

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012822\
 Data File : VX026665.D
 Acq On : 28 Jan 2022 20:36
 Operator : JC/MD
 Sample : N1319-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MH-1D

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\82X011122W.M
 Title : SW846 8260

Signal : TIC: VX026665.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.386	207	213	223	rBV	11489	19663	1.13%	0.239%
2	5.391	694	706	719	rBV	77075	224797	12.91%	2.737%
3	5.556	723	733	753	rVB	134708	382093	21.95%	4.652%
4	5.964	785	800	813	rBV	85551	227636	13.08%	2.772%
5	6.342	854	862	876	rVB2	8213	22001	1.26%	0.268%
6	6.763	922	931	944	rBV	213068	528779	30.38%	6.438%
7	7.799	1093	1101	1113	rBV	737452	1248321	71.72%	15.199%
8	8.549	1217	1224	1234	rBV	123886	193500	11.12%	2.356%
9	8.653	1234	1241	1250	rBV	429676	676027	38.84%	8.231%
10	8.958	1286	1291	1297	rBV	13225	19413	1.12%	0.236%
11	9.250	1333	1339	1345	rBV	33320	50086	2.88%	0.610%
12	9.348	1350	1355	1359	rBV	80606	108487	6.23%	1.321%
13	9.482	1372	1377	1388	rBV	1301702	1740599	100.00%	21.193%
14	9.579	1388	1393	1407	rVB	144011	193695	11.13%	2.358%
15	9.915	1442	1448	1462	rBV	868015	1075423	61.78%	13.094%
16	10.055	1465	1471	1478	rVV	432446	567558	32.61%	6.910%
17	10.640	1562	1567	1574	rBV	30619	39741	2.28%	0.484%
18	11.079	1634	1639	1649	rBV	310730	407088	23.39%	4.957%
19	12.024	1788	1794	1802	rBV	397294	488245	28.05%	5.945%

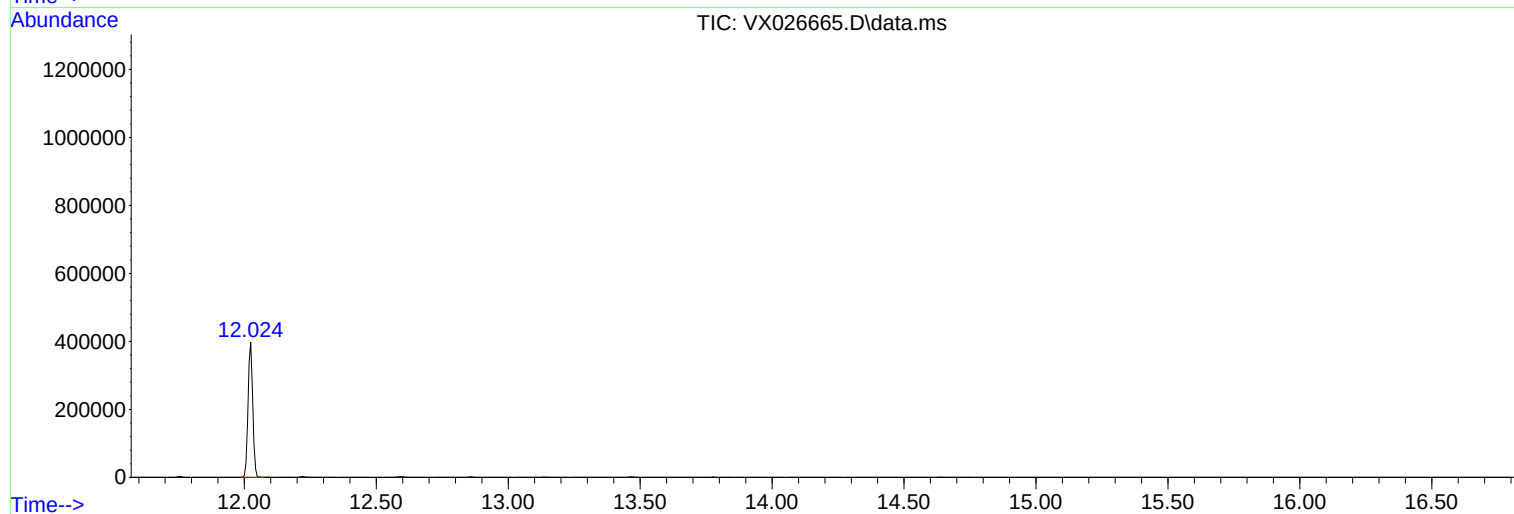
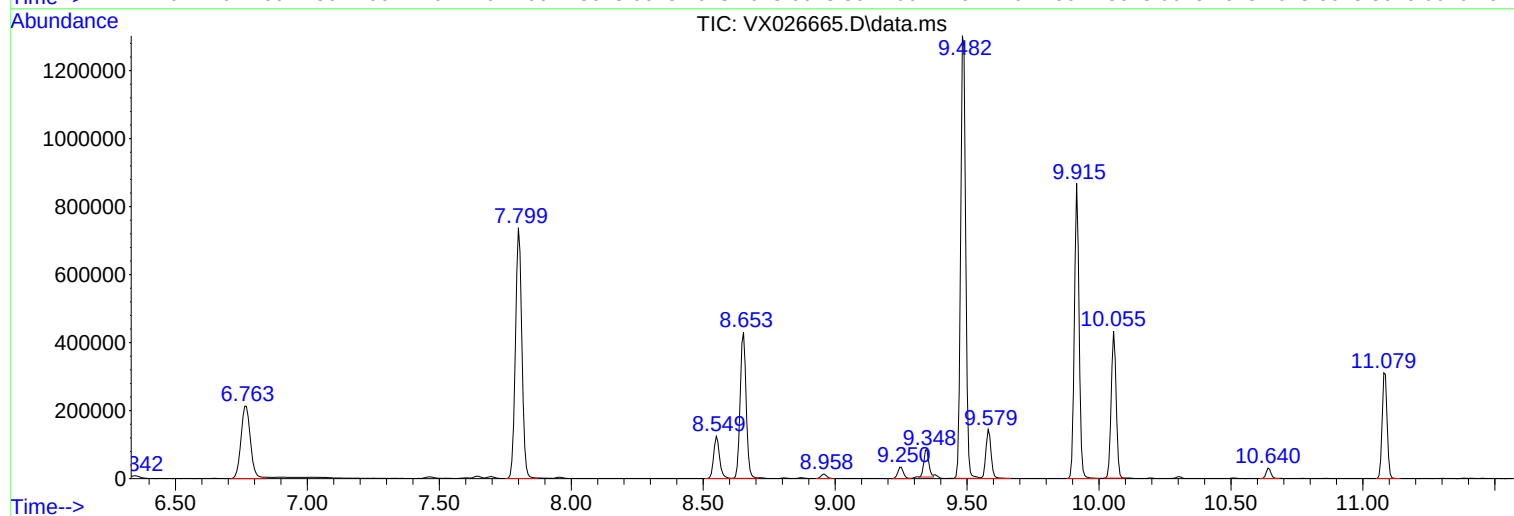
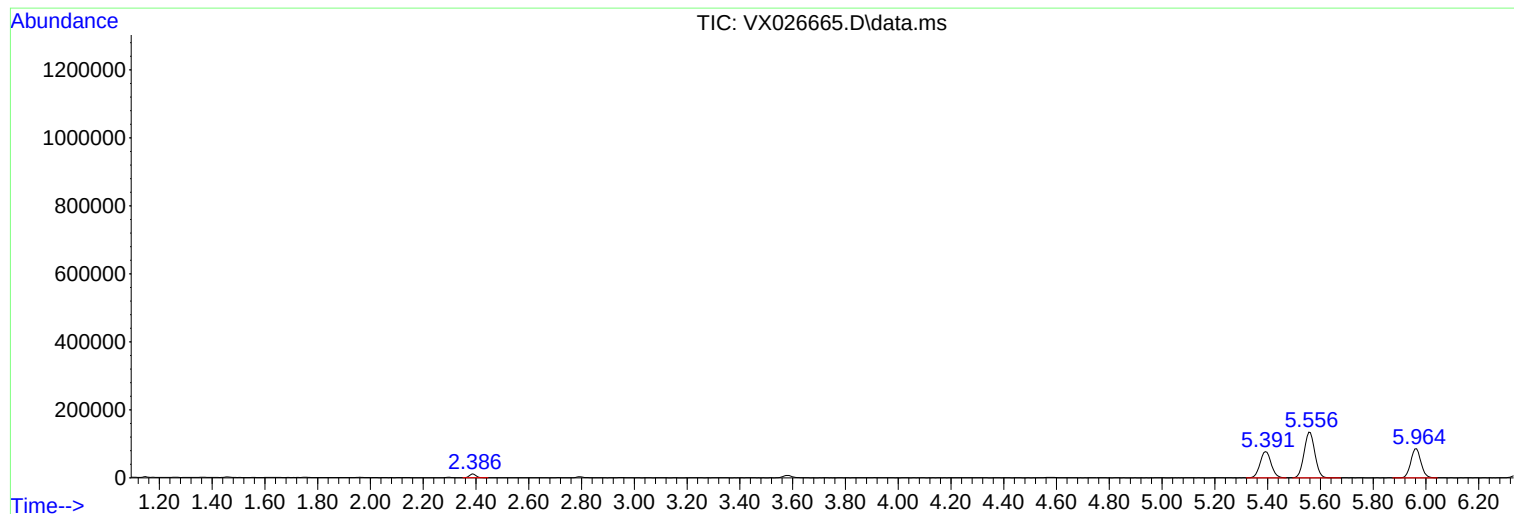
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

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



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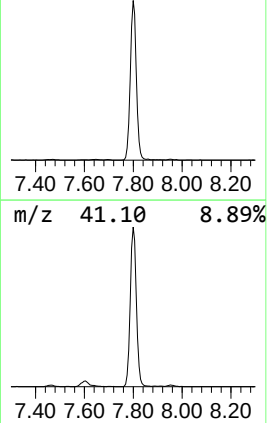
