

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012822\
 Data File : VX026664.D
 Acq On : 28 Jan 2022 20:13
 Operator : JC/MD
 Sample : N1319-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MH-1S

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: VX026664.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	227	rVB	11530	20900	1.25%	0.257%
2	5.391	694	706	720	rBV	78952	227321	13.55%	2.797%
3	5.556	723	733	747	rVB2	137815	388228	23.14%	4.777%
4	5.964	787	800	813	rBV	87167	233489	13.92%	2.873%
5	6.342	851	862	875	rBV2	7529	20457	1.22%	0.252%
6	6.763	921	931	944	rBV	218087	540623	32.22%	6.652%
7	7.799	1094	1101	1113	rBV	711963	1198599	71.44%	14.749%
8	8.549	1217	1224	1234	rBV	120163	184750	11.01%	2.273%
9	8.653	1234	1241	1250	rBV	442236	686207	40.90%	8.444%
10	8.958	1284	1291	1298	rBV	12941	19490	1.16%	0.240%
11	9.244	1333	1338	1345	rBV	32175	47019	2.80%	0.579%
12	9.348	1350	1355	1359	rBV	77783	104260	6.21%	1.283%
13	9.482	1372	1377	1388	rBV	1228204	1677782	100.00%	20.645%
14	9.580	1388	1393	1407	rVB	141930	185873	11.08%	2.287%
15	9.915	1442	1448	1465	rBV	822738	1033861	61.62%	12.722%
16	10.055	1465	1471	1478	rVV	431594	579120	34.52%	7.126%
17	10.640	1562	1567	1579	rBV	31943	41762	2.49%	0.514%
18	11.085	1634	1640	1650	rBV	324775	424847	25.32%	5.228%
19	12.024	1789	1794	1801	rBV	423504	512101	30.52%	6.301%

