Electronic Supplementary Material (ESI) for Molecular BioSystems

Supplementary materials.

Supplementary Figure 1. TDCC
N corresponds to the sample size. Tdcc corresponds to the value of "top-down coeeficient of concordance". Starting from N=2000 TDCC follows saturation trend .

Supplementary Figure 2. Participation of different proteins in the complexes
Shown are the results for one parameter set, which gives the biggest complex in simulation (1586 molecules) and 235 other complexes of the smaller size.
X-axis represents the number of complexes (from 236), which particular protein (Y axis) participates in.

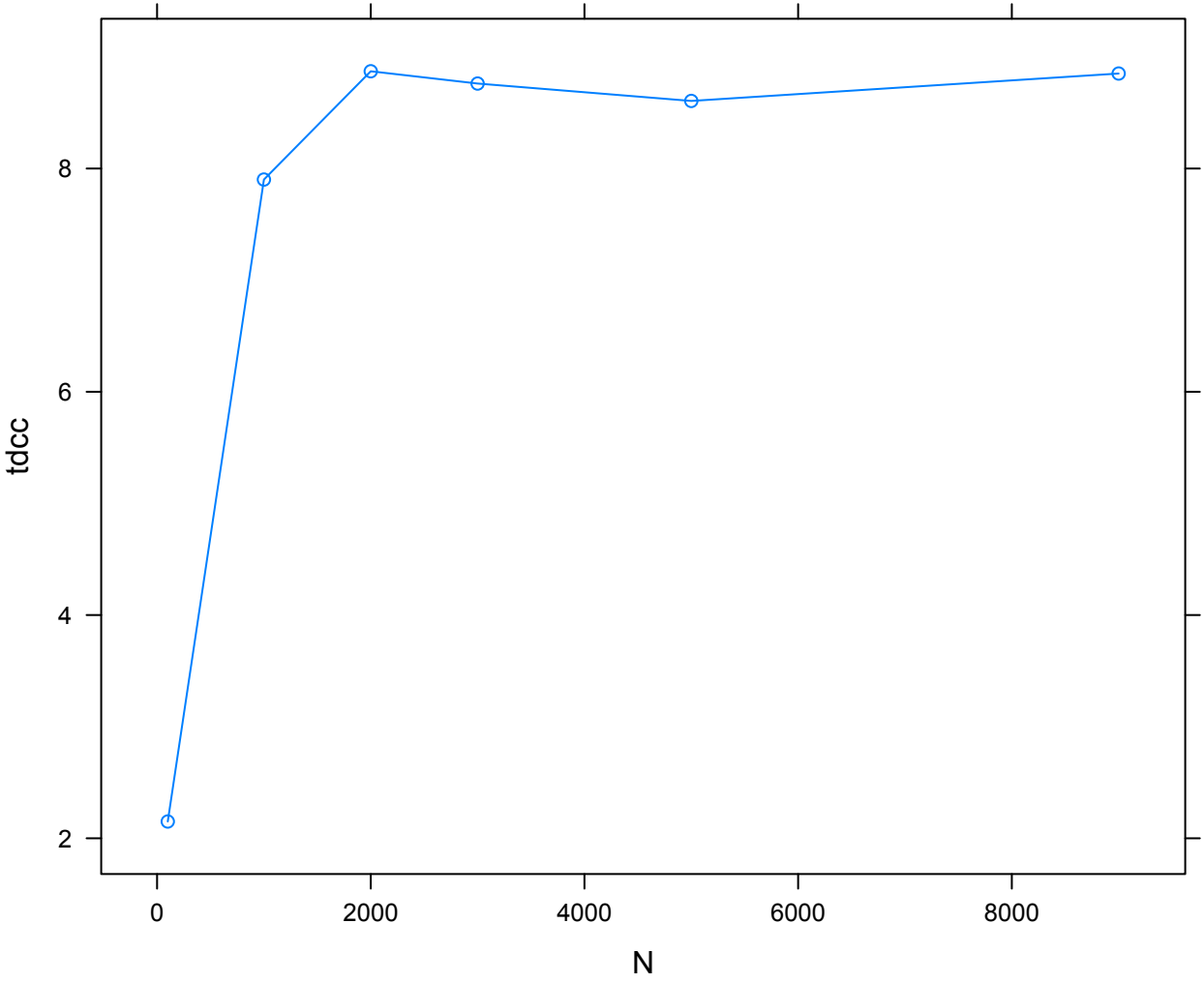
Supplementary Figure 3. Composition of the largest complex
Shown is the brutto composition of the largest (1726 molecules) complex obtained in the 'wild-type' simulation.

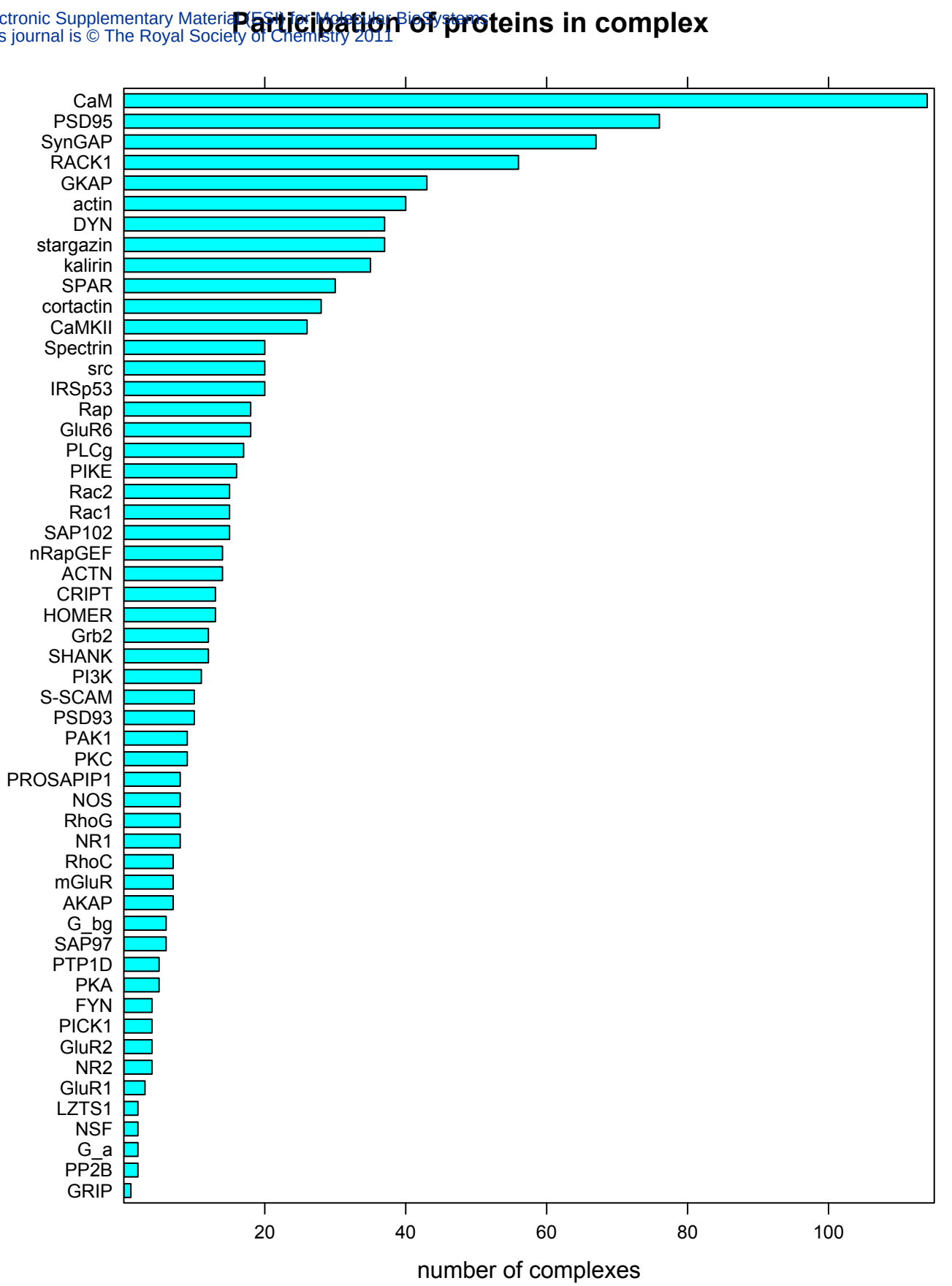
Supplementary Figure 4. Participation of different proteins in the complexes.
Shown are the results for the parameter set that gives the largest complex in PSD95 knock-out simulation (729 molecules) and 211 of other complexes with smaller size.
X-axis represents the number of complexes (from 212), which particular protein (y-axis) participates in.

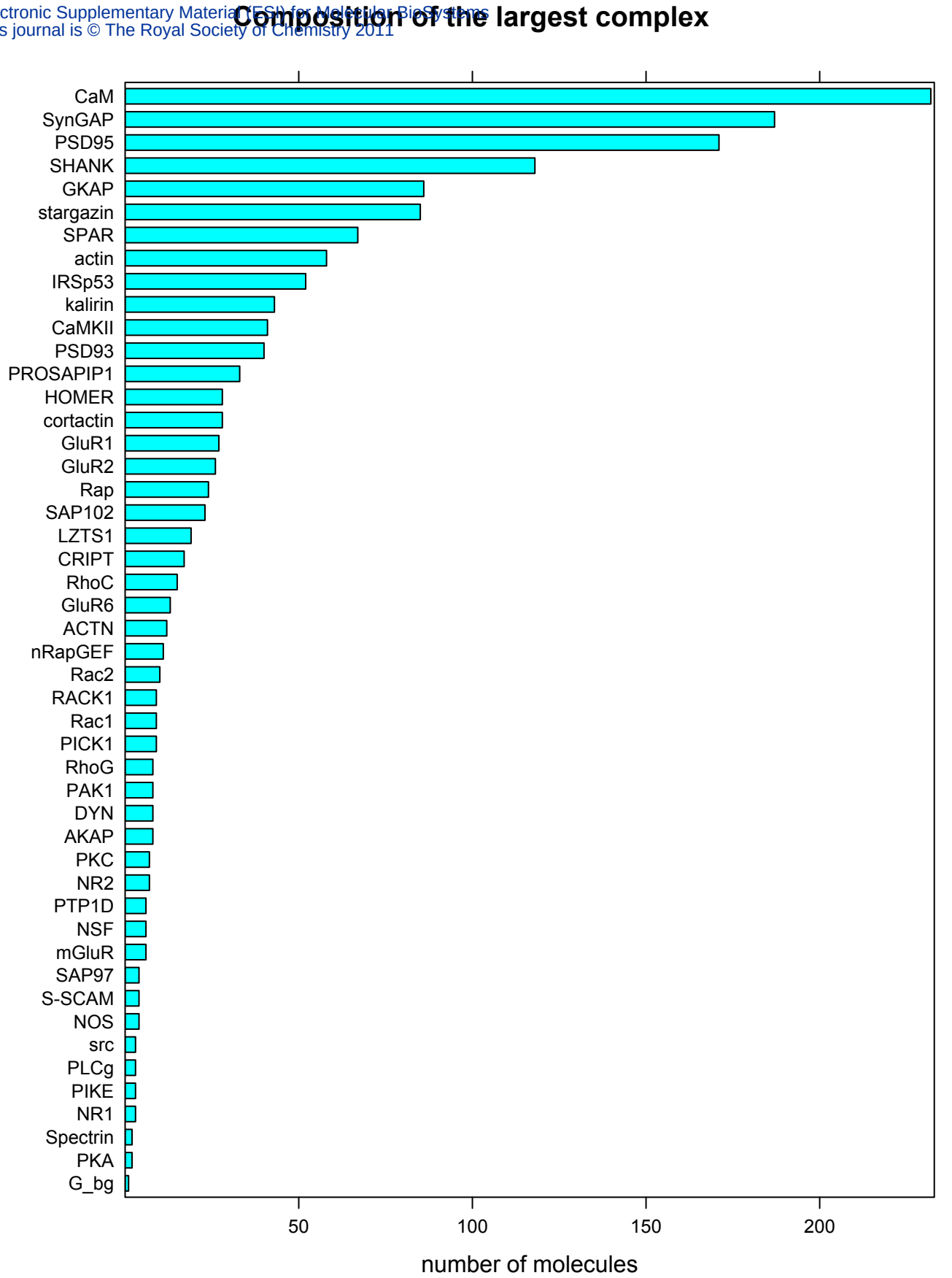
Supplementary Figure 5. Composition of the largest complex
Shown is the brutto formula from PSD95 knock-out simulation.

