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## DATASHEET

### 2,5-Dimethyl-celecoxib

## Product overview

|                    |                                                          |
|--------------------|----------------------------------------------------------|
| <b>Name</b>        | 2,5-Dimethyl-celecoxib                                   |
| <b>Cat No</b>      | HB3717                                                   |
| <b>Purity</b>      | >99%                                                     |
| <b>Description</b> | Shows no COX-2 inhibitory function. Analog of celecoxib. |

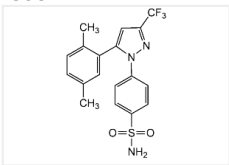
## Biological Data

|                               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
|-------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Biological description</b> | 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 potentially triggers the endoplasmic reticulum stress response (ESR), activating ER stress-associated proteins GRP78/BiP, CHOP/GADD153 and caspase-4. |
|-------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

## Solubility & Handling

|                             |                                                                                                                               |
|-----------------------------|-------------------------------------------------------------------------------------------------------------------------------|
| <b>Storage instructions</b> | Room temperature                                                                                                              |
| <b>Solubility overview</b>  | Soluble in DMSO                                                                                                               |
| <b>Important</b>            | This product is for RESEARCH USE ONLY and is not intended for therapeutic or diagnostic use. Not for human or veterinary use. |

## Chemical Data

|                           |                                                                                                                                     |
|---------------------------|-------------------------------------------------------------------------------------------------------------------------------------|
| <b>Chemical name</b>      | 4-[5-(2,5-dimethylphenyl)-3-(trifluoromethyl)pyrazol-1-yl]benzenesulfonamide                                                        |
| <b>Molecular Weight</b>   | 395.4                                                                                                                               |
| <b>Chemical structure</b> |                                                  |
| <b>Molecular Formula</b>  | C <sub>18</sub> H <sub>16</sub> F <sub>3</sub> N <sub>3</sub> O <sub>2</sub> S                                                      |
| <b>CAS Number</b>         | 457639-26-8                                                                                                                         |
| <b>PubChem identifier</b> | 11545682                                                                                                                            |
| <b>SMILES</b>             | CC1=CC(=C(C=C1)C)C2=CC(=NN2C3=CC=C(C=C3)S(=O)(=O)N)C(F)(F)F                                                                         |
| <b>InChi</b>              | 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) |
| <b>InChiKey</b>           | NTFOSUUWGCDXEF-UHFFFAOYSA-N                                                                                                         |
| <b>MDL number</b>         | MFCD19443858                                                                                                                        |
| <b>Appearance</b>         | White solid                                                                                                                         |