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Chapter 1

ViennaRNA Package core - RNAlib

A Library for folding and comparing RNA secondary structures

Date

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1.1 Introduction

The core of the Vienna RNA Package is formed by a collection of routines for the prediction and comparison of RNA secondary structures. These routines can be accessed through stand-alone programs, such as RNAfold, RNAdistance etc., which should be sufficient for most users. For those who wish to develop their own programs we provide a library which can be linked to your own code.

This document describes the library and will be primarily useful to programmers. However, it also contains details about the implementation that may be of interest to advanced users. The stand-alone programs are described in separate man pages. The latest version of the package including source code and html versions of the documentation can be found at

http://www.tbi.univie.ac.at/~ivo/RNA/

Chapter 2

Folding Routines - Functions for Folding RNA Secondary Structures

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2.1 Calculating Minimum Free Energy Structures

The library provides a fast dynamic programming minimum free energy folding algorithm as described by Zuker & Stiegler (1981).

Associated functions are:

```
float fold (char* sequence, char* structure);
```

Compute minimum free energy and an appropriate secondary structure of an RNA sequence.

```
float circfold (char* sequence, char* structure);
```

Compute minimum free energy and an appropriate secondary structure of a circular RNA sequence.

```
float energy_of_structure(const char *string,
                          const char *structure,
                          int verbosity_level);
```

Calculate the free energy of an already folded RNA using global model detail settings.

```
float energy_of_circ_structure( const char *string,
                                const char *structure,
                                int verbosity_level);
```

Calculate the free energy of an already folded circular RNA.

```
void  update_fold_params(void);
```

Recalculate energy parameters.

```
void  free_arrays(void);
```

Free arrays for mfe folding.

See also

fold.h, cofold.h, 2Dfold.h, Lfold.h, alifold.h and subopt.h for a complete list of available functions.

2.2 Calculating Partition Functions and Pair Probabilities

Instead of the minimum free energy structure the partition function of all possible structures and from that the pairing probability for every possible pair can be calculated, using a dynamic programming algorithm as described by McCaskill (1990). The following functions are provided:

```
float pf_fold ( char* sequence,
                char* structure)
```

Compute the partition function Q of an RNA sequence.

```
void free_pf_arrays (void)
```

Free arrays for the partition function recursions.

```
void update_pf_params (int length)
```

Recalculate energy parameters.

```
char *get_centroid_struct_pl( int length,
                              double *dist,
                              plist *pl);
```

Get the centroid structure of the ensemble.

```
char *get_centroid_struct_pr( int length,
                              double *dist,
                              double *pr);
```

Get the centroid structure of the ensemble.

```
double mean_bp_distance_pr( int length,
                            double *pr);
```

Get the mean base pair distance in the thermodynamic ensemble.

See also

part_func.h, part_func_co.h, part_func_up.h, 2Dpfold.h, LPfold.h, alifold.h and MEA.h for a complete list of available functions.

2.3 Searching for Predefined Structures

We provide two functions that search for sequences with a given structure, thereby inverting the folding routines.

```
float inverse_fold (char *start,
                    char *target)
```

Find sequences with predefined structure.

```
float inverse_pf_fold ( char *start,
                        char *target)
```

Find sequence that maximizes probability of a predefined structure.

The following global variables define the behavior or show the results of the inverse folding routines:

```
char *symbolset
```

This global variable points to the allowed bases, initially "AUGC".

See also

inverse.h for more details and a complete list of available functions.

2.4 Enumerating Suboptimal Structures

```
SOLUTION *subopt (char *sequence,
                  char *constraint,
                  int *delta,
                  FILE *fp)
```

Returns list of subopt structures or writes to fp.

```
SOLUTION *subopt_circ ( char *sequence,
                        char *constraint,
                        int *delta,
                        FILE *fp)
```

Returns list of circular subopt structures or writes to fp.

```
SOLUTION  *zukersubopt(const char *string);
```

Compute Zuker type suboptimal structures.

```
char  *TwoDpfold_pbacktrack ( TwoDpfold_vars *vars,
                              unsigned int d1,
                              unsigned int d2)
```

Sample secondary structure representatives from a set of distance classes according to their Boltzmann probability.

```
char  *alipbacktrack (double *prob)
```

Sample a consensus secondary structure from the Boltzmann ensemble according its probability

.

```
char    *pbacktrack(char *sequence);
```

Sample a secondary structure from the Boltzmann ensemble according its probability

.

```
char    *pbacktrack_circ(char *sequence);
```

Sample a secondary structure of a circular RNA from the Boltzmann ensemble according its probability.

See also

subopt.h, part_func.h, alifold.h and 2Dpfold.h for more detailed descriptions

2.5 Predicting hybridization structures of two molecules

The function of an RNA molecule often depends on its interaction with other RNAs. The following routines therefore allow to predict structures formed by two RNA molecules upon hybridization.

One approach to co-folding two RNAs consists of concatenating the two sequences and keeping track of the concatenation point in all energy evaluations. Correspondingly, many of the cofold() and co_pf_fold() routines below take one sequence string as argument and use the the global variable cut_point to mark the concatenation point. Note that while the *RNAcofold* program uses the '&' character to mark the chain break in its input, you should not use an '&' when using the library routines (set cut_point instead).

In a second approach to co-folding two RNAs, cofolding is seen as a stepwise process. In the first step the probability of an unpaired region is calculated and in a second step this probability of an unpaired region is multiplied with the probability of an interaction between the two RNAs. This approach is implemented for the interaction between a long target sequence and a short ligand RNA. Function pf_unstru() calculates the partition function over all unpaired regions in the input sequence. Function pf_interact(), which calculates the partition function over all possible interactions between two sequences, needs both sequence as separate strings as input.

```
int cut_point
```

Marks the position (starting from 1) of the first nucleotide of the second molecule within the concatenated sequence.

```
float cofold (char *sequence,
              char *structure)
```

Compute the minimum free energy of two interacting RNA molecules.

```
void  free_co_arrays (void)
```

Free memory occupied by cofold()

Partition Function Cofolding

To simplify the implementation the partition function computation is done internally in a null model that does not include the duplex initiation energy, i.e. the entropic penalty for producing a dimer from two monomers). The resulting free energies and pair probabilities are initially relative to that null model. In a second step the free energies can be corrected to include the dimerization penalty, and the pair probabilities can be divided into the conditional pair probabilities given that a re dimer is formed or not formed.

```
cofoldF co_pf_fold( char *sequence,
                    char *structure);
```

Calculate partition function and base pair probabilities.

```
void    free_co_pf_arrays(void);
```

Free the memory occupied by co_pf_fold()

Cofolding all Dimeres, Concentrations

After computing the partition functions of all possible dimeres one can compute the probabilities of base pairs, the concentrations out of start concentrations and sofar and soaway.

```
void  compute_probabilities(
              double FAB,
              double FEA,
              double FEB,
              struct plist  *prAB,
              struct plist  *prA,
              struct plist  *prB,
              int Alength)
```

Compute Boltzmann probabilities of dimerization without homodimers.

```
ConcEnt *get_concentrations(double FEAB,
                            double FEAA,
                            double FEBB,
                            double FEA,
                            double FEB,
                            double * startconc)
```

Given two start monomer concentrations a and b, compute the concentrations in thermodynamic equilibrium of all dimers and the monomers.

Partition Function Cofolding as a stepwise process

In this approach to cofolding the interaction between two RNA molecules is seen as a stepwise process. In a first step, the target molecule has to adopt a structure in which a binding site is accessible. In a second step, the ligand molecule will hybridize with a region accessible to an interaction. Consequently the algorithm is designed as a two step process: The first step is the calculation of the probability that a region within the target is unpaired, or equivalently, the calculation of the free energy needed to expose a region. In the second step we compute the free energy of an interaction for every possible binding site. Associated functions are:

```
pu_contrib *pf_unstru ( char *sequence,
                        int max_w)
```

Calculate the partition function over all unpaired regions of a maximal length.

```
void  free_pu_contrib_struct (pu_contrib *pu)
```

Frees the output of function pf_unstru().

```
interact *pf_interact(
              const char *s1,
              const char *s2,
              pu_contrib *p_c,
              pu_contrib *p_c2,
```

```
              int max_w,
              char *cstruc,
              int incr3,
              int incr5)
```

Calculates the probability of a local interaction between two sequences.

```
void free_interact (interact *pin)
```

Frees the output of function pf_interact().

See also

cofold.h, part_func_co.h and part_func_up.h for more details

2.6 Predicting local structures of large sequences

Local structures can be predicted by a modified version of the fold() algorithm that restricts the span of all base pairs.

```
float Lfold ( const char *string,
              char *structure,
              int maxdist)
```

The local analog to fold().

```
float aliLfold( const char **strings,
                char *structure,
                int maxdist)
```

```
float Lfoldz (const char *string,
              char *structure,
              int maxdist,
              int zsc,
              double min_z)
```

```
plist *pfl_fold (
            char *sequence,
            int winSize,
            int pairSize,
            float cutoffb,
            double **pU,
            struct plist **dpp2,
            FILE *pUfp,
            FILE *spup)
```

Compute partition functions for locally stable secondary structures **(berni! update me)**

See also

Lfold.h and LPfold.h for more details

2.7 Predicting Consensus Structures from Alignment

Consensus structures can be predicted by a modified version of the fold() algorithm that takes a set of aligned sequences instead of a single sequence. The energy function consists of the mean energy averaged over the sequences, plus a covariance term that favors pairs with consistent and compensatory mutations and penalizes pairs that cannot be formed by all structures. For details see Hofacker (2002).

```
float  alifold (const char **strings,
                char *structure)
```

Compute MFE and according consensus structure of an alignment of sequences.

```
float  circalifold (const char **strings,
                    char *structure)
```

Compute MFE and according structure of an alignment of sequences assuming the sequences are circular instead of linear.

```
void    free_alifold_arrays (void)
```

Free the memory occupied by MFE alifold functions.

```
float   energy_of_alistruct (
            const char **sequences,
            const char *structure,
            int n_seq,
            float *energy)
```

Calculate the free energy of a consensus structure given a set of aligned sequences.

```
struct pair_info
```

A base pair info structure.

```
double  cv_fact
```

This variable controls the weight of the covariance term in the energy function of alignment folding algorithms.

```
double  nc_fact
```

This variable controls the magnitude of the penalty for non-compatible sequences in the covariance term of alignment folding algorithms.

See also

alifold.h for more details

2.8 Global Variables for the Folding Routines

The following global variables change the behavior the folding algorithms or contain additional information after folding.

`int noGU`

Global switch to forbid/allow GU base pairs at all.

`int no_closingGU`

GU allowed only inside stacks if set to 1.

`int noLonelyPairs`

Global switch to avoid/allow helices of length 1.

`int tetra_loop`

Include special stabilizing energies for some tri-, tetra- and hexa-loops;.

`int energy_set`

0 = BP; 1=any mit GC; 2=any mit AU-parameter

`float temperature`

Rescale energy parameters to a temperature in degC.

`int dangles`

Switch the energy model for dangling end contributions (0, 1, 2, 3)

`char *nonstandards`

contains allowed non standard base pairs

`int cut_point`

Marks the position (starting from 1) of the first nucleotide of the second molecule within the concatenated sequence.

`float pf_scale`

A scaling factor used by pf_fold() to avoid overflows.

```
int fold_constrained
```

Global switch to activate/deactivate folding with structure constraints.

```
int do_backtrack
```

do backtracking, i.e.

```
char backtrack_type
```

A backtrack array marker for inverse_fold()

include fold_vars.h if you want to change any of these variables from their defaults.

See also

fold_vars.h for a more complete and detailed description of all global variables and how to use them

2.9 Reading Energy Parameters from File

A default set of parameters, identical to the one described in Mathews et.al. (2004), is compiled into the library.

Alternately, parameters can be read from and written to a file.

```
void  read_parameter_file (const char fname[])
```

Read energy parameters from a file.

```
void  write_parameter_file (const char fname[])
```

Write energy parameters to a file.

To preserve some backward compatibility the RNAlib also provides functions to convert energy parameter files from the format used in version 1.4-1.8 into the new format used since version 2.0

```
void convert_parameter_file (
            const char *iname,
            const char *oname,
            unsigned int options)
```

Convert/dump a Vienna 1.8.4 formatted energy parameter file.

See also

read_epars.h and convert_epars.h for detailed description of the available functions

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Chapter 3

Parsing and Comparing - Functions to Manipulate Structures

Representations of Secondary Structures

The standard representation of a secondary structure is the *bracket notation*, where matching brackets symbolize base pairs and unpaired bases are shown as dots. Alternatively, one may use two types of node labels, 'P' for paired and 'U' for unpaired; a dot is then replaced by '(U)', and each closed bracket is assigned an additional identifier 'P'. We call this the expanded notation. In Fontana et al. (1993) a condensed representation of the secondary structure is proposed, the so-called homeomorphically irreducible tree (HIT) representation. Here a stack is represented as a single pair of matching brackets labeled 'P' and weighted by the number of base pairs. Correspondingly, a contiguous strain of unpaired bases is shown as one pair of matching brackets labeled 'U' and weighted by its length. Generally any string consisting of matching brackets and identifiers is equivalent to a plane tree with as many different types of nodes as there are identifiers.

Bruce Shapiro (1988) proposed a coarse grained representation, which, does not retain the full information of the secondary structure. He represents the different structure elements by single matching brackets and labels them as 'H' (hairpin loop), 'I' (interior loop), 'B' (bulge), 'M' (multi-loop), and 'S' (stack). We extend his alphabet by an extra letter for external elements 'E'. Again these identifiers may be followed by a weight corresponding to the number of unpaired bases or base pairs in the structure element. All tree representations (except for the dot-bracket form) can be encapsulated into a virtual root (labeled 'R'), see the example below.

The following example illustrates the different linear tree representations used by the package. All lines show the same secondary structure.

```
a) .((((..(((...)))..((..)))).)).
   (U)(((((U)(U)((((U)(U)(U)P)P)P)(U)(U)(((U)(U)P)P)P)P)(U)P)P)(U)
b) (U)(((U2)((U3)P3)(U2)((U2)P2)P2)(U)P2)(U)
c) (((H)(H)M)B)
   ((((((H)S)((H)S)M)S)B)S)
   (((((((H)S)((H)S)M)S)B)S)E)
```

```
d) (((((((H3)S3)((H2)S2)M4)S2)B1)S2)E2)R)
```

Above: Tree representations of secondary structures. a) Full structure: the first line shows the more convenient condensed notation which is used by our programs; the second line shows the rather clumsy expanded notation for completeness, b) HIT structure, c) different versions of coarse grained structures: the second line is exactly Shapiro's representation, the first line is obtained by neglecting the stems. Since each loop is closed by a unique stem, these two lines are equivalent. The third line is an extension taking into account also the external digits. d) weighted coarse structure, this time including the virtual root.

For the output of aligned structures from string editing, different representations are needed, where we put the label on both sides. The above examples for tree representations would then look like:

```
a) (UU)(P(P(P(P(UU)(UU)(P(P(P(UU)(UU)(UU)P)P)P)(UU)(UU)(P(P(UU)(U...
b) (UU)(P2(P2(U2U2)(P2(U3U3)P3)(U2U2)(P2(U2U2)P2)P2)(UU)P2)(UU)
c) (B(M(HH)(HH)M)B)
   (S(B(S(M(S(HH)S)(S(HH)S)M)S)B)S)
   (E(S(B(S(M(S(HH)S)(S(HH)S)M)S)B)S)E)
d) (R(E2(S2(B1(S2(M4(S3(H3)S3)((H2)S2)M4)S2)B1)S2)E2)R)
```

Aligned structures additionally contain the gap character '_'.

Parsing and Coarse Graining of Structures

Several functions are provided for parsing structures and converting to different representations.

```
char  *expand_Full(const char *structure)
```

Convert the full structure from bracket notation to the expanded notation including root.

```
char *b2HIT (const char *structure)
```

Converts the full structure from bracket notation to the HIT notation including root.

```
char *b2C (const char *structure)
```

Converts the full structure from bracket notation to the a coarse grained notation using the 'H' 'B' 'I' 'M' and 'R' identifiers.

```
char *b2Shapiro (const char *structure)
```

Converts the full structure from bracket notation to the *weighted* coarse grained notation using the 'H' 'B' 'I' 'M' 'S' 'E' and 'R' identifiers.

```
char  *expand_Shapiro (const char *coarse);
```

Inserts missing 'S' identifiers in unweighted coarse grained structures as obtained from b2C().

```
char *add_root (const char *structure)
```

Adds a root to an un-rooted tree in any except bracket notation.

```
char  *unexpand_Full (const char *ffull)
```

Restores the bracket notation from an expanded full or HIT tree, that is any tree using only identifiers 'U' 'P' and 'R'.

```
char  *unweight (const char *wcoarse)
```

Strip weights from any weighted tree.

```
void   unexpand_aligned_F (char *align[2])
```

Converts two aligned structures in expanded notation.

```
void   parse_structure (const char *structure)
```

Collects a statistic of structure elements of the full structure in bracket notation.

See also

RNAstruct.h for prototypes and more detailed description

Distance Measures

A simple measure of dissimilarity between secondary structures of equal length is the base pair distance, given by the number of pairs present in only one of the two structures being compared. I.e. the number of base pairs that have to be opened or closed to transform one structure into the other. It is therefore particularly useful for comparing structures on the same sequence. It is implemented by

```
int bp_distance(const char *str1,
                const char *str2)
```

Compute the "base pair" distance between two secondary structures s1 and s2.

For other cases a distance measure that allows for gaps is preferable. We can define distances between structures as edit distances between trees or their string representations. In the case of string distances this is the same as "sequence alignment". Given a set of edit operations and edit costs, the edit distance is given by the minimum sum of the costs along an edit path converting one object into the other. Edit distances like these always define a metric. The edit operations used by us are insertion, deletion and replacement of nodes. String editing does not pay attention to the matching of brackets, while in tree editing matching brackets represent a single node of the tree. Tree editing is therefore usually preferable, although somewhat slower. String edit distances are always smaller or equal to tree edit distances.

The different level of detail in the structure representations defined above naturally leads to different measures of distance. For full structures we use a cost of 1 for deletion or insertion of an unpaired base and 2 for a base pair. Replacing an unpaired base for a pair incurs a cost of 1.

Two cost matrices are provided for coarse grained structures:

```
/*  Null,    H,    B,    I,    M,    S,    E    */
   {   0,    2,    2,    2,    2,    1,    1},   /* Null replaced */
   {   2,    0,    2,    2,    2, INF,  INF},   /* H    replaced */
   {   2,    2,    0,    1,    2, INF,  INF},   /* B    replaced */
   {   2,    2,    1,    0,    2, INF,  INF},   /* I    replaced */
   {   2,    2,    2,    2,    0, INF,  INF},   /* M    replaced */
   {   1,  INF,  INF,  INF,  INF,    0,  INF},   /* S    replaced */
   {   1,  INF,  INF,  INF,  INF,  INF,    0},   /* E    replaced */


/* Null,    H,    B,    I,    M,    S,    E   */
   {   0,  100,    5,    5,   75,    5,    5},   /* Null replaced */
   { 100,    0,    8,    8,    8, INF,  INF},   /* H    replaced */
   {   5,    8,    0,    3,    8, INF,  INF},   /* B    replaced */
   {   5,    8,    3,    0,    8, INF,  INF},   /* I    replaced */
   {  75,    8,    8,    8,    0, INF,  INF},   /* M    replaced */
   {   5,  INF,  INF,  INF,  INF,    0,  INF},   /* S    replaced */
   {   5,  INF,  INF,  INF,  INF,  INF,    0},   /* E    replaced */
```

The lower matrix uses the costs given in Shapiro (1990). All distance functions use the following global variables:

```
int  cost_matrix;
```

Specify the cost matrix to be used for distance calculations.

```
int   edit_backtrack;
```

Produce an alignment of the two structures being compared by tracing the editing path giving the minimum distance.

```
char *aligned_line[4];
```

Contains the two aligned structures after a call to one of the distance functions with edit_backtrack set to 1.

See also

utils.h, dist_vars.h and stringdist.h for more details

Functions for Tree Edit Distances

```
Tree   *make_tree (char *struc)
```

Constructs a Tree (essentially the postorder list) of the structure 'struc', for use in tree_edit_distance().

```
float   tree_edit_distance (Tree *T1,
                            Tree *T2)
```

Calculates the edit distance of the two trees.

```
void    free_tree(Tree *t)
```

Free the memory allocated for Tree t.

See also

dist_vars.h and treedist.h for prototypes and more detailed descriptions

Functions for String Alignment

```
swString *Make_swString (char *string)
```

Convert a structure into a format suitable for string_edit_distance().

```
float     string_edit_distance (swString *T1,
                                swString *T2)
```

Calculate the string edit distance of T1 and T2.

See also

dist_vars.h and stringdist.h for prototypes and more detailed descriptions

Functions for Comparison of Base Pair Probabilities

For comparison of base pair probability matrices, the matrices are first condensed into probability profiles which are the compared by alignment.

```
float *Make_bp_profile_bppm ( double *bppm,
                              int length)
```

condense pair probability matrix into a vector containing probabilities for upstream paired, downstream paired and unpaired.

```
float profile_edit_distance ( const float *T1,
                              const float *T2)
```

Align the 2 probability profiles T1, T2

.

See also

ProfileDist.h for prototypes and more details of the above functions

Next Page: Utilities

Chapter 4

Utilities - Odds and Ends

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4.1 Producing secondary structure graphs

```
int PS_rna_plot ( char *string,
                  char *structure,
                  char *file)
```

Produce a secondary structure graph in PostScript and write it to 'filename'.

```
int PS_rna_plot_a (
            char *string,
            char *structure,
            char *file,
            char *pre,
            char *post)
```

Produce a secondary structure graph in PostScript including additional annotation macros and write it to 'filename'.

```
int gmlRNA (char *string,
            char *structure,
            char *ssfile,
            char option)
```

Produce a secondary structure graph in Graph Meta Language (gml) and write it to a file.

```
int ssv_rna_plot (char *string,
                  char *structure,
                  char *ssfile)
```

Produce a secondary structure graph in SStructView format.

```
int svg_rna_plot (char *string,
                  char *structure,
                  char *ssfile)
```

Produce a secondary structure plot in SVG format and write it to a file.

```
int xrna_plot ( char *string,
                char *structure,
                char *ssfile)
```

Produce a secondary structure plot for further editing in XRNA.

```
int rna_plot_type
```

Switch for changing the secondary structure layout algorithm.

Two low-level functions provide direct access to the graph lauyouting algorithms:

```
int simple_xy_coordinates ( short *pair_table,
                            float *X,
                            float *Y)
```

Calculate nucleotide coordinates for secondary structure plot the *Simple way*

```
int naview_xy_coordinates ( short *pair_table,
                            float *X,
                            float *Y)
```

See also

PS_dot.h and naview.h for more detailed descriptions.

4.2 Producing (colored) dot plots for base pair probabilities

```
int PS_color_dot_plot ( char *string,
                        cpair *pi,
                        char *filename)
```

```
int PS_color_dot_plot_turn (char *seq,
                            cpair *pi,
                            char *filename,
                            int winSize)
```

```
int PS_dot_plot_list (char *seq,
                      char *filename,
                      plist *pl,
                      plist *mf,
                      char *comment)
```

Produce a postscript dot-plot from two pair lists.

```
int PS_dot_plot_turn (char *seq,
                      struct plist *pl,
                      char *filename,
                      int winSize)
```

See also

PS_dot.h for more detailed descriptions.

4.3 Producing (colored) alignments

```
int PS_color_aln (
            const char *structure,
            const char *filename,
            const char *seqs[],
            const char *names[])
```

4.4 RNA sequence related utilities

Several functions provide useful applications to RNA sequences

```
char  *random_string (int l,
                      const char symbols[])
```

Create a random string using characters from a specified symbol set.

```
int   hamming ( const char *s1,
                const char *s2)
```

Calculate hamming distance between two sequences.

```
void str_DNA2RNA(char *sequence);
```

Convert a DNA input sequence to RNA alphabet.

```
void str_uppercase(char *sequence);
```

Convert an input sequence to uppercase.

4.5 RNA secondary structure related utilities

`char *pack_structure (const char *struc)`

Pack secondary secondary structure, 5:1 compression using base 3 encoding.

