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...METEOR and META are examples of software packages that rely on expert rules as the basis of their predictions. MetabolExpert (**CompuDrug** International) is composed of a knowledge-base tool, at least one database and a prediction tool. Current database modules...

Bridging cheminformatic metabolite prediction and tandem mass spectrometry

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Despite recent technological advances, the analysis of biological samples for metabolite identification purposes often requires prior knowledge of the metabolite masses to successfully acquire high quality mass spectral data in the presence of intense background and interfering matrix signals. This, in turn, necessitates prior knowledge of the metabolite structure, which in most cases can be predicted on the basis of the potential routes of metabolism of those functional groups present in the molecule. The following discussion highlights the significance of knowledge of the metabolite mass in facilitating the detection and structural elucidation of drug metabolites.

The importance of knowledge of drug metabolites to facilitate their identification in biological samples is discussed in light of new strategies based on cheminformatic metabolite predictions with data-dependent tandem mass spectrometry.

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