

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110521\
 Data File : VU045594.D
 Acq On : 06 Nov 2021 05:34
 Operator : SY/MD
 Sample : M4472-07
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 49 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 WC-2-KD

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_U\Method\82U110521W.M
 Title : SW846 8260

Signal : TIC: VU045594.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.292	1214	1229	1243	rBV	122970	260510	9.34%	2.231%
2	5.378	1243	1256	1272	rVB	183247	376213	13.48%	3.221%
3	5.706	1343	1358	1376	rBV	139784	281147	10.08%	2.407%
4	5.912	1409	1422	1438	rBV3	14676	29223	1.05%	0.250%
5	6.076	1454	1473	1477	rBV4	13161	43657	1.56%	0.374%
6	6.253	1515	1528	1564	rVB	301282	610515	21.88%	5.227%
7	6.925	1719	1737	1752	rVB3	11661	34776	1.25%	0.298%
8	7.041	1758	1773	1804	rBV	1085832	1877169	67.27%	16.073%
9	7.738	1972	1990	2003	rBV	157065	263926	9.46%	2.260%
10	7.899	2025	2040	2068	rBV	470531	831771	29.81%	7.122%
11	8.468	2205	2217	2233	rBV2	39141	67521	2.42%	0.578%
12	8.574	2233	2250	2261	rVV	105464	179911	6.45%	1.540%
13	8.729	2282	2298	2320	rVV	1794368	2790502	100.00%	23.893%
14	8.835	2321	2331	2358	rVB	188097	301651	10.81%	2.583%
15	9.211	2430	2448	2480	rBV	1070403	1635273	58.60%	14.002%
16	9.420	2501	2513	2538	rVB	448780	742992	26.63%	6.362%
17	10.073	2705	2716	2727	rBV	34370	51119	1.83%	0.438%
18	10.632	2879	2890	2914	rBV	344803	551113	19.75%	4.719%
19	11.812	3245	3257	3274	rBV	482909	750080	26.88%	6.422%

