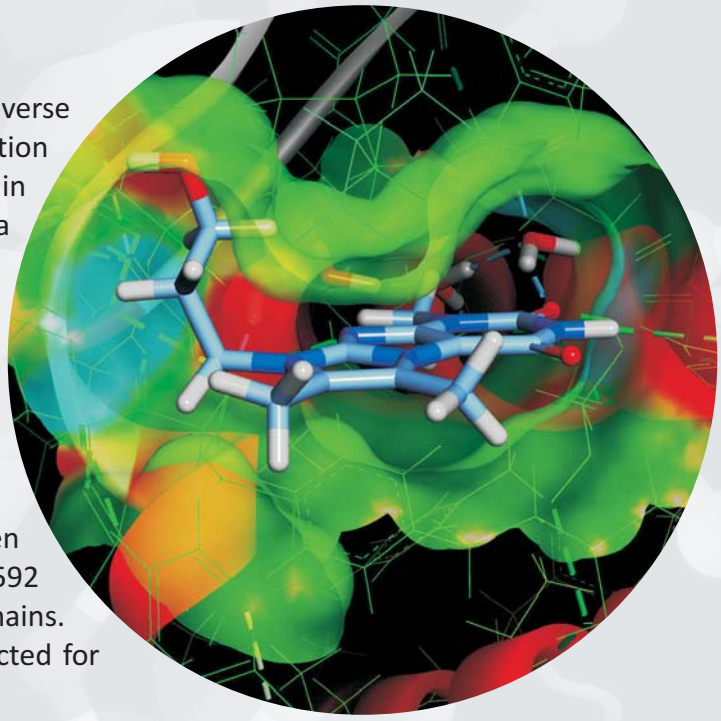
Reaxense

BET Bromodomains Focused Library



Bromodomains are acetyl-lysine recognition modules of a diverse group of proteins that play crucial role in chromatin organization and regulation of gene transcription. Proteins that contain bromodomains have been involved in the development of a large variety of diseases. Bromodomain and extra-terminal (BET) proteins, which belong to a class of proteins collectively called epigenetic "readers", have recently emerged as prospective drug targets for treatment of cancers, inflammatory diseases, and other medical conditions.

Reaxense's BET Bromodomains Focused Library has been designed with flexible molecular docking and comprises 1,592 compounds predicted to have high affinity to BET bromodomains. In addition, a custom subset of compounds has been selected for each of the four BET bromodomain targets.

Features:

- **1,592 compounds focused against BRD2, BRD3, BRD4 and BRDT**
- **Specific compound subset for each target is available**
- **Full Rule of Five (Ro5) compliance**
- **Compounds with reactive and toxic groups filtered out**
- **High diversity over the library**
- **Purity >90%; spectral data available**

