Supporting information to:

On the applicability of computer aided drug discovery to GPCRs: a comparison between molecular models and crystal structure of the β_2-adrenergic receptor

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Table of Contents: **Page**

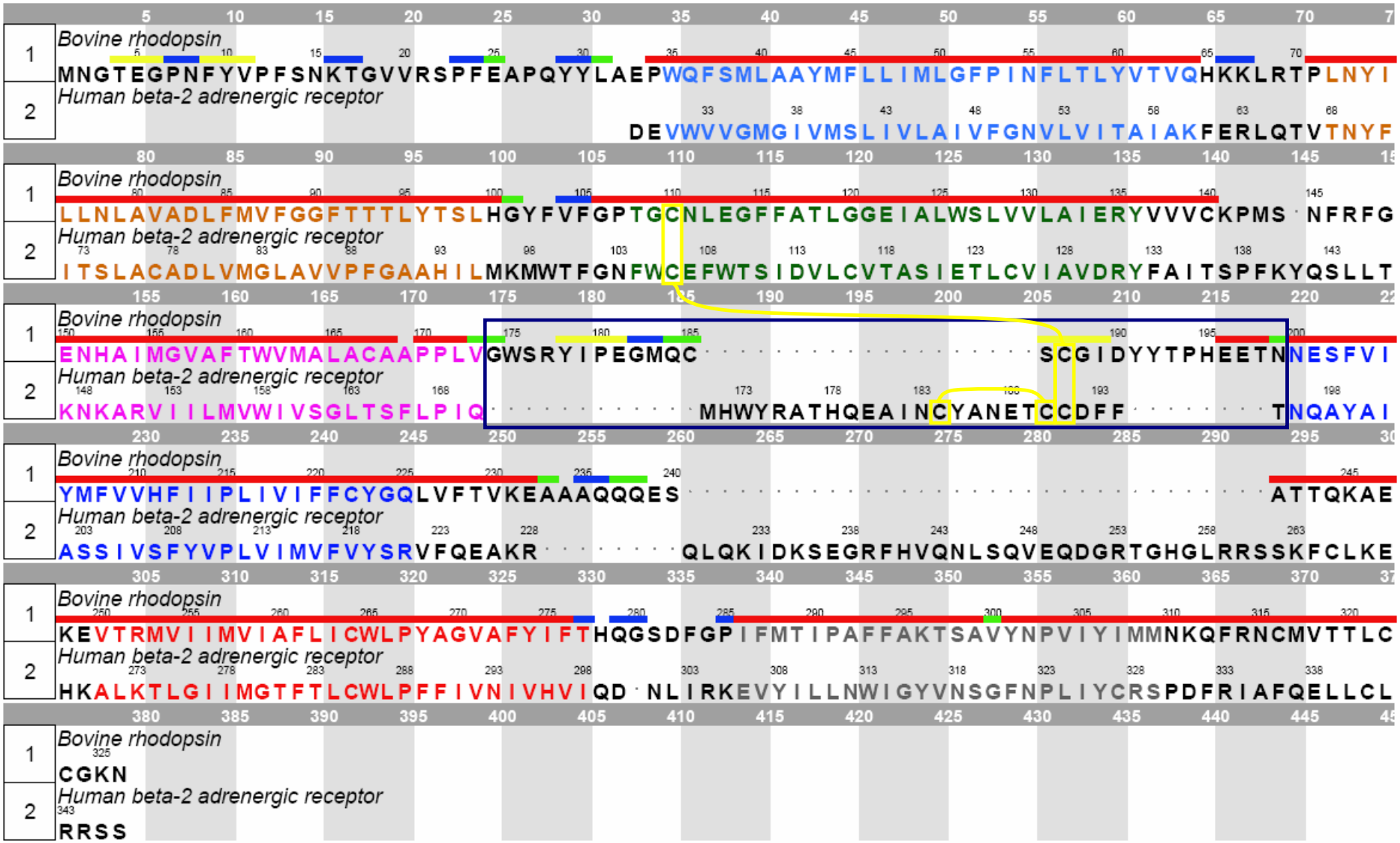

Figure S1. Sequence alignment of bovine rhodopsin and the beta-2 adrenergic receptor utilized for the construction of model 1. The second extracellular loop (blue box) was partially built by homology to rhodopsin. In particular, the conserved Cys in EL2 and the four adjacent residues that in rhodopsin form a beta-strand were aligned with the corresponding residues of the beta2 receptor. The seven transmenbrane regions are color coded (TM1:light blue; TM2, Brown; TM3: green; TM4: purple; TM5: blue; TM6: red; TM7: gray. The figure was produced with MOE (Chemical Computing Group, Montreal, Canada).