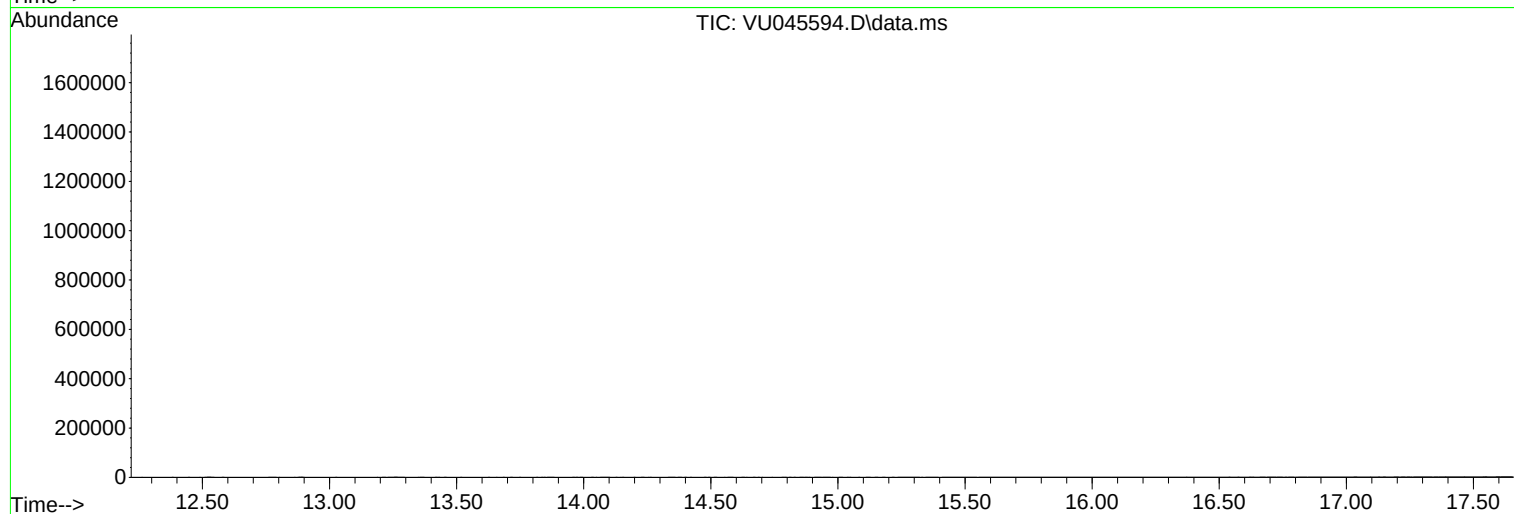
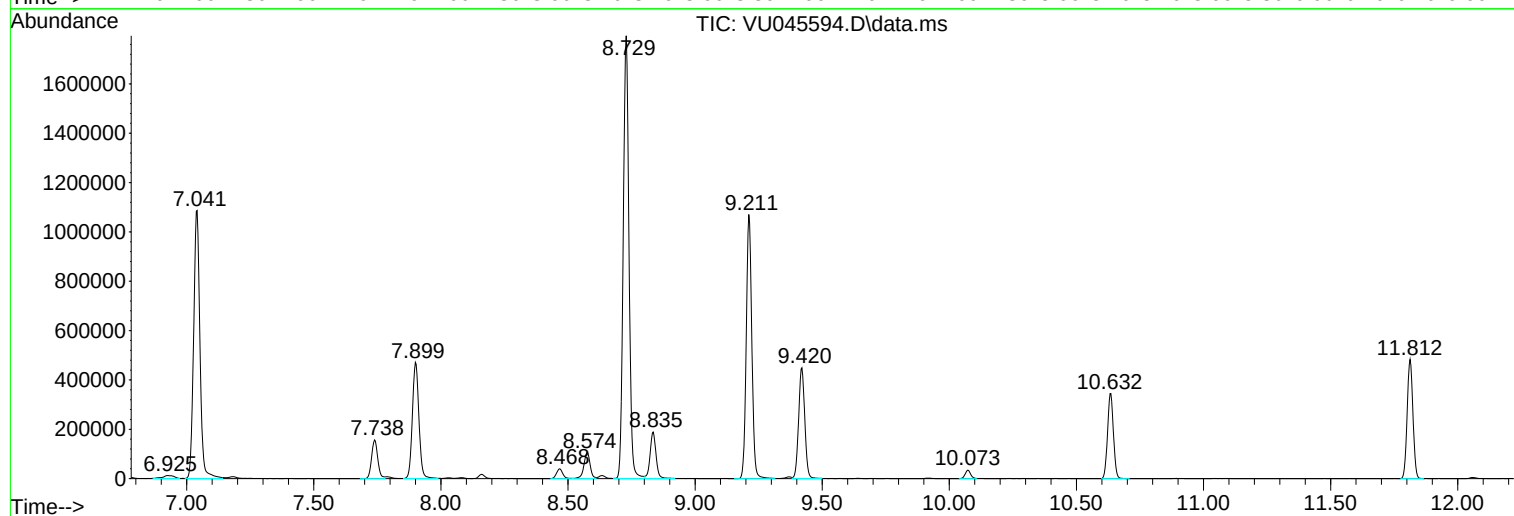
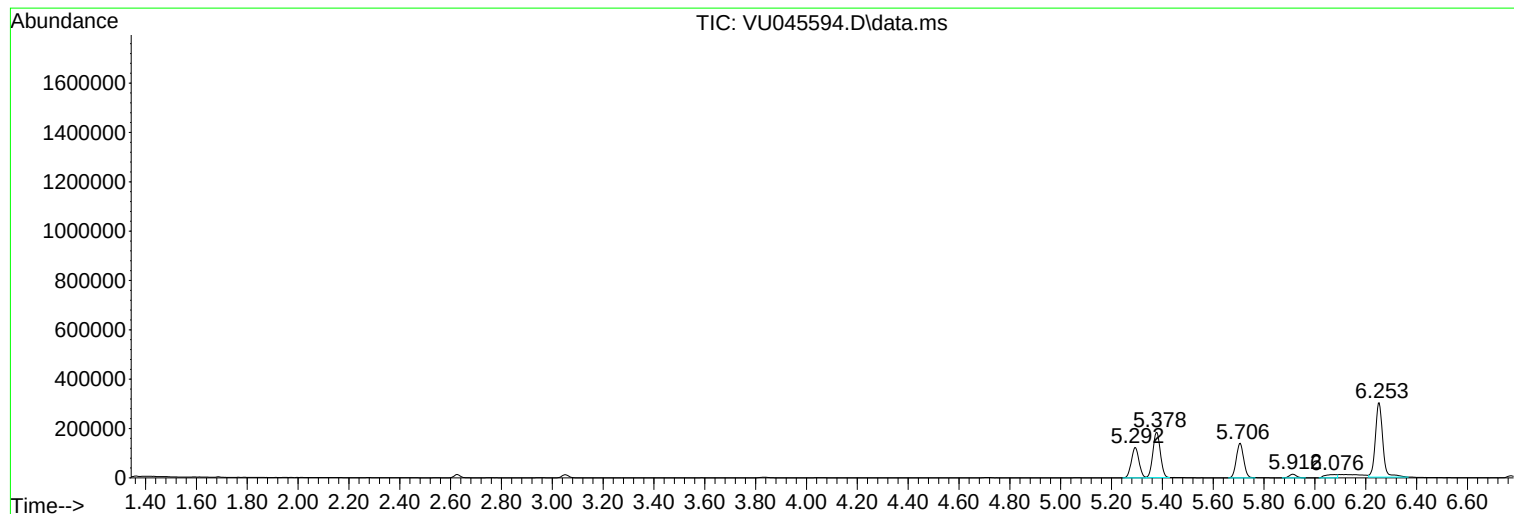
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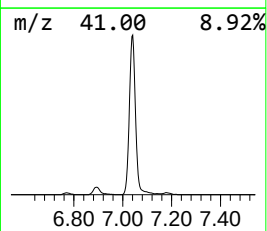
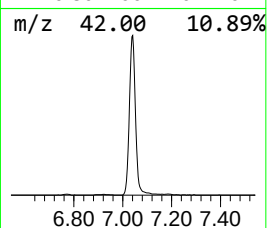
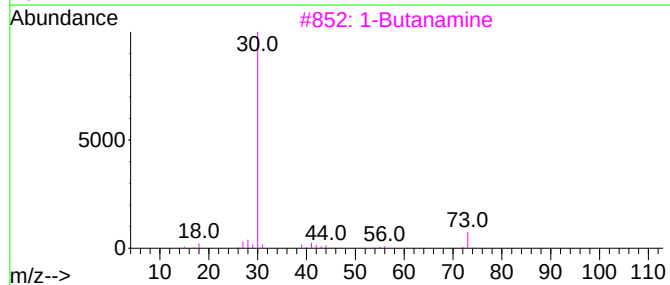
