

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
 Data File : VX027969.D
 Acq On : 04 Apr 2022 19:40
 Operator : JC/MD
 Sample : PB143824ZHE#06
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 PB143824ZHE#06

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % 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\82X032922W.M
 Title : SW846 8260

Signal : TIC: VX027969.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	42	rVB	11965	20324	1.48%	0.311%
2	2.788	272	279	292	rBV	150386	273519	19.90%	4.186%
3	3.574	401	408	418	rBV2	6103	14308	1.04%	0.219%
4	5.391	694	706	719	rBV3	55617	162080	11.79%	2.481%
5	5.556	722	733	748	rVB	100496	282810	20.58%	4.329%
6	5.958	789	799	813	rBV2	56618	149751	10.90%	2.292%
7	6.342	852	862	870	rBV2	6122	15032	1.09%	0.230%
8	6.763	923	931	943	rVB	152595	366453	26.67%	5.609%
9	7.799	1093	1101	1117	rBV	569173	972970	70.80%	14.892%
10	8.549	1214	1224	1234	rBV	91611	139080	10.12%	2.129%
11	8.653	1234	1241	1250	rBV	301958	480455	34.96%	7.354%
12	8.958	1286	1291	1297	rBV	9930	14988	1.09%	0.229%
13	9.244	1332	1338	1345	rBV	23815	35142	2.56%	0.538%
14	9.342	1350	1354	1359	rBV	62098	83718	6.09%	1.281%
15	9.488	1372	1378	1384	rBV	1036860	1374250	100.00%	21.034%
16	9.579	1388	1393	1405	rVB	119635	154483	11.24%	2.365%
17	9.915	1442	1448	1460	rBV	668015	817141	59.46%	12.507%
18	10.055	1463	1471	1478	rBV	318401	424517	30.89%	6.498%
19	10.640	1562	1567	1574	rBV	24760	30554	2.22%	0.468%
20	11.085	1634	1640	1649	rBV	261962	350432	25.50%	5.364%
21	12.024	1789	1794	1805	rBV	307093	371372	27.02%	5.684%

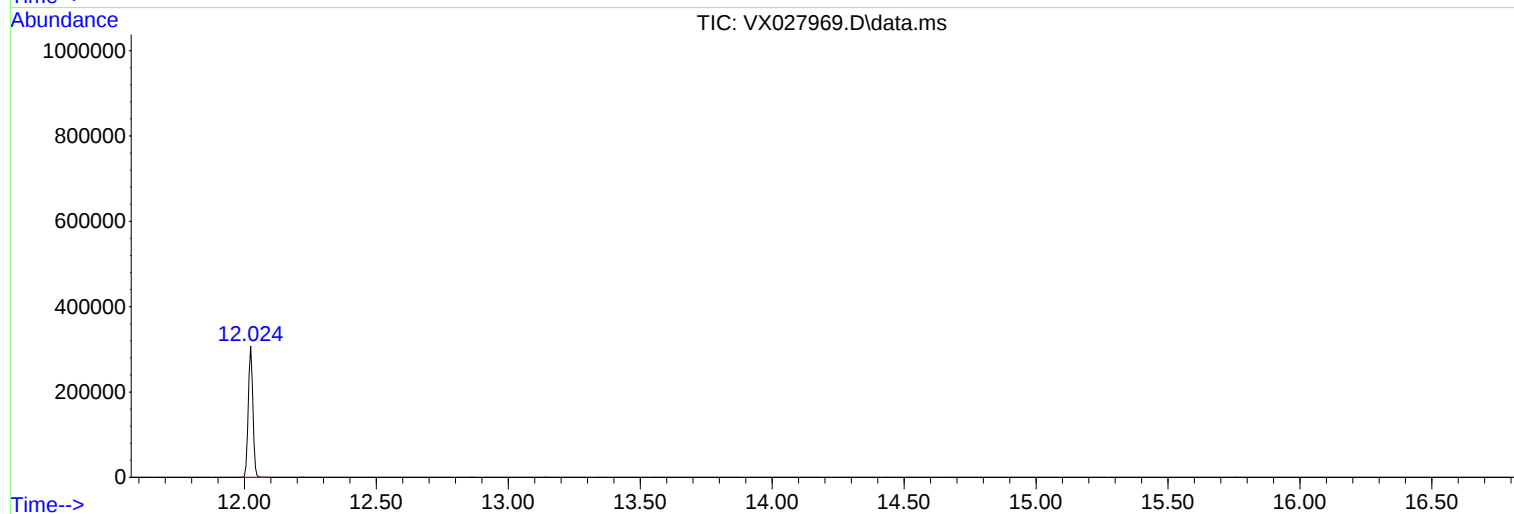
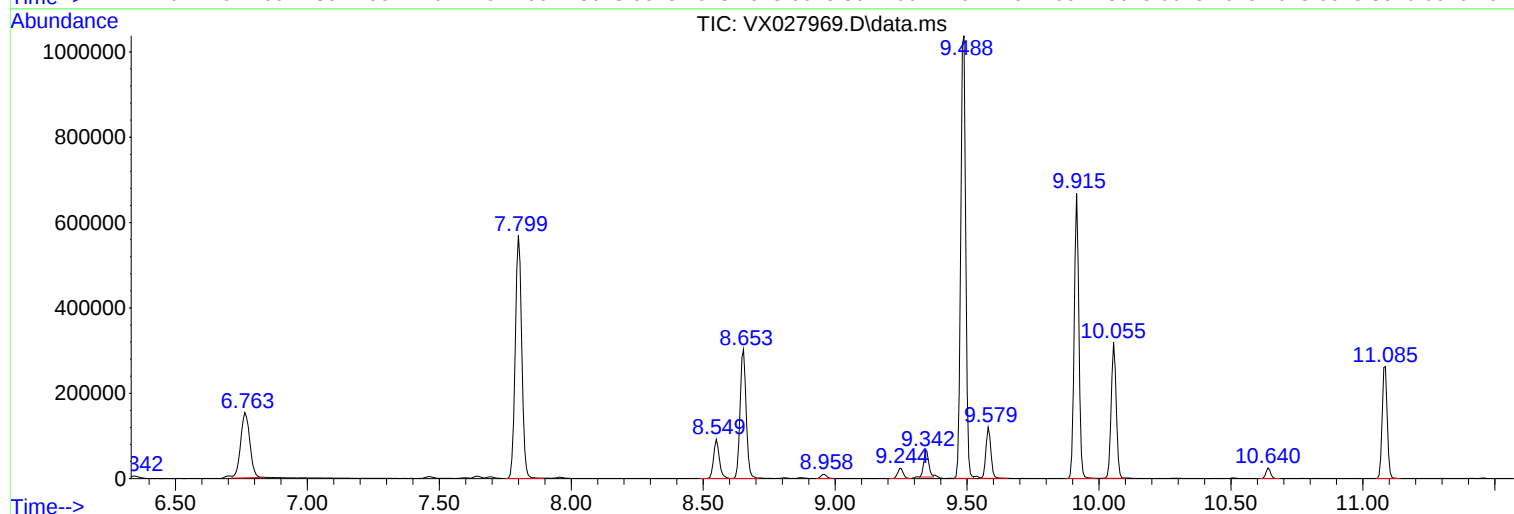
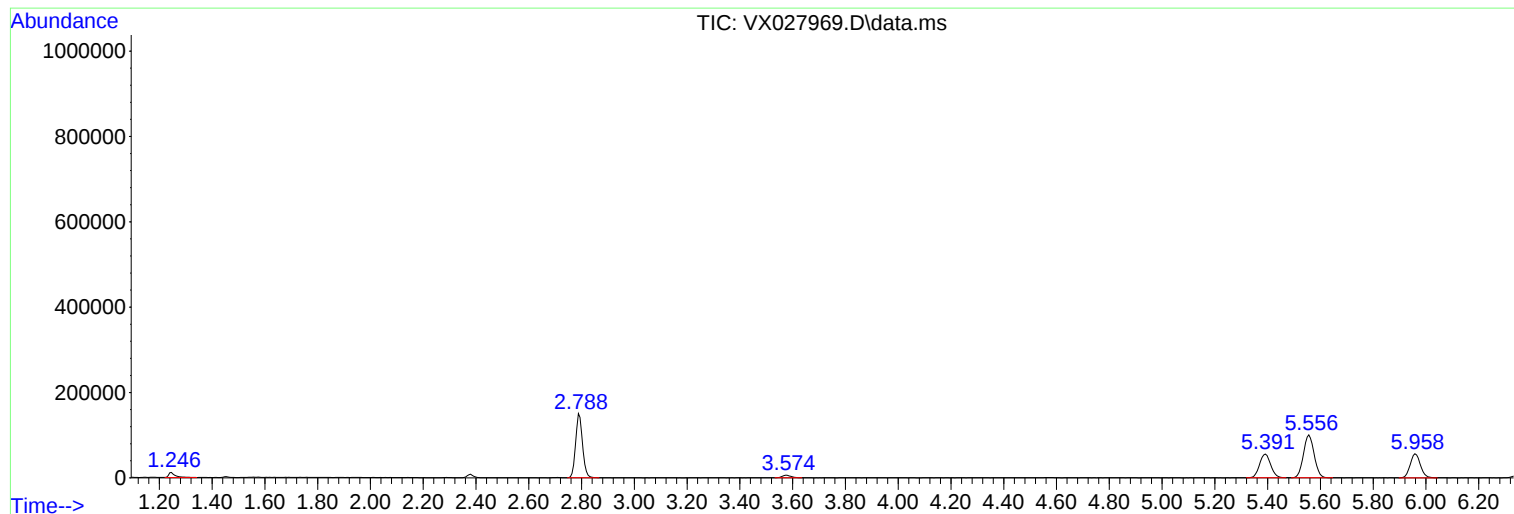
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Quant Title : SW846 8260

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



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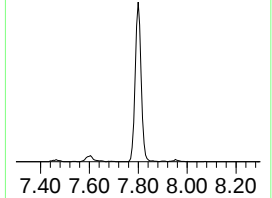
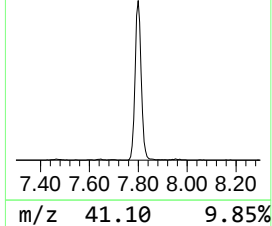
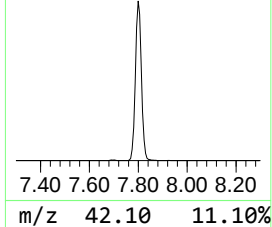
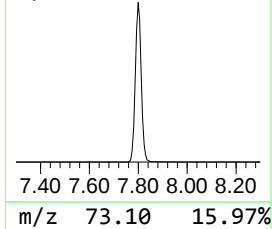
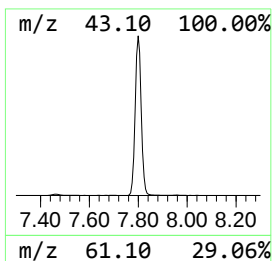
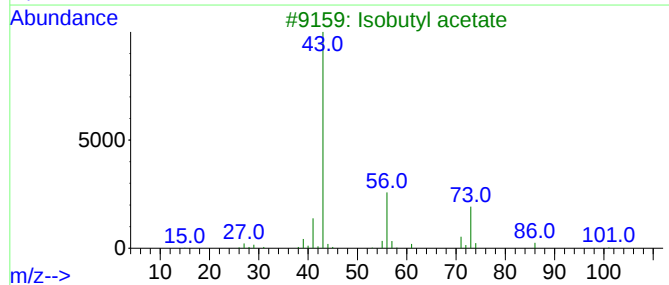
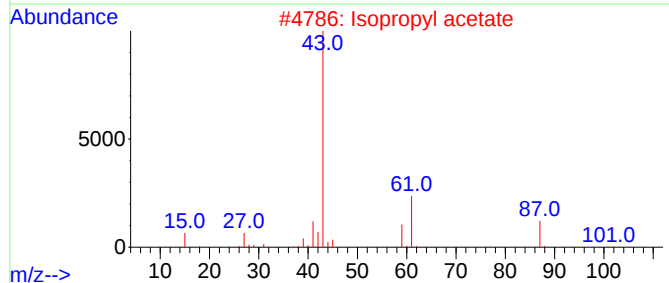
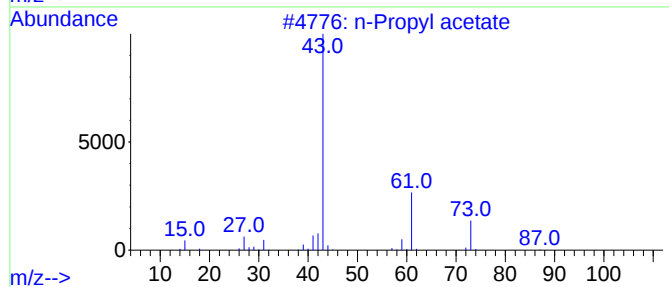
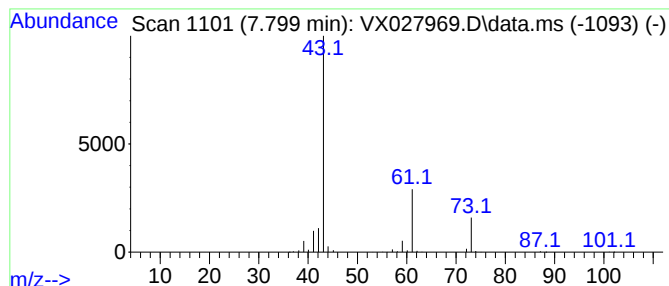
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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	132.76 ug/l	972970	1,4-Difluorobenzene	6.763

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		Isobutyl acetate	116	C6H12O2	000110-19-0	9
4		Isobutylamine	73	C4H11N	000078-81-9	7
5		1-Butanamine	73	C4H11N	000109-73-9	5



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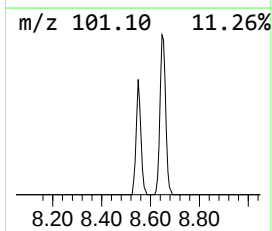
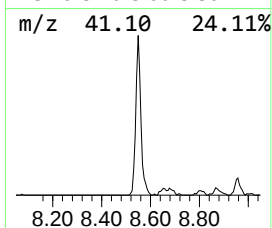
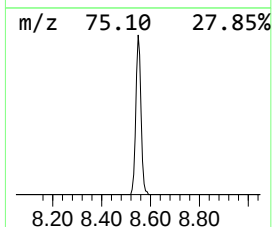
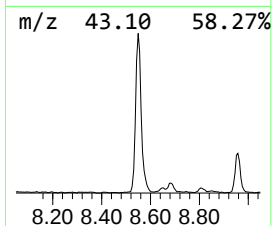
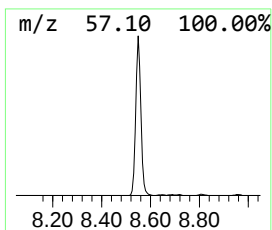
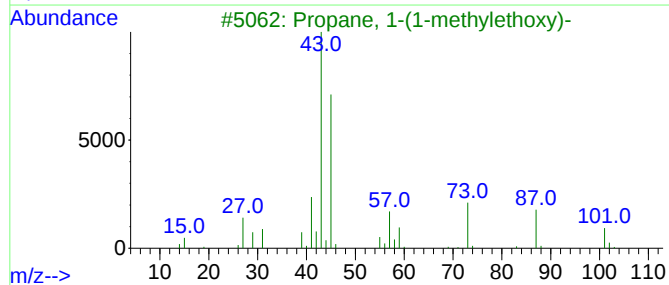
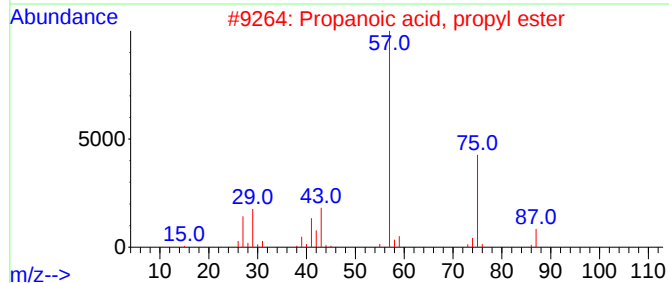
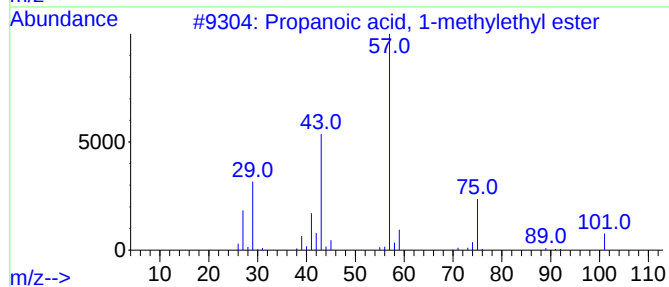
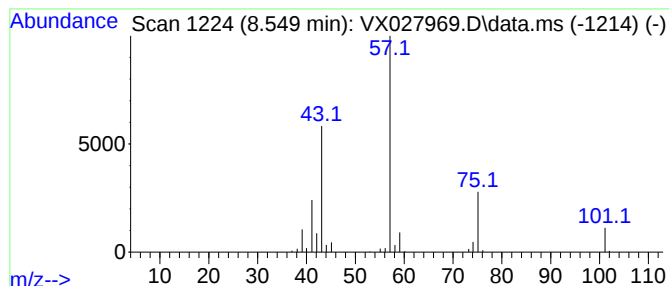
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	16.38 ug/l	139080	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			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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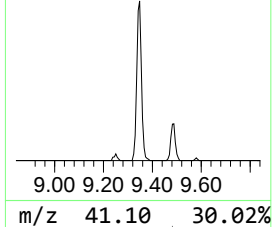
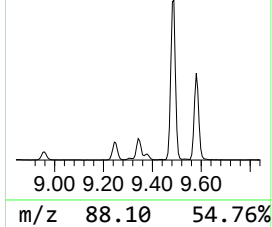