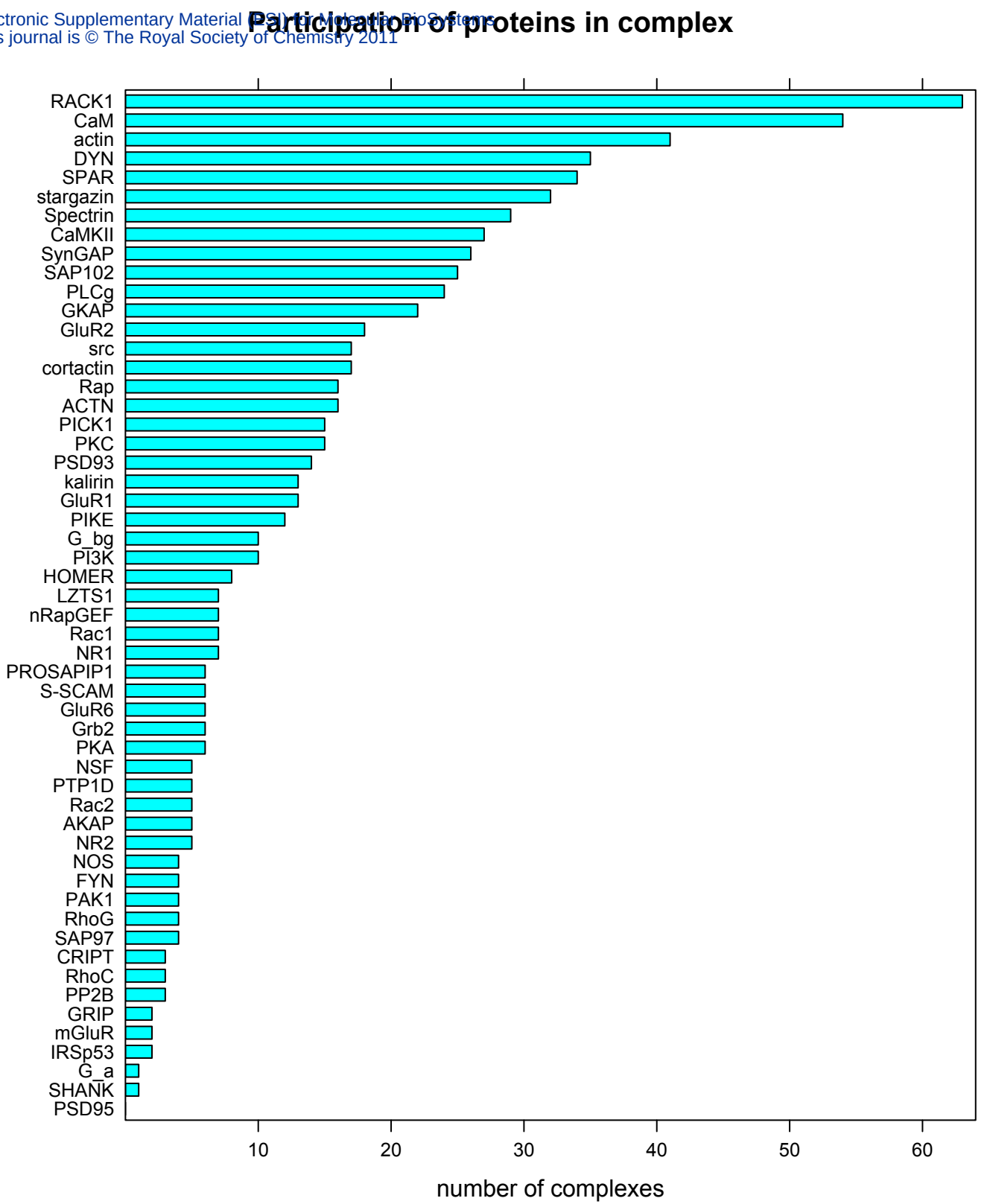
Supplementary Table 1. Rule based model of PSD.

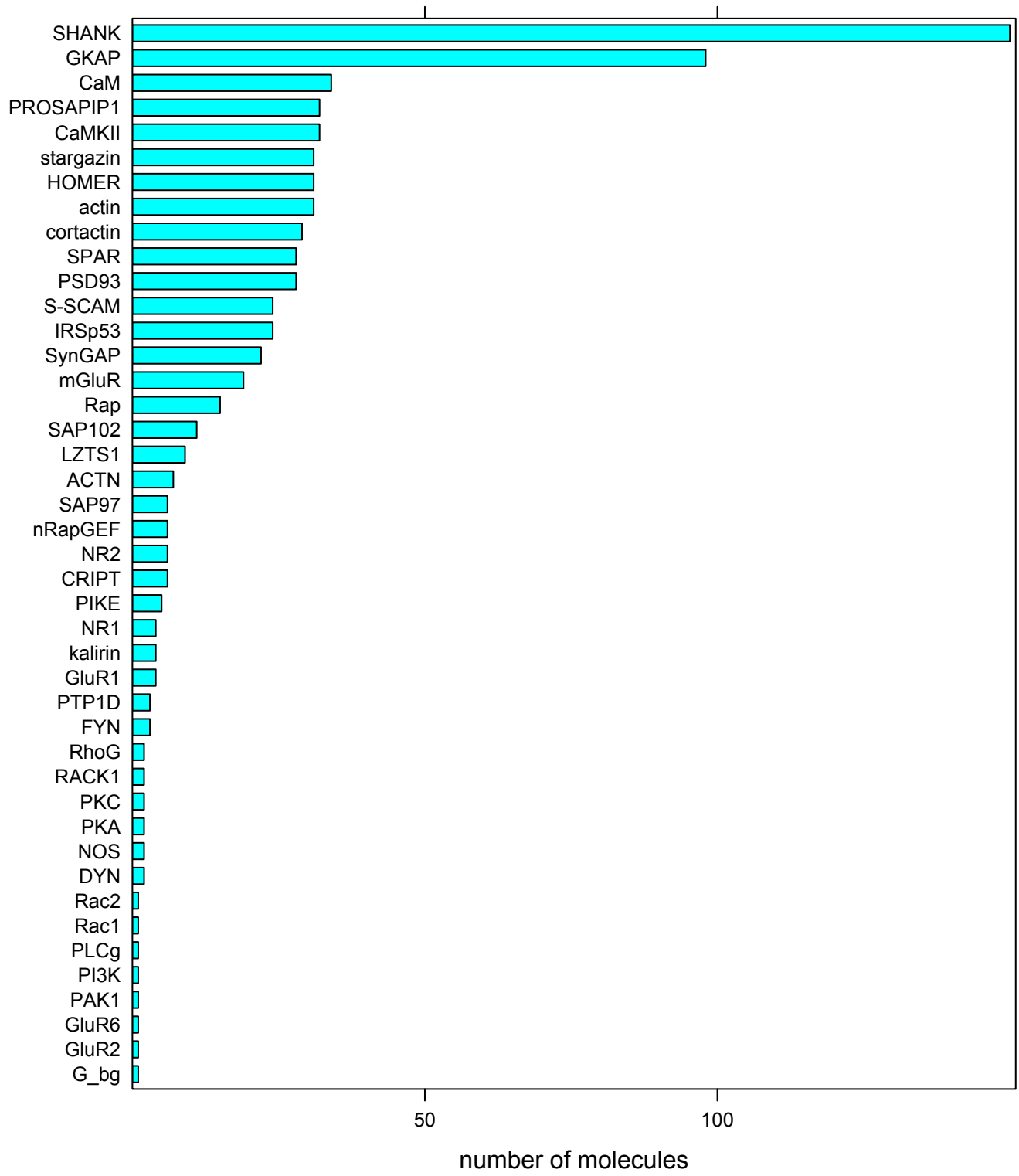
Supplementary Table 2. List of proteins, domains and rules with correspondent literature sources.











