PKfit - A Pharmacokinetic Data Analysis Tool on *R*

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Introduction: Pharmacokinetic (PK) data analysis heavily depends on computer calculation power. In this study, we tried to create a nonlinear regressions tool on R using its available packages and functions. **Methods and Materials**: Design goal of this tool was aimed to be easy-to-use, so a menu-driven interface on RGui was developed. We used *lsoda* function (in *odesolve* package) to solve all differential equations used to define PK models. As for data fitting algorithms, Gauss-Newton algorithm (*nls* function in *stats* package) for non-linear regression, and the Nelder-Mead simplex method (*optim* function in *stats* package) for minimization of weighted sum of squares, as well as the genetic algorithm (*genoud* function in *rgenoud* package) were applied. Users just follow the menu step by step, and then will get the job done. Fourteen pharmacokinetic models: intravenous drug administrations with i.v. bolus or i.v. infusion, extravascular drug administrations, linear with 1^{st}-ordered absorption/elimination or nonlinear (Michaelis-Menten models were built. Two weighting schemes, 1/Cp(obs), and $1/Cp^2$(obs) were also included. The output information included a summarized table (consisting of time, observed and calculated drug plasma/serum concentrations, weighted residuals, area under plasma concentration curve (AUC), and area under the first moment (AUMC), goodness-of-fit, final PK parameter values, and plots such as linear plots, semi-log plots, and residual plots. In the part of simulation, *runif* and *rnorm* functions from *stats* package provide the generation of random uniform distribution derivates and normal distribution derivates for PK parameters, respectively. Further, we also provide the function of Monte-Carlo Simulation. **Results and Discussion**: We called this tool as *PKFit*. It has been announced publicly, and can be downloaded from mirror sites of CRAN (package name: *pkfit*). With only a few examples, most results obtained from in *PKfit* were comparable to those obtained from other two pharmacokinetic programs, *WinNonlin* and *Boomer*. **Conclusion and Future Work**: *PKfit* running on *R* has been built and has been proved that it can provide efficiency and accuracy in data fitting functions. Multiple dosing models or algorithms may be required for further development of *PKfit*.

Keywords: *R*, Pharmacokinetics, Nonlinear Regression, Data Fitting, Simulation

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