

キシダオリジナル ビルディングブロック (K-BB)

- Scaffold別 -



KISHIDA

2021年11月版

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

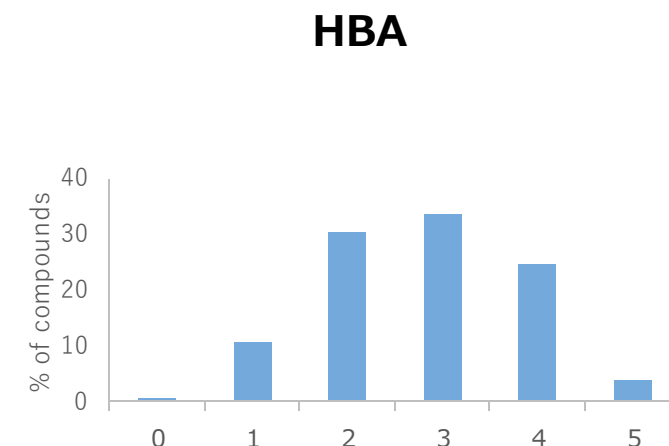
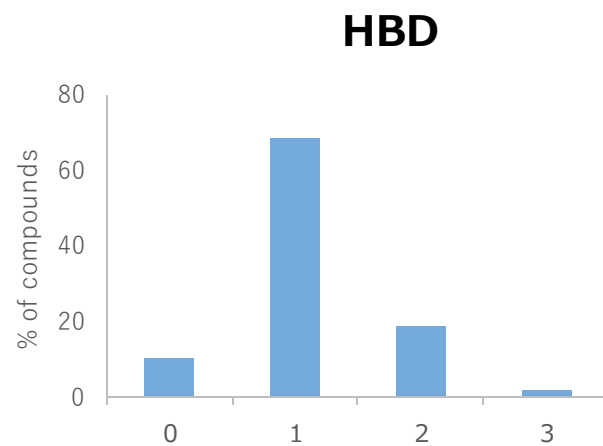
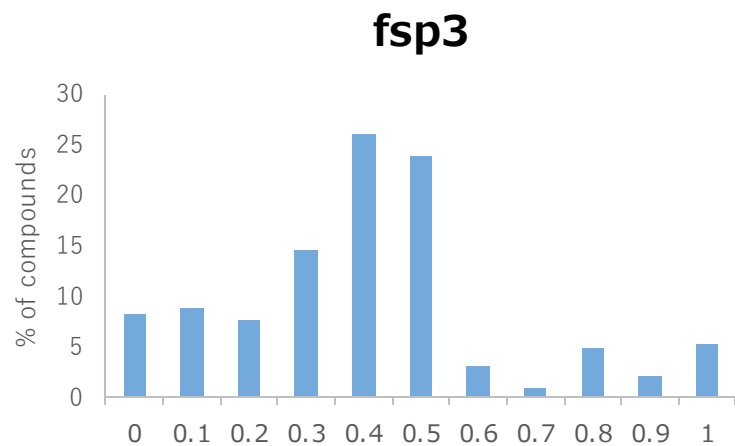
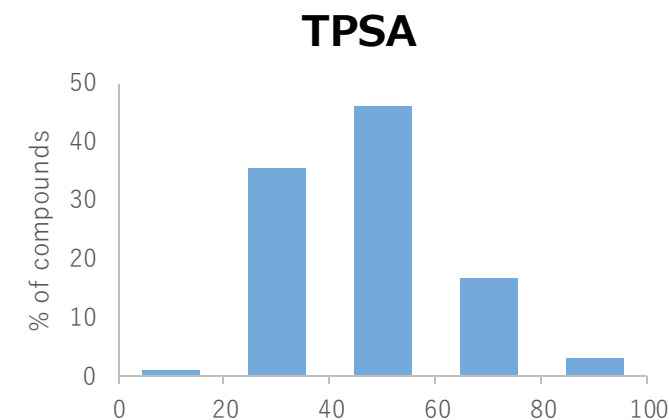
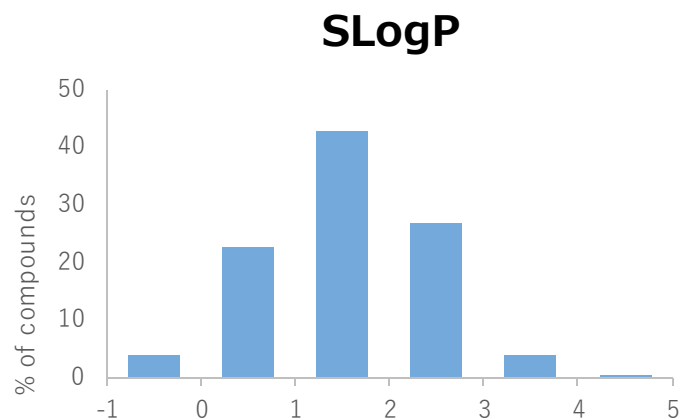
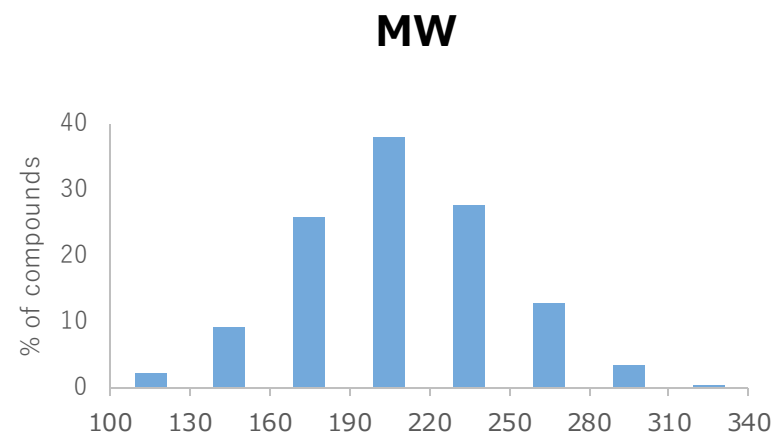
K-BBは、コンセプトは？

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（2021年10月末現在：6,183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、**低価格**にてご提供します。また、**スケールアップ**にも対応可能です
- ◆ 1gでラインナップしています。100, 250, 500mgの**小分け販売**も承ります
- ◆ 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
- ◆ **ラインナップにないBB**のご相談も承ります

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

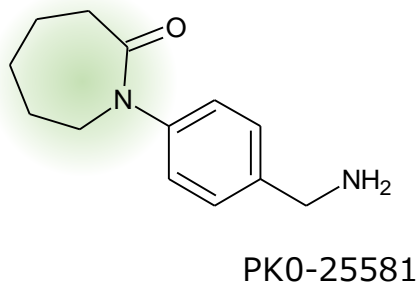
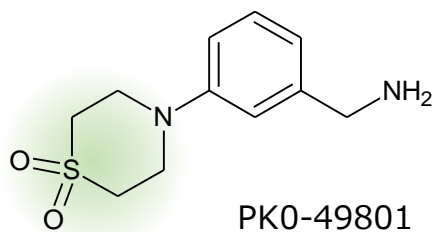
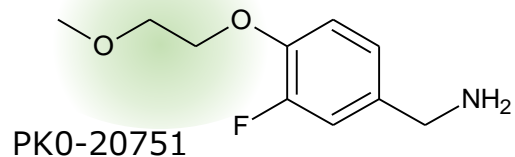
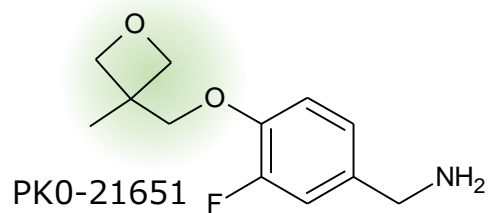
キシダオリジナル ビルディングブロック (K-BB)

-アミン-

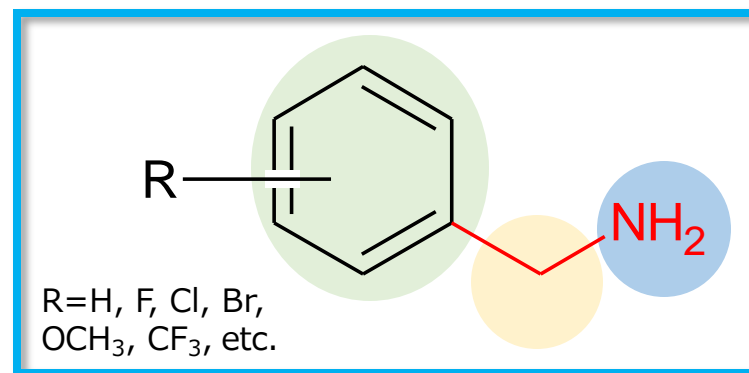
赤字は2021年6月版以降の更新分（新製品）

 は新たに追加したスライド

Benzylamine analogs



35~
analogos

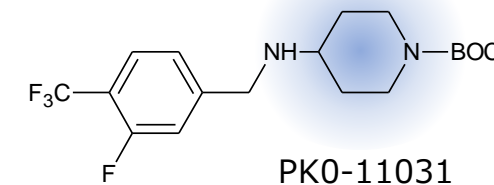
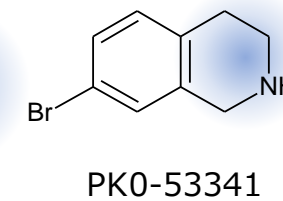
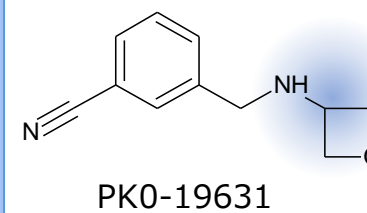


169
(167+2)~
analogos



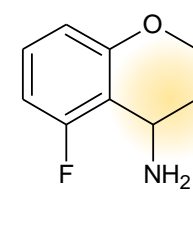
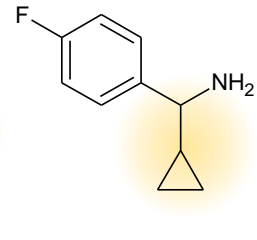
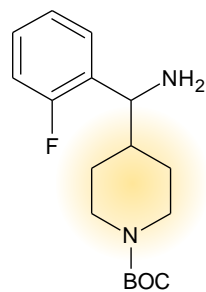
174~
analogos

N-alkyl type



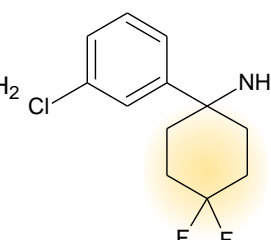
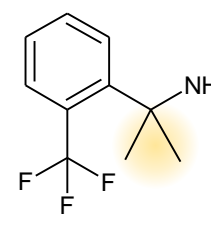
Mono-alkyl type

57~analogos



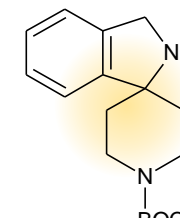
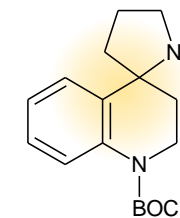
Di-alkyl type

114~analogos

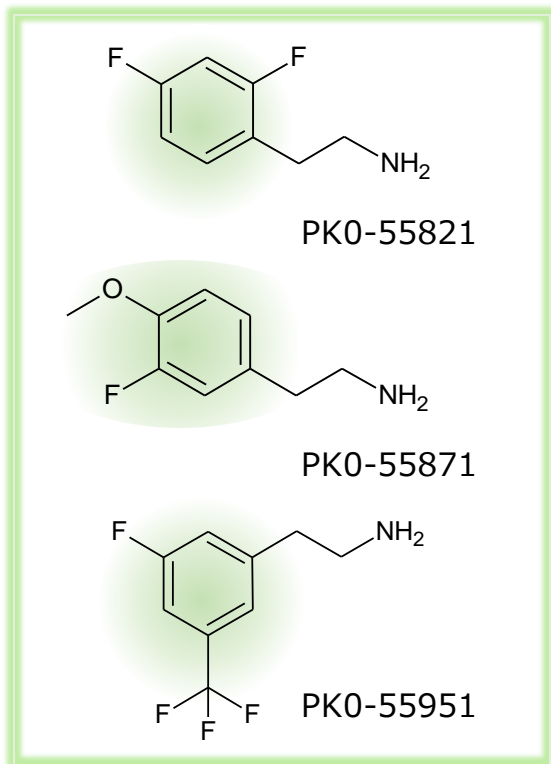


Cyclic type

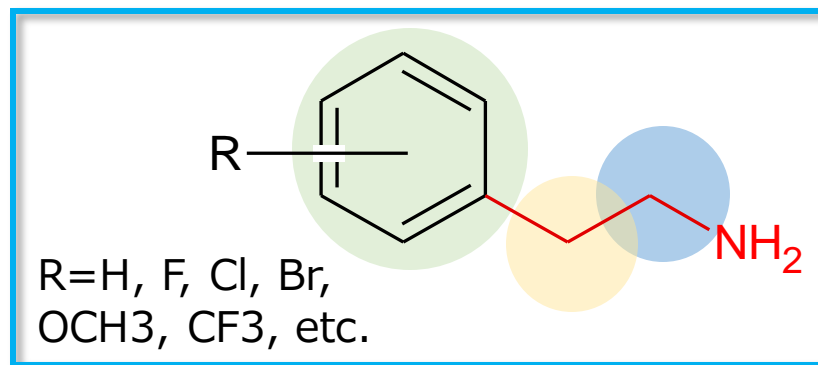
3~analogos



Homo-benzylamine analogs

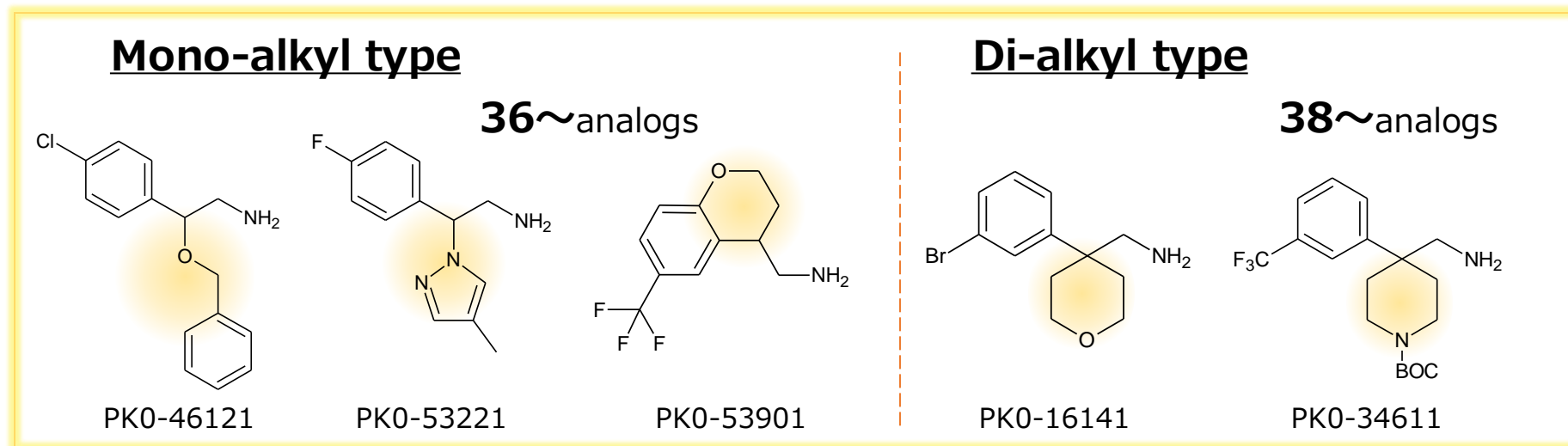
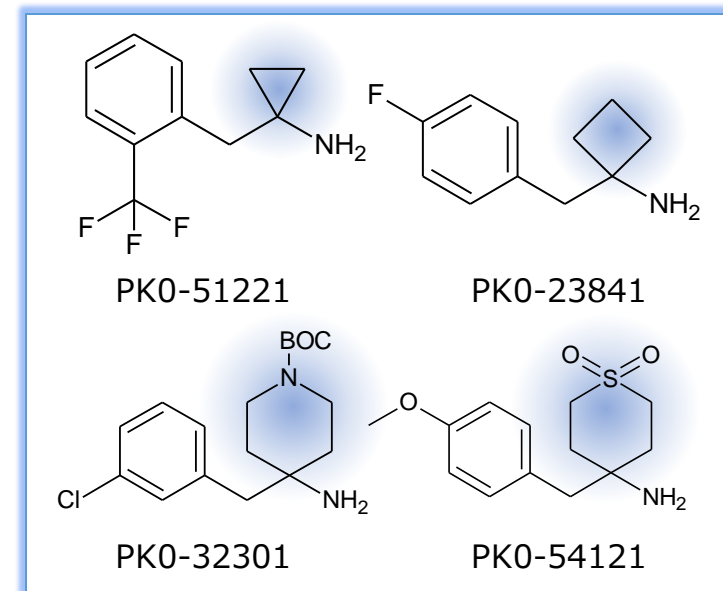


18~
analog

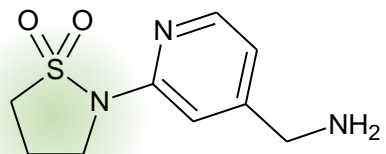


75(74+1)~
analog

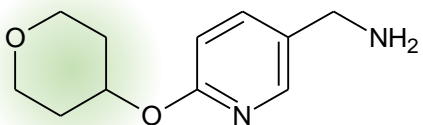
97~
analog



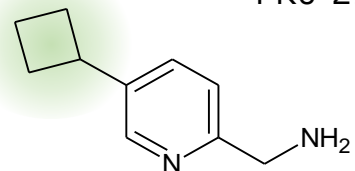
Picolylamine analogs



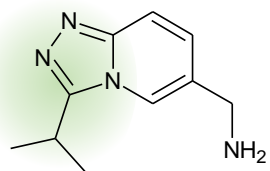
PK0-49701



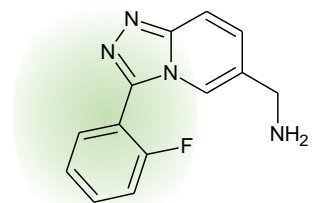
PK0-21201



PK0-53301



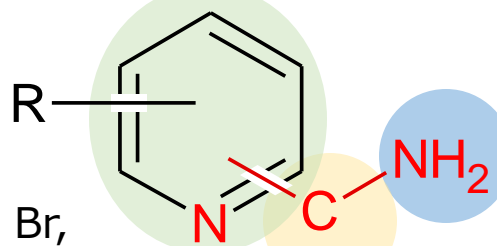
PK0-23061



PK0-22081



80~
analog



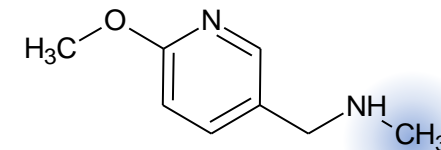
R=H, F, Cl, Br,
OCH3, CF3, etc.



