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Supporting information for article:

Structure of a truncated form of leucine zipper II of JIP3 reveals an unexpected antiparallel coiled-coil arrangement

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Table S1 Details of the JIP3/4-LZII structures and models used for the MD calculations.

Model	chainC/chainD		JIP	chainC/chainD
	#residues	#Na+	#H2O mol.	PDB residues
JIP3- <i>p</i> LZII_1-8	67/67	8	39944	417-483/417-483
JIP3- <i>ap</i> LZII_3-10	56/57	2	41797	430-485/430-486
JIP4- <i>p</i> LZII_1-8	67/62	10	36233	385-451/390-451
JIP4- <i>ap</i> LZII_3-10	54/54	4	40596	408-461/408-461

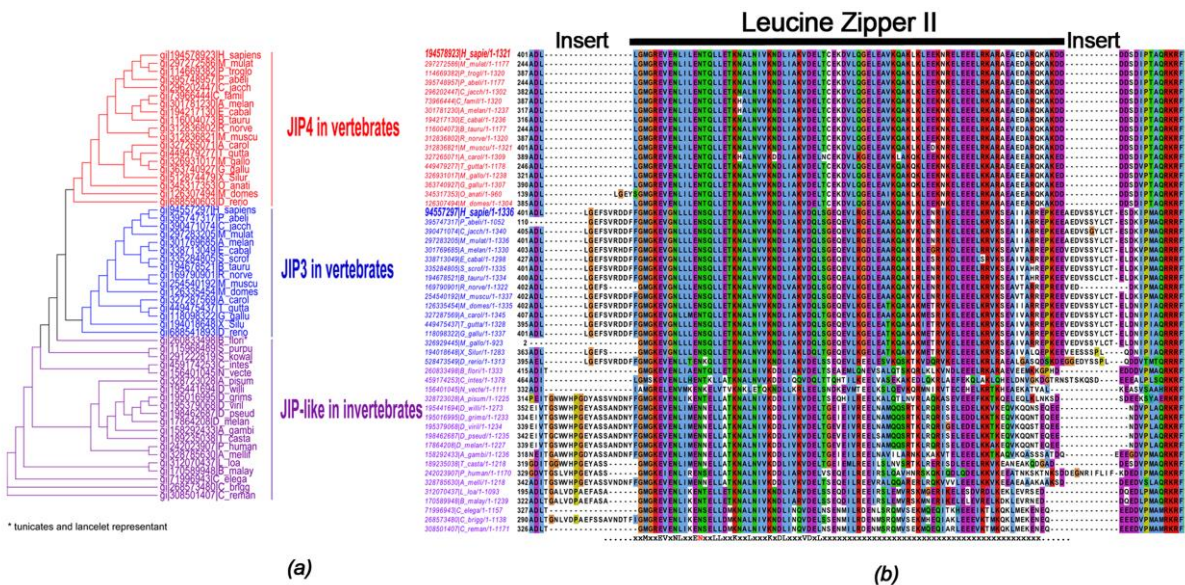


Figure S1 Phylogenetic tree for JIP3 and JIP4 homologs. *(a)* Phylogenetic tree for JIP3 and JIP4 homologs. Tree reconstruction is derived from a multiple sequence alignment of homologs of JIP3 and JIP4 retrieved from different metazoan species. JIP4 and JIP3 orthologs in vertebrates together with JIP-like sequences in invertebrates are indicated in red, blue and purple, respectively. Tree leaves are labelled with the NCBI gene index (gi) of the protein sequence followed by an abbreviated name of the corresponding species. *(b)* Multiple sequence alignment of homologs of JIP3, JIP4 and JIP-like that were used to build the phylogenetic tree in *(a)* focused in the region of the Leucine Zipper II. Gene indexes and abbreviated species names are coloured as in panel *(a)* (represented using Jalview [Waterhouse, A.M., et al. (2009) Jalview Version 2—a multiple sequence alignment editor and analysis workbench. *Bioinformatics* 25: 1189-1191]). Residues strictly conserved are indicated below.

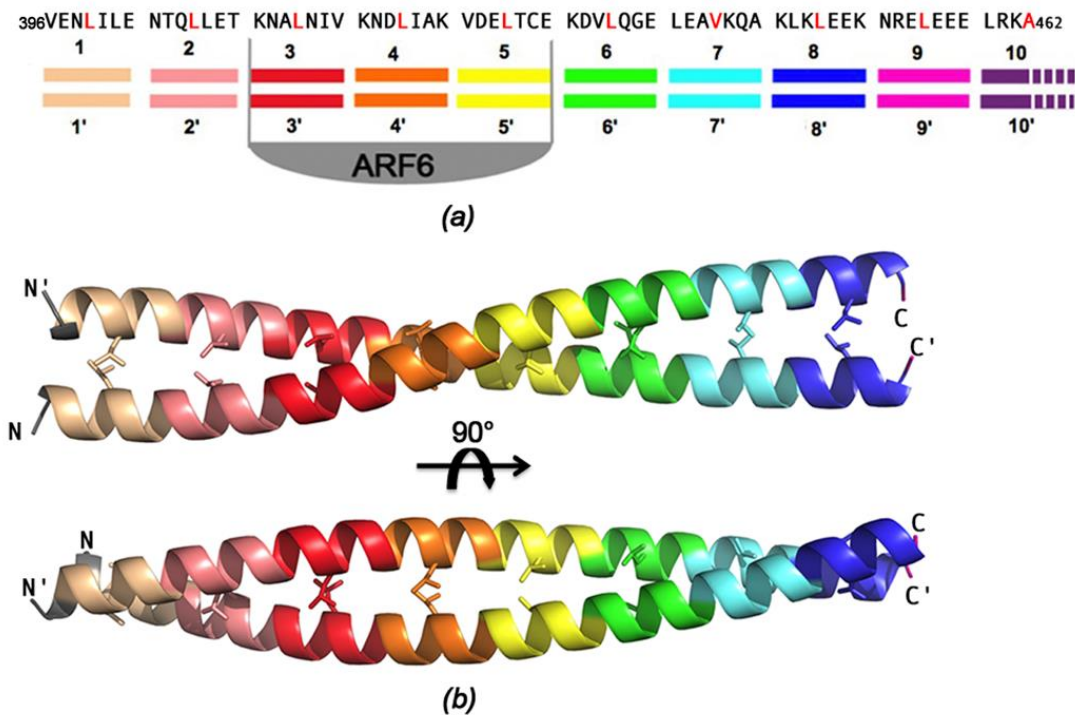


Figure S2 3D structure of the parallel JIP4-LZII_1-10 fragment (a) Schema of the quaternary organization of the parallel JIP4-LZII_1-10 homodimer. The primary sequence of JIP4-LZII_1-10 is reported above. Of note, the ARF6-binding site is indicated in grey. (b) 3D structure of the parallel JIP4-LZII_1-10 fragment (two orthogonal views). Leucine residues at position *d* are indicated in red in (a) and shown in sticks in (b). Heptad repeats are highlighted using a rainbow colour code. Of note no electron density was observed for the heptad repeat 9 and beyond, thus only heptad repeats 1 to 8 were fully modelled.