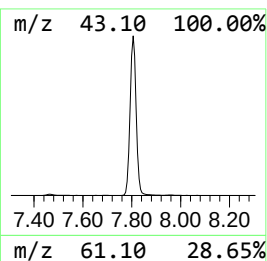
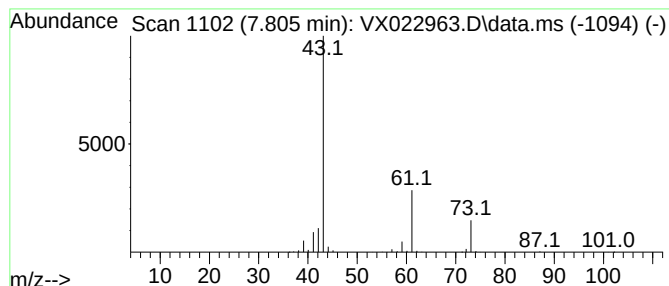
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Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.805	207.52 ug/l	1226500	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		Isobutyl acetate	116	C6H12O2	000110-19-0	9
3		Isopropyl acetate	102	C5H10O2	000108-21-4	9
4		Isobutylamine	73	C4H11N	000078-81-9	7
5		1-Butanamine	73	C4H11N	000109-73-9	5



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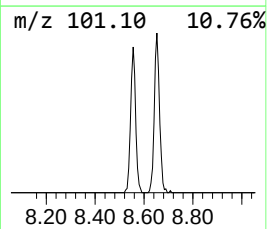
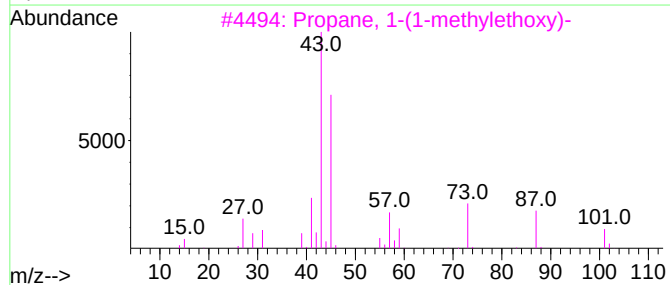
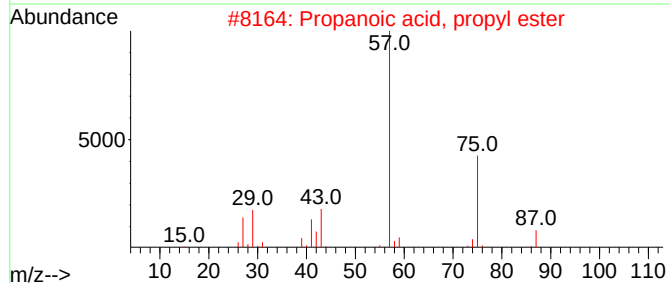
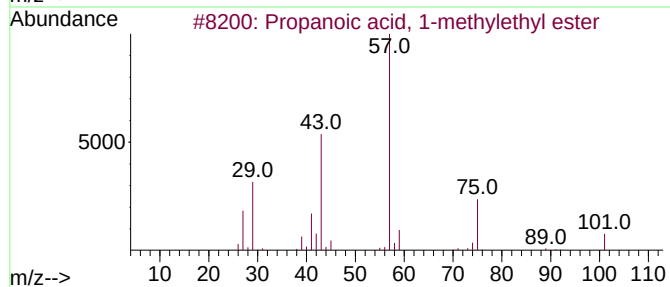
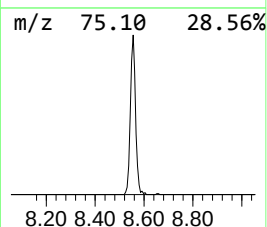
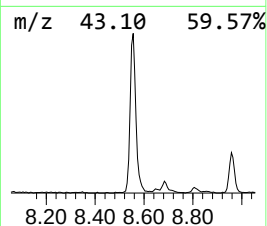
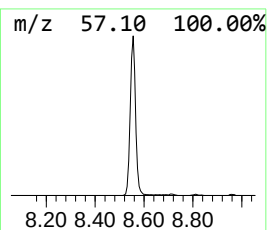
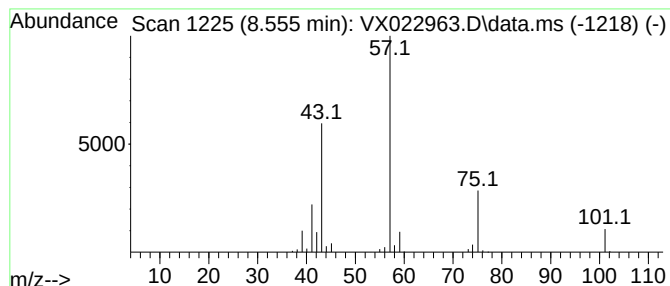
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.555	23.17 ug/l	177190	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	42
3			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
