



## TECHNOLOGY AVAILABLE FOR LICENSING

### A Computational Method for Predicting Protein Interaction Sites

Patent Application #10/678,756

Inventors: Mary Jo Ondrechen, Ronald J. Williams, Robert J. Futrelle, Huyuan Terry Yang, Dagmar Ringe, James Clifton, Ihsan Shehadi, Leonel Murga, Jaeju Ko, David Budil, Wenxu Tong

#### Invention Details:

Theoretical microscopic titration curves are used to identify active sites in proteins of known or unknown structure. The active sites are found in regions where the ionizable residues are partially protonated over a wide pH range. The evaluation of these curves are enhanced by machine learning algorithms, model structures and advanced mathematical analytical procedures. The software method decreases the amount of time to determine protein function, thus decreasing cost for producing new pharmaceuticals.

#### Benefits of the Invention:

The invention is an in-vitro method for pinpointing active sites in large molecules.

#### Advantages:

Quick  
Low cost/decrease time  
Database independent  
Simple

#### Uses:

Determine enzyme active sites  
Determine ligand binding sites  
Aids in predicting protein function  
Assists in the discovery of pharmaceuticals

#### The Bottom Line:

The methods described in the inventions rapidly pinpoint active sites. Identification of active sites enables the rational design of pharmaceuticals and should decrease the time to market.

#### For More Information:

##### Please contact:

**Susan Riley Keyes, Ph.D., J.D.**  
Division of Technology Transfer  
Northeastern University  
360 Huntington Ave, 960 RP  
Boston, MA 02115-5000  
**Phone:** 617-373-8810  
**Fax:** 617-373-8866  
**Email:** s.keyes@neu.edu

or

**Mary Jo Ondrechen, Ph.D.**  
Department of Chemistry  
Northeastern University  
360 Huntington Avenue, 122 Hurtig  
Boston, MA 02115-5000  
**Phone:** 617-373-2856  
**Fax:** 617-373-8795  
**Email:** ondrechen@neu.edu