Rule	Kd_min, nM	Kd_max, nM
'PSD95_oligo' PSD95(NH2), PSD95(NH2) <-> PSD95(NH2!1), PSD95(NH2!1) @ k1,k_1	10	1000
'PSD93_oligo' PSD93(NH2), PSD93(NH2) <-> PSD93(NH2!1), PSD93(NH2!1) @ k1,k_1	10	1000
'PSD95_PSD93' PSD95(psd93),PSD93(psd95) <-> PSD95(psd93!1),PSD93(psd95!1) @ k3,k_3	10	1000
'NR1_dimer' NR1(b),NR1(b) <-> NR1(b!0),NR1(b!0) @ k6,k_6	10	1000
'NR2_dimer' NR2(b),NR2(b) <-> NR2(b!0),NR2(b!0) @ k6,k_6	10	1000
'NR2_NR1' NR1(b),NR2(b) <-> NR1(b!0),NR2(b!0) @ k6,k_6	10	1000
'NR2_spectrin' NR2(SBS~u),Spectrin(NRB) <-> NR2(SBS~u!1),Spectrin(NRB!1) @ k2,k_2	1	5000
'NR1_spectrin' NR1(SBS~u),Spectrin(NRB) <-> NR1(SBS~u!1),Spectrin(NRB!1) @ k4,k_4	1	5000
'NR2_FYN' NR2(TyrP),FYN(SH2) <-> NR2(TyrP!1),FYN(SH2!1) @ k5,k_5	1	100
'NR2_src' NR2(TyrP),src(SH2) <-> NR2(TyrP!1),src(SH2!1) @ k5,k_5	1	100
'NR2_PTP1D' NR2(TyrP),PTP1D(SH2) <-> NR2(TyrP!1),PTP1D(SH2!1) @ k5,k_5	1	100
'NR2_PLCg' NR2(TyrP),PLCg(SH2) <-> NR2(TyrP!1),PLCg(SH2!1) @ k5,k_5	1	100
'NR1_PKC' NR1(SerP),PKC(k) <-> NR1(SerP!1),PKC(k!1) @ k7,k_7	1	100
'NR1_PKA' NR1(SerP),PKA(k) <-> NR1(SerP!1),PKA(k!1) @ k7,k_7	1	100
PDZ12_NR2_PSD95_1'PSD95(PDZ1,PDZ),NR2(c) <-> PSD95(PDZ1!1),NR2(c!1) @ k8,k_8	50	1000
PDZ12_NR2_PSD95_2'PSD95(PDZ2),NR2(c) <-> PSD95(PDZ2!1),NR2(c!1) @ k8,k_8	50	1000
'SAP97_dimer'SAP97(L27),SAP97(L27) <-> SAP97(L27!1),SAP97(L27!1) @ k1,k_1	10	1000
'PDZ12_NR1_SAP97_1'SAP97(PDZ1,PDZ2?),NR2(c) <-> SAP97(PDZ1!1,PDZ2?),NR2(c!1) @ k8,k_8	50	1000
'PDZ12_NR1_SAP97_2'SAP97(PDZ1?,PDZ2),NR2(c) <-> SAP97(PDZ1?,PDZ2!1),NR2(c!1) @ k8,k_8	50	1000
'PDZ12_NR2_PSD93_1'PSD93(PDZ1,PDZ2?),NR2(c) <-> PSD93(PDZ1!1,PDZ2?),NR2(c!1) @ k8,k_8	50	1000
'PDZ12_NR2_PSD93_2'PSD93(PDZ1?,PDZ2),NR2(c) <-> PSD93(PDZ1?,PDZ2!1),NR2(c!1) @ k8,k_8	50	1000
'PDZ12_NR2_SAP102_1'SAP102(PDZ1,PDZ2?),NR2(c) <-> SAP102(PDZ1!1,PDZ2?),NR2(c!1) @ k8,k_8	50	1000
'PDZ12_NR2_SAP102_2'SAP102(PDZ1?,PDZ2),NR2(c) <-> SAP102(PDZ1?,PDZ2!1),NR2(c!1) @ k8,k_8	50	1000
'S-SCAM_NR2' S-SCAM(PDZ1),NR2(c) <-> S-SCAM(PDZ1!1),NR2(c!1) @ k8,k_8	50	1000
'SAP102_Cam' SAP102(H),CaM(h)<-> SAP102(H!1),CaM(h!1) @ k9,k_9	1	100
'SAP102_Cam_PSD95' SAP102(SH3,H!_),PSD95(GK) <-> SAP102(SH3!0,H!_),PSD95(GK!0) @ k10,k_10	1	100
'PSD95_PDZ2_NOS' PSD95(PDZ2),NOS(PDZ) <-> PSD95(PDZ2!1),NOS(PDZ!1) @ k11,k_11	10	1000
'PSD93_DZ2_NOS' PSD93(PDZ2),NOS(PDZ) <-> PSD93(PDZ2!1),NOS(PDZ!1) @ k11,k_11	10	1000
'Spectrin_dim'Spectrin(SL),Spectrin(SL) <-> Spectrin(SL!1),Spectrin(SL!1) @ k1,k_1	10	1000
'Spectrin_RACK1' Spectrin(PH),RACK1(WD) <-> Spectrin(PH!1),RACK1(WD!1) @ k12,k_12	10	1000
'Dynamin_RACK1' DYN(PH),RACK1(WD) <-> DYN(PH!1),RACK1(WD!1) @ k12,k_12	10	1000
'RACK1_PKC' RACK1(WD1),PKC(PH) <-> RACK1(WD1!1),PKC(PH!1) @ k12,k_12	10	1000
'RACK1_src' RACK1(WD6~p),src(SH2) <-> RACK1(WD6~p!1),src(SH2!1) @ k13,k_13	1	100
'RACK1_PLCg' RACK1(WD6~p),PLCg(SH2) <-> RACK1(WD6~p!1),PLCg(SH2!1) @ k13,k_13	1	100
'GluR6_PSD95' PSD95(PDZ1),GluR6(c) <-> PSD95(PDZ1!0),GluR6(c!0) @ k8,k_8	50	1000
'GluR6_SAP102' SAP102(PDZ1),GluR6(c) <-> SAP102(PDZ1!0),GluR6(c!0) @ k8,k_8	50	1000
'GluR6_SAP97' SAP97(PDZ1),GluR6(c) <-> SAP97(PDZ1!0),GluR6(c!0) @ k8,k_8	50	1000
'ACTN_NR1' ACTN(SR),NR1(c0) <-> ACTN(SR!1),NR1(c0!1) @ k14,k_14	3	100
'ACTN_NR2' ACTN(SR),NR2(c0) <-> ACTN(SR!1),NR2(c0!1) @ k14,k_14	3	100

'CaMKII_cluster' CaMKII(c),CaMKII(c) <-> CaMKII(c!0),CaMKII(c!0) @ k1,k_1	1	100
'CaMKII_NR2' CaMKII(k1),NR2(camkbd) <-> CaMKII(k1!1), NR2(camkbd!1) @ k15,k_15	1	500
'CaMKII_ACTN' CaMKII(k2),ACTN(CaMKBD) <-> CaMKII(k2!1),ACTN(CaMKBD!1) @ k16,k_16	1	100
CaMKII_CaM' CaMKII(cam),CaM(h) <-> CaMKII(cam!1),CaM(h!1) @ k17,k_17	1	100
'CaM_NR1' CaM(h),NR1(c0) <-> CaM(h!0),NR1(c0!0) @ k9,k_9	1	100
'CaMKII_NR1' NR1(c0),CaMKII(k1) <-> NR1(c0!1),CaMKII(k1!1) @ k18,k_18	1	100
'CaM_SBS_NR1' CaM(h),NR1(SBS~u) <-> CaM(h!1),NR1(SBS~u!1) @ k9,k_9	1	100
'Cam_Spectrin' CaM(h),Spectrin(NRB) <-> CaM(h!1),Spectrin(NRB!1) @ k9,k_9	1	100
'PDZ3_SynGAP_PSD95'PSD95(PDZ3),SynGAP(c) <-> PSD95(PDZ3!1),SynGAP(c!1) @ k19,k_19	50	1000
'PDZ2_SynGAP_PSD95'PSD95(PDZ2),SynGAP(c) <-> PSD95(PDZ2!1),SynGAP(c!1) @ k8,k_8	50	1000
'PDZ3_IRSp53_PSD95'PSD95(PDZ3),IRSp53(c) <-> PSD95(PDZ3!1),IRSp53(c!1) @ k19,k_19	50	1000
'PDZ3_IRSp53_PSD93'PSD93(PDZ3),IRSp53(c) <-> PSD93(PDZ3!1),IRSp53(c!1) @ k19,k_19	50	1000
'PDZ1_SynGAP_PSD95'PSD95(PDZ1),SynGAP(c) <-> PSD95(PDZ1!1),SynGAP(c!1) @ k8,k_8	50	1000
'PDZ1_stargazin_PSD95'PSD95(PDZ1,PDZ2!_),stargazin(c~u) <-> PSD95(PDZ1!0,PDZ2!_),stargazin(c~u!0) @ k8,k_8	50	1000
'PDZ2_stargazin_PSD95'PSD95(PDZ2,PDZ1!_),stargazin(c~u) <-> PSD95(PDZ2!0,PDZ1!_),stargazin(c~u!0) @ k8,k_8	50	1000
'PDZ1_stargazin_PSD93' PSD93(PDZ1,PDZ2?),stargazin(c~u) <-> PSD93(PDZ1!0,PDZ2?),stargazin(c~u!0) @ k8,k_8	50	1000
'PDZ2_stargazin_PSD93' PSD93(PDZ2,PDZ1?),stargazin(c~u) <-> PSD93(PDZ2!0,PDZ1?),stargazin(c~u!0) @ k8,k_8	50	1000
'PDZ1_stargazin_SAP102' SAP102(PDZ1,PDZ2?),stargazin(c~u) <-> SAP102(PDZ1!0,PDZ2?),stargazin(c~u!0) @ k8,k_8	50	1000
'PDZ2_stargazin_SAP102' SAP102(PDZ2,PDZ1?),stargazin(c~u) <-> SAP102(PDZ2!0,PDZ1?),stargazin(c~u!0) @ k8,k_8	50	1000
'PDZ3_SynGAP_PSD93'PSD93(PDZ3),SynGAP(c) <-> PSD93(PDZ3!1),SynGAP(c!1) @ k19,k_19	50	1000
'PDZ3_SynGAP_SAP97'SAP97(PDZ3),SynGAP(c) <-> SAP97(PDZ3!1),SynGAP(c!1) @ k19,k_19	50	1000
'PDZ1_GluR1_SAP97' SAP97(PDZ1),GluR1(c) <-> SAP97(PDZ1!1),GluR1(c!1) @ k8,k_8	50	1000
'PDZ3_SynGAP_SAP102'SAP102(PDZ3),SynGAP(c) <-> SAP102(PDZ3!1),SynGAP(c!1) @ k19,k_19	50	1000
'PSD95_CaM' PSD95(H),CaM(h)<-> PSD95(H!1),CaM(h!1) @ k9,k_9	1	100
'SAP97_CaM' SAP97(H),CaM(h)<-> SAP97(H!1),CaM(h!1) @ k9,k_9	1	100
'PSD93_CaM' PSD93(H),CaM(h)<-> PSD93(H!1),CaM(h!1) @ k9,k_9	1	100
'SH3_AKAP_PSD95' PSD95(SH3),AKAP(sh3) <-> PSD95(SH3!1),AKAP(sh3!1) @ k20,k_20	1	5000
'SH3_AKAP_SAP97' SAP97(SH3),AKAP(sh3) <-> SAP97(SH3!1),AKAP(sh3!1) @ k20,k_20	1	5000
'SH3_AKAP_SAP102' SAP102(SH3),AKAP(sh3) <-> SAP102(SH3!1),AKAP(sh3!1) @ k20,k_20	1	5000
'SH3_PSD93' PSD93(SH3),AKAP(sh3) <-> PSD93(SH3!1),AKAP(sh3!1) @ k20,k_20	1	5000
'GK_GKAP_PSD95' PSD95(GK),GKAP(GKBD) <-> PSD95(GK!1),GKAP(GKBD!1) @ k21,k_21	1	5000
'GK_GKAP_PSD93' PSD93(GK),GKAP(GKBD) <-> PSD93(GK!1),GKAP(GKBD!1) @ k21,k_21	1	5000
'GK_GKAP_SAP102' SAP102(GK),GKAP(GKBD) <-> SAP102(GK!1),GKAP(GKBD!1) @ k21,k_21	1	5000
'GK_GKAP_SAP97' SAP97(GK),GKAP(GKBD) <-> SAP97(GK!1),GKAP(GKBD!1) @ k21,k_21	1	5000
'S-SCAM_GKAP' S-SCAM(GK),GKAP(GKBD) <-> S-SCAM(GK!1),GKAP(GKBD!1) @ k21,k_21	1	5000
'S-SCAM_nRapGEF' S-SCAM(PDZ2),nRapGEF(c) <-> S-SCAM(PDZ2!1),nRapGEF(c!1) @ k41,k_41	1	5000
'PDZ3_kalirin_PSD95' PSD95(PDZ3),kalirin(c) <-> PSD95(PDZ3!1),kalirin(c!1) @ k19,k_19	50	1000
'PDZ3_kalirin_PSD93' PSD93(PDZ3),kalirin(c) <-> PSD93(PDZ3!1),kalirin(c!1) @ k19,k_19	50	1000
'PDZ3_kalirin_SAP97' SAP97(PDZ3),kalirin(c) <-> SAP97(PDZ3!1),kalirin(c!1) @ k19,k_19	50	1000
'PDZ3_kalirin_SAP102' SAP102(PDZ3),kalirin(c) <-> SAP102(PDZ3!1),kalirin(c!1) @ k19,k_19	50	1000

