



**The Chinese University of Hong Kong**  
**Non-confidential Abstract of Technology Disclosure**

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**Title:**

**3D Protein Binding Interface Prediction Program**

**CUHK Ref. No.:**

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**Inventor(s):**

Professor Sai Ming NGAI, Department of Biology

**Non-confidential abstract:**

All current docking methods starting with rigid-body docking do not perform well on protein complexes with significant conformational change during formation and it is urged that new tactics should consider potential conformational changes(s) during complex formation. At present, there are no visualization programs dedicated to structural perspectives of protein-protein interaction (PPI) study. No single existent program simultaneously provides a handy interface for manipulating molecular objects (protein chains), a quick focus on a particular amino acid residue for the sake of reference/comparison to literature and unambiguous and stereo representation to distinguish among chains or even atoms; and most importantly, interface-related functions are limited.

In this study, we have examined the problem from a kinetic and thermodynamic perspective. We have developed a prediction and visualization program based on the utilization with enhancement to aid PPI studies. Interfaces of nine non-homologous protein complexes with PDB records, equilibrium and association rate constants have been dissected and employed as a guide in the location of protein-protein interaction site. The difficult cases mentioned in (Chen et al. 2003, 52) were then investigated. We found that there is a systematic way helps identify the PPI sites in such difficult cases. We expect formulation of our qualitative identification procedures into automatic validation and analysis can test its classification power upon general PPS site identification for integration into existing docking algorithms to increase sensitivity.

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**For further queries, please contact:**

Mr Billy Lam  
Technology Licensing Coordinator  
*Tel:* (852) 2609 8882  
*Fax:* (852) 2603 5451  
*Email:* [billylam@cuhk.edu.hk](mailto:billylam@cuhk.edu.hk)

*Address:*  
Technology Licensing Office  
The Chinese University of Hong Kong  
Room 226, Pi Ch'iu Bldg, Shatin, New Territories  
Hong Kong SAR