# Small Molecules

**SB431542 (Hydrate)**

Activin/BMP/TGFβ pathway inhibitor;
Inhibits ALK4, ALK5, and ALK7

| | | |
|---|---|---|
| Catalog # | 72232 | 1 mg |
| | 72234 | 10 mg |
| | 100-1051 | 25 mg |

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## Product Description

SB431542 is a selective and potent inhibitor of the transforming growth factor (TGF)-β, Activin, and Nodal pathways. It inhibits the TGF-β type I receptors ALK5 ($IC_{50}$ = 94 nM), ALK4 ($IC_{50}$ = 140 nM), and ALK7 by competing for the ATP binding site. It does not inhibit the bone morphogenetic protein (BMP) type I receptors ALK2, ALK3, and ALK6 (Inman et al.; Laping et al.). This product is supplied as the hydrate form of the molecule.

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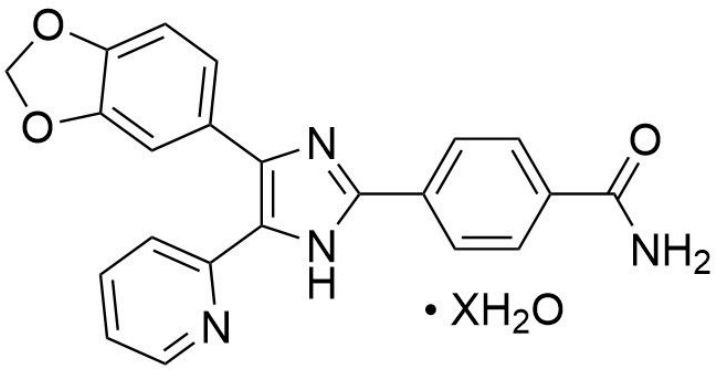
| Molecular Name: | SB431542 (Hydrate) |
| Alternative Names: | SB-431542 |
| CAS Number: | Not applicable |
| Chemical Formula: | $C_{22}H_{16}N_4O_3 \bullet XH_2O$ |
| Molecular Weight: | 384.4 g/mol |
| Purity: | ≥ 98% |
| Chemical Name: | 4-[4-(1,3-benzodioxol-5-yl)-5-(2-pyridinyl)-1H-imidazol-2-yl]-benzamide hydrate |
| Structure: |  |



## Properties

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| Physical Appearance: | A crystalline solid |
| Storage: | Product stable at -20°C as supplied. Protect from prolonged exposure to light.<br>Stable as supplied for 12 months from date of receipt. |
| Solubility: | · DMSO ≤ 50 mM<br>· Absolute ethanol ≤ 5.2 mM<br>For example, to prepare a 10 mM stock solution in DMSO, resuspend 1 mg in 260 µL of DMSO.<br>NOTE: This is based on a molecular weight (MW) of 384.4 g/mol. MW may vary due to variable water content of the molecule. |

Prepare stock solution fresh before use. Information regarding stability of small molecules in solution has rarely been reported, however, as a general guide we recommend storage in DMSO at -20°C. Aliquot into working volumes to avoid repeated freeze-thaw cycles. The effect of storage of stock solution on compound performance should be tested for each application.

Compound has low solubility in aqueous media. For use as a cell culture supplement, stock solution should be diluted into culture medium immediately before use. Avoid final DMSO concentration above 0.1% due to potential cell toxicity.

## Published Applications

REPROGRAMMING
· Replaces SOX2 in the reprogramming of mouse fibroblasts to induced pluripotent stem (iPS) cells (Ichida et al.).
· Increases the efficiency of reprogramming human somatic cells to iPS cells, in combination with PD0325901 (Catalog #72182) and Thiazovivin (Catalog #72252) (Lin et al.).
· Direct lineage reprogramming of fibroblasts to mature neurons, in combination with CHIR99021 (Catalog #72052), ISX-9 (Catalog #73202), Forskolin (Catalog #72112), and I-BET151 (Catalog #73712; Li et al.).
DIFFERENTIATION
· Promotes differentiation of neural progenitor cells from human pluripotent stem cells (PSCs), in combination with either LDN193189 (Catalog #72146) or Noggin (Catalog #78060) (Chambers et al. 2009; Chambers et al. 2012).
· Promotes proliferation and sheet formation of mouse embryonic stem (ES)-derived endothelial cells (Watabe et al.).
· Enhances differentiation of cardiomyocytes from mouse and human PSCs (Kattman et al.).
· Inhibits the self-renewal and causes differentiation of human PSCs, demonstrating the importance of the TGFβ/Activin/Nodal pathway in their maintenance (James et al.; Vallier et al.).

## References

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Chambers SM et al. (2009) Highly efficient neural conversion of human ES and iPS cells by dual inhibition of SMAD signaling. Nat Biotechnol 27(3): 275–80.
Ichida JK et al. (2009) A small molecule inhibitor of TGF-beta signaling replaces Sox2 in reprogramming by inducing Nanog. Cell Stem Cell 5(5): 491–503.
Inman GJ et al. (2002) SB-431542 is a potent and specific inhibitor of transforming growth factor-beta superfamily type I activin receptor-like kinase (ALK) receptors ALK4, ALK5, and ALK7. Mol Pharmacol 62(1): 65–74.
James D et al. (2005) TGFbeta/activin/nodal signaling is necessary for the maintenance of pluripotency in human embryonic stem cells. Development 132(6): 1273–82.
Kattman SJ et al. (2011) Stage-specific optimization of activin/nodal and BMP signaling promotes cardiac differentiation of mouse and human pluripotent stem cell lines. Cell Stem Cell 8(2): 228–40.
Laping NJ et al. (2002) Inhibition of transforming growth factor (TGF)-beta1-induced extracellular matrix with a novel inhibitor of the TGF-beta type I receptor kinase activity: SB-431542. Mol Pharmacol 62(1): 58–64.
Li X et al. (2015) Small-molecule-driven direct reprogramming of mouse fibroblasts into functional neurons. Cell Stem Cell 17(2): 195–203. Lin T et al. (2009) A chemical platform for improved induction of human iPSCs. Nat Methods 6(11): 805–8.
Vallier L et al. (2005) Activin/Nodal and FGF pathways cooperate to maintain pluripotency of human embryonic stem cells. J Cell Sci 118(Pt 19): 4495–509.
Watabe T et al. (2003) TGF-beta receptor kinase inhibitor enhances growth and integrity of embryonic stem cell-derived endothelial cells. J Cell Biol 163(6): 1303–11.

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