

Advanced Metabolomics Bioinformatics, Activity, & SysBio



CHOLINE ADENOSINE TRIPHOSPHATE CHOLESTEROL TESTOSTERONE GLUCOSE
SERINE TRYPTOPHAN PHOSPHOCHOLINE ACYLCARNITINE THREONINE GLYCEROL
PYRUVIC ACID UREA GALACTOSE CHOLINE ADENOSINE CHOLINE LACTIC ACID
TESTOSTERONE GLUCOSE PHOSPHATE CHOLESTEROL OXALOSUCCINIC ACID
PYRUVIC ACID UREA CHOLINE ADENOSINE CHOLINE LACTIC ACID
GLUCOSE CHOLESTEROL OXALOSUCCINIC ACID GALACTOSE GLYCEROL
NICOTINAMIDE ADENINE DINUCLEOTIDE OXALOSUCCINIC ACID GALACTOSE
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2019

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 Scripps Research

Gary Siuzdak



H. Paul Benton



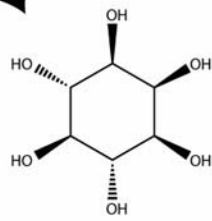
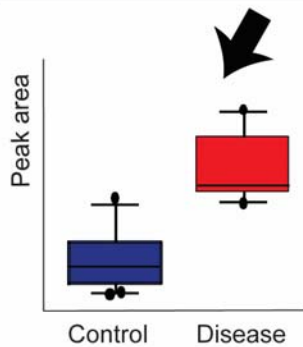
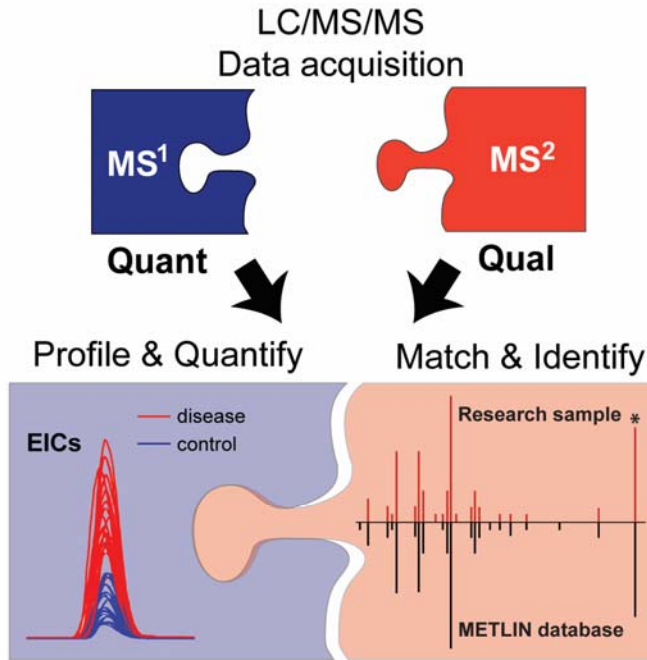
Xavi Domingo



Erica Majumder



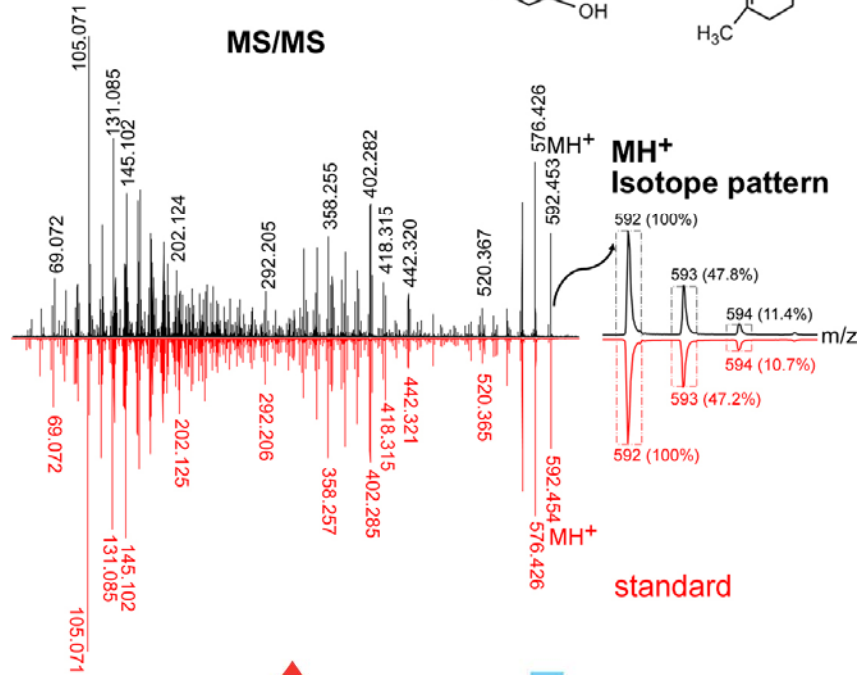
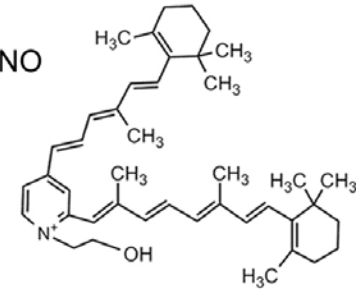
Metabolite ID and Databases



