

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012521\
 Data File : VN065580.D
 Acq On : 25 Jan 2021 16:33
 Operator : JC/MD
 Sample : PB134285TB
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 PB134285TB

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: VN065580.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.502	842	859	877	rVB2	16164	46847	1.70%	0.359%
2	7.550	1788	1807	1818	rBV2	127999	319242	11.60%	2.446%
3	7.624	1818	1830	1849	rVB	249645	594354	21.60%	4.554%
4	7.987	1926	1943	1963	rBV	155637	359323	13.06%	2.753%
5	8.129	1973	1987	2003	rVB2	15060	34540	1.26%	0.265%
6	8.547	2101	2117	2141	rBV	388914	812622	29.54%	6.226%
7	9.151	2291	2305	2316	rBV3	17492	38557	1.40%	0.295%
8	9.235	2316	2331	2367	rVV	1000881	1852048	67.31%	14.190%
9	9.871	2513	2529	2546	rBV	182215	316924	11.52%	2.428%
10	10.058	2573	2587	2606	rBV	614216	1119130	40.68%	8.575%
11	10.251	2637	2647	2661	rVB	18825	32471	1.18%	0.249%
12	10.515	2716	2729	2743	rBV	55555	93187	3.39%	0.714%
13	10.608	2743	2758	2773	rBV	113756	195441	7.10%	1.497%
14	10.733	2785	2797	2815	rVV	1703896	2751373	100.00%	21.081%
15	10.823	2815	2825	2847	rVB	173788	299869	10.90%	2.298%
16	11.138	2908	2923	2940	rBV	1184727	1886919	68.58%	14.457%
17	11.376	2981	2997	3018	rBV	512876	905351	32.91%	6.937%
18	11.849	3133	3144	3157	rBV	40325	65053	2.36%	0.498%
19	12.373	3294	3307	3336	rVB	366251	632758	23.00%	4.848%
20	13.315	3587	3600	3623	rBV	401151	695731	25.29%	5.331%

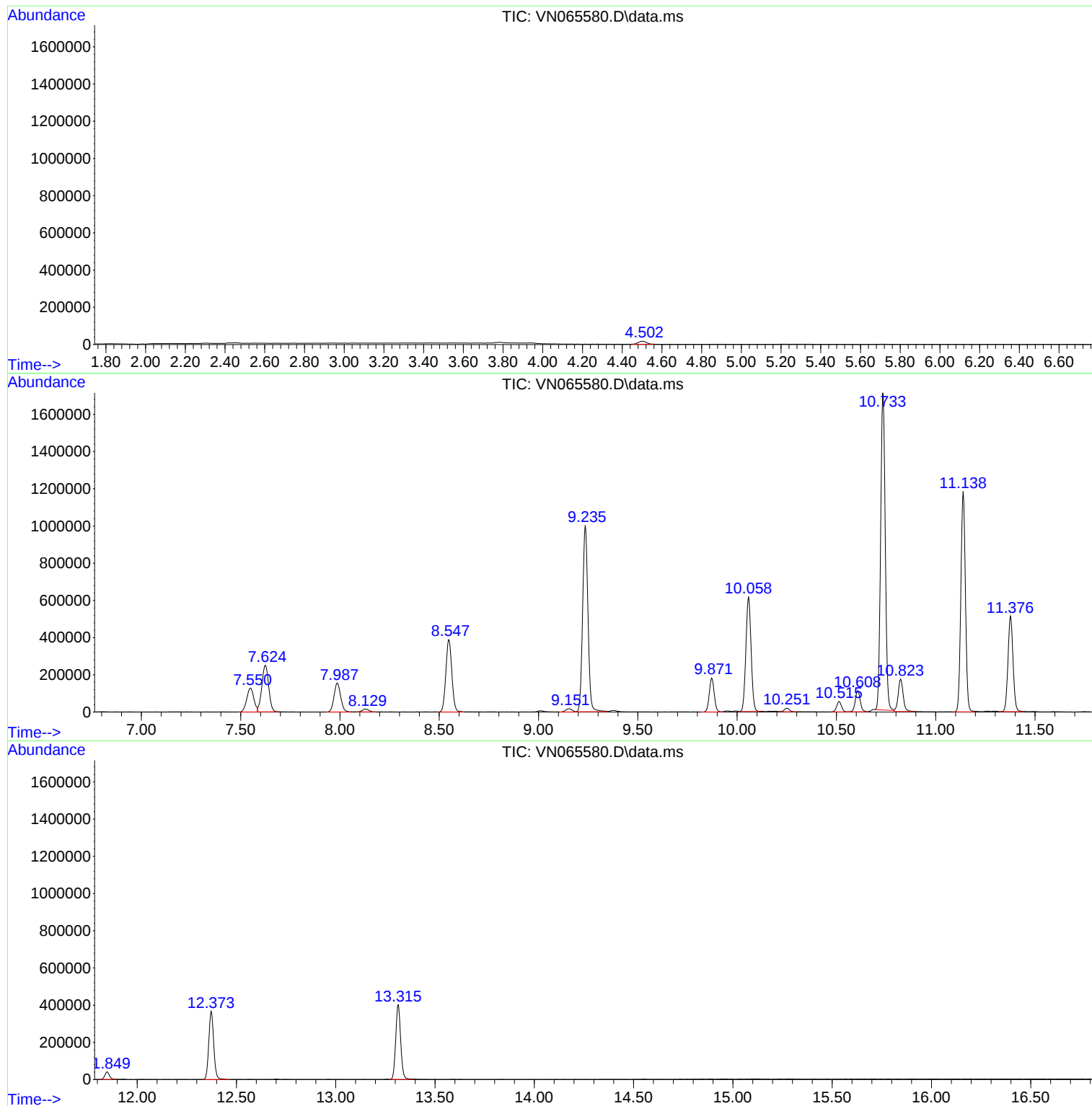
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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



