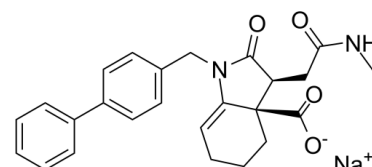


Data Sheet

Product Name:	Fumarate hydratase-IN-2 (sodium salt)
Cat. No.:	CS-5727
Molecular Formula:	C ₂₅ H ₂₅ N ₂ NaO ₄
Molecular Weight:	440.47
Target:	Others
Pathway:	Others
Solubility:	DMSO : 10.66 mg/mL (24.20 mM; Need ultrasonic and warming)



BIOLOGICAL ACTIVITY:

Fumarate hydratase-IN-2 sodium salt (compound 3) is a cell-permeable and competitive **fumarate hydratase** inhibitor ($K_i=4.5 \mu\text{M}$) with nutrient-dependent cytotoxicity ^[1]. IC₅₀ & Target: K_i : 4.5 μM (Fumarate hydratase) ^[1]

References:

[1]. Takeuchi T et al. Identification of fumarate hydratase inhibitors with nutrient-dependent cytotoxicity. J Am Chem Soc. 2015 Jan 21;137(2):564-7.

CAIndexNames:

3aH-Indole-3a-carboxylic acid, 1-([1,1'-biphenyl]-4-ylmethyl)-1,2,3,4,5,6-hexahydro-3-[2-(methylamino)-2-oxoethyl]-2-oxo-, (3R,3aS)-rel-,sodium salt

SMILES:

O=C([O-])[C@]1([C@H](CC(NC)=O)C2=O)C(N2CC(C=C3)=CC=C3C4=CC=CC=C4)=CCCC1.[Na+]

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

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