`char *unpack_structure (const char *packed)`

Unpack secondary structure previously packed with pack_structure()

`short *make_pair_table (const char *structure)`

Create a pair table of a secondary structure.

`short *copy_pair_table (const short *pt)`

Get an exact copy of a pair table.

4.6 Miscellaneous Utilities

`void print_tty_input_seq (void)`

Print a line to *stdout* that asks for an input sequence.

`void print_tty_constraint_full (void)`

Print structure constraint characters to stdout (full constraint support)

`void print_tty_constraint (unsigned int option)`

Print structure constraint characters to stdout.

`int *get_iindx (unsigned int length)`

Get an index mapper array (iindx) for accessing the energy matrices, e.g.

`int *get_indx (unsigned int length)`

Get an index mapper array (indx) for accessing the energy matrices, e.g.

```
void constrain_ptypes (
                const char *constraint,
                unsigned int length,
                char *ptype,
                int *BP,
                int min_loop_size,
                unsigned int idx_type)
```

Insert constraining pair types according to constraint structure string.

```
char  *get_line(FILE *fp);
```

Read a line of arbitrary length from a stream.

```
unsigned int read_record(
                char **header,
                char **sequence,
                char ***rest,
                unsigned int options);
```

Get a data record from stdin.

```
char  *time_stamp (void)
```

Get a timestamp.

```
void warn_user (const char message[])
```

Print a warning message.

```
void nrerror (const char message[])
```

Die with an error message.

```
void   init_rand (void)
```

Make random number seeds.

```
unsigned short xsubi[3];
```

Current 48 bit random number.

```
double urn (void)
```

get a random number from [0..1]

```
int    int_urn (int from, int to)
```

Generates a pseudo random integer in a specified range.

```
void  *space (unsigned size)
```

Allocate space safely.

```
void  *xrealloc ( void *p,
                  unsigned size)
```

Reallocate space safely.

See also

utils.h for a complete overview and detailed description of the utility functions

Next Page: Examples

Chapter 5

Example - A Small Example Program

The following program exercises most commonly used functions of the library.

The program folds two sequences using both the mfe and partition function algorithms and calculates the tree edit and profile distance of the resulting structures and base pairing probabilities.

```
#include  <stdio.h>
#include  <math.h>
#include  "utils.h"
#include  "fold_vars.h"
#include  "fold.h"
#include  "part_func.h"
#include  "inverse.h"
#include  "RNAstruct.h"
#include  "treedist.h"
#include  "stringdist.h"
#include  "ProfileDist.h"

void main()
{
   char *seq1="CGCAGGGAUACCCGCG", *seq2="GCGCCCAUAGGGACGC",
        *struct1,* struct2,* xstruc;
   float e1, e2, tree_dist, string_dist, profile_dist, kT;
   Tree *T1, *T2;
   swString *S1, *S2;
   float **pf1, **pf2;
   FLT_OR_DBL *bppm;
   /* fold at 30C instead of the default 37C */
   temperature = 30.;      /* must be set *before* initializing  */

   /* allocate memory for structure and fold */
   struct1 = (char* ) space(sizeof(char)*(strlen(seq1)+1));
   e1 =  fold(seq1, struct1);

   struct2 = (char* ) space(sizeof(char)*(strlen(seq2)+1));
   e2 =  fold(seq2, struct2);

   free_arrays();     /* free arrays used in fold() */

   /* produce tree and string representations for comparison */
   xstruc = expand_Full(struct1);
```

```
    T1 = make_tree(xstruc);
    S1 = Make_swString(xstruc);
    free(xstruc);

    xstruc = expand_Full(struct2);
    T2 = make_tree(xstruc);
    S2 = Make_swString(xstruc);
    free(xstruc);

    /* calculate tree edit distance and aligned structures with gaps */
    edit_backtrack = 1;
    tree_dist = tree_edit_distance(T1, T2);
    free_tree(T1); free_tree(T2);
    unexpand_aligned_F(aligned_line);
    printf("%s\n%s  %3.2f\n", aligned_line[0], aligned_line[1], tree_dist);

    /* same thing using string edit (alignment) distance */
    string_dist = string_edit_distance(S1, S2);
    free(S1); free(S2);
    printf("%s  mfe=%5.2f\n%s  mfe=%5.2f  dist=%3.2f\n",
           aligned_line[0], e1, aligned_line[1], e2, string_dist);

    /* for longer sequences one should also set a scaling factor for
       partition function folding, e.g: */
    kT = (temperature+273.15)*1.98717/1000.;  /* kT in kcal/mol */
    pf_scale = exp(-e1/kT/strlen(seq1));

    /* calculate partition function and base pair probabilities */
    e1 = pf_fold(seq1, struct1);
    /* get the base pair probability matrix for the previous run of pf_fold() */
    bppm = export_bppm();
    pf1 = Make_bp_profile_bppm(bppm, strlen(seq1));

    e2 = pf_fold(seq2, struct2);
    /* get the base pair probability matrix for the previous run of pf_fold() */
    bppm = export_bppm();
    pf2 = Make_bp_profile(strlen(seq2));

    free_pf_arrays();  /* free space allocated for pf_fold() */

    profile_dist = profile_edit_distance(pf1, pf2);
    printf("%s  free energy=%5.2f\n%s  free energy=%5.2f  dist=%3.2f\n",
           aligned_line[0], e1, aligned_line[1], e2, profile_dist);

    free_profile(pf1); free_profile(pf2);
}
```

In a typical Unix environment you would compile this program using:

```
cc ${OPENMP_CFLAGS} -c example.c -I${hpath}
```

and link using

```
cc ${OPENMP_CFLAGS} -o example -L${lpath} -lRNA -lm
```

where *${hpath}* and *${lpath}* point to the location of the header files and library, respectively.

Note

As default, the RNAlib is compiled with build-in *OpenMP* multithreading support.

Thus, when linking your own object files to the library you have to pass the compiler specific *${OPENMP_CFLAGS}* (e.g. '-fopenmp' for **gcc**) even if your code does not use openmp specific code. However, in that case the *OpenMP* flags may be ommited when compiling example.c

Next Page: References

Chapter 6

References

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Chapter 7

Deprecated List

Global base_pair Do not use this variable anymore!

Global centroid(int length, double ∗dist) This function is deprecated and should not be used anymore as it is not threadsafe!

Global energy_of_circ_struct(const char ∗string, const char ∗structure) This function is deprecated and should not be used in future programs Use energy_of_-circ_structure() instead!

Global energy_of_struct(const char ∗string, const char ∗structure) This function is deprecated and should not be used in future programs! Use energy_of_structure() instead!

Global energy_of_struct_pt(const char ∗string, short ∗ptable, short ∗s, short ∗s1) This function is deprecated and should not be used in future programs! Use energy_of_structure_pt() instead!

Global expHairpinEnergy(int u, int type, short si1, short sj1, const char ∗string) Use exp_E_Hairpin() from loop_energies.h instead

Global expLoopEnergy(int u1, int u2, int type, int type2, short si1, short sj1, short sp1, short sq1) Use exp_E_IntLoop() from loop_energies.h instead

Global get_plist(struct plist ∗pl, int length, double cut_off) { This function is deprecated and will be removed soon!} use assign_plist_from_pr() instead!

Global HairpinE(int size, int type, int si1, int sj1, const char *string) {This function is deprecated and will be removed soon.

Global iindx Do not use this variable anymore!

Global init_co_pf_fold(int length) { This function is deprecated and will be removed soon!}

Global init_pf_fold(int length) This function is obsolete and will be removed soon!

Global initialize_cofold(int length) {This function is obsolete and will be removed soon!}

Global initialize_fold(int length) {This function is deprecated and will be removed soon!}

Global LoopEnergy(int n1, int n2, int type, int type_2, int si1, int sj1, int sp1, int sq1) {This function is deprecated and will be removed soon.

Global Make_bp_profile(int length) This function is deprecated and will be removed soon! See Make_bp_profile_bppm() for a replacement

Global mean_bp_dist(int length) This function is not threadsafe and should not be used anymore. Use mean_bp_distance() instead!

Global pr Do not use this variable anymore!

Global PS_dot_plot(char *string, char *file) This function is deprecated and will be removed soon! Use PS_dot_plot_list() instead!

Chapter 8

Data Structure Index

8.1 Data Structures

Here are the data structures with brief descriptions:

Chapter 9

File Index

9.1 File List

Here is a list of all documented files with brief descriptions:

Chapter 10

Data Structure Documentation

10.1 bondT Struct Reference

base pair

10.1.1 Detailed Description

base pair

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.2 bondTEn Struct Reference

base pair with associated energy

10.2.1 Detailed Description

base pair with associated energy

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.3 cofoldF Struct Reference

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.4 ConcEnt Struct Reference

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.5 constrain Struct Reference

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.6 COORDINATE Struct Reference

this is a workarround for the SWIG Perl Wrapper RNA plot function that returns an array of type COORDINATE

10.6.1 Detailed Description

this is a workarround for the SWIG Perl Wrapper RNA plot function that returns an array of type COORDINATE

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.7 cpair Struct Reference

this datastructure is used as input parameter in functions of PS_dot.c

10.7.1 Detailed Description

this datastructure is used as input parameter in functions of PS_dot.c

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.8 duplexT Struct Reference

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.9 dupVar Struct Reference

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.10 folden Struct Reference

The documentation for this struct was generated from the following file:

- H/data_structures.h

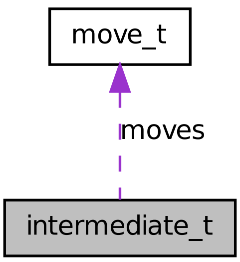
10.11 interact Struct Reference

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.12 intermediate_t Struct Reference

Collaboration diagram for intermediate_t:



The documentation for this struct was generated from the following file:

- H/data_structures.h

10.13 INTERVAL Struct Reference

sequence interval stack element used in subopt.c

10.13.1 Detailed Description

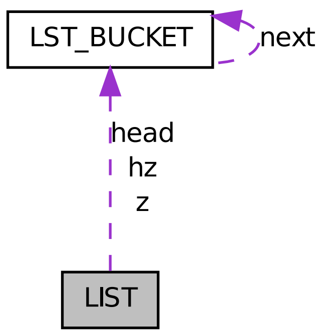
sequence interval stack element used in subopt.c

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.14 LIST Struct Reference

Collaboration diagram for LIST:

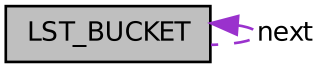


The documentation for this struct was generated from the following file:

- lib/list.h

10.15 LST_BUCKET Struct Reference

Collaboration diagram for LST_BUCKET:



The documentation for this struct was generated from the following file:

- lib/list.h

10.16 model_detailsT Struct Reference

The data structure that contains the complete model details used throughout the calculations.

10.16.1 Detailed Description

The data structure that contains the complete model details used throughout the calculations.

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.17 move_t Struct Reference

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.18 PAIR Struct Reference

base pair data structure used in subopt.c

10.18.1 Detailed Description

base pair data structure used in subopt.c

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.19 pair_info Struct Reference

A base pair info structure.

10.19.1 Detailed Description

A base pair info structure.

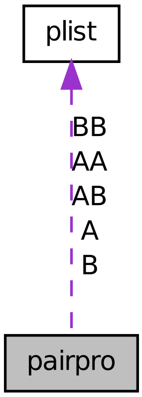
for each base pair (i,j) the structure lists: its probability 'p', an entropy-like measure for its well-definedness 'ent', and in 'bp[]' the frequency of each type of pair. 'bp[0]' contains the number of non-compatible sequences, 'bp[1]' the number of CG pairs, etc.

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.20 pairpro Struct Reference

Collaboration diagram for pairpro:



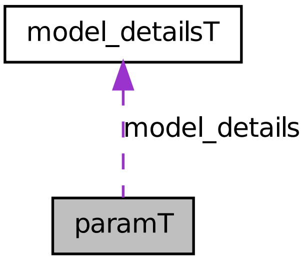
The documentation for this struct was generated from the following file:

- H/data_structures.h

10.21 paramT Struct Reference

The datastructure that contains temperature scaled energy parameters.

Collaboration diagram for paramT:



10.21.1 Detailed Description

The datastructure that contains temperature scaled energy parameters.

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.22 path_t Struct Reference

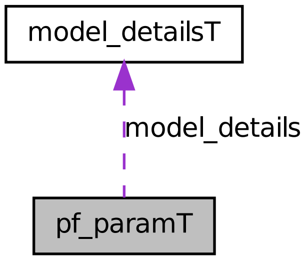
The documentation for this struct was generated from the following file:

- H/data_structures.h

10.23 pf_paramT Struct Reference

The datastructure that contains temperature scaled Boltzmann weights of the energy parameters.

Collaboration diagram for pf_paramT:



10.23.1 Detailed Description

The datastructure that contains temperature scaled Boltzmann weights of the energy parameters.

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.24 plist Struct Reference

this datastructure is used as input parameter in functions of PS_dot.h and others

10.24.1 Detailed Description

this datastructure is used as input parameter in functions of PS_dot.h and others

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.25 Postorder_list Struct Reference

The documentation for this struct was generated from the following file:

- H/dist_vars.h

10.26 pu_contrib Struct Reference

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.27 pu_out Struct Reference

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.28 sect Struct Reference

stack of partial structures for backtracking

10.28.1 Detailed Description

stack of partial structures for backtracking

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.29 snoopT Struct Reference

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.30 SOLUTION Struct Reference

solution element from subopt.c

10.30.1 Detailed Description

solution element from subopt.c

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.31 svm_model Struct Reference

The documentation for this struct was generated from the following file:

- H/svm_utils.h

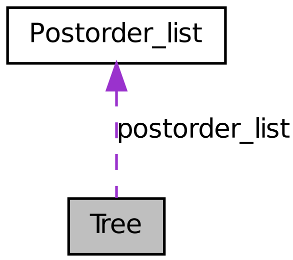
10.32 swString Struct Reference

The documentation for this struct was generated from the following file:

- H/dist_vars.h

10.33 Tree Struct Reference

Collaboration diagram for Tree:



The documentation for this struct was generated from the following file:

- H/dist_vars.h

10.34 TwoDfold_solution Struct Reference

Solution element returned from TwoDfoldList.

10.34.1 Detailed Description

Solution element returned from TwoDfoldList.

This element contains free energy and structure for the appropriate kappa (k), lambda (l) neighborhood The datastructure contains two integer attributes 'k' and 'l' as well as an attribute 'en' of type float representing the free energy in kcal/mol and an attribute 's' of type char* containg the secondary structure representative,

A value of INF in k denotes the end of a list

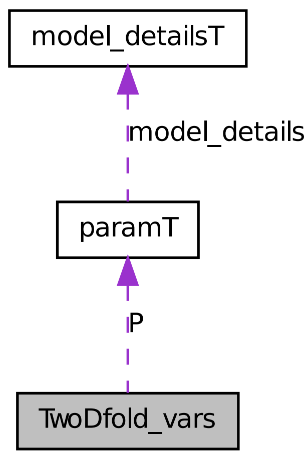
The documentation for this struct was generated from the following file:

- H/data_structures.h

10.35 TwoDfold_vars Struct Reference

Variables compound for 2Dfold MFE folding.

Collaboration diagram for TwoDfold_vars:



10.35.1 Detailed Description

Variables compound for 2Dfold MFE folding.

The documentation for this struct was generated from the following file:

- H/data_structures.h

10.36 TwoDpfold_solution Struct Reference

Solution element returned from TwoDpfoldList.

10.36.1 Detailed Description

Solution element returned from TwoDpfoldList.

This element contains the partition function for the appropriate kappa (k), lambda (l) neighborhood The datastructure contains two integer attributes 'k' and 'l' as well as an attribute 'q' of type #FLT_OR_DBL

A value of INF in k denotes the end of a list

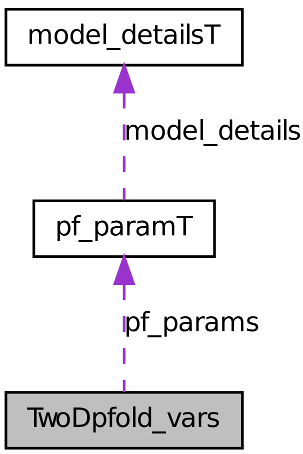
The documentation for this struct was generated from the following file:

- H/data_structures.h

10.37 TwoDpfold_vars Struct Reference

Variables compound for 2Dfold partition function folding.

Collaboration diagram for TwoDpfold_vars:



10.37.1 Detailed Description

Variables compound for 2Dfold partition function folding.

The documentation for this struct was generated from the following file:

- H/data_structures.h

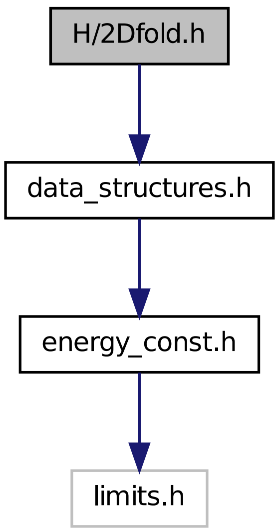
Chapter 11

File Documentation

11.1 H/2Dfold.h File Reference

Compute the minimum free energy (MFE) and secondary structures for a partitioning of the secondary structure space according to the base pair distance to two fixed reference structures basepair distance to two fixed reference structures.

Include dependency graph for 2Dfold.h:



Functions

- TwoDfold_vars ∗ get_TwoDfold_variables (const char ∗seq, const char ∗structure1, const char ∗structure2, int circ)

  Get a structure of type TwoDfold_vars prefilled with current global settings.
- void destroy_TwoDfold_variables (TwoDfold_vars ∗our_variables)

  Destroy a TwoDfold_vars datastructure without memory loss.
- TwoDfold_solution ∗ TwoDfoldList (TwoDfold_vars ∗vars, int distance1, int distance2)

  Compute MFE's and representative for distance partitioning.
- char ∗ TwoDfold_backtrack_f5 (unsigned int j, int k, int l, TwoDfold_vars ∗vars)

  Backtrack a minimum free energy structure from a 5' section of specified length.

11.1.1 Detailed Description

Compute the minimum free energy (MFE) and secondary structures for a partitioning of the secondary structure space according to the base pair distance to two fixed reference structures basepair distance to two fixed reference structures.

11.1.2 Function Documentation

11.1.2.1 TwoDfold_vars∗ get_TwoDfold_variables (const char ∗ *seq,* const char ∗ *structure1,* const char ∗ *structure2,* int *circ*)

Get a structure of type TwoDfold_vars prefilled with current global settings.

This function returns a datastructure of type TwoDfold_vars. The data fields inside the TwoDfold_vars are prefilled by global settings and all memory allocations necessary to start a computation are already done for the convenience of the user

Note

Make sure that the reference structures are compatible with the sequence according to Watson-Crick- and Wobble-base pairing

See also

destroy_TwoDfold_variables(), TwoDfold(), TwoDfold_circ

Parameters

seq	The RNA sequence
structure1	The first reference structure in dot-bracket notation
structure2	The second reference structure in dot-bracket notation
circ	A switch to indicate the assumption to fold a circular instead of linear RNA (0=OFF, 1=ON)

Returns

A datastructure prefilled with folding options and allocated memory

11.1.2.2 void destroy_TwoDfold_variables (**TwoDfold_vars** ∗ *our_variables*)

Destroy a TwoDfold_vars datastructure without memory loss.

This function free's all allocated memory that depends on the datastructure given.

See also

get_TwoDfold_variables()

Parameters

our_-variables	A pointer to the datastructure to be destroyed

11.1.2.3 **TwoDfold_solution**∗ TwoDfoldList (**TwoDfold_vars** ∗ *vars*, int *distance1*, int *distance2*)

Compute MFE's and representative for distance partitioning.

This function computes the minimum free energies and a representative secondary structure for each distance class according to the two references specified in the datastructure 'vars'. The maximum basepair distance to each of both references may be set by the arguments 'distance1' and 'distance2', respectively. If both distance arguments are set to '-1', no restriction is assumed and the calculation is performed for each distance class possible.

The returned list contains an entry for each distance class. If a maximum basepair distance to either of the references was passed, an entry with k=l=-1 will be appended in the list, denoting the class where all structures exceeding the maximum will be thrown into. The end of the list is denoted by an attribute value of INF in the k-attribute of the list entry.

See also

get_TwoDfold_variables(), destroy_TwoDfold_variables(), TwoDfold_solution

Parameters

vars	the datastructure containing all predefined folding attributes
distance1	maximum distance to reference1 (-1 means no restriction)
distance2	maximum distance to reference2 (-1 means no restriction)

11.1.2.4 char* TwoDfold_backtrack_f5 (unsigned int *j*, int *k*, int *l*, TwoDfold_vars * *vars*)

Backtrack a minimum free energy structure from a 5' section of specified length.

This function allows to backtrack a secondary structure beginning at the 5' end, a specified length and residing in a specific distance class. If the argument 'k' gets a value of -1, the structure that is backtracked is assumed to reside in the distance class where all structures exceeding the maximum basepair distance specified in TwoDfoldList() belong to.

Note

The argument 'vars' must contain precalculated energy values in the energy matrices, i.e. a call to TwoDfoldList() preceding this function is mandatory!

See also

TwoDfoldList(), get_TwoDfold_variables(), destroy_TwoDfold_variables()

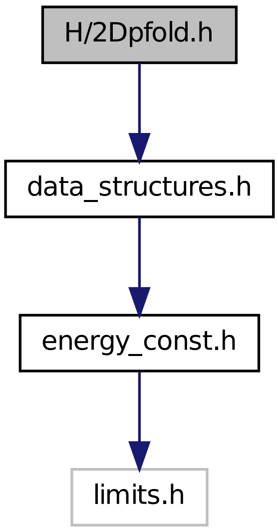
Parameters

j	The length in nucleotides beginning from the 5' end
k	distance to reference1 (may be -1)
l	distance to reference2
vars	the datastructure containing all predefined folding attributes

11.2 H/2Dpfold.h File Reference

Compute the partition function and stochastically sample secondary structures for a partitioning of the secondary structure space according to the base pair distance to two fixed reference structures.

Include dependency graph for 2Dpfold.h:



Functions

- TwoDpfold_vars * get_TwoDpfold_variables (const char *seq, const char *structure1, char *structure2, int circ)

  Get a datastructure containing all necessary attributes and global folding switches.
- TwoDpfold_vars * get_TwoDpfold_variables_from_MFE (TwoDfold_vars *mfe_vars)

  Get the datastructure containing all necessary attributes and global folding switches from a pre-filled mfe-datastructure.
- void destroy_TwoDpfold_variables (TwoDpfold_vars *vars)

  Free all memory occupied by a TwoDpfold_vars datastructure.
- TwoDpfold_solution * TwoDpfoldList (TwoDpfold_vars *vars, int maxDistance1, int maxDistance2)

  Compute the partition function for all distance classes.
- char * TwoDpfold_pbacktrack (TwoDpfold_vars *vars, int d1, int d2)

  Sample secondary structure representatives from a set of distance classes according to their Boltzmann probability.
- char * TwoDpfold_pbacktrack5 (TwoDpfold_vars *vars, int d1, int d2, unsigned int length)

  Sample secondary structure representatives with a specified length from a set of distance classes according to their Boltzmann probability.

11.2.1 Detailed Description

Compute the partition function and stochastically sample secondary structures for a partitioning of the secondary structure space according to the base pair distance to two fixed reference structures.

11.2.2 Function Documentation

11.2.2.1 TwoDpfold_vars* get_TwoDpfold_variables (const char * *seq*, const char * *structure1*, char * *structure2*, int *circ*)

Get a datastructure containing all necessary attributes and global folding switches.

This function prepares all necessary attributes and matrices etc which are needed for a call of TwoDpfoldList. A snapshot of all current global model switches (dangles, temperature and so on) is done and stored in the returned datastructure. Additionally, all matrices that will hold the partition function values are prepared.

Parameters

seq	the RNA sequence in uppercase format with letters from the alphabet {AUCG}
structure1	the first reference structure in dot-bracket notation
structure2	the second reference structure in dot-bracket notation
circ	a switch indicating if the sequence is linear (0) or circular (1)

Returns

the datastructure containing all necessary partition function attributes

11.2.2.2 TwoDpfold_vars* get_TwoDpfold_variables_from_MFE (TwoDfold_vars * *mfe_vars*)

Get the datastructure containing all necessary attributes and global folding switches from a pre-filled mfe-datastructure.

