## National Research Council (NRC) Post-Doctoral Fellowship at the National Institute of Standards and Technology

## **Topics**

Computational Methods for NMR Structural Biology Spectral Fingerprinting of Protein Therapeutics

## **Description**

The efficacy and safety of protein therapeutics depends critically on their High Order Structure (HOS), and changes to HOS during manufacture or storage can render them inactive or promote dangerous immune responses. Methods to measure and characterize HOS are essential for development of new biotherapeutics; for evaluating less expensive "biosimilar" replacements; and for monitoring and improving manufacturing, formulation, and stability. Nuclear magnetic resonance (NMR), which can provide detailed information on structure and dynamics at atomic resolution, is a powerful tool to probe HOS, but typical biomolecular applications use isotopic enrichment, long measurement times, and require extensive and often subjective interactive analysis by an expert.

Our computational methods development has two primary goals. The first goal is continued support of expert-driven biomolecular structure determination by NMR, with an emphasis on spectral reconstruction and quantification. The second goal is to develop computational alternatives to interactive analysis and assignment of spectral features, to provide practical HOS characterization of protein therapeutics via chemometrics and machine learning that is both objective and automated.

## Qualifications

Candidates who have received PhD degrees in chemistry, biophysics or related fields within the last five years are encouraged to apply. A strong background in NMR is preferred, and experience with computational work and software development is required.

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Citizenship Requirement: this NRC Fellowship requires US Citizenship.

Location: Institute of Bioscience and Biotechnology Research, Rockville MD.

Application Procedure: Visit the NRC Research Associateship Program web site for details.

http://sites.nationalacademies.org/PGA/RAP/index.htm

