ChemDiv
The chemistry of cures℠

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Beautiful Chemistry

Exploring Protein Hot Spots
With 'Escape From Flatland' Concepts

Small Molecule Tools For Protein-Protein Interactions

Drug discovery's greatest successes have been unevenly distributed as far as targets are concerned. It is an often-quoted statistic, for example, that more than one third of all currently marketed drugs target G-protein coupled receptors.

The reason for this focus is that G-protein coupled receptors – as well as another area of small-molecule drug discovery's big success, enzyme inhibition – naturally interact with small molecules, and tend to do so in deep pockets that also make good binding sites for drugs.

Protein-protein interactions (PPI), by comparison, can look a lot like maps of the world from Christopher Columbus' time: not particularly detailed, but definitely covering an area that's big. And flat.

But most of proteins' interactions in cells are not with small molecules in deep pockets. They are with other proteins. And so, also like in Christopher Columbus' time, it's clear that ***there are riches to be discovered in that flat expanse***, and researchers have been working on ways to target protein-protein interactions with small molecules.

One way to target such flat interactions is to ***catch them when they are not flat***. Many proteins habitually switch between different conformations, some of which can offer binding opportunities in the form of temporary pockets. And small molecules can induce such conformational changes when they bind to protein surfaces.

Another approach has been to focus on so-called**hotspots**. Even though the overall interaction surface between two proteins is often large, more detailed analysis of how binding occurs has sometimes shown that it is possible to ***disrupt overall binding by focusing in on relatively small areas of interaction*** where a disproportional amount of binding energy is concentrated. Computational methods exist to predict such hotspots, and by focusing on them it is possible to bring the target surface down to a manageable size.

read more

Learn about ChemDiv's Protein-Protein Interaction Tools and Libraries

Design Concepts: Escape from FlatLand℠

Targeted Diversity℠

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June 23-26 - BIO International Convention, San Diego.

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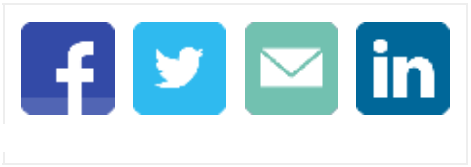

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