*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—U.S. Provisional Patent Application No. 62/011,462 filed 12 June2014

*Licensing Contact:* Kevin W. Chang, Ph.D.; 301–435–5018; *changke@mail.nih.gov*

**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.*

Dated: November 10, 2014.

**Richard U. Rodriguez,**

*Director, Division of Technology Development and Transfer, Office of Technology Transfer, National Institutes of Health.*

[FR Doc. 2014–27083 Filed 11–14–14; 8:45 am]

**BILLING CODE 4140–01–P**

## DEPARTMENT OF HEALTH AND HUMAN SERVICES

### National Institutes of Health

### National Institute of Mental Health: Notice of Closed Meeting

Pursuant to section 10(d) of the Federal Advisory Committee Act, as amended (5 U.S.C. App.), notice is hereby given of the following meeting.

The meeting will be closed to the public in accordance with the provisions set forth in sections 552b(c)(4) and 552b(c)(6), Title 5 U.S.C., as amended. The grant applications and the discussions could disclose confidential trade secrets or commercial property such as patentable material, and personal information concerning individuals associated with the grant applications, the disclosure of which would constitute a clearly unwarranted invasion of personal privacy.

*Name of Committee:* National Institute of Mental Health Special Emphasis Panel; NIMH Career Transition Award for Tenure-Track and Tenured Intramural Investigators (K22).

*Date:* December 2, 2014.

*Time:* 12:30 p.m. to 1:30 p.m.

*Agenda:* To review and evaluate grant applications.

*Place:* National Institutes of Health Neuroscience Center, 6001 Executive Boulevard, Rockville, MD 20852 (Telephone Conference Call).

*Contact Person:* Ingrid Y. Li, Ph.D., Health Science Administrator Division of Extramural Activities, National Institute of Mental Health, NIH Neuroscience Center, 6001 Executive Blvd., Room 6154–C, Bethesda, MD 20892, 301–443–1421, *ili1@mail.nih.gov.*

(Catalogue of Federal Domestic Assistance Program No. 93.242, Mental Health Research Grants, National Institutes of Health, HHS)

Dated: November 7, 2014.

**Carolyn A. Baum,**

*Program Analyst, Office of Federal Advisory Committee Policy.*

[FR Doc. 2014–27060 Filed 11–14–14; 8:45 am]

**BILLING CODE 4140–01–P**

## DEPARTMENT OF HEALTH AND HUMAN SERVICES

### National Institutes of Health

### National Institute of Environmental Health Sciences; Notice of Closed Meeting

Pursuant to section 10(d) of the Federal Advisory Committee Act, as amended (5 U.S.C. App.), notice is hereby given of the following meeting.

The meeting will be closed to the public in accordance with the provisions set forth in sections 552b(c)(4) and 552b(c)(6), Title 5 U.S.C., as amended. The contract proposals and the discussions could disclose confidential trade secrets or commercial property such as patentable material, and personal information concerning individuals associated with the contract proposals, the disclosure of which would constitute a clearly unwarranted invasion of personal privacy.

*Name of Committee:* National Institute of Environmental Health Sciences Special Emphasis Panel; Alternative Toxicological Methods Support Contract for the National Toxicology Program (NTP).

*Date:* December 11, 2014.

*Time:* 1:00 p.m. to 5:00 p.m.

*Agenda:* To review and evaluate contract proposals.

*Place:* National Institute of Environmental Health Sciences, Keystone Building, Conference Room 2166, 530 Davis Drive, Research Triangle Park, NC 27709, (Telephone Conference Call).

*Contact Person:* RoseAnne M. McGee, Scientific Review Officer, Scientific Review Branch, Division of Extramural Research and Training, Nat. Institute of Environmental Health Sciences, P.O. Box 12233, MD EC–30, Research Triangle Park, NC 27709 (919) 541–0752, *mcgee1@niehs.nih.gov.*

(Catalogue of Federal Domestic Assistance Program Nos. 93.115, Biometry and Risk Estimation—Health Risks from Environmental Exposures; 93.142, NIEHS Hazardous Waste Worker Health and Safety Training; 93.143, NIEHS Superfund Hazardous Substances—Basic Research and Education; 93.894, Resources and Manpower Development in the Environmental Health Sciences; 93.113, Biological Response to Environmental Health Hazards; 93.114,