キシダオリジナル
ビルディングブロック（K-BB）

- Scaffold別 -

KISHIDA

本製品は試験研究用途でのみご使用いただけます

2023年8月版

キシダオリジナルビルディングブロック（K-BB）

K-BB は、

創薬研究にご活用いただけるビルディングブロックを、
メディシナルケミストの目線からご提供します



キシダオリジナルビルディングブロック（K-BB）の特徴

K-BBのコンセプトは？

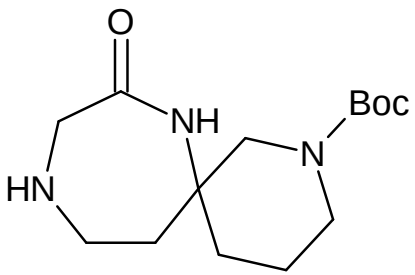
創薬研究に汎用されるScaffoldに加え、**文献・特許情報からトレンドのBB**を
メディシナルケミストの視点でラインナップしています （**2023年7月末：6,363 品**）

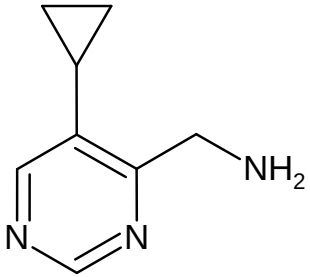
K-BBと他のサプライヤーBBの違いは？

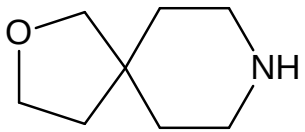
- 創薬の課題（活性・薬効の向上、物性や体内動態の改善など）に**効果が期待できる置換基**を積極的に導入しています.
- BBの主要な置換位置に多種の置換基を導入していますので、「**アナログ群**」として展開性が広く、幅広いSAR取得にご活用いただけます.
- 最適な合成法を精査し、**スケールアップ**にも対応可能です.
- **100mg, 250mg, 1g**の容量をラインナップしています.
- 国内研究者の皆様にタイムリーにお届けできるよう、多くのBBを**在庫化**しています.

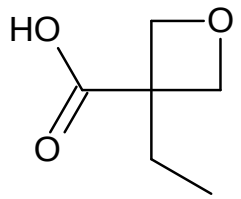
キシダオリジナルビルディングブロック（K-BB）の特徴　～構造・合成の観点から～

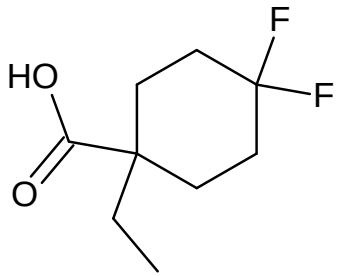
- **マルチファンクション**を有する化合物
- 取り扱いサプライヤー数が限られる化合物
- **スピロ化合物**、**Sp3リッチ**な化合物を多数取り扱い
- 取り扱い困難な**高極性化合物**を取り扱い
- 分子量の小さい化合物（揮発性の高い化合物）
- UV吸収が弱い、または持たない化合物



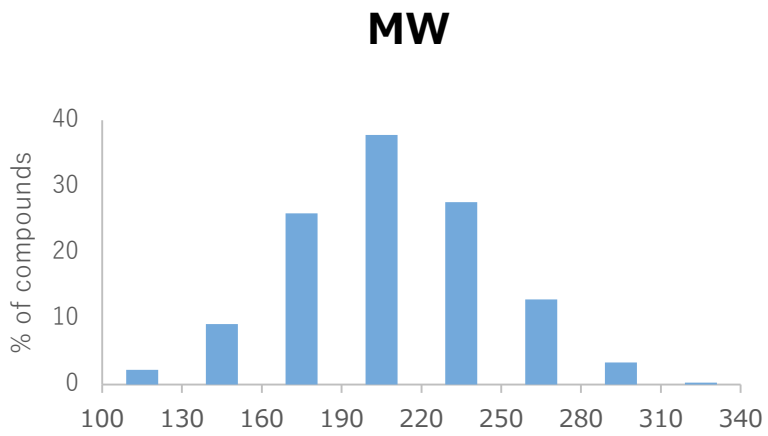


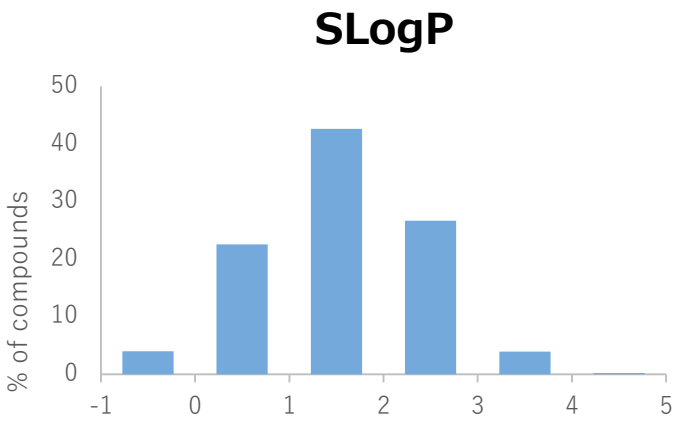


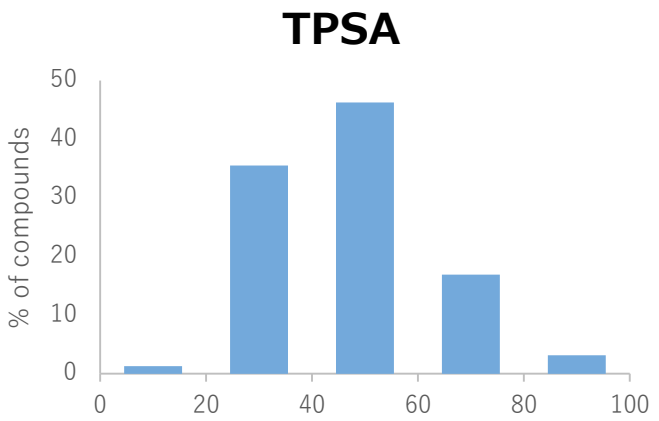


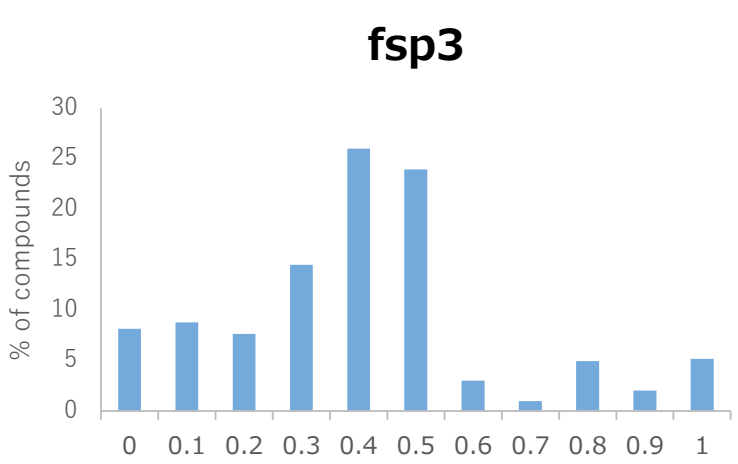


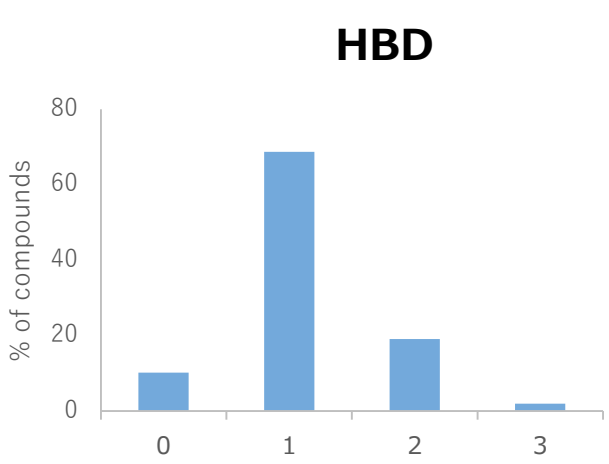
K-BBの計算物性値分布（対象：5093化合物）

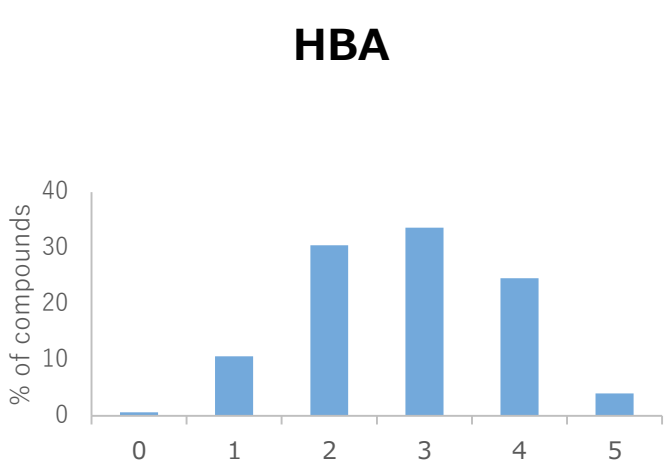






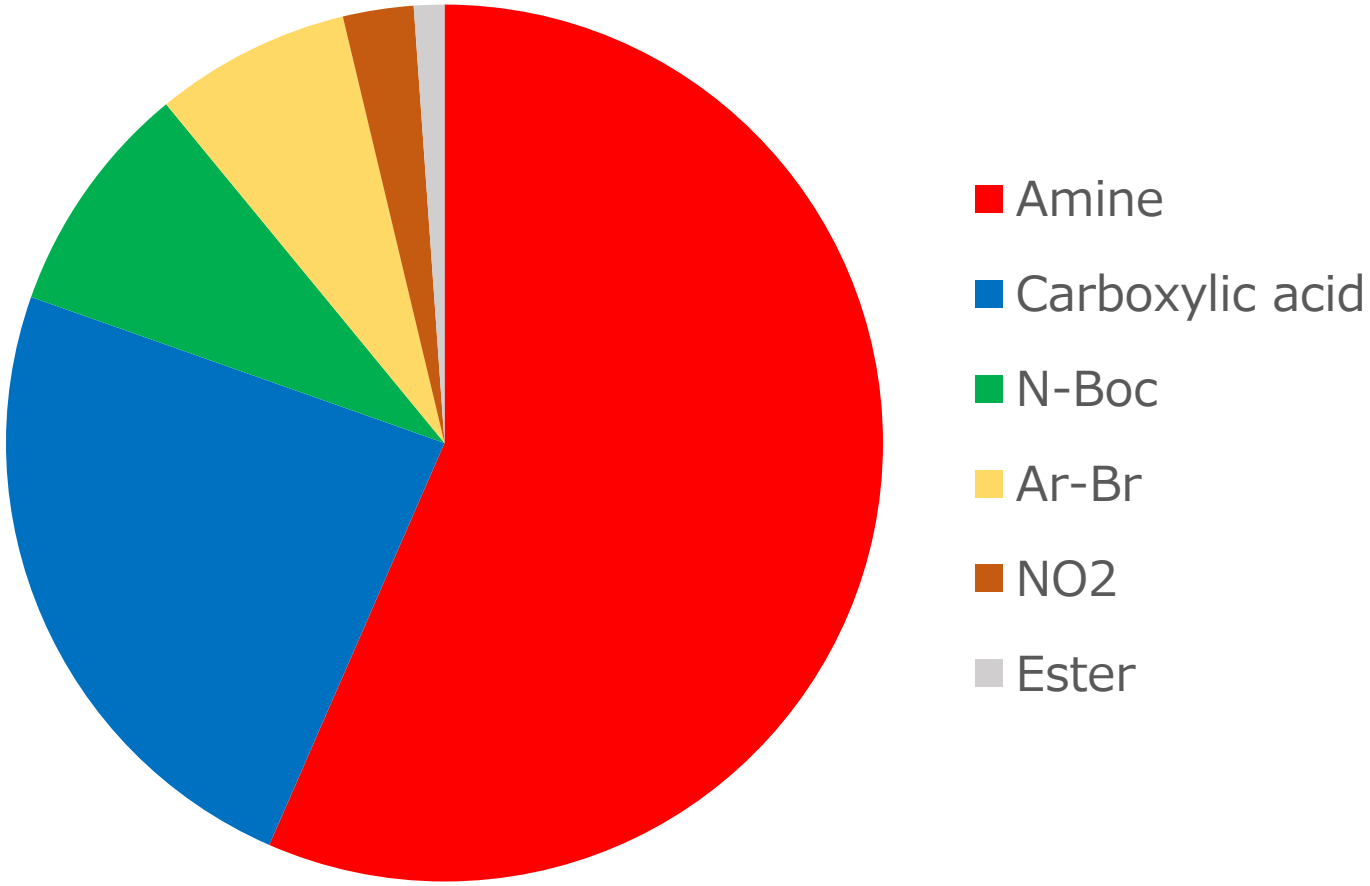






※保護基のあるBBは脱保護した化合物を対象としています.

K-BBの構成（官能基別）



Product lineup

Homo-benzylamine
Imidazole
Benzylamine
Aryl carboxylic acid/ester
Pyrazole
Aniline
3-Hydroxypiperidine
4-Hydroxypiperidine
or 4-Alkoxypiperidine
4-Aminopiperidine
Piperazine
3-Aminopyroridine
3-Hydroxypyroridine
etc.

K-BBの計算物性値分布（Rule of 2：Ro2）

Rule of 2

5,093 compounds

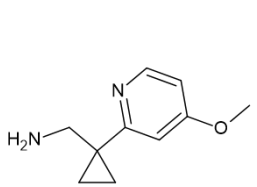
MW <200, clogP <2
HBD ≦2, HBA ≦4

1,905 compounds

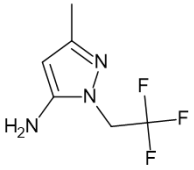
※保護基のあるBBは脱保護した化合物を対象としています.

更に、Fsp3で分類

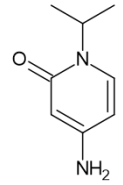
Fsp3 (0.00-0.50) 1,203 compounds



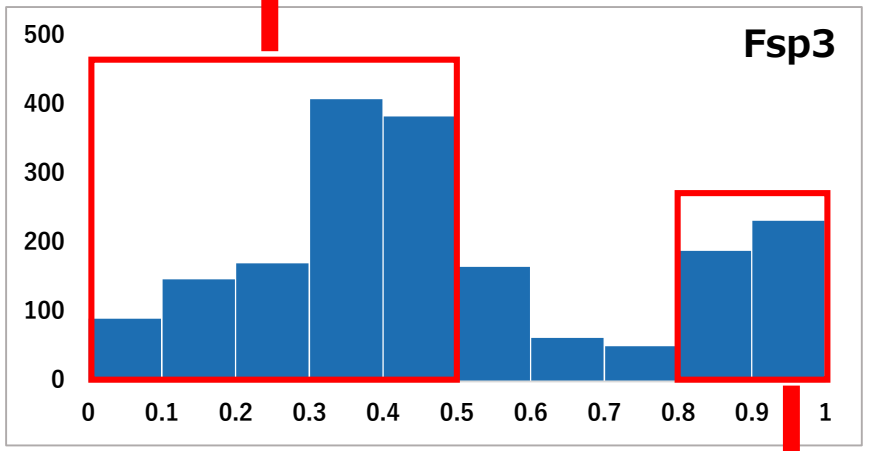
PK0-23021
(0.50)



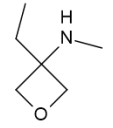
PK0-15181
(0.50)



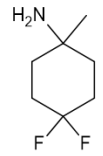
PK0-26751
(0.38)



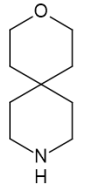
Fsp3 (0.80-1.00) 422 compounds



PK0-14481
(1.00)



PK0-16621
(1.00)



PK0-18011
(1.00)



PK0-27461
(0.86)

K-BBの約4割は「Rule of 2」のクライテリアを満たしています.

Designing novel building blocks is an overlooked strategy to improve compound quality
Drug Discov. Today, 2015, 20(1), 11-17.

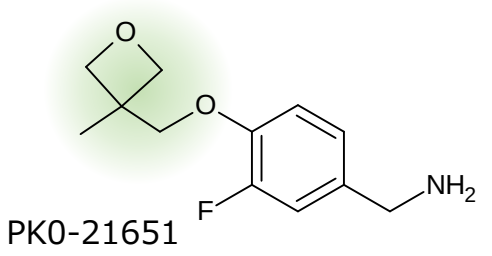
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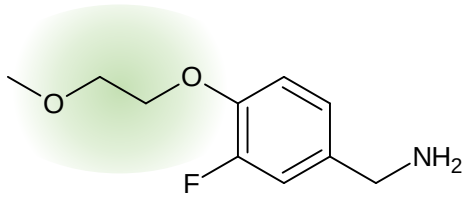
キシダオリジナル
ビルディングブロック（K-BB）

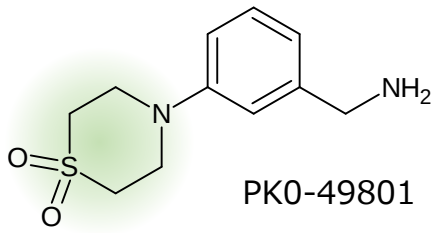
-アミン-

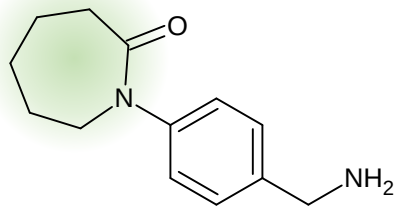
表記の構造式には塩を反映しておりません.

Benzylamine analogs

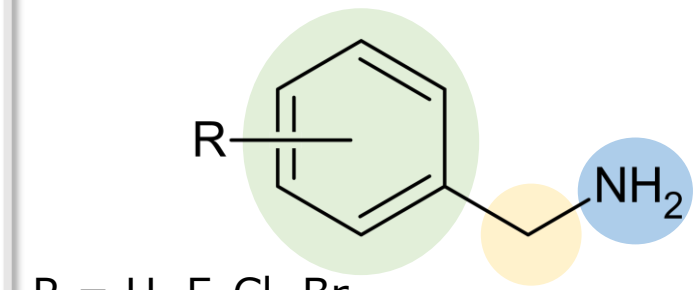

PK0-21651


PK0-20751


PK0-49801


PK0-25581

35 analogs

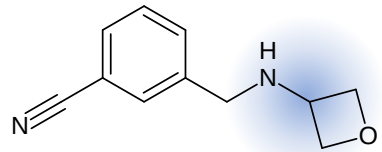


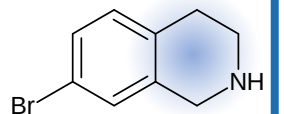
R = H, F, Cl, Br,
OMe, CF_3, etc.

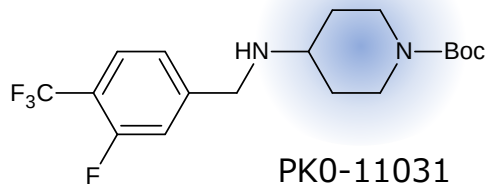
170 analogs

174 analogs

N-alkyl type

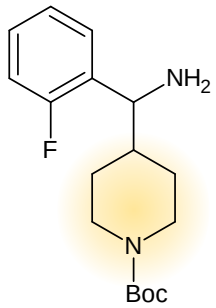

PK0-19631

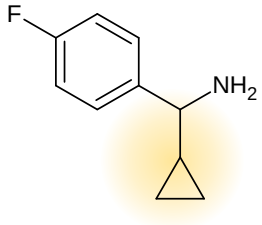

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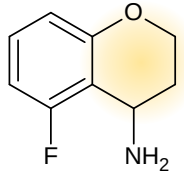

PK0-11031

Mono-alkyl type

57 analogs

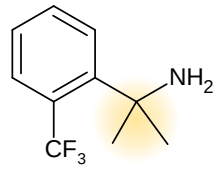

PK0-44741

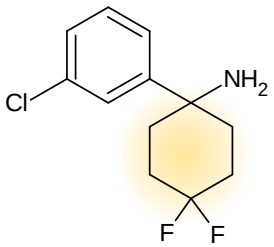

PK0-44451


PK0-52331

Di-alkyl type

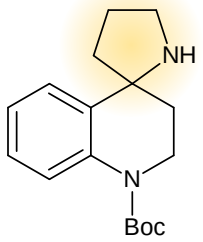
114 analogs

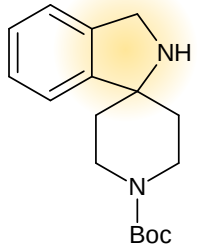

PK0-27021


PK0-44481

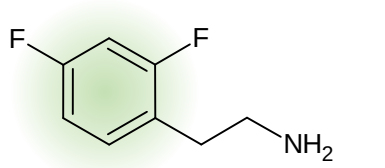
Cyclic type

3 analogs

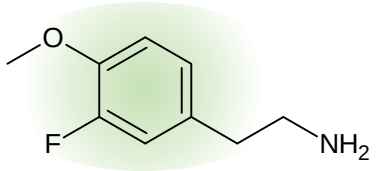

PK0-48941


PK0-48601

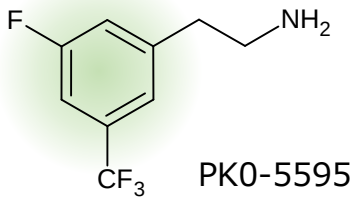
Homo-benzylamine analogs



PK0-55821

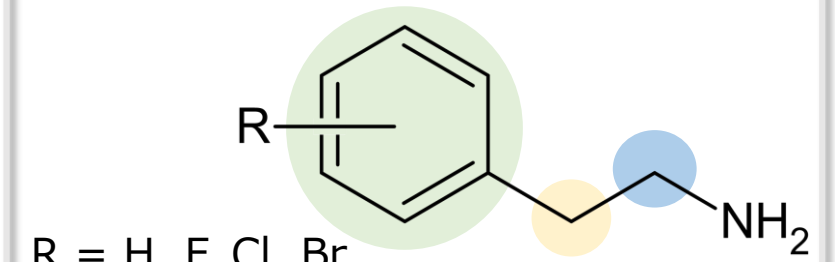


PK0-55871



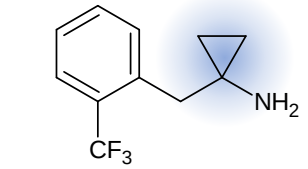
PK0-55951

18 analogs

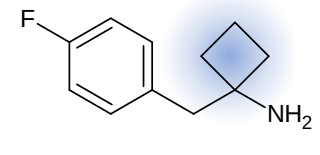


R = H, F, Cl, Br, OMe, CF_3, etc.

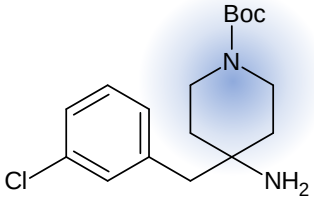
97 analogs



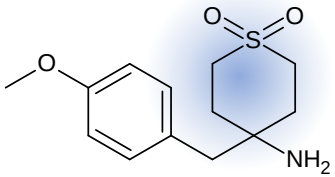
PK0-51221



PK0-23841



PK0-32301

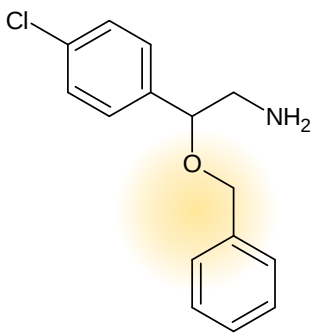


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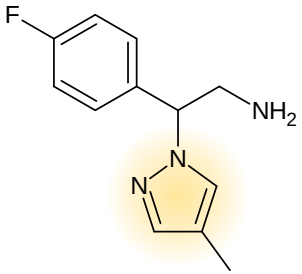
74 analogs

Mono-alkyl type

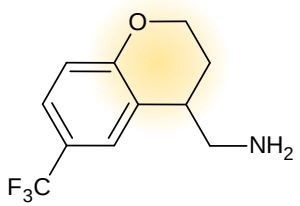
36 analogs



PK0-46121



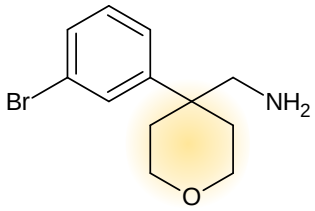
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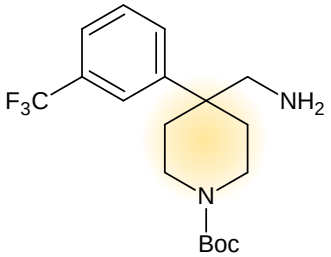
PK0-53901

Di-alkyl type

38 analogs

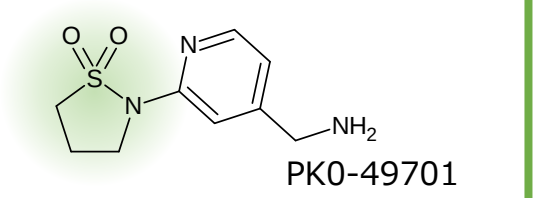


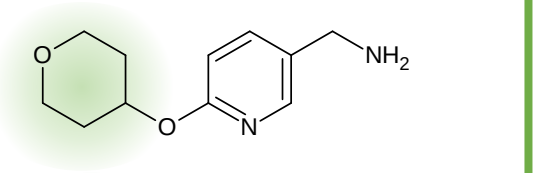
PK0-16141

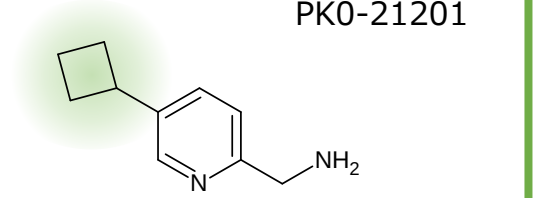


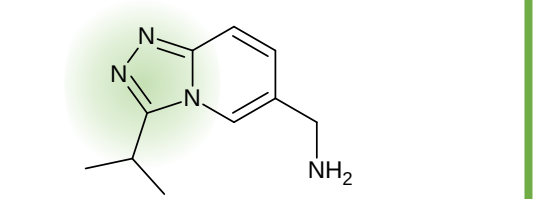
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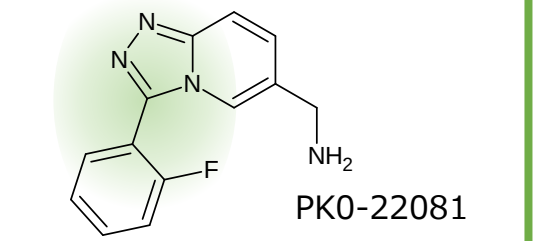
Picolylamine analogs


PK0-49701

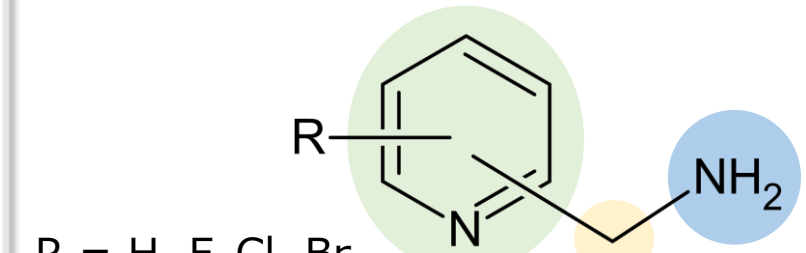

PK0-21201


PK0-53301


PK0-23061

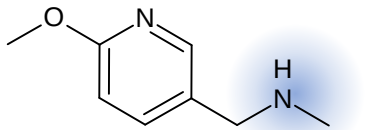

PK0-22081

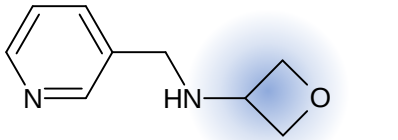
80 analogs

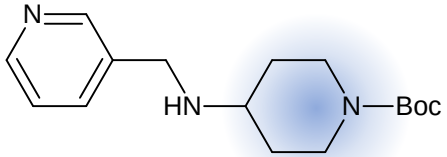


R = H, F, Cl, Br, OMe, CF_3, etc.

55 analogs

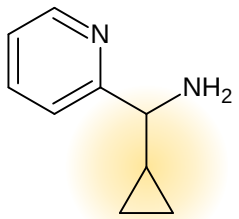

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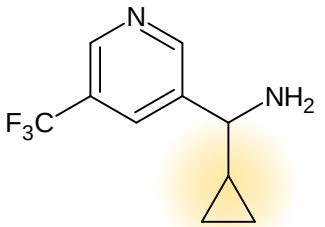

PK0-14801


PK0-10991

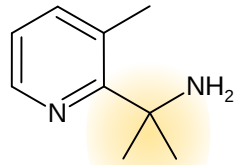
43 analogs

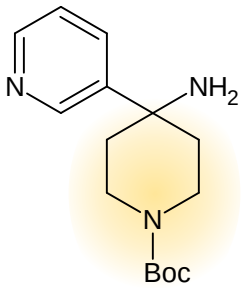
Mono-alkyl type **32** analogs


PK0-44761

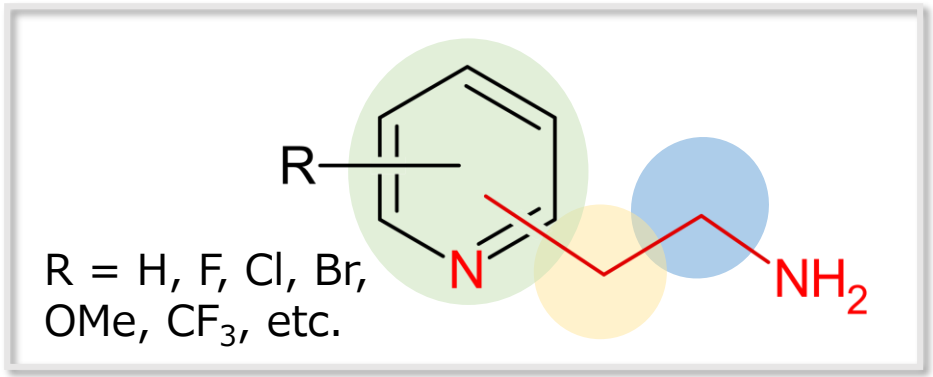

PK0-44831

Di-alkyl type **11** analogs

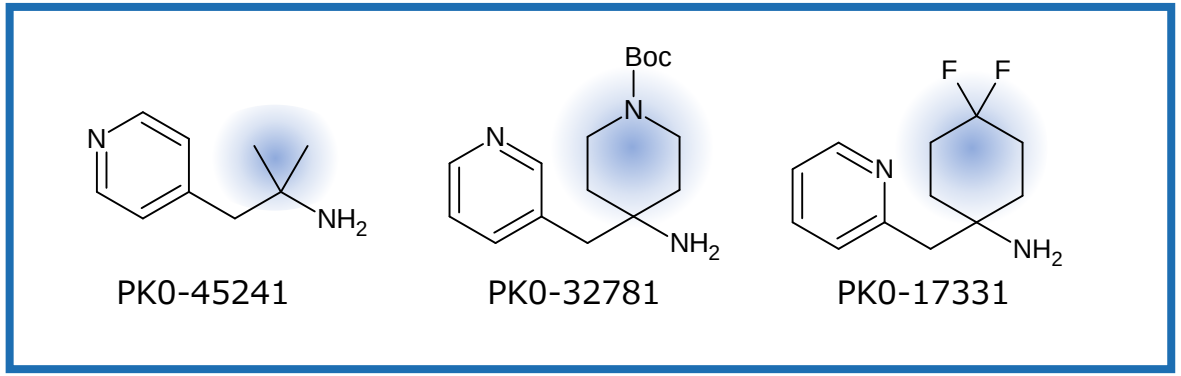

PK0-59041


PK0-34471

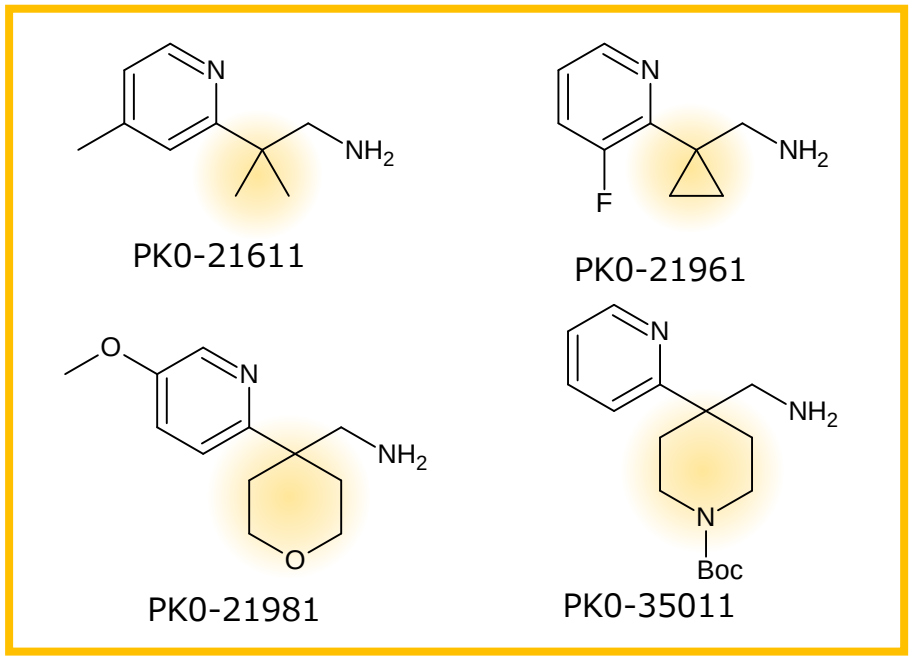
Aminoethylpyridine analogs



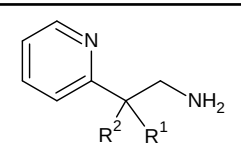
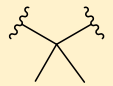
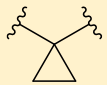
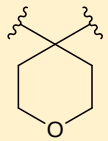
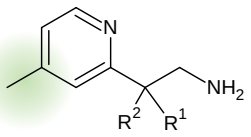
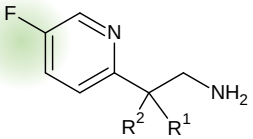
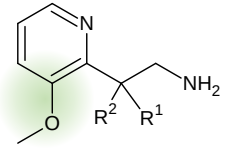
19
analogs



38
analogs

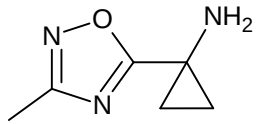


組み合わせにより、幅広いSARを取得できます.

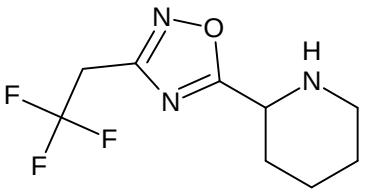
			
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	PK0-21631	PK0-21591	PK0-21601
	PK0-23331	PK0-22501	PK0-38921

Azole-methylamine analogs

Oxadiazoles



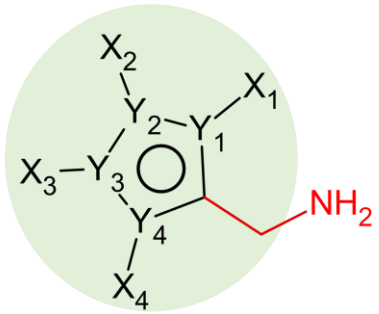
PK0-15321



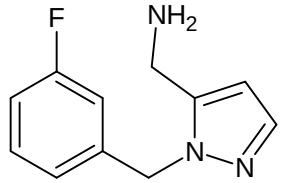
PK0-19971

16
analogs

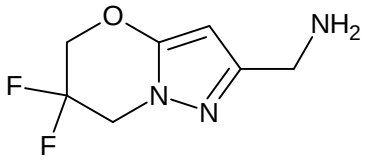
61
analogs



Pyrazoles

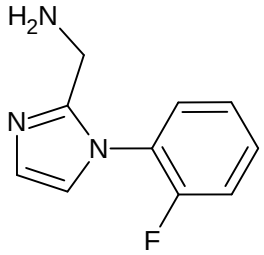


PK0-57831

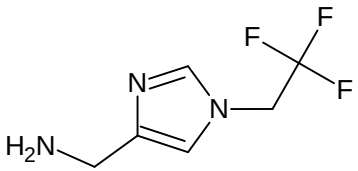


PK0-50441

Imidiazoles



PK0-54531

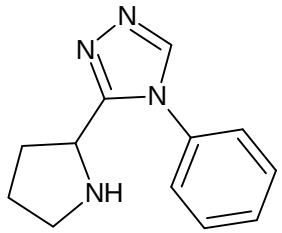


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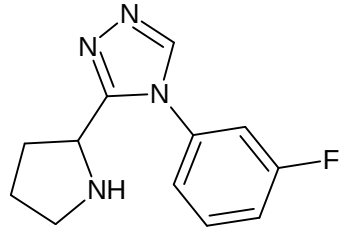
77
analogs

10
analogs

Triazoles

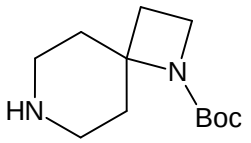


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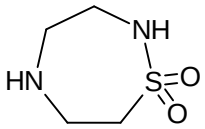


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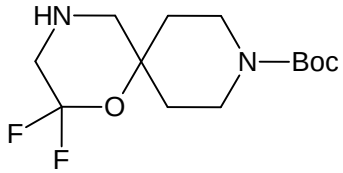
Aliphatic amine analogs



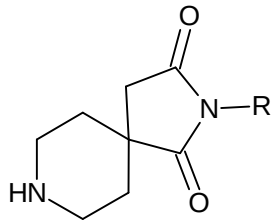
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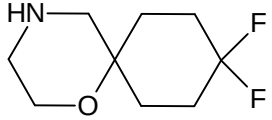
PK0-55131



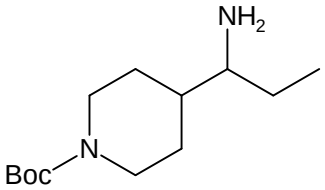
PK0-59081



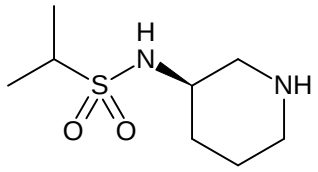
R = Me : PK0-59301
R = Et : PK0-59401



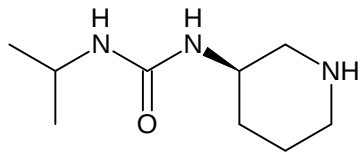
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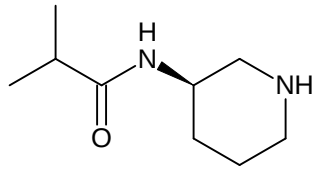
PK0-59521



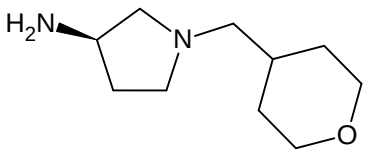
PK0-08771



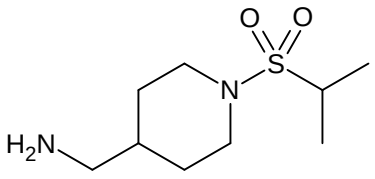
PK0-08961



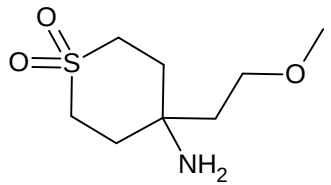
PK0-08101



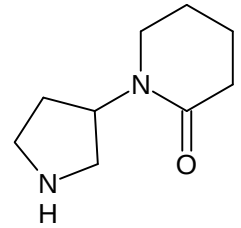
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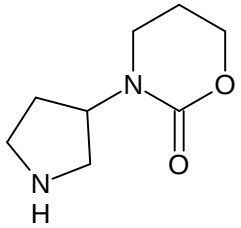
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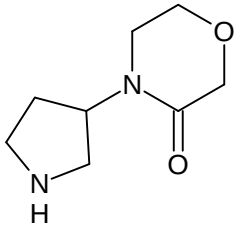
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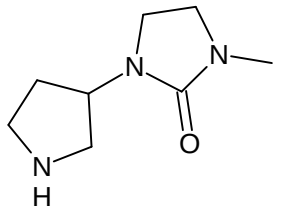
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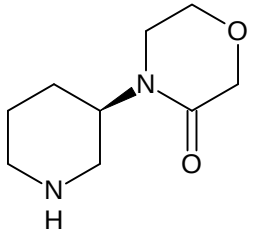
PK0-54131



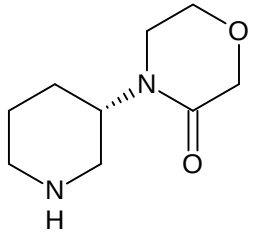
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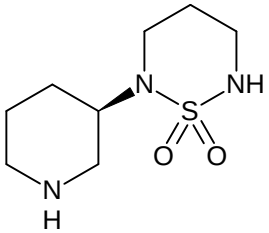
PK0-54151



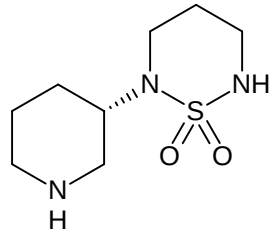
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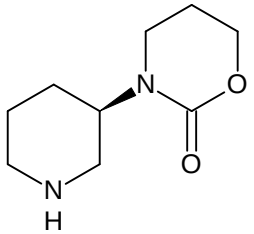
PK0-56581



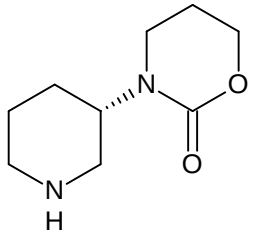
PK0-56831



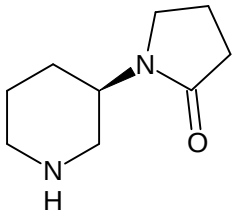
PK0-56851



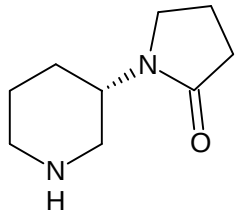
PK0-56811



PK0-56591



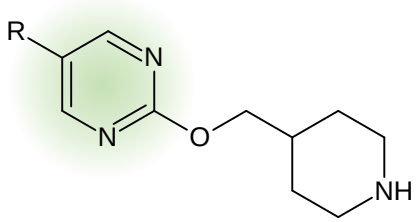
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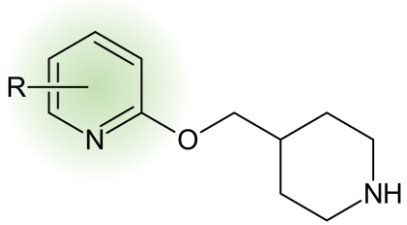
PK0-56611

524
analogs

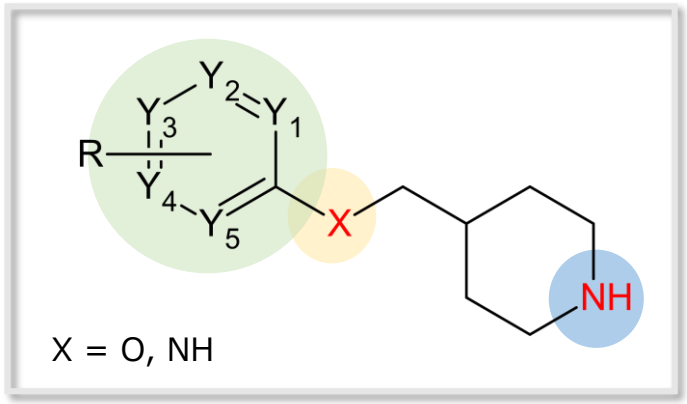
Piperidine analogs



R = H : PK0-55431
R = F : PK0-55621
R = Cl : PK0-55491
R = OMe : PK0-55731



R = 3-F : PK0-55591
R = 3-CF_3 : PK0-55471
R = 6-CF_3 : PK0-55451

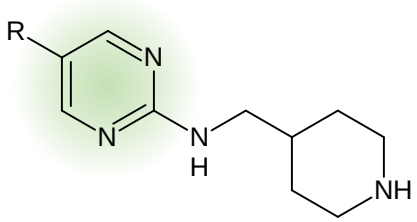


X = O

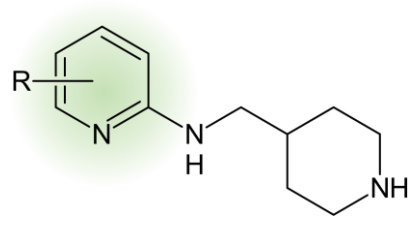
41
analogs
（Ph体含）

X = NH

38
analogs
（Ph体含）



R = H : PK0-55681
R = F : PK0-55581
R = Cl : PK0-55421
R = OMe : PK0-55701

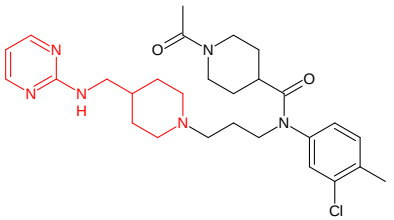


R = H : PK0-55291
R = 3-F : PK0-55531
R = 3-CF_3 : PK0-55401
R = 6-CF_3 : PK0-55381

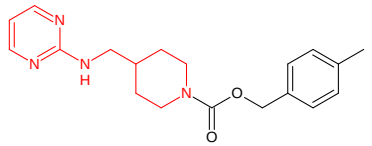
Piperidine analogs ＜参考情報＞

1．高い主活性を示し、細胞毒性との乖離がある、PK0-55681の構造が導入された化合物を報告 (comp.**1**)
Design, synthesis, and biological activity of novel 1,4-disubstituted piperidine/piperazine derivatives as CCR5 antagonist-based HIV-1 entry inhibitors *Bioorg.Med.Chem.Lett.* **2012**, *22*, 3284-3286.

2．高い主活性、hERG活性との選択性を示す、PK0-55681、55291などの構造が導入された化合物を報告 (comp.**2**)
Identification and Characterization of 4-Methylbenzyl 4-[(Pyrimidin-2-ylamino)methyl]piperidine-1-carboxylate, an Orally Bioavailable, Brain Penetrant NR2B Selective *N*-Methyl-D-Aspartate Receptor Antagonist
J.Med.Chem. **2007**, *50*, 807-819.

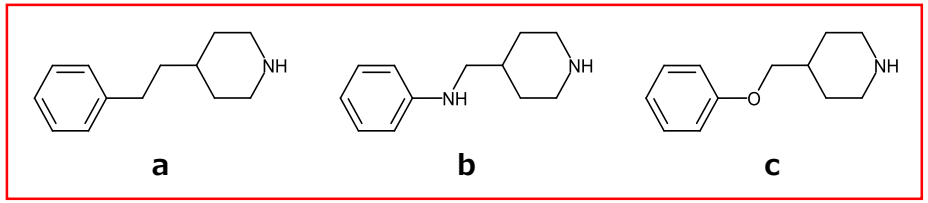


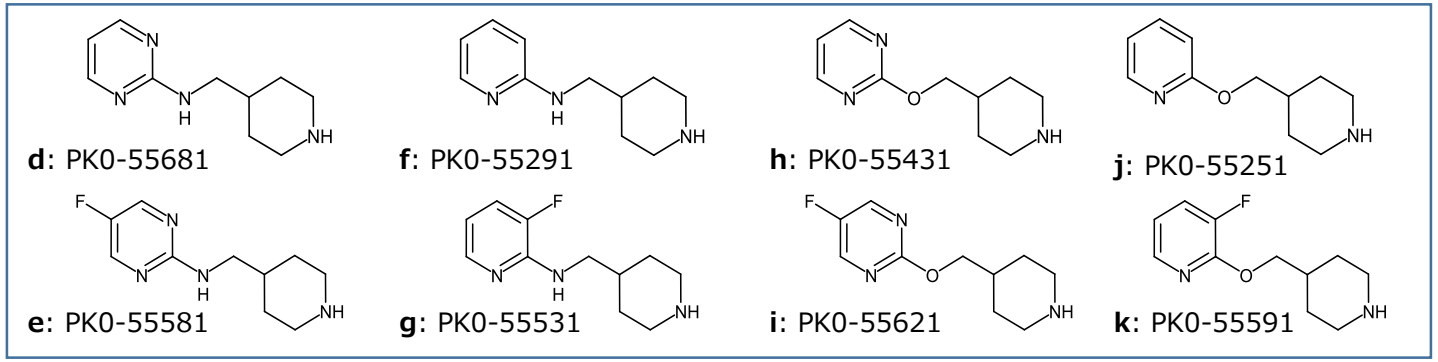
comp.**1**

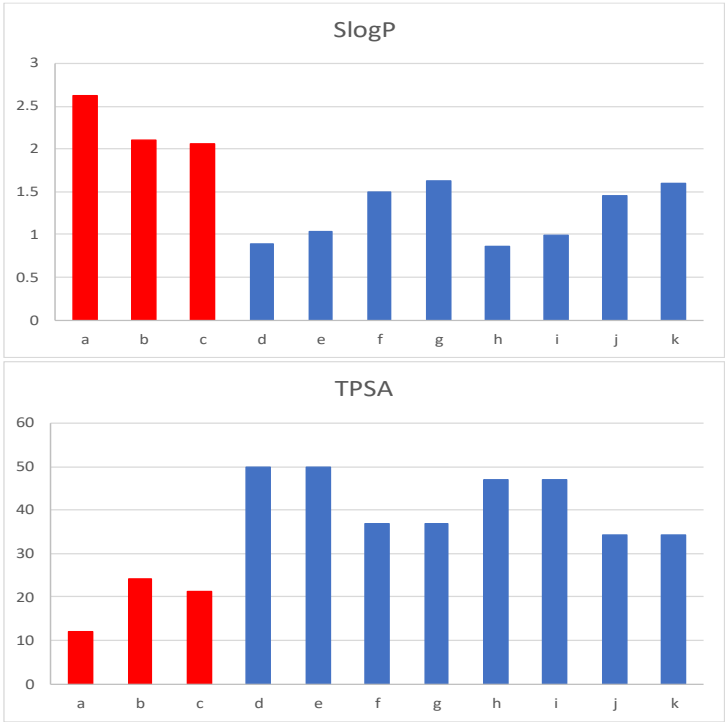


comp.**2**

ヘテロ環の導入した当社のPiperidine analogsの利用により、市販されている化合物a-cに比べ、SlogPの低減とTPSAの向上が期待できます

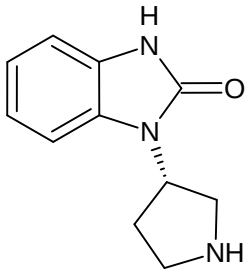




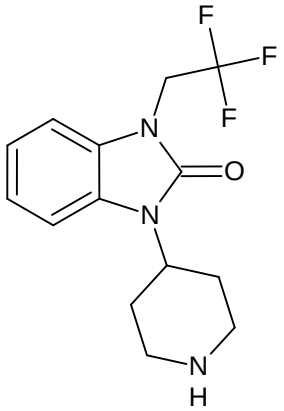


SlogP and TPSA of compd. **a–k**

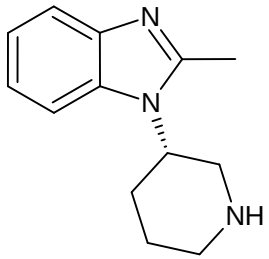
3/4-Aminoepiperidine & 3-Aminopyrrolidine Analogs



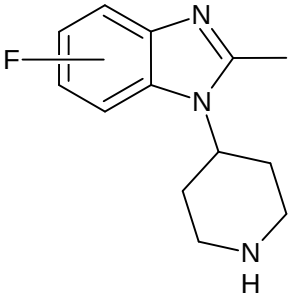
PK0-56661



PK0-55761



PK0-56531

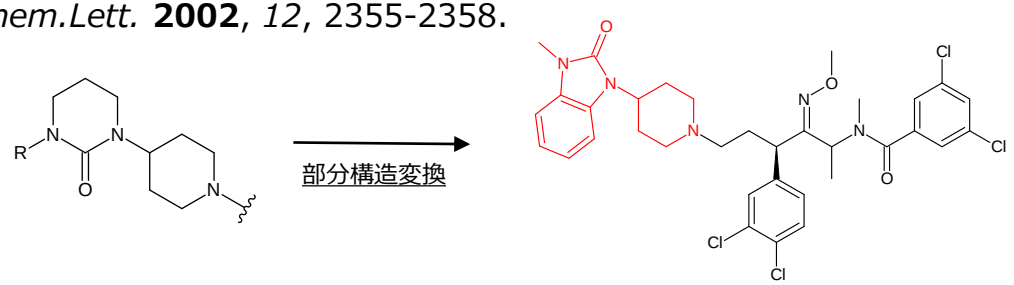


4- ：PK0-57261
5- ：PK0-57251
6- ：PK0-57241
7- ：PK0-57231

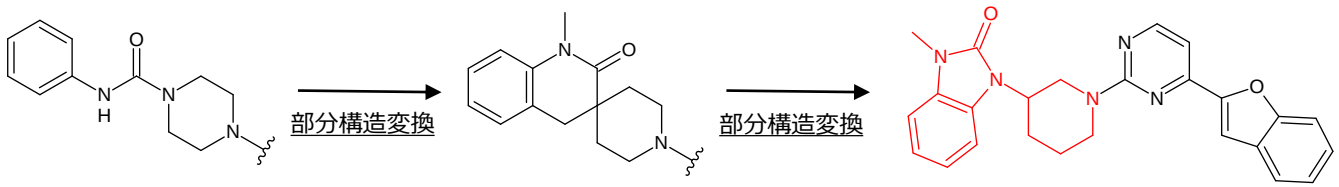
22
analogs

＜参考情報 / K-BB構造が導入されている事例＞

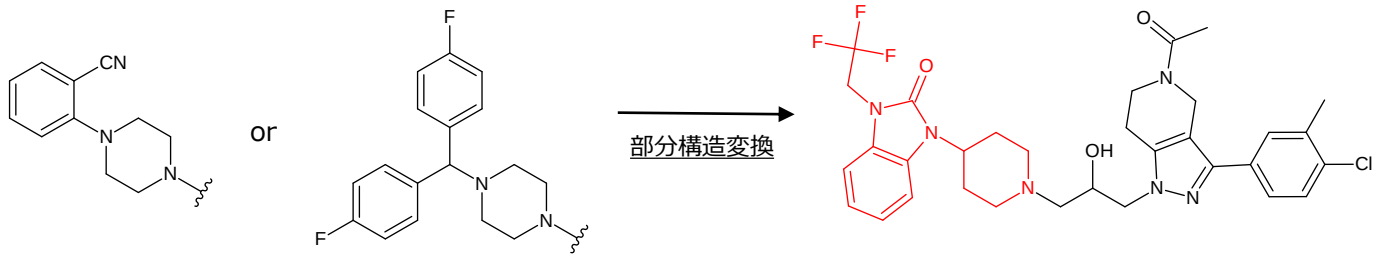
1. 1桁ナノモルのNK1/NK2親和性とNK3に対する選択性を有する化合物群の骨格として導入
Preparation of oxime dual NK1/NK2 antagonists with reduced NK3 affinity
Bioorg.Med.Chem.Lett. **2002**, *12*, 2355-2358.



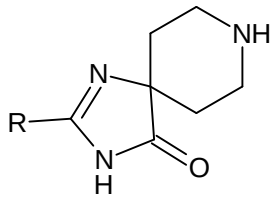
2. PK0-55741、56491などBB構造を含む複数化合物のFAAH阻害活性を報告
Identification of potent, noncovalent fatty acid amide hydrolase (FAAH) inhibitors
Bioorg.Med.Chem.Lett. **2011**, *21*, 2492-2496.



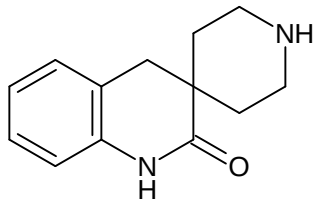
3. 4-arylpiperazine moietyの等価体としてPK0-55761などの導入結果が報告
Discovery and SAR studies of a novel series of noncovalent cathepsin S inhibitors
Bioorg.Med.Chem.Lett. **2005**, *15*, 1687-1691.



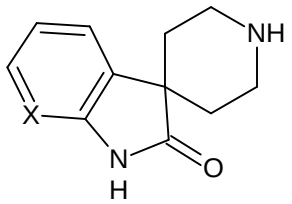
Spiro-piperidine analogs



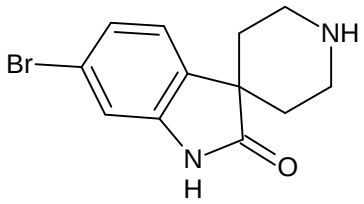
R = Me : PK0-30321
R = Ph : PK0-30261



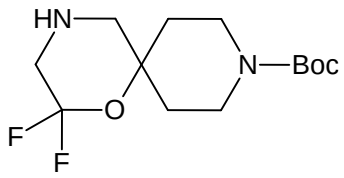
PK0-15451



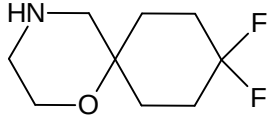
X = CH : PK0-31191
X = N : PK0-51511



PK0-31791



PK0-59081



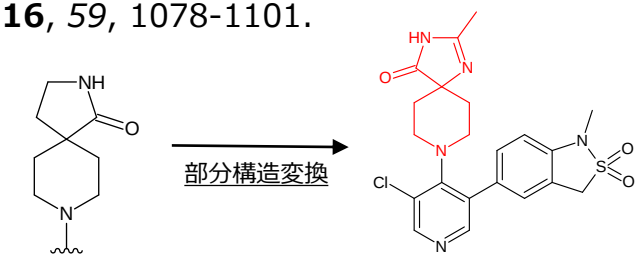
PK0-59481

55
analogs

<参考情報 / K-BB構造が導入されている事例>

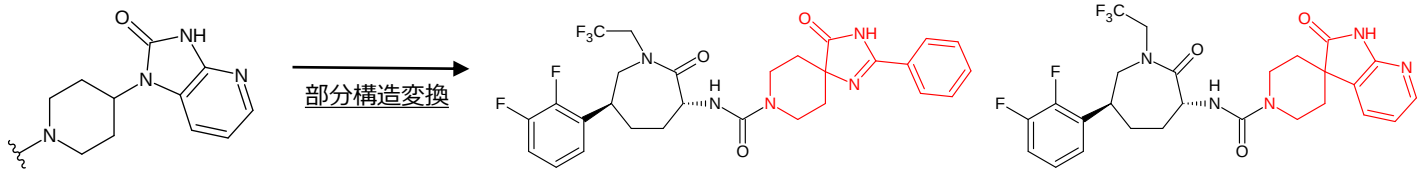
1. 2,8-diazaspiro[4.5]decan-1-one等価体の探索でPK0-30321の導入結果が報告

Discovery of Potent, Selective, and Orally Bioavailable Small-Molecule Modulators of the Mediator Complex-Associated Kinases CDK8 and CDK19
J. Med. Chem. **2016**, *59*, 1078-1101.



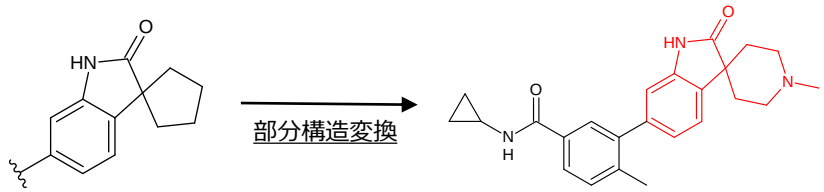
2. Piperidinyl-imidazopyridinone等価体の探索でPK0-30261, 51511などの導入結果が報告

Optimization of azepanone calcitonin gene-related peptide (CGRP) receptor antagonists: Development of novel spiropiperidines
Bioorg.Med.Chem.Lett. **2009**, *19*, 6368-6372.



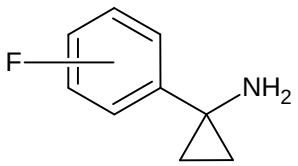
3. Spiroindolone部分の返還でPK0-31791を用いた代替え構造の導入結果が報告

Indolin-2-one p38α inhibitors II: Lead optimisation.
Bioorg.Med.Chem.Lett. **2011**, *21*, 5270-5273.

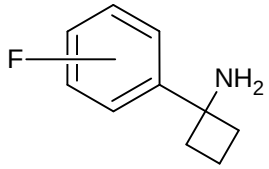


α,α-Disubstituted benzyl/picolylamine analogs

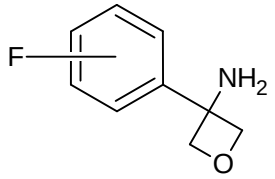
α,α-Disubstituted benzylamine analogs



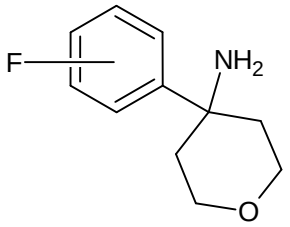
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m- : PK0-09721
p- : PK0-09741



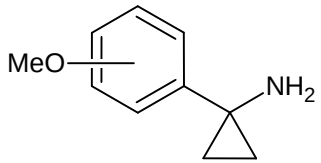
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p- : PK0-09801



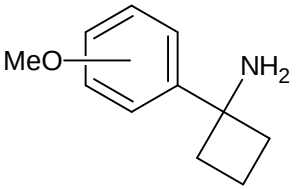
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m- : PK0-11101
p- : PK0-11111



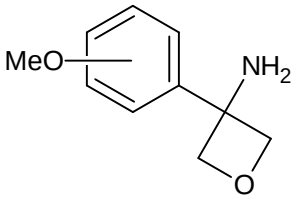
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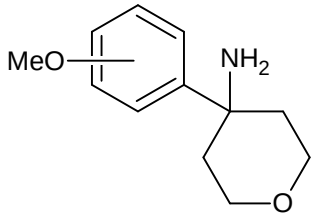
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p- : PK0-10201



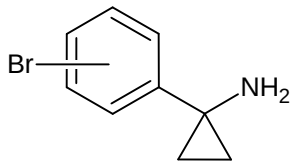
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p- : PK0-10261



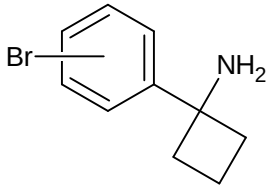
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p- : PK0-11181



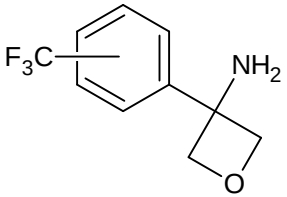
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p- : PK0-16941



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m- : PK0-10001
p- : PK0-10021



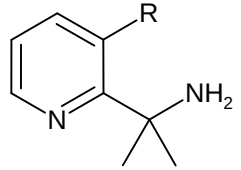
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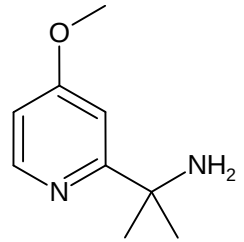
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p- : PK0-12331

109 analogs

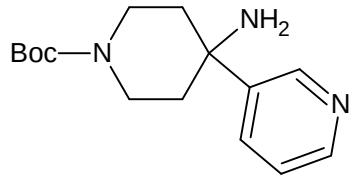
α,α-Disubstituted picolylamine analogs



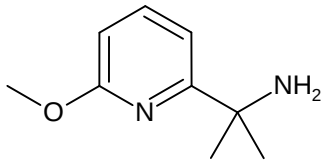
R = F : PK0-58971
R = Me : PK0-59041
R = OMe : PK0-59051



PK0-59181



PK0-34471



PK0-59031

11 analogs

<参考情報 / K-BB構造及び類縁構造が使用されている事例>

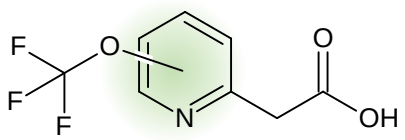
α,α-ジ置換ベンジルアミンによる配座制御により阻害活性が向上
Discovery of isoxazole voltage gated sodium channel blockers for treatment of chronic pain
Bioorg. Med. Chem. Lett. **2009**, *19*, 5334-5338.

キシダオリジナル
ビルディングブロック（K-BB）

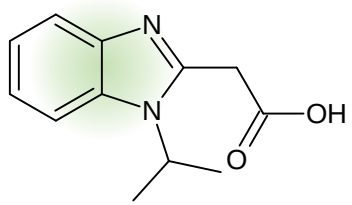
-カルボン酸-

表記の構造式には塩を反映しておりません.

Phenylacetic acid analogs

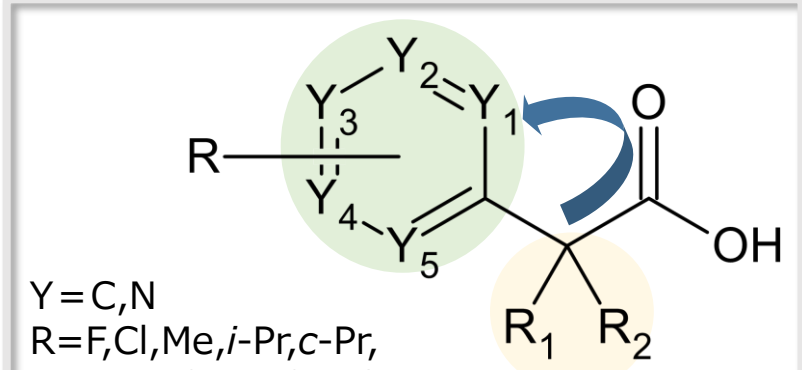


4- : PK0-40741
5- : PK0-40751
6- : PK0-40771

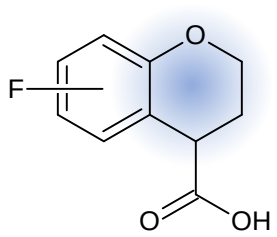


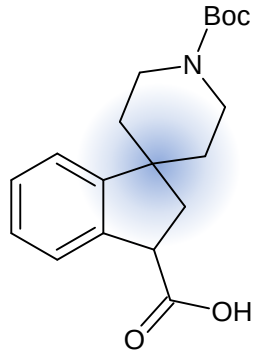
PK0-53931

50
analogs



14
analogs

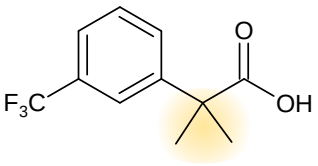




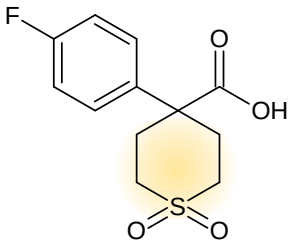
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8- : PK0-52381

PK0-48101

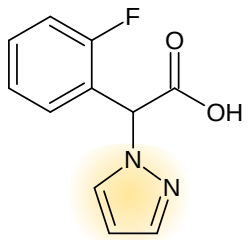
161
analogs



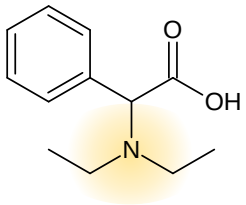
PK0-25631



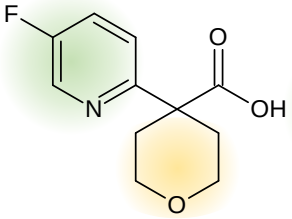
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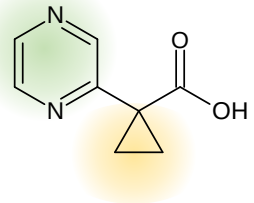
PK0-52691



PK0-51941

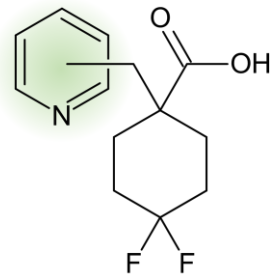


PK0-21701

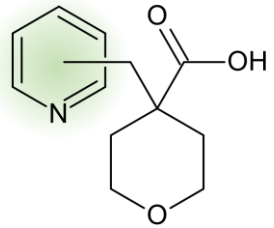


PK0-22151

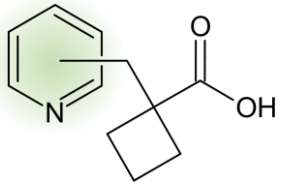
Phenylpropionic acid analogs



2-yl : PK0-17261
3-yl : PK0-17271
4-yl : PK0-17281

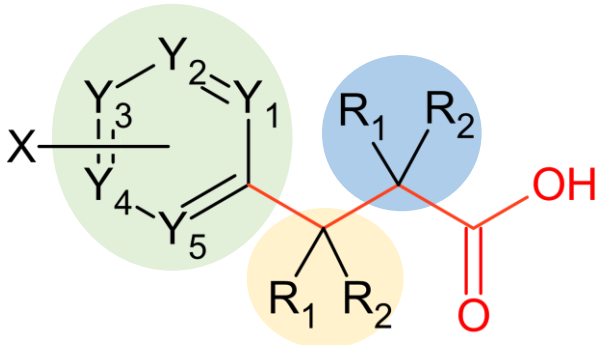


2-yl : PK0-20361
3-yl : PK0-19671
4-yl : PK0-19681



2-yl : PK0-25011
3-yl : PK0-45351
4-yl : PK0-44841

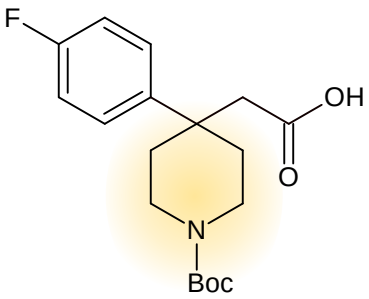
17 analogs



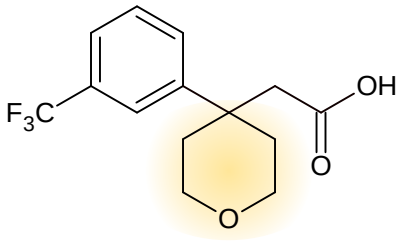
Y=C or N
R=H, F, Cl, Br, Me, OMe, CF_3

93 analogs

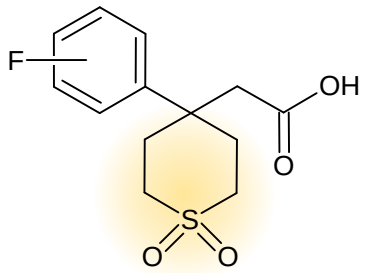
110 analogs



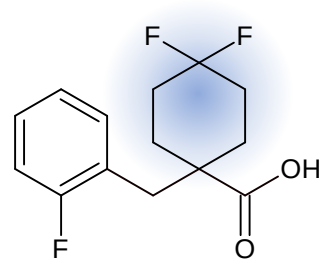
PK0-28321



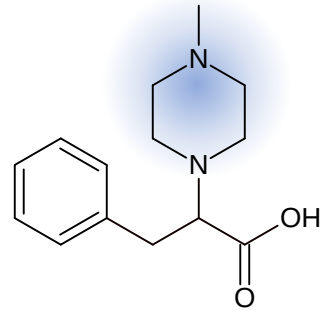
PK0-27591



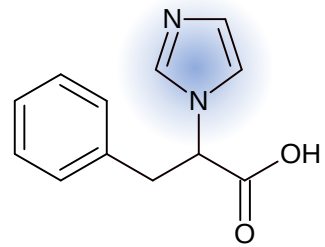
o- : PK0-59251
m- : PK0-59091
p- : PK0-59021



PK0-16591

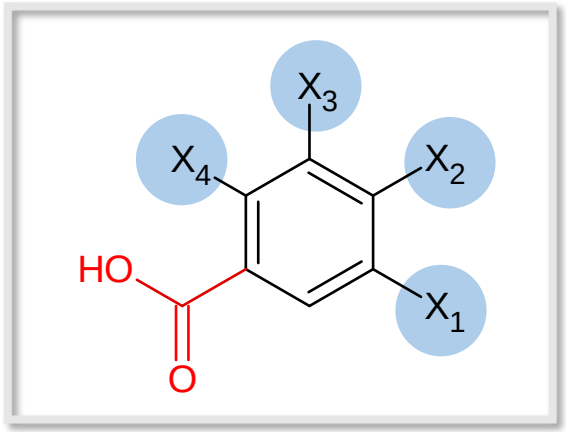


PK0-52211



PK0-57011

Benzoic acid analogs

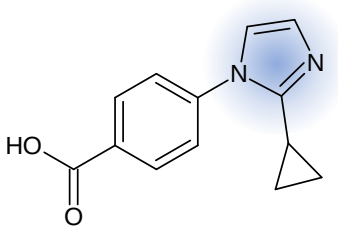


Mono functional

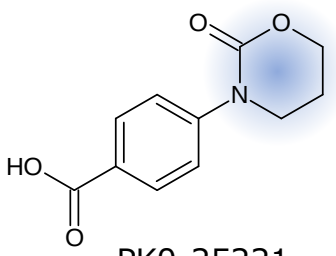
38 analogs

Multi functional

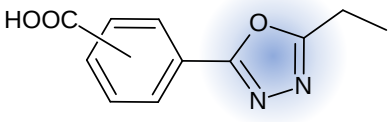
26 analogs



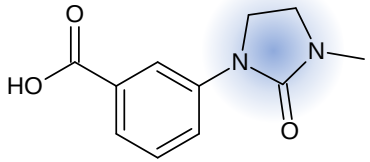
PK0-54651



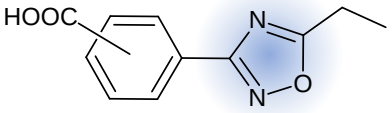
PK0-25221



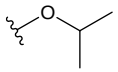
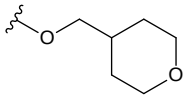
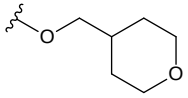
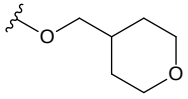
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m- : PK0-57441
p- : PK0-57321



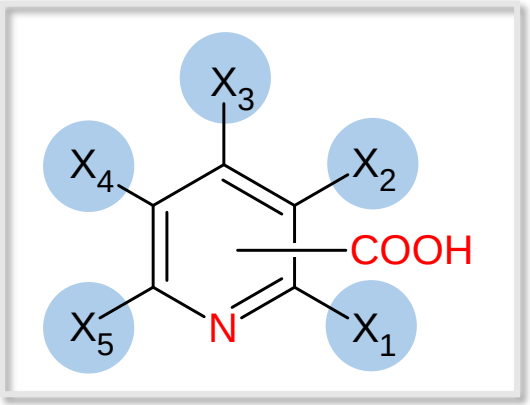
PK0-54631



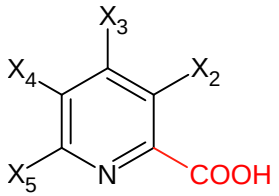
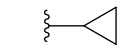
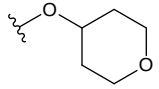
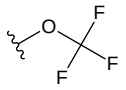
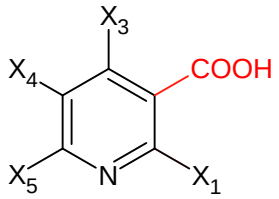
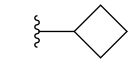
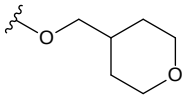
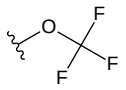
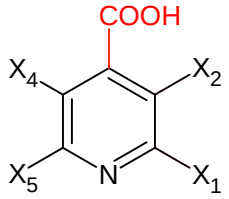
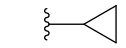
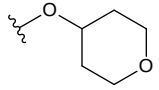
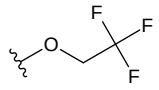
o- : PK0-57311
m- : PK0-57301
p- : PK0-57161

