

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012521\
 Data File : VN065582.D
 Acq On : 25 Jan 2021 17:22
 Operator : JC/MD
 Sample : PB134285ZHE#02
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 PB134285ZHE#02

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_N\methods\82N012521W.M

Title : SW846 8260

Signal : TIC: VN065582.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.499	841	858	879	rBV2	17200	51437	1.89%	0.396%
2	7.550	1789	1807	1818	rBV	129374	323942	11.89%	2.492%
3	7.624	1818	1830	1854	rVB	253872	598853	21.98%	4.606%
4	7.987	1926	1943	1962	rBV2	156447	365563	13.42%	2.812%
5	8.129	1975	1987	2004	rVB2	15448	34338	1.26%	0.264%
6	8.550	2098	2118	2141	rBV	386890	818521	30.04%	6.296%
7	9.151	2291	2305	2317	rBV2	17607	37774	1.39%	0.291%
8	9.235	2317	2331	2362	rVV	970388	1816819	66.69%	13.975%
9	9.872	2516	2529	2546	rBV	181704	314987	11.56%	2.423%
10	10.058	2573	2587	2612	rVB	615758	1134071	41.63%	8.723%
11	10.251	2637	2647	2657	rBV	19241	30935	1.14%	0.238%
12	10.515	2714	2729	2744	rBV	55031	92493	3.39%	0.711%
13	10.608	2745	2758	2774	rBV	113576	191814	7.04%	1.475%
14	10.733	2785	2797	2815	rVV	1672503	2724413	100.00%	20.956%
15	10.823	2815	2825	2849	rVB	174167	293352	10.77%	2.256%
16	11.138	2909	2923	2942	rBV	1194008	1883346	69.13%	14.487%
17	11.376	2983	2997	3018	rBV	523087	910683	33.43%	7.005%
18	11.849	3134	3144	3160	rBV	40287	65142	2.39%	0.501%
19	12.373	3294	3307	3335	rVB	367307	627499	23.03%	4.827%
20	13.315	3586	3600	3625	rBV	396464	684449	25.12%	5.265%

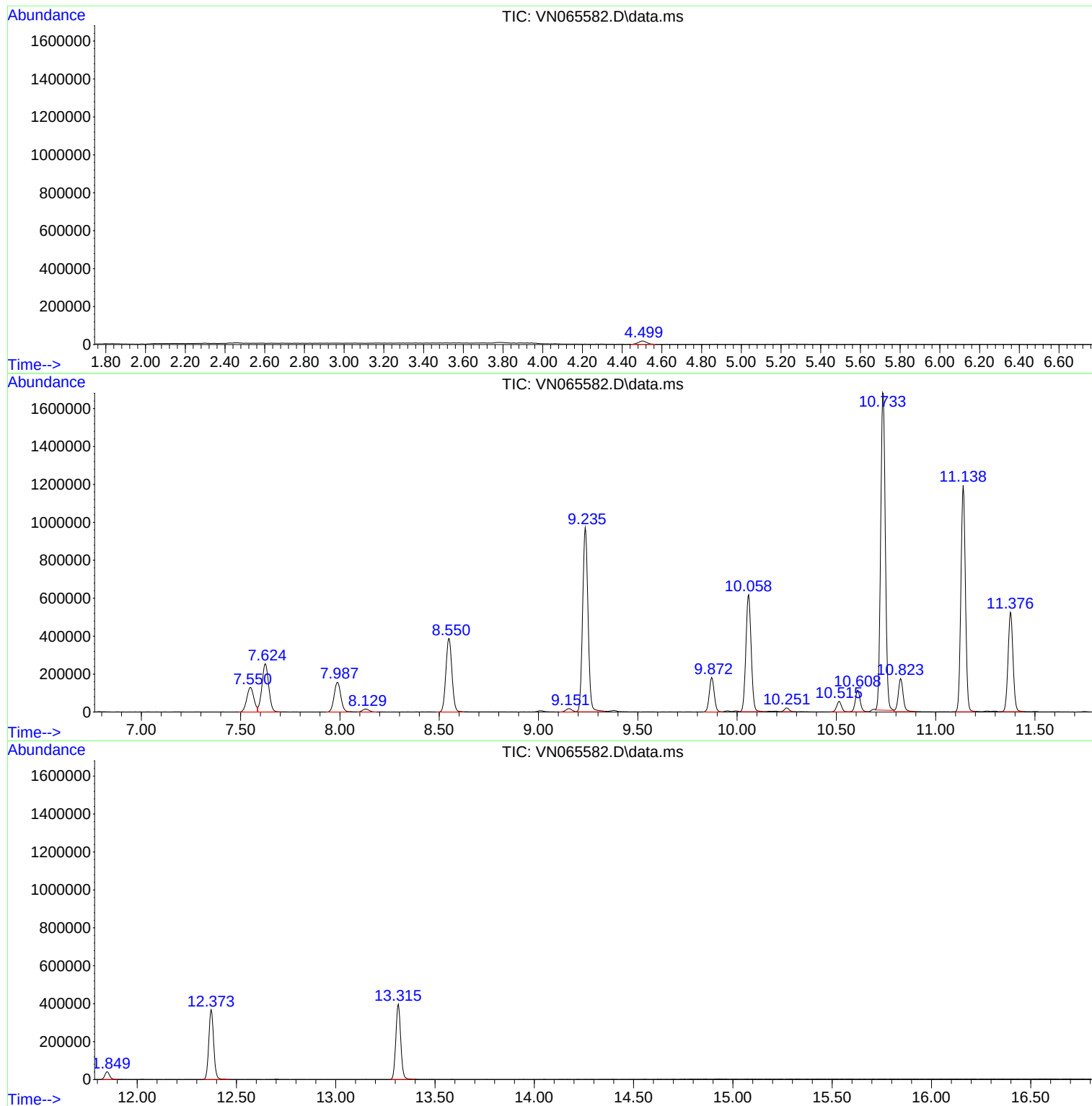
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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



