

Table S2. Transformations for generating anamorelin potential metabolites with Compound Discoverer software for data mining.

Phase I	Desaturation (2H → ∅)
	Dihydrodiol formation (∅ → 2H 2O)
	Ketone formation (O → 2H)
	Oxidation (∅ → O)
	Oxidative deamination to alcohol (2H N → H O)
	Oxidative deamination to ketone (2H N → O)
	Reduction (∅ → 2H)
Phase II	Acetylation (H → 2C 3H O)
	Carnitine conjugation on amine (2H N → 7C 14H N 3O)
	Cysteine conjugation on dihydrodiol (H O → 3C 6H N 2O S)
	Cysteine-Glycine conjugation on dihydrodiol (H O → 5C 9H 2N 3O S)
	Glucuronidation (H → 6C 8H 6O)
	Glutathionylation on dihydrodiol (H O → 10C 16H 3N 6O S)
	Glycine conjugation on amine (H → 2C 3H 2O)
	Methylation (H → C 3H)
	Sulfation (H → H 3O S)
	Sulfation on dihydrodiol (H O → H 3O S)
	Thiol conjugation (H O → H S)
Max # dealkylation	4
Max # Phase II reactions	2
Max # total reactions	5