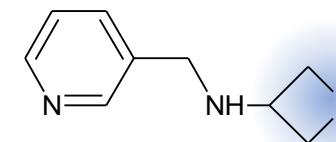
51~
analog



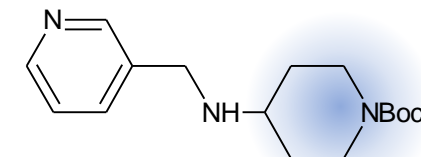
34~
analog



PK0-56061

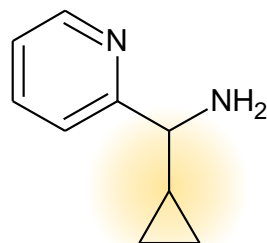


PK0-14801

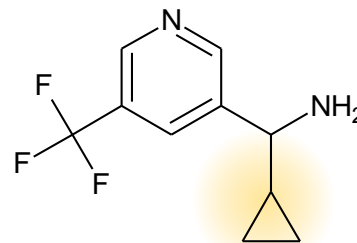


PK0-10991

Mono-alkyl type

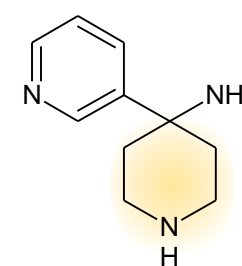


PK0-44761

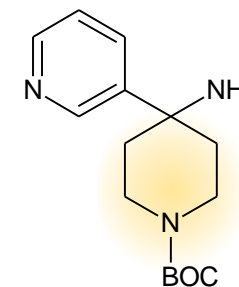


PK0-44831

Di-alkyl type

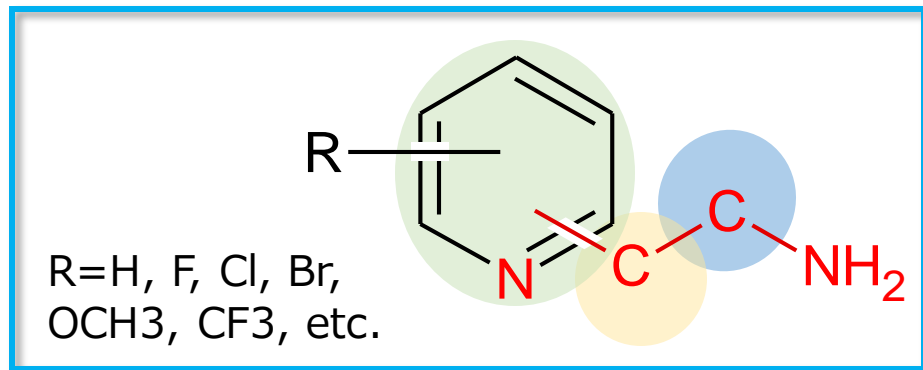


PK0-34501

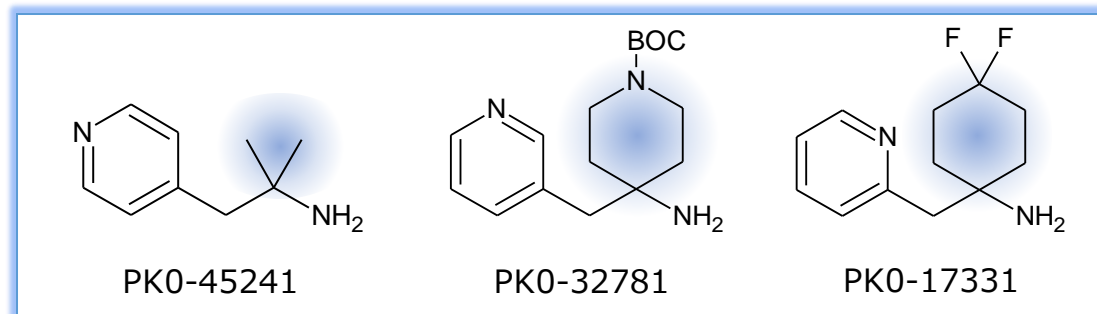


PK0-34471

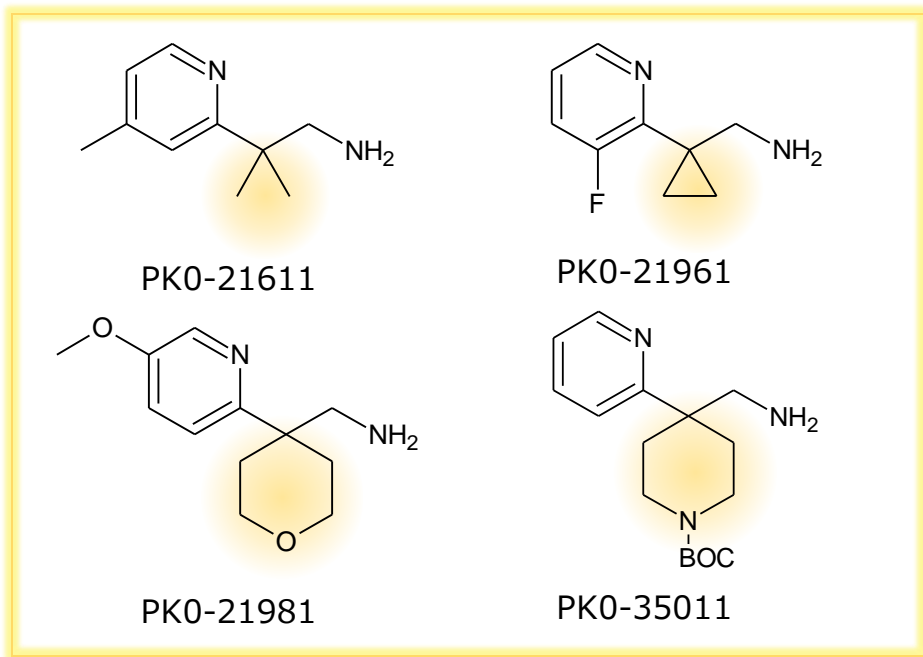
Aminoethylpyridine analogs



19~
 analogs



38~
 analogs

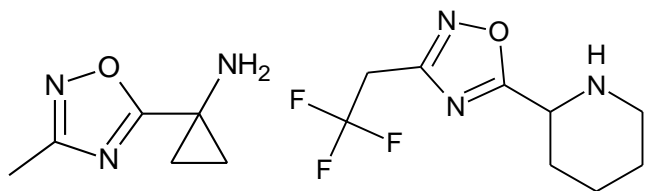


組み合わせにより、幅広いSARを取得できます

	 H_3C CH_3		
	PK0-21611	PK0-22011	PK0-22551
	PK0-21631	PK0-21591	PK0-21601
	PK0-23331	PK0-22501	PK0-38921

Azole-methylamine analogs

Oxadiazoles



PK0-15321

PK0-19971

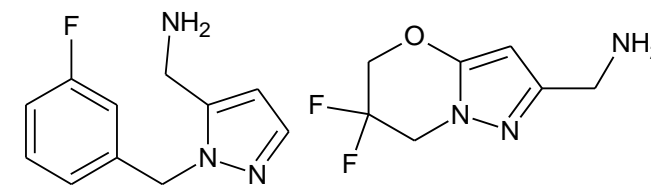
23~
analog



33(23+10)~
analog



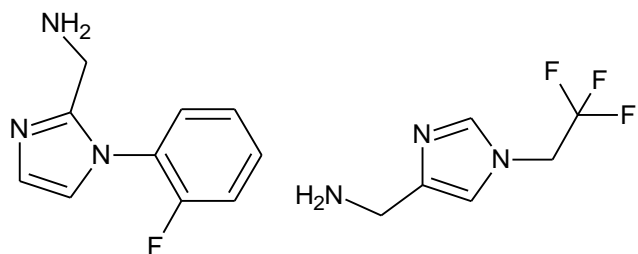
Pyrazoles



PK0-57831

PK0-50441

Imidiazoles



PK0-54531

PK0-30751

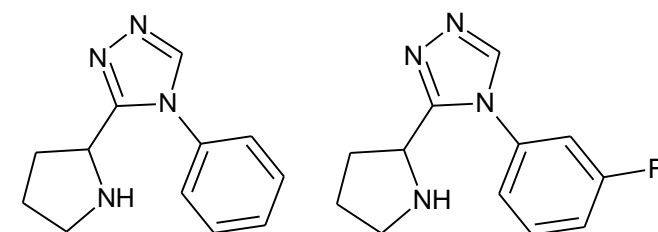
40(34+6)~
analog



4~
analog

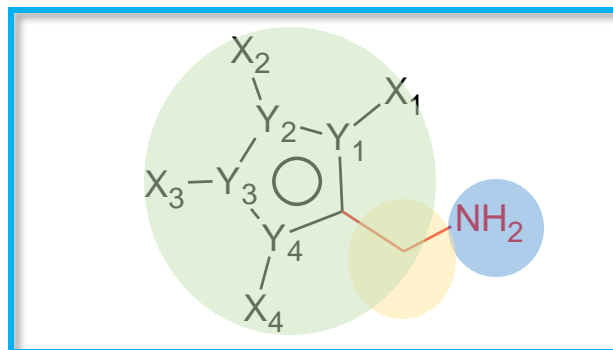


Triazoles

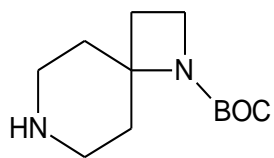


PK0-53601

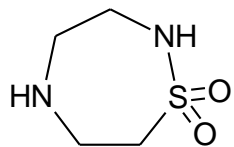
PK0-53801



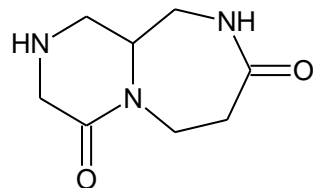
Aliphatic amine analogs



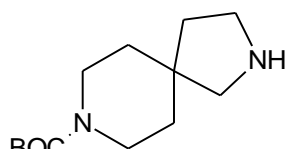
PK0-21751



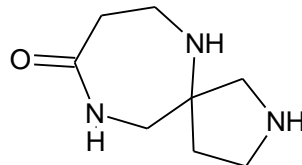
PK0-55131



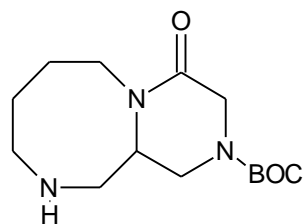
PK0-52841



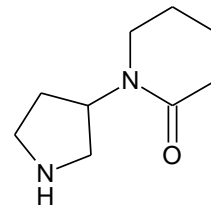
PK0-17991



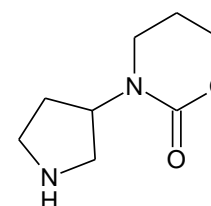
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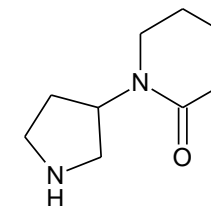
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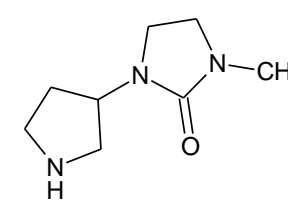
PK0-53811



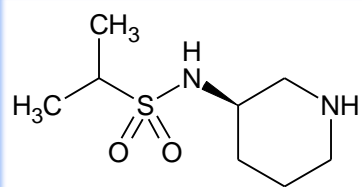
PK0-54131



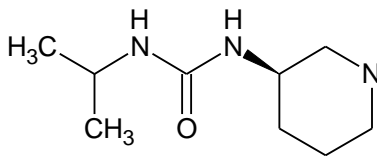
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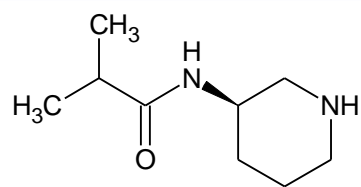
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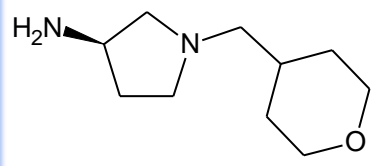
PK0-08771



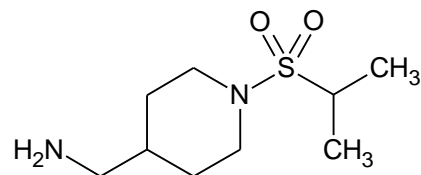
PK0-08961



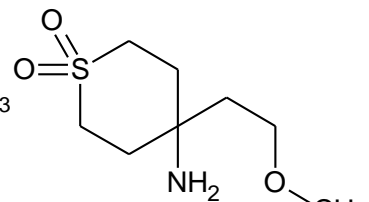
PK0-08101



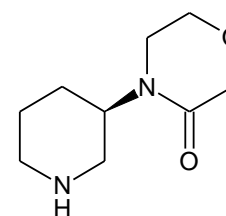
PK0-07301



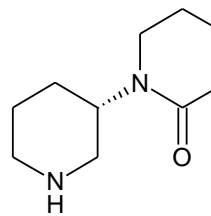
PK0-07761



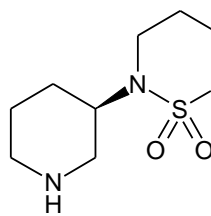
PK0-43521



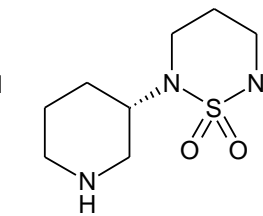
PK0-56801



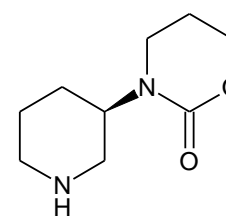
PK0-56581



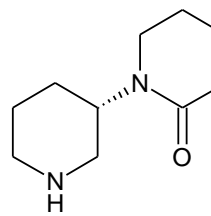
PK0-56831



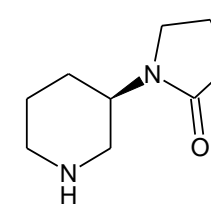
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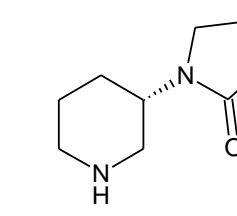
PK0-56811



PK0-56591



PK0-56841

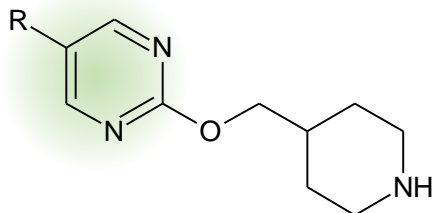


PK0-56611

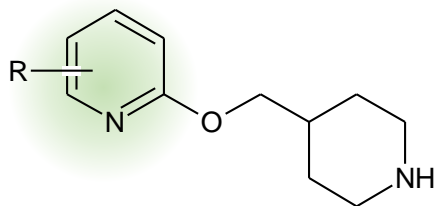


510~
analog

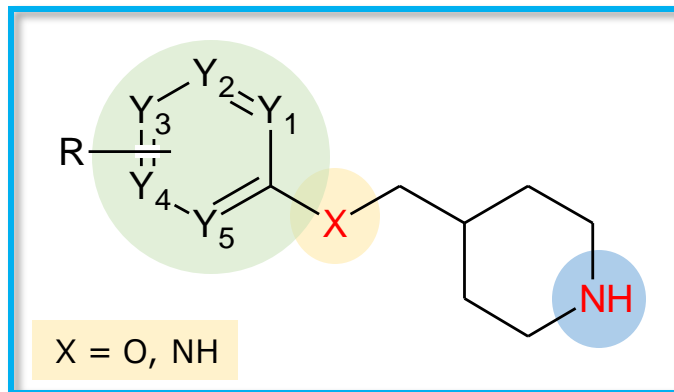
Piperidine analogs



R=H : PK0-55431
R=F : PK0-55621
R=Cl : PK0-55491
R=OCH₃ : PK0-55731



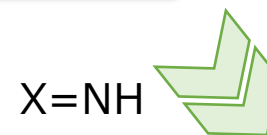
R=3-F : PK0-55591
R=3-CF₃ : PK0-55471
R=6-CF₃ : PK0-55451



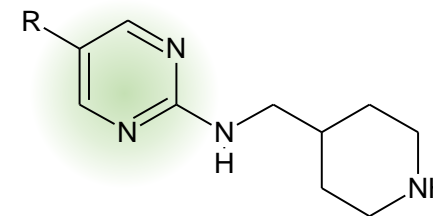
X = O, NH



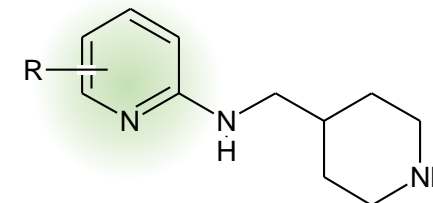
41~
analogs
(Ph体含)



38~
analogs
(Ph体含)



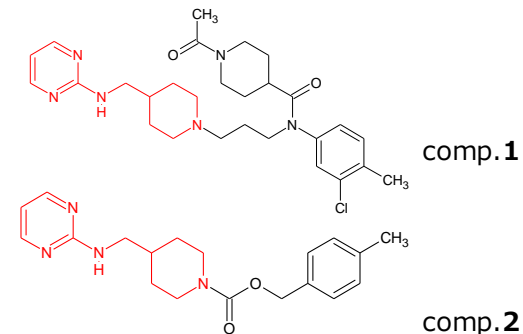
R=H : PK0-55681
R=F : PK0-55581
R=Cl : PK0-55421
R=OCH₃ : PK0-55701



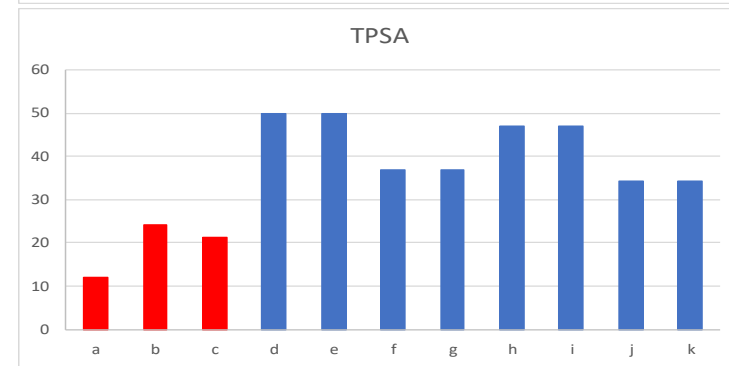
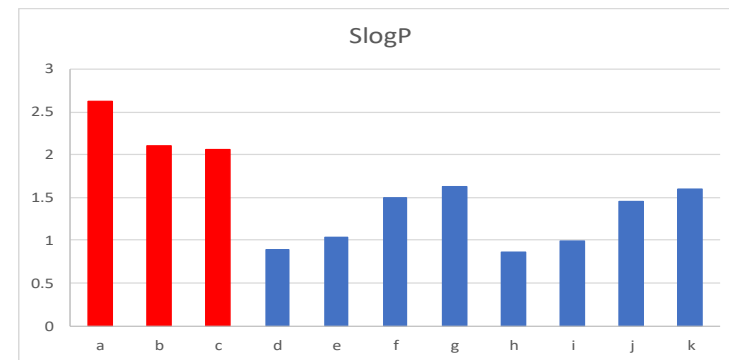
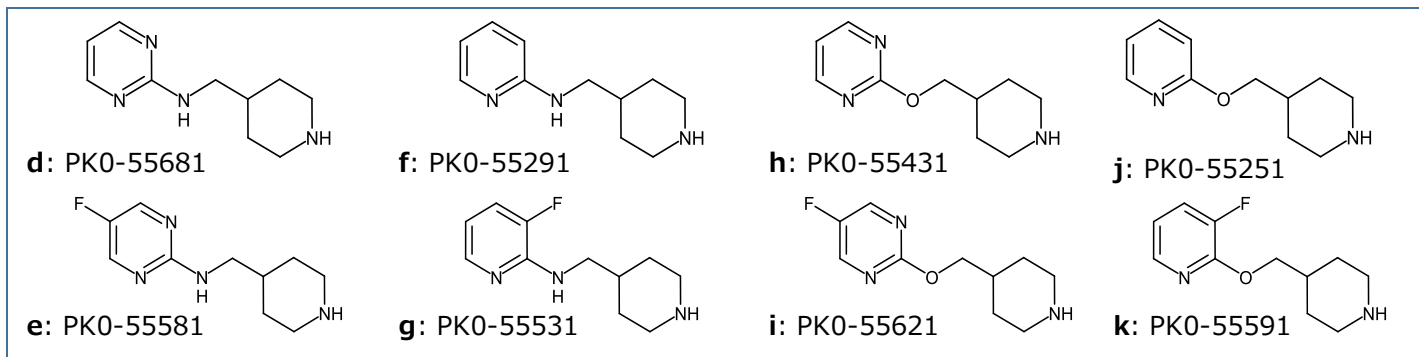
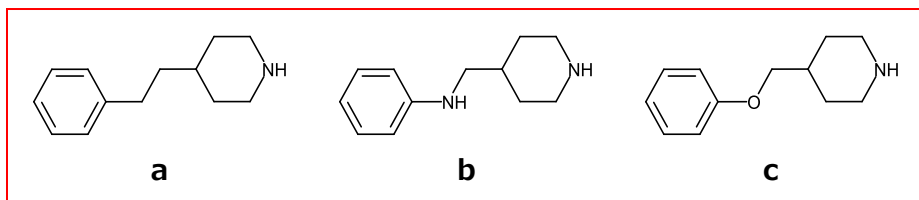
R=H : PK0-55291
R=3-F : PK0-55531
R=3-CF₃ : PK0-55401
R=6-CF₃ : PK0-55381

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

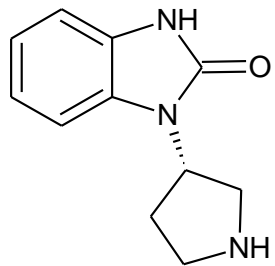


ヘテロ環の導入した当社のPiperidine analogsの利用により、市販されている化合物a-cに比べ、SlogPの低減とTPSAの向上が期待できます

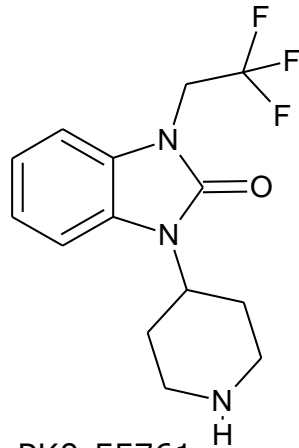


SlogP and TPSA of compd. a-k

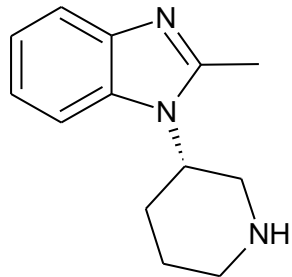
3/4-Aminoepiperidine & 3-amino pyrrolidine analogs



