
 **Protein Informatics Core**   
**Division of Biomedical Informatics & Center for Informatics**  
**CCHRF & UC**  
**Services and Support for Collaborative Efforts**

As part of the proposed Center for Informatics (CI), a new core unit, tentatively called Center for Protein Informatics (CPI), has been created in order to offer services and support for collaborative efforts involving elements of structural bioinformatics, function analysis and prediction, modeling and simulation, as well as related computational protocols focusing primarily on proteins. A preliminary list of these services and types of collaborative efforts supported by CPI is included below (please note that as discussions regarding the overall mission of CI, and CPI in particular, continue, this list is likely to be further modified/extended). For more information please check [Protein Informatics Core](#) web site.

<i>Name</i>	<i>Description</i>	<i>Type</i>
Comprehensive structural and functional analysis of proteins and their families	Identification of available structural information, structure visualization, analysis of functional consequences	Service (possible extensions to further analysis/hypothesis generation)
Advanced and tailored homology/fold recognition searches	Identification of sequence and structure similarity for distant homologs and proteins of unknown structure/function	Service (possible extensions to further analysis/hypothesis generation)
Standard and extended (with loop refinement) homology modeling	Building 3D models for proteins of unknown structure using structural templates, alignments and refinement	Service (possible extensions to further analysis/hypothesis generation)
Analysis of protein flexibility, thermal motions and dynamics	Obtaining approximate description of slow coordinated motions (e.g. hinge motions) and protein dynamics	Service (possible extensions to further analysis/hypothesis generation)
Mapping and analysis of protein-protein and protein-ligand interactions	Analysis and visualization of known physical interactions, simple search for related ligands/interacting partners	Service (possible extensions to further analysis/hypothesis generation)
Mapping and analysis of functional consequences of SNPs in coding regions	Mapping SNPs into known or predicted structures, analysis in terms of stability, folding kinetics and interactions	Service (possible extensions to further analysis/hypothesis generation)
Setting up tailored sequence alignment pipelines	Building tailored databases (e.g. for newly sequenced genomes) for BLAST and related searches	Service (including the use of BMI/CI computational resources)
Setting up comprehensive prediction pipelines	Combining several on- and off-line prediction and analysis tools using scripting and web interfaces	Service (including the use of BMI/CI computational resources)
Setting up molecular dynamics and related simulations	Assisting in building simulation systems, setting force field parameters and preparing simulation runs	Service (including the use of BMI/CI computational resources)

<i>Name</i>	<i>Description</i>	<i>Type</i>
Setting up docking studies	Assisting in choosing docking approach, scoring functions and compound libraries for screening	Service (including the use of BMI/CI computational resources)

The new unit will be offering the above services and other forms of support on the as needed basis. Specific arrangements regarding cost recovery in case of services, extended usage of BMI/CI computational infrastructure and potential grant support for collaborative involvement will be negotiated individually. A web site with further information regarding CPI can be found at <http://folding.chmcc.org>. Please contact:

**Jarek Meller** for inquires regarding the actual services and potential collaborations:

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Or

**Eszter Belcher** for inquires regarding financial aspects of the services, grants and budgets:

Business Director, Division of Biomedical Informatics, CCHRF, ph. 636-0148, e-mail: [bely9d@cchmc.org](mailto:bely9d@cchmc.org).