

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012521\
 Data File : VN065583.D
 Acq On : 25 Jan 2021 17:46
 Operator : JC/MD
 Sample : PB134285ZHE#03
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 PB134285ZHE#03

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: VN065583.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	843	859	881	rVB3	17744	52041	1.92%	0.404%
2	7.550	1788	1807	1817	rBV	126744	313455	11.56%	2.431%
3	7.624	1818	1830	1850	rVB	251173	588670	21.71%	4.565%
4	7.987	1922	1943	1971	rBV	156473	364354	13.44%	2.825%
5	8.129	1975	1987	2001	rVB2	15380	33335	1.23%	0.259%
6	8.547	2102	2117	2139	rVB	388149	807084	29.76%	6.259%
7	9.151	2289	2305	2317	rBV3	18050	38248	1.41%	0.297%
8	9.235	2317	2331	2365	rVV	988350	1818289	67.05%	14.100%
9	9.872	2510	2529	2544	rBV	176491	309093	11.40%	2.397%
10	10.058	2573	2587	2608	rBV	612058	1116970	41.19%	8.662%
11	10.251	2637	2647	2662	rVB	18697	33277	1.23%	0.258%
12	10.511	2716	2728	2742	rBV	53503	90472	3.34%	0.702%
13	10.608	2745	2758	2771	rBV	112796	188757	6.96%	1.464%