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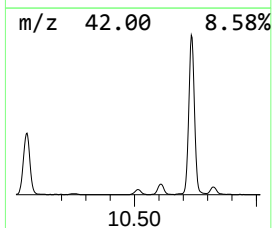
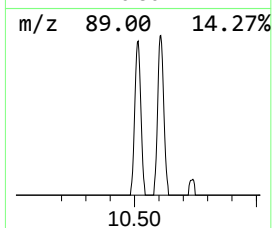
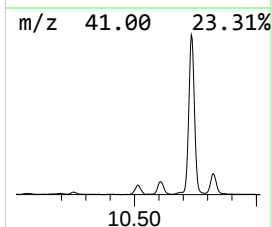
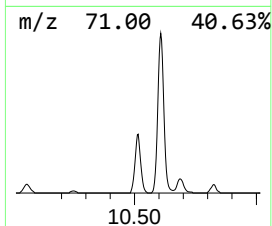
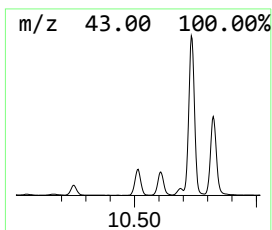
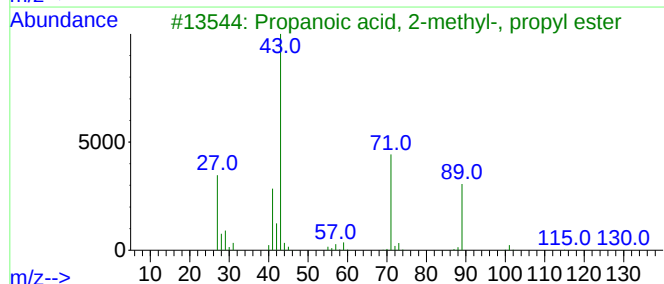
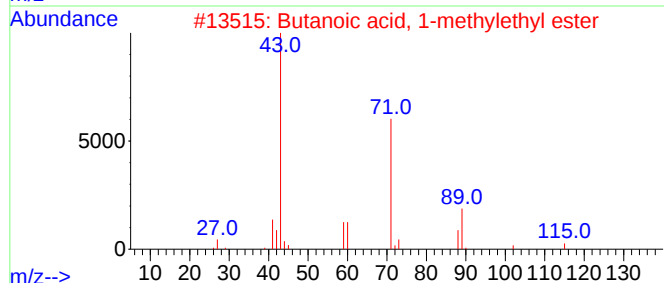
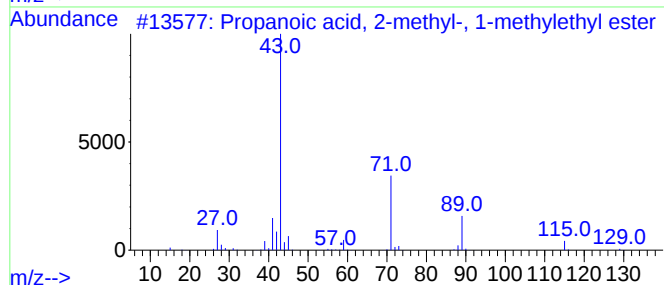
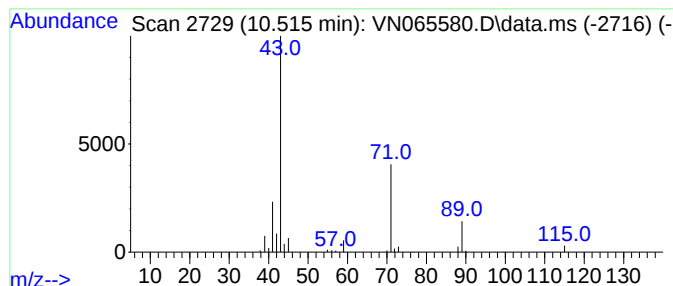
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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	5.15 ug/l	93187	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			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	56
3			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	38
4			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	38
5			Propyl nitrite	89	C3H7NO2	000543-67-9	9



