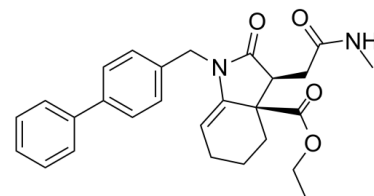


Data Sheet

| | |
|--------------------|---|
| Product Name: | Fumarate hydratase-IN-1 |
| Cat. No.: | CS-5629 |
| CAS No.: | 1644060-37-6 |
| Molecular Formula: | C ₂₇ H ₃₀ N ₂ O ₄ |
| Molecular Weight: | 446.54 |
| Target: | Others |
| Pathway: | Others |
| Solubility: | DMSO : 50 mg/mL (111.97 mM; Need ultrasonic) |



BIOLOGICAL ACTIVITY:

Fumarate hydratase-IN-1 (compound 2) is a cell-permeable **fumarate hydratase** inhibitor. Fumarate hydratase-IN-1 has antiproliferative activity against several cancer cell lines with a mean IC₅₀ of 2.2 μM^[1]. IC₅₀ & Target: Fumarate hydratase^[1] **In Vitro:** Fumarate hydratase-IN-1 inhibits SW620, ACHN, HCT-116, PC3, and SK-MEL-28 cell lines with a mean IC₅₀ of 2.2 μM^[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): 564-567.

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-, ethyl ester, (3R,3aS)-rel-

SMILES:

O=C(OCC)[C@]1([C@H](CC(NC)=O)C2=O)C(N2CC(C=C3)=CC=C3C4=CC=CC=C4)=CCCC1

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

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