ID	X_1	X_2	X_3	X_4
PK0-17461	**F**		**F**	H
PK0-18161	**F**		**F**	H
PK0-20571	**F**		H	H
PK0-20141	H		H	H

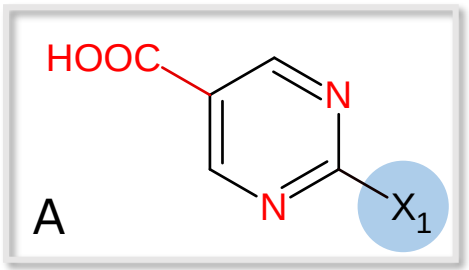
Pyridine-carboxylic acid analogs



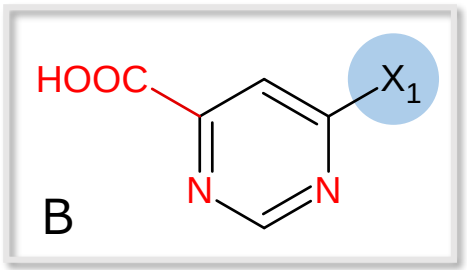
189
analogs

Scaffold	置換基	X1	X2	X3	X4	X5
 **84**～analogs		-	PK0-30991	PK0-30631	PK0-30081	PK0-29681
		-	PK0-21091	PK0-16731	PK0-20241	PK0-20161
		-	PK0-29181	PK0-29171	PK0-28981	PK0-29161
 **62**～analogs		PK0-30111	-	PK0-30641	PK0-49181	PK0-29691
		PK0-20201	-	PK0-22381	PK0-18341	PK0-19511
		PK0-29191	-	PK0-29201	PK0-29001	PK0-28991
 **43**～analogs		PK0-30101	PK0-30091	-	-	-
		PK0-18181	PK0-38431	-	-	-
		PK0-18261	PK0-38811	-	-	-

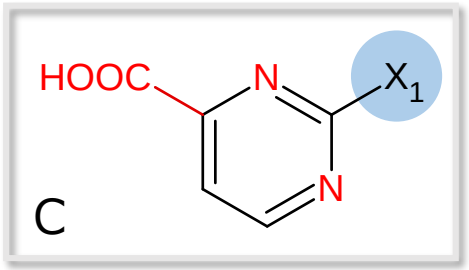
Pyrimidine-carboxylic acid analogs



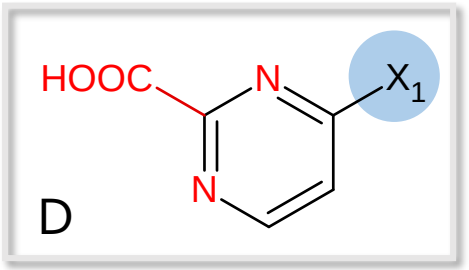
24 analogs



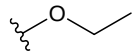
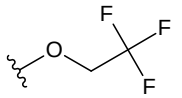
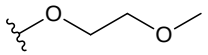
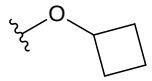
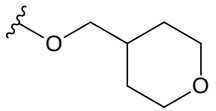
21 analogs



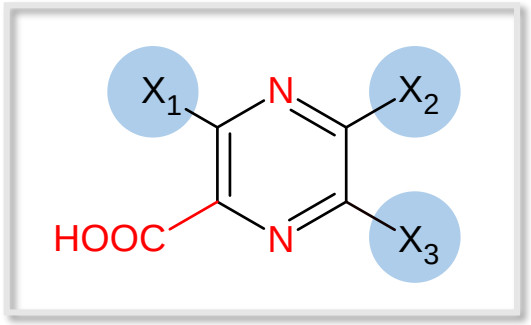
12 analogs



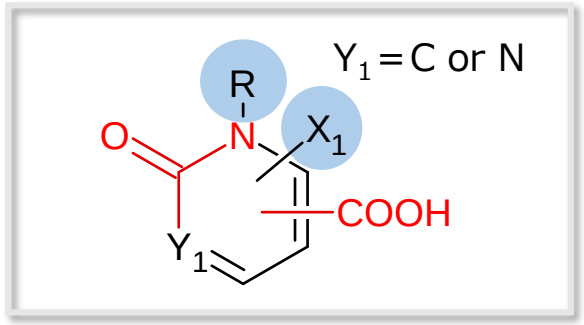
11 analogs

X_1	A型	B型	C型	D型
	PK0-19471	PK0-21481	PK0-43091	PK0-43421
	PK0-21021	PK0-22321	PK0-43741	PK0-49771
	PK0-20651	PK0-22891	PK0-43101	PK0-43781
	PK0-21031	PK0-24841	PK0-43761	PK0-42701
	PK0-21891	PK0-24831	PK0-43731	PK0-43151

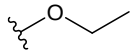
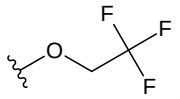
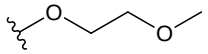
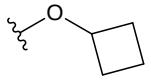
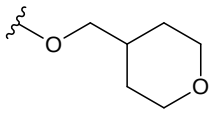
Pyrazine/Pyridone/Pyrimidone-carboxylic acid analogs

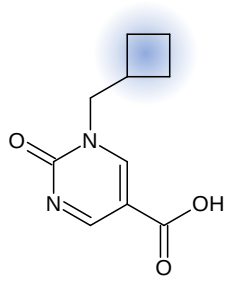


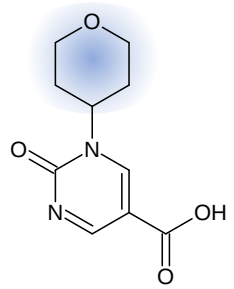
36
analogs

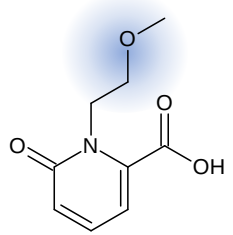


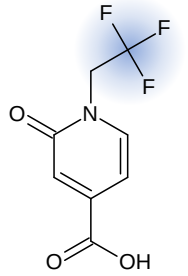
38
analogs

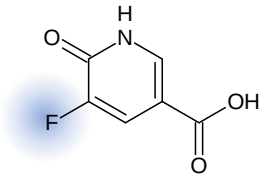
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	PK0-39601	PK0-38061	PK0-39581
	PK0-43181	PK0-39261	PK0-39591
	PK0-41621	PK0-38441	PK0-45001
	PK0-41651	PK0-38841	PK0-40931
	PK0-40951	PK0-38451	PK0-39271

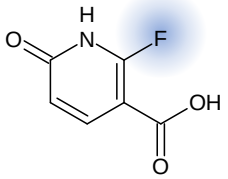

PK0-27341

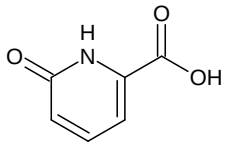

PK0-21941

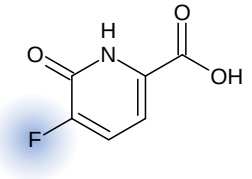

PK0-24871


PK0-23261

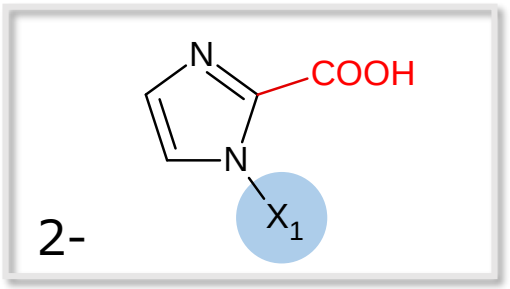

PK0-52451


PK0-52461

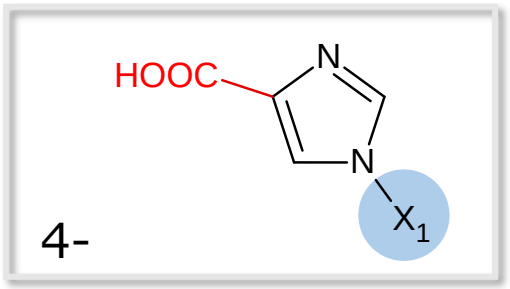

PK0-52261


PK0-52471

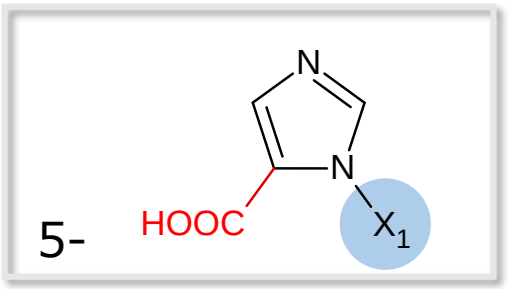
Imidazole-carboxylic acid analogs



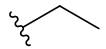
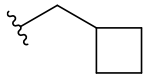
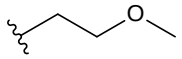
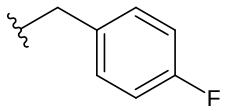
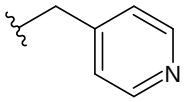
33 analogs



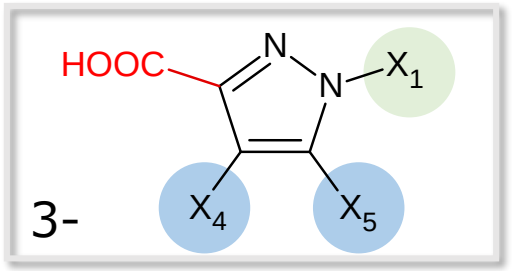
48 analogs



48 analogs

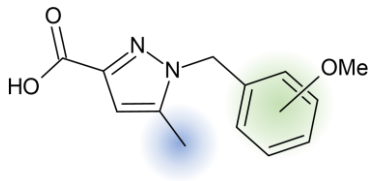
X_1	2-COOH	4-COOH	5-COOH
	**PK0-59431**	PK0-37421	PK0-37431
	PK0-25481	PK0-26181	PK0-37801
	PK0-27001	PK0-26991	PK0-35551
	PK0-25491	PK0-24471	PK0-26391
	PK0-27401	PK0-26241	PK0-30191

Pyrazole-carboxylic acid analogs

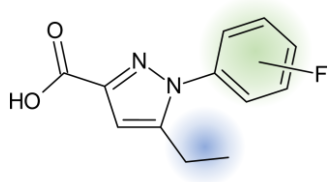


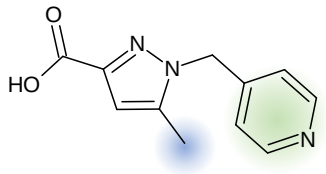
62 analogs

o- : PK0-59271
m- : PK0-59121
p- : PK0-59131

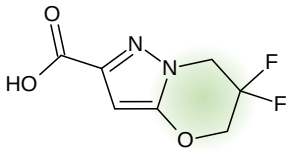


o- : PK0-59411
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p- : PK0-59331

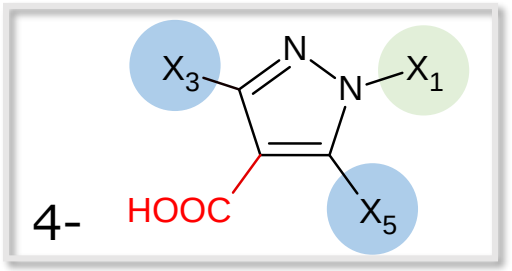




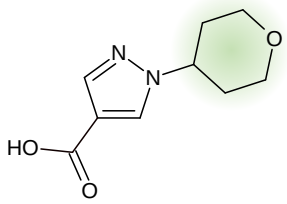
PK0-37691



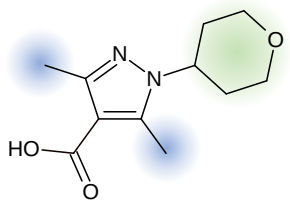
PK0-38871



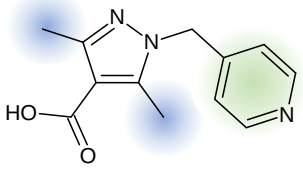
70 analogs



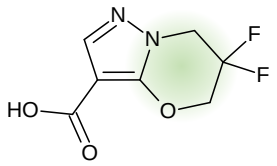
PK0-13341



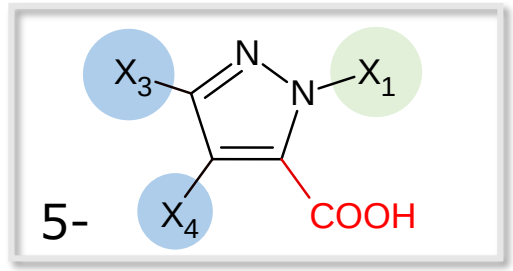
PK0-26151



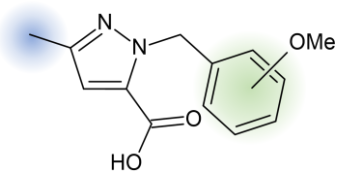
PK0-26761



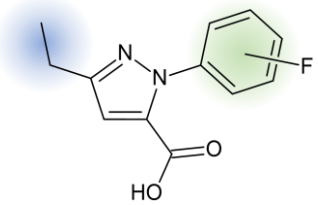
PK0-49321



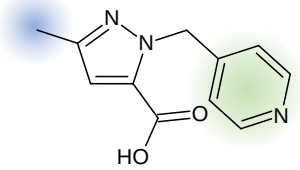
53 analogs



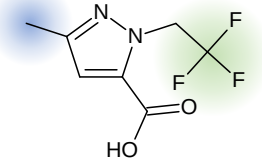
o- : PK0-59281
m- : PK0-59141
p- : PK0-59151



o- : PK0-59421
m- : PK0-59341
p- : PK0-59351



PK0-38131

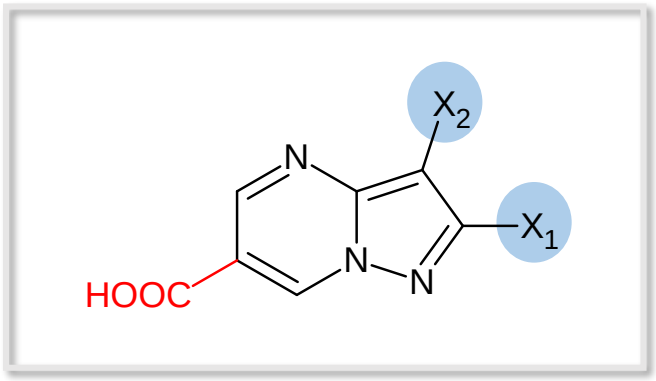


PK0-15191

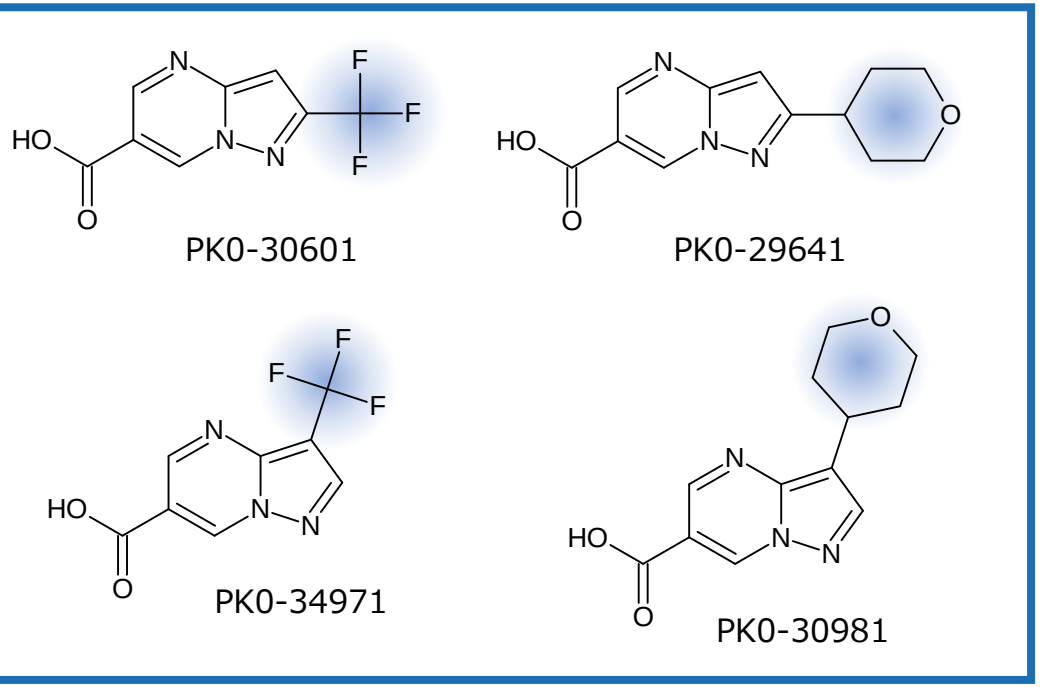
<参考情報 / K-BB構造が導入されている事例>

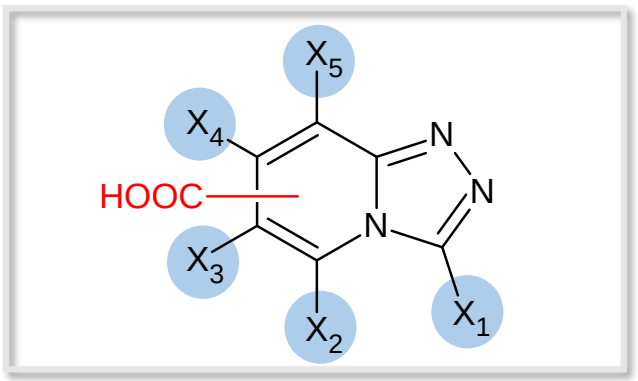
- Preparation of heteroaryl-substituted indole derivatives for restoring mutant p53 function, WO2021231474.
- Preparation of bicyclic heterocyclyl compounds as SOS1 modulators, WO2020180770.

Fused heterocyclic-carboxylic acid analogs (1)

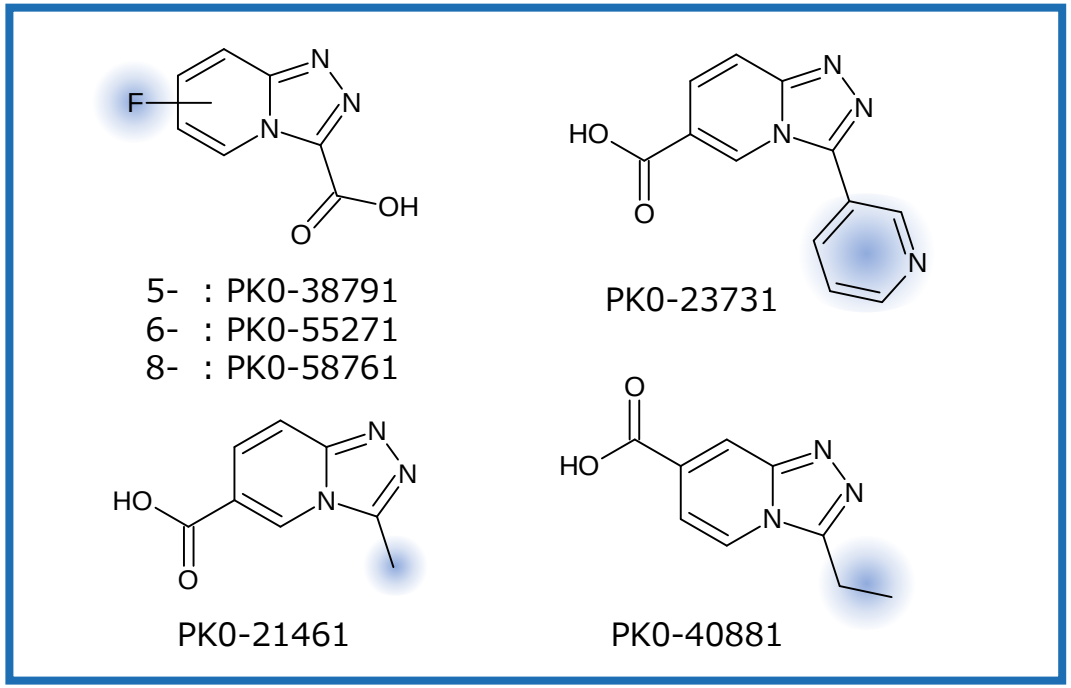


16
analogs

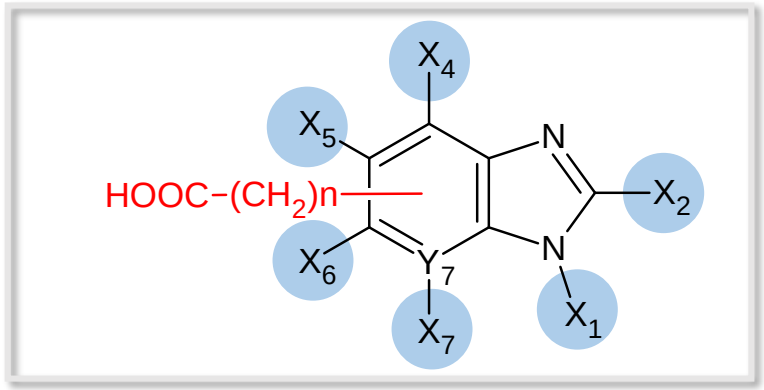




57
analogs

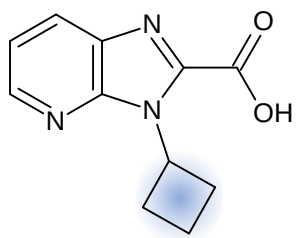


Fused heterocyclic-carboxylic acid analogs (2)

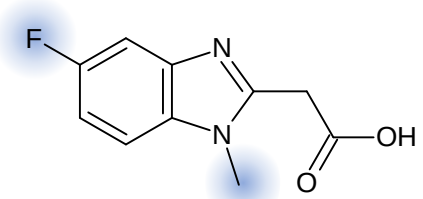


109 analogs

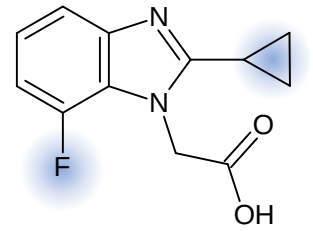
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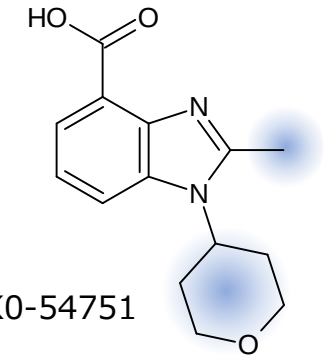
PK0-55211

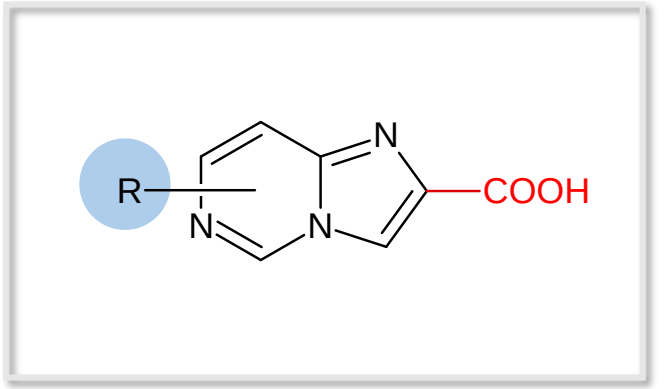


PK0-35581

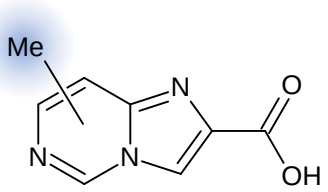


PK0-54751



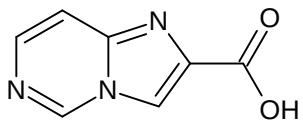


5 analogs

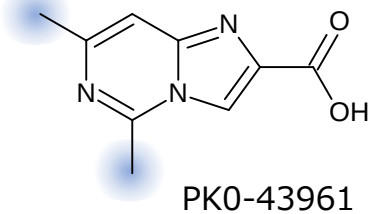


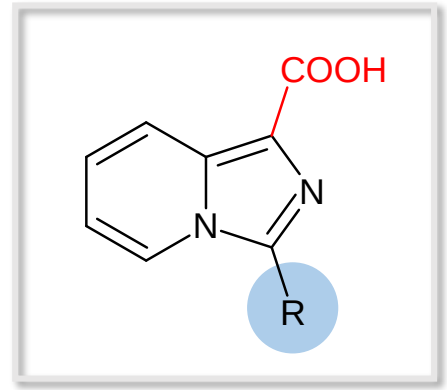
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8- : PK0-43971

