

Supplementary material for:

Suramin induces mitochondrial activation in bloodstage African trypanosomes

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Supplementary figure legends

Figure S1: Summary of metabolite changes of cells grown in the presence ^{13}C -labeled glucose one day after suramin exposure.

Figure S2: Amino acid level changes upon suramin treatment. -log10 fold changes of amino acids detected in the metabolomics are plotted versus the 3 time points analyzed.

Figure S3: Suramin induced proteome changes have an onset later than 24 hours. Correlation of proteome changes upon suramin treatment after 24 hours and 48 hours. The correlation plot uses the respective normalised SILAC ratio, averaged from triplicate experiments.

Figure S4: GO term analysis. Volcano plots of normalised SILAC ratio after 48 hours suramin (35 nM) exposure. -log2 transformed average ratios from triplicate experiments, are plotted against the respective -log10 transformed p-values. Data points are colored for indicated GO terms. Selected data points are annotated.

Figure S5: Correlation of proteome changes upon suramin treatment with proteome differences between BSF and PCF. -log2 transformed abundance shifts after 48 hours suramin (35 nM) exposure, were plotted against corresponding -log2 transformed abundance differences between BSF and PCF (50). Selected GO terms are color indicated. Infinite changes were omitted for clarity. (DH = dehydrogenase, PPDK = pyruvate phosphate dikinase).

Figure S6: Suramin binding to serum proteins. Gel filtration chromatogram of 0.5 ml foetal bovine serum pre-incubated with ^3H -suramin on a 24 ml Superdex 200 column. The black line indicates the relative absorbance at $\lambda=280$ nm and the red line the scintillation count (counts per minute (CPM)) of respective fractions.

Figure S7: Pyruvate transporter overexpression has no effect on suramin sensitivity. Pt1-myc overexpression was detected by western blotting using the myc epitope (A), but did not change potency (EC_{50}) of suramin (B).

Movie S1: 3D segmentation of whole *T. brucei* cell. Plasma membrane and flagellum (purple), glycosomes (orange).

Table S1: High confidence metabolite changes of cells grown in the presence ^{13}C -labeled glucose one day after suramin exposure List of 84 quantified metabolites with the respective \log_2 fold change and corresponding *p*-value

Table S2: Metabolomics analysis at different time points of suramin exposure.

Table S3: High confidence metabolite changes at different time points of suramin exposure List of 65 quantified metabolites.

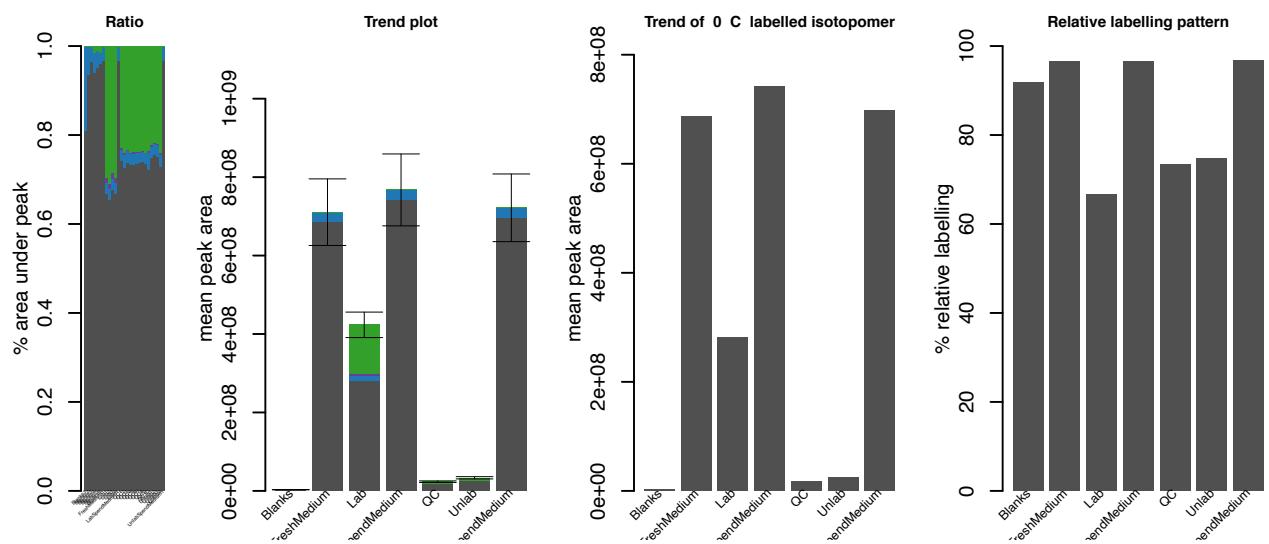
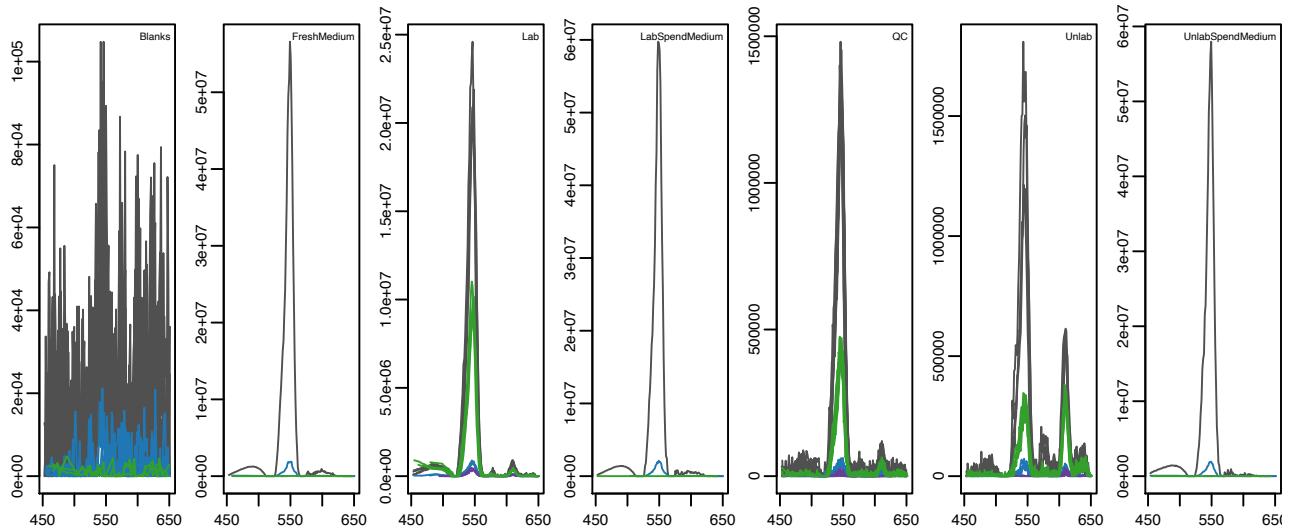
Table S4: SILAC proteomics analysis after 24 hours and 48 hours suramin exposure.

(R)-Lactate

Formula: C₃H₆O₃ Mass: 90.032 Std.RT: 552.6 Ion: NEG

G1

■UL ■+1 ■+2 ■+3

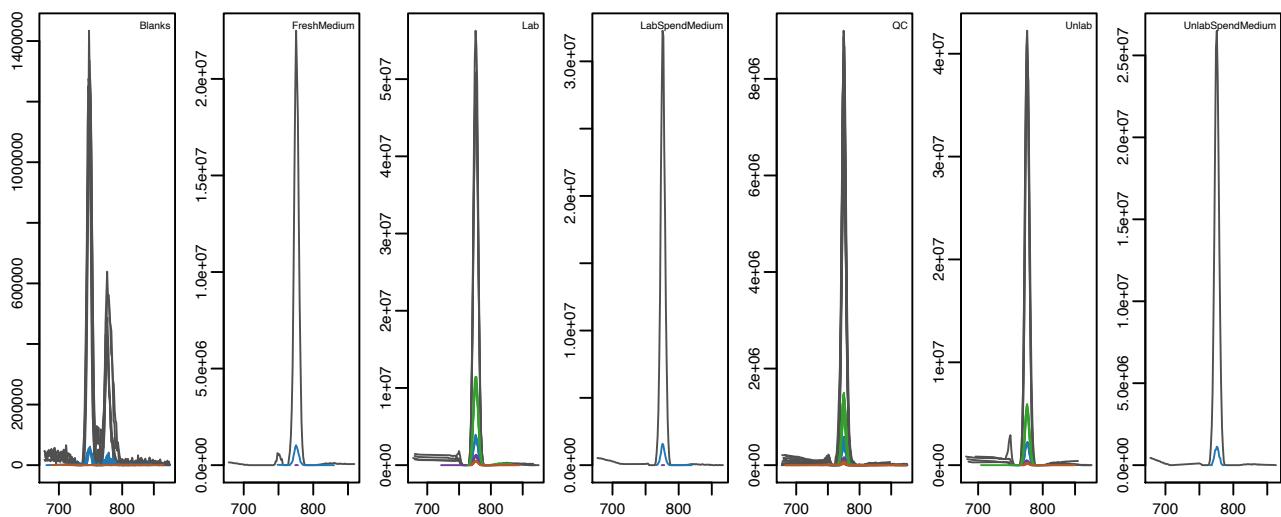


(S)-Malate

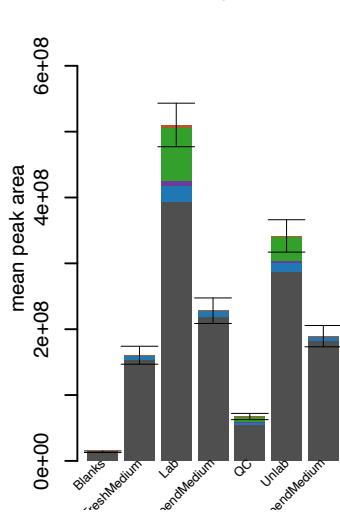
Formula: C₄H₆O₅ Mass: 134.022 Std.RT: 777 Ion: NEG

G1

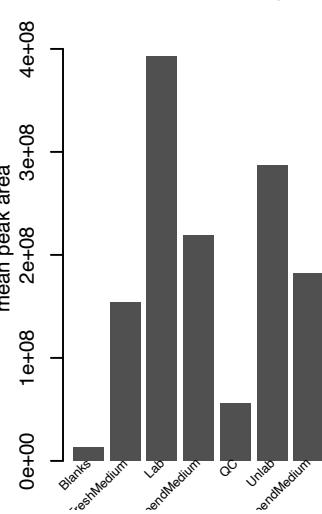
■UL ■+1 ■+2 ■+3 ■+4



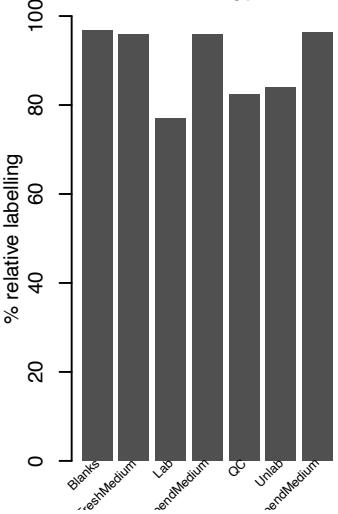
Trend plot



Trend of 0 C labelled isotopomer



Relative labelling pattern

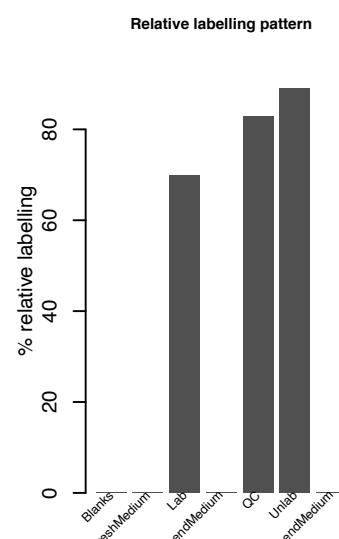
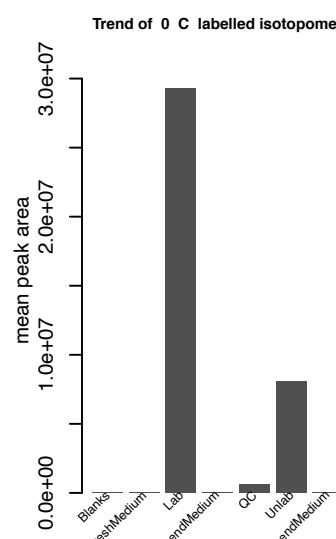
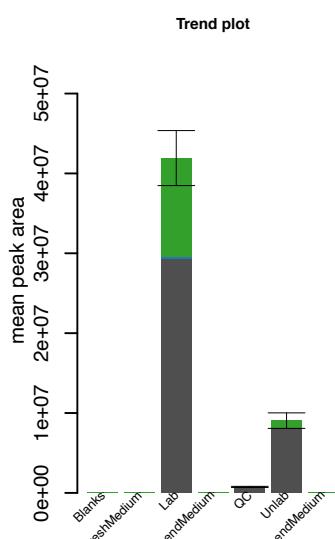
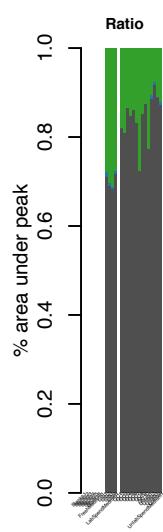
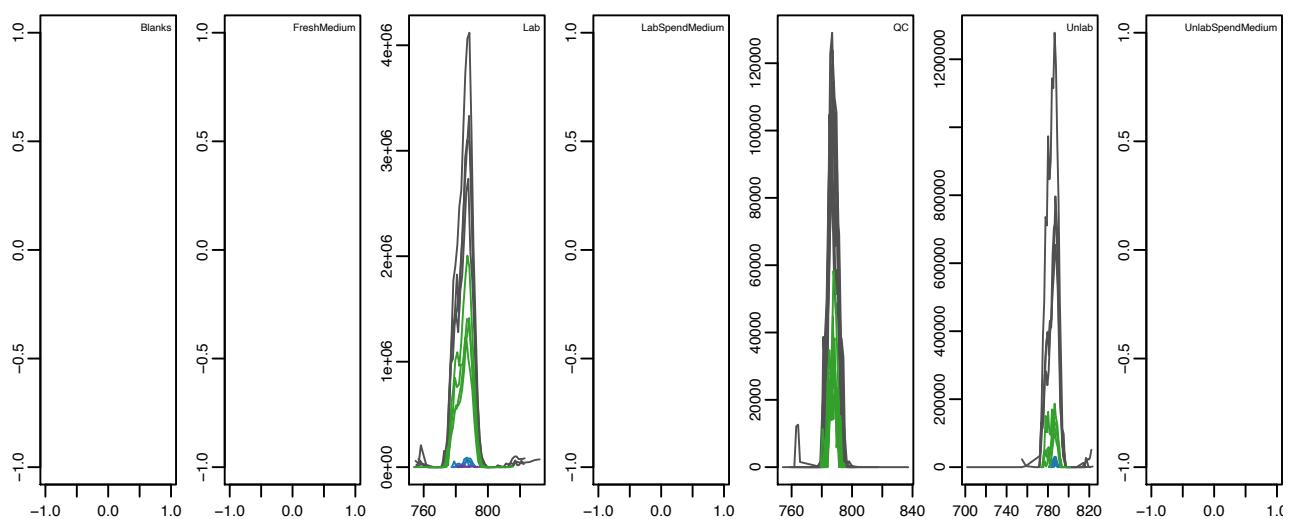


2-phospho-D-glycerate

Formula: C₃H₇O₇P Mass: 185.993 Std.RT: 783 Ion: NEG

G1

■UL ■+1 ■+2 ■+3

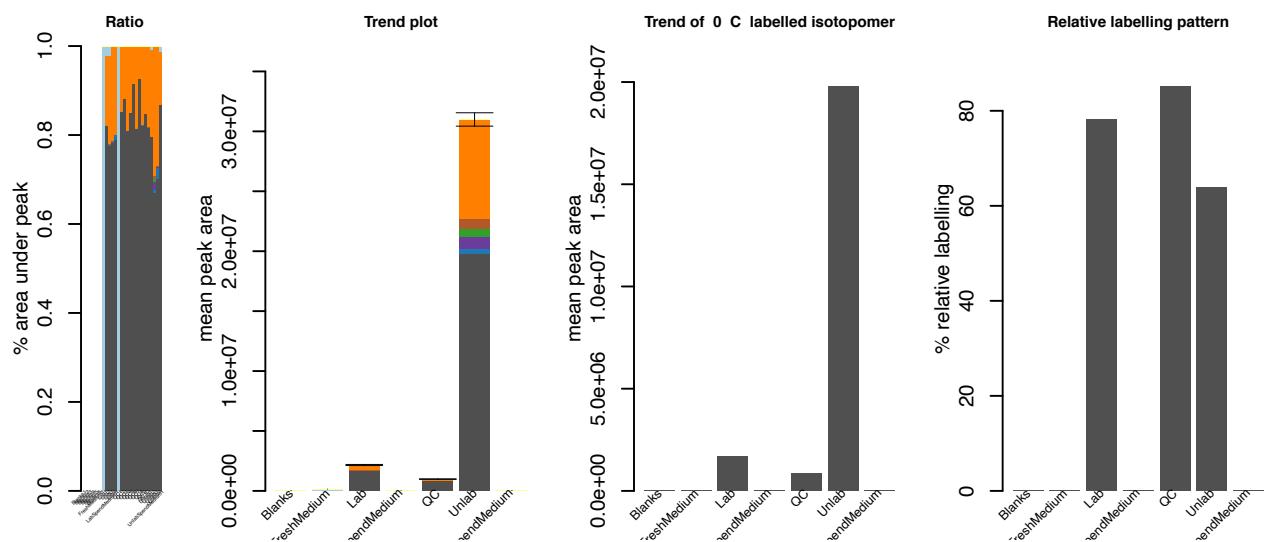
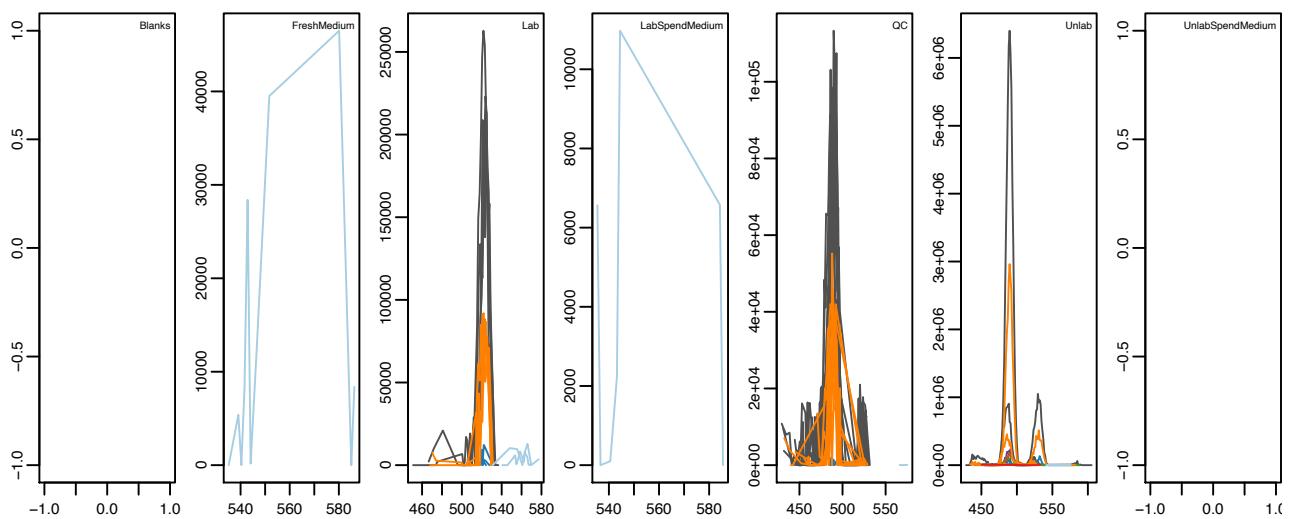


3'_5'-Cyclic AMP

Formula: C10H12N5O6P Mass: 329.053 Std.RT: 526.8 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9 ■+10

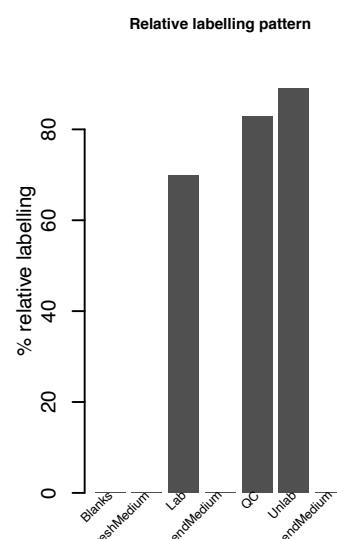
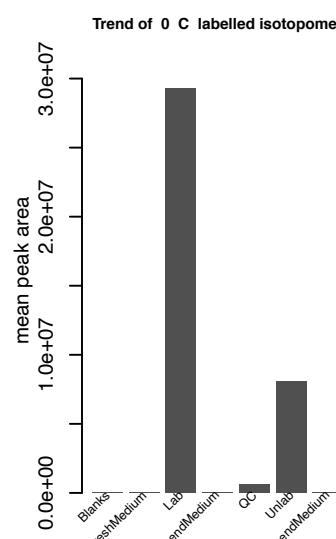
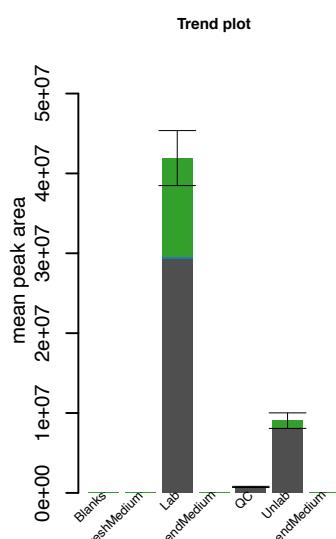
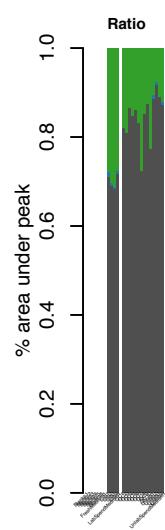
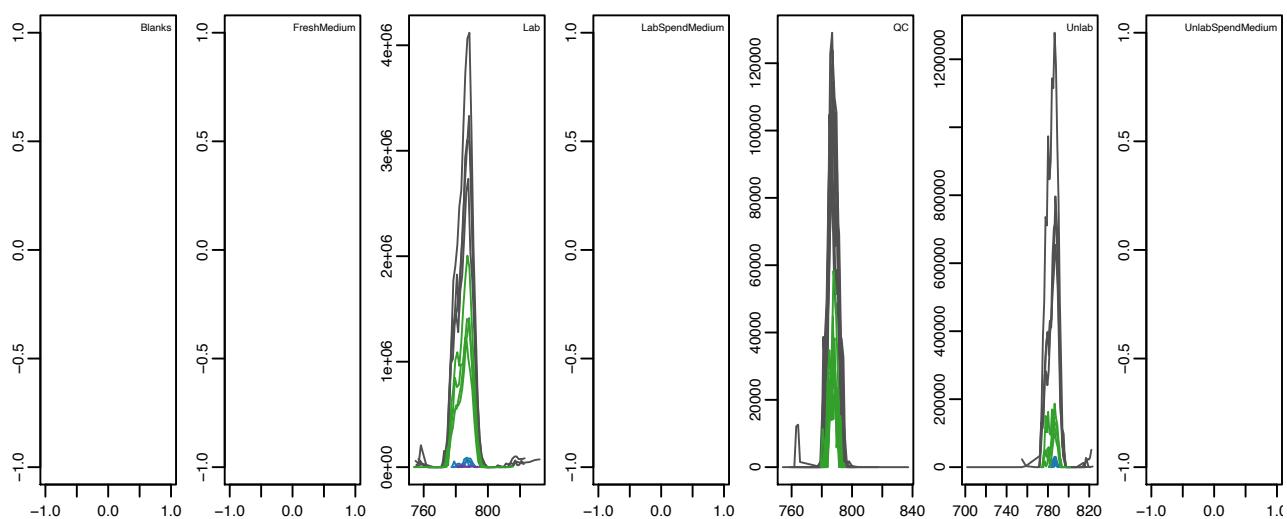


3-Phospho-D-glycerate

Formula: C₃H₇O₇P Mass: 185.993 Std.RT: 788.4 Ion: NEG

G1

■UL ■+1 ■+2 ■+3

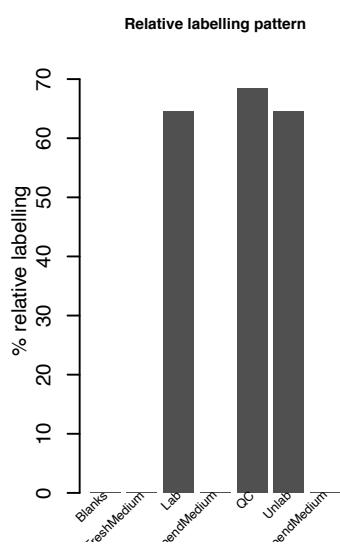
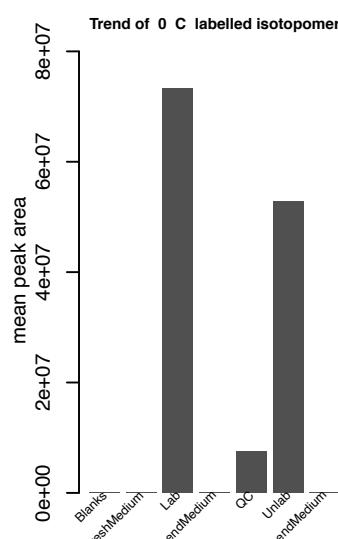
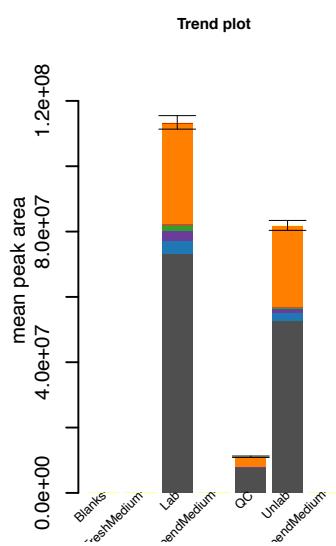
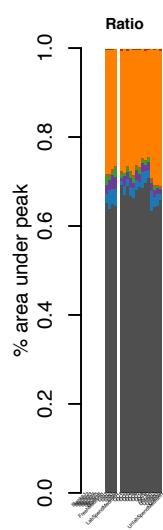
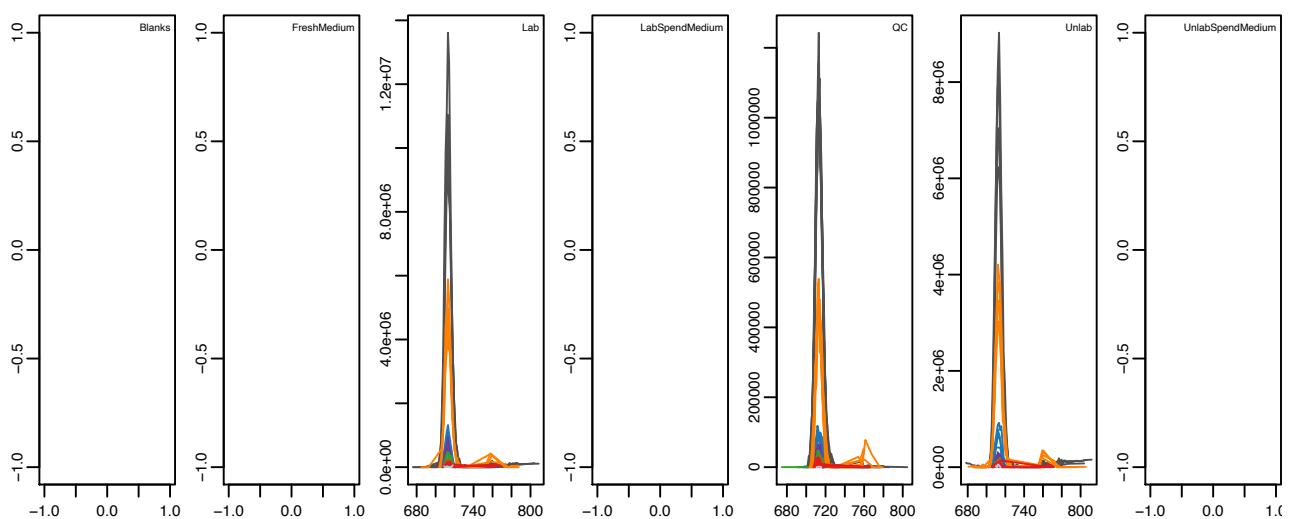


ADP

Formula: C10H15N5O10P2 Mass: 427.029 Std.RT: 714 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9 ■+10

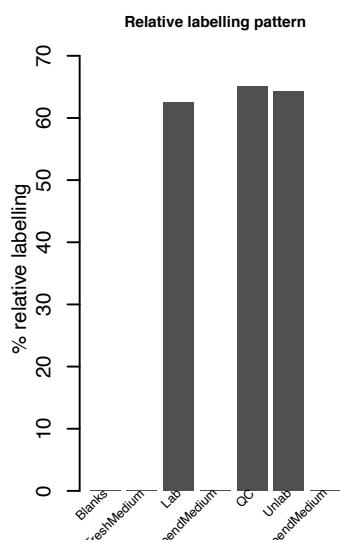
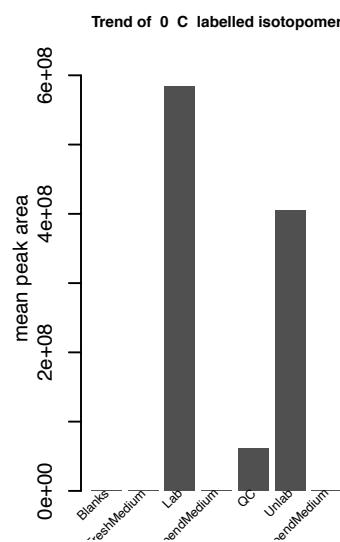
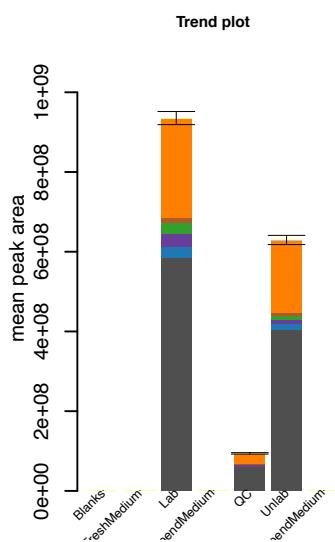
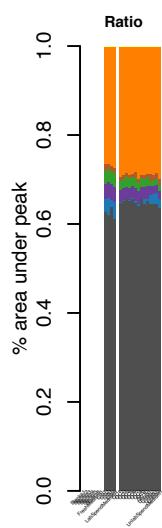
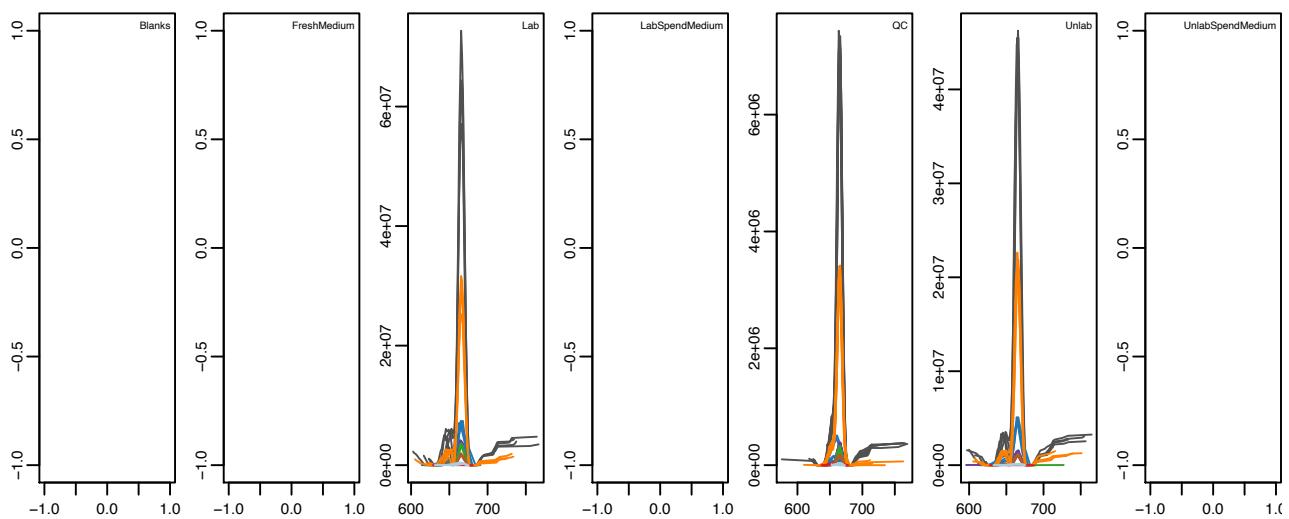


AMP

Formula: C₁₀H₁₄N₅O₇P Mass: 347.063 Std.RT: 670.8 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9 ■+10

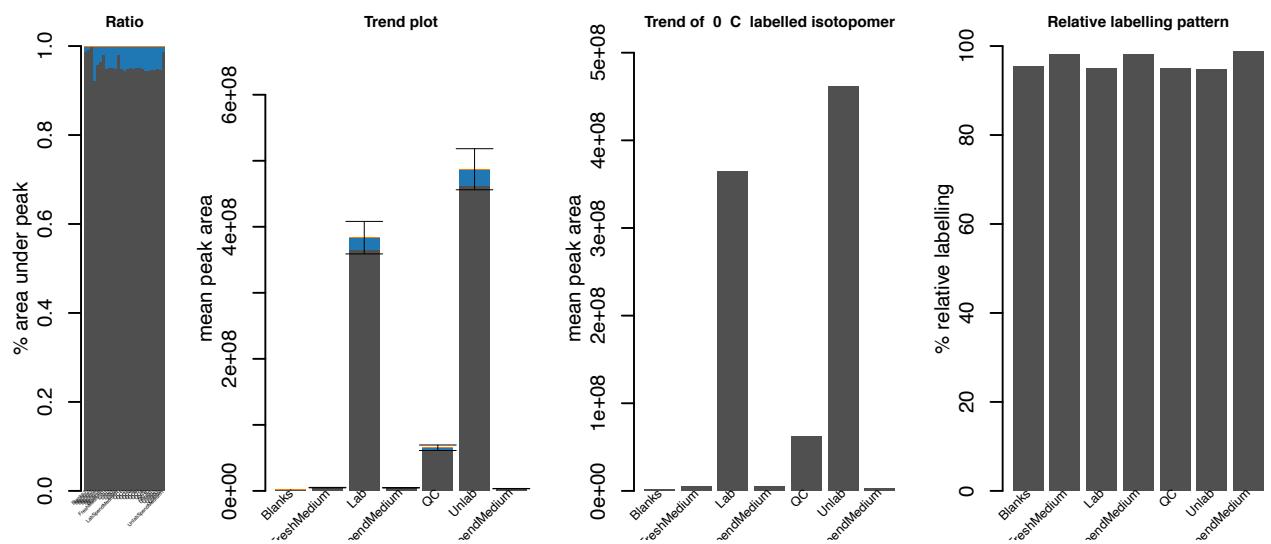
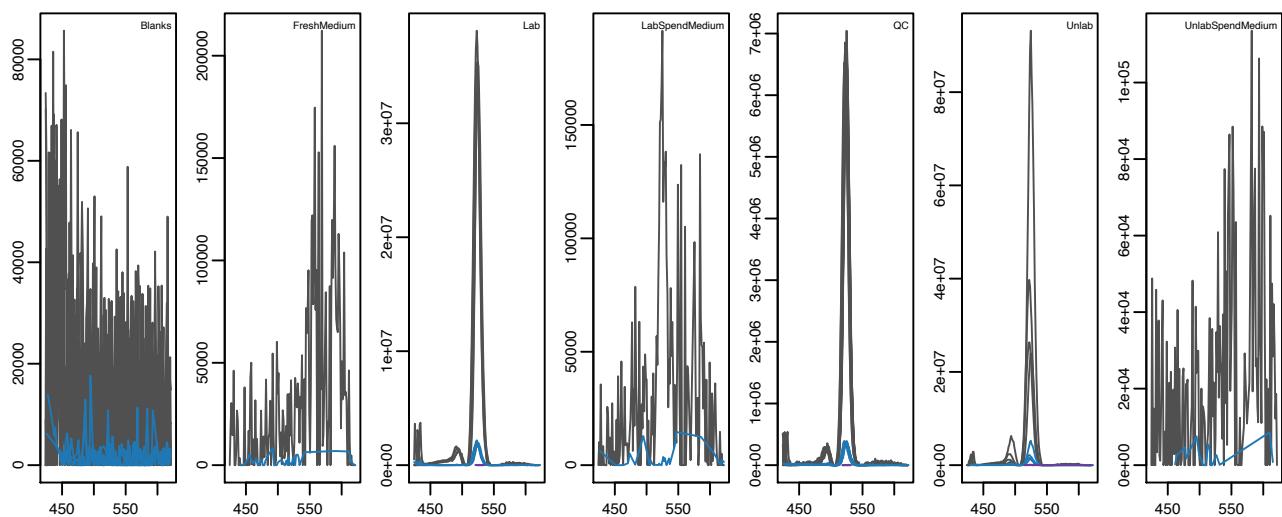


Adenine

Formula: C5H5N5 Mass: 135.054 Std.RT: 523.8 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

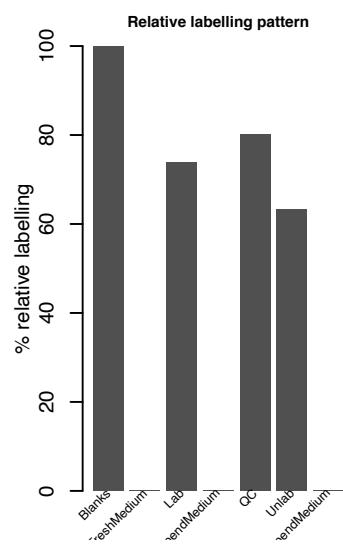
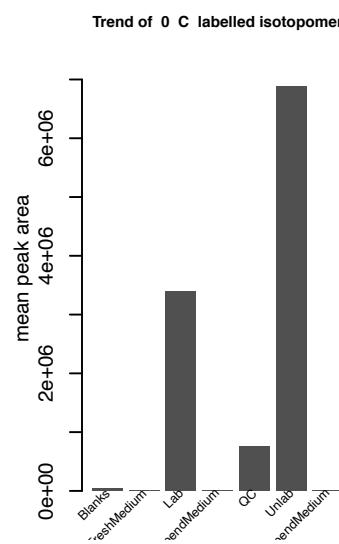
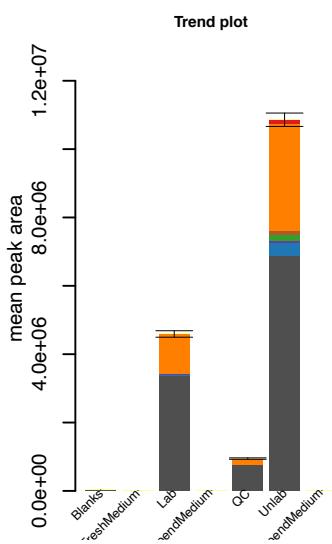
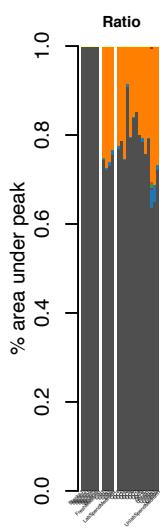
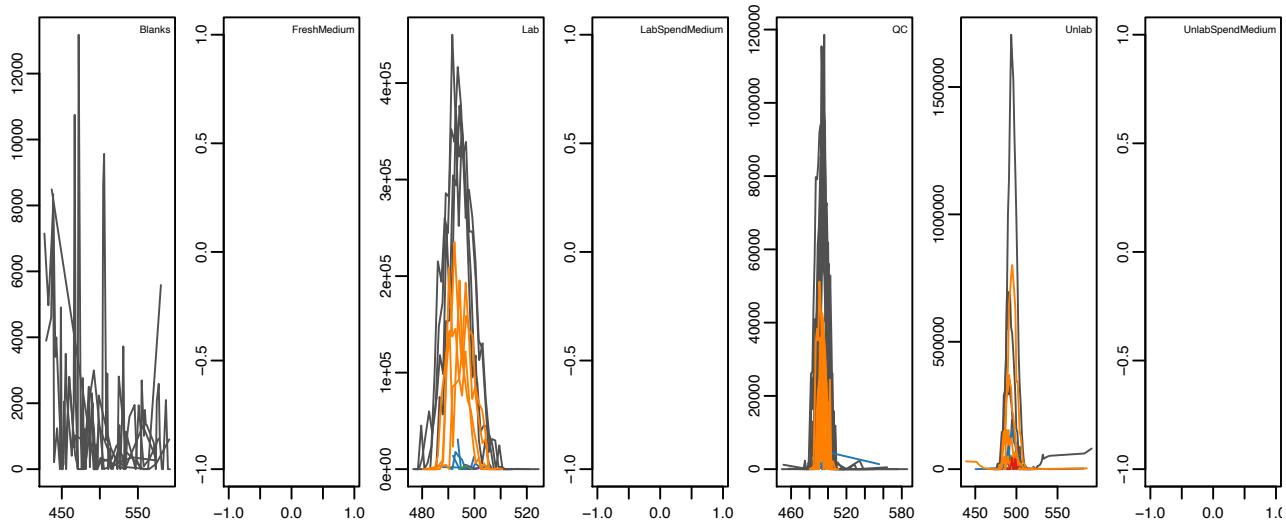


Adenosine

Formula: C₁₀H₁₃N₅O₄ Mass: 267.097 Std.RT: 494.4 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9 ■+10

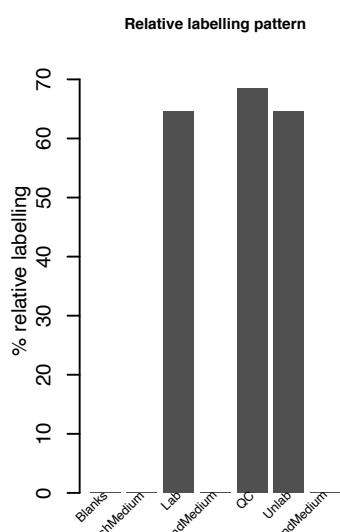
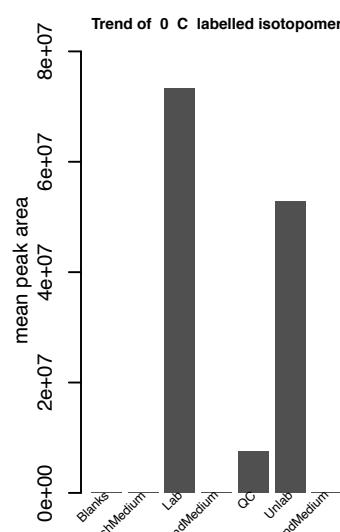
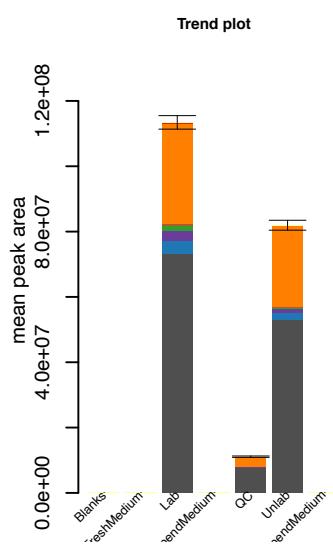
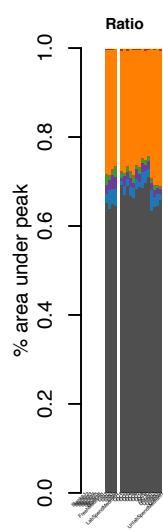
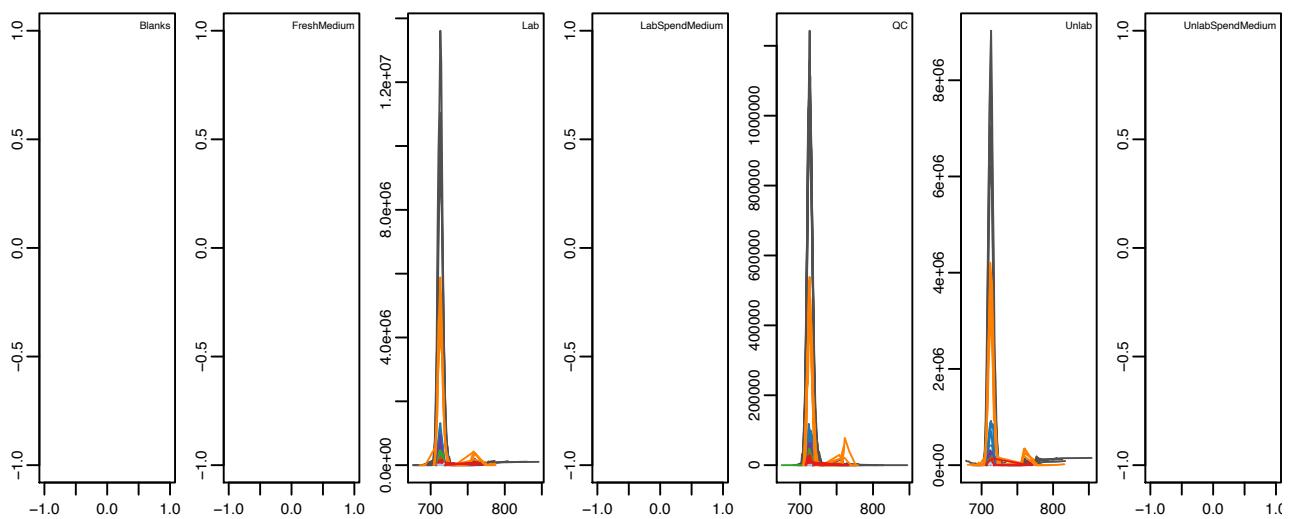


Adenosine 2' 5'-bisphosphate

Formula: C10H15N5O10P2 Mass: 427.029 Std.RT: 761.4 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9 ■+10

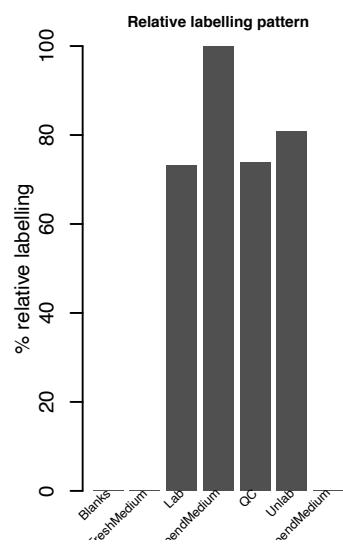
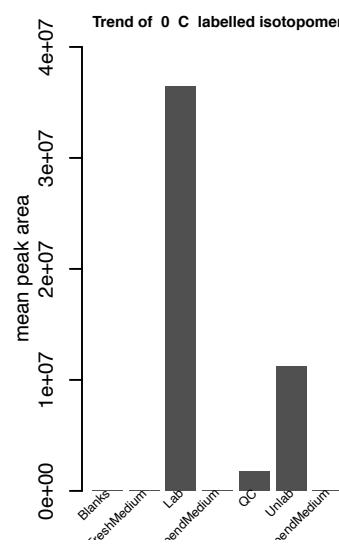
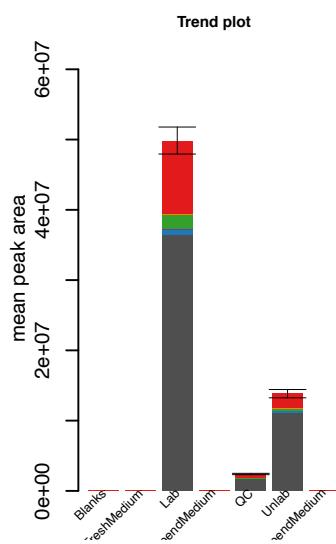
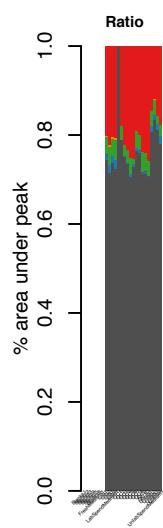
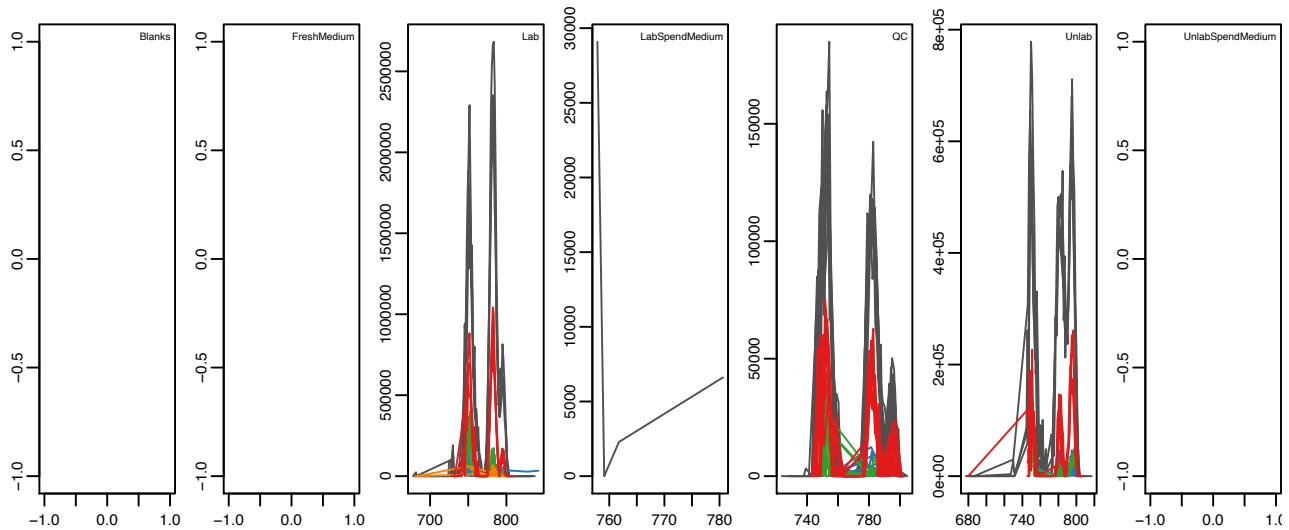


D-Fructose 6-phosphate

Formula: C₆H₁₃O₉P Mass: 260.03 Std.RT: 754.8 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6

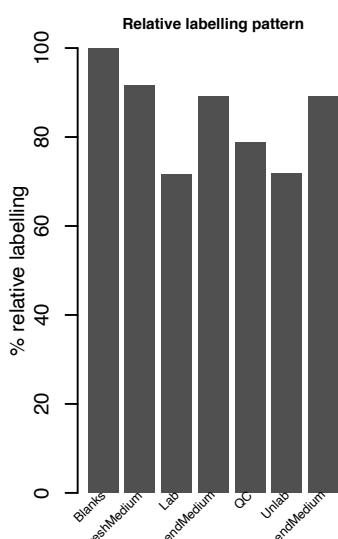
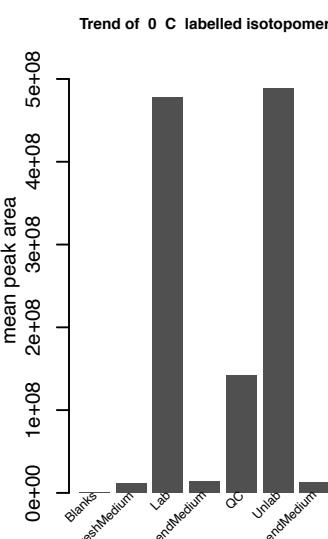
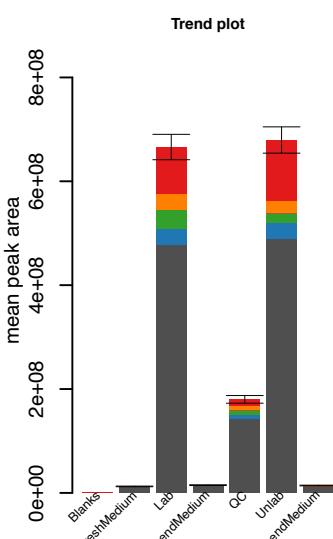
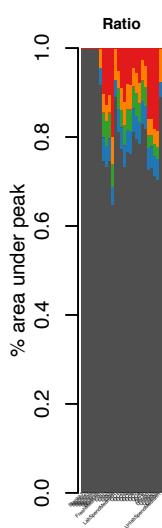
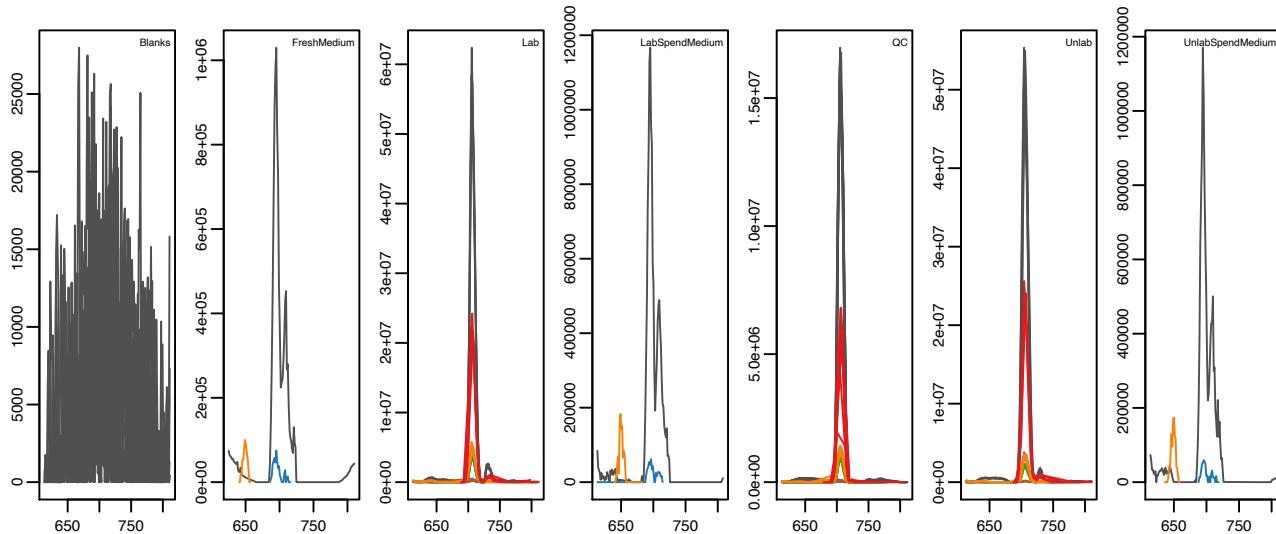


D-Gluconic acid

Formula: C₆H₁₂O₇ Mass: 196.058 Std.RT: 712.8 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6

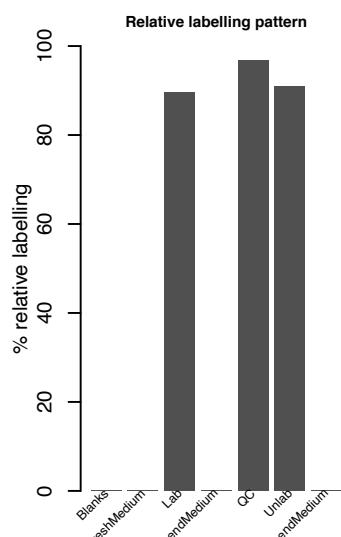
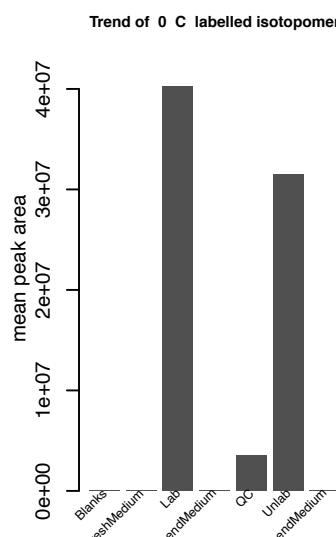
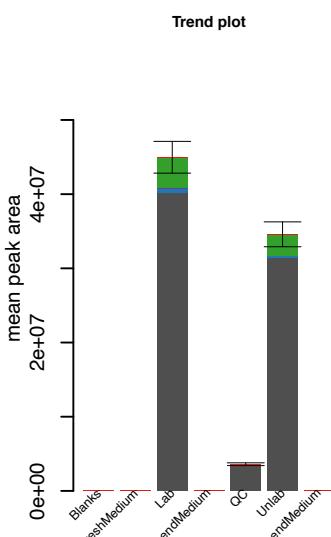
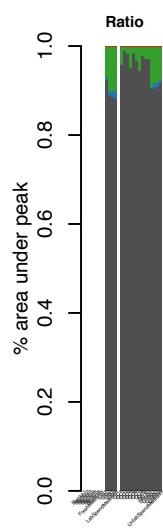
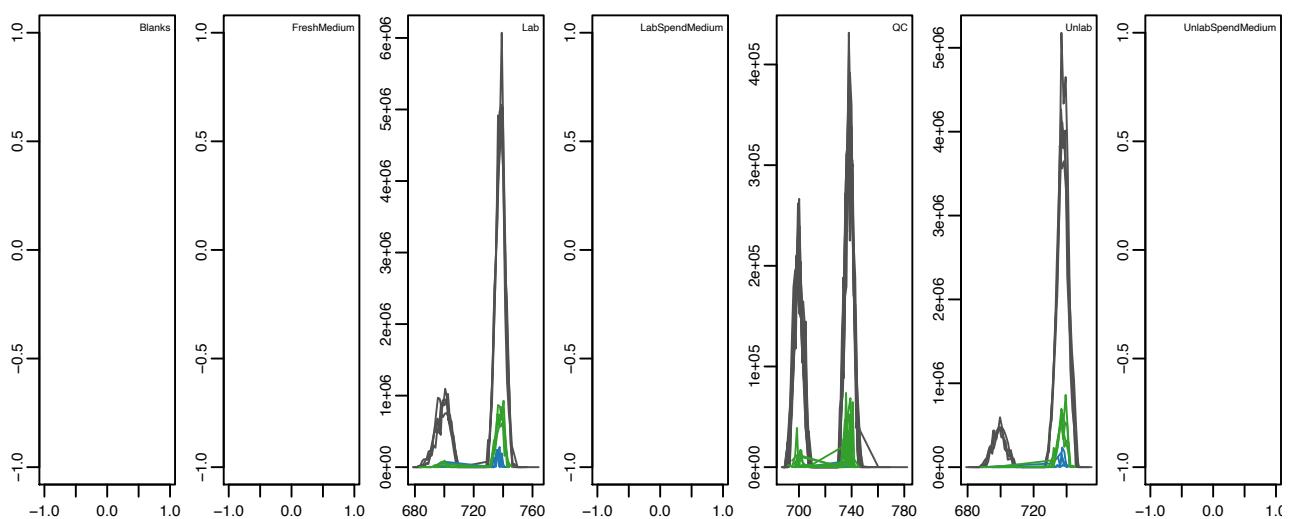


D-Glucosamine-6-phosphate

Formula: C₆H₁₄NO₈P Mass: 259.046 Std.RT: 759 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6

