

# Advanced Metabolomics Bioinformatics, Activity, & Pathways



Annual Conference  
Short Course

CHOLINE ADENOSINE TRIPHOSPHATE CHOLESTEROL TESTOSTERONE GLUCOSE  
SERINE TRYPTOPHAN PHOSPHOCHOLINE ACYLCARNITINE THREONINE GLYCEROL  
PYRUVIC ACID UREA GALACTOSE CHOLINE ADENOSINE CHOLINE MALIC ACID  
TESTOSTERONE GLUCOSE PHOSPHATE CHOLESTEROL OXALOSUCCINIC ACID  
PYRUVIC ACID UREA CHOLINE ADENOSINE CHOLINE LACTIC ACID KETOLGLUTARATE  
GLUCOSE CHOLESTEROL OXALOSUCCINIC ACID GALACTOSE GLYCEROL FUMARATE  
NICOTINAMIDE ADENINE DINUCLEOTIDE OXALOSUCCINIC ACID GALACTOSE GLYCEROL  
SERINE TRYPTOPHAN PHOSPHOCHOLINE ACYLCARNITINE THREONINE GLYCEROL  
PYRUVIC ACID UREA GALACTOSE CHOLINE ADENOSINE CHOLINE MALIC ACID  
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NICOTINAMIDE ADENINE DINUCLEOTIDE OXALOSUCCINIC ACID GALACTOSE GLYCEROL  
SERINE TRYPTOPHAN PHOSPHOCHOLINE ACYLCARNITINE THREONINE GLYCEROL

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Gary Siuzdak



H. Paul Benton



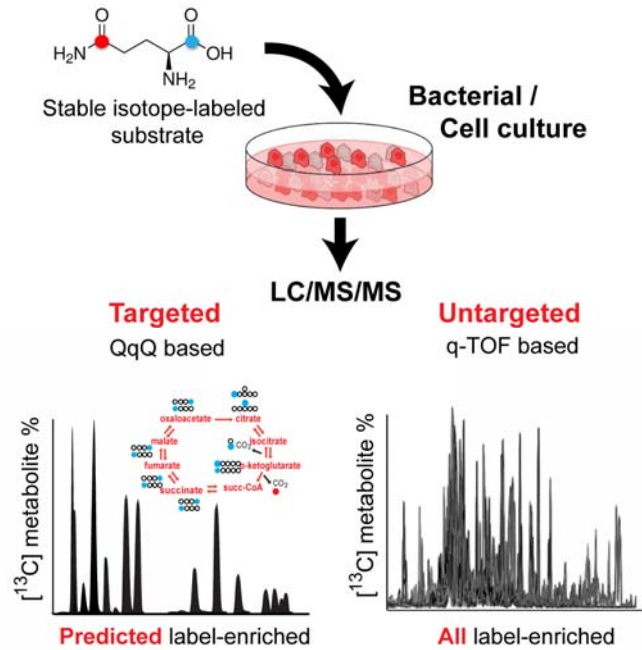
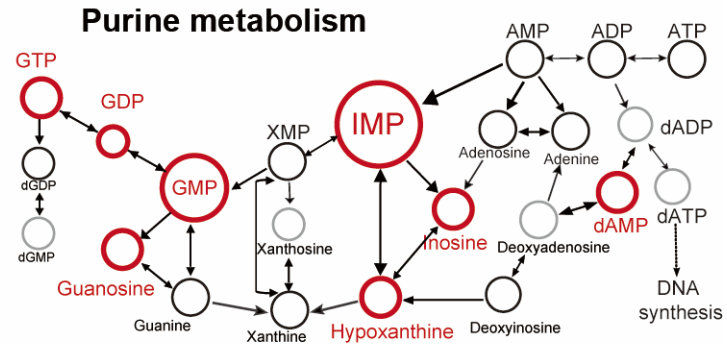
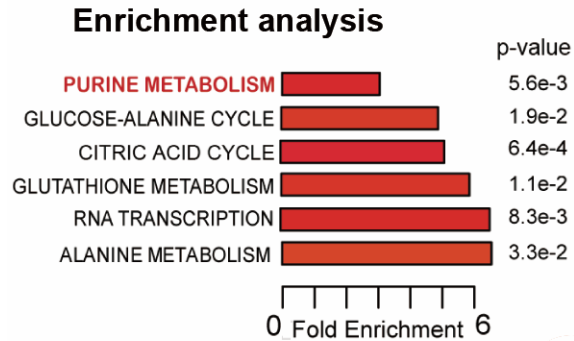
Xavi Domingo



