TERMS AND CONDITIONS FOR USE, REPRODUCTION, AND DISTRIBUTION

1. Definitions.

"License" refers to the terms and conditions for use, reproduction, and distribution as specified in Clauses 1 through 10 of this document.

"Licensor" refers to the copyright owner or authorized entity granting the License.

"Legal Entity" shall mean the union of the acting entity and all other entities that control, are controlled by, or are under common control with that entity. For the purposes of this definition, "control" means (i) the power, direct or indirect, to cause the direction or management of such entity, whether by contract or otherwise, or (ii) ownership of fifty percent (50%) or more of the outstanding shares, or (iii) beneficial ownership of such entity.

"You" (or "Your") shall mean an individual or Legal Entity exercising permissions granted by this License.

"Source" form shall mean the preferred form for making modifications, including but not limited to software source code, documentation source, and configuration files.

"Object" form shall mean any form resulting from mechanical transformation or translation of a Source form, including but not limited to compiled object code, generated documentation, and conversions to other media types.

"Work" shall mean the work of authorship, whether in Source or Object form, made available under the License, as indicated by a copyright notice that is included in or attached to the work (an example is provided in the Appendix below).

"Derivative Works" shall mean any work, whether in Source or Object form, that is based on (or derived from) the Work and for which the editorial revisions, annotations, elaborations, or other modifications represent an original work of authorship. For the purposes of this License, Derivative Works shall not include works that remain separable from or merely link (or bind by name) to the interfaces of, the Work and Derivative Works thereof.

"Contribution" shall mean any work of authorship, including the original version of the Work and any modifications or additions to that Work or Derivative Works thereof, that is intentionally submitted to Licensor for inclusion in the Work by the copyright owner or by an individual or Legal Entity authorized to submit on behalf of the copyright owner. For the purposes of this definition, "submitted" means any form of electronic, verbal, or written communication sent to the Licensor or its representatives, including but not limited to communication on electronic mailing lists, source code control systems, and issue tracking systems that are managed by, or on behalf of, the Licensor for the purpose of discussing and improving the Work, but excluding communication that is conspicuously marked or otherwise designated in writing by the copyright owner as "Not a Contribution."

"Contributor" shall mean Licensor and any individual or Legal Entity on behalf of whom a Contribution has been received by Licensor and subsequently incorporated within the Work.

2. Grant of Copyright License.

Subject to the terms and conditions of this License, each Contributor hereby grants to You a perpetual, worldwide, non-exclusive, no-charge, royalty-free, irrevocable copyright license to reproduce, prepare

Derivative Works of, publicly display, publicly perform, sublicense, and distribute the Work and such Derivative Works in Source or Object form, for all purposes.

3. Redistribution and Modification.

You may use the Work for all purposes, with or without modifications, in Source or Object form.

Your usage is subject to the following conditions:

(a) You must retain all copyright, patent, trademark, and attribution notices from the Source form of the Work in any modifications you make, except for notices that do not pertain to the Derivative Works.

(b) You may add your own attribution notices for internal documentation purposes, if they do not modify the License in any way.

4. Submission of Contributions & Licensing of Additional Data

If you generate additional synthetic binding affinity data that enhances or extends the Work, such data will not be automatically granted an additional license under this agreement. Instead, you must formally notify the Licensor of any such contributions. The Licensor reserves the right to incorporate further clauses regarding these contributions into a revised license. Any modifications to the license will be determined and issued solely by the Licensor to ensure consistency and integrity of the Work's licensing terms. Notwithstanding the above, nothing herein shall supersede or modify the terms of any separate license agreement you may have executed with Licensor regarding such Contributions.

5. Trademarks.

This License does not grant permission to use the trade names, trademarks, service marks, or product names of the Licensor, except as required for reasonable and customary use in describing the origin of the Work and reproducing the content of the NOTICE file.

6. Disclaimer of Warranty.

Unless required by applicable law or agreed to in writing, Licensor provides the Work (and each Contributor provides its Contributions) on an "AS IS" BASIS, WITHOUT WARRANTIES OR CONDITIONS OF ANY KIND, either express or implied, including, without limitation, any warranties or conditions of TITLE, NON-INFRINGEMENT, MERCHANTABILITY, or FITNESS FOR A PARTICULAR PURPOSE. You are solely responsible for determining the appropriateness of using or redistributing the Work and assume any risks associated with Your exercise of permissions under this License.

7. Limitation of Liability.

In no event and under no legal theory, whether in tort (including negligence), contract, or otherwise, unless required by applicable law (such as deliberate and grossly negligent acts) or agreed to in writing, shall any Contributor be liable to You for damages, including any direct, indirect, special, incidental, or consequential damages of any character arising as a result of this License or out of the use or inability

to use the Work (including but not limited to damages for loss of goodwill, work stoppage, computer failure or malfunction, or all other commercial damages or losses), even if such Contributor has been advised of the possibility of such damages. Furthermore, any loss, corruption, or unavailability of synthetic data occurring during access, use, or download from the web portal shall be the sole responsibility of the user ("You"), and the Contributors shall bear no liability for any such issues, including but not limited to accidental deletions, server failures, data corruption, or unauthorized access. It is Your responsibility to ensure appropriate backup and security measures while using or storing synthetic data obtained through the portal.

8. Accepting Warranty or Additional Liability.

You shall redistribute the Work or Derivative Works thereof, for all commercial purposes, consistent with this License. However, you may act only on Your own behalf and on Your sole responsibility, not on behalf of any other Contributor, and only if You agree to indemnify, defend, and hold each Contributor harmless for any liability incurred by, or claims asserted against, such Contributor by reason of your accepting any such warranty or additional liability.

9. Citations

For research related documentation, You have to cite the following (https://doi.org/10.1038/s41597-022-01631-9, https://doi.org/10.1038/s41597-023-02872-y, https://www.devalab.in/AI3/licenses/, and the blog (link: ….), from which the current synthetic data generation has been inspired.

END OF TERMS AND CONDITIONS

APPENDIX:

How to apply the AI3 License to your work.

To apply the AI3 License to your work, attach the following boilerplate notice, with the fields enclosed by brackets "{}" replaced with your own identifying information. (Don't include the brackets!) The text should be enclosed in the appropriate comment syntax for the file format. We also recommend that a file or class name and description of purpose be included on the same "printed page" as the copyright notice for easier identification within third-party archives.

Copyright {2025} {U. Deva Priyakumar}

Licensed under the AI3 License, Version 1.0 (the "License"); you may not use this file except in compliance with the License.

You may obtain a copy of the License at https://www.devalab.in/AI3/licenses/

Unless required by applicable law or agreed to in writing, synthetic data available for usage under the License is distributed on an "AS IS" BASIS, WITHOUT WARRANTIES OR CONDITIONS OF ANY KIND, either express or implied.

See the License for the specific language governing permissions and limitations under the License