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SIMULAID: simulation setup and analysis utilities, written by Mihaly Mezei
Version 02/25/2022; Memory use=1287 Mb; Maximum number of input records=250000
M. Mezei, J. Comp. Chem., Vol 31, 2658-2668 (2010). DOI:10.1002/jcc.21551
NOTE: input prompts showing ? will yield an explanation by typing just a ?
NOTE: input prompts showing + will yield a tip by typing just a +
Conversion files found in directory /simulaid
WARNING: could not determine if this is a cluster headnode
         Functions requiring sizable CPU time should be run on a compute node

SELECT run type:
Print all menu and submenu <F>unctions - - - - - - - - - - -  : f
Geometry <O>ptimization (orientation, smallest sphere) [3]  : o
<C>leanup (sort, renumber, regroup, round charges) - - - -  : c
<S>tructure file and type conversions [15] - - - - - - - - -  : s
<T>rajectory file and type conversions [4] - - - - - - - - -  : t
Atom <N>ame and residue name conversions [4] - - - - - - - -  : n
Trajectory - str<U>cture file conversions (pack/unpack) [4] : u
Conformation <E>dit (trans/rot/cent/algn/add/del, etc.) [15]: e
<M>iscellaneous (seq, RTF, UHBD, tors., Amber sum, etc.)[7] : m
<A>nalyze (TRAJELIX, RMSD, H-bonds, CV, etc.) [17] - - - -  : a
Cluste<R> atoms or data defined by a distance matrix [2] -  : r
Make the input <P>redictable - - - - - - - - - - - - - - -  : p
Open <L>ogfile logging the keyboard inputs - - - - - - - -  : l
<Q>uit Simulaid  - - - - - - - - - - - - - - - - - - - - -  : q  l
"Open logfile logging the keyboard inputs" selected
Name of the log file=seq.inp
File seq.inp (formatted) opened on unit  45
Keyboard inputs will be logged in the file seq.inp
Do you want to make the quizzes predictable (y/n/?) [y]
Interactive quizzes will not depend on the data.
Default options will be used and a message will be printed

SELECT run type:
Print all menu and submenu <F>unctions - - - - - - - - - - -  : f
Geometry <O>ptimization (orientation, smallest sphere) [3]  : o
<C>leanup (sort, renumber, regroup, round charges) - - - -  : c
<S>tructure file and type conversions [15] - - - - - - - - -  : s
<T>rajectory file and type conversions [4] - - - - - - - - -  : t
Atom <N>ame and residue name conversions [4] - - - - - - - -  : n
Trajectory - str<U>cture file conversions (pack/unpack) [4] : u
Conformation <E>dit (trans/rot/cent/algn/add/del, etc.) [15]: e
<M>iscellaneous (seq, RTF, UHBD, tors., Amber sum, etc.)[7] : m
<A>nalyze (TRAJELIX, RMSD, H-bonds, CV, etc.) [17] - - - -  : a
Cluste<R> atoms or data defined by a distance matrix [2] -  : r
Make the input <P>redictable - - - - - - - - - - - - - - -  : p
Open <L>ogfile logging the keyboard inputs - - - - - - - -  : l
<Q>uit Simulaid  - - - - - - - - - - - - - - - - - - - - -  : q  m
"Miscellaneous (seq, RTF, UHBD, tors., Amber sum, etc.)[7]" selected

SELECT miscellaneous file creation:
<E>xtract sequence - - - - - - - - - - - - - - - - - - - -  : e
<C>onvert sequence - - - - - - - - - - - - - - - - - - - -  : c
Create a <G>rasp .crg file - - - - - - - - - - - - - - - -  : g
Create a U<H>BD .dat file  - - - - - - - - - - - - - - - -  : h
Print neighboring PBC cel<L> centers, cell vertices  - - -  : l
Print a PDB file for a <R>ectangle (box) - - - - - - - - -  : r
Torsion <I>nput generation - - - - - - - - - - - - - - - -  : i
Create Charmm RT<F> residue record(s)  - - - - - - - - - -  : f
Summarize <A>mber energy decomposition tables (csv format)  : a
<Q>uit structure-derived file generation - - - - - - - - -  : q  e
"Extract sequence" selected
Name of the input STRUCTURE file=mcd.pdb
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File mcd.pdb (formatted) opened on unit  10
The input format is established as PDB
The PDB format is found to be Brookhaven
Is that OK (y/n) [y]
The input format is established as Brookh. PDB
Do you have charges in the temperature factor column (y/n) [n]
Note: all heteroatoms will be kept and
      only the first of alternate records will be used
Do you want to read chemical symbols from col 77-78 (y/n) [y] n
TITLE MCD - Mast Cell Degranulating Peptide

SELECT MODEL record treatment:
<K>eep MODEL/ENDMDL records  - - - - - - - - - - - - - - - -  : k (default)
<D>elete MODEL/ENDMDL records  - - - - - - - - - - - - - - -  : d
Change ENDMDL to <E>ND and delete MODEL records  - - - - - -  : e
Change ENDMDL to <T>ER and delete MODEL records  - - - - - -  : t
"Keep MODEL/ENDMDL records" selected
REMARK A. Buku, I. Keselman, D. Lupyan, M. Mezei and J.A. Price,
REMARK Chem. Biol. Drug Des, 72, 13-139 (2008).
REMARK DOI:10.1111/j.1747-0285.2008.00684.x
Atom name starting with two upper-case charcters(HG) found
Are both characters part of the chemical symbol (y/n) [n]
Number of atoms found in the input file=    378
Title read:
MCD - Mast Cell Degranulating Peptide
Do you want to replace the title (y/n/+) [n]
Solvent residue name in the input file [HOH]=
Number of solute atoms found=         378
NOTE: no solvent residue HOH was found
Number of residues=          22  solute residues=          22
NOTE: residue numbers are not consecutive
Number of hydrogens in the solute=         200
There are   108 backbone atoms and     270 putative side chain solute atoms
 1    A      1-   378 Resid    1-   22 Resix    1-   22 MW=   2595 <B>=    0.0
The solute contains   22 amino acid residues   0 nucleic acid residues
and     0 unclassified residues
The volume of the solute is estimated to be    3281.29 A^3
Volume of the protein (part) is estimated to be     3281.29 A^3
Dimensions of the solute:
Smallest, middle and largest X coordinate values= -10.8400  -0.2500  10.3400
Smallest, middle and largest Y coordinate values= -12.8900  -1.6750   9.5400
Smallest, middle and largest Z coordinate values= -10.7070   0.8710  12.4490
Volume of enclosing rectangle=    11000.66 A^3


SELECT Output format for sequence list:
<C>harmm sequence input  - - - - - - - - - - - - - - - - - -  : c
PDB <S>SEQRES input  - - - - - - - - - - - - - - - - - - - -  : s
>Title + <1>-char list (FASTA) - - - - - - - - - - - - - - -  : 1
<P>IR  - - - - - - - - - - - - - - - - - - - - - - - - - - -  : p
<G>CG  - - - - - - - - - - - - - - - - - - - - - - - - - - -  : g  1
">Title + 1-char list (FASTA)" selected
Opening file mcd.seq
If the file exists, do you want to overwrite it (y/n) [n] y
File mcd.seq  (formatted) opened on unit  30
1-char sequence (input) list of     22 residues were written to file
    mcd.seq
```