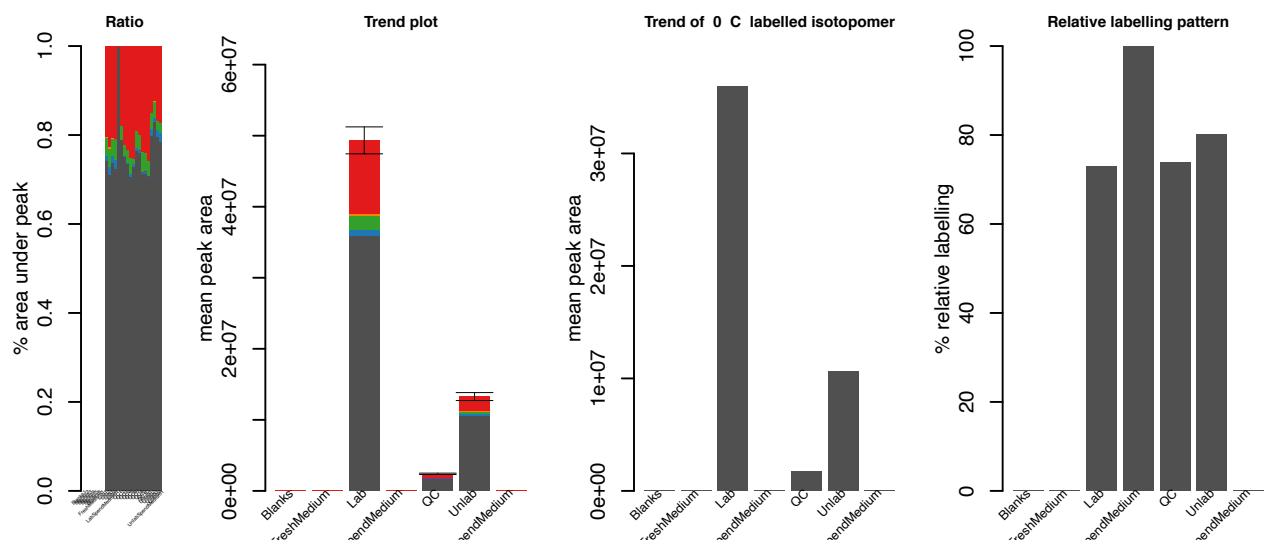
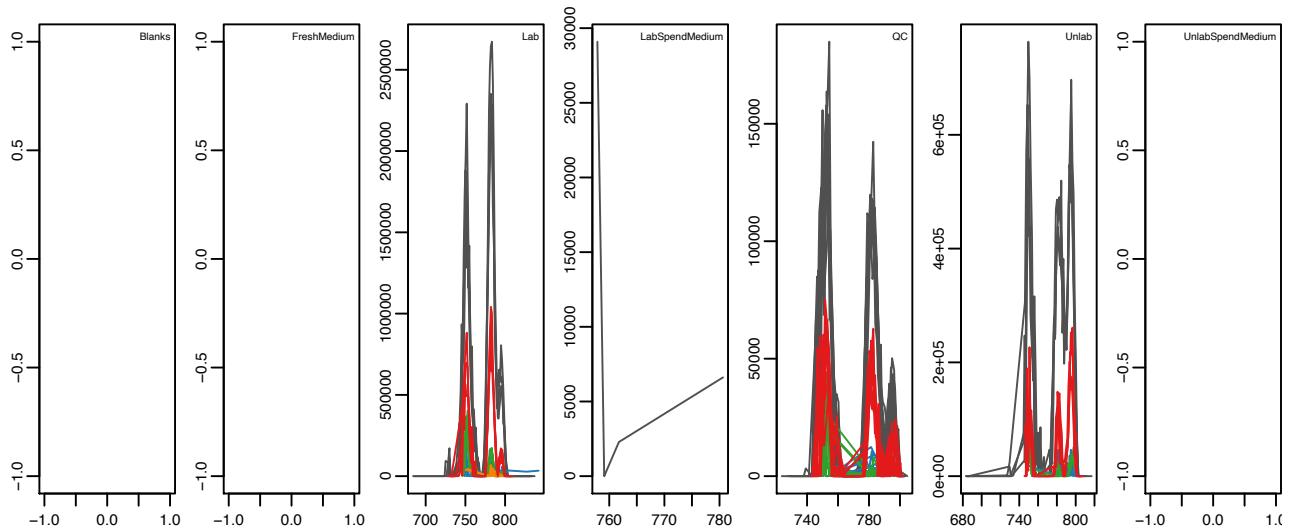


D-glucose 6-phosphate

Formula: C₆H₁₃O₉P Mass: 260.03 Std.RT: 783 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6

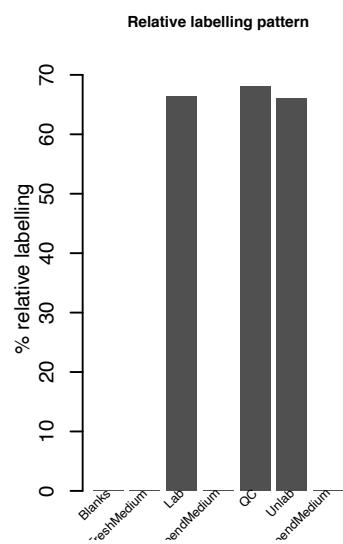
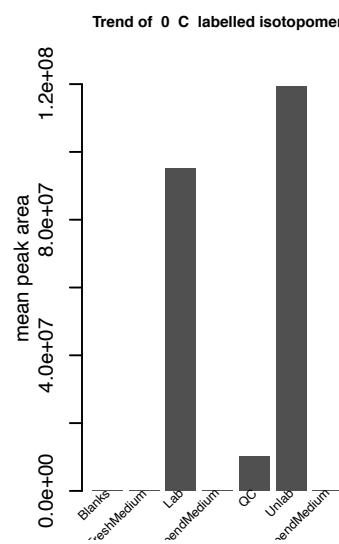
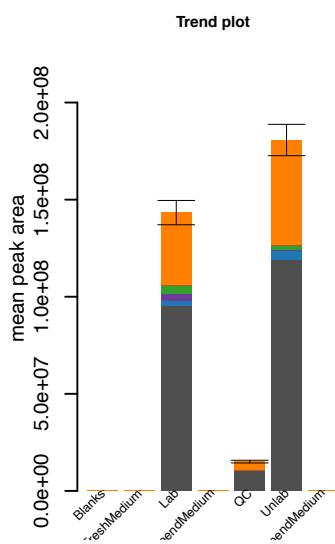
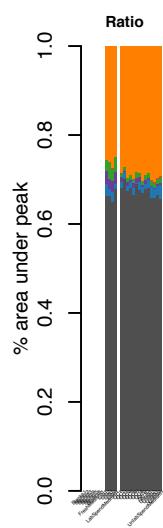
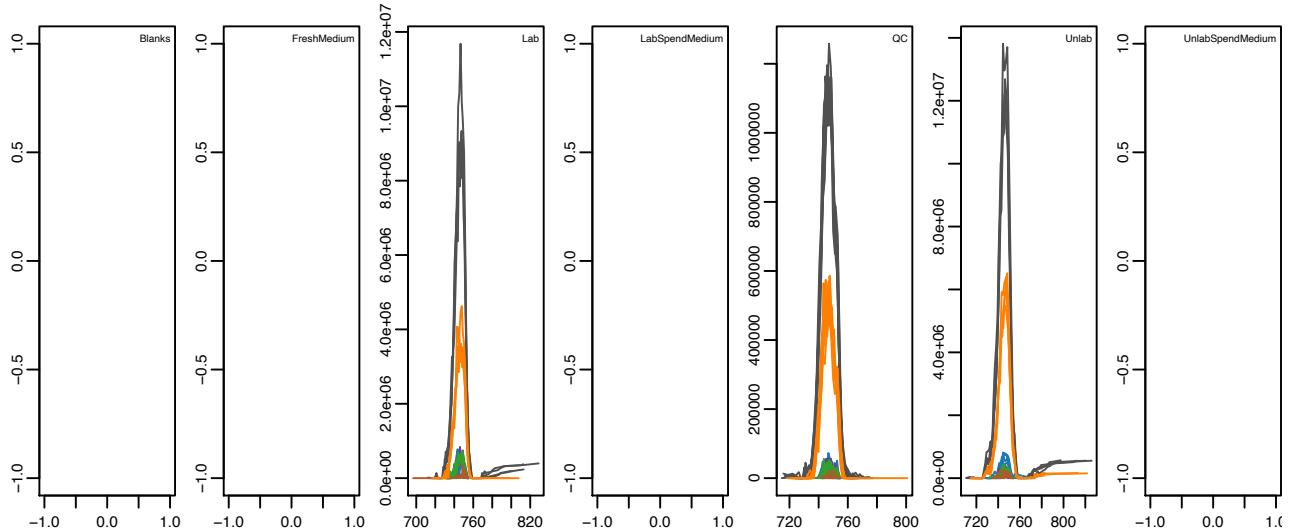


D-ribose 5-phosphate

Formula: C₅H₁₁O₈P Mass: 230.019 Std.RT: 750 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

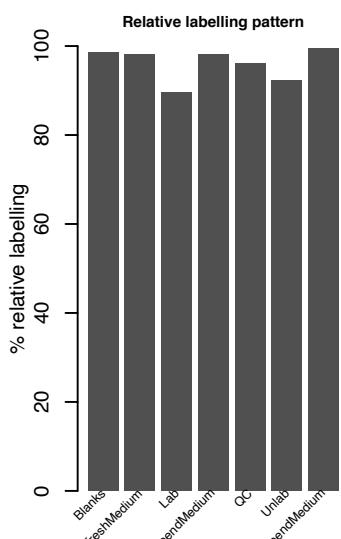
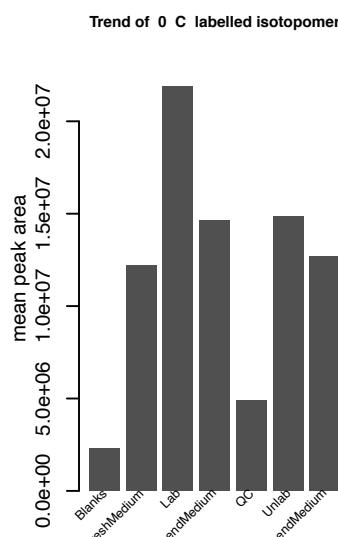
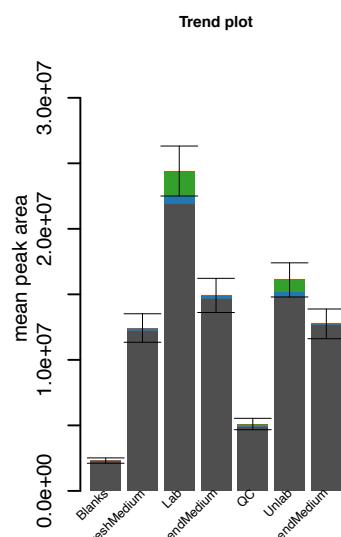
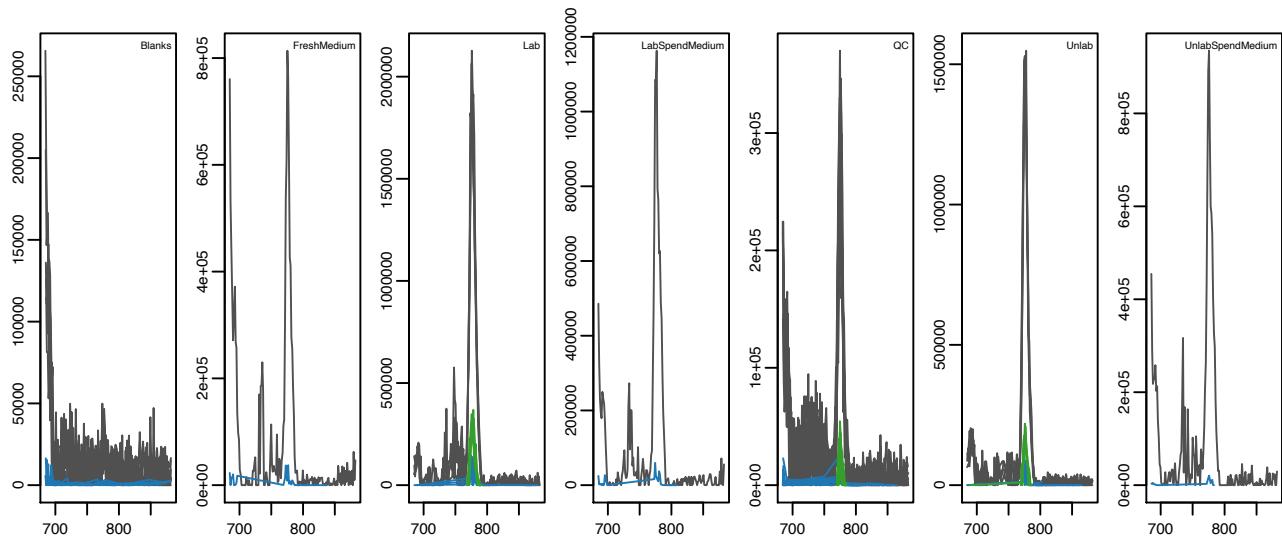


Fumarate

Formula: C₄H₄O₄ Mass: 116.011 Std.RT: 784.2 Ion: NEG

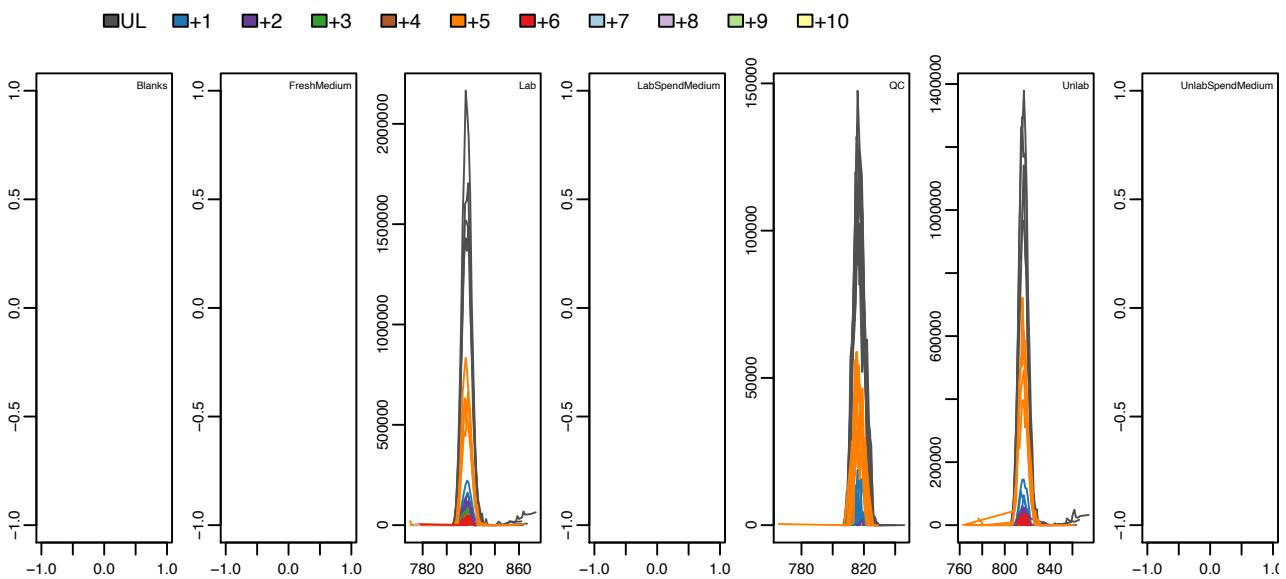
G1

■UL ■+1 ■+2 ■+3 ■+4

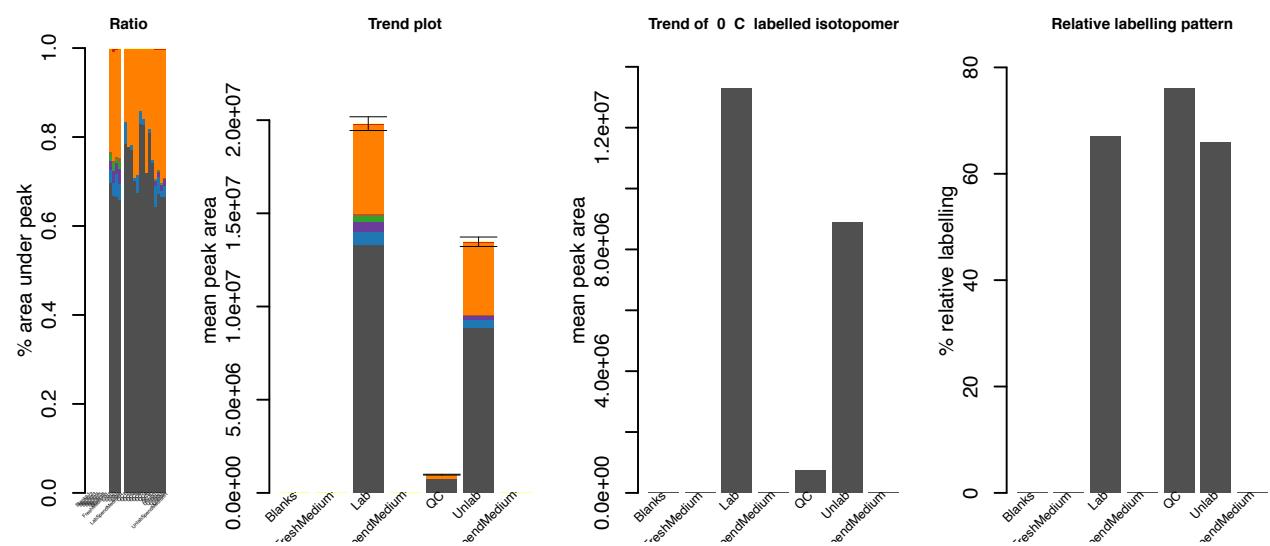


GDP

Formula: C10H15N5O11P2 Mass: 443.024 Std.RT: 816 Ion: NEG



G1

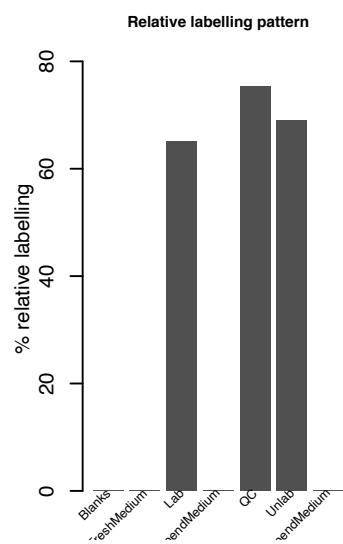
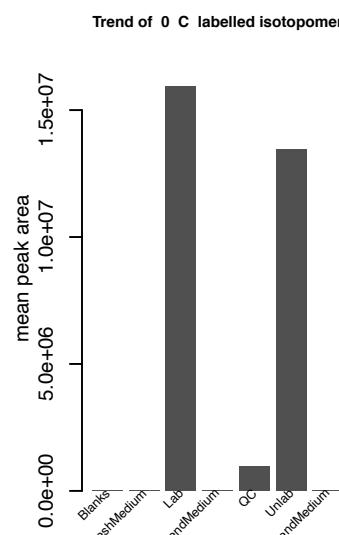
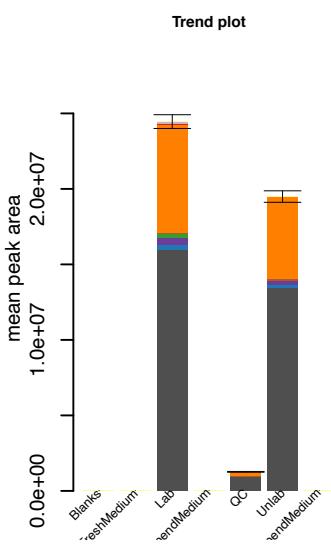
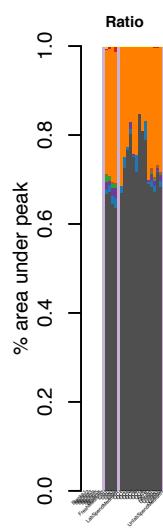
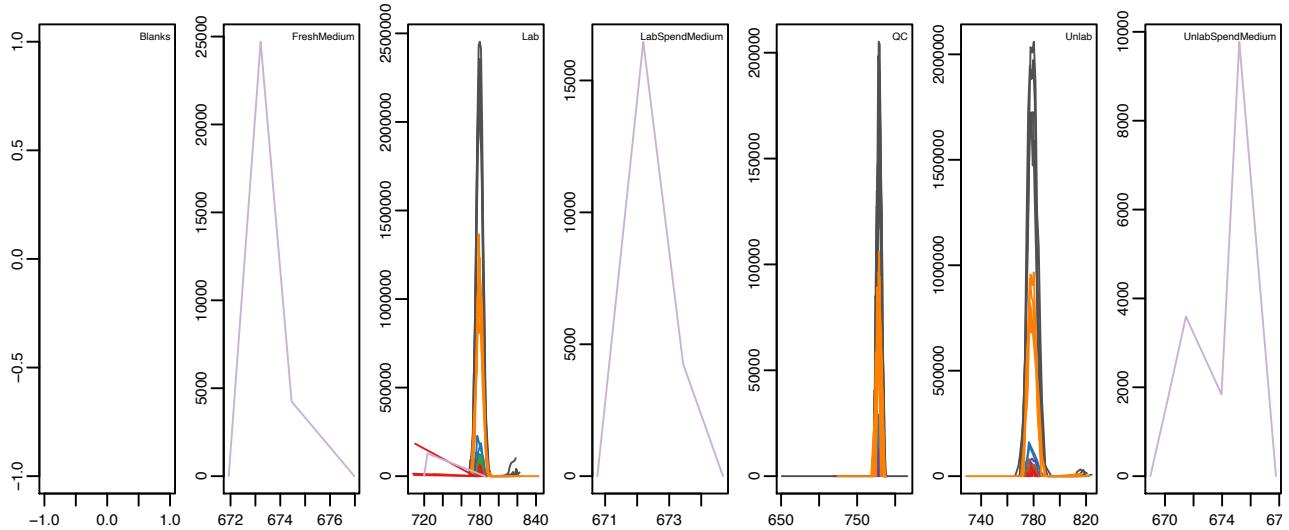


GMP

Formula: C₁₀H₁₄N₅O₈P Mass: 363.058 Std.RT: 747 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9 ■+10

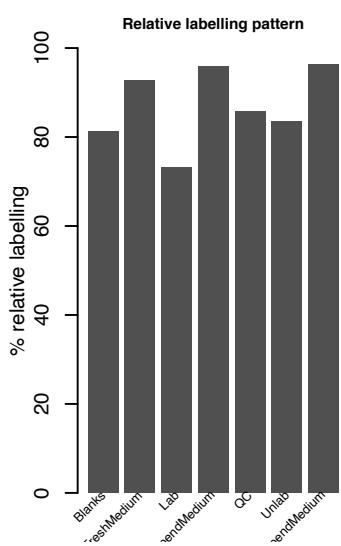
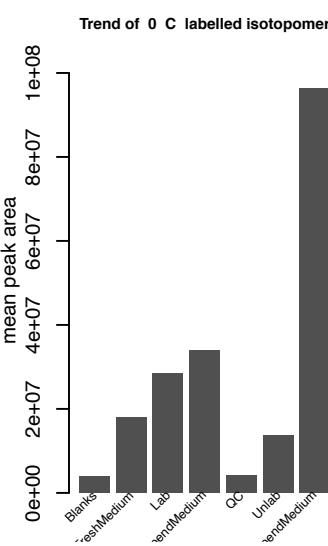
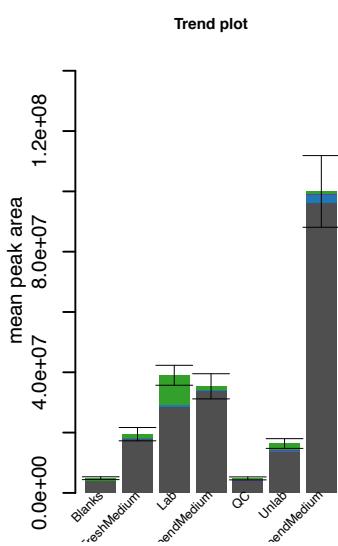
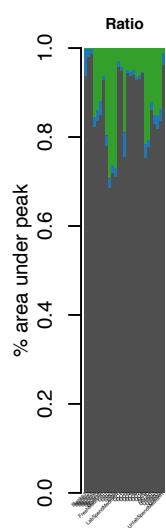
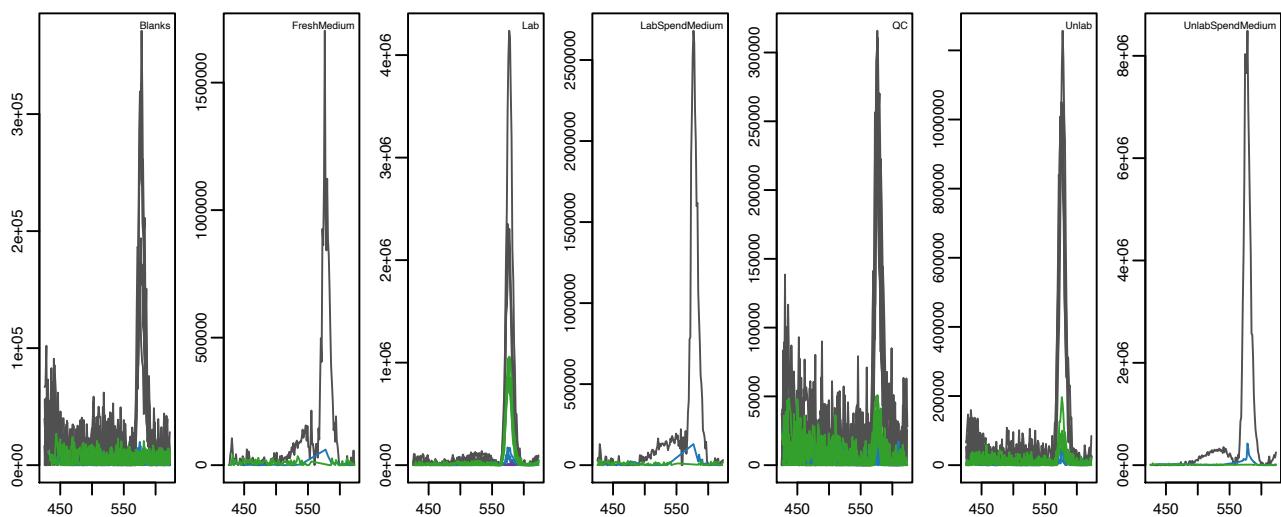


Glycerol

Formula: C₃H₈O₃ Mass: 92.047 Std.RT: 525 Ion: NEG

G1

■UL ■+1 ■+2 ■+3

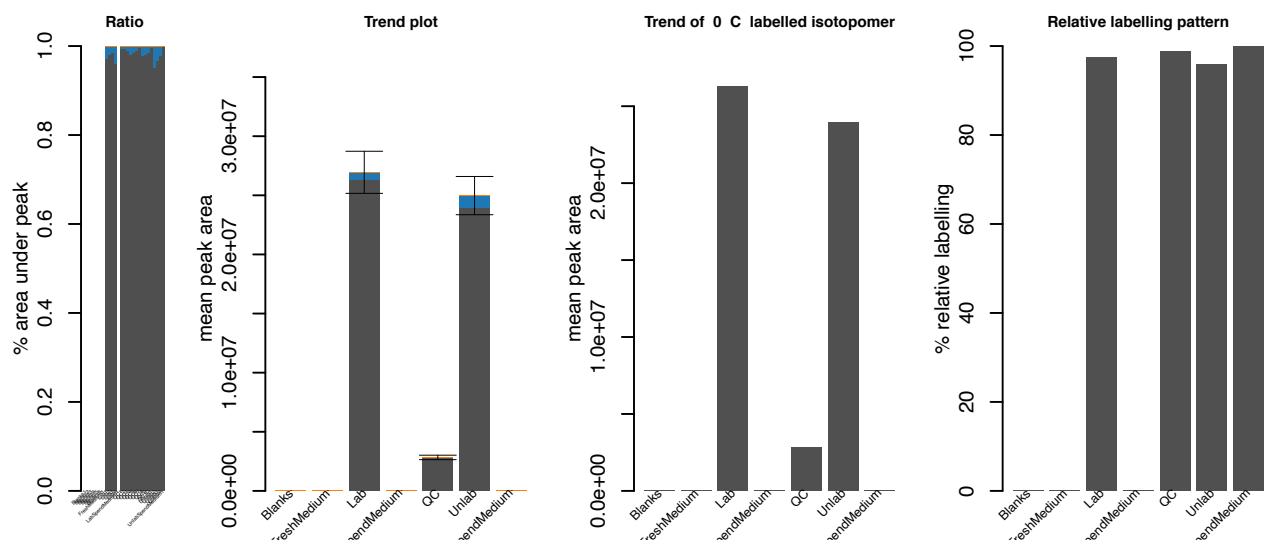
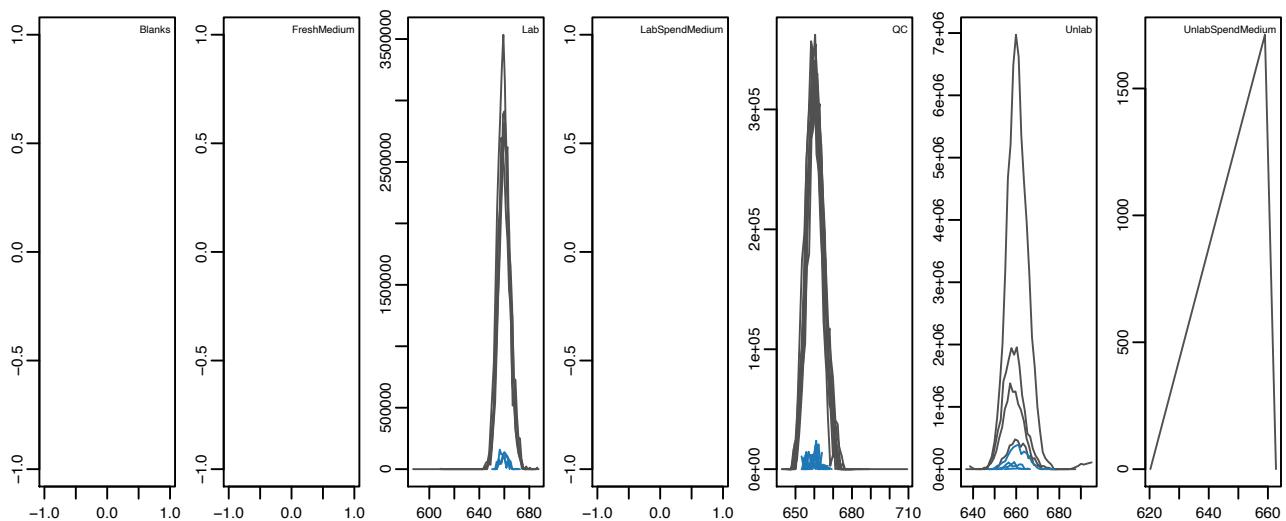


Guanine

Formula: C5H5N5O Mass: 151.049 Std.RT: 664.2 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

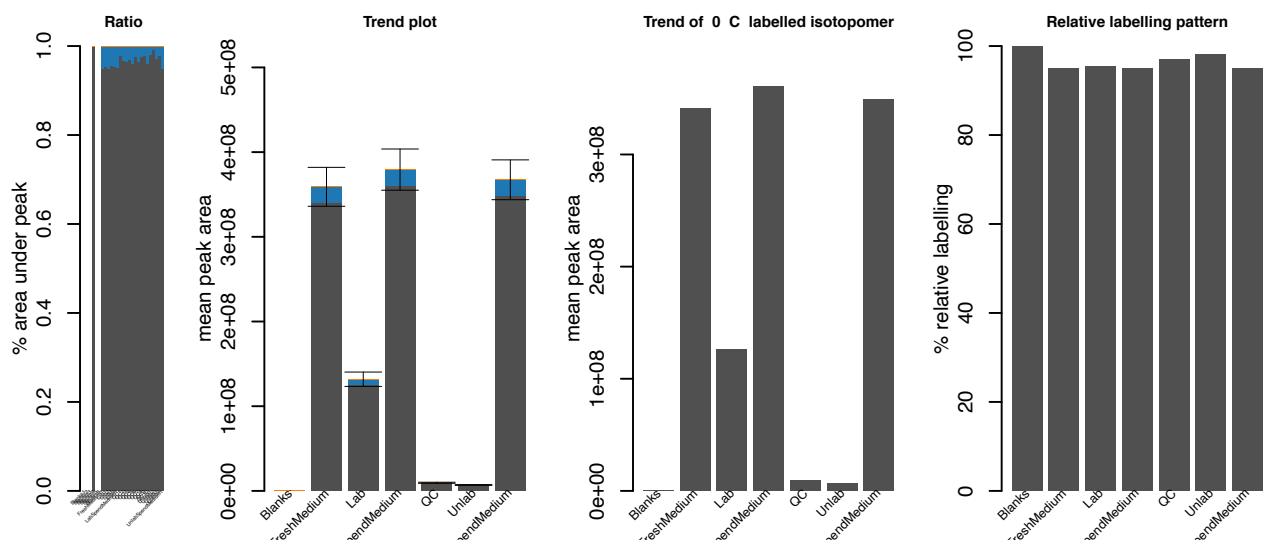
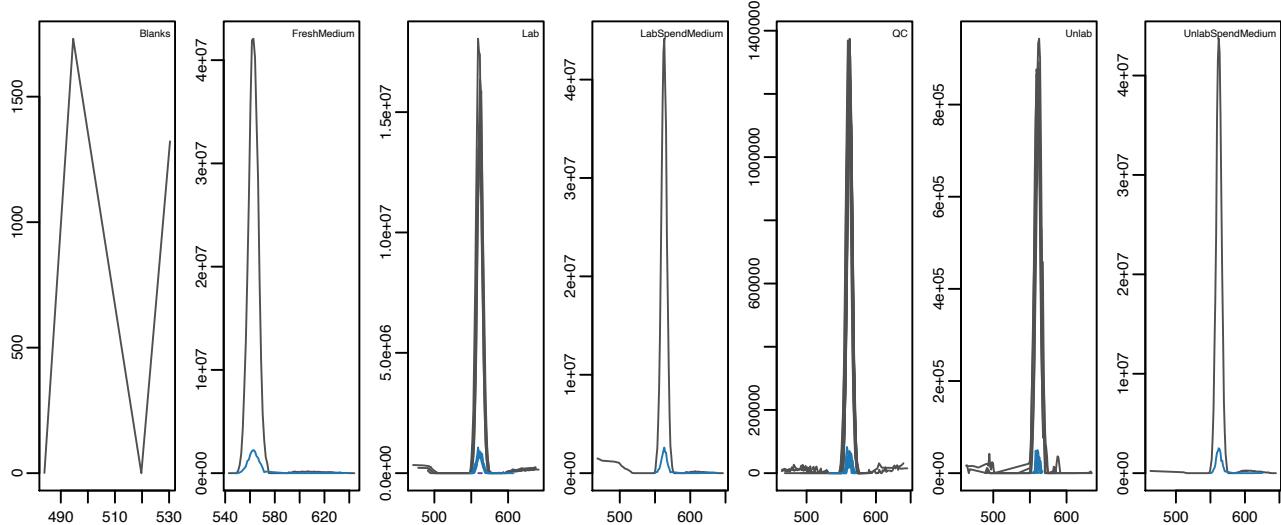


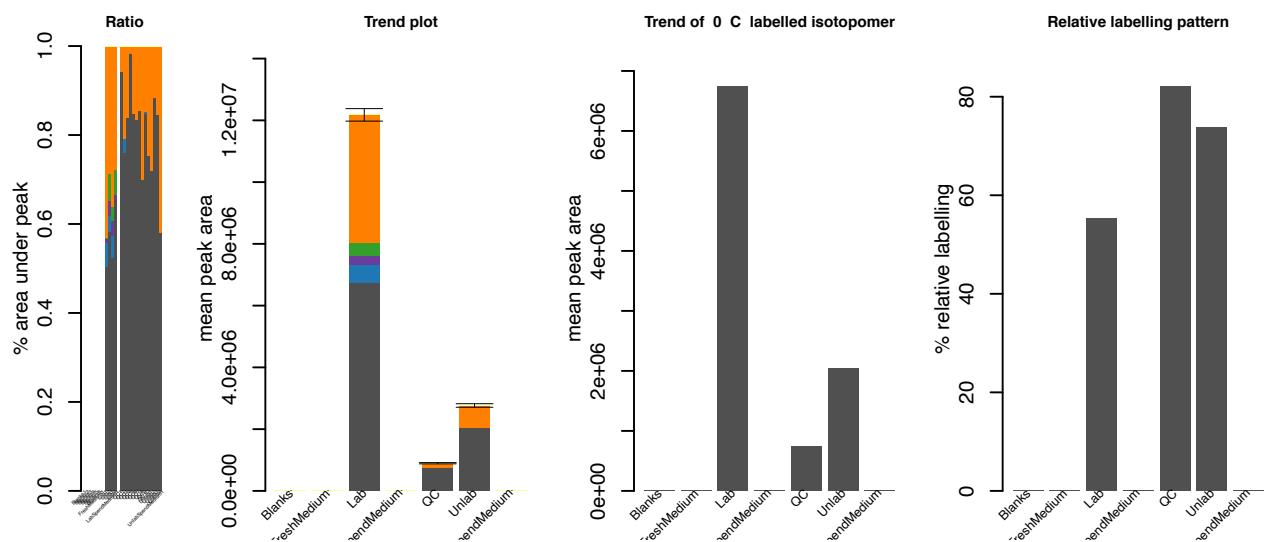
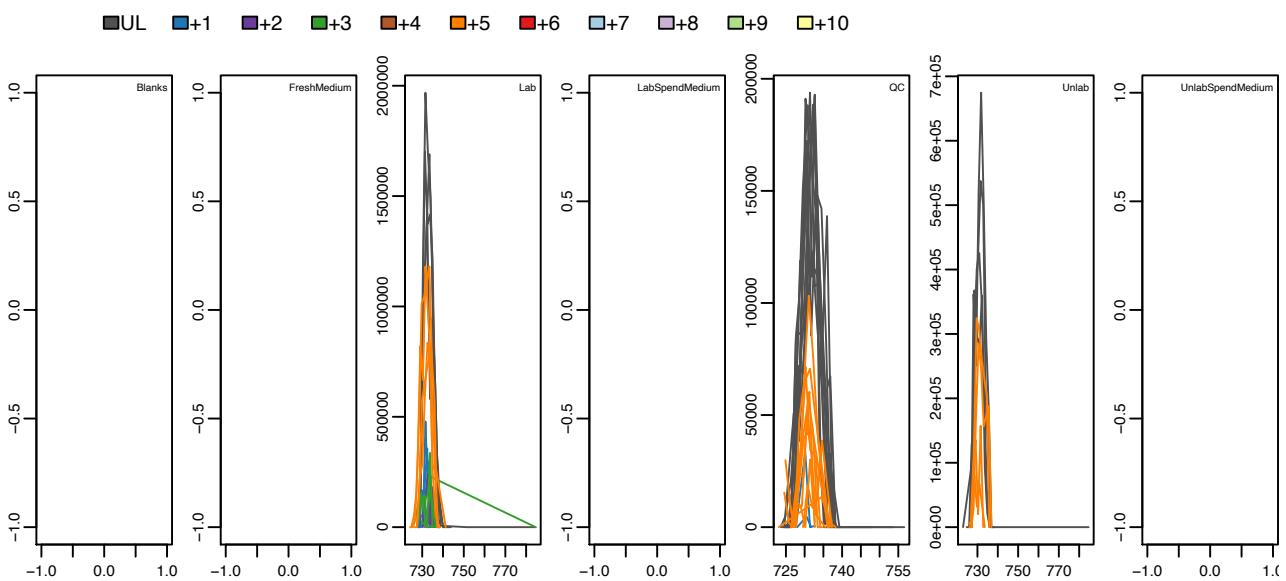
Hypoxanthine

Formula: C5H4N4O Mass: 136.039 Std.RT: 562.2 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5



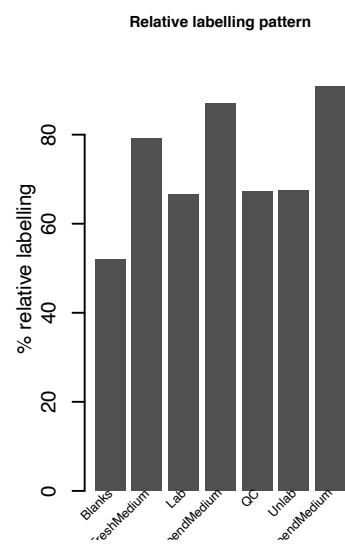
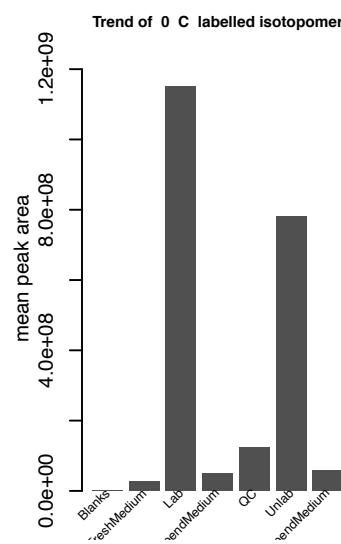
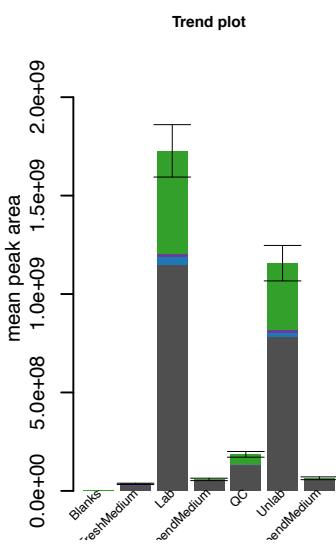
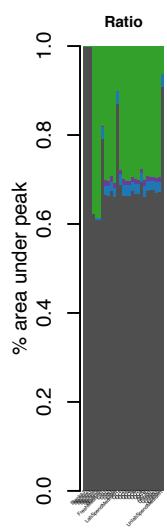
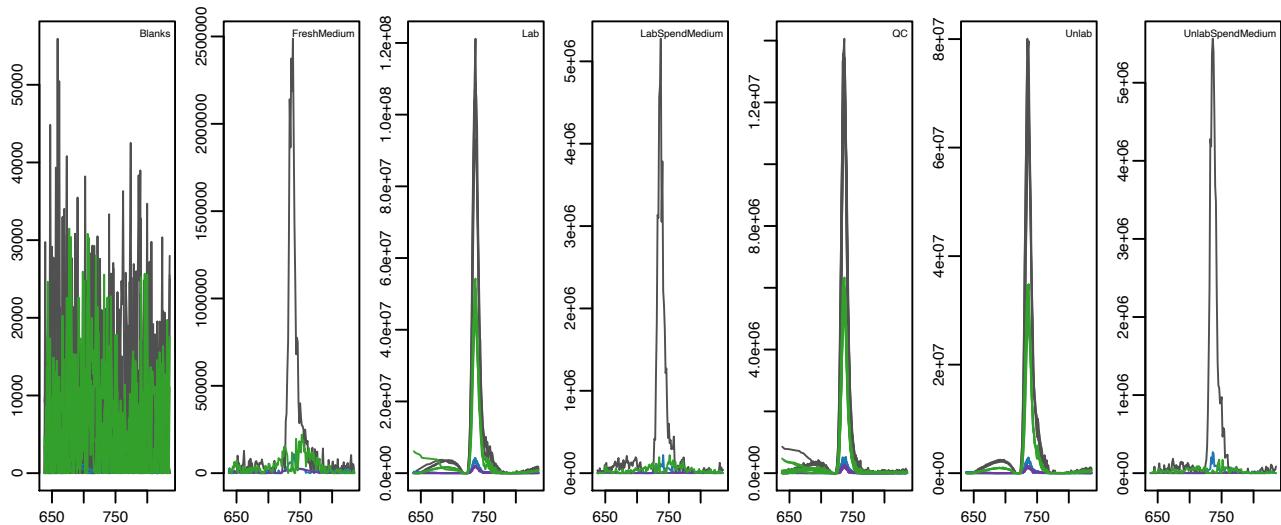
IMPFormula: C₁₀H₁₃N₄O₈P Mass: 348.047 Std.RT: 732.6 Ion: NEG**G1**

L-Alanine

Formula: C3H7NO2 Mass: 89.048 Std.RT: 737.4 Ion: NEG

G1

■UL ■+1 ■+2 ■+3

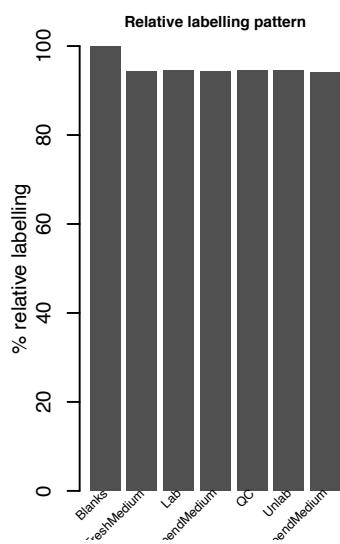
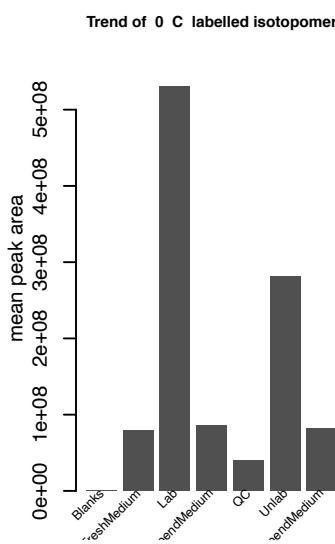
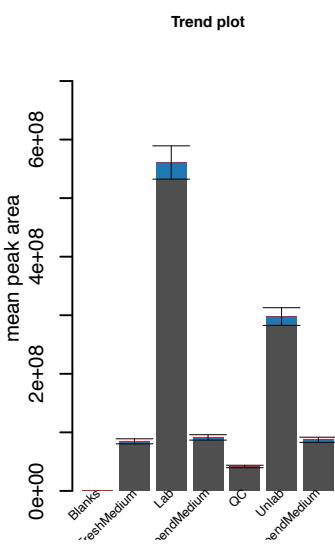
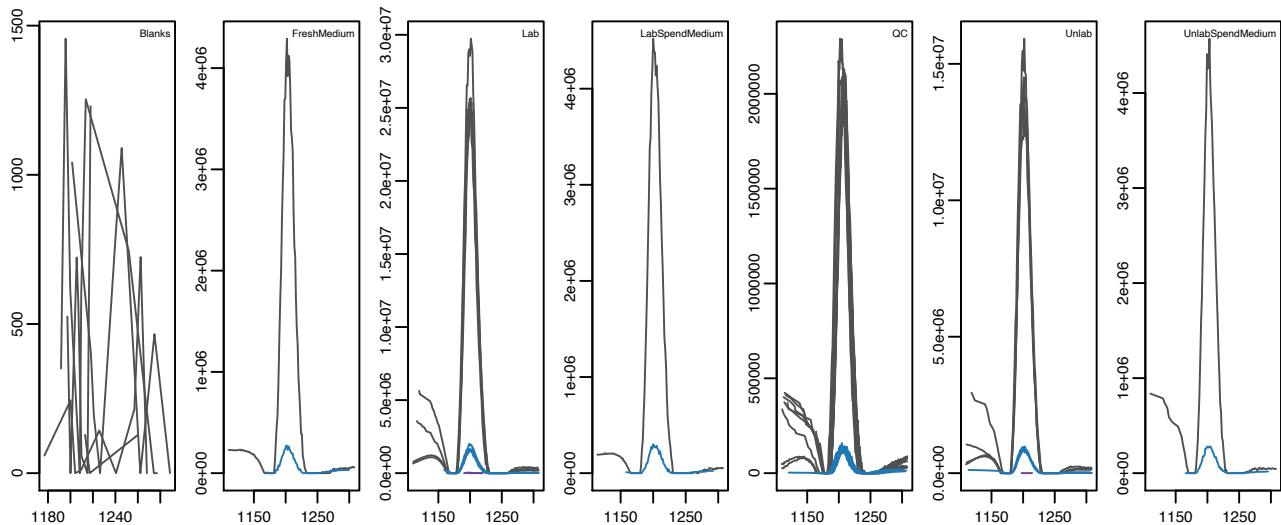


L-Arginine

Formula: C₆H₁₄N₄O₂ Mass: 174.112 Std.RT: 1209.6 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6

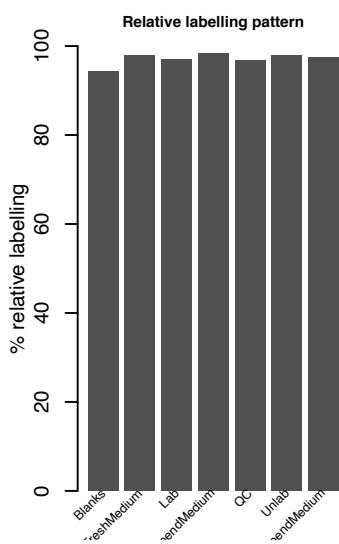
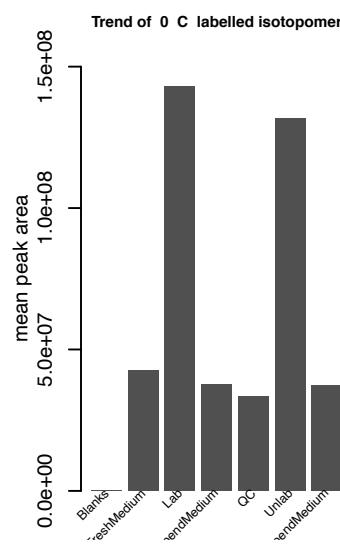
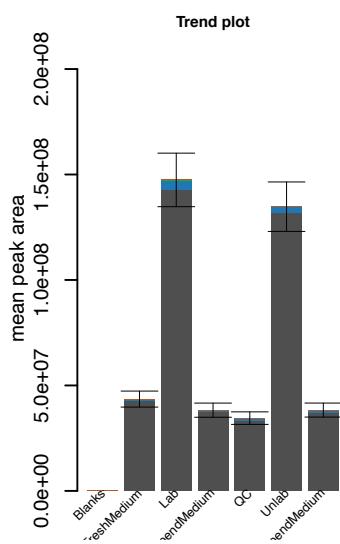
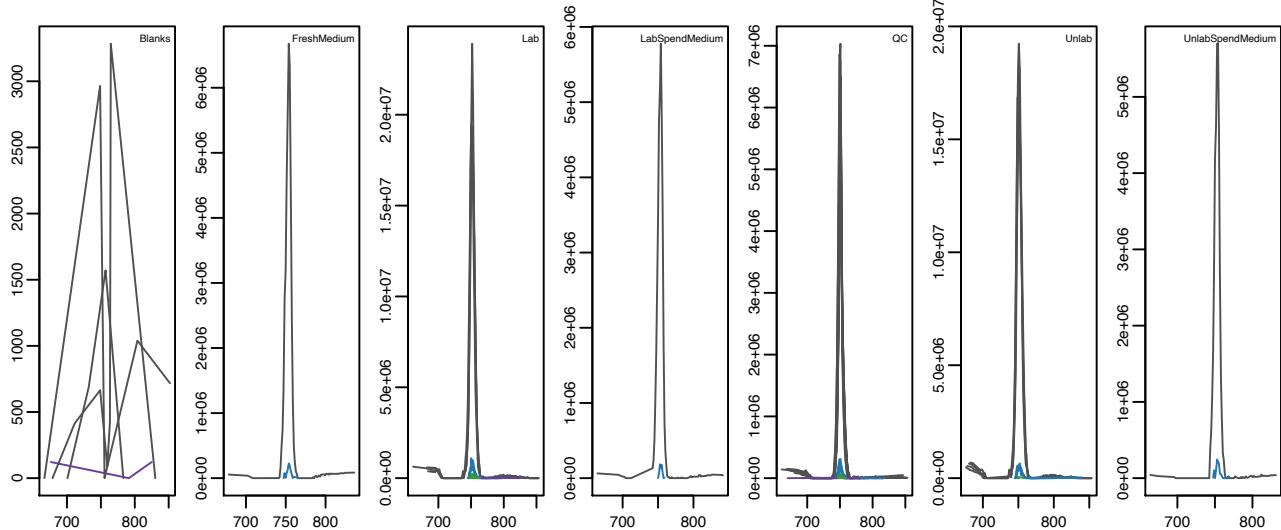


L-Asparagine

Formula: C₄H₈N₂O₃ Mass: 132.053 Std.RT: 754.8 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4

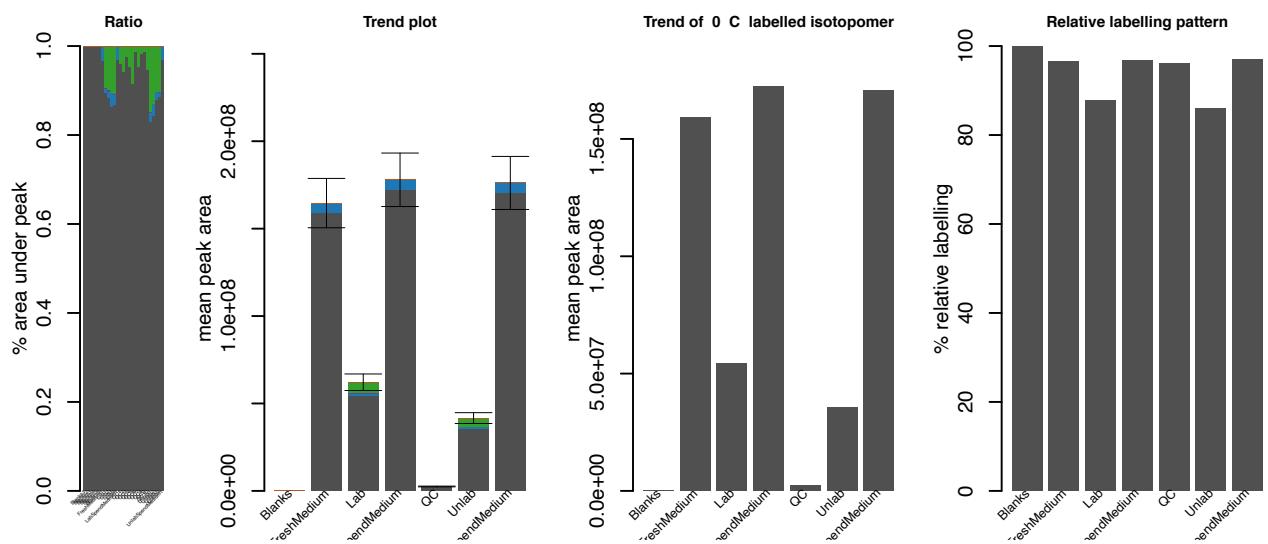
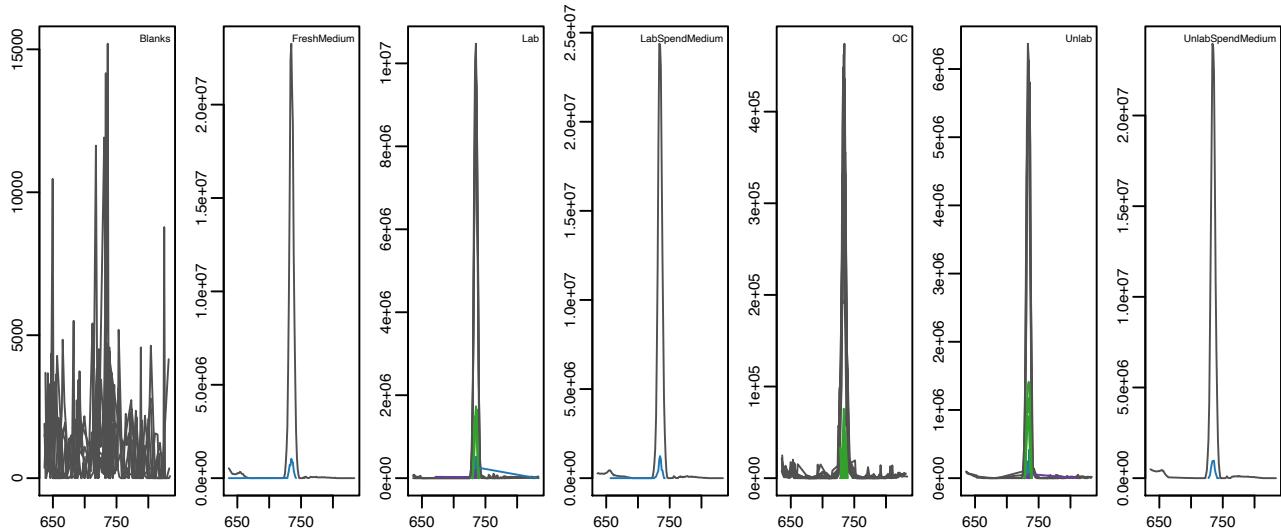


L-Aspartate

Formula: C₄H₇NO₄ Mass: 133.038 Std.RT: 735.6 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4

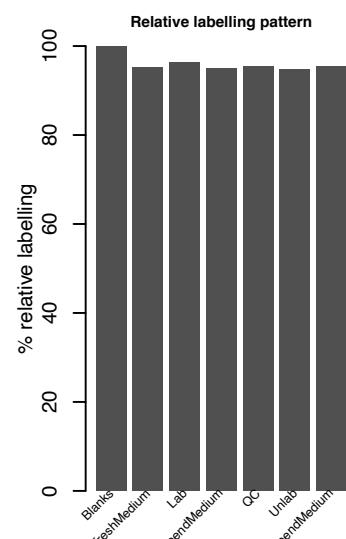
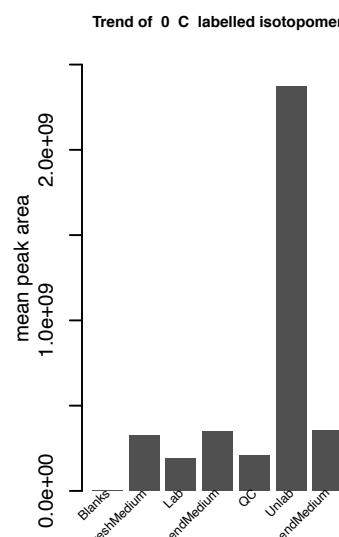
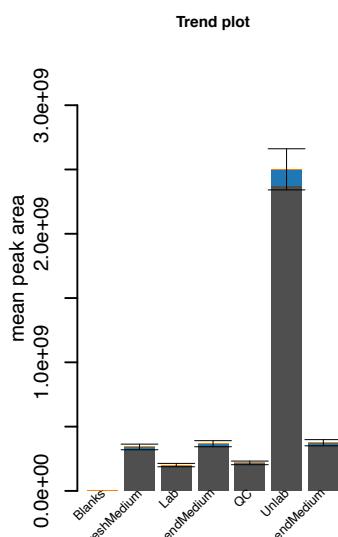
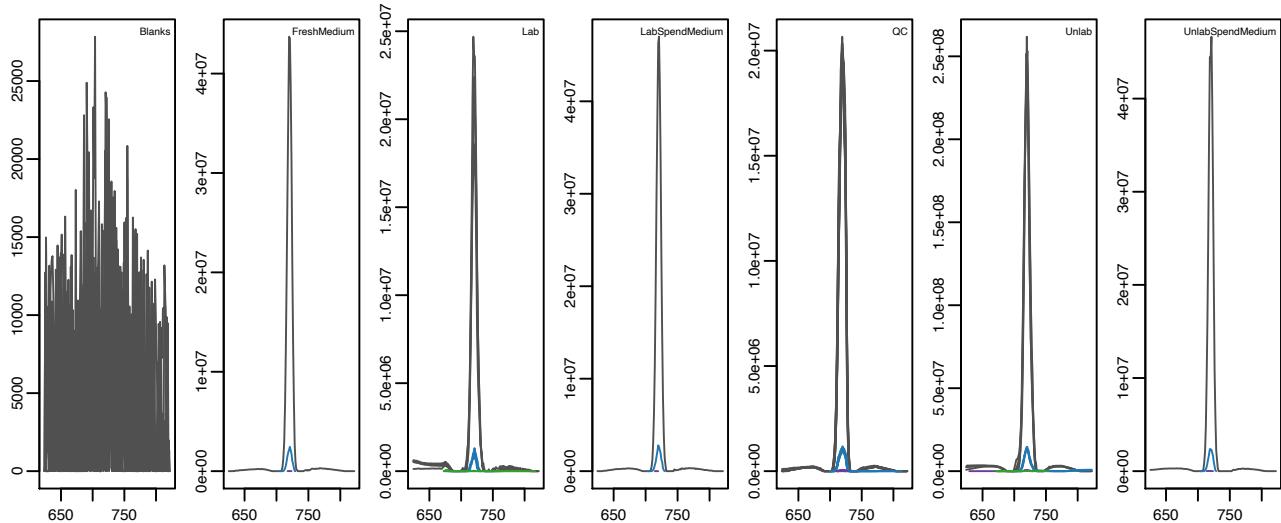


