

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX021519\
 Data File : VX007543.D
 Acq On : 14 Feb 2019 14:09
 Operator : JC/SP
 Sample : K1458-07
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 WC-4

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X020119W.M

Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.611	66	75	80	rBV	26408	61839	1.16%	0.238%
2	2.446	207	212	221	rVB	35676	59603	1.12%	0.229%
3	2.861	271	280	294	rBV	2855755	5334708	100.00%	20.521%
4	5.501	700	713	726	rBV3	284656	817008	15.31%	3.143%
5	5.665	726	740	752	rVV	459357	1268065	23.77%	4.878%
6	6.068	796	806	821	rBV	286472	730853	13.70%	2.811%
7	6.860	925	936	949	rBV	700411	1642427	30.79%	6.318%
8	7.878	1096	1103	1116	rBV	1673373	2868905	53.78%	11.036%
9	8.616	1217	1224	1233	rBV	402720	619319	11.61%	2.382%
10	8.714	1233	1240	1250	rBV	1533630	2363366	44.30%	9.091%
11	9.305	1331	1337	1343	rBV	256728	357266	6.70%	1.374%
12	9.402	1350	1353	1357	rVV	100730	143045	2.68%	0.550%
13	9.543	1370	1376	1382	rBV	1596978	2016692	37.80%	7.757%
14	9.640	1388	1392	1397	rVB	92829	120554	2.26%	0.464%
15	9.969	1441	1446	1457	rBV	1449239	1783525	33.43%	6.861%
16	10.110	1463	1469	1477	rBV	1529465	2088123	39.14%	8.032%
17	10.695	1561	1565	1571	rBV	77056	95063	1.78%	0.366%
18	11.134	1630	1637	1645	rBV	1248143	1632979	30.61%	6.281%
19	12.079	1786	1792	1799	rBV	1558182	1993376	37.37%	7.668%

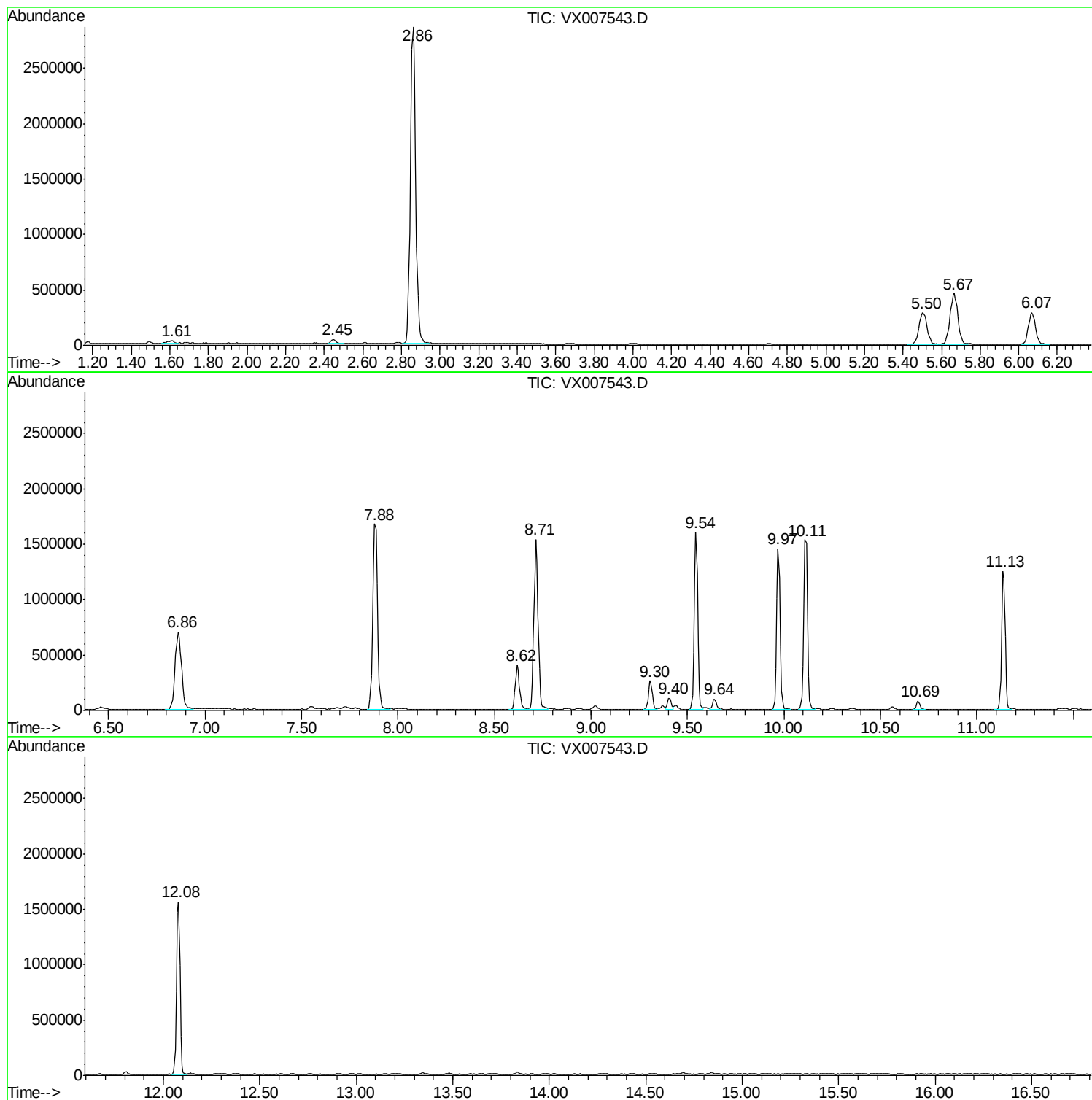
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X020119W.M
Quant Title : SW846 8260