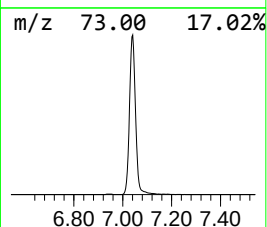
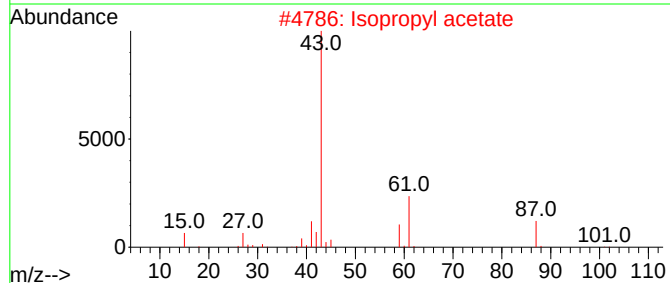
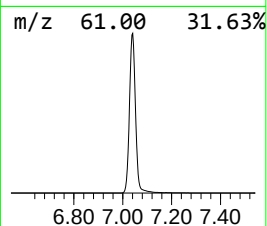
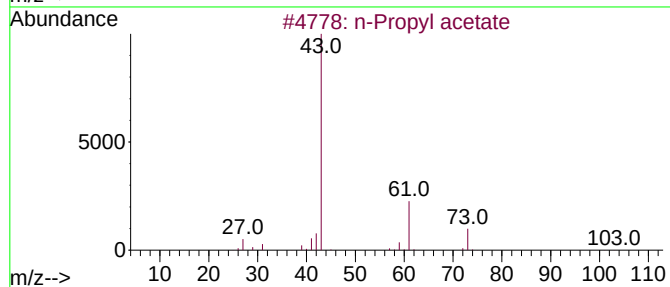
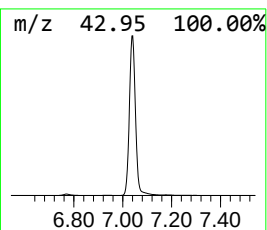
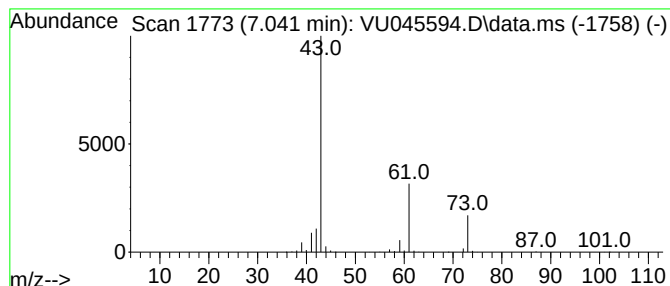
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.M
Quant Title : SW846 8260

