[L2] Explorations into Chemical Reactions and Biochemical Pathways

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The chemoinformatics of chemical reactions is much less developed than the chemoinformatics of molecular structures.

To remedy this situation we need reaction databases that contain much more details on chemical reactions. Methods have been developed to calculate physicochemical effects at the reaction site for the atoms and bonds directly involved in the reaction process. It is shown that these physicochemical effects can quite favourably be used to derive equations for the calculation of data on gas phase reactions and on reactions in solution such as aqueous acidity of alcohols or carboxylic acids or the hydrolysis of amides. Furthermore, it is shown that these physicochemical effects are quite effective for assigning reactions into reaction classes that correspond to chemical knowledge.

Biochemical reactions constitute a particularly interesting and challenging task for increasing our understanding of living species. The BioPath.Database is a rich source of information on biochemical reactions and has been used for a variety of applications of chemical, biological, or medicinal interests. Thus, it was shown that biochemical reactions can be assigned by the physicochemical effects into classes that correspond to the classification of enzymes by the EC numbers. Furthermore, 3D models of reaction intermediates can be used for searching for novel enzyme inhibitors. It was shown in a combined application of chemoinformatics and bioinformatics that essential pathways of diseases can be uncovered. Furthermore, a study showed that bacterial flavor-forming pathways can be discovered.