## **Product** Data Sheet

## hCES2A-IN-1

Molecular Weight: 366.45

Target: Others

Pathway: Others

Storage: Please store the product under the recommended conditions in the Certificate of

Analysis.

## **BIOLOGICAL ACTIVITY**

Description	hCES2A-IN-1 (compound 20w) is a potent hCES2A inhibitor, with an IC $_{50}$ value of 1.6 nM. hCES2A-IN-1, a bysspectin A derivative, shows an approximately 1000-fold improvement over the lead compound bysspectin A $^{[1]}$ .
IC <sub>50</sub> & Target	hCES2A (0.0016 $\pm$ 0.00034 $\mu\text{M}),$ hCES1A (7.26 $\pm$ 0.94 $\mu\text{M})^{[1]}$
In Vitro	hCES2A-IN-1 (compound 20w) exhibits very weak cytotoxicity to the HepG2 cells at concentration less than 10 $\mu$ M <sup>[1]</sup> . hCES2A-IN-1 can inhibit hCES2A-mediated NCEN hydrolysis in living cells in a dose-dependent manner with an IC50 value of 0.052 $\mu$ M, which showed significantly higher inhibition activity than Loperamide with an IC50 value of 1.44 $\mu$ M <sup>[1]</sup> . hCES2A-IN-1 (compound 20w) exhibits favorable metabolic stability. The half-life of compound 20w in phase I or phase II metabolic systems in human liver microsomes are 125.96 min and 97.38 min, respectively <sup>[1]</sup> . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

## **REFERENCES**

[1]. Li W, et al. New bysspectin A derivatives as potent inhibitors of human carboxylesterase 2A. Eur J Med Chem. 2023 Nov 5;259:115708.

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

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