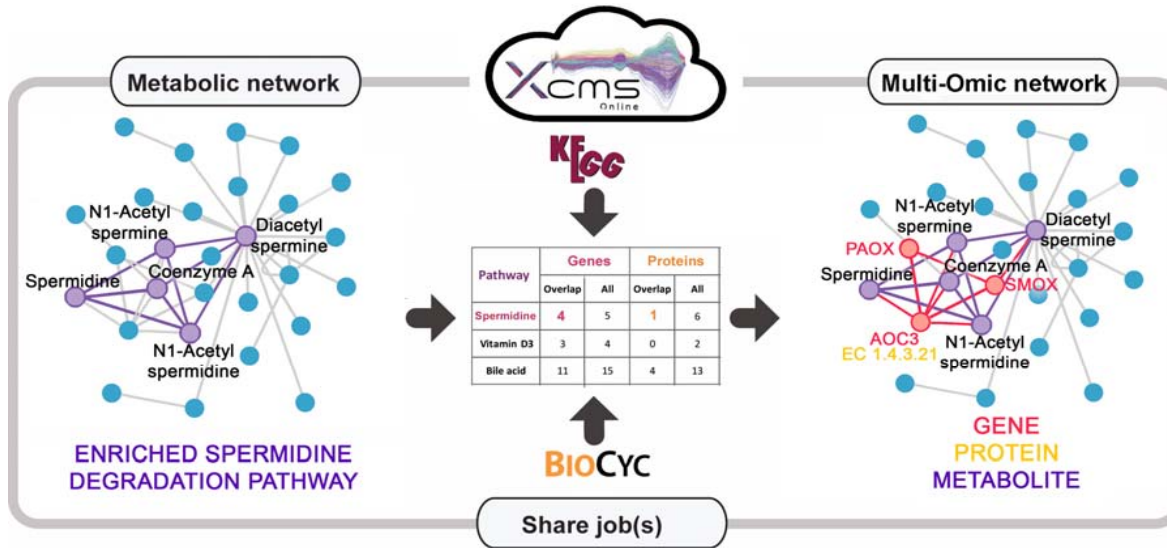
Erica Forsberg



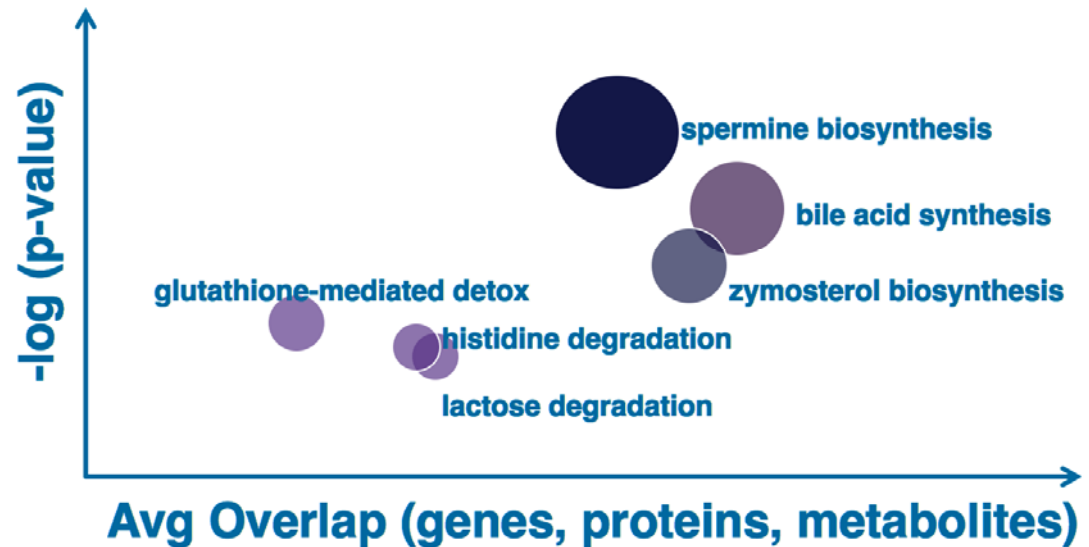
# Pathway Analysis



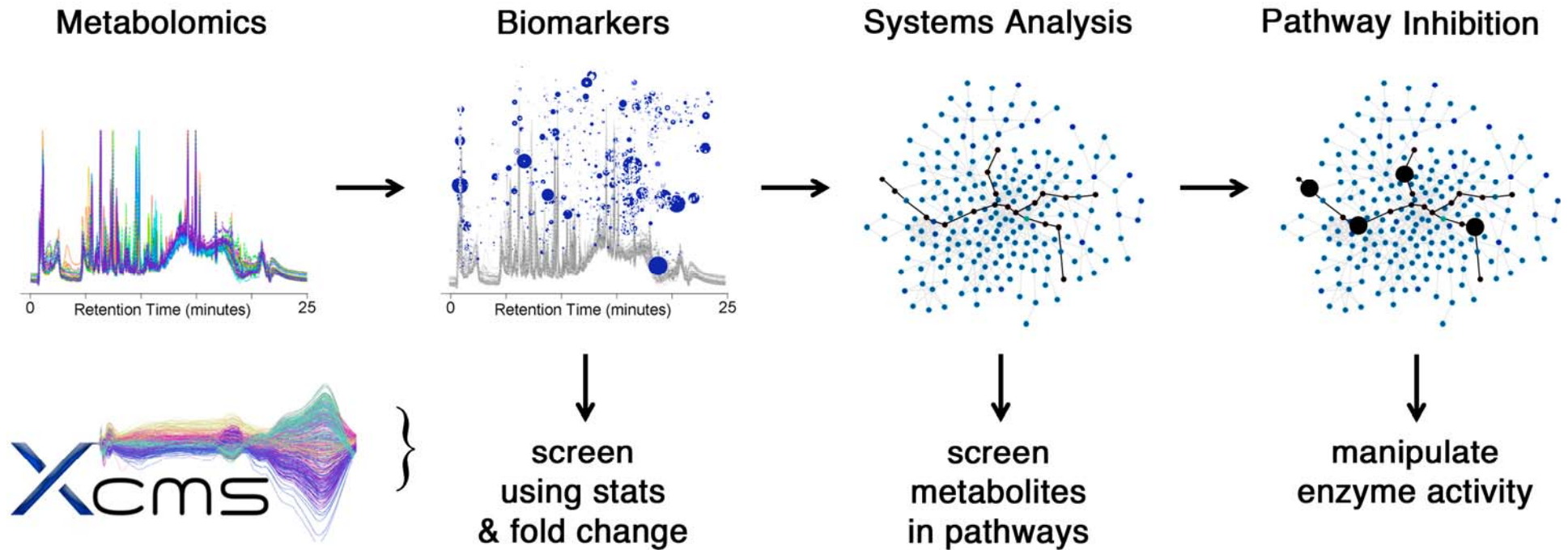
# Systems Biology



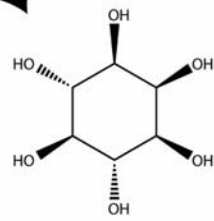
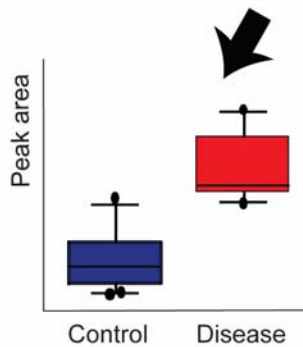
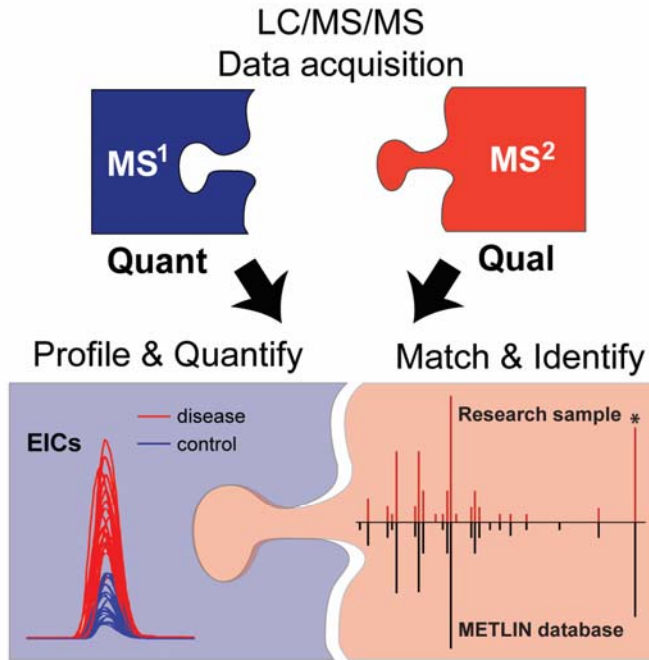
## Multi-Omic Cloud Plot



# Metabolomics Activity Screening



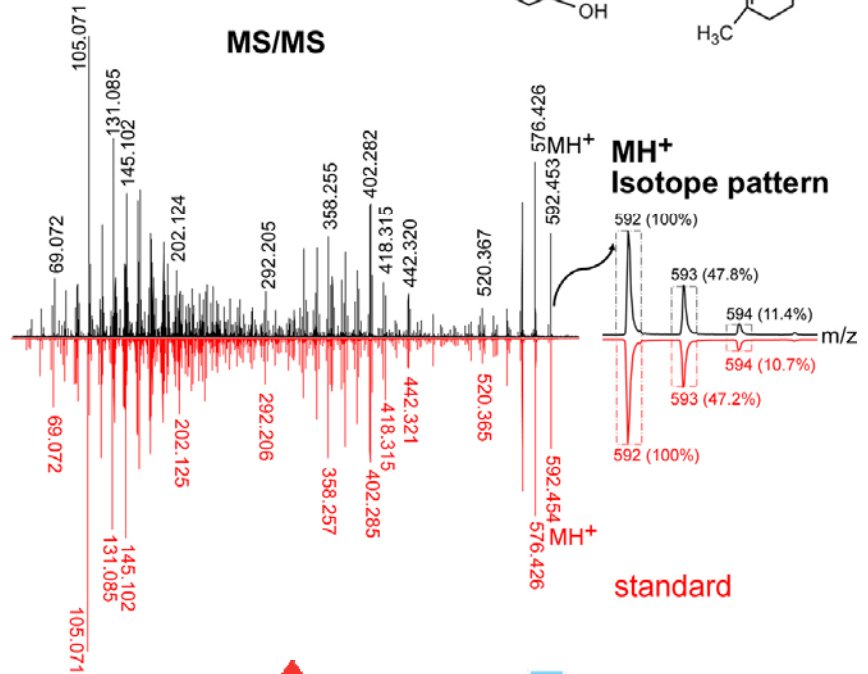
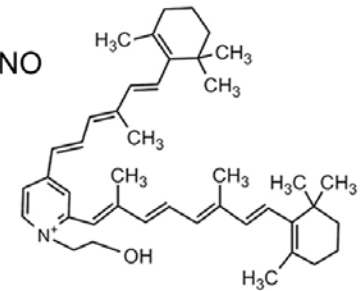
# Metabolite ID and Databases



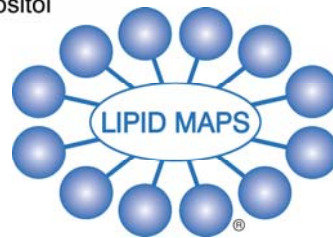
Accurate m/z & retention time

m/z 592.4530 (obs.)  
592.4513 (theo.)  
t<sub>R</sub>(min) 38.9 (obs.)  
39.0 (std.)

