Table S1. β_2AR/GRK5 inter-chain BS^3 and zero-length cross-links, Related to Figures 5 and 6

Validated cross-linked peptides between β_2AR and GRK5 are listed and grouped based on the interface. Cross-linked residue in peptide sequence is highlighted in bold.

Domains (β2AR/GRK5)	Cross-linker type	Charge (z)	Obs. MH+ (Da)	Mass error (ppm)	β2AR sequence	GRK5 sequence	Cross-linked residues (β2AR-GRK5)	Cα-Cα distances in 1st model (Å)	Cα-Cα distances in 2nd model (Å)	Cα-Cα distances in 3rd model (Å)
Cluster 1										
ICL3/NLBD	BS^3	4	1674.89	0.70	VFQEA**KR**	EGGGG**KR**	227-22	10.5	12.7	13.8
ICL3/NLBD	BS^3	3	1669.92	-0.03	QLQ**K**IDK	EGGGG**KR**	232-22	13.5	13.2	15.1
ICL3/NLBD	BS^3	4	1798.02	1.31	QLQ**K**IDK	EGGGG**K**RK	232-22	13.5	13.2	15.1
ICL3/NLBD	BS^3	3	1273.71	0.69	QLQ**K**IDK	**K**GK	232-24	14.2	8.3	9.1
ICL3/NLBD	BS^3	3	1497.91	0.84	QLQ**K**IDK	R**K**GK	232-24	14.2	8.3	9.1
ICL3/NLBD	BS^3	4	1601.83	0.53	ID**K**SEGR	EGGGG**KR**	235-22	15.7	13.5	15.8
ICL3/NLBD	BS^3	3	1273.71	0.69	ID**K**SEGR	**K**GK	235-24	15.7	10	10.6
ICL3/NLBD	BS^3	4	1655.94	-0.27	ID**K**SEGR	**K**GLLQR	235-548	+ND	+ND	+ND
ICL3/CLBD	zero-length	4	2352.25	0.45	.NLSQV**E**QDGR	**K**GLLQR	249-547	+ND	+ND	+ND
Cluster 2										
ICL2/RH-bundle	BS^3	4	3138.72	-1.54	YFAITSPF**K**YQSLLTK	IMT**K**YLTPK	140-108	61.7	29.6	15.9
ICL2/RH-bundle	BS^3	4	2326.31	-1.15	YQSLLT**K**NK	IMT**K**YLTPK	147-108	70.1	37.2	29.3
Cluster 3										
C-term/Cat. domain	BS^3	6	5226.47	2.56	SSL**K**AYGNGY.	MYAC**K**R	348-215	+ND	+ND	+ND
C-term/Cat. domain	BS^3	6	7895.83	8.85	.EKEN**K**LLAED.	QYRVLG**K**	375-194	+ND	+ND	+ND
C-term/Cat. domain	BS^3	5	5060.39	-1.86	.YHVEQE**K**ENK	QPVT**K**NTFR	372-183	+ND	+ND	+ND
C-term/Cat. domain	BS^3	5	4534.15	1.48	.QGPYHVEQE**K**	MLLTKDA**K**	372-426	+ND	+ND	+ND
C-term/Cat. domain	zero-length	4	4646.03	-2.99	.SNGNTG**E**QSG	.FSTV**K**GVNLD.	362-487	+ND	+ND	+ND
Others										
ICL2/Cat. domain	BS^3	4	2322.28	1.60	YQSLLT**K**NK	QPVT**K**NTFR	147-183	15.2	25.9	26.4
ICL3/Cat. domain	BS^3	5	4015.97	1.44	VFQEA**KR**	.FSTV**K**GVNLD.	227-487	43.2	48.2	48.9
ICL3/Cat. domain	BS^3	5	4011.96	-5.05	QLQ**K**IDK	.FSTV**K**GVNLD.	232-487	40.2	46.6	47.5
ICL3/Cat. domain	BS^3	3	2048.04	2.04	ID**K**SEGR	**K**GESMALNEK	235-226	52.6	45.8	45
ICL3/RH-bundle	BS^3	4	2036.11	-0.15	ID**K**SEGR	IMT**K**YLTPK	235-108	43.1	43	31.2
C-term/CLBD	BS^3	5	5181.51	7.30	SSL**K**AYGNGY.	RQHQNNS**K**	348-564	+ND	+ND	+ND
C-term/RH-bundle	BS^3	5	4669.34	2.26	EN**K**LLAEDLP.	IMT**K**YLTPK	375-108	+ND	+ND	+ND
C-term/NLBD	zero-length	3	2304.98	1.95	.SNGNTG**E**QSG	EGGGG**KR**	362-22	+ND	+ND	+ND

+ND Cα-Cα distance is not determined (ND) due to absence of atomic coordinates of one or two cross-linked domains, but the cross-link is plausible based on structural proximity of cross-linked domains in the model.