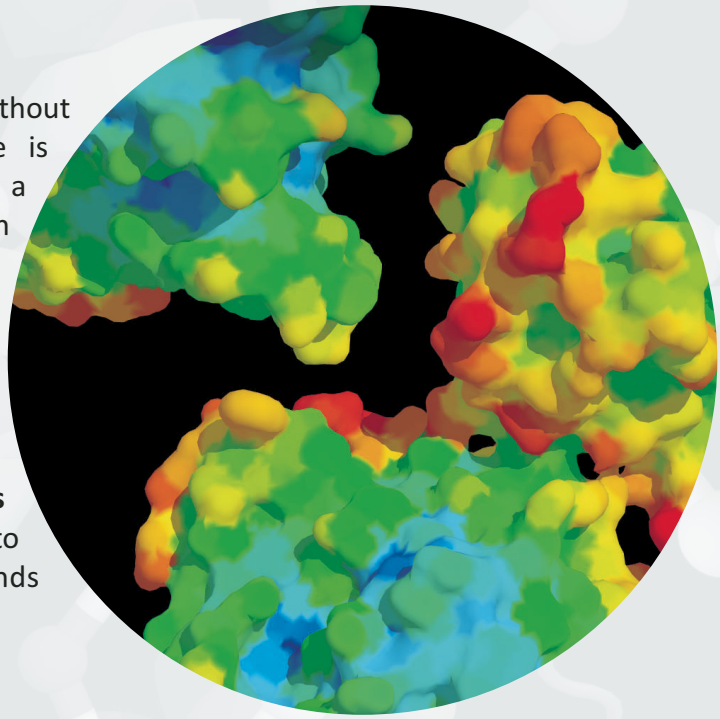
Reaxense

Protein-Protein Interaction Focused Library



Majority of biological processes would not be possible without protein–protein interactions (PPIs). Human interactome is estimated to comprise more than 600,000 PPIs, and only a small part of them has been studied. PPIs are associated with a growing number of diseases and have garnered significant interest in pharmaceutical research offering attractive opportunities for therapeutic intervention. Designing molecules that interfere with the formation of protein complexes is one of the recent challenges in drug design.

Reaxense's PPI Focused Library comprises **1,125 molecules** selected by "Rule-of-Four" compliance and by comparison to TIMBAL database, which is a collection of compounds experimentally confirmed to be PPI inhibitors.

Features:

- **1,125 small PPI inhibitor-like compounds**
- **Full "Rule-of-Four" compliance**
- **Similar to known PPI inhibitors from TIMBAL database**
- **No pan-assay interference (PAINS) compounds**
- **Compounds with reactive and toxic groups filtered out**
- **High diversity over the library**
- **Purity >90%; spectral data available**

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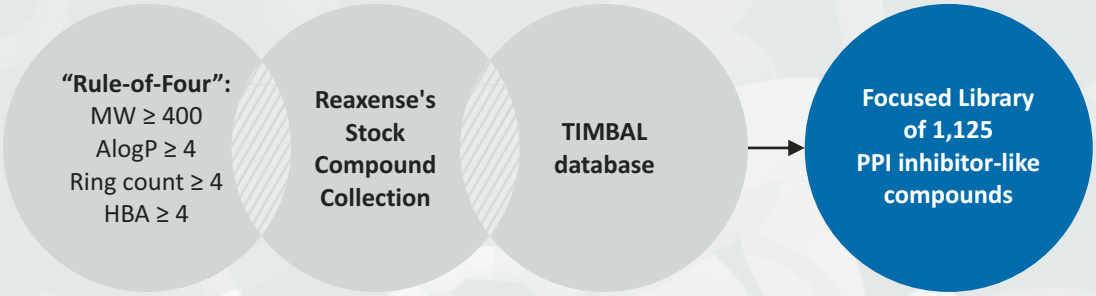
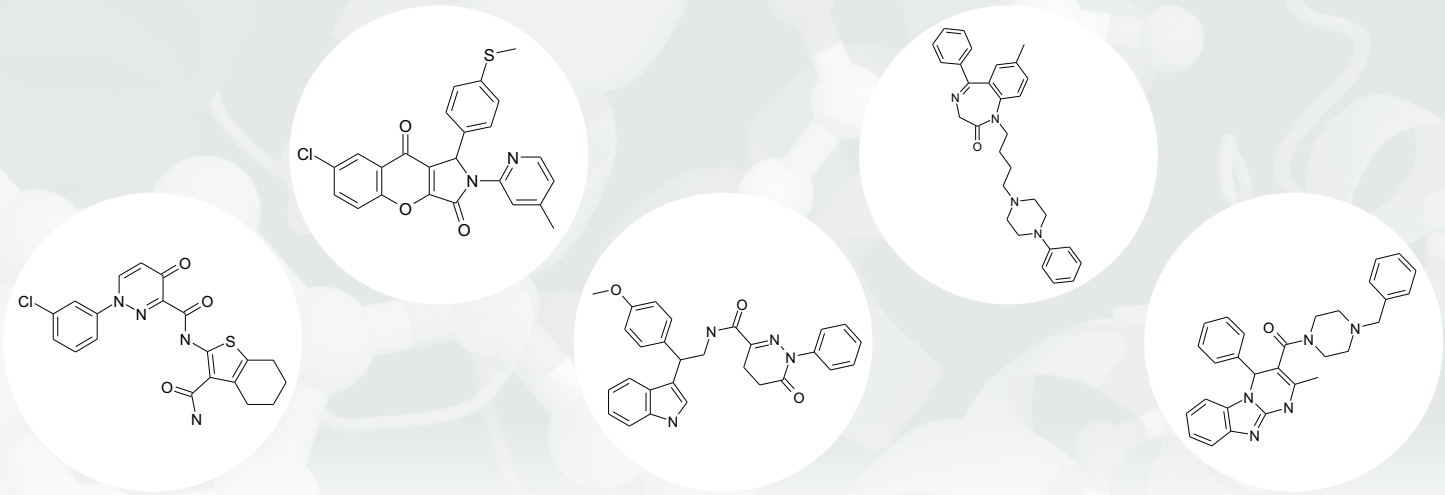
REAXENSE

Design:

Reaxense's Stock Collection of compounds has been filtered by “Rule-of-Four” parameters and screened by similarity (2D fingerprints, $T \geq 0.6$) against TIMBAL database, which is a collection of compounds experimentally confirmed to be PPI inhibitors.



Structure examples:



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