PK0-40341

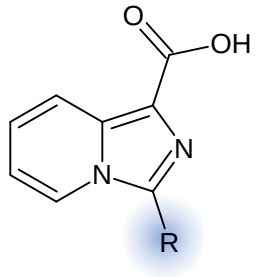


PK0-43961



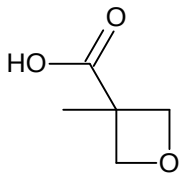


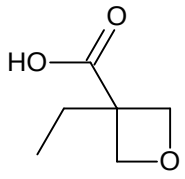
6 analogs

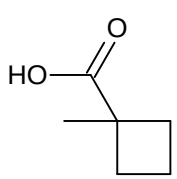


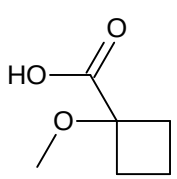
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R = Et : PK0-54441
R = *i*-Pr : PK0-54451
R = *c*-Pr : PK0-54461
R = *c*-Bu : PK0-54671
R =  : PK0-54681

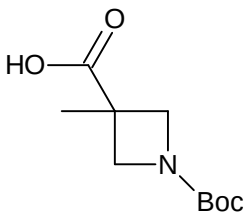
Aliphatic acid analogs

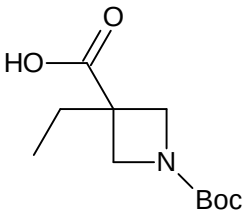

PK0-13561

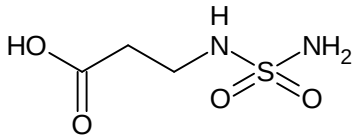

PK0-13681

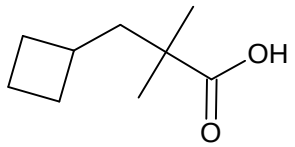

PK0-23451

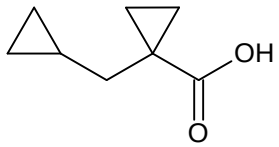

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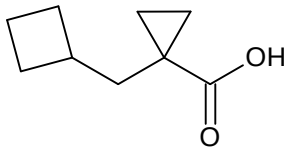

PK0-57171

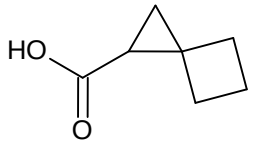

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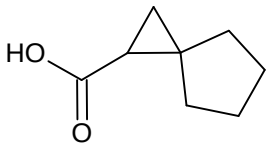

PK0-40361

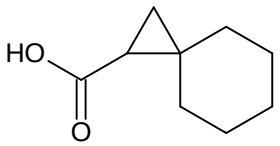

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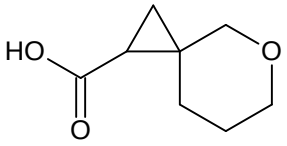

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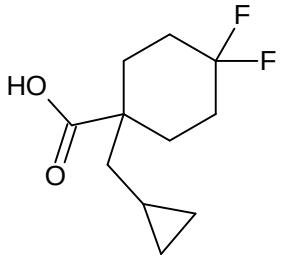

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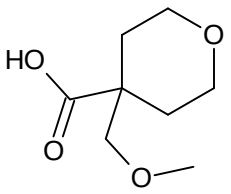

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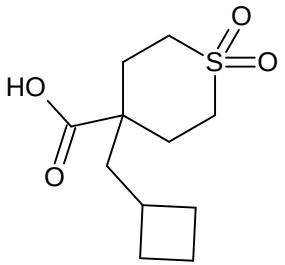

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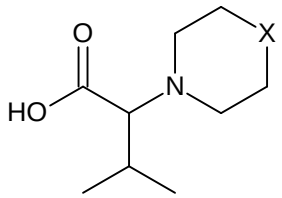

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PK0-30881

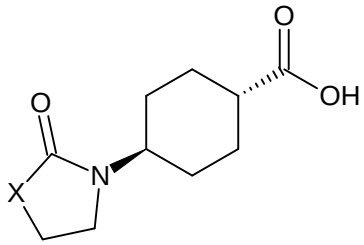

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PK0-19131

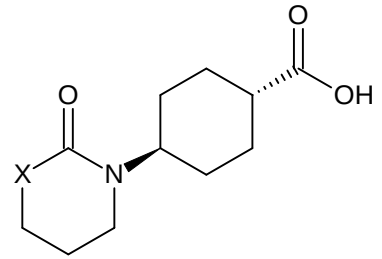

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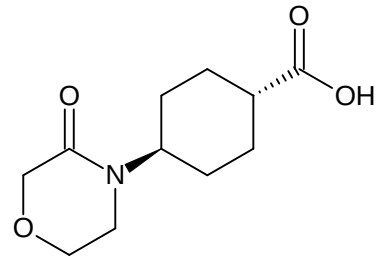
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X = O : PK0-52181
X = NMe : PK0-52191



X = CH_2 : PK0-57051
X = O : PK0-57061
X = NH : PK0-57431



X = CH_2 : PK0-57281
X = O : PK0-57291
X = NH : PK0-57461

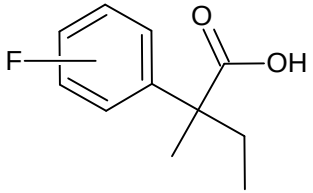

PK0-57471

97
analogs

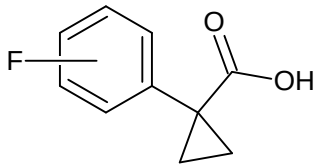
<参考情報>
PK0-57051の構造が活用された報告
cis-1-Oxo-heterocyclyl-4-amido cyclohexane derivatives as NPY5 receptor antagonists
Bioorg. Med. Chem. Lett. **2014**, *24*, 1458-1461.

α,α-Disubstituted phenyl/pyridinylacetic acid analogs

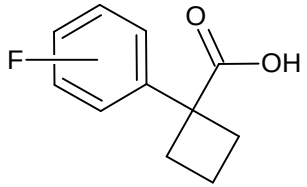
α,α-Disubstituted phenylacetic acid analogs



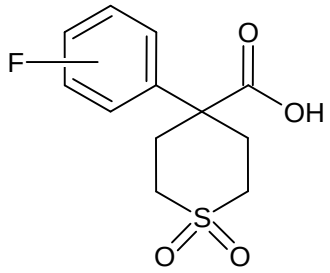
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m- : PK0-55631
p- : PK0-55641



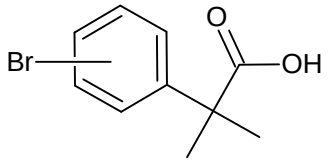
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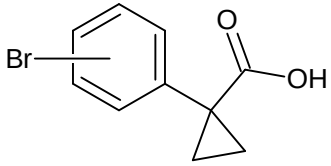
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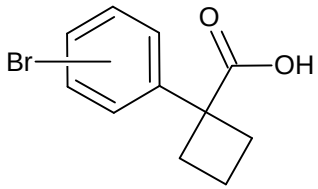
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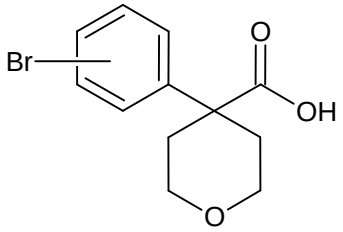
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m- : PK0-08511
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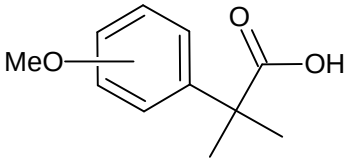
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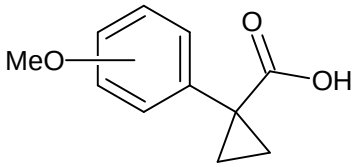
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m- : PK0-10611
p- : PK0-10621



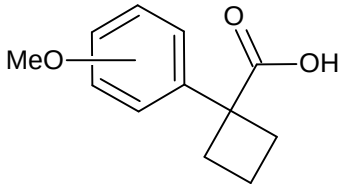
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p- : PK0-16281



o- : PK0-10631
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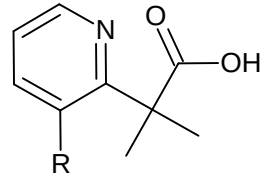
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p- : PK0-10681



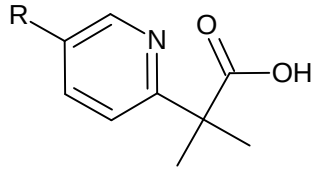
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m- : PK0-10701
p- : PK0-10711

79 analogs

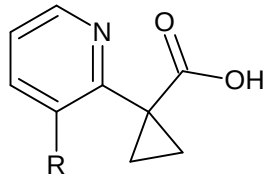
α,α-Disubstituted pyridinylacetic acid analogs



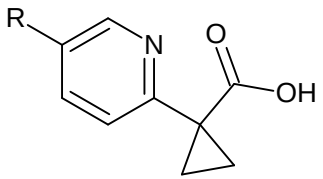
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R = OMe : PK0-23691



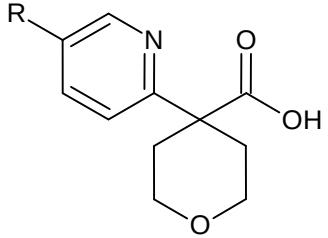
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R = OMe : PK0-22851



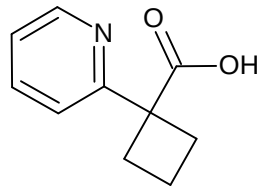
R = F : PK0-21681
R = Cl : PK0-40621
R = Me : PK0-21691
R = OMe : PK0-24051
R = CF_3 : PK0-40631



R = F : PK0-21671
R = Me : PK0-16681
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R = F : PK0-21701
R = OMe : PK0-22731



PK0-40601

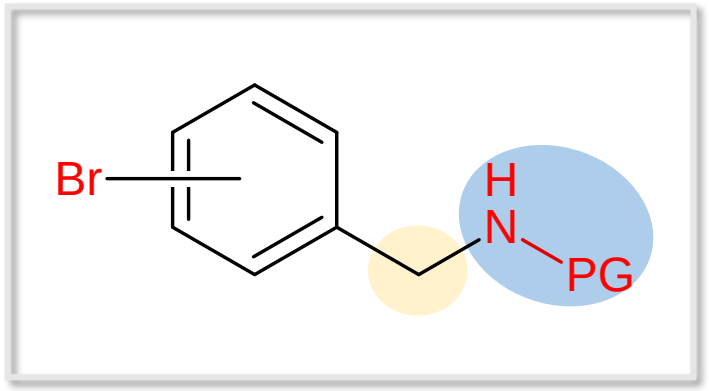
22 analogs

キシダオリジナル
ビルディングブロック（K-BB）

-Br化合物-

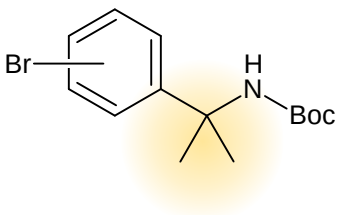
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Br-benzene analogs (1)

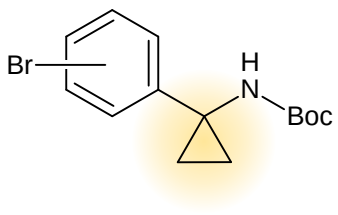


33 analogs

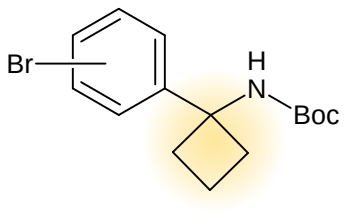
9 analogs



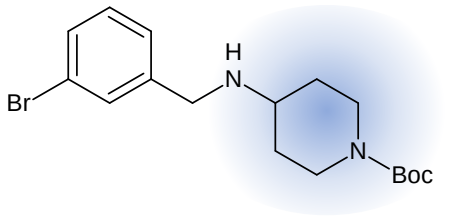
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p- : PK0-08481



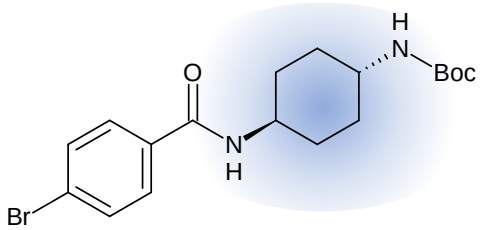
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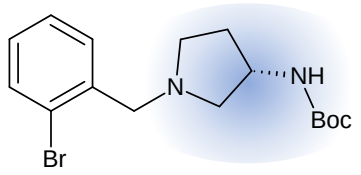
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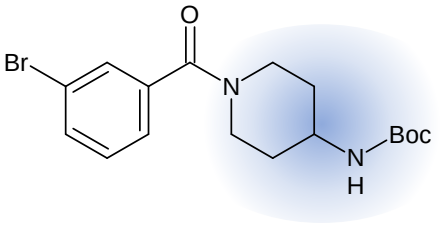
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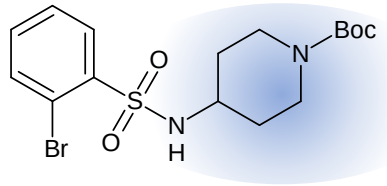
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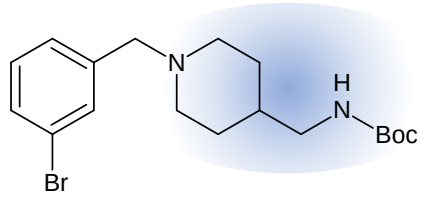
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PK0-03041

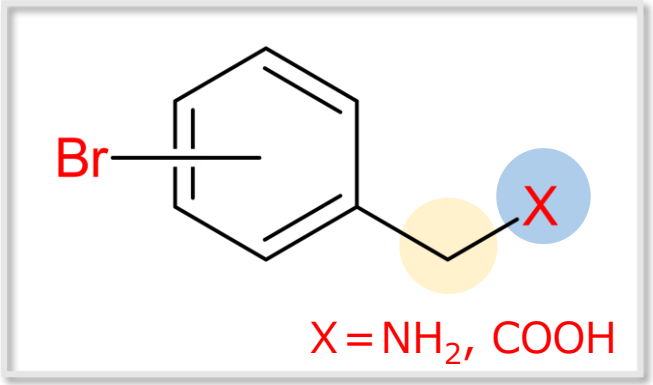


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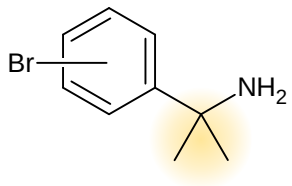
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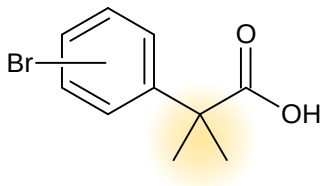


84 analogs

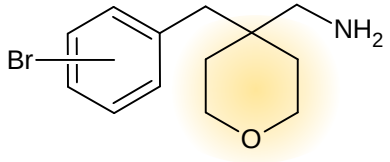
53 analogs



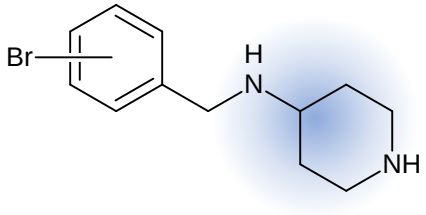
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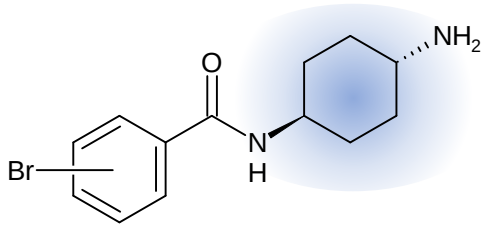
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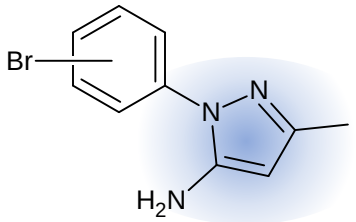
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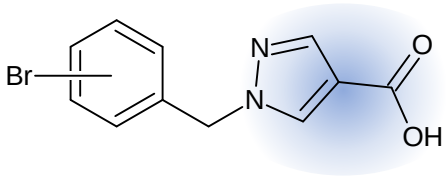
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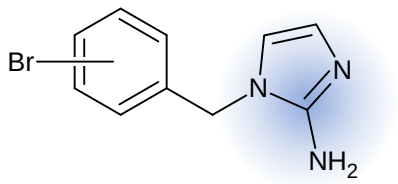
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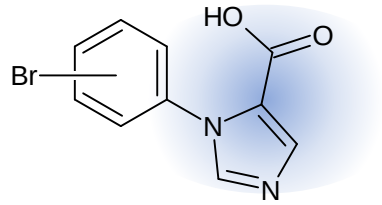
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o- : PK0-12171
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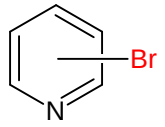
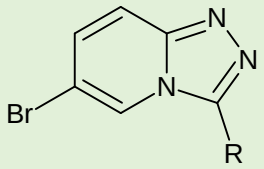
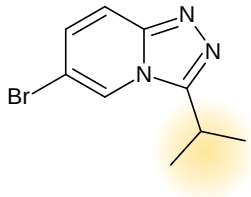
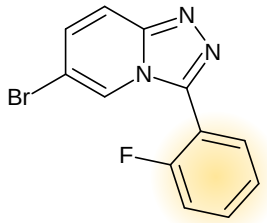
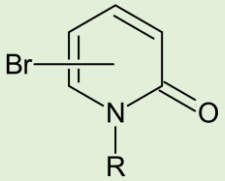
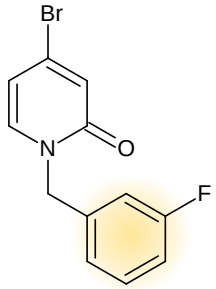
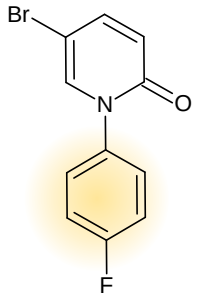
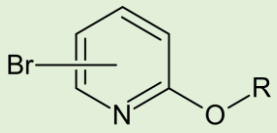
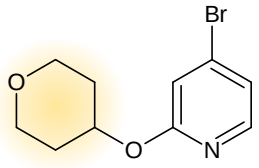
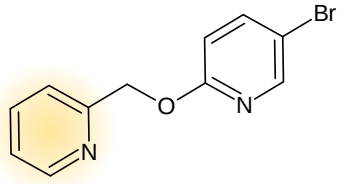


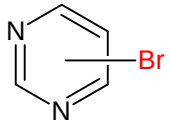
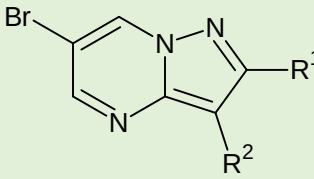
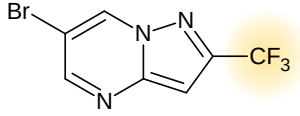
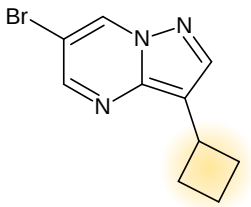
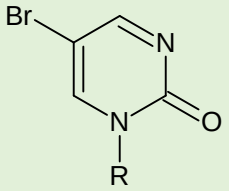
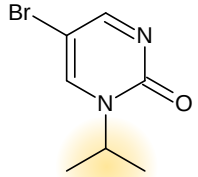
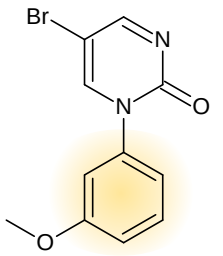
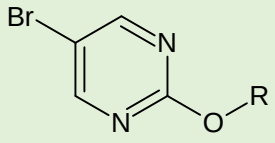
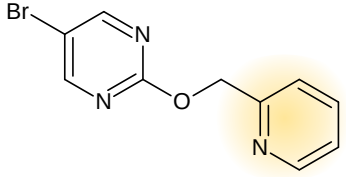
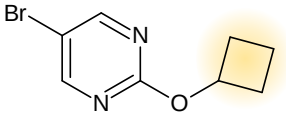
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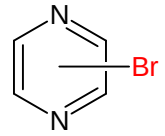
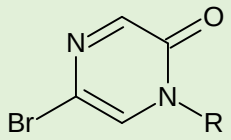
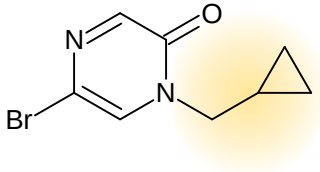
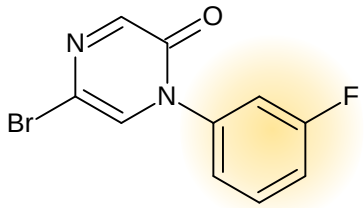
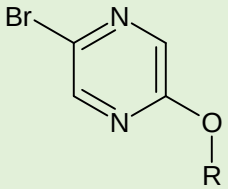
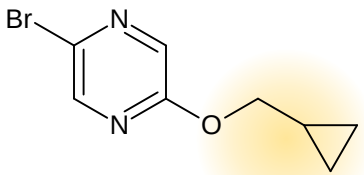
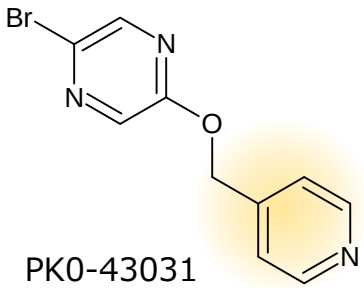
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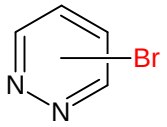
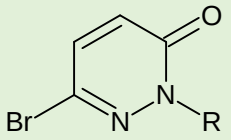
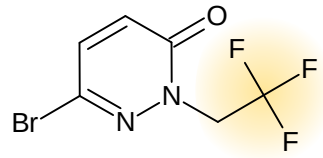
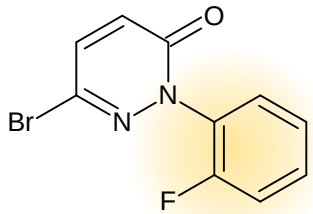
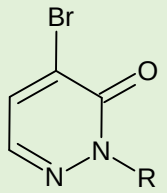
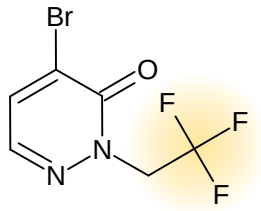
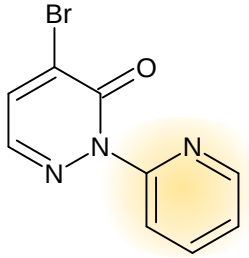
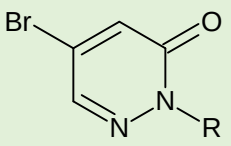
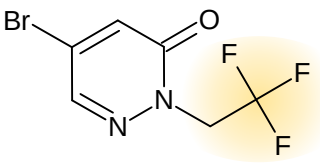
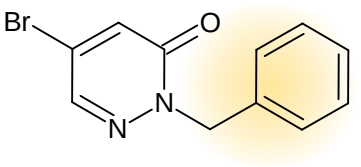
Br-heteroring analogs (1)

	Example-1	Example-2
 **19** analogs	 PK0-18111	 PK0-20011
 **77** analogs	 PK0-39411	 PK0-39431
 **30** analogs	 PK0-42641	 PK0-39881

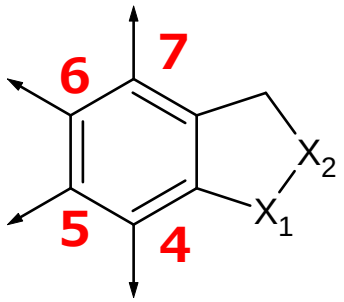
	Example-1	Example-2
 **17** analogs	 PK0-30201	 PK0-30221
 **23** analogs	 PK0-41161	 PK0-39491
 **12** analogs	 PK0-41591	 PK0-41191

Br-heteroring analogs (2)

	Example-1	Example-2
 **23** analogs	 PK0-42151	 PK0-42471
 **17** analogs	 PK0-42291	 PK0-43031

	Example-1	Example-2
 **25** analogs	 PK0-41551	 PK0-49731
 **25** analogs	 PK0-50161	 PK0-50401
 **27** analogs	 PK0-42551	 PK0-41531

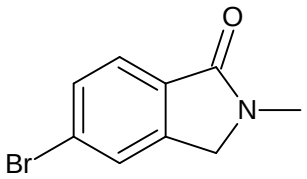
Br-bicyclic analogs (1)



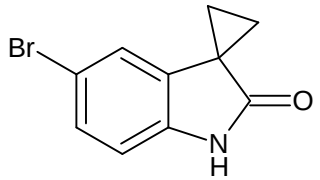
X_1=NH, X_2=CH_2

X_1=CH_2, X_2=NH

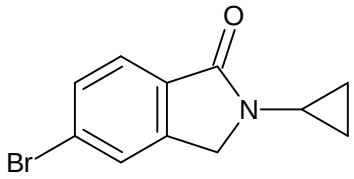
37 analogs



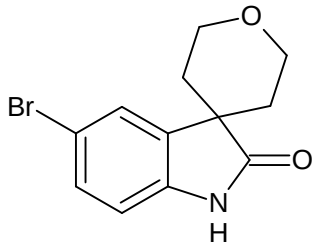
PK0-27621



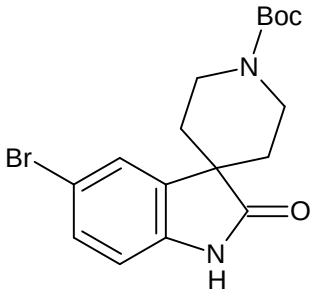
PK0-45911



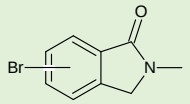
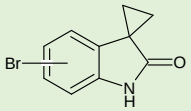
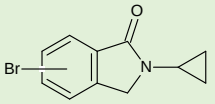
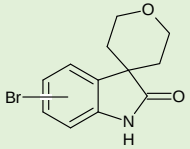
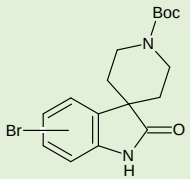
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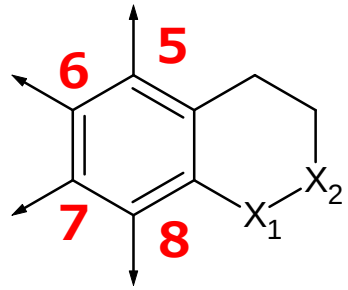
PK0-46271