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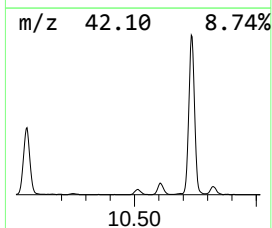
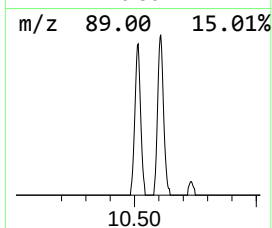
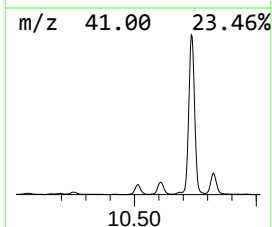
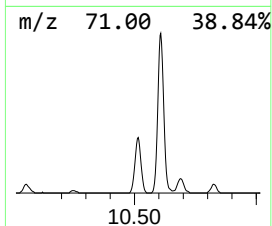
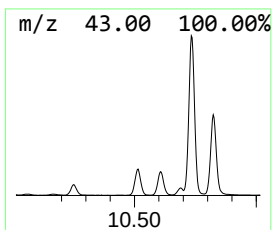
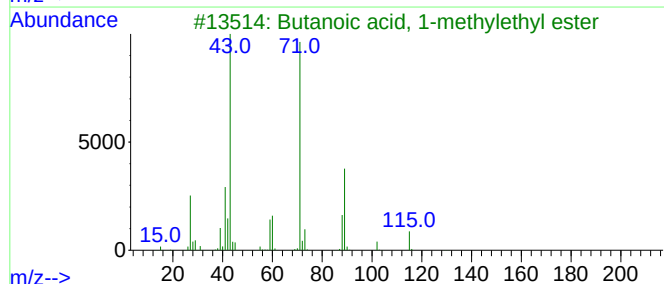
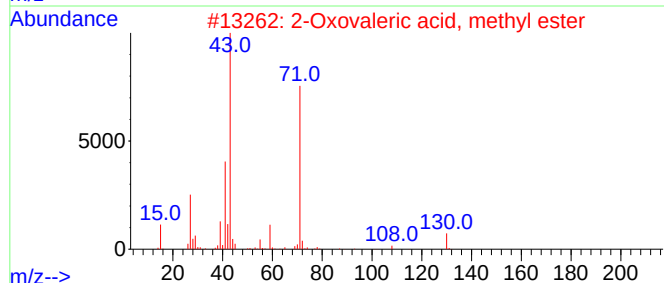
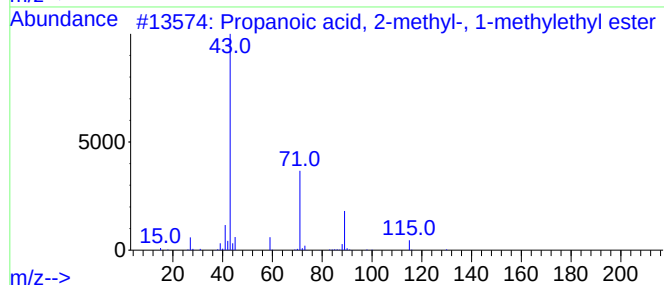
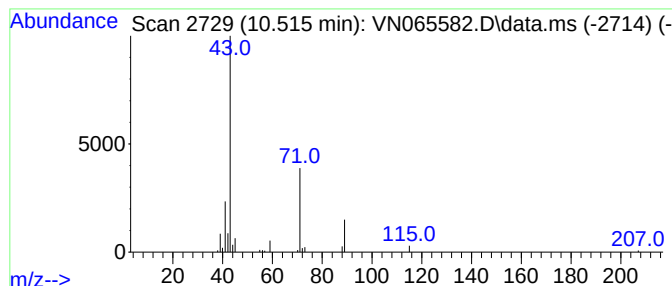
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.515	5.08 ug/l	92493	Chlorobenzene-d5	11.376

