## **Product** Data Sheet

## CYP1B1-IN-5

Cat. No.: HY-152196 CAS No.: 176442-56-1 Molecular Formula:  $C_{_{14}}H_{_8}INO_{_2}$  Molecular Weight: 349.12

Target: Cytochrome P450

Pathway: Metabolic Enzyme/Protease

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

Analysis.

## **BIOLOGICAL ACTIVITY**

Description	$ {\it CYP1B1-IN-5} \ ({\it Compound 6q}) \ is \ a \ potent \ and \ selective \ cytochrome \ P450 \ 1B1 \ ({\it CYP1B1}) \ inhibitor \ with \ an \ IC_{50} \ of \ 4.7 \ nM^{[1]}. $		
IC <sub>50</sub> & Target	CYP1B1 4.7 nM (IC <sub>50</sub> )	CYP1A1 190.7 nM (IC <sub>50</sub> )	CYP1A2 585.7 nM (IC <sub>50</sub> )
In Vitro	CYP1B1-IN-5 (Compound 6q) fits well into the binding pocket of CYP1B1, by forming $\pi$ - $\pi$ stacking interactions with residue Phe231, Phe134 and heme <sup>[1]</sup> . MCE has not independently confirmed the accuracy of these methods. They are for reference only.		

## **REFERENCES**

[1]. Yi L, et al. A new class of CYP1B1 inhibitors derived from bentranil. Bioorg Med Chem Lett. 2022 Dec 21;80:129112.

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

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