TINKER – *Software Tools for Molecular Design*

Version 8.4 February 2018

TINKER is a modular program package for molecular mechanics-based potential energy calculations, geometry optimization, molecular dynamics simulation, free energy calculations, distance geometry and structural analysis. The TINKER license covers the three Tinker codes: Tinker, Tinker-HP and Tinker-OpenMM.

1. On behalf of the Tinker developer community, an informal consortium of researchers also known as the Tinker Core Development Consortium ("**TCDC**") formed by Washington University in Saint Louis (MO, USA), The University of Texas at Austin (TX, USA) and Sorbonne Université (Paris, France) (collectively, TCDC-Members, individually TCDC-Member), the TCDC-Members hereby grant to the **Licensee** (as identified in the signature block below) a non-exclusive, non-sublicensable, non-transferable, revocable, non-commercial license to use the object and source code versions of the software known as "Tinker Software" (the **"Software"**), for internal academic purposes only, including the right and license to incorporate improvements to the Software, for a period of five (5) years subject to the terms and conditions below. All rights, title, interest and copyright to the Software, to all portions thereof, and to any associated documentation shall at all times remain the property of WU, UT Austin and Sorbonne.

2. A member of the TCDC will provide access to the Software to the Licensee, which may install the Software on a local network controlled by the Licensee's responsible official and for the use by the Licensee in accordance with this Agreement. The Software may be used beyond a local network or on a supercomputing center only if indicated by the Licensee in the Research Purpose section below. The Licensee may not sublicense the use of the Software, or make it available to third parties, without the prior written consent of at least one TCDC-Member.

3. The Licensee accepts the Software "as is" and understands that it is experimental in nature. The TCDC and TCDC-Members disclaim any and all representations and warranties, expressed or implied, or statutory, of any kind or nature with respect to the Software, including without limitation any warranty of merchantability or fitness for a particular purpose or non-infringement of any third-party patent, copyright, or any third-party right. The TCDC and all TCDC-Members, their trustees, faculty, staff, students and agents, shall not be liable to Licensee, its successors, assigns, contractors or sublicensees or any third party in any event for any damages or claims, whether direct or indirect, special, consequential or incidental, arising from the use of the Software.

4. Licensee agrees to indemnify, defend, and hold harmless TCDC and TCDC-Members, their personnel, affiliates, and each of their respective trustees, faculty, staff, employees, students, directors, officers, agents, successors and assigns (altogether the "TCDC Indemnitees") from, for and against any and all judgments, settlements, losses, expenses, damages and/or liabilities and any and all court costs, attorneys' fees, and expert witness fees and expenses that a TCDC Indemnitee may incur from any and all allegations, claims, suits, actions or proceedings (the "Claims") arising out of, relating to, or incidental to Licensee's breach of this Agreement or its use, development,

modification, or other exploitation of Software, whether by or through Licensee, and including all Claims for infringement, injury to business, personal injury, and product liability. The obligations set forth in this Section shall survive termination of this Agreement, shall continue even after assignment of rights and responsibilities, and shall not be limited by any provision of this Agreement outside this Section.

5. The Licensee may create computer programs that incorporate or modify the Software or resemble its structure, sequence or organization and may install and use such modified programs on computers for which use of the Software is authorized as described in Section 2. The Licensee may distribute binaries of the modified Software over the public community Tinker web site (www.tinkertools.org). Licensee grants to the TCDC and each TCDC-Member a non-exclusive license, with right to sub-license, to any and all source code that is delivered to the TCDC for possible inclusion in further releases of the Software.

6. The Licensee agrees, in perpetuity, not to disclose the Software to any third party and to use it only for the purposes of this Agreement, unless the TCDC gives prior written consent. In protecting the Software, the Licensee must use at least the same degree of care it uses to protect its own computer programs and other confidential information.

