

SUPPLEMENTARY MATERIAL

Table S1. List of 127 GPCRs that have Common G-Protein Binding Types in the GRAC and gpDB

SWISS-PROT ID	SWISS-PROT AC	G-Protein Binding Type (1: Bind, 0: Not Bind)			
		G _{i/o}	G _{q/11}	G _s	G _{12/13}
5HT1A_HUMAN	P08908	1	0	0	0
5HT1B_HUMAN	P28222	1	0	0	0
5HT1D_HUMAN	P28221	1	0	0	0
5HT1E_HUMAN	P28566	1	0	0	0
5HT1F_HUMAN	P30939	1	0	0	0
5HT5A_HUMAN	P47898	1	0	0	0
AA1R_HUMAN	P30542	1	0	0	0
AA3R_HUMAN	P33765	1	0	0	0
ACM2_HUMAN	P08172	1	0	0	0
ACM4_HUMAN	P08173	1	0	0	0
ADA2B_HUMAN	P18089	1	0	0	0
ADA2C_HUMAN	P18825	1	0	0	0
APJ_HUMAN	P35414	1	0	0	0
CCR10_HUMAN	P46092	1	0	0	0
CCR1_HUMAN	P32246	1	0	0	0
CCR2_HUMAN	P41597	1	0	0	0
CCR3_HUMAN	P51677	1	0	0	0
CCR4_HUMAN	P51679	1	0	0	0
CCR5_HUMAN	P51681	1	0	0	0
CCR6_HUMAN	P51684	1	0	0	0
CCR7_HUMAN	P32248	1	0	0	0
CCR8_HUMAN	P51685	1	0	0	0
CCR9_HUMAN	P51686	1	0	0	0
CNR1_HUMAN	P21554	1	0	0	0
CNR2_HUMAN	P34972	1	0	0	0
CX3C1_HUMAN	P49238	1	0	0	0
CXCR1_HUMAN	P25024	1	0	0	0
CXCR2_HUMAN	P25025	1	0	0	0
CXCR3_HUMAN	P49682	1	0	0	0
CXCR4_HUMAN	P61073	1	0	0	0
CXCR5_HUMAN	P32302	1	0	0	0
CXCR6_HUMAN	O00574	1	0	0	0
DRD2_HUMAN	P14416	1	0	0	0
DRD3_HUMAN	P35462	1	0	0	0

(Table S1) contd.....

SWISS-PROT ID	SWISS-PROT AC	G-Protein Binding Type (1: Bind, 0: Not Bind)			
		G _{i/o}	G _{q/11}	G _s	G _{12/13}
DRD4_HUMAN	P21917	1	0	0	0
EDG1_HUMAN	P21453	1	0	0	0
FPRL1_HUMAN	P25090	1	0	0	0
G109A_HUMAN	Q8TDS4	1	0	0	0
G109B_HUMAN	P49019	1	0	0	0
GALR1_HUMAN	P47211	1	0	0	0
GALR3_HUMAN	O60755	1	0	0	0
GPR44_HUMAN	Q9Y5Y4	1	0	0	0
HRH3_HUMAN	Q9Y5N1	1	0	0	0
HRH4_HUMAN	Q9H3N8	1	0	0	0
MTR1A_HUMAN	P48039	1	0	0	0
MTR1B_HUMAN	P49286	1	0	0	0
NPY2R_HUMAN	P49146	1	0	0	0
NPY4R_HUMAN	P50391	1	0	0	0
NPY5R_HUMAN	Q15761	1	0	0	0
OPRD_HUMAN	P41143	1	0	0	0
OPRK_HUMAN	P41145	1	0	0	0
OPRM_HUMAN	P35372	1	0	0	0
OPRX_HUMAN	P41146	1	0	0	0
OXER1_HUMAN	Q8TDS5	1	0	0	0
P2Y12_HUMAN	Q9H244	1	0	0	0
RL3R1_HUMAN	Q9NSD7	1	0	0	0
RL3R2_HUMAN	Q8TDU9	1	0	0	0
SSR1_HUMAN	P30872	1	0	0	0
SSR2_HUMAN	P30874	1	0	0	0
SSR3_HUMAN	P32745	1	0	0	0
SSR4_HUMAN	P31391	1	0	0	0
SSR5_HUMAN	P35346	1	0	0	0
XCR1_HUMAN	P46094	1	0	0	0
5HT2A_HUMAN	P28223	0	1	0	0
5HT2B_HUMAN	P41595	0	1	0	0
ACM5_HUMAN	P08912	0	1	0	0
ADA1B_HUMAN	P35368	0	1	0	0
ADA1D_HUMAN	P25100	0	1	0	0
BKRB1_HUMAN	P46663	0	1	0	0
BRS3_HUMAN	P32247	0	1	0	0
CLTR1_HUMAN	Q9Y271	0	1	0	0
CLTR2_HUMAN	Q9NS75	0	1	0	0