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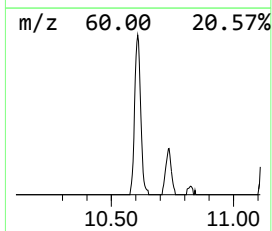
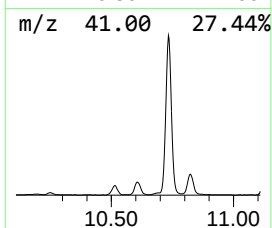
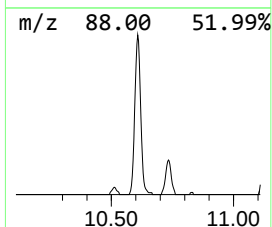
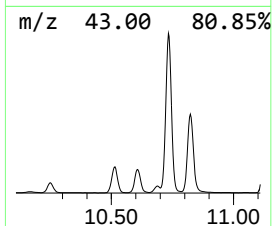
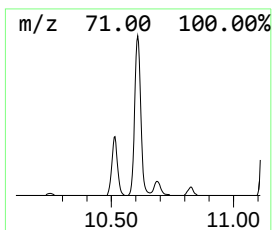
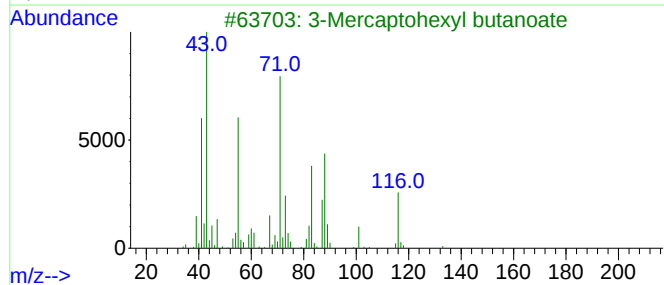
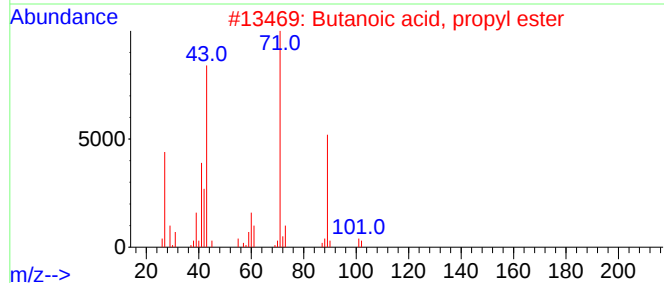
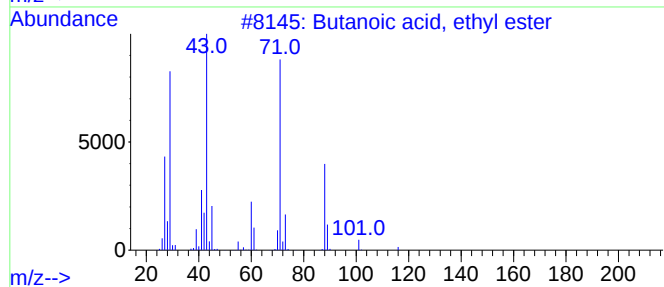
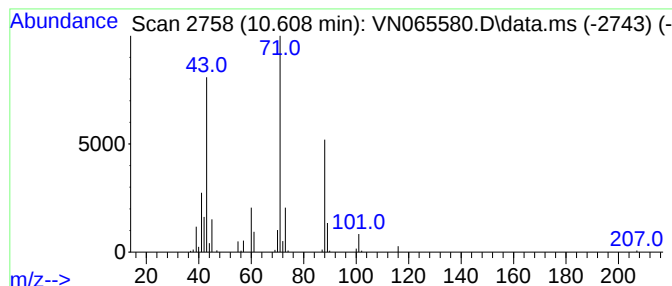
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Quant Title : SW846 8260

