



Some molecular motifs are associated with higher biological activity and are given the "privileged" label when found in molecules that are active at two or more different receptors. Revisiting privileged structures is even more momentous now, when investigators are looking for bi-specific therapeutics and when "rediscovery research" is fueling drug repurposing (1,2).

TimTec new selection of privileged structures includes diverse derivatives of [150 Mesoionic](#), [50 Aminomorpholine](#), and [340 Dihydropyridine](#) compounds available in sets and for cherry-picking.

Mesoionic compounds are "super-charged" having distinct positive and negative areas. These compounds interact well with biomolecules and are able to cross cellular membranes while having lower toxicity and being non-steroidal. Mesoionic compounds are known to have anti-infective, anti-inflammatory, antitumoral activities, and superoxide radical scavenging ability (3).

Aminomorpholines derivatives were previously reported to have anti-inflammatory and antimicrobial activities and neuropharmacological action (4).

Dihydropyridines are quite famous L-type calcium channel blockers with the long list of brand and generic drug names backing up their blood pressure lowering action. From chemistry perspective, these are pyridine-based structures. The therapeutic activity of Dihydropyridines in the treatment of hypertension was established in early 1970-s. These structures are still under exploration for the well-studied and, now, new targets potentially becoming neuroprotective medicines and anticancer agents (5).

Additional collections of privileged structures round up the following fragments derivatives:

[Benzhydryl](#) ;
[Biphenyl](#) ;
[Aza-\(and diaza-\)biphenyl](#) ;
[Anilino-pyridine, pyrimidine, or triaz-ine](#) ;
[Phenylpiperazine](#) .

Discounted price depends on the final number of compounds selected and a required sample

size. Structural info is available in a variety of formats. You can request any other structure- or fragment- based selection for us to assemble custom sets.

References:

1. Jarvis L.M. Two for the Price of One. CEN, Dec 17, 2012.
2. Thayer A. M. Drug Repurposing. CEN, Oct 1, 2012.
3. Senff-Ribeiro A, Echevarria A, et al. Effect of a new 1,3,4-thiadiazolium mesoionic compound (MI-D) on B16-F10 murine melanoma. *Melanoma Res.* 2003 Oct;13(5):465-71. PMID:14512788
Rodrigues R F, da Silva E F. A comparative study of mesoionic compounds in *Leishmania* sp. and toxicity evaluation. *Euro. J of Med Chem.* Vol 42, Issue 7, July 2007, Pages 1039–1043
Senff-Ribeiro A., Echevarria A., et al. Antimelanoma activity of 1,3,4-thiadiazolium mesoionics: a structure-activity relationship study. *Anti-Cancer Drugs.* 15(3):269-275, March 2004.
Deshpande SR, Pai KV, Pai RS. Design and synthesis of certain mesoionic sydnonyl styrylketones as potential nonsteroidal antiinflammatory agents. *Arzneimittelforschung.* 2011;61(3):180-5. doi: 10.1055/s-0031-1296186.
Pires Ado R, Noleto GR, et al. Interaction of 1,3,4-thiadiazolium mesoionic derivatives with mitochondrial membrane and scavenging activity: Involvement of their effects on mitochondrial energy-linked functions. *Chem Biol Interact.* 2011 Jan 15;189(1-2):17-25. doi: 10.1016/j.cbi.2010.09.030.
4. Vigorita MG, Previterra T, et al. N-trifluoroacetyl derivatives as pharmacological agents. V. Evaluation of antiinflammatory and antimicrobial activities of some N-heterocyclic trifluoroacetamides. *Farmaco.* 1990 Feb;45(2):223-35. PMID: 2133997
Mustafa Y., Hüseyin Ü., et al. Spectroscopic study, antimicrobial activity and crystal structures of N-(2-hydroxy-5-nitrobenzalidene)4-aminomorpholine and N-(2-hydroxy-1-naphthylidene)4-aminomorpholine. *J of Mol Str.* Vol 738, Issues 1–3, 14 March 2005, Pages 253–260.
Kalm MJ. 4-Aminomorpholines. *J. Med. Chem.*, 1964, 7 (4), pp 427–433. DOI: 10.1021/jm00334a007
5. Goncharova RI, Dubur GY. Comparative study of the genetic activity of analogs of nucleotide bases and redox coenzymes. I. Absence of mutagenic effect of some derivatives of purine, pyrimidine, and dihydropyridine in experiments with *Drosophila melanogaster*. *Sov Genet.* 1971 Jun;7(6):779-82. PMID:5005877
Ghorab MM, Al-Said MS, Nissan YM. Dapsone in heterocyclic chemistry, part V: synthesis, molecular docking and anticancer activity of some novel sulfonylbiscompounds carrying biologically active dihydropyridine, dihydroisoquinoline, 1,3-dithiolan, 1,3-dithian, acrylamide, pyrazole, pyrazolopyrimidine and benzochromenemotives. *Chem Pharm Bull (Tokyo).* 2012;60(8):1019-28. PMID: 22863706
Fernández-Morales JC, Arranz-Tagarro JA, et al. Stabilizers of neuronal and mitochondrial calcium cycling as a strategy for developing a medicine for Alzheimer's disease. *ACS Chem Neurosci.* 2012 Nov 21;3(11):873-83. doi: 10.1021/cn3001069. PMID:23173068