pubs.acs.org/jcim

Correction to Computational Comparison of Imidazoline Association with the I2 Binding Site in Human Monoamine Oxidases

Livia Basile, Matteo Pappalardo, Salvatore Guccione,* Danilo Milardi, and Rona R. Ramsay* *J. Chem. Inf. Model.* **2014**, 54 (4), 1200–1207. DOI: 10.1021/ci400346k

This corrects the caption to Figure 1. It should read as follows: Comparison of the MAO A (PDB ID: 2Z5X,¹⁷ blue) active site cavity with that of MAO B-TCP-2-BFI (PDB ID: 2XCG,¹⁴ magenta). The FAD cofactors are shown in line form. The residues in contact with 2-BFI (cyan) are displayed in stick format: Pro102, Ile199, Gln206, Ile316, and Tyr326 in MAO B (magenta) with the equivalent residues Ala111, Phe208, Gln215, Ile325, and Ile335 in MAO A (blue). Residues 109–112 of the loop at the entrance to the active site cavity in MAO A are shown in blue stick format.



Published: July 8, 2014