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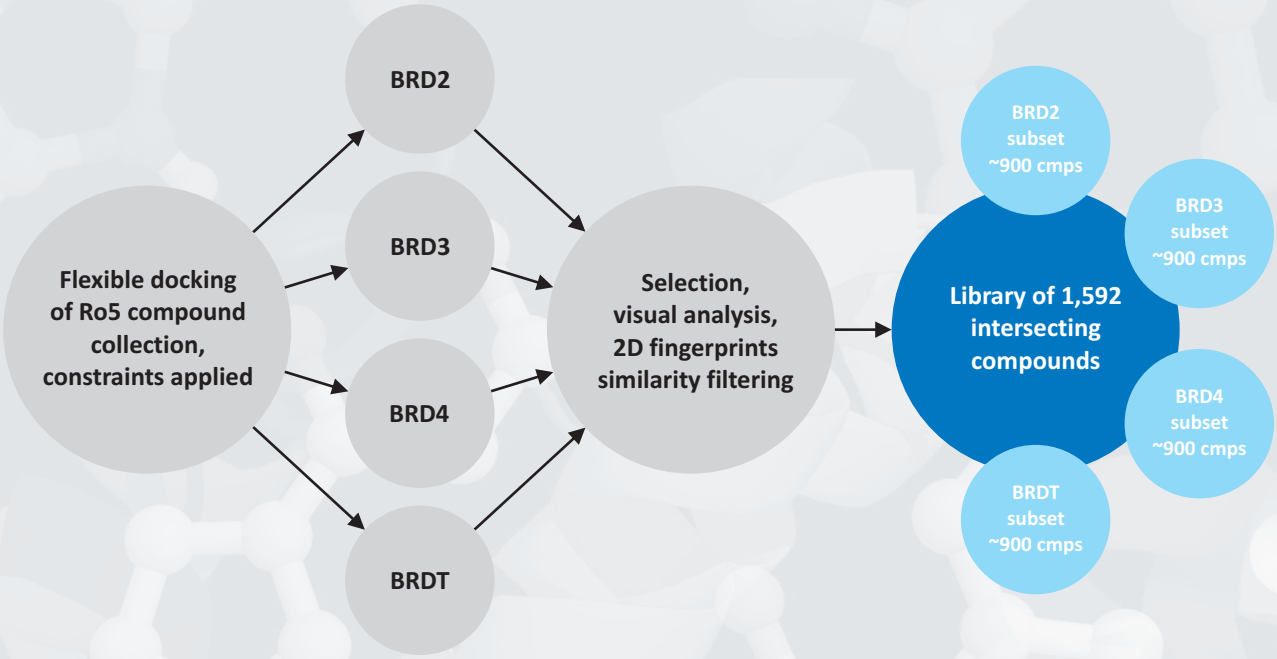
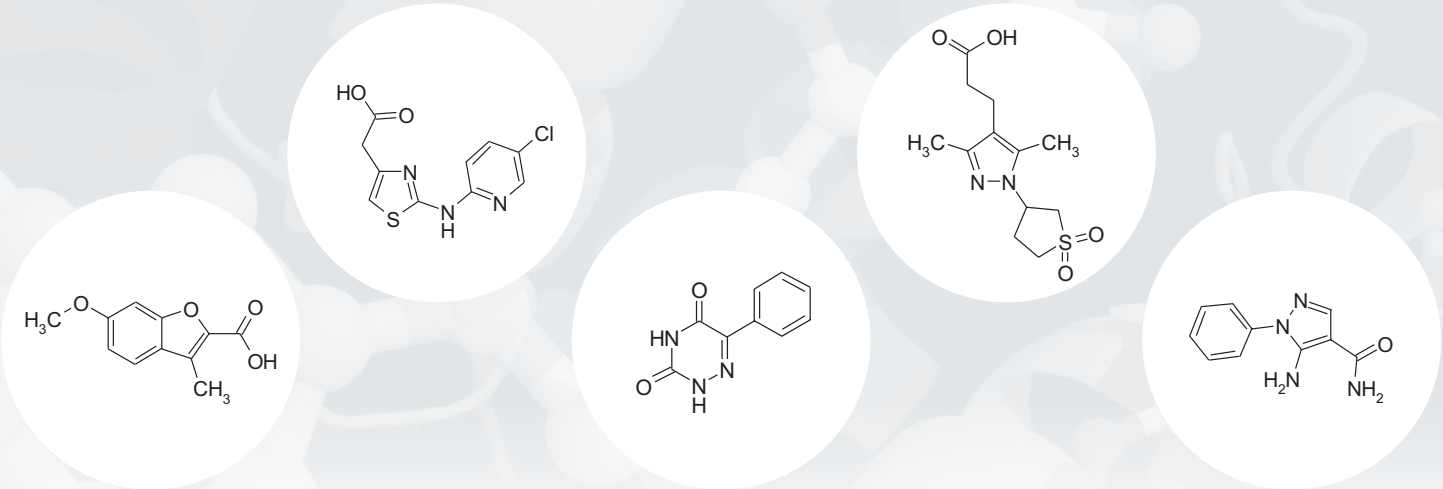
Design:

Flexible docking of Reaxense Ro5 compound collection to each of BET bromodomain target (BRD2, BRD3, BRD4 and BRDT) has been applied. Hydrogen bond (HB) constraints have been assigned to retain only those compounds able to form at least one HB with key amino acid residues and conservative water molecules of the target's binding site. After the docking, the compounds with the highest scores are selected and a visual analysis of the protein-ligand complexes and 2D fingerprints (MOLPRINT2D) Tanimoto similarity filtering is performed. Lastly, the resulting set of compounds from each target has been merged into a single library of 1,592 compounds predicted to bind any of the four proteins with high affinity. Best-scored, non-overlapping compound subsets for either BRD2, BRD3, BRD4 and BRDT are also available in order to probe selective binding.



Structure examples:



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