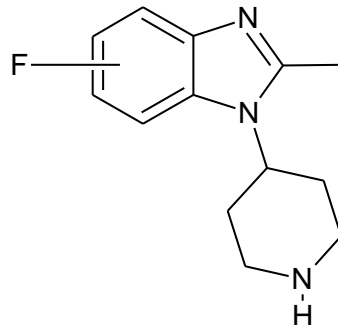
PK0-56661



PK0-55761



PK0-56531



4-: PK0-57261

5-: PK0-57251

6-: PK0-57241

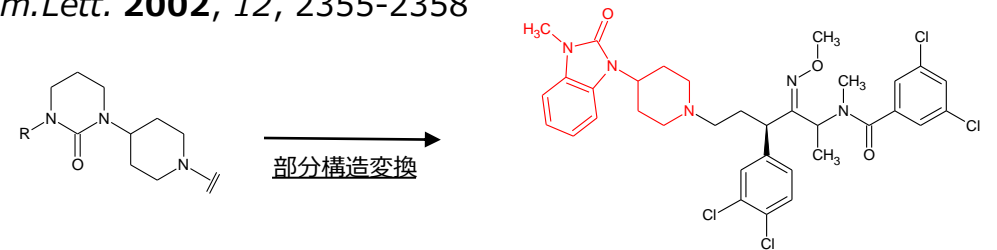
7-: PK0-57231



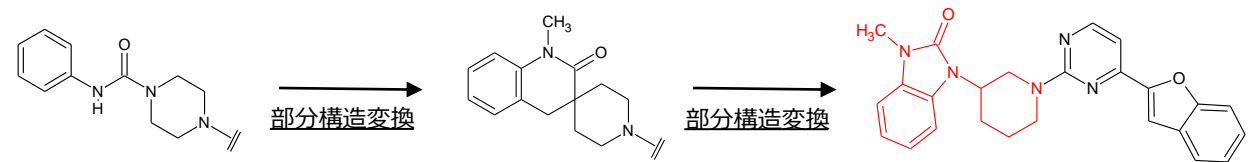
22~
analogues

<参考情報 / K-BB構造が導入されている事例>

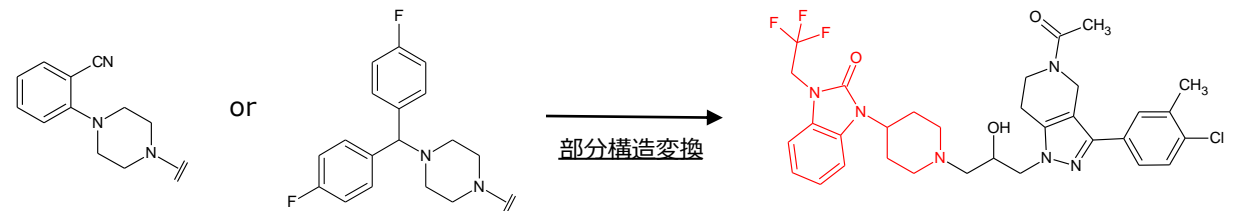
1. 1桁ナノモルのNK1/NK2親和性とNK3に対する選択性を有する化合物群の骨格として導入
Preparation of oxime dual NK1/NK2 antagonists with reduced NK3 affinity
Bioorg.Med.Chem.Lett. **2002**, *12*, 2355-2358



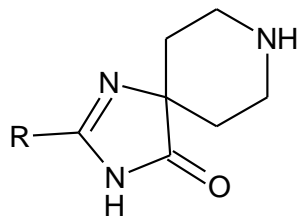
2. PK0-55741、56491などBB構造を含む複数化合物のFAAH阻害活性を報告
Identification of potent, noncovalent fatty acid amide hydrolase (FAAH) inhibitors
Bioorg.Med.Chem.Lett. **2011**, *21*, 2492-2496



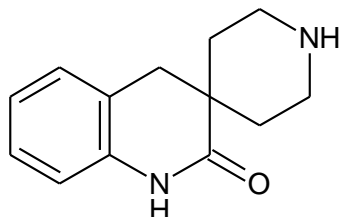
3. 4-arylpiperazine moietyの等価体としてPK0-55761などの導入結果が報告
Discovery and SAR studies of a novel series of noncovalent cathepsin S inhibitors
Bioorg.Med.Chem.Lett. **2005**, *15*, 1687-1691



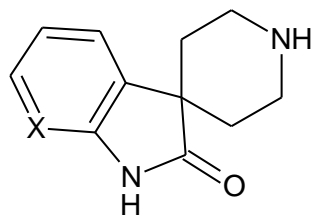
Spiro-piperidine analogs



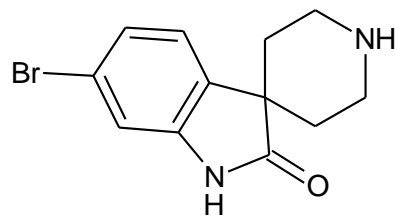
R=Me; PK0-30321
R=Ph; PK0-30261



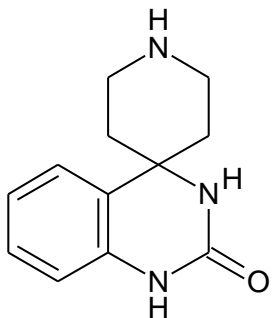
PK0-15451



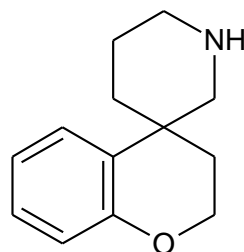
X=CH; PK0-31191
X=N; PK0-51511



PK0-31791



PK0-57891



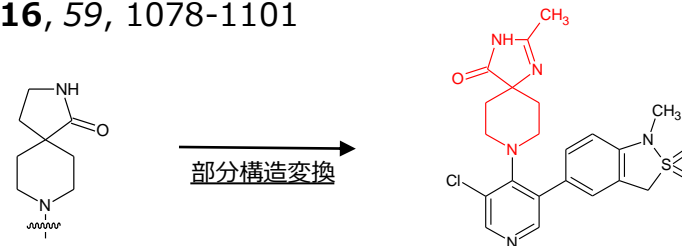
PK0-57681



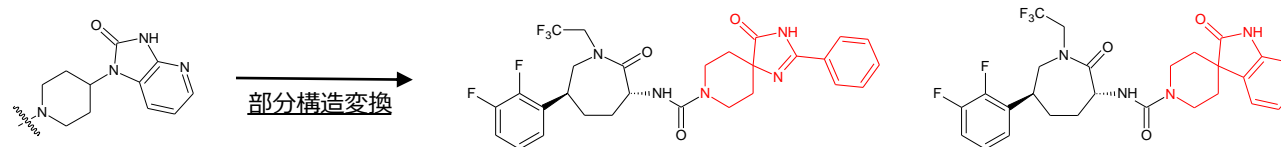
48(46+2)~
analog

<参考情報 / K-BB構造が導入されている事例>

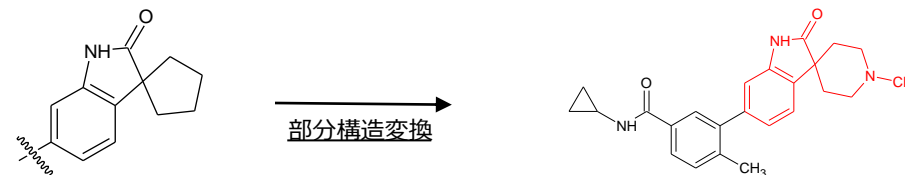
- 2,8-diazaspiro[4.5]decan-1-one等価体の探索でPK0-30321の導入結果が報告
Discovery of Potent, Selective, and Orally Bioavailable Small-Molecule Modulators of the Mediator Complex-Associated Kinases CDK8 and CDK19
J. Med. Chem. **2016**, *59*, 1078-1101



- 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 spiro-piperidines
Bioorg. Med. Chem. Lett. **2009**, *19*, 6368-6372



- Spiroindolone部分の返還でPK0-31791を用いた代替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



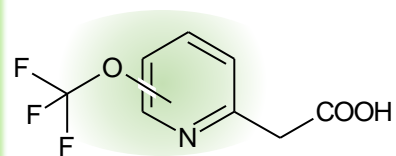
キシダオリジナル ビルディングブロック (K-BB)

-カルボン酸-

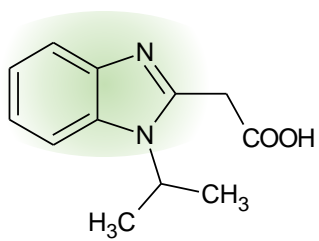
赤字は2021年6月版以降の更新分（新製品）

は新たに追加したスライド

Phenylacetic acid analogs

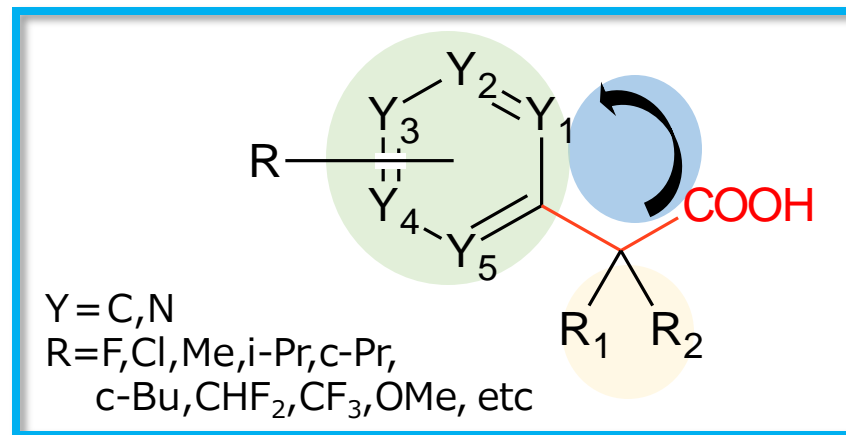


4- : PK0-40741
5- : PK0-40751
6- : PK0-40771



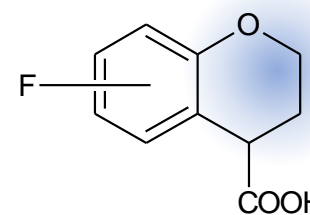
PK0-53931

50~
analog

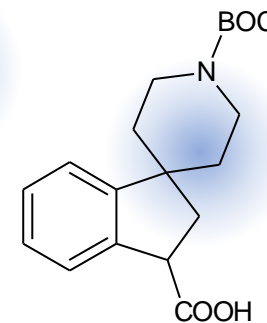


10
(6+4)~
analog

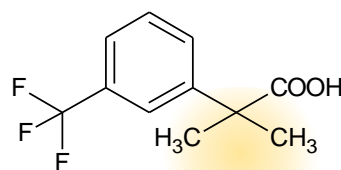
157(145+12)~
analog



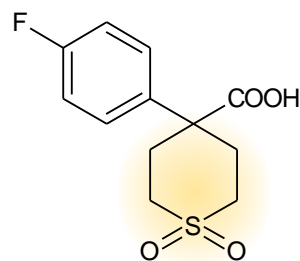
5-: PK0-52511
6-: PK0-52521
7-: PK0-52531
8-: PK0-52381



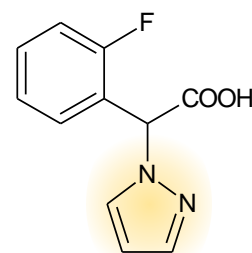
PK0-48101



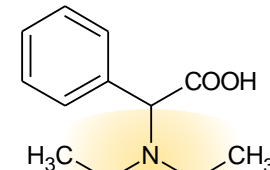
PK0-25631



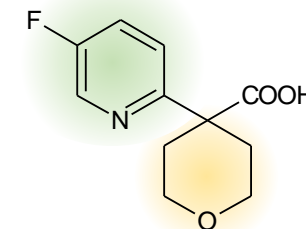
PK0-53761



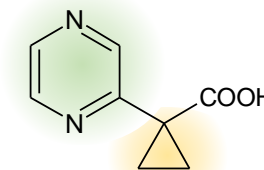
PK0-52691



PK0-51941

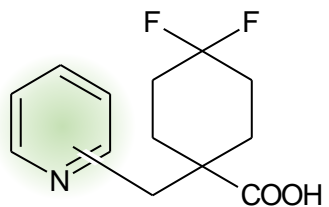


PK0-21701

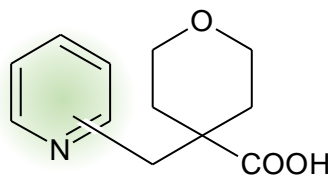


PK0-22151

Phenylpropionic acid analogs



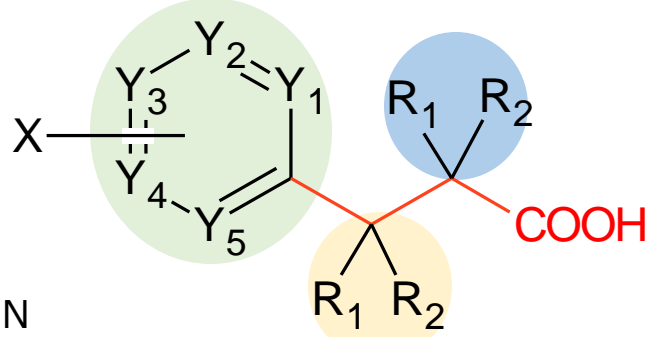
2-yl : PK0-17261
3-yl : PK0-17271
4-yl : PK0-17281



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



17~
analog



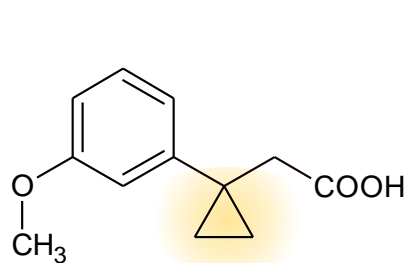
Y = C or N
R = H, F, Cl, Br, Me, OMe, CF₃



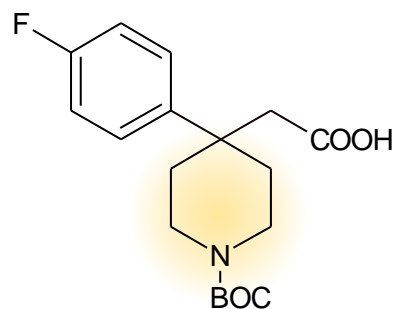
93~
analog



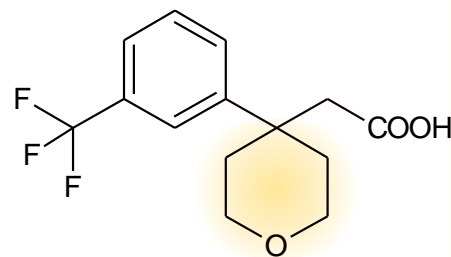
107~
analog



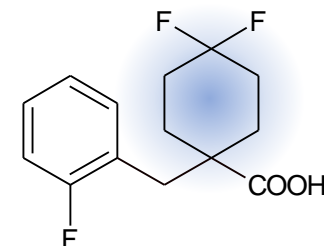
PK0-50681



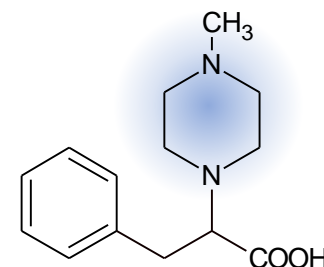
PK0-28321



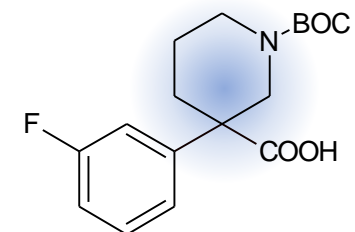
PK0-27591



PK0-16591

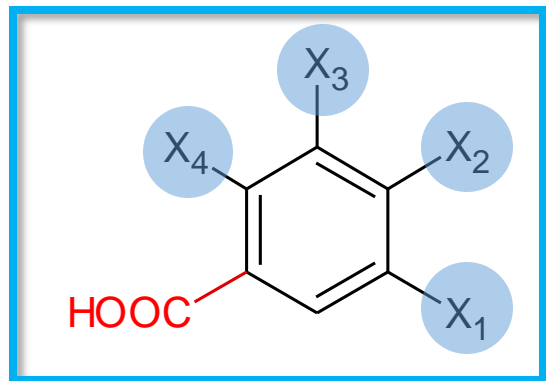


PK0-52211



PK0-54201

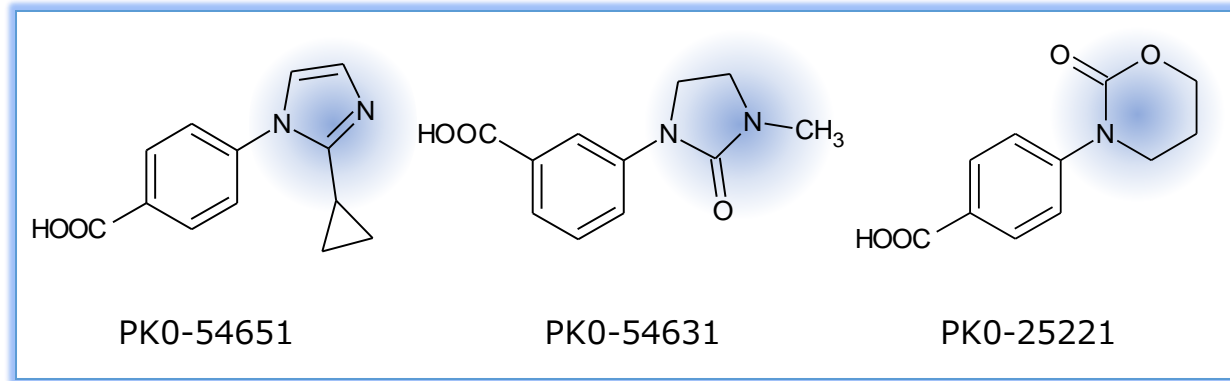
Benzoic acid analogs



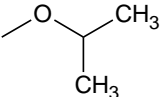
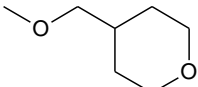
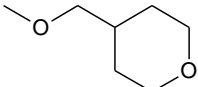
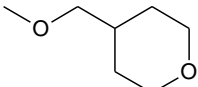
Mono functional



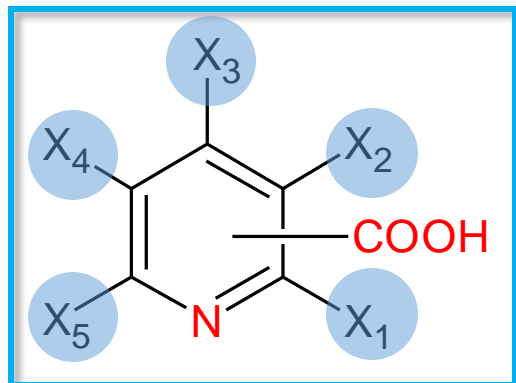
38(27+11)~
analogs



Multi functional  **26~**
analogs

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

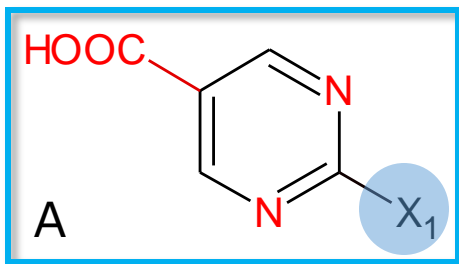
Pyridine-carboxylic acid analogs



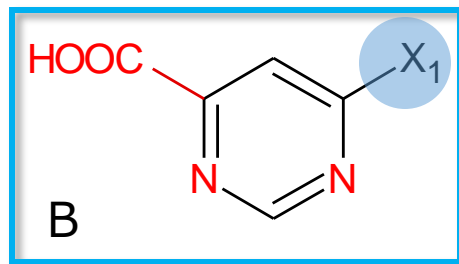
189~
analogs

		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	-	-	-

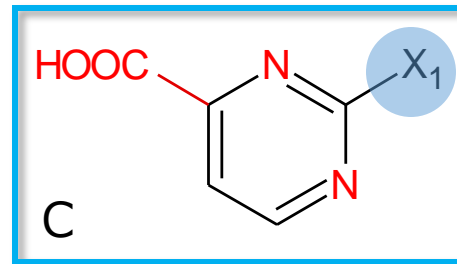
Pyrimidine-carboxylic acid analogs



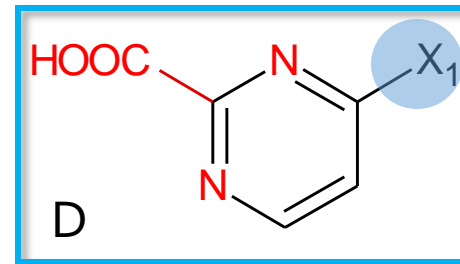
23~
analog



19~
analog



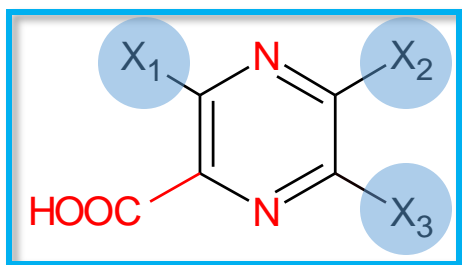
11~
analog



11~
analog

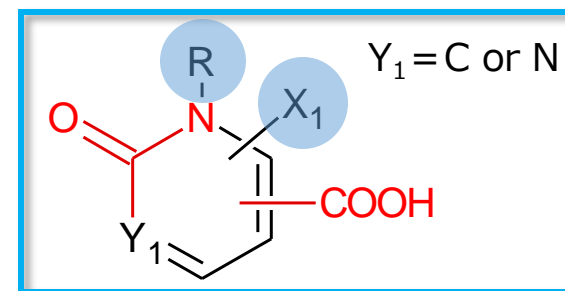
X ₁	A型	B型	C型	D型
-OEt	PK0-19471	PK0-21481	PK0-43091	PK0-43421
-OCH ₂ CF ₃	PK0-21021	PK0-22321	PK0-43741	PK0-49771
-OCH ₂ CH ₂ OCH ₃	PK0-20651	PK0-22891	PK0-43101	PK0-43781
	PK0-21031	PK0-24841	PK0-43761	PK0-42701
	PK0-21891	PK0-24831	PK0-43731	PK0-43151