Accurate m/z & retention time

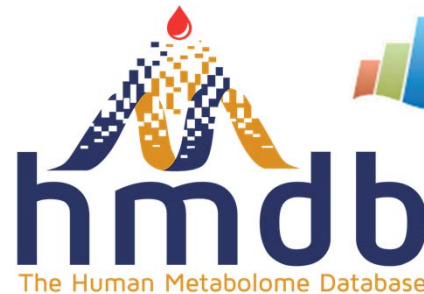
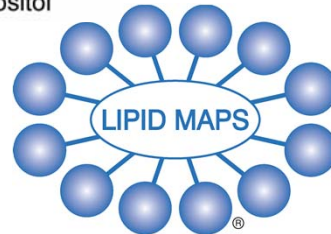
m/z	592.4530 (obs.)
	592.4513 (theo.)
t _R (min)	38.9 (obs.)
	39.0 (std.)

C₄₂H₅₈NO

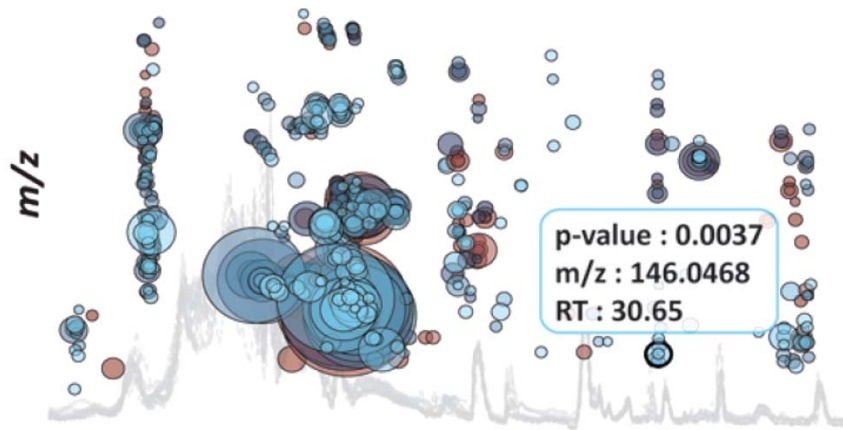


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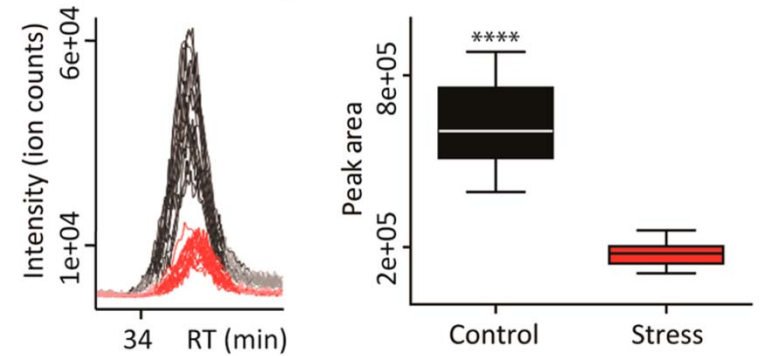
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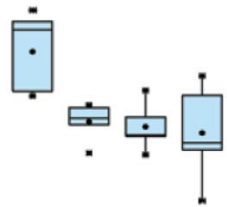
Statistics



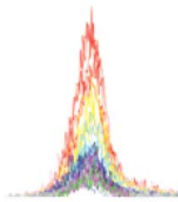
Welch t-test
Control vs. Nitric oxide stress
m/z = 171.0055



