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 671 times
2) trial_fasta.png, downloaded 674 times
3) trial_fasta.txyz, downloaded 686 times