Pyrazine/Pyridone/Pyrimidone-carboxylic acid analogs

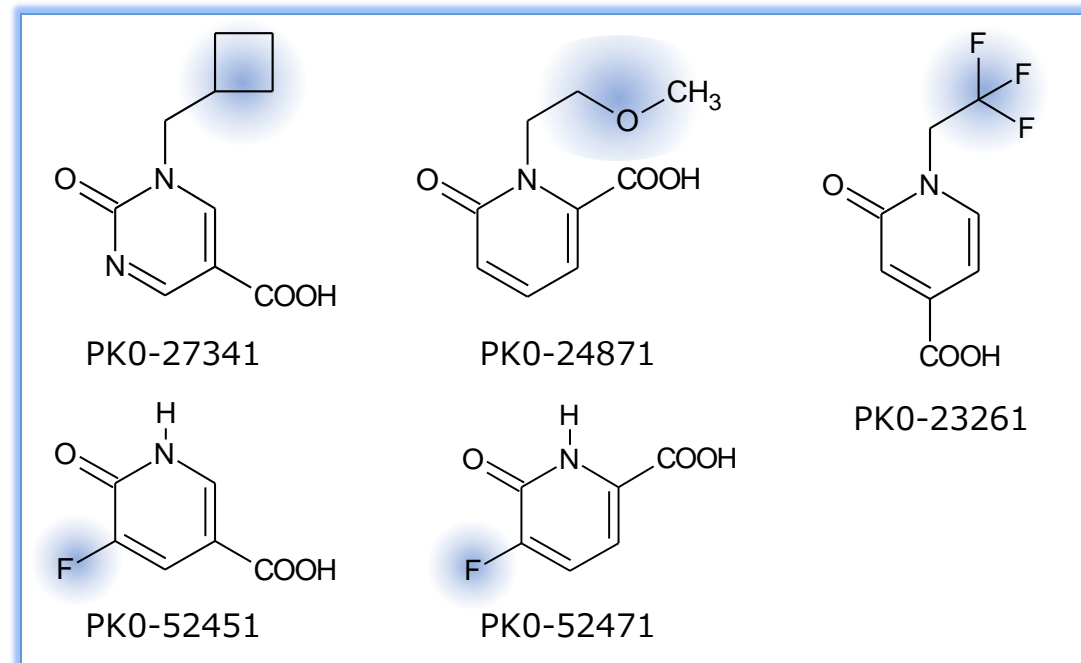


33~
analog

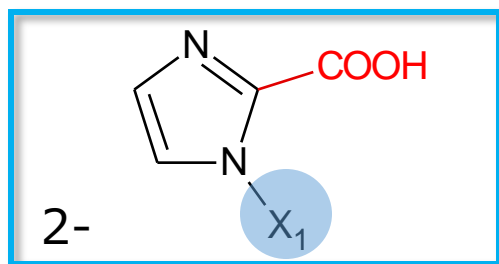
	X_1	X_2	X_3
-OEt	PK0-39601	PK0-38061	PK0-39581
-OCH ₂ CF ₃	PK0-43181	PK0-39261	PK0-39591
-OCH ₂ CH ₂ OCH ₃	PK0-41621	PK0-38441	PK0-45001
	PK0-41651	PK0-38841	PK0-40931
	PK0-40951	PK0-38451	PK0-39271



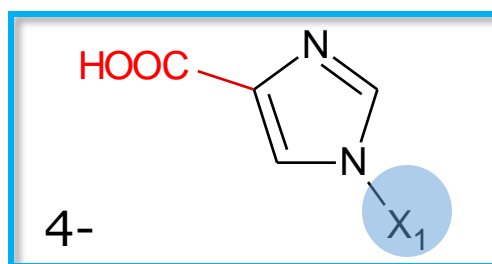
38~
analog



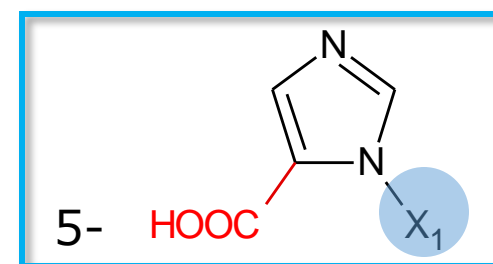
Imidazole-carboxylic acid analogs



32(31+1)~
analog



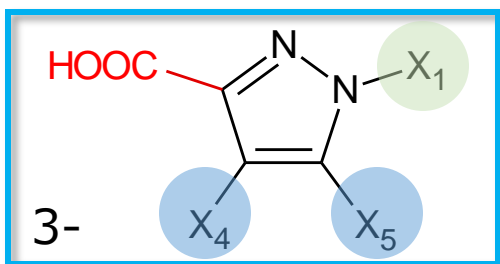
48~
analog



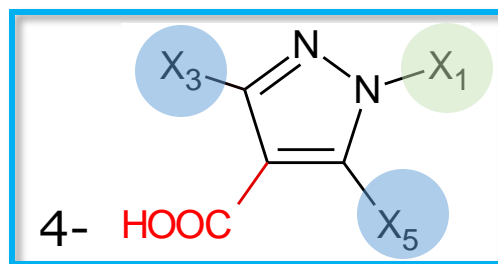
48~
analog

X_1	2-COOH	4-COOH	5-COOH
-Et	PK0-26861	PK0-37421	PK0-37431
	PK0-25481	PK0-26181	PK0-37801
-CH ₂ CH ₂ OCH ₃	PK0-27001	PK0-26991	PK0-35551
	PK0-25491	PK0-24471	PK0-26391
	PK0-27401	PK0-26241	PK0-30191

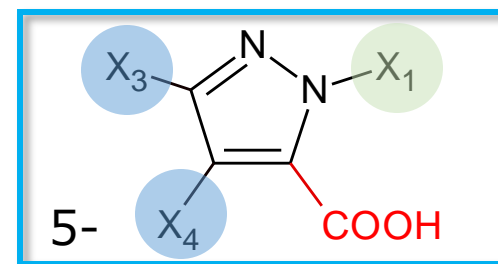
Pyrazole-carboxylic acid analogs



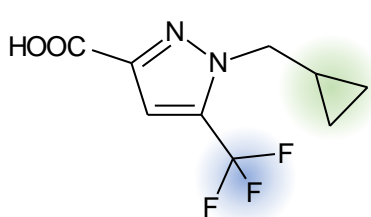
49~
analog



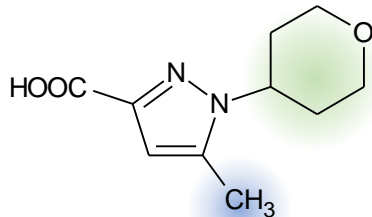
70~
analog



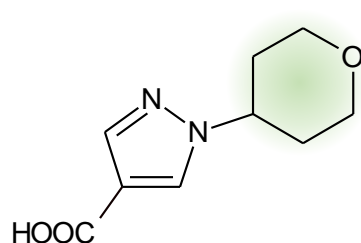
40~
analog



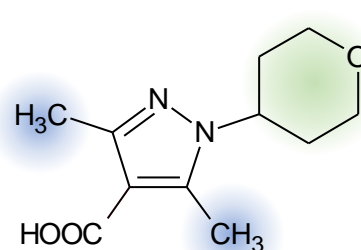
PK0-37381



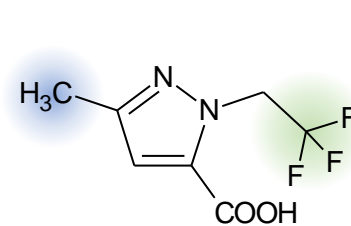
PK0-13591



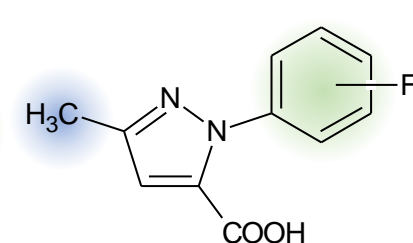
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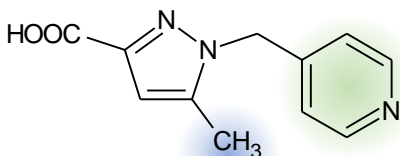
PK0-26151



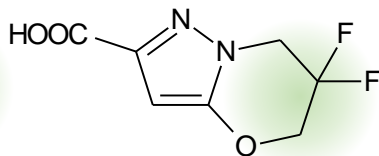
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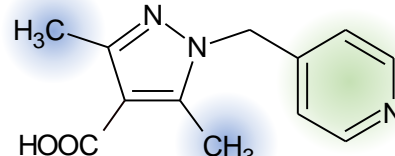
o- : PK0-36021
m- : PK0-36031
p- : PK0-36041



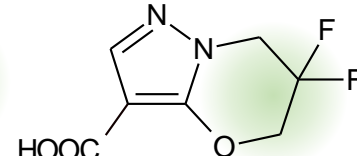
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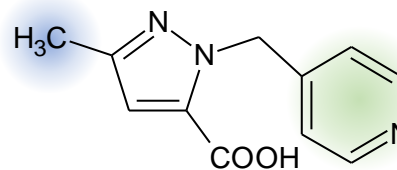
PK0-38871



PK0-26761

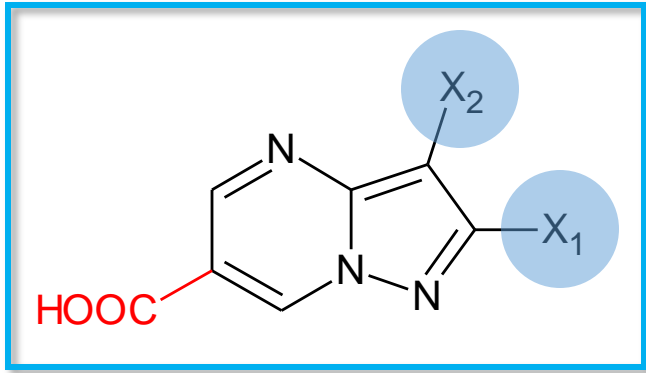


PK0-49321

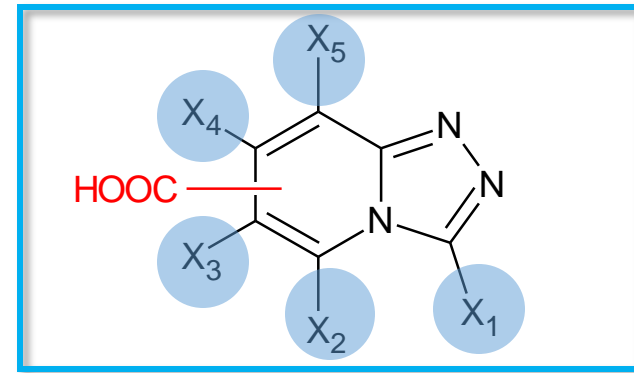


PK0-38131

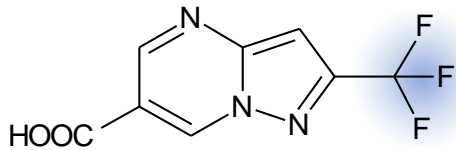
Fused heterocyclic-carboxylic acid analogs (1)



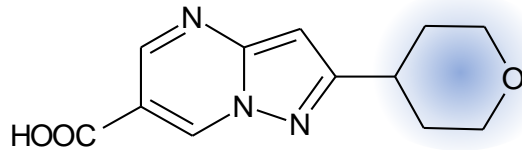
16~
analog



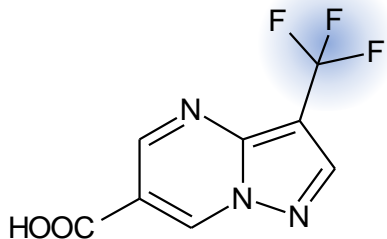
55~
analog



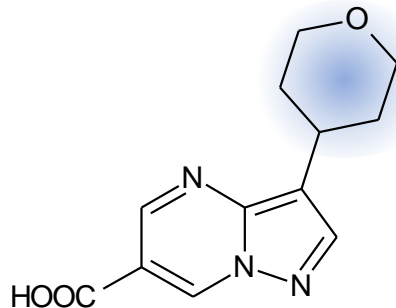
PK0-30601



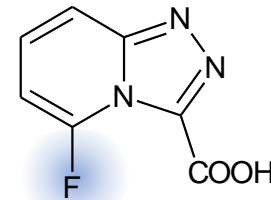
PK0-29641



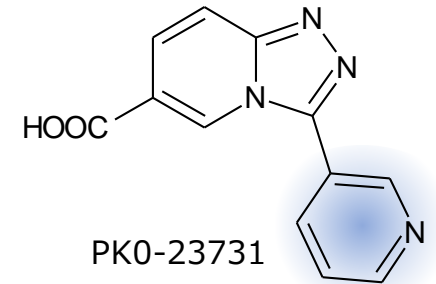
PK0-34971



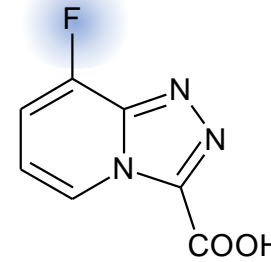
PK0-30981



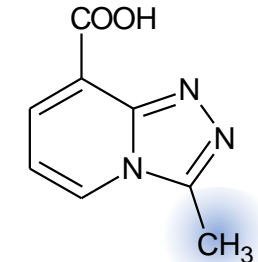
PK0-38791



PK0-23731

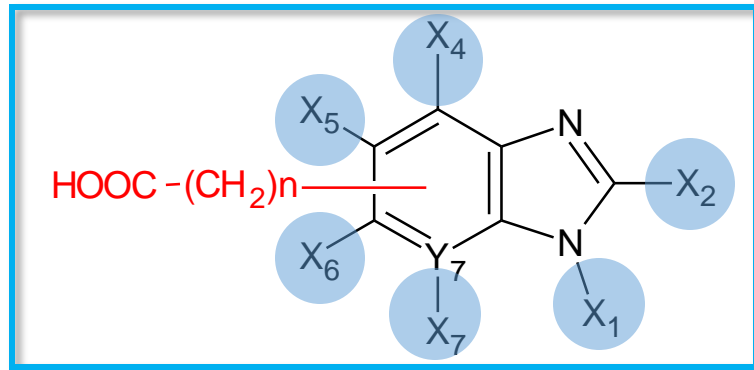


PK0-37661

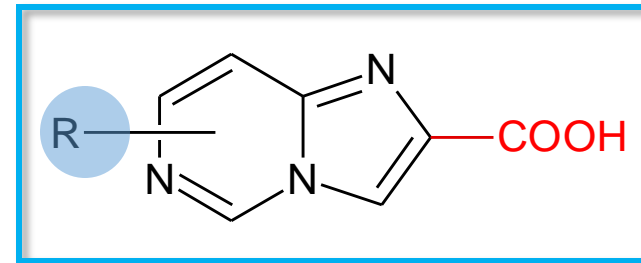


PK0-38011

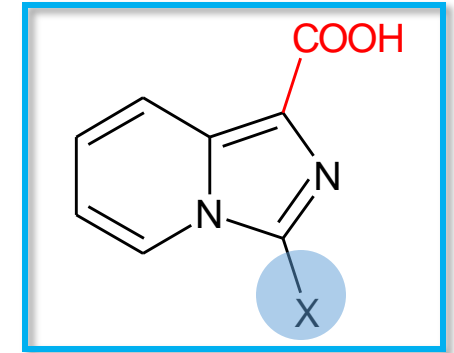
Fused heterocyclic-carboxylic acid analogs (2)



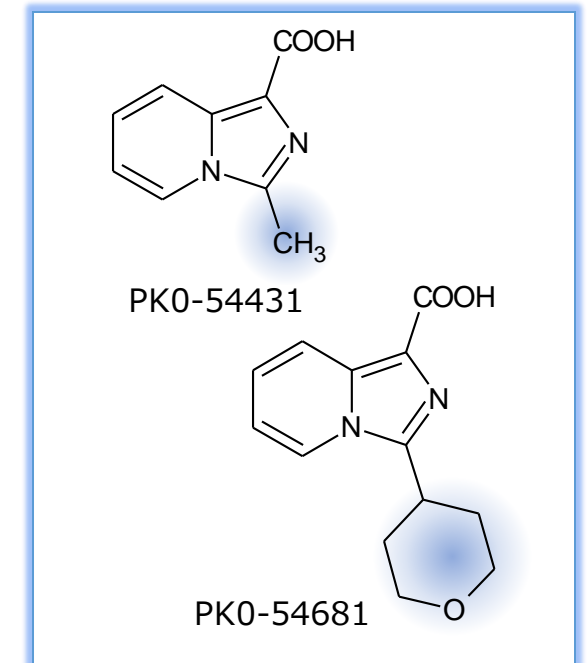
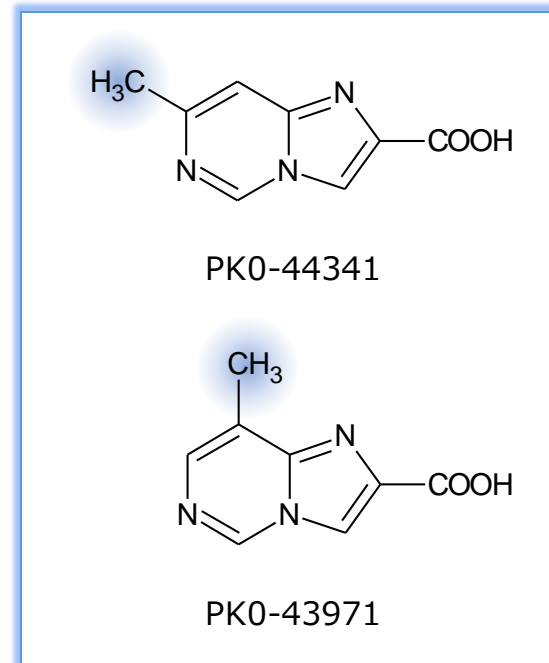
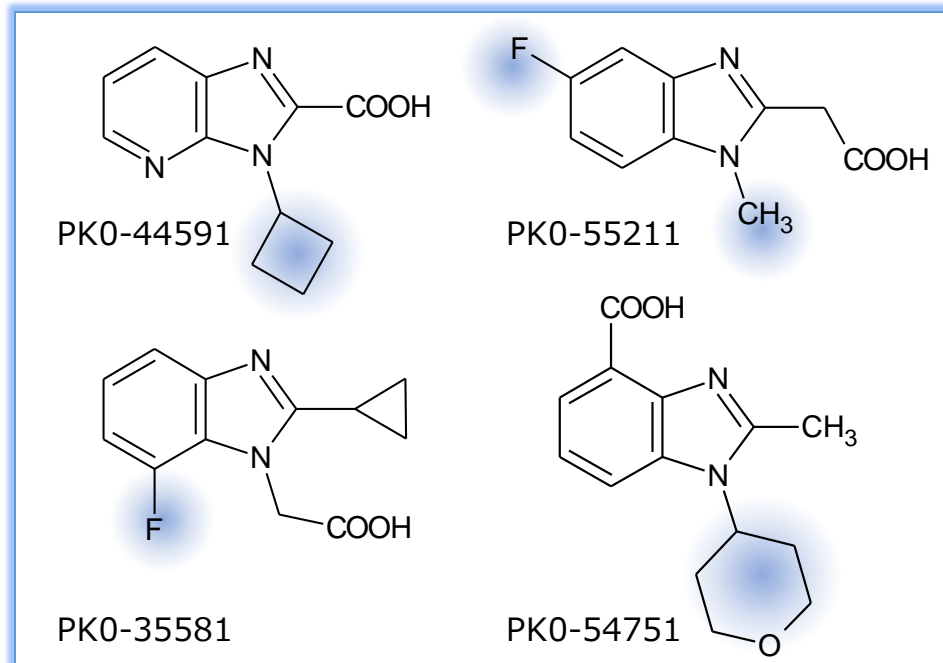
109~
analogs



5~
analogs

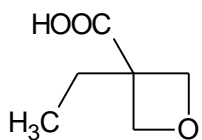


6~
analogs

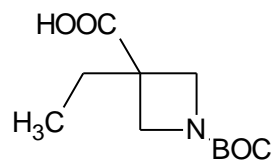


Aliphatic acid analogs

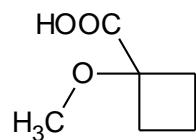
NEW!