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.
7.041	153.74 ug/l	1877170	1,4-Difluorobenzene	6.253

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	4
5			N-Acetyllethylenediamine	102	C4H10N2O	001001-53-2	4



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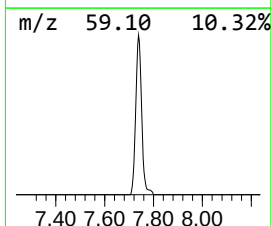
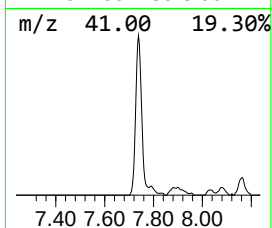
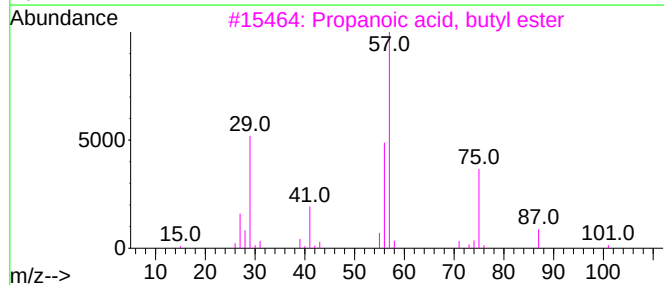
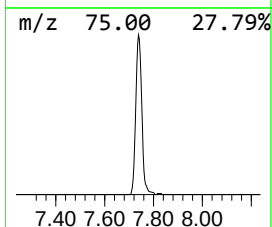
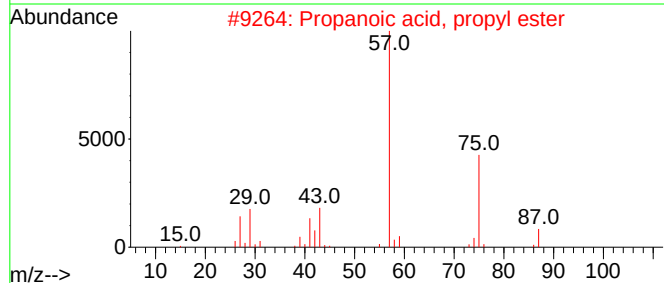
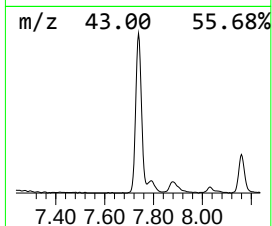
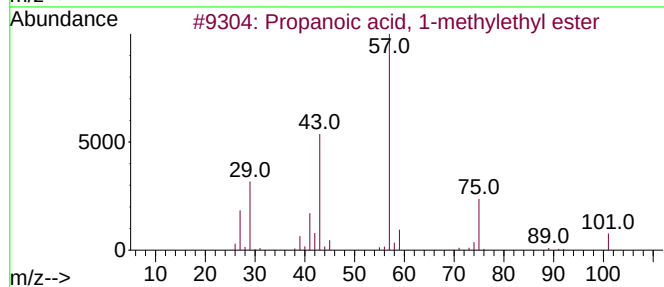
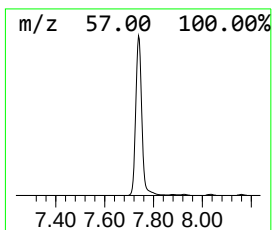
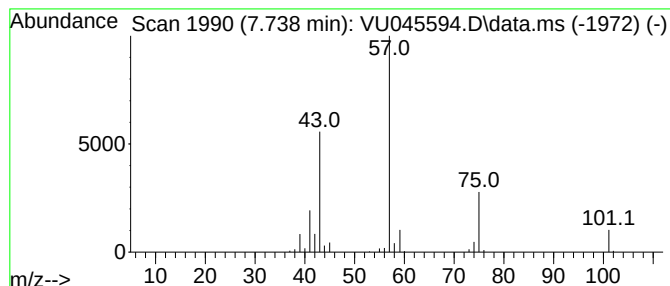
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.738	21.61 ug/l	263926	1,4-Difluorobenzene	6.253