L-Glutamate

Formula: C5H9NO4 Mass: 147.053 Std.RT: 723.6 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

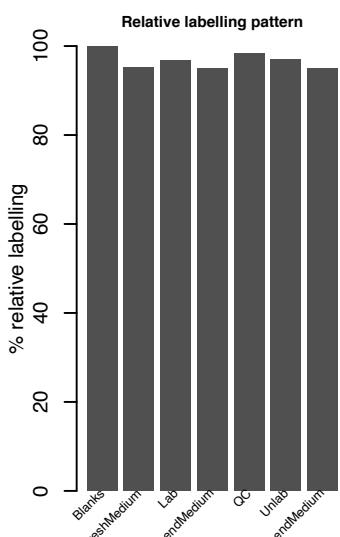
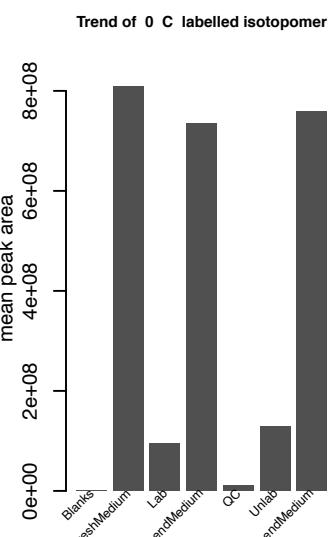
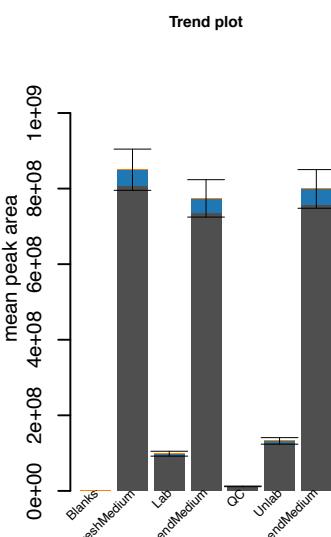
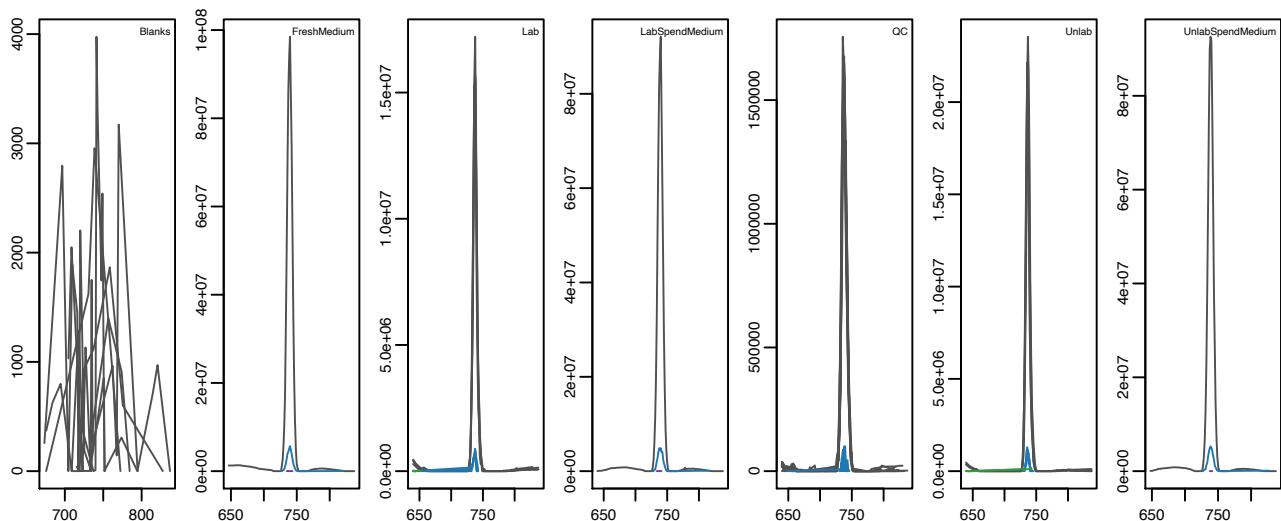


L-Glutamine

Formula: C5H10N2O3 Mass: 146.069 Std.RT: 739.2 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

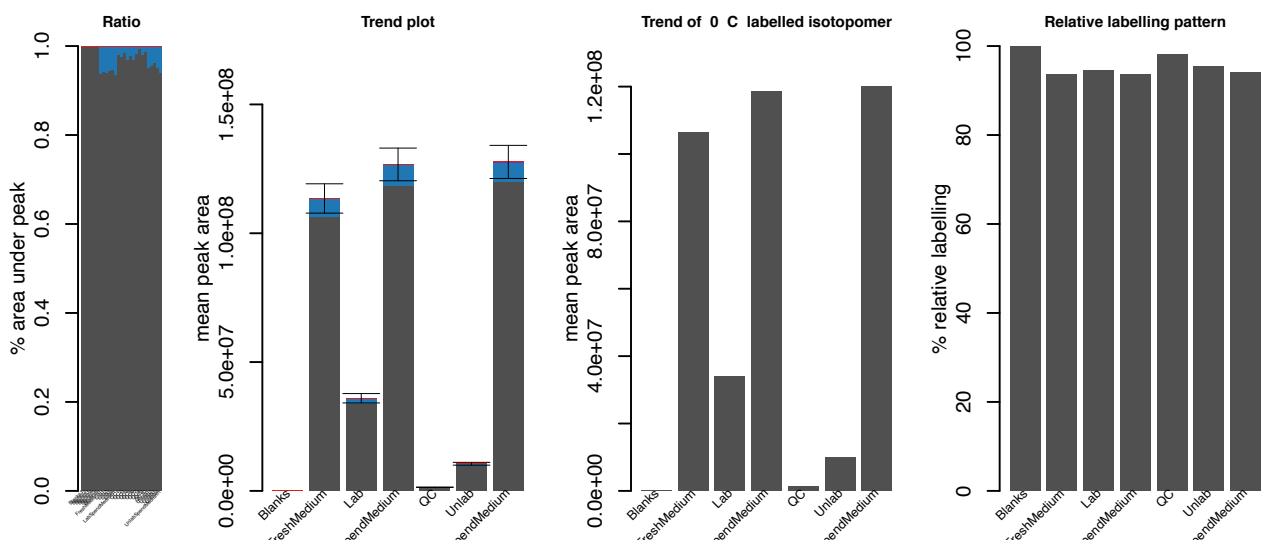
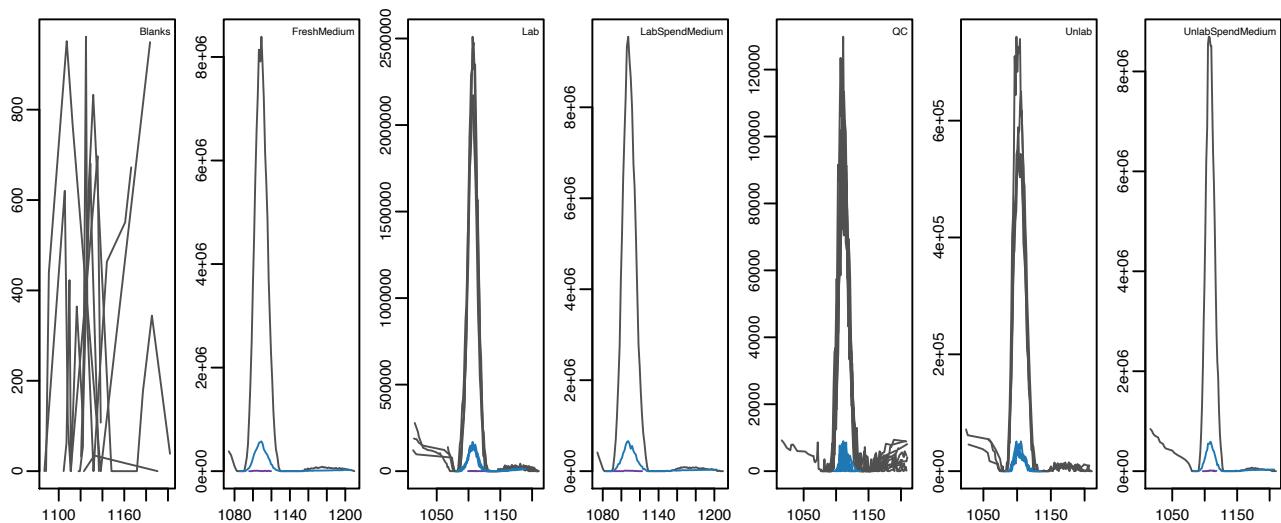


L-Lysine

Formula: C₆H₁₄N₂O₂ Mass: 146.106 Std.RT: 1111.8 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6

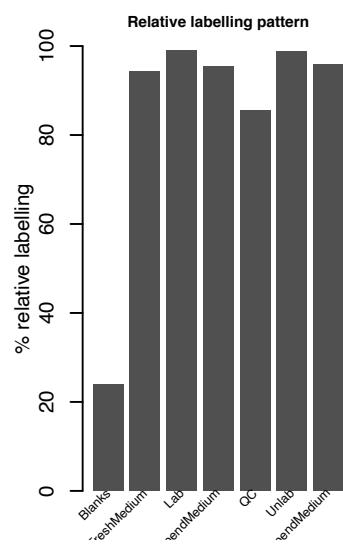
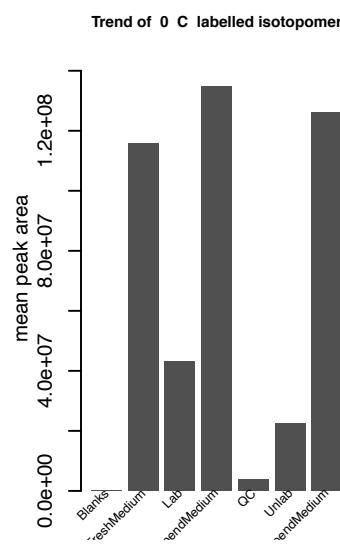
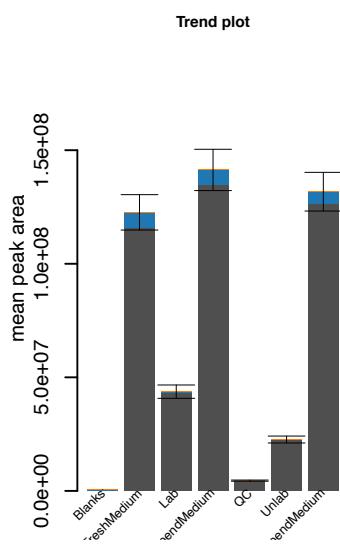
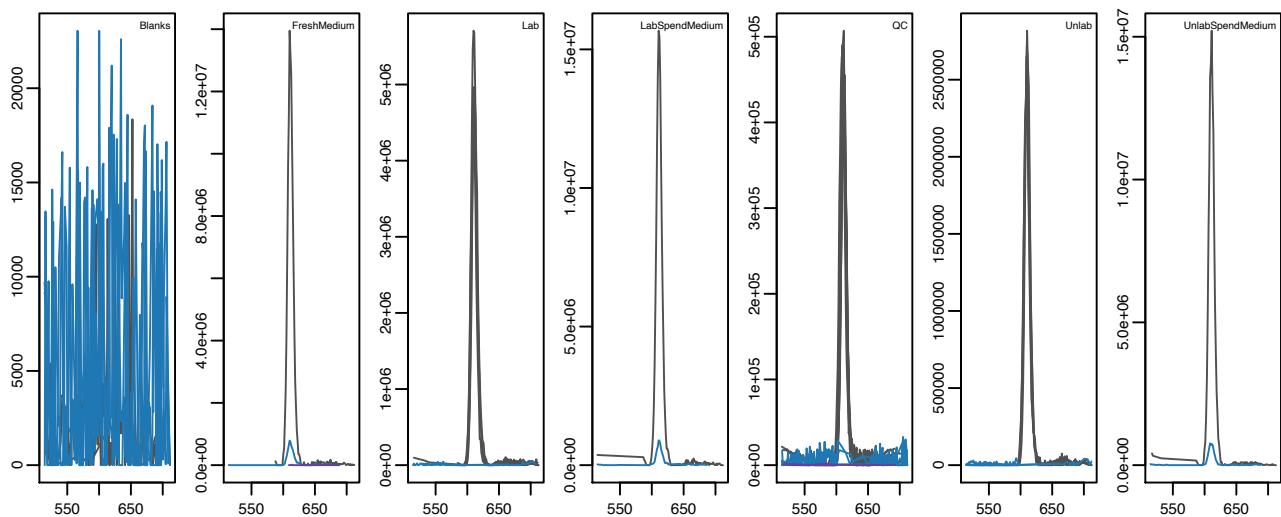


L-Methionine

Formula: C₅H₁₁NO₂S Mass: 149.051 Std.RT: 613.8 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

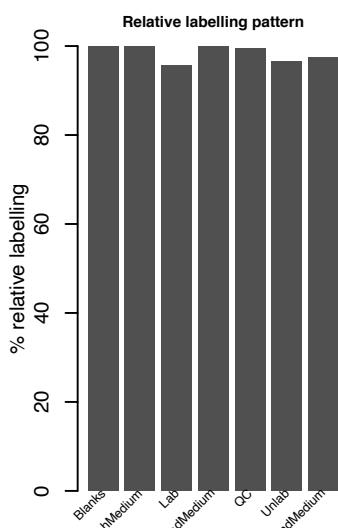
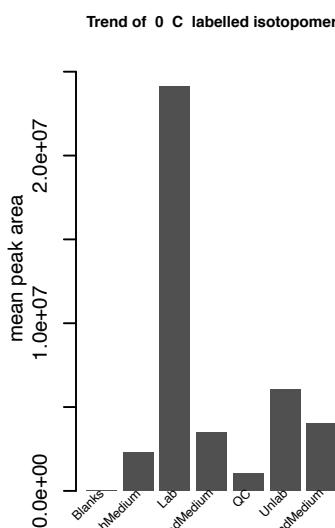
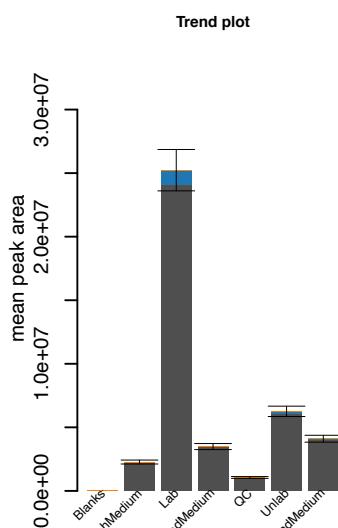
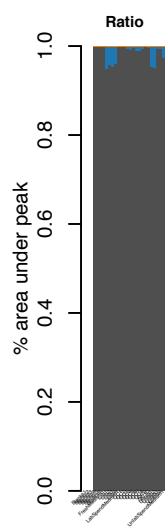
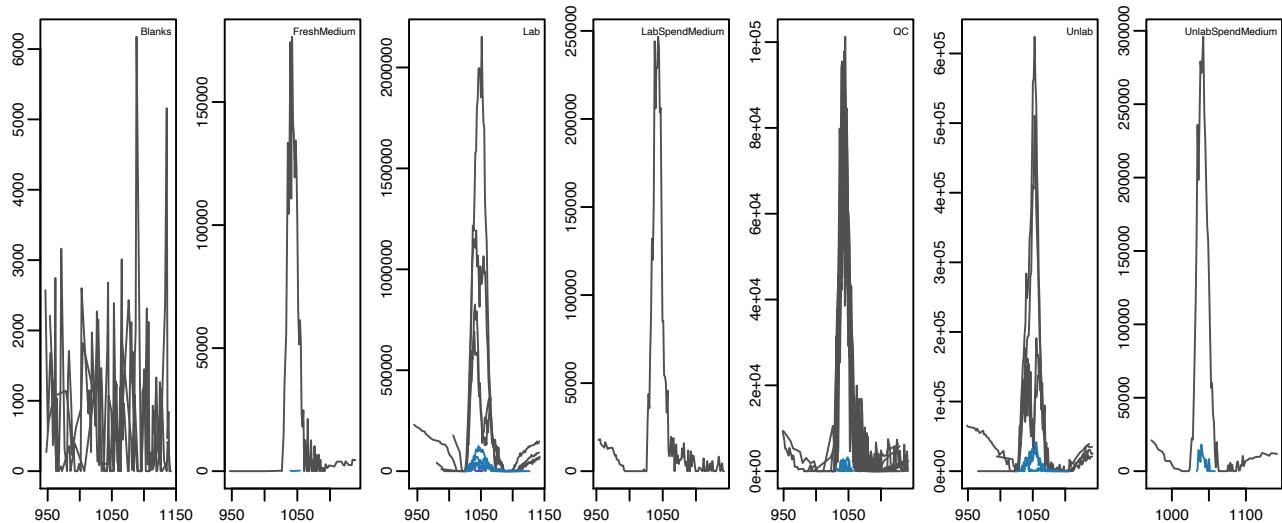


L-Ornithine

Formula: C5H12N2O2 Mass: 132.09 Std.RT: 1044 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

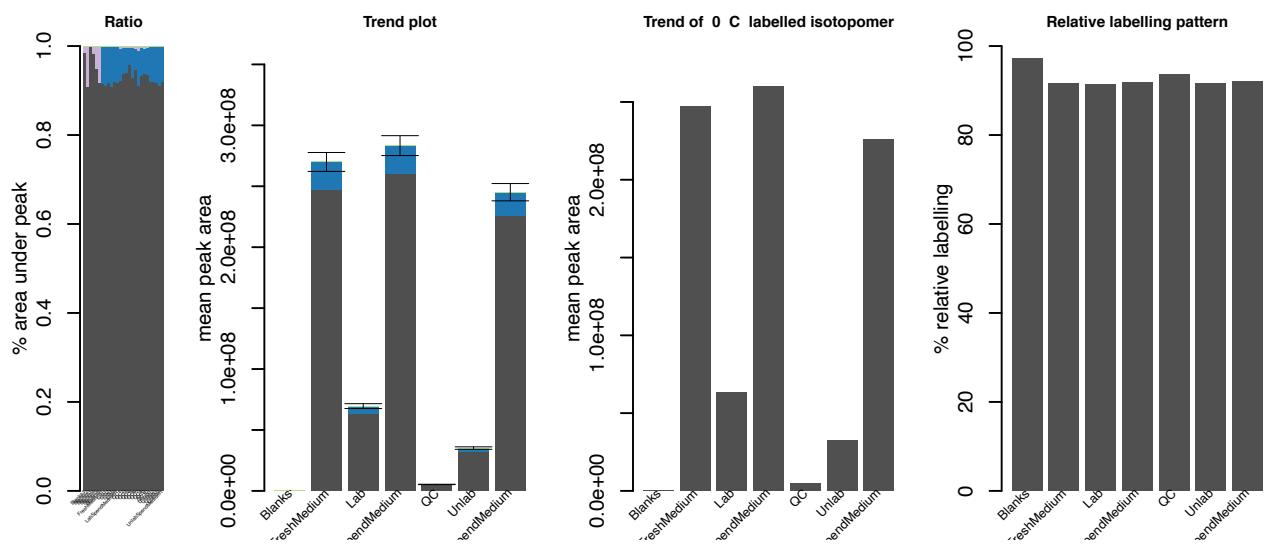
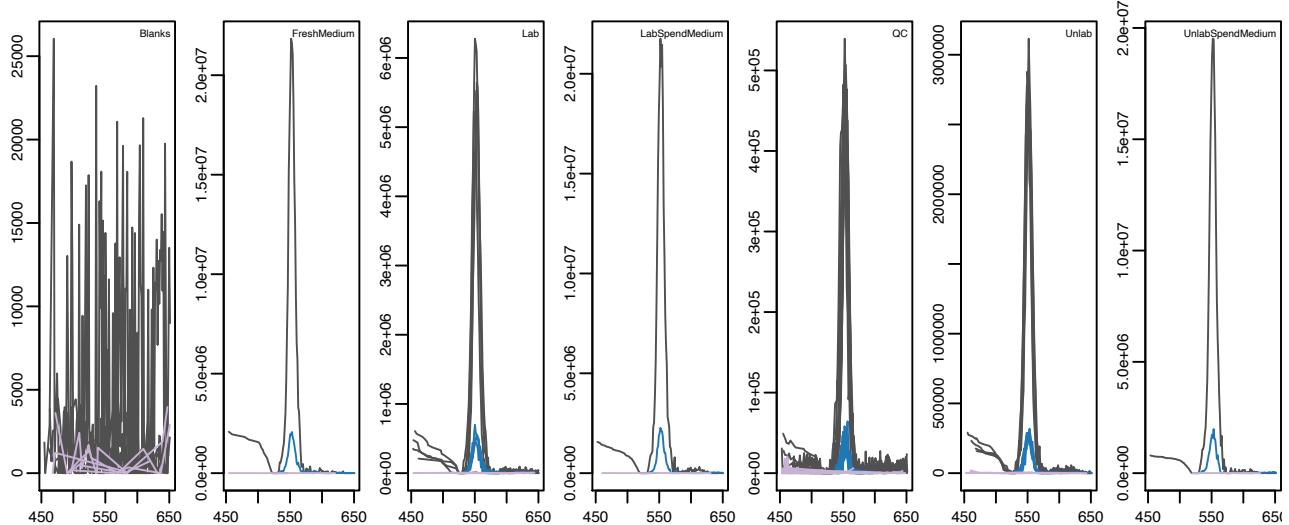


L-Phenylalanine

Formula: C9H11NO2 Mass: 165.079 Std.RT: 552.6 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9

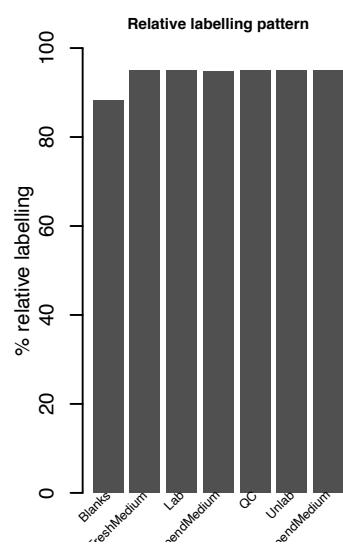
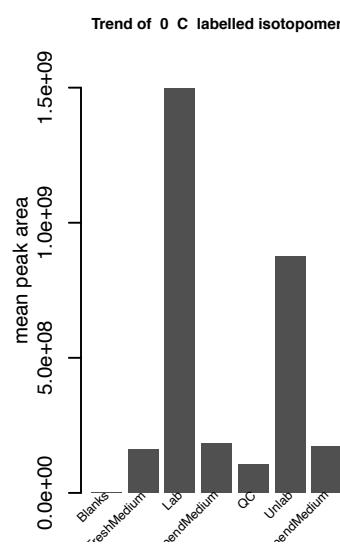
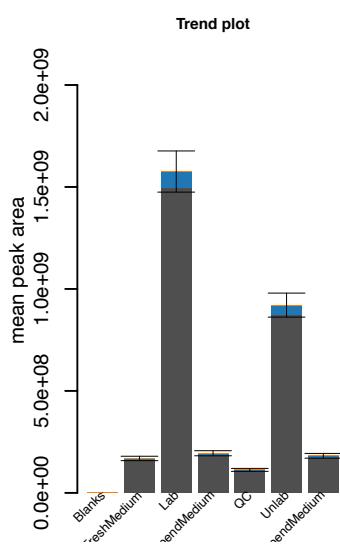
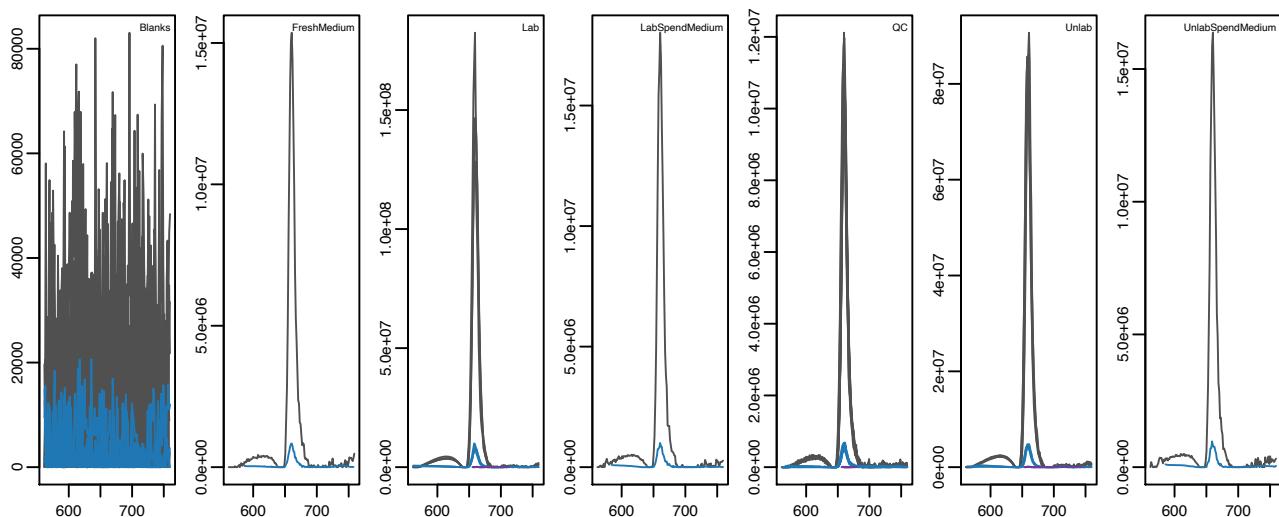


L-Proline

Formula: C5H9NO2 Mass: 115.063 Std.RT: 661.2 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

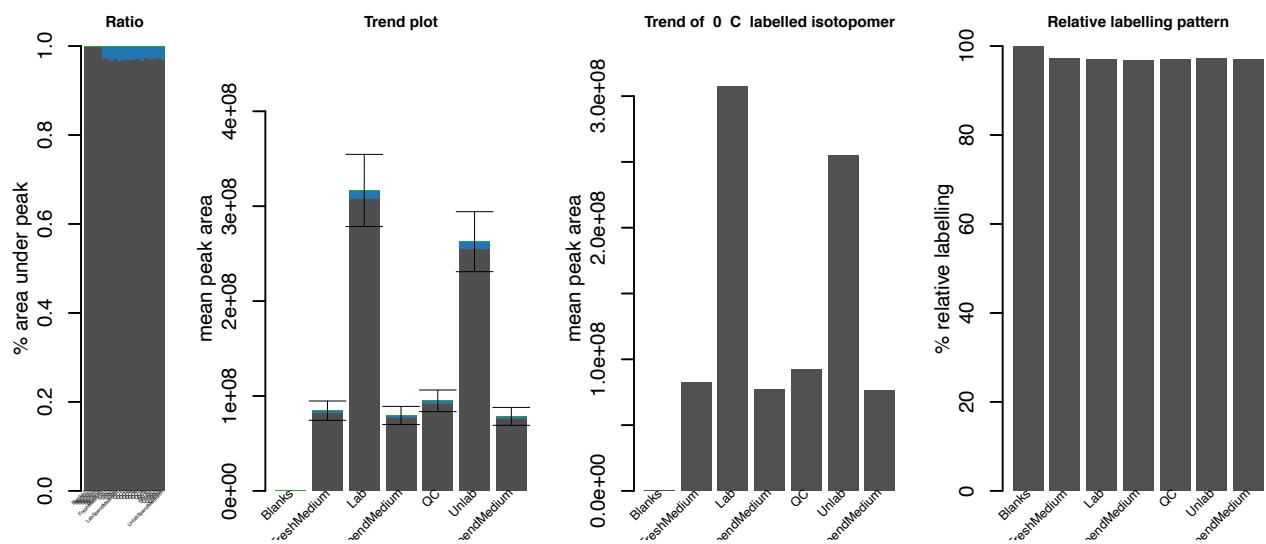
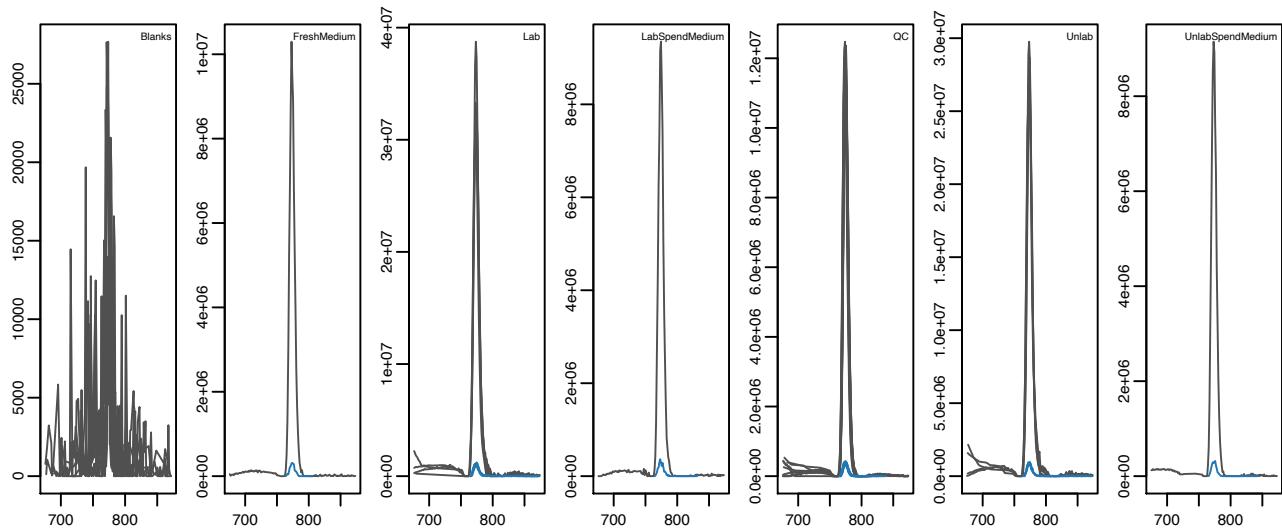


L-Serine

Formula: C3H7NO3 Mass: 105.043 Std.RT: 775.2 Ion: NEG

G1

■UL ■+1 ■+2 ■+3

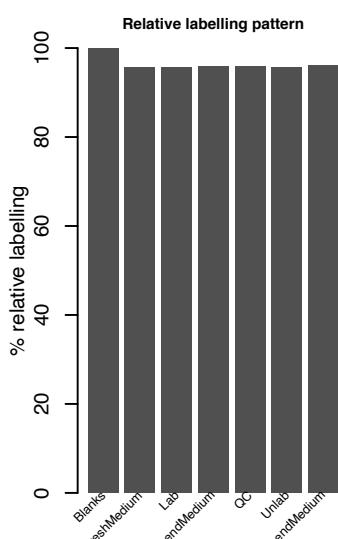
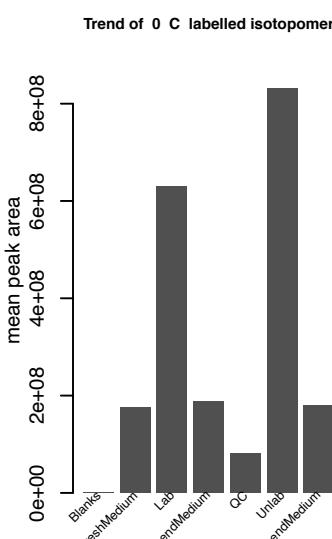
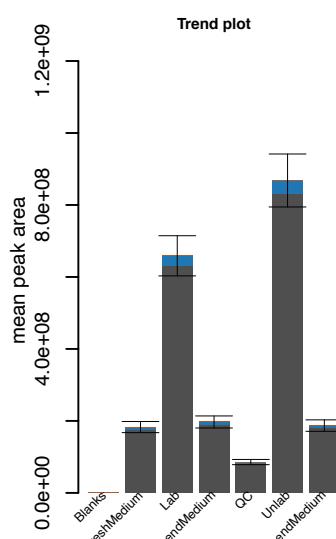
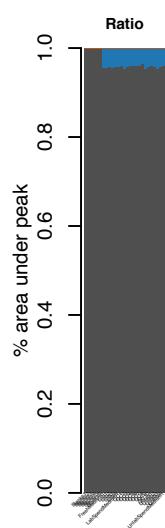
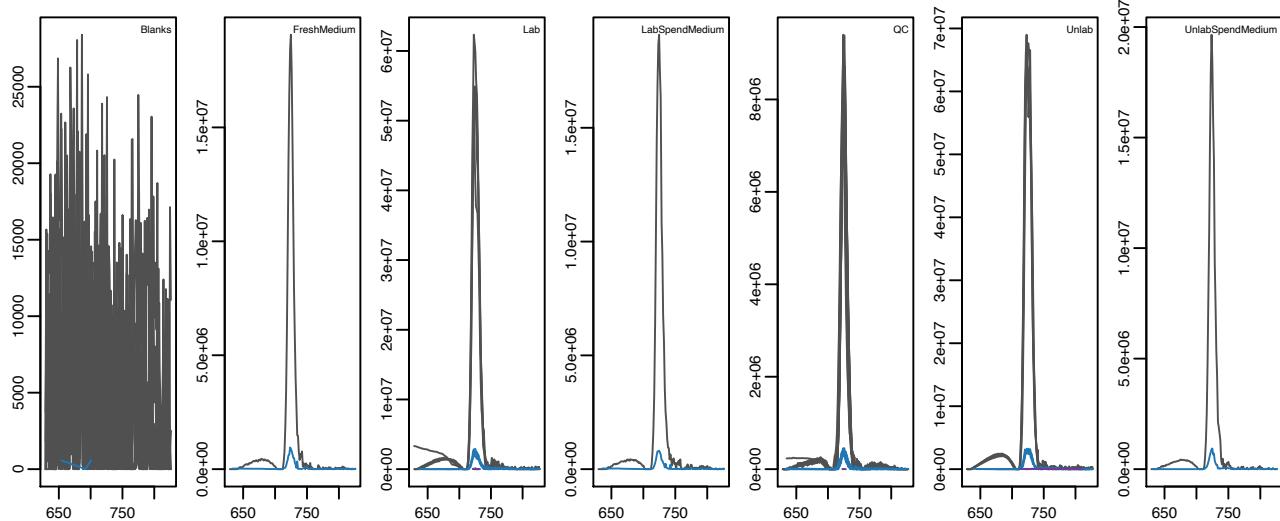


L-Threonine

Formula: C₄H₉NO₃ Mass: 119.058 Std.RT: 728.4 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4

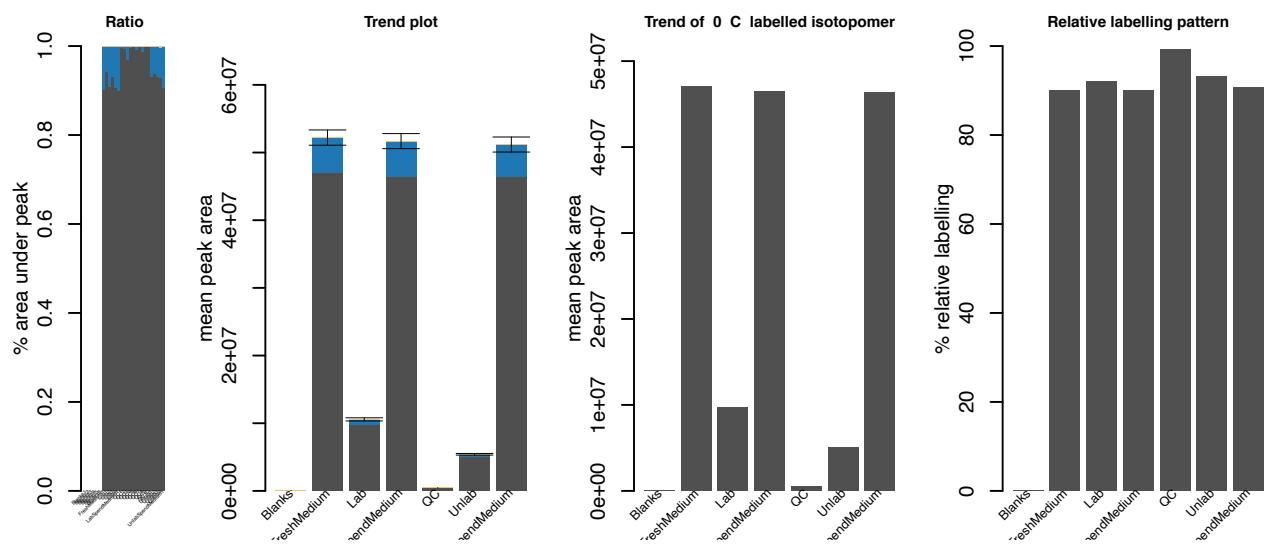
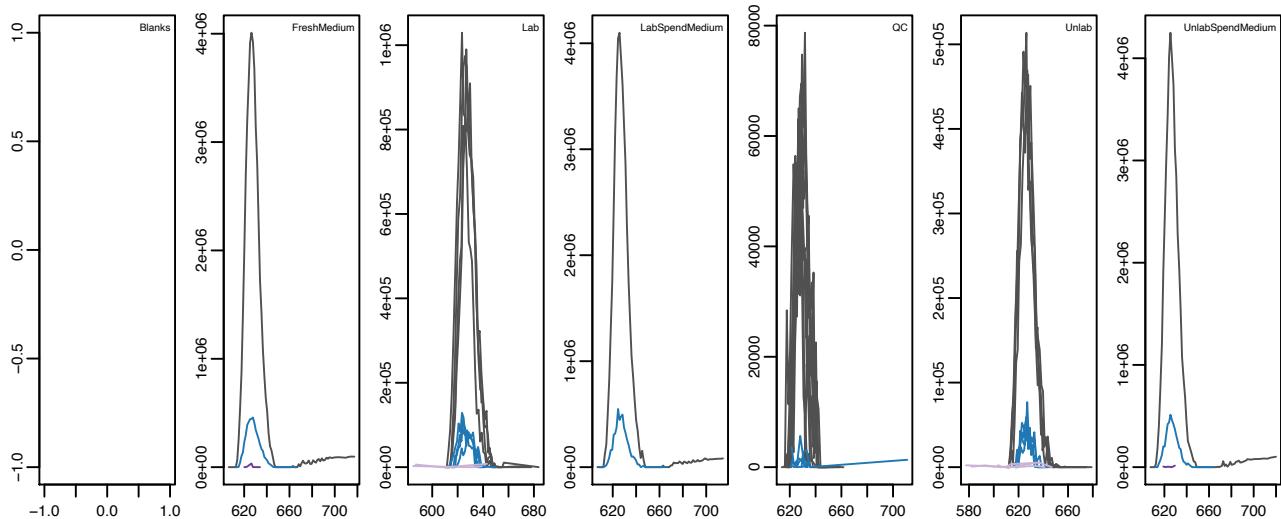


L-Tryptophan

Formula: C11H12N2O2 Mass: 204.09 Std.RT: 630 Ion: NEG

G1

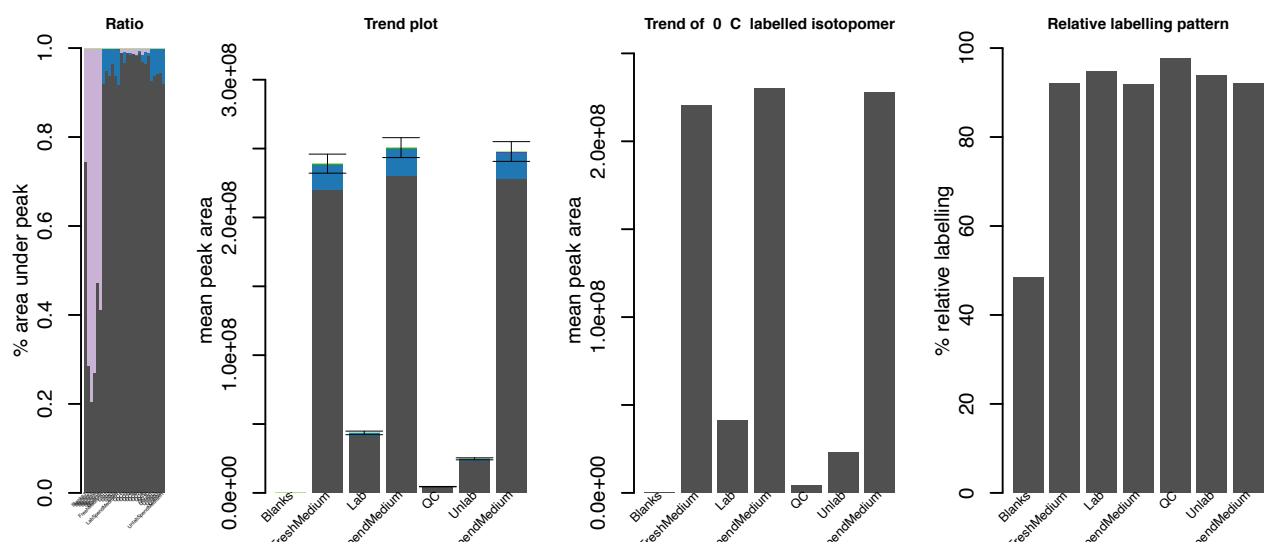
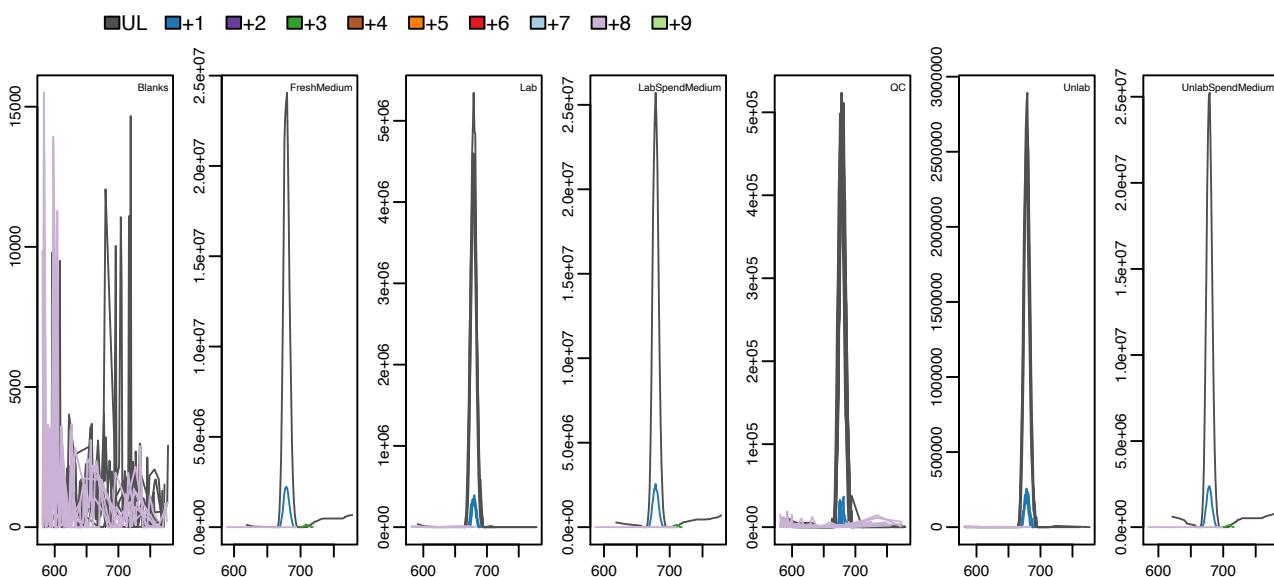
■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9 ■+10 ■+11



L-Tyrosine

Formula: C9H11NO3 Mass: 181.074 Std.RT: 680.4 Ion: NEG

G1

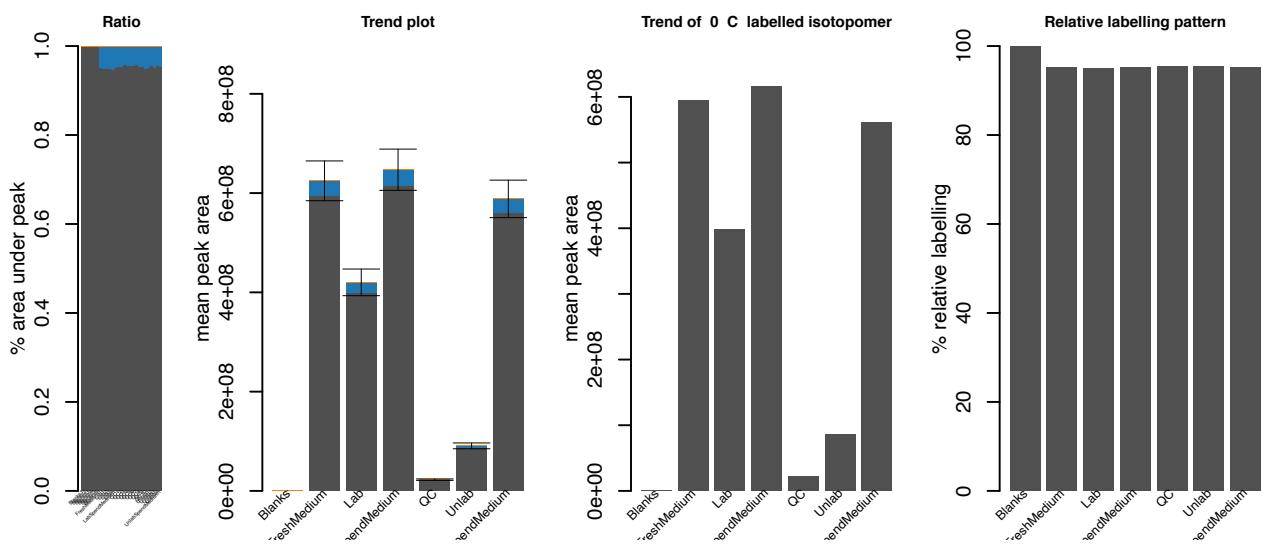
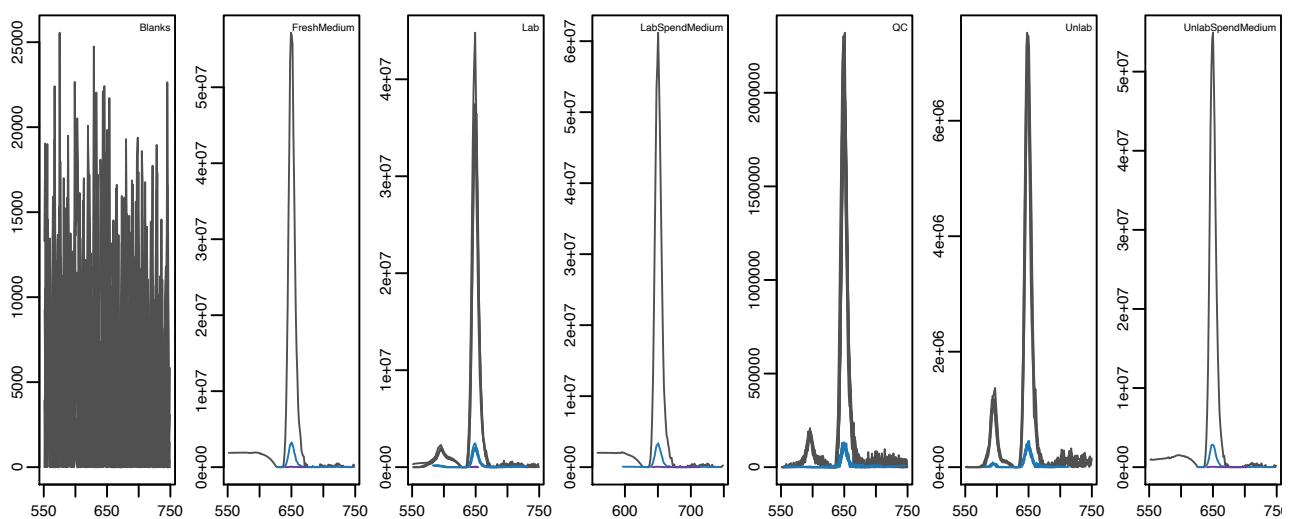


L-Valine

Formula: C5H11NO2 Mass: 117.079 Std.RT: 651 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

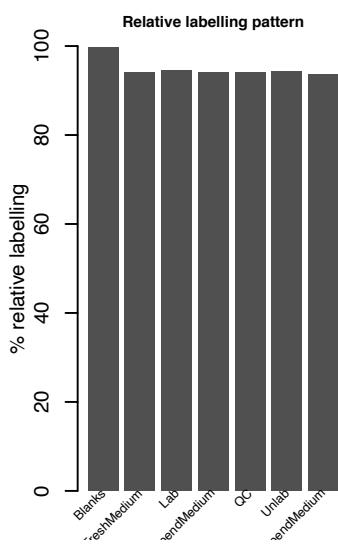
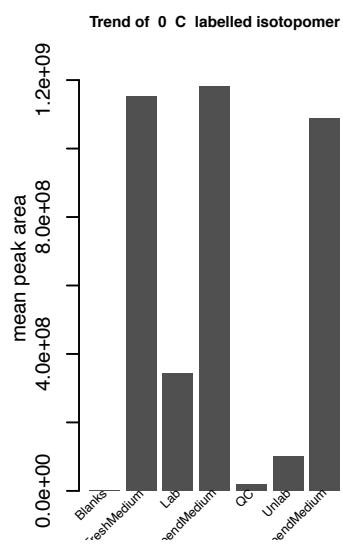
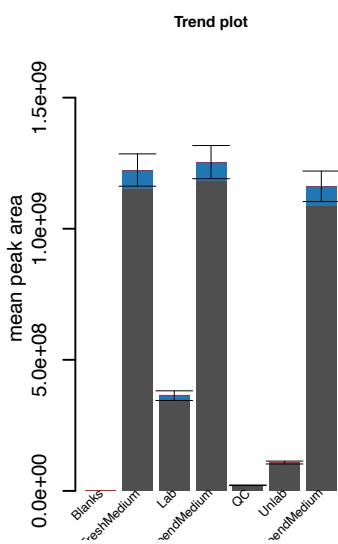
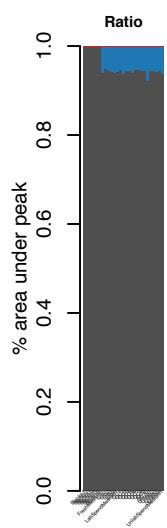
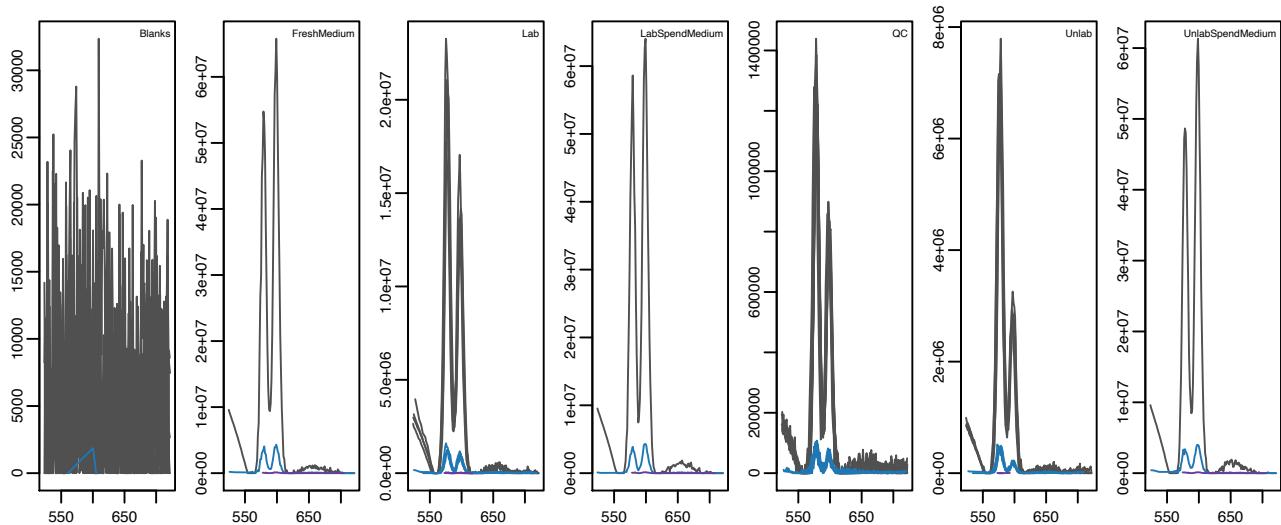


L-isoleucine

Formula: C6H13NO2 Mass: 131.095 Std.RT: 623.4 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6

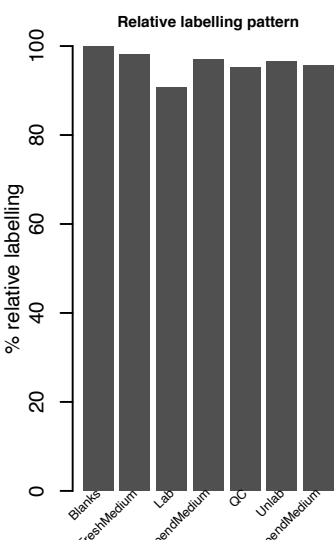
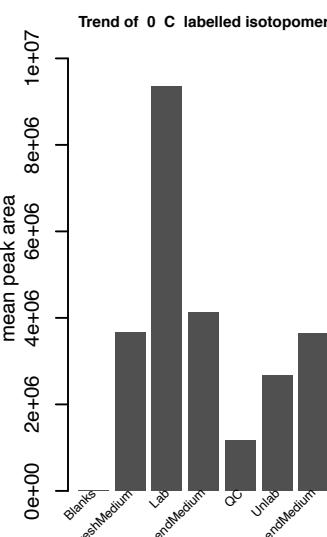
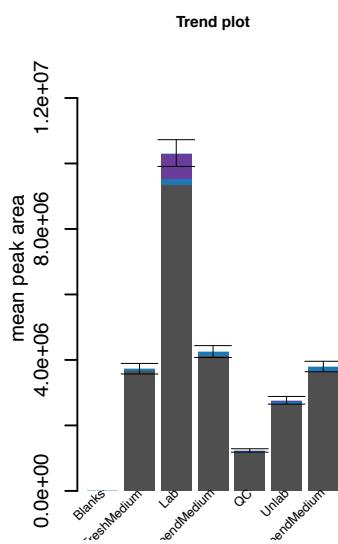
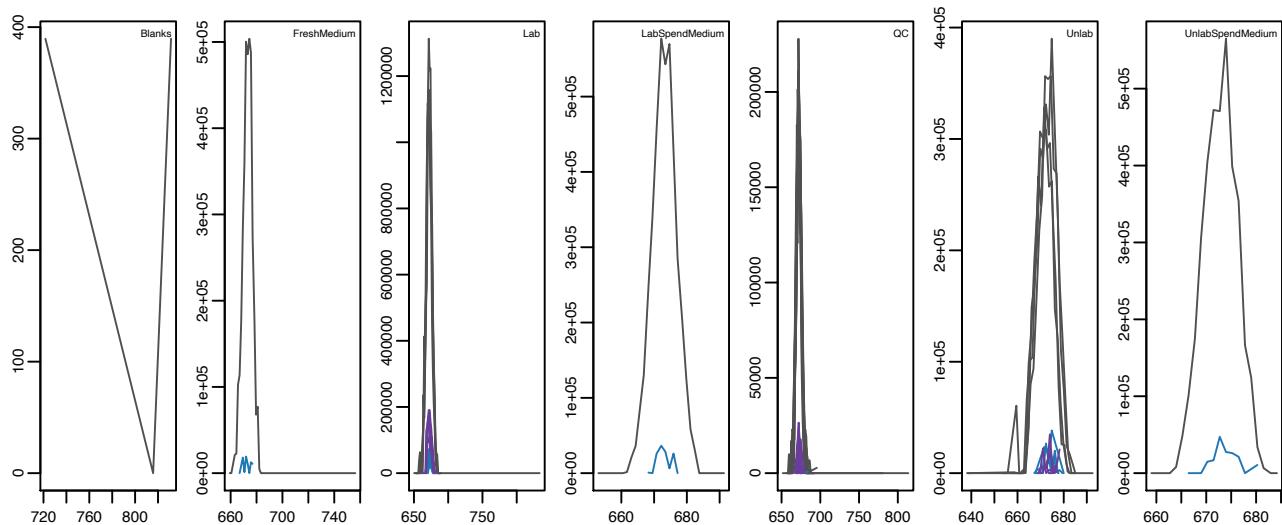


N-Acetylornithine

Formula: C7H14N2O3 Mass: 174.1 Std.RT: 735 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7

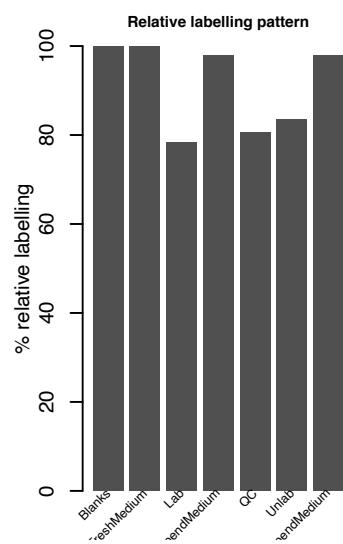
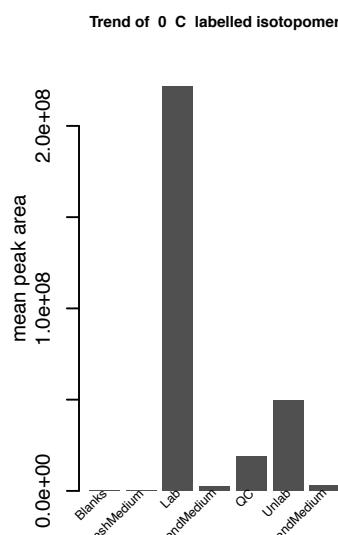
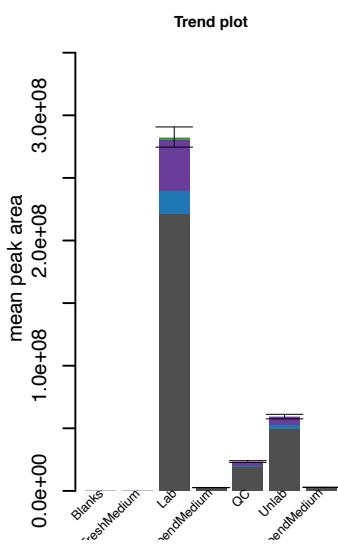
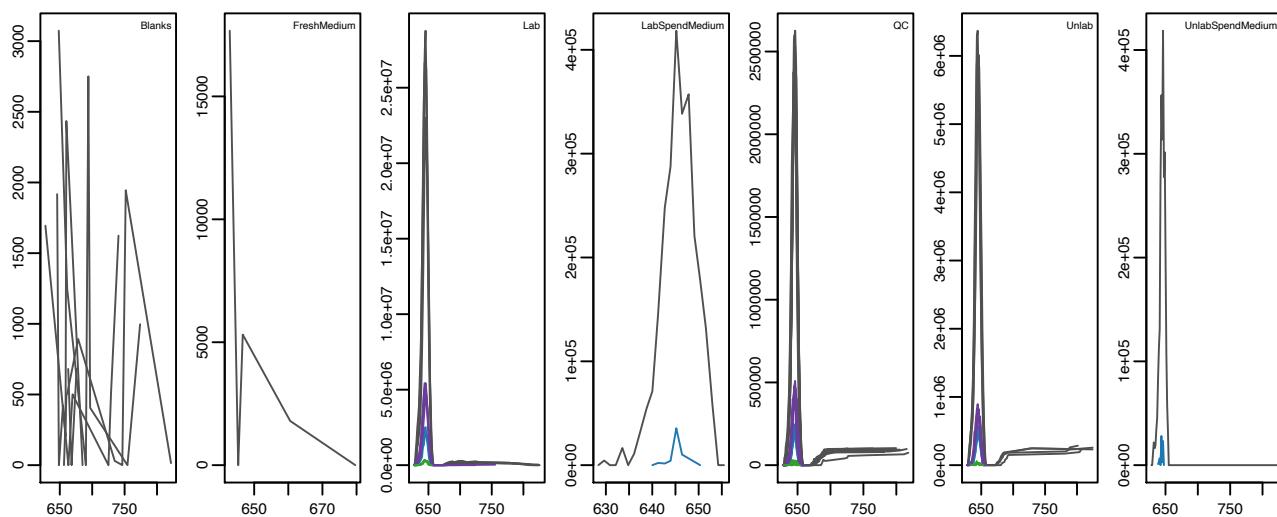