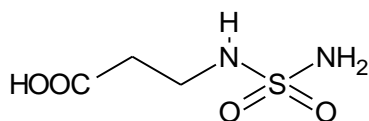
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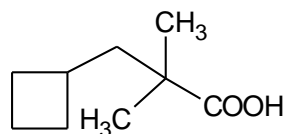
PK0-57181



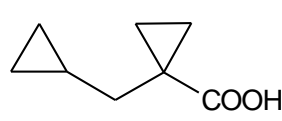
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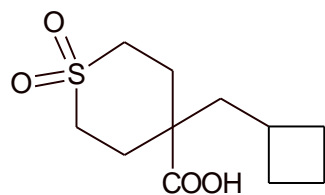
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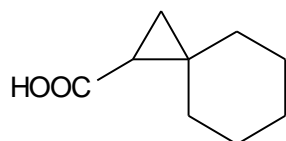
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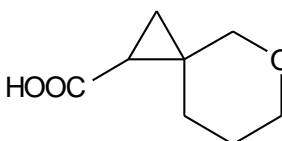
PK0-28291



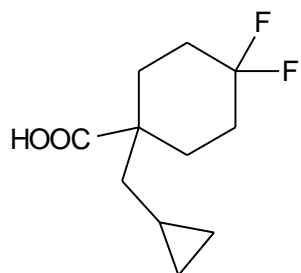
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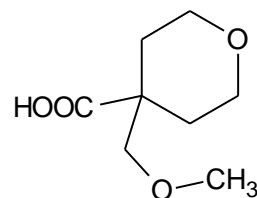
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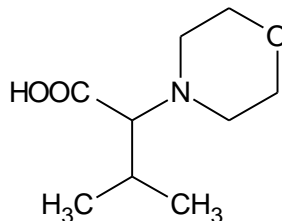
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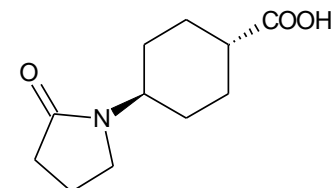
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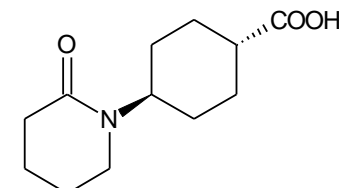
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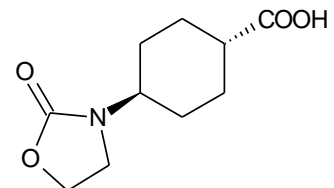
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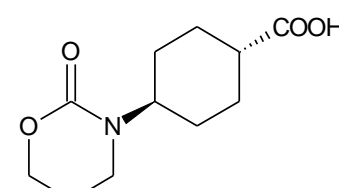
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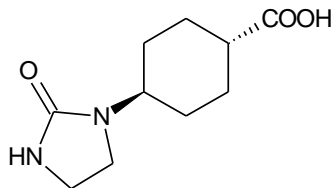
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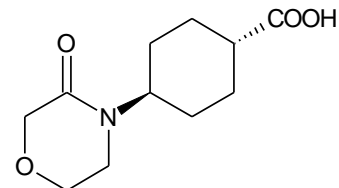
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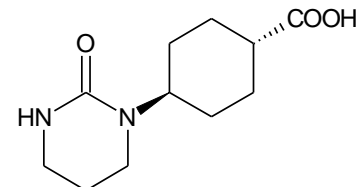
PK0-57291



PK0-57431



PK0-57471



PK0-57461



95~
analog

<参考情報>

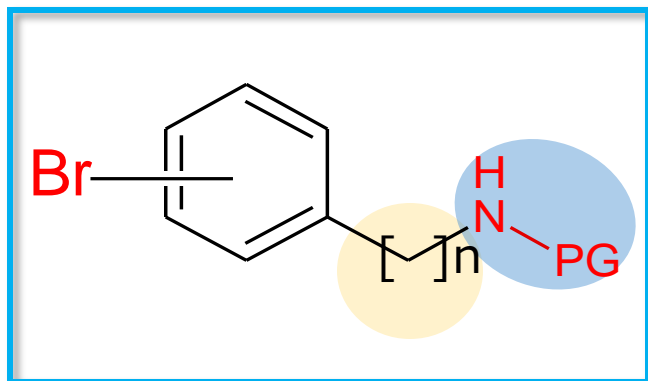
PK0-57051の構造が活用された報告

cis-1-Oxo-heterocyclyl-4-amido cyclohexane derivatives as NPY5 receptor antagonists *Bioorg. Med. Chem. Lett.* **2014**, *24*, 1458-1461

キシダオリジナル
ビルディングブロック (K-BB)

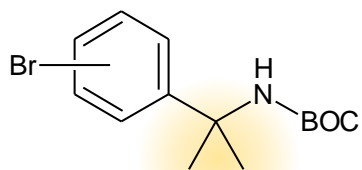
-Br化合物-

Br-benzene analogs (1)

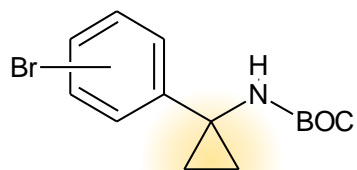


33~
analog

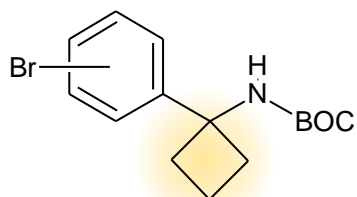
9~
analog



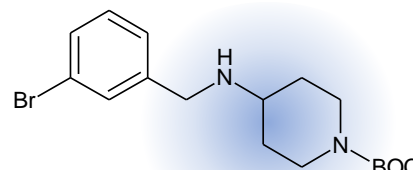
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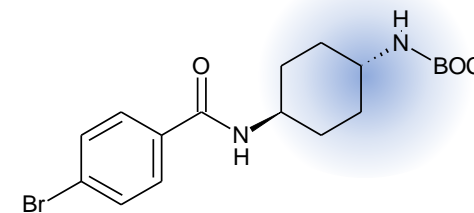
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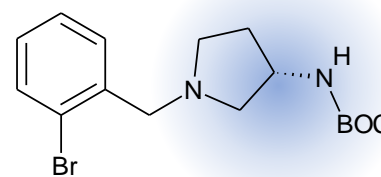
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m- : PK0-10051
p- : PK0-10071



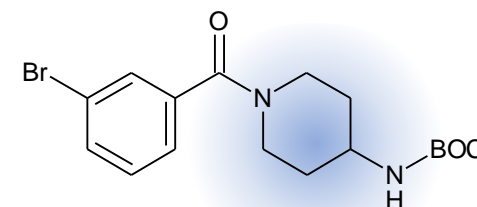
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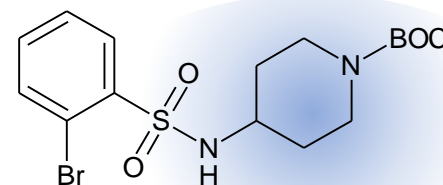
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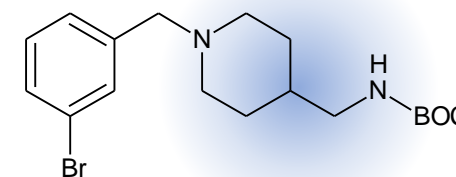
PK0-06021



PK0-03041

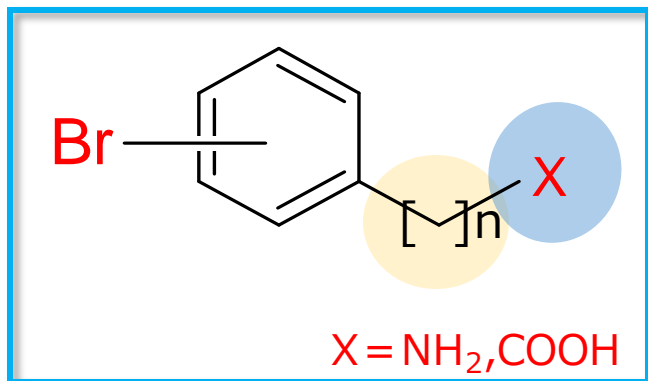


PK0-01971



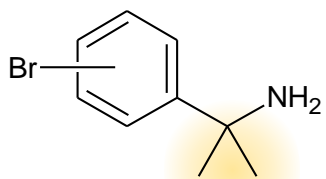
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Br-benzene analogs (2)

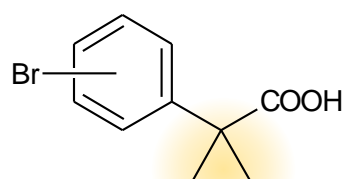


84~
analog

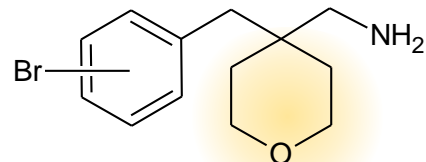
53~
analog



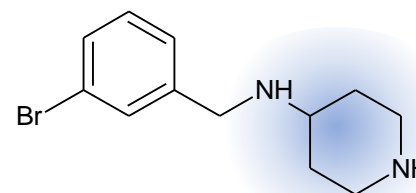
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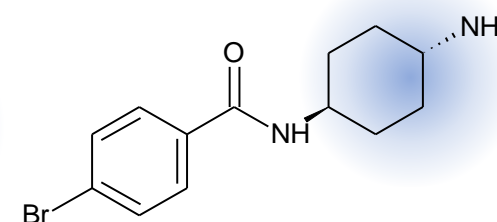
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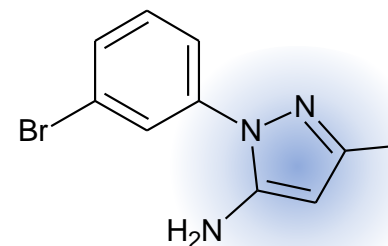
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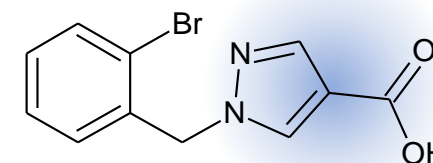
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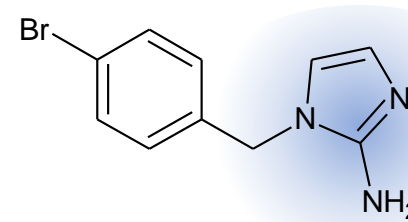
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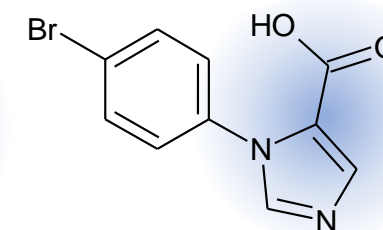
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PK0-12171

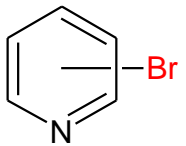
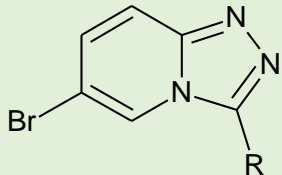
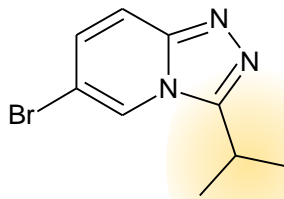
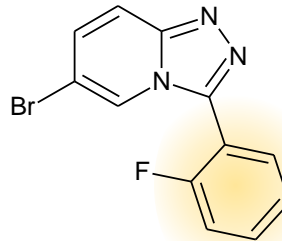
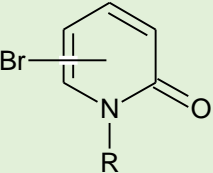
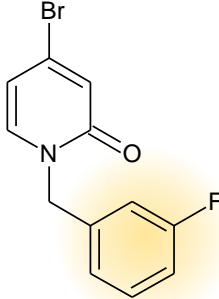
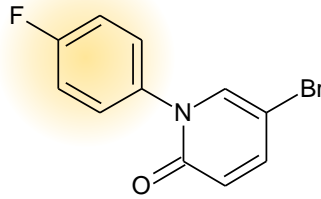
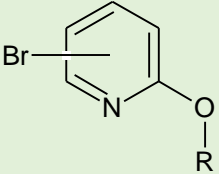
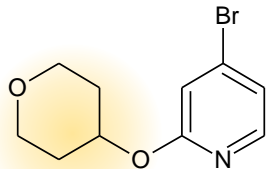
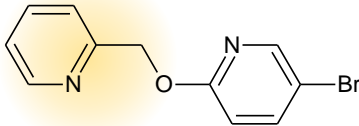


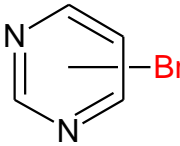
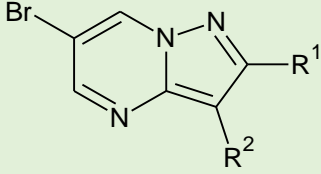
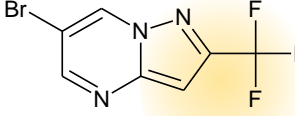
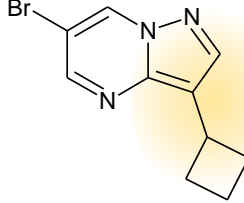
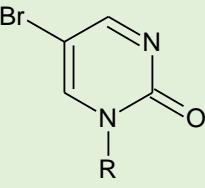
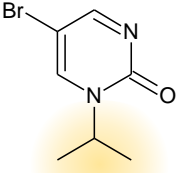
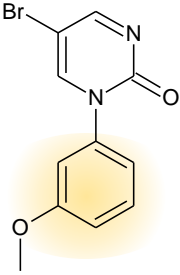
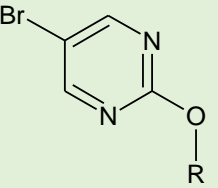
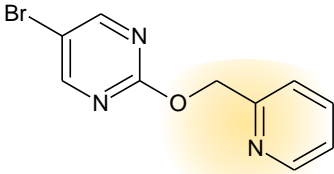
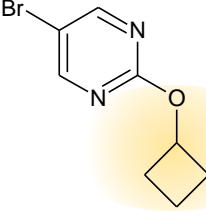
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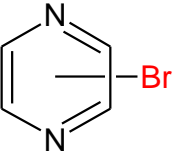
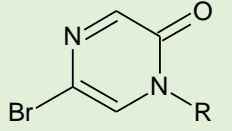
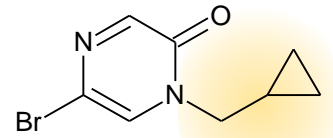
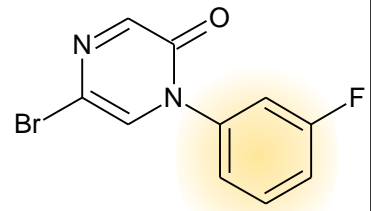
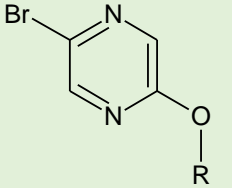
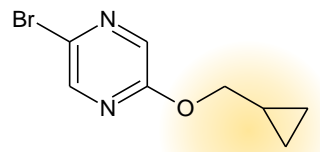
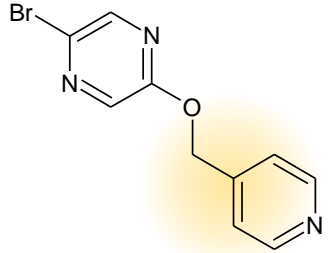
PK0-24581

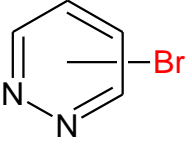
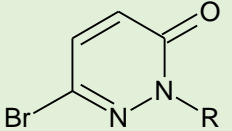
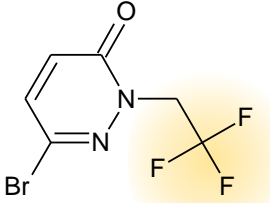
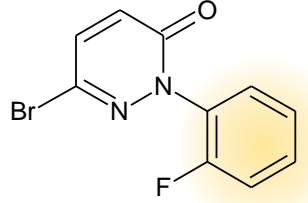
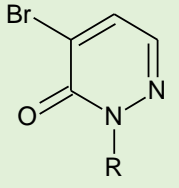
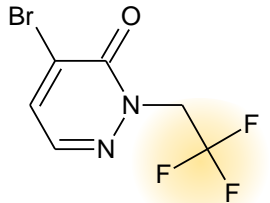
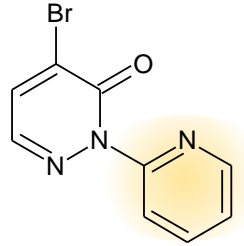
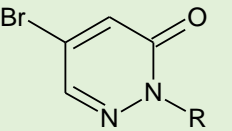
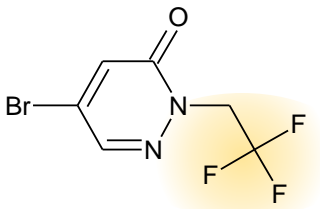
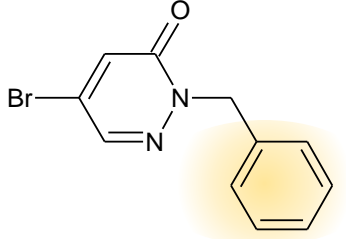
Br-heteroring analogs (1)

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

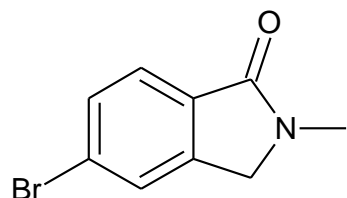
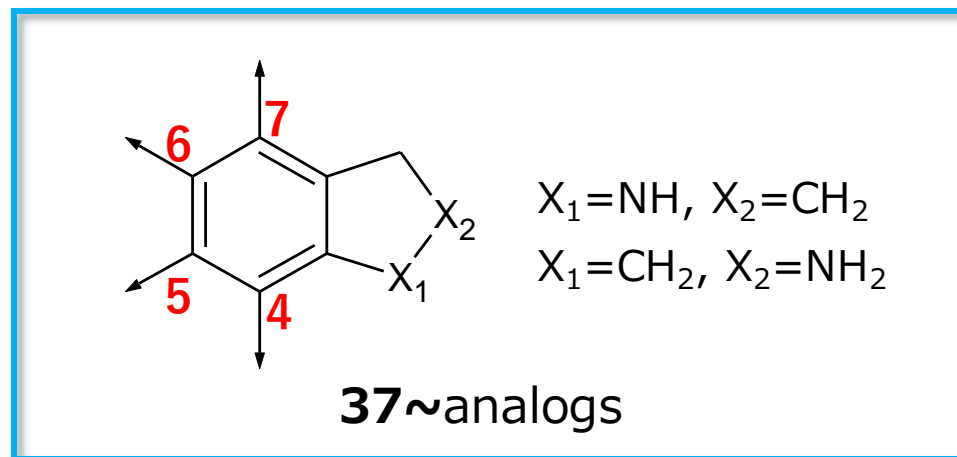
	Example-1	Example-2
 17~analogs	 PK0-30201	 PK0-30221
 23~analogs	 PK0-41161	 PK0-39491
 12~analogs	 PK0-41591	 PK0-41191

Br-heteroring analogs (2)

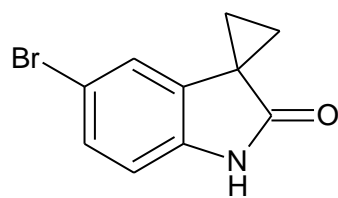
	Example-1	Example-2
 23~analogs	 PK0-42151	 PK0-42471
 17~analogs	 PK0-42291	 PK0-43031