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2			2-Oxovaleric acid, methyl ester	130	C6H10O3	1000353-27-4	42
3			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	39
4			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	38
5			Cyanoic acid, ethyl ester	71	C3H5NO	000627-48-5	9



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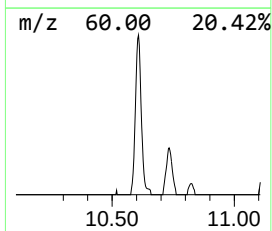
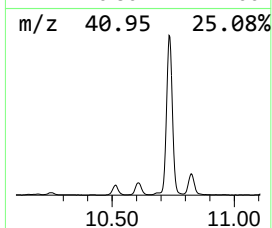
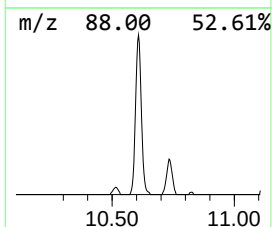
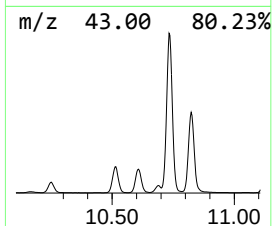
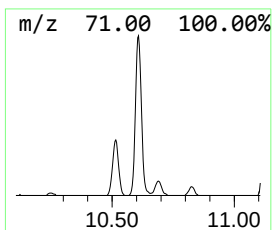
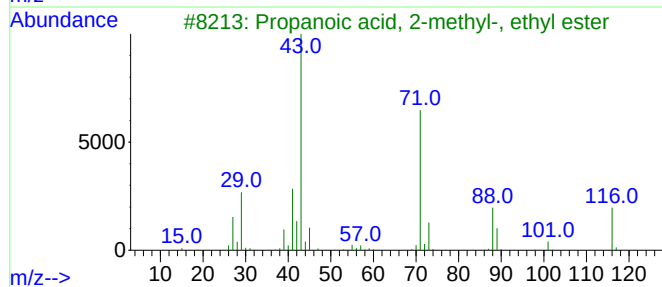
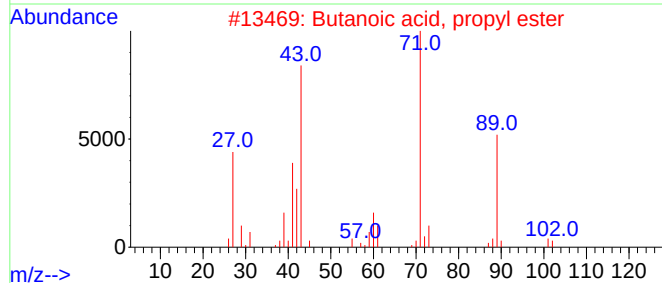
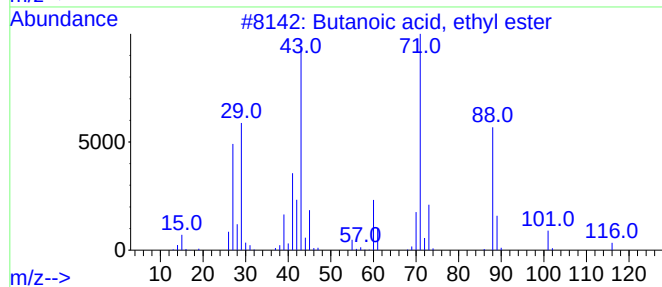
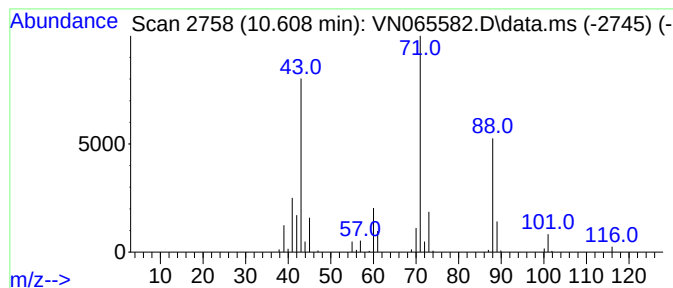
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Quant Title : SW846 8260

