Structure-based design of riboswitch ligands and selective NMT inhibitors

Ruth Brenk
Department of Biomedicine, University of Bergen, Norway

Structure-based ligand design is an integral part of modern drug discovery. This approach makes use of the knowledge of the crystal structure of the target for the design of new ligands. In my group, we develop computational methods for structure-based design and apply such methods for the design of new ligands. In this seminar, I will report on different aspects of structure-based drug discovery. One the one hand side, I will present our ongoing efforts to design riboswitch ligands. Riboswitches are part of the 5' untranslated region of mRNA. With little precedence for drug design efforts for RNA, they can be considered to be challenging targets. One the other side, I will present an approach on how to dissect molecular driving forces to design selective inhibitors which is an import goal in many drug discovery projects.