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

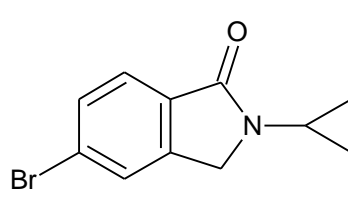
Br-bicyclic analogs (1)



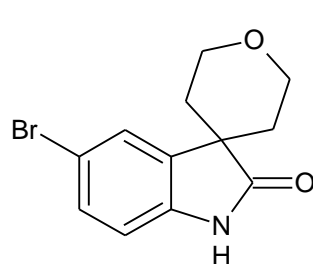
PK0-27621



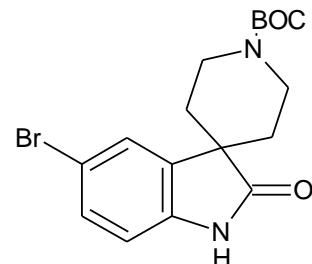
PK0-45911



PK0-27641



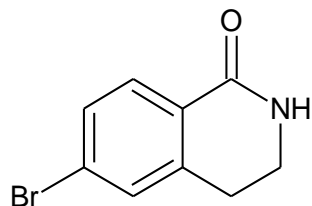
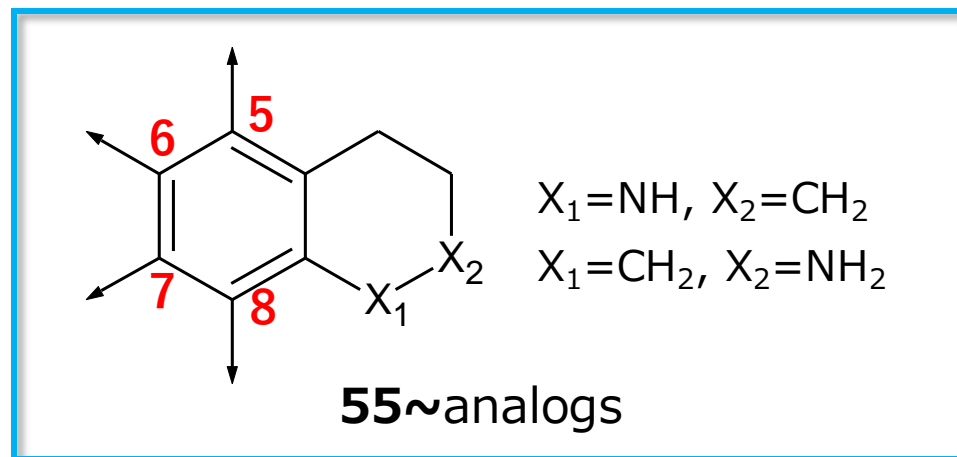
PK0-46271



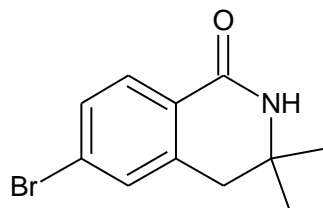
PK0-31741

	4-Br	5-Br	6-Br	7-Br
	PK0-27631	PK0-27621	PK0-27891	PK0-32711
	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

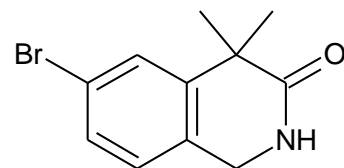
Br-bicyclic analogs (2)



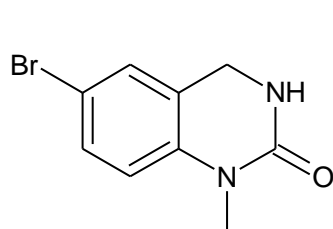
PK0-36311



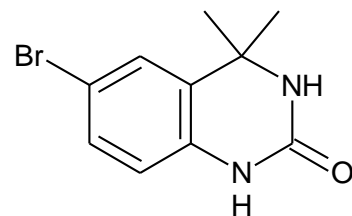
PK0-49051



PK0-37901



PK0-37081



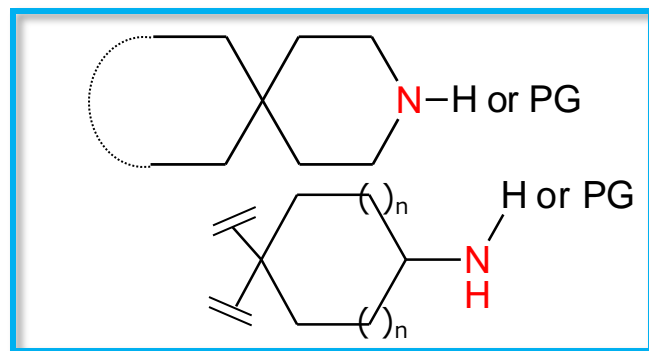
PK0-43461

	5-Br	6-Br	7-Br	8-Br
	PK0-36321	PK0-36311	PK0-36301	PK0-38961
	PK0-49711	PK0-49051	PK0-49041	PK0-49261
	PK0-43471	PK0-37901	PK0-37101	PK0-37911
	PK0-37091	PK0-37081	PK0-37071	PK0-37881
	PK0-49851	PK0-43461	PK0-38491	PK0-45971

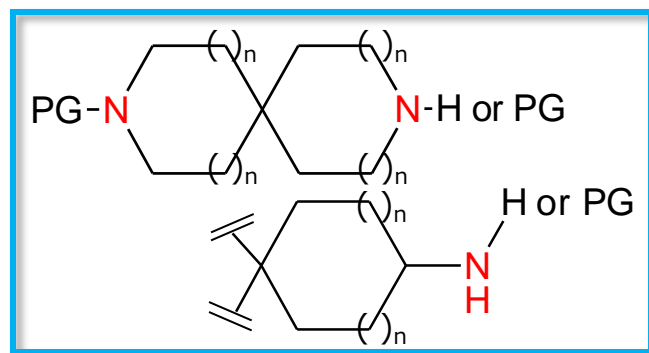
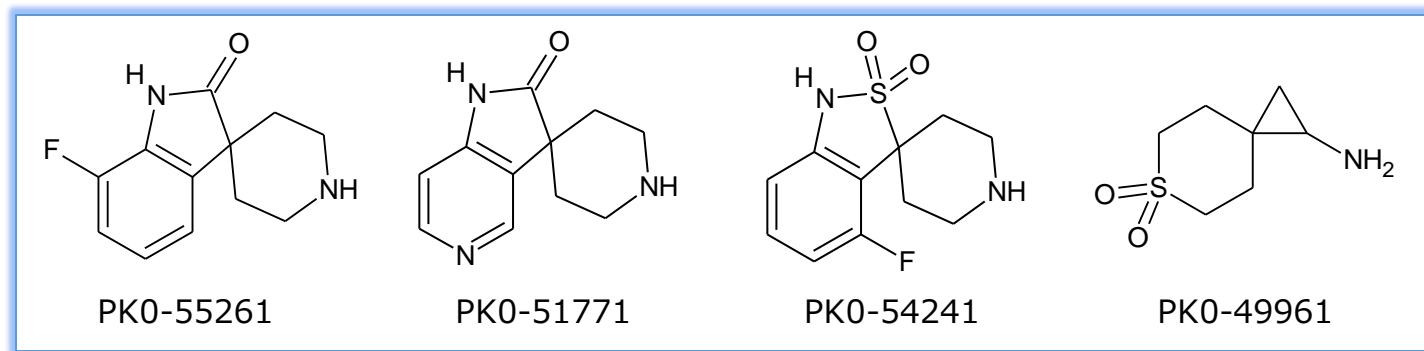
キシダオリジナル ビルディングブロック (K-BB)

-スピロ骨格化合物-

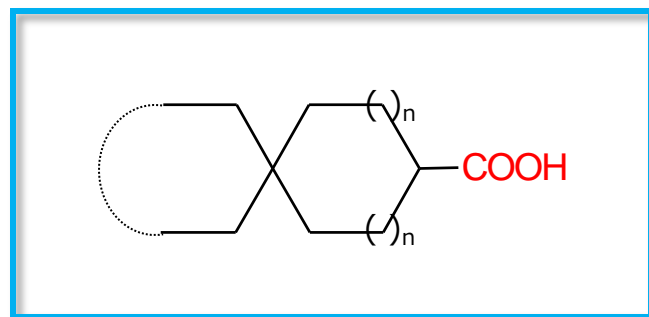
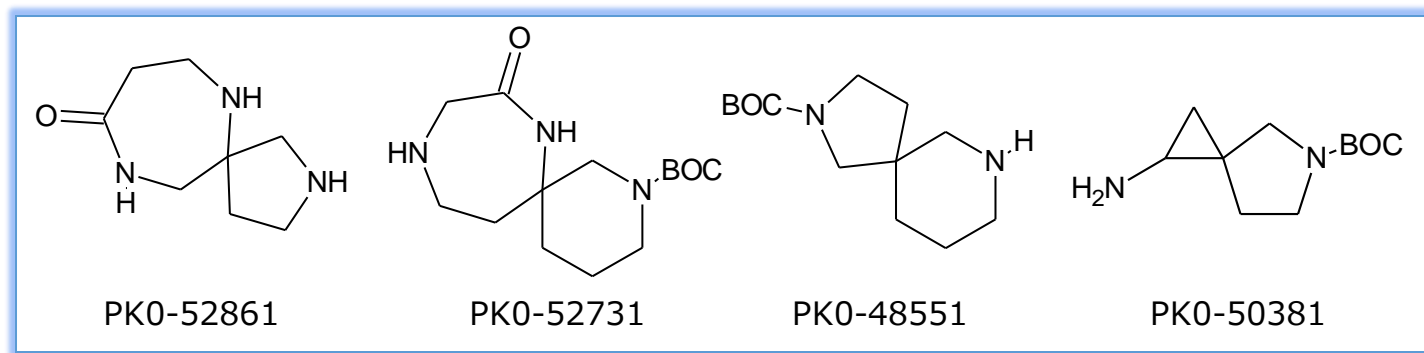
Spiro compounds (1)



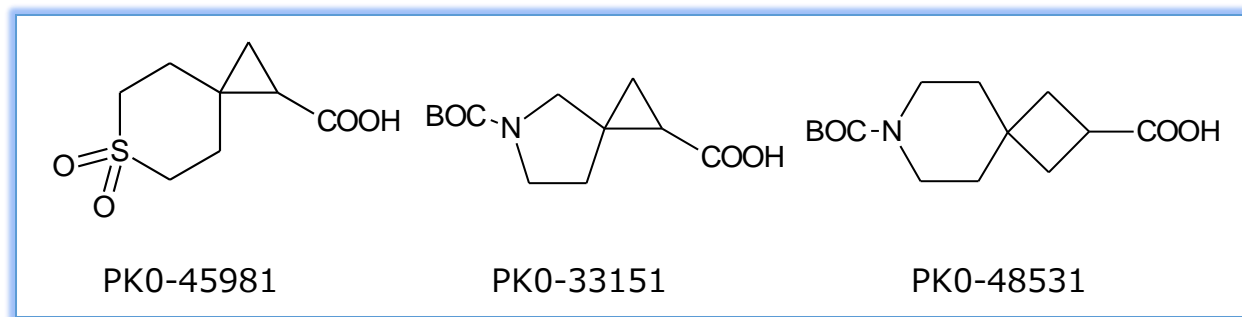
➤➤
218
(216+2)~
analog



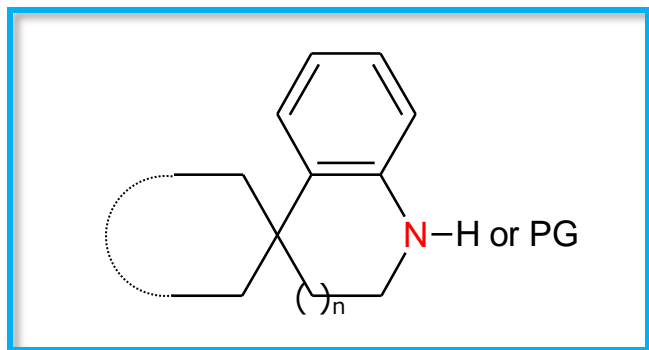
➤➤
150~
analog



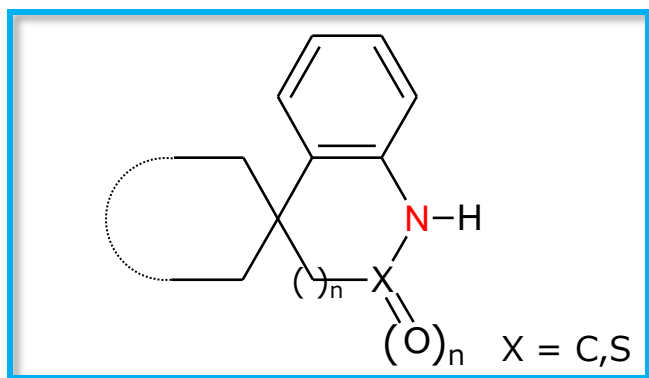
➤➤
19~
analog



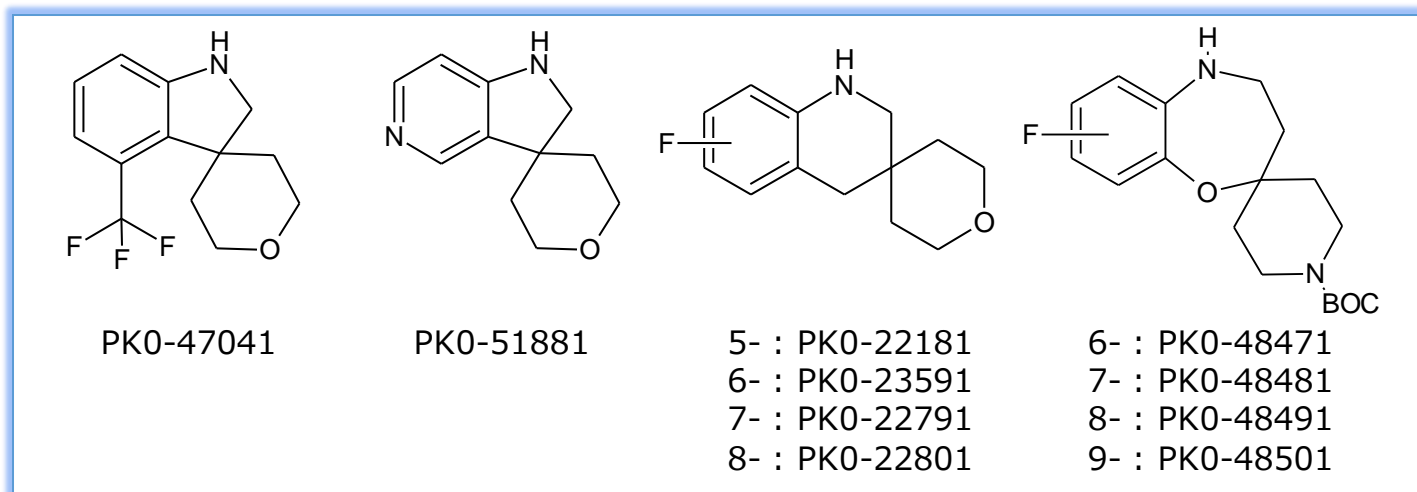
Spiro compounds (2)



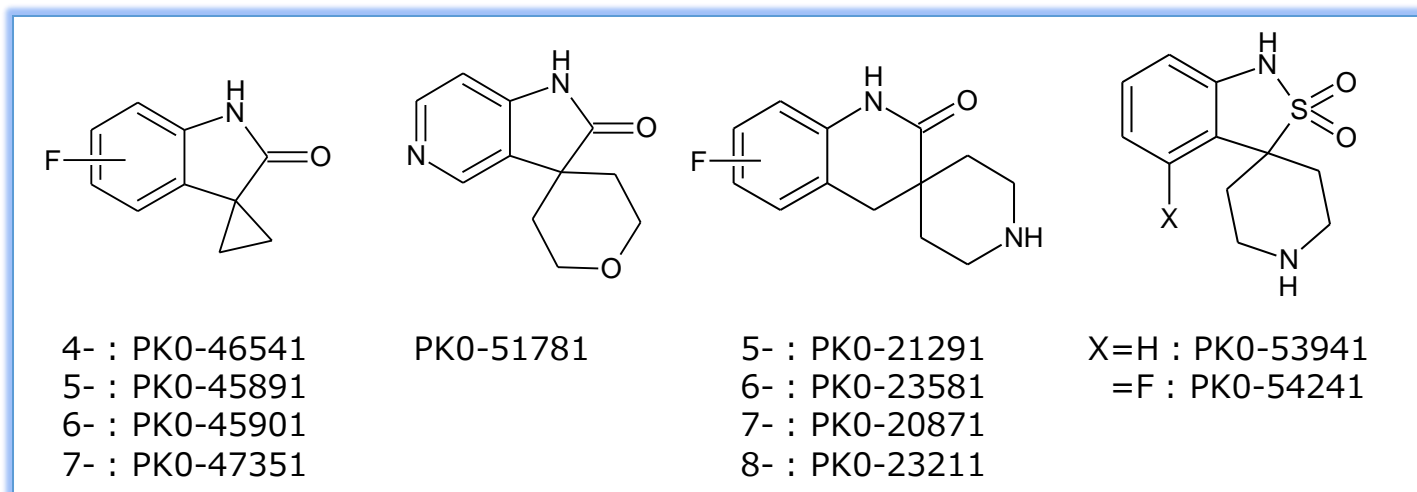
»
109~
 analogs



»
112~
 analogs



6- : PK0-23591
 7- : PK0-48481
 8- : PK0-48491
 8- : PK0-22801
 9- : PK0-48501



5- : PK0-45891
 6- : PK0-45901
 7- : PK0-20871
 8- : PK0-23211
 =F : PK0-54241

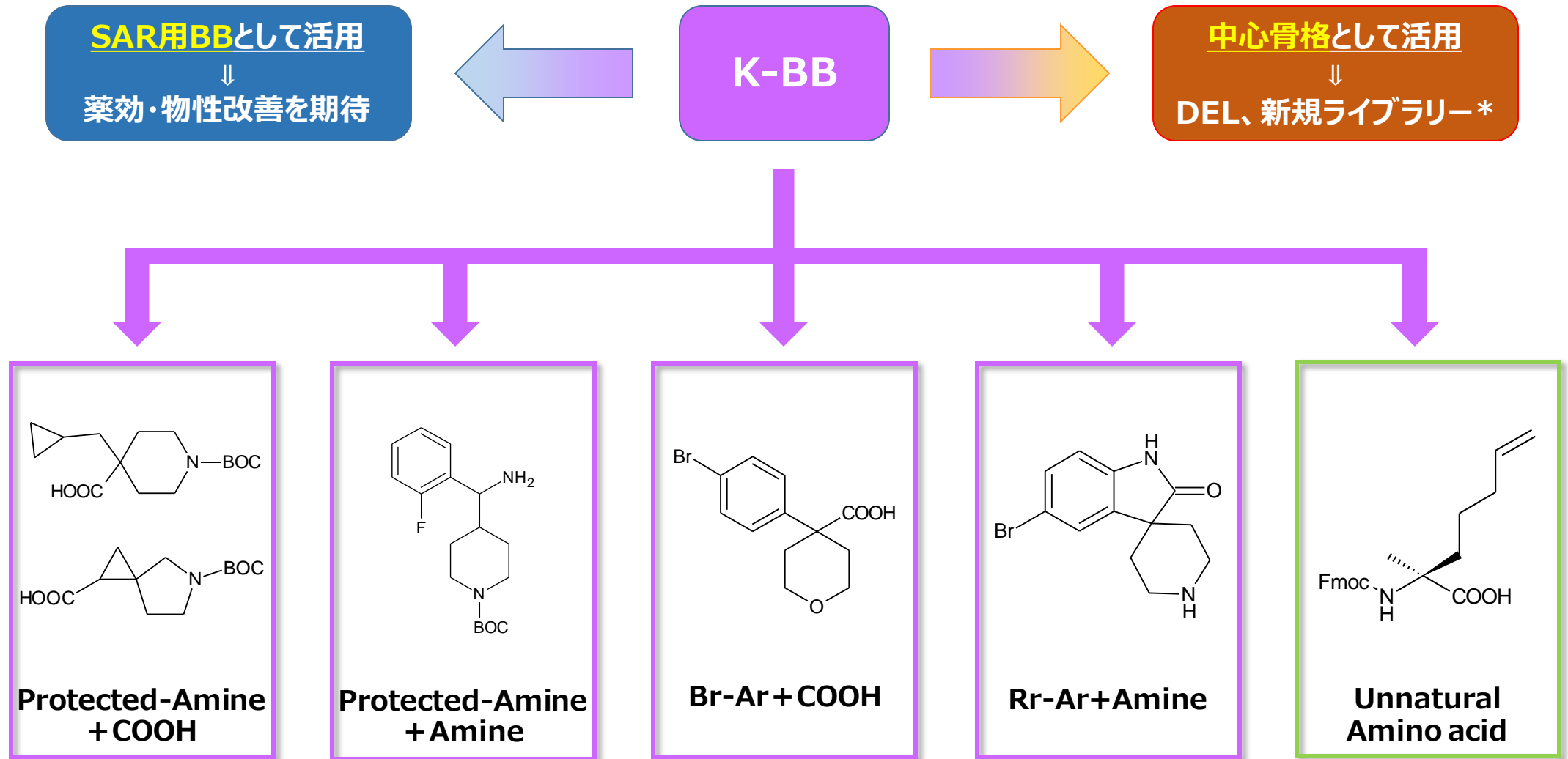
キシダオリジナル ビルディングブロック (K-BB)

