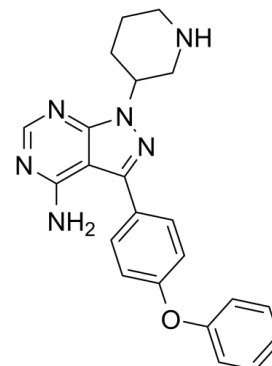


## Data Sheet

Product Name:	Btk inhibitor 1
Cat. No.:	CS-1800
CAS No.:	1412418-47-3
Molecular Formula:	C <sub>22</sub> H <sub>22</sub> N <sub>6</sub> O
Molecular Weight:	386.45
Target:	Btk
Pathway:	Protein Tyrosine Kinase/RTK
Solubility:	DMSO : 50 mg/mL (129.38 mM; Need ultrasonic)



### BIOLOGICAL ACTIVITY:

Btk inhibitor 1 (Ibrutinib analog racemate) Ibrutinib is a covalent and irreversible Ibrutinib **Bruton's tyrosine kinase (BTK)** inhibitor and is the racemate of Btk inhibitor 1 R enantiomer. Btk inhibitor 1 R enantiomer (Compound 14 in the reference) can be used in synthesis of Ibrutinib and ibrutinib-based activity-based probes (ABPs)<sup>[1]</sup>.

### References:

[1]. Liu N, et al. Direct and two-step bioorthogonal probes for Bruton's tyrosine kinase based on ibrutinib: a comparative study. *Org Biomol Chem*. 2015 May 14;13(18):5147-57.

### CAIndexNames:

1H-Pyrazolo[3,4-d]pyrimidin-4-amine, 3-(4-phenoxyphenyl)-1-(3-piperidinyl)-

### SMILES:

NC1=C2C(N(C3CNCCC3)N=C2C4=CC=C(OC5=CC=CC=C5)C=C4)=NC=N1

**Caution: Product has not been fully validated for medical applications. For research use only.**

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