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	10.79 ug/l	195441	Chlorobenzene-d5	11.376

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	43
3			3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	42
4			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	42
5			Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	38



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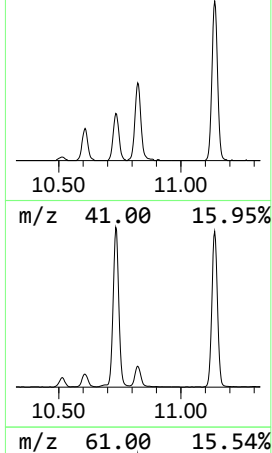
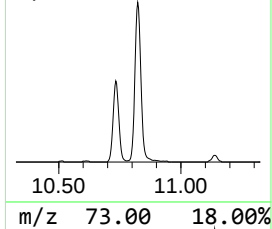
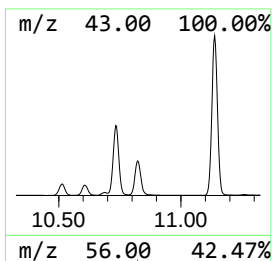
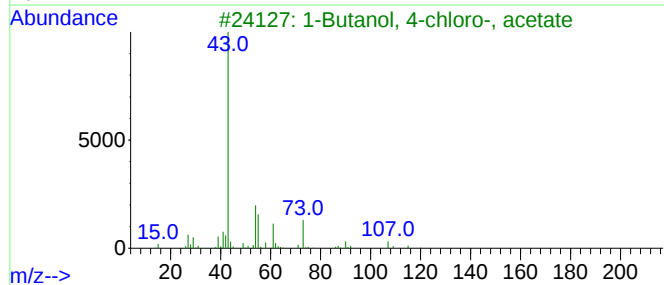
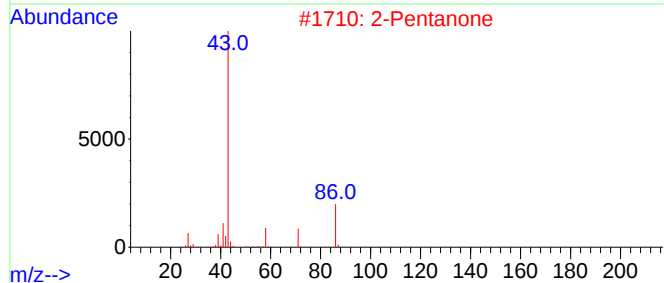
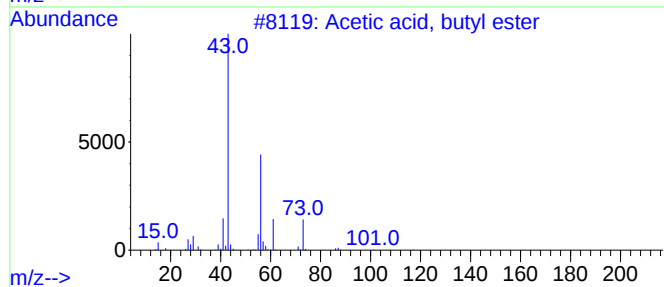
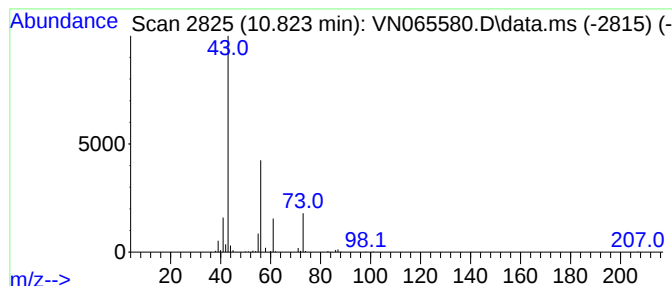
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Acetic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.823	16.56 ug/l	299869	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			2-Pentanone	86	C5H10O	000107-87-9	9
3			1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	9
4			Isobutyl acetate	116	C6H12O2	000110-19-0	9
5			Isobutylamine	73	C4H11N	000078-81-9	7



