

## **Computer-aided Drug Design**

Farzin Hadizadeh, Pharm.D, Ph.D

*Department of Medicinal Chemistry, Pharmacy Faculty, MUMS, Mashhad, Iran*

The low cost of the powerful desktop computers gives the medicinal chemists the ability to "design" the molecule on the basis of an estimated fit onto a receptor or have similar spatial characteristics found in the prototypical lead compound. Of course, this assumes that the molecular structure of the receptor is known in enough detail for a reasonable estimation of its three-dimensional shape. When a good understanding of the geometry of the active site is known, databases containing the three-dimensional coordinates of the chemicals in the database can be searched rapidly by computer programs that select candidates likely to fit in the active site. There have been dramatic successes with use of this approach.