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



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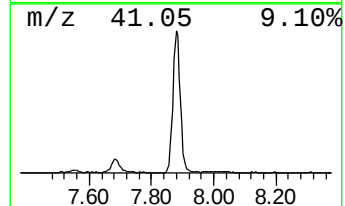
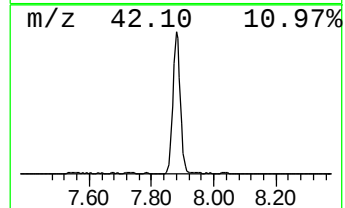
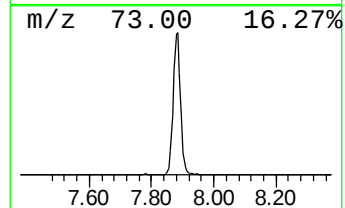
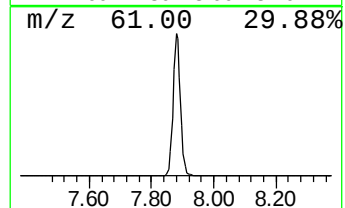
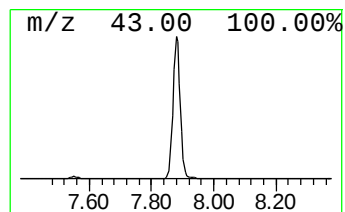
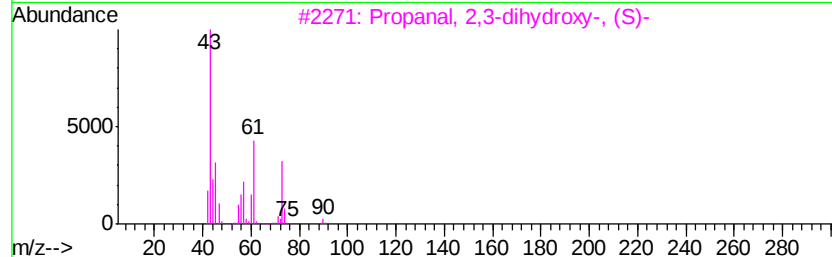
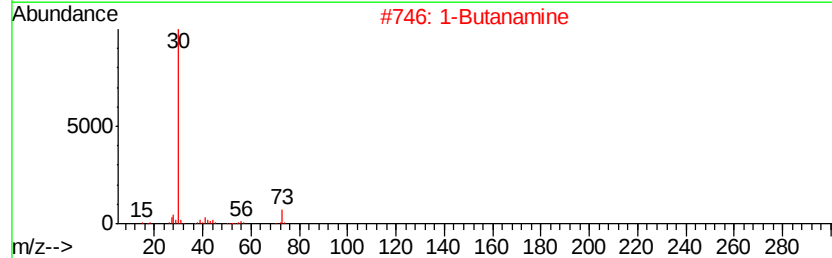
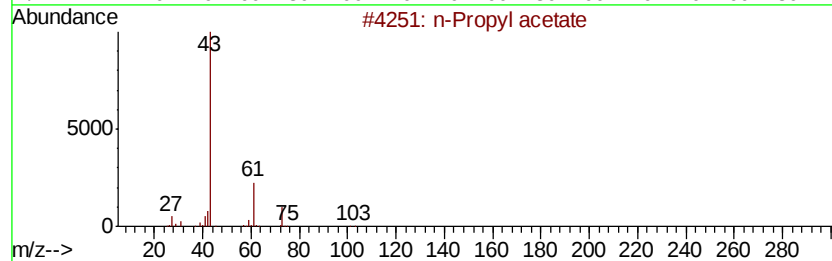
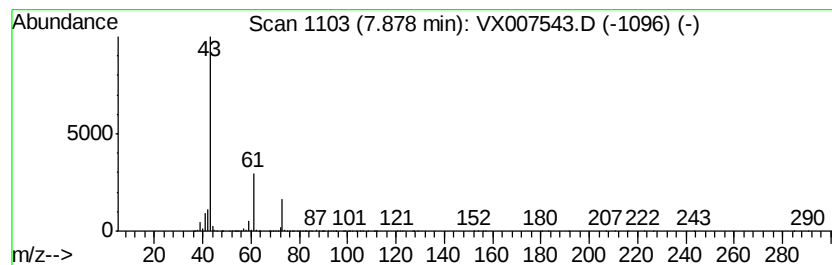
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Quant Title : SW846 8260