N2-Acetyl-L-lysine

Formula: C₈H₁₆N₂O₃ Mass: 188.116 Std.RT: 727.2 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8

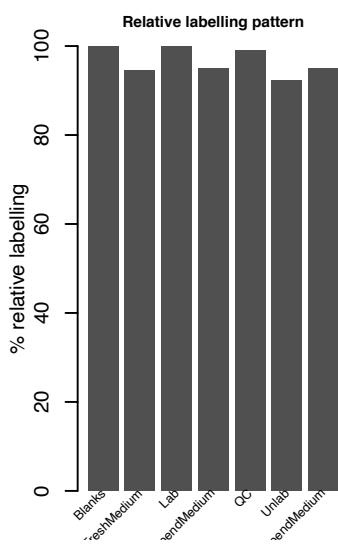
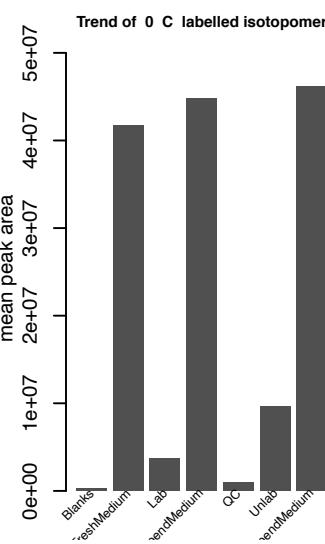
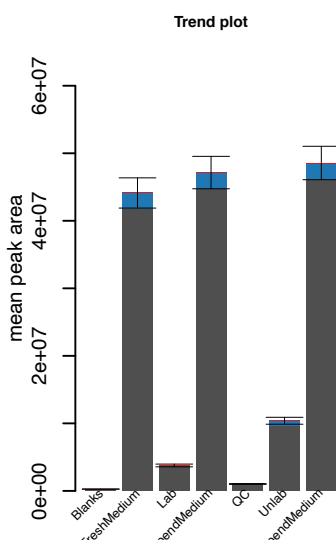
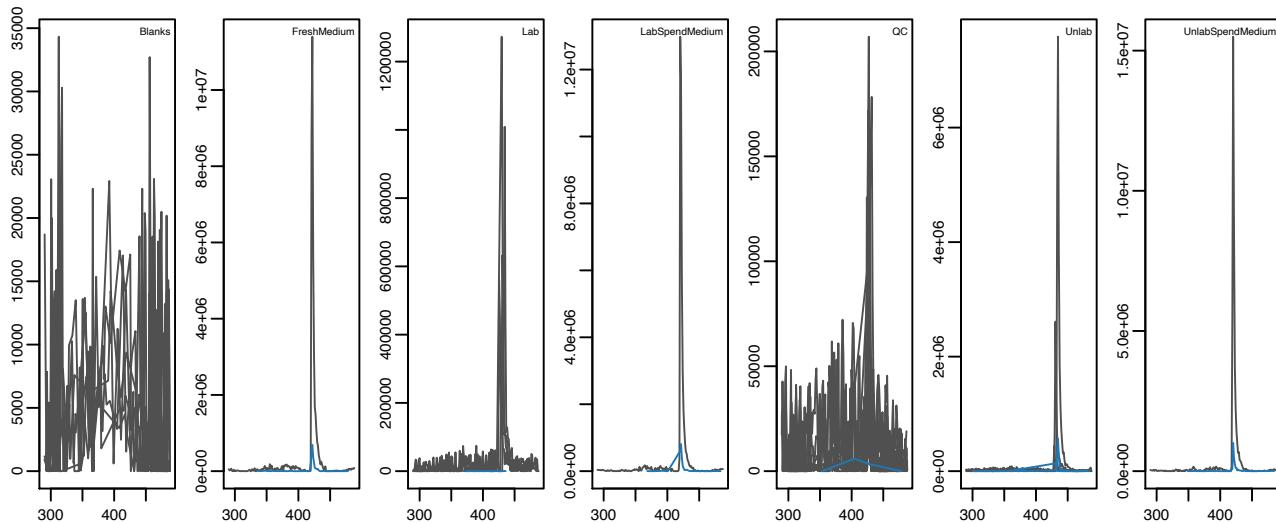


Nicotinamide

Formula: C₆H₆N₂O Mass: 122.048 Std.RT: 389.4 Ion: NEG

G1

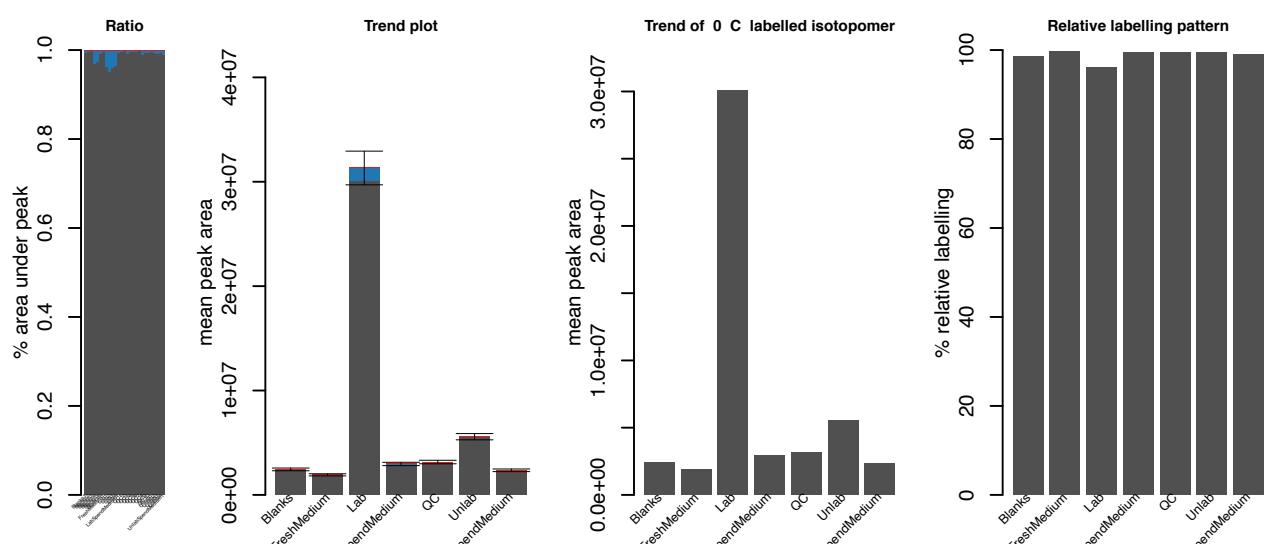
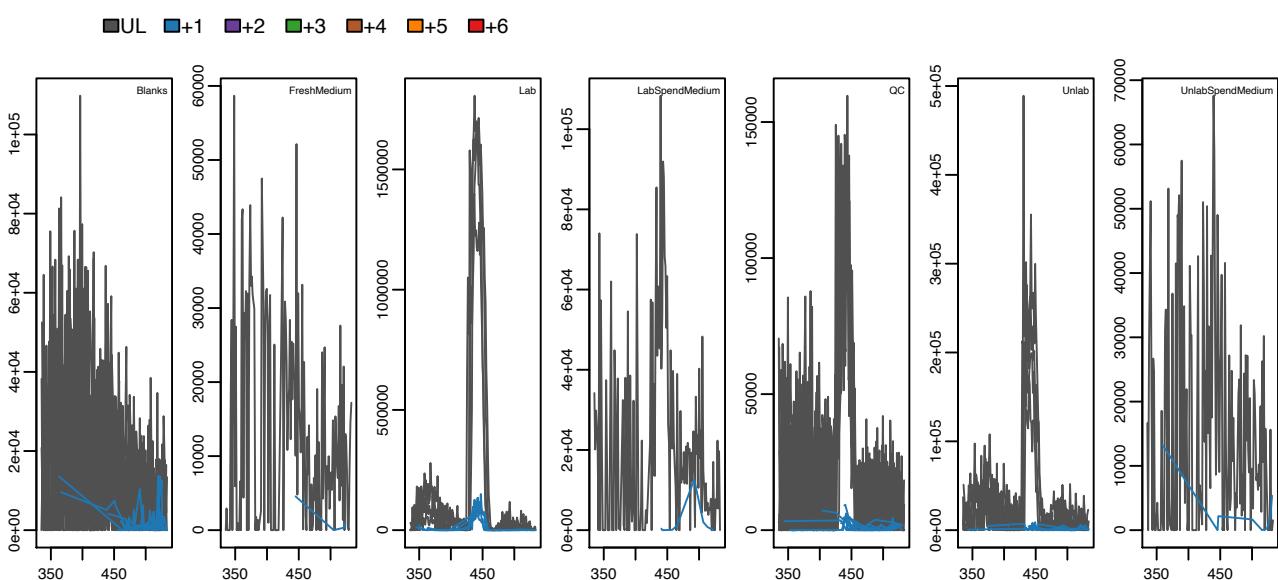
■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6



Nicotinate

Formula: C₆H₅NO₂ Mass: 123.032 Std.RT: 435 Ion: NEG

G1

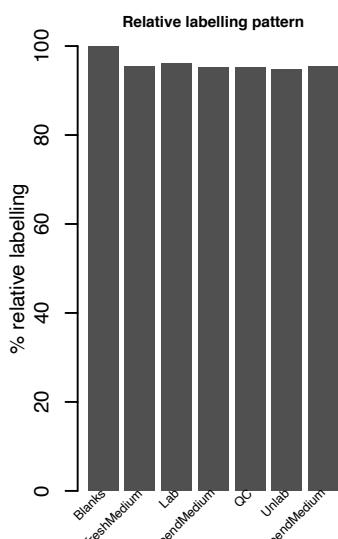
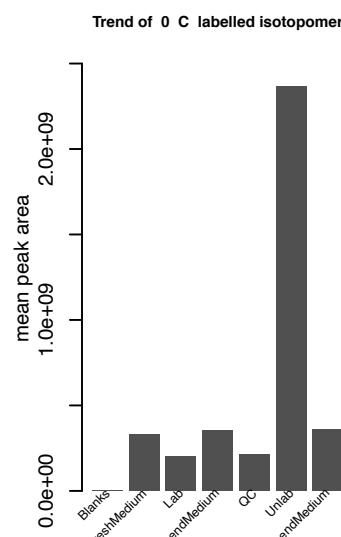
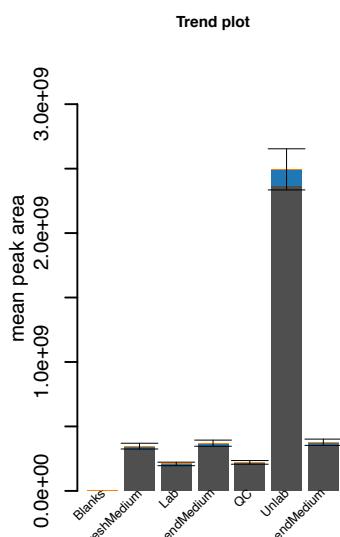
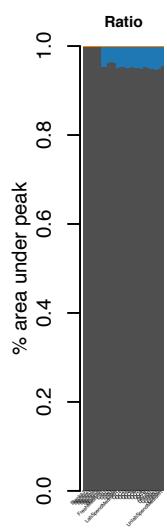
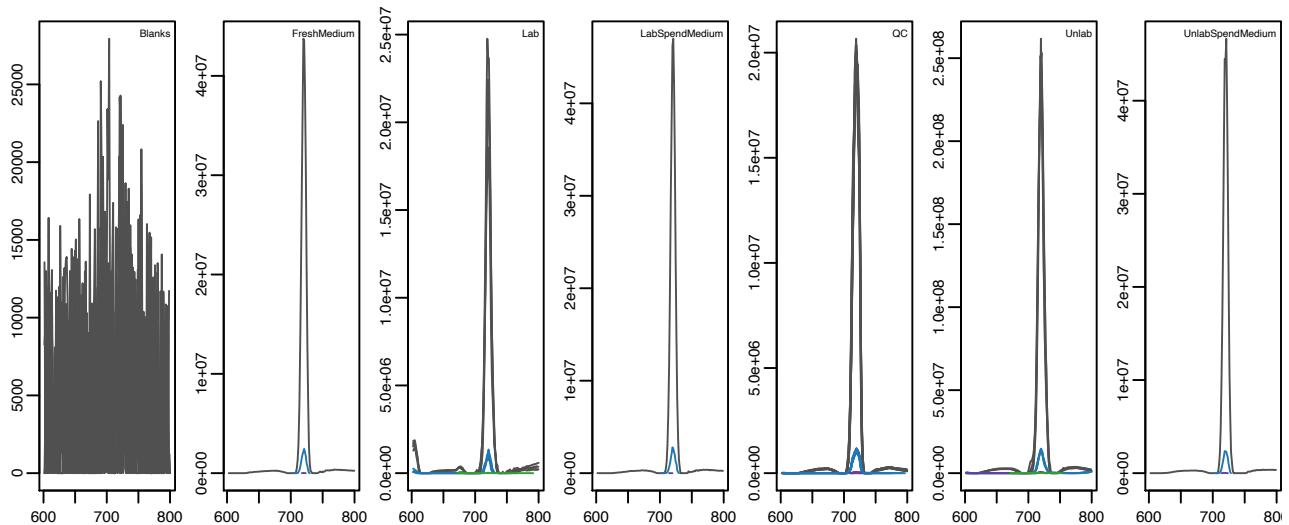


O-Acetyl-L-serine

Formula: C5H9NO4 Mass: 147.053 Std.RT: 701.4 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

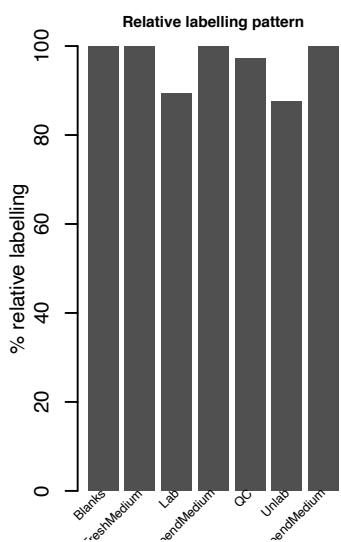
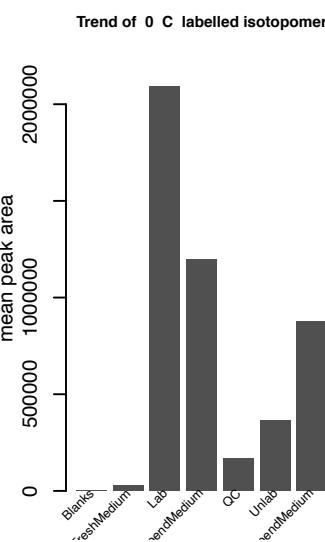
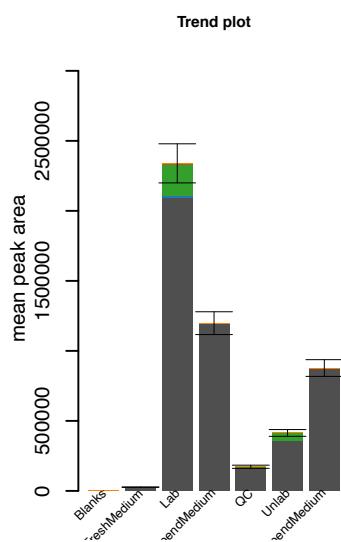
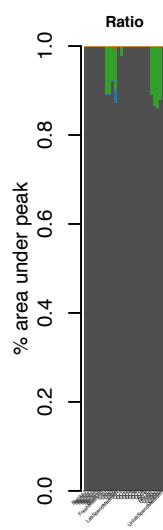
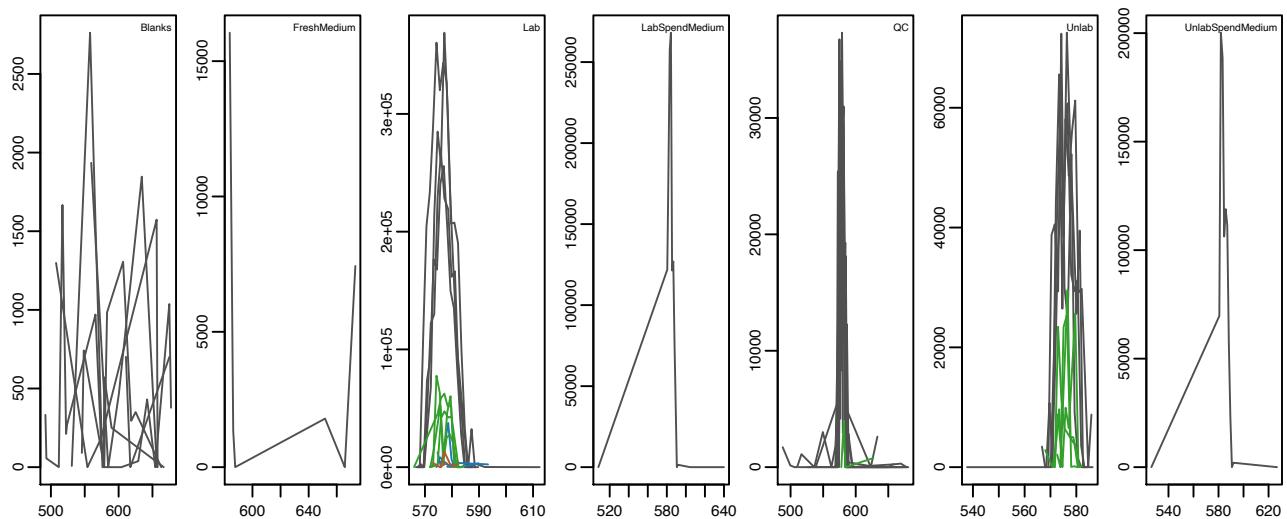


Orotate

Formula: C5H4N2O4 Mass: 156.017 Std.RT: 586.8 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

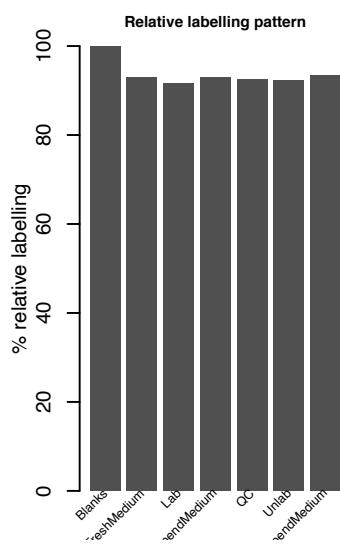
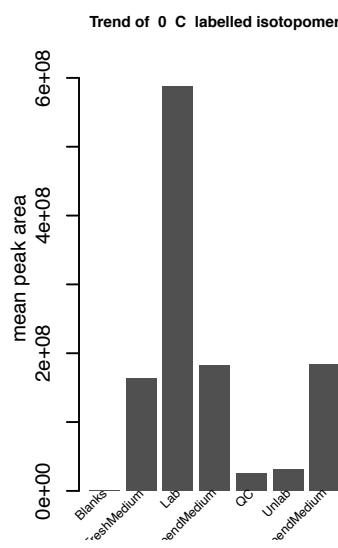
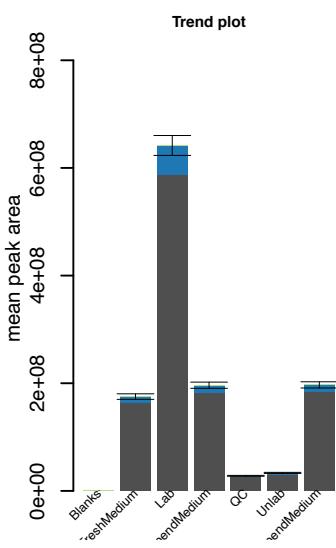
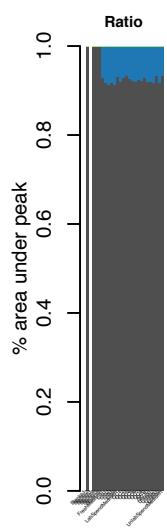
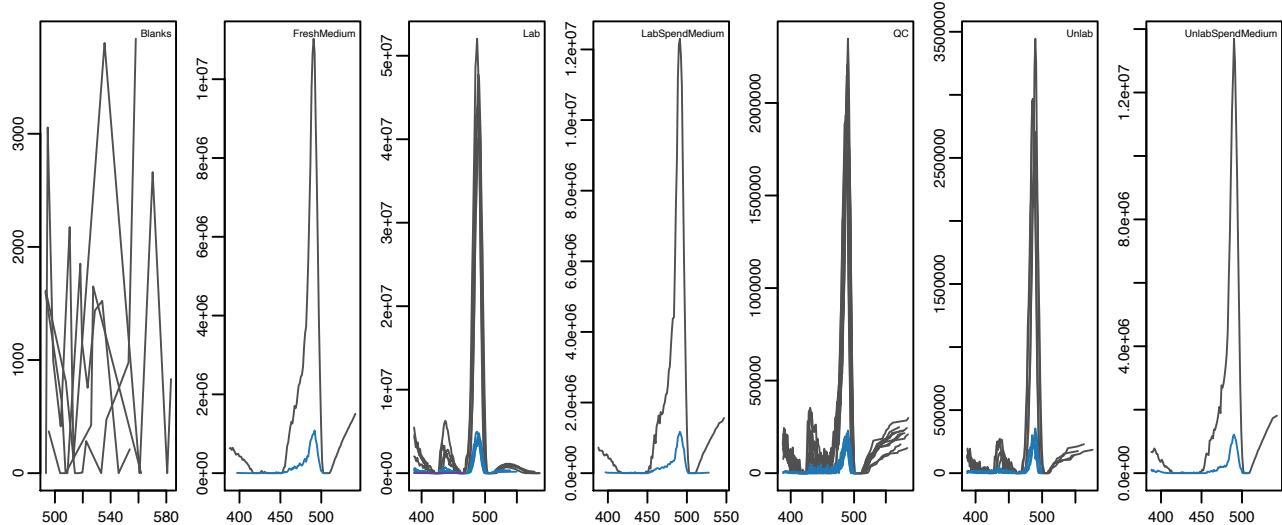


Pantothenate

Formula: C9H17NO5 Mass: 219.111 Std.RT: 487.2 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9

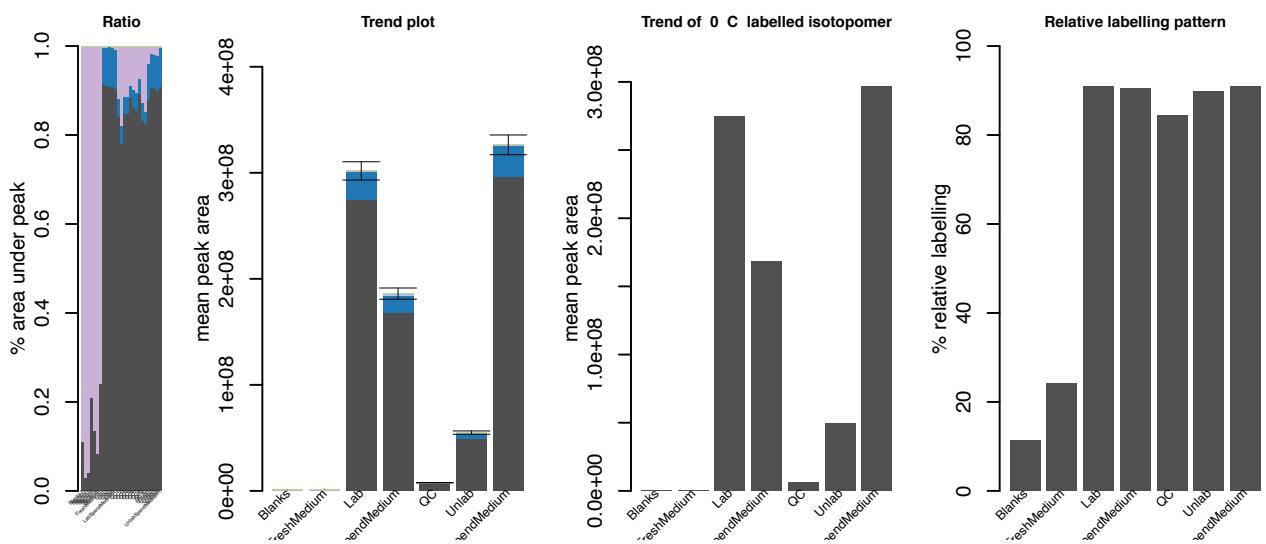
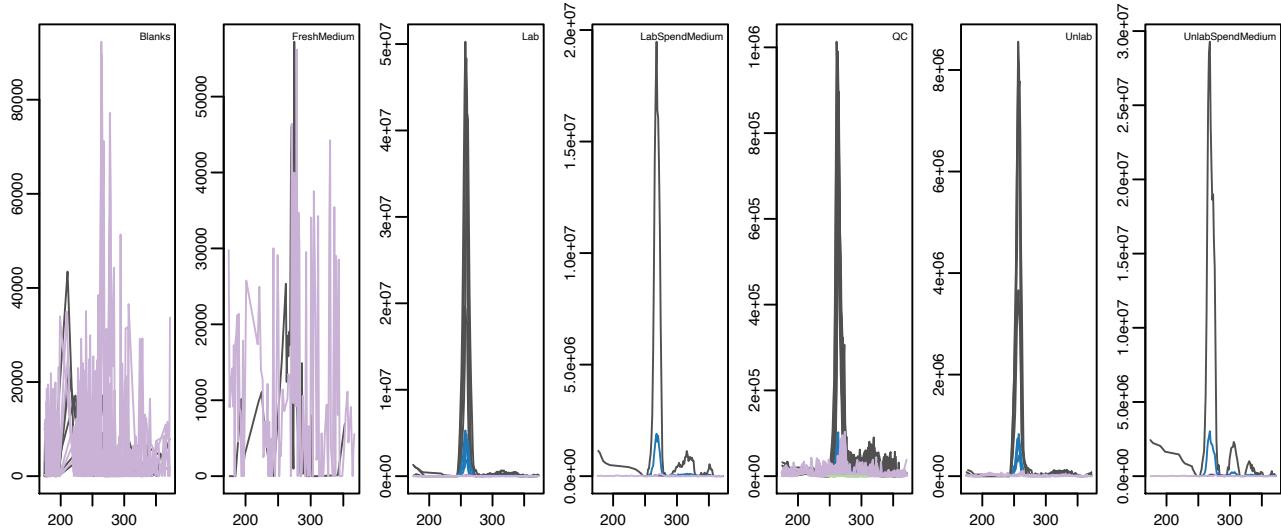


Phenylpyruvate

Formula: C9H8O3 Mass: 164.047 Std.RT: 274.2 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9

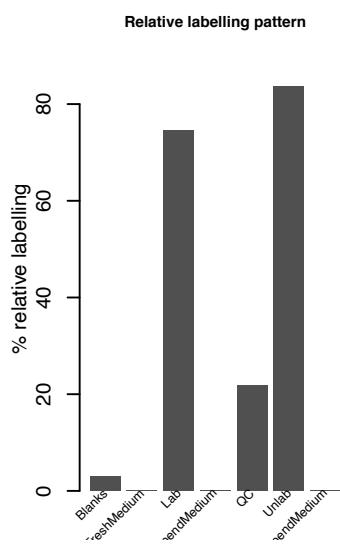
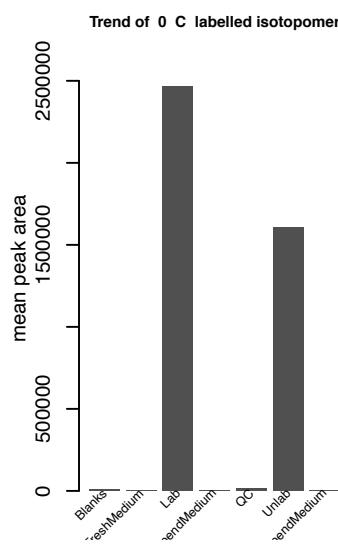
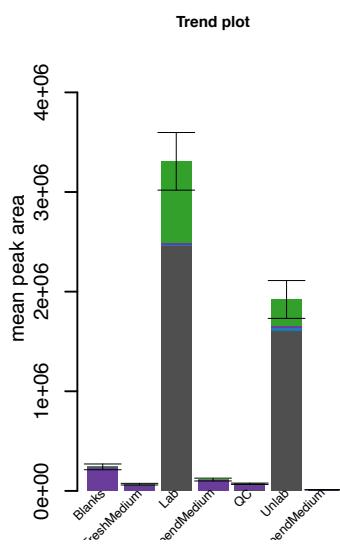
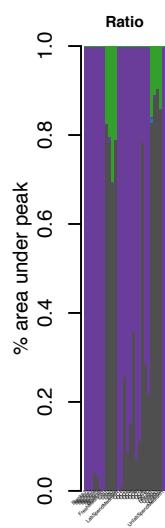
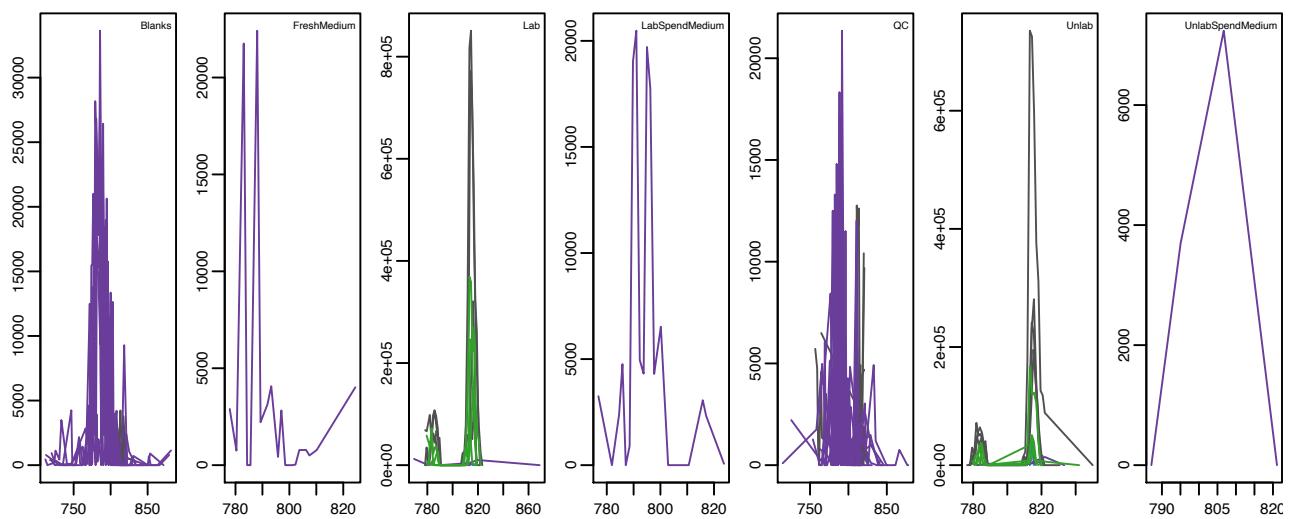


Phosphoenolpyruvate

Formula: C₃H₅O₆P Mass: 167.982 Std.RT: 811.8 Ion: NEG

G1

■UL ■+1 ■+2 ■+3

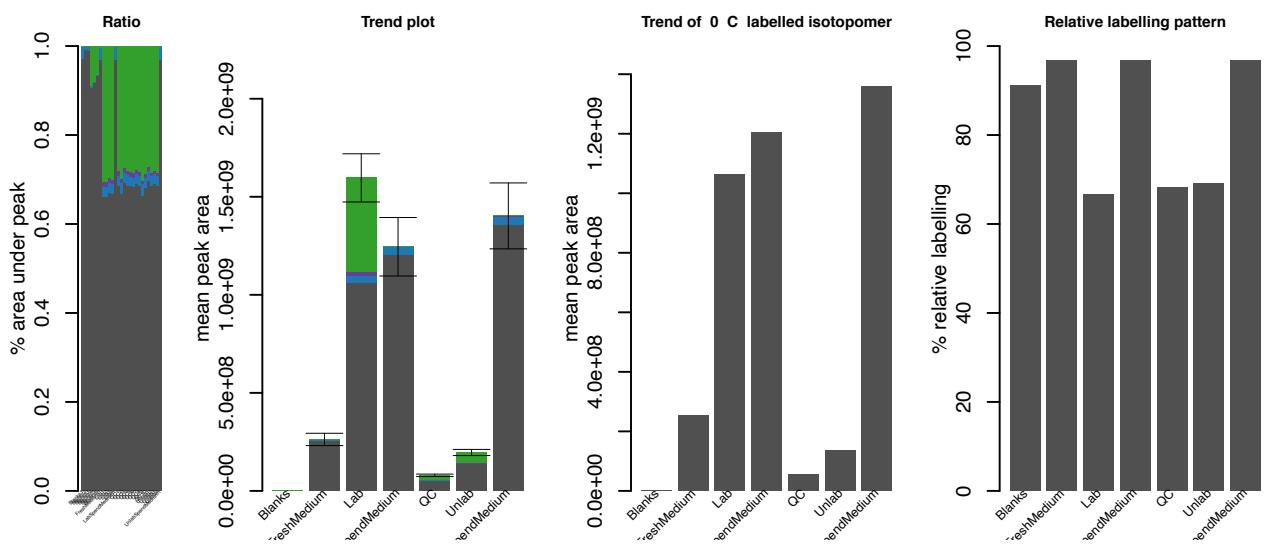
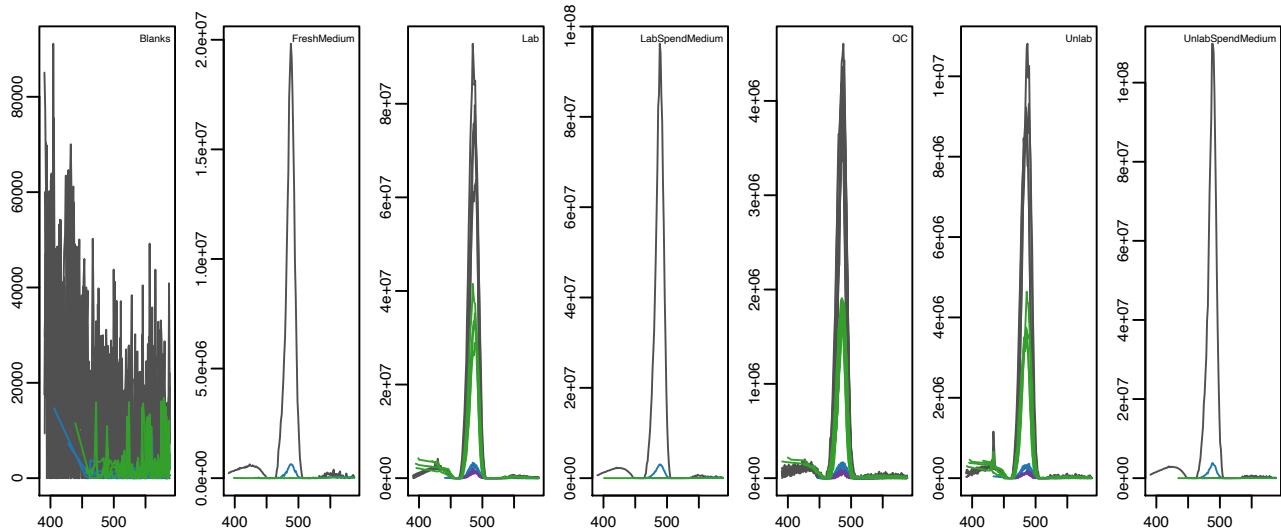


Pyruvate

Formula: C₃H₄O₃ Mass: 88.016 Std.RT: 490.2 Ion: NEG

G1

■UL ■+1 ■+2 ■+3

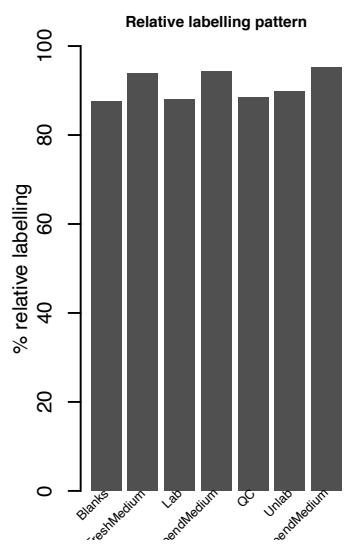
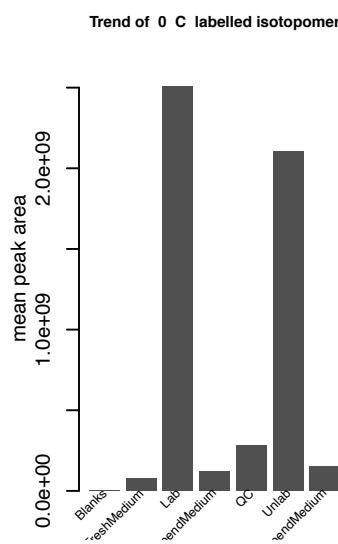
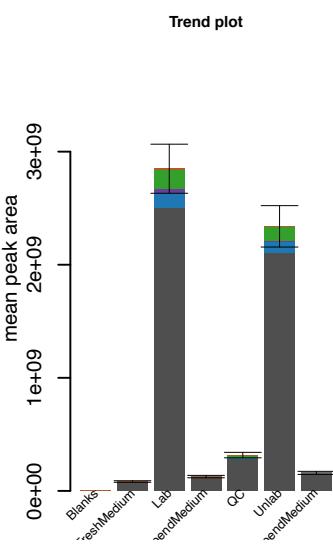
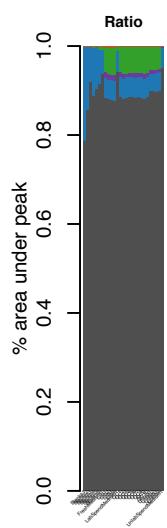
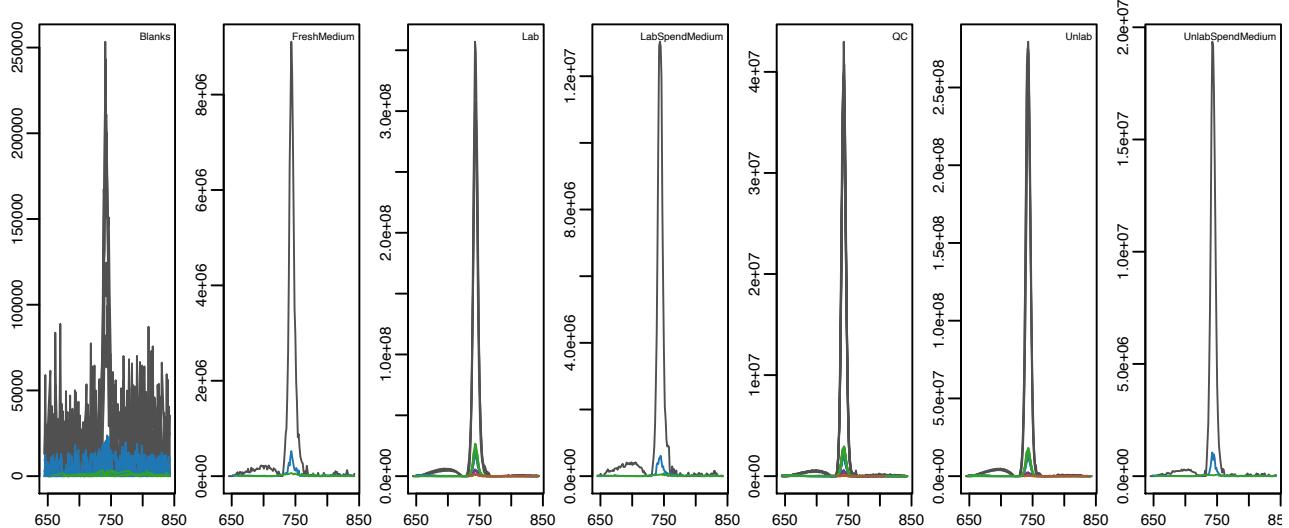


Succinate

Formula: C₄H₆O₄ Mass: 118.027 Std.RT: 744.6 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4

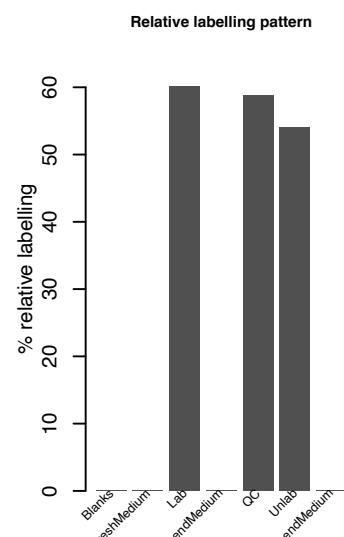
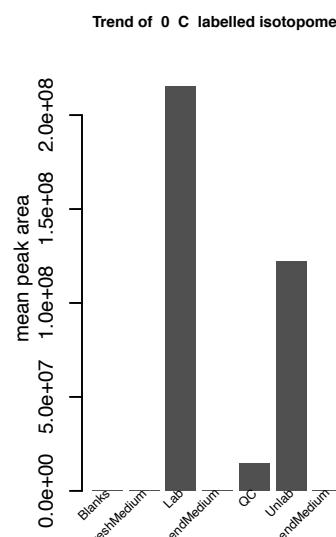
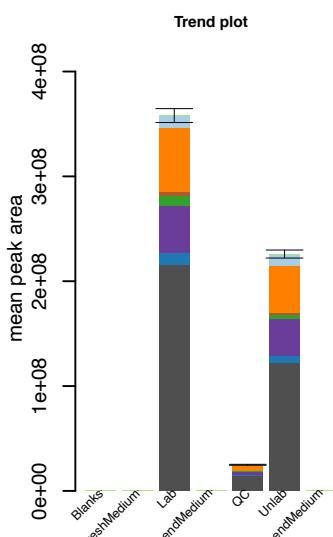
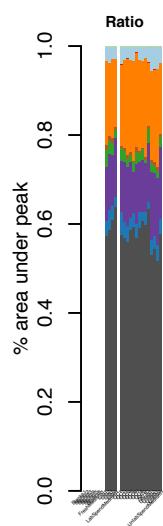
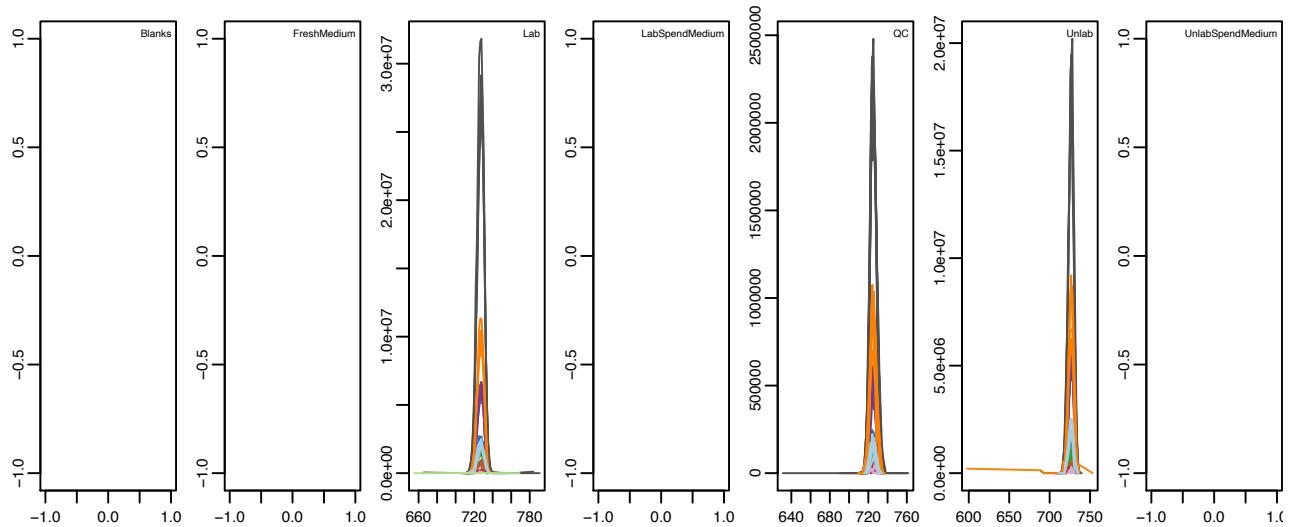


UMP

Formula: C9H13N2O9P Mass: 324.036 Std.RT: 694.8 Ion: NEG

G1

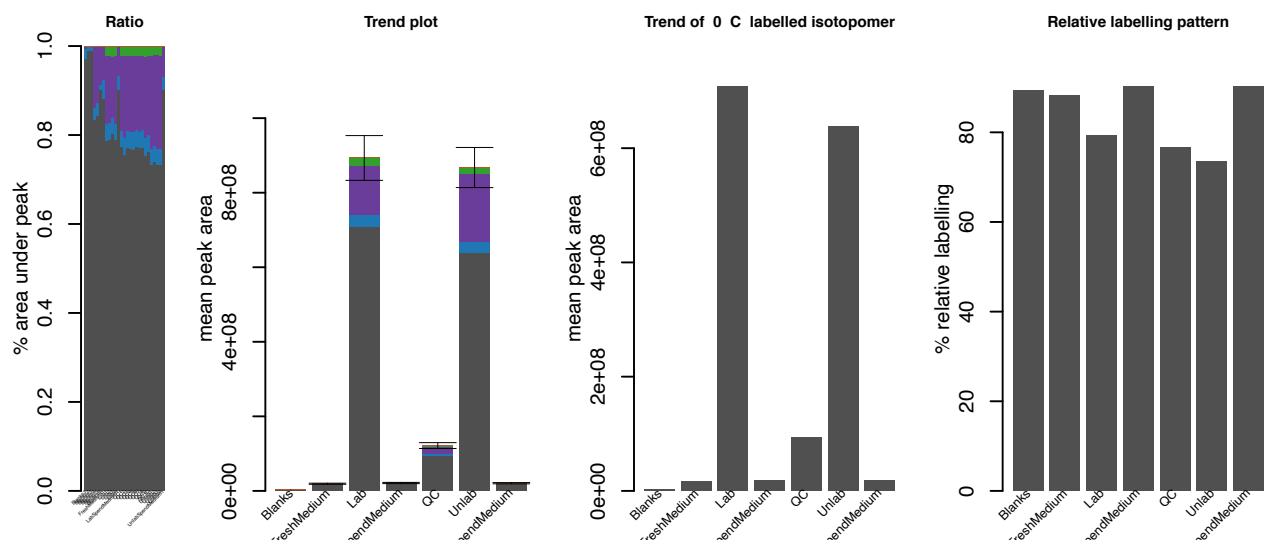
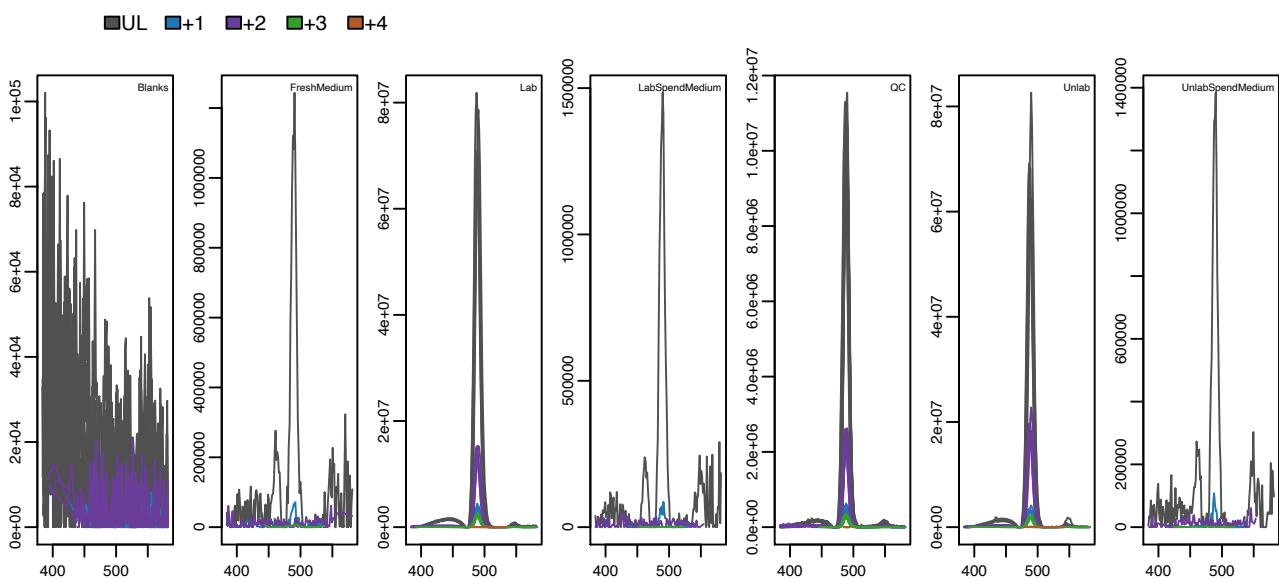
■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9



Uracil

Formula: C4H4N2O2 Mass: 112.027 Std.RT: 483.6 Ion: NEG

G1

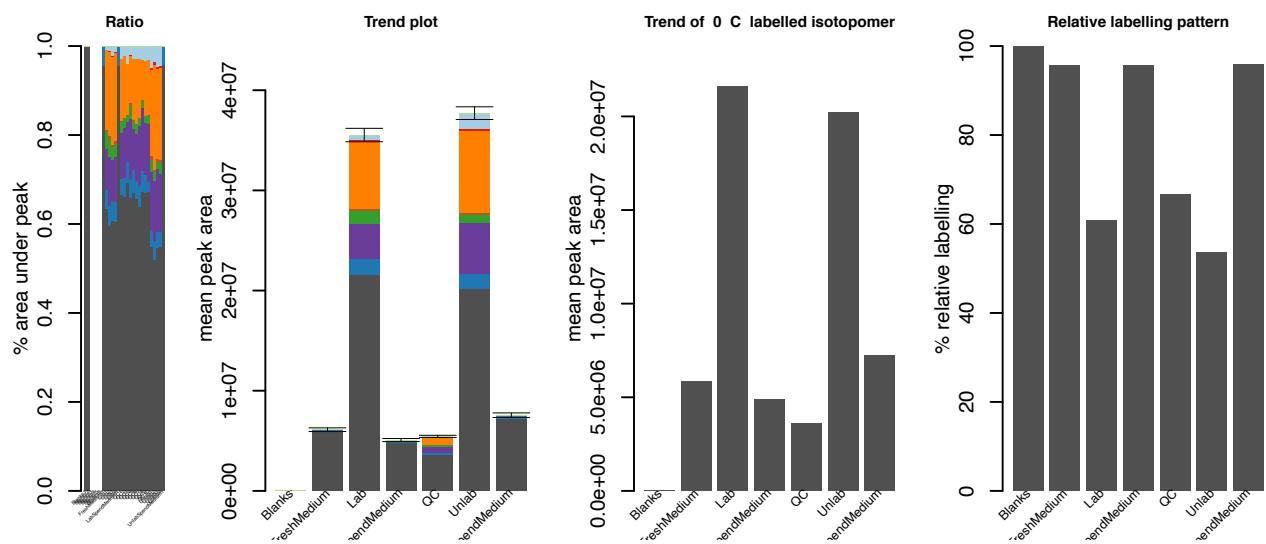
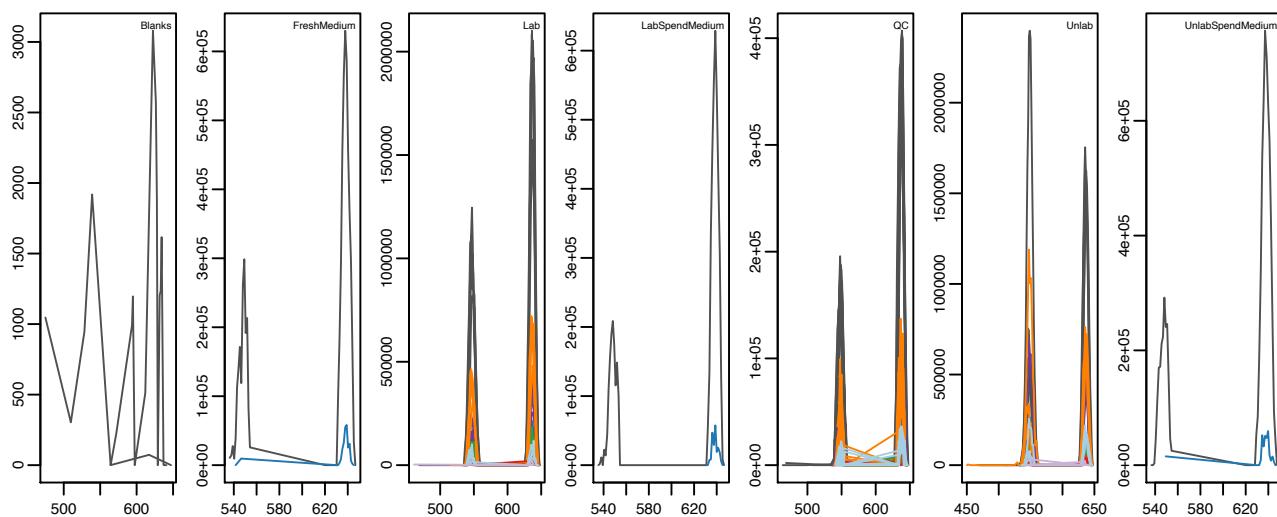


Uridine

Formula: C9H12N2O6 Mass: 244.07 Std.RT: 549 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9

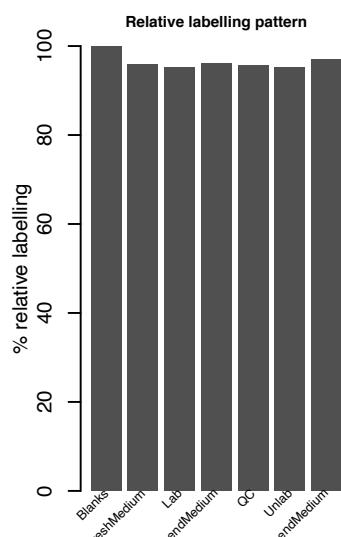
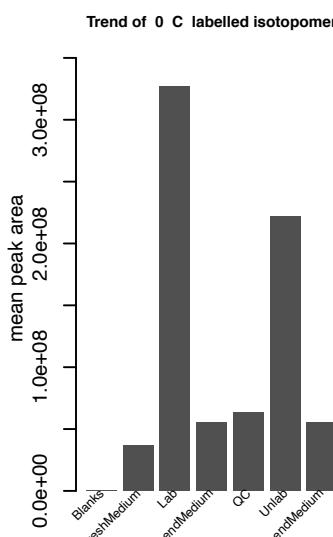
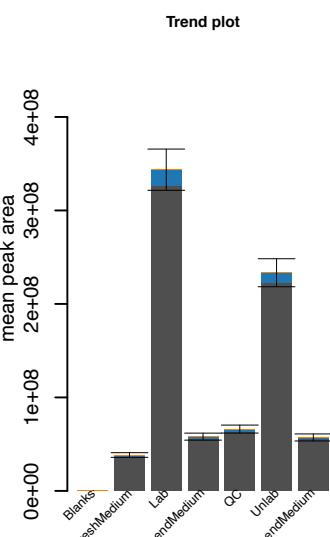
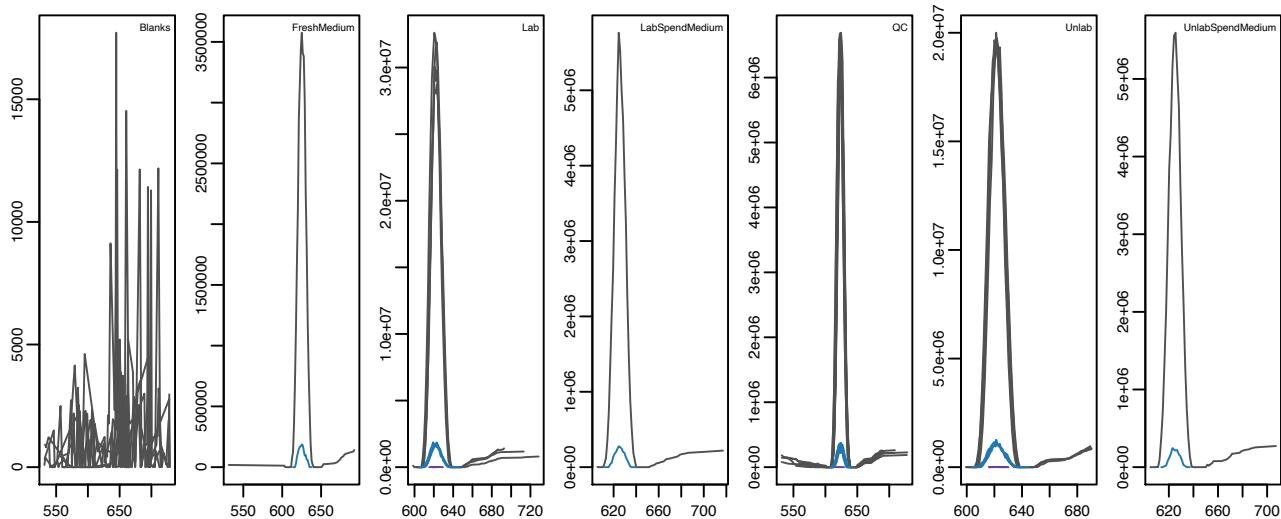


Xanthine

Formula: C₅H₄N₄O₂ Mass: 152.033 Std.RT: 630.6 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

