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.