This function actually does the same as get_TwoDpfold_variables but takes its switches and settings from a pre-filled MFE equivalent datastructure

See also

get_TwoDfold_variables(), get_TwoDpfold_variables()

Parameters

mfe_vars	the pre-filled mfe datastructure

Returns

the datastructure containing all necessary partition function attributes

11.2.2.3 void destroy_TwoDpfold_variables (TwoDpfold_vars * *vars*)

Free all memory occupied by a TwoDpfold_vars datastructure.

This function free's all memory occupied by a datastructure obtained from from get_-TwoDpfold_variables() or get_TwoDpfold_variables_from_MFE()

See also

get_TwoDpfold_variables(), get_TwoDpfold_variables_from_MFE()

Parameters

vars	the datastructure to be free'd

11.2.2.4 TwoDpfold_solution* TwoDpfoldList (TwoDpfold_vars * *vars*, int *maxDistance1*, int *maxDistance2*)

Compute the partition function for all distance classes.

This function computes the partition functions for all distance classes according the two reference structures specified in the datastructure 'vars'. Similar to TwoDfoldList() the arguments maxDistance1 and maxDistance2 specify the maximum distance to both reference structures. A value of '-1' in either of them makes the appropriate distance restrictionless, i.e. all basepair distancies to the reference are taken into account during computation. In case there is a restriction, the returned solution contains an entry where the attribute k=l=-1 contains the partition function for all structures exceeding the restriction. A values of INF in the attribute 'k' of the returned list denotes the end of the list

See also

get_TwoDpfold_variables(), destroy_TwoDpfold_variables(), TwoDpfold_solution

Parameters

vars	the datastructure containing all necessary folding attributes and matrices
maxDistance1	the maximum basepair distance to reference1 (may be -1)
maxDistance2	the maximum basepair distance to reference2 (may be -1)

Returns

a list of partition funtions for the appropriate distance classes

11.2.2.5 char* TwoDpfold_pbacktrack (TwoDpfold_vars * *vars*, int *d1*, int *d2*)

Sample secondary structure representatives from a set of distance classes according to their Boltzmann probability.

If the argument 'd1' is set to '-1', the structure will be backtracked in the distance class where all structures exceeding the maximum basepair distance to either of the references reside.

Note

The argument 'vars' must contain precalculated partition function matrices, i.e. a call to TwoDpfoldList() preceding this function is mandatory!

See also

TwoDpfoldList()

Parameters

vars	the datastructure containing all necessary folding attributes and matrices
d1	the distance to reference1 (may be -1)
d2	the distance to reference2

Returns

a sampled secondary structure in dot-bracket notation

11.2.2.6 char* TwoDpfold_pbacktrack5 (TwoDpfold_vars * *vars*, int *d1*, int *d2*, unsigned int *length*)

Sample secondary structure representatives with a specified length from a set of distance classes according to their Boltzmann probability.

This function does essentially the same as TwoDpfold_pbacktrack with the only difference that partial structures, i.e. structures beginning from the 5' end with a specified length of the sequence, are backtracked

Note

The argument 'vars' must contain precalculated partition function matrices, i.e. a call to TwoDpfoldList() preceding this function is mandatory!
This function does not work (since it makes no sense) for circular RNA sequences!

See also

TwoDpfold_pbacktrack(), TwoDpfoldList()

Parameters

vars	the datastructure containing all necessary folding attributes and matrices
d1	the distance to reference1 (may be -1)
d2	the distance to reference2
length	the length of the structure beginning from the 5' end

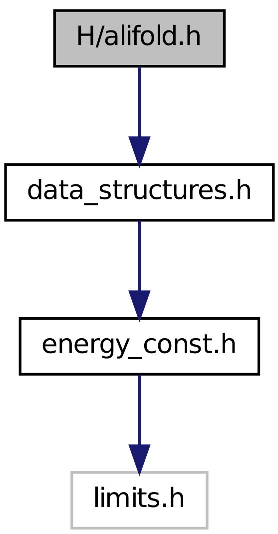
Returns

a sampled secondary structure in dot-bracket notation

11.3 H/alifold.h File Reference

compute various properties (consensus MFE structures, partition function, Boltzmann distributed stochastic samples, ...) for RNA sequence alignments

Include dependency graph for alifold.h:



Functions

- void update_alifold_params (void)

  Update the energy parameters for alifold function.
- float alifold (const char **strings, char *structure)

  Compute MFE and according consensus structure of an alignment of sequences.
- float circalifold (const char **strings, char *structure)

  Compute MFE and according structure of an alignment of sequences assuming the sequences are circular instead of linear.
- void free_alifold_arrays (void)

  Free the memory occupied by MFE alifold functions.

- int get_mpi (char ∗Alseq[ ], int n_seq, int length, int ∗mini)

  Get the mean pairwise identity in steps from ?to?(ident)
- float ∗∗ readribosum (char ∗name)

  Read a ribosum or other user-defined scoring matrix.
- float energy_of_alistruct (const char ∗∗sequences, const char ∗structure, int n_-seq, float ∗energy)

  Calculate the free energy of a consensus structure given a set of aligned sequences.
- void encode_ali_sequence (const char ∗sequence, short ∗S, short ∗s5, short ∗s3, char ∗ss, unsigned short ∗as, int circ)

  Get arrays with encoded sequence of the alignment.
- void alloc_sequence_arrays (const char ∗∗sequences, short ∗∗∗S, short ∗∗∗S5, short ∗∗∗S3, unsigned short ∗∗∗a2s, char ∗∗∗Ss, int circ)

  Allocate memory for sequence array used to deal with aligned sequences.
- void free_sequence_arrays (unsigned int n_seq, short ∗∗∗S, short ∗∗∗S5, short ∗∗∗S3, unsigned short ∗∗∗a2s, char ∗∗∗Ss)

  Free the memory of the sequence arrays used to deal with aligned sequences.
- float alipf_fold_par (const char ∗∗sequences, char ∗structure, plist ∗∗pl, pf_-paramT ∗parameters, int calculate_bppm, int is_constrained, int is_circular)
- float alipf_fold (const char ∗∗sequences, char ∗structure, plist ∗∗pl)

  The partition function version of alifold() works in analogy to pf_fold().
- float alipf_circ_fold (const char ∗∗sequences, char ∗structure, plist ∗∗pl)
- FLT_OR_DBL ∗ export_ali_bppm (void)

  Get a pointer to the base pair probability array.
- char ∗ alipbacktrack (double ∗prob)

  Sample a consensus secondary structure from the Boltzmann ensemble according its probability

  .

Variables

- double cv_fact

  This variable controls the weight of the covariance term in the energy function of alignment folding algorithms.
- double nc_fact

  This variable controls the magnitude of the penalty for non-compatible sequences in the covariance term of alignment folding algorithms.

11.3.1 Detailed Description

compute various properties (consensus MFE structures, partition function, Boltzmann distributed stochastic samples, ...) for RNA sequence alignments

11.3.2 Function Documentation

11.3.2.1 void update_alifold_params (void)

Update the energy parameters for alifold function.

Call this to recalculate the pair matrix and energy parameters after a change in folding parameters like temperature

11.3.2.2 float alifold (const char ** *strings*, char * *structure*)

Compute MFE and according consensus structure of an alignment of sequences.

This function predicts the consensus structure for the aligned 'sequences' and returns the minimum free energy; the mfe structure in bracket notation is returned in 'structure'.

Sufficient space must be allocated for 'structure' before calling alifold().

Parameters

strings	A pointer to a NULL terminated array of character arrays
structure	A pointer to a character array that may contain a constraining consensus structure (will be overwritten by a consensus structure that exhibits the MFE)

Returns

The free energy score in kcal/mol

11.3.2.3 float circalifold (const char ** *strings*, char * *structure*)

Compute MFE and according structure of an alignment of sequences assuming the sequences are circular instead of linear.

Parameters

strings	A pointer to a NULL terminated array of character arrays
structure	A pointer to a character array that may contain a constraining consensus structure (will be overwritten by a consensus structure that exhibits the MFE)

Returns

The free energy score in kcal/mol

11.3.2.4 int get_mpi (char * *Alseq[ ]*, int *n_seq*, int *length*, int * *mini*)

Get the mean pairwise identity in steps from ?to?(ident)

Parameters

Alseq	

n_seq	The number of sequences in the alignment
length	The length of the alignment
mini	

Returns

The mean pairwise identity

11.3.2.5 float energy_of_alistruct (const char ** *sequences,* const char * *structure,* int *n_seq,* float * *energy*)

Calculate the free energy of a consensus structure given a set of aligned sequences.

Parameters

sequences	The NULL terminated array of sequences
structure	The consensus structure
n_seq	The number of sequences in the alignment
energy	A pointer to an array of at least two floats that will hold the free energies (energy[0] will contain the free energy, energy[1] will be filled with the covariance energy term)

Returns

free energy in kcal/mol

11.3.2.6 void encode_ali_sequence (const char * *sequence,* short * *S,* short * *s5,* short * *s3,* char * *ss,* unsigned short * *as,* int *circ*)

Get arrays with encoded sequence of the alignment.

this function assumes that in S, S5, s3, ss and as enough space is already allocated (size must be at least sequence length+2)

Parameters

sequence	The gapped sequence from the alignment
S	pointer to an array that holds encoded sequence
s5	pointer to an array that holds the next base 5' of alignment position i
s3	pointer to an array that holds the next base 3' of alignment position i
ss	
as	
circ	assume the molecules to be circular instead of linear (circ=0)

11.3.2.7 void alloc_sequence_arrays (const char ** *sequences*, short *** *S*, short *** *S5*, short *** *S3*, unsigned short *** *a2s*, char *** *Ss*, int *circ*)

Allocate memory for sequence array used to deal with aligned sequences.

Note that these arrays will also be initialized according to the sequence alignment given

See also

free_sequence_arrays()

Parameters

sequences	The aligned sequences
S	A pointer to the array of encoded sequences
S5	A pointer to the array that contains the next 5' nucleotide of a sequence position
S3	A pointer to the array that contains the next 3' nucleotide of a sequence position
a2s	A pointer to the array that contains the alignment to sequence position mapping
Ss	A pointer to the array that contains the ungapped sequence
circ	assume the molecules to be circular instead of linear (circ=0)

11.3.2.8 void free_sequence_arrays (unsigned int *n_seq*, short *** *S*, short *** *S5*, short *** *S3*, unsigned short *** *a2s*, char *** *Ss*)

Free the memory of the sequence arrays used to deal with aligned sequences.

This function frees the memory previously allocated with alloc_sequence_arrays()

See also

alloc_sequence_arrays()

Parameters

n_seq	The number of aligned sequences
S	A pointer to the array of encoded sequences
S5	A pointer to the array that contains the next 5' nucleotide of a sequence position
S3	A pointer to the array that contains the next 3' nucleotide of a sequence position
a2s	A pointer to the array that contains the alignment to sequence position mapping
Ss	A pointer to the array that contains the ungapped sequence

11.3.2.9 float alipf_fold_par (const char ** *sequences*, char * *structure*, plist ** *pl*, pf_paramT * *parameters*, int *calculate_bppm*, int *is_constrained*, int *is_circular*)

Parameters

sequences	
structure	
pl	
parameters	
calculate_-bppm	
is_-constrained	
is_circular	

Returns

11.3.2.10 float alipf_fold (const char ** *sequences*, char * *structure*, plist ** *pl*)

The partition function version of alifold() works in analogy to pf_fold().

Pair probabilities and information about sequence covariations are returned via the 'pi' variable as a list of pair_info structs. The list is terminated by the first entry with pi.i = 0.

Parameters

sequences	
structure	
pl	

Returns

11.3.2.11 float alipf_circ_fold (const char ** *sequences*, char * *structure*, plist ** *pl*)

Parameters

sequences	
structure	
pl	

Returns

11.3.2.12 FLT_OR_DBL* export_ali_bppm (void)

Get a pointer to the base pair probability array.

Accessing the base pair probabilities for a pair (i,j) is achieved by

```
FLT_OR_DBL *pr = export_bppm(); pr_ij = pr[iindx[i]-j];
```

See also

get_iindx()

Returns

A pointer to the base pair probability array

11.3.2.13 char* alipbacktrack (double * *prob*)

Sample a consensus secondary structure from the Boltzmann ensemble according its probability

.

Parameters

prob	to be described (berni)

Returns

A sampled consensus secondary structure in dot-bracket notation

11.3.3 Variable Documentation

11.3.3.1 double cv_fact

This variable controls the weight of the covariance term in the energy function of alignment folding algorithms.

Default is 1.

11.3.3.2 double nc_fact

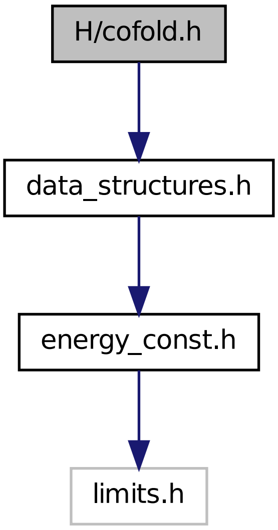
This variable controls the magnitude of the penalty for non-compatible sequences in the covariance term of alignment folding algorithms.

Default is 1.

11.4 H/cofold.h File Reference

MFE version of cofolding routines.

Include dependency graph for cofold.h:



Functions

- float cofold (const char ∗sequence, char ∗structure)

    Compute the minimum free energy of two interacting RNA molecules.
- void free_co_arrays (void)

    Free memory occupied by cofold()
- void update_cofold_params (void)

    Recalculate parameters.
- SOLUTION ∗ zukersubopt (const char ∗string)

    Compute Zuker type suboptimal structures.
- void get_monomere_mfes (float ∗e1, float ∗e2)

    get_monomer_free_energies
- void export_cofold_arrays (int ∗∗f5_p, int ∗∗c_p, int ∗∗fML_p, int ∗∗fM1_p, int ∗∗fc_p, int ∗∗indx_p, char ∗∗ptype_p)

    Export the arrays of partition function cofold.
- void initialize_cofold (int length)

    allocate arrays for folding

11.4.1 Detailed Description

MFE version of cofolding routines. This file includes (almost) all function declarations within the **RNAlib** that are related to MFE Cofolding... This also includes the Zuker suboptimals calculations, since they are implemented using the cofold routines.

11.4.2 Function Documentation

11.4.2.1 float cofold (const char * *sequence*, char * *structure*)

Compute the minimum free energy of two interacting RNA molecules.

The code is analog to the fold() function. If cut_point ==-1 results should be the same as with fold().

Parameters

sequence	The two sequences concatenated
structure	Will hold the barcket dot structure of the dimer molecule

Returns

minimum free energy of the structure

11.4.2.2 SOLUTION* zukersubopt (const char * *string*)

Compute Zuker type suboptimal structures.

Compute Suboptimal structures according to M. Zuker, i.e. for every possible base pair the minimum energy structure containing the resp. base pair. Returns a list of these structures and their energies.

Parameters

string	RNA sequence

Returns

List of zuker suboptimal structures

11.4.2.3 void get_monomere_mfes (float * *e1*, float * *e2*)

get_monomer_free_energies

Export monomer free energies out of cofold arrays

Parameters

e1	A pointer to a variable where the energy of molecule A will be written to
e2	A pointer to a variable where the energy of molecule B will be written to

11.4.2.4 void export_cofold_arrays (int ∗∗ *f5_p,* int ∗∗ *c_p,* int ∗∗ *fML_p,* int ∗∗ *fM1_p,* int ∗∗ *fc_p,* int ∗∗ *indx_p,* char ∗∗ *ptype_p*)

Export the arrays of partition function cofold.

Export the cofold arrays for use e.g. in the concentration Computations or suboptimal secondary structure backtracking

Parameters

f5_p	A pointer to the 'f5' array, i.e. array conatining best free energy in interval [1,j]
c_p	A pointer to the 'c' array, i.e. array containing best free energy in interval [i,j] given that i pairs with j
fML_p	A pointer to the 'M' array, i.e. array containing best free energy in interval [i,j] for any multiloop segment with at least one stem
fM1_p	A pointer to the 'M1' array, i.e. array containing best free energy in interval [i,j] for multiloop segment with exactly one stem
fc_p	A pointer to the 'fc' array, i.e. array ...
indx_p	A pointer to the indexing array used for accessing the energy matrices
ptype_p	A pointer to the ptype array containing the base pair types for each possibility (i,j)

11.4.2.5 void initialize_cofold (int *length*)

allocate arrays for folding

Deprecated

{This function is obsolete and will be removed soon!}

11.5 H/convert_epars.h File Reference

Functions and definitions for energy parameter file format conversion.

Defines

- #define VRNA_CONVERT_OUTPUT_ALL 1U

  Flag to indicate printing of a complete parameter set.
- #define VRNA_CONVERT_OUTPUT_HP 2U

  Flag to indicate printing of hairpin contributions.
- #define VRNA_CONVERT_OUTPUT_STACK 4U

  Flag to indicate printing of base pair stack contributions.
- #define VRNA_CONVERT_OUTPUT_MM_HP 8U

  Flag to indicate printing of hairpin mismatch contribution.

- #define VRNA_CONVERT_OUTPUT_MM_INT 16U

    Flag to indicate printing of interior loop mismatch contribution.
- #define VRNA_CONVERT_OUTPUT_MM_INT_1N 32U

    Flag to indicate printing of 1:n interior loop mismatch contribution.
- #define VRNA_CONVERT_OUTPUT_MM_INT_23 64U

    Flag to indicate printing of 2:3 interior loop mismatch contribution.
- #define VRNA_CONVERT_OUTPUT_MM_MULTI 128U

    Flag to indicate printing of multi loop mismatch contribution.
- #define VRNA_CONVERT_OUTPUT_MM_EXT 256U

    Flag to indicate printing of exterior loop mismatch contribution.
- #define VRNA_CONVERT_OUTPUT_DANGLE5 512U

    Flag to indicate printing of 5' dangle conctribution.
- #define VRNA_CONVERT_OUTPUT_DANGLE3 1024U

    Flag to indicate printing of 3' dangle contribution.
- #define VRNA_CONVERT_OUTPUT_INT_11 2048U

    Flag to indicate printing of 1:1 interior loop contribution.
- #define VRNA_CONVERT_OUTPUT_INT_21 4096U

    Flag to indicate printing of 2:1 interior loop contribution.
- #define VRNA_CONVERT_OUTPUT_INT_22 8192U

    Flag to indicate printing of 2:2 interior loop contribution.
- #define VRNA_CONVERT_OUTPUT_BULGE 16384U

    Flag to indicate printing of bulge loop contribution.
- #define VRNA_CONVERT_OUTPUT_INT 32768U

    Flag to indicate printing of interior loop contribution.
- #define VRNA_CONVERT_OUTPUT_ML 65536U

    Flag to indicate printing of multi loop contribution.
- #define VRNA_CONVERT_OUTPUT_MISC 131072U

    Flag to indicate printing of misc contributions (such as terminalAU)
- #define VRNA_CONVERT_OUTPUT_SPECIAL_HP 262144U

    Flag to indicate printing of special hairpin contributions (tri-, tetra-, hexa-loops)
- #define VRNA_CONVERT_OUTPUT_VANILLA 524288U

    Flag to indicate printing of given parameters only

    Note

    This option overrides all other output options, except VRNA_CONVERT_OUTPUT_-DUMP !
- #define VRNA_CONVERT_OUTPUT_NINIO 1048576U

    Flag to indicate printing of interior loop asymmetry contribution.
- #define VRNA_CONVERT_OUTPUT_DUMP 2097152U

    Flag to indicate dumping the energy contributions from the library instead of an input file.

Functions

- void convert_parameter_file (const char *iname, const char *oname, unsigned int options)

    Convert/dump a Vienna 1.8.4 formatted energy parameter file.

11.5.1 Detailed Description

Functions and definitions for energy parameter file format conversion.

11.5.2 Function Documentation

11.5.2.1 void convert_parameter_file (const char * *iname*, const char * *oname*, unsigned int *options*)

Convert/dump a Vienna 1.8.4 formatted energy parameter file.

The options argument allows to control the different output modes.

Currently available options are:

VRNA_CONVERT_OUTPUT_ALL, VRNA_CONVERT_OUTPUT_HP, VRNA_CONVERT_-OUTPUT_STACK

VRNA_CONVERT_OUTPUT_MM_HP, VRNA_CONVERT_OUTPUT_MM_INT, VRNA_-CONVERT_OUTPUT_MM_INT_1N

VRNA_CONVERT_OUTPUT_MM_INT_23, VRNA_CONVERT_OUTPUT_MM_MULTI, VRNA_CONVERT_OUTPUT_MM_EXT

VRNA_CONVERT_OUTPUT_DANGLE5, VRNA_CONVERT_OUTPUT_DANGLE3, VRNA_-CONVERT_OUTPUT_INT_11

VRNA_CONVERT_OUTPUT_INT_21, VRNA_CONVERT_OUTPUT_INT_22, VRNA_-CONVERT_OUTPUT_BULGE

VRNA_CONVERT_OUTPUT_INT, VRNA_CONVERT_OUTPUT_ML, VRNA_CONVERT_-OUTPUT_MISC

VRNA_CONVERT_OUTPUT_SPECIAL_HP, VRNA_CONVERT_OUTPUT_VANILLA, VRNA_-CONVERT_OUTPUT_NINIO

VRNA_CONVERT_OUTPUT_DUMP

The defined options are fine for bitwise compare- and assignment-operations, e. g.: pass a collection of options as a single value like this:

```
convert_parameter_file(ifile, ofile, option_1 | option_2 | option_n)
```

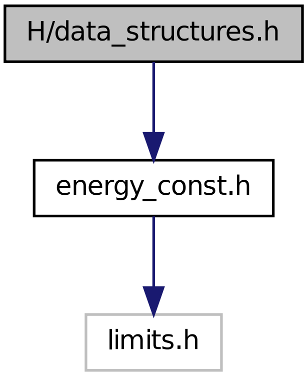
Parameters

iname	The input file name (If NULL input is read from stdin)
oname	The output file name (If NULL output is written to stdout)
options	The options (as described above)

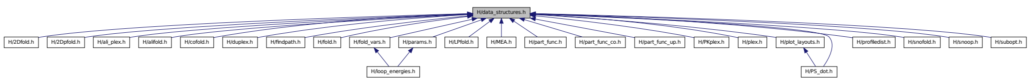
11.6 H/data_structures.h File Reference

All datastructures and typedefs shared among the Vienna RNA Package can be found here.

Include dependency graph for data_structures.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct plist

  this datastructure is used as input parameter in functions of PS_dot.h and others
- struct cpair

  this datastructure is used as input parameter in functions of PS_dot.c
- struct COORDINATE

  this is a workarround for the SWIG Perl Wrapper RNA plot function that returns an array of type COORDINATE
- struct sect

  stack of partial structures for backtracking
- struct bondT

base pair

- struct bondTEn

  base pair with associated energy
- struct model_detailsT

  The data structure that contains the complete model details used throughout the calculations.
- struct paramT

  The datastructure that contains temperature scaled energy parameters.
- struct pf_paramT

  The datastructure that contains temperature scaled Boltzmann weights of the energy parameters.
- struct PAIR

  base pair data structure used in subopt.c
- struct INTERVAL

  sequence interval stack element used in subopt.c
- struct SOLUTION

  solution element from subopt.c
- struct cofoldF
- struct ConcEnt
- struct pairpro
- struct pair_info

  A base pair info structure.
- struct move_t
- struct intermediate_t
- struct path_t
- struct pu_contrib
- struct interact
- struct pu_out
- struct constrain
- struct duplexT
- struct folden
- struct snoopT
- struct dupVar
- struct TwoDfold_solution

  Solution element returned from TwoDfoldList.
- struct TwoDfold_vars

  Variables compound for 2Dfold MFE folding.
- struct TwoDpfold_solution

  Solution element returned from TwoDpfoldList.
- struct TwoDpfold_vars

  Variables compound for 2Dfold partition function folding.

Defines

- #define MAXALPHA 20

  Maximal length of alphabet.
- #define MAXDOS 1000

  Maximum density of states discretization for subopt.

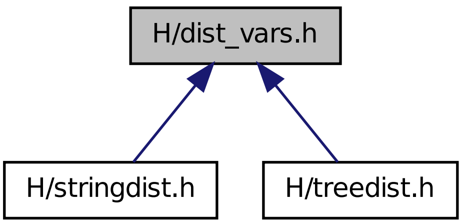
11.6.1 Detailed Description

All datastructures and typedefs shared among the Vienna RNA Package can be found here.

