# **Product data sheet**



| MedKoo Cat#: 558446   |  | _                      |
|---|--|------------------------|
| Name: GW779439X   |  |                        |
| CAS: 551919-98-3  |  | \                      |
| Chemical Formula: C <sub>22</sub> H <sub>21</sub> F <sub>3</sub> N <sub>8</sub> |  | N                      |
| Exact Mass: 454.1841  |  | N N                    |
| Molecular Weight: 454.4612  |  |                        |
| Product supplied as:  | Powder                                     | ] —N N—(/ >>—NH        |
| Purity (by HPLC):   | ≥ 98%                                      | ] \_/ \ <del>_</del> / |
| Shipping conditions   | Ambient temperature                        | ] F-√                  |
| Storage conditions:   | Powder: -20°C 3 years; 4°C 2 years.        | ] F F                  |
|   | In solvent: -80°C 3 months; -20°C 2 weeks. | ' '                    |

## 1. Product description:

GW779439X is a cyclin dependent kinase inhibitor.

## 2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

| Solvent | Max Conc. mg/mL | Max Conc. mM |
|---------|-----------------|--------------|
| DMSO    | 31.25           | 68.76        |

4. Stock solution preparation table:

| Concentration / Solvent Volume / Mass | 1 mg    | 5 mg     | 10 mg    |
|---------------------------------------|---------|----------|----------|
| 1 mM                                  | 2.20 mL | 11.00 mL | 22.00 mL |
| 5 mM                                  | 0.44 mL | 2.20 mL  | 4.40 mL  |
| 10 mM                                 | 0.22 mL | 1.10 mL  | 2.20 mL  |
| 50 mM                                 | 0.04 mL | 0.22 mL  | 0.44 mL  |

#### 5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of "Calculator"

#### 6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

1. Schaenzer AJ, Wlodarchak N, Drewry DH, Zuercher WJ, Rose WE, Ferrer CA, Sauer JD, Striker R. GW779439X and Its Pyrazolopyridazine Derivatives Inhibit the Serine/Threonine Kinase Stk1 and Act As Antibiotic Adjuvants against β-Lactam-Resistant Staphylococcus aureus. ACS Infect Dis. 2018 Oct 12;4(10):1508-1518. doi: 10.1021/acsinfecdis.8b00136. Epub 2018 Aug 15. PMID: 30059625; PMCID: PMC6779124.

In vivo study

TBD

#### 7. Bioactivity

#### Biological target:

GW779439X is a pyrazolopyridazine identified in an inhibitor of the S. aureus PASTA kinase Stk1. GW779439X potentiates the activity of  $\beta$ -lactam antibiotics against various MRSA and MSSA isolates, some even crossing the breakpoint from resistant to sensitive. GW779439X is an AURKA inhibitor and induces apoptosis by the caspases 3/7 pathway.

#### In vitro activity

As can be seen in Table 1, GW779439X was able to potentiate the activity of all  $\beta$ -lactams tested, particularly the penicillinase-resistant penicillins oxacillin and nafcillin to an MIC considered susceptible to these agents.

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Reference: ACS Infect Dis. 2018 Oct 12;4(10):1508-1518. https://pubmed.ncbi.nlm.nih.gov/30059625/

In vivo activity

TBD

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.