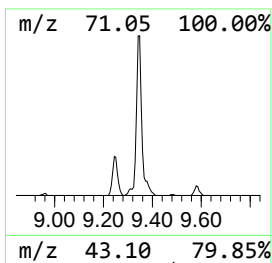
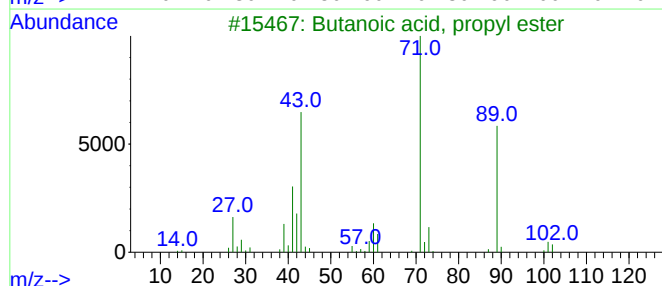
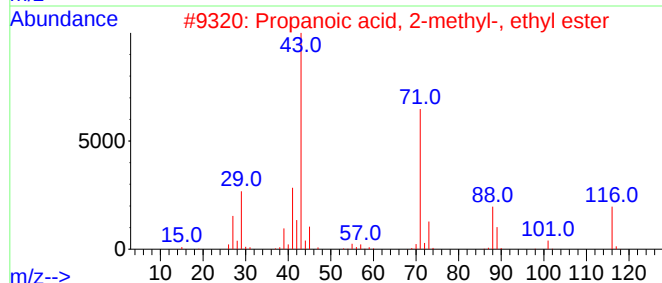
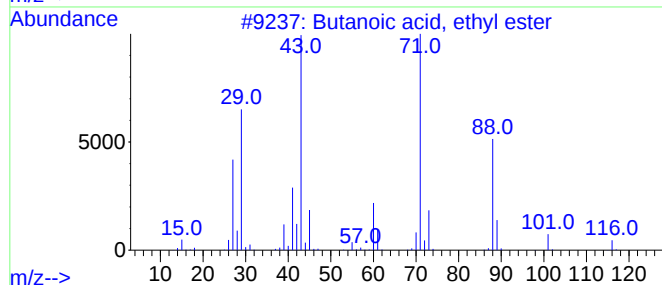
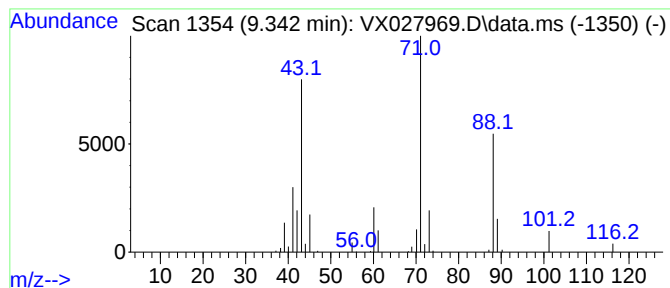
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	9.86 ug/l	83718	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			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	59
3			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	53
4			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	38
5			4-Butoxy-2-butanone	144	C8H16O2	030536-44-8	28



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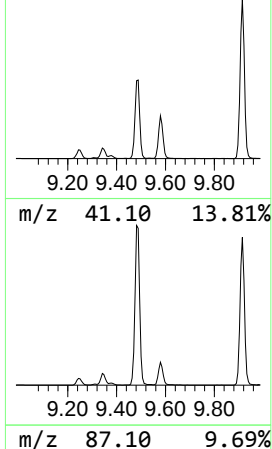
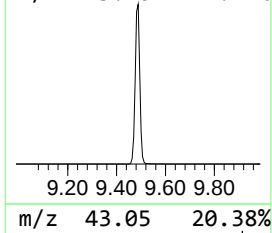
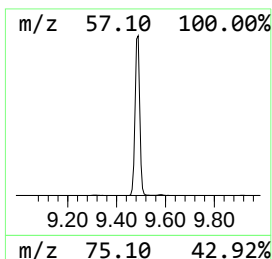
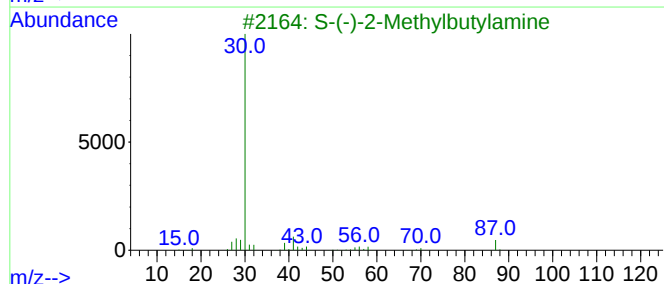
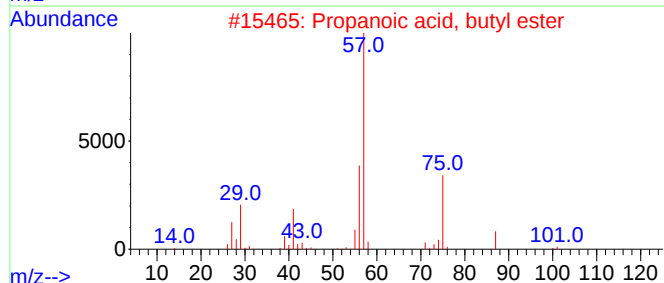