'kalirin_Rac1' kalirin(GEF1),Rac1(gef) <-> kalirin(GEF1!1),Rac1(gef!1) @ k22,k_22	1	100
'kalirin_Rac2' kalirin(GEF1),Rac2(gef) <-> kalirin(GEF1!1),Rac2(gef!1) @ k22,k_22	1	100
'kalirin_RhoG' kalirin(GEF1),RhoG(gef) <-> kalirin(GEF1!1),RhoG(gef!1) @ k22,k_22	1	100
'kalirin_RhoC' kalirin(GEF1),RhoC(gef) <-> kalirin(GEF1!1),RhoC(gef!1) @ k22,k_22	1	100
'PDZ3_CRIPT_PSD95' PSD95(PDZ3),CRIPT(c) <-> PSD95(PDZ3!1),CRIPT(c!1) @ k19,k_19	50	1000
'PDZ3_CRIPT_PSD93' PSD93(PDZ3),CRIPT(c) <-> PSD93(PDZ3!1),CRIPT(c!1) @ k19,k_19	50	1000
'PDZ3_CRIPT_SAP97' SAP97(PDZ3),CRIPT(c) <-> SAP97(PDZ3!1),CRIPT(c!1) @ k19,k_19	50	1000
'PDZ3_CRIPT_SAP102' SAP102(PDZ3),CRIPT(c) <-> SAP102(PDZ3!1),CRIPT(c!1) @ k19,k_19	50	1000
'Rac1_PAK' Rac1(pak),PAK1(PBD) <-> Rac1(pak!0),PAK1(PBD!0) @ k24,k_24	1	100
'GK_SPAR_PSD95' PSD95(GK),SPAR(GKBD) <-> PSD95(GK!1),SPAR(GKBD!1) @ k21,k_21	1	5000
'GK_SPAR_PSD93' PSD93(GK),SPAR(GKBD) <-> PSD93(GK!1),SPAR(GKBD!1) @ k21,k_21	1	5000
'GK_SPAR_SAP97' SAP97(GK),SPAR(GKBD) <-> SAP97(GK!1),SPAR(GKBD!1) @ k21,k_21	1	5000
'GK_SPAR_SAP102' SAP102(GK),SPAR(GKBD) <-> SAP102(GK!1),SPAR(GKBD!1) @ k21,k_21	1	5000
'SPAR_Rap'SPAR(GAP),Rap(gap) <-> SPAR(GAP!1),Rap(gap!1) @ k24,k_24	1	100
'Rap_nRapGEF' nRapGEF(RA),Rap(gef) <-> nRapGEF(RA!1),Rap(gef!1) @ k42,k_42	1	1000
'SPAR_actin' SPAR(Act1),actin(act1) <-> SPAR(Act1!0),actin(act1!0) @ k25,k_25	1	5000
'PDZ_GKAP_Shank' SHANK(PDZ),GKAP(c) <-> SHANK(PDZ!1),GKAP(c!1) @ k27,k_27	10	1000
'PDZ_PROSAPIP1_Shank' SHANK(PDZ),PROSAPIP1(c) <-> SHANK(PDZ!1),PROSAPIP1(c!1) @ k27,k_27	10	1000
'PROSAPIP1_SPAR' PROSAPIP1(CC1),SPAR(CC) <-> PROSAPIP1(CC1!1),SPAR(CC!1) @ k37,k_37	1	1000
'PROSAPIP1_dimer' PROSAPIP1(CC),PROSAPIP1(CC) <-> PROSAPIP1(CC!0),PROSAPIP1(CC!0) @ k37,k_37	1	1000
'PROSAPIP_LZTS1' PROSAPIP1(CC2),LZTS1(CC) <-> PROSAPIP1(CC2!1),LZTS1(CC!1) @ k37,k_37	1	1000
'LZTS1_SPAR' LZTS1(CC1),SPAR(CC) <-> LZTS1(CC1!1),SPAR(CC!1) @ k37,k_37	1	1000
'Shank_mGluR' SHANK(PDZ),mGluR(c) <-> SHANK(PDZ!1),mGluR(c!1) @ k27,k_27	10	1000
'Shank_dimer' SHANK(SAM1),SHANK(SAM1) <-> SHANK(SAM1!1),SHANK(SAM1!1) @ k1,k_1	1	100
'Shank_oligo' SHANK(SAM2),SHANK(SAM2) <-> SHANK(SAM2!1),SHANK(SAM2!1) @ k1,k_1	1	100
'Shank_Homer' SHANK(PRD),HOMER(EVH1) <-> SHANK(PRD!1),HOMER(EVH1!1) @ k28,k_28	50	1000
'HOMER_dimer' HOMER(CC),HOMER(CC) <-> HOMER(CC!1),HOMER(CC!1) @ k37,k_37	1	1000
'HOMER_mGluR' HOMER(EVH1),mGluR(PRD) <->HOMER(EVH1!1),mGluR(PRD!1) @ k28,k_28	50	1000
'HOMER_PIKE' HOMER(EVH1),PIKE(PRD1) <-> HOMER(EVH1!1),PIKE(PRD1!1) @ k28,k_28	50	1000
'PIKE_PLCg' PIKE(PRD2),PLCg(SH3) <-> PIKE(PRD2!1),PLCg(SH3!1) @ k29,k_29	50	1000
'PIKE_PI3K' PIKE(PRD3),PI3K(SH3) <-> PIKE(PRD3!1),PI3K(SH3!1) @ k29,k_29	50	1000
'mGluR_CaM' mGluR(CaMBD),CaM(h) <-> mGluR(CaMBD!0),CaM(h!0) @ k9,k_9	1	100
'Shank_IRSp53' SHANK(PRD),IRSp53(SH3) <-> SHANK(PRD!1),IRSp53(SH3!1) @ k29,k_29	50	1000
'AKAP_PKA' AKAP(r),PKA(R) <-> AKAP(r!0),PKA(R!0) @ k30,k_30	1	5000
'AKAP_PKC' AKAP(c),PKC(akap) <-> AKAP(c!0),PKC(akap!0) @ k31,k_31	50	1000
'Shank_cortactin' SHANK(PRD),cortactin(SH3) <-> SHANK(PRD!0),cortactin(SH3!0) @ k29,k_29	50	1000
'Dynamin_cortactin' DYN(PRD),cortactin(SH3) <-> DYN(PRD!0),cortactin(SH3!0) @ k29,k_29	50	1000
'Dynamin_Src' DYN(PRD),src(SH3) <-> DYN(PRD!0),src(SH3!0) @ k29,k_29	50	1000
'Dynamin_FYN' DYN(PRD),FYN(SH3) <-> DYN(PRD!0),FYN(SH3!0) @ k29,k_29	50	1000
'Dynamin_PLCg' DYN(PRD),PLCg(SH3) <-> DYN(PRD),PLCg(SH3) @ k29,k_29	50	1000

'PLCg_G_bg' PLCg(PH),G_bg(PHB) <-> PLCg(PH!1),G_bg(PHB!1) @ k40,k_40	10	1000
'G_bg_G_a' G_bg(PHB),G_a(bg) <-> G_bg(PHB!1),G_a(bg!1) @ k31,k_31	50	1000
'Dynamin_Grb2' DYN(PRD),Grb2(SH3) <-> DYN(PRD!1),Grb2(SH3!1) @ k29,k_29	50	1000
'PI3K_Grb2' PI3K(PRD),Grb2(SH3) <-> PI3K(PRD!1),Grb2(SH3!1) @ k29,k_29	50	1000
'PI3K_Src' PI3K(PRD),src(SH3) <-> PI3K(PRD!0),src(SH3!0) @ k29,k_29	50	1000
'Dynamin_dimer' DYN(CC),DYN(CC) <-> DYN(CC!0),DYN(CC!0) @ k37,k_37	1	1000
'cortactin_actin' cortactin(NTA),actin(cort) <-> cortactin(NTA!0),actin(cort!0) @ k32,k_32	1	5000
'ACTN_ actin' ACTN(ABD),actin(actn) <-> ACTN(ABD!0),actin(actn!0) @ k33,k_33	1	5000
'AKAP_PP2B' AKAP(sh3),PP2B(akap) <-> AKAP(sh3!1),PP2B(akap!1) @ k34,k_34	1	5000
'GluR1_GluR2' GluR1(N2),GluR2(N1) <-> GluR1(N2!1),GluR2(N1!1) @ k23,k_23	1	100
'GluR1_GluR1' GluR1(N1),GluR1(N1) <-> GluR1(N1!1),GluR1(N1!1) @ k23,k_23	1	100
'GluR2_GluR2' GluR2(N2),GluR2(N2) <-> GluR2(N2!1),GluR2(N2!1) @ k23,k_23	1	100
'stargazin_GluR1' stargazin(glur),GluR1(starg) <-> stargazin(glur!1),GluR1(starg!1) @ k35,k_35	1	5000
'Pick1_GluR2' PICK1(PDZ),GluR2(c~u) <-> PICK1(PDZ!1),GluR2(c~u!1) @ k27,k_27	10	1000
'GRIP_PDZ45_Glur2' GRIP(PDZ4~u,PDZ5),GluR2(c~u) <-> GRIP(PDZ4~u,PDZ5!1),GluR2(c~u!1) @ k36,k_36	1	5000
'GluR2_NSF' GluR2(c1),NSF(g) <-> GluR2(c1!1),NSF(g!1) @ k39,k_39	1	1000
'GRIP_dimer' GRIP(PDZ6),GRIP(PDZ6) <-> GRIP(PDZ6),GRIP(PDZ6) @ k38,k_38	1	100
'GluR2_PKC' GluR2(K),PKC(k) <-> GluR2(K!1),PKC(k!1) @ k7,k_7	1	100

