Software License Agreement for ‘*Group Contribution Method’*

The software *Group Contribution Method* is designed to estimate the standard Gibbs free energy of formation (ΔfG'°) and reaction (ΔrG'°) for the majority of the biochemical compounds and reactions found in the *i*JR904 and *i*AF 1260 genome-scale metabolic models of Escherichia coli and in the Kyoto Encyclopedia of Genes and Genomes and University of Minnesota Biocatalysis and Biodegradation Database.

1. This is an agreement between Licensor and Licensee, who is being licensed to use the software *Group Contribution Method*.
2. Licensee acknowledges that this is only a limited non-exclusive license. Licensor is and remains the owner of all titles, rights, copyright and interests in the software *Group Contribution Method*.
3. The software *Group Contribution Method* is licensed at no charge for the purposes of scientific research. Any distribution, modification and usage for commercial purposes of the software *Group Contribution Method* without written authorization of licensor are prohibited and may lead to legal action.
4. Licensee agrees to defend and indemnify Licensor and hold Licensor harmless from all claims, losses, damages, or expenses connected with or resulting from use of the software *Group Contribution Method.*
5. The Licensor is not responsible for any accuracy of calculated results.
6. Licensor has the right to terminate this License Agreement and Licensee’s right to use the software *Group Contribution Method* upon any breach by Licensee.
7. This License Agreement is valid without Licensor’s signature. It becomes effective upon the earlier of Licensee’s signature or Licensee’s use of the software.
8. Licensee agrees to cite the following work(s) as acknowledgement to the Licensor.

Jankowski, M.D., Henry, C.S., Broadbelt, L.J. and Hatzimanikatis, V., "Group Contribution Method for Thermodynamic Analysis of Complex Metabolic Networks", *Biophysical Journal*, **2008**, 95, 1487-1499

Finley, S.D., Broadbelt, L.J., and Hatzimanikatis, V., "Thermodynamic Analysis of Biodegradation Pathways", *Biotechnology and Bioengineering*, **2009**, 103, 532-541.

Henry, C.S., Jankowski, M.D., Broadbelt, L.J. and Hatzimanikatis, V., "Genome-Scale Thermodynamic Analysis of Escherichia coli Metabolism", *Biophysical J.*, **2006**, 90(4), 1453-1461.

Licensee Name: \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ (Print)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ (Signature)

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

**Please Email, fax or mail the licensing agreement back to Professor Vassily Hatzimanikatis.**

**F: +41-(0)21-693-98-75  
E:** [**vassily.hatzimanikatis@epfl.ch**](javascript:void(location.href='mailto:'+String.fromCharCode(118,97,115,115,105,108,121,46,104,97,116,122,105,109,97,110,105,107,97,116,105,115,64,101,112,102,108,46,99,104)+'?'))

Contact address:

Prof. Linda J. Broadbelt

Department of Chemical and Biological Engineering

Northwestern University

Tech E-136, 2145 Sheridan Rd.

Evanston, IL 60208-3120, USA

T: +1-847-491-5351

F: +1-847-491-3728

E: [broadbelt@northwestern.edu](mailto:broadbelt@northwestern.edu)

Prof. Vassily Hatzimanikatis

Ecole polytechnique fédérale de Lausanne  
Institut des sciences et ingénierie chimiques  
EPFL SB ISIC LCSB,CH H4 625 (Bât. CH),Station 6  
CH-1015 Lausanne, Switzerland

T: +41-(0)21-693-98-70