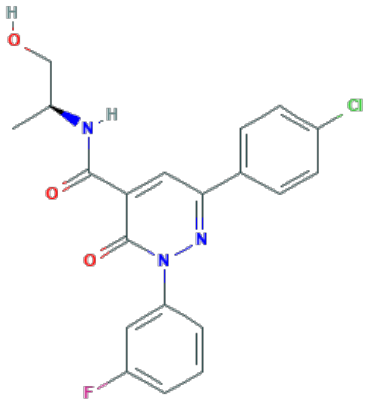
CD BioGlyco

SUITE 201, 17 Ramsey Road, Shirley, NY 11967, USA

Tel: 1-631-637-6119 | Email: info@bioglyco.com

Product Information

AhR inhibitor, AHR antagonist 1, Purity ≥98%



Cat. No.: X24-09-YM457

Size: 5 mg; 10 mg; 50 mg; 100 mg

MDL: MFCD31736303

CAS Number: 2162982-11-6

Compound CID: 132168144

Synonym: 2162982-11-6; BAY2335218; BAY-218; BS-16509; HY-111449; BAY-218; BAY 218; 6-(4-Chlorophenyl)-2-(3-fluorophenyl)-*N*-[(2*S*)-1-hydroxypropan-2-yl]-3-oxopyridazine-4-carboxamide; AhR inhibitor

This product is for research use only and is not intended for diagnostic use.

Product Information

Description	AHR antagonist 1, soluble in DMSO and ethanol and insoluble in water, is an effective metabolism inhibitor, that has the ability to prevent the pathway of cell metabolism by inhibiting AhR. The molecular weight of the compound is 401.82, and its molecular formula is $C_{20}H_{17}ClFN_3O_3$.
Molecular Weight	401.82
Molecular Formula	$C_{20}H_{17}ClFN_3O_3$
IUPAC Name	6-(4-Chlorophenyl)-2-(3-fluorophenyl)-*N*-[(2*S*)-1-hydroxypropan-2-yl]-3-oxopyridazine-4-carboxamide
InChI	InChI=1S/C20H17ClFN3O3/c1-12(11-26)23-19(27)17-10-18(13-5-7-14(21)8-6-13)24-25(20(17)28)16-4-2-3-15(22)9-16/h2-10,12,26H,11H2,1H3,(H,23,27)/t12-/m0/s1
InChI Key	RFGRNBWAUZSMBN-LBPRGKRZSA-N
Canonical SMILES	CC(CO)NC(=O)C1=CC(=NN(C1=O)C2=CC(=CC=C2)F)C3=CC=C(C=C3)Cl
Isomeric SMILES	C[C@@H](CO)NC(=O)C1=CC(=NN(C1=O)C2=CN(N=C2)C)C3=CC=C(C=C3)Cl
Form	Lyophilized powder
Purity	≥98%
Impurities	Free from inappropriate visible particulates, foreign matter, discoloration, or other defects.
Solubility	*In vitro*: DMSO: 76 mg/mL (189.14 mM); Water: insoluble; Ethanol: 19 mg/mL (47.28 mM)
Identity	Confirmed by NMR/HPLC/MS.
Stability	In its lyophilized form, the chemical remains stable for 36 months.

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Quality Level	Research grade
Applications	AHR antagonist 1 plays a key role in cancer biology and immune regulation, providing a tool to study the receptor’s contribution to various pathologies.
Storage	Store at -20ºC, and keep desiccated.