A challenge for metabolite analysis solutions are their ability to process data and to efficiently report the results. Some software solutions incorporate the use of prediction algorithms to generate structures of possible metabolites of a given parent compound, which can then be utilized further downstream during data processing. Although these software packages have matured, there are inherent limitations to these solutions:

- Only as reliable as their prediction algorithms for generating possible metabolites
- Limited prediction databases
- Typically for mammalian species

Here, we describe a user created biotransformation database to augment a pre-existing prediction algorithm as part of the structure generation process. This new interface is integrated into the MetaSense™ software solution.

**INTRODUCTION**

**UNCOMMON BIOTRANSFORMATIONS**

Phase 1 and 2 metabolism often overlap between mammals and plants, however, conjugations found in plants can be quite different. Moreover, the environmental fate of agrochemicals are of high interest and these reactions are not well documented [1-3]. The table represents some reactions which are described to be unique to plant metabolism for pesticides, herbicides, and insecticides.

**UNIQUE USERS INITIATED BIOTRANSFORMATIONS**

- Reactions are drawn and atoms are mapped between the left side of the reaction and the product side within the chemical drawing application found in MetaSense™
- The system recognizes cleavages and conjugations, including various oxidations, reductions, and multiple products
- Generic reactions are updated to a SpectrusDB database where several user reactions can be contained and multiple databases can be created
- During analysis of metabolite datasets, MetaSense™ can use its native prediction engine in addition to several user created reaction databases

**SUMMARY**

- ACD/Labs has developed an interface for user-defined metabolic reactions to address the lack of well represented biotransformations
- User reactions are drawn in a generic biotransformation scheme and are uploaded to a SpectrusDB database
- User created metabolic reactions can be seamlessly integrated to work with the pre-existing prediction engine
- Integration of user created metabolic reactions allows for increased chemical coverage during analysis of xenobiotic metabolism studies with the MetaSense™ solution