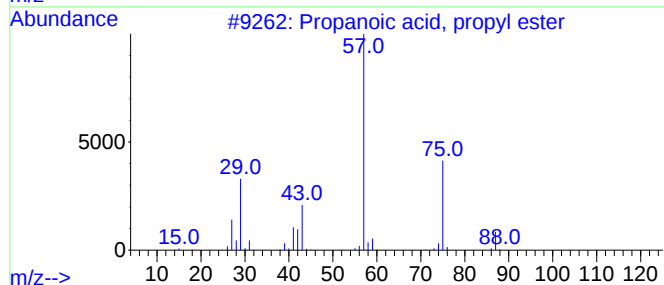
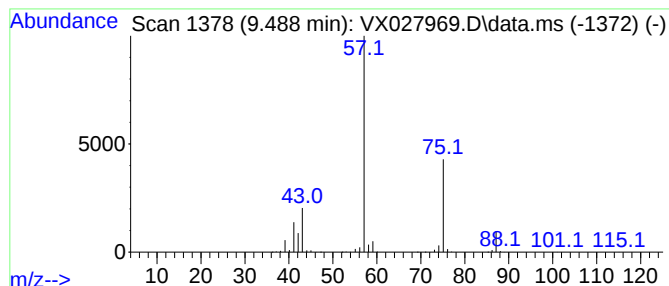
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.488	161.86 ug/l	1374250	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	40
3			S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	9
4			Isobutyl ether	130	C8H18O	000628-55-7	9
5			2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9



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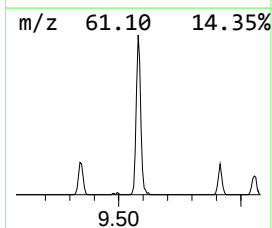
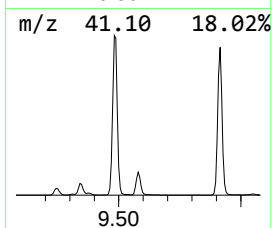
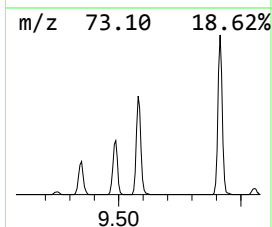
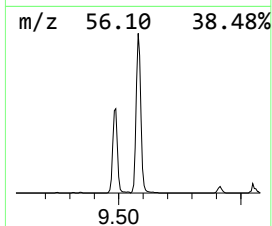
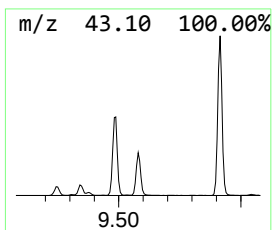
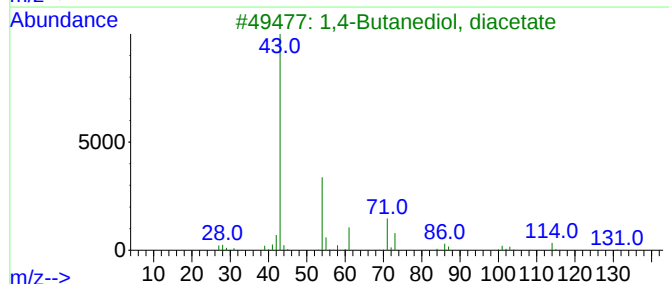
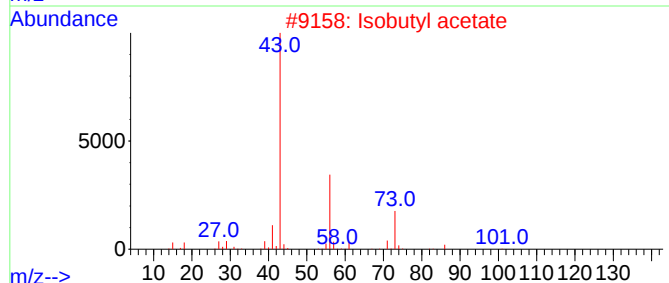
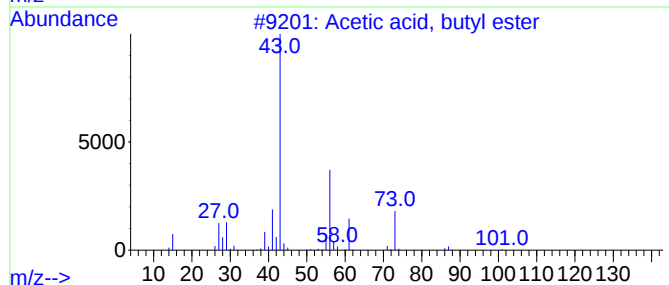
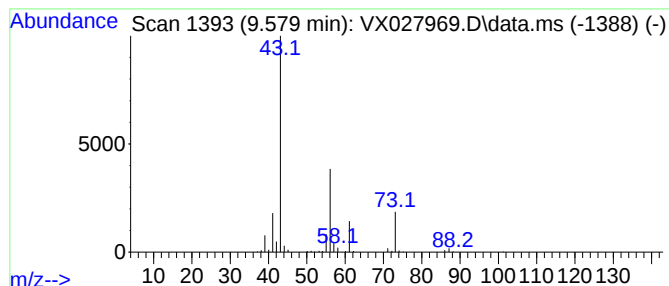
