## PAD-IN-2

| Cat. No.:          | HY-135304   |       |          |  |  |
|--------------------|---|-------|----------|--|--|
| CAS No.:           | 2304852-21-7  |       |          |  |  |
| Molecular Formula: | C <sub>27</sub> H <sub>28</sub> CIN <sub>5</sub> O <sub>2</sub> |       |          |  |  |
| Molecular Weight:  | 490   |       |          |  |  |
| Target:            | Protein Arginine Deiminase                                      |       |          |  |  |
| Pathway:           | Epigenetics   | 5     |          |  |  |
| Storage:           | Powder  | -20°C | 3 years  |  |  |
|                    |   | 4°C   | 2 years  |  |  |
|                    | In solvent  | -80°C | 6 months |  |  |
|                    |   | -20°C | 1 month  |  |  |

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### SOLVENT & SOLUBILITY

| In Vitro                     | DMSO : 70 mg/mL (142.86 mM; Need ultrasonic)  |                               |           |            |            |  |  |
|------------------------------|---|-------------------------------|-----------|------------|------------|--|--|
| Preparing<br>Stock Solutions |   | Solvent Mass<br>Concentration | 1 mg      | 5 mg       | 10 mg      |  |  |
|                              | Preparing<br>Stock Solutions  | 1 mM                          | 2.0408 mL | 10.2041 mL | 20.4082 mL |  |  |
|                              |   | 5 mM                          | 0.4082 mL | 2.0408 mL  | 4.0816 mL  |  |  |
|                              |   | 10 mM                         | 0.2041 mL | 1.0204 mL  | 2.0408 mL  |  |  |
|                              | Please refer to the solubility information to select the appropriate solvent.   |                               |           |            |            |  |  |
| In Vivo                      | 1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 5.25 mg/mL (10.71 mM); Clear solution |                               |           |            |            |  |  |
|                              | 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)<br>Solubility: ≥ 5.25 mg/mL (10.71 mM); Clear solution         |                               |           |            |            |  |  |

| BIOLOGICAL ACTIV |   |
|------------------|---|
| DIOLOGICAL ACTIV |   |
| Description      | PAD-IN-2 is a potent pad4 inhibitor (IC <sub>50</sub> : <1 μM). PAD-IN-2 can be used in the research of auto-immune diseases and cancers, such as rheumatoid arthritis, vasculitis, systemic lupus erythematosis, cutaneous lupus erythematosis, ulcerative colitis, cystic fibrosis, asthma, multiple sclerosis and psoriasis <sup>[1]</sup> . |
| In Vitro         | PAD-IN-2 (Example-57, 1 h) inhibits PAD4 activity with an IC <sub>50</sub> value <1 μM (determined by ammonia release biochemical assay) <sup>[1]</sup> .<br>MCE has not independently confirmed the accuracy of these methods. They are for reference only.  |

# Product Data Sheet

CI

'NH<sub>2</sub>

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### REFERENCES

[1]. Hallur, Gurulingappa, et al. Heterocyclic compounds as pad4 inhibitors. Patent WO2019058393 A1.

#### Caution: Product has not been fully validated for medical applications. For research use only.

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