Supplementary Material 2.

Coordinates files of receptor- ligand complexes (PDB format)

B2_ norepinephrine.pdb

D2_dopamine.pdb.

Coordinates, limited to residues lining the predicted binding sites, of the β_2-norepinephrine and D_2-dopamine complexes. Amino-acids are numbered according to the Ballesteros and Weinstein convention and, the numbering of residues, *e.g.* 3.32 may appear as 332 when displayed using a program to view the structure.

Interaction map files (Autodock format)

β_2-AR: *B2_site_C.map, B2_site_HA.map, B2_site_HD.map; B2_ligand_C.map*, *B2_ligand_HA.map, B2_ligand_HD.map*

D_2: *D2_site_C.map, D2_site_HA.map, D2_site_HD.map, D2_ligand_C.map, D2_ligand_HA.map, D2_ligand_HD.map*

Interaction maps computed from the β_2-norepinephrine (B2_) and D_2-dopamine (D2_) complexes from either the ligand (_ligand_) or the binding site (_site_). These maps predict location favorable for interactions with hydrophobic (_C), hydrogen-bond donor (_HD) and hydrogen-bond acceptors (_HA) atoms. The maps can be viewed with respect to the corresponding structure of the binding site (see Coordinates files above) or with respect to the complete model structures (available form http://www.abo.fi/fak/mnf/bkf/research/johnson/structures.html) using for example the graphics program Bodil, available from www.abo.fi/bodil.

Tutorial: visualisation of "*B2_ norepinephrine.pdb"* and *"B2_ligand_C.map"* using Bodil

Start Bodil (Opens the window "Bodil")

In the window "Bodil":
Select in the menu: View -> 3Dview (Opens the window "3Dview")
View -> StructureEditor (Opens the window "Structure Editor")
View -> File -> and pick the files "B2_ norepinephrine.pdb" and "B2_ligand_C.map"
(The file *B2_ligand_C.map* will be recognized as Autodock format)

In the window "Structure Editor":
(left panel) Select (left click) "Grid_B2_ligand_C"
(right panel) Right-click on "Grid_B2_ligand_C" and select "Limits" (Opens the window "GridLimit")

In the window "GridLimit":
set "Visible point value - Max" (box on the top-right) to e.g 100.0 (press 'enter' after typing the value) and click OK
(This window can also be used to set limits to the region displayed)

In the window "Structure Editor":
Add -> ContourHi and set the "minimum contour value" to e.g 0.10
(In Figure 6, the minimum contour value has been set to 0.10 to display _C and to 0.15 to display _HA and _HD)

The maps together with the molecular complex appears on the "3Dview window" and can be *e.g* rotated (right mouse button) or zoomed (middle+right mouse button)

To color the maps:
In the window "Structure Editor", right panel:
Select (left click) Contour0.10 and right click over it. Select Setcolor and pick a suitable color for the map. Double click on an empty region of the 3Dview window to cancel the selection mode.

To hide/unhide an item:
In the window "Structure Editor", left panel: *right click on an item.*

To delete an item:
In the window "Structure Editor": *middle click on an item, click OK.*