11.7 H/dist_vars.h File Reference

Global variables for Distance-Package.

This graph shows which files directly or indirectly include this file:



Data Structures

- struct Postorder_list
- struct Tree
- struct swString

Variables

- int edit_backtrack

  Produce an alignment of the two structures being compared by tracing the editing path giving the minimum distance.
- char $*$ aligned_line [4]

Contains the two aligned structures after a call to one of the distance functions with edit_backtrack set to 1.

- int cost_matrix

Specify the cost matrix to be used for distance calculations.

11.7.1 Detailed Description

Global variables for Distance-Package.

11.7.2 Variable Documentation

11.7.2.1 int edit_backtrack

Produce an alignment of the two structures being compared by tracing the editing path giving the minimum distance.

set to 1 if you want backtracking

11.7.2.2 int cost_matrix

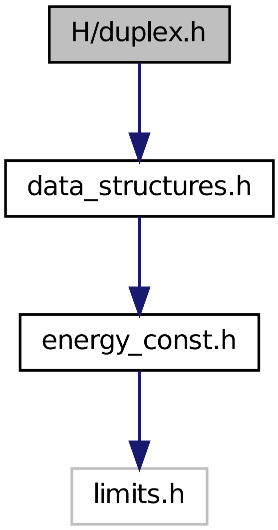
Specify the cost matrix to be used for distance calculations.

if 0, use the default cost matrix (upper matrix in example), otherwise use Shapiro's costs (lower matrix).

11.8 H/duplex.h File Reference

Duplex folding function declarations...

Include dependency graph for duplex.h:



11.8.1 Detailed Description

Duplex folding function declarations...

11.9 H/edit_cost.h File Reference

global variables for Edit Costs included by treedist.c and stringdist.c

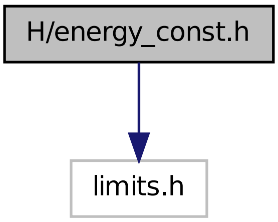
11.9.1 Detailed Description

global variables for Edit Costs included by treedist.c and stringdist.c

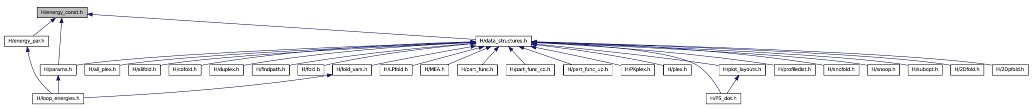
11.10 H/energy_const.h File Reference

energy constants

Include dependency graph for energy_const.h:



This graph shows which files directly or indirectly include this file:



Defines

- #define GASCONST 1.98717

  The gas constant.
- #define K0 273.15

  0 deg Celsius in Kelvin
- #define INF (INT_MAX/10)

  Infinity as used in minimization routines.
- #define FORBIDDEN 9999

  forbidden
- #define BONUS 10000

  bonus contribution
- #define NBPAIRS 7

  The number of distinguishable base pairs.
- #define TURN 3

  The minimum loop length.
- #define MAXLOOP 30

  The maximum loop length.

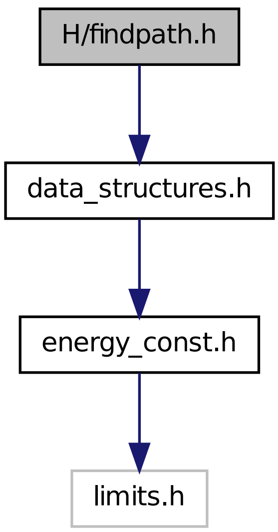
11.10.1 Detailed Description

energy constants

11.11 H/findpath.h File Reference

Compute direct refolding paths between two secondary structures.

Include dependency graph for findpath.h:



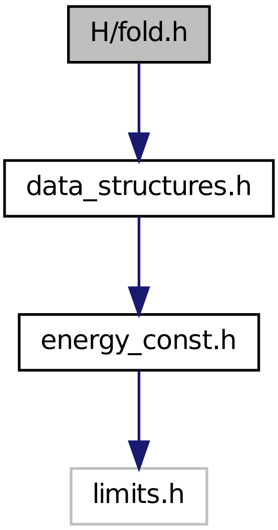
11.11.1 Detailed Description

Compute direct refolding paths between two secondary structures.

11.12 H/fold.h File Reference

MFE calculations and energy evaluations for single RNA sequences.

Include dependency graph for fold.h:



Functions

- float fold_par (const char ∗sequence, char ∗structure, paramT ∗parameters, int is_constrained, int is_circular)

  Compute minimum free energy and an appropriate secondary structure of an RNA sequence.
- float fold (const char ∗sequence, char ∗structure)

  Compute minimum free energy and an appropriate secondary structure of an RNA sequence.
- float circfold (const char ∗sequence, char ∗structure)

  Compute minimum free energy and an appropriate secondary structure of a circular RNA sequence.
- float energy_of_structure (const char ∗string, const char ∗structure, int verbosity_- level)

  Calculate the free energy of an already folded RNA using global model detail settings.
- float energy_of_struct_par (const char ∗string, const char ∗structure, paramT ∗parameters, int verbosity_level)

  Calculate the free energy of an already folded RNA.
- float energy_of_circ_structure (const char ∗string, const char ∗structure, int verbosity_- level)

Calculate the free energy of an already folded circular RNA.

- float energy_of_circ_struct_par (const char ∗string, const char ∗structure, paramT ∗parameters, int verbosity_level)

  Calculate the free energy of an already folded circular RNA.
- int energy_of_structure_pt (const char ∗string, short ∗ptable, short ∗s, short ∗s1, int verbosity_level)

  Calculate the free energy of an already folded RNA.
- int energy_of_struct_pt_par (const char ∗string, short ∗ptable, short ∗s, short ∗s1, paramT ∗parameters, int verbosity_level)

  Calculate the free energy of an already folded RNA.
- void free_arrays (void)

  Free arrays for mfe folding.
- void parenthesis_structure (char ∗structure, bondT ∗bp, int length)

  Create a dot-backet/parenthesis structure from backtracking stack.
- void parenthesis_zuker (char ∗structure, bondT ∗bp, int length)

  Create a dot-backet/parenthesis structure from backtracking stack obtained by zuker suboptimal calculation in cofold.c.
- void update_fold_params (void)

  Recalculate energy parameters.
- void assign_plist_from_db (plist ∗∗pl, const char ∗struc, float pr)

  Create a plist from a dot-bracket string.
- int LoopEnergy (int n1, int n2, int type, int type_2, int si1, int sj1, int sp1, int sq1)
- int HairpinE (int size, int type, int si1, int sj1, const char ∗string)
- void initialize_fold (int length)

  Allocate arrays for folding

  .
- float energy_of_struct (const char ∗string, const char ∗structure)

  Calculate the free energy of an already folded RNA.
- int energy_of_struct_pt (const char ∗string, short ∗ptable, short ∗s, short ∗s1)

  Calculate the free energy of an already folded RNA.
- float energy_of_circ_struct (const char ∗string, const char ∗structure)

  Calculate the free energy of an already folded circular RNA.

Variables

- int logML

  if nonzero use logarithmic ML energy in energy_of_struct
- int uniq_ML

  do ML decomposition uniquely (for subopt)
- int cut_point

  brief set to first pos of second seq for cofolding
- int eos_debug

  brief verbose info from energy_of_struct

11.12.1 Detailed Description

MFE calculations and energy evaluations for single RNA sequences. This file includes (almost) all function declarations within the RNAlib that are related to MFE folding...

11.12.2 Function Documentation

11.12.2.1 float fold_par (const char ∗ *sequence,* char ∗ *structure,* paramT ∗ *parameters,* int *is_constrained,* int *is_circular*)

Compute minimum free energy and an appropriate secondary structure of an RNA sequence.

The first parameter given, the RNA sequence, must be *uppercase* and should only contain an alphabet Σ that is understood by the RNAlib

(e.g. $\Sigma = \{A,U,C,G\}$)

The second parameter, *structure*, must always point to an allocated block of memory with a size of at least $\mathrm{strlen}(\mathrm{sequence})+1$

If the third parameter is NULL, global model detail settings are assumed for the folding recursions. Otherwise, the provided parameters are used.

The fourth parameter indicates whether a secondary structure constraint in enhanced dot-bracket notation is passed through the structure parameter or not. If so, the characters " | x < > " are recognized to mark bases that are paired, unpaired, paired upstream, or downstream, respectively. Matching brackets " ( ) " denote base pairs, dots "." are used for unconstrained bases.

To indicate that the RNA sequence is circular and thus has to be post-processed, set the last parameter to non-zero

After a successful call of fold_par(), a backtracked secondary structure (in dot-bracket notation) that exhibits the minimum of free energy will be written to the memory *structure* is pointing to. The function returns the minimum of free energy for any fold of the sequence given.

Note

OpenMP: Passing NULL to the 'parameters' argument involves access to several global model detail variables and thus is not to be considered threadsafe

See also

fold(), circfold(), model_detailsT, set_energy_model(), get_scaled_parameters()

Parameters

sequence	RNA sequence
structure	A pointer to the character array where the secondary structure in dot-bracket notation will be written to
parameters	A data structure containing the prescaled energy contributions and the model details. (NULL may be passed, see OpenMP notes above)

is_-constrained	Switch to indicate that a structure contraint is passed via the structure argument (0==off)
is_circular	Switch to (de-)activate postprocessing steps in case RNA sequence is circular (0==off)

Returns

the minimum free energy (MFE) in kcal/mol

11.12.2.2 float fold (const char * *sequence*, char * *structure*)

Compute minimum free energy and an appropriate secondary structure of an RNA sequence.

This function essentially does the same thing as fold_par(). However, it takes its model details, i.e. temperature, dangles, tetra_loop, noGU, no_closingGU, fold_constrained, noLonelyPairs from the current global settings within the library

Use fold_par() for a completely threadsafe variant

See also

fold_par(), circfold()

Parameters

sequence	RNA sequence
structure	A pointer to the character array where the secondary structure in dot-bracket notation will be written to

Returns

the minimum free energy (MFE) in kcal/mol

11.12.2.3 float circfold (const char * *sequence*, char * *structure*)

Compute minimum free energy and an appropriate secondary structure of a circular RNA sequence.

This function essentially does the same thing as fold_par(). However, it takes its model details, i.e. temperature, dangles, tetra_loop, noGU, no_closingGU, fold_constrained, noLonelyPairs from the current global settings within the library

Use fold_par() for a completely threadsafe variant

See also

fold_par(), circfold()

Parameters

sequence	RNA sequence
structure	A pointer to the character array where the secondary structure in dot-bracket notation will be written to

Returns

the minimum free energy (MFE) in kcal/mol

11.12.2.4 float energy_of_structure (const char * *string,* const char * *structure,* int *verbosity_level*)

Calculate the free energy of an already folded RNA using global model detail settings.

If verbosity level is set to a value >0, energies of structure elements are printed to stdout

Note

OpenMP: This function relies on several global model settings variables and thus is not to be considered threadsafe. See energy_of_struct_par() for a completely threadsafe implementation.

See also

energy_of_struct_par(), energy_of_circ_structure()

Parameters

string	RNA sequence
structure	secondary structure in dot-bracket notation
verbosity_-level	a flag to turn verbose output on/off

Returns

the free energy of the input structure given the input sequence in kcal/mol

11.12.2.5 float energy_of_struct_par (const char * *string,* const char * *structure,* paramT * *parameters,* int *verbosity_level*)

Calculate the free energy of an already folded RNA.

If verbosity level is set to a value >0, energies of structure elements are printed to stdout

See also

energy_of_circ_structure(), energy_of_structure_pt(), get_scaled_parameters()

Parameters

string	RNA sequence in uppercase letters

structure	Secondary structure in dot-bracket notation
parameters	A data structure containing the prescaled energy contributions and the model details.
verbosity_-level	A flag to turn verbose output on/off

Returns

The free energy of the input structure given the input sequence in kcal/mol

11.12.2.6 float energy_of_circ_structure (const char * *string*, const char * *structure*, int *verbosity_level*)

Calculate the free energy of an already folded circular RNA.

Note

OpenMP: This function relies on several global model settings variables and thus is not to be considered threadsafe. See energy_of_circ_struct_par() for a completely threadsafe implementation.

If verbosity level is set to a value >0, energies of structure elements are printed to stdout

See also

energy_of_circ_struct_par(), energy_of_struct_par()

Parameters

string	RNA sequence
structure	Secondary structure in dot-bracket notation
verbosity_-level	A flag to turn verbose output on/off

Returns

The free energy of the input structure given the input sequence in kcal/mol

11.12.2.7 float energy_of_circ_struct_par (const char * *string*, const char * *structure*, paramT * *parameters*, int *verbosity_level*)

Calculate the free energy of an already folded circular RNA.

If verbosity level is set to a value >0, energies of structure elements are printed to stdout

See also

energy_of_struct_par(), get_scaled_parameters()

Parameters

string	RNA sequence
structure	Secondary structure in dot-bracket notation
parameters	A data structure containing the prescaled energy contributions and the model details.
verbosity_-level	A flag to turn verbose output on/off

Returns

The free energy of the input structure given the input sequence in kcal/mol

11.12.2.8 int energy_of_structure_pt (const char * *string*, short * *ptable*, short * *s*, short * *s1*, int *verbosity_level*)

Calculate the free energy of an already folded RNA.

If verbosity level is set to a value >0, energies of structure elements are printed to stdout

Note

OpenMP: This function relies on several global model settings variables and thus is not to be considered threadsafe. See energy_of_struct_pt_par() for a completely threadsafe implementation.

See also

make_pair_table(), energy_of_struct_pt_par()

Parameters

string	RNA sequence
ptable	the pair table of the secondary structure
s	encoded RNA sequence
s1	encoded RNA sequence
verbosity_-level	a flag to turn verbose output on/off

Returns

the free energy of the input structure given the input sequence in 10kcal/mol

11.12.2.9 int energy_of_struct_pt_par (const char * *string*, short * *ptable*, short * *s*, short * *s1*, paramT * *parameters*, int *verbosity_level*)

Calculate the free energy of an already folded RNA.

If verbosity level is set to a value >0, energies of structure elements are printed to stdout

See also

make_pair_table(), energy_of_struct_par(), get_scaled_parameters()

Parameters

string	RNA sequence in uppercase letters
ptable	The pair table of the secondary structure
s	Encoded RNA sequence
s1	Encoded RNA sequence
parameters	A data structure containing the prescaled energy contributions and the model details.
verbosity_-level	A flag to turn verbose output on/off

Returns

The free energy of the input structure given the input sequence in 10kcal/mol

11.12.2.10 void parenthesis_structure (char * *structure*, bondT * *bp*, int *length*)

Create a dot-backet/parenthesis structure from backtracking stack.

Note

This function is threadsafe

11.12.2.11 void parenthesis_zuker (char * *structure*, bondT * *bp*, int *length*)

Create a dot-backet/parenthesis structure from backtracking stack obtained by zuker suboptimal calculation in cofold.c.

Note

This function is threadsafe

11.12.2.12 void assign_plist_from_db (plist ** *pl*, const char * *struc*, float *pr*)

Create a plist from a dot-bracket string.

The dot-bracket string is parsed and for each base pair an entry in the plist is created. The probability of each pair in the list is set by a function parameter.

The end of the plist is marked by sequence positions i as well as j equal to 0. This condition should be used to stop looping over its entries

This function is threadsafe

Parameters

pl	A pointer to the plist that is to be created
struc	The secondary structure in dot-bracket notation
pr	The probability for each base pair

11.12.2.13 int LoopEnergy (int *n1*, int *n2*, int *type*, int *type_2*, int *si1*, int *sj1*, int *sp1*, int *sq1*)

Deprecated

{This function is deprecated and will be removed soon.

Use E_IntLoop() instead!}

11.12.2.14 int HairpinE (int *size*, int *type*, int *si1*, int *sj1*, const char * *string*)

Deprecated

{This function is deprecated and will be removed soon.

Use E_Hairpin() instead!}

11.12.2.15 void initialize_fold (int *length*)

Allocate arrays for folding

.

Deprecated

{This function is deprecated and will be removed soon!}

11.12.2.16 float energy_of_struct (const char * *string*, const char * *structure*)

Calculate the free energy of an already folded RNA.

Note

This function is not entirely threadsafe! Depending on the state of the global variable eos_debug it prints energy information to stdout or not...

Deprecated

This function is deprecated and should not be used in future programs! Use energy_of_structure() instead!

See also

energy_of_structure, energy_of_circ_struct(), energy_of_struct_pt()

Parameters

string	RNA sequence
structure	secondary structure in dot-bracket notation

Returns

the free energy of the input structure given the input sequence in kcal/mol

11.12.2.17 int energy_of_struct_pt (const char * *string*, short * *ptable*, short * *s*, short * *s1*)

Calculate the free energy of an already folded RNA.

Note

This function is not entirely threadsafe! Depending on the state of the global variable eos_debug it prints energy information to stdout or not...

Deprecated

This function is deprecated and should not be used in future programs! Use energy_of_structure_pt() instead!

See also

make_pair_table(), energy_of_structure()

Parameters

string	RNA sequence
ptable	the pair table of the secondary structure
s	encoded RNA sequence
s1	encoded RNA sequence

Returns

the free energy of the input structure given the input sequence in 10kcal/mol

11.12.2.18 float energy_of_circ_struct (const char * *string*, const char * *structure*)

Calculate the free energy of an already folded circular RNA.

Note

This function is not entirely threadsafe! Depending on the state of the global variable eos_debug it prints energy information to stdout or not...

Deprecated

This function is deprecated and should not be used in future programs Use energy_of_circ_structure() instead!

See also

energy_of_circ_structure(), energy_of_struct(), energy_of_struct_pt()

Parameters

string	RNA sequence
structure	secondary structure in dot-bracket notation

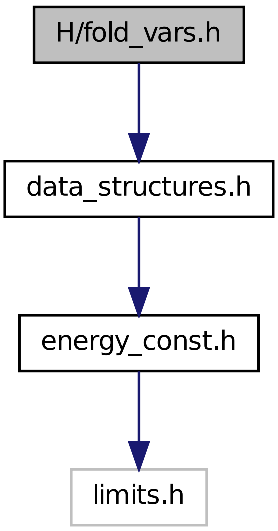
Returns

the free energy of the input structure given the input sequence in kcal/mol

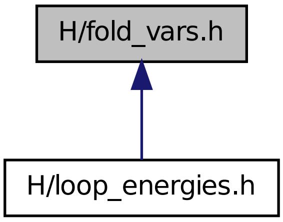
11.13 H/fold_vars.h File Reference

Here all all declarations of the global variables used throughout RNAlib.

Include dependency graph for fold_vars.h:



This graph shows which files directly or indirectly include this file:



Functions

- void set_model_details (model_detailsT *md)

    Set default model details.

Variables

- int fold_constrained

    Global switch to activate/deactivate folding with structure constraints.
- int noLonelyPairs

    Global switch to avoid/allow helices of length 1.
- int dangles

    Switch the energy model for dangling end contributions (0, 1, 2, 3)
- int noGU

    Global switch to forbid/allow GU base pairs at all.
- int no_closingGU

    GU allowed only inside stacks if set to 1.
- int tetra_loop

    Include special stabilizing energies for some tri-, tetra- and hexa-loops;.
- int energy_set

    0 = BP; 1=any mit GC; 2=any mit AU-parameter
- int circ

    backward compatibility variable.
- int csv

    generate comma seperated output
- int oldAliEn

    use old alifold energies (with gaps)

- int ribo

  use ribosum matrices
- char * RibosumFile

  warning this variable will vanish in the future ribosums will be compiled in instead
- char * nonstandards

  contains allowed non standard base pairs
- double temperature

  Rescale energy parameters to a temperature in degC.
- int james_rule

  interior loops of size 2 get energy 0.8Kcal and no mismatches, default 1
- int logML

  use logarithmic multiloop energy function
- int cut_point

  Marks the position (starting from 1) of the first nucleotide of the second molecule within the concatenated sequence.
- bondT * base_pair

  Contains a list of base pairs after a call to fold().
- FLT_OR_DBL * pr

  A pointer to the base pair probability matrix.
- int * iindx

  index array to move through pr.
- double pf_scale

  A scaling factor used by pf_fold() to avoid overflows.
- int do_backtrack

  do backtracking, i.e.
- char backtrack_type

  A backtrack array marker for inverse_fold()

11.13.1 Detailed Description

Here all all declarations of the global variables used throughout RNAlib.

11.13.2 Function Documentation

11.13.2.1 void set_model_details (model_detailsT * *md*)

Set default model details.

Use this function if you wish to initialize a model_detailsT data structure with its default values, i.e. the global model settings

See also

Parameters

md	A pointer to the data structure that shall be initialized

11.13.3 Variable Documentation

11.13.3.1 int noLonelyPairs

Global switch to avoid/allow helices of length 1.

Disallow all pairs which can only occur as lonely pairs (i.e. as helix of length 1). This avoids lonely base pairs in the predicted structures in most cases.

11.13.3.2 int dangles

Switch the energy model for dangling end contributions (0, 1, 2, 3)

If set to 0 no stabilizing energies are assigned to bases adjacent to helices in free ends and multiloops (so called dangling ends). Normally (dangles = 1) dangling end energies are assigned only to unpaired bases and a base cannot participate simultaneously in two dangling ends. In the partition function algorithm pf_fold() these checks are neglected. If dangles is set to 2, all folding routines will follow this convention. This treatment of dangling ends gives more favorable energies to helices directly adjacent to one another, which can be beneficial since such helices often do engage in stabilizing interactions through co-axial stacking.

If dangles = 3 co-axial stacking is explicitly included for adjacent helices in mutli-loops. The option affects only mfe folding and energy evaluation (fold() and energy_of_structure()), as well as suboptimal folding (subopt()) via re-evaluation of energies. Co-axial stacking with one intervening mismatch is not considered so far.

Default is 2 in most algorithms, partition function algorithms can only handle 0 and 2

11.13.3.3 int tetra_loop

Include special stabilizing energies for some tri-, tetra- and hexa-loops;.

default is 1.

11.13.3.4 int energy_set

0 = BP; 1=any mit GC; 2=any mit AU-parameter

If set to 1 or 2: fold sequences from an artificial alphabet ABCD..., where A pairs B, C pairs D, etc. using either GC (1) or AU parameters (2); default is 0, you probably don't want to change it.

11.13.3.5 int circ

backward compatibility variable.

. this does not effect anything

11.13.3.6 char* nonstandards

contains allowed non standard base pairs

Lists additional base pairs that will be allowed to form in addition to GC, CG, AU, UA, GU and UG. Nonstandard base pairs are given a stacking energy of 0.

11.13.3.7 double temperature

Rescale energy parameters to a temperature in degC.

Default is 37C. You have to call the update_..._params() functions after changing this parameter.

11.13.3.8 int cut_point

Marks the position (starting from 1) of the first nucleotide of the second molecule within the concatenated sequence.

To evaluate the energy of a duplex structure (a structure formed by two strands), concatenate the to sequences and set it to the first base of the second strand in the concatenated sequence. The default value of -1 stands for single molecule folding. The cut_point variable is also used by PS_rna_plot() and PS_dot_plot() to mark the chain break in postscript plots.

11.13.3.9 bondT* base_pair

Contains a list of base pairs after a call to fold().

base_pair[0].i contains the total number of pairs.

Deprecated

Do not use this variable anymore!

11.13.3.10 FLT_OR_DBL* pr

A pointer to the base pair probability matrix.

Deprecated

Do not use this variable anymore!

11.13.3.11 int* iindx

index array to move through pr.

The probability for base i and j to form a pair is in pr[iindx[i]-j].

Deprecated

Do not use this variable anymore!

11.13.3.12 double pf_scale

A scaling factor used by pf_fold() to avoid overflows.

Should be set to approximately $exp((-F/kT)/length)$, where F is an estimate for the ensemble free energy, for example the minimum free energy. You must call update_pf_-params() after changing this parameter.

If pf_scale is -1 (the default) , an estimate will be provided automatically when computing partition functions, e.g. pf_fold() The automatic estimate is usually insufficient for sequences more than a few hundred bases long.

11.13.3.13 int do_backtrack

do backtracking, i.e.

compute secondary structures or base pair probabilities

If 0, do not calculate pair probabilities in pf_fold(); this is about twice as fast. Default is 1.

