

## How to Obtain AutoDock 3.05 Software

1. Using a typewriter or block print lettering, complete all of the requested information in the attached Software License Agreement and sign under the heading "Recipient Scientist" on the last page. Include your institutional email address to receive the ftp instructions. Post-Docs and Graduate Students need to have the principal investigator of their lab sign as the "Recipient Scientist".
2. Have the agreement signed by an officer of your institution. Examples of authorized officials are President, Vice President for Research, Vice Provost, Legal Counsel, Director of Technology Transfer, or some other designated officer authorized to legally bind your institution.
3. Check your application to be sure it has all of the requested information and signatures. If we receive an incomplete or unreadable application, it will delay your receipt of the software.
4. Fax and **mail** 1 original signed Agreement to:  
The Scripps Research Institute  
Office of Technology Development  
10550 N. Torrey Pines Road, TPC-9  
La Jolla, CA 92037 U.S.A.  
Phone: (858) 784-8496  
FAX: (858) 784-9910
5. Upon receipt of the completed Agreement, you will receive, by email, instructions to ftp the files. Any questions regarding the completion of this License Agreement should be directed to: Melissa Wetjen, Office of Technology Development, Phone: (858) 784-8496 or Email: [mwetjen@scripps.edu](mailto:mwetjen@scripps.edu)

## AUTODOCK 3.05 SOFTWARE TRANSFER AGREEMENT

THIS SOFTWARE LICENSE AGREEMENT ("Agreement") is made by and between The Scripps Research Institute ("TSRI"), having an address at 10550 N. Torrey Pines Road, La Jolla, CA 92037 and

\_\_\_\_\_, having an address at \_\_\_\_\_ ("Recipient") and \_\_\_\_\_ ("Recipient Scientist").

### RECITALS

- A. TSRI is the owner of the Software (as defined below).
- B. TSRI desires to grant to Recipient and Recipient desires to obtain from TSRI a non-exclusive license to use the Software solely in accordance with the terms and on the conditions set forth in this Agreement.

NOW, THEREFORE, the parties hereto agree as follows:

#### 1. DEFINITIONS.

1.1 "Software" shall mean the AutoDock computer program in machine readable source code form.

#### 2. GRANT OF RIGHTS.

The License granted for Software under this Agreement authorizes Recipient on a nonexclusive basis to use \_\_\_\_\_ copy(ies) of the Software. Recipient may retain one additional copy of the Software for archival purposes. Recipient agrees to use the Software for internal non-commercial research purposes only, and shall not distribute or transfer the Software to anyone not under the Recipient Scientist's direct supervision or beyond the Recipient Scientist's laboratory.

#### 3. DELIVERY.

3.1 Software. TSRI shall deliver to Recipient a master copy of the Software licensed hereunder in source code form, suitable for reproduction, in electronic files only.

#### 4. MODIFICATIONS.

4.1 Other Modifications. Recipient may, from time to time, request that TSRI incorporate certain features, enhancements or modifications into the Software. TSRI may, in its sole discretion, undertake to incorporate such changes, which shall be the sole property of TSRI, and distribute the Software so modified to all or any of TSRI's licensees. Any modifications or derivative works based on the Software are considered part of the Software and ownership thereof is retained by TSRI.

**5. COPIES AND RECORDS.** Recipient agrees to maintain appropriate records of the number and location of all copies of the Software.

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mark, or legend appearing on any of the Software or output generated by the Software, and to reproduce and include same on each copy of the Software.

6.2 Protection of Ownership. Recipient agrees to use its best efforts, consistent with the practices and procedures Recipient takes to protect Recipient's own most valuable proprietary information and materials, and will take all reasonable steps to protect the Software and any pertinent documentation and associated trade secrets against any unauthorized use, reproduction, disclosure or distribution.

6.3 Research Publications, including scientific papers, films, videotapes and CDs, by the Recipient Scientist resulting from the use of the Software should cite Professor Arthur Olson, the author of the Software, and the following publications:

- 1) Goodsell, D.S. and Olson, A.J. (1990) Automated Docking of Substrates to Proteins by Simulated Annealing. *Proteins: Structure, Function, and Genetics* 8:195-202.
- 2) Morris, G.M., Goodsell, D.S., Huey, R. and Olson, A.J. (1996) Distributed Automated Docking of Flexible Ligands to Proteins: Parallel Applications of AutoDock 2.4. *J. Computer-Aided Molecular Design* 10:293-304.
- 3) Morris, G.M., Goodsell, D.S., Halliday, R.S., Huey, R., Hart, W.E., Belew, R.K., Olson, A.J. (1998) Automated docking using Lamarckian genetic algorithm and an empirical binding free energy function. *J. Comp. Chem.* 19:1639-1662.