Initial Conditions:
%init: 0 * (PSD95(NH2,PDZ1,PDZ2,PDZ3,GK,SH3,H,psd93))
%init: 10 * (SAP97(L27,PDZ1,PDZ2,PDZ3,GK,SH3,H))
%init: 10 * (NR2(c,b,c0,SBS~u,K,camkbd,TyrP))
%init: 10 * (NR1(c,b,c0,SBS~u,K,SerP))
%init: 37 * (SAP102(L27,PDZ1,PDZ2,PDZ3,GK,H,SH3))
%init: 50 * (PSD93(L27,PDZ1,PDZ2,PDZ3,GK,H,SH3,NH2,psd95))
%init: 360 * (SynGAP(c))
%init: 150 * (GKAP(c,GKBD))
%init: 150 * (SHANK(PDZ,SAM1,SAM2,PRD))
%init: 60 * (HOMER(EVH1,CC))
%init: 80 * (IRSp53(c,SH3))
%init: 100 * (cortactin(SH3,NTA))
%init: 20 * (AKAP(sh3,r,c))
%init: 1000 * (CaM(h))
%init: 20 * (PKA(R,k))
%init: 20 * (PKC(akap,k,PH,Ser~p))
%init: 1000 * (actin(cort,actn,act1,act2,a,a1))
%init: 20 * (PP2B(akap))
%init: 30 * (GluR1(N1,N2,starg,c))

```
%init: 30 * (GluR2(c~u,N1,N2,K,c1))
%init: 20 * (mGluR(PRD,c,CaMBD))
%init: 150 * (stargazin(c~u,glur))
%init: 40 * (PICK1(PDZ))
%init: 30 * (GRIP(PDZ4~u,PDZ5,PDZ6))
%init: 100 * (ACTN(SR,ABD,CaMKBD))
%init: 100 * (DYN(PRD,CC,PH))
%init: 30 * (src(SH3,SH2))
%init: 30 * (Grb2(SH3))
%init: 40 * (PLCg(SH3,SH2,PH))
%init: 100 * (kalirin(c,GEF1,NH2~u))
%init: 100 * (Rac1(gef,pak))
%init: 100 * (Rac2(gef))
%init: 100 * (RhoG(gef))
%init: 100 * (RhoC(gef))
%init: 5600 * (CaMKII(k,k1,k2,cam,c))
%init: 100 * (PAK1(PBD))
%init: 100 * (SPAR(GKBD,GAP,Act1,Act2,CC))
%init: 100 * (Spectrin(NRB,SL,PH))
%init: 20 * (FYN(SH2,SH3))
%init: 100 * (PTP1D(SH2))
%init: 20 * (NOS(PDZ))
%init: 200 * (RACK1(WD,WD1,WD6~p))
%init: 40 * (PI3K(PRD,SH3))
%init: 40 * (G_bg(PHB))
%init: 40 * (G_a(bg))
%init: 40 * (GluR6(c))
%init: 40 * (CRIPT(c))
%init: 40 * (NSF(g))
%init: 40 * (S-SCAM(PDZ1,GK,PDZ2))
%init: 40 * (nRapGEF(c,RA))
%init: 40 * (PROSAPIP1(c,CC1,CC,CC2))
%init: 20 * (LZTS1(CC,CC1))
%init: 50 * (Rap(gap,gef))
%init: 40 * (PIKE(PRD1,PRD2,PRD3))

# Simulation:
%obs: NR1(b!_,c!_)
%obs: NR2(b,SBS!_,c!_,c0!_)
%obs: PSD95(PDZ1!_,PDZ2!_)
```

```
%obs: GluR1(c!_,N2!_,N1!_,starg!_)
%obs: SHANK(PDZ!_,SAM1!_,SAM2!_,PRD!_)
```

Prot1	domain	prot2	domain	rule	1 model	PMID		kinetics	pmed for kine	notes
NR2A/NR2B	C-term	Veli	PDZ	NR2©,Veli(PDZ) <-> NR2(C!1),Veli(PDZ!1) @ 1.0,0.1	-	10341223	AP	the affinity of PL–PDZ domain inter- actions is ι	17855605	Many PDZ domain–ligand interactions are promiscuous and display modest a
NR2A/NR2B	SBS(spectrin	Spectrin	NRB	NR2_spectrin' NR2(SBS~u!1),Spectrin(NRB!1) <-> NR	+	9670010	AP			
NR2A/NR2B	C-term	CAMKII	k	'CaMKII_NR2' CaMKII(k),NR2(c) <-> CaMKII(k!1),NR2	+	9751209	AP			
NR2A/NR2B	SBS	Src	SH2	NR2_src' NR2(SBS-Tyr~u),src(SH2) <-> NR2(SBS~p!1	+	10458595	AP			potential binding sites for Src SH2 domains are present in NR2A at Tyr1292-,
NR2A/NR2B	SBS	PLCg	SH2	NR2_PLCg' NR2(SBS-Tyr~u),PLCg(SH2) <-> NR2(SBS	+	10458595, 9(	AP			
NR2	SBS	fyn	SH2	'NR2_Fyn' NR2(SBS-Tyr~u),fyn(SH2) <-> NR2(SBS~p	+	9670010, 10(	AP	10-1000 nM		UNDERSTANDING BIOLOGY USING PEPTIDES
NR1	SBS	PKC	k	NR1_PKC' NR1(SBS-Ser~u,K),PKC(k) <-> NR1(SBS-Se	+	9670010	AP			American Peptide Symposia, 2006, Volume 9, Part 8, 559-560, DOI: 10.1007/978-0-387-(
NR1	SBS	PKA	k	NR1_PKA' NR1(SBS-Ser~u,K),PKA(k) <-> NR1(SBS-Se	+	9670010	AP			
NR1	SBS	Spectrin	NRB	NR1_spectrin' NR1(SBS~u!1),Spectrin(NRB!1) <-> NR	+	9670010	AP			
NR2A/NR2B	C-term	Chapsin-110/	PDZ12	'PDZ12_NR2dim_PSD93'PSD93(PDZ1,PDZ2),NR2(c,b?)	+	10336672	AP			
NR2A/NR2B	C-term	PSD95	PDZ12	'PDZ12_NR2dim_PSD95'PSD95(PDZ1,PDZ2),NR2(c,b?)	+	10336672	AP			
NR2A/NR2B	C-term	SAP1102	PDZ12	'PDZ12_NR2dim_SAP102'SAP102(PDZ1,PDZ2),NR2(c,b	+	10336672	AP			
NR2A/NR2B	C-term	SAP97	PDZ12		+		AP			
NR2B	C0	ACTN	rod	'ACTN_NR2' ACTN(rod),NR2(c0) <-> ACTN(rod!1),NR2	+	9009191	AP	Kd of 30-100 nM		Wyszynski et al,1997
NR1	C0	ACTN	rod	'ACTN_NR1' ACTN(rod),NR1(c0) <-> ACTN(rod!1),NR1	+	9009191	AP	Kd of 30-100 nM		Wyszynski et al,1997
NR1	C0	CaM	h	'CaM_NR1' CaM(h),NR1(c0) <-> CaM(h!0),NR1(c0!0) @	+	9009191	AP	Kd of 90nM		Wyszynski et al,1998
NR2B	C-term	tubulin	NRB	NR2_tubulin' NR2©,tubulin(NRB) <-> NR2(c!1),tubulin	-	10037467	AP			
NR1	C-term	tubulin	NRB	NR1_tubulin' NR1©,tubulin(NRB) <-> NR1(c!1),tubulin	-	10037467	AP			
NR2B	SBS	PTPiD	SH2	'NR2_PTP1D' NR2(SBS-Tyr~u),PTP1D(SH2) <-> NR2(S	-	10381539	AP			
PSD95	NH2	PSD95	NH2	'PSD95_oligo' PSD95(NH2), PSD95(NH2) <-> PSD95(N	+	10364172	AP			
PSD95	GK	SAP102	SH3	'SAP102_Cam_PSD95' SAP102(SH3,H),CaM(h),PSD95(	+	10026200	AP			
PSD95	PDZ2	nNOS	PDZ	PDZ2_NOS' **PSD95**(PDZ2),**NOS**(PDZ) <-> **PSD95**(PDZ	+	8922396	AP	IC50 ~0.2 uM	17855605	
PSD95	PDZ2/PDZ1	Stargazin	C-term	'PDZ1_stargazin_PSD95'PSD95(PDZ1),stargazin(c) <-:	+	11140673	AP	PDZ domain 2 and SAP102 as having the strong	17855605	
PSD95	PDZ2/PDZ3	SynGap	C-term	'PDZ3_SynGAP_PSD95'PSD95(PDZ3),SynGAP(c) <-> P	+		OS	IC50, ~□8 □uM	17855605	
PSD95	PDZ3	IRSp53	C-term	PDZ3_IRSp53_PSD93'PSD93(PDZ3),IRSp53(c) <-> PS	+		OS			
PSD95	GK	GKAP	GKBD	'GK_GKAP_PSD95' PSD95(GK),GKAP(GKBD) <-> PSD9	+		OS			
PSD95	PDZ3	Kalirin	C-term	'PDZ3_kalirin_PSD95' PSD95(PDZ3),kalirin(c) <-> PSD	+		OS			
PSD95	GK	SPAR	GKBD	'GK_SPAR_PSD95' PSD95(GK),SPAR(GKBD) <-> PSD9	+		OS			
Spectrin	SL	Spectrin	SL	Spectrin_dim'SpectrinSPL),Spectrin(SL) <-> Spectrin(S	+	4016576	AP			
Spectrin		Tubulin			-	4016576	AP			
Spectrin		GAP43			-	10521589	AP			
Spectrin	PH	RACK1	WD	Spectrin_RACK1' Spectrin(PH),RACK1(WD) <-> Spectr	+	10529223	AP			
fyn	SH2	NR2	SBS~u	'NR2_Fyn' NR2(SBS~u),fyn(SH2) <-> NR2(SBS~p!1),f	+	9670010, 10(	OS			
Src	SH2	RACK1	WD6	'RACK1_src' RACK1(WD6~p),src(SH2) <-> RACK1(WD	+	11279199	AP	We observed concentration-dependent, saturabl	9584165	
Src	SH2	PSD95	PDZ3???		-		AP	Significant sequence similarity with the G protein β-subunit		
Src	SH3	PI3K	PRD	'PI3K_Src' PI3K(PRD),src(SH3) <-> PI3K(PRD!0),src(S	+	10830300	AP			
Src	SH3	Dynamin	PRD	'Dynamin_Src' DYN(PRD),src(SH3) <-> DYN(PRD!0),sr	+	9539797	AP			
PTP1D		Grb2			-	10386953[uic	AP			
PTP1D	PTP	PI3K			-	10386953[uic	AP			
PLCg	SH3	Dynamin	PRD	'Dynamin_PLCg' DYN(PRD),PLCg(SH3) <-> DYN(PRD),	+	8206897	AP			
PLCg	PH	G_bg	PHB(PH-bindi	'PLCg_G_bg' PLCg(PH),G_bg(PHB) <-> PLCg(PH!1),G_	+	10220275	AP	All PH domains tested (PH domains of ras-specific guanine nucleotide exchange factor (ras-GRF), phospholipase (PLC) gamma1, and Son o		
PKC	Ser~p	14-3-3	SerP	'PKC_14-3-3'14-3-3(pSer~u!1),PKC(Ser~p!1) <-> 14-	+	10433554, 1(	AP			
PKC	akap	AKap150	c	'AKAP_PKC' AKAP(c),PKC(akap) <-> AKAP(c!0),PKC(ak	+	9202019	AP			
PKC	PH	RACK1	WD	'RACK1_PKC' RACK1(WD1,WD6~u),PKC(PH) <-> RACK	+	11387319	AP			
PKC		Dynamin		no direct binding?	-	8063723	AP	It had an optimum phosphorylation rate of 1.42 +/- 0.02 mumol/mg/min and a concentration giving half-maximal activity (S0.5) of 0.14 +		
PKC	c	Yotiao			-	10945988	AP			
SAP97	L27	SAP97	L27	'SAP97_dimer'SAP97(L27),SAP97(L27) <-> SAP97(L27	+		OS			
SAP97	PDZ12	NR1	C-term	PDZ12_NR1dim_SAP97'SAP97(PDZ1,PDZ2),NR1(c,b?),	+		OS			
SAP97	PDZ3	SynGAP	C-term	'PDZ3_SynGAP_SAP97'SAP97(PDZ3),SynGAP(c) <-> S	+		OS			
SAP97	PDZ1	GluR1	C-term	'PDZ1_GluR1_SAP97' SAP97(PDZ1),GluR1(c) <-> SAP9	+		OS			
SAP97	SH3	AKAP	sh3	'SH3/GK(CaM)_AKAP_SAP97' SAP97(SH3,GK?,H),CaM(	+		OS			
SAP97	PDZ3	Kalirin	C-term	'PDZ3_kalirin_SAP97' SAP97(PDZ3),kalirin(c) <-> SAP	+		OS			
SAP97	GK	SPAR	GKBD	'GK_SPAR_SAP97' SAP97(GK),SPAR(GKBD) <-> SAP97	+		OS			
SAP97	GK	GKAP	GKBD	'GK_GKAP_SAP97' SAP97(GK),GKAP(GKBD) <-> SAP97	+		OS			
SAP97	PDZ2/PDZ1	Stargazin		PDZ1_stargazin_SAP97' SAP97(PDZ1),stargazin(c) <->	-	11140673	AP			
SAP102	H	CaM	h	'SAP102_Cam_PSD95' SAP102(SH3,H),CaM(h),PSD95(	+	10026200	AP			
SAP102	PDZ12	NR2	C-term	'PDZ12_NR2dim_SAP102'SAP102(PDZ1,PDZ2),NR2(c,b	+		OS			
SAP102	PDZ12	NR1	C-term	PDZ12_NR1dim_SAP102'SAP102(PDZ1,PDZ2),NR1(c,b	+		OS			
SAP102	PDZ3	SynGAP	C-term	PDZ3_SynGAP_SAP102'SAP102(PDZ3),SynGAP(c) <->	+		OS			
SAP102	PDZ3	Kalirin	C-term	'PDZ3_kalirin_SAP102' SAP102(PDZ3),kalirin(c) <-> SA	+		OS			
SAP102	GK	SPAR	GKBD	'GK_SPAR_SAP102' SAP102(GK),SPAR(GKBD) <-> SAP	+		OS			
SAP102	GK	GKAP	GKBD	'GK_GKAP_SAP102' SAP102(GK),GKAP(GKBD) <-> SAP	+		OS			
PSD93/Chaps	PDZ2	NOS	PDZ	'PSD93_DZ2_NOS' PSD93(PDZ2),NOS(PDZ) <-> PSD9	+	8922396	OS			
GluR6	C-term	PSD95	PDZ1	'GluR6_PSD95' PSD95(PDZ1),GluR6(c) <-> PSD95(PDZ	+	9808460	AP			
GluR6	C-term	SAp97	PDZ1	'GluR6_SAP102' SAP102(PDZ1,PDZ2?,GK?,PDZ3?,SH3?	+	9808460	AP			
GluR6	C-term	SAP102	PDZ1	'GluR6_SAP97' SAP97(PDZ1),GluR6(c) <-> SAP97(PDZ	+	9808460	AP			
Shank	PRD	Cortactin	SH3	'Shank_cortactin' SHANK(PRD),cortactin(SH3) <-> SHA	+	10433268	AP			
Shank	PDZ	Gkap	C-term	'PDZ_GKAP_Shank' SHANK(PDZ),GKAP(c) <-> SHANK(	+	10488079	AP	1.0 microM	20715264	
Shank	PRD	Homer	EVH1	'Shank_Homer' SHANK(PRD),HOMER(EVH1) <-> SHAN	+	10433269	AP			
Shank	SAM	Shank	SAM	'Shank_dimer' SHANK(SAM),SHANK(SAM) <-> SHANK(	+	10433268	AP			
Homer	EVH1	mGlur	PRD	'HOMER_mGluR' HOMER(EVH1),mGluR(PRD) <->HOME	+	10433269	AP	Well known examples include the interactions of	12857736	
Homer	CC	Homer	CC	'HOMER_dimer' HOMER(CC),HOMER(CC) <-> HOMER((	+	9808458	AP			
Cortactin	NTA	actin	cort	'cortactin_actin' cortactin(NTA),actin(cort) <-> cortacti	+	10433268	AP			
Cortactin		Rac1		no direct binding?	-	9683637	AP			