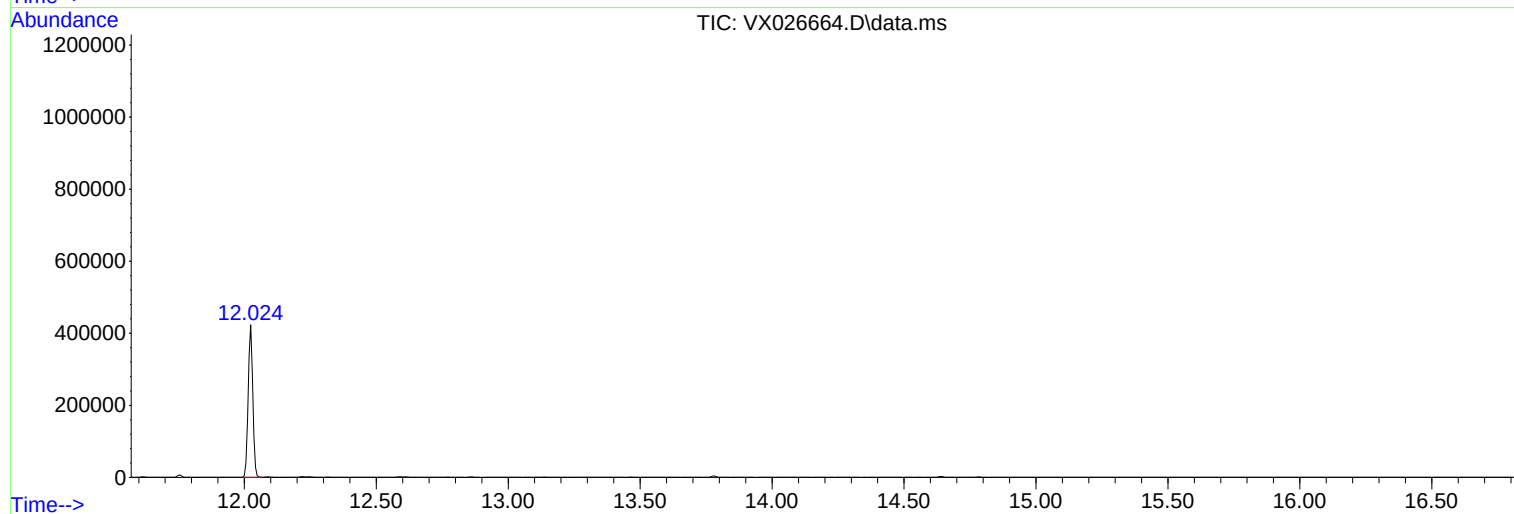
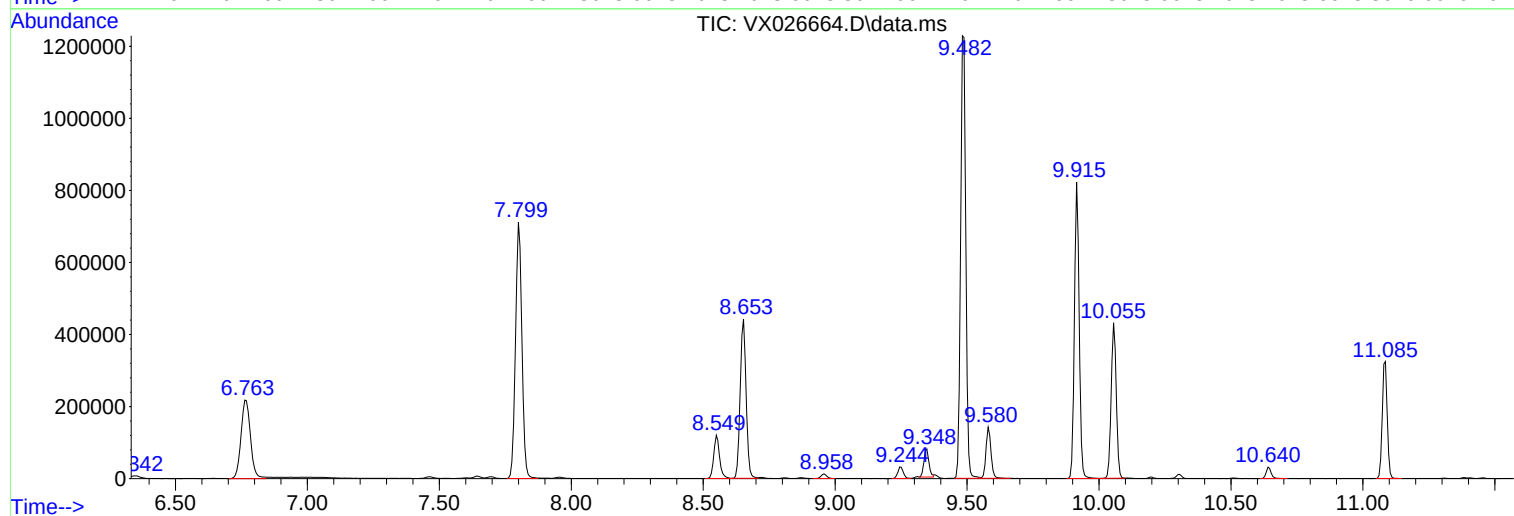
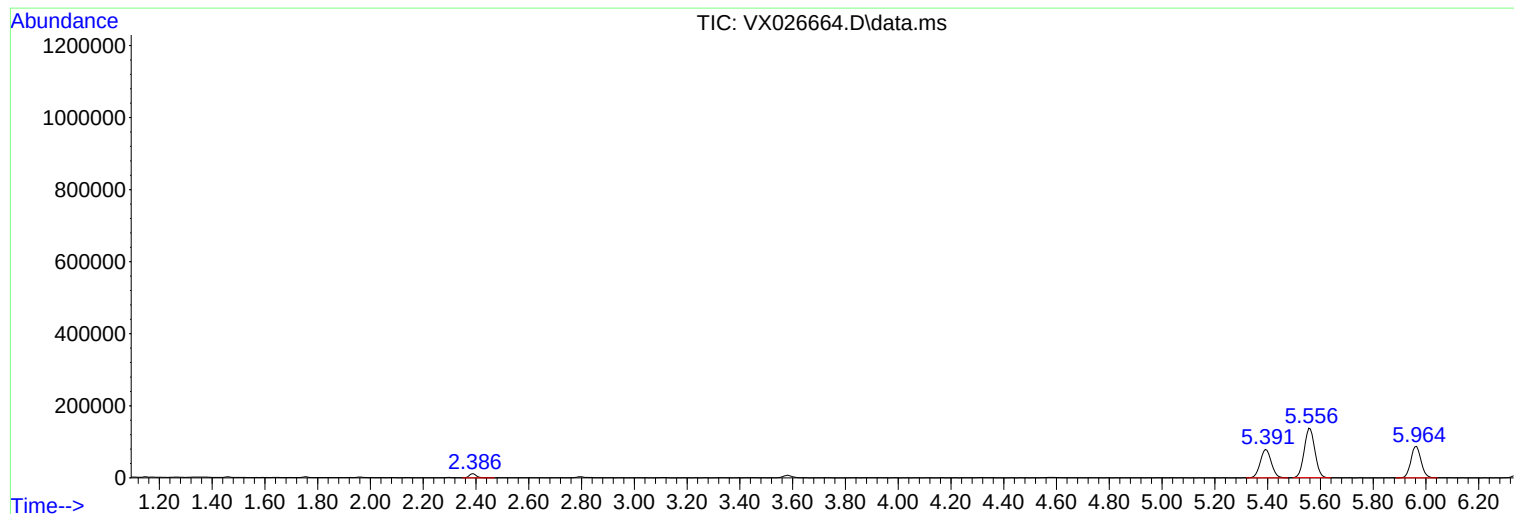
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Quant Title : SW846 8260