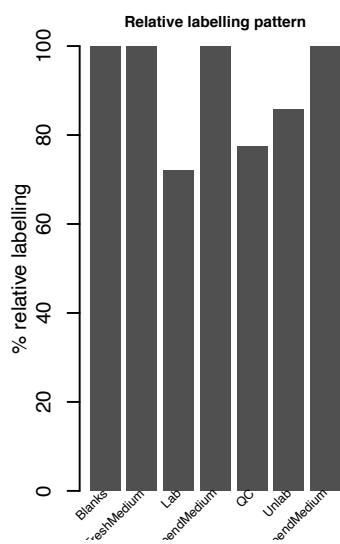
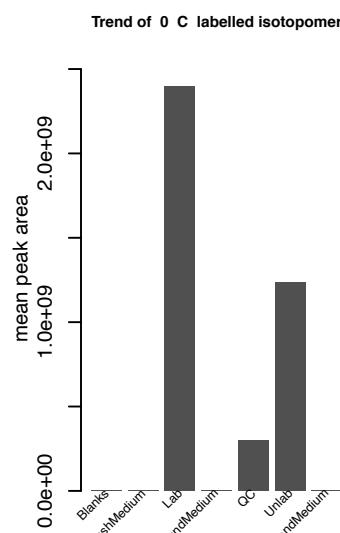
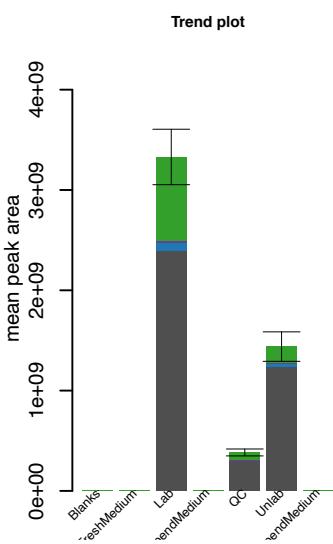
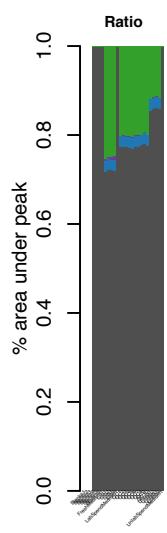
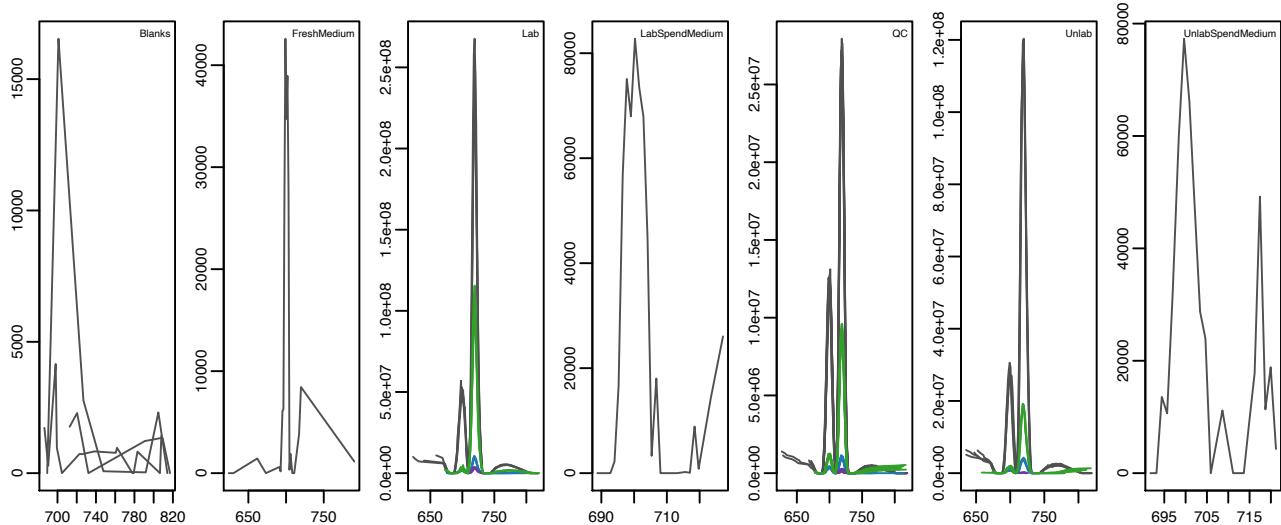


sn-Glycerol 3-phosphate

Formula: C₃H₉O₆P Mass: 172.014 Std.RT: 720.6 Ion: NEG

G1

■UL ■+1 ■+2 ■+3

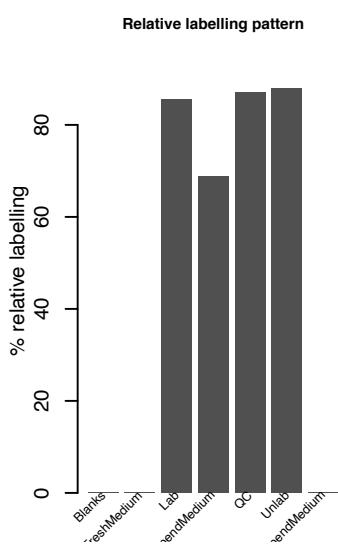
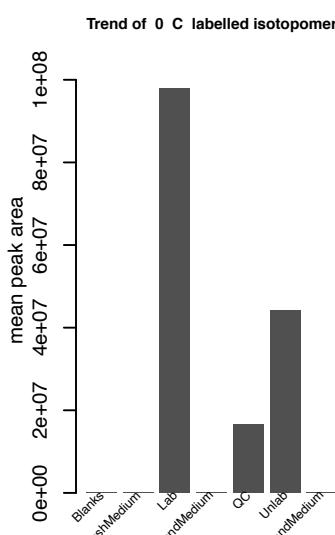
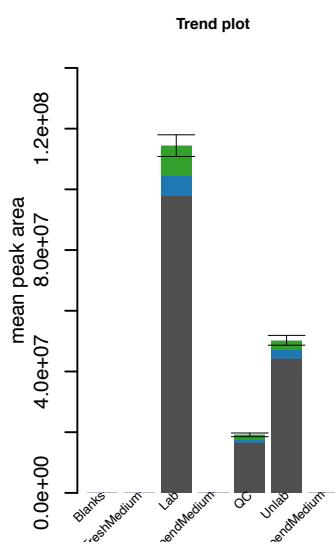
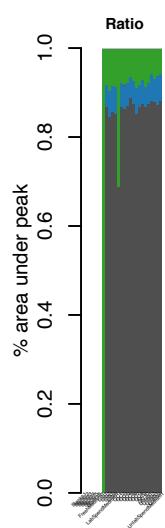
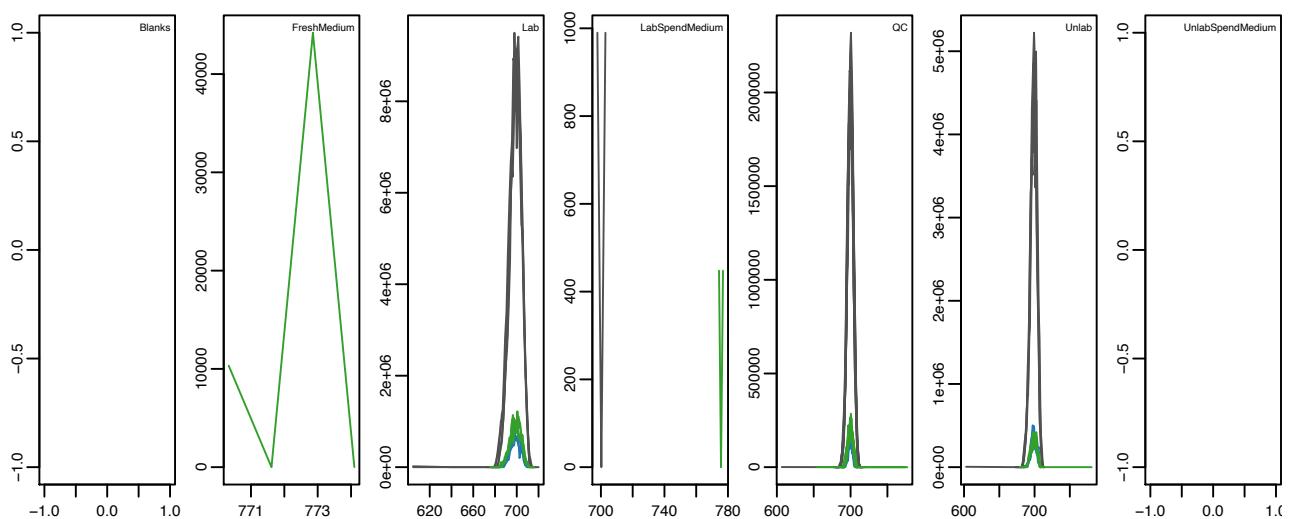


sn-glycero-3-Phosphocholine

Formula: C₈H₂₀NO₆P Mass: 257.103 Std.RT: 700.8 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8

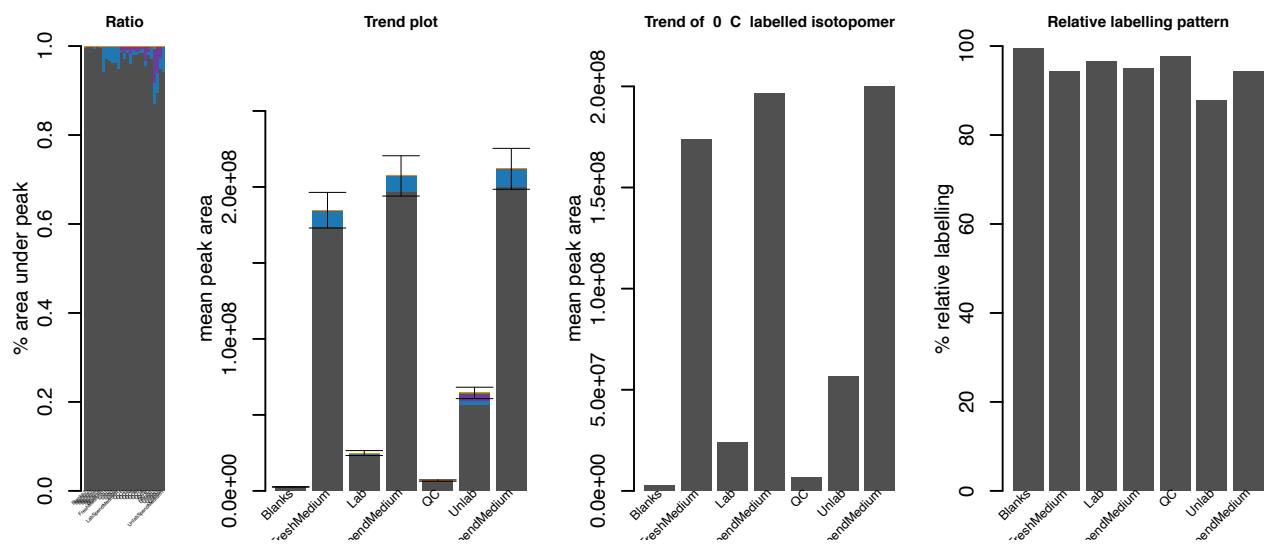
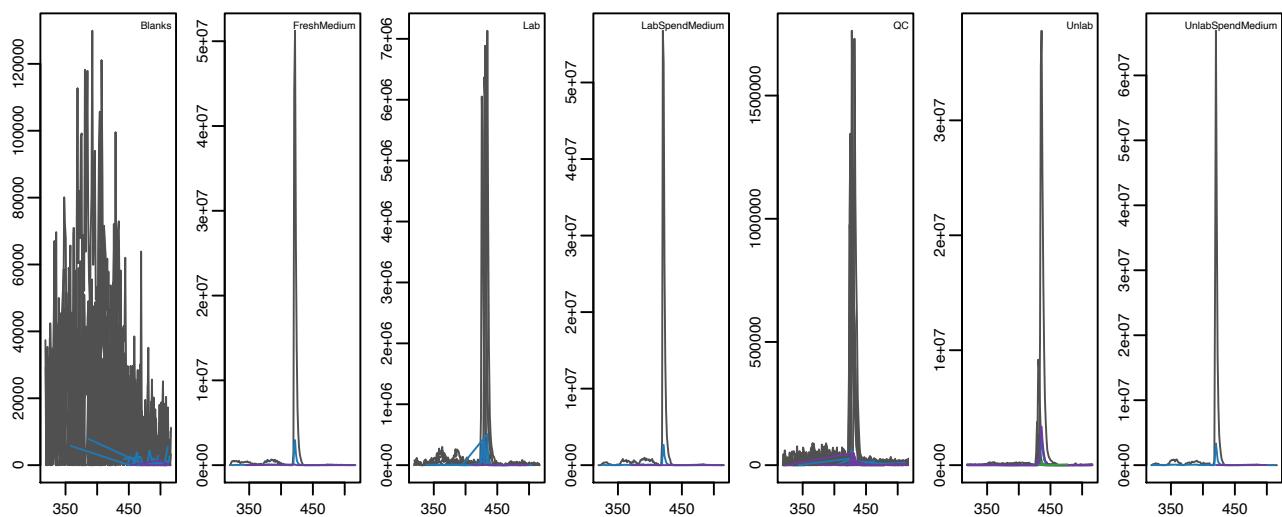


thymine

Formula: C5H6N2O2 Mass: 126.043 Std.RT: 418.2 Ion: NEG

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

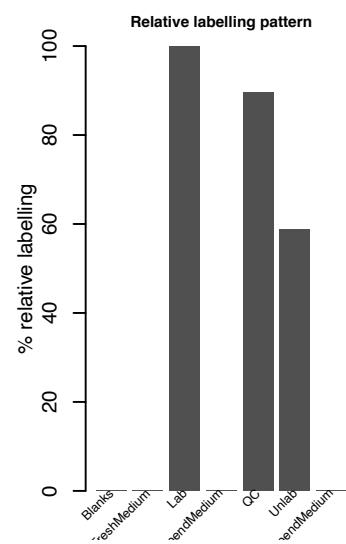
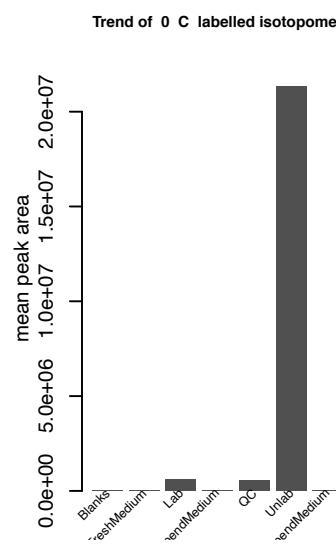
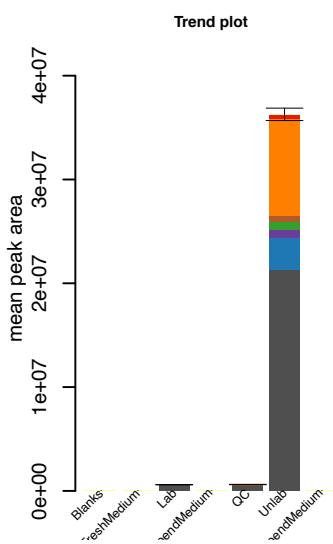
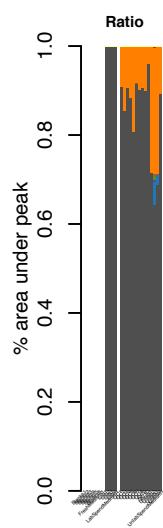
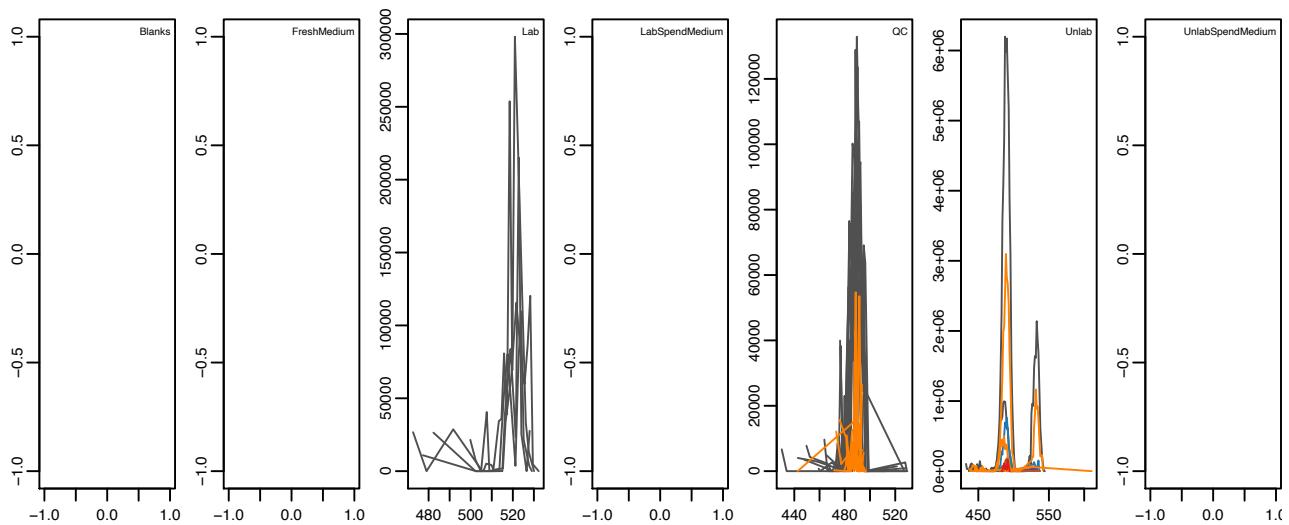


3'_5'-Cyclic AMP

Formula: C10H12N5O6P Mass: 329.053 Std.RT: 526.8 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9 ■+10

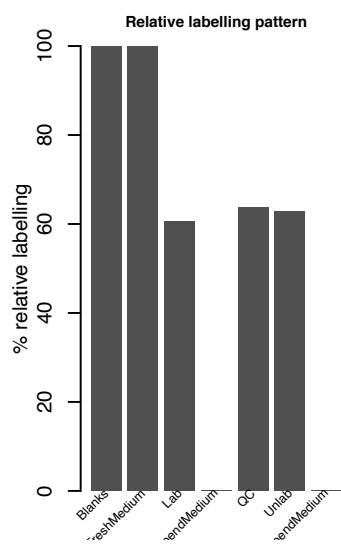
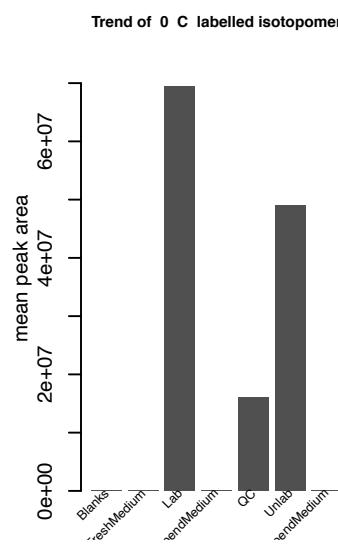
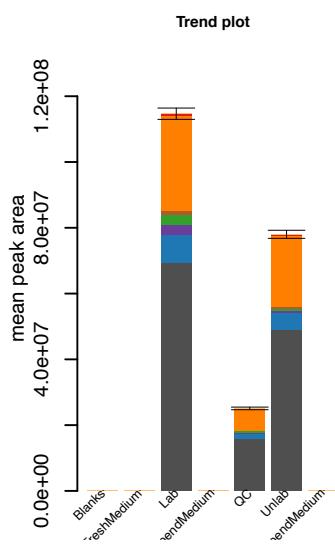
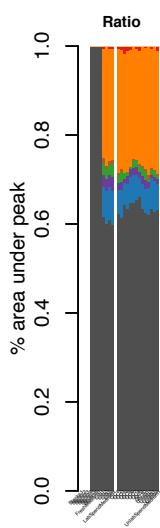
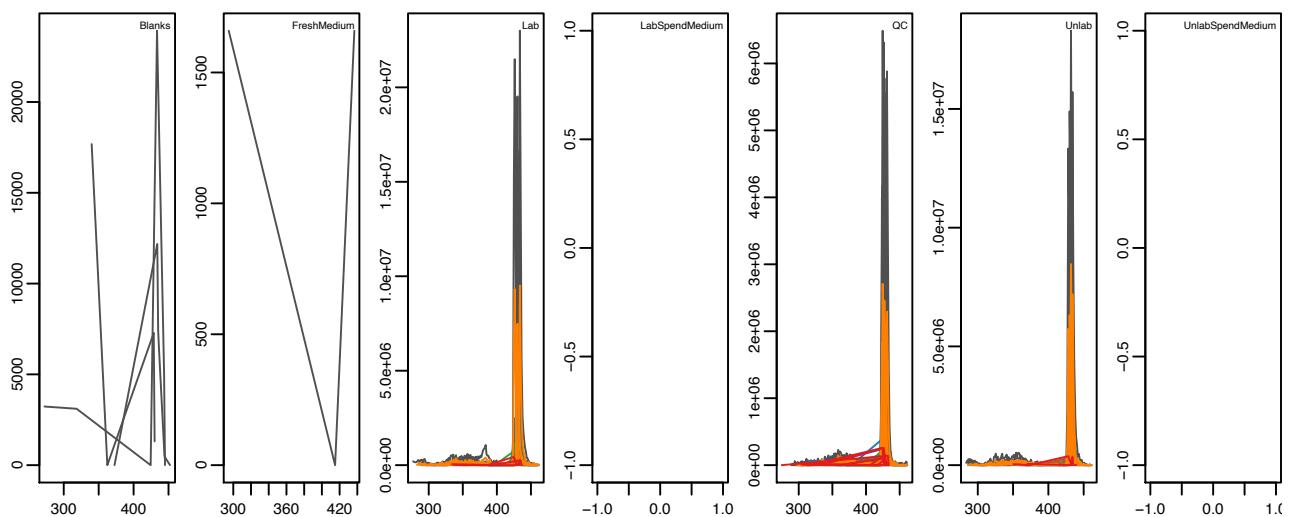


5'-Methylthioadenosine

Formula: C11H15N5O3S Mass: 297.09 Std.RT: 363 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9 ■+10 ■+11

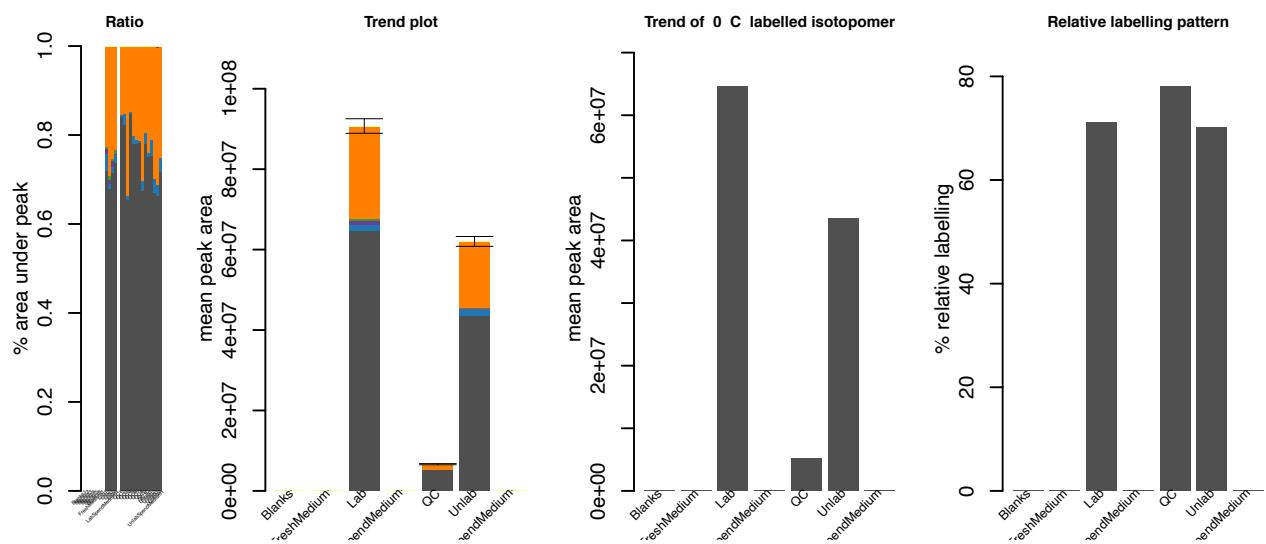
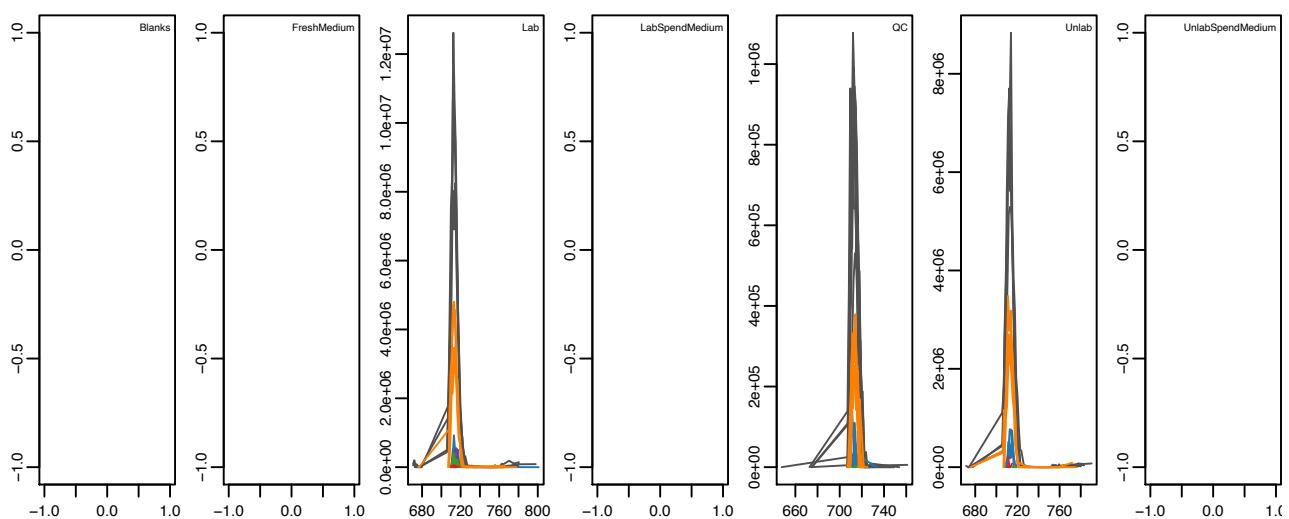


ADP

Formula: C10H15N5O10P2 Mass: 427.029 Std.RT: 714 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9 ■+10

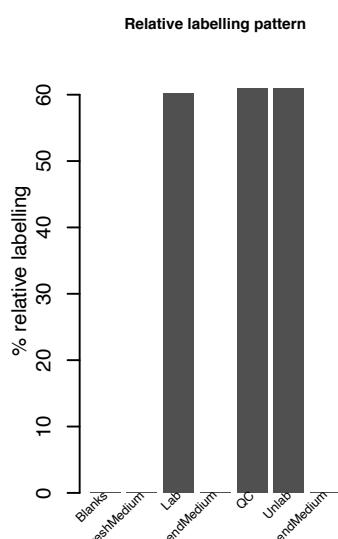
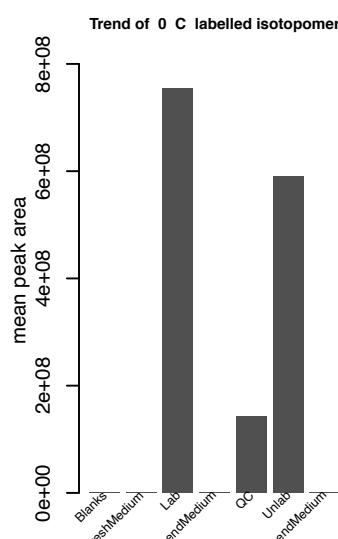
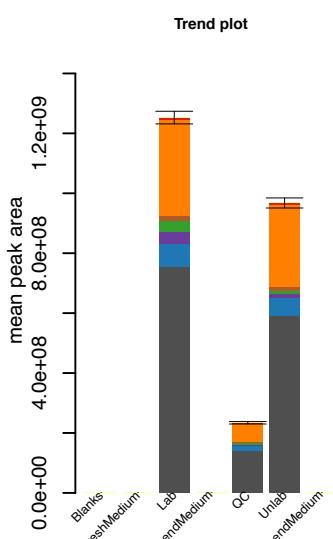
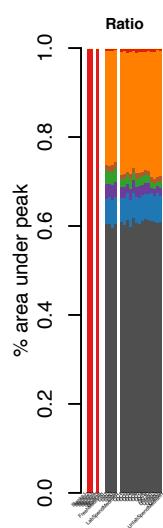
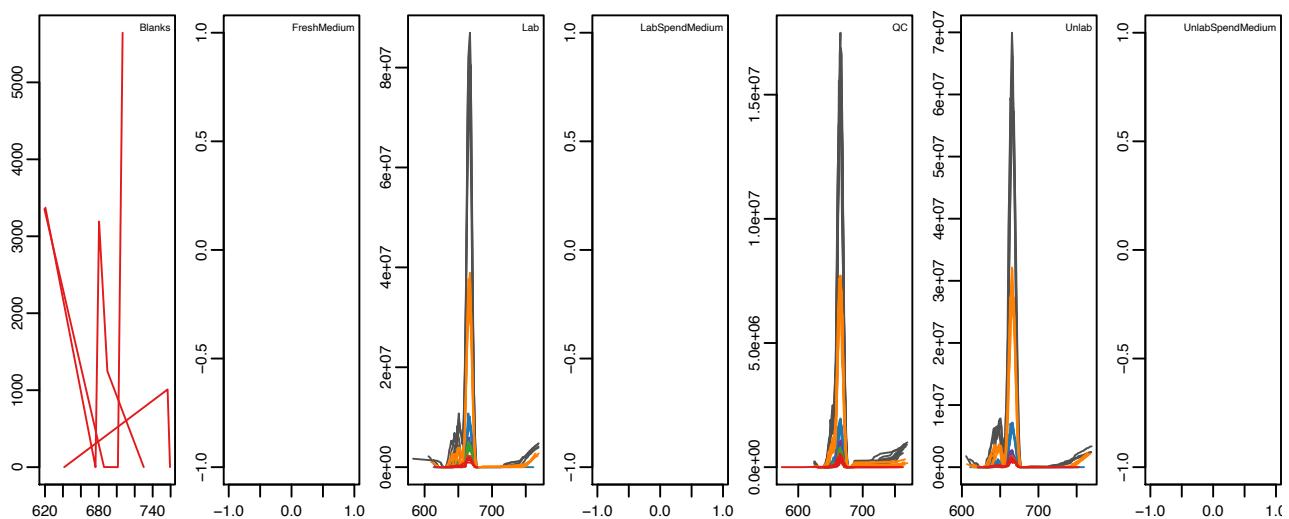


AMP

Formula: C₁₀H₁₄N₅O₇P Mass: 347.063 Std.RT: 670.8 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9 ■+10

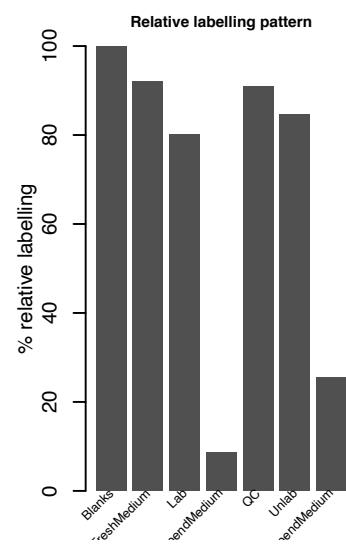
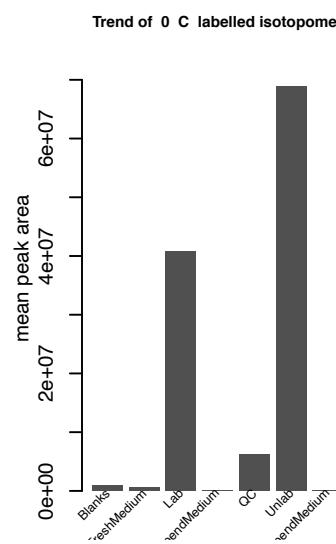
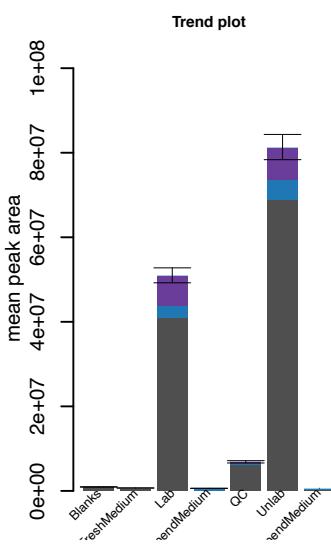
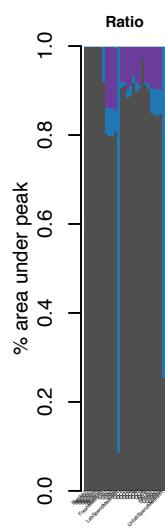
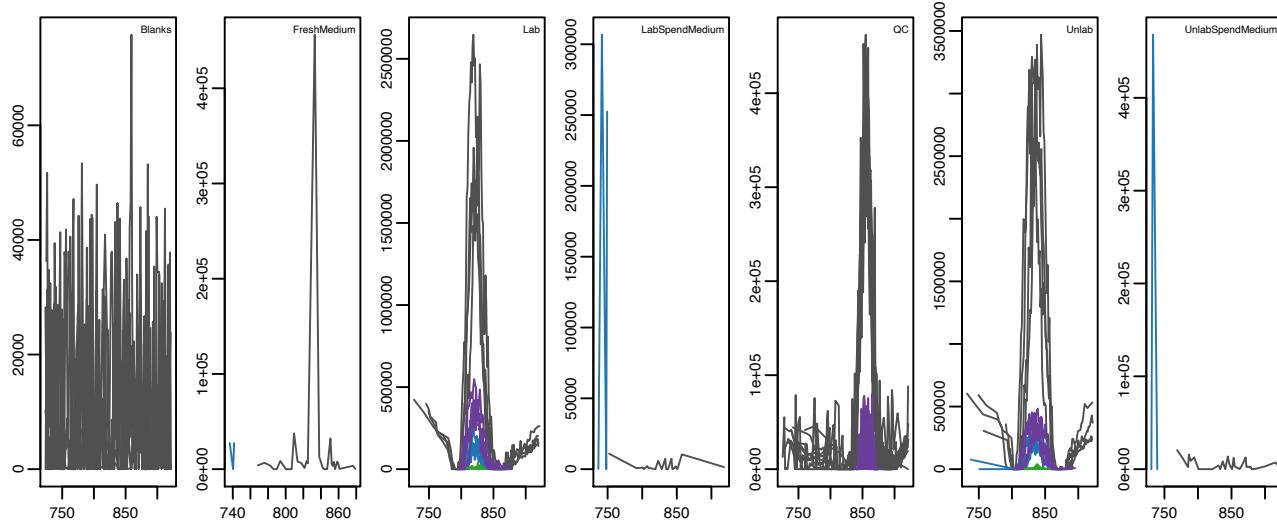


Acetylcholine

Formula: C₇H₁₅NO₂ Mass: 145.11 Std.RT: 823.2 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7

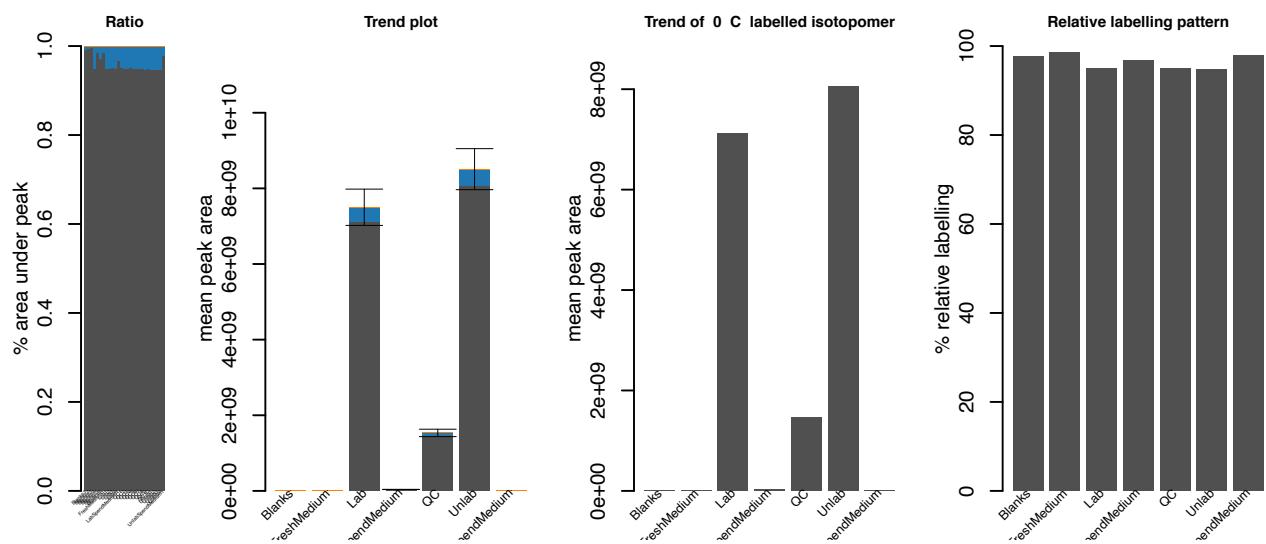
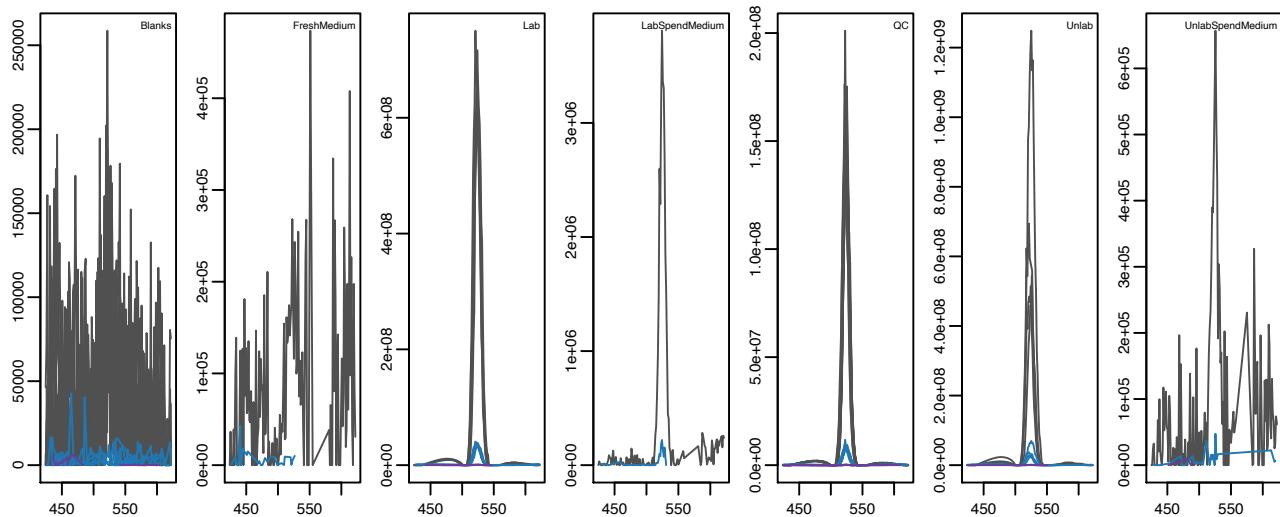


Adenine

Formula: C5H5N5 Mass: 135.054 Std.RT: 523.8 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

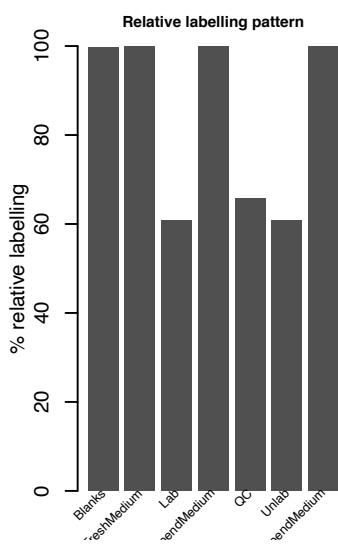
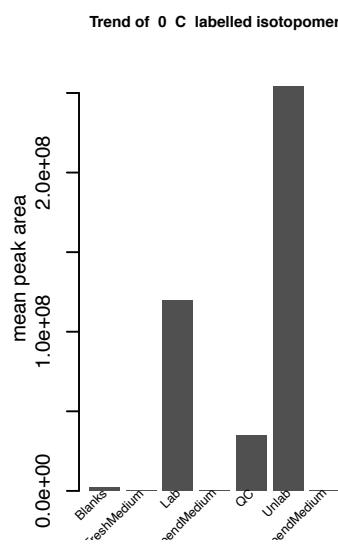
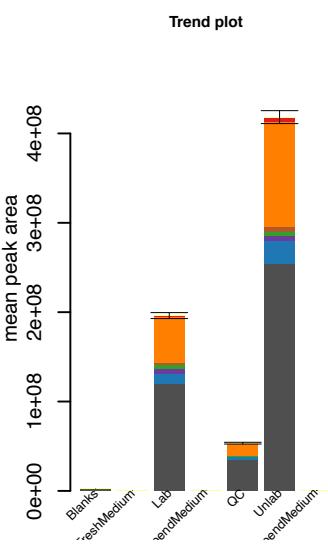
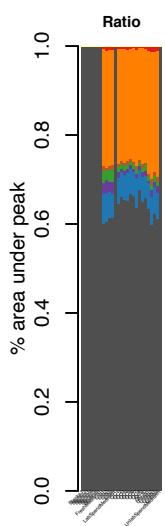
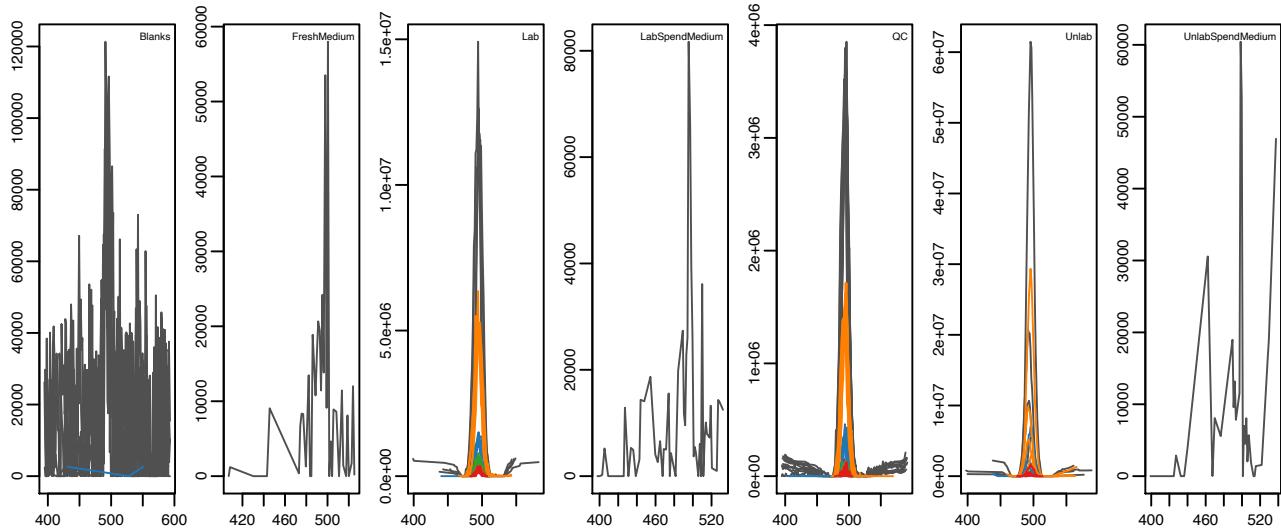


Adenosine

Formula: C₁₀H₁₃N₅O₄ Mass: 267.097 Std.RT: 494.4 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9 ■+10

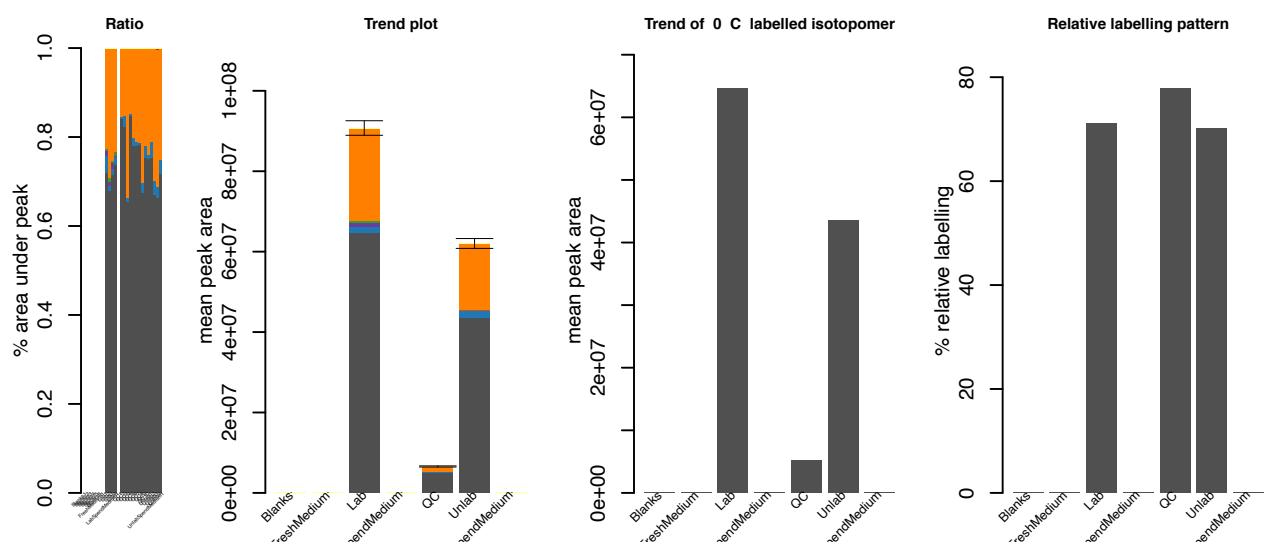
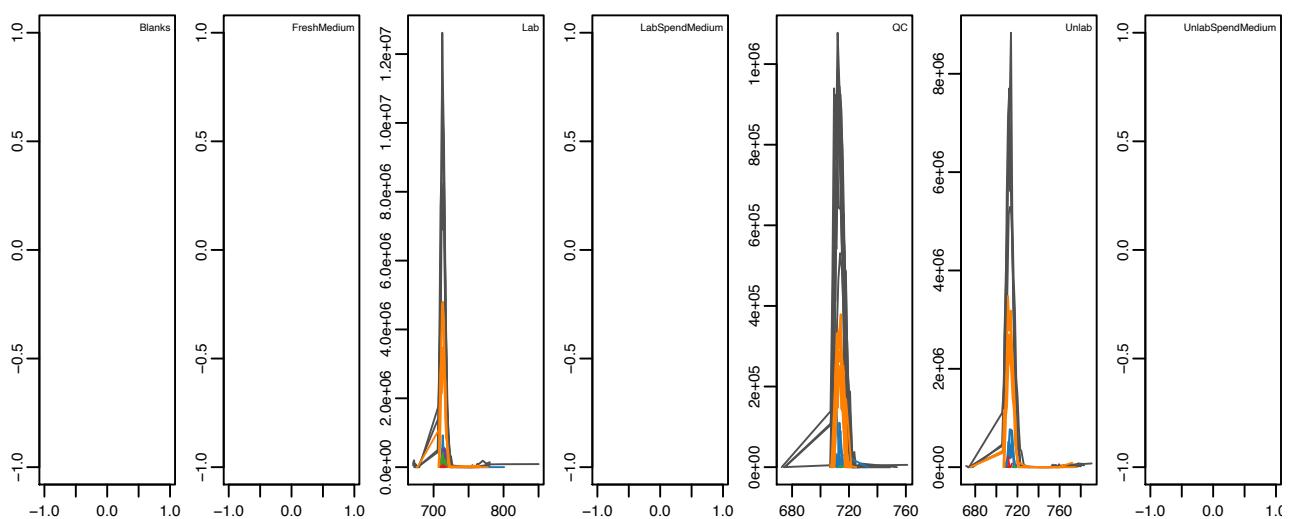


Adenosine 2'–5'-bisphosphate

Formula: C₁₀H₁₅N₅O₁₀P₂ Mass: 427.029 Std.RT: 761.4 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9 ■+10

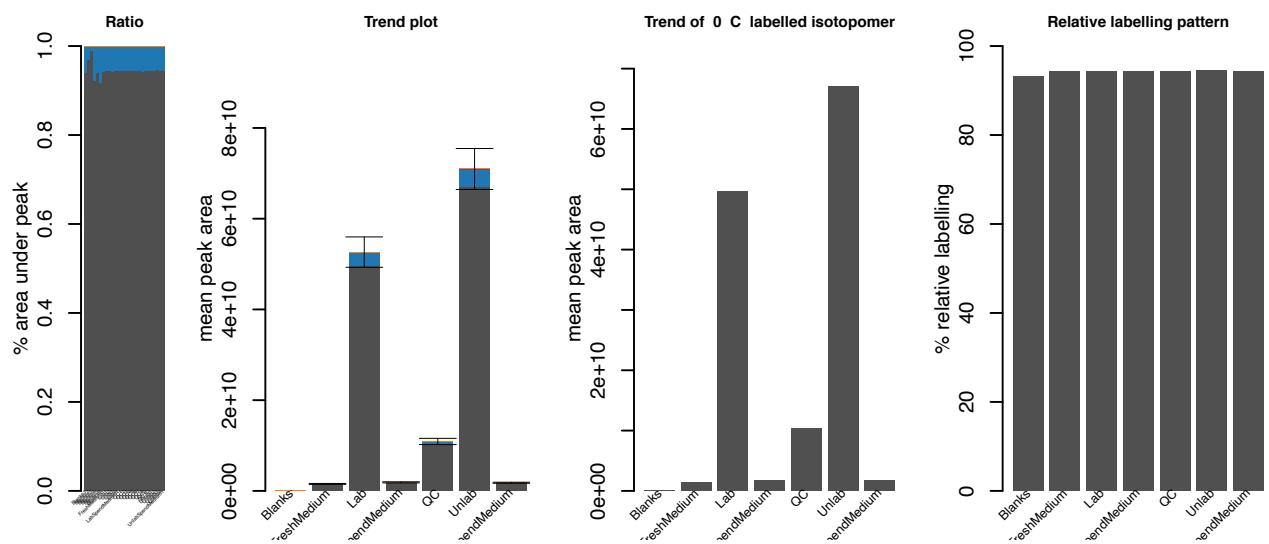
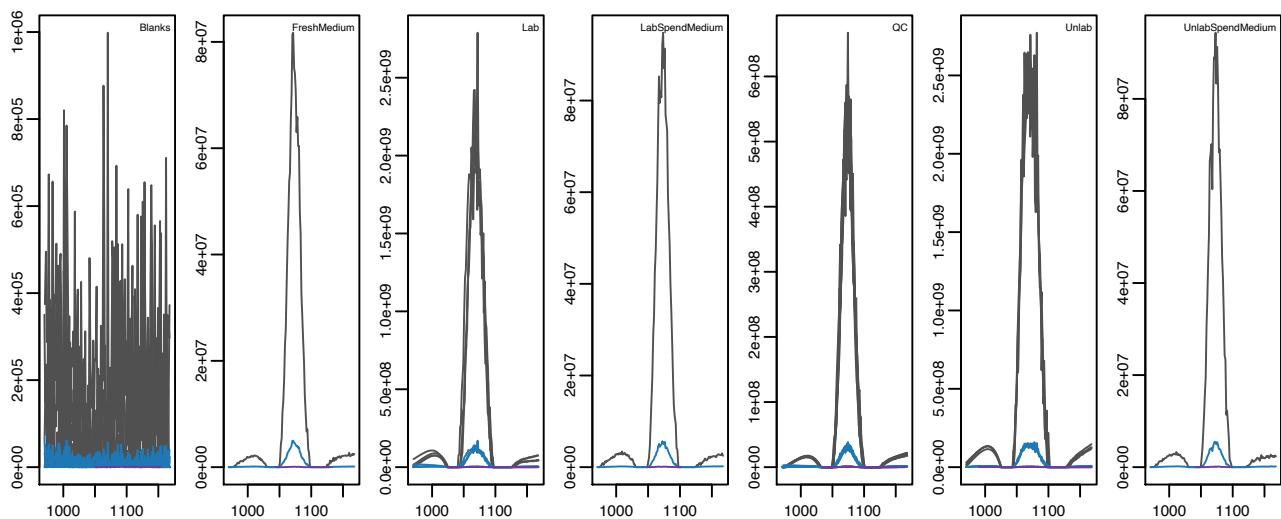


Choline

Formula: C₅H₁₃NO Mass: 103.1 Std.RT: 1069.8 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

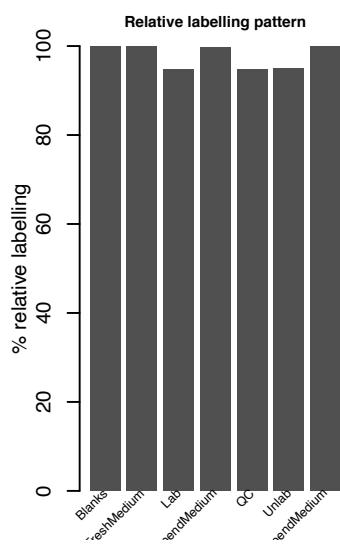
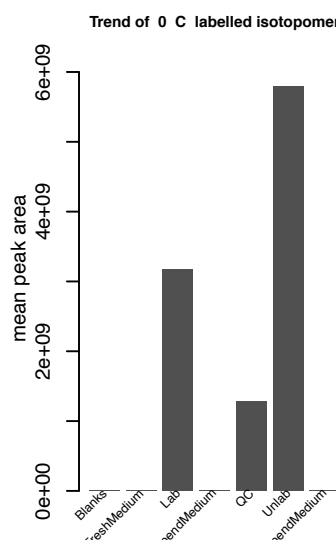
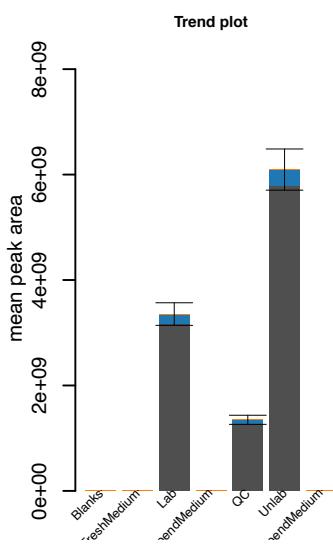
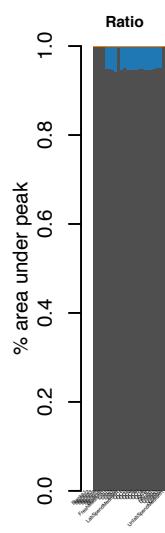
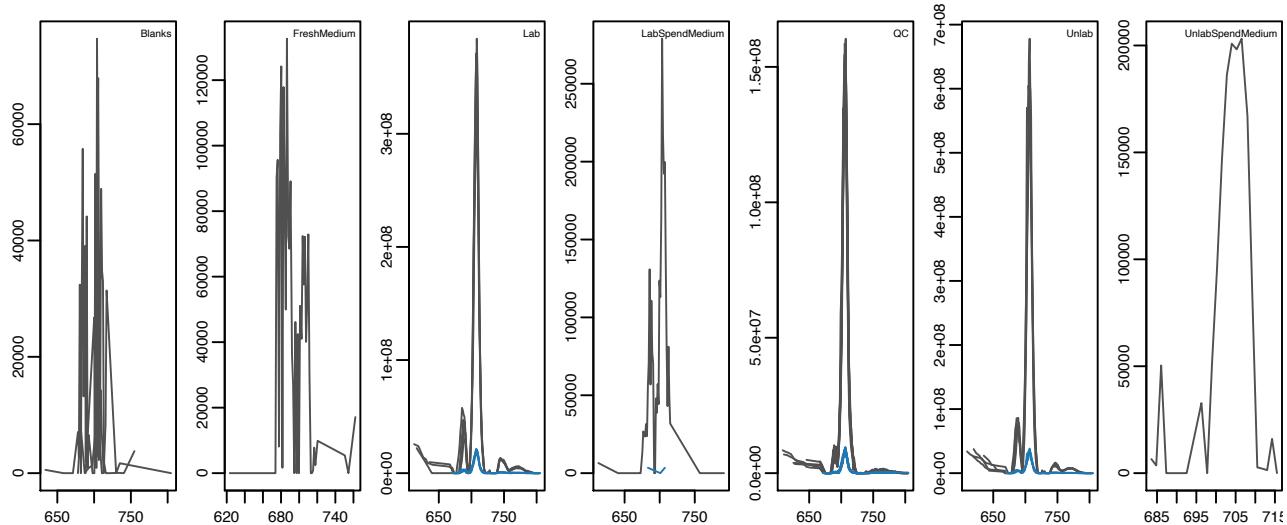


Choline phosphate

Formula: C5H14NO4P Mass: 183.066 Std.RT: 706.2 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

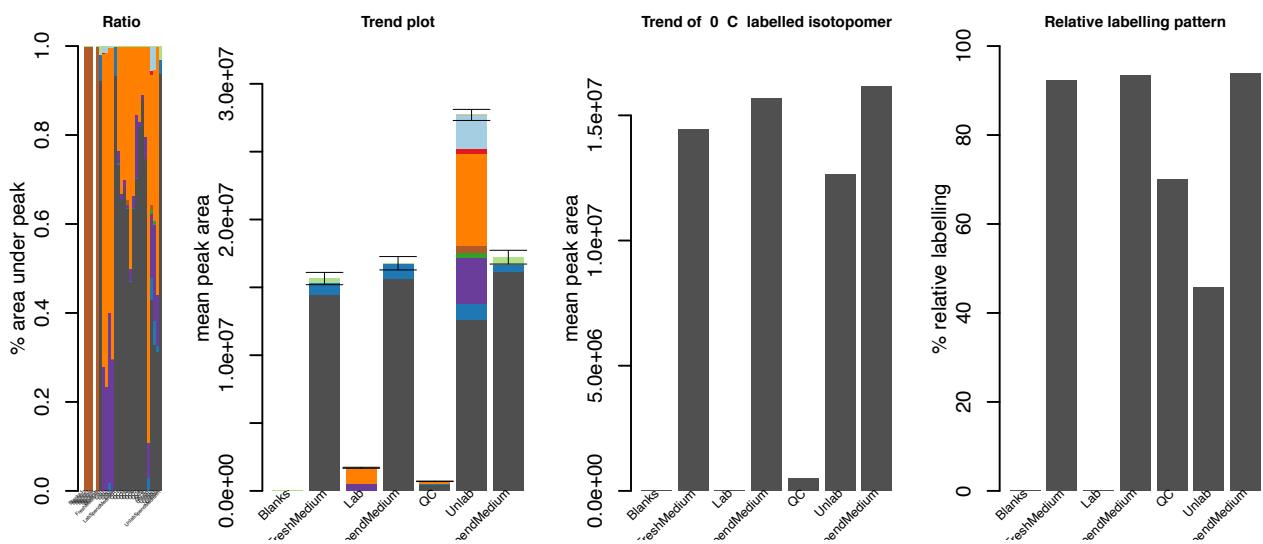
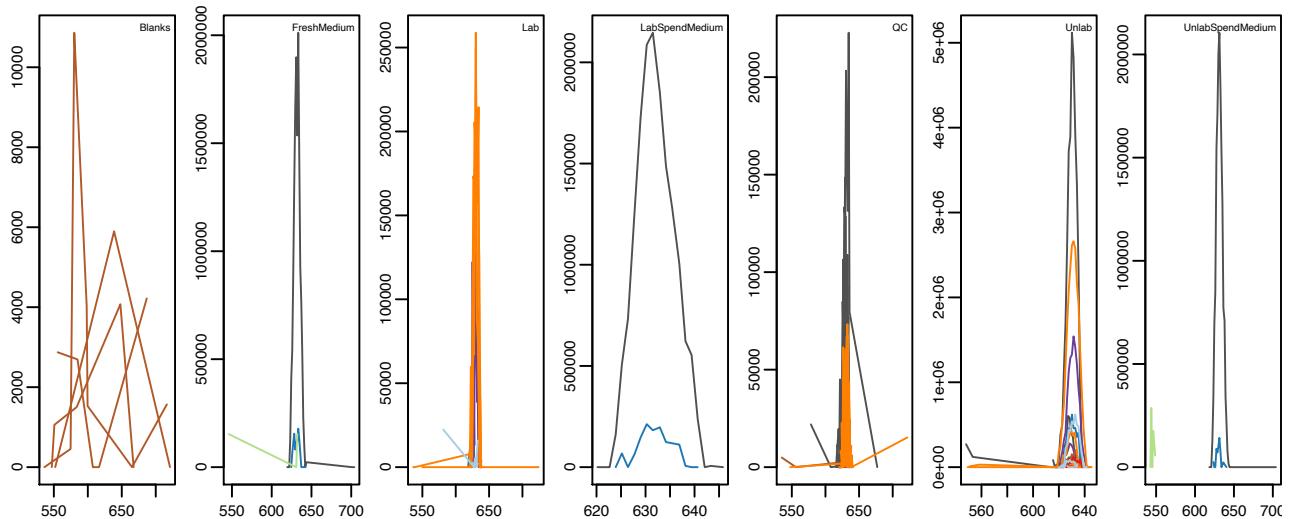


