[Billing Code 4140-01-P]

DEPARTMENT OF HEALTH AND HUMAN SERVICES

National Institutes of Health

Government-Owned Inventions; Availability for Licensing

AGENCY: National Institutes of Health, HHS

ACTION: Notice

SUMMARY: The inventions listed below are owned by an agency of the U.S. Government and are available for licensing in the U.S. in accordance with 35 U.S.C. 209 and 37 CFR Part 404 to achieve expeditious commercialization of results of federally-funded research and development. Foreign patent applications are filed on selected inventions to extend market coverage for companies and may also be available for licensing.

FOR FURTHER INFORMATION: Licensing information and copies of the U.S. patent applications listed below may be obtained by writing to the indicated licensing contact at the Office of Technology Transfer, National Institutes of Health, 6011 Executive Boulevard, Suite 325, Rockville, Maryland 20852-3804; telephone: 301-496-7057; fax: 301-402-0220. A signed Confidential Disclosure Agreement will be required to receive copies of the patent applications.

SUPPLEMENTARY INFORMATION: Technology descriptions follow.

Heterocyclic Compounds for the Treatment of Hepatitis C Virus

Description of Technology: The vast majority of people infected with Hepatitis C Virus (HCV) will have chronic infection. Over decades, this can lead to liver disease and liver cancer. In fact, HCV infection is the leading cause of liver transplants in the U.S. Several new drugs have recently come into the market that have changed the HCV treatment paradigm. However, the effectiveness of these new drugs can vary depending on the HCV genotype. Furthermore, all oral, interferon free therapeutic regimens for HCV infection will need combinations of drugs that target different aspects of the HCV life cycle. Thus, there is still the need for additional new therapeutics against HCV.

The subject technologies are aryloxazole based small molecules that are potent inhibitors of HCV infection and replication. The compounds exhibit synergy with currently available therapeutics for HCV and represent a new class of anti-HCV compounds. The compounds affect the entry step of HCV infection, a step not targeted by currently available therapeutics against HCV.

Potential Commercial Applications: Prevention and treatment of HCV infection.

Competitive Advantages:

• Potent inhibitors of HCV infection and replication.

• Show synergistic effect with currently available HCV therapeutics.

• Represent new class of HCV inhibitors that target the entry step of HCV infection.

Development Stage:

• Early-stage

• In vitro data available

Inventors: Jake Tsanyang Liang (NIDDK), Zongyi Hu (NIDDK), Juan Jose Marugan (NCATS), Noel Terrance Southhall (NCATS), Xin Hu (NCATS), Jingbo Xiao (NCATS), Shanshan He (NIDDK), Marc Ferrer-Alegre (NCATS), Wei Zhang (NCATS)

Intellectual Property: HHS Reference No. E-161-2014/0 - US Provisional Patent Application No. 62/011,462 filed 12 June2014

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Autodock Vina Software Process for Efficient Large-Scale Cognate Ligand Screening

Description of Technology: The invention pertains to software processes, additions, and docking approaches to Autodock Vina that speeds the rate and efficiency of analyzing ligand interactions with a receptor by cognate ligands and rewards conformations in the scoring algorithm for residue interactions that are based on the biological data. The score is multiplied by a weighting factor to control the degree of ligand-residue interactions that are considered. This multiplier is then added to the docking score for confirmation. This new scoring mechanism is used to score each compound in each generation of the evolutionary genetic algorithm. This docking

approach can be used to score and rank compounds in large-scale virtual screening applications. The software includes logic for converting SDF formatted to an Autodock Vina compatible format (containing approx. 25,000 compounds each) and submits the job to the portable batch system on the computing cluster to convert into PDBC files (a concatenated filed type). Modified Vina software stores the analyzed binding pocket in RAM that does not have to be recomputed upon every docking process. This increases the efficiency of the docking algorithm by several orders of magnitude. The software on the head node intelligently monitors memory usage, CPU usage and docking speed. Based on this information, the head node elastically controls the load on each node.

Potential Commercial Applications:

• Drug screening

• Ligand identification

Competitive Advantages:

• Speed

• Batch processing

• Efficient CPU processing

Development Stage: In vitro data available

Inventors: Marvin Gershengorn, Umesh Padia, Janak Padia, Elizabeth Geras-Raaka (all of NIDDK)

Intellectual Property: HHS Reference No. E-289-2014/0 - Software Tool. Patent protection is not being pursued for this technology.

Licensing Contact: Michael Shmilovich, Esq.; 301-435-5019; shmilovm@mail.nih.gov

Collaborative Research Opportunity: The National Institutes of Diabetes and Digestive and Kidney Diseases is seeking statements of capability or interest from parties interested in collaborative research to further develop, evaluate or commercialize Cognate Ligand Identification. For collaboration opportunities, please contact Anna Amar at 301-451-2305 or aamar@mail.nih.gov.

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Richard U. Rodriguez, M.B.A.
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Division of Technology Development and Transfer
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