References

- 1 Palczewski, K. et al. (2000) Crystal structure of Rhodopsin: A G-Protein-coupled receptor. Science 289, 739-745
- 2 Strader, C.D. et al. (1989) Structural basis of β-adrenergic receptor function. FASEB J. 3, 1825-1832
- 3 Liaw, C.W. et al. (1997) Localization of agonist- and antagonist-binding domains of human corticotropin releasing factor receptors. Mol. Endocrinol. 11, 2048–2053
- 4 Wlodawer, A. et al. (1998) Inhibitors of HIV protease: a major success of structure-based design. Ann. Rev. Biophys. Biomol. Struct. 27, 249-284

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The optimal fragmentation principle - Reply A

Initial letter: Johnson, D.E. (2001) The optimal fragmentation principle. Drug Discovery Today 6, 175 Response from Dale Johnson

Both Peter Bach and Ann Richard make excellent points in their replies to my letter. As Bach states, there is a need for a single platform for current predictive tools - one that enables a user to combine approaches, use different databases or add personal information. A secure web-based approach might be a reasonable solution.

Richard points out that a major limiting factor in the development of models and predictive systems is access to quality data. In many cases it is also a problem of the 'existence' of quality data. In addition to sharing proprietary information, there is also a crucial need to create new databases from mechanistic screening approaches that can be used to fill gaps in chemical space in databases or chemical libraries (especially in the drug discovery area) and to provide researchers immediate access to screens where confirmation algorithms can be applied to predictive results.

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