4			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	23
5			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	22



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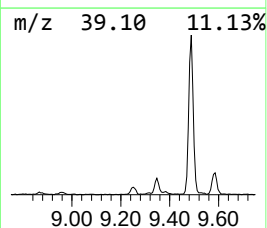
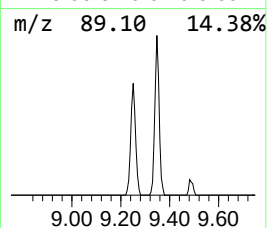
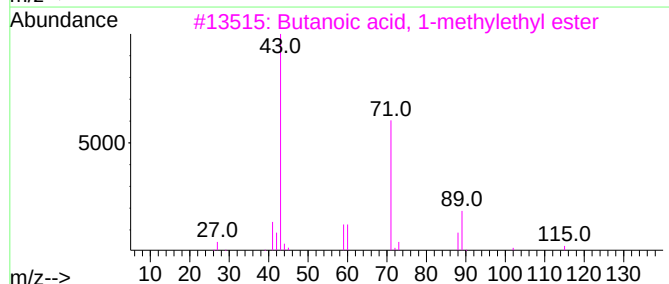
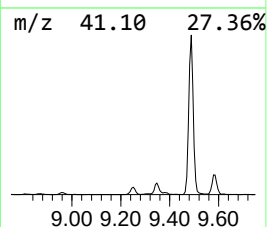
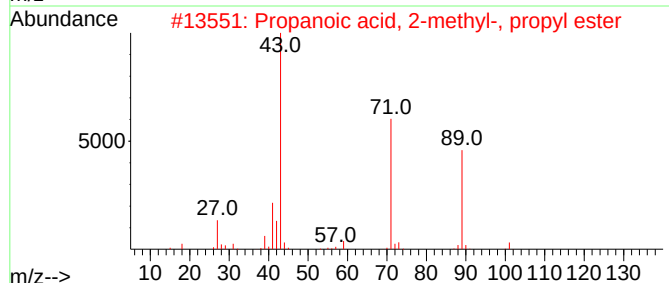
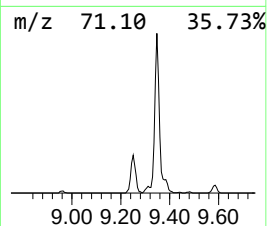
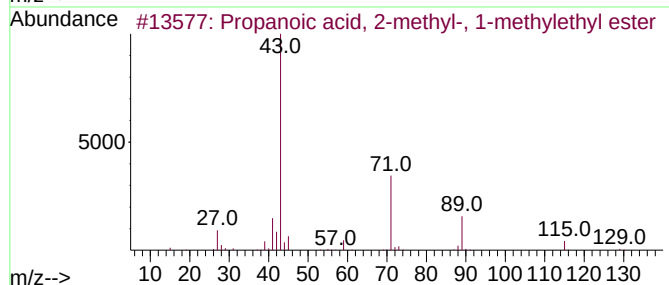
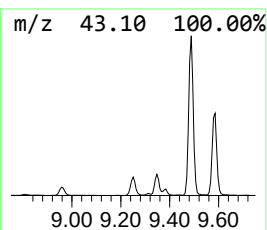
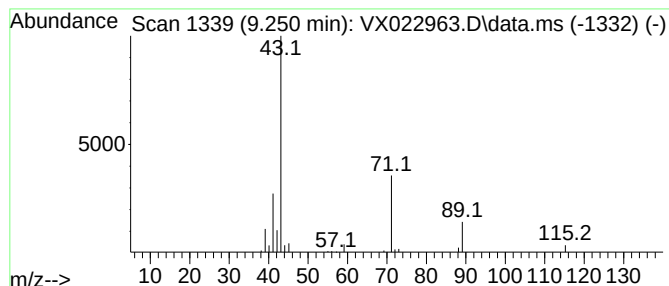
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Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.250	5.84 ug/l	44650	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	72
4			Sulfurous acid, pentyl 2-propyl ...	194	C8H18O3S	1000309-11-5	38
5			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	28



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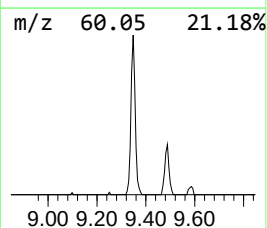
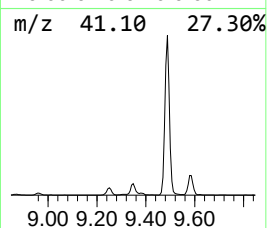
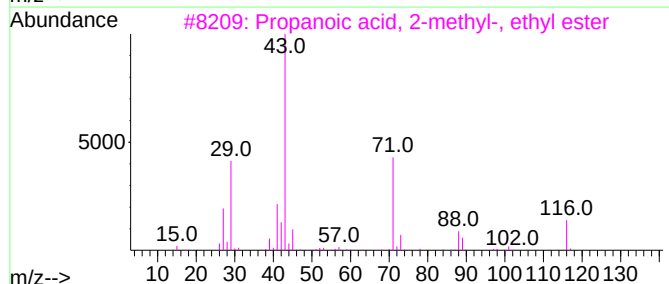