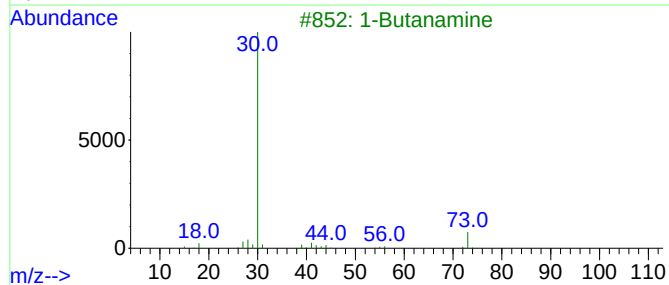
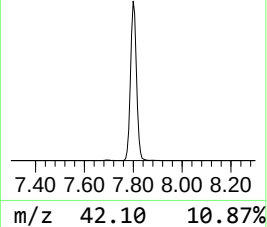
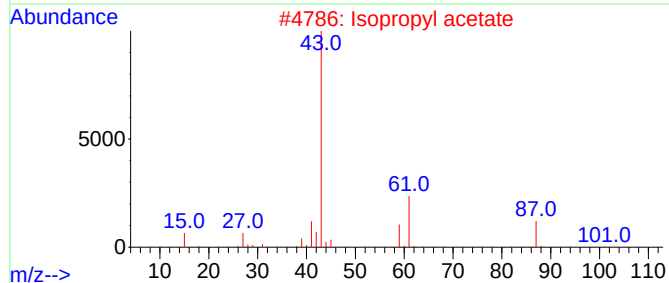
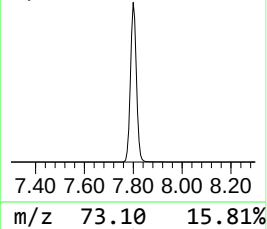
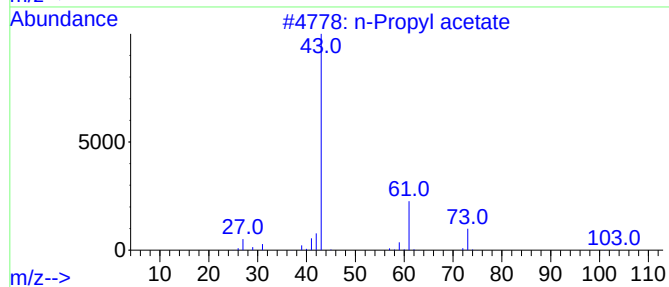
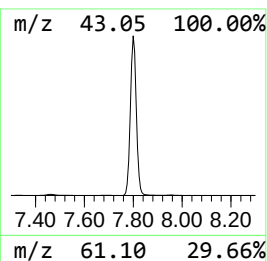
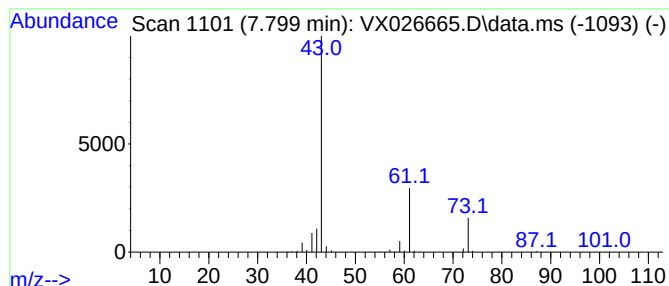
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
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TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	118.04 ug/l	1248320	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	5
5			Hydrogen azide	43	HN3	007782-79-8	4



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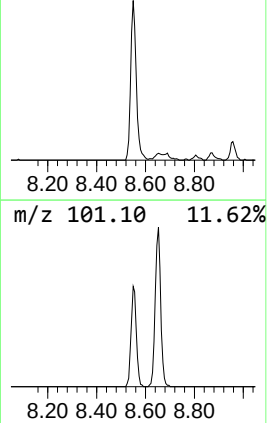
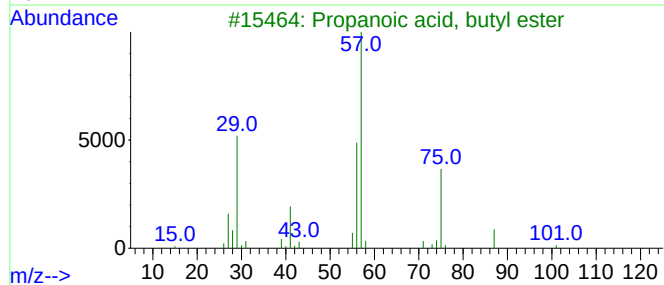
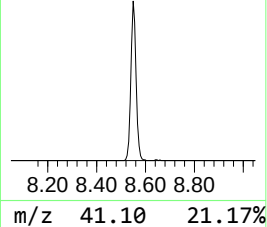
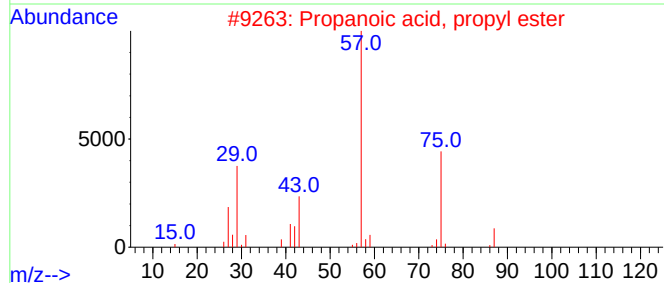
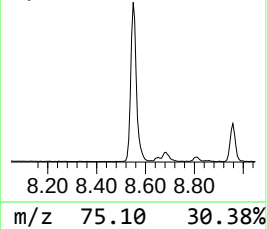
