Special Issue

Fragment-to-Lead Optimization in Drug Discovery

Message from the Guest Editors

Fragment-based lead discovery (FBLD) has developed remarkably in the last two decades, becoming an effective approach for the identification of lead compounds and a complementary method to high throughput screening in drug discovery. FBLD aims for the detection of reversible and irreversible small molecules (fragments) binding to a biological target and their optimization to higher affinity compounds (leads). A major challenge in FBLD is the transition from fragment hits to leads. Several approaches based on computational and experimental methods have successfully driven the optimization of fragments to viable lead series for different molecular targets and their improvement will be fundamental to broaden the application and success of FBLD in drug discovery. This Special Issue on Molecules aims to provide a venue for current research and state-of-the-art developments for lead generation from fragments. Reviews and original research articles focusing on any aspect of fragment-to-lead optimization are welcome.

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As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts and novel materials. Pushing the boundaries of the discipline, we invite papers on multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

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