11.13.3.14 char backtrack_type

A backtrack array marker for inverse_fold()

If set to 'C': force (1,N) to be paired, 'M' fold as if the sequence were inside a multi-loop. Otherwise ('F') the usual mfe structure is computed.

11.14 H/inverse.h File Reference

Inverse folding routines.

Functions

- float inverse_fold (char *start, const char *target)

  Find sequences with predefined structure.
- float inverse_pf_fold (char *start, const char *target)

  Find sequence that maximizes probability of a predefined structure.

Variables

- char ∗ symbolset

  This global variable points to the allowed bases, initially "AUGC".
- float final_cost

  when to stop inverse_pf_fold()
- int give_up

  default 0: try to minimize structure distance even if no exact solution can be found
- int inv_verbose

  print out substructure on which inverse_fold() fails

11.14.1 Detailed Description

Inverse folding routines.

11.14.2 Function Documentation

11.14.2.1 float inverse_fold (char ∗ *start,* const char ∗ *target*)

Find sequences with predefined structure.

This function searches for a sequence with minimum free energy structure provided in the parameter 'target', starting with sequence 'start'. It returns 0 if the search was successful, otherwise a structure distance in terms of the energy difference between the search result and the actual target 'target' is returned. The found sequence is returned in 'start'. If give_up is set to 1, the function will return as soon as it is clear that the search will be unsuccessful, this speeds up the algorithm if you are only interested in exact solutions.

Parameters

start	The start sequence
target	The target secondary structure in dot-bracket notation

Returns

The distance to the target in case a search was unsuccessful, 0 otherwise

11.14.2.2 float inverse_pf_fold (char ∗ *start,* const char ∗ *target*)

Find sequence that maximizes probability of a predefined structure.

This function searches for a sequence with maximum probability to fold into the provided structure 'target' using the partition function algorithm. It returns $-kT \cdot \log(p)$ where p is the frequency of 'target' in the ensemble of possible structures. This is usually much slower than inverse_fold().

Parameters

start	The start sequence
target	The target secondary structure in dot-bracket notation

Returns

The distance to the target in case a search was unsuccessful, 0 otherwise

11.14.3 Variable Documentation

11.14.3.1 char∗ symbolset

This global variable points to the allowed bases, initially "AUGC".

It can be used to design sequences from reduced alphabets.

11.15 H/Lfold.h File Reference

Predicting local MFE structures of large sequences.

Functions

- float Lfold (const char ∗string, char ∗structure, int maxdist)

  The local analog to fold().
- float aliLfold (const char ∗∗strings, char ∗structure, int maxdist)
- float Lfoldz (const char ∗string, char ∗structure, int maxdist, int zsc, double min_z)

11.15.1 Detailed Description

Predicting local MFE structures of large sequences.

11.15.2 Function Documentation

11.15.2.1 float Lfold (const char ∗ *string*, char ∗ *structure*, int *maxdist*)

The local analog to fold().

Computes the minimum free energy structure including only base pairs with a span smaller than 'maxdist'

Parameters

string	
structure	
maxdist	

11.15.2.2 float aliLfold (const char ** *strings*, char * *structure*, int *maxdist*)

Parameters

strings	
structure	
maxdist	

Returns

11.15.2.3 float Lfoldz (const char * *string*, char * *structure*, int *maxdist*, int *zsc*, double *min_z*)

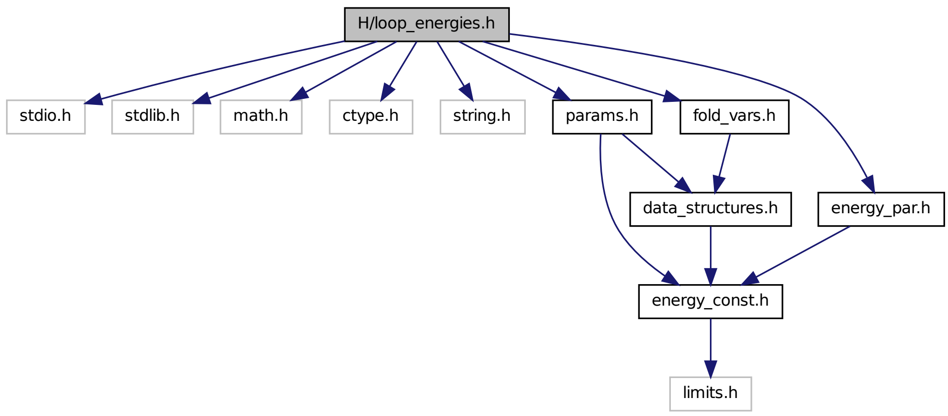
Parameters

string	
structure	
maxdist	
zsc	
min_z	

11.16 H/loop_energies.h File Reference

Energy evaluation for MFE and partition function calculations.

Include dependency graph for loop_energies.h:



Functions

- PRIVATE int E_IntLoop (int n1, int n2, int type, int type_2, int si1, int sj1, int sp1, int sq1, paramT *P)
- PRIVATE int E_Hairpin (int size, int type, int si1, int sj1, const char *string, paramT *P)
- PRIVATE int E_Stem (int type, int si1, int sj1, int extLoop, paramT *P)
- PRIVATE double exp_E_Stem (int type, int si1, int sj1, int extLoop, pf_paramT *P)
- PRIVATE double exp_E_Hairpin (int u, int type, short si1, short sj1, const char *string, pf_paramT *P)
- PRIVATE double exp_E_IntLoop (int u1, int u2, int type, int type2, short si1, short sj1, short sp1, short sq1, pf_paramT *P)

11.16.1 Detailed Description

Energy evaluation for MFE and partition function calculations. This file contains functions for the calculation of the free energy ΔG of a hairpin- [E_Hairpin()] or interior-loop [E_IntLoop()] .

The unit of the free energy returned is $10^{-2} * \mathrm{kcal/mol}$

In case of computing the partition function, this file also supplies functions which return the Boltzmann weights $e^{-\Delta G/kT}$ for a hairpin- [exp_E_Hairpin()] or interior-loop [exp_E_IntLoop()].

11.16.2 Function Documentation

11.16.2.1 PRIVATE int E_IntLoop (int *n1*, int *n2*, int *type*, int *type_2*, int *si1*, int *sj1*, int *sp1*, int *sq1*, paramT * *P*)

Compute the Energy of an interior-loop

This function computes the free energy ΔG of an interior-loop with the following structure:

```
      3'  5'
      |   |
      U - V
  a_n       b_1
   .         .
   .         .
   .         .
  a_1       b_m
      X - Y
      |   |
      5'  3'
```

This general structure depicts an interior-loop that is closed by the base pair (X,Y). The enclosed base pair is (V,U) which leaves the unpaired bases a_1-a_n and b_1-b_n that constitute the loop. In this example, the length of the interior-loop is $(n+m)$ where n or m may be 0 resulting in a bulge-loop or base pair stack. The mismatching nucleotides for the closing pair (X,Y) are:

5'-mismatch: a_1

3'-mismatch: b_m

and for the enclosed base pair (V,U):

5'-mismatch: b_1

3'-mismatch: a_n

Note

Base pairs are always denoted in 5'->3' direction. Thus the enclosed base pair must be 'turned arround' when evaluating the free energy of the interior-loop

See also

scale_parameters()
paramT

Note

This function is threadsafe

Parameters

n1	The size of the 'left'-loop (number of unpaired nucleotides)
n2	The size of the 'right'-loop (number of unpaired nucleotides)
type	The pair type of the base pair closing the interior loop
type_2	The pair type of the enclosed base pair
si1	The 5'-mismatching nucleotide of the closing pair
sj1	The 3'-mismatching nucleotide of the closing pair
sp1	The 3'-mismatching nucleotide of the enclosed pair
sq1	The 5'-mismatching nucleotide of the enclosed pair
P	The datastructure containing scaled energy parameters

Returns

The Free energy of the Interior-loop in dcal/mol

11.16.2.2 PRIVATE int E_Hairpin (int *size*, int *type*, int *si1*, int *sj1*, const char ∗ *string*, paramT ∗ *P*)

Compute the Energy of a hairpin-loop

To evaluate the free energy of a hairpin-loop, several parameters have to be known. A general hairpin-loop has this structure:

```
  a3 a4
a2      a5
a1      a6
  X - Y
  |   |
  5'  3'
```

where X-Y marks the closing pair [e.g. a **(G,C)** pair]. The length of this loop is 6 as there are six unpaired nucleotides (a1-a6) enclosed by (X,Y). The 5' mismatching nucleotide is a1 while the 3' mismatch is a6. The nucleotide sequence of this loop is "a1.a2.a3.a4.a5.a6"

Note

The parameter sequence should contain the sequence of the loop in capital letters of the nucleic acid alphabet if the loop size is below 7. This is useful for unusually stable tri-, tetra- and hexa-loops which are treated differently (based on experimental data) if they are tabulated.

See also

scale_parameters()
paramT

Warning

Not (really) thread safe! A threadsafe implementation will replace this function in a future release!
Energy evaluation may change due to updates in global variable "tetra_loop"

Parameters

size	The size of the loop (number of unpaired nucleotides)
type	The pair type of the base pair closing the hairpin
si1	The 5'-mismatching nucleotide
sj1	The 3'-mismatching nucleotide
string	The sequence of the loop
P	The datastructure containing scaled energy parameters

Returns

The Free energy of the Hairpin-loop in dcal/mol

11.16.2.3 PRIVATE int E_Stem (int *type*, int *si1*, int *sj1*, int *extLoop*, paramT $*$ *P*)

Compute the energy contribution of a stem branching off a loop-region

This function computes the energy contribution of a stem that branches off a loop region. This can be the case in multiloops, when a stem branching off increases the degree of the loop but also *immediately interior base pairs* of an exterior loop contribute free energy. To switch the bahavior of the function according to the evaluation of a multiloop- or exterior-loop-stem, you pass the flag 'extLoop'. The returned energy contribution consists of a TerminalAU penalty if the pair type is greater than 2, dangling end contributions of mismatching nucleotides adjacent to the stem if only one of the si1, sj1 parameters is greater than 0 and mismatch energies if both mismatching nucleotides are positive values. Thus, to avoid incooperating dangling end or mismatch energies just pass a negative number, e.g. -1 to the mismatch argument.

This is an illustration of how the energy contribution is assembled:

```
        3'   5'
        |    |
        X - Y
  5'-si1      sj1-3'
```

Here, (X,Y) is the base pair that closes the stem that branches off a loop region. The nucleotides si1 and sj1 are the 5'- and 3'- mismatches, respectively. If the base pair type of (X,Y) is greater than 2 (i.e. an A-U or G-U pair, the TerminalAU penalty will be included in the energy contribution returned. If si1 and sj1 are both nonnegative numbers, mismatch energies will also be included. If one of sij or sj1 is a negtive value, only 5' or 3' dangling end contributions are taken into account. To prohibit any of these mismatch contributions to be incoorporated, just pass a negative number to both, si1 and sj1. In case the argument extLoop is 0, the returned energy contribution also includes the *internal-loop-penalty* of a multiloop stem with closing pair type.

See also

E_MLstem()
E_ExtLoop()

Note

This function is threadsafe

Parameters

type	The pair type of the first base pair un the stem
si1	The 5'-mismatching nucleotide
sj1	The 3'-mismatching nucleotide
extLoop	A flag that indicates whether the contribution reflects the one of an exterior loop or not
P	The datastructure containing scaled energy parameters

Returns

The Free energy of the branch off the loop in dcal/mol

11.16.2.4 PRIVATE double exp_E_Stem (int *type,* int *si1,* int *sj1,* int *extLoop,* pf_paramT ∗ *P*)

Compute the Boltzmann weighted energy contribution of a stem branching off a loop-region

This is the partition function variant of E_Stem()

See also

E_Stem()

Note

This function is threadsafe

Returns

The Boltzmann weighted energy contribution of the branch off the loop

11.16.2.5 PRIVATE double exp_E_Hairpin (int *u*, int *type*, short *si1*, short *sj1*, const char * *string*, pf_paramT * *P*)

Compute Boltzmann weight $e^{-\Delta G/kT}$ of a hairpin loop

multiply by scale[u+2]

See also

get_scaled_pf_parameters()
pf_paramT
E_Hairpin()

Warning

Not (really) thread safe! A threadsafe implementation will replace this function in a future release!
Energy evaluation may change due to updates in global variable "tetra_loop"

Parameters

u	The size of the loop (number of unpaired nucleotides)
type	The pair type of the base pair closing the hairpin
si1	The 5'-mismatching nucleotide
sj1	The 3'-mismatching nucleotide
string	The sequence of the loop
P	The datastructure containing scaled Boltzmann weights of the energy parameters

Returns

The Boltzmann weight of the Hairpin-loop

11.16.2.6 PRIVATE double exp_E_IntLoop (int *u1*, int *u2*, int *type*, int *type2*, short *si1*, short *sj1*, short *sp1*, short *sq1*, pf_paramT * *P*)

Compute Boltzmann weight $e^{-\Delta G/kT}$ of interior loop

multiply by scale[u1+u2+2] for scaling

See also

get_scaled_pf_parameters()
pf_paramT
E_IntLoop()

Note

This function is threadsafe

Parameters

u1	The size of the 'left'-loop (number of unpaired nucleotides)
u2	The size of the 'right'-loop (number of unpaired nucleotides)
type	The pair type of the base pair closing the interior loop
type2	The pair type of the enclosed base pair
si1	The 5'-mismatching nucleotide of the closing pair
sj1	The 3'-mismatching nucleotide of the closing pair
sp1	The 3'-mismatching nucleotide of the enclosed pair
sq1	The 5'-mismatching nucleotide of the enclosed pair
P	The datastructure containing scaled Boltzmann weights of the energy parameters

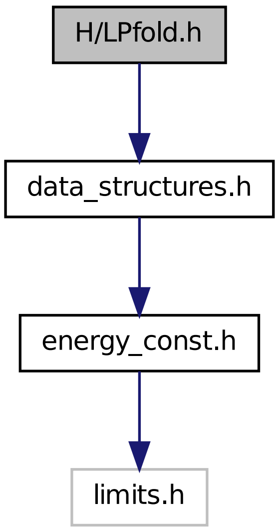
Returns

The Boltzmann weight of the Interior-loop

11.17 H/LPfold.h File Reference

Function declarations of partition function variants of the Lfold algorithm.

Include dependency graph for LPfold.h:



Functions

- void update_pf_paramsLP (int length)
- plist ∗ pfl_fold (char ∗sequence, int winSize, int pairSize, float cutoffb, double ∗∗pU, struct plist ∗∗dpp2, FILE ∗pUfp, FILE ∗spup)

  *Compute partition functions for locally stable secondary structures **(berni! update me)***
- void putoutpU_prob (double ∗∗pU, int length, int ulength, FILE ∗fp, int energies)

  Writes the unpaired probabilities (pU) or opening energies into a file.
- void putoutpU_prob_bin (double ∗∗pU, int length, int ulength, FILE ∗fp, int energies)

  Writes the unpaired probabilities (pU) or opening energies into a binary file.
- void init_pf_foldLP (int length)

  Dunno if this function was ever used by external programs linking to RNAlib, but it was declared PUBLIC before.

11.17.1 Detailed Description

Function declarations of partition function variants of the Lfold algorithm.

11.17.2 Function Documentation

11.17.2.1 void update_pf_paramsLP (int *length*)

Parameters

length	

11.17.2.2 plist∗ pfl_fold (char ∗ *sequence,* int *winSize,* int *pairSize,* float *cutoffb,* double ∗∗ *pU,* struct plist ∗∗ *dpp2,* FILE ∗ *pUfp,* FILE ∗ *spup*)

Compute partition functions for locally stable secondary structures **(berni! update me)**

pfl_fold computes partition functions for every window of size 'winSize' possible in a RNA molecule, allowing only pairs with a span smaller than 'pairSize'. It returns the mean pair probabilities averaged over all windows containing the pair in 'pl'. 'winSize' should always be $>=$ 'pairSize'. Note that in contrast to Lfold(), bases outside of the window do not influence the structure at all. Only probabilities higher than 'cutoffb' are kept.

If 'pU' is supplied (i.e is not the NULL pointer), pfl_fold() will also compute the mean probability that regions of length 'u' and smaller are unpaired. The parameter 'u' is supplied in 'pup[0][0]'. On return the 'pup' array will contain these probabilities, with the entry on 'pup[x][y]' containing the mean probability that x and the y-1 preceding bases are unpaired. The 'pU' array needs to be large enough to hold n+1 float∗ entries, where n is the sequence length.

If an array dpp2 is supplied, the probability of base pair (i,j) given that there already exists a base pair (i+1,j-1) is also computed and saved in this array. If pUfp is given (i.e. not NULL), pU is not saved but put out imediately. If spup is given (i.e. is not NULL), the pair probabilities in pl are not saved but put out imediately.

Parameters

sequence	RNA sequence
winSize	size of the window
pairSize	maximum size of base pair
cutoffb	cutoffb for base pairs
pU	array holding all unpaired probabilities
dpp2	array of dependent pair probabilities
pUfp	file pointer for pU
spup	file pointer for pair probabilities

Returns

list of pair probabilities

11.17.2.3 void putoutpU_prob (double ∗∗ *pU,* int *length,* int *ulength,* FILE ∗ *fp,* int *energies*)

Writes the unpaired probabilities (pU) or opening energies into a file.

Can write either the unpaired probabilities (accessibilities) pU or the opening energies -log(pU)kT into a file

Parameters

pU	pair probabilities
length	length of RNA sequence
ulength	maximum length of unpaired stretch
fp	file pointer of destination file
energies	switch to put out as opening energies

11.17.2.4 void putoutpU_prob_bin (double ** *pU*, int *length*, int *ulength*, FILE * *fp*, int *energies*)

Writes the unpaired probabilities (pU) or opening energies into a binary file.

Can write either the unpaired probabilities (accessibilities) pU or the opening energies -log(pU)kT into a file

Parameters

pU	pair probabilities
length	length of RNA sequence
ulength	maximum length of unpaired stretch
fp	file pointer of destination file
energies	switch to put out as opening energies

11.17.2.5 void init_pf_foldLP (int *length*)

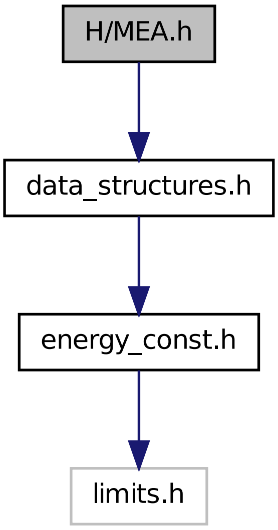
Dunno if this function was ever used by external programs linking to RNAlib, but it was declared PUBLIC before.

Anyway, never use this function as it will be removed soon and does nothing at all

11.18 H/MEA.h File Reference

Computes a MEA (maximum expected accuracy) structure.

Include dependency graph for MEA.h:



Functions

- float MEA (plist *p, char *structure, double gamma)

  Computes a MEA (maximum expected accuracy) structure.

11.18.1 Detailed Description

Computes a MEA (maximum expected accuracy) structure.

11.18.2 Function Documentation

11.18.2.1 float MEA (plist * *p,* char * *structure,* double *gamma*)

Computes a MEA (maximum expected accuracy) structure.

The algorithm maximizes the expected accuracy

$$A(S) = \sum_{(i,j) \in S} 2\gamma p_{ij} + \sum_{i \notin S} p_i^u$$

Higher values of γ result in more base pairs of lower probability and thus higher sensitivity. Low values of γ result in structures containing only highly likely pairs (high specificity). The code of the MEA function also demonstrates the use of sparse dynamic programming scheme to reduce the time and memory complexity of folding.

11.19 H/mm.h File Reference

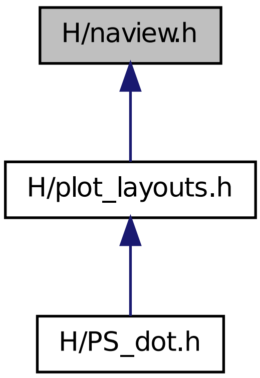
Several Maximum Matching implementations.

11.19.1 Detailed Description

Several Maximum Matching implementations. This file contains the declarations for several maximum matching implementations

11.20 H/naview.h File Reference

This graph shows which files directly or indirectly include this file:

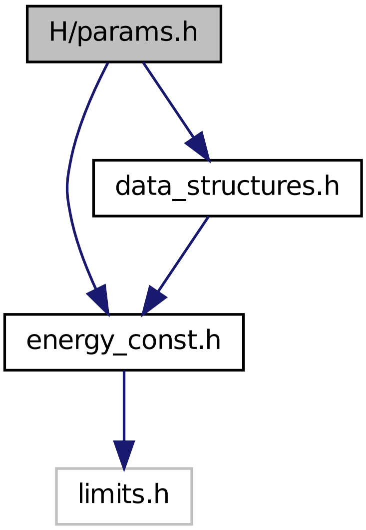


11.20.1 Detailed Description

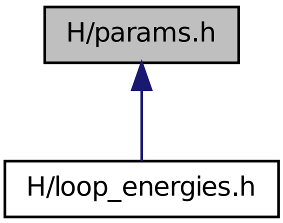
11.21 H/params.h File Reference

Several functions to obtain (pre)scaled energy parameter data containers.

Include dependency graph for params.h:



This graph shows which files directly or indirectly include this file:



Functions

- paramT * scale_parameters (void)

  Get precomputed energy contributions for all the known loop types.

- paramT * get_scaled_parameters (double temperature, model_detailsT md)

  Get precomputed energy contributions for all the known loop types.
- pf_paramT * get_scaled_pf_parameters (void)

  get a datastructure of type pf_paramT which contains the Boltzmann weights of several energy parameters scaled according to the current temperature
- pf_paramT * get_boltzmann_factors (double temperature, double betaScale, model_detailsT md, double pf_scale)

  Get precomputed Boltzmann factors of the loop type dependent energy contributions with independent thermodynamic temperature.
- pf_paramT * get_boltzmann_factor_copy (pf_paramT *parameters)

  Get a copy of already precomputed Boltzmann factors.
- pf_paramT * get_scaled_alipf_parameters (unsigned int n_seq)

  Get precomputed Boltzmann factors of the loop type dependent energy contributions (alifold variant)
- pf_paramT * get_boltzmann_factors_ali (unsigned int n_seq, double temperature, double betaScale, model_detailsT md, double pf_scale)

  Get precomputed Boltzmann factors of the loop type dependent energy contributions (alifold variant) with independent thermodynamic temperature.

11.21.1 Detailed Description

Several functions to obtain (pre)scaled energy parameter data containers.

11.21.2 Function Documentation

11.21.2.1 paramT* scale_parameters (void)

Get precomputed energy contributions for all the known loop types.

Note

OpenMP: This function relies on several global model settings variables and thus is not to be considered threadsafe. See get_scaled_parameters() for a completely threadsafe implementation.

Returns

A set of precomputed energy contributions

11.21.2.2 paramT* get_scaled_parameters (double *temperature*, model_detailsT *md*)

Get precomputed energy contributions for all the known loop types.

Call this function to retrieve precomputed energy contributions, i.e. scaled according to the temperature passed. Furthermore, this function assumes a data structure that contains the model details as well, such that subsequent folding recursions are able to retrieve the correct model settings

See also

model_detailsT, set_model_details()

Parameters

temperature	The temperature in degrees Celcius
md	The model details

Returns

precomputed energy contributions and model settings

11.21.2.3 pf_paramT* get_scaled_pf_parameters (void)

get a datastructure of type pf_paramT which contains the Boltzmann weights of several energy parameters scaled according to the current temperature

Returns

The datastructure containing Boltzmann weights for use in partition function calculations

11.21.2.4 pf_paramT* get_boltzmann_factors (double *temperature*, double *betaScale*, model_detailsT *md*, double *pf_scale*)

Get precomputed Boltzmann factors of the loop type dependent energy contributions with independent thermodynamic temperature.

This function returns a data structure that contains all necessary precalculated Boltzmann factors for each loop type contribution.

In contrast to get_scaled_pf_parameters(), this function enables setting of independent temperatures for both, the individual energy contributions as well as the thermodynamic temperature used in $exp(-\Delta G/kT)$

See also

get_scaled_pf_parameters(), get_boltzmann_factor_copy()

Parameters

dangle_-model	The dangle model to be used (possible values: 0 or 2)
temperature	The temperature in degC used for (re-)scaling the energy contributions
alpha	A scaling value that is used as a multiplication factor for the absolute temperature of the system

Returns

A set of precomputed Boltzmann factors

11.21.2.5 pf_paramT* get_boltzmann_factor_copy (pf_paramT * *parameters*)

Get a copy of already precomputed Boltzmann factors.