Prot1	domain	prot2	domain	rule	PMID	kinetics	PMID	notes
NR2A/NR2B	SBS(spectrin	Spectrin	NRB	NR2_spectrin' NR2(SBS~u),Spectrin(NRB) <-> NR2(SBS~u!1),Spectrin(NRB!1) @ k2,k_2	9670010			
NR2A/NR2B	camkbd	CAMKII	k	'CaMKII_NR2' CaMKII(k1),NR2(camkbd) <-> CaMKII(k1!1), NR2(camkbd!1) @ k15,k_15	9751209			
NR2A/NR2B	TyrP	Src	SH2	NR2_src' NR2(TyrP),src(SH2) <-> NR2(TyrP!1),src(SH2!1) @ k5,k_5	10458595			potential binding sites for Src SH2 domains are present in
NR2A/NR2B	TyrP	PLCg	SH2	'NR2_PLCg' NR2(TyrP),PLCg(SH2) <-> NR2(TyrP!1),PLCg(SH2!1) @ k5,k_5	10458595, 9231720			
NR2	TyrP	FYN	SH2	'NR2_FYN' NR2(TyrP),FYN(SH2) <-> NR2(TyrP!1),FYN(SH2!1) @ k5,k_5	9670010, 10458595	10-1000 nM		UNDERSTANDING BIOLOGY USING PEPTIDES
NR1	SerP	PKC	k	'NR1_PKC' NR1(SerP),PKC(k) <-> NR1(SerP!1),PKC(k!1) @ k7,k_7	9670010			American Peptide Symposia, 2006, Volume 9, Part 8, 559-560, DOI: 10.
NR1	SerP	PKA	k	'NR1_PKA' NR1(SerP),PKA(k) <-> NR1(SerP!1),PKA(k!1) @ k7,k_7	9670010			
NR1	SBS	Spectrin	NRB	'NR1_spectrin' NR1(SBS~u),Spectrin(NRB) <-> NR1(SBS~u!1),Spectrin(NRB!1) @ k4,k_4	9670010			
NR1	b	NR2	b	'NR2_NR1' NR1(b),NR2(b) <-> NR1(b!0),NR2(b!0) @ k6,k_6	17959602			
NR2A/NR2B	C-term	Chapsin-110/PSD93	PDZ12	PDZ12_NR2_PSD93_1'PSD93(PDZ1),NR2(c) <-> PSD93(PDZ1!1),NR2(c!1) @ k8,k_8	10336672			
NR2A/NR2B	C-term	PSD95	PDZ12	PDZ12_NR2_PSD93_1'PSD93(PDZ1),NR2(c) <-> PSD93(PDZ1!1),NR2(c!1) @ k8,k_8	10336672			
NR2A/NR2B	C-term	SAP102	PDZ12	PDZ12_NR2_SAP102_1'SAP102(PDZ1),NR2(c) <-> SAP102(PDZ1!1),NR2(c!1) @ k8,k_8	10336672			
NR2B	C0	ACTN	SR(rod)	'ACTN_NR2' ACTN(SR),NR2(c0) <-> ACTN(SR!1),NR2(c0!1) @ k14,k_14	9009191	Kd of 30-100 nM		Wyszynski et al,1997
NR1	C0	ACTN	SR(rod)	'ACTN_NR1' ACTN(SR),NR1(c0) <-> ACTN(SR!1),NR1(c0!1) @ k14,k_14	9009191	Kd of 30-100 nM		Wyszynski et al,1997
NR1	C0	CaM	h	'CaM_NR1' CaM(h),NR1(c0) <-> CaM(h!0),NR1(c0!0) @ k9,k_9	9009191	Kd of 90nM		Wyszynski et al,1998
NR2B	TyrP	PTPiD	SH2	'NR2_PTP1D' NR2(TyrP),PTP1D(SH2) <-> NR2(TyrP!1),PTP1D(SH2!1) @ k5,k_5	10381539			
PSD95	NH2	PSD95	NH2	'PSD95_oligo' PSD95(NH2), PSD95(NH2) <-> PSD95(NH2!1), PSD95(NH2!1) @ k1,k_1	10364172			
PSD95	GK	SAP102	SH3	'SAP102_Cam_PSD95' SAP102(SH3,H!_),PSD95(GK) <-> SAP102(SH3!0,H!_),PSD95(GK!0) @ k10,k_10	10026200			
PSD95	PDZ2	nNOS	PDZ	'PSD95_PDZ2_NOS' PSD95(PDZ2),NOS(PDZ) <-> PSD95(PDZ2!1),NOS(PDZ!1) @ k11,k_11	8922396	IC50 ~0.2 uM	17855605	
PSD95	PDZ2/PDZ1	Stargazin	C-term	'PDZ1_stargazin_PSD95'PSD95(PDZ1,PDZ2!_),stargazin(c~u) <-> PSD95(PDZ1!0,PDZ2!_),stargazin(c~u!0) @ k8	11140673	PDZ domain 2 and SAP102 as having the stron	17855605	
PSD95	PDZ1/PDZ2/P	SynGap	C-term	'PDZ3_SynGAP_PSD95'PSD95(PDZ3),SynGAP(c) <-> PSD95(PDZ3!1),SynGAP(c!1) @ k19,k_19	9581761	IC50, ~□8 □uM	17855605	
PSD95	PDZ3	IRSp53	C-term	'PDZ3_IRSp53_PSD95'PSD95(PDZ3),IRSp53(c) <-> PSD95(PDZ3!1),IRSp53(c!1) @ k19,k_19	15255944			
PSD95	GK	GKAP	GKBD	'GK_GKAP_PSD95' PSD95(GK),GKAP(GKBD) <-> PSD95(GK!1),GKAP(GKBD!1) @ k21,k_21	10433269			
PSD95	PDZ3	Kalirin	C-term	'PDZ3_kalirin_PSD95' PSD95(PDZ3),kalirin(c) <-> PSD95(PDZ3!1),kalirin(c!1) @ k19,k_19	14627644			
PSD95	SH3	AKAP	sh3	'SH3_AKAP_PSD95' PSD95(SH3),AKAP(sh3) <-> PSD95(SH3!1),AKAP(sh3!1) @ k20,k_20	10939335			
PSD95	PDZ3	CRIPT	c	'PDZ3_CRIPT_PSD95' PSD95(PDZ3),CRIPT(c) <-> PSD95(PDZ3!1),CRIPT(c!1) @ k19,k_19	9581762			
PSD95	GK	SPAR	GKBD	'GK_SPAR_PSD95' PSD95(GK),SPAR(GKBD) <-> PSD95(GK!1),SPAR(GKBD!1) @ k21,k_21	11502259			
PSD93	NH2	PSD93	NH2	'PSD93_oligo' PSD93(NH2), PSD93(NH2) <-> PSD93(NH2!1), PSD93(NH2!1) @ k1,k_1	10364172			
PSD93	PDZ2	NOS	PDZ	'PSD93_DZ2_NOS' PSD93(PDZ2),NOS(PDZ) <-> PSD93(PDZ2!1),NOS(PDZ!1) @ k11,k_11	8922396			
PSD93	PDZ3	IRSp53	c	'PDZ3_IRSp53_PSD93'PSD93(PDZ3),IRSp53(c) <-> PSD93(PDZ3!1),IRSp53(c!1) @ k19,k_19	15255944			
PSD93	PDZ1/PDZ2	Stargazin	c	'PDZ1_stargazin_PSD93' PSD93(PDZ1,PDZ2?),stargazin(c~u) <-> PSD93(PDZ1!0,PDZ2?),stargazin(c~u!0) @ k8,l	15136571			
PSD93	PDZ3	SynGap	c	'PDZ3_SynGAP_PSD93'PSD93(PDZ3),SynGAP(c) <-> PSD93(PDZ3!1),SynGAP(c!1) @ k19,k_19	9581761			
PSD93	SH3	AKAP	sh3	'SH3_PSD93' PSD93(SH3),AKAP(sh3) <-> PSD93(SH3!1),AKAP(sh3!1) @ k20,k_20	10939335			
PSD93	GK	GKAP	GKBD	'GK_GKAP_PSD93' PSD93(GK),GKAP(GKBD) <-> PSD93(GK!1),GKAP(GKBD!1) @ k21,k_21	14724236			
PSD93	PDZ3	Kalirin	c	'PDZ3_kalirin_PSD93' PSD93(PDZ3),kalirin(c) <-> PSD93(PDZ3!1),kalirin(c!1) @ k19,k_19	14627644			
PSD93	PDZ3	CRIPT	c	'PDZ3_CRIPT_PSD93' PSD93(PDZ3),CRIPT(c) <-> PSD93(PDZ3!1),CRIPT(c!1) @ k19,k_19	9581762			
PSD93	GK	SPAR	GKBD	'GK_SPAR_PSD93' PSD93(GK),SPAR(GKBD) <-> PSD93(GK!1),SPAR(GKBD!1) @ k21,k_21	11502259			
PSD93	psd95	PSD95	psd93	'PSD95_PSD93' PSD95(psd93),PSD93(psd95) <-> PSD95(psd93!1),PSD93(psd95!1) @ k3,k_3				
Spectrin	SL	Spectrin	SL	'Spectrin_dim'Spectrin(SL),Spectrin(SL) <-> Spectrin(SL!1),Spectrin(SL!1) @ k1,k_1	4016576			
Spectrin	PH	RACK1	WD	'Spectrin_RACK1' Spectrin(PH),RACK1(WD) <-> Spectrin(PH!1),RACK1(WD!1) @ k12,k_12	10529223			