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



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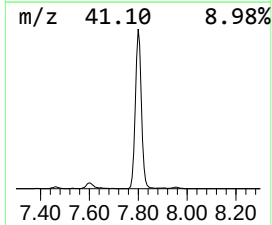
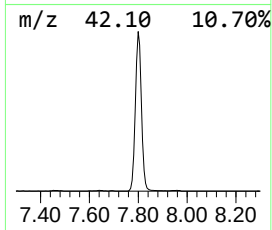
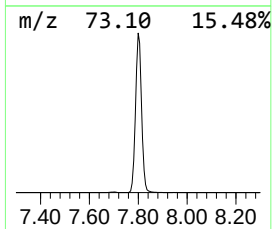
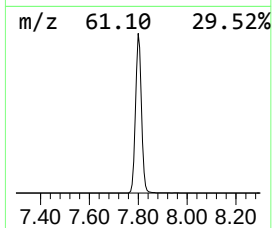
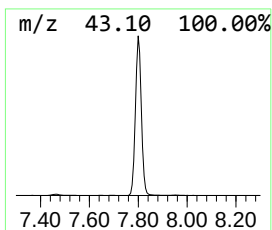
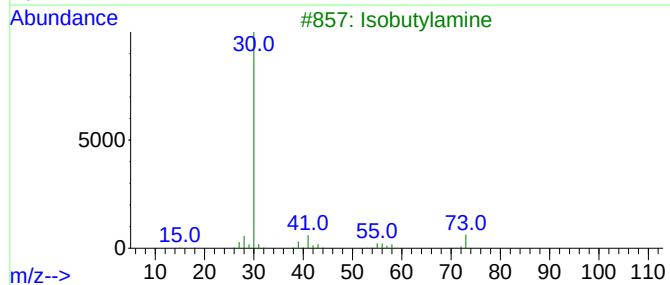
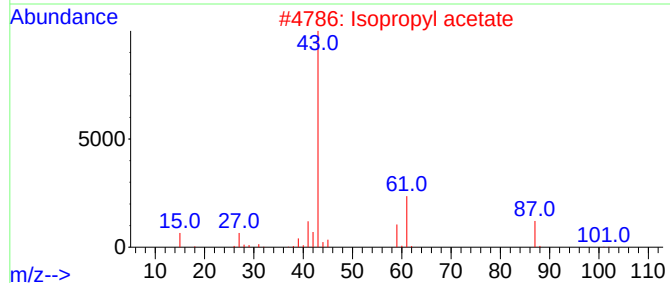
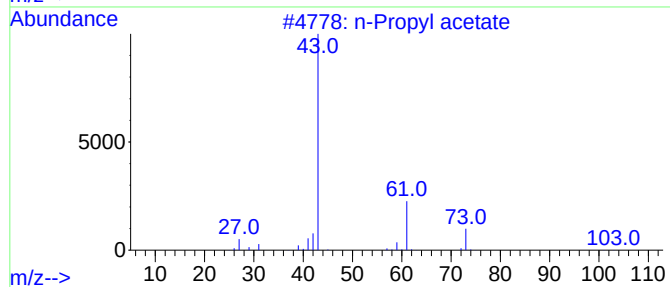
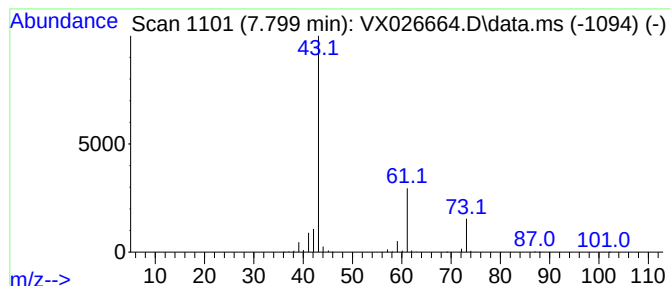
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