See also

get_boltzmann_factors(), get_scaled_pf_parameters()

Parameters

parameters	The input data structure that shall be copied

Returns

A copy of the provided Boltzmann factor dataset

11.21.2.6 pf_paramT* get_scaled_alipf_parameters (unsigned int *n_seq*)

Get precomputed Boltzmann factors of the loop type dependent energy contributions (alifold variant)

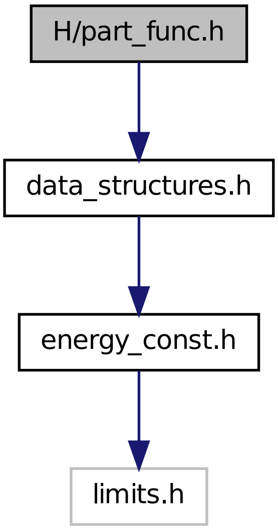
11.21.2.7 pf_paramT* get_boltzmann_factors_ali (unsigned int *n_seq*, double *temperature*, double *betaScale*, model_detailsT *md*, double *pf_scale*)

Get precomputed Boltzmann factors of the loop type dependent energy contributions (alifold variant) with independent thermodynamic temperature.

11.22 H/part_func.h File Reference

Partition function of single RNA sequences.

Include dependency graph for part_func.h:



Functions

- float pf_fold_par (const char ∗sequence, char ∗structure, pf_paramT ∗parameters, int calculate_bppm, int is_constrained, int is_circular)

  Compute the partition function Q for a given RNA sequence.
- float pf_fold (const char ∗sequence, char ∗structure)

  Compute the partition function Q of an RNA sequence.
- float pf_circ_fold (const char ∗sequence, char ∗structure)

  Compute the partition function of a circular RNA sequence.
- char ∗ pbacktrack (char ∗sequence)

  Sample a secondary structure from the Boltzmann ensemble according its probability.
- char ∗ pbacktrack_circ (char ∗sequence)

  Sample a secondary structure of a circular RNA from the Boltzmann ensemble according its probability.
- void free_pf_arrays (void)

  Free arrays for the partition function recursions.
- void update_pf_params (int length)

  Recalculate energy parameters.
- FLT_OR_DBL ∗ export_bppm (void)

Get a pointer to the base pair probability array.

- void assign_plist_from_pr (plist ∗∗pl, FLT_OR_DBL ∗probs, int length, double cutoff)

  Create a plist from a probability matrix.

- int get_pf_arrays (short ∗∗S_p, short ∗∗S1_p, char ∗∗ptype_p, FLT_OR_DBL ∗∗qb_p, FLT_OR_DBL ∗∗qm_p, FLT_OR_DBL ∗∗q1k_p, FLT_OR_DBL ∗∗qln_p)

  Get the pointers to (almost) all relavant computation arrays used in partition function computation.

- double get_subseq_F (int i, int j)

  Get the free energy of a subsequence from the q[] array.

- char ∗ get_centroid_struct_pl (int length, double ∗dist, plist ∗pl)

  Get the centroid structure of the ensemble.

- char ∗ get_centroid_struct_pr (int length, double ∗dist, FLT_OR_DBL ∗pr)

  Get the centroid structure of the ensemble.

- double mean_bp_distance (int length)

  Get the mean base pair distance of the last partition function computation.

- double mean_bp_distance_pr (int length, FLT_OR_DBL ∗pr)

  Get the mean base pair distance in the thermodynamic ensemble.

- void bppm_to_structure (char ∗structure, FLT_OR_DBL ∗pr, unsigned int length)

  Create a dot-bracket like structure string from base pair probability matrix.

- char bppm_symbol (const float ∗x)

  Get a pseudo dot bracket notation for a given probability information.

- void init_pf_fold (int length)

  Allocate space for pf_fold()

- char ∗ centroid (int length, double ∗dist)
- double mean_bp_dist (int length)

  get the mean pair distance of ensemble

- double expLoopEnergy (int u1, int u2, int type, int type2, short si1, short sj1, short sp1, short sq1)
- double expHairpinEnergy (int u, int type, short si1, short sj1, const char ∗string)

Variables

- int st_back

  a flag indicating that auxilary arrays are needed throughout the computations which are necessary for stochastic backtracking

11.22.1 Detailed Description

Partition function of single RNA sequences. This file includes (almost) all function declarations within the **RNAlib** that are related to Partion function folding...

Note

If you plan on using the functions provided from this section of the RNAlib concurrently via **OpenMP** you have to place a *COPYIN* clause right before your *PARALLEL* directive! Otherwise, some functions may not behave as expected. A complete list of variables that have to be passed to the *COPYIN* clause can be found in the detailed description of each function below.

11.22.2 Function Documentation

11.22.2.1 float pf_fold_par (const char * *sequence*, char * *structure*, pf_paramT * *parameters*, int *calculate_bppm*, int *is_constrained*, int *is_circular*)

Compute the partition function Q for a given RNA sequence.

If *structure* is not a NULL pointer on input, it contains on return a string consisting of the letters " . , | { } ( ) " denoting bases that are essentially unpaired, weakly paired, strongly paired without preference, weakly upstream (downstream) paired, or strongly up- (down-)stream paired bases, respectively. If fold_constrained is not 0, the *structure* string is interpreted on input as a list of constraints for the folding. The character "x" marks bases that must be unpaired, matching brackets " ( ) " denote base pairs, all other characters are ignored. Any pairs conflicting with the constraint will be forbidden. This is usually sufficient to ensure the constraints are honored. If tha parameter calculate_-bppm is set to 0 base pairing probabilities will not be computed (saving CPU time), otherwise after calculations took place pr will contain the probability that bases *i* and *j* pair.

Note

The global array pr is deprecated and the user who wants the calculated base pair probabilities for further computations is advised to use the function export_bppm()

See also

pf_circ_fold(), bppm_to_structure(), export_bppm(), get_boltzmann_factors()

Parameters

sequence	The RNA sequence input
structure	A pointer to a char array where a base pair probability information can be stored in a pseudo-dot-bracket notation (may be NULL, too)
parameters	Data structure containing the precalculated Boltzmann factors
calculate_-bppm	Switch to Base pair probability calculations on/off (0==off)
is_-constrained	Switch to indicate that a structure contraint is passed via the structure argument (0==off)
is_circular	Switch to (de-)activate postprocessing steps in case RNA sequence is circular (0==off)

Returns

The Gibbs free energy of the ensemble ($G = -RT \cdot \log(Q)$) in kcal/mol

11.22.2.2 float pf_fold (const char * *sequence*, char * *structure*)

Compute the partition function Q of an RNA sequence.

If *structure* is not a NULL pointer on input, it contains on return a string consisting of the letters " . , | { } ( ) " denoting bases that are essentially unpaired, weakly paired, strongly paired without preference, weakly upstream (downstream) paired, or strongly up- (down-)stream paired bases, respectively. If fold_constrained is not 0, the *structure* string is interpreted on input as a list of constraints for the folding. The character "x" marks bases that must be unpaired, matching brackets " ( ) " denote base pairs, all other characters are ignored. Any pairs conflicting with the constraint will be forbidden. This is usually sufficient to ensure the constraints are honored. If do_backtrack has been set to 0 base pairing probabilities will not be computed (saving CPU time), otherwise pr will contain the probability that bases *i* and *j* pair.

Note

The global array pr is deprecated and the user who wants the calculated base pair probabilities for further computations is advised to use the function export_bppm()

See also

pf_circ_fold(), bppm_to_structure(), export_bppm()

Parameters

sequence	The RNA sequence input
structure	A pointer to a char array where a base pair probability information can be stored in a pseudo-dot-bracket notation (may be NULL, too)

Returns

The Gibbs free energy of the ensemble ($G = -RT \cdot \log(Q)$) in kcal/mol

11.22.2.3 float pf_circ_fold (const char * *sequence*, char * *structure*)

Compute the partition function of a circular RNA sequence.

See also

pf_fold(), pf_fold_par()

Parameters

sequence	The RNA sequence input
structure	A pointer to a char array where a base pair probability information can be stored in a pseudo-dot-bracket notation (may be NULL, too)

Returns

The Gibbs free energy of the ensemble ($G = -RT \cdot \log(Q)$) in kcal/mol

11.22.2.4 char* pbacktrack (char * *sequence*)

Sample a secondary structure from the Boltzmann ensemble according its probability

.

Note

You have to call pf_fold() first in order to fill the partition function matrices
OpenMP notice:
This function relies on passing the following variables to the appropriate *COPYIN* clause *(additionally to the ones needed by pf_fold())*:
pstruc, sequence

Parameters

sequence	The RNA sequence

Returns

A sampled secondary structure in dot-bracket notation

11.22.2.5 char* pbacktrack_circ (char * *sequence*)

Sample a secondary structure of a circular RNA from the Boltzmann ensemble according its probability.

This function does the same as pbacktrack() but assumes the RNA molecule to be circular

Note

OpenMP notice:
This function relies on passing the following variables to the appropriate *COPYIN* clause *(additionally to the ones needed by pf_fold())*:
pstruc, sequence

Parameters

sequence	The RNA sequence

Returns

A sampled secondary structure in dot-bracket notation

11.22.2.6 void free_pf_arrays (void)

Free arrays for the partition function recursions.

Call this function if you want to free all allocated memory associated with the partition function forward recursion.

Note

Successive calls of pf_fold(), pf_circ_fold() already check if they should free any memory from a previous run.

OpenMP notice:

This function should be called before leaving a thread in order to avoid leaking memory

See also

pf_fold(), pf_circ_fold()

11.22.2.7 void update_pf_params (int *length*)

Recalculate energy parameters.

Call this function to recalculate the pair matrix and energy parameters after a change in folding parameters like temperature

11.22.2.8 FLT_OR_DBL∗ export_bppm (void)

Get a pointer to the base pair probability array.

Accessing the base pair probabilities for a pair (i,j) is achieved by

```
FLT_OR_DBL *pr = export_bppm(); pr_ij = pr[iindx[i]-j];
```

Note

Call pf_fold() before using this function!

See also

pf_fold(), pf_circ_fold(), get_iindx()

Returns

A pointer to the base pair probability array

11.22.2.9 void assign_plist_from_pr (plist ∗∗ *pl*, FLT_OR_DBL ∗ *probs*, int *length*, double *cutoff*)

Create a plist from a probability matrix.

The probability matrix given is parsed and all pair probabilities above the given threshold are used to create an entry in the plist

The end of the plist is marked by sequence positions i as well as j equal to 0. This condition should be used to stop looping over its entries

Note

This function is threadsafe

Parameters

pl	A pointer to the plist that is to be created
probs	The probability matrix used for creting the plist
length	The length of the RNA sequence
cutoff	The cutoff value

11.22.2.10 int get_pf_arrays (short ∗∗ *S_p*, short ∗∗ *S1_p*, char ∗∗ *ptype_p*, FLT_OR_DBL ∗∗ *qb_p*, FLT_OR_DBL ∗∗ *qm_p*, FLT_OR_DBL ∗∗ *q1k_p*, FLT_OR_DBL ∗∗ *qln_p*)

Get the pointers to (almost) all relavant computation arrays used in partition function computation.

Note

In order to assign meaningful pointers, you have to call pf_fold first!

See also

pf_fold(), pf_circ_fold()

Parameters

S_p	A pointer to the 'S' array (integer representation of nucleotides)
S1_p	A pointer to the 'S1' array (2nd integer representation of nucleotides)
ptype_p	A pointer to the pair type matrix
qb_p	A pointer to the Q^B matrix
qm_p	A pointer to the Q^M matrix
q1k_p	A pointer to the 5' slice of the Q matrix ($q1k(k) = Q(1,k)$)
qln_p	A pointer to the 3' slice of the Q matrix ($qln(l) = Q(l,n)$)

Returns

Non Zero if everything went fine, 0 otherwise

11.22.2.11 char∗ get_centroid_struct_pl (int *length*, double ∗ *dist*, plist ∗ *pl*)

Get the centroid structure of the ensemble.

This function is a threadsafe replacement for centroid() with a 'plist' input

The centroid is the structure with the minimal average distance to all other structures

$< d(S) >= \sum_{(i,j) \in S} (1 - p_{ij}) + \sum_{(i,j) \notin S} p_{ij}$

Thus, the centroid is simply the structure containing all pairs with $p_i j > 0.5$ The distance of the centroid to the ensemble is written to the memory adressed by *dist*.

Parameters

length	The length of the sequence

dist	A pointer to the distance variable where the centroid distance will be written to
pl	A pair list containing base pair probability information about the ensemble

Returns

The centroid structure of the ensemble in dot-bracket notation

11.22.2.12 char* get_centroid_struct_pr (int *length*, double * *dist*, FLT_OR_DBL * *pr*)

Get the centroid structure of the ensemble.

This function is a threadsafe replacement for centroid() with a probability array input

The centroid is the structure with the minimal average distance to all other structures

$<d(S)>=\sum_{(i,j)\in S}(1-p_{ij})+\sum_{(i,j)\notin S}p_{ij}$

Thus, the centroid is simply the structure containing all pairs with $p_ij>0.5$ The distance of the centroid to the ensemble is written to the memory adressed by *dist*.

Parameters

length	The length of the sequence
dist	A pointer to the distance variable where the centroid distance will be written to
pr	A upper triangular matrix containing base pair probabilities (access via iindx get_iindx())

Returns

The centroid structure of the ensemble in dot-bracket notation

11.22.2.13 double mean_bp_distance (int *length*)

Get the mean base pair distance of the last partition function computation.

Note

To ensure thread-safety, use the function mean_bp_distance_pr() instead!

See also

mean_bp_distance_pr()

Parameters

length	

Returns

mean base pair distance in thermodynamic ensemble

11.22.2.14 double mean_bp_distance_pr (int *length*, FLT_OR_DBL * *pr*)

Get the mean base pair distance in the thermodynamic ensemble.

This is a threadsafe implementation of mean_bp_dist() !

$<d> = \sum_{a,b} p_a p_b d(S_a, S_b)$

this can be computed from the pair probs $p_i j$ as

$<d> = \sum_{ij} p_{ij}(1 - p_{ij})$

Note

This function is threadsafe

Parameters

length	The length of the sequence
pr	The matrix containing the base pair probabilities

Returns

The mean pair distance of the structure ensemble

11.22.2.15 void init_pf_fold (int *length*)

Allocate space for pf_fold()

Deprecated

This function is obsolete and will be removed soon!

11.22.2.16 char* centroid (int *length*, double * *dist*)

Deprecated

This function is deprecated and should not be used anymore as it is not threadsafe!

See also

get_centroid_struct_pl(), get_centroid_struct_pr()

11.22.2.17 double mean_bp_dist (int *length*)

get the mean pair distance of ensemble

Deprecated

This function is not threadsafe and should not be used anymore. Use mean_bp_-distance() instead!

11.22.2.18 double expLoopEnergy (int *u1*, int *u2*, int *type*, int *type2*, short *si1*, short *sj1*, short *sp1*, short *sq1*)

Deprecated

Use exp_E_IntLoop() from loop_energies.h instead

11.22.2.19 double expHairpinEnergy (int *u*, int *type*, short *si1*, short *sj1*, const char ∗ *string*)

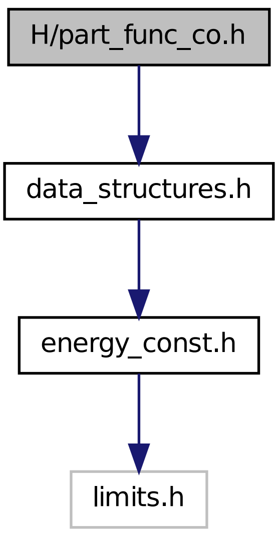
Deprecated

Use exp_E_Hairpin() from loop_energies.h instead

11.23 H/part_func_co.h File Reference

Partition function for two RNA sequences.

Include dependency graph for part_func_co.h:



Functions

- cofoldF co_pf_fold (char ∗sequence, char ∗structure)

  Calculate partition function and base pair probabilities.
- cofoldF co_pf_fold_par (char ∗sequence, char ∗structure, pf_paramT ∗parameters, int calculate_bppm, int is_constrained)

  Calculate partition function and base pair probabilities.
- FLT_OR_DBL ∗ export_co_bppm (void)

  Get a pointer to the base pair probability array.
- void free_co_pf_arrays (void)

  Free the memory occupied by co_pf_fold()
- void update_co_pf_params (int length)

  Recalculate energy parameters.
- void update_co_pf_params_par (int length, pf_paramT ∗parameters)

  Recalculate energy parameters.
- void compute_probabilities (double FAB, double FEA, double FEB, struct plist ∗prAB, struct plist ∗prA, struct plist ∗prB, int Alength)

  Compute Boltzmann probabilities of dimerization without homodimers.
- ConcEnt ∗ get_concentrations (double FEAB, double FEAA, double FEBB, double FEA, double FEB, double ∗startconc)

  Given two start monomer concentrations a and b, compute the concentrations in thermodynamic equilibrium of all dimers and the monomers.
- plist ∗ get_plist (struct plist ∗pl, int length, double cut_off)

  DO NOT USE THIS FUNCTION ANYMORE.
- void init_co_pf_fold (int length)

  DO NOT USE THIS FUNCTION ANYMORE.

Variables

- int mirnatog

  Toggles no intrabp in 2nd mol.
- double F_monomer [2]

  Free energies of the two monomers.

11.23.1 Detailed Description

Partition function for two RNA sequences. As for folding one RNA molecule, this computes the partition function of all possible structures and the base pair probabilities. Uses the same global pf_scale variable to avoid overflows.

To simplify the implementation the partition function computation is done internally in a null model that does not include the duplex initiation energy, i.e. the entropic penalty for producing a dimer from two monomers). The resulting free energies and pair probabilities are initially relative to that null model. In a second step the free energies can be corrected to include the dimerization penalty, and the pair probabilities can be divided into the conditional pair probabilities given that a re dimer is formed or not formed.

After computing the partition functions of all possible dimeres one can compute the probabilities of base pairs, the concentrations out of start concentrations and sofar and soaway.

Dimer formation is inherently concentration dependent. Given the free energies of the monomers A and B and dimers AB, AA, and BB one can compute the equilibrium concentrations, given input concentrations of A and B, see e.g. Dimitrov & Zuker (2004)

11.23.2 Function Documentation

11.23.2.1 cofoldF co_pf_fold (char * *sequence*, char * *structure*)

Calculate partition function and base pair probabilities.

This is the cofold partition function folding. The second molecule starts at the cut_point nucleotide.

Note

OpenMP: Since this function relies on the global parameters do_backtrack, dangles, temperature and pf_scale it is not threadsafe according to concurrent changes in these variables! Use co_pf_fold_par() instead to circumvent this issue.

See also

co_pf_fold_par()

Parameters

sequence	Concatenated RNA sequences
structure	Will hold the structure or constraints

Returns

cofoldF structure containing a set of energies needed for concentration computations.

11.23.2.2 cofoldF co_pf_fold_par (char * *sequence*, char * *structure*, pf_paramT * *parameters*, int *calculate_bppm*, int *is_constrained*)

Calculate partition function and base pair probabilities.

This is the cofold partition function folding. The second molecule starts at the cut_point nucleotide.

See also

get_boltzmann_factors(), co_pf_fold()

Parameters

sequence	Concatenated RNA sequences
structure	Pointer to the structure constraint
parameters	Data structure containing the precalculated Boltzmann factors
calculate_-bppm	Switch to turn Base pair probability calculations on/off (0==off)
is_-constrained	Switch to indicate that a structure contraint is passed via the structure argument (0==off)

Returns

cofoldF structure containing a set of energies needed for concentration computations.

11.23.2.3 FLT_OR_DBL* export_co_bppm (void)

Get a pointer to the base pair probability array.

Accessing the base pair probabilities for a pair (i,j) is achieved by

```
FLT_OR_DBL *pr = export_bppm(); pr_ij = pr[iindx[i]-j];
```

See also

get_iindx()

Returns

A pointer to the base pair probability array

11.23.2.4 void update_co_pf_params (int *length*)

Recalculate energy parameters.

This function recalculates all energy parameters given the current model settings.

Note

This function relies on the global variables pf_scale, dangles and temperature. Thus it might not be threadsafe in certain situations. Use update_co_pf_params_-par() instead.

See also

get_boltzmann_factors(), update_co_pf_params_par()

Parameters

length	Length of the current RNA sequence

11.23.2.5 void update_co_pf_params_par (int *length*, pf_paramT ∗ *parameters*)

Recalculate energy parameters.

This function recalculates all energy parameters given the current model settings. It's second argument can either be NULL or a data structure containing the precomputed Boltzmann factors. In the first scenario, the necessary data structure will be created automatically according to the current global model settings, i.e. this mode might not be threadsafe. However, if the provided data structure is not NULL, threadsafety for the model parameters dangles, pf_scale and temperature is regained, since their values are taken from this data structure during subsequent calculations.

See also

get_boltzmann_factors(), update_co_pf_params()

Parameters

length	Length of the current RNA sequence
parameters	data structure containing the precomputed Boltzmann factors

11.23.2.6 void compute_probabilities (double *FAB*, double *FEA*, double *FEB*, struct plist ∗ *prAB*, struct plist ∗ *prA*, struct plist ∗ *prB*, int *Alength*)

Compute Boltzmann probabilities of dimerization without homodimers.

Given the pair probabilities and free energies (in the null model) for a dimer AB and the two constituent monomers A and B, compute the conditional pair probabilities given that a dimer AB actually forms. Null model pair probabilities are given as a list as produced by assign_plist_from_pr(), the dimer probabilities 'prAB' are modified in place.

Parameters

FAB	free energy of dimer AB
FEA	free energy of monomer A
FEB	free energy of monomer B
prAB	pair probabilities for dimer
prA	pair probabilities monomer
prB	pair probabilities monomer
Alength	Length of molecule A

11.23.2.7 ConcEnt∗ get_concentrations (double *FEAB*, double *FEAA*, double *FEBB*, double *FEA*, double *FEB*, double ∗ *startconc*)

Given two start monomer concentrations a and b, compute the concentrations in thermodynamic equilibrium of all dimers and the monomers.

This function takes an array 'startconc' of input concentrations with alternating entries for the initial concentrations of molecules A and B (terminated by two zeroes), then computes the resulting equilibrium concentrations from the free energies for the dimers. Dimer free energies should be the dimer-only free energies, i.e. the FcAB entries from the cofoldF struct.

Parameters

FEAB	Free energy of AB dimer (FcAB entry)
FEAA	Free energy of AA dimer (FcAB entry)
FEBB	Free energy of BB dimer (FcAB entry)
FEA	Free energy of monomer A
FEB	Free energy of monomer B
startconc	List of start concentrations [a0],[b0],[a1],[b1],...,[an][bn],[0],[0]

Returns

ConcEnt array containing the equilibrium energies and start concentrations

11.23.2.8 plist* get_plist (struct plist * *pl,* int *length,* double *cut_off*)

DO NOT USE THIS FUNCTION ANYMORE.

Deprecated

{ This function is deprecated and will be removed soon!} use assign_plist_from_pr() instead!

11.23.2.9 void init_co_pf_fold (int *length*)

DO NOT USE THIS FUNCTION ANYMORE.

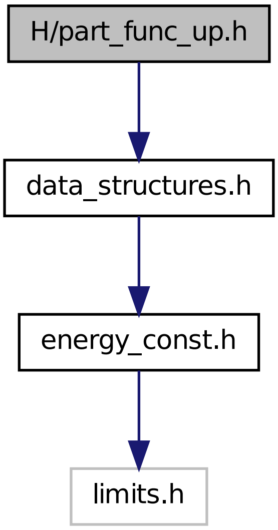
Deprecated

{ This function is deprecated and will be removed soon!}

11.24 H/part_func_up.h File Reference

Partition Function Cofolding as stepwise process.