PK0-31741

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	PK0-46571	PK0-45911	PK0-46771	PK0-47161
	PK0-27651	PK0-27641	PK0-27901	PK0-32721
	PK0-46921	PK0-46271	PK0-46931	PK0-47221
	PK0-33081	PK0-31741	PK0-31751	PK0-32641

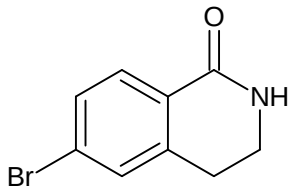
Br-bicyclic analogs (2)



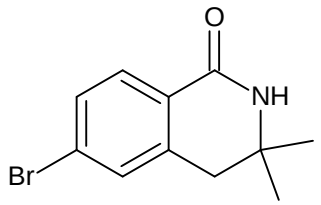
X_1=NH, X_2=CH_2

X_1=CH_2, X_2=NH

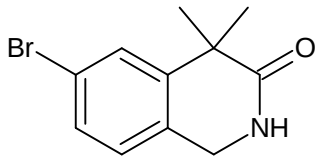
55 analogs



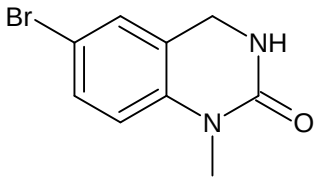
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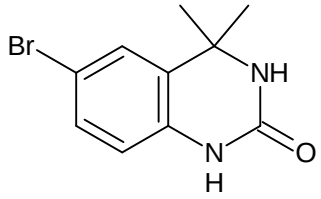
PK0-49051



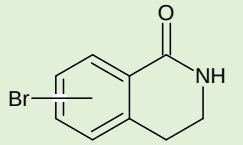
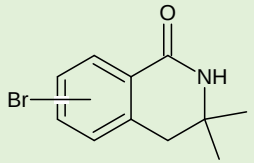
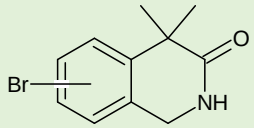
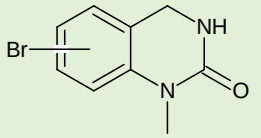
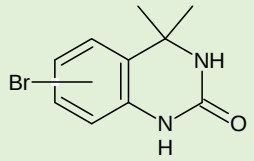
PK0-37901



PK0-37081



PK0-43461

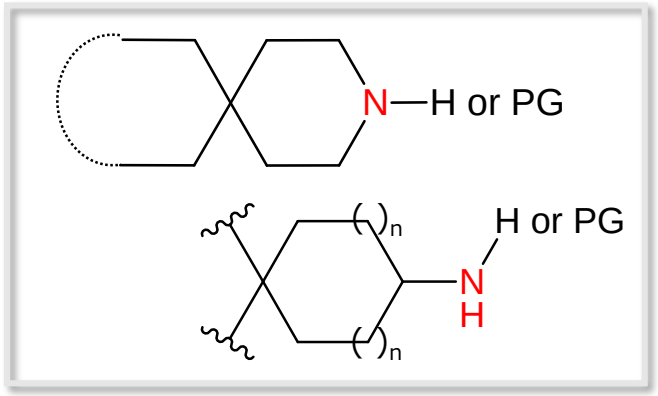
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	PK0-49711	PK0-49051	PK0-49041	PK0-49261
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	PK0-37091	PK0-37081	PK0-37071	PK0-37881
	PK0-49851	PK0-43461	PK0-38491	PK0-45971

キシダオリジナル
ビルディングブロック（K-BB）

-スピロ骨格化合物-

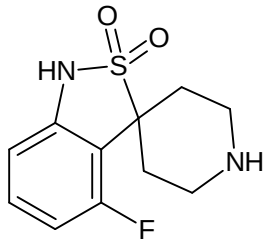
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Spiro compounds (1)



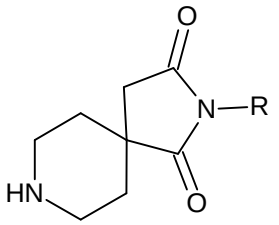
224 analogs

PK0-49961

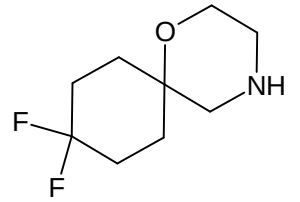


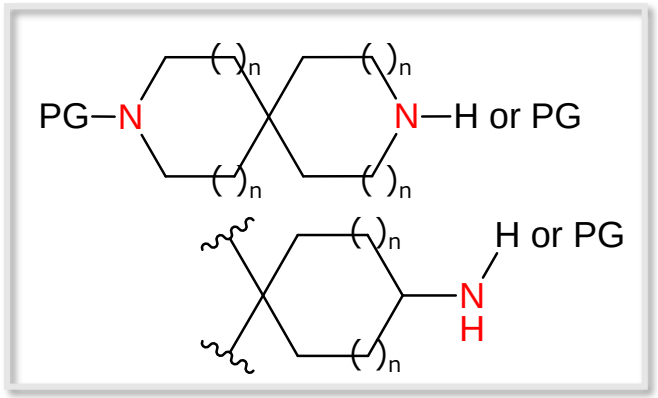
PK0-54241

R = Me : PK0-59301
R = Et : PK0-59401



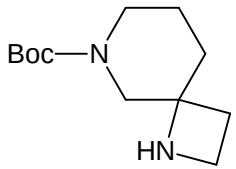
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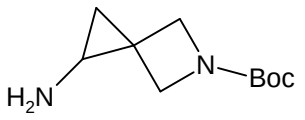


151 analogs

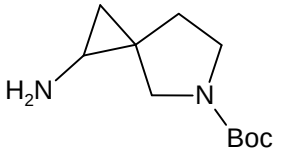
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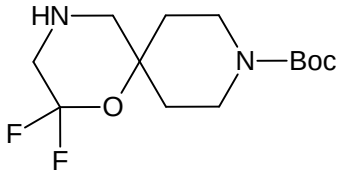
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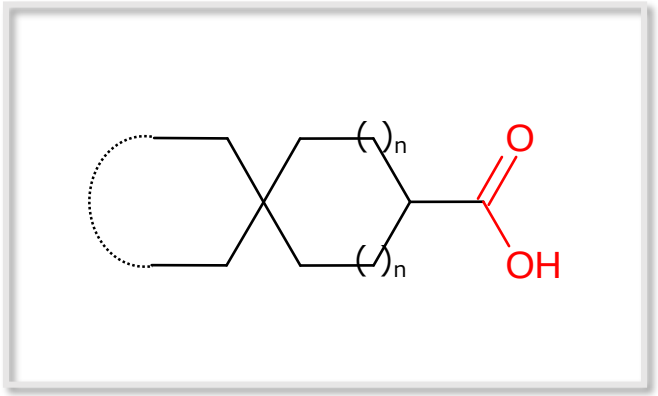


PK0-50381



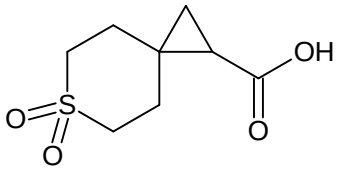
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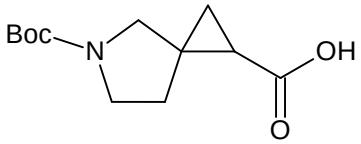


19 analogs

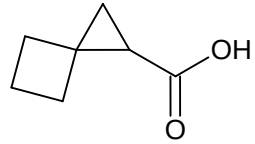
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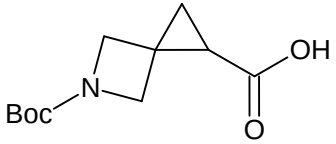
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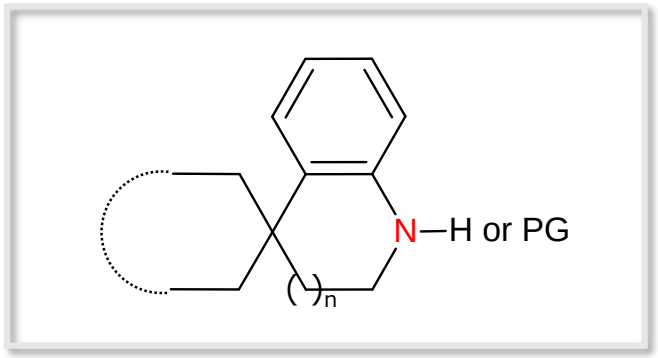
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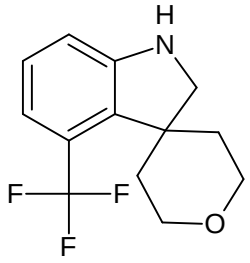
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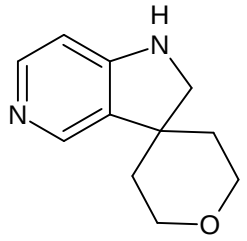
Spiro compounds (2)



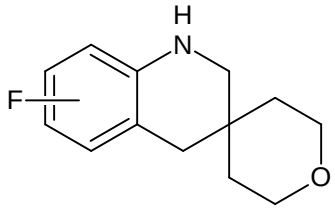
110
analogs



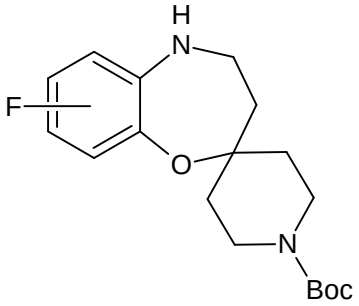
PK0-47041



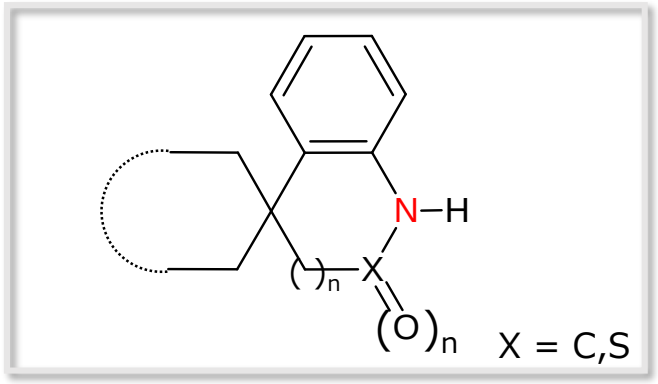
PK0-51881



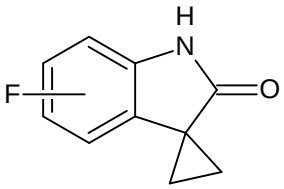
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6- : PK0-23591
7- : PK0-22791
8- : PK0-22801



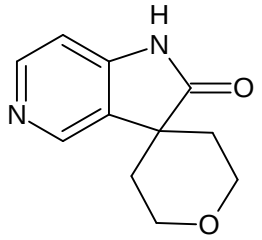
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7- : PK0-48481
8- : PK0-48491
9- : PK0-48501



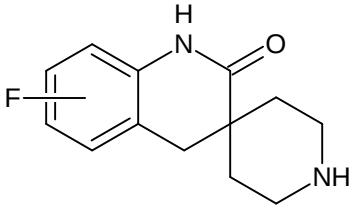
115
analogs



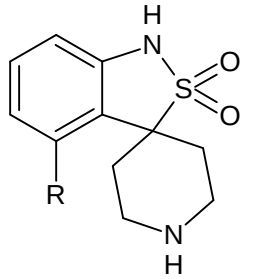
4- : PK0-46541
5- : PK0-45891
6- : PK0-45901
7- : PK0-47351



PK0-51781

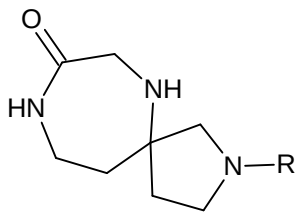


5- : PK0-21291
6- : PK0-23581
7- : PK0-20871
8- : PK0-23211

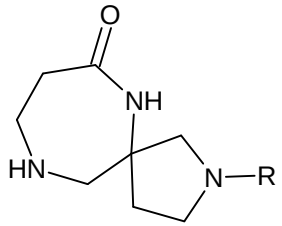


R = H : PK0-53941
R = F : PK0-54241

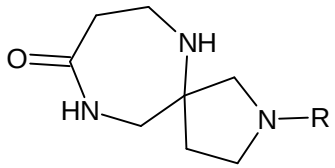
Spiro compounds – オリジナリティが高いBB –



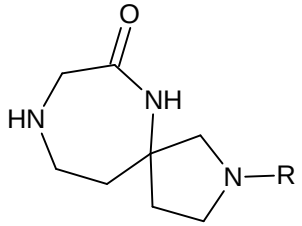
R = H : PK0-52701
R = Boc : PK0-52721



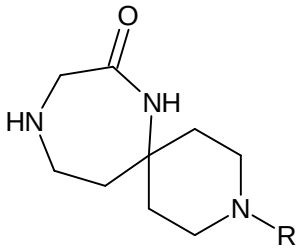
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R = Boc : PK0-52431



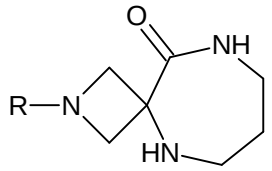
R = H : PK0-52861
R = Boc : PK0-52921



R = H : PK0-52661
R = Boc : PK0-52561

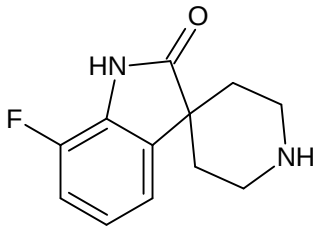


R = H : PK0-52671
R = Boc : PK0-52571

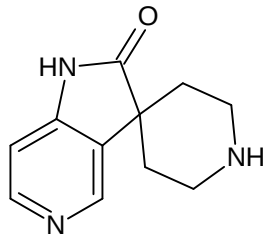


R = H : PK0-52851
R = Boc : PK0-52911

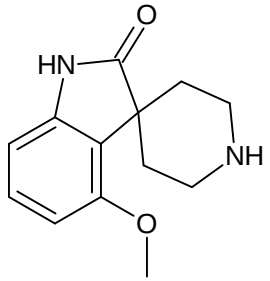
etc.



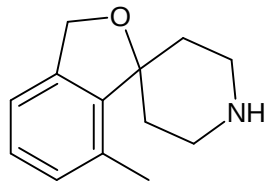
PK0-55261



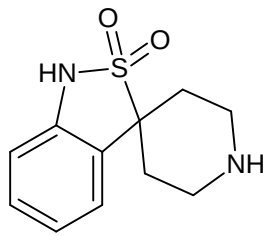
PK0-51771



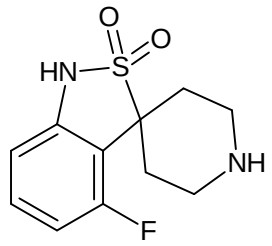
PK0-51651



PK0-50541

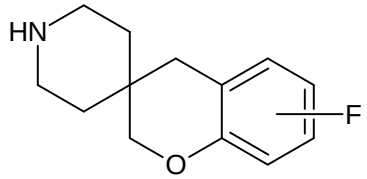


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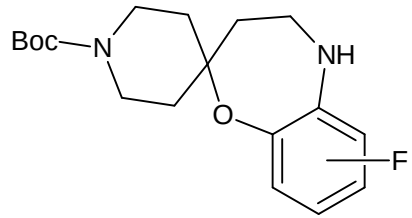


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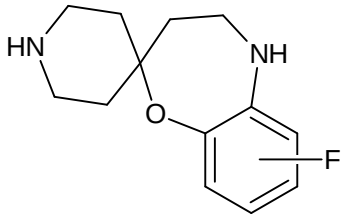
etc.



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7- : PK0-53121
8- : PK0-53111

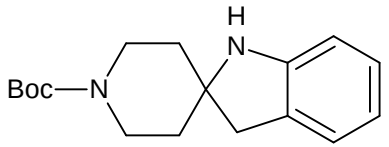


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7- : PK0-48481
8- : PK0-48491
9- : PK0-48501



6- : PK0-48571
7- : PK0-48251
8- : PK0-48581
9- : PK0-48591

etc.



R = H : PK0-48341
R = Boc : PK0-48331

etc.

キシダオリジナル
ビルディングブロック（K-BB）

-中心骨格化合物-

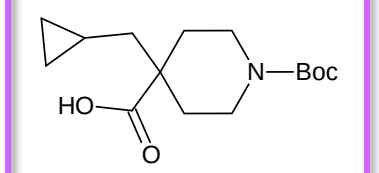
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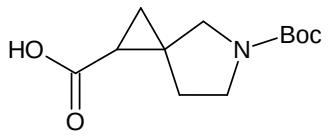
Multi-functional building blocks

SAR用BBとして活用
⇓
薬効・物性改善を期待

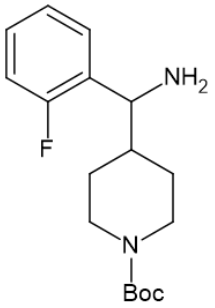
Multi-functional K-BB

中心骨格として活用
⇓
DEL、新規ライブラリー＊

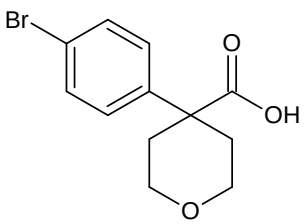




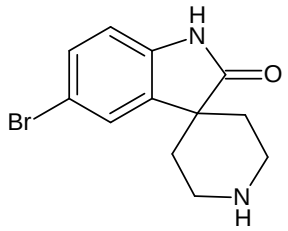
Protected-Amine ＋COOH



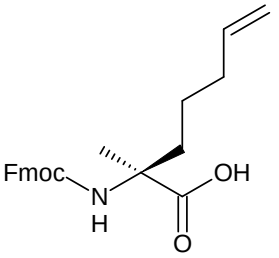
Protected-Amine ＋Amine



Br-Ar＋COOH



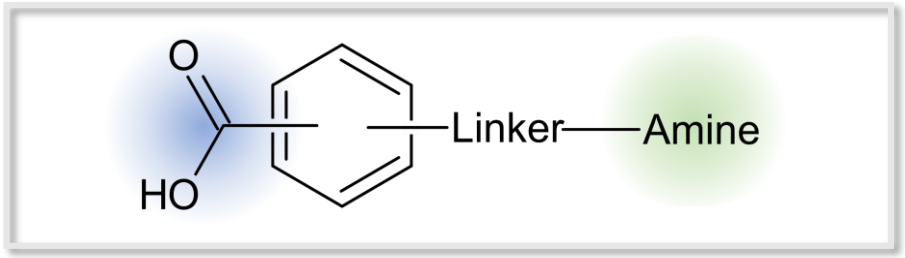
Br-Ar+Amine



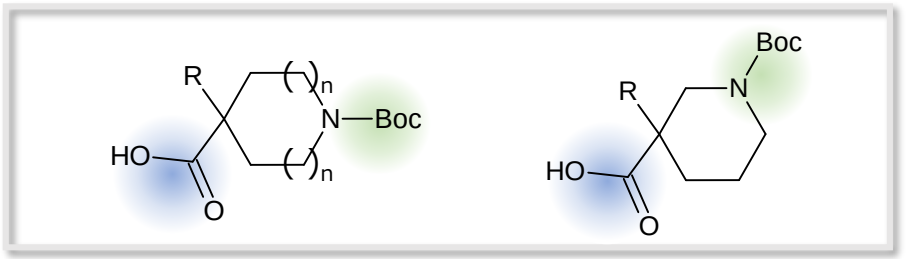
Unnatural Amino acid

＊お客様がお持ちのBBと組み合わせることで、オリジナルライブラリーの作製が可能です.
当社のパラレル合成サービスもご利用いただけます.

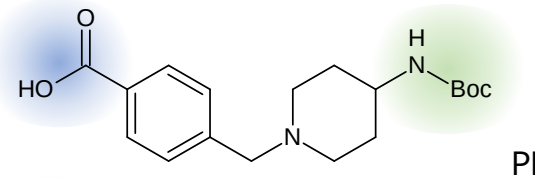
“Protected amine + COOH” analogs



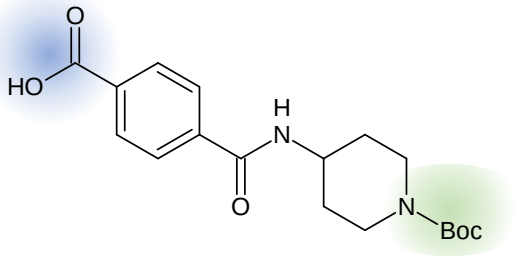
10
analogs



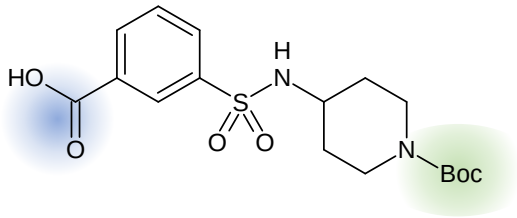
40
analogs



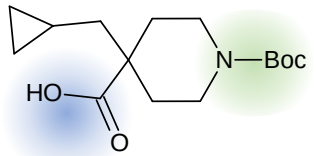
PK0-03641



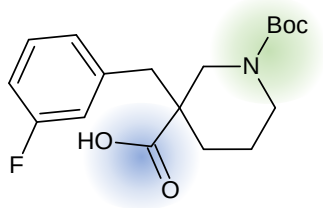
PK0-02081



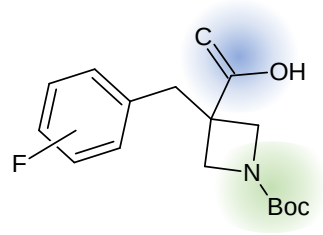
PK0-02011



PK0-31981

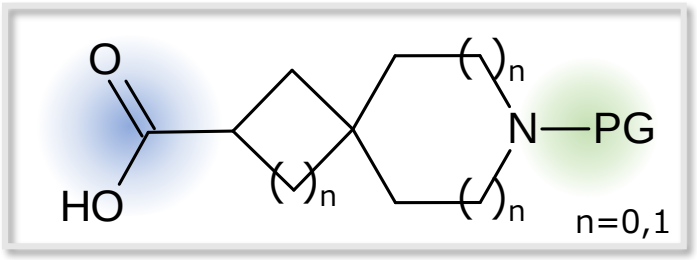


PK0-53681

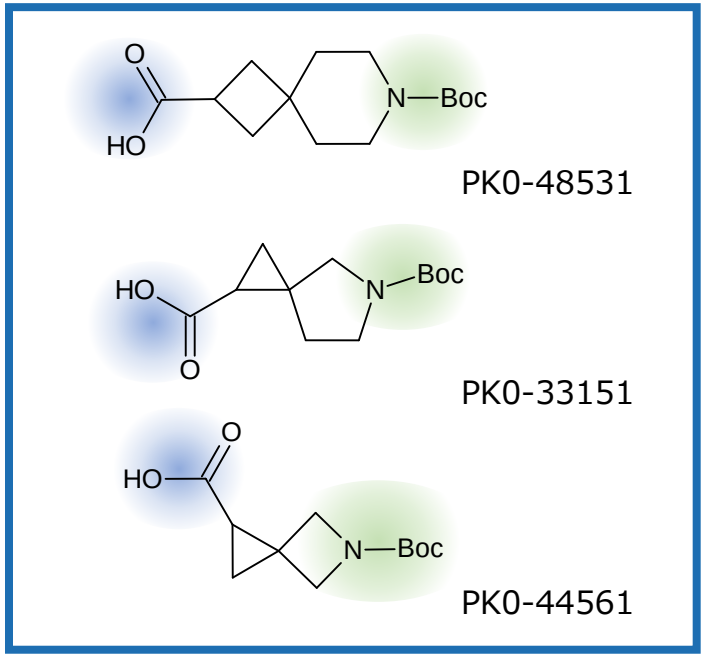


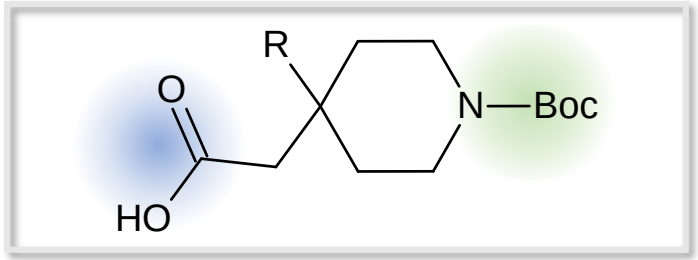
2- : PK0-55171
3- : PK0-55181
4- : PK0-55191