(Table S1) contd.....

SWISS-PROT ID	SWISS-PROT AC	G-Protein Binding Type (1: Bind, 0: Not Bind)			
		G _{i/o}	G _{q/11}	G _s	G _{12/13}
GHSR_HUMAN	Q92847	0	1	0	0
GNRHR_HUMAN	P30968	0	1	0	0
HRH1_HUMAN	P35367	0	1	0	0
MCHR2_HUMAN	Q969V1	0	1	0	0
NMBR_HUMAN	P28336	0	1	0	0
NMUR1_HUMAN	Q9HB89	0	1	0	0
NTR1_HUMAN	P30989	0	1	0	0
NTR2_HUMAN	O95665	0	1	0	0
OX1R_HUMAN	O43613	0	1	0	0
OX2R_HUMAN	O43614	0	1	0	0
P2RY1_HUMAN	P47900	0	1	0	0
P2RY2_HUMAN	P41231	0	1	0	0
P2RY4_HUMAN	P51582	0	1	0	0
P2RY6_HUMAN	Q15077	0	1	0	0
PE2R1_HUMAN	P34995	0	1	0	0
PF2R_HUMAN	P43088	0	1	0	0
PRLHR_HUMAN	P49683	0	1	0	0
TRFR_HUMAN	P34981	0	1	0	0
UR2R_HUMAN	Q9UKP6	0	1	0	0
V1BR_HUMAN	P47901	0	1	0	0
5HT6R_HUMAN	P50406	0	0	1	0
5HT7R_HUMAN	P34969	0	0	1	0
AA2AR_HUMAN	P29274	0	0	1	0
AA2BR_HUMAN	P29275	0	0	1	0
ACTHR_HUMAN	Q01718	0	0	1	0
ADRB1_HUMAN	P08588	0	0	1	0
ADRB2_HUMAN	P07550	0	0	1	0
DRD1_HUMAN	P21728	0	0	1	0
HRH2_HUMAN	P25021	0	0	1	0
MC3R_HUMAN	P41968	0	0	1	0
MC4R_HUMAN	P32245	0	0	1	0
MC5R_HUMAN	P33032	0	0	1	0
MSHR_HUMAN	Q01726	0	0	1	0
PD2R_HUMAN	Q13258	0	0	1	0
PE2R2_HUMAN	P43116	0	0	1	0
PE2R4_HUMAN	P35408	0	0	1	0
PI2R_HUMAN	P43119	0	0	1	0
TAAR1_HUMAN	Q96RJ0	0	0	1	0

(Table S1) contd.....