-中心骨格化合物-

赤字は2021年6月版以降の更新分（新製品）

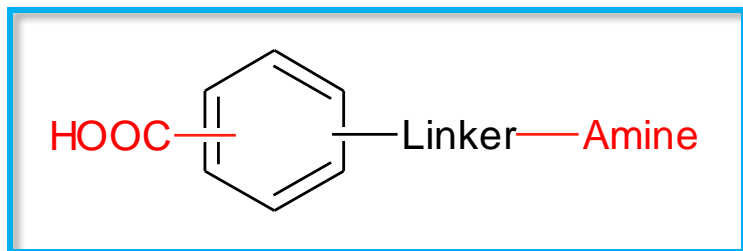
 は新たに追加したスライド

コンセプト

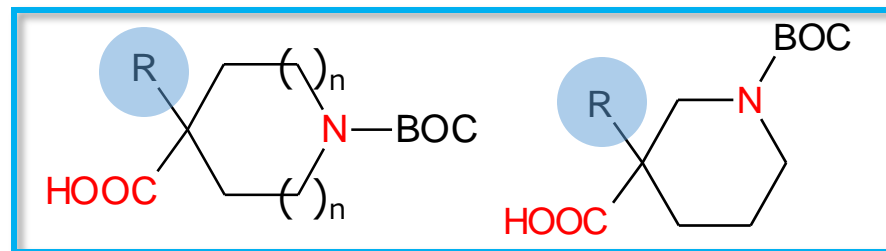
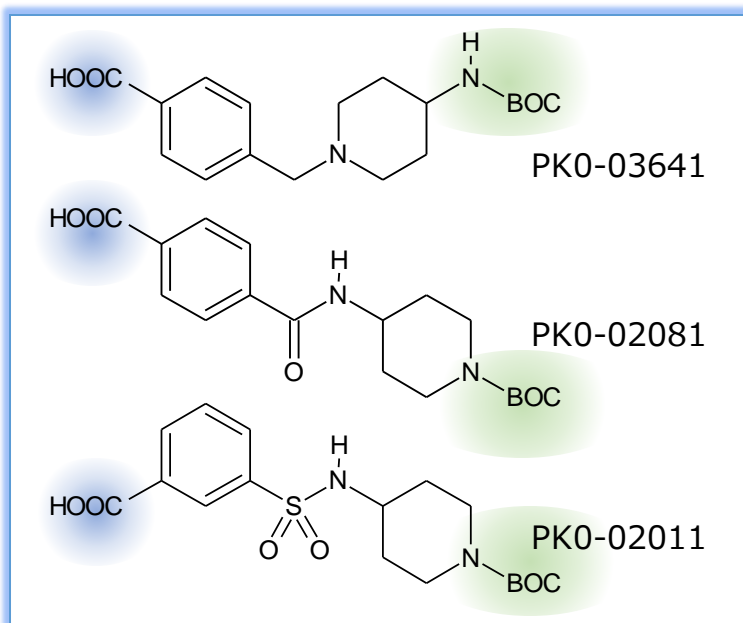


*お客様がお持ちのBBと組み合わせることで、オリジナルライブラリーの作製が可能です
当社のパラレル合成サービスもご利用いただけます

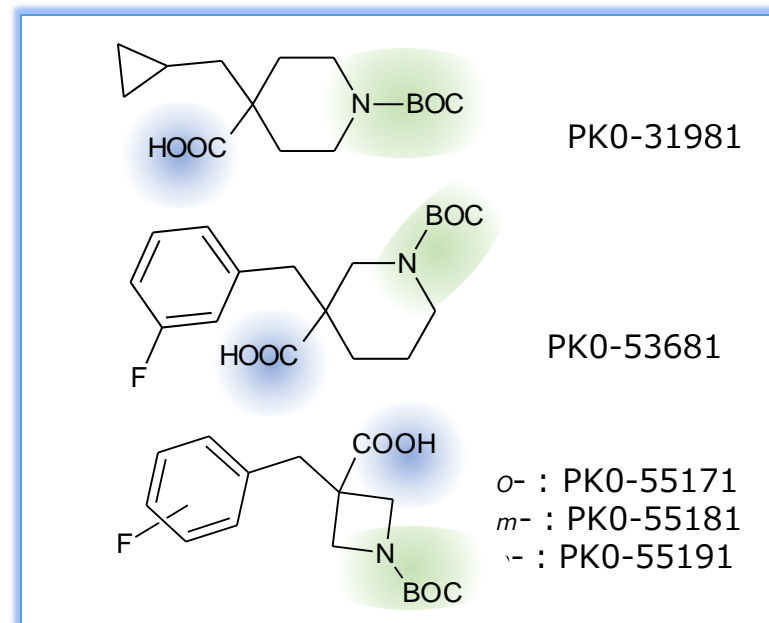
“Protected amine + COOH” analogs



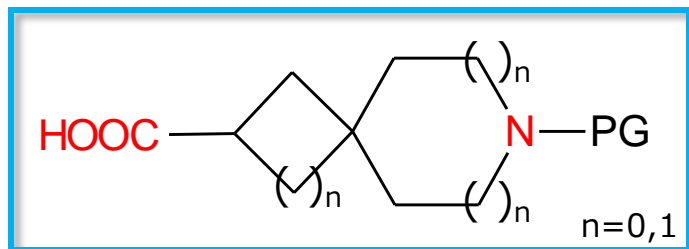
10~
analog



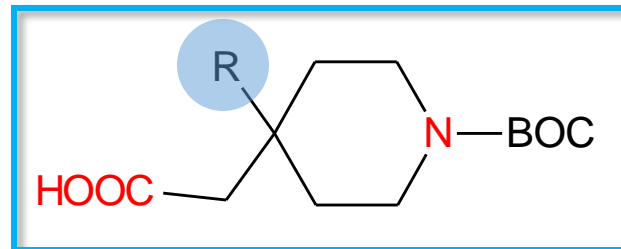
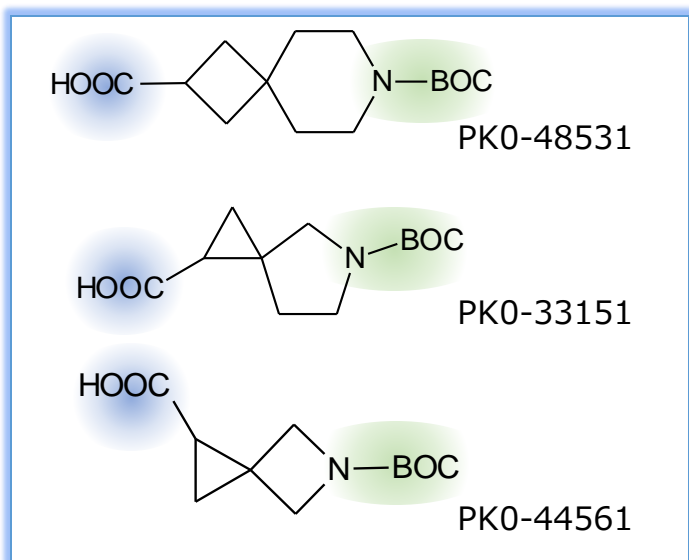
38~
analog



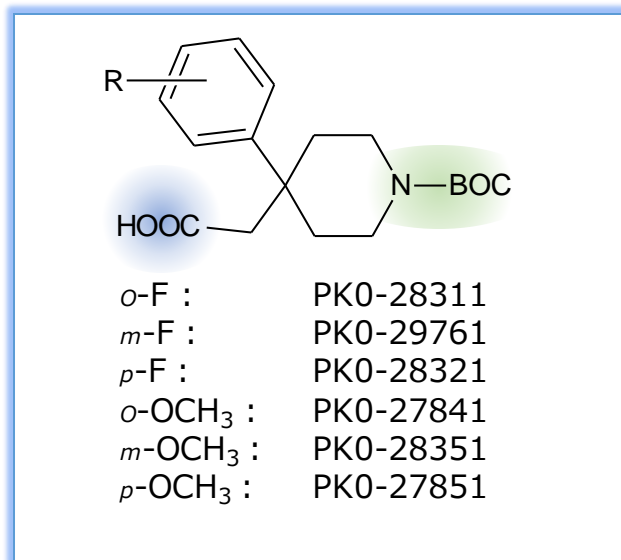
"Protected amine + COOH" analogs



8~
analog



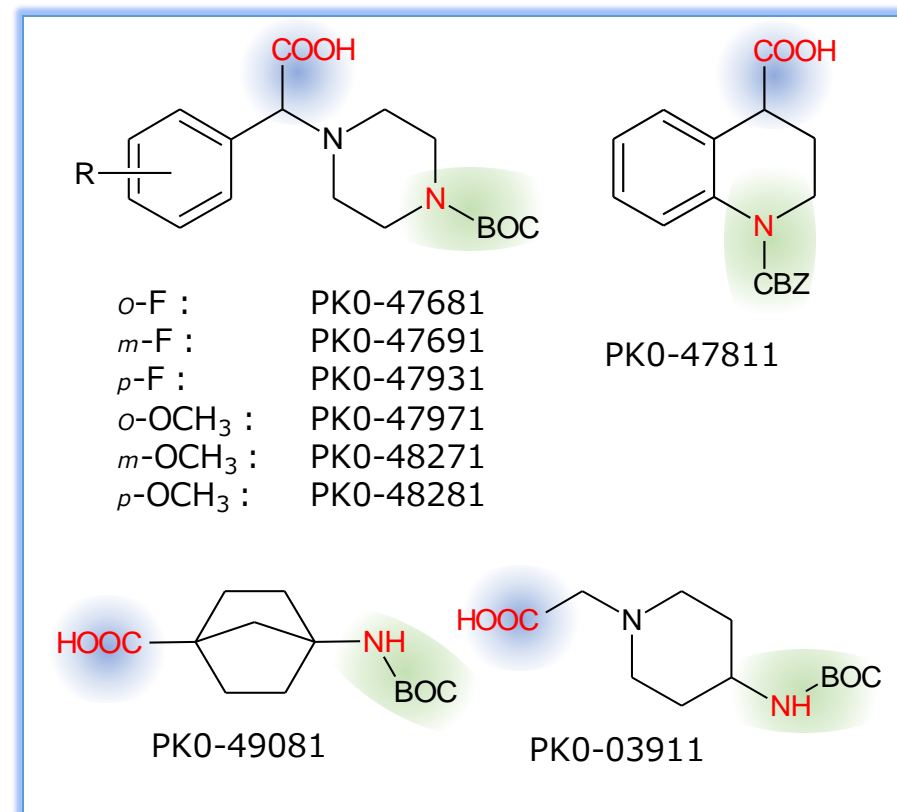
17~
analog



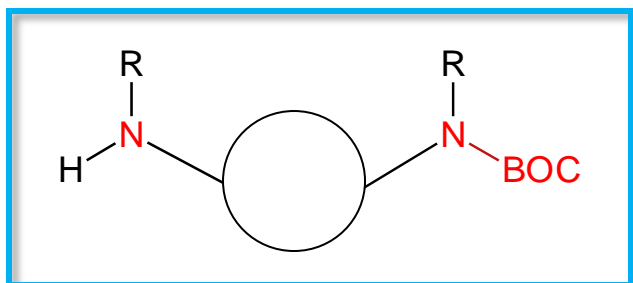
Others



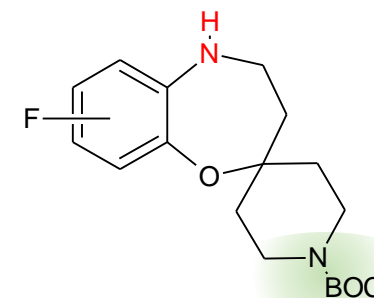
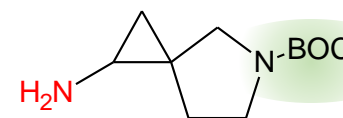
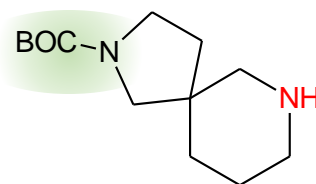
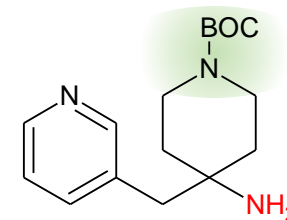
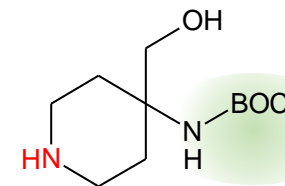
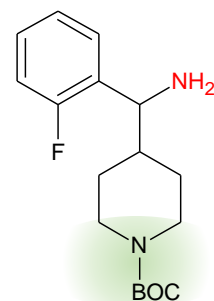
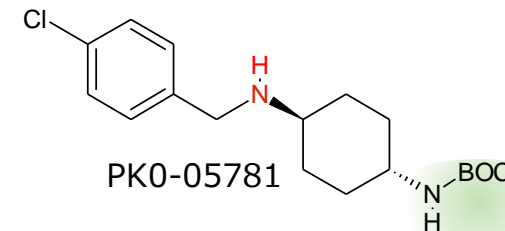
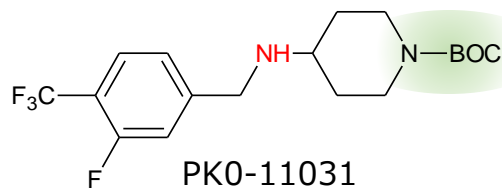
11~
analog



