

NAME

chess2flya -- Chemical shift prediction for RNA

SYNOPSIS

chess2flya [-h] [-c num] [-f statistics-file] [-s sequence-file] [-w macro-file]

DESCRIPTION

The program CHES2FLYA uses as input a file with RNA sequence and secondary structure information in the .ct file format. This can be created manually or e.g. on [www.rnasoft.ca](http://www.rnasoft.ca). CHES2FLYA uses chemical shift statistics (statfile.tab) that were evaluated considering the neighbouring nucleotides and their position in the secondary structure (loop, bulge, stem, mismatch,...). Using these input data, CHES2FLYA generates a file (cyana.prot) containing predicted chemical shifts of all nucleotides of RNAs. Additionally an angle restraint file (cyana.aco) and a sequence file (cyana.seq) are prepared. These files can be used for automated assignment with the FLYA algorithm within CYANA.

The following options are available:

-h help  
-c prediction interval defined by the percentage of resonances in it [1-11] (default: 2)  
1: 50%, 2: 60%, 3: 70%, 4: 80%, 5: 90%, 6: 95%, 7: 98%, 8: 99%, 9: 99.5%, 10: 99.8%, 11: 99.9%  
-f input file with statistics table (default: statfile.tab)  
-s input file with RNA sequence and secondary structure (default: rna.ct)  
The file has to be in .ct format and can be created e.g. on <http://www.rnasoft.ca/>.  
-w output CYANA macro to generate Watson-Crick H-bond restraints (default: none)

FILES

chess2flya	script to start chess2flya
chess.flya.Linux	executable for Linux, called by chess2flya
chess.flya.Darwin	executable for Mac, called by chess2flya
statfile.tab	RNA chemical shift statistics table
FZL4.ct	example file with RNA sequence and secondary structure; can be created e.g. on <a href="http://www.rnasoft.ca/">http://www.rnasoft.ca/</a>
rnaflya.cya	example CYANA macro to run CHES2FLYA and FLYA automated assignment
rna.lib	additional CYANA library with rules for expected NOESY peaks
*.peaks	example input peak lists for FLYA

EXAMPLES

Run CHES2FLYA alone:

```
./chess2flya -s FZL4.ct -w wc.cya
```

Run CHES2FLYA and FLYA:

```
cyana rnaflya
```

REFERENCE

When reporting results obtained with CHES2FLYA, please cite this publication:

Aeschbacher, T., Schmidt, E., Blatter, M., Maris, C., Duss, O., Allain, F. H.-T., Guentert, P. & Schubert, M. Automated and assisted RNA resonance assignment using NMR chemical shift statistics. Nucl. Acids Res. 41, e172 (2013)

BUGS

On some computers it is necessary to increase the stacksize with the Unix command:  
limit stacksize unlimited

The input file with chemical shift statistics must not exceed 20000 lines. Other input files must not exceed 10000 lines.