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			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	25
4			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
5			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10



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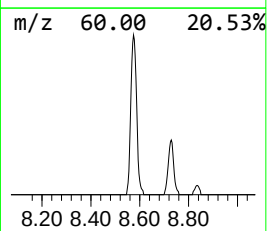
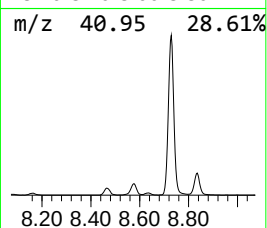
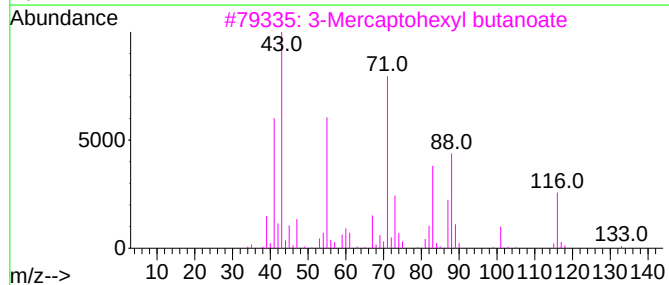
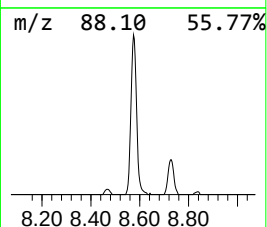
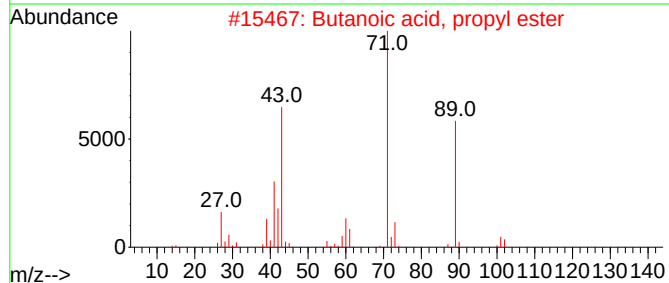
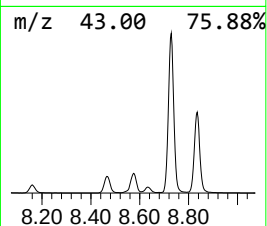
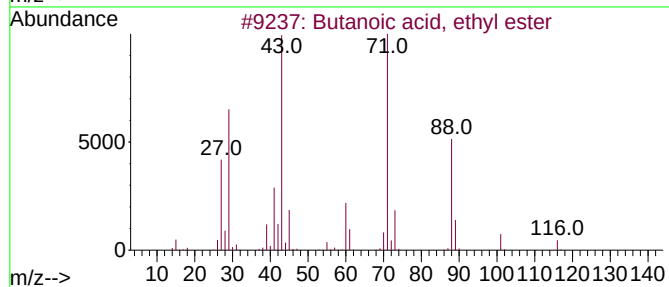
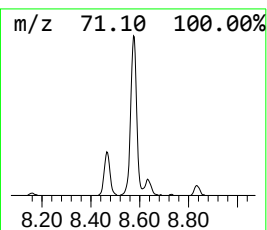
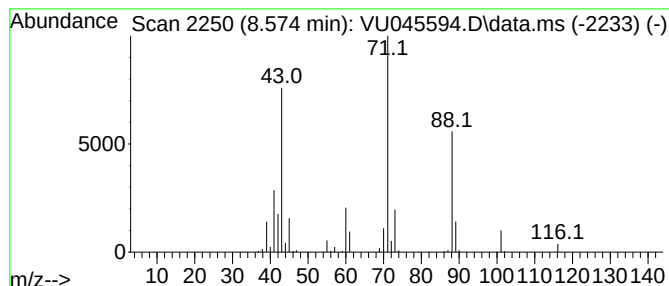
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Quant Title : SW846 8260