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

Peak Number 2 Butanoic acid, ethyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.608	10.53 ug/l	191814	Chlorobenzene-d5	11.376

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	95
2			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50
3			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	42
4			Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	38
5			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	35



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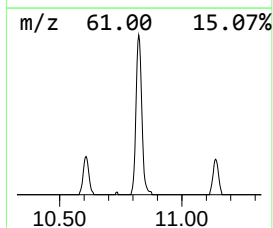
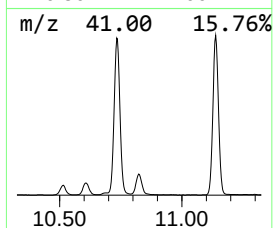
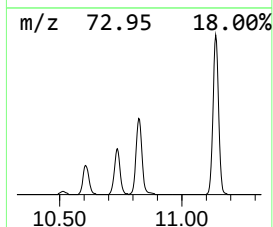
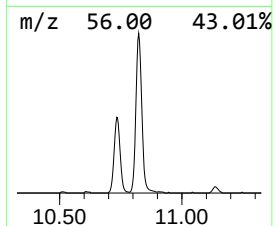
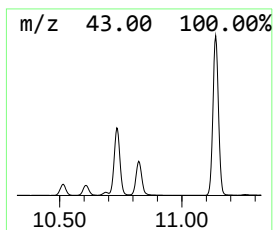
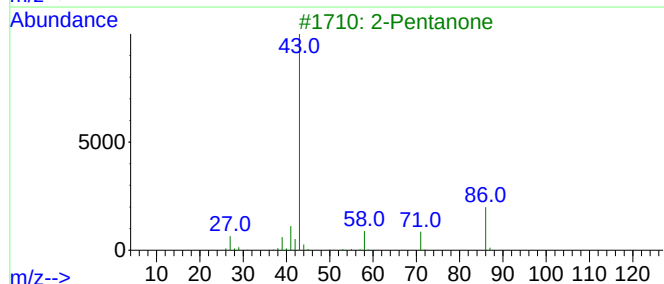
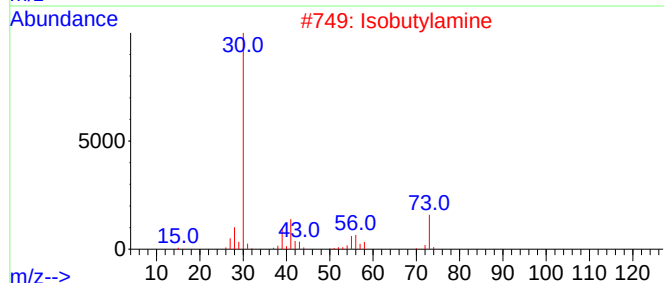
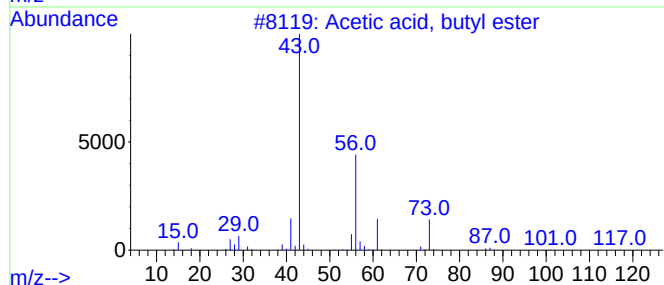
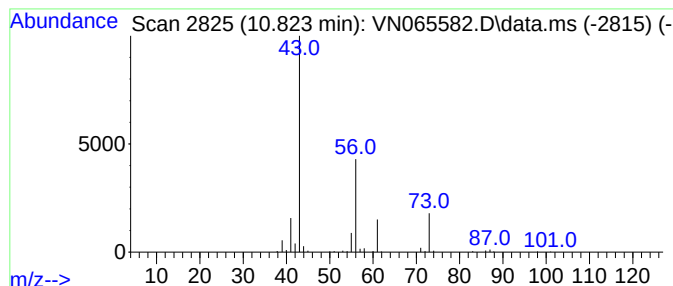
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Peak Number 3 Acetic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.823	16.11 ug/l	293352	Chlorobenzene-d5	11.376

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2			Isobutylamine	73	C4H11N	000078-81-9	9
3			2-Pentanone	86	C5H10O	000107-87-9	9
4			Isopropyl acetate	102	C5H10O2	000108-21-4	9
5			1-Propanol, 3-chloro-, acetate	136	C5H9ClO2	000628-09-1	9



