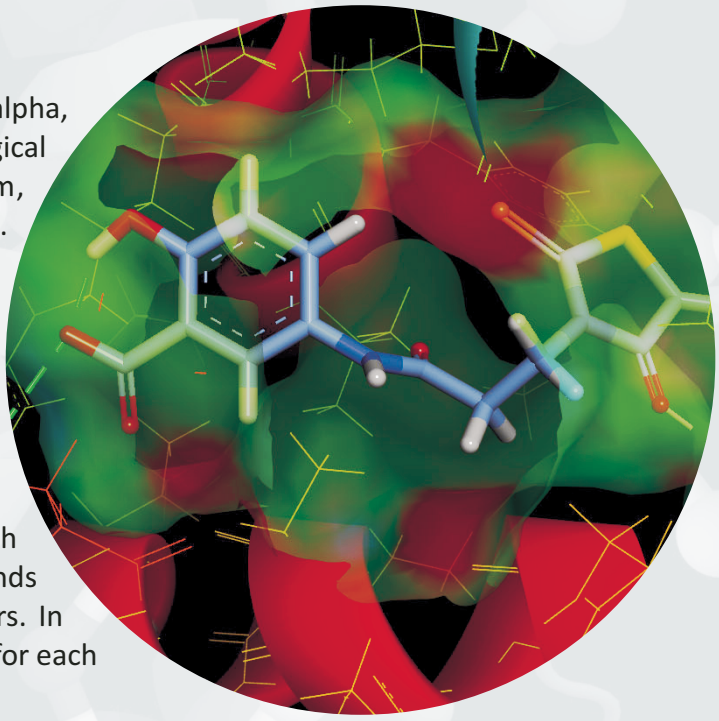
Reaxense

ROR Nuclear Receptors Focused Library



Retinoic acid receptor-related orphan receptors (RORs) alpha, beta, and gamma play critical roles in a variety of physiological processes, which include regulation of metabolism, development and immunity as well as the circadian rhythm. Several reports have presented evidence for a potential role of RORs in pathologies such as osteoporosis, several autoimmune diseases, asthma, cancer, and obesity. This stimulated the development of RORs synthetic ligands and opened up the possibility of chemotherapeutic intervention for these receptors.

Reaxense's RORs Focused Library has been designed with flexible molecular docking and comprises 1,158 compounds predicted to bind RORα, RORβ and RORγ nuclear receptors. In addition, a custom subset of compounds has been selected for each of the three ROR targets.

Features:

- **1,158 compounds focused against RORα, RORβ and RORγ**
- **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**

5000 Yonge Street, Suite 1901
Toronto, Ontario
M2N 7E9
CANADA

Email: rxinfo@reaxense.com
Phone: +1-855-745-5570
Fax: +1-866-608-0550
www.reaxense.com