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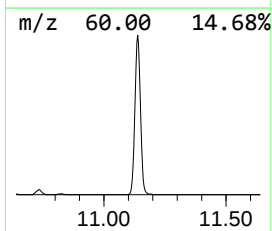
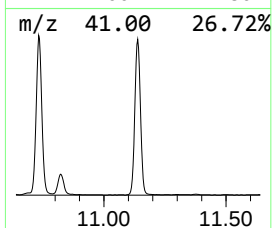
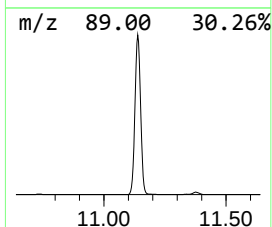
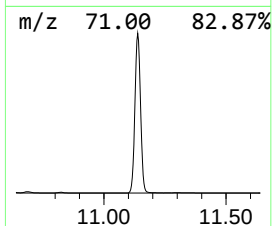
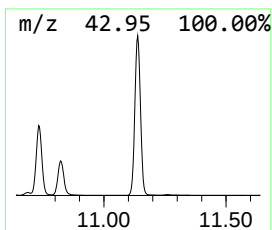
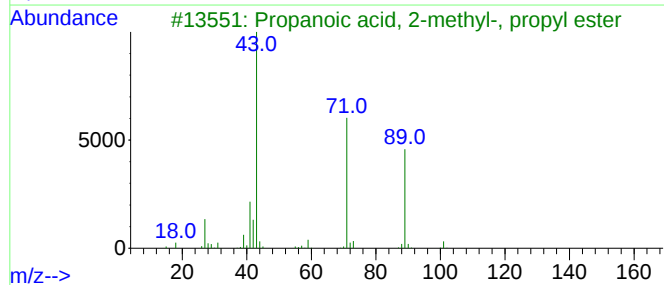
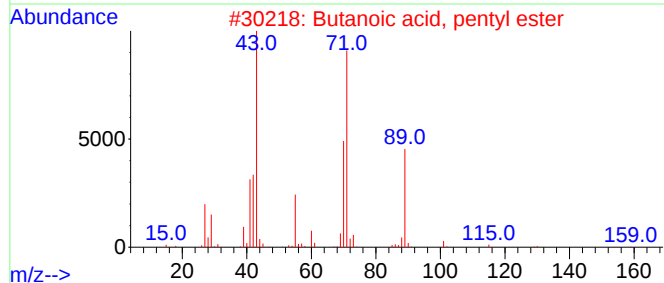
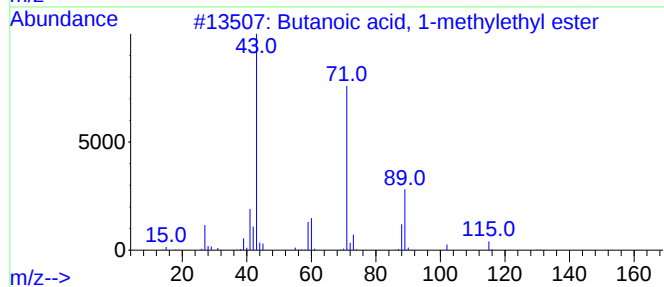
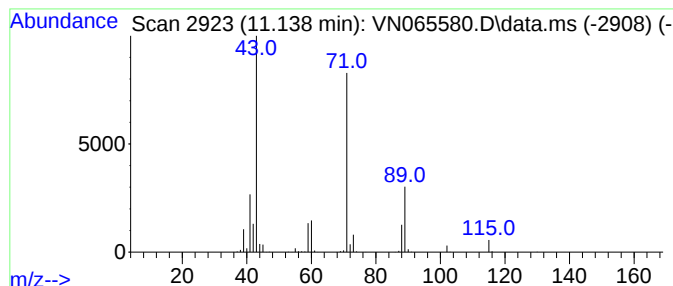
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Peak Number 4 Butanoic acid, 1-methylethy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.138	104.21 ug/l	1886920	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, propyl ester	130	C7H14O2	000105-66-8	50
5			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	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	93187	3	11.376	905351	50.0
Butanoic acid, ...	10.608	10.8	ug/l	195441	3	11.376	905351	50.0
Acetic acid, bu...	10.823	16.6	ug/l	299869	3	11.376	905351	50.0
Butanoic acid, ...	11.138	104.2	ug/l	1886920	3	11.376	905351	50.0