Corrigendum: Cloud-based simulations on Google Exacycle reveal ligand modulation of GPCR activation pathways

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In the version of this Article originally published, Figure 4 displayed incorrectly drawn chemical structures for five of the ligands. The correct structures were, however, used in the calculations. The hemiaminal group previously depicted in compounds **2**–**4** should have been a β-amino alcohol, compound **7** contained an extra benzylic carbon and compound **8** had an extra ring. The corresponding PubChem CID numbers for the correct ligands are as follows. Agonists: **1**, 19044758; **2**, 44216210; **3**, 44209282; **4**, 44213610. Antagonists: **5**, 15020513; **6**, 19823514; **7**, 44209768; **8**, 44209764. These drawing errors have now been corrected in the online versions of this Article. Additionally, the 'Inverse agonist' label at the top of Fig. 4b has been changed to 'Antagonist' as this was the original designation for this set of the GPCR ligand database used for docking (E. A. Gatica and C. N. Cavasotto, *J. Chem. Inf. Model.* **52,** 1–6; 2012). Some ligands, particularly carazolol used in this study, may have inverse agonist activity.

For all calculations, functional groups were protonated according to pH = 7. Stereochemistry is not depicted in the figure because stereoisomer activity for these compounds has not been elucidated. The structures in Figure 4 are each representative of many ligands that define a 3D chemotype and share a similar binding pose in protein conformations with similar progress scores. Stereoisomers were enumerated for up to four chiral centers and docked. The isomer with the highest score, or approximated binding affinity, was selected for a given protein conformation. Different protein conformations score isomers differently, and protein conformations with the same progress score may select different isomers of the same compound. Further experiments on the known agonist and antagonist ligands would be needed in order to determine the activities of stereoisomers, as has been done for albuterol and fenoterol (R. Seifert and S. Dove, *Mol. Pharmacol.* **75,** 13–18; 2009).