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Molecular simulations of peptides and proteins with Molecular Fragment Dynamics (MFD)

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Molecular Fragment Dynamics (MFD) is a mesoscopic simulation technique based on dissipative particle dynamics. The method has been shown to successfully describe the phase behaviour and interfacial tensions of large chemical systems in good agreement with experimental results [1]. Unlike molecular mechanics a MFD simulation is based on "coarse-grained" molecular fragments rather than "fine-grained" atom types.

The current MFD fragment definition is based on a SMILES like one-dimensional line notation which is visualized with the Structure Diagram Generator of the Chemistry Development Kit (CDK) [2]. For an extension of the MFD technique to chemical ensembles containing peptides and proteins an appropriate molecular fragment cheminformatics tool for their design is in need.

This work provides an editor for the construction of peptides and proteins from molecular fragments. It includes building blocks for all 20 proteinogenic amino acids, their charged species and disulfide bonds. A flexible input of one-letter and three-letter amino acid codes is supported. Additionally, the editor has the capability to set charges of side chains manually or automatically.

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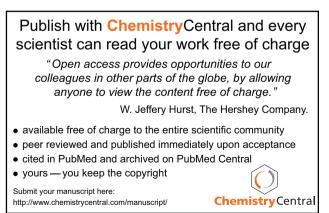
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