7. The user agrees that any reports or published results obtained with the Software will acknowledge its use by the appropriate citation. Considering the use of Tinker, any published work which utilizes Tinker shall give appropriate acknowledgement to the Tinker developer community's contribution by including the following main reference:

"**TINKER 8: A Modular Software Package for Molecular Design and Simulation**. Joshua A. Rackers, Marie L. Laury, Chao Lu, Zhi Wang, Louis Lagardère, Jean-Philip Piquemal, Pengyu Ren, Jay W. Ponder, ***Journal of Chemical Theory and Computation***, *14*, 5273-5289, **2018**, DOI 10.1021/acs.jctc.8b00529"

Considering the use of the specific Tinker-OpenMM code, included in the Tinker distribution, any published work which utilizes Tinker-OpenMM shall give, in addition to the main Tinker reference, appropriate acknowledgement to the Tinker-OpenMM developer community's contribution by including the following reference:

"**Tinker-OpenMM: Absolute and Relative Alchemical Free Energies using AMOEBA on GPUs**. Matthew Harger, Daniel Li, Zhi Wang Kevin Dalby, Louis Lagardère, Jean-Philip Piquemal , Jay Ponder, Pengyu Ren, ***Journal of Computational Chemistry***, *38*, 2047-2055, **2017**, DOI 10.1002/jcc.24853"

Considering the use of the specific Tinker-HP code, included in the Tinker distribution, any published work which utilizes Tinker-HP shall give, in addition to the main Tinker reference, appropriate acknowledgement to the Tinker-HP developer community's contribution by including the following reference:

"**Tinker-HP: a Massively Parallel Molecular Dynamics Package for Multiscale Simulations of Large Complex Systems with Advanced Polarizable Force Fields,** Louis Lagardère, Luc-Henri Jolly, Filippo Lipparini, Félix Aviat, Benjamin Stamm, Zhifeng F. Jing, Matthew Harger, G. Andres Cisneros, Nohad Gresh, Yvon Maday, Pengyu Ren, Jay W. Ponder, Jean-Philip Piquemal, ***Chemical Science***, *9*, 956-972, **2017**, DOI: 10.1039/c7sc04531j"

8. This license may be terminated upon twenty days' notice for any breach of this Agreement, provided that that breach has not been corrected prior to the expiry of such notice.

9. Commercial use of the Software, or derivative works based thereon, REQUIRES A COMMERCIAL LICENSE. Should Licensee wish to make commercial use of the Software, Licensee will contact one of the contacts that will act on behalf of the TCDC: for North America and rest of world outside of Europe: Washington University in Saint Louis (contact:OTM@dom.wustl.edu,ref: case 017551); for Europe, Sorbonne Université (contact: entreprisestransfert@sorbonne-universite.fr) to negotiate an appropriate license. Commercial Purposes include any sale, lease, license, or other transfer of the Software in its entirety or in part, to another entity. Commercial Purposes also includes, without limitation, uses of the Software by any entity, including Licensee, to perform any service for sale or contract research, to produce or manufacture products for sale.

10. Notice. Any notices or disclosures required or provided by the terms of this agreement shall be in writing and shall be delivered personally or sent by certified or registered mail, return receipt requested, postage prepaid or by internationally-recognized express mail service providing evidence of delivery. The effective date of any notice shall be the date of first receipt by the receiving Party or the date of refusal of receipt. Notices shall be sent to the addresses and addressees given below:

For North and South America and outside of Europe, preferably:

Washington University in Saint Louis (MO, USA)

Technical Contact:
Washington University in Saint Louis
Department of Chemistry
Campus Box 1134
One Brookings Drive
Saint Louis, MO 63130
c/o: Prof. Jay W. Ponder

The University of Texas at Austin (TX, USA)

Technical Contact:
Department of Biomedical Engineering
Cockrell School of Engineering
The University of Texas at Austin
107 W. Dean Keeton, BME Building
1 University Station, C0800
c/o: Prof. Pengyu Ren

For Europe, preferably:

Sorbonne Université (Paris, France)

Technical Contact:
Laboratoire de Chimie Théorique (LCT, UMR 7616)
CC 137, 4, Place Jussieu F-75252 Paris cedex 05
c/o: Prof. Jean-Philip Piquemal

Administrative Contact:
Sorbonne Université
Direction de la Recherche et du Transfert de Technologies
Tour Zamansky
4, Place Jussieu, 75252 Paris cedex 05
c/o: Mrs. Sophie Cluet - Ref. Sorbonne: X17/1504

Please Sign and Complete the Research Description on the following page.

Licensee:

_____(Signature);_____(Name and Title)

_____(Name and Title of Responsible Official,
if not Signing Authority)

_____(Organization)_____(Address)

_____(Email Address)_____(Date)

Description of Research Purpose:

In addition to the describing the Research Purpose, please address the following questions.

(1) How many users will have access to the Software?
(2) Will the Software be installed on a single or multiple computer(s)?
(3) Will users be able to use the Software beyond a local network?
(4) Will the Software be installed at a supercomputing center?