Include dependency graph for part_func_up.h:



Functions

- pu_contrib ∗ pf_unstru (char ∗sequence, int max_w)

  Calculate the partition function over all unpaired regions of a maximal length.
- interact ∗ pf_interact (const char ∗s1, const char ∗s2, pu_contrib ∗p_c, pu_contrib ∗p_c2, int max_w, char ∗cstruc, int incr3, int incr5)

  Calculates the probability of a local interaction between two sequences.
- void free_interact (interact ∗pin)

  Frees the output of function pf_interact().
- void free_pu_contrib_struct (pu_contrib ∗pu)

  Frees the output of function pf_unstru().

11.24.1 Detailed Description

Partition Function Cofolding as stepwise process. In this approach to cofolding the interaction between two RNA molecules is seen as a stepwise process. In a first step, the target molecule has to adopt a structure in which a binding site is accessible. In a second step, the ligand molecule will hybridize with a region accessible to an interaction. Consequently the algorithm is designed as a two step process: The first step is the calculation of the probability that a region within the target is unpaired, or equivalently, the calculation of the free energy needed to expose a region. In the second step we compute the free energy of an interaction for every possible binding site.

11.24.2 Function Documentation

11.24.2.1 pu_contrib* pf_unstru (char * *sequence*, int *max_w*)

Calculate the partition function over all unpaired regions of a maximal length.

You have to call function pf_fold() providing the same sequence before calling pf_unstru(). If you want to calculate unpaired regions for a constrained structure, set variable 'structure' in function 'pf_fold()' to the constrain string. It returns a pu_contrib struct containing four arrays of dimension [i = 1 to length(sequence)][j = 0 to u-1] containing all possible contributions to the probabilities of unpaired regions of maximum length u. Each array in pu_contrib contains one of the contributions to the total probability of being unpaired: The probability of being unpaired within an exterior loop is in array pu_contrib->E, the probability of being unpaired within a hairpin loop is in array pu_contrib->H, the probability of being unpaired within an interior loop is in array pu_contrib->I and probability of being unpaired within a multi-loop is in array pu_contrib->M. The total probability of being unpaired is the sum of the four arrays of pu_contrib.

This function frees everything allocated automatically. To free the output structure call free_pu_contrib().

Parameters

sequence	
max_w	

Returns

11.24.2.2 interact* pf_interact (const char * *s1*, const char * *s2*, pu_contrib * *p_c*, pu_contrib * *p_c2*, int *max_w*, char * *cstruc*, int *incr3*, int *incr5*)

Calculates the probability of a local interaction between two sequences.

The function considers the probability that the region of interaction is unpaired within 's1' and 's2'. The longer sequence has to be given as 's1'. The shorter sequence has to be given as 's2'. Function pf_unstru() has to be called for 's1' and 's2', where the probabilities of being unpaired have to be given in 'p_c' and 'p_c2', respectively. If you do not want to include the probabilities of being unpaired for 's2' set 'p_c2' to NULL. If variable 'cstruc' is not NULL, constrained folding is done: The available constrains for intermolecular interaction are: '.' (no constrain), 'x' (the base has no intermolecular interaction) and '|' (the corresponding base has to be paired intermolecularily).

The parameter 'w' determines the maximal length of the interaction. The parameters 'incr5' and 'incr3' allows inclusion of unpaired residues left ('incr5') and right ('incr3') of the region of interaction in 's1'. If the 'incr' options are used, function pf_unstru() has to be called with w=w+incr5+incr3 for the longer sequence 's1'.

It returns a structure of type interact which contains the probability of the best local interaction including residue i in Pi and the minimum free energy in Gi, where i is the position in sequence 's1'. The member Gikjl of structure interact is the best interaction between region [k,i] k<i in longer sequence 's1' and region [j,l] j<l in 's2'. Gikjl_wo is Gikjl without the probability of beeing unpaired.

Use free_interact() to free the returned structure, all other stuff is freed inside pf_-interact().

Parameters

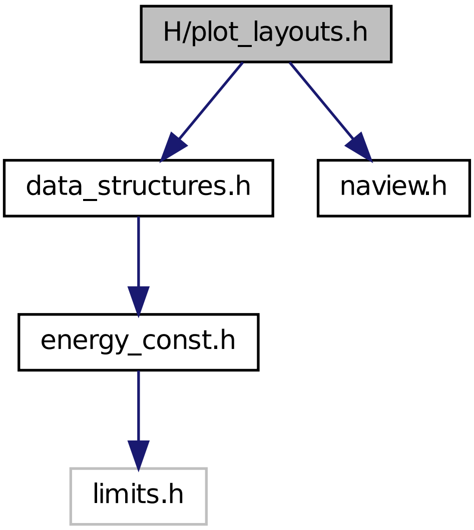
s1	
s2	
p_c	
p_c2	
max_w	
cstruc	
incr3	
incr5	

Returns

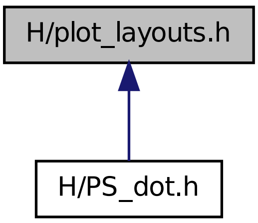
11.25 H/plot_layouts.h File Reference

Secondary structure plot layout algorithms.

Include dependency graph for plot_layouts.h:



This graph shows which files directly or indirectly include this file:



Defines

- #define VRNA_PLOT_TYPE_SIMPLE 0

  Definition of Plot type simple

- #define VRNA_PLOT_TYPE_NAVIEW 1

  Definition of Plot type Naview
- #define VRNA_PLOT_TYPE_CIRCULAR 2

  Definition of Plot type Circular

Functions

- int simple_xy_coordinates (short ∗pair_table, float ∗X, float ∗Y)

  Calculate nucleotide coordinates for secondary structure plot the Simple way
- int simple_circplot_coordinates (short ∗pair_table, float ∗x, float ∗y)

  Calculate nucleotide coordinates for Circular Plot

Variables

- int rna_plot_type

  Switch for changing the secondary structure layout algorithm.

11.25.1 Detailed Description

Secondary structure plot layout algorithms. c Ronny Lorenz The ViennaRNA Package

11.25.2 Define Documentation

11.25.2.1 #define VRNA_PLOT_TYPE_SIMPLE 0

Definition of Plot type *simple*

This is the plot type definition for several RNA structure plotting functions telling them to use **Simple** plotting algorithm

See also

rna_plot_type, PS_rna_plot_a(), PS_rna_plot(), svg_rna_plot(), gmlRNA(), ssv_-rna_plot(), xrna_plot()

11.25.2.2 #define VRNA_PLOT_TYPE_NAVIEW 1

Definition of Plot type *Naview*

This is the plot type definition for several RNA structure plotting functions telling them to use **Naview** plotting algorithm

See also

rna_plot_type, PS_rna_plot_a(), PS_rna_plot(), svg_rna_plot(), gmlRNA(), ssv_-rna_plot(), xrna_plot()

11.25.2.3 #define VRNA_PLOT_TYPE_CIRCULAR 2

Definition of Plot type *Circular*

This is the plot type definition for several RNA structure plotting functions telling them to produce a **Circular plot**

See also

rna_plot_type, PS_rna_plot_a(), PS_rna_plot(), svg_rna_plot(), gmlRNA(), ssv_-rna_plot(), xrna_plot()

11.25.3 Function Documentation

11.25.3.1 int simple_xy_coordinates (short * *pair_table*, float * *X*, float * *Y*)

Calculate nucleotide coordinates for secondary structure plot the *Simple way*

See also

make_pair_table(), rna_plot_type, simple_circplot_coordinates(), naview_xy_coordinates(), PS_rna_plot_a(), PS_rna_plot, svg_rna_plot()

Parameters

pair_table	The pair table of the secondary structure
X	a pointer to an array with enough allocated space to hold the x coordinates
Y	a pointer to an array with enough allocated space to hold the y coordinates

Returns

length of sequence on success, 0 otherwise

11.25.3.2 int simple_circplot_coordinates (short * *pair_table*, float * *x*, float * *y*)

Calculate nucleotide coordinates for *Circular Plot*

This function calculates the coordinates of nucleotides mapped in equal distancies onto a unit circle.

Note

In order to draw nice arcs using quadratic bezier curves that connect base pairs one may calculate a second tangential point P^t in addition to the actual R^2 coordinates. the simplest way to do so may be to compute a radius scaling factor rs in the interval $[0,1]$ that weights the proportion of base pair span to the actual length of the sequence. This scaling factor can then be used to calculate the coordinates for P^t, i.e. $P^t_x[i] = X[i] * rs$ and $P^t_y[i] = Y[i] * rs$.

See also

make_pair_table(), rna_plot_type, simple_xy_coordinates(), naview_xy_coordinates(), PS_rna_plot_a(), PS_rna_plot, svg_rna_plot()

Parameters

pair_table	The pair table of the secondary structure
x	a pointer to an array with enough allocated space to hold the x coordinates
y	a pointer to an array with enough allocated space to hold the y coordinates

Returns

length of sequence on success, 0 otherwise

11.25.4 Variable Documentation

11.25.4.1 int rna_plot_type

Switch for changing the secondary structure layout algorithm.

Current possibility are 0 for a simple radial drawing or 1 for the modified radial drawing taken from the *naview* program of Bruccoleri & Heinrich (1988).

Note

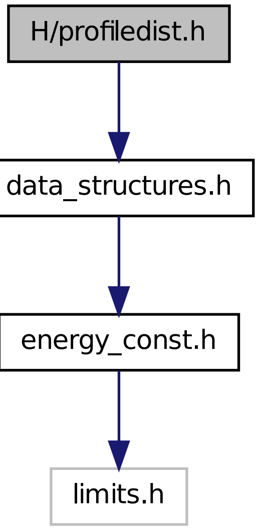
To provide thread safety please do not rely on this global variable in future implementations but pass a plot type flag directly to the function that decides which layout algorithm it may use!

See also

VRNA_PLOT_TYPE_SIMPLE, VRNA_PLOT_TYPE_NAVIEW, VRNA_PLOT_TYPE_-CIRCULAR

11.26 H/profiledist.h File Reference

Include dependency graph for profiledist.h:



Functions

- float profile_edit_distance (const float ∗T1, const float ∗T2)

  Align the 2 probability profiles T1, T2

  .
- float ∗ Make_bp_profile_bppm (FLT_OR_DBL ∗bppm, int length)

  condense pair probability matrix into a vector containing probabilities for upstream paired, downstream paired and unpaired.
- void print_bppm (const float ∗T)

  print string representation of probability profile
- void free_profile (float ∗T)

  free space allocated in Make_bp_profile
- float ∗ Make_bp_profile (int length)

11.26.1 Detailed Description

11.26.2 Function Documentation

11.26.2.1 float profile_edit_distance (const float * *T1*, const float * *T2*)

Align the 2 probability profiles T1, T2

.

This is like a Needleman-Wunsch alignment, we should really use affine gap-costs ala Gotoh

11.26.2.2 float* Make_bp_profile_bppm (FLT_OR_DBL * *bppm*, int *length*)

condense pair probability matrix into a vector containing probabilities for upstream paired, downstream paired and unpaired.

This resulting probability profile is used as input for profile_edit_distance

Parameters

bppm	A pointer to the base pair probability matrix
length	The length of the sequence

Returns

The bp profile

11.26.2.3 void free_profile (float * *T*)

free space allocated in Make_bp_profile

Backward compatibility only. You can just use plain free()

11.26.2.4 float* Make_bp_profile (int *length*)

Note

This function is NOT threadsafe

See also

Make_bp_profile_bppm()

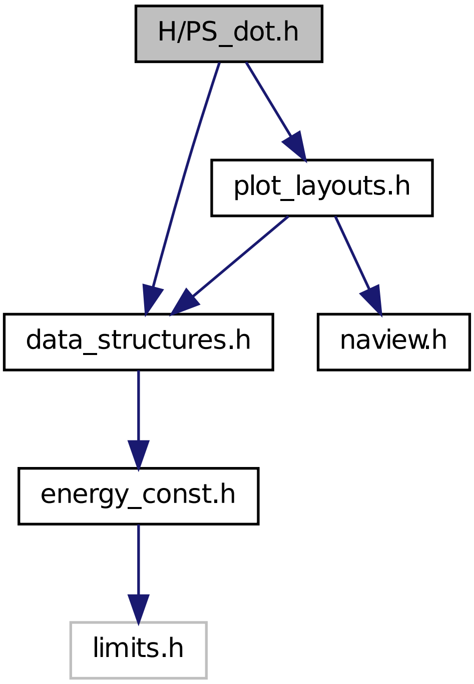
Deprecated

This function is deprecated and will be removed soon! See Make_bp_profile_-bppm() for a replacement

11.27 H/PS_dot.h File Reference

Various functions for plotting RNA secondary structures, dot-plots and other visualizations.

Include dependency graph for PS_dot.h:



Functions

- int PS_rna_plot (char ∗string, char ∗structure, char ∗file)

  Produce a secondary structure graph in PostScript and write it to 'filename'.
- int PS_rna_plot_a (char ∗string, char ∗structure, char ∗file, char ∗pre, char ∗post)

  Produce a secondary structure graph in PostScript including additional annotation macros and write it to 'filename'.
- int gmlRNA (char ∗string, char ∗structure, char ∗ssfile, char option)

  Produce a secondary structure graph in Graph Meta Language (gml) and write it to a file.
- int ssv_rna_plot (char ∗string, char ∗structure, char ∗ssfile)

  Produce a secondary structure graph in SStructView format.
- int svg_rna_plot (char ∗string, char ∗structure, char ∗ssfile)

  Produce a secondary structure plot in SVG format and write it to a file.
- int xrna_plot (char ∗string, char ∗structure, char ∗ssfile)

Produce a secondary structure plot for further editing in XRNA.

- int PS_dot_plot_list (char ∗seq, char ∗filename, plist ∗pl, plist ∗mf, char ∗comment)

  Produce a postscript dot-plot from two pair lists.
- int aliPS_color_aln (const char ∗structure, const char ∗filename, const char ∗seqs[ ], const char ∗names[ ])

  PS_color_aln for duplexes.
- int PS_dot_plot (char ∗string, char ∗file)

  Wrapper to PS_dot_plot_list.

11.27.1 Detailed Description

Various functions for plotting RNA secondary structures, dot-plots and other visualizations.

11.27.2 Function Documentation

11.27.2.1 int PS_rna_plot (char ∗ *string,* char ∗ *structure,* char ∗ *file*)

Produce a secondary structure graph in PostScript and write it to 'filename'.

Note that this function has changed from previous versions and now expects the structure to be plotted in dot-bracket notation as an argument. It does not make use of the global base_pair array anymore.

Parameters

string	The RNA sequence
structure	The secondary structure in dot-bracket notation
file	The filename of the postscript output

Returns

1 on success, 0 otherwise

11.27.2.2 int PS_rna_plot_a (char ∗ *string,* char ∗ *structure,* char ∗ *file,* char ∗ *pre,* char ∗ *post*)

Produce a secondary structure graph in PostScript including additional annotation macros and write it to 'filename'.

Same as PS_rna_plot() but adds extra PostScript macros for various annotations (see generated PS code). The 'pre' and 'post' variables contain PostScript code that is verbatim copied in the resulting PS file just before and after the structure plot. If both arguments ('pre' and 'post') are NULL, no additional macros will be printed into the PostScript.

Parameters

string	The RNA sequence
structure	The secondary structure in dot-bracket notation
file	The filename of the postscript output
pre	PostScript code to appear before the secondary structure plot
post	PostScript code to appear after the secondary structure plot

Returns

1 on success, 0 otherwise

11.27.2.3 int gmlRNA (char ∗ *string,* char ∗ *structure,* char ∗ *ssfile,* char *option*)

Produce a secondary structure graph in Graph Meta Language (gml) and write it to a file.

If 'option' is an uppercase letter the RNA sequence is used to label nodes, if 'option' equals *'X'* or *'x'* the resulting file will coordinates for an initial layout of the graph.

Parameters

string	The RNA sequence
structure	The secondary structure in dot-bracket notation
ssfile	The filename of the gml output
option	The option flag

Returns

1 on success, 0 otherwise

11.27.2.4 int ssv_rna_plot (char ∗ *string,* char ∗ *structure,* char ∗ *ssfile*)

Produce a secondary structure graph in SStructView format.

Write coord file for SStructView

Parameters

string	The RNA sequence
structure	The secondary structure in dot-bracket notation
ssfile	The filename of the ssv output

Returns

1 on success, 0 otherwise

11.27.2.5 int svg_rna_plot (char ∗ *string,* char ∗ *structure,* char ∗ *ssfile*)

Produce a secondary structure plot in SVG format and write it to a file.

Parameters

string	The RNA sequence
structure	The secondary structure in dot-bracket notation
ssfile	The filename of the svg output

Returns

1 on success, 0 otherwise

11.27.2.6 int xrna_plot (char ∗ *string,* char ∗ *structure,* char ∗ *ssfile*)

Produce a secondary structure plot for further editing in XRNA.

Parameters

string	The RNA sequence
structure	The secondary structure in dot-bracket notation
ssfile	The filename of the xrna output

Returns

1 on success, 0 otherwise

11.27.2.7 int PS_dot_plot_list (char ∗ *seq,* char ∗ *filename,* plist ∗ *pl,* plist ∗ *mf,* char ∗ *comment*)

Produce a postscript dot-plot from two pair lists.

This function reads two plist structures (e.g. base pair probabilities and a secondary structure) as produced by assign_plist_from_pr() and assign_plist_from_db() and produces a postscript "dot plot" that is written to 'filename'.

Using base pair probabilities in the first and mfe structure in the second plist, the resulting "dot plot" represents each base pairing probability by a square of corresponding area in a upper triangle matrix. The lower part of the matrix contains the minimum free energy structure.

See also

assign_plist_from_pr(), assign_plist_from_db()

Parameters

seq	The RNA sequence
filename	A filename for the postscript output
pl	The base pair probability pairlist
mf	The mfe secondary structure pairlist
comment	A comment

Returns

1 if postscript was successfully written, 0 otherwise

11.27.2.8 int PS_dot_plot (char * *string*, char * *file*)

Wrapper to PS_dot_plot_list.

Produce postscript dot-plot

Reads base pair probabilities produced by pf_fold() from the global array pr and the pair list base_pair produced by fold() and produces a postscript "dot plot" that is written to 'filename'. The "dot plot" represents each base pairing probability by a square of corresponding area in a upper triangle matrix. The lower part of the matrix contains the minimum free energy

Note

DO NOT USE THIS FUNCTION ANYMORE SINCE IT IS NOT THREADSAFE

Deprecated

This function is deprecated and will be removed soon! Use PS_dot_plot_list() instead!

11.28 H/read_epars.h File Reference

Functions to read and write energy parameter sets from/to files.

Functions

- void read_parameter_file (const char fname[ ])

  Read energy parameters from a file.
- void write_parameter_file (const char fname[ ])

  Write energy parameters to a file.

11.28.1 Detailed Description

Functions to read and write energy parameter sets from/to files.

11.28.2 Function Documentation

11.28.2.1 void read_parameter_file (const char *fname[ ]*)

Read energy parameters from a file.

Parameters

fname	The path to the file containing the energy parameters

11.28.2.2 void write_parameter_file (const char *fname[ ]*)

Write energy parameters to a file.

Parameters

fname	A filename (path) for the file where the current energy parameters will be written to

11.29 H/RNAstruct.h File Reference

Parsing and Coarse Graining of Structures.

Functions

- char ∗ b2HIT (const char ∗structure)

  Converts the full structure from bracket notation to the HIT notation including root.
- char ∗ b2C (const char ∗structure)

  Converts the full structure from bracket notation to the a coarse grained notation using the 'H' 'B' 'I' 'M' and 'R' identifiers.
- char ∗ b2Shapiro (const char ∗structure)

  Converts the full structure from bracket notation to the weighted coarse grained notation using the 'H' 'B' 'I' 'M' 'S' 'E' and 'R' identifiers.
- char ∗ add_root (const char ∗structure)

  Adds a root to an un-rooted tree in any except bracket notation.
- char ∗ expand_Shapiro (const char ∗coarse)

  Inserts missing 'S' identifiers in unweighted coarse grained structures as obtained from b2C().
- char ∗ expand_Full (const char ∗structure)

  Convert the full structure from bracket notation to the expanded notation including root.
- char ∗ unexpand_Full (const char ∗ffull)

  Restores the bracket notation from an expanded full or HIT tree, that is any tree using only identifiers 'U' 'P' and 'R'.
- char ∗ unweight (const char ∗wcoarse)

  Strip weights from any weighted tree.
- void unexpand_aligned_F (char ∗align[2])

  Converts two aligned structures in expanded notation.
- void parse_structure (const char ∗structure)

  Collects a statistic of structure elements of the full structure in bracket notation.

Variables

- int loop_size [STRUC]

  contains a list of all loop sizes.
- int helix_size [STRUC]

  contains a list of all stack sizes.
- int loop_degree [STRUC]

  contains the corresponding list of loop degrees.
- int loops

  contains the number of loops (and therefore of stacks).
- int unpaired

  contains the number of unpaired bases.
- int pairs

  contains the number of base pairs in the last parsed structure.

11.29.1 Detailed Description

Parsing and Coarse Graining of Structures. Example:

```
*   .((..(((...)))..((..)))).   is the bracket or full tree
*   becomes expanded:   - expand_Full() -
*   ((U)(((U)(U)((((U)(U)(U)P)P)P)(U)(U)(((U)(U)P)P)P)P)(U)R)
*   HIT:                - b2HIT() -
*   ((U1)((U2)((U3)P3)(U2)((U2)P2)P2)(U1)R)
*   Coarse:             - b2C() -
*   ((H)((H)M)R)
*   becomes expanded:   - expand_Shapiro() -
*   (((((H)S)((H)S)M)S)R)
*   weighted Shapiro:   - b2Shapiro() -
*   ((((((H3)S3)((H2)S2)M4)S2)E2)R)
*
```

11.29.2 Function Documentation

11.29.2.1 char∗ b2HIT (const char ∗ *structure*)

Converts the full structure from bracket notation to the HIT notation including root.

Parameters

structure	

Returns

11.29.2.2 char∗ b2C (const char ∗ *structure*)

Converts the full structure from bracket notation to the a coarse grained notation using the 'H' 'B' 'I' 'M' and 'R' identifiers.

Parameters

structure	

Returns

11.29.2.3 char∗ b2Shapiro (const char ∗ *structure*)

Converts the full structure from bracket notation to the *weighted* coarse grained notation using the 'H' 'B' 'I' 'M' 'S' 'E' and 'R' identifiers.

Parameters

structure	

Returns

11.29.2.4 char∗ add_root (const char ∗ *structure*)

Adds a root to an un-rooted tree in any except bracket notation.

Parameters

structure	

Returns

11.29.2.5 char∗ expand_Shapiro (const char ∗ *coarse*)

Inserts missing 'S' identifiers in unweighted coarse grained structures as obtained from b2C().

Parameters

coarse	

Returns

11.29.2.6 char* expand_Full (const char * *structure*)

Convert the full structure from bracket notation to the expanded notation including root.

Parameters

structure	

Returns

11.29.2.7 char* unexpand_Full (const char * *ffull*)

Restores the bracket notation from an expanded full or HIT tree, that is any tree using only identifiers 'U' 'P' and 'R'.

Parameters

ffull	

Returns

11.29.2.8 char* unweight (const char * *wcoarse*)

Strip weights from any weighted tree.

Parameters

wcoarse	

Returns

11.29.2.9 void unexpand_aligned_F (char * *align[2]*)

Converts two aligned structures in expanded notation.

Takes two aligned structures as produced by tree_edit_distance() function back to bracket notation with '_' as the gap character. The result overwrites the input.

Parameters

align	

11.29.2.10 void parse_structure (const char * *structure*)

Collects a statistic of structure elements of the full structure in bracket notation.

The function writes to the following global variables: loop_size, loop_degree, helix_size, loops, pairs, unpaired

Parameters

structure	

Returns

11.29.3 Variable Documentation

11.29.3.1 int loop_size[STRUC]

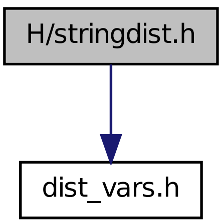
contains a list of all loop sizes.

loop_size[0] contains the number of external bases.

11.30 H/stringdist.h File Reference

Functions for String Alignment.

Include dependency graph for stringdist.h:



Functions

- swString * Make_swString (char *string)

  Convert a structure into a format suitable for string_edit_distance().
- float string_edit_distance (swString *T1, swString *T2)

  Calculate the string edit distance of T1 and T2.

11.30.1 Detailed Description

Functions for String Alignment.