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

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	110.85 ug/l	1198600	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		Isobutylamine	73	C4H11N	000078-81-9	7
4		1-Butanamine	73	C4H11N	000109-73-9	7
5		Isobutyl acetate	116	C6H12O2	000110-19-0	4



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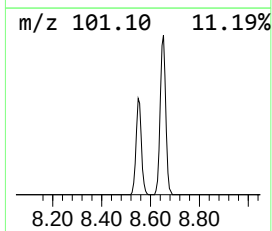
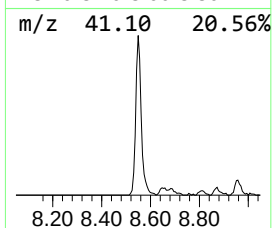
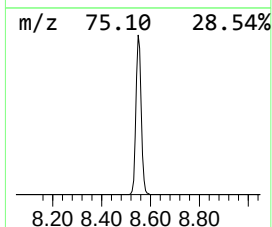
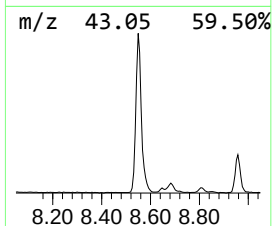
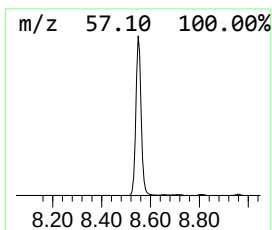
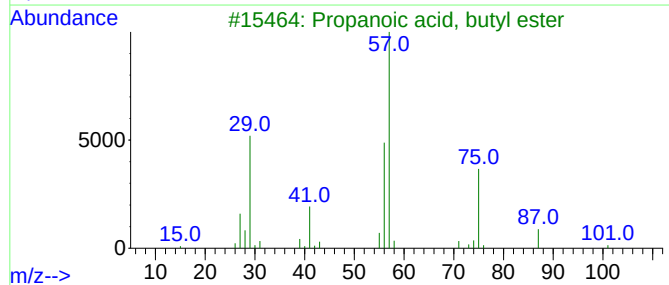
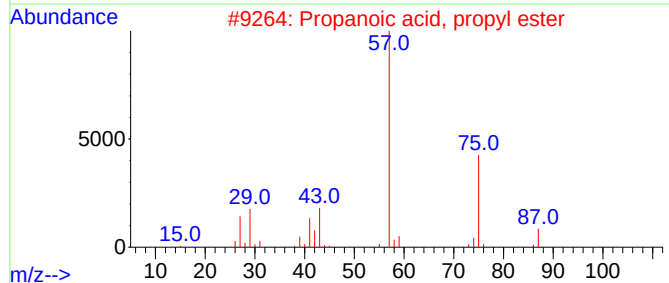
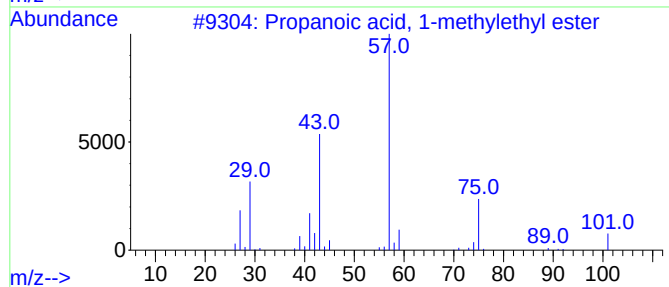
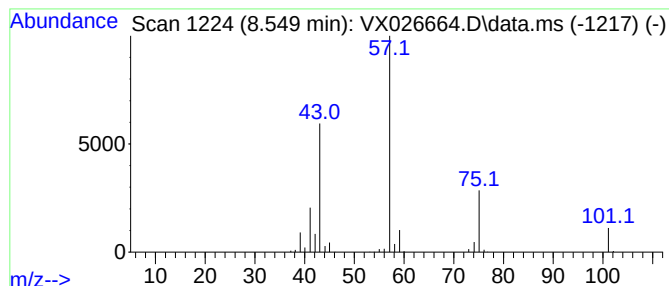
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	15.95 ug/l	184750	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	28