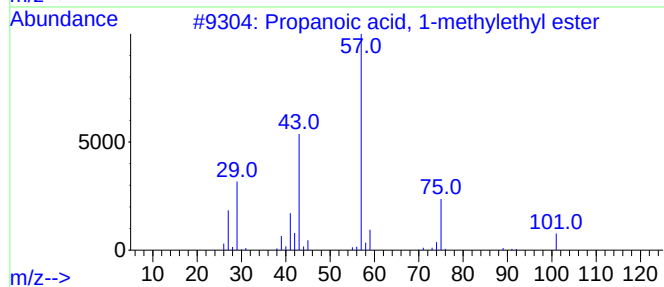
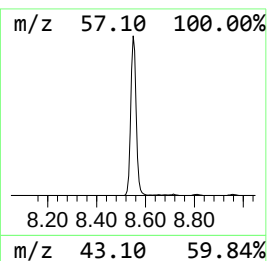
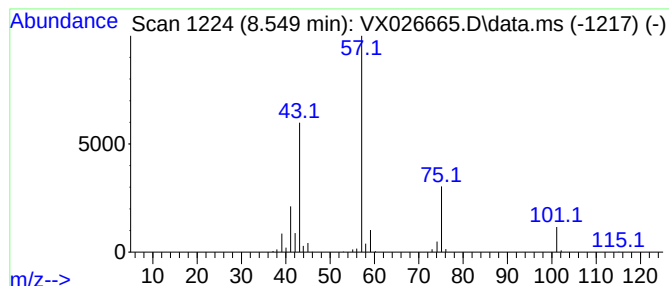
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	17.05 ug/l	193500	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
3			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
4			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10



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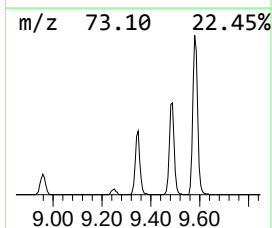
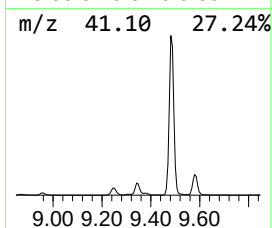
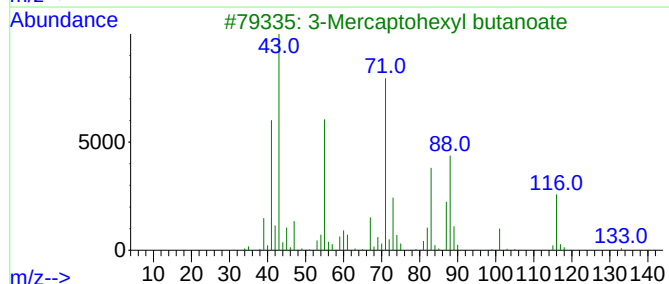
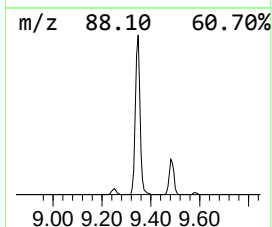
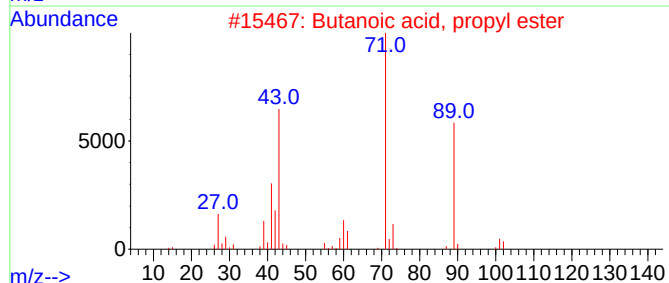
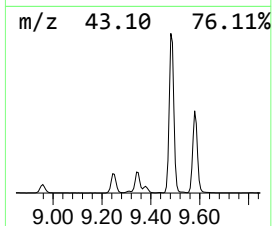
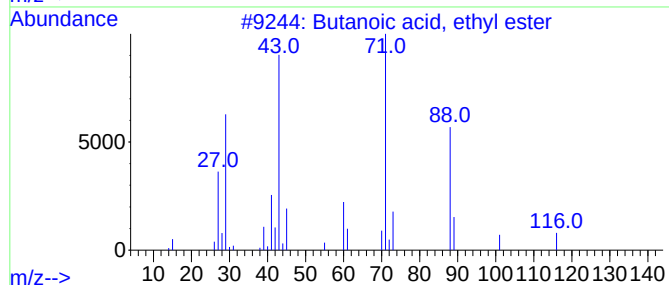
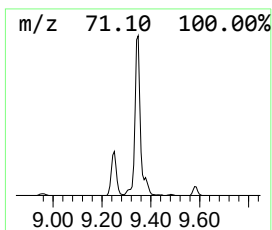
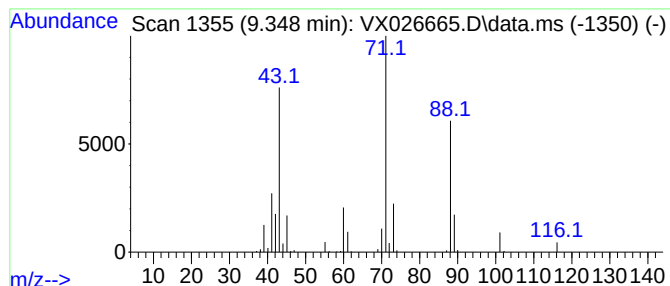