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

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.88	87.34 ug/l	2868910	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2		1-Butanamine	73	C4H11N	000109-73-9	9
3		Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	9
4		Isopropyl acetate	102	C5H10O2	000108-21-4	9
5		Isobutylamine	73	C4H11N	000078-81-9	4



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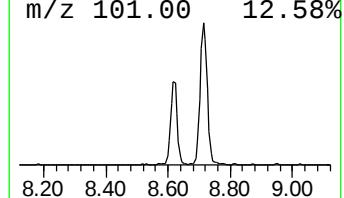
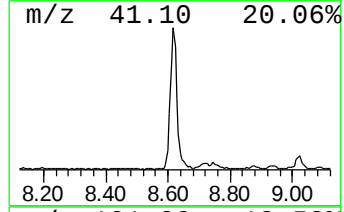
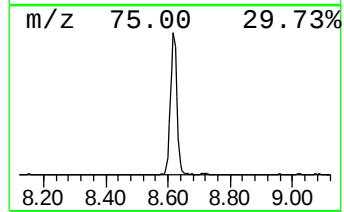
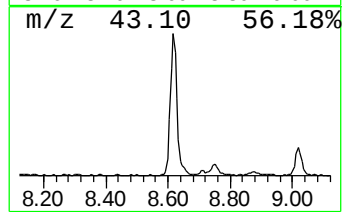
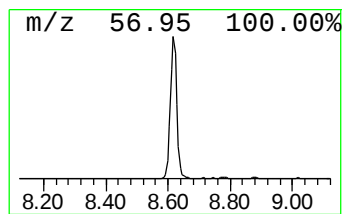
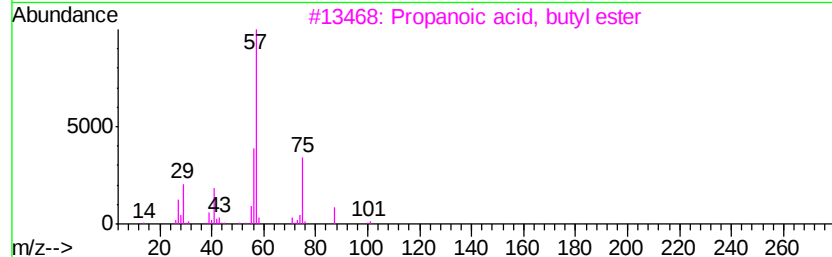
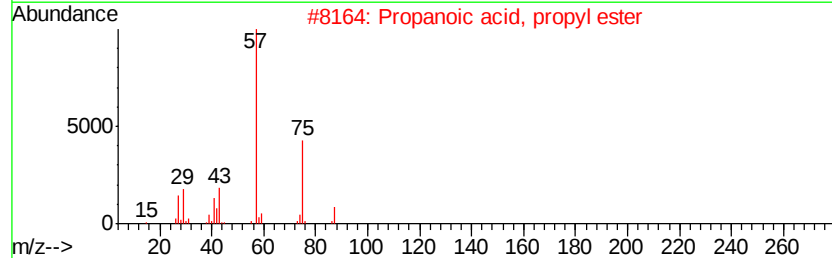
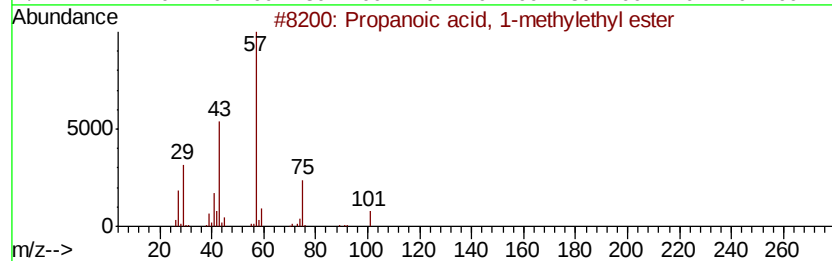
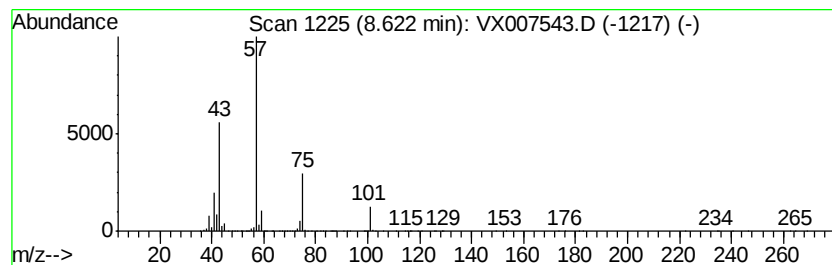
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Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.62	14.83 ug/l	619319	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
3		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
4		Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	12