4			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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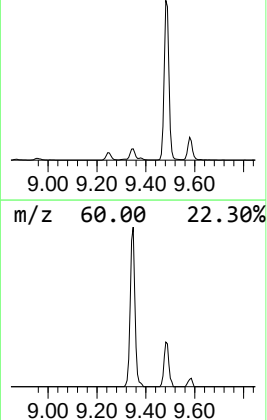
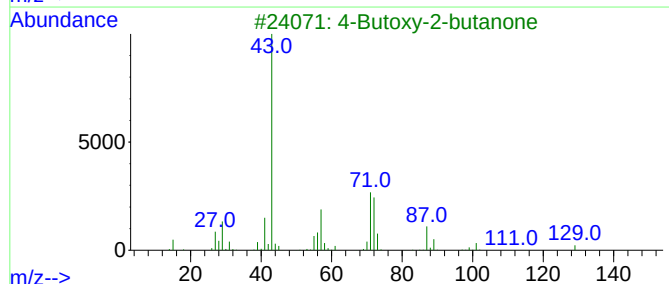
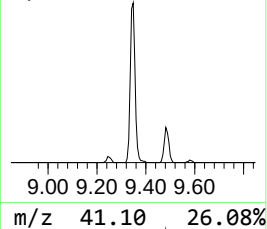
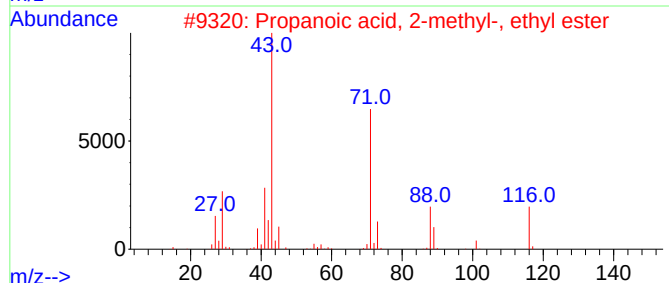
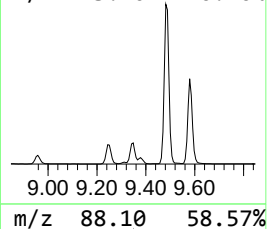
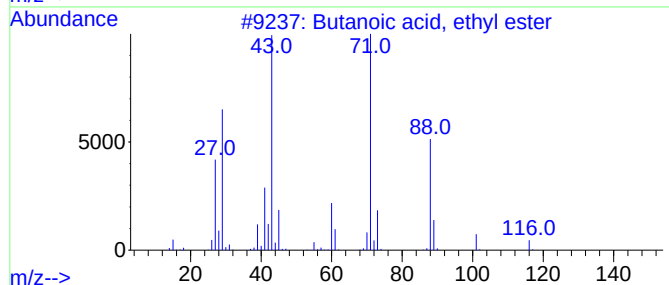
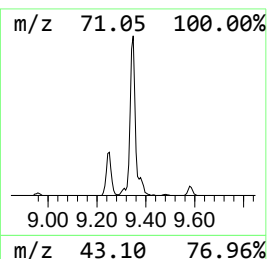
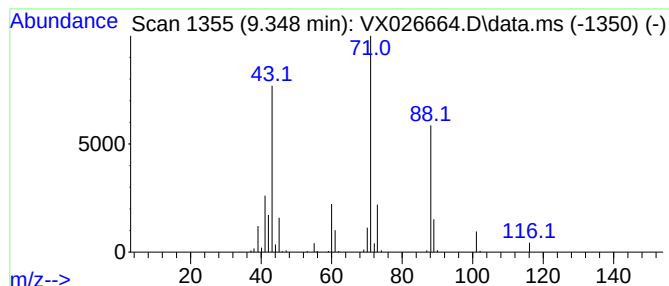
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.348	9.00 ug/l	104260	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	95
2			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	53
3			4-Butoxy-2-butanone	144	C8H16O2	030536-44-8	42
4			Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	38
5			3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	37