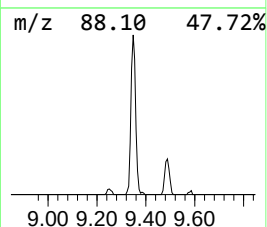
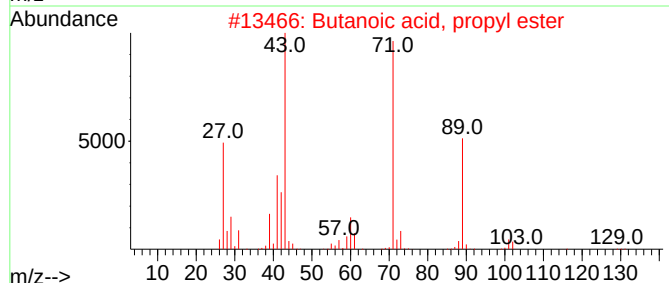
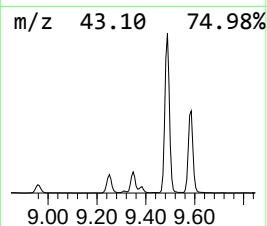
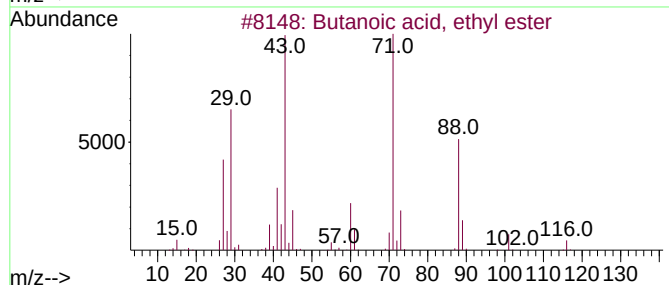
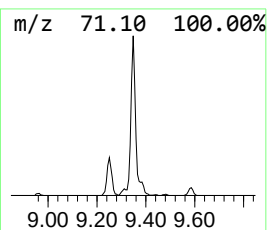
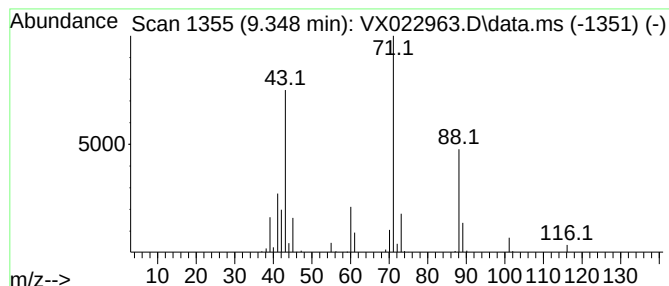
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Peak Number 4 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.348	12.96 ug/l	99098	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			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50
3			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	47
4			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	38
5			Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	38



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Instrument :
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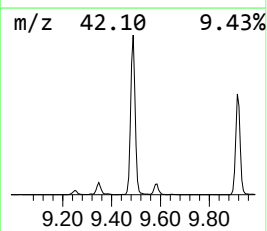
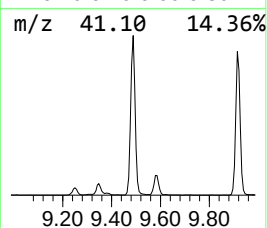
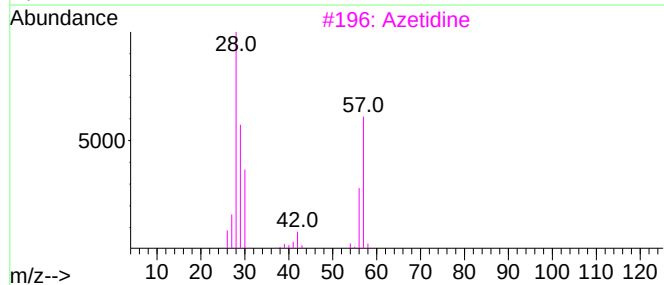
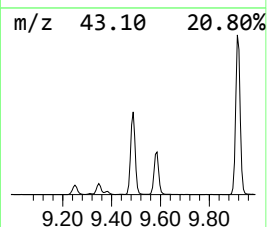
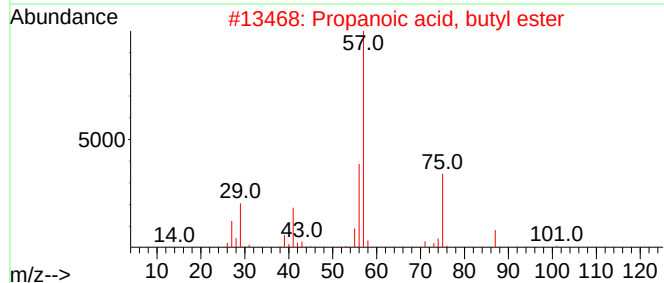
