AUTOMATED DESIGN

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Innovative bioactive agents fuel sustained drug discovery and the development of new medicines. Future success in chemical biology and pharmaceutical research will fundamentally rely on the combination of advanced synthetic and analytical technologies that are embedded in a theoretical framework that provides a rationale for the interplay between chemical structure and biological effect. A driving role in this setting falls on leading edge concepts in computer-assisted molecular design and engineering, by providing access to a virtually infinite source of novel tool compounds and lead structures, and guiding experimental screening campaigns. We will present concepts and ideas for the representation of molecular structure, predictive models of structure-activity relationships, automated molecular design, and discuss *de novo* design approaches that have proven their usefulness and will contribute to future drug discovery by generating innovative bioactive agents. Emphasis will be put on methods for fragment- and reaction-based compound generation. As we are currently witnessing strong renewed interest in bioactive natural products we will showcase natural-product inspired molecular design methods and their prospective application.

Selected references:

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3. Friedrich, L., Rodrigues, T., C. S. Neuhaus, Schneider, P. and Schneider, G. (2016) From complex natural products to simple synthetic mimetics by computational de novo design. *Angew. Chem. Int. Ed*. 55, 6789–6792.
4. Rodrigues, T., Reker, D., Welin, M., Caldera, M., Brunner, C., Gabernet, G., Schneider, P., Walse, B. and Schneider, G. (2015) De novo fragment design for drug discovery and chemical biology. *Angew. Chem. Int. Ed*. 54, 15079–15083.