Supporting Information



Supporting Figure S1: RMSD Vs Time for all replicas of AhR different termini. (A) AhR Canon; (B) NC Trunc; (C) N- Trunc; (D) C-Trunc.



Supporting Figure S2: RMSD Vs Time for all replicas of different PAS-B domains simulated. (A) AhR; (B) AhR - reduced C300-C313 Bond; (C) D. Suzukii JHR; (D) HIF1 α ; (E) NCOA1; (F) HIF2 α ;

NCOA1_PAS-B	GHMTGVE	SFM	TKQDTTGK:	IISID TSS	LRAAGRTG	WEDLVRI	KCIYAFFQPQGR <mark>E</mark> F	SY	56
D.Suzukii_JHR_PAS-B	QPE	PYQLEYH	TRHLIDGS	IIDCDQRI	GLVAGYMK	DEVRNL	-SPFCFMHLDDVR-	-W	53
AhR_PAS-B	IF	RTKNFIFR	TKHKLDFT	PIGCDAKG	RIVLGYTE	AELCTR	GSGYQFIHAADML-	- Y	53
HIF1a_PAS-B	[SKTFL	SRHSLDMKI	SYCDERI	TELMGYEP	EELLGR	-SIYEYYHALDSD-	-H	49
HIF2a_PAS-B	GEFKGL	SKTFL	SEHSMDMK	TYCDDRI	TELIGYHP	EELLGR	-SAYEFYHALDSE-	-N	55
		:	· · · ·	*	*	*	. : : : .		
NCOA1_PAS-B	ARQLFQ	VMT-RGT	ASSPSYRE	LNDGTML	SAHTRCKL	.CYPQSPI	DMQPFIMGIHIIDR	EH	115
D.Suzukii_JHR_PAS-B	VIVALR	MYDCNSD	YGESCYRL	SRNGRFI	YLHTKGFL	EIDRGT	NKVHSFLCVNTLLC)EE	113
AhR_PAS-B	CAESHI	MIK-TGE	SGMIVFRL	TKNNRWT	WVQSNARL	LYKNG-	-RPDYIIVTQRPLT	DE	110
HIF1a_PAS-B	LTKTHH	MFT-KGQ	VTTGQYRM	AKRGGYV	WVETQATV	IYNTKN:	SQPQCIVCVNYVVS		106
HIF2a_PAS-B	MTKSHQN	ILCT-KGQ	VVSGQYRM	AKHGGYV	WLETQGTV	IYNPRNI	LQPQCIMCVNYVLS	EI	114
		: .	*		.:. :		:: :		
NCOA1_PAS-B	SG-	117							
D.Suzukii_JHR_PAS-B	AGR	116							
AhR_PAS-B	E	111							
HIF1a_PAS-B		106							
HIF2a_PAS-B	EK-	116							

Supporting Figure S3: Sequence alignment for all five different PAS-B domains: . indicates weak similarity, : indicates strong similarity and * indicates complete conservation (identity).



Supporting Figure S4: 3D structural alignment for all five different PAS-B domains investigated in this study: Orange boxes indicate the structurally conserved areas, In grey, the conservation and Backbone RMSD graphs per residue..



Supporting Figure S5: HIF2a Hydrogen bond in the conformation showing buried Y281, the red line indicate the backbone interactions.