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In silico enzyme selectivity predictions of four major phase II drug metabolism enzymes

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The liver is the main site of drug metabolism in human body. Drug metabolism in liver, converting lipophilic substrates into more polar products which are easily excreted form, occurs in two steps, phase I and phase II. Especially, phase II metabolism is important because it is fast pathway for drug elimination and closely related with excretion, but still practical models are not available. Generally, phase II transformations conjugate a highly polar group to the substrates, then produce more hydrophilic products than its substrates. We categorized these metabolic reactions into four major classes. The reactions are glucuronidation, sulfation, N-acetylation and glutathione conjugation, and enzymes responsible for those reactions are UDP-glucoronosyl transferase (UGT), sulfotransferase (SULT), N-acetyltransferase (NAT) and glutathione transferase (GST) respectively. We made four *in silico* substrate classification models using random forest method. ECFP_4 is selected as molecular descriptor. ECFPs are topological fingerprints for molecular characterization using Morgan algorithm to capture molecular features. These models effectively predict phase II transformational fate of a drug molecule. And we also found that suggestion of important substructure features is possible by statistical analysis of random forest models.

Biography

Hyoungjun Son is a graduate student and currently Ph.D candidate at Yonsei University.