CHEMMEDCHEM

CHEMISTRY ENABLING DRUG DISCOVERY

09/2007

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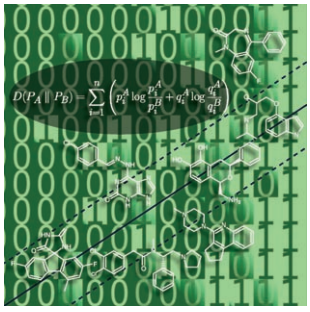
Some articles in this issue have already appeared online in Wiley InterScience. See www.chemmedchem.org under EarlyView®

COVER PICTURE

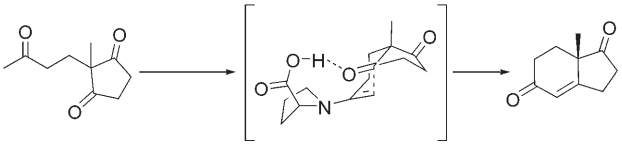


The cover picture shows a bit pattern reflecting relative frequencies of a molecular fingerprint and molecules belonging to different activity classes. A divergence function is derived that captures differences in bit frequencies between active and database compounds. The function is applied to establish a linear relationship (black line) between bit divergence and expected compound recall in similarity searching. For a fingerprint, a screening database, and set of known active reference molecules, the linear model can be used to estimate the probability to identify hits in similarity search calculations. For details, see the Full Paper by M. Vogt and J. Bajorath on p. 1311 ff.

NEWS

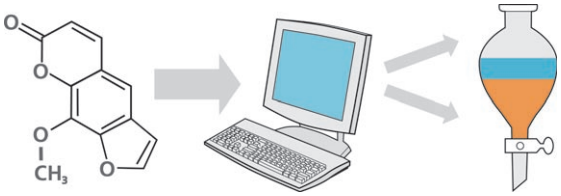
REVIEWS

MINIREVIEWS

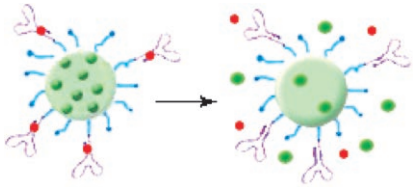


Despite considerable efforts to explore and extend the scope of asymmetric organocatalytic reactions throughout the last years, their use in medicinal and process chemistry is still rather low. This minireview highlights some of the recent developments in the rapidly evolving field of organocatalysis recently presented at the Schering Foundation organized symposium on "Organocatalysis".

COMMUNICATIONS



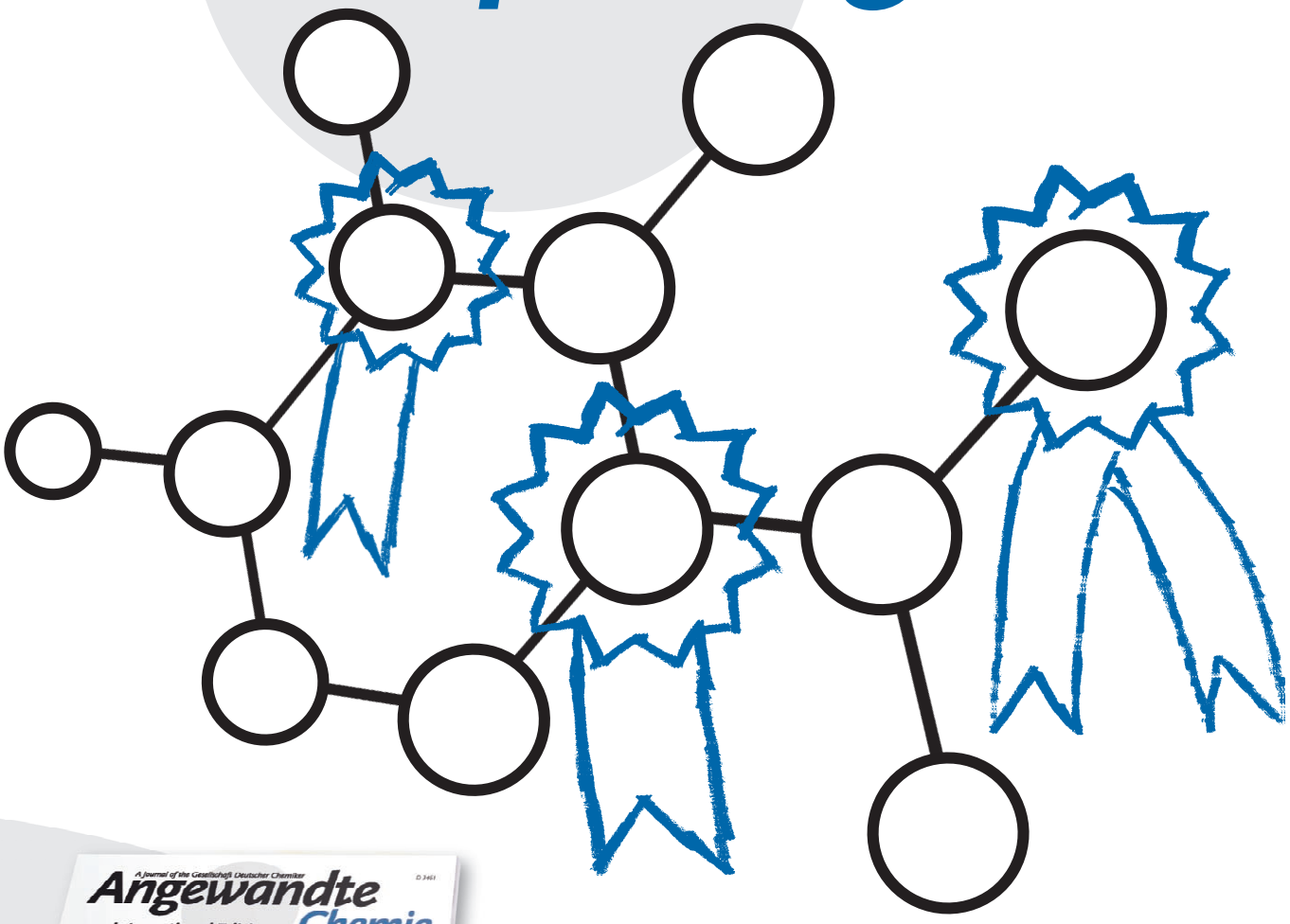
The lipophilicity of 14556 library compounds at Bayer Schering was modeled using Gaussian process methodology. In a blind test with 7013 new drug-discovery molecules from the last few months, 81% were predicted correctly within one log unit, compared with only 44% achieved by commercial software. Predicted error bars exhibit close to ideal statistical properties, thereby allowing assessment of the model's domain of applicability.



Herein we report a novel targeted drug delivery system consisting of nanoparticle–aptamer bioconjugates, which can carry both hydrophobic and hydrophilic chemotherapeutic drugs simultaneously, and deliver them selectively in a targeted and temporally distinct manner. This work provides a robust platform for targeted co-delivery of chemotherapeutic agents with the hope of both leveraging the synergistic effects of multiple drugs and also potentially suppressing the likelihood of drug resistance by the treated tissues.

FULL PAPERS

Incredibly prestigious!



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service@wiley-vch.de
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* Author to whom correspondence should be addressed.

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