SWISS-PROT ID	SWISS-PROT AC	G-Protein Binding Type (1: Bind, 0: Not Bind)			
		G _{i/o}	G _{q/11}	G _s	G _{12/13}
V2R_HUMAN	P30518	0	0	1	0
C5AR_HUMAN	P21730	1	1	0	0
LT4R1_HUMAN	Q15722	1	1	0	0
LT4R2_HUMAN	Q9NPC1	1	1	0	0
MCHR1_HUMAN	Q99705	1	1	0	0
OXYR_HUMAN	P30559	1	1	0	0
PAR2_HUMAN	P55085	1	1	0	0
PAR3_HUMAN	O00254	1	1	0	0
PAR4_HUMAN	Q96R10	1	1	0	0
PTAFR_HUMAN	P25105	1	1	0	0
P2Y11_HUMAN	Q96G91	0	1	1	0
LSHR_HUMAN	P22888	1	1	1	0
EDG8_HUMAN	Q9H228	1	0	0	1
PAR1_HUMAN	P25116	1	1	0	1
EDG4_HUMAN	Q9HBW0	1	1	0	1
EDG2_HUMAN	Q92633	1	1	0	1
TSHR_HUMAN	P16473	1	1	1	1

Table S2 (A). List of the Numerical Values for the 20 Amino Acid Residues for the Amino Acid Properties that are Effective for Discriminating G_i/o Binding Type

Res. Num.	Position 94 (TM2)	Position 109 (EL1)	Position 138 (IL2)	Position 144 (IL2)	Position 145 (IL2)	Position 211 (TM5)	Position 259 (TM6)	Position 263 (TM6)
Amino Acid	Transfer Free Energy (AcWI-X-LL Peptides from Bilayer Interface to Water)	Normalized Frequency of C-Terminal Helix	Slopes Tripeptide	Refractivity	Hydrophobicity Coefficient (RP-HPLC, C18 with 0.1%TFA/MeCN/H ₂ O)	Normalized Frequency of Extended Structure	Transfer Free Energy (CHP/Water)	Normalized Average Hydrophobicity Scale
A	4.08	1.20	-0.393	4.34	0.06	0.790	-0.48	0.02
C	4.49	1.11	-0.222	35.77	0.49	1.268	-0.32	0.77
D	3.02	0.61	-0.247	12.00	-0.20	0.530	-0.75	-1.04
E	2.23	1.24	-0.260	17.26	-0.10	0.643	-0.71	-1.14
F	5.38	1.10	-0.189	29.40	4.80	1.052	1.03	1.35
G	4.24	0.42	-0.570	0.00	0.21	0.725	0.00	-0.80
H	4.08	1.77	-0.244	21.81	-2.24	0.864	-0.51	0.26
I	4.52	0.98	-0.144	19.06	3.48	1.361	0.81	1.81
K	3.77	1.83	-0.294	21.29	-1.62	0.735	-0.09	-0.41
L	4.81	1.13	-0.281	18.78	3.50	1.111	1.02	1.14
M	4.48	1.57	-0.274	21.64	0.21	1.092	0.81	1.00
N	3.83	0.59	-0.268	13.28	0.25	0.832	-0.87	-0.77
P	3.80	0.00	-	10.93	0.71	1.249	2.03	-0.09
Q	3.67	1.22	-0.291	17.56	0.31	1.038	-0.32	-1.10
R	3.91	1.25	-0.317	26.66	-0.85	1.087	-0.06	-0.42
S	4.12	0.96	-0.280	6.35	-0.62	1.093	0.05	-0.97
T	4.11	0.75	-0.152	11.01	0.65	1.214	-0.35	-0.77
V	4.18	1.25	-0.080	13.92	1.59	1.428	0.56	1.13
W	6.10	0.40	-0.206	42.53	2.29	1.114	0.66	1.71
Y	5.19	0.73	-0.155	31.53	1.89	1.340	1.24	1.11

TM: Transmembrane, IL: Intracellular Loop, EL: Extracellular Loop

Res. Num.: Sequential number of residues in rhodopsin which were used as template for structural alignment to each GPCR.

