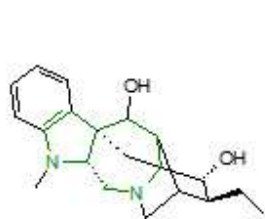
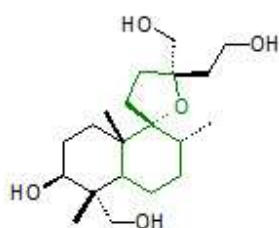
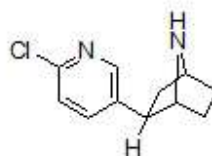


ASINEX's BioDesign approach incorporates key structural features of known pharmacologically relevant natural products (e.g. alkaloids and other secondary metabolites) into synthetically feasible medicinal chemistry scaffolds. In order to identify the privileged pharmacophoric elements, ring systems and linkers, we have carried out statistical analyses of structural features of natural products, marketed drugs, and drug candidates. Our research shows that saturated, fused ring, spiro, and bridged systems with a tendency towards multiple chiral centers are highly privileged among natural products and marketed drugs yet these structures are very poorly represented in commercial libraries. Our medicinal chemists have, in turn, addressed this market need by incorporating these privileged elements into the design of novel synthetic molecules with high molecular framework diversity, multiple stereogenic centers (≥ 2), and degree of saturation ($Fsp3 > 0.5$).

**Ajmaline****Lagochilin****Epibatidine**

[1] Oxygen-containing fragments in natural products. Zoya Titarenko, Natalya Vasilevich, Vladimir Zernov, Michael Kirpichenok, Dmitry Genis; *J. Comput. Aided Mol. Des.*, 2013, Feb;27(2), pp 125-160, DOI: 10.1007/s10822-012-9629-z

[2] Lessons from natural products chemistry can offer novel approaches for synthetic chemistry in drug discovery. Natalya I Vasilevich, Roman V Kombarov, Dmitry V Genis, Michael A Kirpichenok; *J. Med. Chem.*, 2012, 55 (16), pp 7003–7009, DOI: 10.1021/jm300344v

[3] A minimalist fragment approach for the design of natural-product-like synthetic scaffolds. Dmitry Genis, Mikhail Kirpichenok, Roman Kombarov; *Drug Discovery Today*, 2012, Volume 17, 21–22, pp 1170–1174, DOI: 10.1016/j.drudis.2012.05.013.

[4] BioCores: identification of a drug/natural product-based privileged structural motif for small-molecule lead discovery. Kombarov Roman, Altieri Andrea, Genis Dmitry, Kirpichenok Mikhail, Kochubey Valery, Rakitina Natalia, Titarenko Zoya; *Molecular Diversity*, 2010 14(1), pp 193-200; DOI: 10.1007/s11030-009-9157-5.