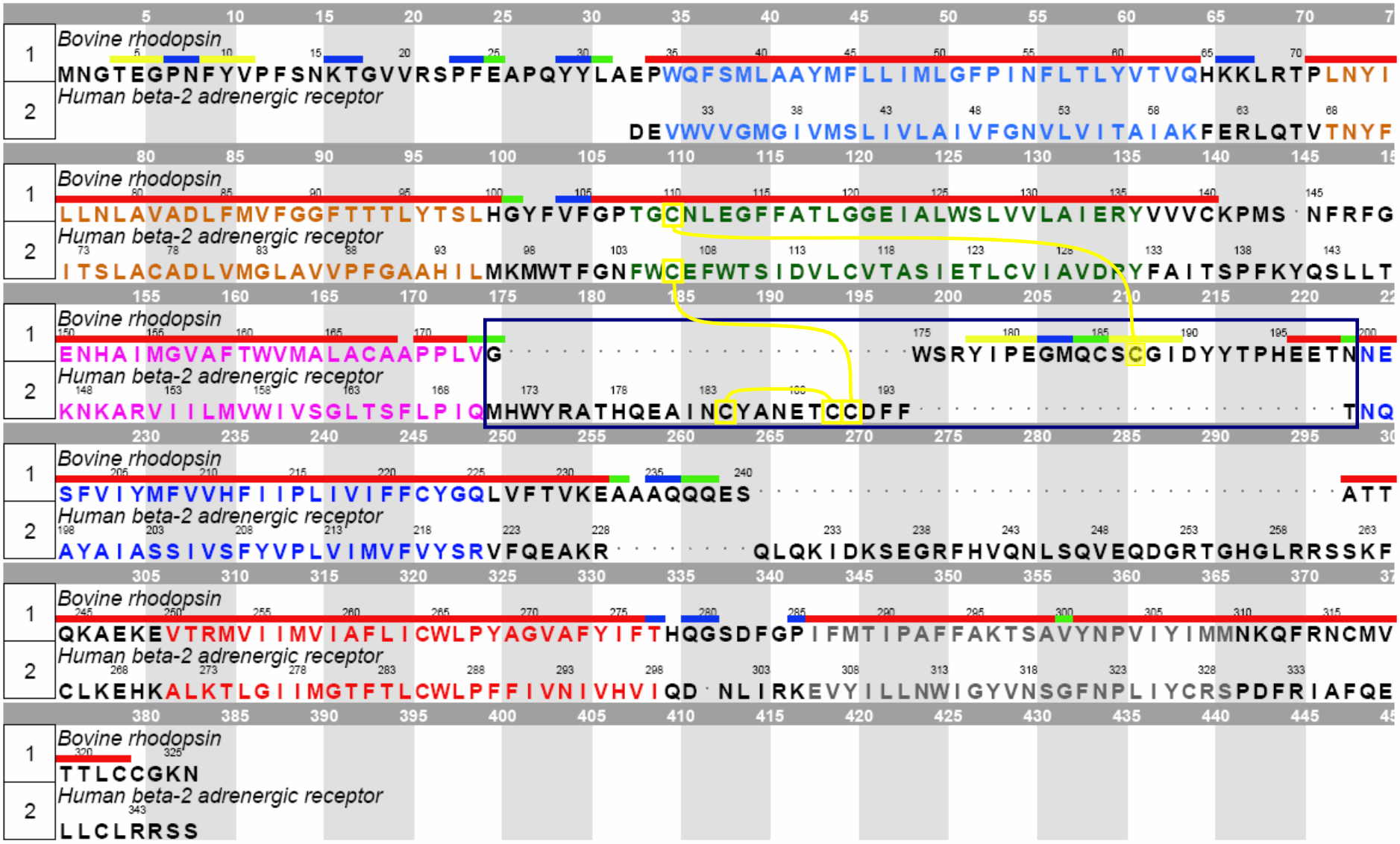

Figure S2. Sequence alignment of bovine rhodopsin and the beta-2 adrenergic receptor utilized for the construction of model 2. The second extracellular loop (blue box) was built completely de novo, without any alignment between the sequences of rhodopsin and the beta2 receptor. The seven transmenbrane regions are color coded (TM1:light blue; TM2, Brown; TM3: green; TM4: purple; TM5: blue; TM6: red; TM7: gray. The figure was produced with MOE (Chemical Computing Group, Montreal, Canada).

Figure S3. The docking region, represented here in purple, was defined as a cubic box with a side of 26 Å and centered on Val114(3.33). The latter is located in a central position within the 7TM helical bundle, and is represented here in space filling mode.