“Protected amine + COOH” analogs

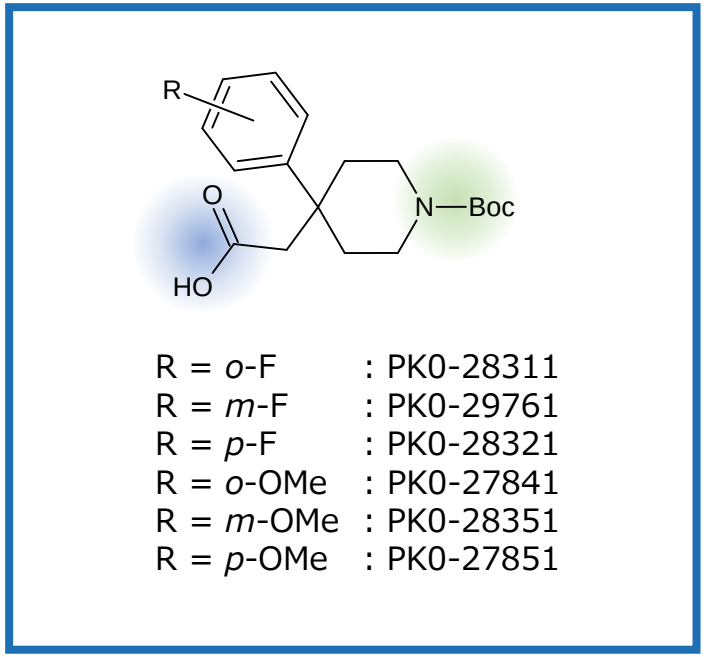


8 analogs



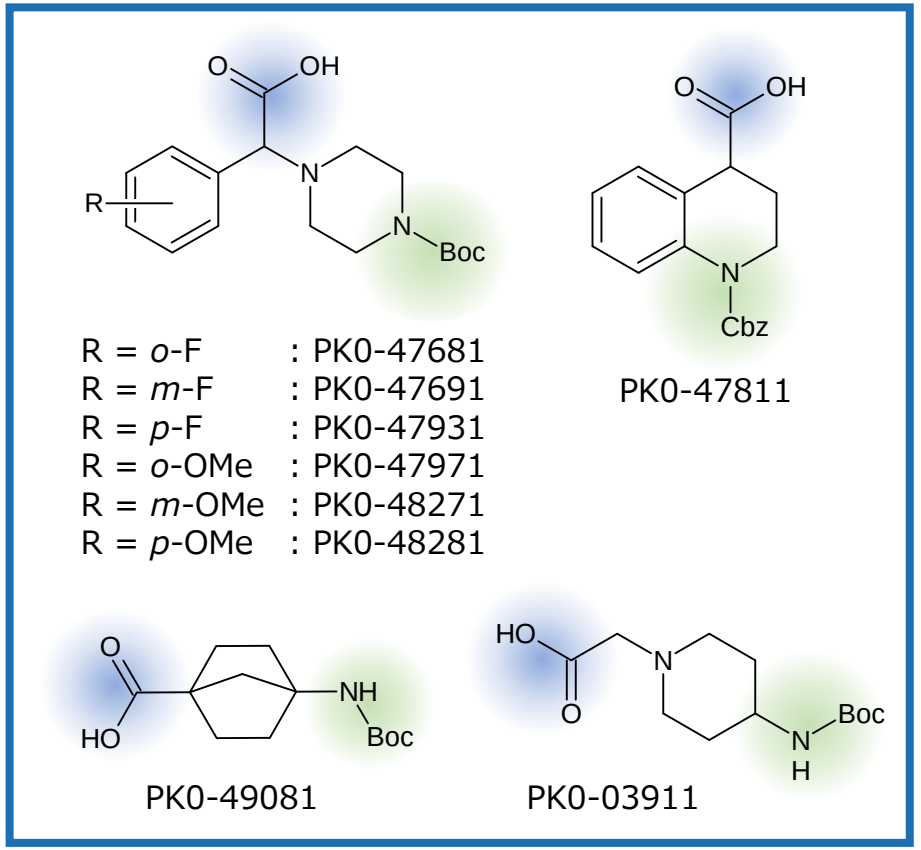


17 analogs

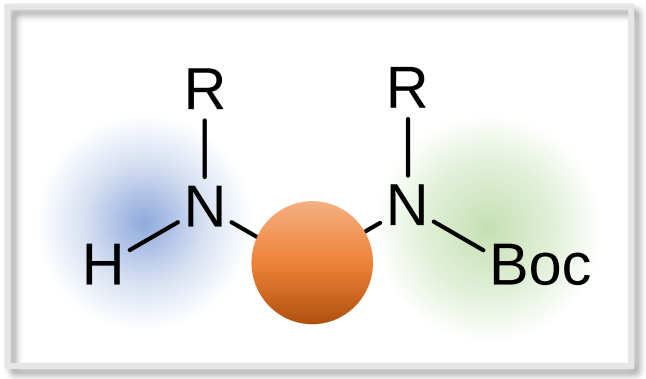


Others

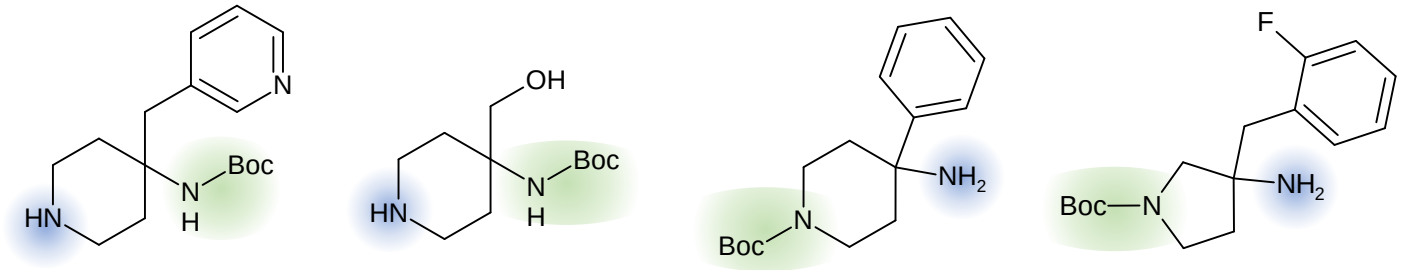
11 analogs



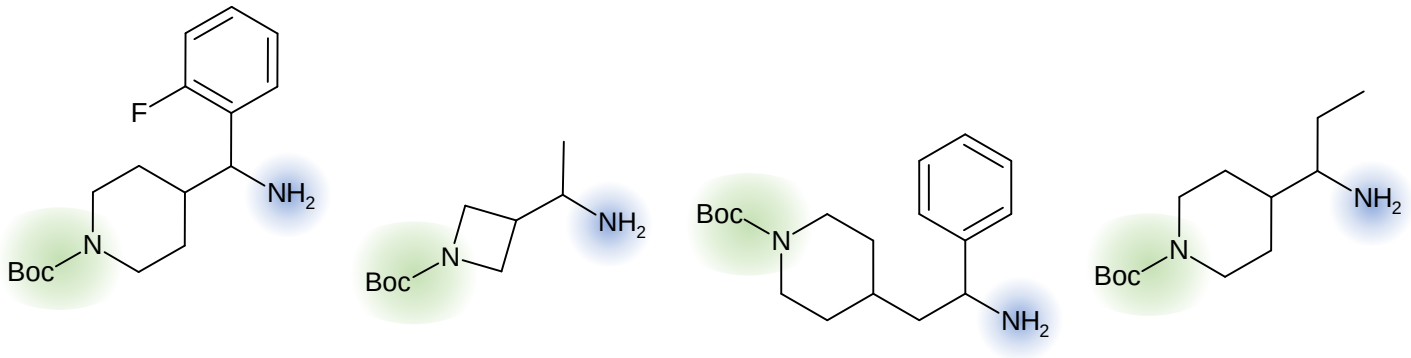
“Protected amine + Amine” analogs



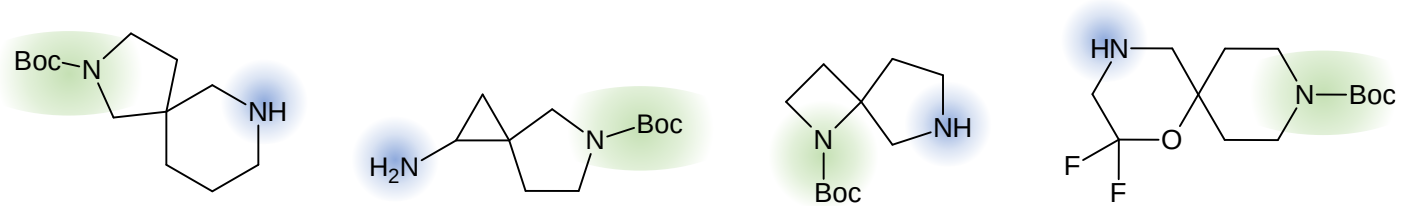
448
analogs



PK0-32781　PK0-24211　PK0-31841　PK0-31841



PK0-44741　PK0-48211　PK0-45731　PK0-59521



PK0-48551　PK0-50381　PK0-52621　PK0-59081

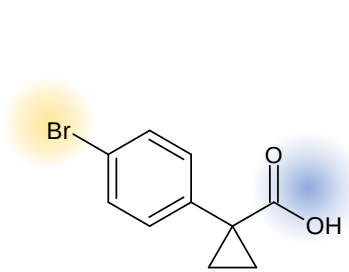
＜参考情報 / K-BB構造及び類縁構造が使用されている事例＞

***N*-Boc-ジアミン化合物をPROTACリンカーとして利用**
Direct-to-Biology Accelerates PROTAC Synthesis and the Evaluation of Linker Effects on Permeability and Degradation
ACS Med. Chem. Lett. **2022**, 13, 1182-1190.

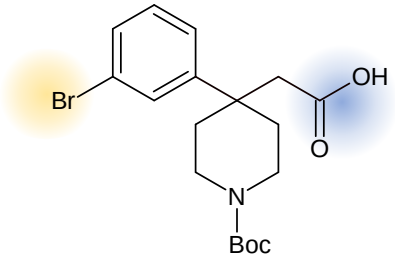
“Bromide + COOH” analogs

Br + Alkyl-COOH

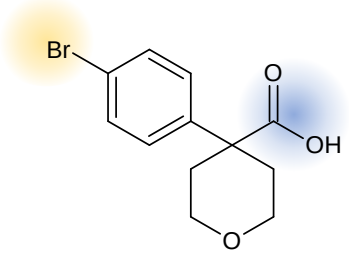
26 analogs



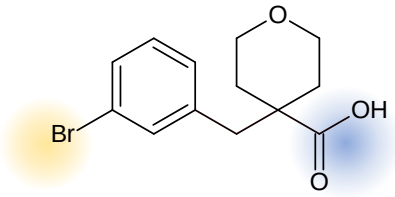
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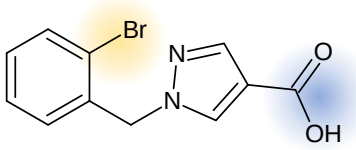
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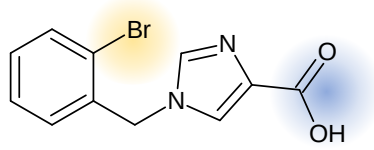
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Br + Heteroaryl-COOH

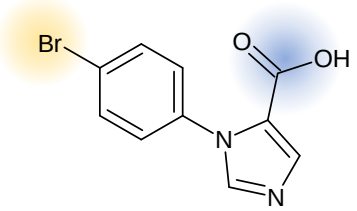
26 analogs



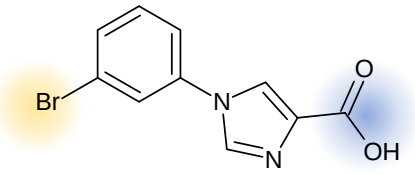
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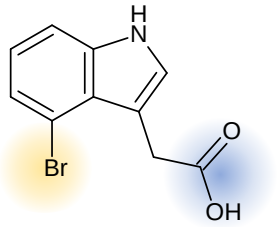
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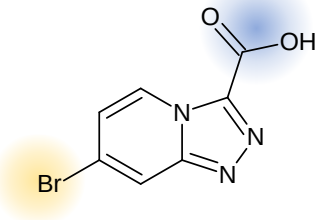
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PK0-26281



PK0-38221

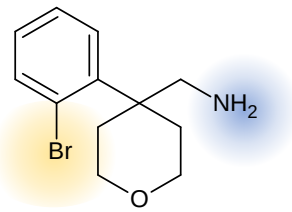


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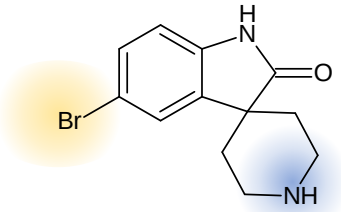
“Bromide + Amine” analogs

Br + Free-Amine

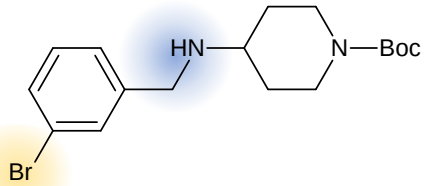
112 analogs



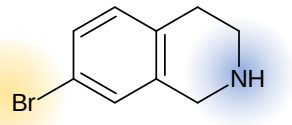
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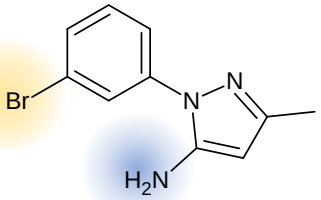
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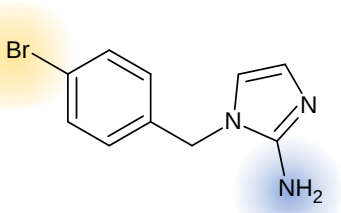
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PK0-53341



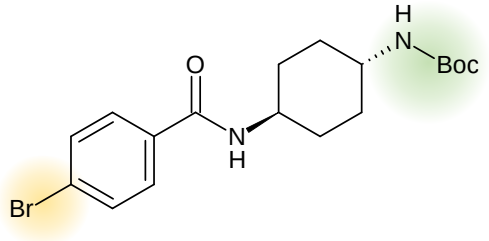
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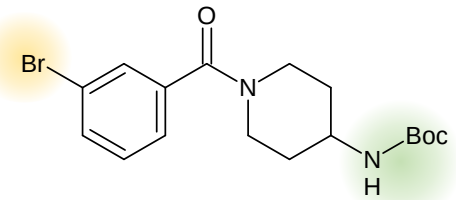
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Br + Protected-Amine

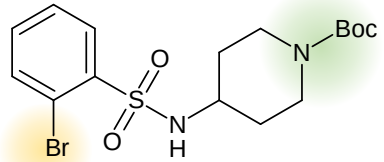
40 analogs



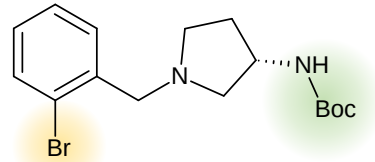
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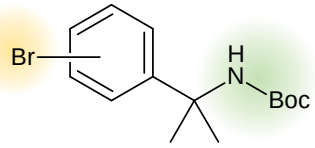
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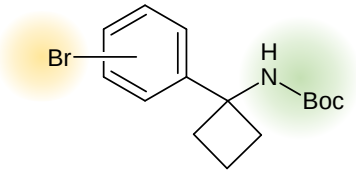
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PK0-06021



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m-: PK0-09951
p- : PK0-08481

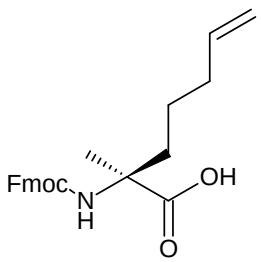


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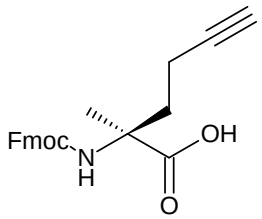
Unnatural amino acid

N-Protected Unnatural Amino Acid

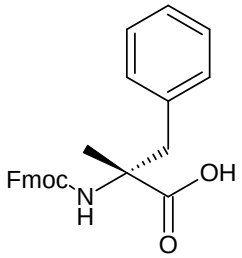
55 analogs



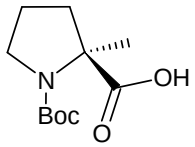
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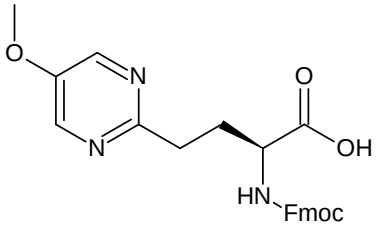
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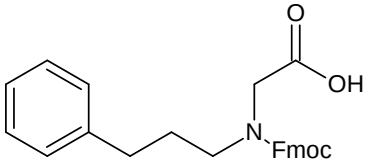
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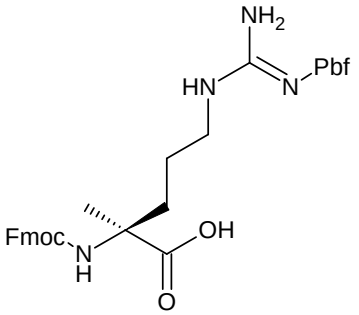
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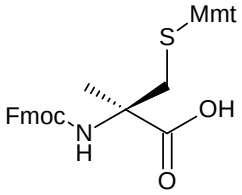
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Side Chain & *N*-Protected Unnatural Amino Acid

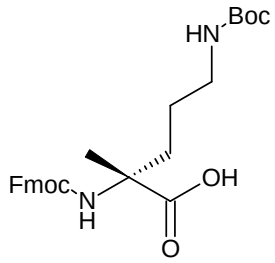
25 analogs



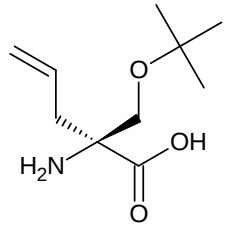
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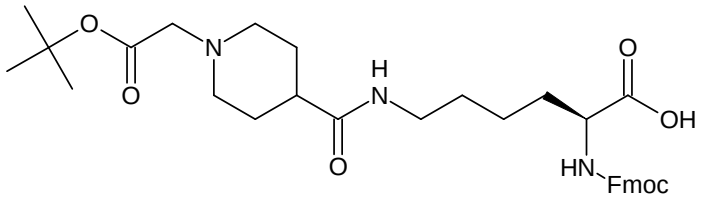
KUA-00501



KUA-00661



KUA-01391

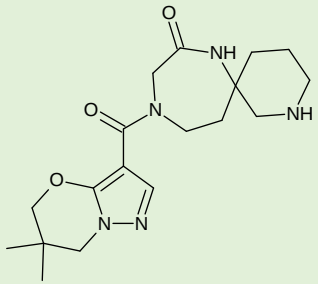


KUP-10071

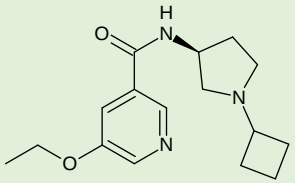
当社のアミノ酸事業での取り扱っている**ユニークな非天然型アミノ酸**です
KUA化合物は、当社が特許使用権を有する丸岡触媒を用いて合成しています

Kishida original virtual library（K-LB)

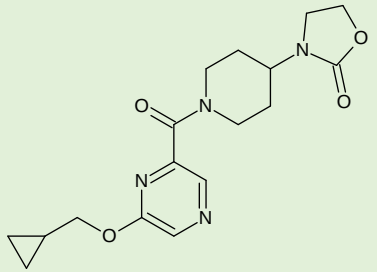
2-component Library



MW 361.45
Fsp3 0.72

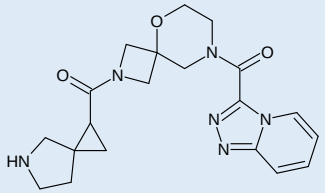


MW 289.38
Fsp3 0.63

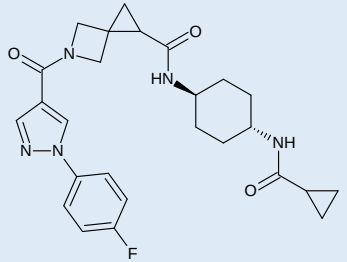


MW 346.39
Fsp3 0.65

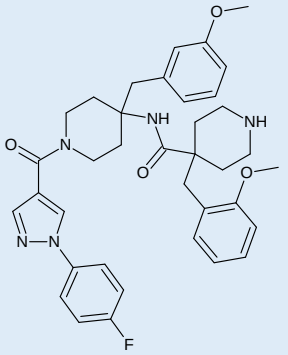
3-component Library



MW 396.45
Fsp3 0.60



MW 479.56
Fsp3 0.54



MW 639.77
Fsp3 0.38

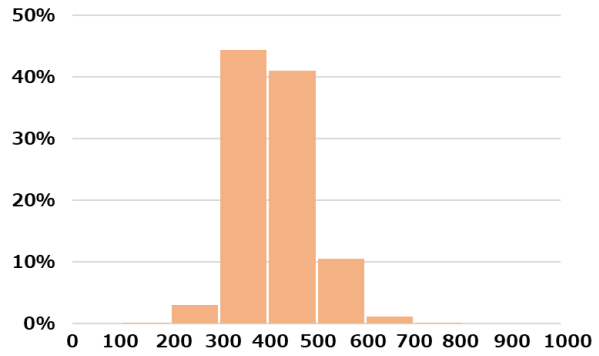
K-LBの特徴

- 2成分結合ライブラリー：**約500万化合物**
- 3成分結合ライブラリー：**約30万化合物**
- 構成素子：**キシダオリジナルビルディングブロック (K-BB)**
- 反応形式：**縮合反応（アミド化）**
- ファイル形式：SD file

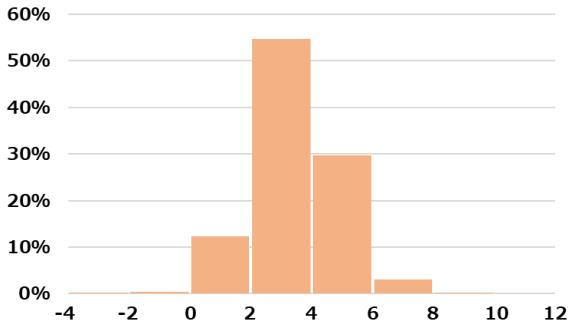
Kishida original virtual library（K-LB）の物理化学的特性分布