14	10.733	2785	2797	2815	rVV	1678901	2711948	100.00%	21.030%
15	10.823	2815	2825	2848	rVB	173001	294489	10.86%	2.284%
16	11.138	2910	2923	2942	rBV	1171517	1853652	68.35%	14.374%
17	11.376	2980	2997	3018	rVB	526169	903517	33.32%	7.006%
18	11.849	3133	3144	3157	rBV	40442	66373	2.45%	0.515%
19	12.373	3294	3307	3333	rVB	364157	628258	23.17%	4.872%
20	13.315	3587	3600	3620	rBV	402074	683167	25.19%	5.298%

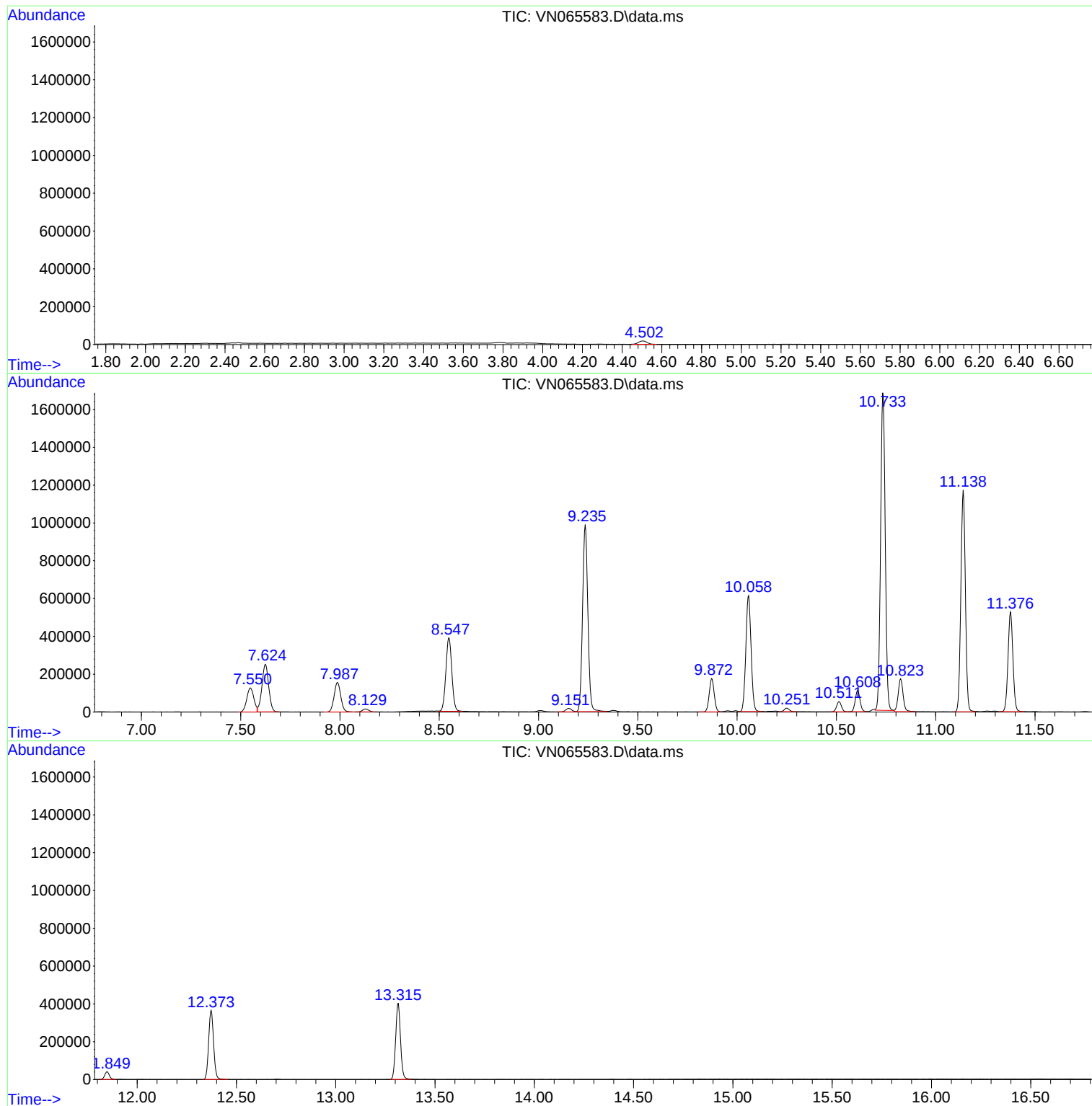
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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



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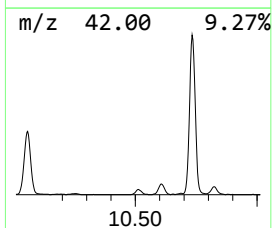
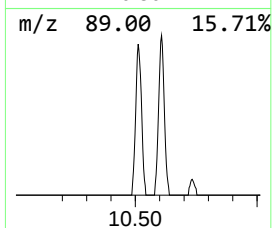
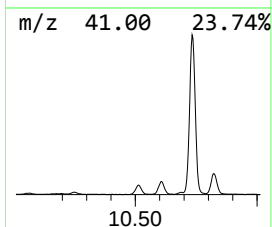
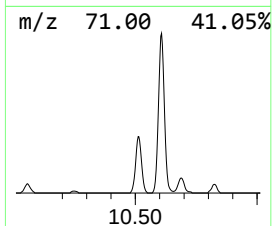
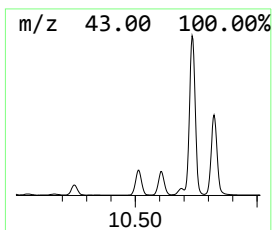
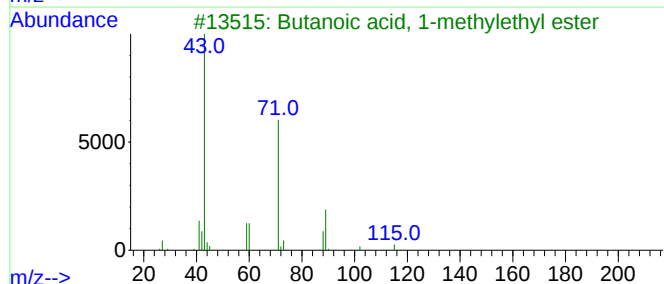
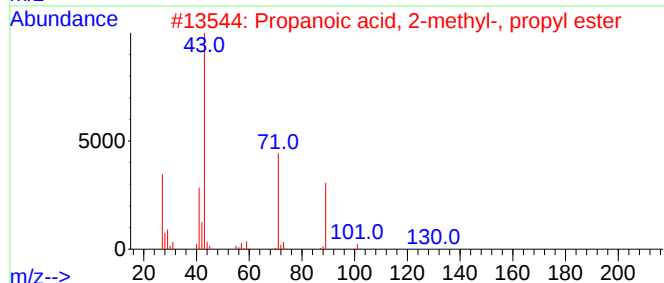
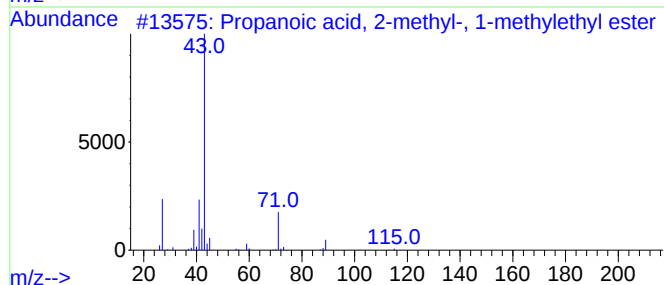
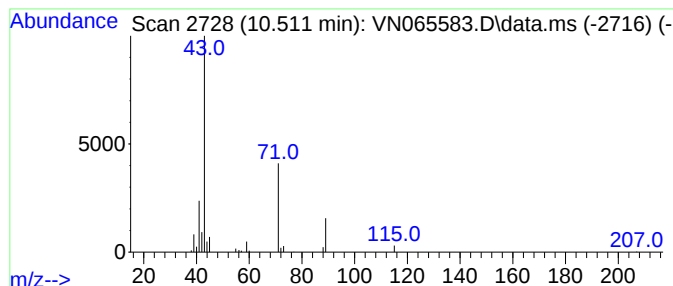
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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.
