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DATASHEET

2,5-Dimethyl-celecoxib

Product overview

Name 2,5-Dimethyl-celecoxib

Cat No HB3717 **Purity** >99%

Description Shows no COX-2 inhibitory function. Analog of celecoxib.

Biological Data

Biological description Close structural analog of the selective cyclooxygenase-2 (COX-2) inhibitor celecoxib, that lacks

COX-2 inhibitory function. Anti-proliferative, anti-tumorigenic and anti-angiogenic. Potent apoptosis inducer in many cancer cell lines. Down-regulates the expression of survivin, cyclins, MMPs and inhibits cyclin-dependent kinase activity. Modulates PDK-1, AKT, GSK3beta, p70 S6K, PKA and MAPKAP-K1alpha.Reduces phosphorylation of ERK1/2 but not AKT T-308 or AKT S-473. Increases intracellular free calcium levels and potently triggers the endoplasmatic reticulum stress response (ESR), activating ER stress-associated proteins GRP78/BiP, CHOP/GADD153 and caspase-4.

Solubility & Handling

Solubility overview Soluble in DMSO Storage instructions Room temperature

Storage of solutions Prepare and use solutions on the same day if possible. Store solutions at -20°C for up to one month if

storage is required. Equilibrate to RT and ensure the solution is precipitate free before use.

Shipping Conditions Stable for ambient temperature shipping. Follow storage instructions on receipt.

Important This product is for RESEARCH USE ONLY and is not intended for therapeutic or diagnostic use. Not

for human or veterinary use.

Chemical Data

Chemical name Molecular Weight Chemical structure 4-[5-(2,5-dimethylphenyl)-3-(trifluoromethyl)pyrazol-1-yl]benzenesulfonamide 395.4



Molecular Formula $C_{18}H_{16}F_3N_3O_2S$ **CAS Number** 457639-26-8 **PubChem identifier** 11545682

SMILES CC1=CC(=C(C=C1)C)C2=CC(=NN2C3=CC=C(C=C3)S(=O)(=O)N)C(F)(F)FInChi

InChI=1S/C18H16F3N3O2S/c1-11-3-4-12(2)15(9-11)16-10-17(18(19,20)21)23-24(16)13-5-7-14(8-6

-13)27(22,25)26/h3-10H,1-2H3,(H2,22,25,26)

InChiKey NTFOSUUWGCDXEF-UHFFFAOYSA-N

MDL number MFCD19443858 **Appearance** White solid