Cytidine

Formula: C9H13N3O5 Mass: 243.086 Std.RT: 633.6 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9

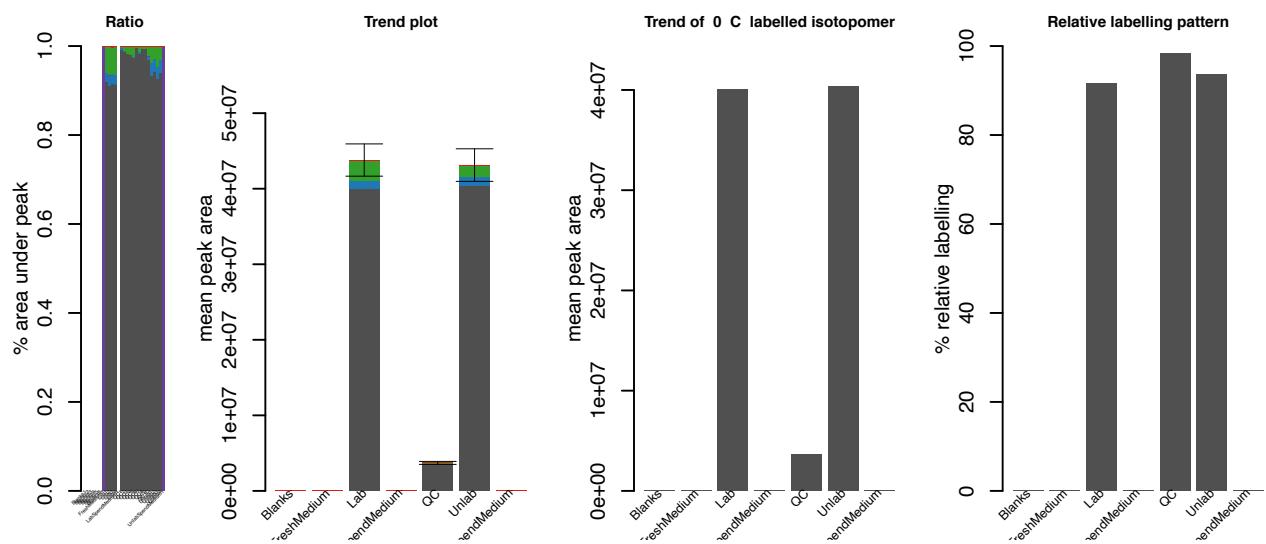
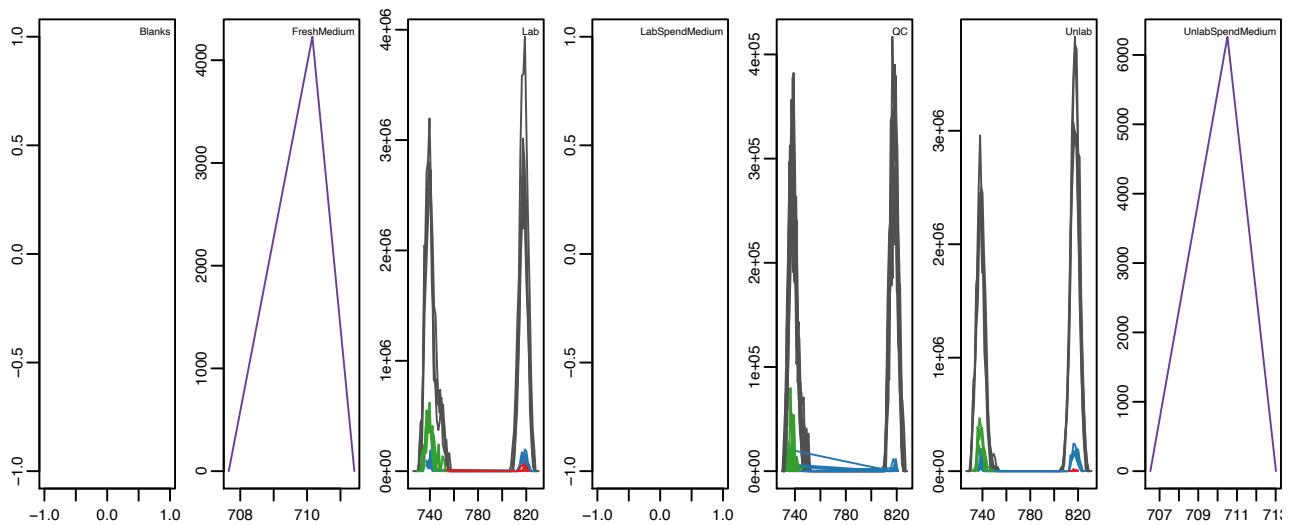


D-Glucosamine-6-phosphate

Formula: C₆H₁₄NO₈P Mass: 259.046 Std.RT: 759 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6

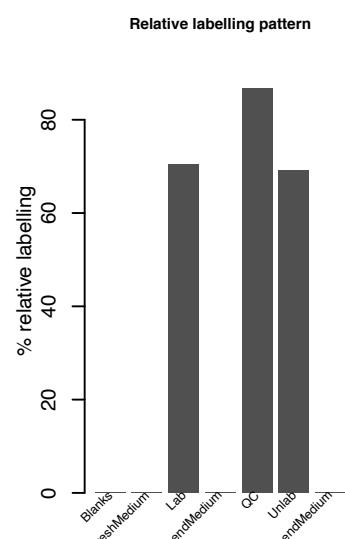
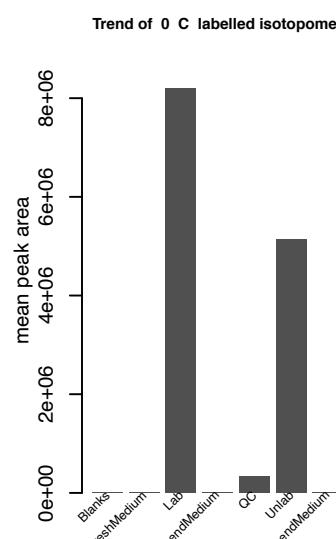
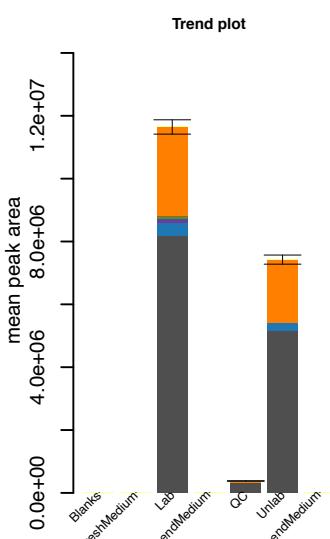
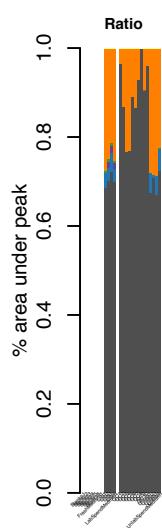
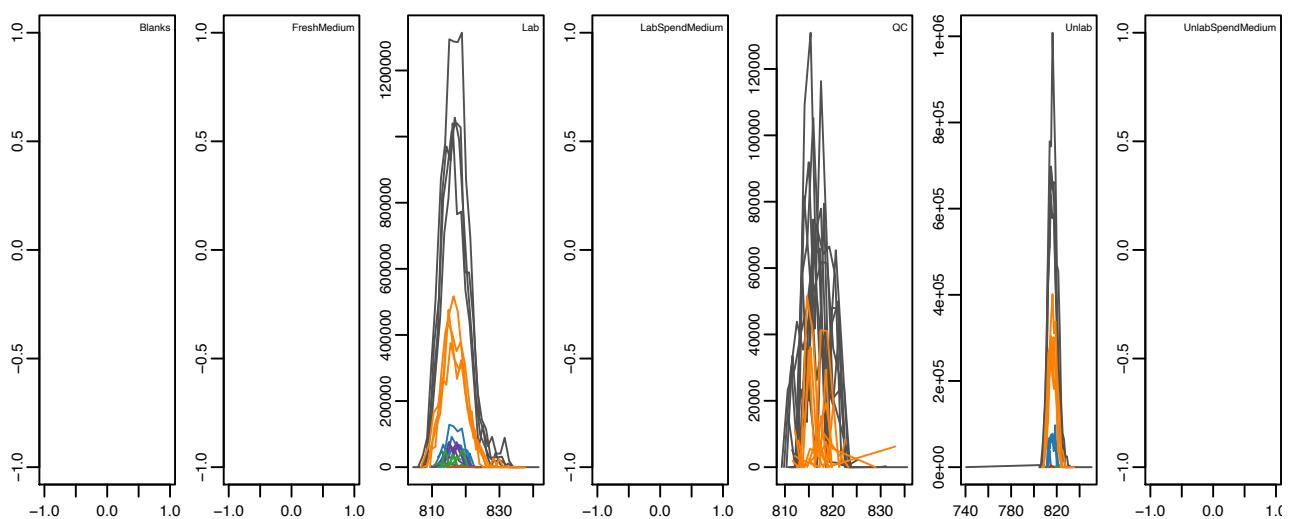


GDP

Formula: C10H15N5O11P2 Mass: 443.024 Std.RT: 816 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9 ■+10

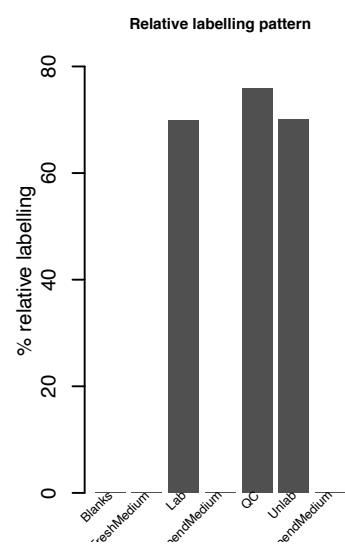
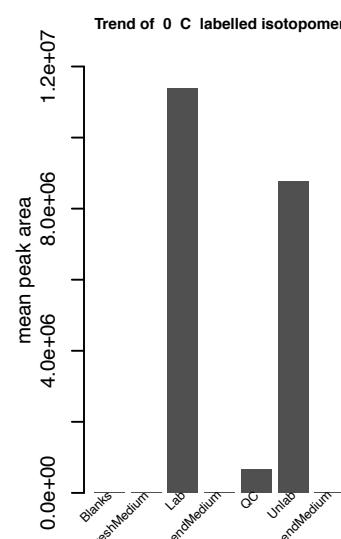
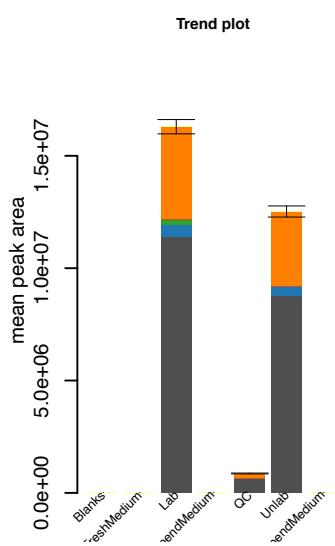
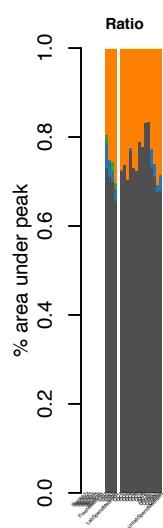
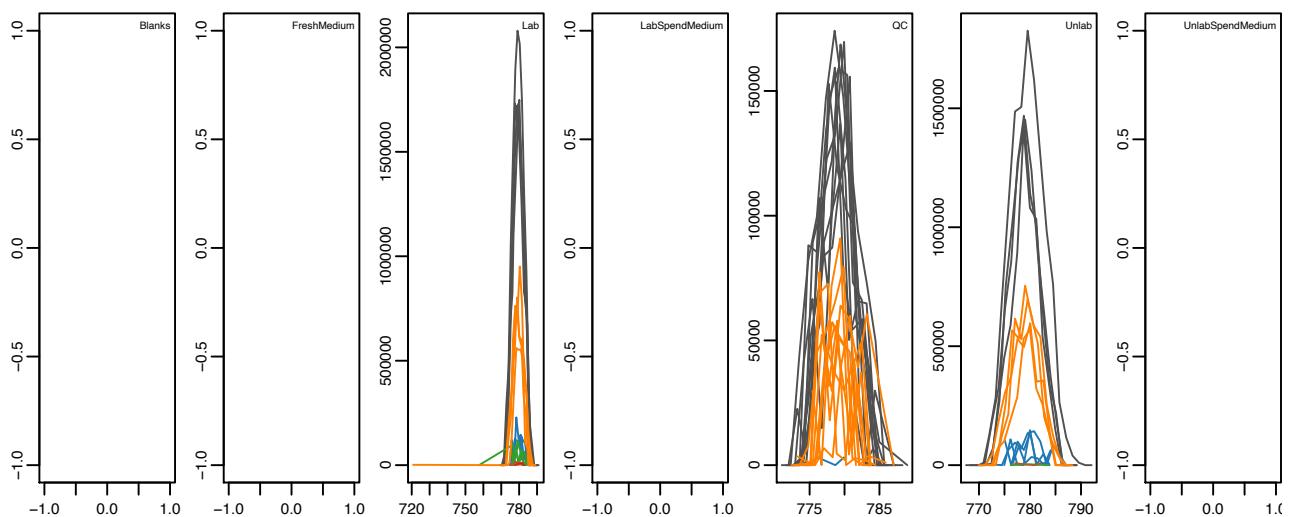


GMP

Formula: C10H14N5O8P Mass: 363.058 Std.RT: 747 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9 ■+10

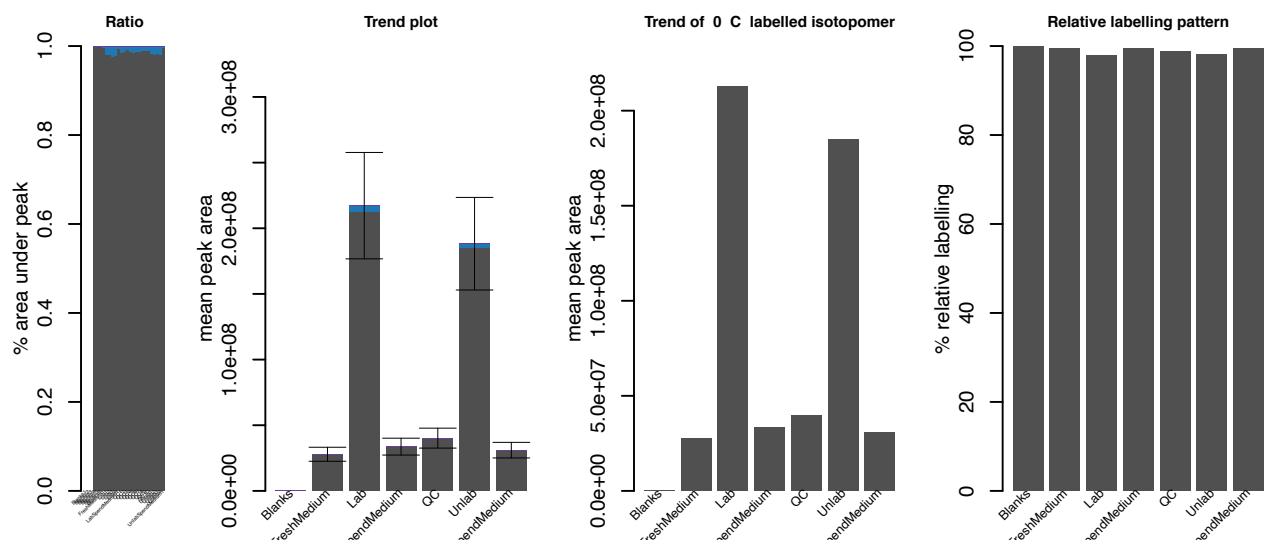
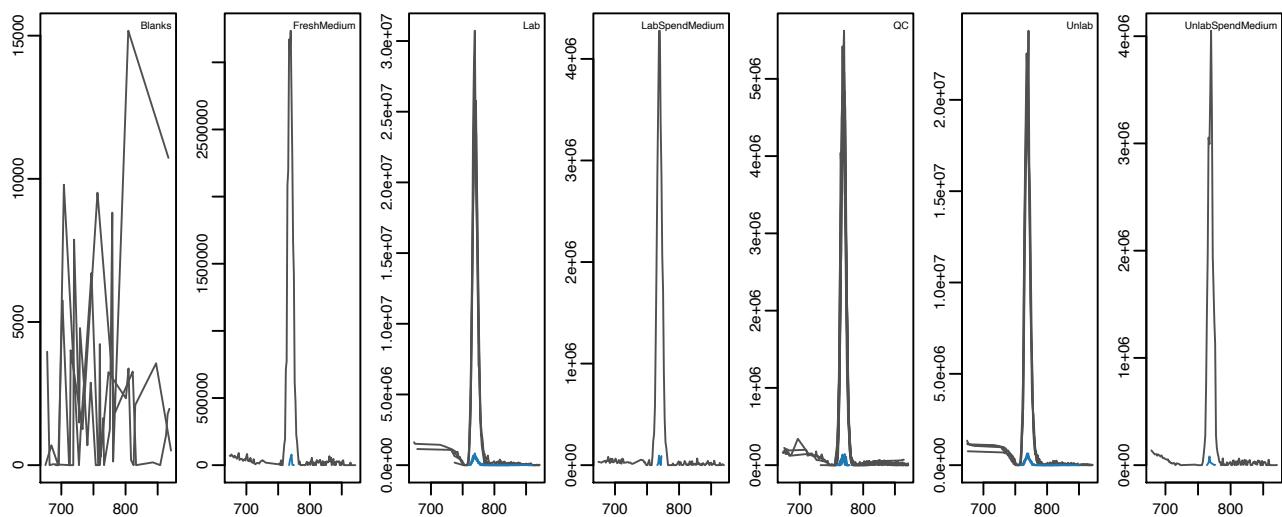


Glycine

Formula: C₂H₅NO₂ Mass: 75.032 Std.RT: 772.8 Ion: POS

G1

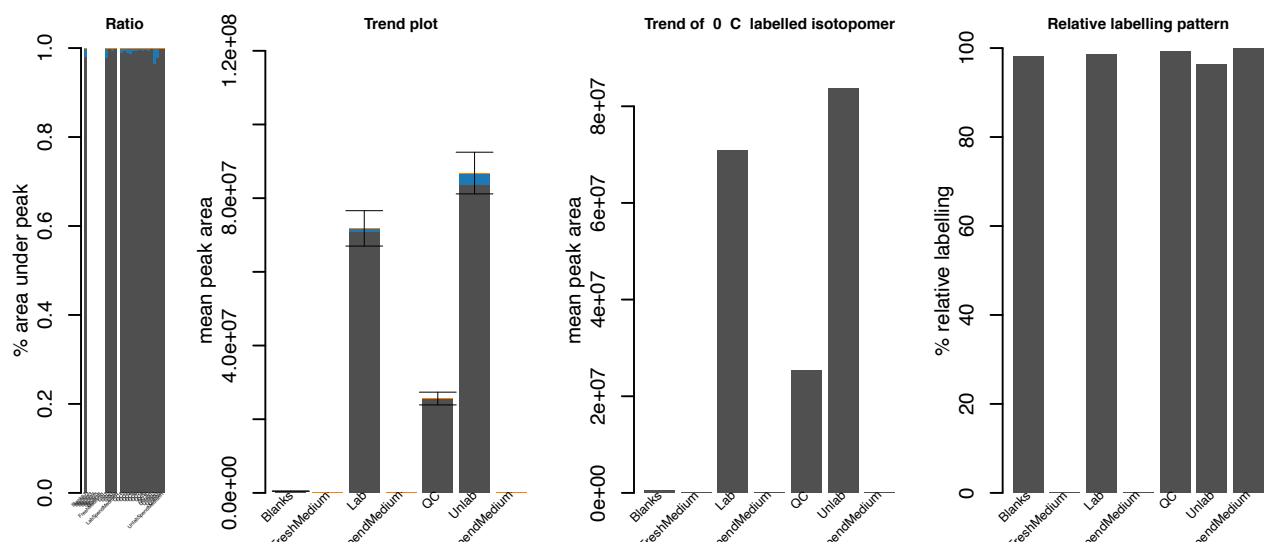
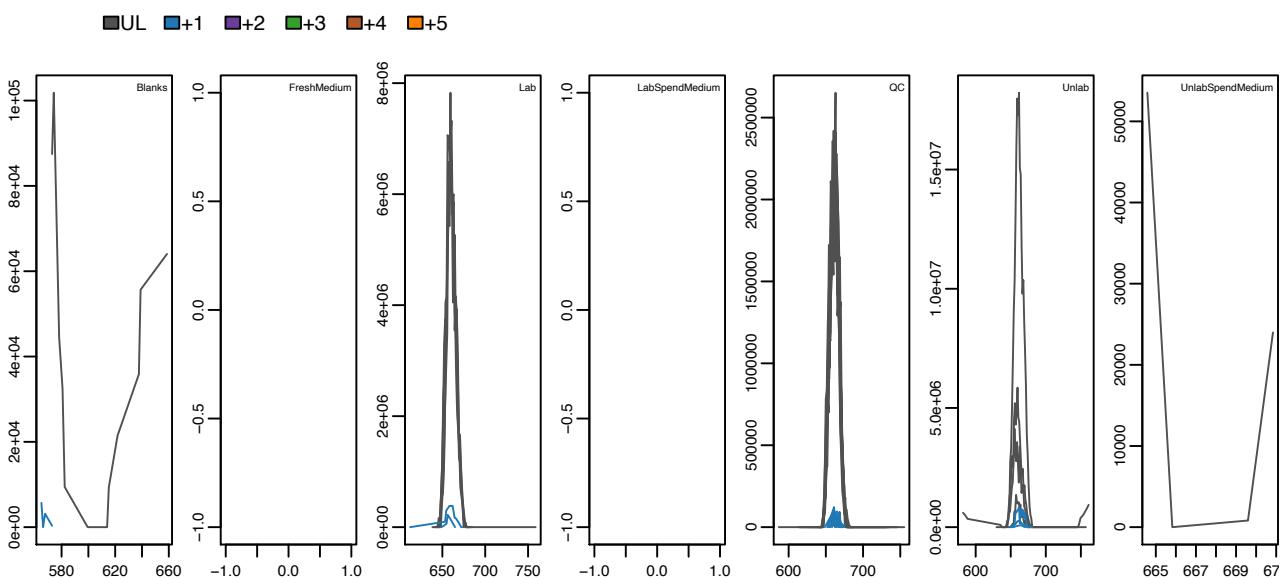
■UL ■+1 ■+2



Guanine

Formula: C5H5N5O Mass: 151.049 Std.RT: 664.2 Ion: POS

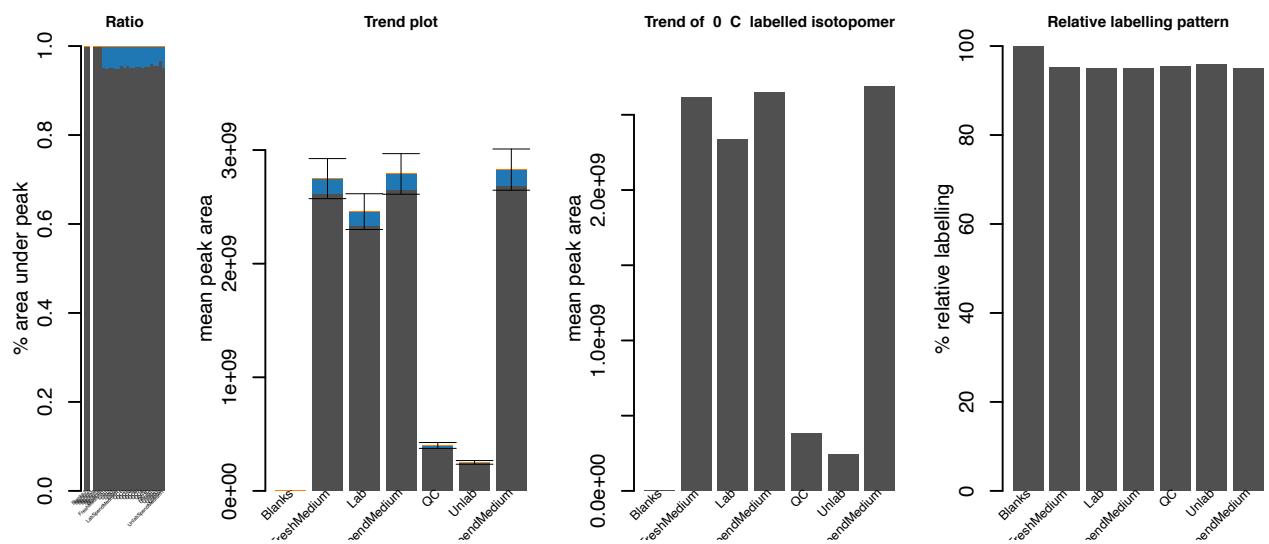
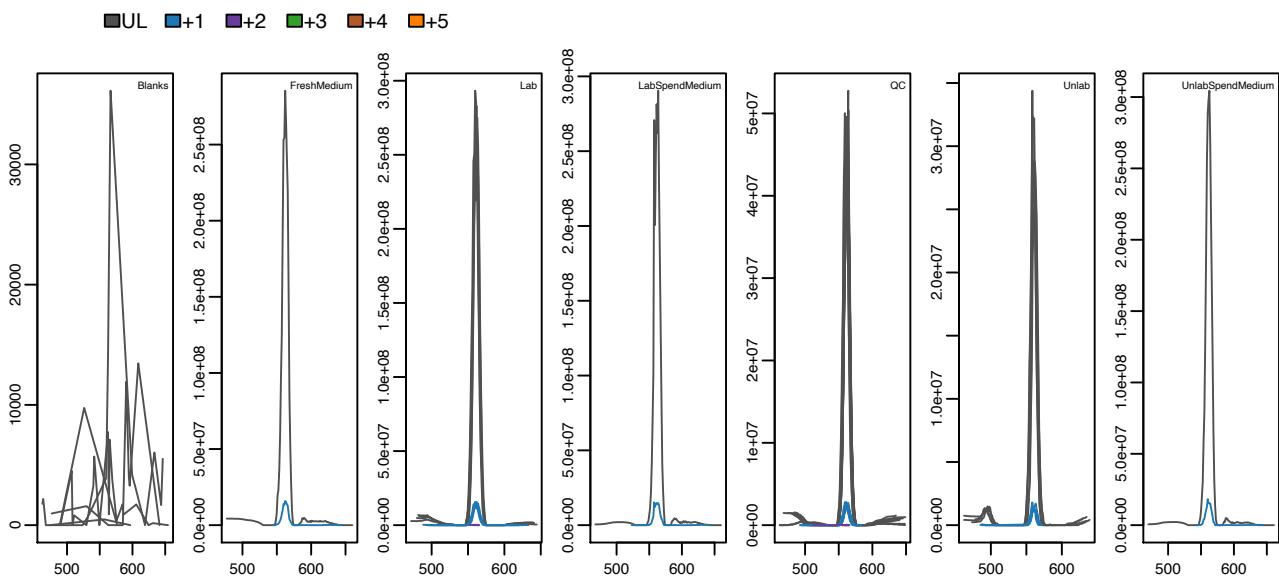
G1



Hypoxanthine

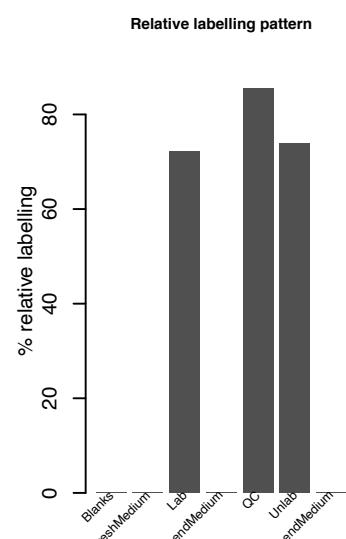
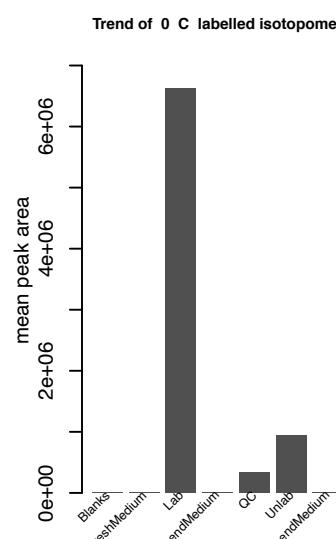
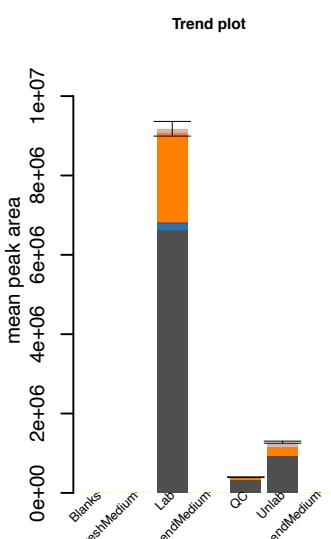
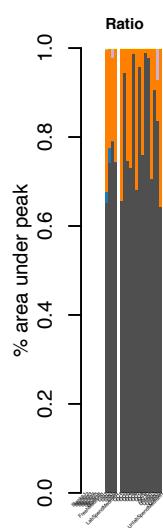
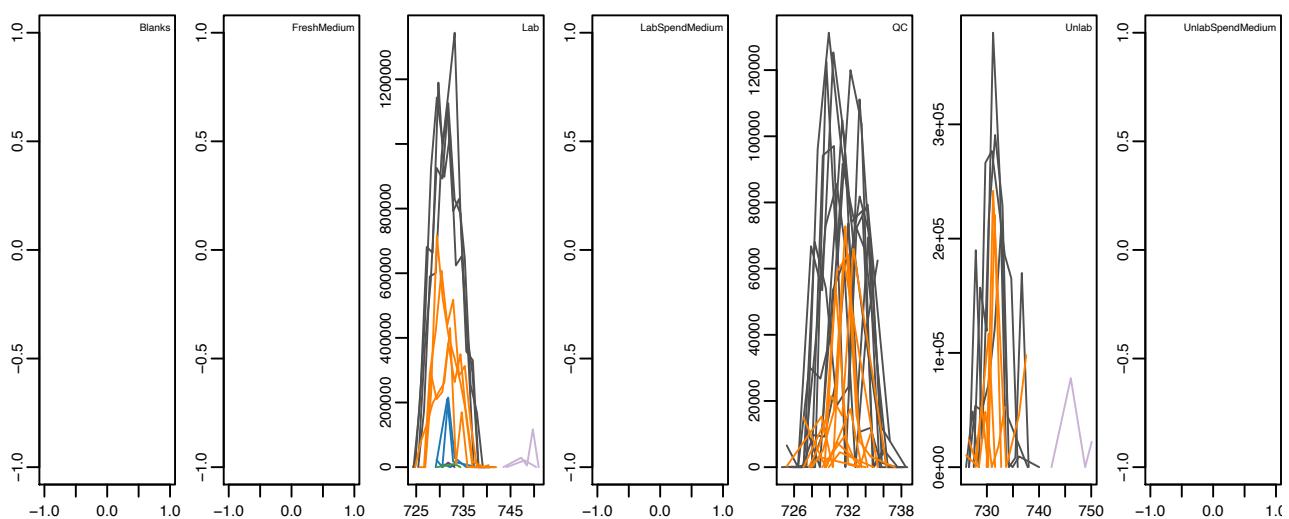
Formula: C5H4N4O Mass: 136.039 Std.RT: 562.2 Ion: POS

G1



IMPFormula: C₁₀H₁₃N₄O₈P Mass: 348.047 Std.RT: 732.6 Ion: POS**G1**

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9 ■+10

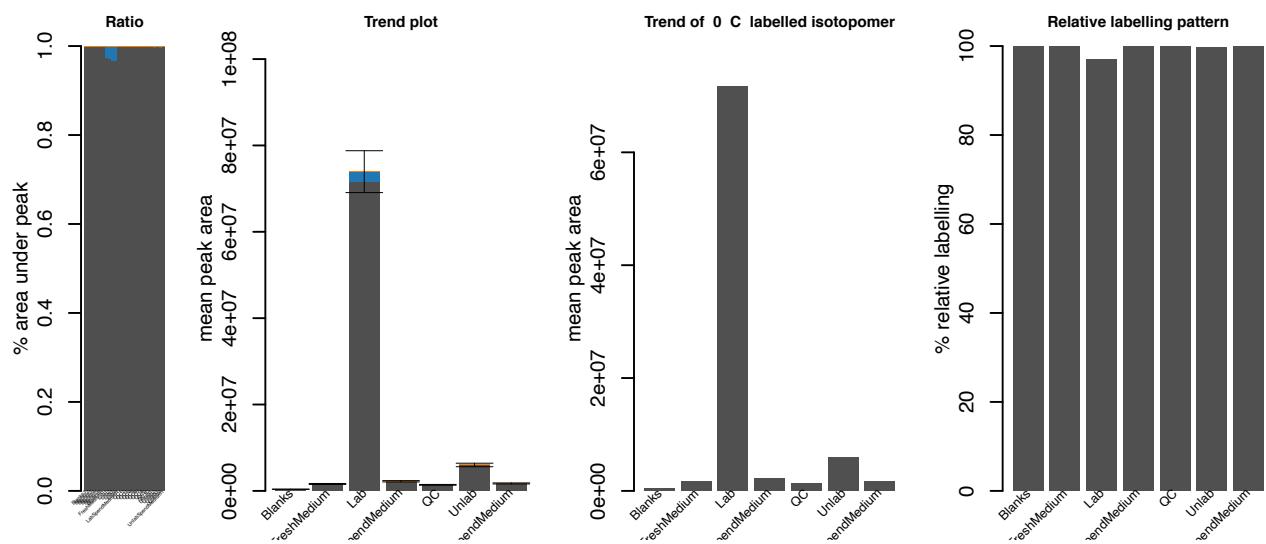
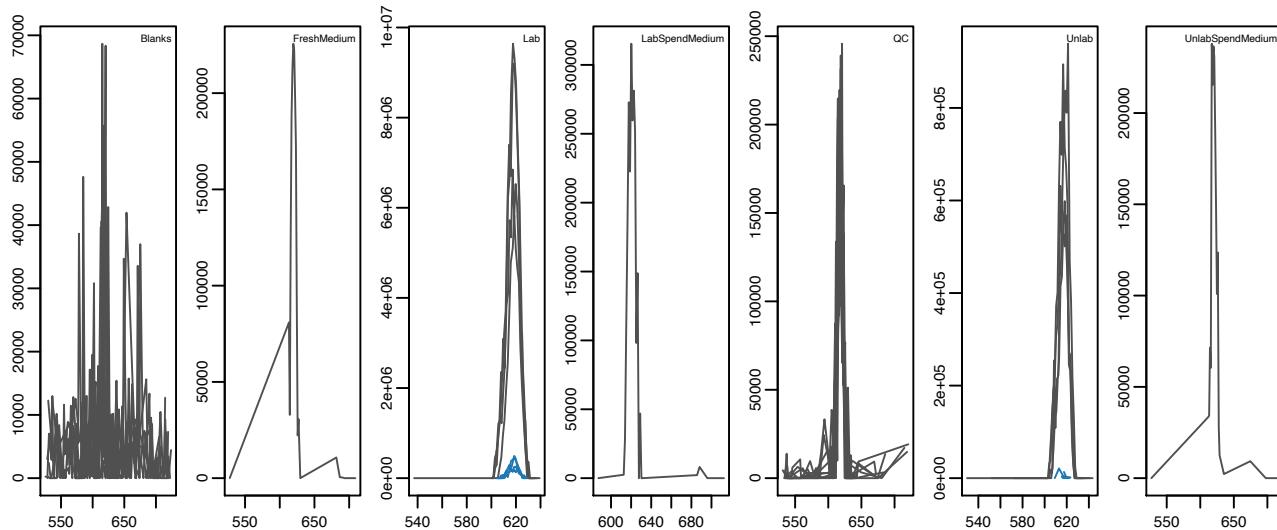


Imidazole-4-acetate

Formula: C5H6N2O2 Mass: 126.043 Std.RT: 625.2 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

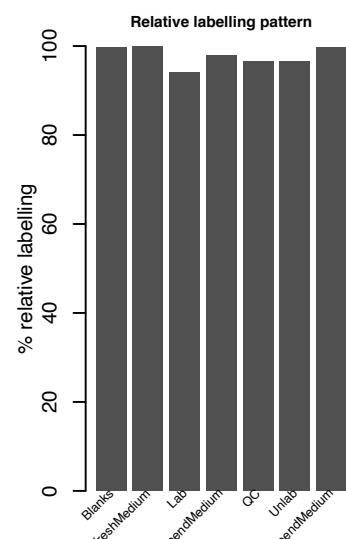
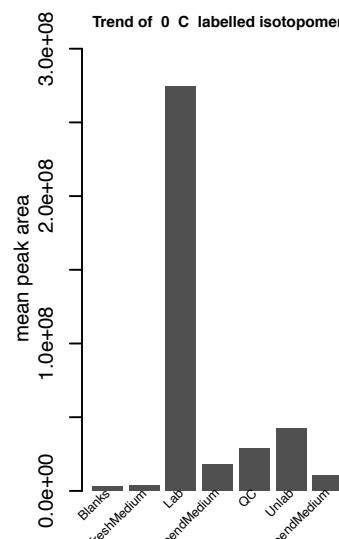
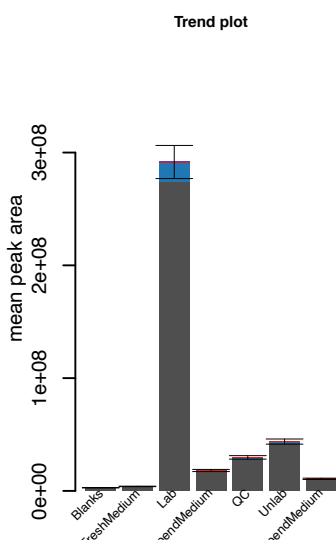
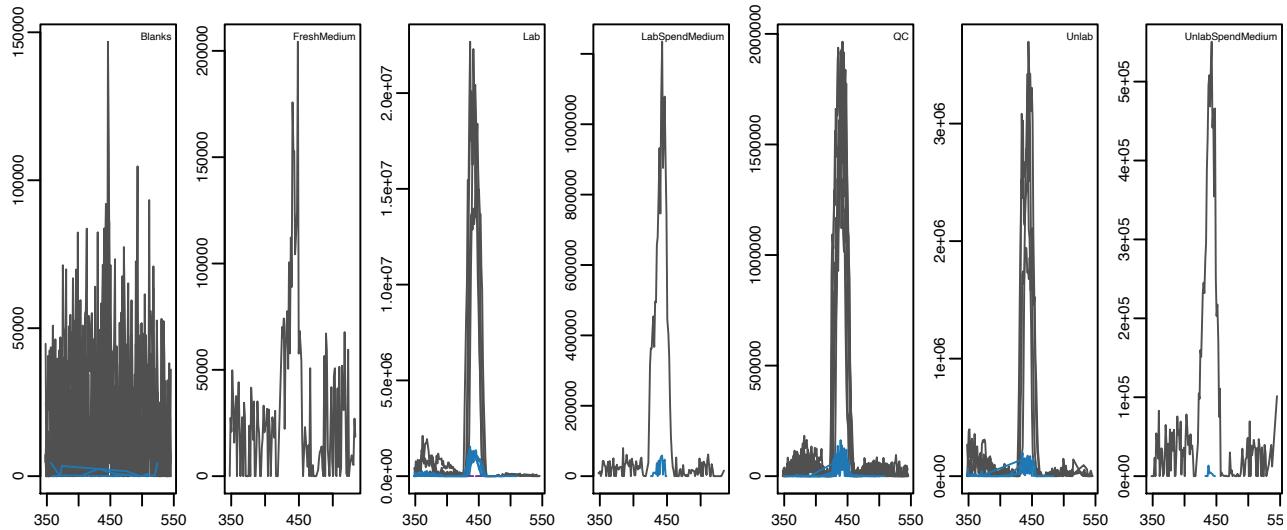


Isonicotinic acid

Formula: C₆H₅NO₂ Mass: 123.032 Std.RT: 447.6 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6

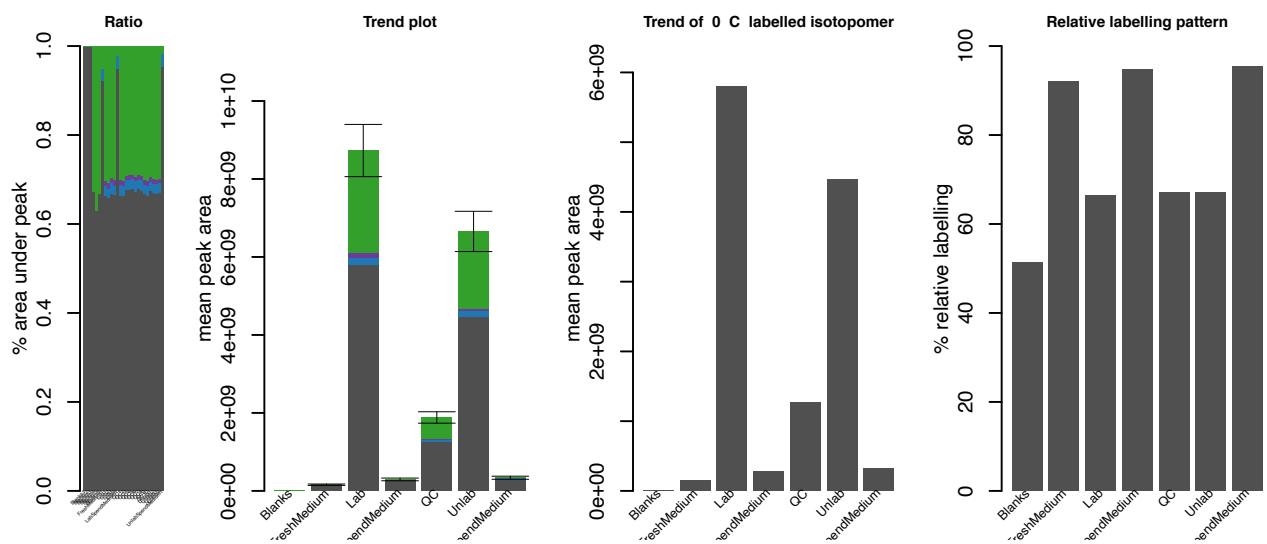
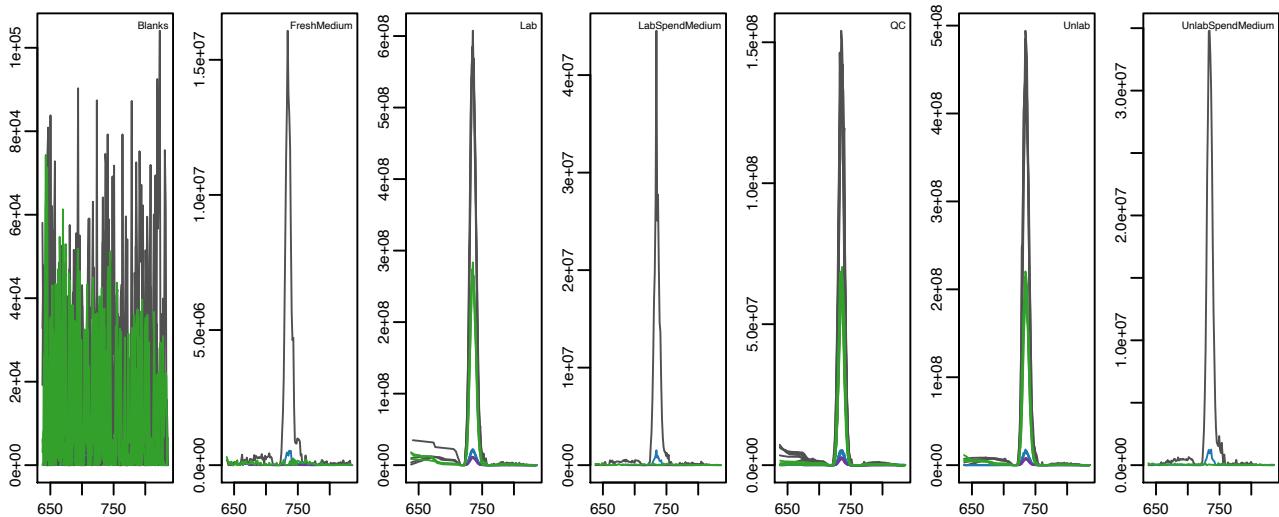


L-Alanine

Formula: C3H7NO2 Mass: 89.048 Std.RT: 737.4 Ion: POS

G1

■UL ■+1 ■+2 ■+3

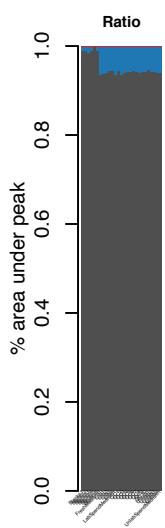
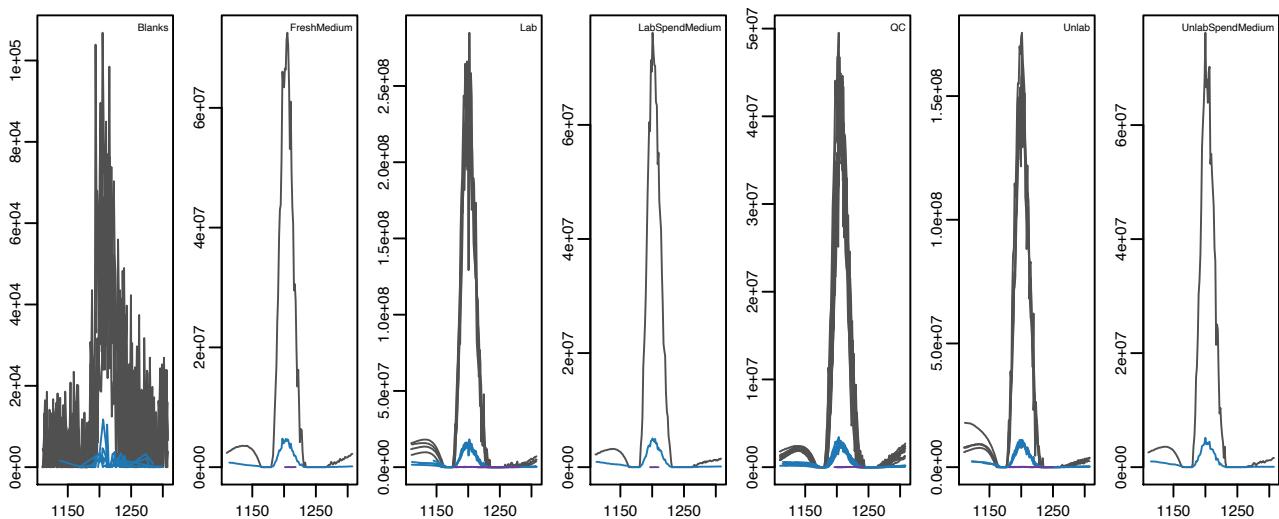


L-Arginine

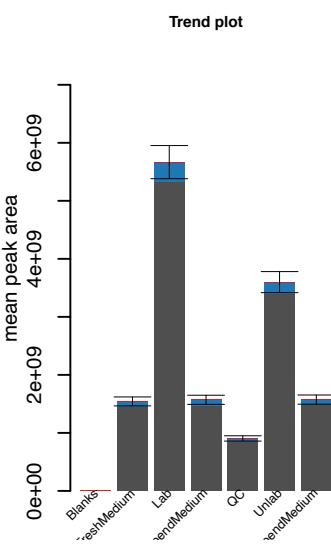
Formula: C₆H₁₄N₄O₂ Mass: 174.112 Std.RT: 1209.6 Ion: POS

G1

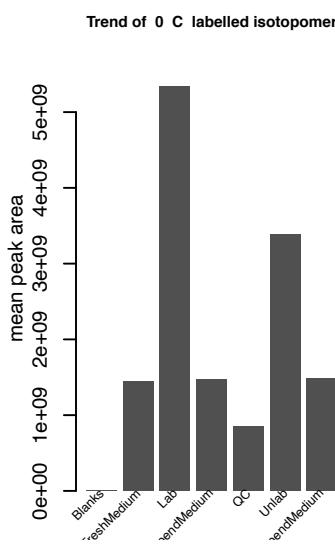
■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6



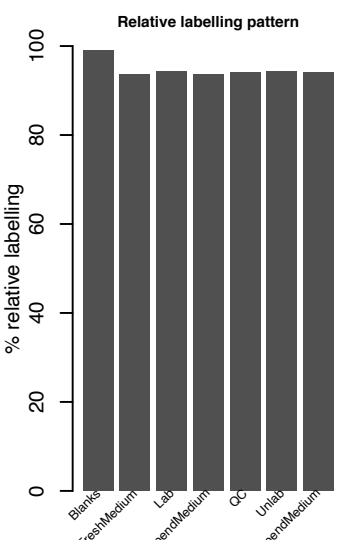
Trend plot



Trend of 0 C labelled isotopomer



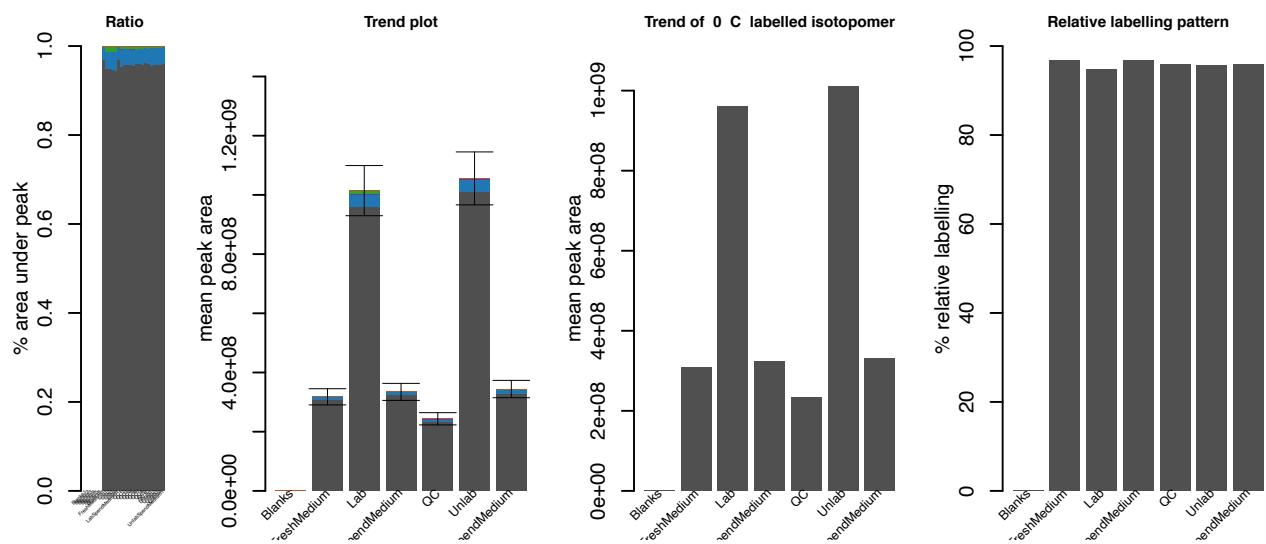
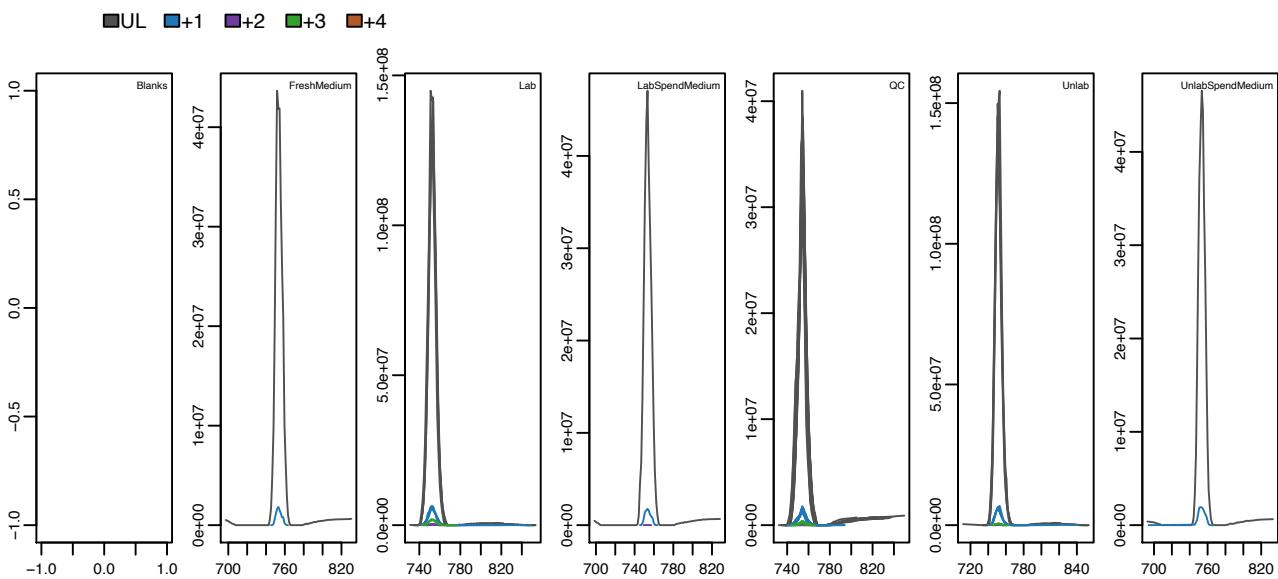
Relative labelling pattern



L-Asparagine

Formula: C4H8N2O3 Mass: 132.053 Std.RT: 754.8 Ion: POS

G1

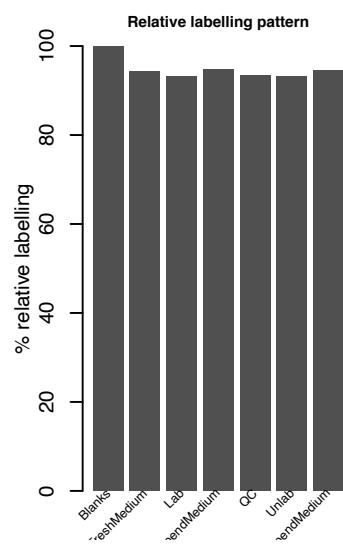
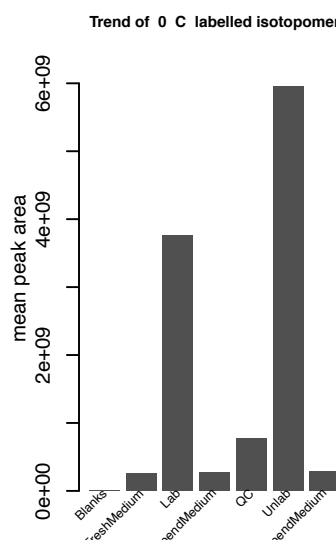
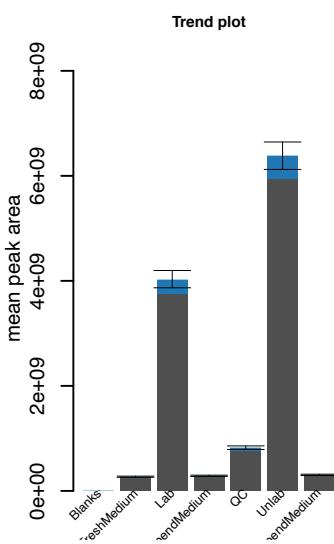
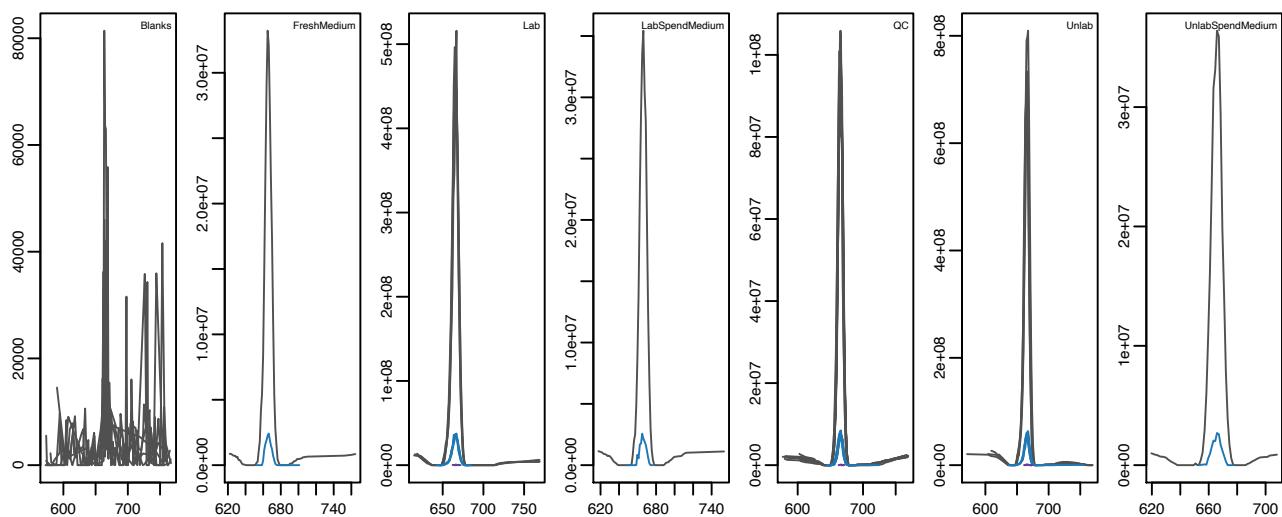


L-Carnitine

Formula: C₇H₁₅NO₃ Mass: 161.105 Std.RT: 670.8 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7