## **7. CONFIDENTIALITY.**

7.1 Acknowledgement. Recipient hereby acknowledges and agrees that the Software constitutes and contains valuable proprietary products and trade secrets of TSRI embodying substantial creative efforts and confidential information, ideas, and expressions. Accordingly, Recipient agrees to treat (and take precautions to ensure that its employees treat) the Software as confidential, not to disclose or permit to any third party or entity access to the Software or any portion thereof without the written permission of a duly authorized representative of TSRI.

7.2 Injunctive Relief. Recipient acknowledges that the unauthorized use, transfer or disclosure of the Software or copies thereof will (i) substantially diminish the value to TSRI of the trade secrets and other proprietary interests that are the subject of this Agreement; (ii) render TSRI's remedy at law for such unauthorized use, disclosure or transfer inadequate; and (iii) cause irreparable injury in a short period of time. If Recipient breaches any of its obligations with respect to the use or confidentiality of the Software, TSRI shall be entitled to seek equitable relief to protect its interests therein, including, but not limited to, preliminary and permanent injunctive relief.

7.3 Survival. Recipient's obligations under this Article 7 will survive the termination of this Agreement or of any license granted under this Agreement for whatever reason.

## **8. WARRANTIES; SUPERIOR RIGHTS.**

8.1 Government Rights. Recipient understands that the Software may have been developed under a funding agreement with the Government of the United States of America and, if so, that the Government may have certain rights relative thereto. This Agreement is explicitly made subject to the Government's rights under any such agreement and any applicable law or regulation, if any. To the extent that there is a conflict between any such agreement, applicable law or regulation and this Agreement, the terms of such Government agreement, applicable law or regulation shall prevail.

8.2 Disclaimer of Warranties. ANY INFORMATION, MATERIALS OR SERVICES FURNISHED BY TSRI PURSUANT TO THIS AGREEMENT ARE ON AN "AS IS" BASIS. TSRI DOES NOT REPRESENT OR WARRANT THAT ALL ERRORS IN THE SOFTWARE WILL BE CORRECTED. THERE ARE NO WARRANTIES RESPECTING THE SOFTWARE OR SERVICES PROVIDED HEREUNDER, EITHER EXPRESS OR IMPLIED, INCLUDING BUT NOT LIMITED TO ANY WARRANTY OF DESIGN, MERCHANTABILITY, FITNESS FOR A PARTICULAR PURPOSE, EVEN IF TSRI HAS BEEN INFORMED OF SUCH PURPOSE OR THAT THE SOFTWARE WILL NOT INFRINGE ANY PATENT, COPYRIGHT, TRADEMARK, OR OTHER PROPRIETARY RIGHTS. NO AGENT OF TSRI IS AUTHORIZED TO ALTER OR EXCEED THE WARRANTY OBLIGATIONS OF TSRI AS SET FORTH HEREIN.

## **9. INDEMNIFICATION.**

Except to the extent prohibited by law, Recipient shall indemnify and hold harmless, TSRI, its trustees, officers, agents and employees from and against any claims, demands, or causes of action whatsoever, including without limitation those arising on account of Recipient's modification or enhancement of the Software or otherwise caused by, or arising out of, or resulting from, the exercise or practice of the license granted hereunder by Recipient, its sublicensees, if any, its subsidiaries or their officers, employees, agents or representatives.

**10. NONASSIGNABILITY.** Any and all assignments of this Agreement or any rights granted hereunder by Recipient without the prior written consent of TSRI are void except (i) to an affiliate of Recipient or (ii) as expressly permitted hereunder.

**11. GOVERNING LAW; JURISDICTION AND VENUE.** The validity, interpretation, construction and performance of this Agreement shall be governed by the laws of the State of California.

**12. SEVERABILITY.** If any provision of this Agreement shall be held by a court of competent jurisdiction to be illegal, invalid or unenforceable, the remaining provisions shall remain in full force and effect. This Agreement and its exhibits contain the entire understanding and agreement between the parties respecting the subject matter hereof. This Agreement may not be supplemented, modified, amended, released or discharged except by an instrument in writing signed by each party's duly authorized representative. All captions and headings in this Agreement are for purposes of convenience only and shall not affect the construction or interpretation of any of its provisions. Any waiver by either party of any default or breach hereunder shall not constitute a waiver of any provision of this Agreement or of any subsequent default or breach of the same or a different kind.

IN WITNESS WHEREOF, the parties have caused their duly authorized representatives to execute this Agreement as of the date first set forth above.

**Recipient:**

By: \_\_\_\_\_

(Authorized Official)

Name/Title: \_\_\_\_\_

Date: \_\_\_\_\_

**TSRI:**

By: \_\_\_\_\_

Name/Title: Jennifer L. Dyer, Director, Technology Development

Date: \_\_\_\_\_

**Acknowledge and Agree:**

By: \_\_\_\_\_

(Recipient Scientist)

Name/Title: \_\_\_\_\_

Date: \_\_\_\_\_

Department: \_\_\_\_\_

Fax: \_\_\_\_\_

Address: \_\_\_\_\_

\_\_\_\_\_

\_\_\_\_\_

Email: \_\_\_\_\_

(to receive ftp instructions)