Build topology of lignin polymer via LigninBuilder for Gromacs.

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Documented by: Xinjie Tong

1. In linux, create a repository:
   Eg. /home/xtong3/repos/
   And clone it to there :
   git clone git@github.com:jvermaas/LigninBuilder.git
   Ref:Vermaas, Josh V., et al. "Automated Transformation of Lignin Topologies into Atomic Structures with LigninBuilder."
2. UseLigninBuilder/libraries/ *library.txt as a template
   To build a simple G tetramer. It is as the following.
   GG_bo4_tetramer.txt

```
STARTING NEW POPULATION.....
************************************** CHAIN #1****************************************
MW:
Branch:
Distance Metric:
0  0  4  -  3  0  0  0  0  0  0
Monomer List:
1: 3
2: 3
3: 3
4: 3
Bond List:
Monomer_I    Monomer_II    Pos_Mon_I    Bond_type
1            2             1            1
2            3             1            1
3            4             1            1
#
```

Can be blank

In order: the number of monomer
Syringly(S), p-hydroxyphenyl(P), guaiacyl(G),

- (a double dash)
the number of bonds:
$\beta-o-4, \beta-o-5, 5-5, 4-o-5, \beta-1, \alpha-o-4$ *or* $\beta-o-4, \beta-\beta$

Monomer code

$\beta-o-4$ *from* C_β *of monomer* 1 *to* O4 *of monomer* 2. *equal to* (2 1 2 1)

Table S1: Linkage codes created through the individual position and bond codes listed in Table 1 are enumerated here in their combinations found in the tested lignin libraries.

Linkage Codes			
Position Code	Bond Code	Bond Type	Modification Site
1	1	β-O-4	C_β
1	2	β-5	C_β
1	5	β-1	C_β
1	7	β-β	C_β
1	8	β-O-4	C_β (Only for β-O-4/α-O-4 combo)
2	1	β-O-4	O_4 (4-O-β)
2	4	4-O-5	O_4
3	3	5-5	C_5
3	4	4-O-5	C_5 (5-O-4)
4	6	α-O-4	C_α (Only for β-O-4/α-O-4 combo)

Table 1. Monomer, Bond, and Position Codes That Specify Lignin Topology in a Way That Is Readable by LigninBuilder[a]

monomer codes		bond codes		position codes	
code no.	monomer	code no.	bond	code no.	position
1	S	1	*β*-O-4	1	C_β
2	H	2	*β*-5	2	O_4
3	G	3	5-5	3	C_5
		4	4-O-5	4	C_α
		5	*β*-1	5	C_1
		6	*α*-O-4		
		7	*β*-*β*		

3. Install Namd:
    1. Download https://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=NAMD Namd version 2.13(2018-11-09)
       Linux-x86_64-multicore (64-bit Intel/AMD single node)
    2. Extract it.
    3. go to extracted folder (cd NAMD_2.10_Linux-x86_64-multicore)
    4. then copy NAMD binary file to bin folder (sudo cp namd2 /usr/local/bin/namd2)
    5. Add to ~/.bashrc export PATH=/usr/local/bin:$PATH

4. Open VMD

   In TKConsole, use commands:

   lappend auto_path /home/xtong3/repos/LigninBuilder/LigninBuilderPlugin
   package require ligninbuilder

   ::ligninbuilder::buildfromlibrary "/home/xtong3/repos/LigninBuilder/libraries/GG_bo4_tetramer.txt" GG_bo4_tetramer
   ::ligninbuilder::minimizestructures GG_bo4_tetramer namd2 "+p8"

   It will generate all outputs in a new folder named GG_bo4_tetramer namd2\
   If input contains 100 lignins, then output file should be L0-L99.psf
   And par_lignin.prm is parameter files.

5. Use PyTopol to convert Charmm parameter to topology in Gromacs

   https://github.com/resal81/PyTopol/wiki/PyTopol-Installation

   $ git clone https://github.com/resal81/PyTopol.git
   $ cd PyTopol
   $ export PYTHONPATH=`pwd`:$PYTHONPATH
   $ cd scripts

   Copy psf and prm files to the same directory as psf2top.py then run:
   python psf2top.py -p L0.psf -c par_lignin.prm
   Rename the output top.top and itp_mol_01.itp to desired name.

   I renamed to GG_bo4_tetramer_types.itp and GG_bo4_tetramer.itp respectively.
   Since the former contains atomtypes and the latter is a normal itp file.
   And I deleted extra useless lines started from [dihedrals] in GG_bo4_tetramer_types.itp

   Copy L0.pdb to GG_bo4_tetramer.pdb and seperately save all new *itp/top/pdb in
   ~/repos/simulation_topologies/gromacs_top/charmm36-nov2018.ff/LIGNIN_BUILDER_TOP/GG_bo4_tetramer_TOP

   Note:
   A.If you come across"ValueError: for dihedral CLG2R6B-CLG2R61-CLG2R61-CLG3C51 no parameter was found",
   You can add another .prm at the end of command. I had this issue when built a b-o-5 tetramer
   python psf2top.py -p L0.psf -c par_lignin.prm extraterms-par_lignin.prm

   (bo4,b-o-5,bo4 tetramer)
   STARTING NEW POPULATION.....
   ********** CHAIN #1**********
   MW:
   Branch:
   Distance Metric:
   0 0 4 - 2 1 0 0 0 0 0
   Monomer List:
   1: 3

2: 3
3: 3
4: 3

Bond List:

Monomer_I	Monomer_II	Pos_Mon_I	Bond_type
1	2	1	1
2	3	1	2
3	4	1	1

#

B.You need to delete the first directive in top.top because in default force field alread has that otherwise will give an err or.
[defaults] ;

;nbfunc	comb-rule	gen-pairs	fudgeLJ	fudgeQQ
1	2	yes	1.0	1.0

Step 4 you can create a tcl file named build.tcl and put the following text in it.
Then you can simply run in vmd console in two lines:
$ source build.tcl
$ build lib_prefix

build.tcl code as following

```
lappend auto_path /home/xtong3/repos/LigninBuilder/LigninBuilderPlugin

proc build {lib_prefix} {

package require ligninbuilder

::ligninbuilder::buildfromlibrary "/home/xtong3/repos/LigninBuilder/libraries/$lib_prefix.txt" $lib_prefix
::ligninbuilder::minimizestructures $lib_prefix namd2 "+p8"

}
```