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Expanding the toolbox of protein-templated reactions for early drug discovery

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Stellingen

Expanding the toolbox of protein-templated reactions for early drug discovery

M. Yagiz Unver

1. Kinetic target-guided synthesis has the potential to speed up the early stages of the drug-discovery process significantly.

Angew. Chem. Int. Ed **2017**, *56*, 7358–7378, Chapters 1–3.

2. Use of protein-templated reactions for hit identification/optimization and dynamic combinatorial chemistry for lead optimization would be a powerful combination to accelerate early drug discovery.

Chem. Soc. Rev **2015**, *44*, 2455–2488, Chapters 1–5.

3. Docking and modeling programs give more accurate results if people use them without prejudice.
4. If the NMR spectrum of a compound is very complicated to interpret due to the presence of rotamers or diastereomers, NMR interpretation should not be a requirement to publish the work as long as the compound is pure and its chemical identity is confirmed by means of other analytical techniques.

Chapter 3

5. Imagination is the main building block in the field of target-guided synthesis.
6. Doing a PhD in the field of medicinal chemistry requires an open-minded mentality towards all life sciences especially if you start from an organic-chemistry background.
7. Modeling and docking programs do not always give you active compounds; they help you, however, to eliminate many of the inactive ones.
8. Selecting the best hit by using protein-templated reactions is like the cherry on the cake, since identifying an active compound from scratch is already a great achievement.
9. Reproducibility in enzymatic assays should carefully be checked as it affects lead optimization.

Bioorg. Med. Chem. Lett. **2016**, *26*, 2764–2767