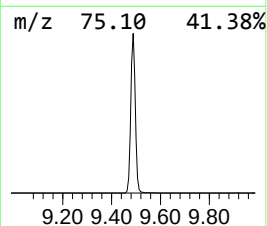
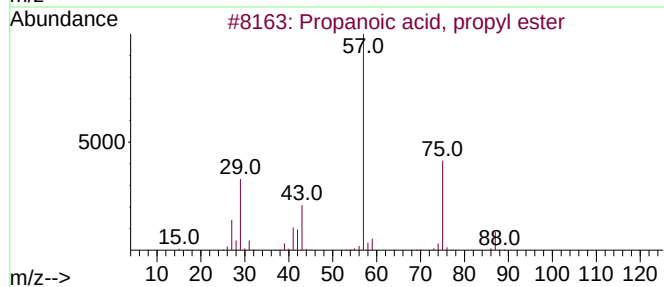
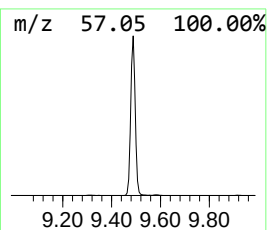
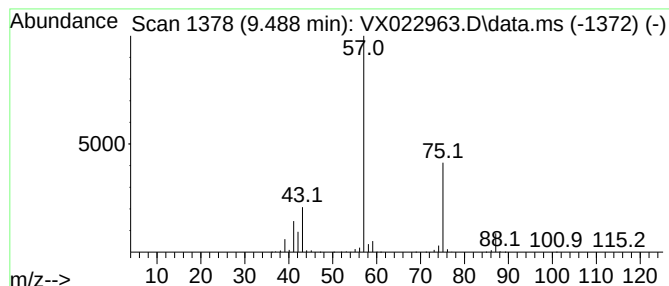
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Peak Number 5 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.488	215.19 ug/l	1645620	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	38
3			Azetidine	57	C3H7N	000503-29-7	9
4			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5			Isobutyl ether	130	C8H18O	000628-55-7	9



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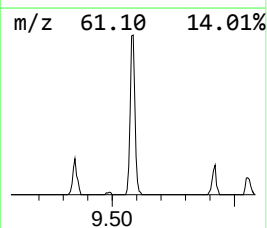
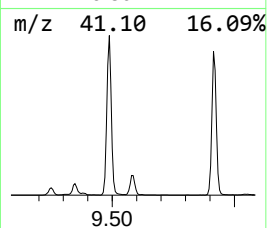
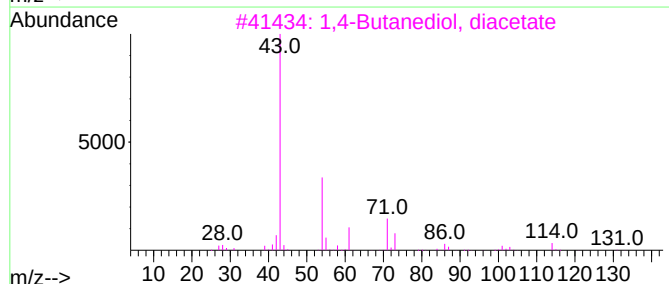
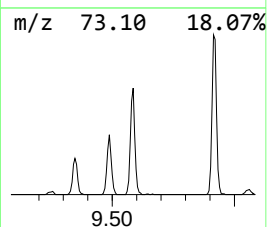
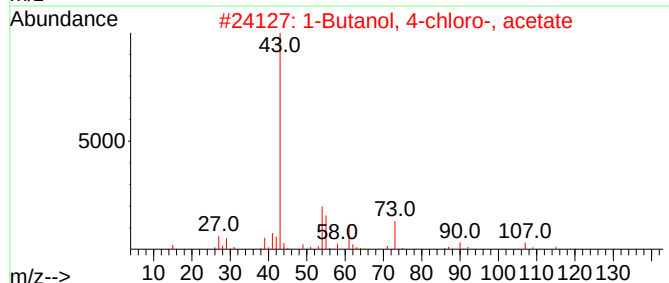
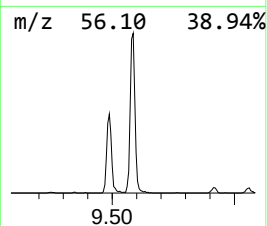
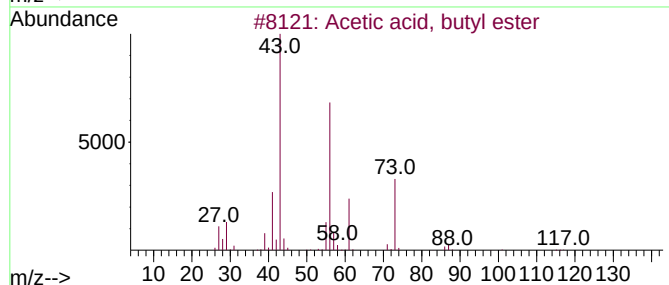
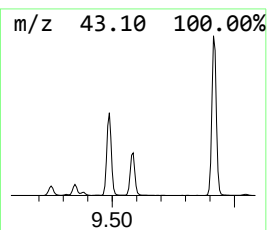
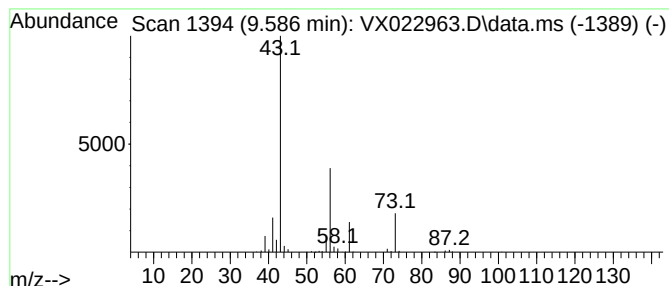
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Quant Title : SW846 8260