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Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.574	12.11 ug/l	179911	Chlorobenzene-d5	9.420

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			3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	45
4			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	40
5			Butanoic acid, 2-methylbutyl ester	158	C9H18O2	051115-64-1	37



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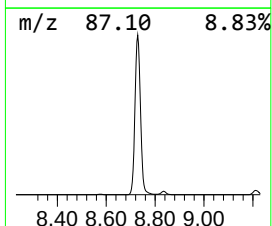
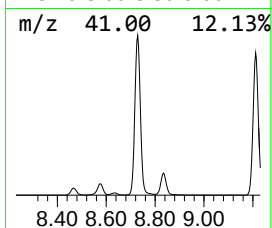
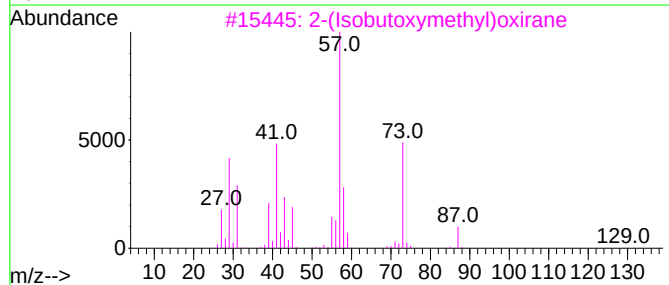
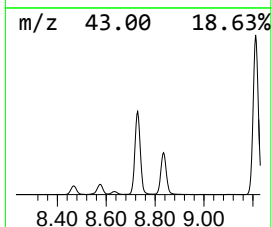
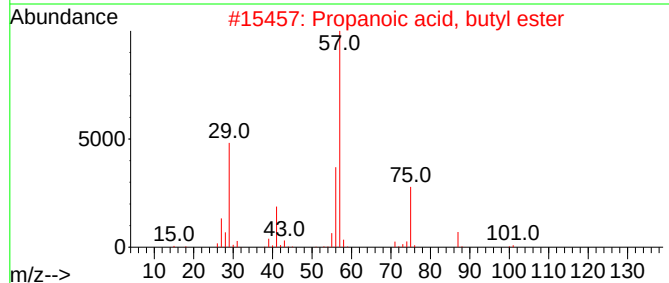
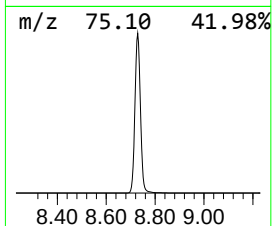
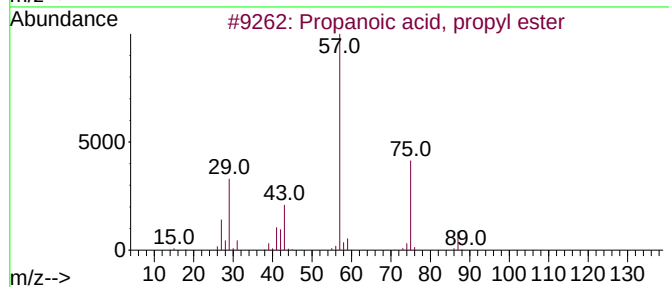
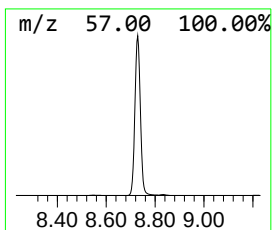
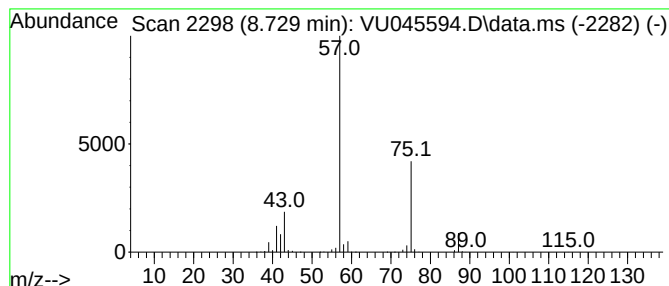
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.729	187.79 ug/l	2790500	Chlorobenzene-d5	9.420

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	28
3			2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5			1-Penten-3-ol	86	C5H10O	000616-25-1	7