10.511	5.01 ug/l	90472	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			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78
3			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	64
4			Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	45
5			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	38



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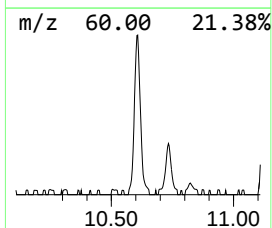
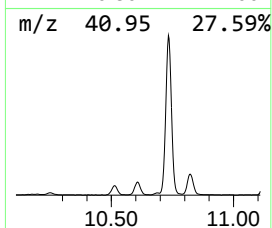
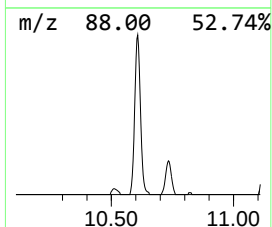
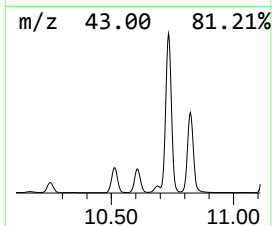
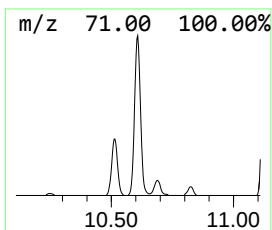
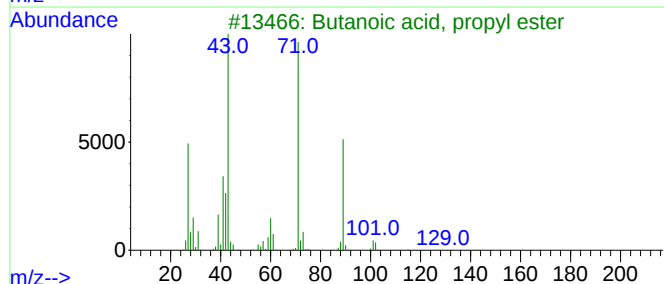
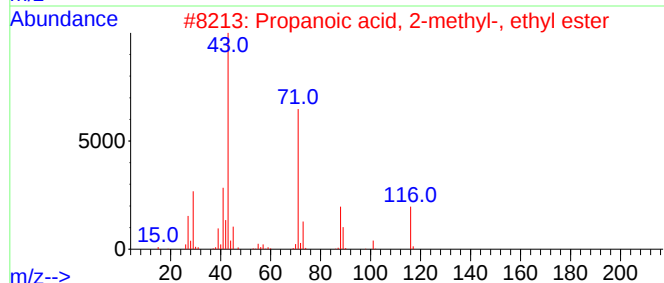
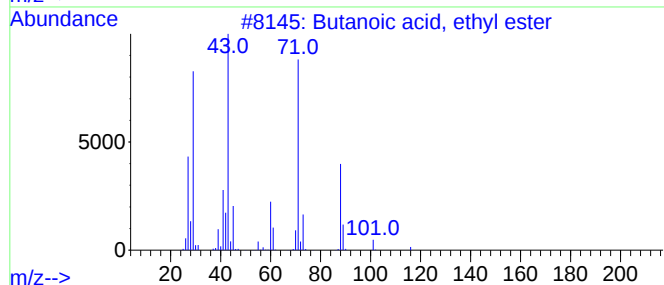
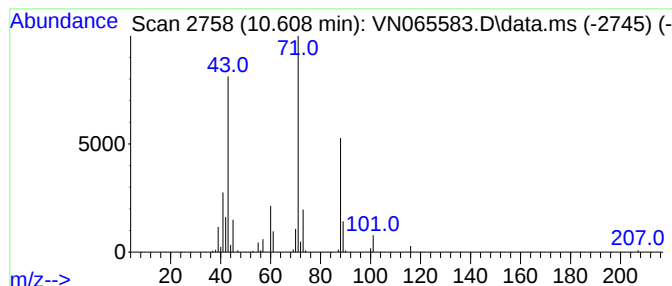
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Quant Title : SW846 8260

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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	10.45 ug/l	188757	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			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	53