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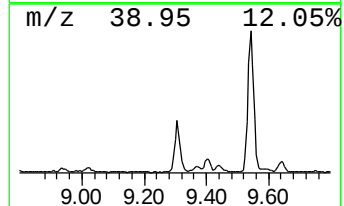
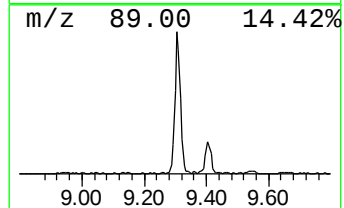
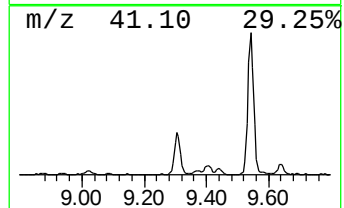
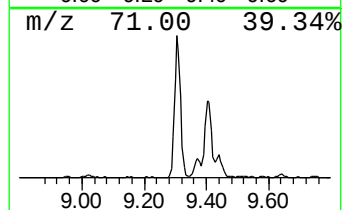
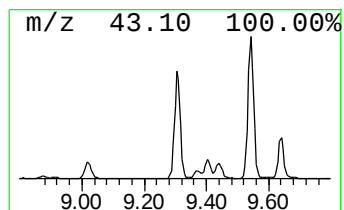
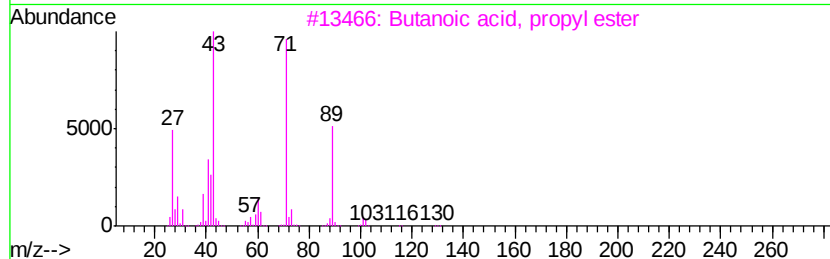
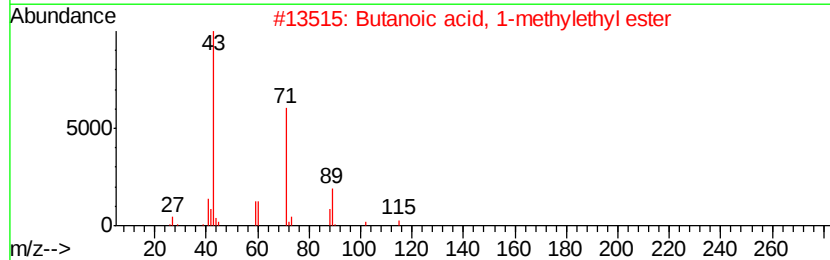
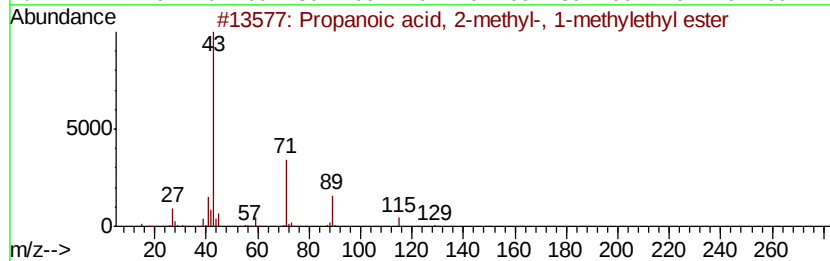
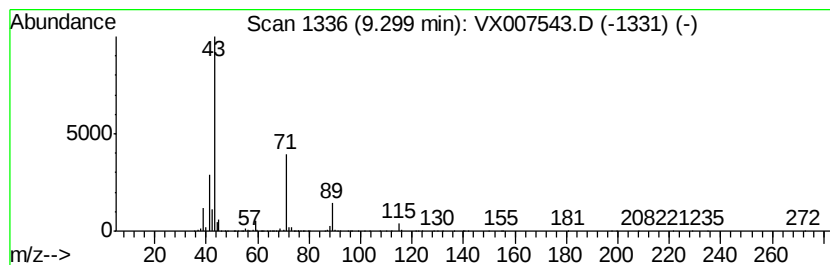
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Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.30	8.55 ug/l	357266	Chlorobenzene-d5	10.12

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	72
3		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	45
4		3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42
5		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	39



