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Supplementary Information

Revisiting the Homology Modeling of G-Protein Coupled Receptors: β_1-Adrenoceptor as An Example

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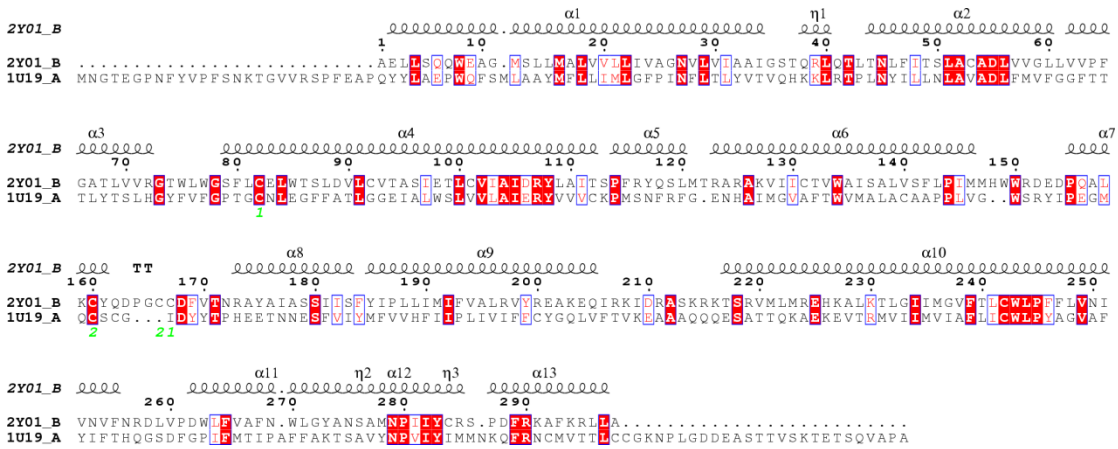

Figure S1. Aligned sequences of Bt_Rho and Mg_adrb1 with the gap opening penalty and gap extension penalty set to 10 and 3.

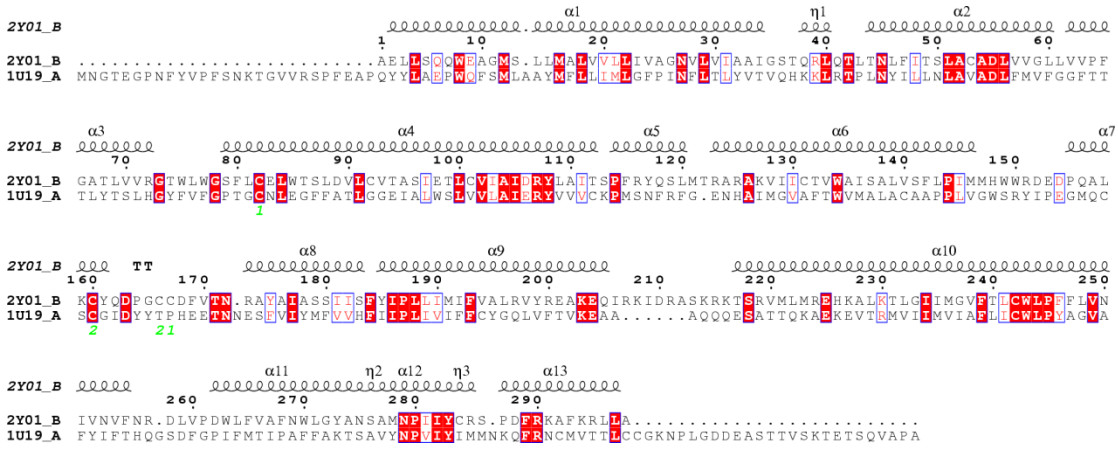

Figure S2. Aligned sequences of Bt_Rho and Mg_adrb1 with the gap opening penalty and gap extension penalty set to 10 and 1.

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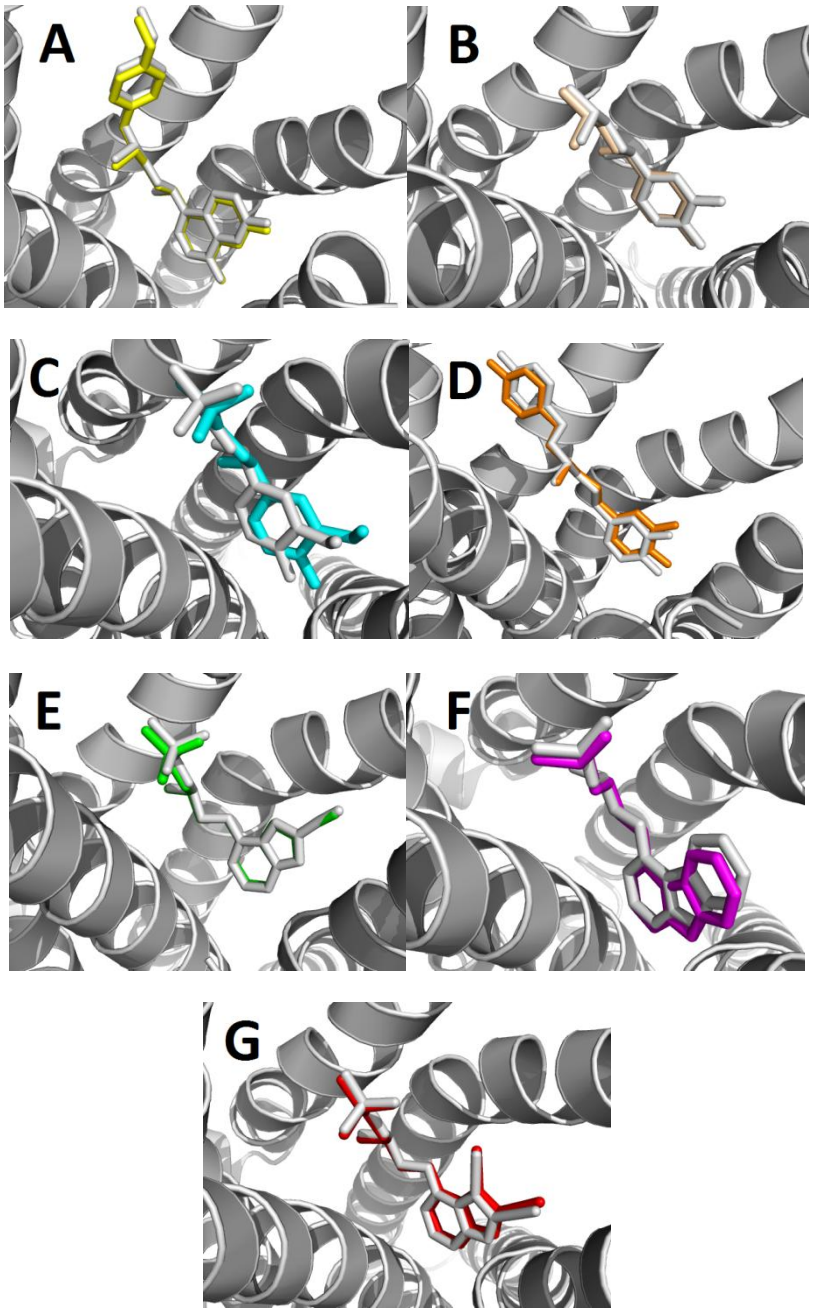