3			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	43
4			3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	42
5			Ethyl 6-bromohexanoate	222	C8H15BrO2	025542-62-5	38



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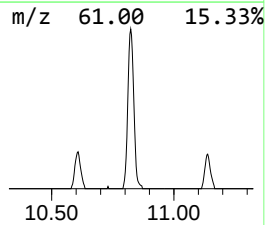
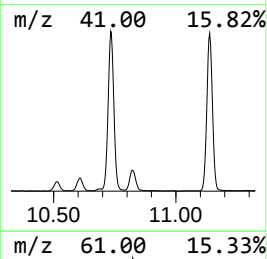
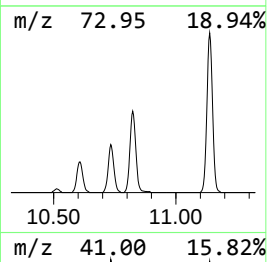
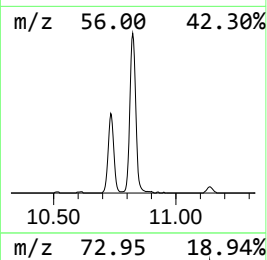
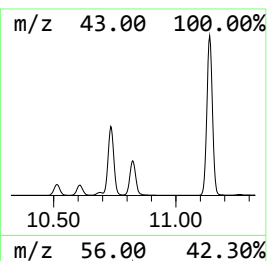
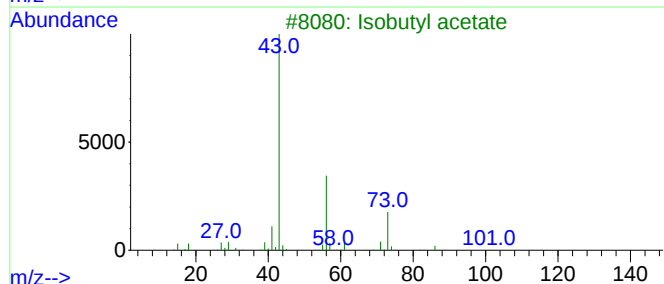
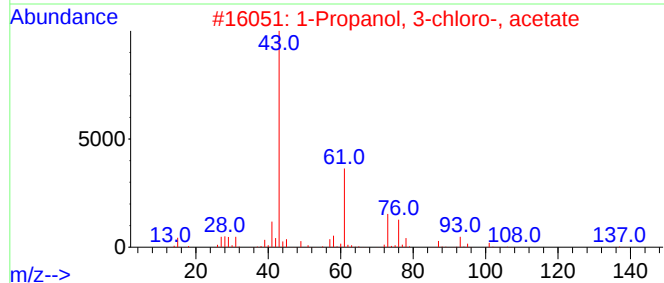
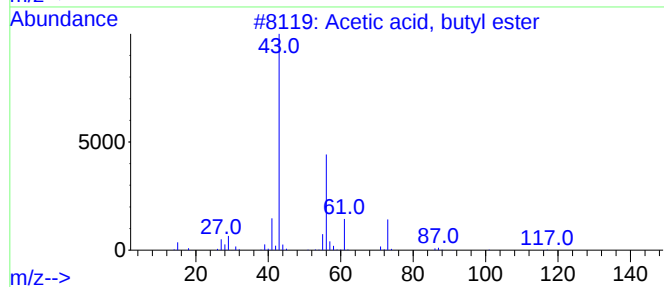
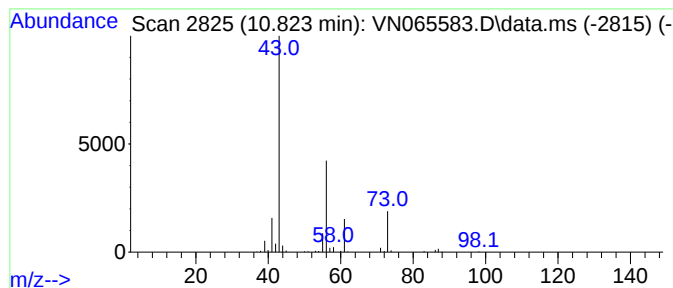
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Peak Number 3 Acetic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.823	16.30 ug/l	294489	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			1-Propanol, 3-chloro-, acetate	136	C5H9ClO2	000628-09-1	9
3			Isobutyl acetate	116	C6H12O2	000110-19-0	9
4			Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	9