"Protected amine + Amine" analogs

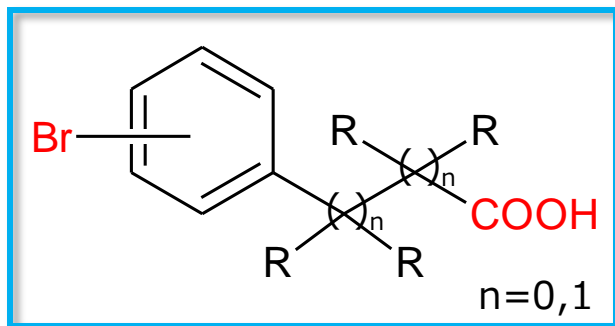


449
(439+10)~
analog

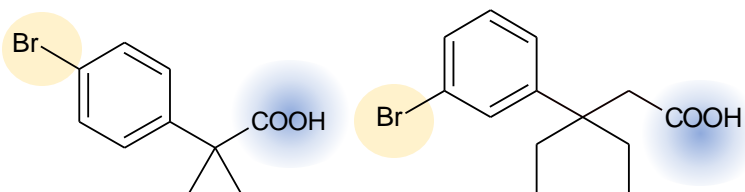


6- : PK0-48471
7- : PK0-48481
8- : PK0-48491
9- : PK0-48501

"Bromide + COOH" analogs

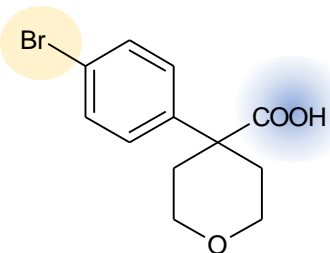


26~
analogs

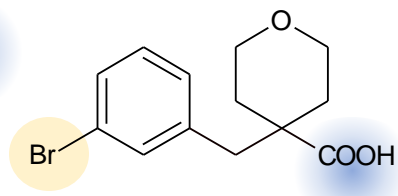


PK0-10591

PK0-28341



PK0-16281

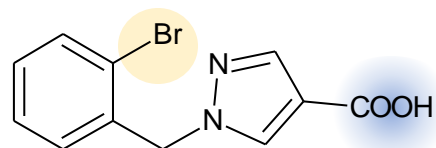


PK0-18511

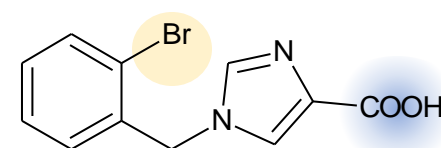
Br + Heteroaryl-COOH



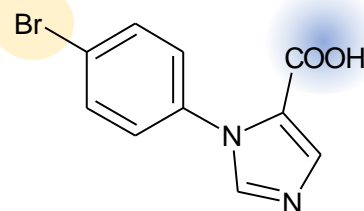
25~
analogs



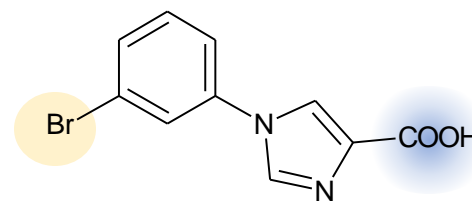
PK0-12171



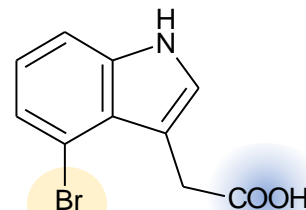
PK0-26201



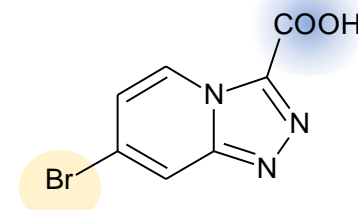
PK0-24581



PK0-26281



PK0-38221



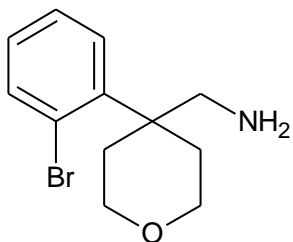
PK0-35891

"Bromide + Amine" analogs

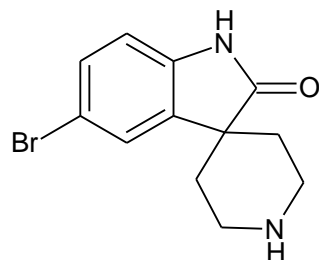
Br + Free-Amine



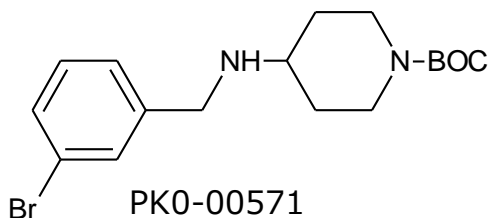
112~
analogs



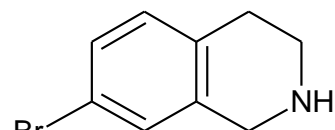
PK0-16851



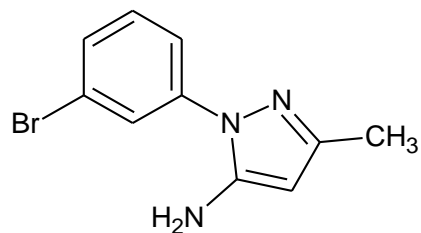
PK0-31781



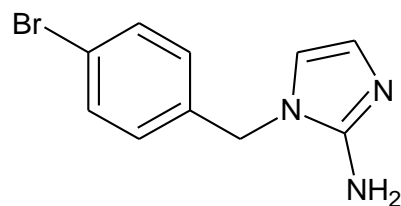
PK0-00571



PK0-53341



PK0-11621

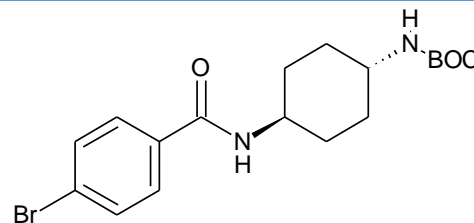


PK0-31661

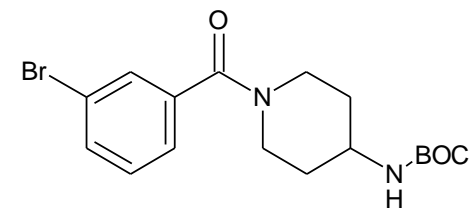
Br + Protected-Amine



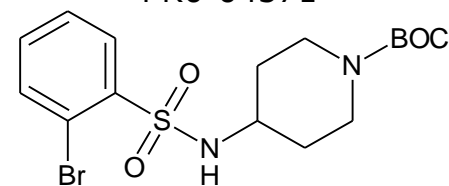
40~
analogs



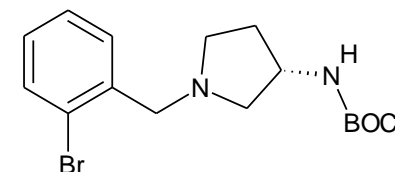
PK0-04571



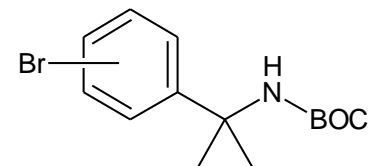
PK0-03041



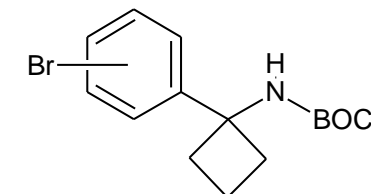
PK0-01971



PK0-06021

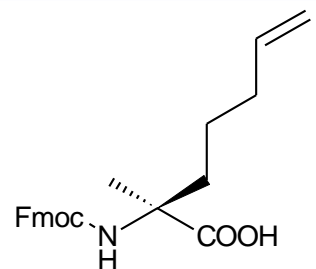


o- : PK0-09931
m- : PK0-09951
p- : PK0-08481

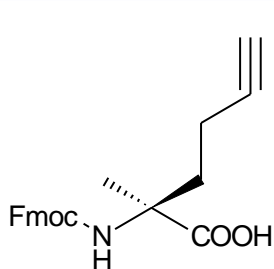


o- : PK0-10031
m- : PK0-10051
p- : PK0-10071

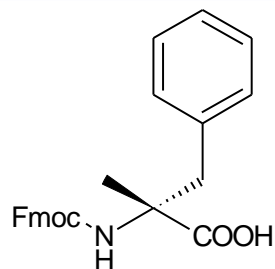
Unnatural Amino Acid

N-Protected
Unnatural Amino Acid55~
analogs

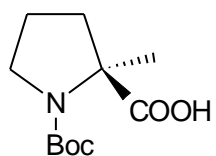
KUA-00061



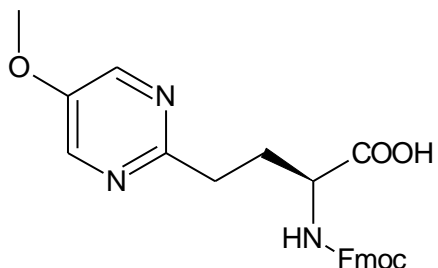
KUA-00181



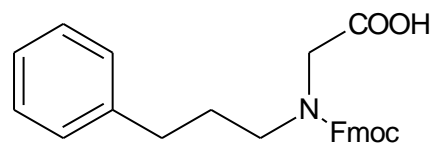
KUA-00711



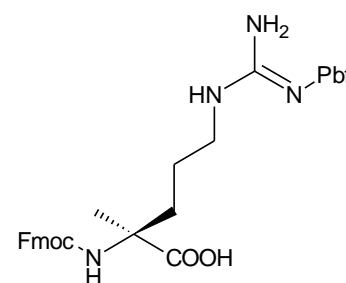
KUA-00721



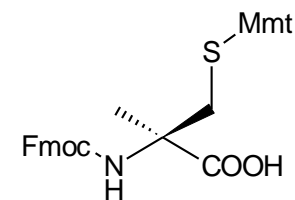
KUP-10031



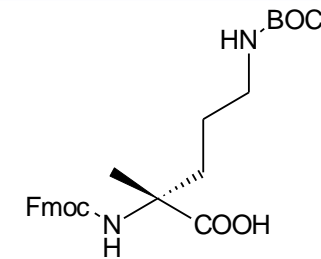
KUP-10351

Side Chain & N-Protected
Unnatural Amino Acid25~
analogs

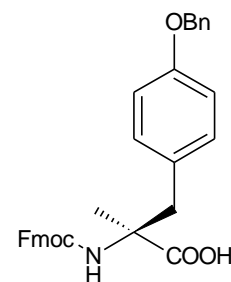
KUA-00391



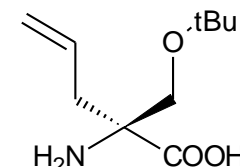
KUA-00501



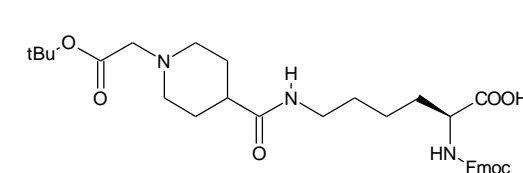
KUA-00661



KUA-00831



KUA-01391



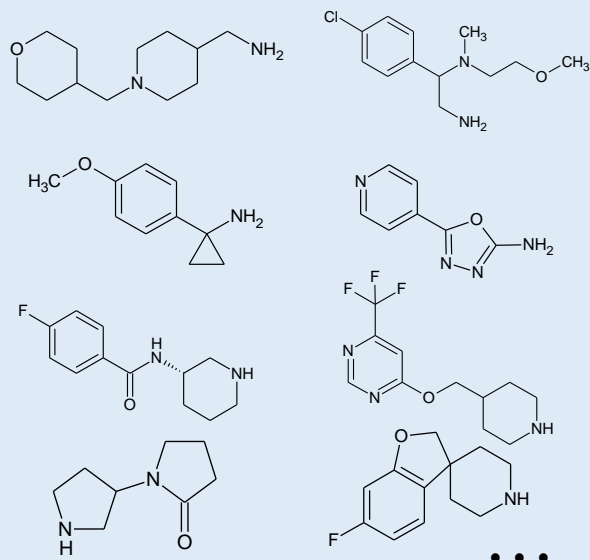
KUP-10071

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

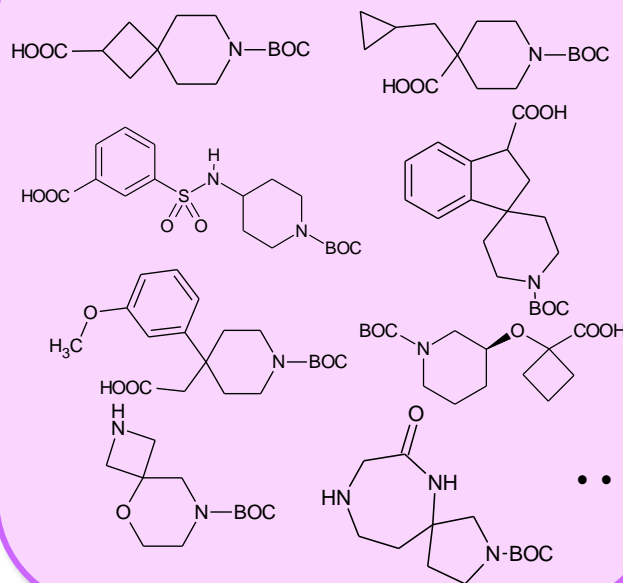
KISHIDA ORIGINAL VIRTUAL LIBRARY (K-LB)

K-LBは、**K-BBを構成因子とする**バーチャルライブラリーです

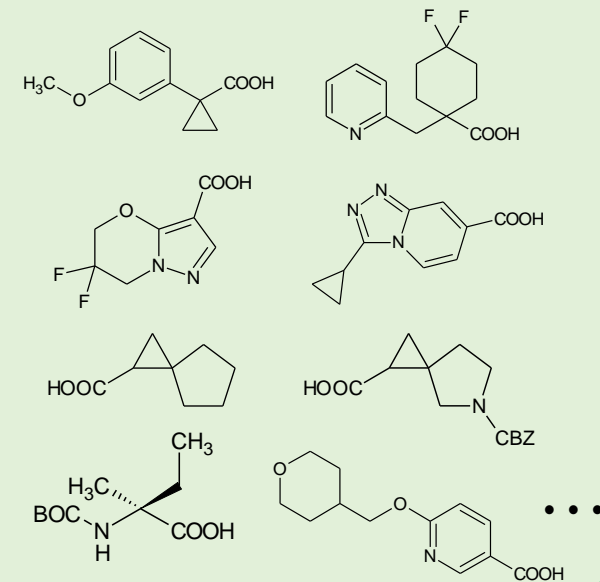
アミンBB



中心骨格BB



カルボン酸BB

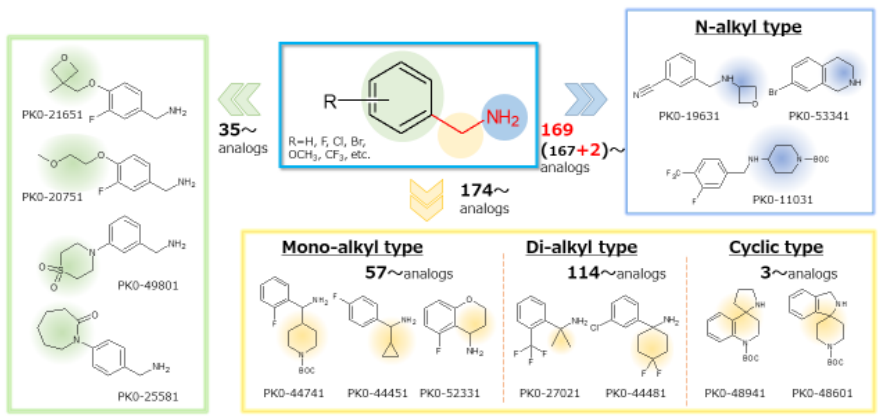


3成分結合型バーチャルライブラリー

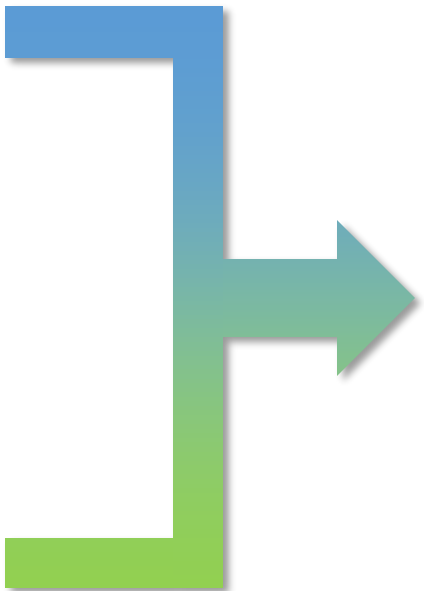
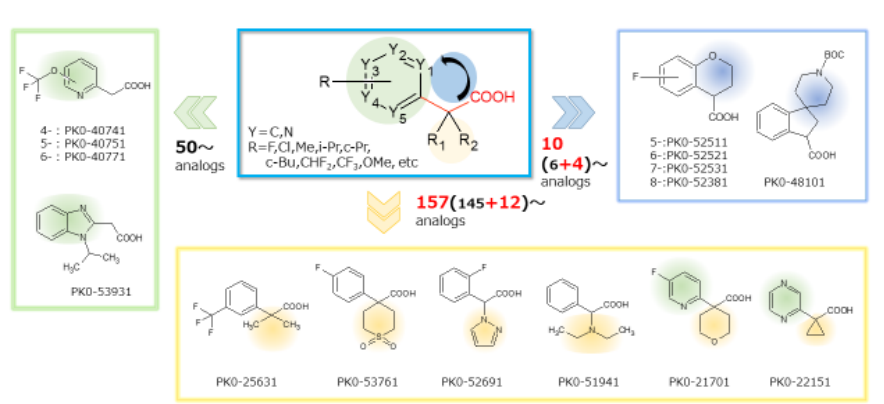
KISHIDA ORIGINAL VIRTUAL LIBRARY (K-LB)

お客様所有の試薬との組み合わせにより、新たなライブラリーの作製も可能です

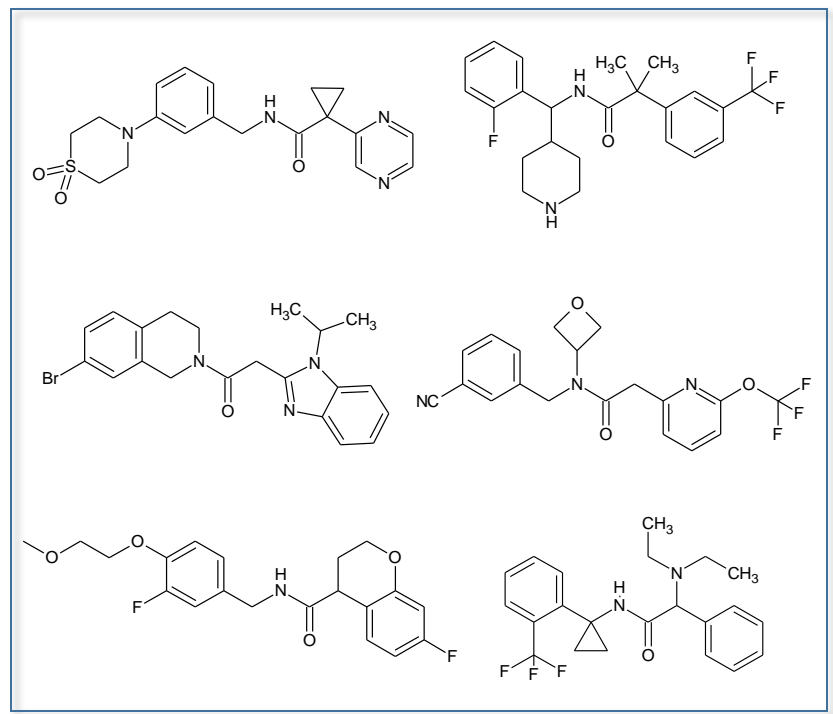
Benzylamine analogs



Phenylacetic acid analogs

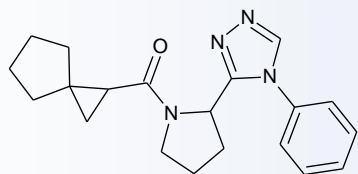
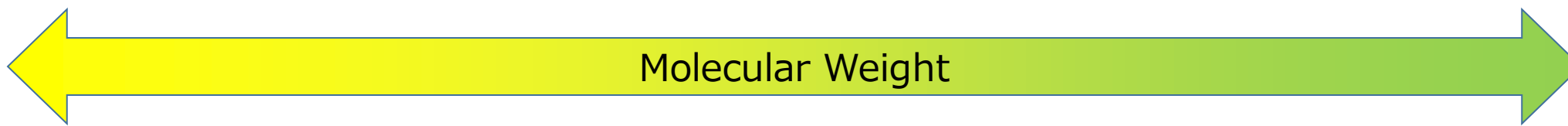


2成分結合型バーチャルライブラリー

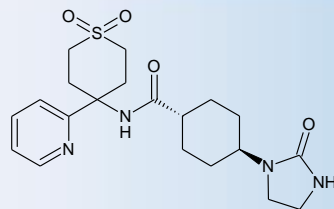


KISHIDA ORIGINAL VIRTUAL LIBRARY (K-LB)

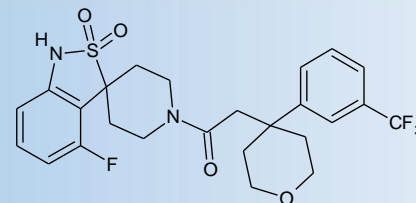
幅広い分子量を占める、2or3成分結合型バーチャルライブラリー
ユニークなBBの組み合わせにより、新規性の高いヒット化合物が取得できます



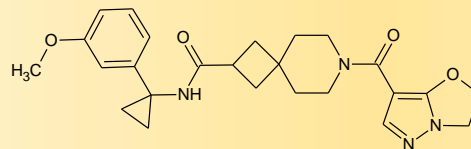
MW 336.4



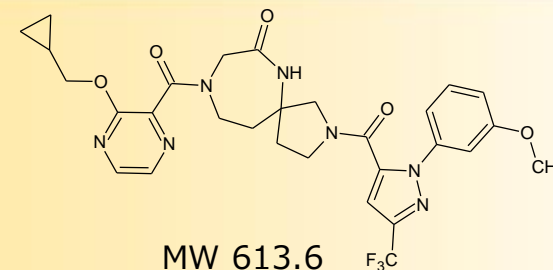
MW 407.5



MW 526.5



MW 448.5

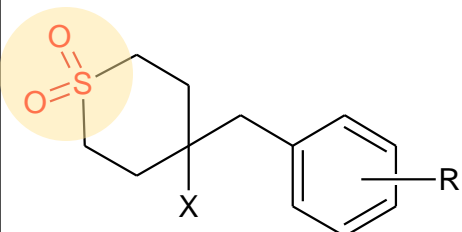


MW 613.6

キシダオリジナル ビルディングブロック (K-BB)

-その他-

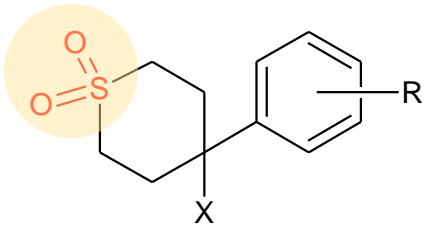
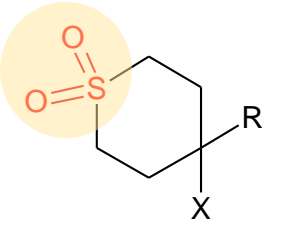
Tetrahydrothiopyran dioxide analogs

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



61~
analog

緑字はScifinderで提供サプライヤーが限られた製品です

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
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 ₂ CH ₂ OCH ₃		PK0-43521	PK0-42761
2-Py-CH ₂		PK0-42791	PK0-42771
3-Py-CH ₂	PK0-53531	PK0-43511	

<参考情報>

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

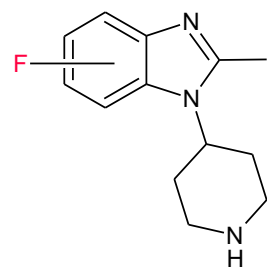
5-Chloroindoloyl glycine amide inhibitors of glycogen phosphorylase: synthesis, in vitro, in vivo, and X-ray crystallographic characterization.
Bioorg.Med.Chem.Lett. **2005**, 15, 459-465

Fluoro-containing BBs for ^{19}F -NMR screening

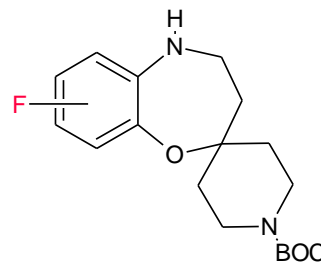
各種のScaffoldに対して、
フッ素原子を積極的に導入



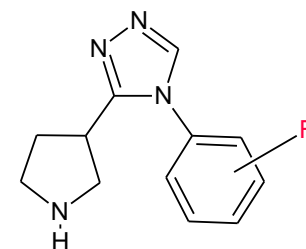
1842
(1818+24)~
analog



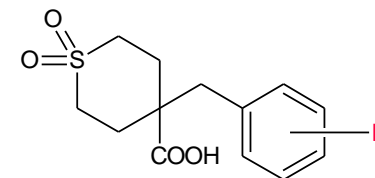
4-: PK0-57261
5-: PK0-57251
6-: PK0-57241
7-: PK0-57231



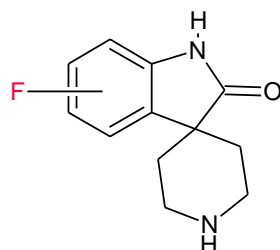
6- : PK0-48471
7- : PK0-48481
8- : PK0-48491
9- : PK0-48501



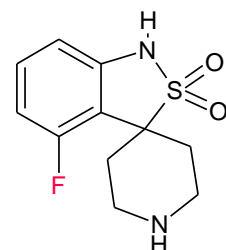
2-: PK0-54271
3-: PK0-54281
4-: PK0-54291



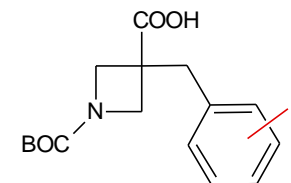
2-: PK0-41751
3-: PK0-41991
4-: PK0-41761



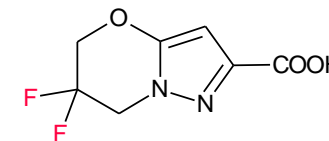
4-: PK0-47851
5-: PK0-32651
6-: PK0-31761
7-: PK0-55261



PK0-54241



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



PK0-38871

NEW! 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が掲載されました

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(19) 14299-14310

参考情報

K-BB・K-LBをご利用いただいた研究論文

<K-BB>

1. A combination of ^{19}F NMR and surface plasmon resonance for site-specific hit selection and validation of fragment molecules that bind to the ATP-binding site of a kinase. Satoru Nagatoishi et al., *Bioorg.Med.Chem.* **2018**, 26(8) 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. Kazuyoshi Ikeda, Yuichiro Kezuka, Takamasa Nonaka, Tomoki Yonezawa, Masanori Osawa, and Etsuko Katoh *J.Med.Chem.* **2021**, 64(19) 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. Yogo Shimizu et al., *Scientific Reports*, **2021**, 11, 7420