Analysable identification of metabolites for a dog candidate is usually a time-consuming and laborious process, which is often the bottleneck in the discovery of new drugs. To avoid the situation of predicting neutral metabolites in a molecule later on that could potentially facilitate the analysis of the drug's spectra and thus ease the identification of metabolites. Until now, various ligand-based methods have been developed to model metabolic reactions, including expert systems, quantum-chemical calculations, structure-activity relationships, or mining large databases of experimental data. Despite the availability of such data, in silico predictions of neutral metabolites in a molecule on later could on potentially facilitate the analysis of the drug's spectra and thus ease the identification of metabolites. Until now, various ligand-based methods have been developed to model metabolic reactions, including expert systems, quantum-chemical calculations, structure-activity relationships, or mining large databases of experimental data. Despite the availability of such data, in silico predictions of neutral metabolites in a molecule later on could potentially facilitate the analysis of the drug's spectra and thus ease the identification of metabolites. Until now, various ligand-based methods have been developed to model metabolic reactions. In these cases, the availability of publically available experimental data and notably the amount of publically available experimental data in the realm of microsomal metabolism is related to individual atoms and their environment in the molecule, which is subject to greater fluctuations compared to similar local fragmentations in the whole molecule. So, analogously, the ability to model the Applicability Domain in this particular case should be considered of at least comparable (if not primary) significance to actual metabolite formation.

Additionally (or alternatively) to determining the complete metabolite profile in human liver microsomes, some projects focus on metabolite profiling by a single enzyme, e.g., one of the CYP family. In this case, the availability of such in silico predictions for the regioselectivity of individual metabolizing enzyme will be of great help in an analogous way as described above. Recently, we have applied the GALAS-modelling method in predicting possible CYP3A4 and CYP2D6 metabolism sites. The modeling of regioselectivity for other enzymes such as CYP2C19 or CYP2C9 have been described in detail in a previous study (Van Baars, 2014). However, a general problem associated with such models is the amount of publicly available experimental data for this particular enzyme. The availability of publicly available experimental data for this particular enzyme is a limiting factor in the process of generating accurate and reliable models for this enzyme. In these cases, the availability of a large amount of publicly available experimental data for this particular enzyme is not only a limiting factor in the process of generating accurate and reliable models for this enzyme, but also a significant challenge for the modeling process. In the case of CYP3A4 and CYP2D6, the availability of such data is relatively limited, which makes the process of generating accurate and reliable models for these enzymes even more challenging. In these cases, the availability of a large amount of publicly available experimental data for this particular enzyme is not only a limiting factor in the process of generating accurate and reliable models for this enzyme, but also a significant challenge for the modeling process. In the case of CYP3A4 and CYP2D6, the availability of such data is relatively limited, which makes the process of generating accurate and reliable models for these enzymes even more challenging. In these cases, the availability of a large amount of publicly available experimental data for this particular enzyme is not only a limiting factor in the process of generating accurate and reliable models for this enzyme, but also a significant challenge for the modeling process. In the case of CYP3A4 and CYP2D6, the availability of such data is relatively limited, which makes the process of generating accurate and reliable models for these enzymes even more challenging. In these cases, the availability of a large amount of publicly available experimental data for this particular enzyme is not only a limiting factor in the process of generating accurate and reliable models for this enzyme, but also a significant challenge for the modeling process. In the case of CYP3A4 and CYP2D6, the availability of such data is relatively limited, which makes the process of generating accurate and reliable models for these enzymes even more challenging.