5			1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	9



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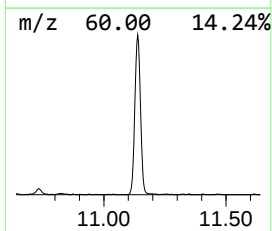
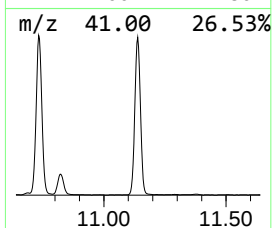
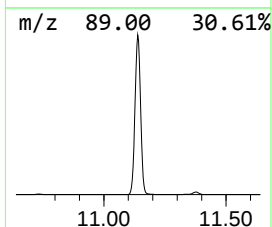
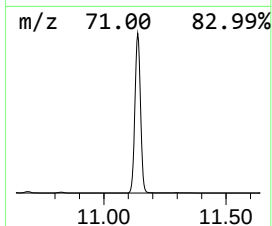
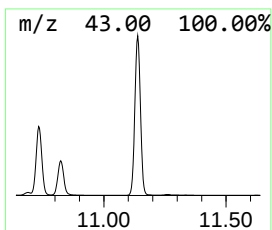
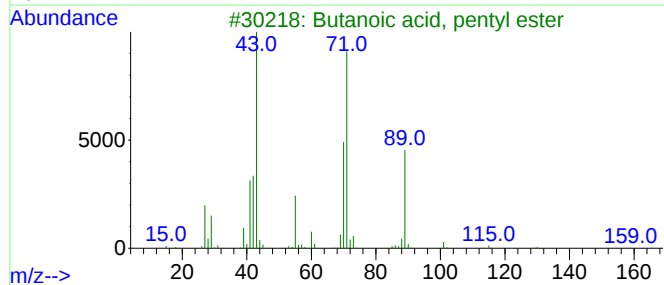
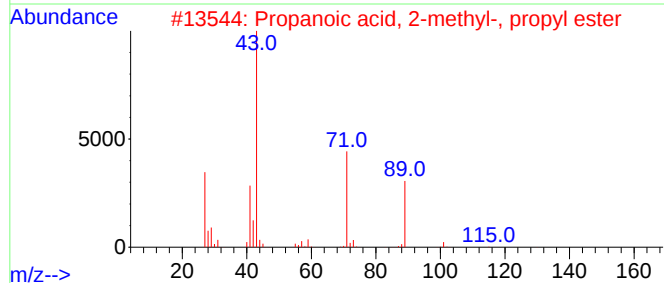
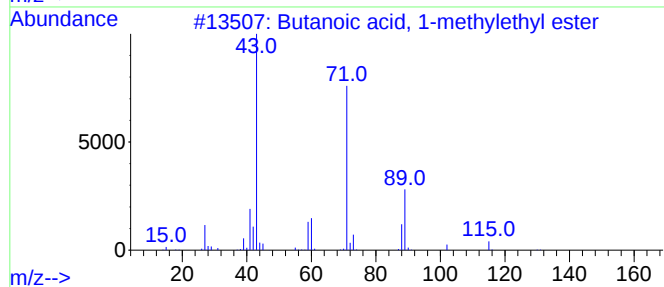
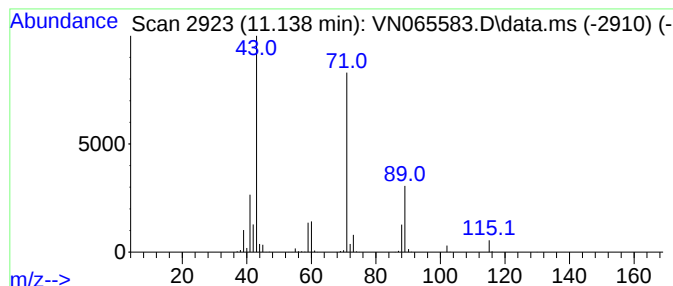
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.138	102.58 ug/l	1853650	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			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
4			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	56
5			Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	10.511	5.0	ug/l	90472	3	11.376	903517	50.0
Butanoic acid, ...	10.608	10.4	ug/l	188757	3	11.376	903517	50.0
Acetic acid, bu...	10.823	16.3	ug/l	294489	3	11.376	903517	50.0
Butanoic acid, ...	11.138	102.6	ug/l	1853650	3	11.376	903517	50.0