Table S2 (B). List of the Numerical Values for the 20 Amino Acid Residues for the Amino Acid Properties that are Effective for Discriminating Gq/11 Binding Type

Res. Num.	Position 98 (EL1)	Position 101 (EL1)	Position 134 (IL2)	Position 143 (IL2)	Position 273 (TM6)	Position 307 (TM7)	Position 307 (TM7)
Amino Acid	van der Waals Parameter Epsilon	Retention Coefficient in NaH ₂ PO ₄	Optimized Side Chain Interaction	Average Side Chain Orientation Angle	Relative Preference Value at C1	Size	Number of Atoms in the Side Chain Labelled 2+1
A	0.025	1.0	4.55	87	1.1	2.5	0
C	0.100	4.6	-0.78	104	1.6	3.0	0
D	0.100	-0.5	2.85	71	0.4	2.5	1
E	0.100	1.1	5.16	72	0.8	5.0	1
F	0.390	12.6	4.37	108	0.7	6.5	1
G	0.025	0.2	9.14	90	0.2	0.5	0
H	0.100	-2.2	4.48	90	3.4	6.0	1
I	0.190	7.0	2.10	105	0.7	5.5	1
K	0.200	-3.0	10.68	65	2.0	7.0	1
L	0.190	9.6	3.24	104	0.7	5.5	2
M	0.190	4.0	2.18	100	1.0	6.0	1
N	0.100	-3.0	5.56	70	1.2	5.0	1
P	0.170	3.1	5.14	78	0.0	5.5	0
Q	0.100	-2.0	4.15	66	2.1	6.0	1
R	0.200	-2.0	5.97	81	1.0	7.5	1
S	0.025	-2.9	6.78	83	1.7	3.0	0
T	0.100	-0.6	8.60	83	1.0	5.0	0
V	0.150	4.6	3.81	94	0.7	5.0	0
W	0.560	15.1	1.97	94	0.0	7.0	1
Y	0.390	6.7	2.40	83	1.2	7.0	1

TM: Transmembrane, IL: Intracellular Loop, EL: Extracellular Loop

Res. Num.: Sequential number of residues in rhodopsin which were used as template for structural alignment to each GPCR.

Table S2 (C). List of the Numerical Values for the 20 Amino Acid Residues for the Amino Acid Properties that are Effective for Discriminating Gs Binding Type

Res. Num.	Position 149 (IL2)	Position 170 (TM4)	Position 170 (TM4)	Position 171 (TM4)	Position 230 (IL3)	Position 233 (IL3)
Amino Acid	Hydrophilicity	Hydropathy Scale Based on Self-Information Values in the Two-State Model (36% Accessibility)	Optimized Average Non-Bonded Energy per Atom	Free Energy Change of Epsilon(i) to Alpha(Rh)	Normalized Positional Residue Frequency at Helix Termini N1	Average Relative Fractional Occurrence in AL(i)
A	-0.5	5	-2.49	-0.07	1.10	0.82
C	-1.0	224	-3.13	0.17	0.26	0.00
D	3.0	45	8.86	-0.80	1.14	2.64
E	3.0	-8	4.04	-0.63	2.30	2.62
F	-2.5	117	-6.64	0.40	0.90	0.00
G	0.0	-47	-0.56	0.27	0.55	1.63
H	-0.5	-50	4.22	-0.49	0.83	0.00
I	-1.8	83	-10.87	0.06	1.06	2.32
K	3.0	-38	-9.97	-0.45	1.08	2.86
L	-1.8	82	-7.16	-0.17	0.84	0.00
M	-1.3	83	-4.96	0.03	0.90	0.00
N	0.2	-77	2.27	-0.57	0.72	2.07
P	0.0	-103	5.19	-0.47	1.67	0.00
Q	0.2	-67	1.79	-0.26	1.31	0.00
R	3.0	-57	2.55	-0.40	1.05	2.60
S	0.3	-41	-1.60	-0.11	0.81	1.23
T	-0.4	79	-4.75	0.09	0.77	2.48
V	-1.5	117	-3.97	-0.11	0.76	1.62
W	-3.4	130	-17.84	-0.61	1.26	0.00
Y	-2.3	27	9.25	-0.61	0.99	1.90

TM: Transmembrane, IL: Intracellular Loop, EL: Extracellular Loop

Res. Num.: Sequential number of residues in rhodopsin which were used as template for structural alignment to each GPCR.