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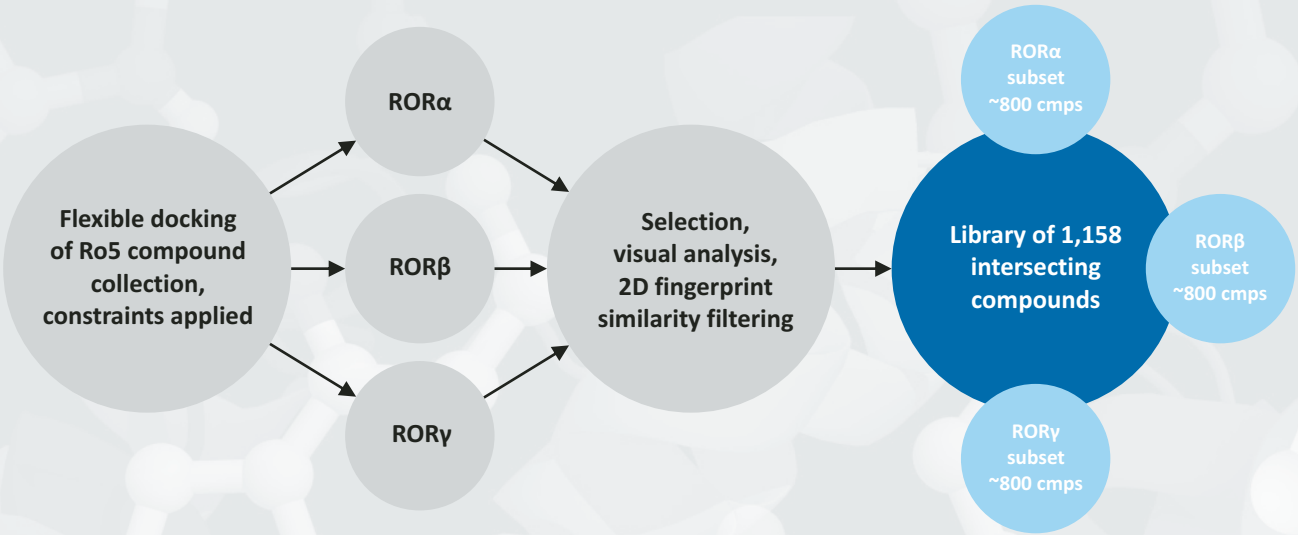
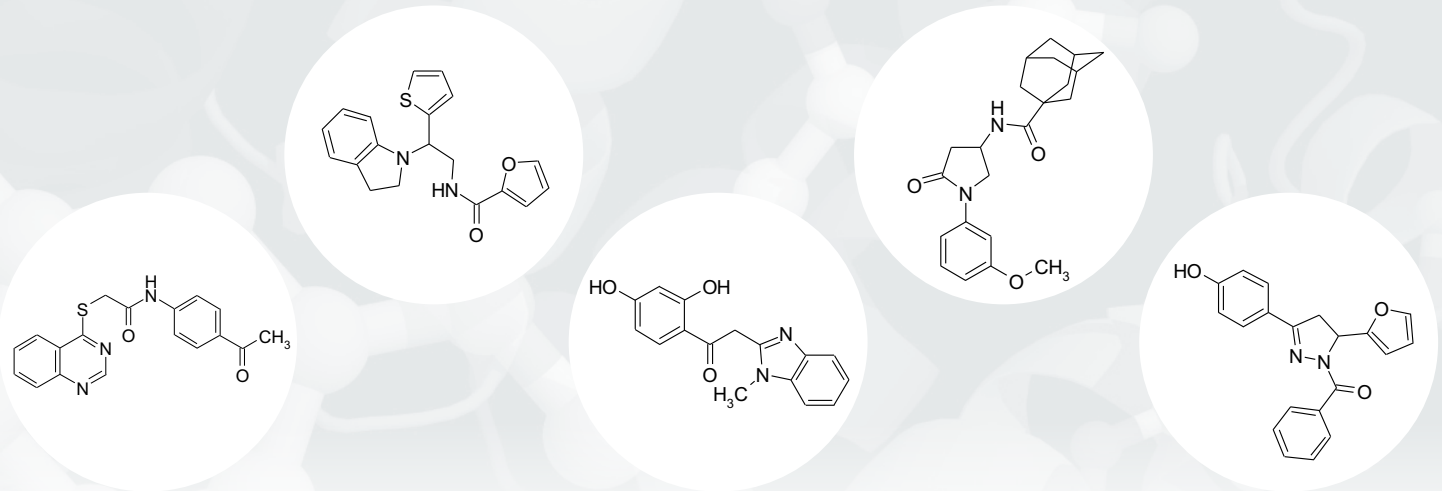
Design:

Flexible docking of the Reaxense Ro5 compound collection to each of ROR nuclear receptor target (RORα, RORβ and RORγ) 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 fingerprint (MOLPRINT2D) Tanimoto similarity filtering is performed. Lastly, the resulting set of compounds from each target has been merged into a single library of 1,158 compounds predicted to bind any of the three proteins with high affinity. Best-scored, non-overlapping compound subsets for either RORα, RORβ or RORγ are also available in order to probe selective binding.



Structure examples:



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