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Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.348	9.56 ug/l	108487	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	94
2			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50
3			3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	45
4			4-Butoxy-2-butanone	144	C8H16O2	030536-44-8	42
5			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	42



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Instrument :
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ClientSampleId :
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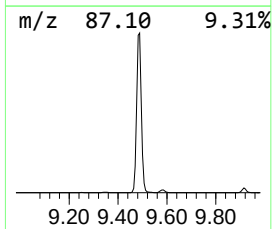
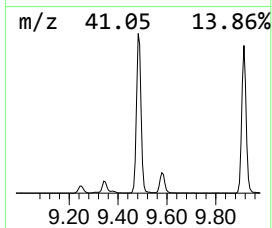
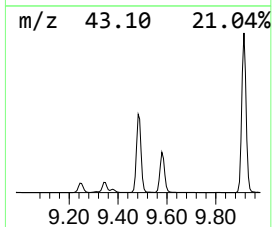
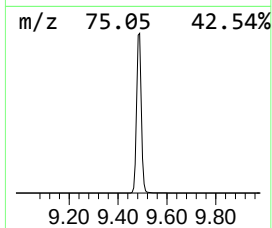
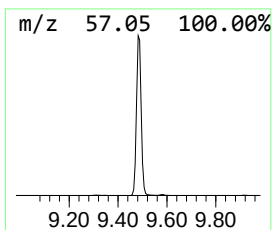
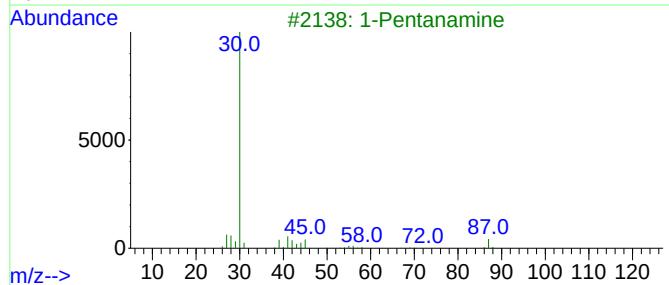
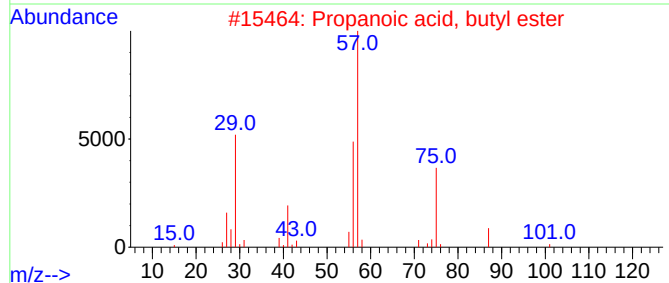
