

**Supporting Information**

# Development of covalent ligands for G protein-coupled receptors: a case for the human adenosine A<sub>3</sub> receptor

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- Figure S1. Overlay of a view from crystal structure of compound **2** (mustard carbon sticks) bound to human adenosine A<sub>1</sub> receptor (mustard; PDB: 5UEN) and the hA<sub>3</sub>AR (violet) homology model docking with **17b** (violet carbon sticks).

## Supplementary data

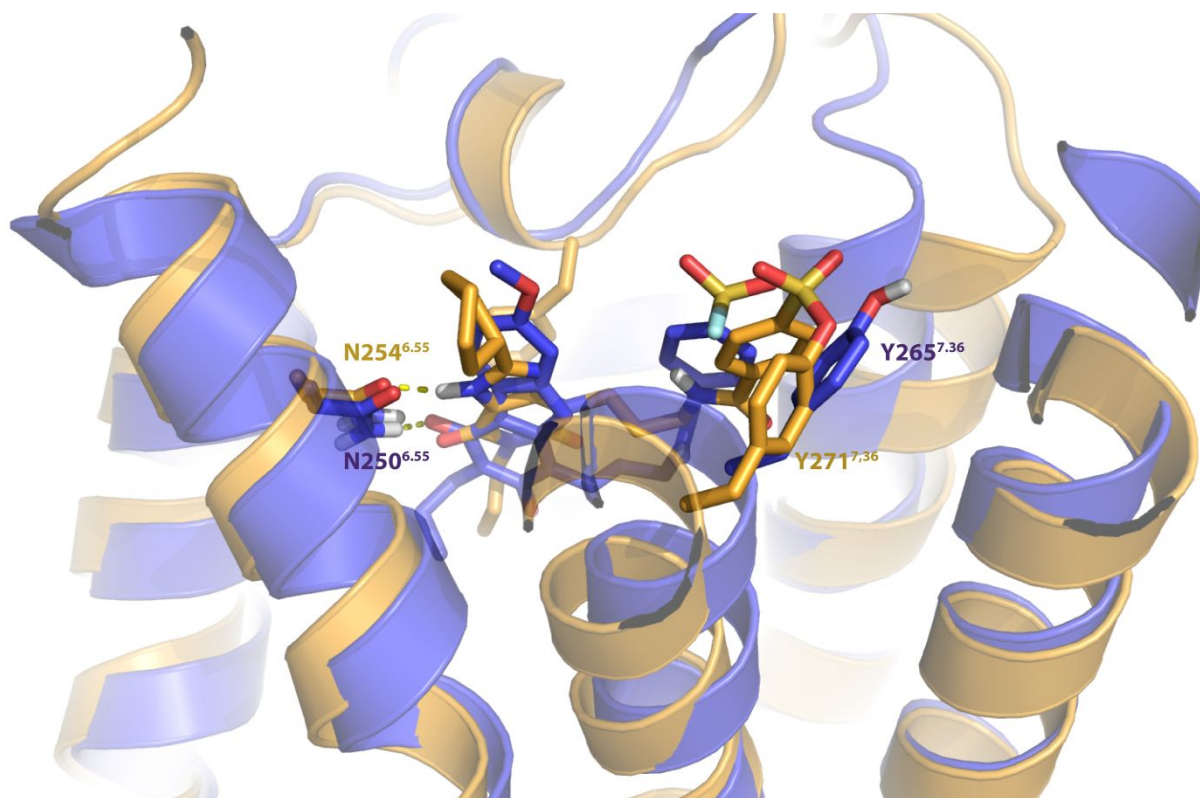


Figure S1. Overlay of a view from crystal structure of compound **2** (mustard carbon sticks) bound to human adenosine A<sub>1</sub> receptor (mustard; PDB: 5UEN)<sup>1</sup> and the hA<sub>3</sub>AR (violet) homology model docking with **17b** (violet carbon sticks). Atoms color code: red = oxygen, blue = nitrogen, white = hydrogen, yellow = sulfur, cyan = fluorine. Hydrogen bonds between ligands and relevant amino acid residues are indicated by dashed lines.

## REFERENCES:

1. Glukhova, A.; Thal, D. M.; Nguyen, A. T.; Vecchio, E. A.; Jorg, M.; Scammells, P. J.; May, L. T.; Sexton, P. M.; Christopoulos, A. Structure of the adenosine A<sub>1</sub> receptor reveals the basis for subtype selectivity. *Cell* **2017**, 168, 867-877.