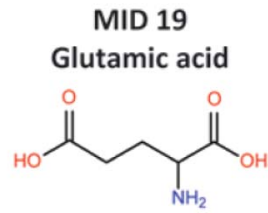
Box-Plot



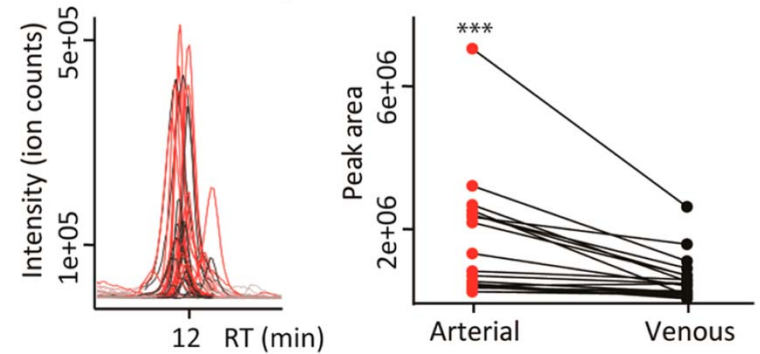
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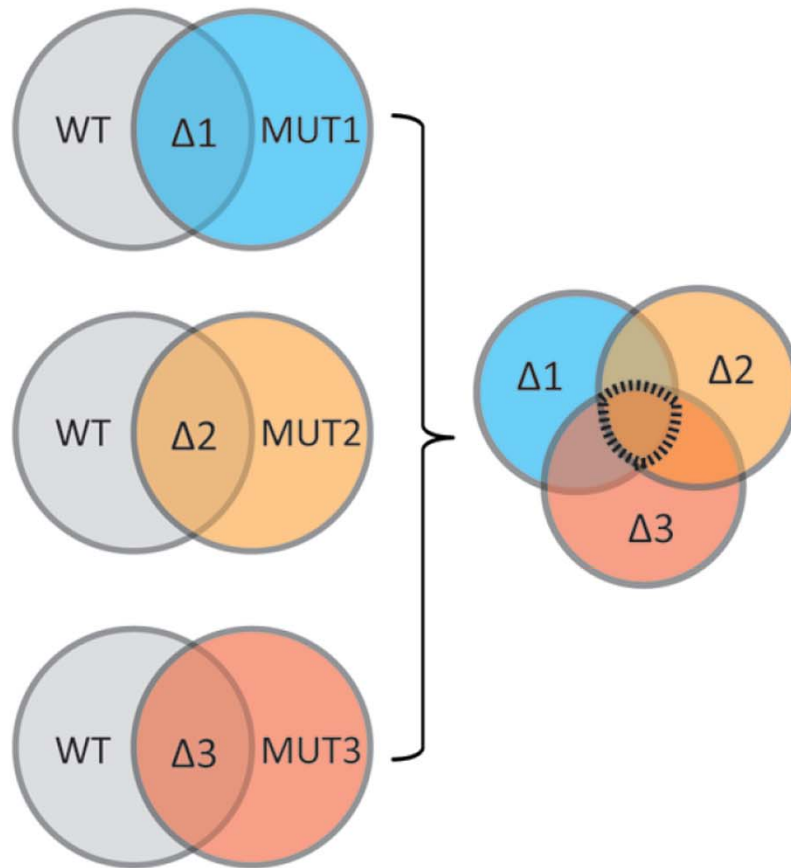