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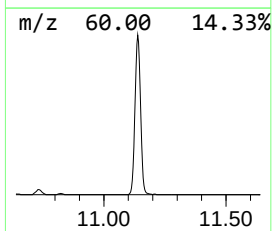
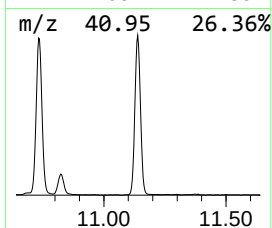
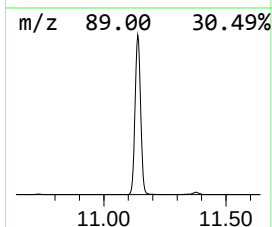
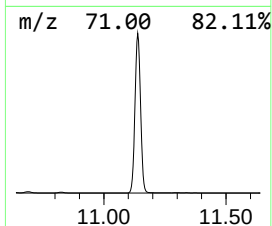
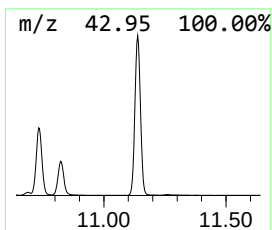
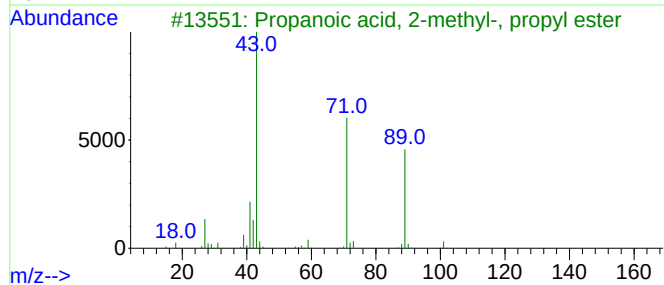
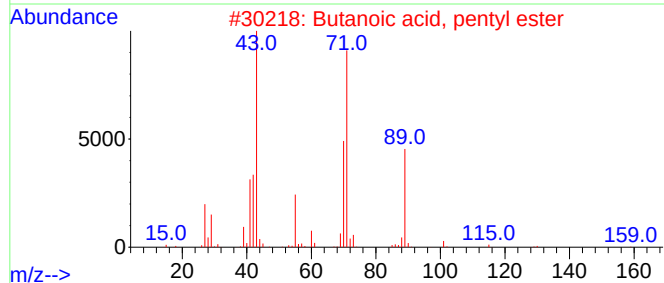
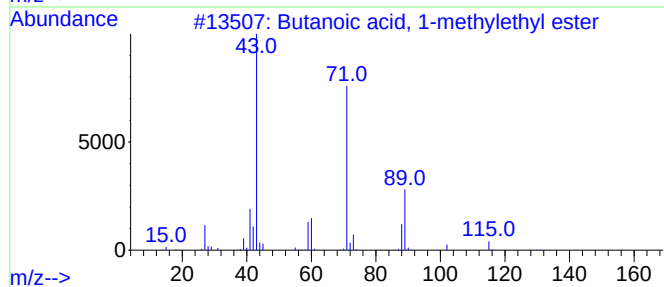
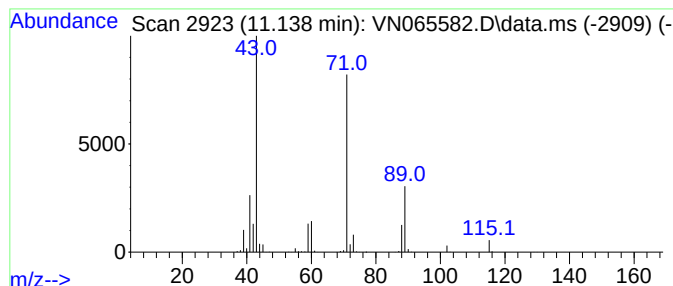
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Peak Number 4 Butanoic acid, 1-methylethy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.139	103.40 ug/l	1883350	Chlorobenzene-d5	11.376

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	95
2			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
3			Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	56
4			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	45
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	45



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	10.515	5.1	ug/l	92493	3	11.376	910683	50.0
Butanoic acid, ...	10.608	10.5	ug/l	191814	3	11.376	910683	50.0
Acetic acid, bu...	10.823	16.1	ug/l	293352	3	11.376	910683	50.0
Butanoic acid, ...	11.139	103.4	ug/l	1883350	3	11.376	910683	50.0