Src	SH2	RACK1	WD6	'RACK1_src' RACK1(WD6~p),src(SH2) <-> RACK1(WD6~p!1),src(SH2!1) @ k13,k_13	11279199	We observed concentration-dependent, saturat	9584165	
Src	SH3	PI3K	PRD	'PI3K_Src' PI3K(PRD),src(SH3) <-> PI3K(PRD!0),src(SH3!0) @ k29,k_29	10830300			
Src	SH3	Dynamin	PRD	'Dynamin_Src' DYN(PRD),src(SH3) <-> DYN(PRD!0),src(SH3!0) @ k29,k_29	9539797			
PLCg	SH3	Dynamin	PRD	'Dynamin_PLCg' DYN(PRD),PLCg(SH3) <-> DYN(PRD),PLCg(SH3) @ k29,k_29	8206897			
PLCg	PH	G_bg	PHB(PH-bindi	'PLCg_G_bg' PLCg(PH),G_bg(PHB) <-> PLCg(PH!1),G_bg(PHB!1) @ k40,k_40	10220275	All PH domains tested (PH domains of ras-specific guanine nucleotide exchange factor (ras-GRF), phospholipase (PLC) g		
PKC	akap	AKAP	c	'AKAP_PKC' AKAP(c),PKC(akap) <-> AKAP(c!0),PKC(akap!0) @ k31,k_31	9202019			
PKC	PH	RACK1	WD	'RACK1_PKC' RACK1(WD1),PKC(PH) <-> RACK1(WD1!1),PKC(PH!1) @ k12,k_12	11387319			
SAP97	L27	SAP97	L27	'SAP97_dimer'SAP97(L27),SAP97(L27) <-> SAP97(L27!1),SAP97(L27!1) @ k1,k_1	16815335			
SAP97	PDZ3	SynGAP	C-term	'PDZ3_SynGAP_SAP97'SAP97(PDZ3),SynGAP(c) <-> SAP97(PDZ3!1),SynGAP(c!1) @ k19,k_19	9581761			
SAP97	PDZ1	GluR1	C-term	'PDZ1_GluR1_SAP97' SAP97(PDZ1),GluR1(c) <-> SAP97(PDZ1!1),GluR1(c!1) @ k8,k_8	18842882			
SAP97	SH3	AKAP	sh3	'SH3_AKAP_SAP97' SAP97(SH3),AKAP(sh3) <-> SAP97(SH3!1),AKAP(sh3!1) @ k20,k_20	10939335			
SAP97	PDZ3	Kalirin	C-term	'PDZ3_kalirin_SAP97' SAP97(PDZ3),kalirin(c) <-> SAP97(PDZ3!1),kalirin(c!1) @ k19,k_19	14627644			
SAP97	GK	SPAR	GKBD	'GK_SPAR_SAP97' SAP97(GK),SPAR(GKBD) <-> SAP97(GK!1),SPAR(GKBD!1) @ k21,k_21	11502259			
SAP97	PDZ3	CRIPT	c	'PDZ3_CRIPT_SAP97' SAP97(PDZ3),CRIPT(c) <-> SAP97(PDZ3!1),CRIPT(c!1) @ k19,k_19	9581762			
SAP97	GK	GKAP	GKBD	'GK_GKAP_SAP97' SAP97(GK),GKAP(GKBD) <-> SAP97(GK!1),GKAP(GKBD!1) @ k21,k_21	11060025			
SAP102	H	CaM	h	'SAP102_Cam' SAP102(H),CaM(h)<-> SAP102(H!1),CaM(h!1) @ k9,k_9	10026200			
SAP102	PDZ12	NR2	C-term	PDZ12_NR2_SAP102_1'SAP102(PDZ1),NR2(c) <-> SAP102(PDZ1!1),NR2(c!1) @ k8,k_8	10336672			
SAP102	PDZ3	SynGAP	C-term	'PDZ3_SynGAP_SAP102'SAP102(PDZ3),SynGAP(c) <-> SAP102(PDZ3!1),SynGAP(c!1) @ k19,k_19	9581761			
SAP102	PDZ3	Kalirin	C-term	'PDZ3_kalirin_SAP102' SAP102(PDZ3),kalirin(c) <-> SAP102(PDZ3!1),kalirin(c!1) @ k19,k_19	14627644			
SAP102	GK	SPAR	GKBD	'GK_SPAR_SAP102' SAP102(GK),SPAR(GKBD) <-> SAP102(GK!1),SPAR(GKBD!1) @ k21,k_21	11502259			
SAP102	PDZ2/PDZ1	Stargazin	c	'PDZ1_stargazin_SAP102' SAP102(PDZ1,PDZ2?),stargazin(c~u) <-> SAP102(PDZ1!0,PDZ2?),stargazin(c~u!0) @ k	**15136571**			
SAP102	SH3	AKAP	sh3	'SH3_AKAP_SAP102' SAP102(SH3),AKAP(sh3) <-> SAP102(SH3!1),AKAP(sh3!1) @ k20,k_20	10939335			
SAP102	PDZ3	CRIPT	c	'PDZ3_CRIPT_SAP102' SAP102(PDZ3),CRIPT(c) <-> SAP102(PDZ3!1),CRIPT(c!1) @ k19,k_19	9581762			
SAP102	GK	GKAP	GKBD	'GK_GKAP_SAP102' SAP102(GK),GKAP(GKBD) <-> SAP102(GK!1),GKAP(GKBD!1) @ k21,k_21	11060025			
GluR6	C-term	PSD95	PDZ1	'GluR6_PSD95' PSD95(PDZ1),GluR6(c) <-> PSD95(PDZ1!0),GluR6(c!0) @ k8,k_8	9808460			
GluR6	C-term	SAp97	PDZ1	'GluR6_SAP97' SAP97(PDZ1),GluR6(c) <-> SAP97(PDZ1!0),GluR6(c!0) @ k8,k_8	9808460			
GluR6	C-term	SAP102	PDZ1	'GluR6_SAP102' SAP102(PDZ1),GluR6(c) <-> SAP102(PDZ1!0),GluR6(c!0) @ k8,k_8	9808460			
Shank	PRD	Cortactin	SH3	'Shank_cortactin' SHANK(PRD),cortactin(SH3) <-> SHANK(PRD!0),cortactin(SH3!0) @ k29,k_29	10433268			
Shank	PDZ	GKAP	C-term	'PDZ_GKAP_Shank' SHANK(PDZ),GKAP(c) <-> SHANK(PDZ!1),GKAP(c!1) @ k27,k_27	10488079	1.0 microM	20715264	
Shank	PRD	Homer	EVH1	'Shank_Homer' SHANK(PRD),HOMER(EVH1) <-> SHANK(PRD!1),HOMER(EVH1!1) @ k28,k_28	10433269			
Shank	PDZ	mGlur	c	'Shank_mGluR' SHANK(PDZ),mGluR(c) <-> SHANK(PDZ!1),mGluR(c!1) @ k27,k_27	10433269			
Shank	PRD	IRSp53	SH3	'Shank_IRSp53' SHANK(PRD),IRSp53(SH3) <-> SHANK(PRD!1),IRSp53(SH3!1) @ k29,k_29	15255944			
Shank	PDZ	PROSAPIP1	c	'PDZ_PROSAPIP1_Shank' SHANK(PDZ),PROSAPIP1(c) <-> SHANK(PDZ!1),PROSAPIP1(c!1) @ k27,k_27	16439662			
Shank	SAM	Shank	SAM	'Shank_dimer' SHANK(SAM1),SHANK(SAM1) <-> SHANK(SAM1!1),SHANK(SAM1!1) @ k1,k_1	10433268, 16439662			
Homer	EVH1	mGlur	PRD	'HOMER_mGluR' HOMER(EVH1),mGluR(PRD) <->HOMER(EVH1!1),mGluR(PRD!1) @ k28,k_28	10433269, 10433269	Well known examples include the interactions c	12857736	
Homer	EVH1	PIKE	PRD1	'HOMER_PIKE' HOMER(EVH1),PIKE(PRD1) <-> HOMER(EVH1!1),PIKE(PRD1!1) @ k28,k_28	10851183			
Homer	CC	Homer	CC	'HOMER_dimer' HOMER(CC),HOMER(CC) <-> HOMER(CC!1),HOMER(CC!1) @ k37,k_37	9808458			
Cortactin	NTA	actin	cort	'cortactin_actin' cortactin(NTA),actin(cort) <-> cortactin(NTA!0),actin(cort!0) @ k32,k_32	10433268			
Cortactin	SH3	Dynamin	PRD	'Dynamin_cortactin' DYN(PRD),cortactin(SH3) <-> DYN(PRD!0),cortactin(SH3!0) @ k29,k_29	11018064	dissociation equilibrium constant (Kd) of His-co	15671060	
CaMKII	c	CAMKII	c	'CaMKII_cluster' CaMKII(c),CAMKII(c) <-> CaMKII(c!0),CaMKII(c!0) @ k1,k_1	18005004			
