



**What is necessary about the structural  
properties of a SBDD target?**

- High-resolution structure available
  - Resolution of  $< 2.5 \text{ \AA}$  [1]
  - Homology models less trustworthy
    - can still be useful, perhaps to guide structure determination
- Experimental structures/homology models can be refined by molecular dynamics simulation

- unique structural motifs, favouring specificity

- “Druggable”
  - precedence - previously targeted
  - structure-based
    - cavities or pockets
    - comparing physicochemical and geometric properties of pocket with known druggable targets
- as a caveat, concept is about history and does not account for innovation



[1] Anderson, A. The Progress of Structure-Based Drug Design. *Chemistry & Biology* 2003, 10 (9), 787-797. <https://doi.org/10.1016/j.chenbi.2003.09.002>

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