Subject: Computational Chemistry
Posted by ruthamcau on Mon, 16 Sep 2019 14:02:38 GMT
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I'm doing undergraduate research with my professor at my university on computational chemistry and my task is to run energy minimization calculations with molecular mechanics for the protein, fibronectin. I'm using TINKER for energy calculations, however, it requires a third-party molecular editor that can generate coordinate files (i.e. .xyz, .pdb, etc. in the appropriate file format. Is there someone with experience with computational chemistry? I'm interested in building coordinates for this particular peptide sequence,

YAVTGRGDSPASSKPISINYRTEIG KPSQMC

The problem is that I can't find a decent molecular editor, if there is one that I could just input the peptide sequence without having to manually construct it that would be very helpful.

Subject: Re: Computational Chemistry
Posted by nbehrnd on Tue, 17 Sep 2019 14:44:46 GMT
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Dear ruthamcau,

the single-letter abbreviation in your example is used by the Fasta format [1]. This is one of the file formats openbabel [2] accepts as input; available for free, either with a GUI, or to run on CLI / script with bindings to languages like Python, C++. Beside .xyz and .pdb, the .txyz for TINKER equally is one of the formats openbabel may write. As option, openbabel itself may offer /a guess/ about the conformation with forcefields like UFF or MMFF94 but intended for small molecules.

Avogadro [3] may be on first sight less interesting for you because it lacks an export to TINKER, and allowing you to construct via GUI (build -> insert) peptides by three-letter, RNA/DNA by single-letter buttons. But under «extensions» you have multiple templates to set up input files of quite a number of quantum chemical programs; as such complementary to pure openbabel.

Continuing with a programmatic approach to handle peptide sequences, I would mention Biopython [4] and the more general introduction to Python for Bioscientists by Ekmekci et al. in PLOS Computational Bioploy [5, openaccess] (e.g., exercise #10).

Good luck,
Norwid

[1] https://en.wikipedia.org/wiki/FASTA_format
[2] http://openbabel.org/wiki/Main_Page

[3] http://avogadro.cc/
[4] https://biopython.org/
[5] https://doi.org/10.1371/journal.pcbi.1004867

## File Attachments

1) trial_fasta.xyz, downloaded 528 times
2) trial_fasta.png, downloaded 515 times
3) trial_fasta.txyz, downloaded 534 times