

MATERIALS TRANSFER AGREEMENT

Provider:

Molecular Networks GmbH – Computerchemie
Henkestraße 91
91052 Erlangen
Germany

Recipient:

U.S. Environmental Protection Agency (EPA)
Office of Research and Development (ORD)
National Center for Computational Toxicology (NCCT)

1. Provider agrees to transfer to Recipient's Investigator named below the following Research Material:

- 3D molecular models (single and multi-conformational models) of ToxCast chemicals generated by Provider's proprietary software applications CORINA and ROTATE
- MOSES.Script (Linux) – software for identifying and generating features for ToxCast and Tox21 chemicals
- MOSES.StructuralFeatures – software for generating structural features for ToxCast and Tox21 chemicals
- MOSES.MetabolicFeatures – software for generating metabolic features for ToxCast and Tox21 chemicals
- ADRIANA.Code (Windows XP, Linux) – software for computing physico-chemical descriptors of ToxCast and Tox21 chemicals
- MetaboGen – predictions for ToxCast and Tox21 chemicals
- IsoCYP – predictions for ToxCast and Tox21 chemicals

2. Recipient agrees to transfer to the Provider the following Research Results after internal EPA review, but prior to final publication: Structural alerts, structural categories, computational models on toxicity and metabolism and associated algorithms and training sets developed by EPA's National Center for Computational Toxicity within the ToxCast and Tox21 research projects with material transferred by the Provider (see paragraph 1). Furthermore, publicly releasable data on toxicity, metabolism and adverse reactions of interest to the Provider, collected during the course of the ToxCast project, will be made available from the Recipient to the Provider after internal EPA review, but prior to final publication. All pre-publication information provided by the Recipient to the Provider, as described above, shall be treated as confidential by the Provider until confirmation of final publication or written notification of release by the Recipient. After final publication or

written notification of release by the Recipient, the Provider may freely use the Research Results including their use in commercial applications.

Recipient agrees to provide Provider with qualified feedback from time to time and in a reasonable level of detail regarding the usability, usefulness and functionality of the software applications provided with the Research Material.

3. This Research Material may not be used in human subjects. The Research Material will be used only for research purposes by Recipient's investigator in his/her laboratory, for the research project described below. This Research Material will not be used for screening, production or sale, for which a commercialization license may be required. Recipient agrees to comply with all Federal rules and regulations applicable to the Research Project and the handling of the Research Material.

3(a). Were Research Materials collected according to 45 C.F.R. Part 46, "Protection of Human Subjects?"

Yes (Please provide Assurance Number: _____)

No

Not Applicable (Materials not collected from humans)

4. This Research Material will be used by Recipient's investigator solely in connection with the following research project ("Research Project") described with specificity as follows (*use an attachment page if necessary*):

- ToxCast and Tox21 research projects within EPA's National Center for Computational Toxicology.

5. In all oral presentations or written publications concerning the Research Project, Recipient will acknowledge Provider's contribution of this Research Material unless requested otherwise. To the extent permitted by law, Recipient agrees to treat as confidential, any of Provider's written information about this Research Material that is stamped "CONFIDENTIAL" for a period of five (5) years from the date of its disclosure to recipient. The foregoing shall not apply to information that is or becomes publicly available or which is disclosed to Recipient without a confidentiality obligation. Any oral disclosures from Provider to Recipient which Provider wishes to be treated as confidential shall be identified as being Confidential at the time of the disclosure and by written notice delivered to Recipient within thirty (30) days after the date of the oral disclosure. Recipient may publish or otherwise publicly disclose the results of the Research Project, but if Provider has given Confidential information to Recipient, such public disclosure may be made only after Provider has had thirty (30) days to review the proposed disclosure to determine if it includes any Confidential information, to the extent such review period is permitted by law.

6. This Research Material represents a significant investment on the part of Provider and is considered proprietary to Provider. Recipient's investigator therefore agrees to retain control over this Research Material and further agrees not to transfer the Research Material to other people not under his/her direct supervision without advance written approval of Provider. Provider reserves the right to distribute the Research Material to others and to use it for its own purposes. When the Research Project is completed, the Research Material will be returned to the Provider or disposed, if directed by Provider.

7. This Research Material is provided as a service to the research community. It is being supplied to Recipient with no warranties, express or implied, including any warranty of merchantability or fitness for a particular purpose. Provider makes no representations that the use of the Research Material will not infringe any patent or proprietary rights of third parties.

8. Recipient shall retain title to any patent or other intellectual property rights in inventions made by its employees in the course of the Research Project. However, if said inventions contain any portion of the Research Material, are derived from the Research Material, or could not have been produced but for the use of the Research Material, Recipient agrees to contact the Provider to determine what ownership interests, if any, the Provider may have, and, where applicable, to negotiate in good faith the terms of a commercial license. Inventorship for a patent application or a commercialized product based on said inventions shall be determined according to United States patent law. The preparation of one or more joint peer reviewed manuscripts is encouraged.

9. When Provider is the EPA: Recipient agrees not to claim, infer, or imply endorsement by the Government of the United States of America (hereinafter referred to as "Government") of the Research Project, the institution or personnel conducting the Research Project or any resulting product(s). Recipient agrees to hold the Government harmless and to indemnify the Government for all liabilities, demands, damages, expenses and losses arising out of Recipient's use for any purpose of the Research Material.

10. When Recipient is the EPA: Provider will not be liable to EPA for any claims or damages arising from EPA's use of the Research Material.

11. The Provider shall have the right to terminate this Agreement at any time if Recipient breaches any of the terms of this Agreement.

12. All notices pertaining to or required by this Agreement shall be in writing and shall be signed by an authorized representative and shall be delivered by hand (including private courier mail service) or sent by certified mail, return receipt requested, with postage prepaid, addressed as follows: