

## **structure-based design**

*in drug design*

Structure-based design is a design strategy for new chemical entities based on the three-dimensional (*3D*) structure of the target obtained by X-ray or nuclear magnetic resonance (*NMR*) studies, or from protein homology models.

**Source:**

PAC, 1997, 69, 1137 (*Glossary of terms used in computational drug design (IUPAC Recommendations 1997)*) on page 1150