Table S3. Compound Discoverer processing settings for generating dipyanone putative metabolites.

Dipyanone	
Phase I reactions	Cyclisation 1 (–H → +O) Cyclisation 2 (–4C –8H –O → ø) Dehydration (–2H –O → ø) Desaturation (–2H → ø) Dihydrodiol formation (ø → +2H +2O) Hydration (ø → +2H +O) Ketone formation (–O → +2H) Oxidation (ø → +O) Oxidative deamination to alcohol (–2H –N → +H +O) Oxidative deamination to ketone (–3H –N → +O) Reduction (ø → 2H)
Phase II reactions	Acetylation (–H → +2C +3H +O) Cysteine conjugation (–H → +3C +6H +N +2O +S) Cysteine-Glycine conjugation (–H → +5C +9H +2N +3O +S) Glucuronide conjugation (–H → +6C +9H +6O) GSH conjugation (–H → +10C +15H +3N +6O +S) Methylation (–H → +C +3H) Sulfation (–H → +H +3O +S)
Max number of dealkylations	3
Max number of phase II reactions	2
Max number of all steps	5
Adducts	$[M+H]^+$ $[M-H]^-$