

[L4] Analyzing Promiscuity at the Level of Active Compounds and Targets

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In the context of polypharmacology, promiscuity is defined as the ability of small molecules to specifically interact with multiple targets. In addition, promiscuity can also be viewed as a characteristic feature of targets by considering their ability to recognize structurally diverse molecules as well as compounds with multi-target activities.

Promiscuity estimates can be obtained through systematic mining of compound activity data. Currently available volumes of activity data already are so large that it should be possible to derive statistically sound trends from their analysis. However, confidence criteria must be carefully considered when drawing conclusions from compound data mining. Herein, the results of recent promiscuity analyses are presented in context including studies that view promiscuity from a target perspective.