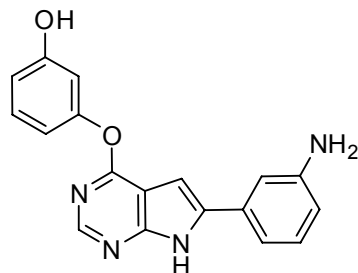


3-[[6-(3-aminophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]oxy]-phenol (TWS119) - glycogen synthase kinase-3 (GSK-3) inhibitor



Chemical Formula: C₁₈H₁₄N₄O₂
Molecular Weight: 318.33

- Ref. 1: Dessalew et al. **Investigation of potential glycogen synthase kinase 3 inhibitors using pharmacophore mapping and virtual screening.** *Chemical Biology & Drug Design* (2006), 68, 154-165
To investigate the identification of new potential glycogen synthase kinase-3 inhibitors, a pharmacophore mapping study was carried out using a set of 21 structurally diverse glycogen synthase kinase-3 inhibitors. The best hypothesis was used to screen electronically the NCI2000 database. The hits obtained were docked into glycogen synthase kinase-3 β active site. A total of five novel potential leads were proposed after: (i) visual examination of how well they dock into the glycogen synthase kinase-3 β -binding site, (ii) comparative analysis of their FlexX, G-Score, PMF-Score, ChemScore and D-Scores values, (iii) comparison of their best fit value with the known inhibitors and (iv) examination of the how the hits retain interactions with the important amino acid residues of glycogen synthase kinase-3 β -binding site.
- Ref. 2: Ding et al. **Synthetic small molecules that control stem cell fate.** *Proceedings of the National Academy of Sciences of the United States of America* (2003), 100, 7632-7637
A high-throughput phenotypic cell-based screen of kinase-directed combinatorial libraries led to the discovery of **TWS119**, a 4,6-disubstituted pyrrolopyrimidine that can induce neurogenesis in murine ESCs. The target of **TWS119** was shown to be glycogen synthase kinase-3 β (GSK-3 β) by both affinity-based and biochemical methods. This study provides evidence that GSK-3 β is involved in the induction of mammalian neurogenesis in ESCs. This and such other molecules are likely to provide insights into the molecular mechanisms that control stem cell fate and may ultimately be useful to *in vivo* stem cell biology and therapy.

OTAVA catolg no.	CAS RN	Amount	Delivery time	Purity
7070707013	601514-19-6	1 mg 5 mg 25 mg 100 mg	In-stock In-stock In-stock In-stock	≥ 95% by HPLC, ¹³ C NMR & ¹ H NMR
