

**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

- “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.chembi.2003.09.002>

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