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ALS Vial : 25 Sample Multiplier: 1

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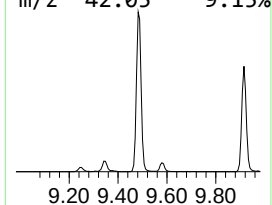
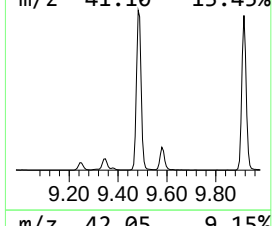
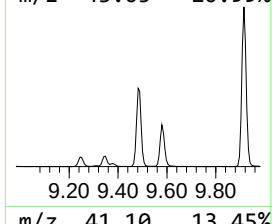
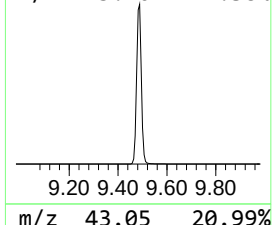
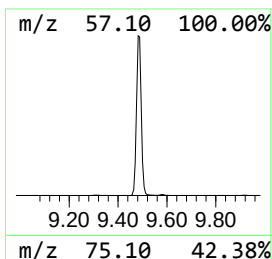
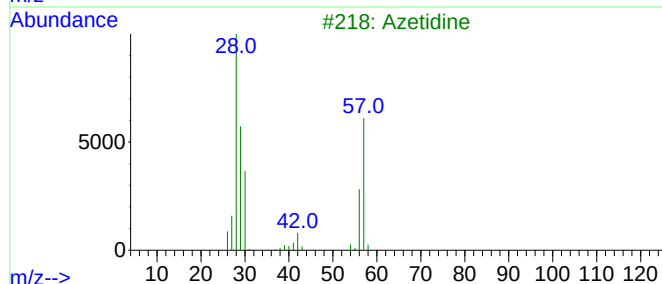
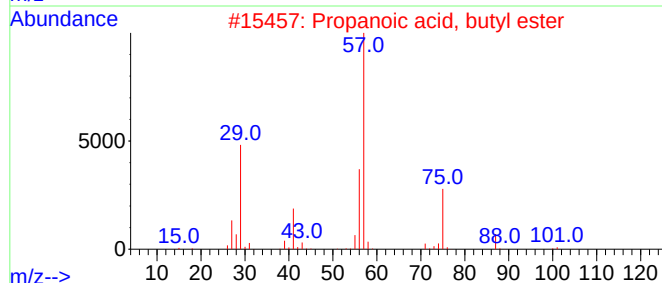
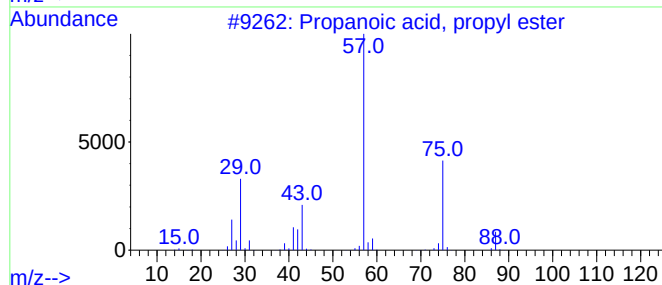
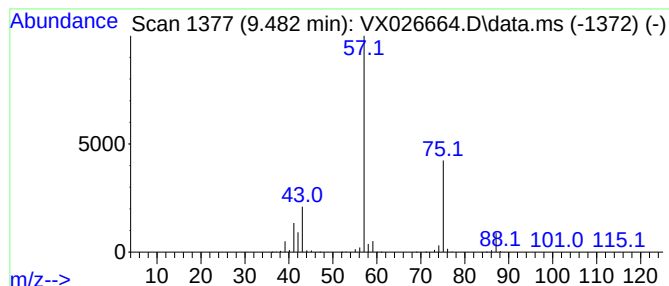
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Quant Title : SW846 8260

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

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	144.86 ug/l	1677780	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			Azetidine	57	C3H7N	000503-29-7	9
4			2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
5			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9