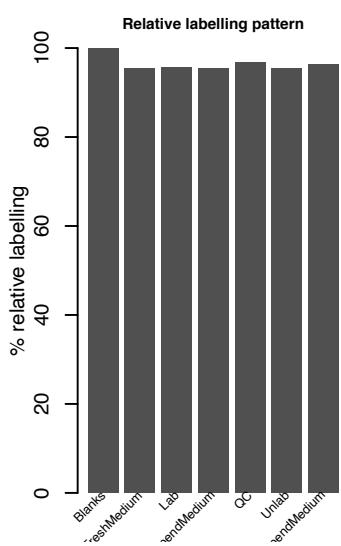
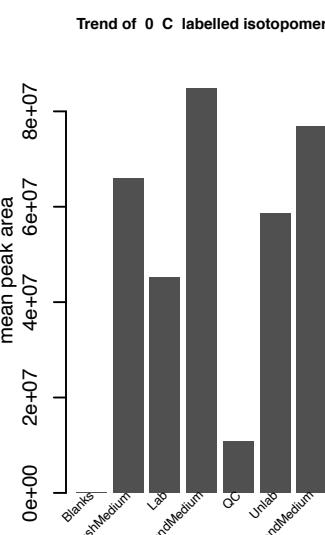
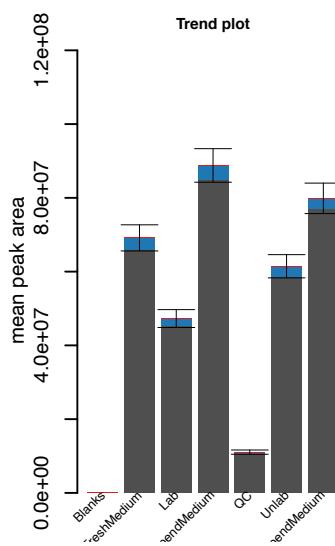
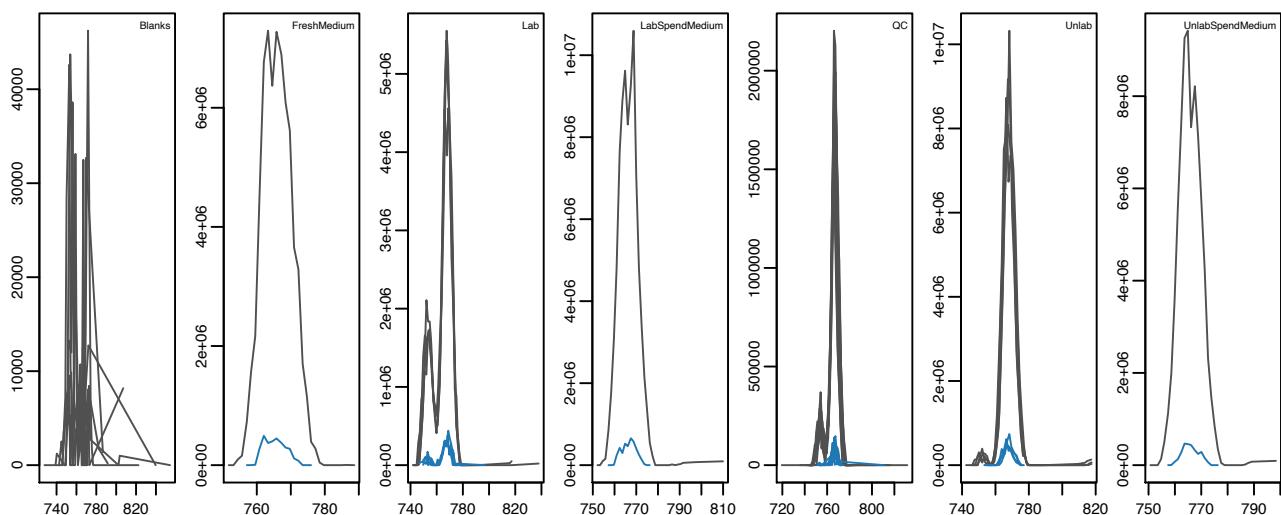


L-Citrulline

Formula: C₆H₁₃N₃O₃ Mass: 175.096 Std.RT: 767.4 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6

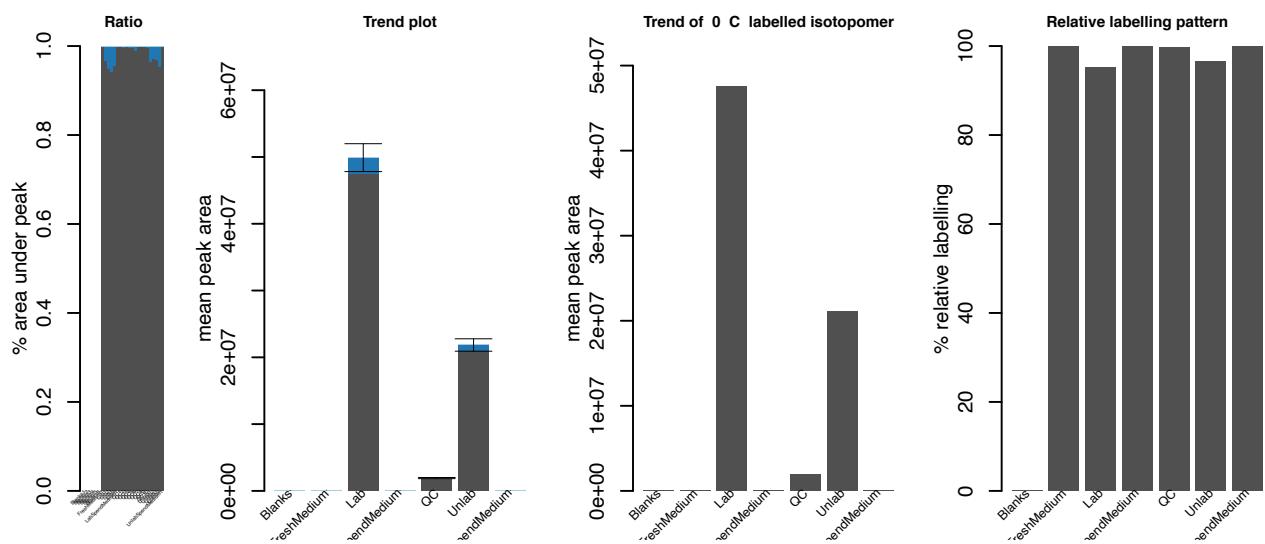
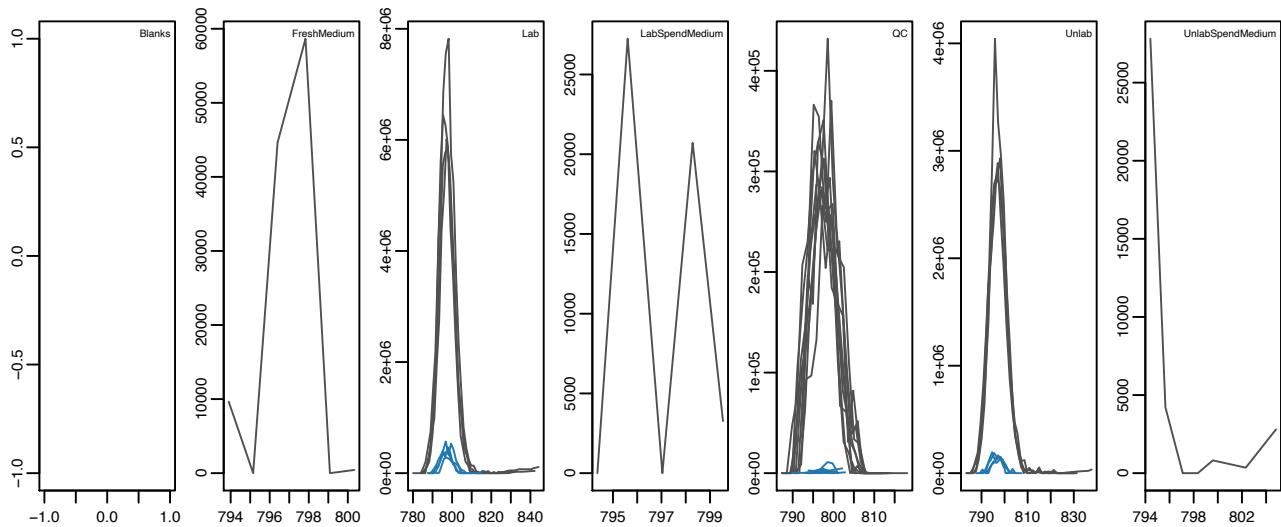


L-Cystathionine

Formula: C₇H₁₄N₂O₄S Mass: 222.067 Std.RT: 798.6 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7

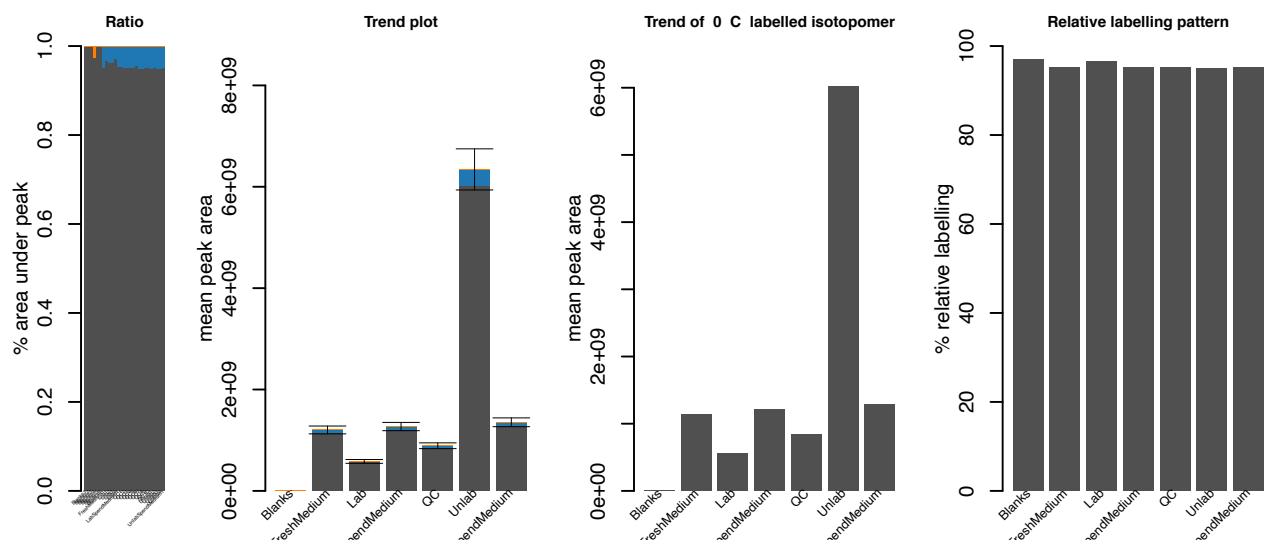
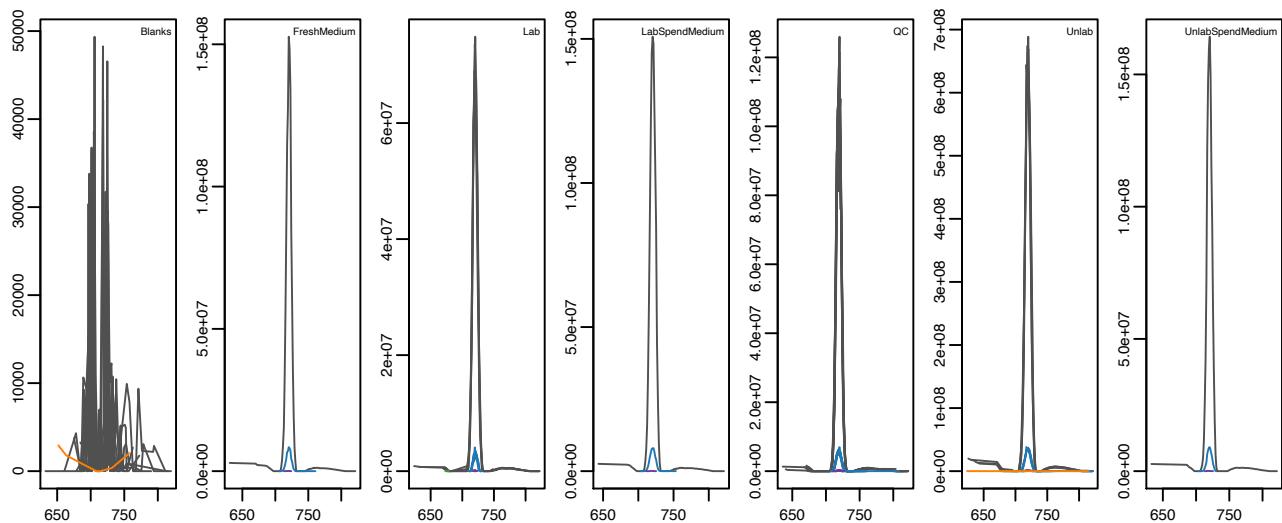


L-Glutamate

Formula: C5H9NO4 Mass: 147.053 Std.RT: 723.6 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

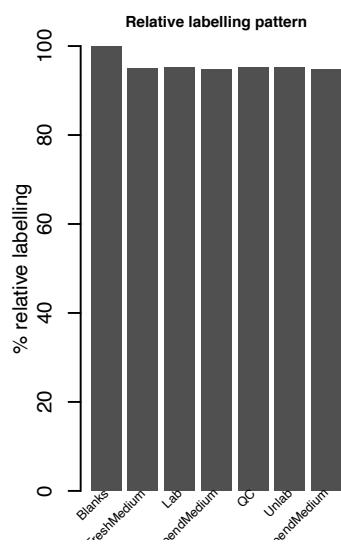
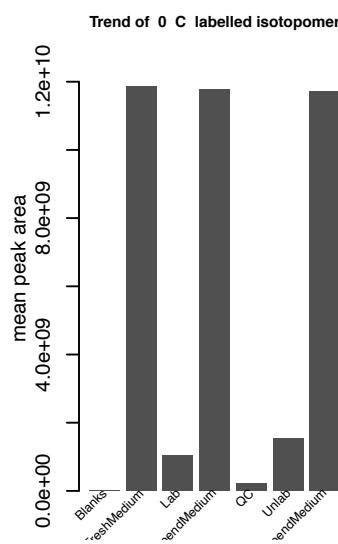
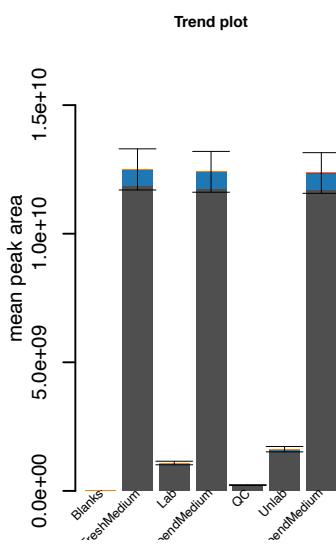
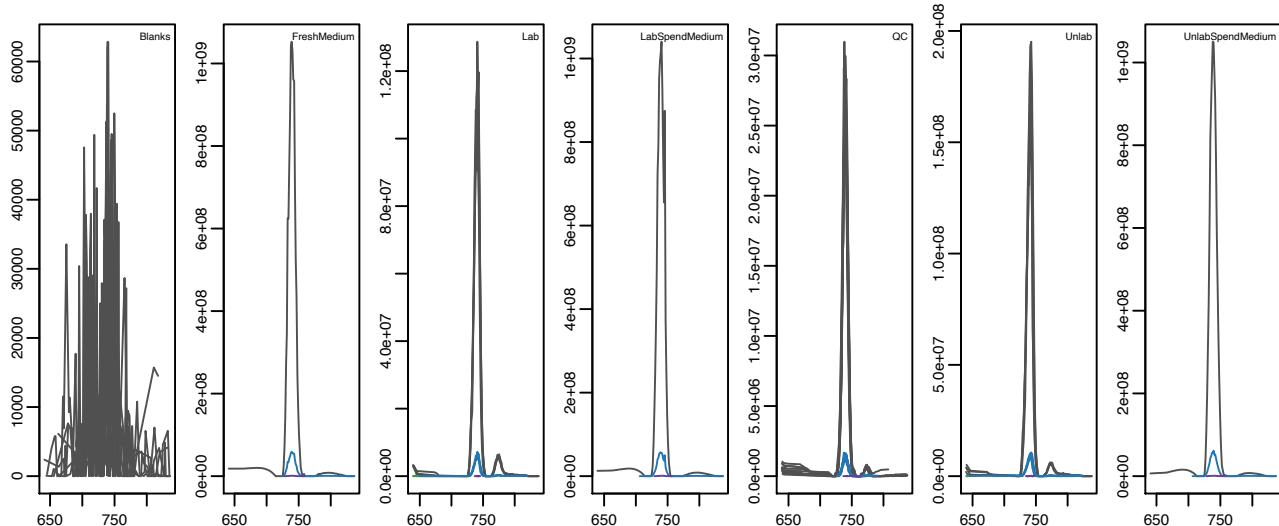


L-Glutamine

Formula: C5H10N2O3 Mass: 146.069 Std.RT: 739.2 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

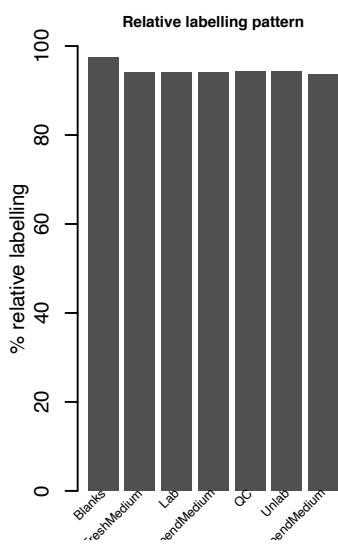
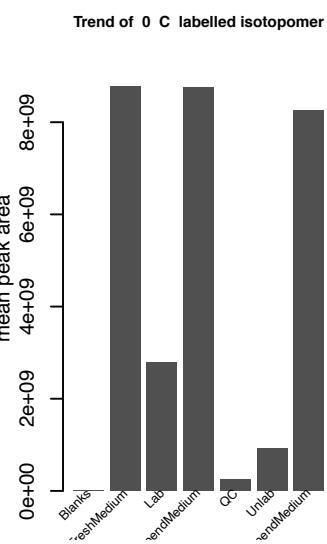
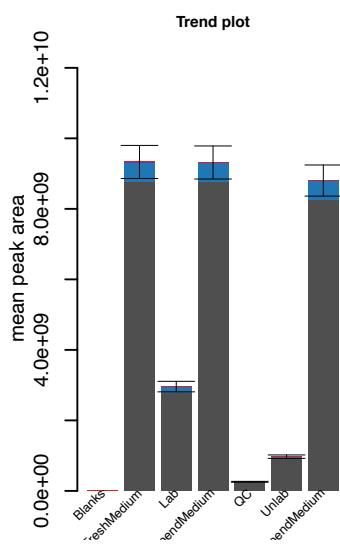
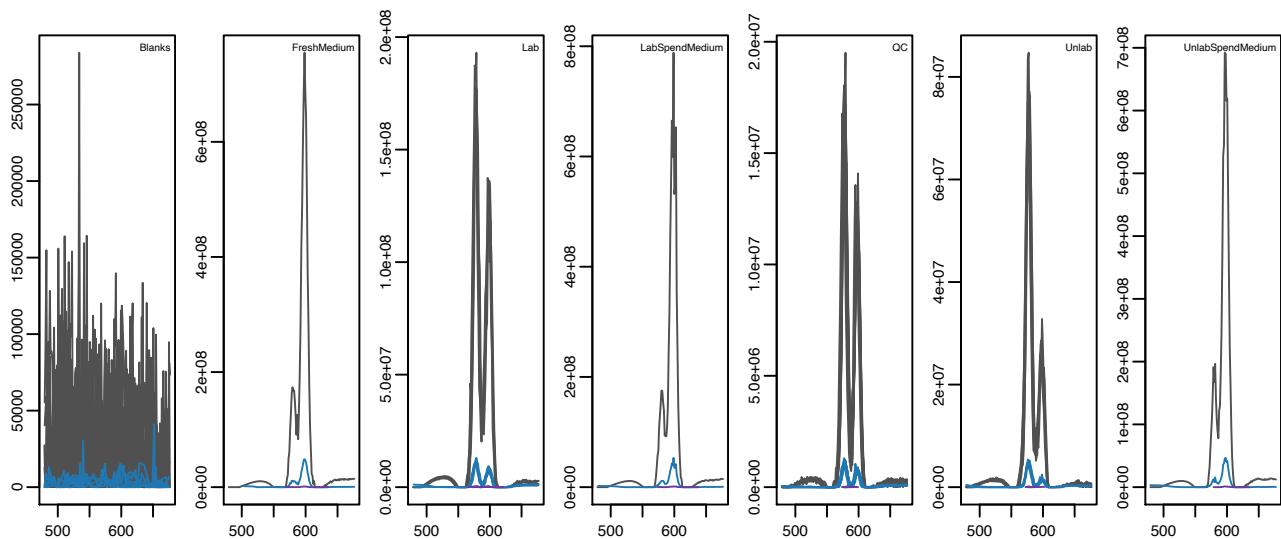


L-Leucine

Formula: C₆H₁₃NO₂ Mass: 131.095 Std.RT: 578.4 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6

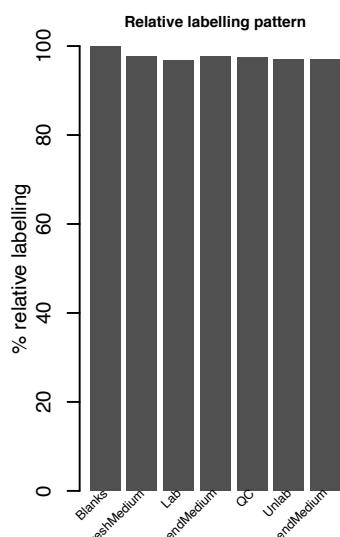
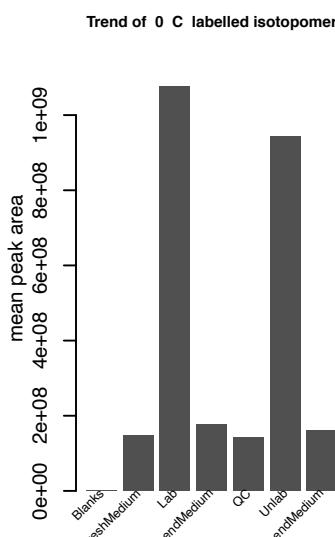
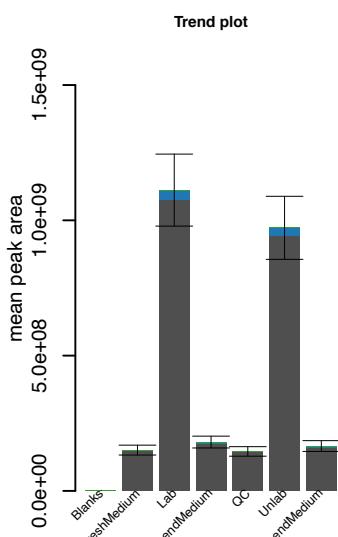
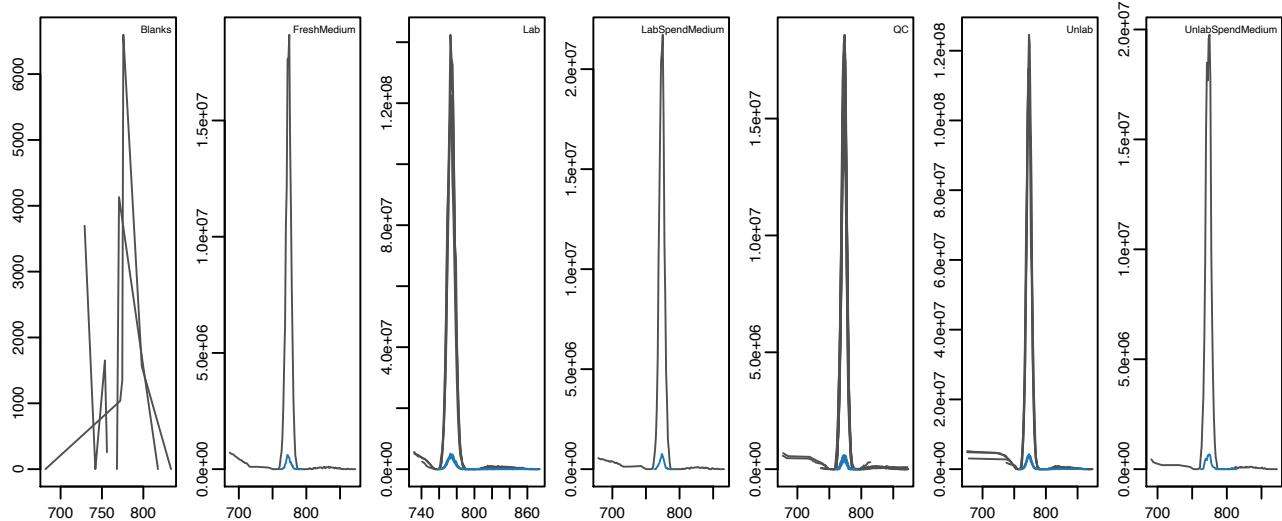


L-Serine

Formula: C3H7NO3 Mass: 105.043 Std.RT: 775.2 Ion: POS

G1

■UL ■+1 ■+2 ■+3

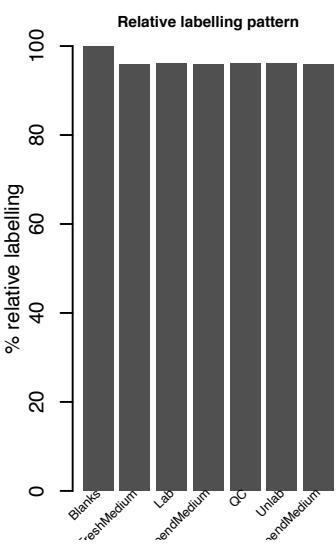
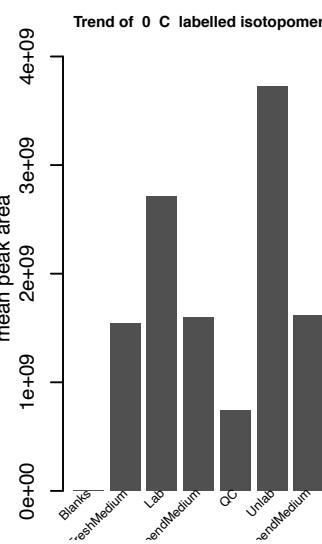
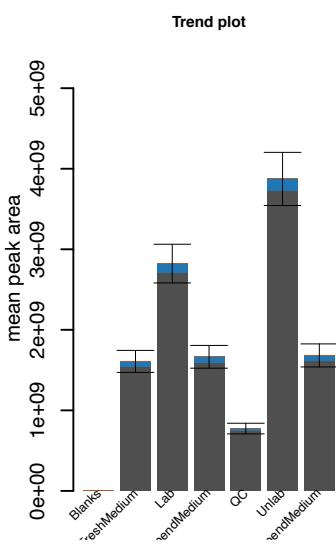
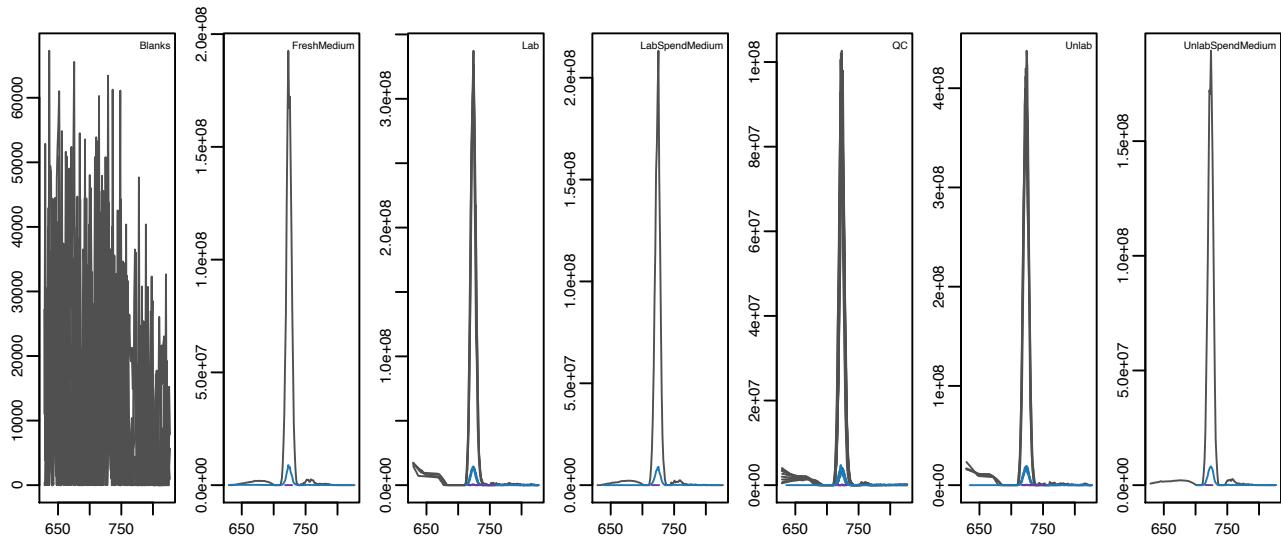


L-Threonine

Formula: C₄H₉NO₃ Mass: 119.058 Std.RT: 728.4 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4

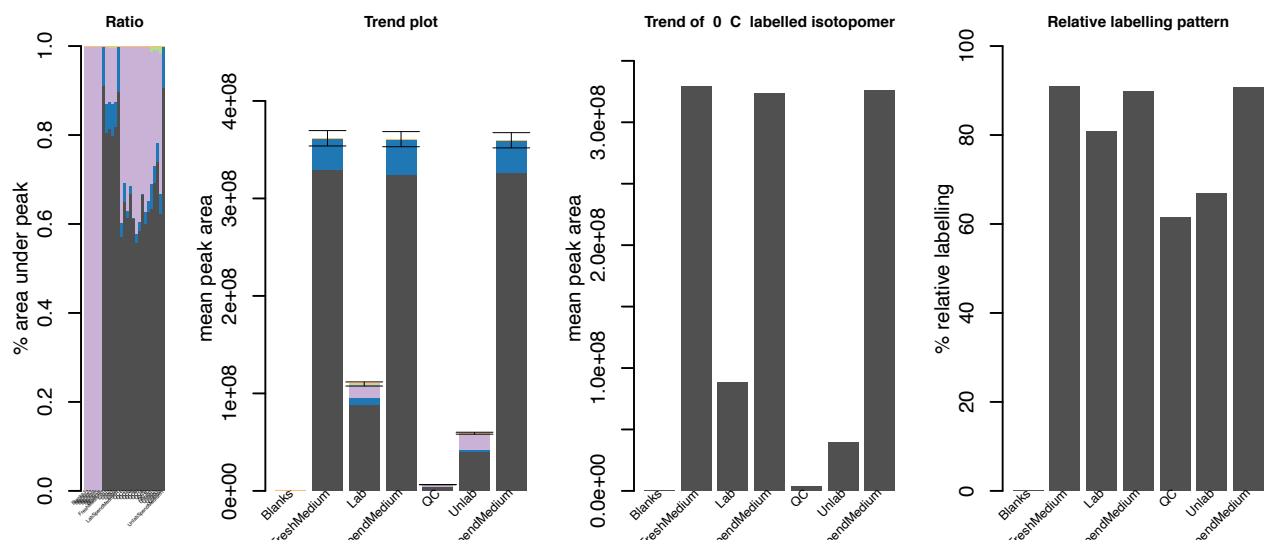
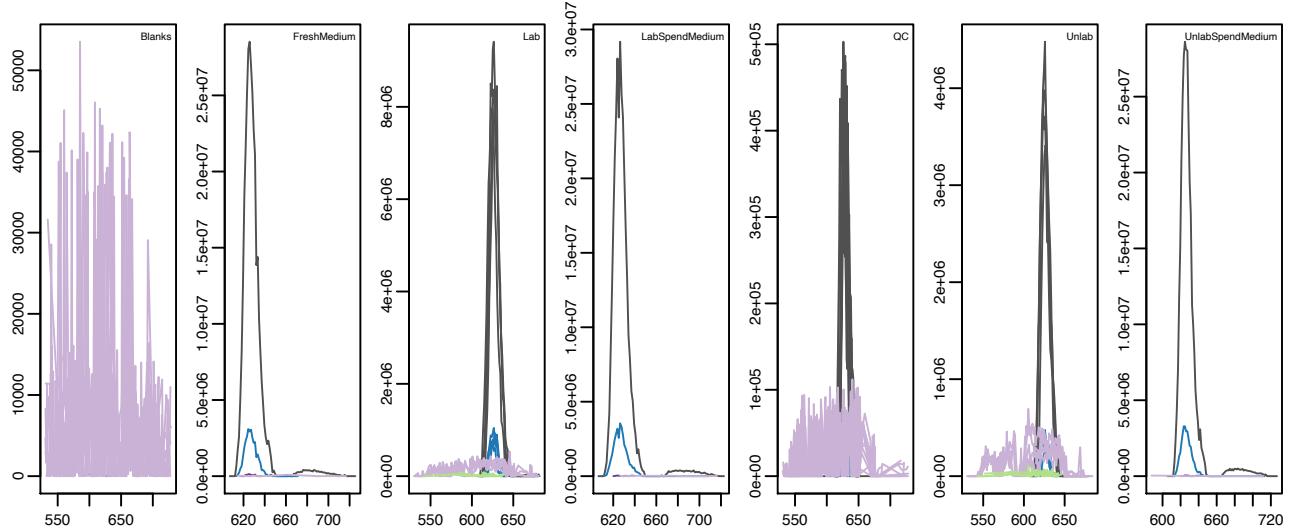


L-Tryptophan

Formula: C₁₁H₁₂N₂O₂ Mass: 204.09 Std.RT: 630 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9 ■+10 ■+11

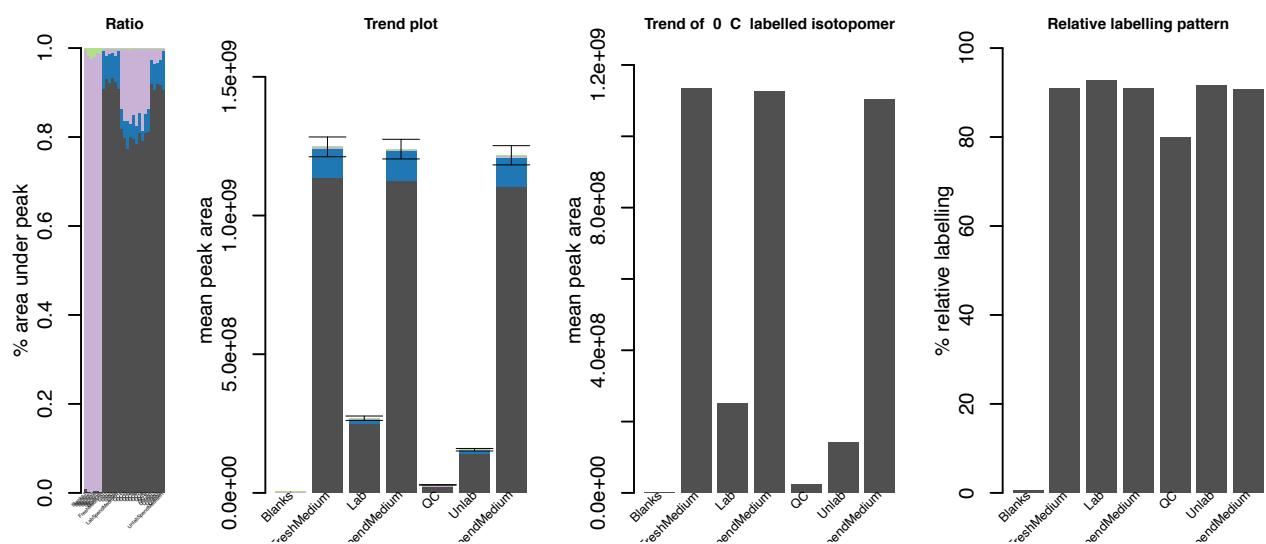
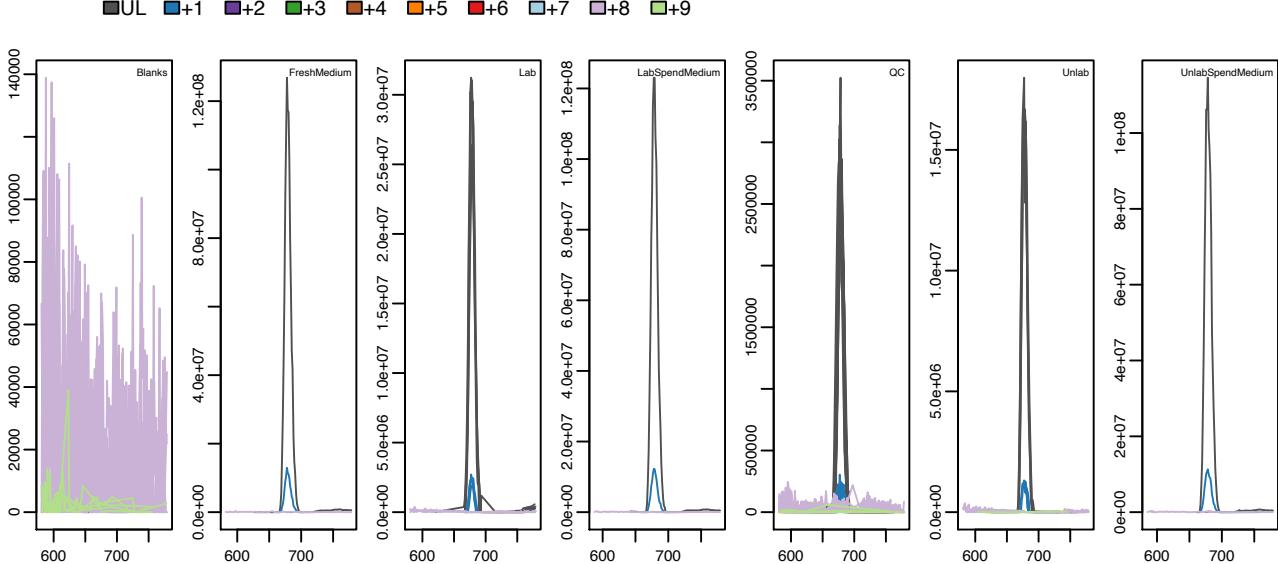


L-Tyrosine

Formula: C9H11NO3 Mass: 181.074 Std.RT: 680.4 Ion: POS

G1

■ 1 ■ 2 ■ 3 ■ 4 ■ 5 ■ 6 ■ 7 ■ 8 ■ 9

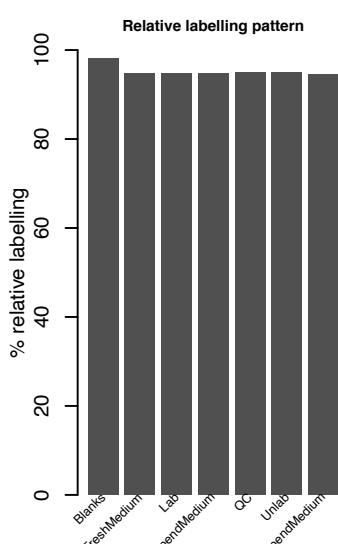
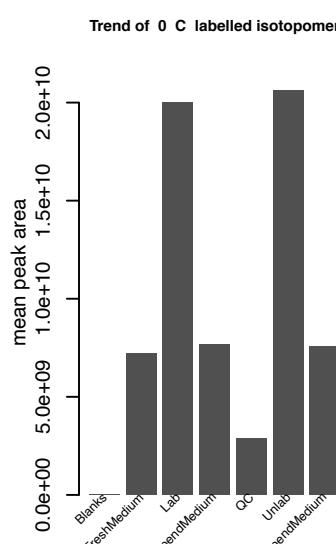
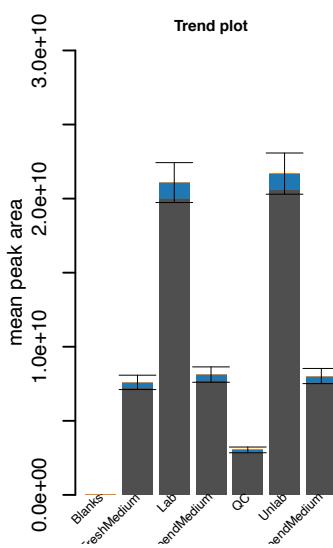
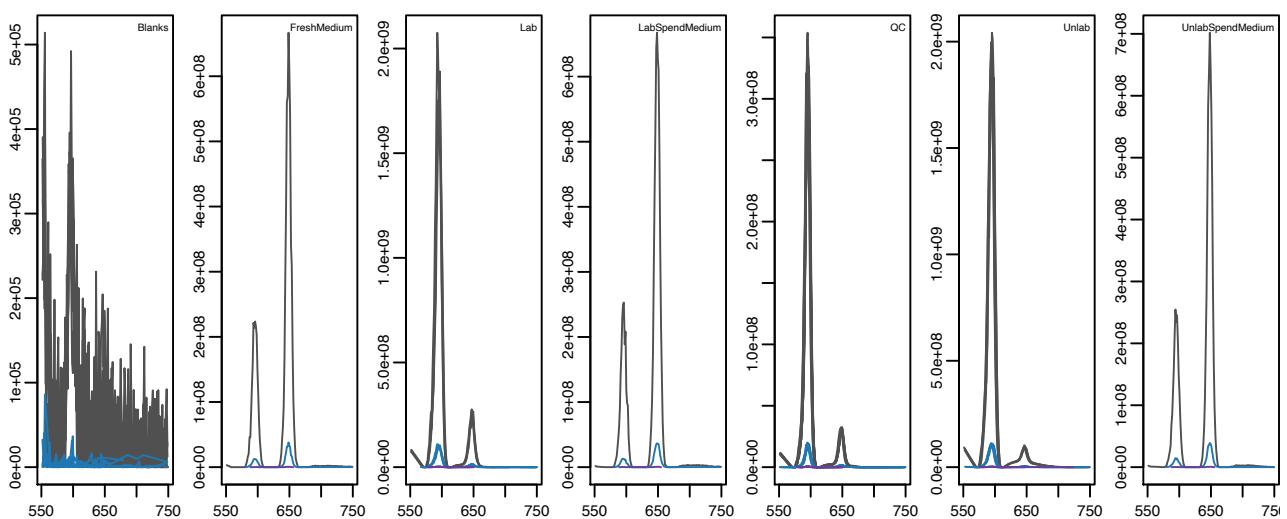


L-Valine

Formula: C5H11NO2 Mass: 117.079 Std.RT: 651 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

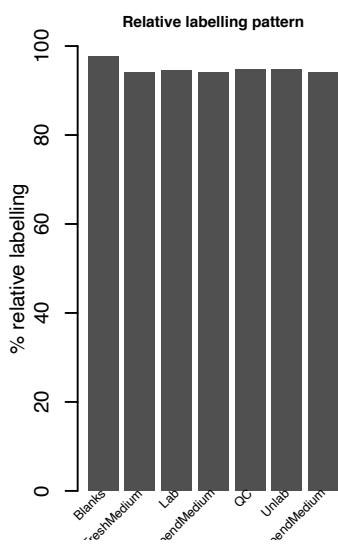
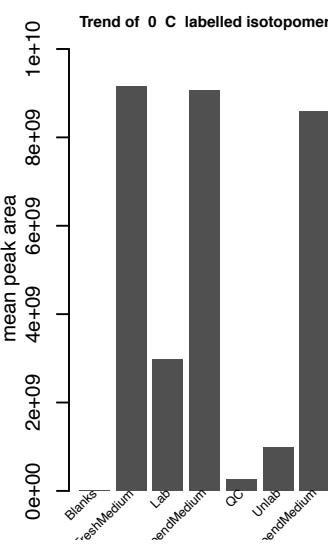
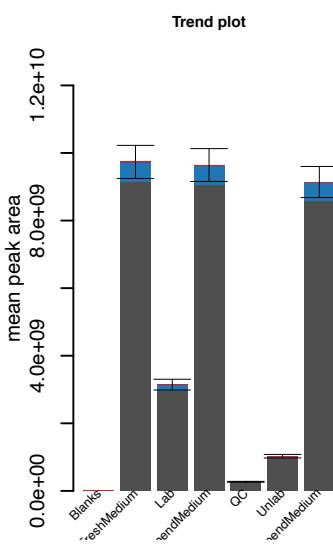
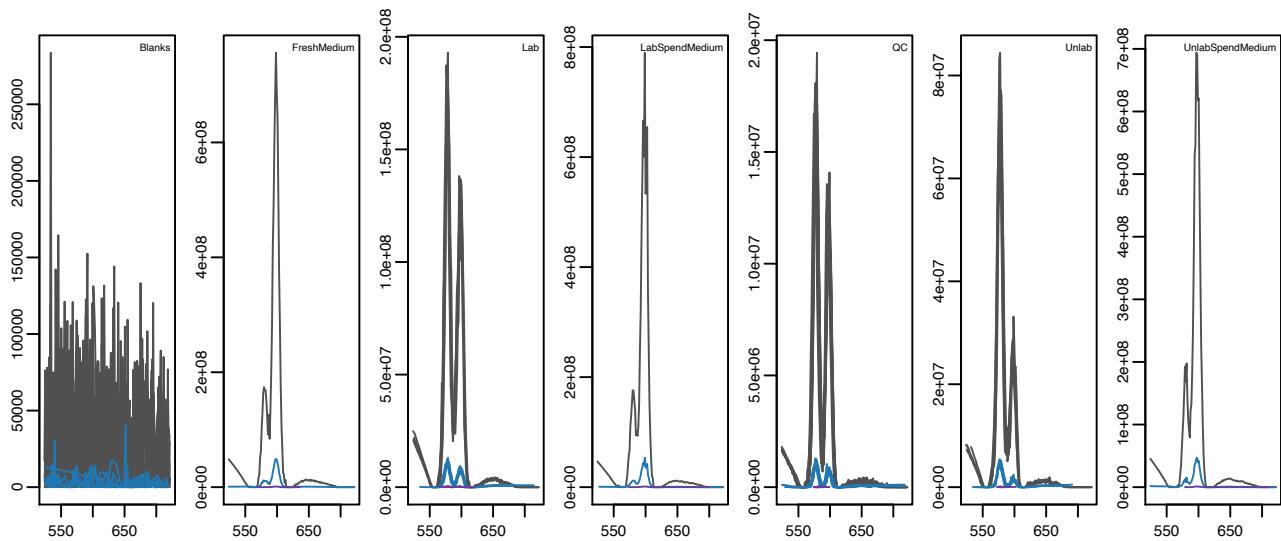


L-isoleucine

Formula: C₆H₁₃NO₂ Mass: 131.095 Std.RT: 623.4 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6

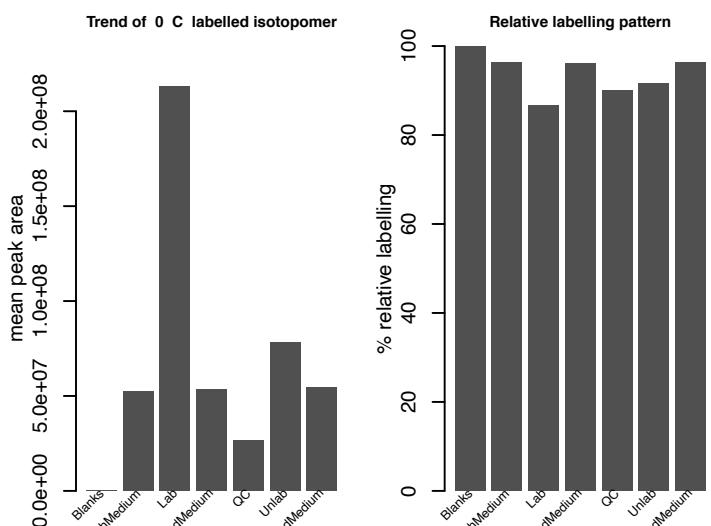
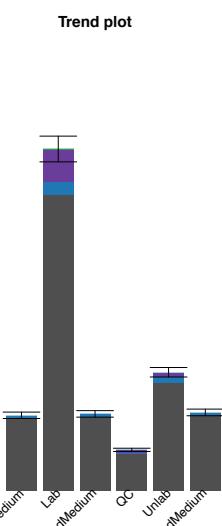
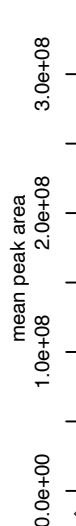
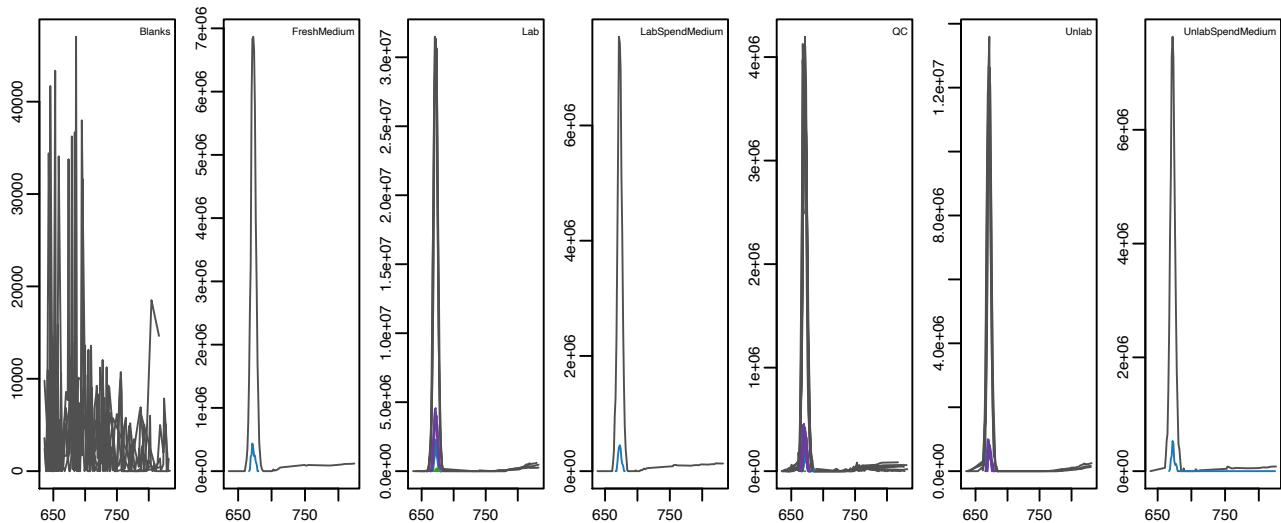


N-Acetylornithine

Formula: C7H14N2O3 Mass: 174.1 Std.RT: 735 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7

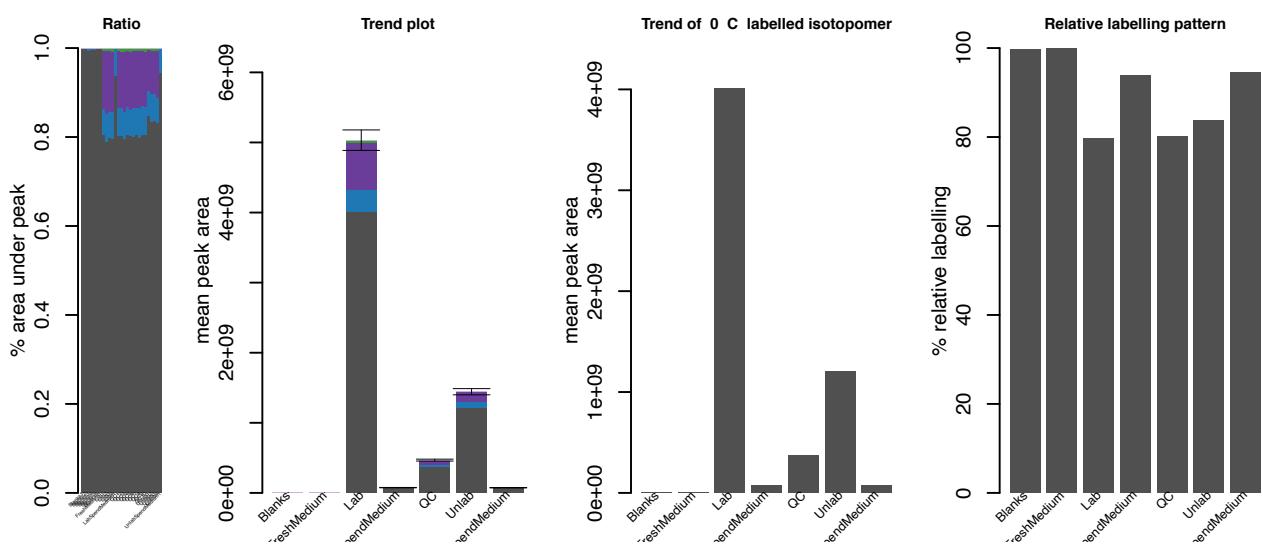
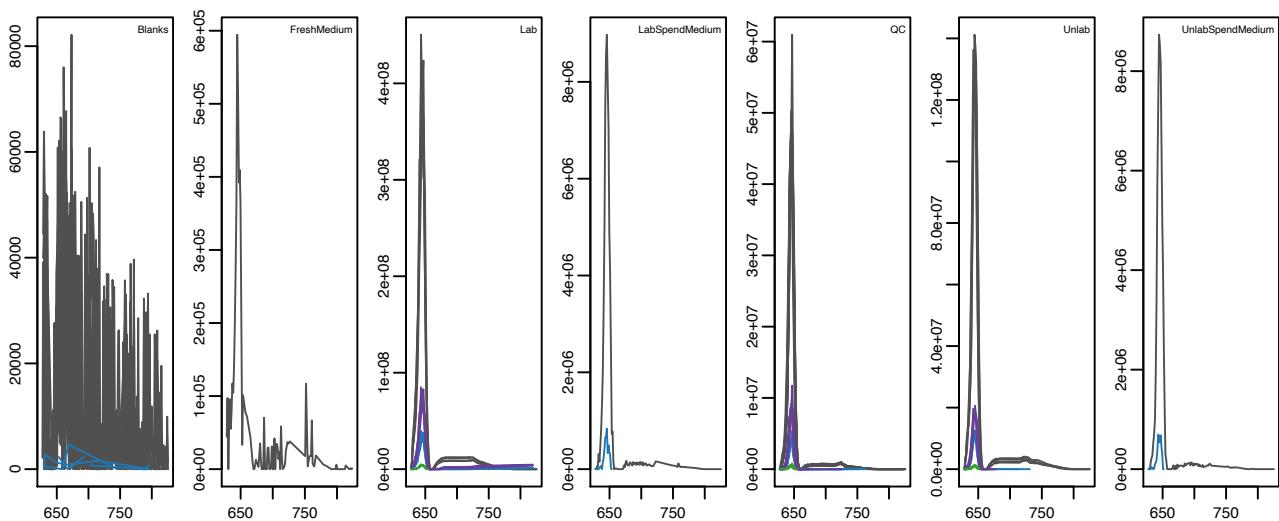


N₂-Acetyl-L-lysine

Formula: C8H16N2O3 Mass: 188.116 Std.RT: 727.2 Ion: POS

G1

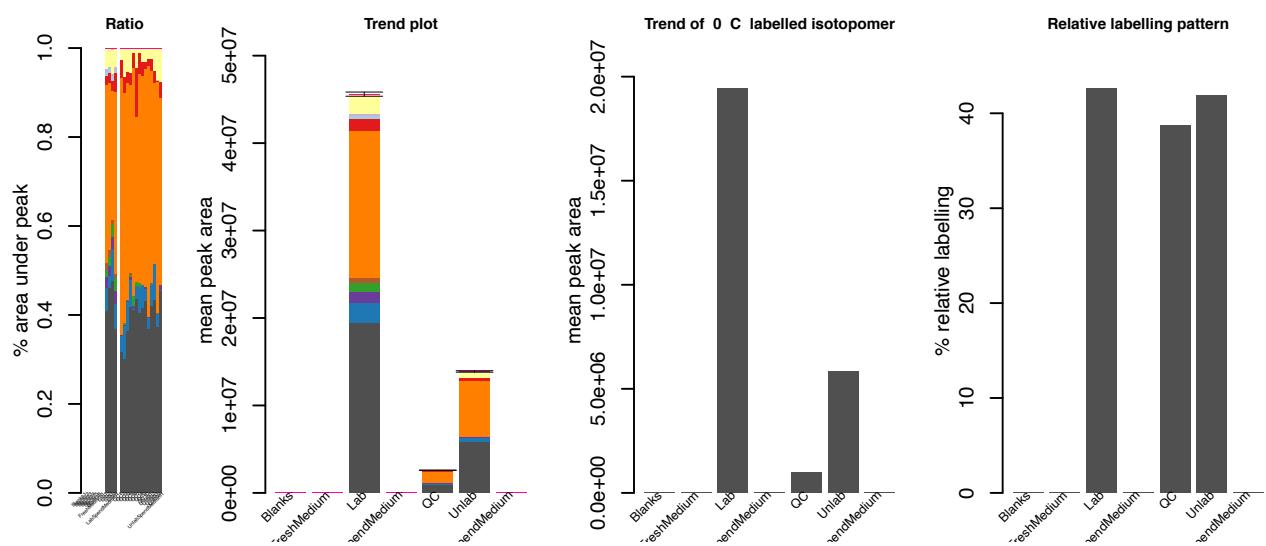
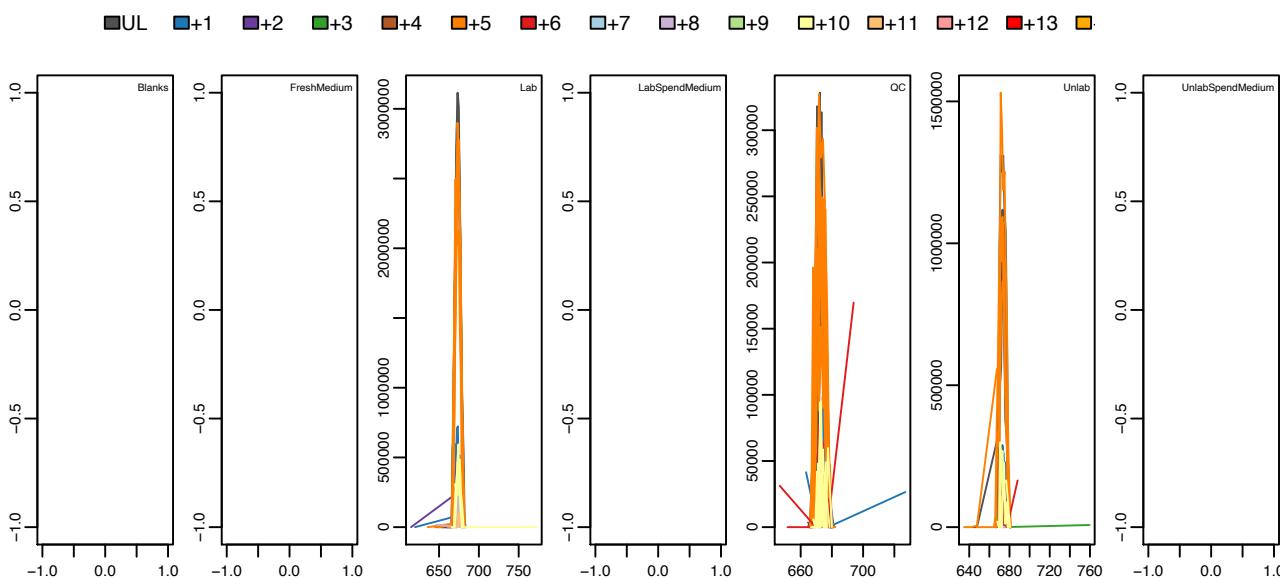
■UL □+1 □+2 □+3 □+4 □+5 □+6 □+7 □+8



NAD+

Formula: C₂₁H₂₇N₇O₁₄P₂ Mass: 663.109 Std.RT: 678 Ion: POS

G1

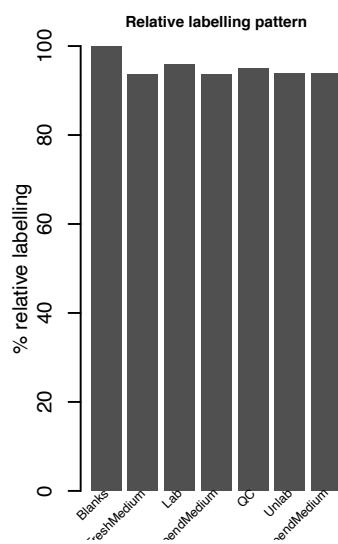
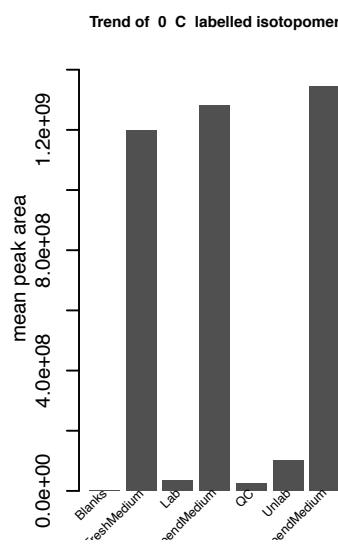
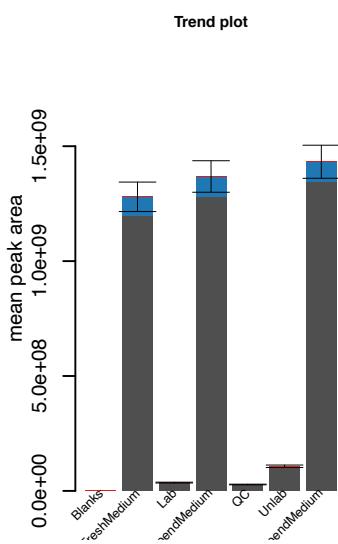
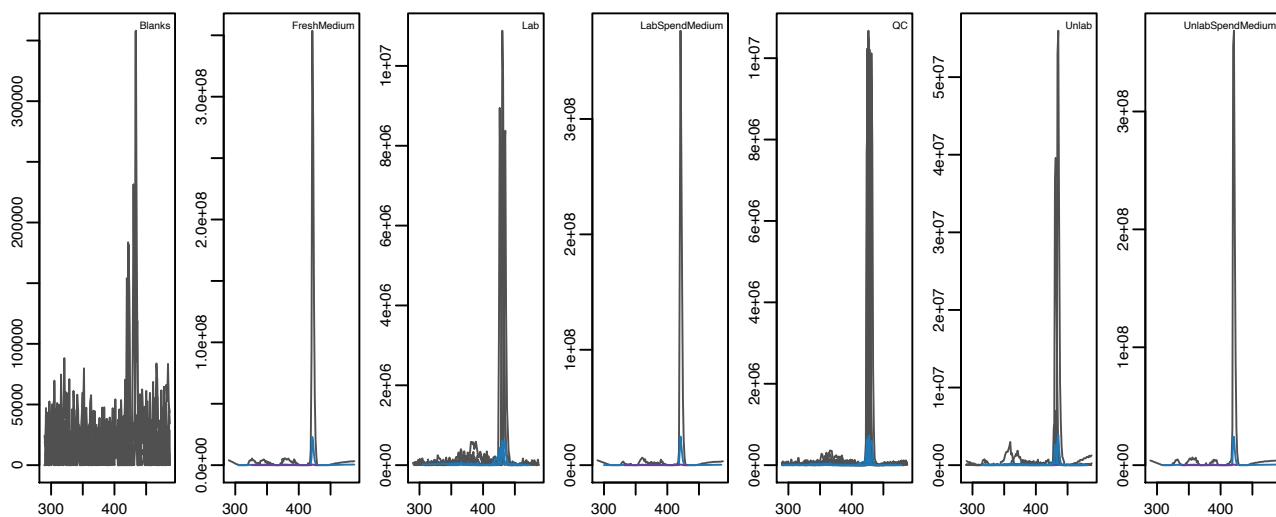


Nicotinamide

Formula: C₆H₆N₂O Mass: 122.048 Std.RT: 389.4 Ion: POS

G1

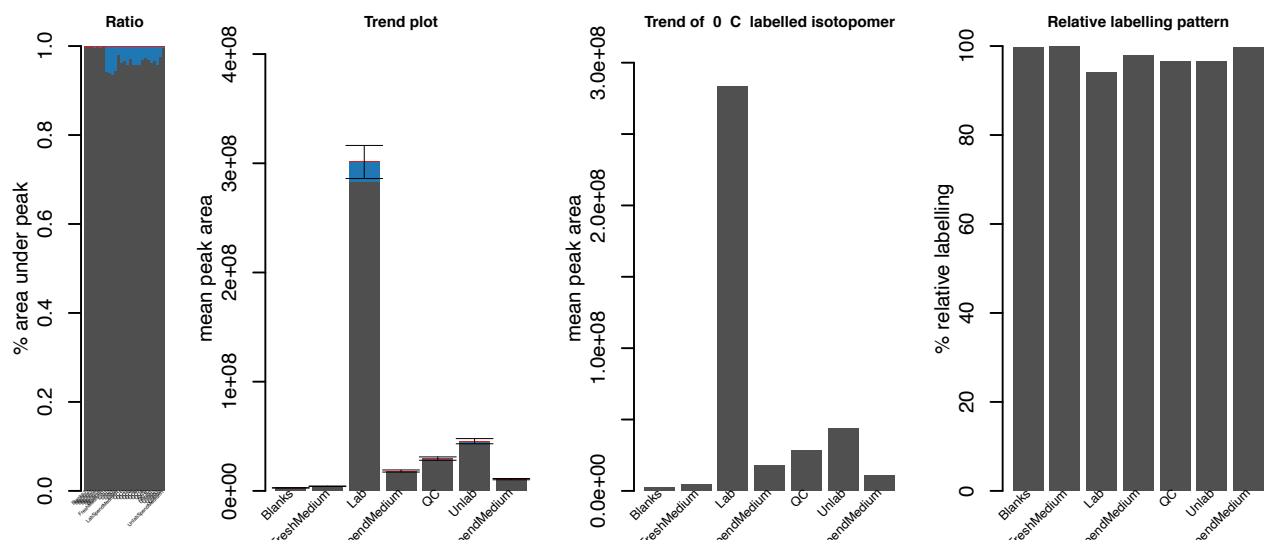
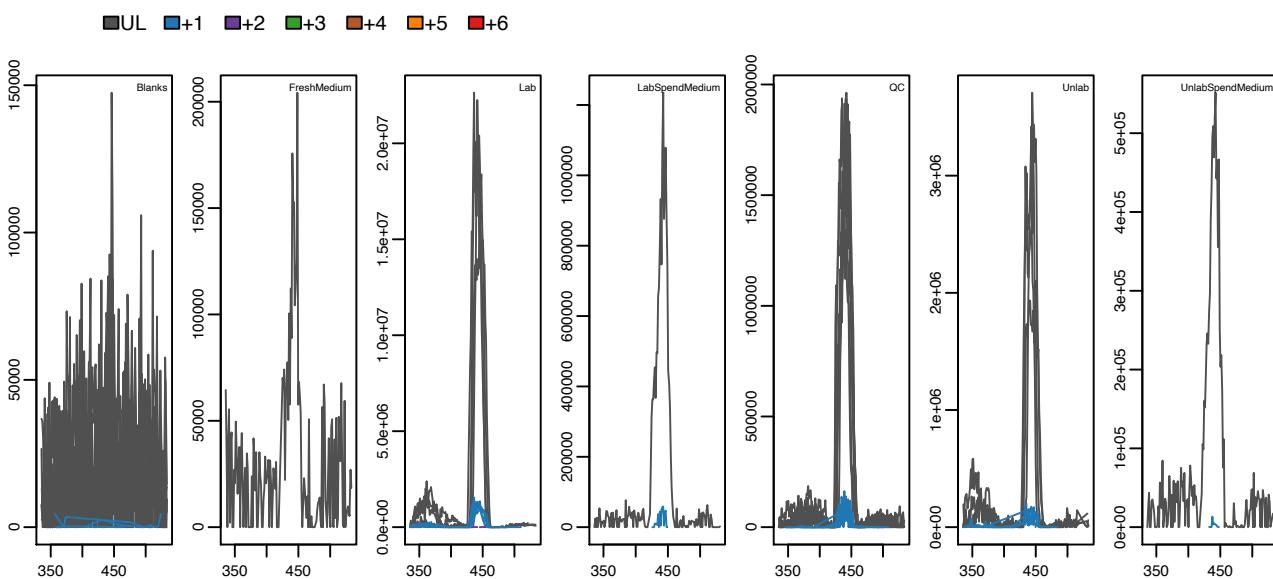
■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6



Nicotinate

Formula: C6H5NO2 Mass: 123.032 Std.RT: 435 Ion: POS

G1

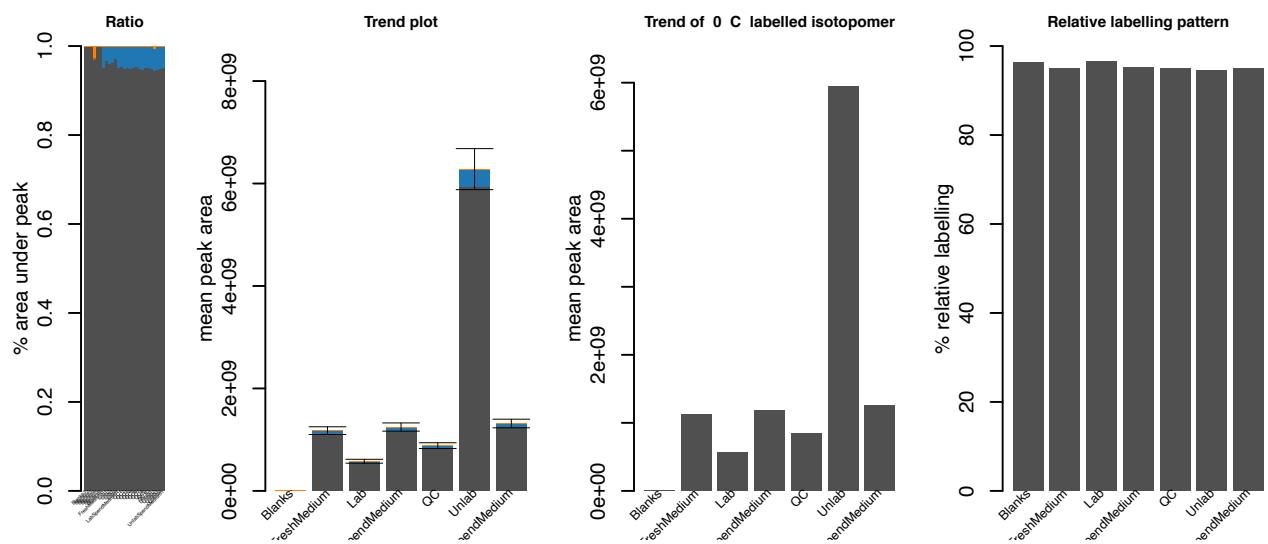
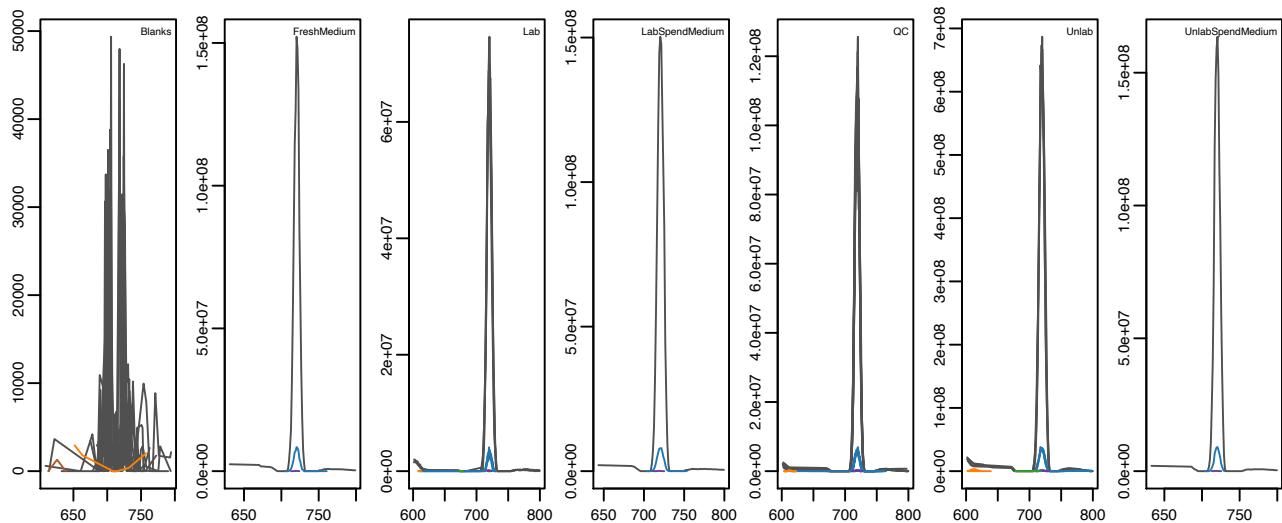


O-Acetyl-L-serine

Formula: C5H9NO4 Mass: 147.053 Std.RT: 701.4 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

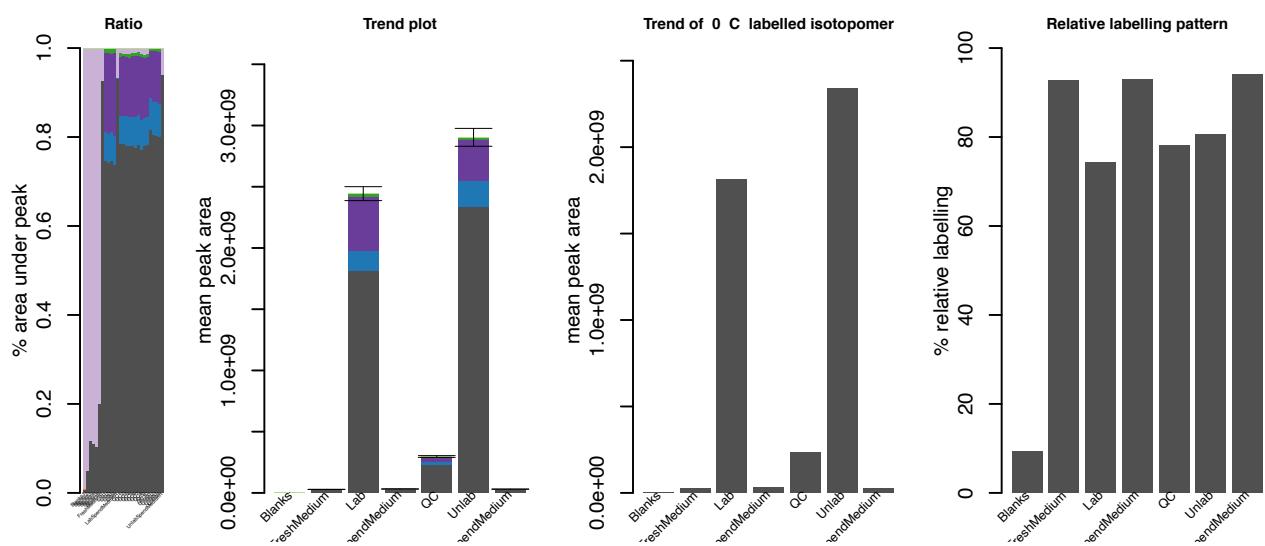
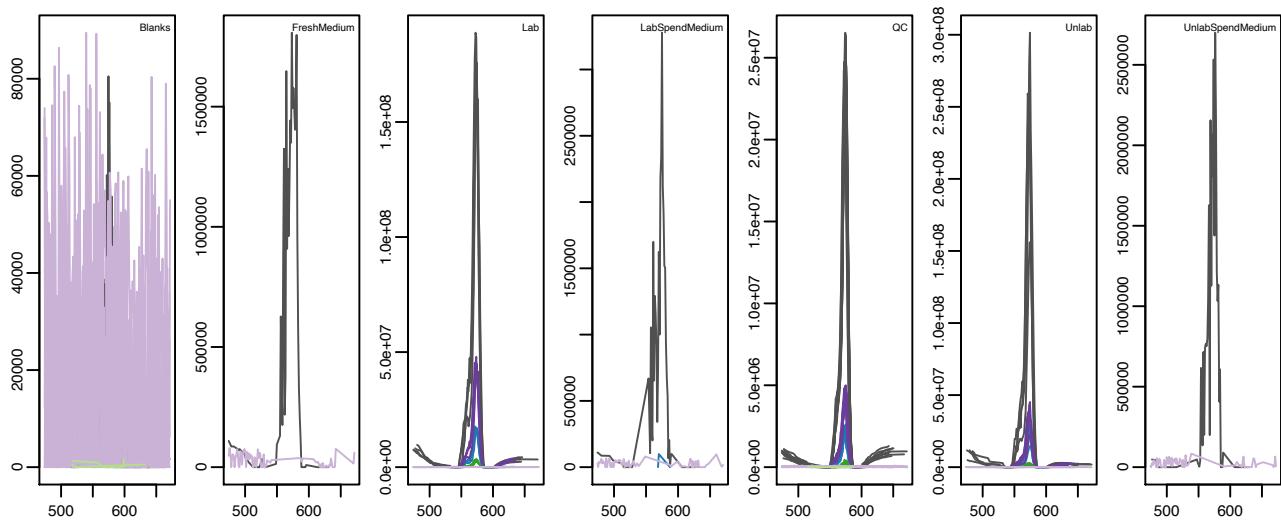


O-Acetyl carnitine

Formula: C9H17NO4 Mass: 203.116 Std.RT: 573.6 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9

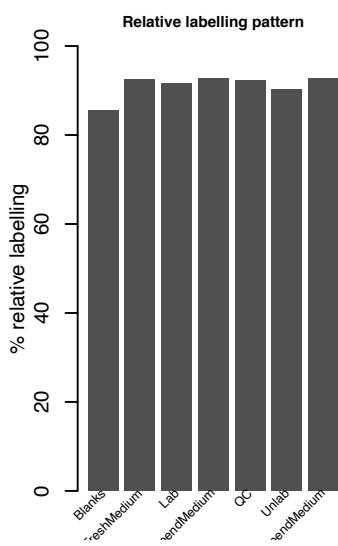
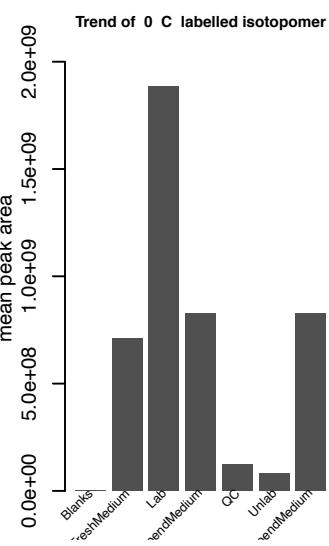
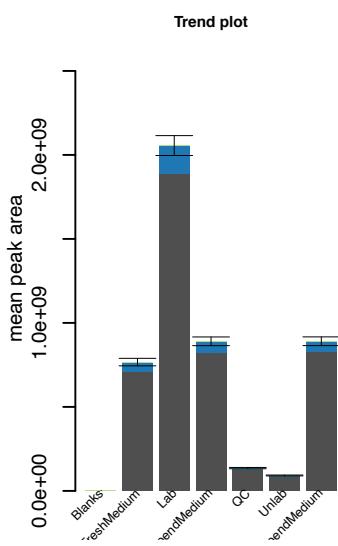
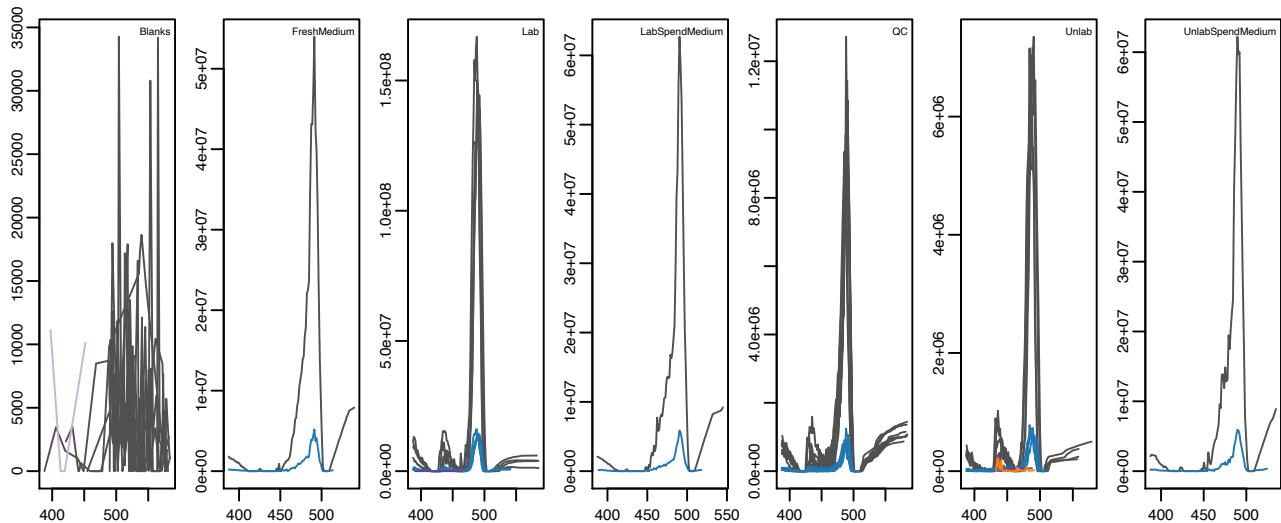


Pantothenate

Formula: C9H17NO5 Mass: 219.111 Std.RT: 487.2 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9

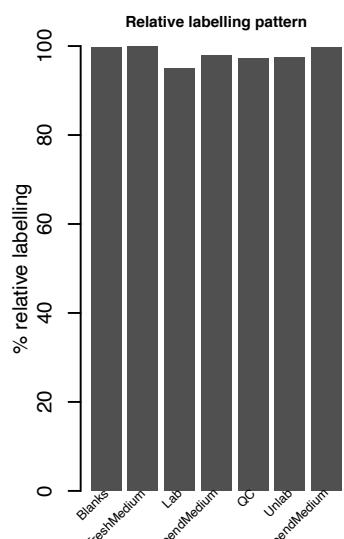
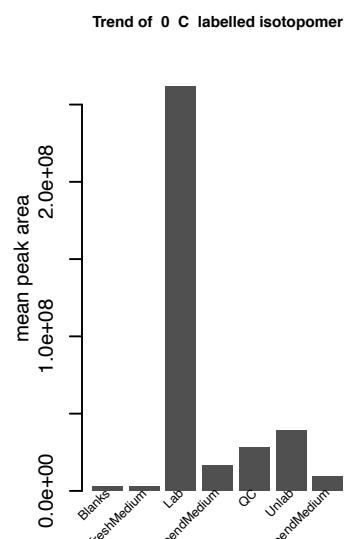
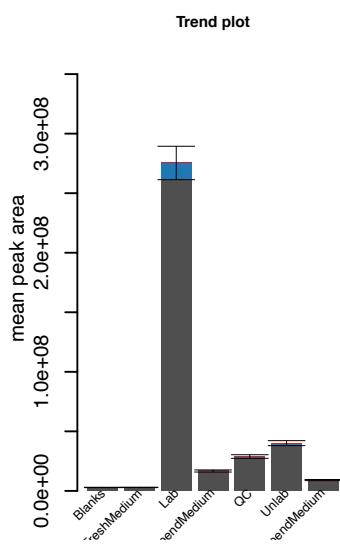
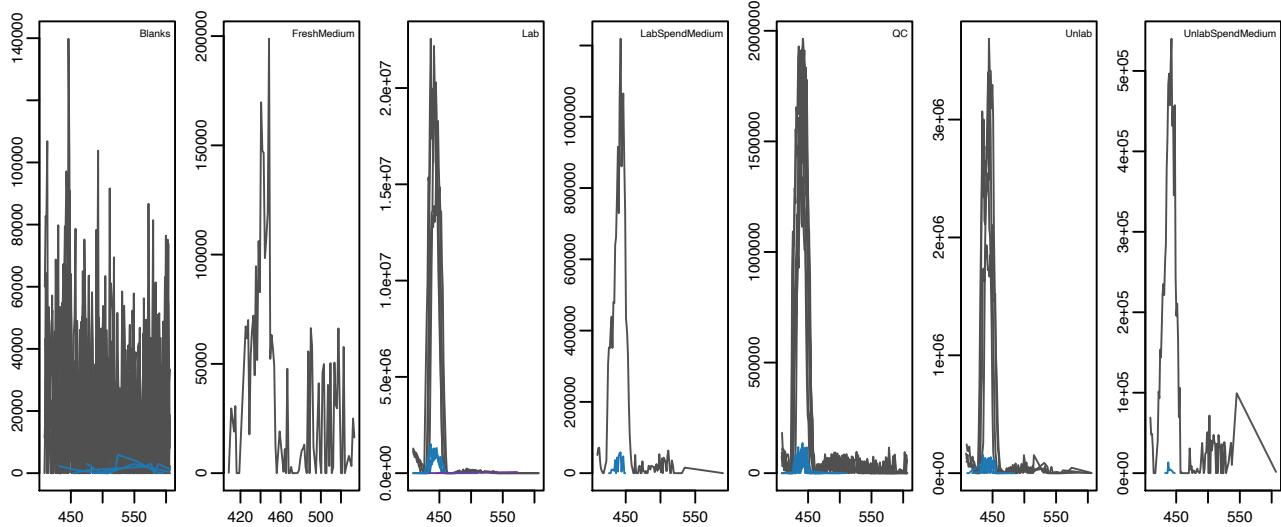


Picolinic acid

Formula: C₆H₅NO₂ Mass: 123.032 Std.RT: 508.2 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6

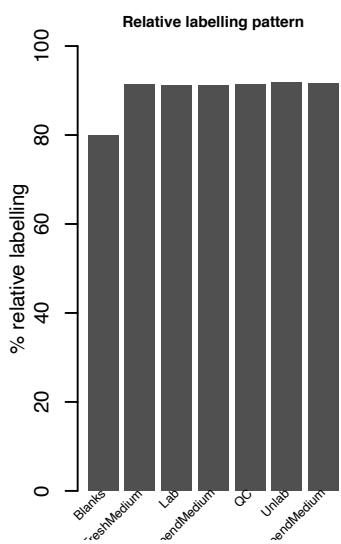
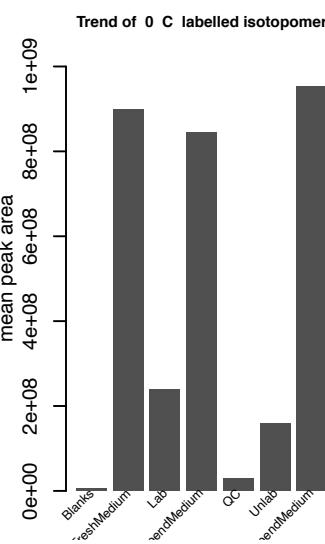
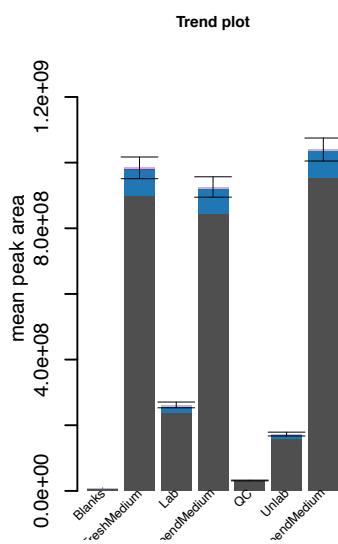
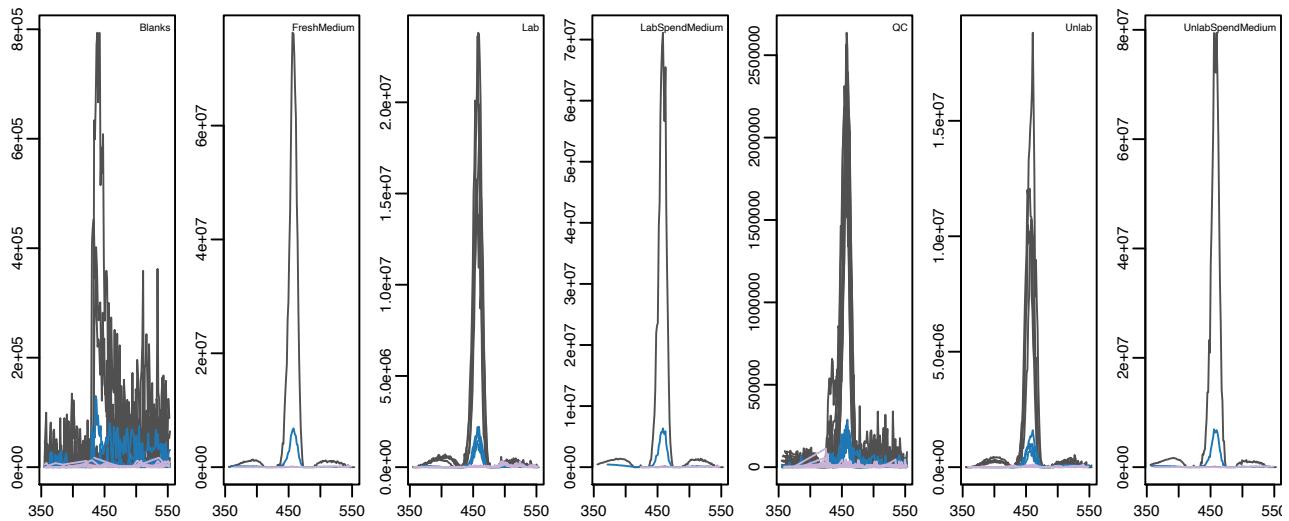


Pyridoxal

Formula: C₈H₉NO₃ Mass: 167.058 Std.RT: 454.8 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8

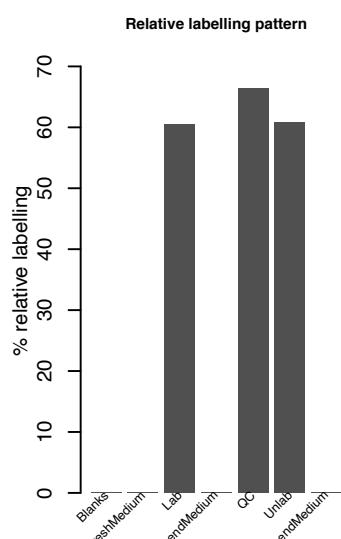
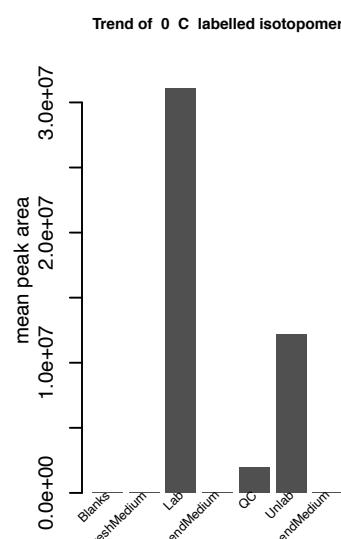
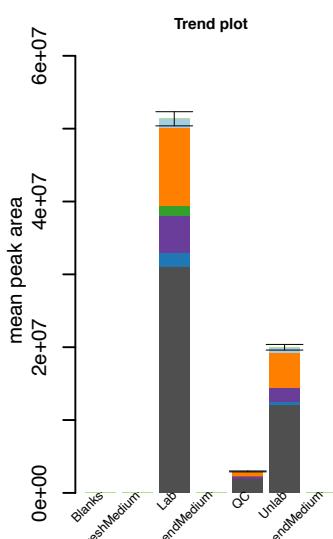
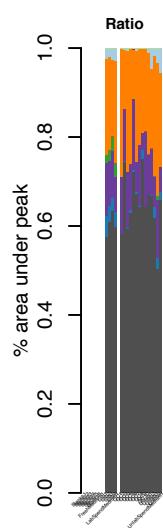
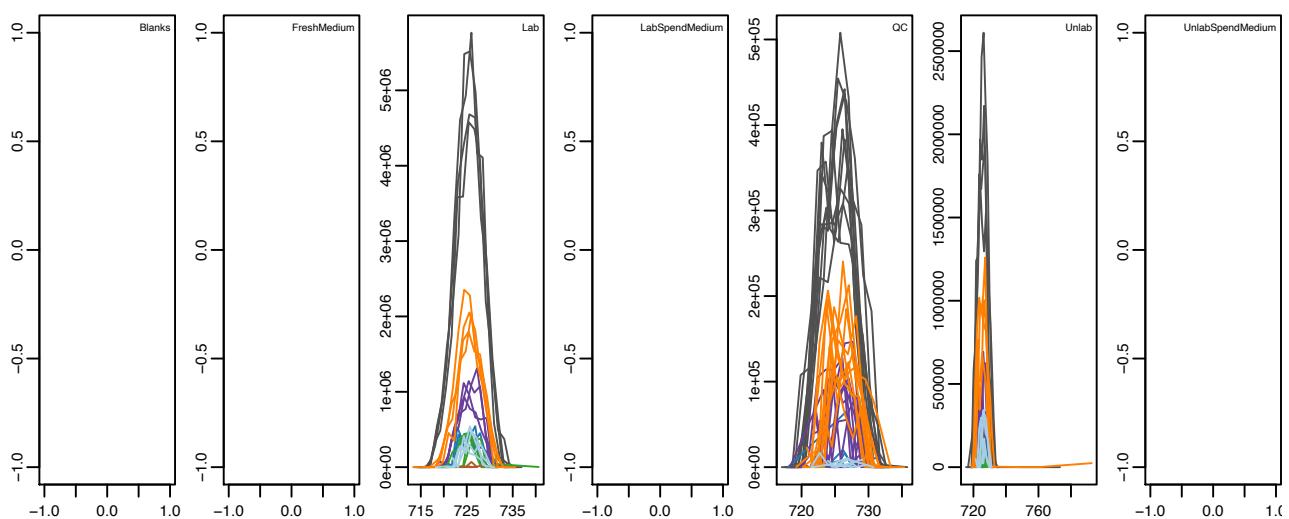


UMP

Formula: C9H13N2O9P Mass: 324.036 Std.RT: 694.8 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9

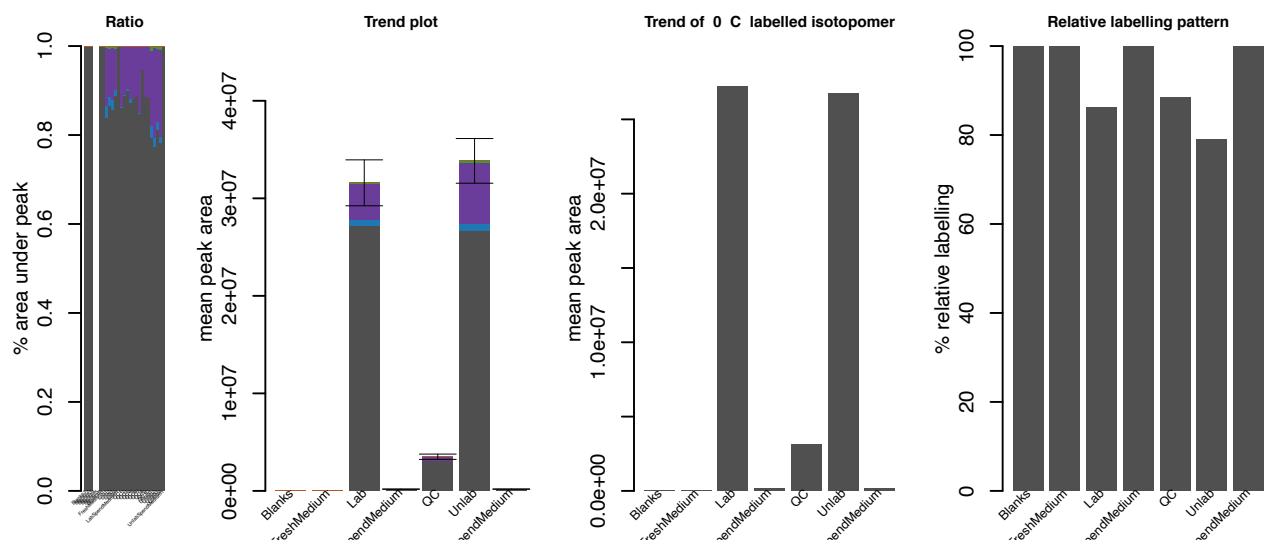
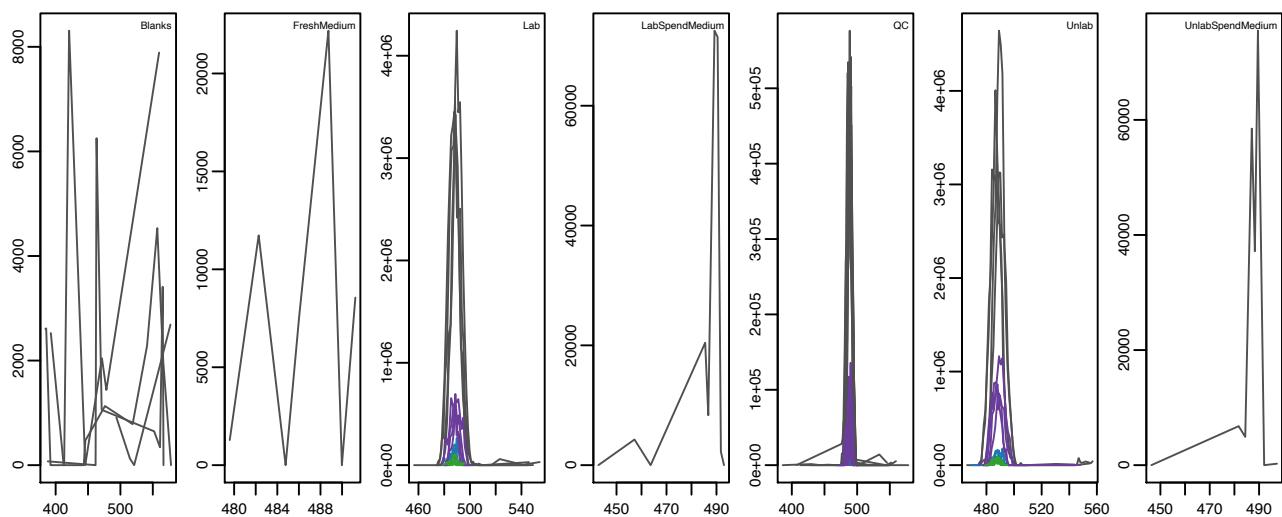


Uracil

Formula: C4H4N2O2 Mass: 112.027 Std.RT: 483.6 Ion: POS

G1

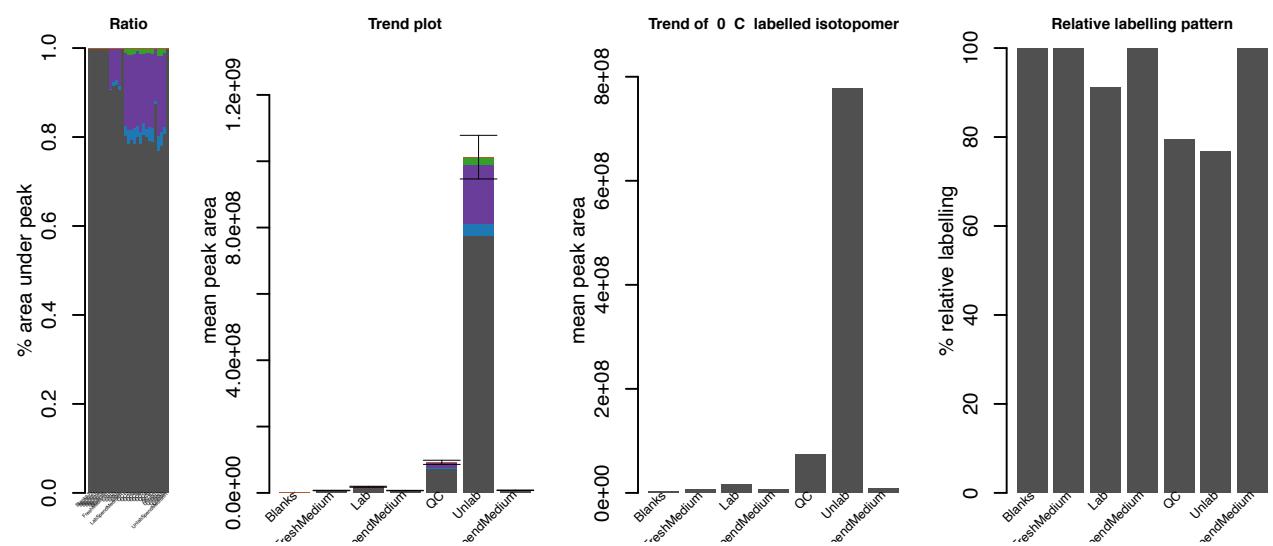
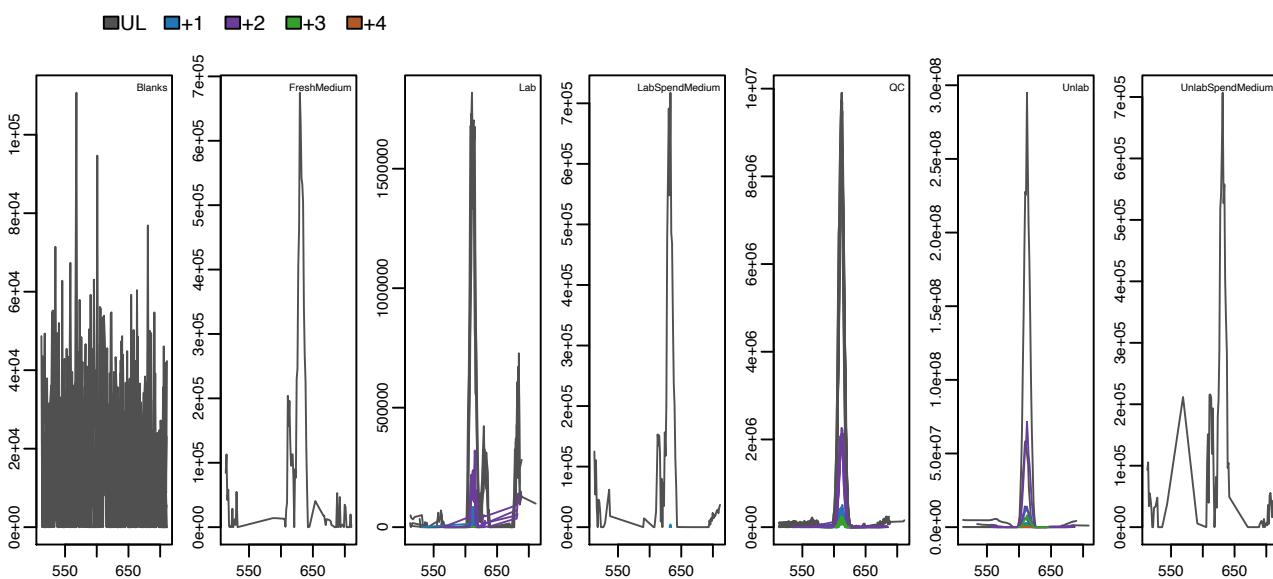
■UL ■+1 ■+2 ■+3 ■+4



cytosine

Formula: C4H5N3O Mass: 111.043 Std.RT: 612.6 Ion: POS

G1

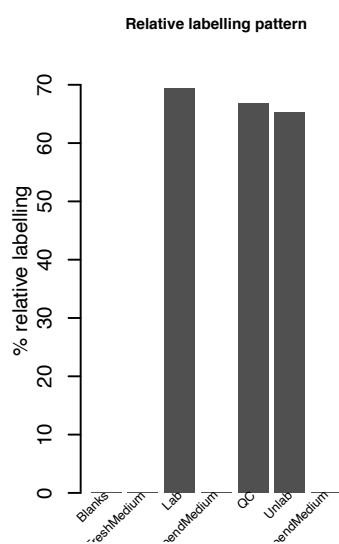
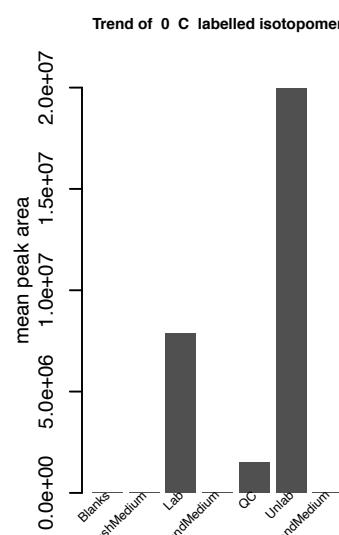
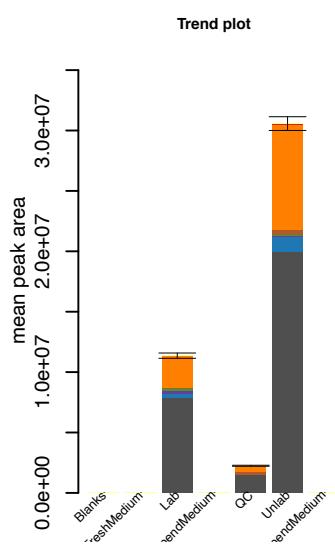
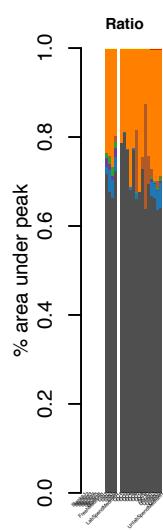
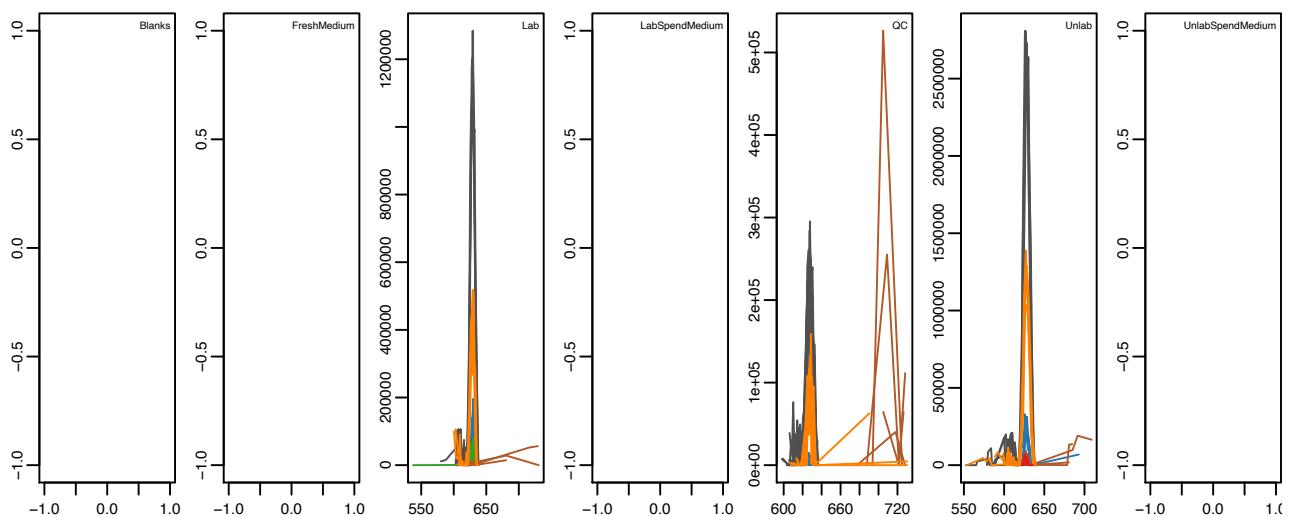


dAMP

Formula: C10H14N5O6P Mass: 331.068 Std.RT: 632.4 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8 ■+9 ■+10

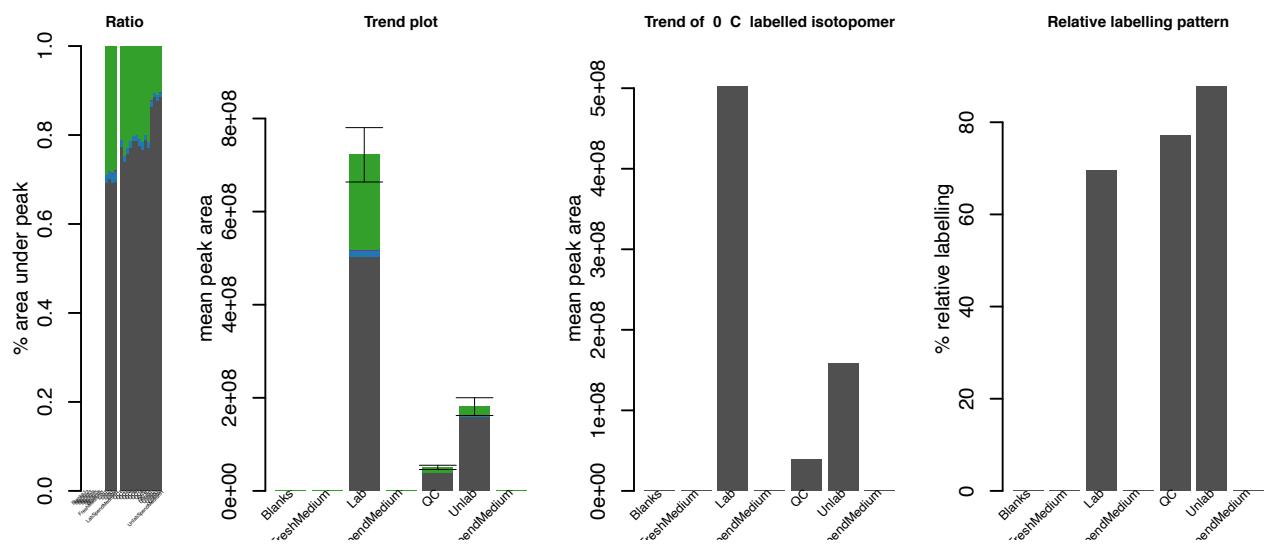
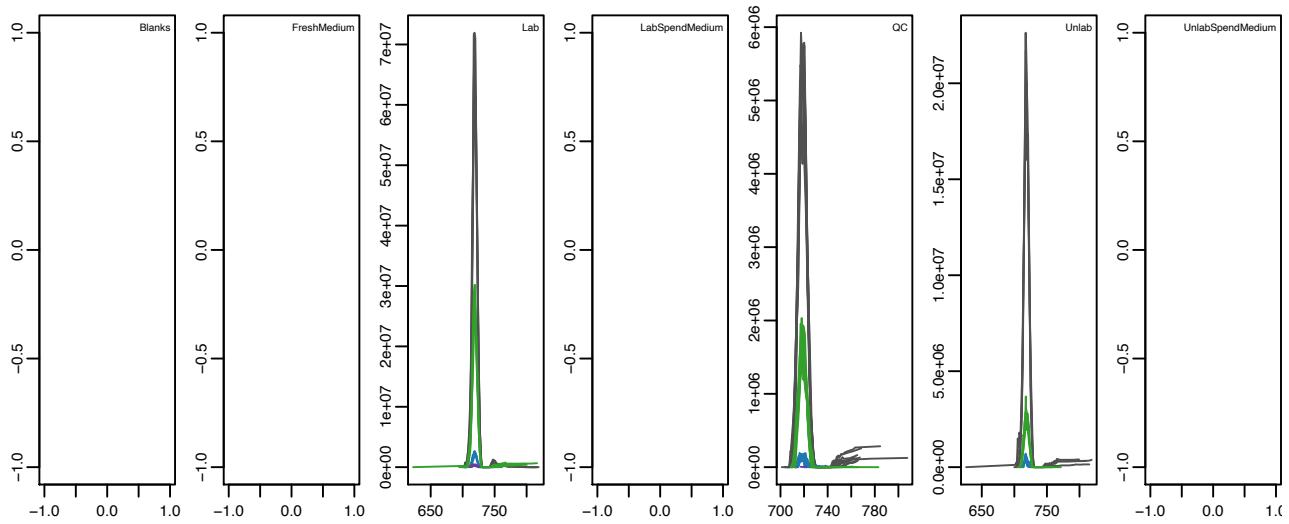


sn-Glycerol 3-phosphate

Formula: C₃H₉O₆P Mass: 172.014 Std.RT: 720.6 Ion: POS

G1

■UL ■+1 ■+2 ■+3

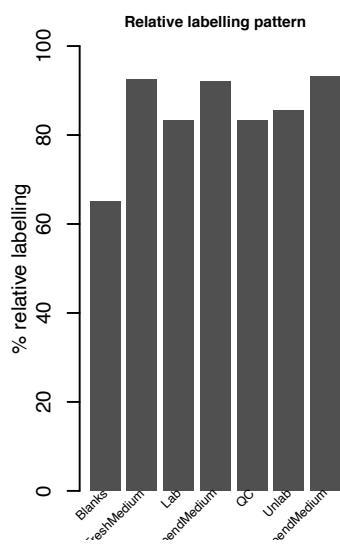
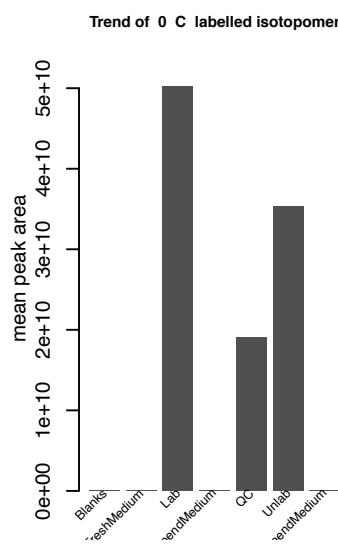
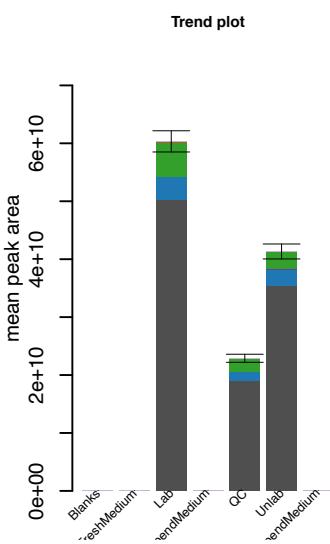
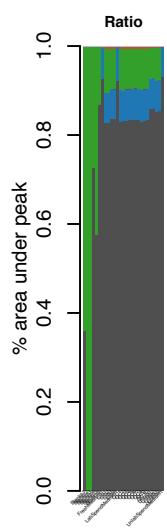
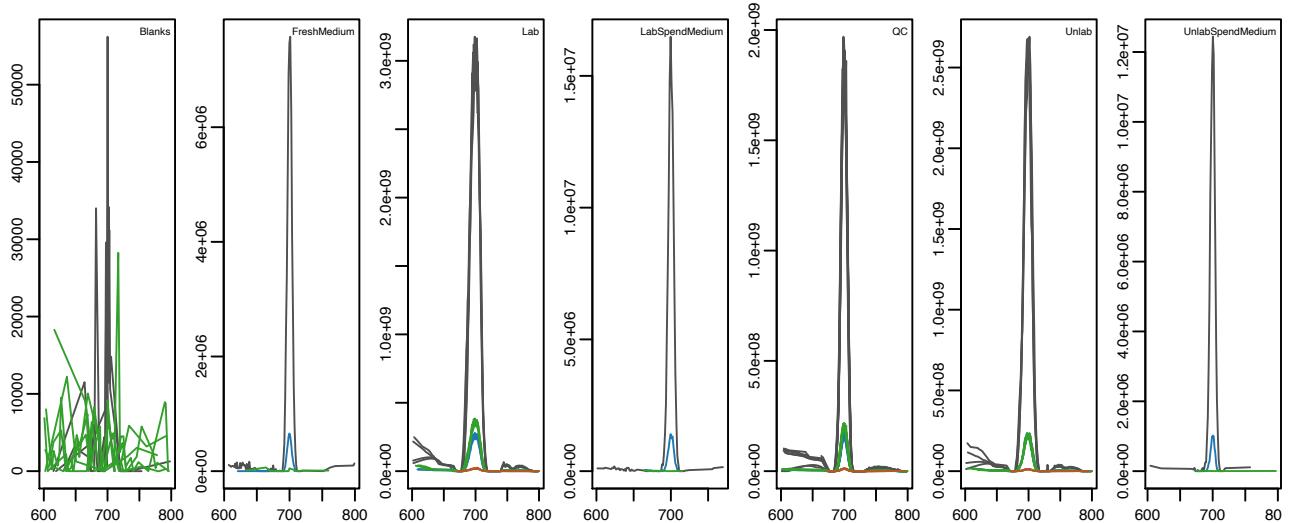


sn-glycero-3-Phosphocholine

Formula: C₈H₂₀NO₆P Mass: 257.103 Std.RT: 700.8 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5 ■+6 ■+7 ■+8

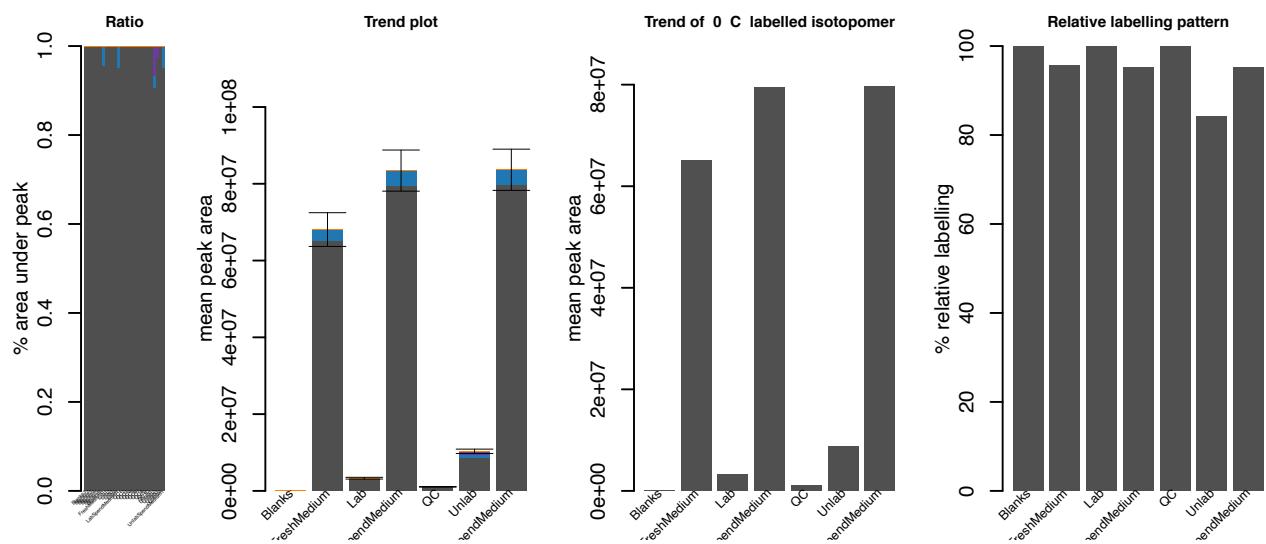
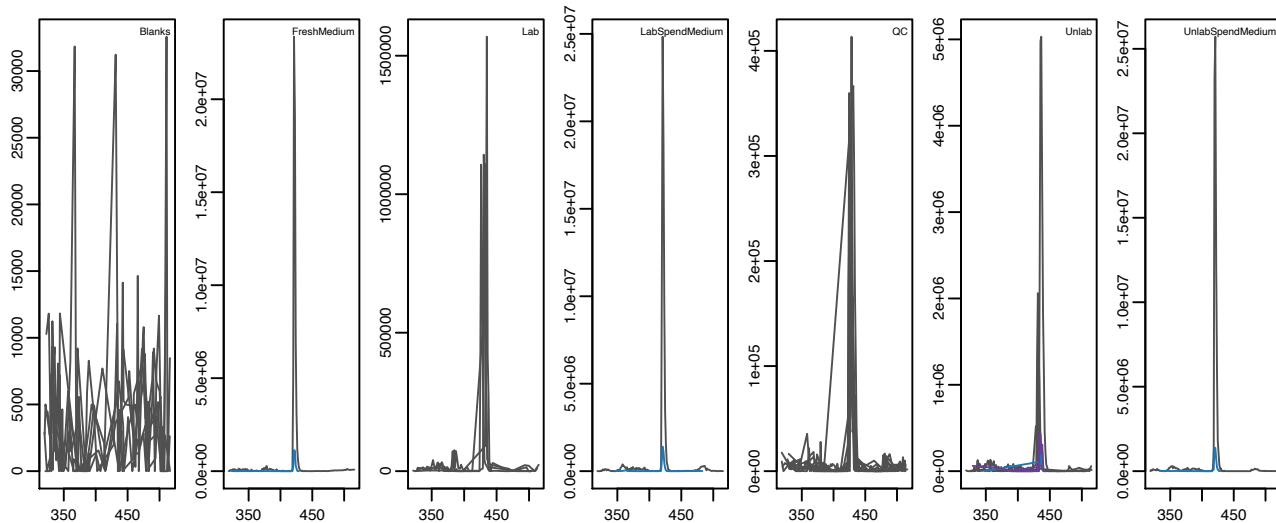


thymine

Formula: C5H6N2O2 Mass: 126.043 Std.RT: 418.2 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5



trans-4-Hydroxy-L-proline

Formula: C5H9NO3 Mass: 131.058 Std.RT: 720.6 Ion: POS

G1

■UL ■+1 ■+2 ■+3 ■+4 ■+5

