

## Supplementary Material (Table)

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Authors:

Meekyum Olivia Kim<sup>1,\*</sup>, Sara E. Nichols<sup>1,2,3</sup>, Yi Wang<sup>4,\*</sup> †, J. Andrew McCammon<sup>1,2,3,4</sup>

<sup>1</sup> Department of Chemistry and Biochemistry, University of California San Diego, La Jolla, CA 92093, USA

<sup>2</sup> Department of Pharmacology, University of California San Diego, La Jolla, CA 92093, USA

<sup>3</sup> Center for Theoretical Biological Physics, University of California San Diego, La Jolla, CA 92093, USA

<sup>4</sup> Howard Hughes Medical Institute, University of California San Diego, La Jolla, CA 92093, USA

\* To whom correspondence should be addressed:

Meekyum Olivia Kim, [mok007@ucsd.edu](mailto:mok007@ucsd.edu);

Yi Wang, [yiwang@phy.cuhk.edu.hk](mailto:yiwang@phy.cuhk.edu.hk)

† Current address: Department of Physics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong



**Supplementary Table 1** *p*-Values for AUC of 36 receptor models, displayed with protonation and rotameric states of two histidines in each model. The letter F in protonation and rotameric state name represents a flipped state. Receptors with *p*-Values less than 0.05 (boldfaced) differ in their ability to distinguish the actives and decoys in VS with statistical significance compared to others.