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In zipfile: **inverse\_prov\_PBPK\_model\_start\_here.zip**

initialDistribution.m

main.m

makeJacobianIndex.m

PBPK\_model.m \*

twiceLSmethod.m

**[1]Yasunori Aoki, Ken Hayami, Hans De Sterck, Akihiko Konagaya: Cluster Newton Method for Sampling Multiple Solutions of Underdetermined Inverse Problems:Application to a Parameter Identification Problem in Pharmacokinetics, SIAM J. Scientific Computing, 36 (1), B14-B44 (2014); available at [10.1137/120885462](https://doi.org/10.1137/120885462) and [NII-2011-002E](https://doi.org/10.1137/120885462)**

**[2] Arikuma T, Yoshikawa S, Azuma R, Watanabe K, Muramatsu K, Konagaya A.: Drug interaction prediction using ontology-driven hypothetical assertion framework for pathway generation followed by numerical simulation, BMC Bioinformatics, vol. 9 (Suppl 6), S11 (2008); available at [doi:10.1186/1471-2105-9-S6-S11](https://doi.org/10.1186/1471-2105-9-S6-S11)**

\* Arikuma irinotecan PBPK model was originally written by Takeshi Arikuma in GNU Octave in 2008, and then rewritten and improved by Yasunori Aoki in Matlab in 2011.

The following MATLAB codes of **Yoshida's Cluster Newton**

**Method**[3], **Gaudreau's Cluster Newton Method**[4] are published as some derivatives of the original cluster under the Academic Free License, version 3.0 specified below. The following references should be cited when publishing related topics with these codes, respectively.

[3]Yoshida K, Maeda K, Kusuhara H, Konagaya A: Estimation of feasible solution space using Cluster Newton Method: application to pharmacokinetic analysis of irinotecan with physiologically-based pharmacokinetic models, BMC Systems Biology 2013, 7 (Suppl 3): S3 (2013); available at [doi:10.1186/1752-0509-7-S3-S3](https://doi.org/10.1186/1752-0509-7-S3-S3)

[4]Philippe Gaudreau, Ken Hayami, Y. Aoki, Hassan Safouhi, Akihiko Konagaya:  
Improvements to the cluster Newton method for underdetermined inverse problems.J. Computational Applied Mathematics283:122-141(2015); available at [doi:10.1016/j.cam.2015.01.014](https://doi.org/10.1016/j.cam.2015.01.014) and [NII-2013-002E](https://doi.org/10.1016/j.cam.2015.01.014)

In zipfile: **invprob\_140127.zip**

main\_dS.m

main\_bet.m

main.m

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