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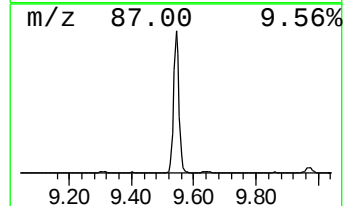
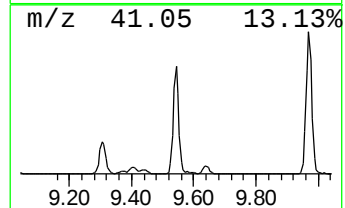
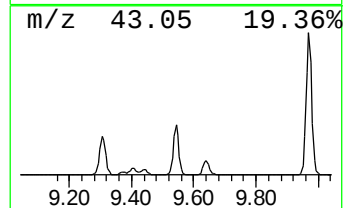
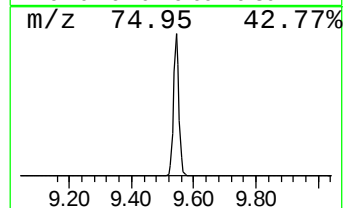
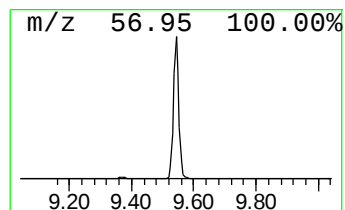
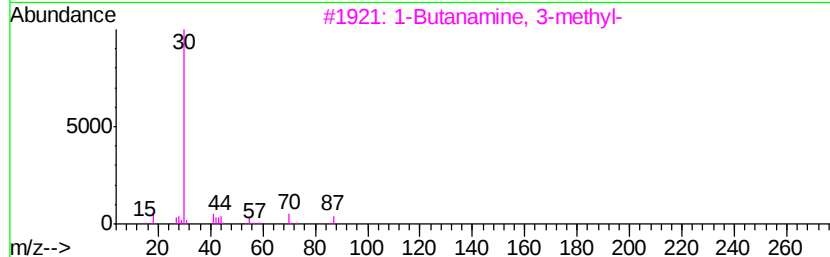
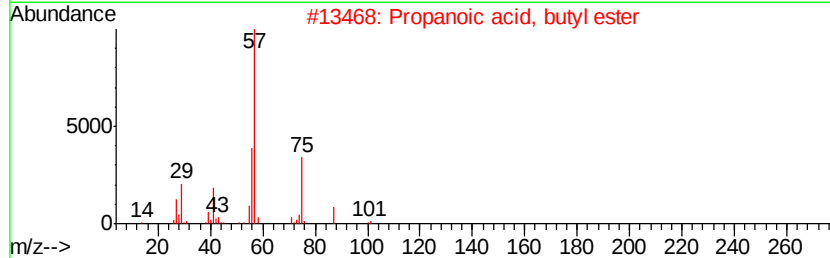
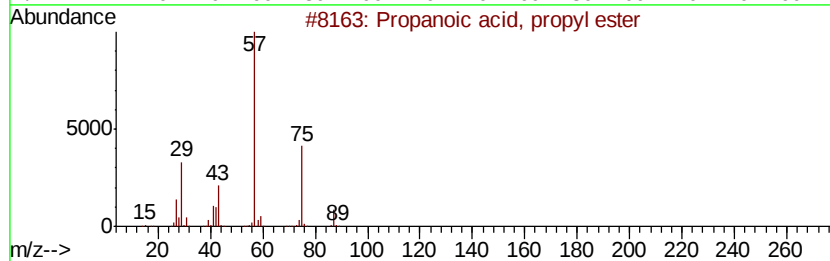
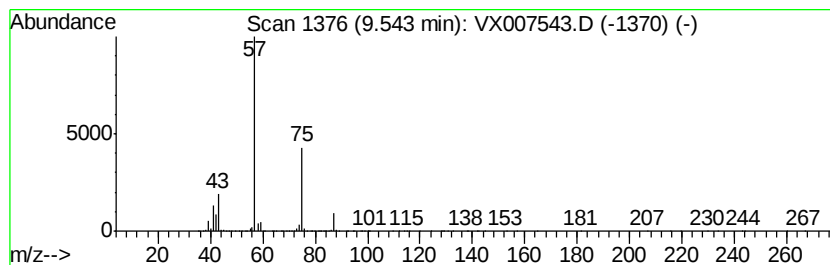
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Peak Number 4 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.54	48.29 ug/l	2016690	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	40
3		1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	9
4		1-Penten-3-ol	86	C5H10O	000616-25-1	7
5		1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	7