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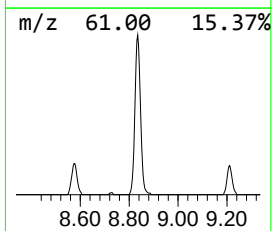
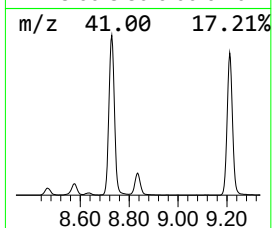
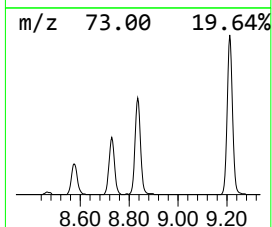
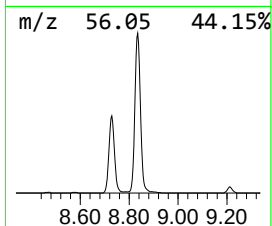
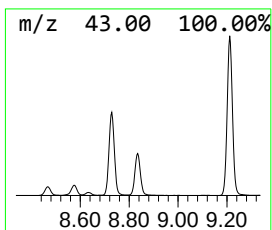
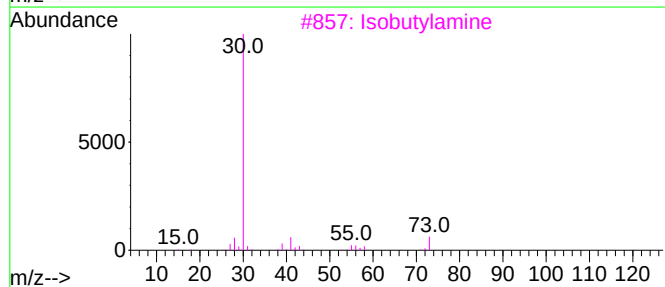
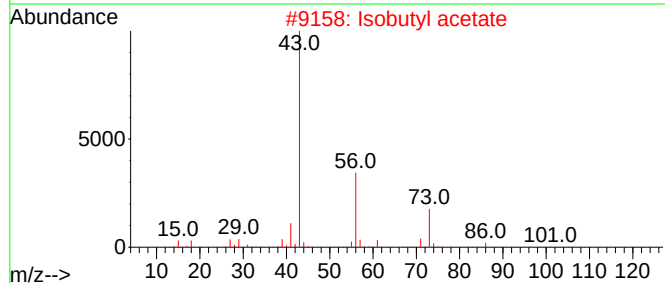
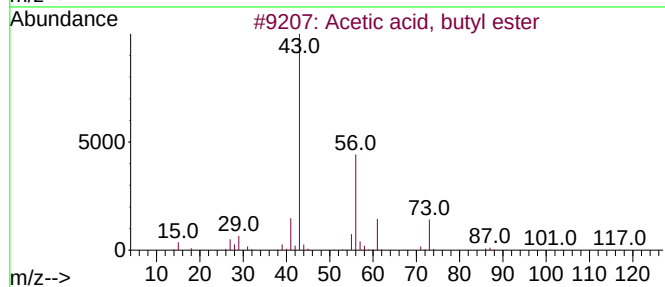
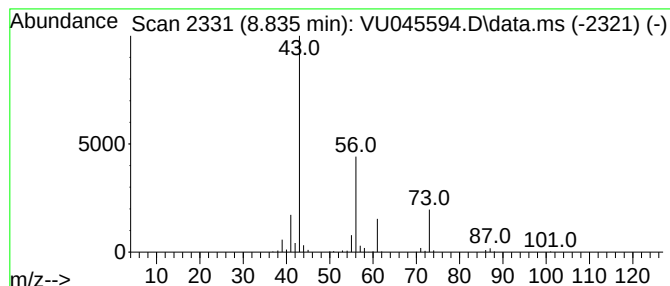
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Peak Number 5 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.835	20.30 ug/l	301651	Chlorobenzene-d5	9.420

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			Isobutylamine	73	C4H11N	000078-81-9	9
4			2-Pentanone	86	C5H10O	000107-87-9	9
5			Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	9



