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## Background

The Biology and Chemistry Library Project is an object oriented C++ programming library. The library is designed to simulate biological molecules – proteins and peptides in particular – as well as small chemicals such as therapeutics. It comprises mathematical methods to evaluate the energy of these molecules in their natural environment. Vanderbilt seeks to advance this research and to publish and enable adoption of research codes in furtherance of its public interest mission.

Distribution of research codes as a research courtesy is facilitated by licensing these codes for development and use. Development of these codes was supported, in part, by the following: the National Institute of Health (NIH) and the National Science Foundation (NSF).

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This Agreement embodies the entire understanding of the parties and supersedes all previous communications, representations, or understandings, either oral or written, between the parties relating to the subject matter hereof.

# ATTACHMENT A

## **Software Code**

The Biology and Chemistry Library Project software ("Software") is an object oriented C++ programming library developed in the Meiler laboratory at Vanderbilt. The library is designed to simulate biological molecules – proteins and peptides in particular – as well as small chemicals such as therapeutics. It comprises mathematical methods to evaluate the energy of these molecules in their natural environment, manipulate conformation and chemical structure of the molecules, model biological processes such as protein folding and protein-small molecule interactions, determine protein structure de novo from no or sparse/low-resolution diverse experimental data, and correlate structural data with various properties such as NMR spectra or biological activities. The Software is comprised of several Modules.

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