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Title: Machine learning for early stage drug discovery

Abstract: Fuelled by the success of machine learning in a wide range of domains, there is significant interest in the application of machine learning to early stage drug discovery in areas from designing novel compounds to screening libraries of compounds against a specific target. However, many existing machine learning methods either do not account for the 3D structure of the protein at all or struggle to capture meaningful spatial information from it. I will describe how our structure-aware models for compound design and virtual screening can facilitate the design of compounds which conform to a specified design hypothesis and help uncover key protein-ligand interactions which can be used to aid molecule design.