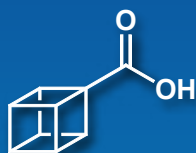
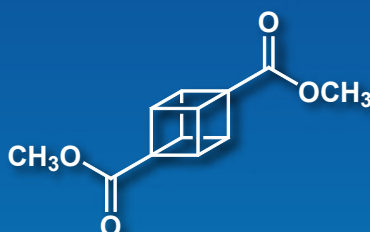


Cubane Building Blocks as Benzene Bioisosteres



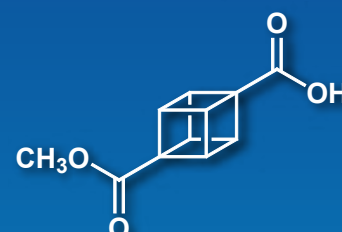
Cubane-1-carboxylic Acid

100mg
[C3808]



Dimethyl Cubane-1,4-dicarboxylate

100mg / 1g / 5g
[D5542]



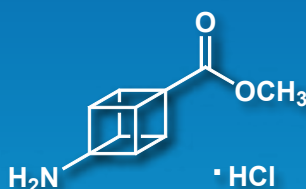
4-(Methoxycarbonyl)cubane-1-carboxylic Acid

100mg
[M3466]



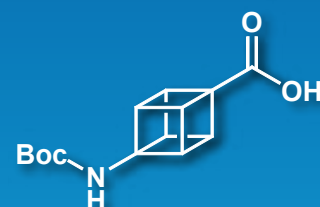
Cubane-1-amine Hydrochloride

50mg
[C3810]



Methyl 4-Amino-1-cubane-carboxylate Hydrochloride

100mg
[M3505]



4-(Boc-amino)-1-cubane-carboxylic Acid

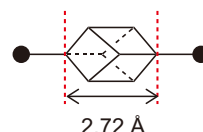
100mg
[B6415]

Cubanes have been proposed as possible bioisosteres of benzene in drug design because the diagonal distance of the skeleton is almost the same as the diameter of benzene.¹⁾ The introduction of a cubane skeleton in place of the benzene ring is expected to improve solubility and pharmacokinetics by changing the planar molecules containing benzene rings to less planar molecules.²⁾ We have a lineup of cubanes with various substituents useful as building blocks for drug discovery research.

1,4-substituted benzene



1,4-disubstituted cubane



bioisosterism

- References** 1) B. A. Chalmers, C. M. Williams, *et al.*, *Angew. Chem. Int. Ed.* **2016**, *55*, 3580. <https://doi.org/10.1002/anie.201510675>
2) T. A. Reekie, M. Kassiou, *et al.*, *J. Med. Chem.* **2019**, *62*, 1078. <https://doi.org/10.1021/acs.jmedchem.8b00888>

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