

Resource Summary Report

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Program DynaFit

RRID:SCR_008444

Type: Tool

Proper Citation

Program DynaFit (RRID:SCR_008444)

Resource Information

URL: <http://www.biokin.com/dynafit/>

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Description: Program DynaFit Analysis of (bio)chemical kinetics and equilibria Welcome to the DynaFit home page. Purpose Symbolic Notation Bibliographic Reference Numerical Methods Minimum System Requirements Purpose The main purpose of the program DynaFit is to perform nonlinear least-squares regression of chemical kinetic, enzyme kinetic, or ligand-receptor binding data. The experimental data can be either initial reaction velocities in dependence on the concentration of varied species (e.g., inhibitor concentration vs. velocity), or the reaction progress curves (e.g., time vs. absorbance). Symbolic Notation The main advantage in using the program DynaFit is in the ability to characterize the (bio)chemical reacting system in terms of symbolic, or stoichiometric, equations. For example, the "slow, tight" inhibition of a dissociative dimeric enzyme is described by the following text: Monomer Monomer $\rightleftharpoons$ Enzyme : k1 k2 Enzyme Inhibitor $\rightleftharpoons$ Complex : k3 k4 Enzyme Substrate $\rightleftharpoons$ ReactiveX : k5 k6 ReactiveX $\rightarrow$ Product Enzyme : k7 k8 The names of chemical species (Monomer, Enzyme, etc.) are entirely arbitrary and can be freely chosen by the investigator. Bibliographic Reference If you publish any results obtained by using DYNAFIT, please cite the following reference: Kuzmic, P. (1996) Anal. Biochem. 237, 260-273. Program DYNAFIT for the Analysis of Enzyme Kinetic Data: Application to HIV Proteinase ABSTRACT A computer program with the code name DYNAFIT was developed for fitting either the initial velocities, or the time-course of enzyme reactions, to an arbitrary molecular mechanism represented symbolically by a set of chemical equations. Seven numerical tests and five graphical tests are applied to judge the goodness of fit. Experimental data on the inhibition of the dissociative dimeric proteinase from HIV were used in four test examples. A set of initial velocities was analyzed to see if a tight-binding inhibitor could bind to the HIV proteinase monomer. Three different sets of progress curves were analyzed (i) to determine the kinetic properties of an irreversible inhibitor; (ii) to investigate the dissociation and denaturation mechanism for the protease dimer; and (iii) to investigate the inhibition mechanism for a transient inhibitor. See a MEDLINE abstract with related references concerning the kinetics of HIV-1 protease. Numerical Methods The nonlinear regression

module uses the Levenberg-Marquardt algorithm [1]. The time-course of (bio)chemical reactions is computed by the numerical integration of simultaneous first-order ordinary differential equations, using the Livermore Solver of ODE Systems (LSODE, [2]). The composition of complex mixtures at equilibrium (e.g., in the concentration jump experiment where a complex mixture is incubated prior to the addition of a reagent) is computed by solving simultaneous nonlinear algebraic equations, namely, the mass balance equations for the component species, by using the multidimensional Newton-Raphson method [3].

References G. A. F. Seber and C. J. Wild (1989) Nonlinear Regression, Wiley, New York, p. 624. A. C. Hindmarsh (1983) ODEPACK: a systematized collection of ODE solvers; in Scientific Computing, ed. R. S. Stepleman et al., North Holland, Amsterdam, pp. 55--64. E. Kreyszig (1993) Advanced Engineering Mathematics; 7th ed., John Wiley, New York, p. 929. Minimum System Requirements DynaFit for Windows Intel Pentium III or Celeron class 800 MHz or faster processor Microsoft Windows XP (SP1) or 2000 (SP2) 128 MB RAM 20 MB Hard Disk Space Ethernet Network Interface Card required for license activation(1) CD/DVD-ROM drive required for software installation(2) (1) The Network Interface Card is used to compute a unique Computer ID, tied to a particular DynaFit license. Essentially the Computer ID required for license activation is an encrypted Media Access Control (MAC address) associated with the given Network Card. (2) CD/DVD-ROM is not required if the software is being installed by using the downloadable installer file dynafit-install.zip. Sponsor. This work has been supported by the NIH, grant No. R43 AI52587-02 and the U.S. Department of Defense, U.S. Army Medical Research and Materials Command, Ft. Detrick, MD, administered by the Pacific Telehealth & Technology Hui, Honolulu, HI, contract No. V549P-6073.

Synonyms: DynaFit

Resource Type: software resource

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Alternate IDs: nif-0000-30477

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Ratings and Alerts

No rating or validation information has been found for Program DynaFit.

No alerts have been found for Program DynaFit.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 132 mentions in open access literature.

Listed below are recent publications. The full list is available at [ASWG](#) .

Lang L, et al. (2026) Making HEDS or tails of glutaredoxin catalysis: Direct reduction of bis(2-hydroxyethyl) disulfide as a non-glutathione disulfide substrate. *Redox biology*, 93, 104149.

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K??hn S, et al. (2025) SNAP-tag2 for faster and brighter protein labeling. *Nature chemical biology*, 21(11), 1754.

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Wilhelm J, et al. (2025) Improving split-HaloTag through computational protein engineering. *Protein science : a publication of the Protein Society*, 34(5), e70123.

Teixeira LR, et al. (2024) Water and chloride as allosteric inhibitors in WNK kinase osmosensing. *eLife*, 12.

Fagnani L, et al. (2024) Mechanism of non-competitive inhibition of the SARS-CoV-2 3CL protease dimerization: Therapeutic and clinical promise of the lichen secondary metabolite perlatolinic acid. *Heliyon*, 10(19), e38445.

Singla A, et al. (2024) Structural basis for Retriever-SNX17 assembly and endosomal sorting. *bioRxiv* : the preprint server for biology.

Kuznetsova AA, et al. (2024) Substrate Specificity Diversity of Human Terminal Deoxynucleotidyltransferase May Be a Naturally Programmed Feature Facilitating Its Biological Function. *International journal of molecular sciences*, 25(2).

Ito K, et al. (2024) The Swi5-Sfr1 complex regulates Dmc1- and Rad51-driven DNA strand exchange proceeding through two distinct three-stranded intermediates by different mechanisms. *Nucleic acids research*, 52(20), 12517.

Singla A, et al. (2024) Structural basis for Retriever-SNX17 assembly and endosomal sorting. *Nature communications*, 15(1), 10193.

Osterberg MK, et al. (2024) Coupling of zinc and GTP binding drives G-domain folding in *Acinetobacter baumannii* ZigA. *Biophysical journal*, 123(8), 979.