SL-93. Natural Product-like Gem-dimethyl Moiety

The gem-dimethyl moiety is one of the most commonly occurring structural elements found in many pharmacologically relevant natural products (e.g. taxanes, statins) [1]. This element is also successfully used by medicinal chemists for improving potency and pharmacokinetic properties of drug candidates. Three-dimensional character of this element in combination with adjacent O, N heteroatoms translates into a broad diversity of molecular shapes and can

facilitate the formation of a bioactive conformation upon binding to a target protein.

Enrichment of the screening library with small molecules containing this important pharmacophore can contribute to the discovery of potent hits against multiple targets.

H ₃ C	H ₃ C CH ₃	H ₃ C O H CH ₃
LAS 33789622	LAS 51391705	LAS 54571711
CH ₃ NH CH ₃ CH ₃ CH ₃ CH ₃	F	H ₃ C CH ₃ CH ₃ CH ₃ CH ₃ BDE 31969949

Signature Library 93

Formats	Supplementary Information
80 compounds per plate	SL#93_gem-dimethyl.sdf
0.1 mg; 1 mg; 2 mg dry film/powder	
0.1 μmol; 1 μmol DMSO solutions	

References:

1. J Med Chem. 2018 Mar 22;61(6):2166-2210. doi: 10.1021/acs.jmedchem.7b00315

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