Figure S3. Docking poses of **s**even extracted ligands docked to the crystal structure of Mg_Adrb1. (A) Carmoterol, (B) isoprenaline, (C) salbultamol, (D) dobutamine, (E) cyanopindolol, (F) carazolol, (G)iodocyanopindolol. Crystal structure of Mg_Adrb1 and its ligands are shown in white.

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Table S1. Every seven TMs of one hundred models built by structures in active and inactive states were compared with the crystal structure of Mg_Adrb1 in active state.

Template	RMSD/Å	
	Active Template	Inactive Template
Hs_A2a	1.51±0.01	1.53±0.01
Bt_Opn/Bt_Rho	1.53±0.01	1.54±0.01
Hs_Adrb2	0.62±0.03	0.67±0.03

Table S2. Every seven TMs of one hundred models built by structures in active and inactive states were compared with the crystal structure of Mg_Adrb1 in inactive state.

Template	RMSD/Å	
	Active Template	Inactive Template
Hs_A2a	1.46±0.01	1.38±0.02
Bt_Opn/Bt_Rho	1.49±0.01	1.50±0.01
Hs_Adrb2	0.59±0.02	0.55±0.02

Table S3. Detailed results of molecular docking experiments with Autodock4.2.

Templates	Ligand(Crystal sturcture resolution)							
	Dobutamine(2.50Å)		Salbutamol(3.05Å)		Isoprenaline(2.85Å)		Carmoterol(2.60Å)	
	RMSD	Energy	RMSD	Energy	RMSD	Energy	RMSD	Energy
self	0.5±0.01	-8.03±0.01	0.82±0.01	-6.51±0.00	0.36±0.01	-6.26±0.00	0.46±0.01	-10.19±0.00
Hs_Adrb2	**1.04±0.04**	-6.03±0.00	**0.78±0.00**	-4.86±0.00	3.10±0.04	-4.86±0.00	**1.46±0.01**	-7.77±0.00
Tp_Rho	2.68±0.02	-4.17±0.00	4.74±0.00	-6.42±0.00	4.04±0.01	**-5.18±0.00**	4.13±0.01	-4.97±0.00
Hs_Aa2ar	5.69±0.00	-5.45±0.00	4.18±0.00	-5.21±0.00	4.36±0.06	-4.44±0.01	2.75±0.00	-4.50±0.00
Multiple1	1.24±0.01	-7.42±0.00	1.09±0.00	**-6.49±0.00**	**1.27±0.00**	-4.58±0.00	1.97±0.01	**-7.96±0.00**
Multiple2	1.93±0.01	-4.96±0.00	1.82±0.00	-3.53±0.00	2.48±0.01	-3.82±0.00	3.2±0.01	-5.25±0.00

Templates	Ligand(Crystal sturcture resolution)					
	Cyanopindolol(2.70Å)		Carazolol(3.00Å)		Indocyanopindolol(2.65Å)	
	RMSD	Energy	RMSD	Energy	RMSD	Energy
self	0.35±0.02	-8.57±0.00	0.53±0.00	-9.86±0.00	0.28±0.01	-9.28±0.00
Hs_Adrb2	**0.60±0.02**	**-8.06±0.00**	0.73±0.00	-8.33±0.00	**0.53±0.01**	**-9.02±0.00**
Tp_Rho	3.26±0.00	-5.11±0.00	4.92±0.01	-6.07±0.00	1.97±0.00	-5.92±0.00
Hs_Aa2ar	6.02±0.00	-5.54±0.01	4.69±1.15	-5.78±0.01	5.61±0.00	-5.36±0.00
Multiple1	3.04±0.00	-4.62±0.00	**0.63±0.00**	**-9.97±0.00**	0.77±0.00	-10.4±0.00
Multiple2	3.83±0.00	-5.02±0.01	1.99±0.00	-5.23±0.00	5.63±0.02	-5.42±0.00