1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C_{20}H_{20}Cl_{2}N_{8}O_{3}.HCl.\frac{1}{4}H_{2}O

Batch Molecular Weight: 550.31

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Desiccate at RT

2. ANALYTICAL DATA

HPLC: Shows 99.7% purity

\textsuperscript{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

\begin{tabular}{ccc}
 & Carbon & Hydrogen & Nitrogen \\
Theoretical & 43.65 & 4.3 & 20.36 \\
Found & 43.32 & 4.39 & 20.68 \\
\end{tabular}
Product Name: TH 5427 hydrochloride
Catalog No.: 6534
Batch No.: 1
IUPAC Name: 7-{[5-(3,4-Dichlorophenyl)-1,3,4-oxadiazol-2-yl]methyl}-1,3-dimethyl-8-(piperazine-1-yl)-1H-purine-2,6-dione hydrochloride

Description:
Potent nudix hydrolase 5 (NUDT5) inhibitor (IC₅₀ = 29 nM). Displays >650-fold selectivity for NUDT5 over MTH1. Inhibits ATP synthesis, chromatin remodeling, gene expression and proliferation in progesterin-treated breast cancer cells in vitro.

Physical and Chemical Properties:
Batch Molecular Formula: C₆₀H₅₀Cl₂N₉O₅.HCl.1¼H₂O
Batch Molecular Weight: 550.31
Physical Appearance: White solid
Minimum Purity: >98%

Storage: Desiccate at RT

Solubility & Usage Info:
water to 100 mM
DMSO to 100 mM

Stability and Solubility Advice:
Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:
SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.
SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

Licensing Information:
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References: