

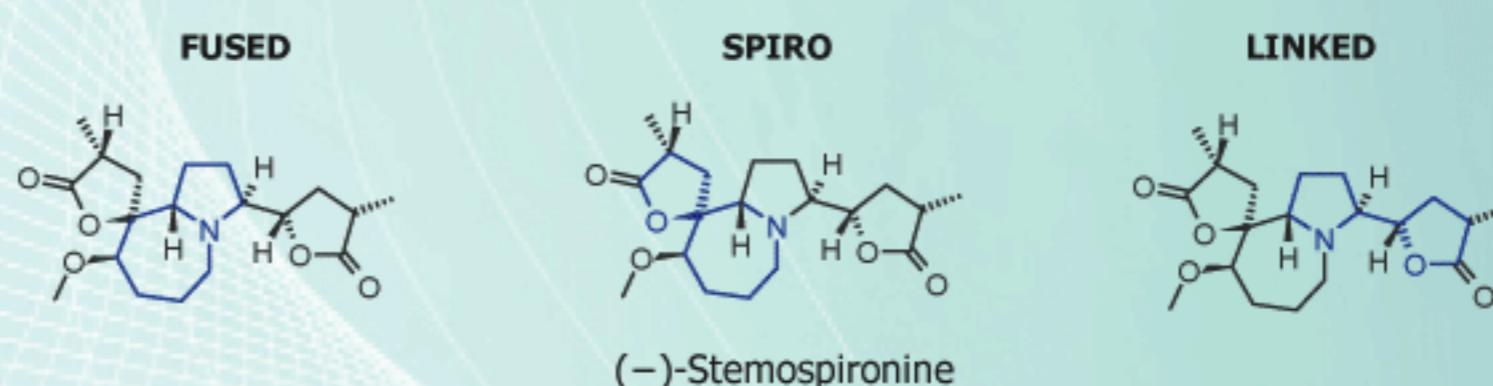
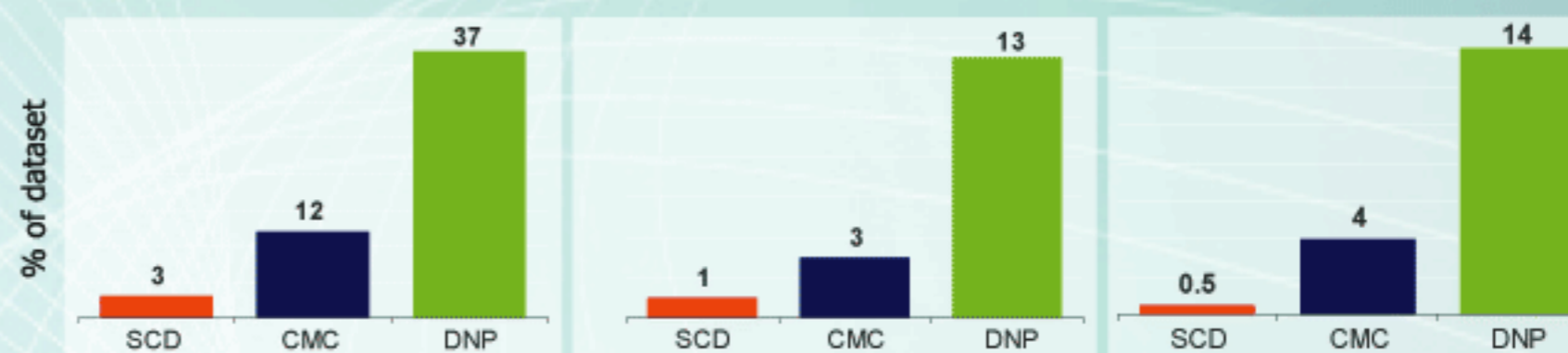
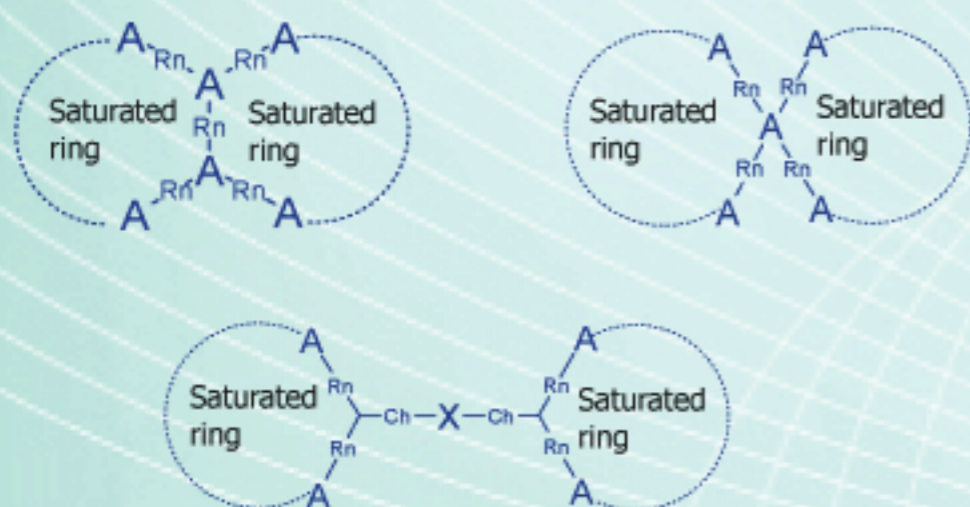
ASINEX MINIMALIST LIBRARY 2011

17000 compounds / 175 scaffolds

High Skeletal Diversity & Pharmacophore Density Inspired by Nature

ASINEX is continuing to develop a compendium of **natural product-like** libraries by incorporating structural features of pharmacologically relevant natural products into the scaffold skeletons of the synthetic compounds. In order to identify privileged pharmacophores, ring systems and linkers, we have carried out a statistical analysis of natural product alkaloids, marketed drugs and commercial libraries. It was found that **saturated linked, fused, spiro** and **bridged** ring systems, with a tendency towards chirality, are highly privileged among natural products and marketed drugs, but at the same time are poorly represented in commercial libraries.

