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Assignment of protonation states and geometries to macromolecular structures using Unary Quadratic Optimization

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A method is presented for assigning protonation states and hydrogen atom geometry to macromolecular structures. Tautomer and ionization state (including metal ligation) are taken into account during a large scale free energy optimization. This discrete optimization is performed with a Unary Quadratic Optimization procedure. The thermodynamic theory and the results of several computational validation experiments will be presented.