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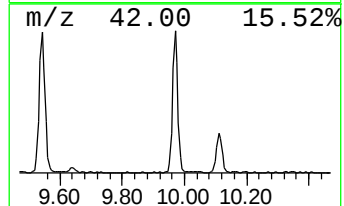
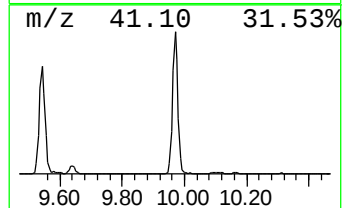
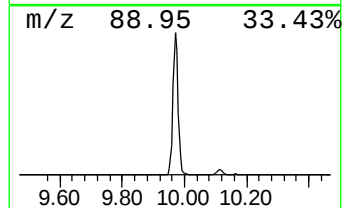
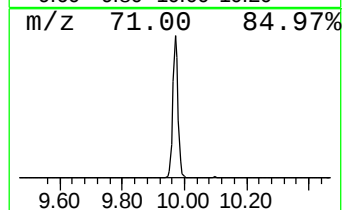
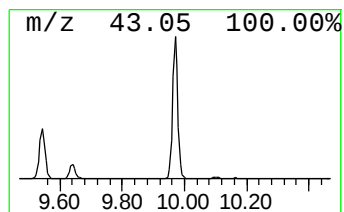
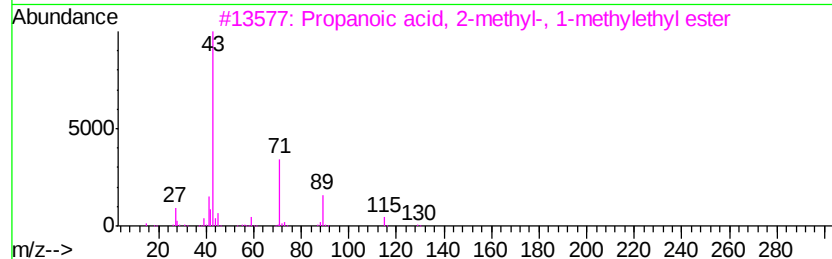
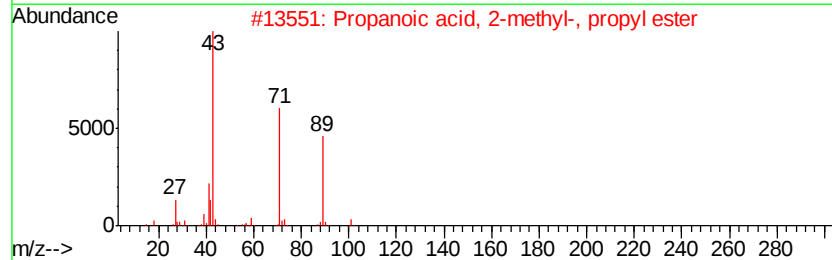
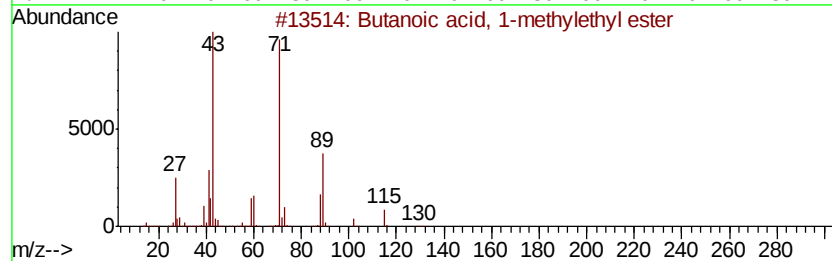
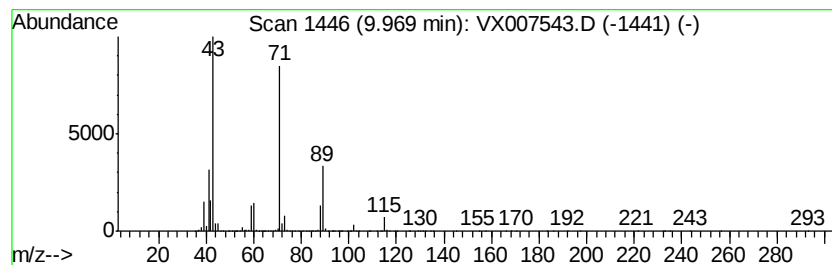
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Peak Number 5 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.97	42.71 ug/l	1783530	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
2		Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	72
3		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
4		Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72
5		Propanoic acid, 2-methyl-, pentyl...	158	C9H18O2	002445-72-9	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	7.88	87.3	ug/l	2868910	2	6.86	1642430	50.0
Propanoic acid, 1...	8.62	14.8	ug/l	619319	3	10.12	2088120	50.0
Propanoic acid, 2...	9.30	8.6	ug/l	357266	3	10.12	2088120	50.0
Propanoic acid, p...	9.54	48.3	ug/l	2016690	3	10.12	2088120	50.0
Butanoic acid, 1-...	9.97	42.7	ug/l	1783530	3	10.12	2088120	50.0