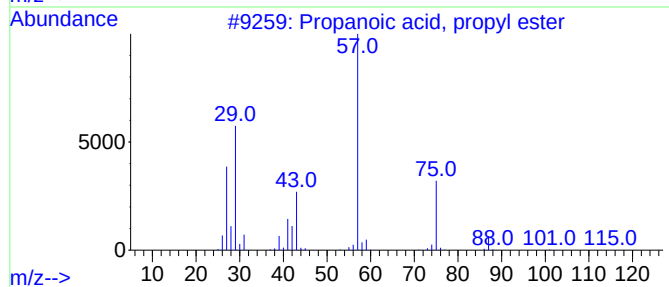
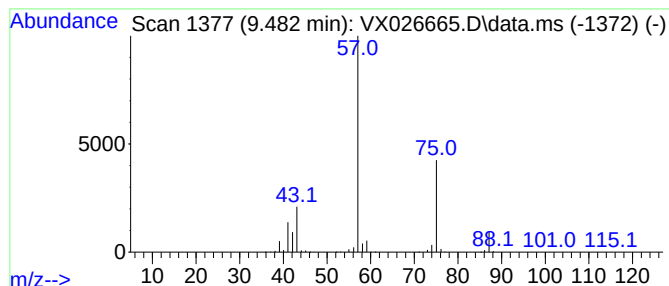
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	153.34 ug/l	1740600	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			1-Pentanamine	87	C5H13N	000110-58-7	10
4			Azetidine	57	C3H7N	000503-29-7	9
5			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9



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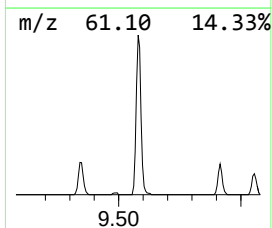
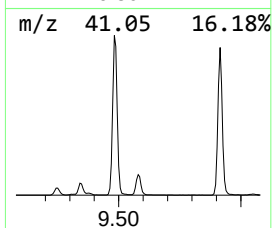
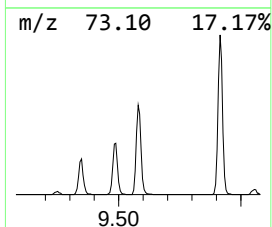
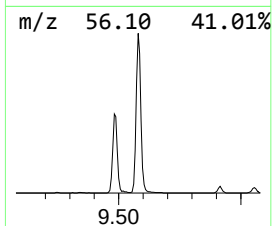
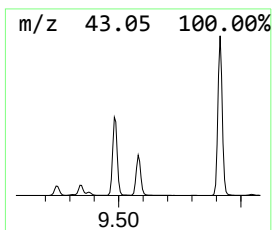
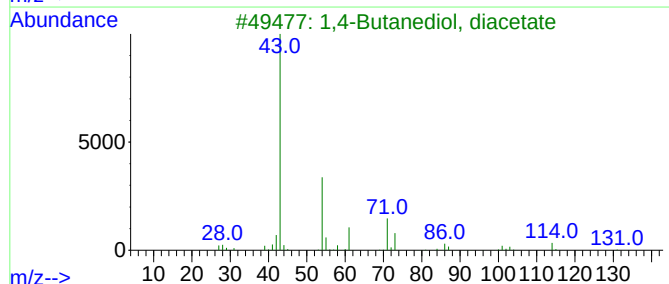
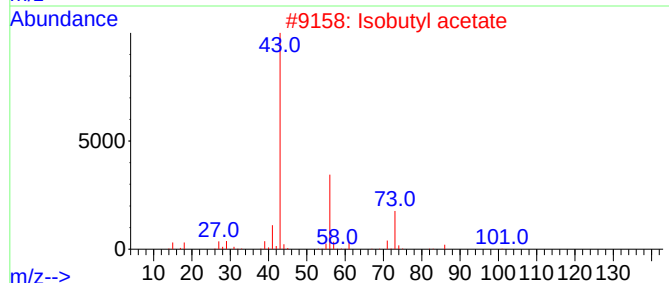
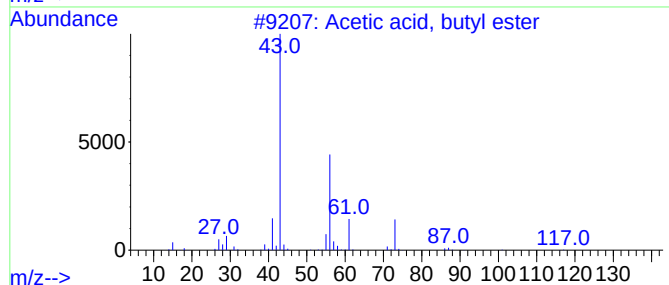
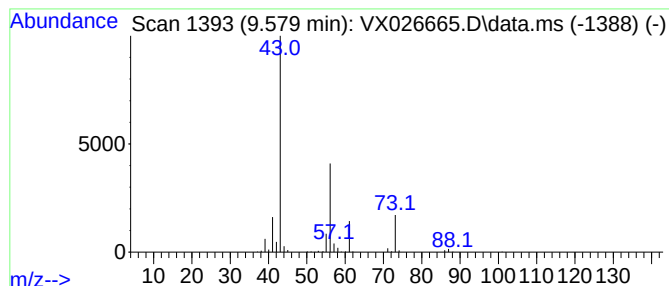
