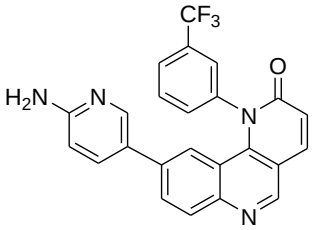
## Torin 2

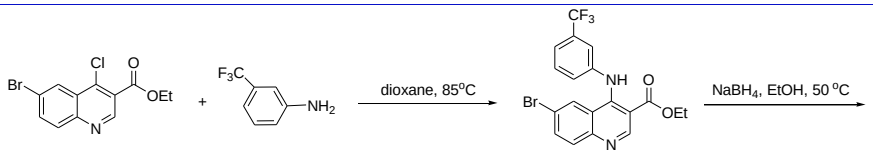


Chemical Formula: $C_{24}H_{15}F_3N_4O$
Molecular Weight: 432.40

| Category | Parameter | Description |
|---|---|---|
| Compound | Name | Torin 2 |
| | Citation | *J Med Chem*. **2011**, *54(5):*1473-80 |
| | Chemical descriptors | O=C1N(C2=CC(C(F)(F)F)=CC=C2)C3=C(C=C1)C=NC4=CC=C(C5=CN=C(N)C=C5)C=C43 |
| | Chemical name | 9-(6-aminopyridin-3-yl)-1-(3-(trifluoromethyl)phenyl)benzo[h][1,6]naphthyridin-2(1H)-one |
| | Availability | Tocris Bioscience<br>http://www.tocris.com/dispprod.php?ItemId=294892 |
| *In vitro* profiling | Primary target (potency) | **mTORC1** ($IC_{50}$ of 2.1 nM) |
| | Other target (potency) | Invitrogen Lipid Kinase panel:<br>**PI4K β** ($IC_{50}$ of 18.3nM),<br>**PI3K-C2 α** ($IC_{50}$ of 28.1nM),<br>**PI3K-C2β** ($IC_{50}$ of 24.5nM),<br>**hVPS34** ($IC_{50}$ of 8.58nM),<br>**P110 α/p85α** ($IC_{50}$ of 4.68 nM),<br>**P110δ/P85α** ($IC_{50}$ of 17.5 nM),<br>**P110γ** ($IC_{50}$ of 5.67 nM),<br>**DNA-PK** ($IC_{50}$ of 0.5 nM) |
| | Selectivity | Torin2 exhibit excellent overall selectivity (S(5) score(1 μM) = 2%) in a panel of 440 kinases (Ambit KinomeScan™ technology) and has strong binding to mTOR (4.6% control), CSNK1E (2.7% control), several PI3Ks, CSF1R (2.4% control) and MKNK2 (0.9% control). |
| | Potential reactivity | |
| | SAR | *J Med Chem*. **2011**, *54(5):*1473-80, Table 2 |
| | Mechanism of inhibition | ATP-competitive |
| | Structure of target-probe complex | |
| Cellular profiling | Validation of cellular target | |
| | Validation of cellular specificity | 800-fold selectivity over PI3K |
| Pharmacodynamics | | |

Pharmacokinetics

| $C_{max}$ (ng/mL) I.V./P.O. | $T_{max}$ (h) PO | AUC (h*ng/mL) I.V./P.O. | $T_{1/2}$ (h) I.V. | CL (mL/min/Kg) I.V. | $V_{ss}$ (L/Kg) I.V. | F (%) P.O. |
|---|---|---|---|---|---|---|
| 1540/3968 | 0.25 | 850/4311 | 0.72 | 19.6 | 1.0 | 51 |




Synthetic scheme