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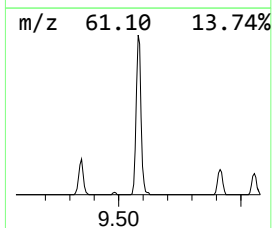
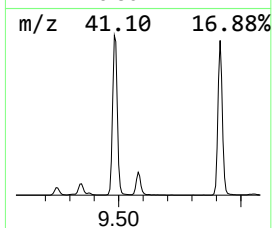
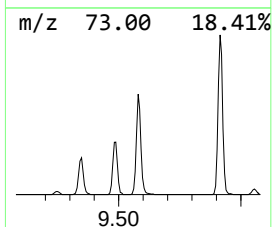
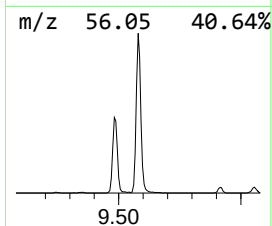
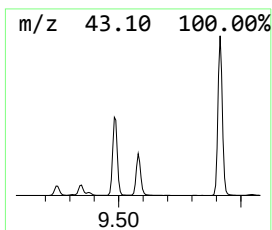
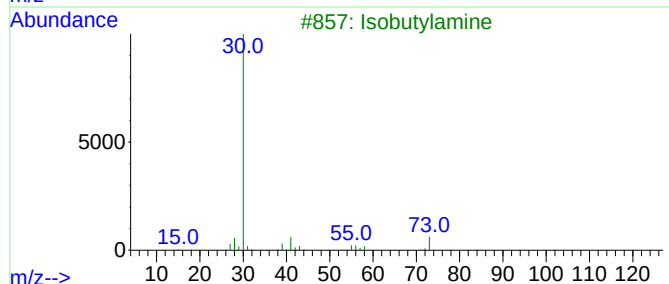
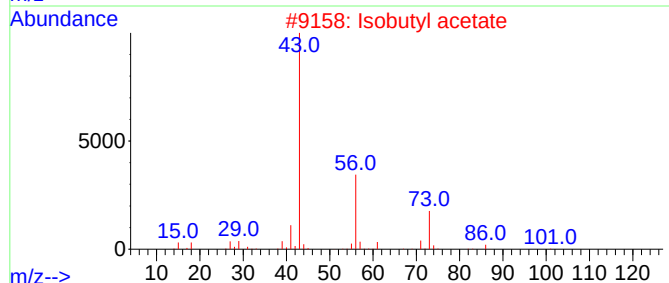
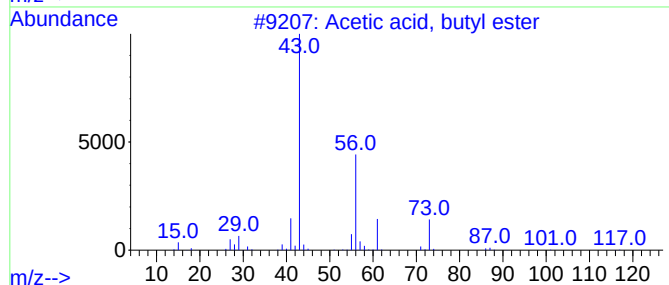
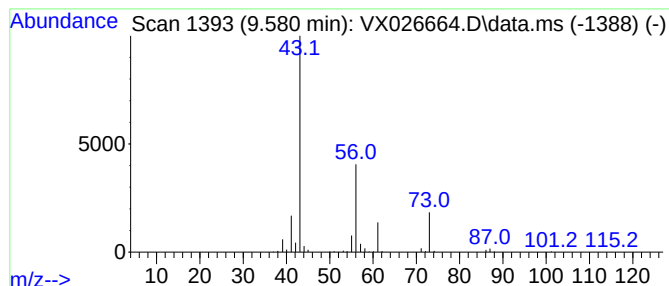
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	16.05 ug/l	185873	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	39
3			Isobutylamine	73	C4H11N	000078-81-9	9
4			Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9
5			1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	9



