Supplemental Data

Supplemental Tables

Table S1

Quality check of the homology model of the Kir6.2Δ1-25 tetramer. The calculations have been done using What If (swift.cmbi.ru.nl), MolProbity (smb.slac.stanford.edu) and the JCSG protein structure validation server (www.jcsg.org).

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<th>Ramachandran Plot</th>
<th>Planarity</th>
<th>Proline Puckering</th>
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<td>Residues in most favored regions</td>
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Table S2

The 20 best docking results obtained for the docking of M2 onto Kir6.2Δ1-25. The best docking model of each cluster is highlighted in bold.

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<th>(\theta_{Kir6.2})</th>
<th>(E_{M2-Kir6.2})</th>
<th>M2 interface</th>
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Table S3

The 20 best docking results obtained for the docking of M2$^{Δ458-466}$ onto Kir6.2$^{Δ1-25}$. The best docking model of each cluster is highlighted in bold.

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<th>$θ_{Kir6.2}$</th>
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SUPPLEMENTAL FIGURES

Figure S1

Comparison of the homodimer organization in the crystal structures of κ-OR, μ-OR and CXCR4, and in the docking model of CXCR4. Helices not involved in the interface are in white. Helix IV of the CXCR4 docking model is colored for comparison with the crystal structure. For clarity, only the transmembrane helices and the in-plane helix VIII are displayed.
Figure S2

Comparison of the β2 crystal structures bound to an agonist (BI-167107; PDB entry 3SN6) or an inverse agonist (carazolol; PDB entry 2RH1). A– Superimposition of the PDB entries 3NS6 and 2RH1. B– PDB entry 2RH1 colored as a function of the Cα RMSD with the PDB entry 3SN6. For clarity, only the β2 structure is shown.
Figure S3

Schematic representation of the potential molecular mechanism of M2Kir6.2Δ1-25. 1– The ligand binds the M2 binding site. 2– A slight conformational change occurs at the tip of the M2 helix I. 3– A slight conformational change occurs at the M2 C-terminus. 4– The conformational change occurring in M2 modifies the Kir6.2 N-terminus conformation. Potentially, an interaction with the Kir6.2 turn E³²²-Y³²⁶ is affected too. The regular gating mechanism of Kir6.2 is by-passed. 5– The modifications are transmitted to the closest gate of Kir6.2 by the regular gating mechanism of the channel.