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Peak Number 5 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.579	17.06 ug/l	193695	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			Isobutyl acetate	116	C6H12O2	000110-19-0	40
3			1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	17
4			Isobutylamine	73	C4H11N	000078-81-9	9
5			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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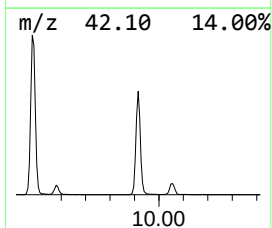
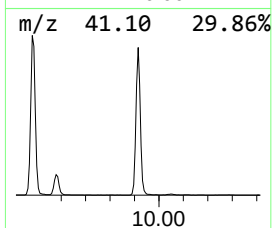
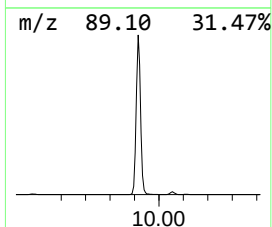
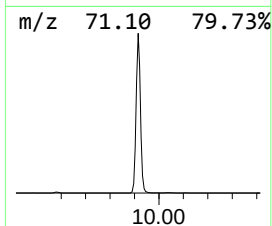
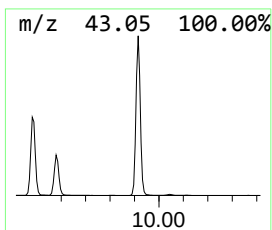
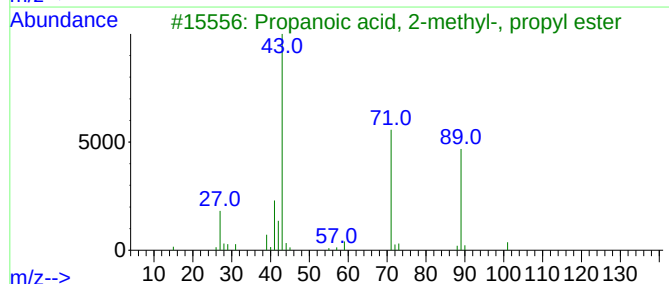
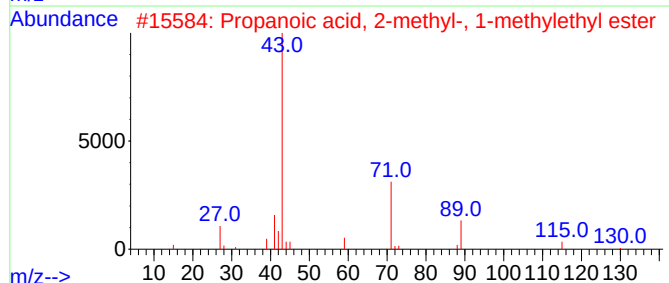
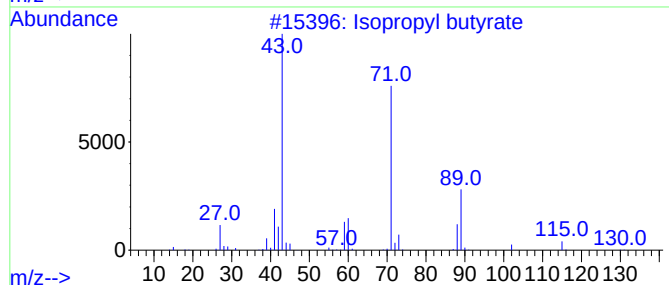
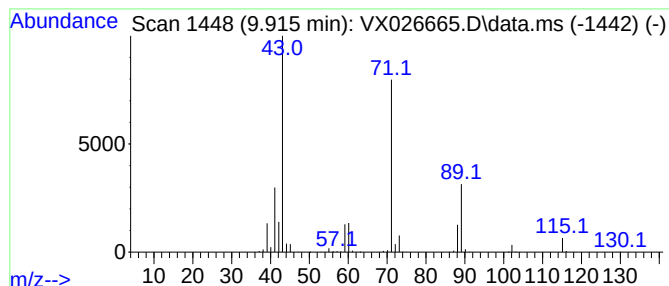
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	94.74 ug/l	1075420	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	95
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
3			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72
5			Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012822\
Data File : VX026665.D
Acq On : 28 Jan 2022 20:36
Operator : JC/MD
Sample : N1319-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MH-1D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.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
n-Propyl acetate	7.799	118.0	ug/l	1248320	2	6.769	528779	50.0
Propanoic acid,...	8.549	17.1	ug/l	193500	3	10.055	567558	50.0
Butanoic acid, ...	9.348	9.6	ug/l	108487	3	10.055	567558	50.0
Propanoic acid,...	9.482	153.3	ug/l	1740600	3	10.055	567558	50.0
Acetic acid, bu...	9.579	17.1	ug/l	193695	3	10.055	567558	50.0
Isopropyl butyrate	9.915	94.7	ug/l	1075420	3	10.055	567558	50.0