CaMKII	cam	CaM	h	CaMKII_CaM' CaMKII(cam),CaM(h) <-> CaMKII(cam!1),CaM(h!1) @ k17,k_17	18005004			
CaMKII	k1	NR1	c0	'CaMKII_NR1' NR1(c0),CaMKII(k1) <-> NR1(c0!1),CaMKII(k1!1) @ k18,k_18	18005004			
CaMKII	k2	ACTN	CBD	'CaMKII_ACTN' CaMKII(k2),ACTN(CaMKBD) <-> CaMKII(k2!1),ACTN(CaMKBD!1) @ k16,k_16	16120608			
CaM	h	PSD93	H	'PSD93_CaM' PSD93(H),CaM(h)<-> PSD93(H!1),CaM(h!1) @ k9,k_9	10026200			
CaM	h	SAP97	H	'SAP97_CaM' SAP97(H),CaM(h)<-> SAP97(H!1),CaM(h!1) @ k9,k_9	15044483			
CaM	h	PSD95	H	'PSD95_CaM' PSD95(H),CaM(h)<-> PSD95(H!1),CaM(h!1) @ k9,k_9	18005004			
CaM	h	mGluR	CaMBD	'mGluR_CaM' mGluR(CaMBD),CaM(h) <-> mGluR(CaMBD!0),CaM(h!0) @ k9,k_9	10469171			
CaM	h	NR1	SBS	'CaM_SBS_NR1' CaM(h),NR1(SBS~u) <-> CaM(h!1),NR1(SBS~u!1) @ k9,k_9	9952395			
CaM	h	Spectrin	NRB	'Cam_Spectrin' CaM(h),Spectrin(NRB) <-> CaM(h!1),Spectrin(NRB!1) @ 1.0,0.1	9670010			
RACK1	WD6	PLCg	SH2	'RACK1_PLCg' RACK1(WD6~p),PLCg(SH2) <-> RACK1(WD6~p!1),PLCg(SH2!1) @ k13,k_13	10529223			
Dynamin	PRD	FYN	SH3	'Dynamin_FYN' DYN(PRD),FYN(SH3) <-> DYN(PRD!0),FYN(SH3!0) @ k29,k_29	9111080			
Dynamin	PRD	Grb2	SH3	'Dynamin_Grb2' DYN(PRD),Grb2(SH3) <-> DYN(PRD!1),Grb2(SH3!1) @ k29,k_29	9111080			
Dynamin	CC	Dynamin	CC	'Dynamin_dimer' DYN(CC),DYN(CC) <-> DYN(CC!0),DYN(CC!0) @ k37,k_37	10329695			
Dynamin	PH	RACK1	WD	'Dynamin_RACK1' DYN(PH),RACK1(WD) <-> DYN(PH!1),RACK1(WD!1) @ k12,k_12	10529223	Dynamin-1 competes with the binding of RACK	12359736	
S-SCAM	PDZ1	NR2	c	'S-SCAM_NR2' S-SCAM(PDZ1),NR2(c) <-> S-SCAM(PDZ1!1),NR2(c!1) @ k8,k_8	9694864			
S-SCAM	GK	GKAP	GKBD	'S-SCAM_GKAP' S-SCAM(GK),GKAP(GKBD) <-> S-SCAM(GK!1),GKAP(GKBD!1) @ k21,k_21	9694864			
S-SCAM	PDZ2	nRapGEF	c	'S-SCAM_nRapGEF' S-SCAM(PDZ2),nRapGEF(c) <-> S-SCAM(PDZ2!1),nRapGEF(c!1) @ k41,k_41	9694864			
Kalirin	GEF1	Rac1	gef	'kalirin_Rac1' kalirin(GEF1),Rac1(gef) <-> kalirin(GEF1!1),Rac1(gef!1) @ k22,k_22	19403804, 14627644			
Kalirin	GEF1	Rac2	gef	'kalirin_Rac2' kalirin(GEF1),Rac2(gef) <-> kalirin(GEF1!1),Rac2(gef!1) @ k22,k_22	19403804, 14627644			
Kalirin	GEF1	RhoG	gef	'kalirin_RhoG' kalirin(GEF1),RhoG(gef) <-> kalirin(GEF1!1),RhoG(gef!1) @ k22,k_22	19403804, 14627644			
Kalirin	GEF1	RhoC	gef	'kalirin_RhoC' kalirin(GEF1),RhoC(gef) <-> kalirin(GEF1!1),RhoC(gef!1) @ k22,k_22	19403804, 14627644			
Rac1	pak	PAK1	PBD	'Rac1_PAK' Rac1(pak),PAK1(PBD) <-> Rac1(pak!0),PAK1(PBD!0) @ k24,k_24	12167697			
SPAR	CC	LZTS1	CC1	'LZTS1_SPAR' LZTS1(CC1),SPAR(CC) <-> LZTS1(CC1!1),SPAR(CC!1) @ k37,k_37	15703396			
SPAR	GAP	Rap	gap	'SPAR_Rap'SPAR(GAP),Rap(gap) <-> SPAR(GAP!1),Rap(gap!1) @ k24,k_24	20547063, 17961154			
SPAR	CC	PROSAPIP1	CC1	'PROSAPIP1_SPAR' PROSAPIP1(CC1),SPAR(CC) <-> PROSAPIP1(CC1!1),SPAR(CC!1) @ k37,k_37	17961154			
SPAR	Act1	actin	act1	'SPAR_actin' SPAR(Act1),actin(act1) <-> SPAR(Act1!0),actin(act1!0) @ k25,k_25	17961154			
nRapGEF	RA	Rap	gef	'Rap_nRapGEF' nRapGEF(RA),Rap(gef) <-> nRapGEF(RA!1),Rap(gef!1) @ k42,k_42	21686267			
PROSAPIP1	CC	PROSAPIP1	CC	'PROSAPIP1_dimer' PROSAPIP1(CC),PROSAPIP1(CC) <-> PROSAPIP1(CC!0),PROSAPIP1(CC!0) @ k37,k_37	16522626			
PROSAPIP1	CC2	LZTS1	CC	'PROSAPIP_LZTS1' PROSAPIP1(CC2),LZTS1(CC) <-> PROSAPIP1(CC2!1),LZTS1(CC!1) @ k37,k_37	16522626			
PIKE	PRD2	PLCg	SH3	'PIKE_PLCg' PIKE(PRD2),PLCg(SH3) <-> PIKE(PRD2!1),PLCg(SH3!1) @ k29,k_29	16567124			
PIKE	PRD3	PI3K	SH3	'PIKE_PI3K' PIKE(PRD3),PI3K(SH3) <-> PIKE(PRD3!1),PI3K(SH3!1) @ k29,k_29	20419274			
AKAP	sh3	PP2B	akap	'AKAP_PP2B' AKAP(sh3),PP2B(akap) <-> AKAP(sh3!1),PP2B(akap!1) @ k34,k_34	21498812			
AKAP	r	PKA	R	'AKAP_PKA' AKAP(r),PKA(R) <-> AKAP(r!0),PKA(R!0) @ k30,k_30	21498812			
PI3K	PRD	Grb2	SH3	'PI3K_Grb2' PI3K(PRD),Grb2(SH3) <-> PI3K(PRD!1),Grb2(SH3!1) @ k29,k_29	19665053			
ACTN	ABD	actin	actn	'ACTN_ actin' ACTN(ABD),actin(actn) <-> ACTN(ABD!0),actin(actn!0) @ k33,k_33	21666840			
G_bg	PHB	G_a	bg	'G_bg_G_a' G_bg(PHB),G_a(bg) <-> G_bg(PHB!1),G_a(bg!1) @ k31,k_31				
GluR1	N2	GuR2	N1	'GluR1_GluR2' GluR1(N2),GluR2(N1) <-> GluR1(N2!1),GluR2(N1!1) @ k23,k_23				
GluR1	N1	GluR1	N1	'GluR1_GluR1' GluR1(N1),GluR1(N1) <-> GluR1(N1!1),GluR1(N1!1) @ k23,k_23				
GluR2	N2	GluR2	N2	'GluR2_GluR2' GluR2(N2),GluR2(N2) <-> GluR2(N2!1),GluR2(N2!1) @ k23,k_23				
GluR1	starg	stragazin	glur	'stargazin_GluR1' stargazin(glur),GluR1(starg) <-> stargazin(glur!1),GluR1(starg!1) @ k35,k_35	15136571			
GluR2	c	PICK1	PDZ	'Pick1_GluR2' PICK1(PDZ),GluR2(c~u) <-> PICK1(PDZ!1),GluR2(c~u!1) @ k27,k_27	21527319			
GluR2	c	GRIP	PDZ/PDZ54	'GRIP_PDZ45_Glur2' GRIP(PDZ4~u,PDZ5),GluR2(c~u) <-> GRIP(PDZ4~u,PDZ5!1),GluR2(c~u!1) @ k36,k_36	20547835			
GluR2	c	NSF	g	'GluR2_NSF' GluR2(c1),NSF(g) <-> GluR2(c1!1),NSF(g!1) @ k39,k_39	21106836			
GluR2	K	PKC	k	'GluR2_PKC' GluR2(K),PKC(k) <-> GluR2(K!1),PKC(k!1) @ k7,k_7	20547835			
GRIP	PDZ6	GRIP	PDZ6	'GRIP_dimer' GRIP(PDZ6),GRIP(PDZ6) <-> GRIP(PDZ6),GRIP(PDZ6) @ k38,k_38	20547835			