

Exploring Activity Cliffs from a Chemoinformatics viewpoint

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The activity cliff concept experiences considerable interest in medicinal chemistry and chemoinformatics. Activity cliffs are defined as pairs or groups of structurally similar or analogous active compounds having large differences in potency. Depending on the research field, views on activity cliffs partly differ. While interpretability and utility of activity cliff information is considered to be of critical importance in medicinal chemistry, large-scale exploration and prediction of activity cliffs are of special interest in chemoinformatics. Much emphasis has recently been put on making activity cliff information accessible for medicinal chemistry applications. Herein, different approaches to the analysis and prediction of activity cliffs are discussed that are of particular relevance from a chemoinformatics viewpoint.