11.30.2 Function Documentation

11.30.2.1 swString* Make_swString (char * *string*)

Convert a structure into a format suitable for string_edit_distance().

Parameters

string	

Returns

11.30.2.2 float string_edit_distance (swString * *T1*, swString * *T2*)

Calculate the string edit distance of T1 and T2.

Parameters

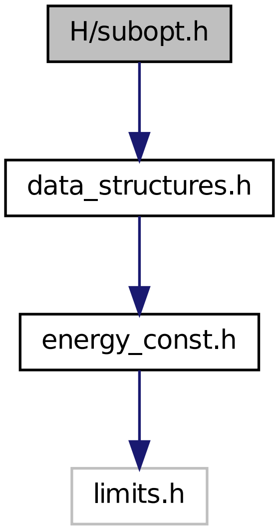
T1	
T2	

Returns

11.31 H/subopt.h File Reference

RNAsubopt and density of states declarations.

Include dependency graph for subopt.h:



Functions

- SOLUTION * subopt (char *seq, char *sequence, int delta, FILE *fp)

  Returns list of subopt structures or writes to fp.
- SOLUTION * subopt_circ (char *seq, char *sequence, int delta, FILE *fp)

  Returns list of circular subopt structures or writes to fp.

Variables

- int subopt_sorted

  Sort output by energy.
- double print_energy

  printing threshold for use with logML

11.31.1 Detailed Description

RNAsubopt and density of states declarations.

11.31.2 Function Documentation

11.31.2.1 SOLUTION∗ subopt (char ∗ *seq*, char ∗ *sequence*, int *delta*, FILE ∗ *fp*)

Returns list of subopt structures or writes to fp.

This function produces **all** suboptimal secondary structures within 'delta' ∗ 0.01 kcal/mol of the optimum. The results are either directly written to a 'fp' (if 'fp' is not NULL), or (fp==NULL) returned in a SOLUTION ∗ list terminated by an entry were the 'structure' pointer is NULL.

Parameters

seq	
sequence	
delta	
fp	

Returns

11.31.2.2 SOLUTION∗ subopt_circ (char ∗ *seq*, char ∗ *sequence*, int *delta*, FILE ∗ *fp*)

Returns list of circular subopt structures or writes to fp.

This function is similar to subopt() but calculates secondary structures assuming the RNA sequence to be circular instead of linear

Parameters

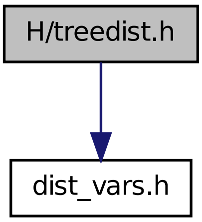
seq	
sequence	
delta	
fp	

Returns

11.32 H/treedist.h File Reference

Functions for Tree Edit Distances.

Include dependency graph for treedist.h:



Functions

- Tree ∗ make_tree (char ∗struc)

    Constructs a Tree (essentially the postorder list) of the structure 'struc', for use in tree_edit_distance().
- float tree_edit_distance (Tree ∗T1, Tree ∗T2)

    Calculates the edit distance of the two trees.
- void print_tree (Tree ∗t)

    Print a tree (mainly for debugging)
- void free_tree (Tree ∗t)

    Free the memory allocated for Tree t.

11.32.1 Detailed Description

Functions for Tree Edit Distances.

11.32.2 Function Documentation

11.32.2.1 Tree∗ make_tree (char ∗ *struc*)

Constructs a Tree (essentially the postorder list) of the structure 'struc', for use in tree_edit_distance().

Parameters

struc	may be any rooted structure representation.

Returns

11.32.2.2 float tree_edit_distance (Tree * *T1*, Tree * *T2*)

Calculates the edit distance of the two trees.

Parameters

T1	
T2	

Returns

11.32.2.3 void free_tree (Tree * *t*)

Free the memory allocated for Tree t.

Parameters

t	

11.33 H/utils.h File Reference

Various utility- and helper-functions used throughout the Vienna RNA package.

Defines

- #define VRNA_INPUT_ERROR 1U

  Output flag of get_input_line(): "An ERROR has occured, maybe EOF".
- #define VRNA_INPUT_QUIT 2U

  Output flag of get_input_line(): "the user requested quitting the program".
- #define VRNA_INPUT_MISC 4U

  Output flag of get_input_line(): "something was read".
- #define VRNA_INPUT_FASTA_HEADER 8U

  Input/Output flag of get_input_line():
  if used as input option this tells get_input_line() that the data to be read should comply with the FASTA format.
- #define VRNA_INPUT_SEQUENCE 16U

  Input flag for get_input_line():
  Tell get_input_line() that we assume to read a nucleotide sequence.
- #define VRNA_INPUT_CONSTRAINT 32U

Input flag for get_input_line():
Tell get_input_line() that we assume to read a structure constraint.

- #define VRNA_INPUT_NO_TRUNCATION 256U

  Input switch for get_input_line(): "do not trunkate the line by eliminating white spaces at end of line".
- #define VRNA_INPUT_NO_REST 512U

  Input switch for read_record(): "do fill rest array".
- #define VRNA_INPUT_NO_SPAN 1024U

  Input switch for read_record(): "never allow data to span more than one line".
- #define VRNA_INPUT_NOSKIP_BLANK_LINES 2048U

  Input switch for read_record(): "do not skip empty lines".
- #define VRNA_INPUT_BLANK_LINE 4096U

  Output flag for read_record(): "read an empty line".
- #define VRNA_INPUT_NOSKIP_COMMENTS 128U

  Input switch for get_input_line(): "do not skip comment lines".
- #define VRNA_INPUT_COMMENT 8192U

  Output flag for read_record(): "read a comment".
- #define VRNA_CONSTRAINT_PIPE 1U

  pipe sign '|' switch for structure constraints (paired with another base)
- #define VRNA_CONSTRAINT_DOT 2U

  dot '.
- #define VRNA_CONSTRAINT_X 4U

  'x' switch for structure constraint (base must not pair)
- #define VRNA_CONSTRAINT_ANG_BRACK 8U

  angle brackets '$<$', '$>$' switch for structure constraint (paired downstream/upstream)
- #define VRNA_CONSTRAINT_RND_BRACK 16U

  round brackets '(',')' switch for structure constraint (base i pairs base j)
- #define VRNA_CONSTRAINT_MULTILINE 32U

  constraint may span over several lines
- #define VRNA_CONSTRAINT_NO_HEADER 64U

  do not print the header information line
- #define VRNA_CONSTRAINT_ALL 128U

  placeholder for all constraining characters
- #define MIN2(A, B) ((A) $<$ (B) ? (A) : (B))

  Get the minimum of two comparable values.
- #define MAX2(A, B) ((A) $>$ (B) ? (A) : (B))

  Get the maximum of two comparable values.
- #define MIN3(A, B, C) (MIN2((MIN2((A),(B))) ,(C)))

  Get the minimum of three comparable values.
- #define MAX3(A, B, C) (MAX2((MAX2((A),(B))) ,(C)))

  Get the maximum of three comparable values.
- #define XSTR(s) STR(s)

  Stringify a macro after expansion.
- #define STR(s) #s

Stringify a macro argument.

- #define FILENAME_MAX_LENGTH 80

  Maximum length of filenames that are generated by our programs.
- #define FILENAME_ID_LENGTH 42

  Maximum length of id taken from fasta header for filename generation.

Functions

- void ∗ space (unsigned size)

  Allocate space safely.
- void ∗ xrealloc (void ∗p, unsigned size)

  Reallocate space safely.
- void nrerror (const char message[])

  Die with an error message.
- void warn_user (const char message[])

  Print a warning message.
- void init_rand (void)

  Make random number seeds.
- double urn (void)

  get a random number from [0..1]
- int int_urn (int from, int to)

  Generates a pseudo random integer in a specified range.
- char ∗ time_stamp (void)

  Get a timestamp.
- char ∗ random_string (int l, const char symbols[])

  Create a random string using characters from a specified symbol set.
- int hamming (const char ∗s1, const char ∗s2)

  Calculate hamming distance between two sequences.
- int hamming_bound (const char ∗s1, const char ∗s2, int n)

  Calculate hamming distance between two sequences up to a specified length.
- char ∗ get_line (FILE ∗fp)

  Read a line of arbitrary length from a stream.
- unsigned int get_input_line (char ∗∗string, unsigned int options)

  Retrieve a line from 'stdin' savely while skipping comment characters and other features This function returns the type of input it has read if recognized.
- unsigned int read_record (char ∗∗header, char ∗∗sequence, char ∗∗∗rest, unsigned int options)

  Get a data record from stdin.
- char ∗ pack_structure (const char ∗struc)

  Pack secondary secondary structure, 5:1 compression using base 3 encoding.
- char ∗ unpack_structure (const char ∗packed)

  Unpack secondary structure previously packed with pack_structure()
- short ∗ make_pair_table (const char ∗structure)

Create a pair table of a secondary structure.

- short ∗ copy_pair_table (const short ∗pt)

  Get an exact copy of a pair table.
- short ∗ alimake_pair_table (const char ∗structure)

  Pair table for snoop align.
- short ∗ make_pair_table_snoop (const char ∗structure)

  returns a newly allocated table, such that: table[i]=j if (i.j) pair or 0 if i is unpaired, table[0] contains the length of the structure.
- int bp_distance (const char ∗str1, const char ∗str2)

  Compute the "base pair" distance between two secondary structures s1 and s2.
- void print_tty_input_seq (void)

  Print a line to stdout that asks for an input sequence.
- void print_tty_input_seq_str (const char ∗s)

  Print a line with a user defined string and a ruler to stdout.
- void print_tty_constraint_full (void)

  Print structure constraint characters to stdout (full constraint support)
- void print_tty_constraint (unsigned int option)

  Print structure constraint characters to stdout.
- void str_DNA2RNA (char ∗sequence)

  Convert a DNA input sequence to RNA alphabet.
- void str_uppercase (char ∗sequence)

  Convert an input sequence to uppercase.
- int ∗ get_iindx (unsigned int length)

  Get an index mapper array (iindx) for accessing the energy matrices, e.g.
- int ∗ get_indx (unsigned int length)

  Get an index mapper array (indx) for accessing the energy matrices, e.g.
- void constrain_ptypes (const char ∗constraint, unsigned int length, char ∗ptype, int ∗BP, int min_loop_size, unsigned int idx_type)

  Insert constraining pair types according to constraint structure string.

Variables

- unsigned short xsubi [3]

  Current 48 bit random number.

11.33.1 Detailed Description

Various utility- and helper-functions used throughout the Vienna RNA package.

11.33.2 Define Documentation

11.33.2.1 #define VRNA_INPUT_FASTA_HEADER 8U

Input/Output flag of get_input_line():

if used as input option this tells get_input_line() that the data to be read should comply with the FASTA format.

the function will return this flag if a fasta header was read

11.33.2.2 #define VRNA_INPUT_SEQUENCE 16U

Input flag for get_input_line():

Tell get_input_line() that we assume to read a nucleotide sequence.

11.33.2.3 #define VRNA_INPUT_CONSTRAINT 32U

Input flag for get_input_line():

Tell get_input_line() that we assume to read a structure constraint.

11.33.2.4 #define VRNA_CONSTRAINT_DOT 2U

dot '.

' switch for structure constraints (no constraint at all)

11.33.2.5 #define FILENAME_MAX_LENGTH 80

Maximum length of filenames that are generated by our programs.

This definition should be used throughout the complete ViennaRNA package wherever a static array holding filenames of output files is declared.

11.33.2.6 #define FILENAME_ID_LENGTH 42

Maximum length of id taken from fasta header for filename generation.

this has to be smaller than FILENAME_MAX_LENGTH since in most cases, some suffix will be appended to the ID

11.33.3 Function Documentation

11.33.3.1 void* space (unsigned *size*)

Allocate space safely.

Parameters

size	The size of the memory to be allocated in bytes

Returns

A pointer to the allocated memory

11.33.3.2 void∗ xrealloc (void ∗ *p*, unsigned *size*)

Reallocate space safely.

Parameters

p	A pointer to the memory region to be reallocated
size	The size of the memory to be allocated in bytes

Returns

A pointer to the newly allocated memory

11.33.3.3 void nrerror (const char *message[ ]*)

Die with an error message.

See also

warn_user()

Parameters

message	The error message to be printed before exiting with 'FAILURE'

11.33.3.4 void warn_user (const char *message[ ]*)

Print a warning message.

Print a warning message to *stderr*

Parameters

message	The warning message

11.33.3.5 double urn (void)

get a random number from [0..1]

Note

Usually implemented by calling *erand48()*.

Returns

A random number in range [0..1]

11.33.3.6 int int_urn (int *from,* int *to*)

Generates a pseudo random integer in a specified range.

Parameters

from	The first number in range
to	The last number in range

Returns

A pseudo random number in range [from, to]

11.33.3.7 char∗ time_stamp (void)

Get a timestamp.
Returns a string containing the current date in the format

```
Fri Mar 19 21:10:57 1993
```

Returns

A string containing the timestamp

11.33.3.8 char∗ random_string (int *l,* const char *symbols[ ]*)

Create a random string using characters from a specified symbol set.

Parameters

l	The length of the sequence
symbols	The symbol set

Returns

A random string of length 'l' containing characters from the symbolset

11.33.3.9 int hamming (const char * *s1*, const char * *s2*)

Calculate hamming distance between two sequences.

Calculate the number of positions in which

Parameters

s1	The first sequence
s2	The second sequence

Returns

The hamming distance between s1 and s2

11.33.3.10 int hamming_bound (const char * *s1*, const char * *s2*, int *n*)

Calculate hamming distance between two sequences up to a specified length.

This function is similar to hamming() but instead of comparing both sequences up to their actual length only the first 'n' characters are taken into account

Parameters

s1	The first sequence
s2	The second sequence

Returns

The hamming distance between s1 and s2

11.33.3.11 char* get_line (FILE * *fp*)

Read a line of arbitrary length from a stream.

Returns a pointer to the resulting string. The necessary memory is allocated and should be released using *free()* when the string is no longer needed.

Parameters

fp	A file pointer to the stream where the function should read from

Returns

A pointer to the resulting string

11.33.3.12 unsigned int get_input_line (char ** *string*, unsigned int *options*)

Retrieve a line from 'stdin' savely while skipping comment characters and other features This function returns the type of input it has read if recognized.

An option argument allows to switch between different reading modes.

Currently available options are:

#VRNA_INPUT_NOPRINT_COMMENTS, VRNA_INPUT_NOSKIP_COMMENTS, #VRNA_-INPUT_NOELIM_WS_SUFFIX

pass a collection of options as one value like this:

```
get_input_line(string, option_1 | option_2 | option_n)
```

If the function recognizes the type of input, it will report it in the return value. It also reports if a user defined 'quit' command (@-sign on 'stdin') was given. Possible return values are:

VRNA_INPUT_FASTA_HEADER, VRNA_INPUT_ERROR, VRNA_INPUT_MISC, VRNA_-INPUT_QUIT

Parameters

string	A pointer to the character array that contains the line read
options	A collection of options for switching the functions behavior

Returns

A flag with information about what has been read

11.33.3.13 unsigned int read_record (char ** *header*, char ** *sequence*, char *** *rest*, unsigned int *options*)

Get a data record from stdin.

This function may be used to obtain complete datasets from stdin. A dataset is always defined to contain at least a sequence. If data on stdin starts with a fasta header, i.e. a line like

```
>some header info
```

then read_record() will assume that the sequence that follows the header may span over several lines. To disable this behavior and to assign a single line to the argument 'sequence' one can pass VRNA_INPUT_NO_SPAN in the 'options' argument. If no fasta header is read in the beginning of a data block, a sequence must not span over multiple lines!

Unless the options VRNA_INPUT_NOSKIP_COMMENTS or VRNA_INPUT_NOSKIP_-BLANK_LINES are passed, a sequence may be interrupted by lines starting with a comment character or empty lines.

A sequence is regarded as completely read if it was either assumed to not span over multiple lines, a secondary structure or structure constraint follows the sequence on the next line or a new header marks the beginning of a new sequence...

All lines following the sequence (this includes comments) and not initiating a new dataset are available through the line-array 'rest'. Here one can usually find the structure constraint or other information belonging to the current dataset. Filling of 'rest' may be prevented by passing VRNA_INPUT_NO_REST to the options argument.

Note

This function will exit any program with an error message if no sequence could be read!

The main purpose of this function is to be able to easily parse blocks of data from stdin in the header of a loop where all calculations for the appropriate data is done inside the loop. The loop may be then left on certain return values, e.g.:

```
char *id, *seq, **rest;
int  i;
while(!(read_record(&id, &seq, &rest, 0) & (VRNA_INPUT_ERROR | VRNA_INPUT_QUIT))){
  if(id) printf("%s\n", id);
  printf("%s\n", seq);
  if(rest)
    for(i=0;rest[i];i++)
      printf("%s\n", rest[i]);
}
```

In the example above, the while loop will be terminated when read_record() returns either an error or a user initiated quit request.

As long as data is read from stdin, the id is printed if it is available for the current block of data. The sequence will be printed in any case and if some more lines belong to the current block of data each line will be printed as well.

Note

Do not forget to free the memory occupied by header, sequence and rest!

Parameters

header	A pointer which will be set such that it points to the header of the record
sequence	A pointer which will be set such that it points to the sequence of the record
rest	A pointer which will be set such that it points to an array of lines which also belong to the record
options	Some options which may be passed to alter the behavior of the function, use 0 for no options

Returns

A flag with information about what the function actually did read

11.33.3.14 char* pack_structure (const char * *struc*)

Pack secondary secondary structure, 5:1 compression using base 3 encoding.

Returns a binary string encoding of the secondary structure using a 5:1 compression scheme. The string is NULL terminated and can therefore be used with standard string functions such as strcmp(). Useful for programs that need to keep many structures in memory.

Parameters

struc	The secondary structure in dot-bracket notation

Returns

The binary encoded structure

11.33.3.15 char∗ unpack_structure (const char ∗ *packed*)

Unpack secondary structure previously packed with pack_structure()

Translate a compressed binary string produced by pack_structure() back into the familiar dot-bracket notation.

Parameters

packed	The binary encoded packed secondary structure

Returns

The unpacked secondary structure in dot-bracket notation

11.33.3.16 short∗ make_pair_table (const char ∗ *structure*)

Create a pair table of a secondary structure.

Returns a newly allocated table, such that table[i]=j if (i.j) pair or 0 if i is unpaired, table[0] contains the length of the structure.

Parameters

structure	The secondary structure in dot-bracket notation

Returns

A pointer to the created pair_table

11.33.3.17 short∗ copy_pair_table (const short ∗ *pt*)

Get an exact copy of a pair table.

Parameters

pt	The pair table to be copied

Returns

A pointer to the copy of 'pt'

11.33.3.18 short* alimake_pair_table (const char * *structure*)

Pair table for snoop align.

11.33.3.19 short* make_pair_table_snoop (const char * *structure*)

returns a newly allocated table, such that: table[i]=j if (i.j) pair or 0 if i is unpaired, table[0] contains the length of the structure.

The special pseudoknotted H/ACA-mRNA structure is taken into account.

11.33.3.20 int bp_distance (const char * *str1*, const char * *str2*)

Compute the "base pair" distance between two secondary structures s1 and s2.

The sequences should have the same length. dist = number of base pairs in one structure but not in the other same as edit distance with open-pair close-pair as move-set

Parameters

str1	First structure in dot-bracket notation
str2	Second structure in dot-bracket notation

Returns

The base pair distance between str1 and str2

11.33.3.21 void print_tty_input_seq (void)

Print a line to *stdout* that asks for an input sequence.

There will also be a ruler (scale line) printed that helps orientation of the sequence positions

11.33.3.22 void print_tty_input_seq_str (const char * *s*)

Print a line with a user defined string and a ruler to stdout.

(usually this is used to ask for user input) There will also be a ruler (scale line) printed that helps orientation of the sequence positions

Parameters

s	A user defined string that will be printed to stdout

11.33.3.23 void print_tty_constraint_full (void)

Print structure constraint characters to stdout (full constraint support)

11.33.3.24 void print_tty_constraint (unsigned int *option*)

Print structure constraint characters to stdout.

(constraint support is specified by option parameter)

Currently available options are:

VRNA_CONSTRAINT_PIPE (paired with another base)

VRNA_CONSTRAINT_DOT (no constraint at all)

VRNA_CONSTRAINT_X (base must not pair)

VRNA_CONSTRAINT_ANG_BRACK (paired downstream/upstream)

VRNA_CONSTRAINT_RND_BRACK (base i pairs base j)

pass a collection of options as one value like this:

```
print_tty_constraint(option_1 | option_2 | option_n)
```

Parameters

option	Option switch that tells which constraint help will be printed

11.33.3.25 void str_DNA2RNA (char * *sequence*)

Convert a DNA input sequence to RNA alphabet.

This function substitudes *T* and *t* with *U* and *u*, respectively

Parameters

sequence	The sequence to be converted

11.33.3.26 void str_uppercase (char * *sequence*)

Convert an input sequence to uppercase.

Parameters

sequence	The sequence to be converted

11.33.3.27 int* get_iindx (unsigned int *length*)

Get an index mapper array (iindx) for accessing the energy matrices, e.g.

in partition function related functions.

Access of a position "(i,j)" is then accomplished by using

```
(i,j) ~ iindx[i]-j
```

This function is necessary as most of the two-dimensional energy matrices are actually one-dimensional arrays throughout the ViennaRNAPackage

Consult the implemented code to find out about the mapping formula ;)

See also

get_indx()

Parameters

length	The length of the RNA sequence

Returns

The mapper array

11.33.3.28 int* get_indx (unsigned int *length*)

Get an index mapper array (indx) for accessing the energy matrices, e.g.

in MFE related functions.

Access of a position "(i,j)" is then accomplished by using

```
(i,j) ~ indx[j]+i
```

This function is necessary as most of the two-dimensional energy matrices are actually one-dimensional arrays throughout the ViennaRNAPackage

Consult the implemented code to find out about the mapping formula ;)

See also

get_iindx()

Parameters

length	The length of the RNA sequence

Returns

The mapper array

11.33.3.29 void constrain_ptypes (const char * *constraint*, unsigned int *length*, char * *ptype*, int * *BP*, int *min_loop_size*, unsigned int *idx_type*)

Insert constraining pair types according to constraint structure string.

See also

get_indx(), get_iindx()

Parameters

constraint	The structure constraint string
length	The actual length of the sequence (constraint may be shorter)
ptype	A pointer to the basepair type array
min_loop_-size	The minimal loop size (usually TURN)
idx_type	Define the access type for base pair type array (0 = indx, 1 = iindx)

11.33.4 Variable Documentation

11.33.4.1 unsigned short xsubi[3]

Current 48 bit random number.

This variable is used by urn(). These should be set to some random number seeds before the first call to urn().

See also

urn()

11.34 lib/1.8.4_epars.h File Reference

Free energy parameters for parameter file conversion.

11.34.1 Detailed Description

Free energy parameters for parameter file conversion. This file contains the free energy parameters used in ViennaRNAPackage 1.8.4. They are summarized in:

D.H.Mathews, J. Sabina, M. ZUker, D.H. Turner "Expanded sequence dependence of thermodynamic parameters improves prediction of RNA secondary structure" JMB, 288, pp 911-940, 1999

Enthalpies taken from:

A. Walter, D Turner, J Kim, M Lyttle, P M"uller, D Mathews, M Zuker "Coaxial stckaing of helices enhances binding of oligoribonucleotides.." PNAS, 91, pp 9218-9222, 1994

D.H. Turner, N. Sugimoto, and S.M. Freier. "RNA Structure Prediction", Ann. Rev. Biophys. Biophys. Chem. 17, 167-192, 1988.

John A.Jaeger, Douglas H.Turner, and Michael Zuker. "Improved predictions of secondary structures for RNA", PNAS, 86, 7706-7710, October 1989.

L. He, R. Kierzek, J. SantaLucia, A.E. Walter, D.H. Turner "Nearest-Neughbor Parameters for GU Mismatches...." Biochemistry 1991, 30 11124-11132

A.E. Peritz, R. Kierzek, N, Sugimoto, D.H. Turner "Thermodynamic Study of Internal Loops in Oligoribonucleotides..." Biochemistry 1991, 30, 6428--6435

11.35 lib/1.8.4_intloops.h File Reference

Free energy parameters for interior loop contributions needed by the parameter file conversion functions.

11.35.1 Detailed Description

Free energy parameters for interior loop contributions needed by the parameter file conversion functions.

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