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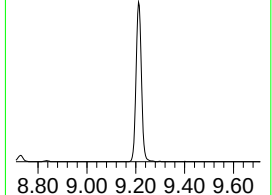
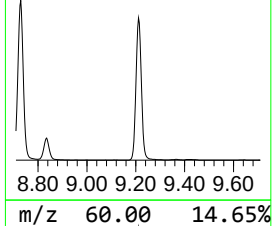
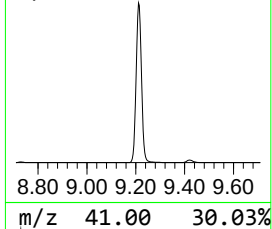
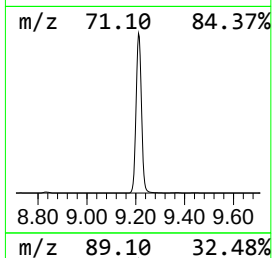
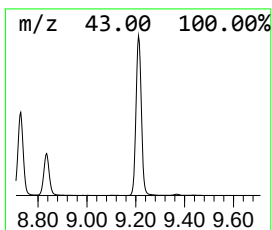
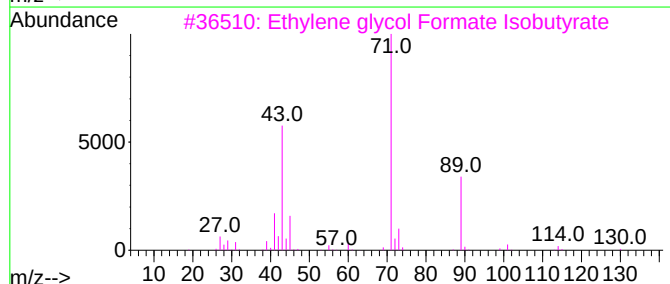
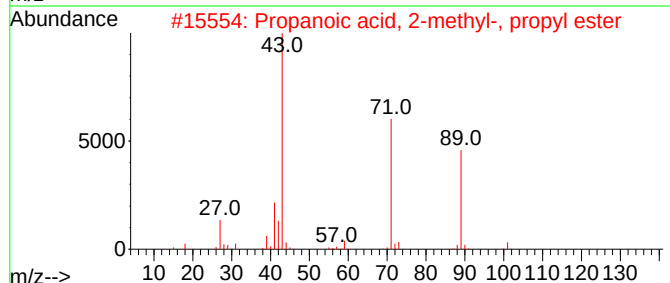
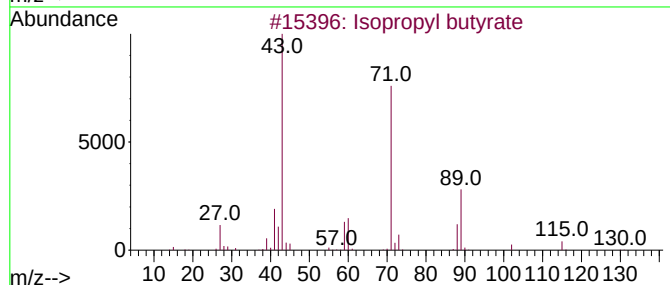
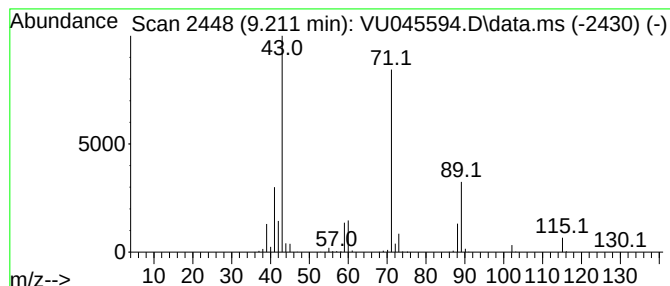
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.M
Quant Title : SW846 8260

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.
9.211	110.05 ug/l	1635270	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	94
2			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3			Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
4			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
5			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110521\
Data File : VU045594.D
Acq On : 06 Nov 2021 05:34
Operator : SY/MD
Sample : M4472-07
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
WC-2-KD

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.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	7.041	153.7	ug/l	1877170	2	6.253	610515	50.0
Propanoic acid,...	7.738	21.6	ug/l	263926	2	6.253	610515	50.0
Butanoic acid, ...	8.574	12.1	ug/l	179911	3	9.420	742992	50.0
Propanoic acid,...	8.729	187.8	ug/l	2790500	3	9.420	742992	50.0
Acetic acid, bu...	8.835	20.3	ug/l	301651	3	9.420	742992	50.0
Isopropyl butyrate	9.211	110.1	ug/l	1635270	3	9.420	742992	50.0