Fragment-based Drug Discovery: Lessons and Outlook (Methods and Principles in Medicinal Chemistry)

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From its origins as a niche technique more than 15 years ago, fragment-based approaches have become a major tool for drug and ligand discovery, often yielding results where other methods have failed. Written by the pioneers in the field, this book provides a comprehensive overview of current methods and applications of fragment-based discovery, as well as an outlook on where the field is headed.

The first part discusses basic considerations of when to use fragment-based methods, how to select targets, and how to build libraries in the chemical fragment space. The second part describes established, novel and emerging methods for fragment screening, including empirical as well as computational approaches. Special cases of fragment-based screening, e. g. for complex target systems and for covalent inhibitors are also discussed. The third part presents several case studies from recent and on-going drug discovery projects for a variety of target classes, from kinases and phosphatases to targeting protein-protein interaction and epigenetic targets.

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