Wilcoxon signed-rank test
Arterial vs. venous blood
m/z = 309.2796

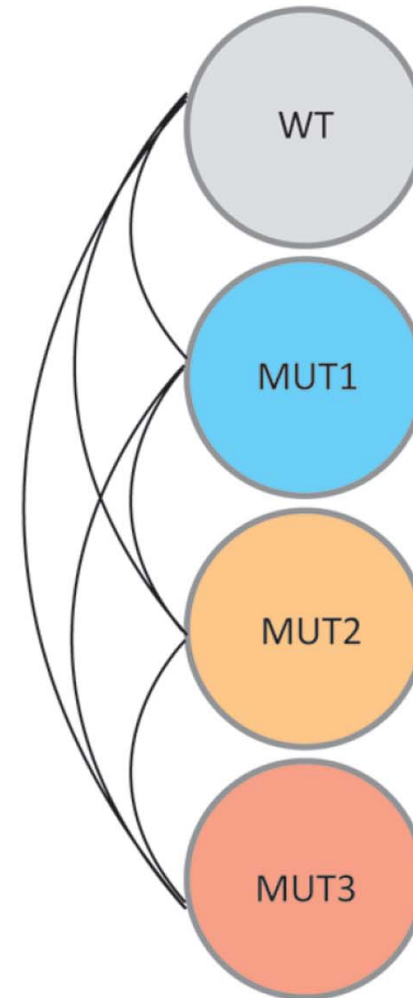


Multi-Group and Meta Analyses

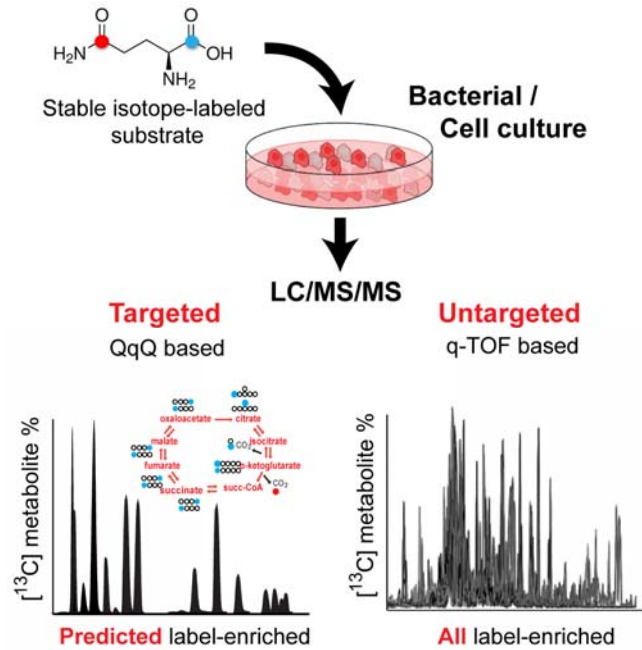
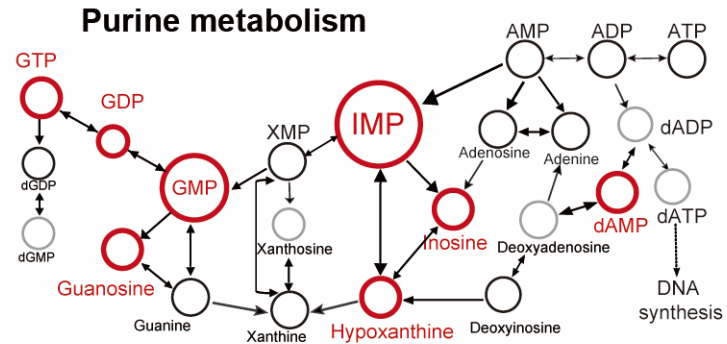
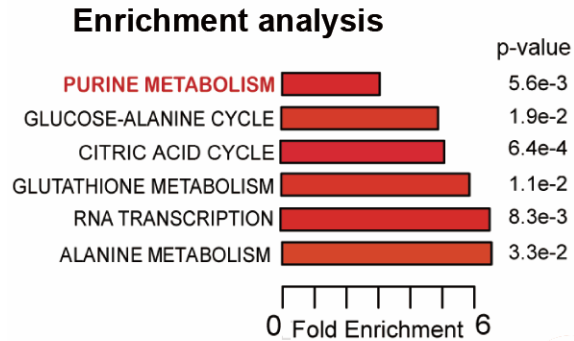
Meta-analysis of independent two-group comparisons



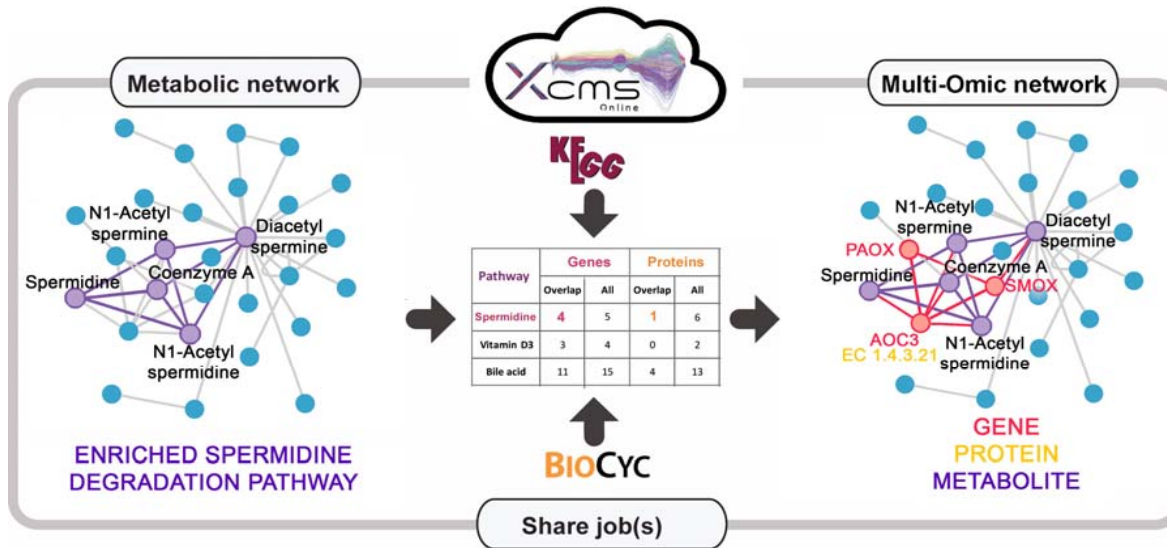
Multigroup analysis



Pathway Analysis



Systems Biology



Multi-Omic Cloud Plot