2-Component Library

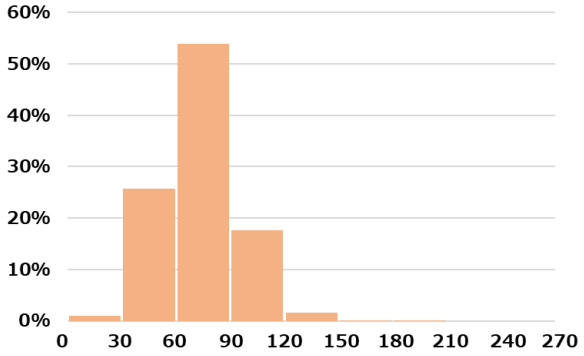
MW



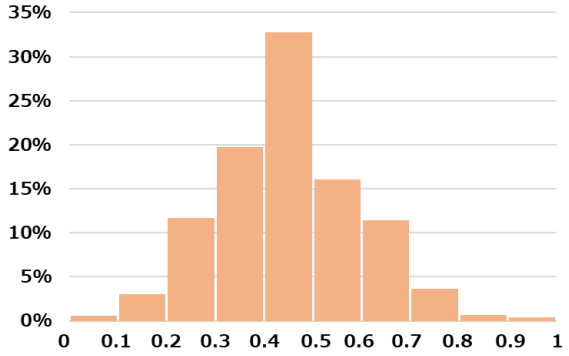
SlogP



TPSA

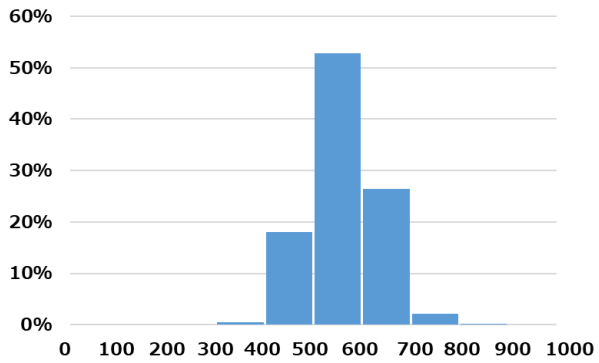


Fsp3

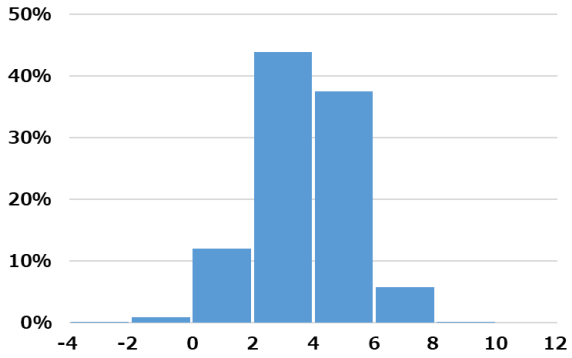


3-Component Library

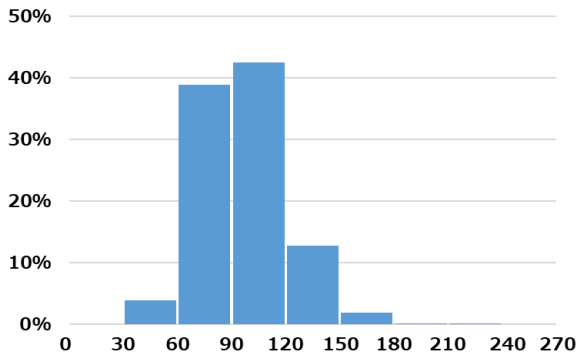
MW



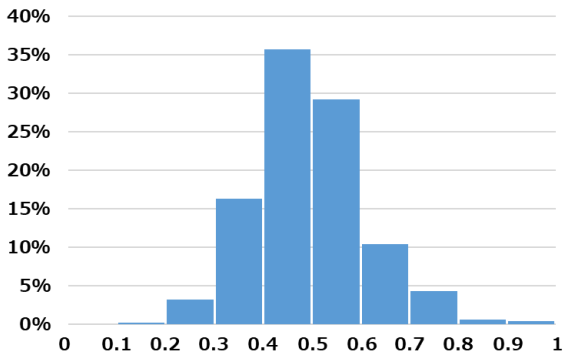
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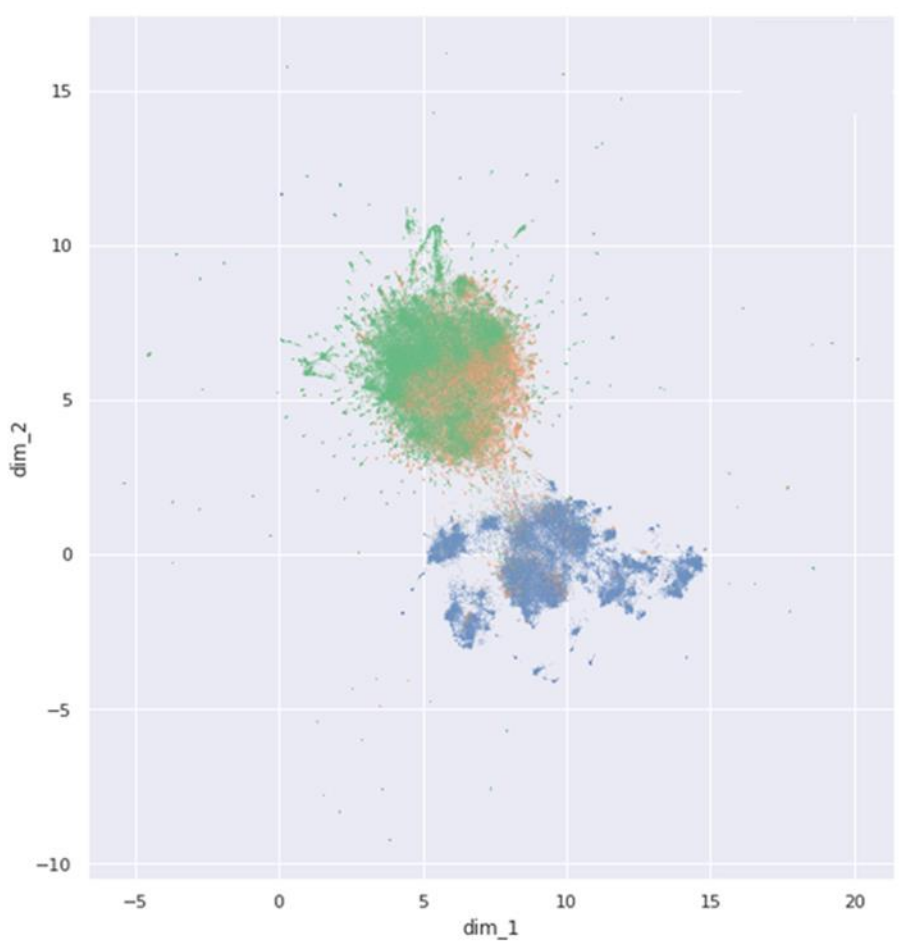
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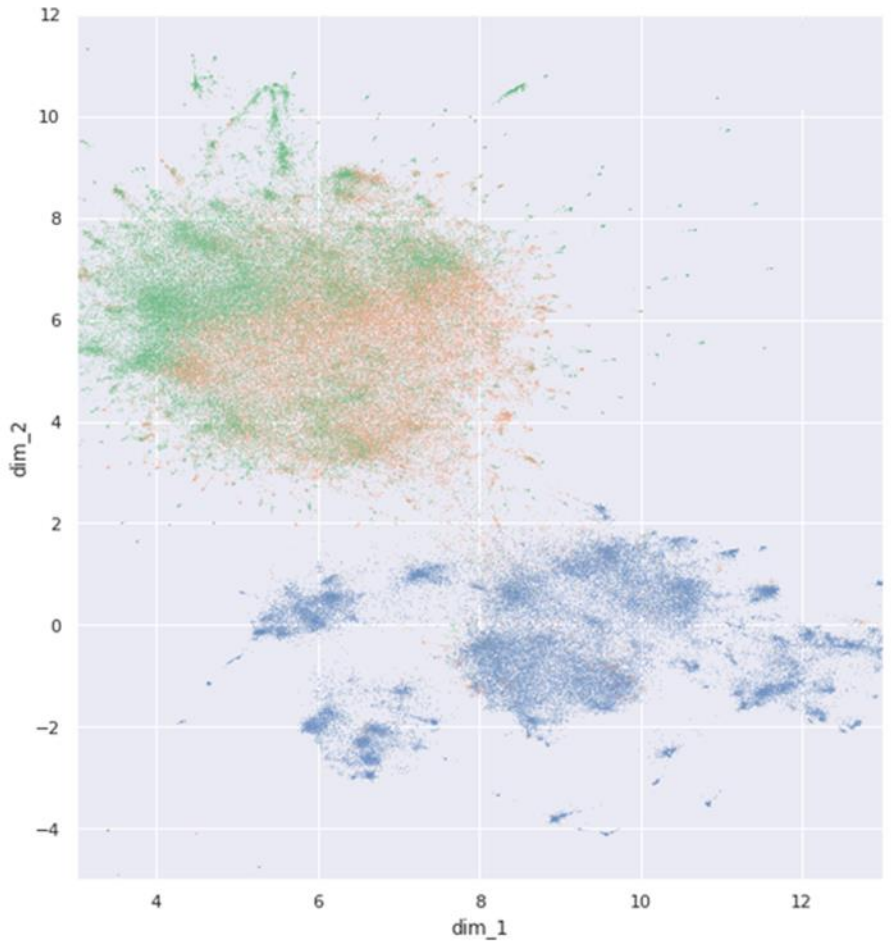


Fsp3



Chemical space

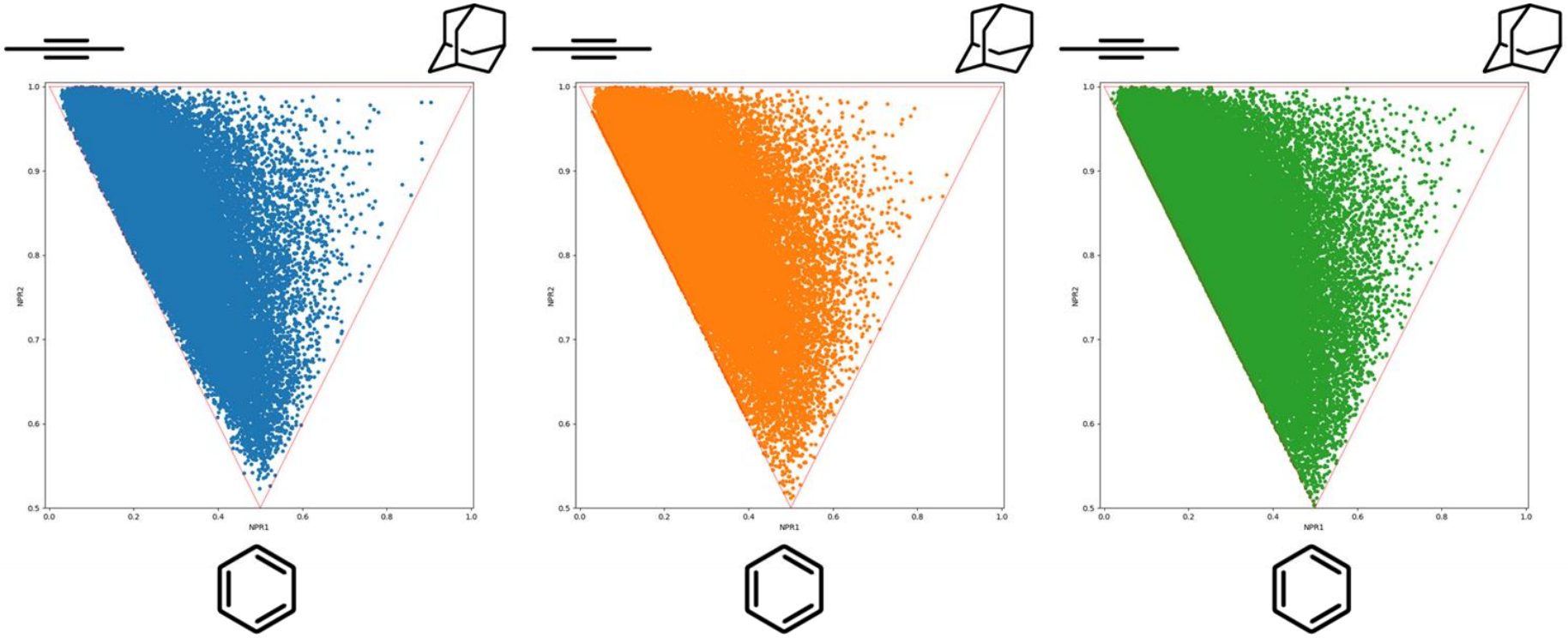






市販品ライブラリー及び公共データベースとの比較より、K-LBは異なるケミカルスペースを保有している

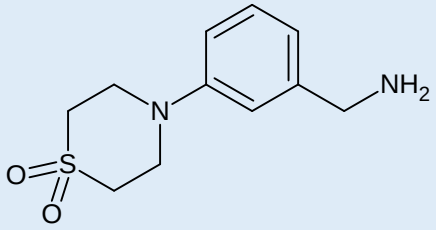
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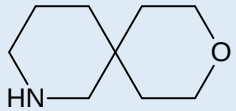


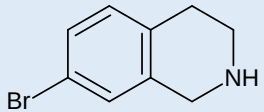
３次元構造の分布に大きな差はなし

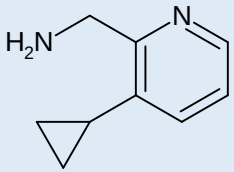
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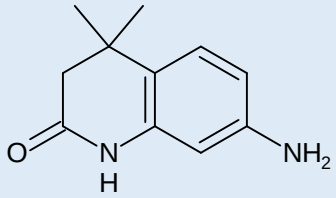
Amines





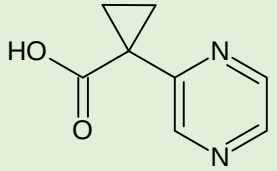


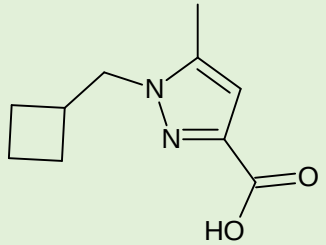


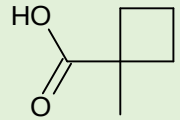


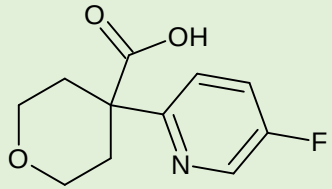
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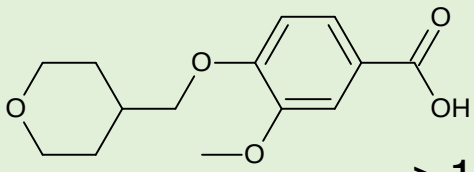
Carboxylic acids









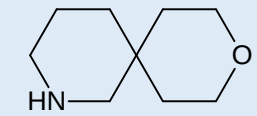


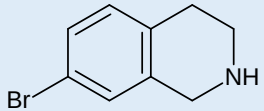
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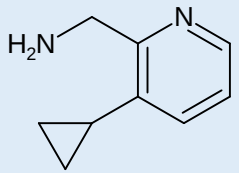
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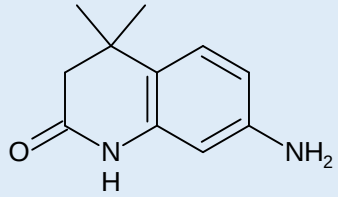
3-Component library

Amines

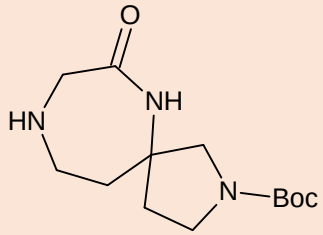


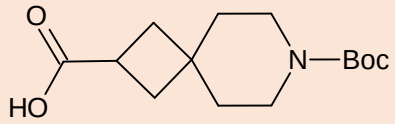


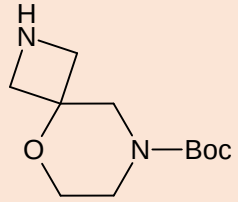


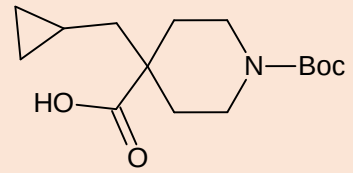


Bi-functional BBs

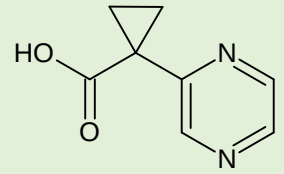


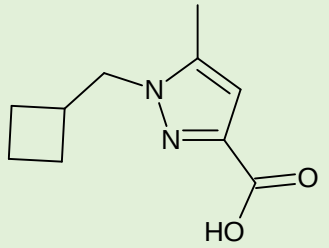


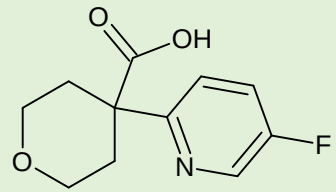


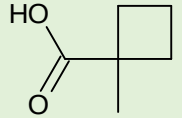


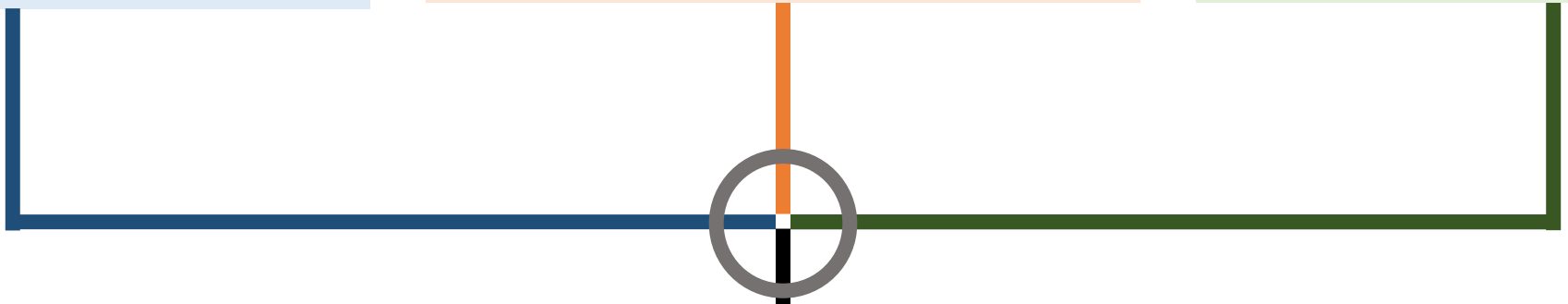
Carboxylic acids











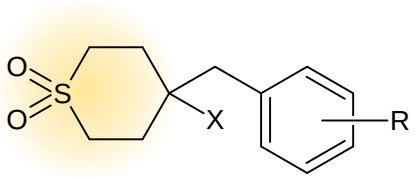
3-component Library

キシダオリジナル
ビルディングブロック（K-BB）

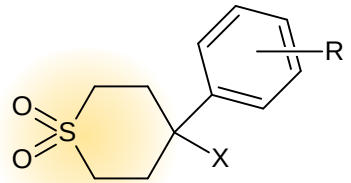
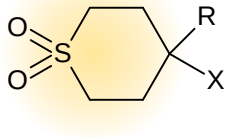
-その他-

表記の構造式には塩を反映しておりません.

Tetrahydrothiopyran dioxide analogs

Structure	R	X=NH_2	X=COOH
	H	PK0-39661	PK0-32691
	o-OMe	PK0-43231	PK0-43211
	m-OMe	PK0-54111	PK0-41781
	p-OMe	PK0-54121	PK0-41331
	o-Cl	PK0-41811	PK0-41771
	m-Cl	PK0-53991	PK0-42001
	p-Cl	PK0-43531	PK0-43481
	o-F	PK0-41791	PK0-41751
	m-F	PK0-42021	PK0-41991
	p-F	PK0-41801	PK0-41761
	o-CF_3	PK0-43541	PK0-42011
	m-CF_3	PK0-45381	PK0-43491
	p-CF_3	PK0-45391	PK0-43501

65
analogs

Structure	R	X=NH_2	X=COOH
	H	PK0-49861	PK0-49721
	o-Cl	PK0-53781	PK0-53971
	m-Cl	PK0-53581	PK0-53981
	p-Cl	PK0-53541	PK0-53771
	o-F	PK0-53561	PK0-53951
	m-F	PK0-53571	PK0-53961
	p-F	PK0-53401	PK0-53761
	Me	PK0-39651	PK0-32681
	Et	PK0-42381	PK0-41981
	iBu	PK0-42781	PK0-42351
	CH_2-cPr	PK0-43221	PK0-42361
	CH_2-cBu	PK0-42391	PK0-42371
	$CH_2CH_2OCH_3$	PK0-43521	PK0-42761
	2-Py-CH_2	PK0-42791	PK0-42771
	3-Py-CH_2	PK0-53531	PK0-43511

青字はScifinderで提供サプライヤーが限られた製品です.

＜参考情報＞

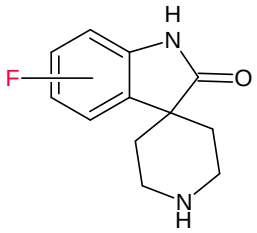
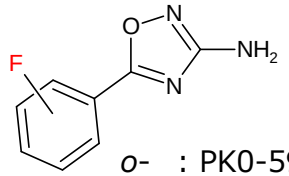
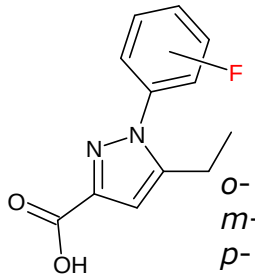
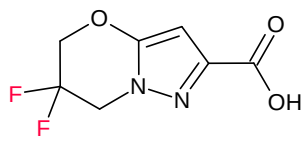
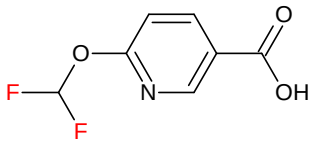
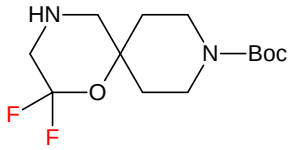
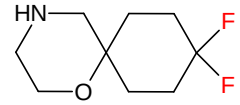
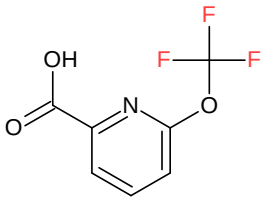
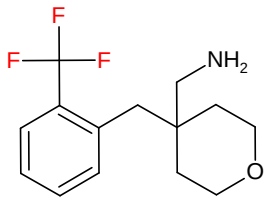
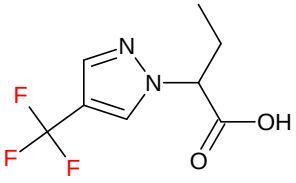
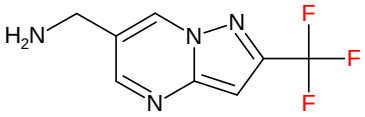
Tetrahydrothiopyran dioxide骨格の導入が、薬効・非薬効に効果的だった事例

5-Chloroindoloyl glycine amide inhibitors of glycogen phosphorylase: synthesis, in vitro, in vivo, and X-ray crystallographic characterization.
Bioorg. Med. Chem. Lett. **2005**, *15*, 459-465.

Fluorinated building blocks

各種のScaffoldに対して、
フッ素原子を積極的に導入

1912
analogs

種類	構造例
モノフルオロ	 4- : PK0-47851 5- : PK0-32651 6- : PK0-31761 7- : PK0-55261  *o*- : PK0-59201 *m*- : PK0-59211 *p*- : PK0-59221  *o*- : PK0-59411 *m*- : PK0-59321 *p*- : PK0-59331
ジフルオロ	 PK0-38871  PK0-28881  PK0-59081  PK0-59481
トリフルオロ	 PK0-29161  PK0-59551  PK0-59601  PK0-59751

当社のBBを活用したFBDDにより、ヒット化合物を取得した論文

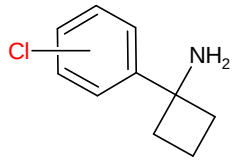
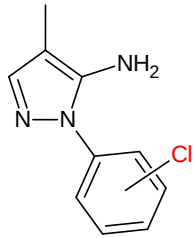
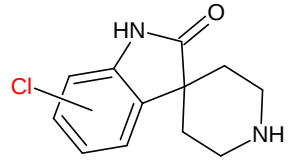
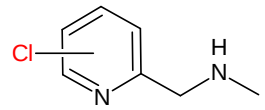
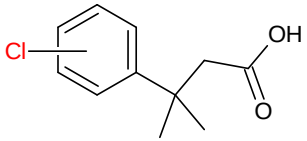
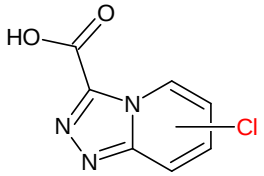
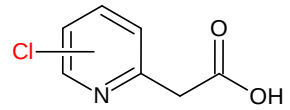
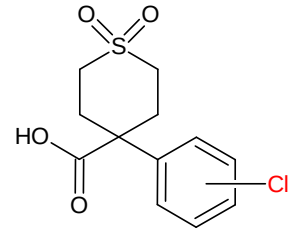
Comprehensive approach of ^{19}F nuclear magnetic resonance, enzymatic, and In Silico methods for site-specific hit selection and validation of fragment molecules that inhibit Methionine γ-Lyase activity. Kazuyoshi Ikeda, Yuichiro Kezuka, Takamasa Nonaka, Tomoki Yonezawa, Masanori Osawa, and Etsuko Katoh *J.Med.Chem.* **2021**, *64*, 14299-14310.

Chlorinated building blocks

クロル基導入の効果

- 酸性度の上昇 (塩基性度の低下)
- Me基と近いファンデルワールス半径
- “acceptor”または”donor”として機能
- 配座制御
- 疎水性相互作用の増大

313
analogs

種類	構造例			
アミン	 *o*- : PK0-09901 *m*- : PK0-09921	 *o*- : PK0-14681 *m*- : PK0-14311 *p*- : PK0-14321	 4- : PK0-31771 5- : PK0-32191 6- : PK0-31231 7- : PK0-41011	 3- : PK0-55991 4- : PK0-58791 5- : PK0-54771 6- : PK0-54571
カルボン酸	 *o*- : PK0-27091 *m*- : PK0-27101 *p*- : PK0-27111	 5- : PK0-36701 6- : PK0-37651 8- : PK0-37671	 3- : PK0-47471 5- : PK0-47311 6- : PK0-46101	 *o*- : PK0-53971 *m*- : PK0-53981 *p*- : PK0-53771

<参考情報>
創薬研究における塩素原子の効果（Magic Chloro）
“Magic Chloro”: Profound Effects of the Chlorine Atom in Drug Discovery
J. Med. Chem. 2023, 66, 5305-5331.

参考情報

K-BB・K-LBをご活用いただいた研究論文

K-BB

1. A combination of19F NMR and surface plasmonresonance for site-specific hit selection and validation of fragment molecules that bind to the ATP-binding site of a kinase. *Bioorg.Med.Chem.* **2018**, *26*, 1929-1938.

2. Comprehensive approach of ^{19}F nuclear magnetic resonance, enzymatic, and In Silico methods for site-specific hit selection and validation of fragment molecules that inhibit Methionine γ-Lyase activity. *J.Med.Chem.* **2021**, *64*, 14299-14310.

K-LB

1. Identification of novel inhibitors of Keap1/Nrf2 by a promising method combining protein–protein interaction-oriented library and machine learning. *Scientific Reports*, **2021**, *11*, 7420.

2. DLiP-PPI library: An integrated chemical database of small-to-medium-sized molecules targeting protein-protein interactions. *Front. Chem.*, **2023**, *10*, 1090643.

3. Applying deep learning to iterative screening of medium-sized molecules for protein-protein interaction-targeted drug discovery. *Chem. Commun.*, **2023**, *59*, 6722.