

## Supplementary Material

### Reference:

Bindewald E, Hayes R, Yaroslava G, Yingling Y, Kasprzak W and Shapiro BA:  
RNAJunction: A Database of RNA Junctions and Kissing Loops For Three-Dimensional Structural Analysis  
and Nanodesign. Nucleic Acids Research, 2008 (database issue).

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## 1. Attribute Overview of RNAJunction relational database tables

Relation	Attribute	Description
<b>motifs</b>		
		general information about each junction
	MOTIF_ID	unique integer to identify each junction, also referred to as junction id (jid)
	PDB_ID	identifier for original structures from Protein Data Bank (PDB)
	N_STRANDS	integer, number of strands, equal to the number of helices
	LILLEY	Lilley Classification, see help/lilley_help.php
	FINGERPRINT	colon delimited integers, value for each angle in junction
	LOOP_LEN_SUM	total number of unpaired bases in junction (not to exceed 50)
	KLOOP	TRUE/FALSE, indicates if junction is kissing loop
	INTERNAL_HEL	TRUE/FALSE, indicates if junction has loops within its helices
	FILENAME	filename, max 300 characters
	MD_SIM	TRUE/FALSE, indicates if junction has had molecular dynamics simulations performed
	DATASET	1 character (A,B,C) to denote the helix fit parameter A=most strict, B=med. strict, C = least
	ST_HELIXENDS	BOOLEAN, indicates presence of non-standard base pairs in helices
	REP_FLAG	BOOLEAN, indicates if structure is representative structure (old method)
	MIN_RMSD	Double, rmsd (in angstroms) for minimized structure compared to original structure
	CLUSTER	Varchar(200), name of the seq/structure cluster to which entry belongs
<b>strands</b>		
		detailed information about each strand
	STRAND_ID	unique integer to identify each strand
	NAME_ID5	label for first nucleotide in strand (5' end)
	NAME_ID3	label for last nucleotide in strand (3' end)
	NUM_ID5_ORIG	label for first nucleotide in strand (5' end) from original pdb file
	NUM_ID3_ORIG	label for last nucleotide in strand (3' end) from original pdb file
	NAME2_ID5	label for first paired nucleotide on 5' side of the loop region
	NAME2_ID3	label for first paired nucleotide on 3' side of the loop region
	NUM2_ID5_ORIG	label for first paired nucleotide on 5' side of the loop region from original pdb file
	NUM2_ID3_ORIG	label for first paired nucleotide on 3' side of the loop region from original pdb file
	SEQ2	sequence of strand for the loop region only
	SEQ2_LEN	length of sequence for the loop region only
	SEQ	sequence of strand max 300 nucleotides
	SEQ_LEN	length of sequence
	STRAND_C	name of strand, from original PDB file
	MOTIF_ID	unique integer to identify each junction, also referred to as junction id (jid)
<b>helices</b>		
		detailed information about each helix
	HELIX_ID	unique integer to identify each helix
	INID	Index of first residue of incoming strand (internal counting)
	OUTID	Index of last residue of outgoing strand (internal counting)
	INID2	index of residue of incoming strand of first base pair of helix (internal counting)
	OUTID2	index of residue of outgoing strand of first base pair of helix (internal counting)
	INID2_ORIG	Index of residue of incoming strand corresponding to first base pair of helix (PDB counting)
	OUTID2_ORIG	Index of residue of outgoing strand corresponding to first base pair of helix (PDB counting)
	INSEQ_CHAR	name of incoming strand
	OUTSEQ_CHAR	name of outgoing strand
	HBX	x coordinate for branch descriptor artifact (generated by junctionscan)
	HBY	y coordinate for branch descriptor artifact (generated by junctionscan)

HBZ	z coordinate for branch descriptor artifact (generated by junctionscan)
HXX	x coordinate for the x direction of the helix orientation artifact (generated by junctionscan)
HXY	y coordinate for the x direction of the helix orientation artifact (generated by junctionscan)
HXZ	z coordinate for the x direction of the helix orientation artifact (generated by junctionscan)
HYX	x coordinate for the y direction of the helix orientation artifact (generated by junctionscan)
HYY	y coordinate for the y direction of the helix orientation artifact (generated by junctionscan)
HYZ	z coordinate for the y direction of the helix orientation artifact (generated by junctionscan)
HZX	x coordinate for the z direction of the helix orientation artifact (generated by junctionscan)
HZY	y coordinate for the z direction of the helix orientation artifact (generated by junctionscan)
HZZ	z coordinate for the z direction of the helix orientation artifact (generated by junctionscan)
MOTIF_ID	unique integer to identify each junction, also referred to as junction id (jid)

angles	value and position for each angle
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ANGLE_ID	unique integer to identify each angle
ANGLE	the value of the angle, in degrees
POSITION	the position of the angle in the junctions fingerprint (natural number)
MOTIF_ID	unique integer to identify each junction, also referred to as junction id (jid)

