Recent progress on cheminformatics approaches to epigenetic drug discovery

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Abstract

The ability of epigenetic markers to affect genome function has enabled transformative changes in drug discovery, especially in cancer and other emerging therapeutic areas. Concordant with the introduction of the term 'epi-informatics', the size of the epigenetically relevant chemical space has grown substantially and so did the number of applications of cheminformatic methods to epigenetics. Recent progress in epi-informatics has improved our understanding of the structure–epigenetic activity relationships and boosted the development of models predicting novel epigenetic agents. Herein, we review the advances in computational approaches to drug discovery of small molecules with epigenetic modulation profiles, summarize the current chemogenomics data available for epigenetic targets, and provide a perspective on the greater utility of biomedical knowledge mining as a means to advance the epigenetic drug discovery.

Biography

Zoe sessions is a third-year undergraduate at the university of north carolina at chapel hill. She is pursuing her chemistry b.s. and is looking to complete her phd in pharmaceutical sciences following hier 2022 graduation. This is her first publication