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 CHESS2FLYA 1.0  Thomas Aeschbacher & Markus Blatter 2013
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-------------------------------------------------------------------------

The program CHESS2FLYA uses as input a file with secondary structure information in the .ct file format.
This can be created manually or e.g. on "www.rnasoft.ca". chess2flya creates then a .prot file containing
chemical shift prediction of all nucleotides of RNAs. Additionally an angle restraint file (.aco file),
a sequence file (.seq file) are prepared. These files are then used as an input for FLYA automated assignment
algorithm within CYANA (P.Guntert). chess2flya requires the statistics file Statfile.tab.


Usage: chess2flya [options]

#############################################################################################
        -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      file with statistics table (default Statfile.tab)
        -s      file with RNA sequence and secondary structure (default rnass.ct)
                The file has to be in the .ct format and can be created e.g. on http://www.rnasoft.ca/ .
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./chess2flya -h                 #--> Help appears
./chess2flya                    #--> Creates 60% prediction itervals for each shift of the secondary structure file 'rnass.ct' (Standard input file)
./chess2flya -s 'input.ct'      #--> Creates 60% prediction itervals for each shift of the secondary structure file 'input.ct'
./chess2flya -s 'input.ct' -c 3 #--> Creates 70% prediction itervals for each shift of the secondary structure file 'input.ct'

######################
# Given example:
# RNA stemloop FZL4
######################
cd CHESS2FLYA/demo
../chess2flya -s FZL4.ct -f ../Statfile.tab  #--> generates: cyana.aco, cyana.prot, cyana.seq, cyana.wc

#############################################################################################
#----------------------------------FLYA----(Peter Guntert)----------------------------------#
#############################################################################################
# requires Cyana3.9

# Unpack the FLYA.tar file by
tar -xvf FLYA.tar

# FLYA uses two directories, one with the original input data ("orig"), one for the
# actual calculation with the name of the project ("FZL4")
# "orig" should be accessible from "FZL4" via "../orig"
  mkdir FZL4                    #--> already created from the tar file
  mkdir orig                    #--> already created from the tar file

#required files in these direcctories:
# peak lists of the 1H-13C HSQC, 2D TOCSY and 2D NOESY spectra and for comparison also
# the assigned shift lists (if available) in xeasy format
./orig/FZL4_HSQC_PeakList
./orig/FZL4_NOESY_PeakList
./orig/FZL4_TOCSY_PeakList
./orig/FZL4_HSQC_ShiftList
./orig/FZL4_NOESY_ShiftList
./orig/FZL4_TOCSY_ShiftList
./orig/FZL4.aco                 #--> from cp ./CHESS2FLYA/cyana.aco ./orig/FZL4.aco
./orig/FZL4.prot                #--> from cp ./CHESS2FLYA/cyana.prot ./orig/FZL4.prot
./orig/FZL4.wc                  #--> from cp ./CHESS2FLYA/cyana.wc ./orig/FZL4.wc


# CYANA run macros
./FZL4/PREP.cya                 #--> please see the content of PREP.cya at the end
./FZL4/init.cya                 #--> please see the content of init.cya at the end
./FZL4/FLYA.cya                 #--> please see the content of FLYA.cya at the end
./FZL4/FZL4.seq                 #--> from cp ./CHESS2FLYA/cyana.seq ./orig/FZL4.seq


# in FZL4 directory:
# source CYANA 3.9 (or later) executables and run PREP.cya followed by FLYA.cya

 cyana PREP.cya                 -->  this will generate the following files:
                                stat.prot
                                ref.prot
                                NOESY.peaks
                                TOCSY.peaks
                                C13H1.peaks
                                all.aco

 cyana FLYA.cya                 -->  this will generate the following files:
                                flya.tab
                                flya.prot
                                TOCSY_exp.peaks
                                TOCSY_asn.peaks
                                NOESY_exp.peaks
                                NOESY_asn.peaks
                                C13H1_exp.peaks
                                C13H1_asn.peaks
                                flya.txt



#######################################--PREP.cya--#######################################
dir     := ../orig
input   := FZL4_NOESY_PeakList,FZL4_TOCSY_PeakList,FZL4_HSQC_PeakList
spectra := NOESY,TOCSY,C13H1
format  := NOESY H1 H2, TOCSY H1 H2, C13H1 C H

read prot $dir/FZL4.prot unknown=warn
write prot stat.prot

read prot $dir/FZL4_NOESY_ShiftList| unknown=warn
read prot $dir/FZL4_TOCSY_ShiftList| unknown=warn add
read prot $dir/FZL4_HSQC_ShiftList| unknown=warn add
write prot ref.prot

do i 1 length('spectra')
  read prot ref.prot
  read peaks $dir/$input(i)| format="$format(i)"
  write peaks $spectra(i) names
end do

read $dir/FZL4.aco unknown=warn
write all.aco

system "cp -a $dir/FZL4.wc wc.cya"
#############################################################################################

#######################################--FLYA.cya--#######################################
#noesy:=NOESY
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#scalar:=TOCSY,C13H1
calibration :=                      # NOE calibration parameters
structures  := 500,20               # number of initial, final structures
steps       := 10000                 # number of torsion angle dynamics steps
upl_values  := 2.4,5.2
randomseed  := 57923                 # random number generator seed
run_assign_reference:=ref.prot
run_assign_iterations:=15000
run_assign_population:=100
run_assign_statistics:=stat.prot
analyze_assign_group:="SugarC: C1\' H1\' / CONSOLIDATED, BasesC: C2 H2 C5 H5  C6 H6 C8 H8 / CONSOLIDATED, StemC: 1..8 14..21 C2 H2 C5 H5  C6 H6 C8 H8 C1\'
H1\' / CONSOLIDATED, AllC: CONSOLIDATED, Sugar: C1\' H1\', Bases: C2 H2 C5 H5  C6 H6 C8 H8, Stem: 1..8 14..21 C2 H2 C5 H5  C6 H6 C8 H8 C1\' H1\', ALL: *"

if (.not.existfile('start.pdb')) then
  ./init
  read aco all.aco
  wc
  sugarbond
  calc_all 100 #vtfmin
  overview start.ovw structures=20 pdb
end if

flya refprot=ref.prot noesy=$noesy scalar=$scalar runs=50 plot=
##############################################################################################

#######################################--init.cya--#########################################
path:=.,$cyanadir/macro
name:=FZL4
cyanalib
read seq $name.seq
noesy:=NOESY
scalar:=TOCSY,C13H1

tolerance:=0.02,0.02,0.3
assigncs_accH:=tolerance(1)
assigncs_accC:=tolerance(3)
assigncs_accN:=tolerance(3)

command NOESY_expect peaks
  atoms select "C1\' H1\' C2 H2 C5 H5  C6 H6 C8 H8 - C*"
  spectrum $peaks append distance=4.0 structures=20 probability=0.9
  spectrum $peaks append distance=6.0 structures=20 probability=0.8
  spectrum $peaks append distance=9.0 structures=20 probability=0.5
  spectrum $peaks append distance=14.0 structures=20 probability=0.3 write
#  atom select "*"
#  spectrum $peaks append distance=6.0 structures=20 probability=0.01
end

command TOCSY_expect peaks
  atoms select "H5 H6 URA RCYT"
  spectrum $peaks skipdiagonal append write
end

command C13H1_select
  atoms select "C1\' H1\' C2 H2 C5 H5  C6 H6 C8 H8"
end
##############################################################################################
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