Recent patent applications in computational biotechnologies

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With the prevalence of genomic and proteomic data, modern research in experimental biotech has become a human-guided, computer-assisted endeavor. A wide range of molecular and structural bioinformatics methods and resources is available and the number of therapeutically relevant macromolecular entities is growing rapidly. This highlights the need for using computer-aided techniques for the identification and efficient optimization of novel hit compounds. **Table 1** is an attempt to catalog recent patents for *in silico* prediction tools, compound collections, some ligand-based prediction methods, characterization/simulation of three-dimensional targets and homology modeling tools together with all-atom molecular dynamics methodology for the analysis of macromolecular structures and interfaces. Different applications and approaches facilitating the drug discovery process are reported. This review should help readers find patented computer tools useful for facilitating rapid and cost-effective identification of new hit compounds.

COMPETING FINANCIAL INTERESTS
The author declares no competing financial interests.

Table 1 Recent patent applications in computational biotechnologies

Patent number	Description	Assignee	Inventor	Priority application date	Publication date
WO 2012096015	Nucleic acid information processing device and processing method thereof.	Japan Software Management Co. Ltd. (Japan), Bioinformatics Institute for Global Good (Tokyo), Nasu H, Tsujimoto A, Yamakawa T, Ono H	Nasu H, Tsujimoto A, Yamakawa T, Ono H	1/11/2011	7/19/2012
WO 2011153372	Methods and systems for simulations of complex biological networks using gene expression indexing in computational models. A method has been developed for using genome-wide transcription profile (that is, gene-expression level) values to derive a gene expression index used as a kinetic value for every biological reaction and process assigned to each and every gene.	University of Texas (Austin, TX, USA), Phelix CF	Phelix CF	6/2/2010	12/8/2011
US 2011282910	Template-constrained fragment alignment used to identify fragments of similar shape and activity in drug development. A computer-implemented drug discovery method utilizing a specifically programmed computer for aligning in three dimensions molecular fragments derived from molecules in a molecular database to a specified three-dimensional template.	Cramer RD	Cramer RD	1/29/2010	11/17/2011
US 2011172981	High-throughput, ensemble-based docking and elucidation of three-dimensional structural confirmations of flexible biomolecular targets.	University of Michigan (Ann Arbor, MI, USA)	Al-Hashimi Hashim M, Stelzer A, Andricioaei I, Aaron F	9/26/2008	7/14/2011
WO 2011061548	A method for computational drug design using an evolutionary algorithm, comprising evaluating virtual molecules according to vector distance (VD) to at least one achievement objective that defines a desired ideal molecule.	University of Dundee (UK), Besnard J	Besnard J	11/20/2009	5/26/2011
CA 2769045	Method for binding-site identification by ligand competitive saturation simulation.	University of Maryland (College Park, MD, USA)	Mackerell AD, Guvench O	5/4/2009	11/11/2010
US 20100068217	Computational protocols for the design of epitope-protein scaffolds, which elicit selected neutralizing antibodies and related compositions and uses.	Kwong PD, Ofek G, Guenaga J, Wyatt R, Yang ZY, Zhou T, Nabel GJ, Tang M, Schief W, Baker D	Kwong PD, Ofek G, Guenaga J, Wyatt R, Yang ZY, Zhou T, Nabel GJ, Tang M, Schief W, Baker D	8/25/2006	3/18/2010
US 2009271159	Apparatus and method for integrating a physical molecular model with a computer-based visualization and simulation model.	Molysym (Cambridge, MA, USA)	Sherman BH, Green DF, Ruping KH, Donaldson KD	12/31/2002	10/29/2009
WO 2009120371	Computationally designed inhibitors of amyloidosis.	University of Washington (Seattle), Daggett V, Law P	Daggett V, Law P	3/27/2008	10/1/2009

Source: US Patent and Trademark Office, Espacenet, JP and EP patent offices. The status of each application is slightly different from country to country.

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