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.586	24.70 ug/l	188858	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2			1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	17
3			1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	17
4			Isobutylamine	73	C4H11N	000078-81-9	9
5			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062521\
Data File : VX022963.D
Acq On : 26 Jun 2021 08:08
Operator : JC/MD
Sample : M2832-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 56 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-3-WC

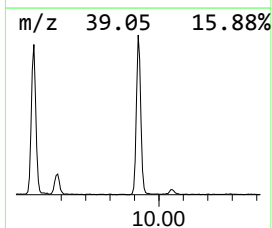
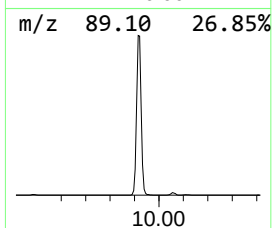
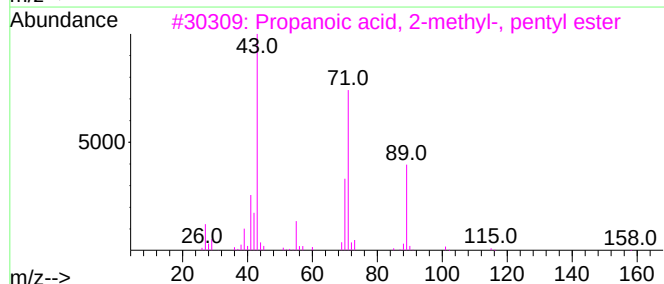
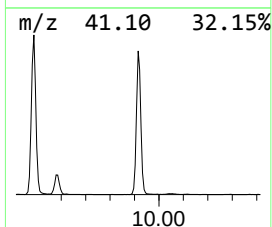
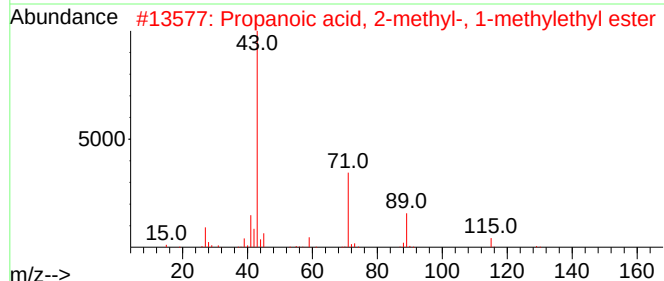
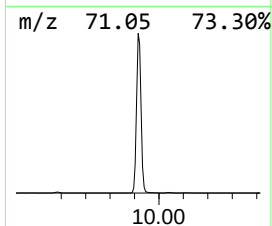
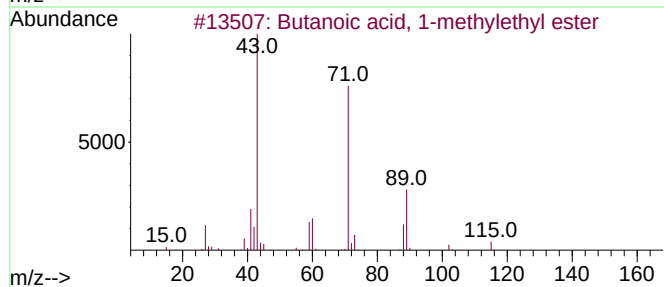
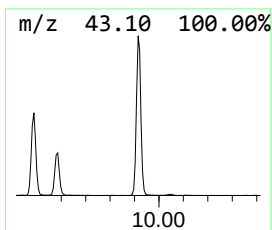
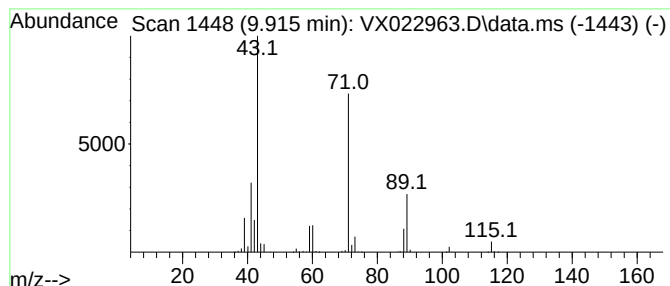
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Quant Title : SW846 8260

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	129.03 ug/l	986696	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	94
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
3			Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
5			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062521\
Data File : VX022963.D
Acq On : 26 Jun 2021 08:08
Operator : JC/MD
Sample : M2832-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 56 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-3-WC

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.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	7.805	207.5	ug/l	1226500	2	6.769	295517	50.0
Propanoic acid,...	8.555	23.2	ug/l	177190	3	10.055	382362	50.0
Propanoic acid,...	9.250	5.8	ug/l	44650	3	10.055	382362	50.0
Butanoic acid, ...	9.348	13.0	ug/l	99098	3	10.055	382362	50.0
Propanoic acid,...	9.488	215.2	ug/l	1645620	3	10.055	382362	50.0
Acetic acid, bu...	9.586	24.7	ug/l	188858	3	10.055	382362	50.0
Butanoic acid, ...	9.915	129.0	ug/l	986696	3	10.055	382362	50.0