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.579	18.20 ug/l	154483	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			1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	17
4			Isobutylamine	73	C4H11N	000078-81-9	9
5			Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9



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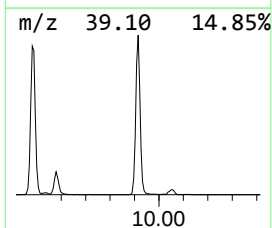
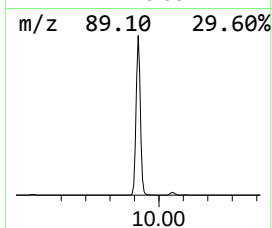
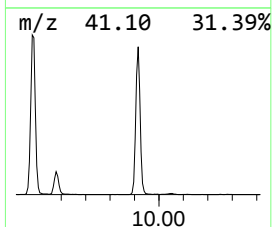
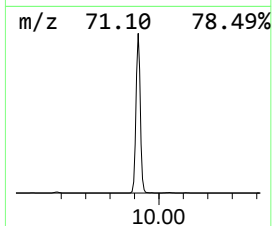
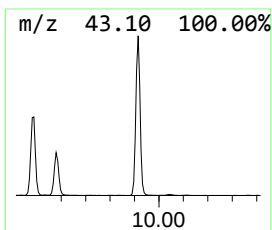
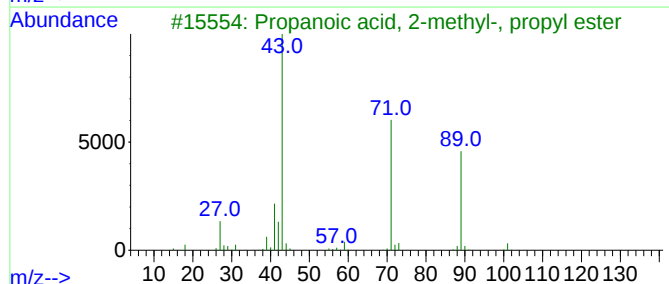
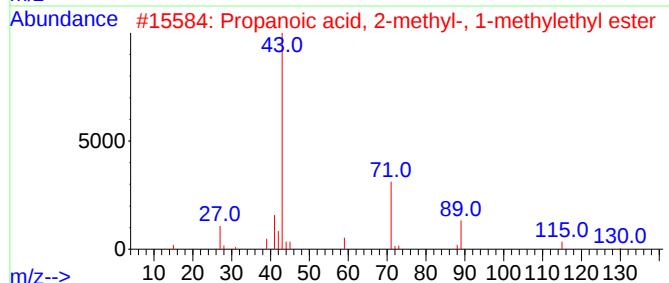
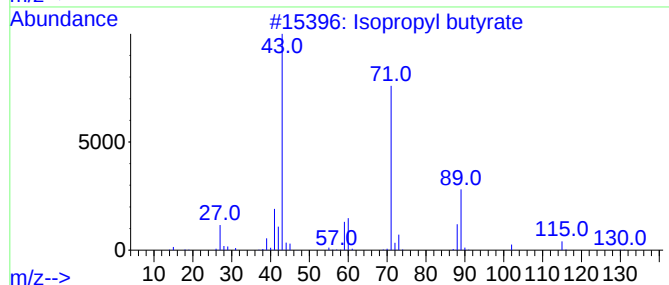
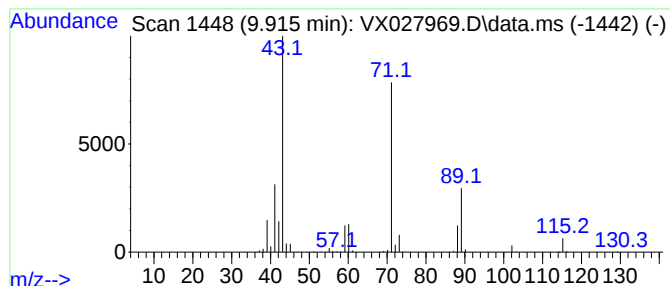
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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	96.24 ug/l	817141	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	94
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, butyl ester	144	C8H16O2	000109-21-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027969.D
Acq On : 04 Apr 2022 19:40
Operator : JC/MD
Sample : PB143824ZHE#06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB143824ZHE#06

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.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	132.8	ug/l	972970	2	6.763	366453	50.0
Propanoic acid,...	8.549	16.4	ug/l	139080	3	10.055	424517	50.0
Butanoic acid, ...	9.342	9.9	ug/l	83718	3	10.055	424517	50.0
Propanoic acid,...	9.488	161.9	ug/l	1374250	3	10.055	424517	50.0
Acetic acid, bu...	9.579	18.2	ug/l	154483	3	10.055	424517	50.0
Isopropyl butyrate	9.915	96.2	ug/l	817141	3	10.055	424517	50.0