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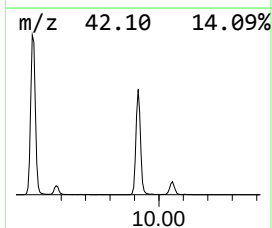
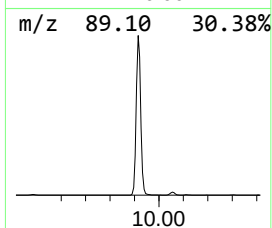
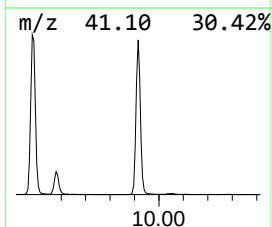
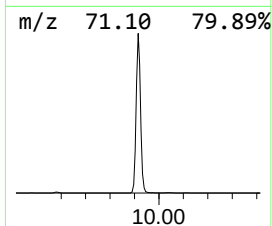
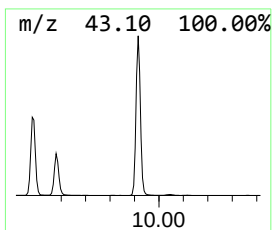
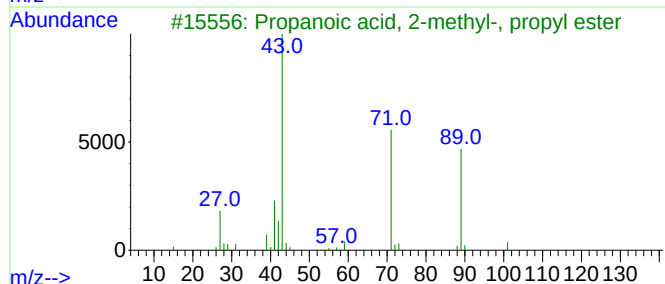
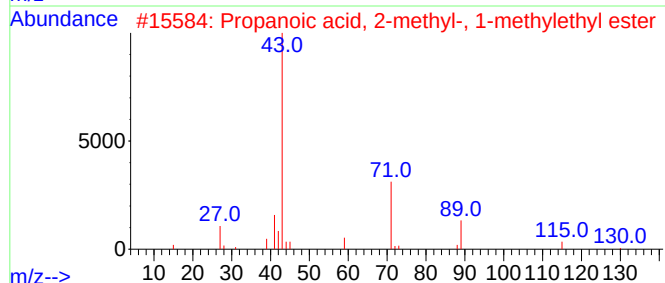
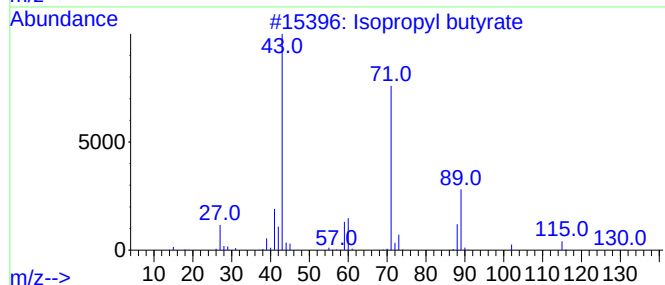
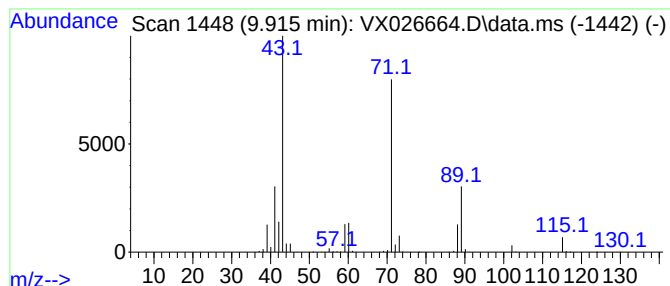
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

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

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	89.26 ug/l	1033860	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
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			Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
5			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012822\
Data File : VX026664.D
Acq On : 28 Jan 2022 20:13
Operator : JC/MD
Sample : N1319-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MH-1S

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.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
n-Propyl acetate	7.799	110.8	ug/l	1198600	2	6.769	540623	50.0
Propanoic acid,...	8.549	15.9	ug/l	184750	3	10.055	579120	50.0
Butanoic acid, ...	9.348	9.0	ug/l	104260	3	10.055	579120	50.0
Propanoic acid,...	9.482	144.9	ug/l	1677780	3	10.055	579120	50.0
Acetic acid, bu...	9.580	16.1	ug/l	185873	3	10.055	579120	50.0
Isopropyl butyrate	9.915	89.3	ug/l	1033860	3	10.055	579120	50.0