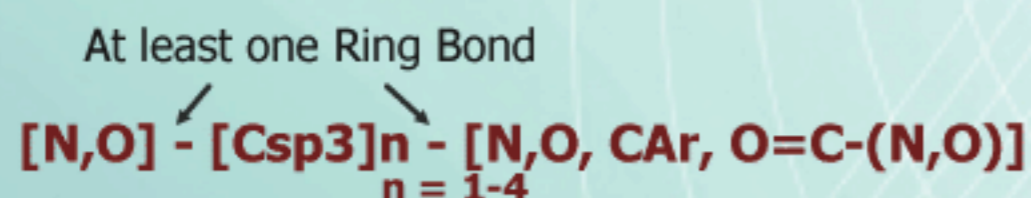
ASINEX Minimalist Scaffolds



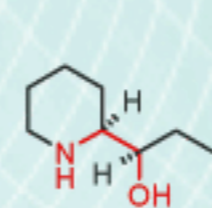
(-)-Stemospironine

We also have identified the most occurring 2D structural elements among natural products which we have called "minimalist fragments".

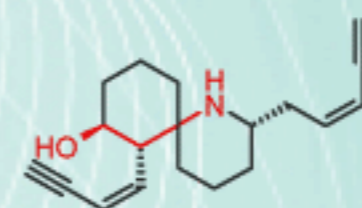
Minimalist Fragments



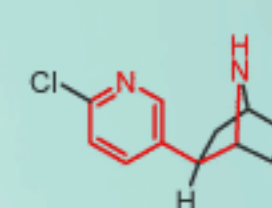
Minimalist Fragments in Natural Products



Conhydrine



Histrionicotoxin 283A

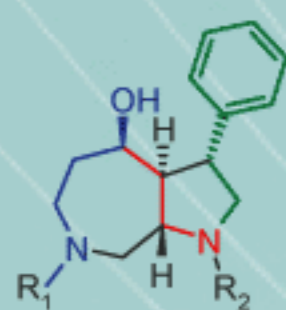


Epibatidine

Incorporation of minimalist fragments into conformationally constrained saturated cyclic systems leads to natural product-like scaffolds with a **high density of multiple pharmacophoric features** and increased protein binding properties [1]. All scaffolds are properly functionalized and the position of heteroatoms and functional groups within the framework emulates the corresponding molecular patterns of pharmacologically relevant marine toxins, carbohydrates and alkaloids. Moreover the Minimalist Library provides a very rich source of original **peptidomimetic scaffolds** and is ideal for probing challenging target classes including:

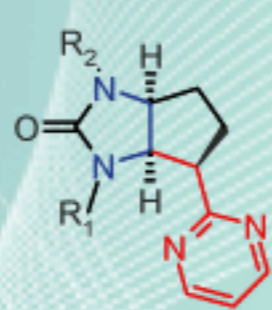
Protein-protein interactions, Proteases, Ion Channels, Antibacterial / Antiviral targets.

ASINEX Minimalist Scaffolds



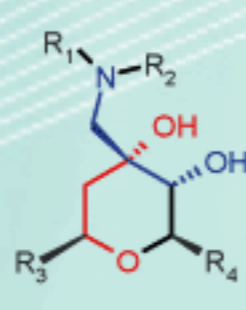
BD 248

58 compounds



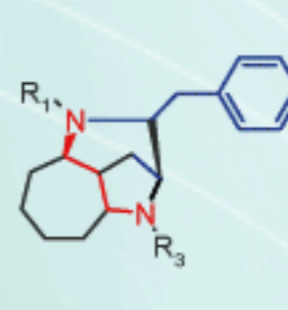
BD 441

64 compounds



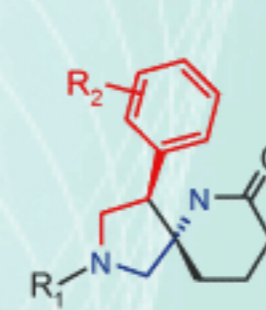
BD 573

88 compounds



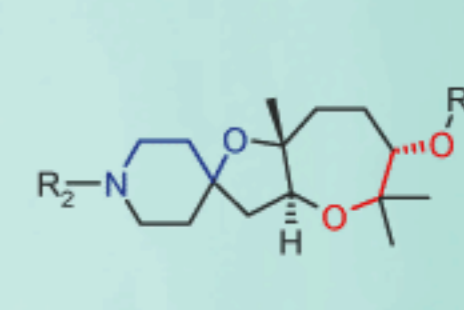
BD 318

1033 compounds



BD 328

317 compounds



BD 373

35 compounds

High density of minimalist fragments per molecule

To achieve this result, we deliberately exploited the advantages of modern **stereo-controlled biomimetic transformations**. All final compounds are without undesirable functionalities and have been optimized in terms of physico-chemical parameters and tested for chemical stability and solubility.

The final compounds possessing MW < 275 Da represent a very valuable source of unique, three-dimensional, **fragment-like** molecules which have been specifically refined and tested for solubility in aqueous media at high concentrations. ASINEX supports further follow-up optimization by providing corresponding synthetic protocols and intermediates.

Library specifics:

Quality: min.purity of 90%, avg. of 95% (LC-MS, NMR), stored as dry powder

ASINEX's MINIMALIST LIBRARY is only available upon request, please contact us at:

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