

## Supporting information

### **Serotonin 2A receptor (5-HT<sub>2A</sub>R) activation by 25H-NBOMe positional isomers: in vitro functional evaluation and molecular docking**

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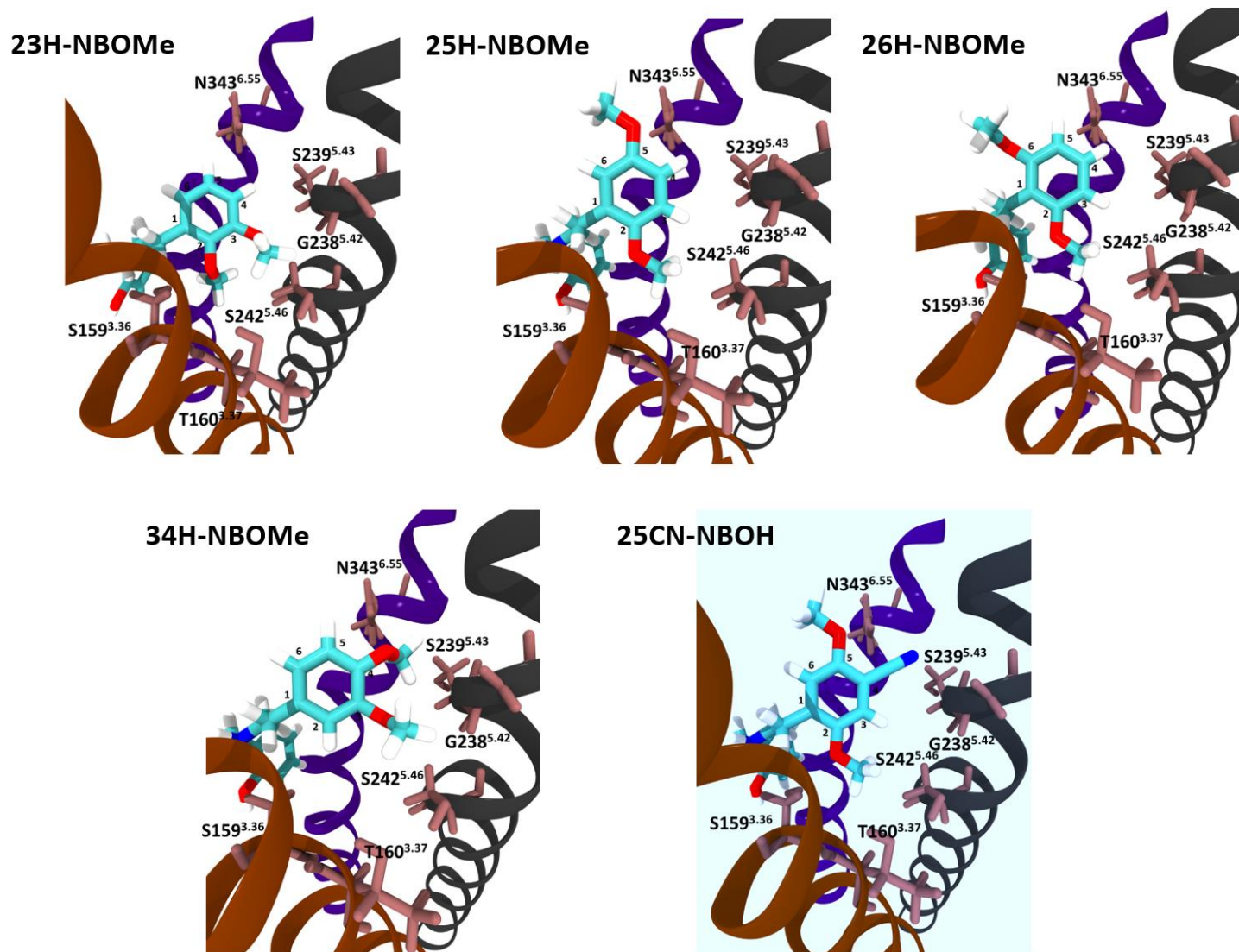
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## **CONTENT**

**Figure S1**                      **Visual representation of the docking of 25CN-NBOH and 23H-, 25H-, 26H-, and 34H-NBOMe in the binding pocket of the 5-HT<sub>2A</sub>R.**



**Figure S1:** Visual representation of the docking of 25CN-NBOH, and 23H-, 25H-, 26H-, and 34H-NBOMe in the binding pocket of the 5-HT<sub>2A</sub>R (PDB: 6WHA)<sup>1</sup>. The specified residues are those specifically hypothesized to interact with the specific methoxy groups on the phenyl group of the phenethylamine moiety.

## REFERENCE

1. Kim, K.; Che, T.; Panova, O.; DiBerto, J. F.; Lyu, J.; Krumm, B. E.; Wacker, D.; Robertson, M. J.; Seven, A. B.; Nichols, D. E.; Shoichet, B. K.; Skiniotis, G.; Roth, B. L., Structure of a Hallucinogen-Activated Gq-Coupled 5-HT<sub>2A</sub> Serotonin Receptor. *Cell* **2020**, 182 (6), 1574-1588 e19.