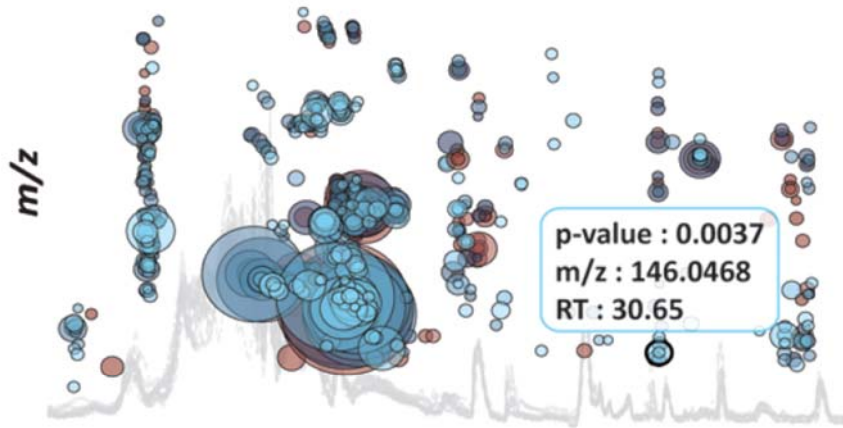
C<sub>42</sub>H<sub>58</sub>NO



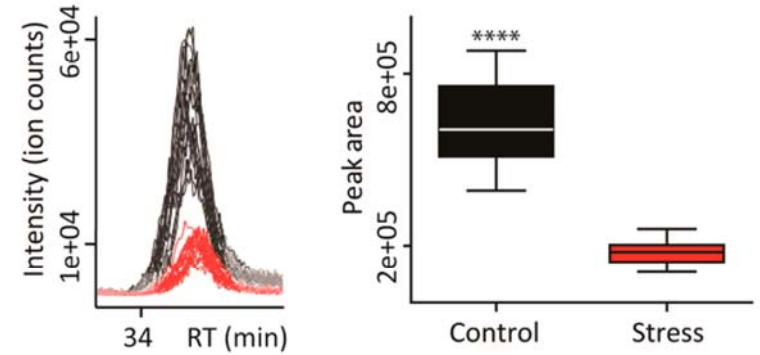
CHOLINE ADENOSINE TRIPHOSPHATE CHOLESTEROL TESTOSTERONE  
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PYRUVIC ACID UREA GALACTOSE CHOLINE ADENOSINE CYCLOSERINE  
GLUCONIC ACID GALACTONIC ACID  
NICOTINAMIDE ADENINE DINUCLEOTIDE OXALOSUCCLIC ACID GALACTOSE  
SERINE TRYPTOPHAN PHOSPHOCHOLINE ACYLCARNITINE THIAMINE  
**METLIN**



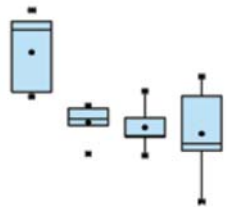
# Statistics



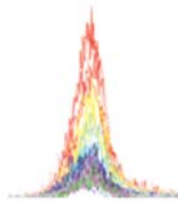
Welch t-test  
Control vs. Nitric oxide stress  
m/z = 171.0055



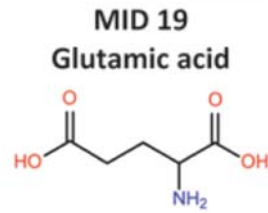
Box-Plot



EIC



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Wilcoxon signed-rank test  
Arterial vs. venous blood  
m/z = 309.2796

