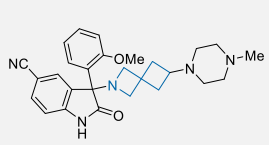
Unique 3D-shaped Spirocycles to Explore Novel Chemical Space

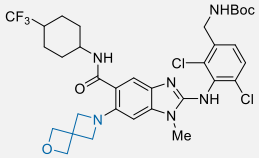
Introduction

Conformational rigidification of flexible compounds by introducing a ring is a popular strategy in drug design. The resulting cyclic analogues usually have a reduced conformational entropy penalty upon binding to a protein target. A conformational restriction can also be imposed by introduction of a spirocyclic ring. Spirocyclic systems are 3D-shaped, in strict contrast to flatten benzene compounds.[1-6] It is especially true for polycyclic compounds. In this context, *Enamine* offers a library of innovative three-cyclic scaffolds for drug design.

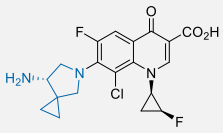
Unique Spirocycles in drug discovery



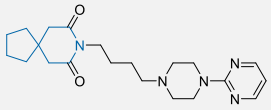
Antivasopressin agent
US2015/344489
AbbVie



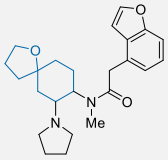
mPGES-1 inhibitor
WO 2012/076673 A1
Boehringer Ingelheim



Sitafloxacin
Fluoroquinolone antibiotic
Daiichi Sankyo Co.

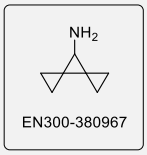


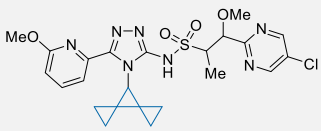
Buspirone
Treatment of anxiety disorders
Mead Johnson



Enadoline
Highly selective k-opioid agonist

Case studies



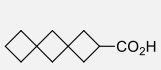


Agonist of the APJ receptor
WO2018/93580, 2018, A1
Amgen Inc.

Unique properties:

- 3D-shaped;
- Fsp^3-rich;
- conformationally restricted;
- functionalization of pharmacophores;
- entry into novel chemical space.

We offer: more than 50 of three-cyclic building blocks from stock on a 5-10 g scale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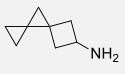
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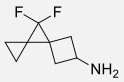
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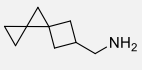
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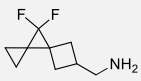
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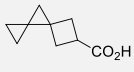
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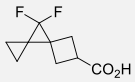
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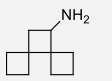
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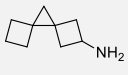
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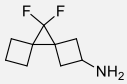
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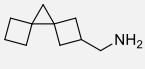
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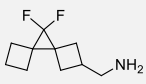
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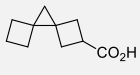
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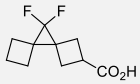
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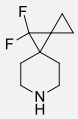
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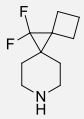
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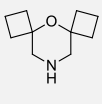
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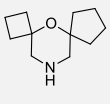
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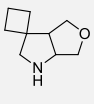
EN300-251624

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EN300-216727

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