LARMOR^{D} v1.0

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Purpose:	LARMOR^{D} is a simple and efficiency program predicting non-exchangeable ^{1}H and protonated ^{13}C RNA chemical shifts.
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Main Reference:	A Simple and Fast Approach for Predicting ^{1}H and ^{13}C Chemical Shifts: Toward Chemical Shift-Guided Simulations of RNA, **A.T. Frank, S.M. Law, and C.L. Brooks III**, *To Be Submitted*, 2014
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Source Files and Installation

- Makefile
- lib/
- src/
- tests/

LARMOR^{D} is written in C++ and can be compiled by issuing:

```
make
```

at the command line. An executable called “larmord” will be generated and can be found in the directory called “bin/”

To remove all object files and the executables issue:

```
make clean
```

Command Line Arguments

```
Usage:   larmord [-options] <PDBfile(s)>
Options: [-csfile CSfile]
         [-parmfile PARAMfile]
         [-trj TRAJfile]
         [-skip frames] [-start frame] [-stop frame]
         [-identification ID]
```

The LARMOR^{D} program requires at least one PDB file (`<PDBfile(s)>`) as input along with other optional arguments (`[-options]`). The order in which the required/optional arguments are provided does not matter.

`<PDBfile(s)>`

In its most basic form of usage, one or more PDB formatted files maybe be supplied to LARMOR^{D} for secondary structure element (SSE) analysis. The PDB files can take on any name and do not need to be of the same molecule. Also, a molecule can contain multiple chains.

Example 1:

```
larmord file.1.pdb
```

Example 2:

```
larmord file.1.pdb file.2.pdb file.3.pdb ... file.N.pdb
```

Example 3:

```
larmord a.pdb b.pdb c.pdb ... n.pdb
```

[-options]

The following are options that can be specified at the command line.

-trj TRAJfile

This option allows a CHARMM (binary) trajectory file to be analyzed. Only a single PDB file can be used with this option (or only the first PDB file is used if more than one is provided) and the number of atoms in the PDB must match the number of atoms in the trajectory file. Multiple trajectories (of the same molecule) can also be analyzed with multiple "-trj" arguments. Note that the first and second columns in the output represent the frame count and the simulation time, respectively.

Example 5:

```
larmord –trj file.1.dcd file.1.pdb
```

Example 6:

```
larmord –trj file.1.dcd –trj file.2.dcd file.1.pdb
```

[-skip frames] [-start frame] [-stop frame]

These options can be used to skip simulation frames and/or control which simulation frames to start/stop on.

-identification ID

This options specifying ID tag to be included in output. Default is "None"

Example 7:

```
larmord –identification SRL file.pdb
```

Example 7 Output:

```
0 1 7 URA C5' 64.508 0 66.3 SRL
0 1 7 URA H5' 4.23158 0 3.78 SRL
0 1 7 URA H5'' 4.19069 0 3.58 SRL
0 1 7 URA C4' 82.9541 0 83.1 SRL
0 1 7 URA H4' 4.35532 0 4 SRL
0 1 7 URA C1' 92.928 0 93.1 SRL
…
```

-csfile CSfile

This option supplies path to file that specifying the nuclei for which LARMOR^{D} will predict chemical shifts.

Chemical shifts file format [residue name, residue, nucleus, measured chemical shifts, error]:

```
CYT 6 C1' 91.438 0.00
URA 7 C1' 92.388 0.00
CYT 8 C1' 89.297 0.00
ADE 9 C1' 85.504 0.00
GUA 10 C1' 81.3 0.00
GUA 1 C1' 89.246 0.00
GUA 2 C1' 90.258 0.00
…
```

Example 8:

```
larmord file.pdb
```

Example 8 Out:

```
0 1 7 URA C5' 64.508 0 66.3 None
0 1 7 URA H5' 4.23158 0 3.78 None
0 1 7 URA H5'' 4.19069 0 3.58 None
0 1 7 URA C4' 82.9541 0 83.1 None
0 1 7 URA H4' 4.35532 0 4 None
0 1 7 URA C1' 92.928 0 93.1 None
…
```

Example 9:

```
larmord -csfile measured_shifts.dat file.pdb
```

Example 9 Out:

```
0 1 7 URA C4' 82.9541 79.743 83.1 None
0 1 7 URA H4' 4.35532 4.166 4 None
0 1 7 URA C1' 92.928 92.388 93.1 None
0 1 7 URA H1' 5.52637 5.344 5.6 None
0 1 7 URA H6 7.81604 7.447 7.85 None
0 1 7 URA C5 105.411 101.297 103.5 None
…
```

-parmfile PARAMfile

This option allows the user to supply a file containing the parameters that should be used to predict chemical shifts; supplied parameters will override the default parameters hardcoded into LARMOR^{D}.

parameter file [NMR-active nucleus, residue name of neighboring atom *j*, atom name of *j*, alpha for *j*]
(see Eq. 1):

```
H4' GUA C1' 0.709970102502
H4' GUA C2' 1.75726958963
H4' GUA C3' 0.820067830994
H4' GUA C4' -0.0
H4' GUA C5' 1.19834177254
H4' GUA P 1.41704358137
…
```

$$\delta_i^{\text{pred}} = \delta_i^{\text{ref}} + \sum_{j=1}^{N} \alpha_j r_{ij}^{-3} \quad (1)$$