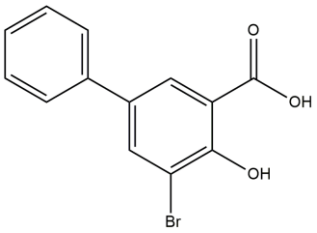
NSC109116

09/19

ALTERNATE NAME: 3-bromo-5-phenylsalicylic acid; 5-Bromo-4-hydroxy-[1,1'-biphenyl]-3-carboxylic acid; 3-bromo-2-hydroxy-5-phenylbenzoic acid; AKR1C1 Inhibitor; Aldo-Keto Reductase family 1 member C1 Inhibitor; 5-PBSA

CATALOG #:
B2911-1 1 mg
B2911-5 5 mg

STRUCTURE:



MOLECULAR FORMULA: $C_{13}H_9BrO_3$

MOLECULAR WEIGHT: 293.1

CAS NUMBER: 4906-68-7

APPEARANCE: A crystalline solid

PURITY: >97%

SOLUBILITY:
~0.1 mg/ml in Ethanol
~12.5 mg/ml in DMSO
~15 mg/ml in DMF

DESCRIPTION: NSC109116 is an inhibitor of human 20α-hydroxysteroid dehydrogenase (AKR1C1), an aldo-keto reductase (AKR) enzyme. AKR1C1 metabolizes progesterone to an inactive form, 20α-hydroxy progesterone. NSC109116 is a salicylic compound that selectively inhibits AKR1C1 (K_i = 4 nM) over AKR1C2. It potently inhibits the metabolism of progesterone in bovine aortic endothelial cells overexpressing AKR1C1 with an IC_{50} of 460 nM.

STORAGE TEMPERATURE: -20°C. Store in the dark. Product is light sensitive.

HANDLING: Do not take internally. Wear gloves and mask when handling the product! Avoid contact by all modes of exposure.

REFERENCES:

1. El-Kabbani, O., Scammells, P.J., Gosling, J., et al. Structure-guided design, synthesis, and evaluation of salicylic acid-based inhibitors targeting a selectivity pocket in the active site of human 20α-hydroxysteroid dehydrogenase (AKR1C1). Journal of Medicinal Chemistry 52, 3259-3264 (2009).
2. Zhang, Y., Dufort, I., Rheault, P., et al. Characterization of a human 20α-hydroxysteroid dehydrogenase. Journal of Molecular Endocrinology 25, 221-228 (2000).

RELATED PRODUCTS:

Progesterone (Cat. No. 2913)
AKR1C3 Inhibitor II (Cat. No. 2404)
Megestrol acetate (Cat. No. B2193)
AKR1C3 Inhibitor III (Cat. No. 2424)
AKR1C3 Inhibitor I (Cat. No. 2403)

DISCLAIMER: ***FOR RESEARCH USE ONLY! Not to be used on humans.***