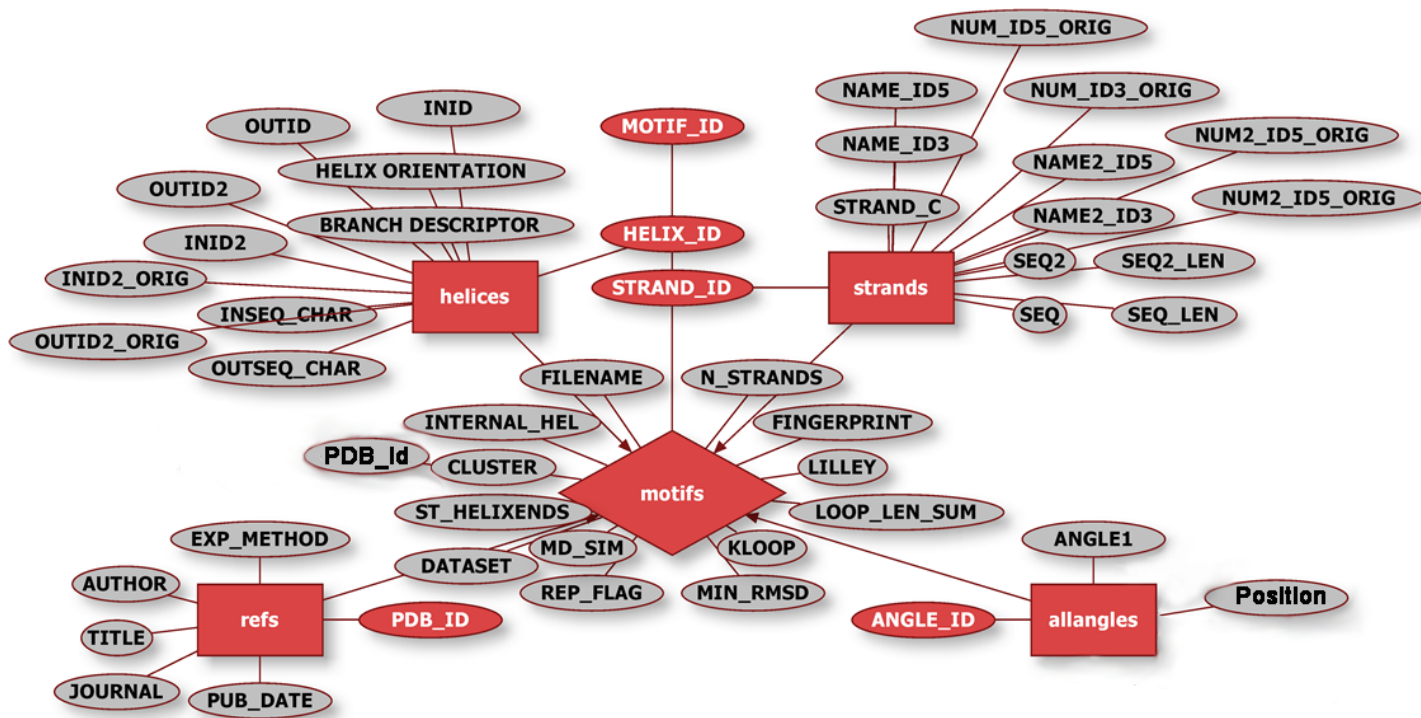
md_sims	results of molecular dynamics simulations
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SIM_ID	unique integer to identify each simulation filename for the graphical representation the junctions conformational changes with respect to time
ANGLE_PLOT	
RMSD	root mean square deviation
SOLVENT_METHOD	implicit of explicit
ST_DEV_ANGLE	standard deviation for the change in angle
ETOT	the junction's total energy after being minimized
MED_STRUC	motif_id for the median junction as per the simulation
MIN_STRUC	motif_id for the minimum junction as per the simulation
MAX_STRUC	motif_id for the maximum junction as per the simulation
ORIG_STRUC	motif_id for the original junction

refs	source for each pdb file cited
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PDB_ID	identifier for original structures from Protein Data Bank (PDB)
AUTHOR	authors on original structure's publication
TITLE	title of the original structure's publication
JOURNAL	journal in which the original structure was published
PUB_DATE	date on which the original structure was published
EXP_METHOD	Enum('ELECTRON_MICROSCOPY','FIBER_DIFFRACTION','FLUORESCENCE_TRANSFER','NMR','X-RAY_DIFFRACTION','UNAVAILABLE')

**Figure S1:** Entity Relationship Diagram of RNAJunction database



**Figure S2:** Geometry of Corridor Filter

