

Supplement table 2. Bioinformatics databases that were queried for identified metabolites.

Database	Underlying principle	Approximate total metabolites
KEGG RPAIR	Atomic mapping	6000
KEGG REACTION	Enzymes and non- Enzymatic reactions	6000
KEGG PATHWAY	Metabolic Pathway	6000
KEGG LIGAND	Chemical compounds	20000
PubChem	Chemical compounds	40 million
HumanCyc	Enzymatic reaction and pathway	900
Reactome	Biochemical Reaction, Literature curated	600
EHMN	Reconstructed Metabolic network	3000
BIGG-UCSD	Reconstructed Metabolic network	1100
ChEBI	Chemical compounds	55000
MetaCyc compound	Chemical compounds	8000
MetaCyc reaction	Metabolic reaction	6000
MetaCyc pathway	Metabolic pathway	6000
HMDB	Human Specific Metabolites	8000