Molecular Cell, Volume *24*

Supplemental Data

Molecular Basis of AKAP Specificity

for PKA Regulatory Subunits

Matthew G. Gold, Birgitte Lygren, Pawel Dokurno, Naoto Hoshi, George McConnachie, Kjetil Taskén, Cathrine R. Carlson, John D. Scott, and David Barford

Table S1. Structural comparison of RIIα D/D molecules

	R.m.s.d. (Å) for equivalent Cα-atoms			
D/D Protomer	[1]Apo 1	[2]AKAP-*IS* 1	AKAP-*IS* 2	Ordered region
Apo 1	-	0.48	0.48	^{5}Ala 4 – ^{5}Ala 50
Apo 2	0.22	0.51	0.53	^{5}Ala 3 – ^{5}Ala 50
Apo 3	0.24	0.51	0.50	^{5}Ala 4 – ^{5}Ala 49
Apo 4	0.23	0.55	0.54	Ile 3 – His 49
Apo 5	0.20	0.50	0.50	Ile 3 – ^{5}Ala 50
Apo 6	0.14	0.48	0.46	^{5}Ala 3 – ^{5}Ala 50
Apo 7	0.19	0.44	0.48	Gln 4 – ^{5}Ala 48
Apo 8	0.26	0.55	0.49	Ile 3 – His 49
AKAP-*IS* 1	-	-	0.51	Ile 5 – Arg 43
AKAP-*IS* 2	-	-	-	Ile 3 – Arg 43
[3]NMR D/D 1	1.03	0.95	0.82	
NMR D/D 2	1.03	0.95	0.82	
[4]NMR D/D-HT31 1	1.65	1.22	1.07	
NMR D/D-HT31 2	0.86	0.84	0.73	

[1]Apo: Apo RII D/D
[2]AKAP-*IS*: RII D/D – AKAP-*IS* complex
[3]NMR D/D: NMR structure of apo RIIα D/D

[4]NMR D/D-HT31: NMR structure of RIIα D/D-HT31 complex
[5]Denotes side chain built as Ala

Rmsd (Å) for equivalent Cα-atoms

Apo-RII dimer vs. AKAP-*IS*-RII dimer: 0.62 Å
Apo-RII dimer (X-ray) vs. Apo-RII dimer (NMR): 1.25 Å
AKAP-*IS*-RII (X-ray) vs. Ht31-RII (NMR): 1.44 Å