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 Enzyme : k1 k2 Enzyme Inhibitor Complex : k3 k4 Enzyme Substrate ReactiveX : k5 k6 ReactiveX --> 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, plase 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 simultaous 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.

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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 118 mentions in open access literature.

Listed below are recent publications. The full list is available at FDI Lab - SciCrunch.org.

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

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

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.

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

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Orris B, et al. (2023) Guanine-containing ssDNA and RNA induce dimeric and tetrameric SAMHD1 in cryo-EM and binding studies. bioRxiv : the preprint server for biology.

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Orris B, et al. (2023) Guanine-containing ssDNA and RNA induce dimeric and tetrameric structural forms of SAMHD1. Nucleic acids research, 51(22), 12443.

Humphreys JM, et al. (2023) Hydrostatic Pressure Sensing by WNK kinases. Molecular biology of the cell, 34(11), ar109.

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Phycoerythrobilin-Binding Orange Fluorescent Proteins. bioRxiv : the preprint server for biology.

Harrison SA, et al. (2023) Comparative analysis of the physical properties of murine and human S100A7: Insight into why zinc piracy is mediated by human but not murine S100A7. The Journal of biological chemistry, 299(11), 105292.

Kramer DA, et al. (2023) The intrinsically disordered cytoplasmic tail of a dendrite branching receptor uses two distinct mechanisms to regulate the actin cytoskeleton. eLife, 12.

Kosinski R, et al. (2022) The role of DNA nanostructures in the catalytic properties of an allosterically regulated protease. Science advances, 8(1), eabk0425.

Zhang Y, et al. (2022) SifR is an Rrf2-family quinone sensor associated with catechol iron uptake in Streptococcus pneumoniae D39. The Journal of biological chemistry, 298(7), 102046.

Pose M, et al. (2022) Fluorescent detection of hydrogen sulfide (H2S) through the formation of pyrene excimers enhances H2S quantification in biochemical systems. The Journal of biological chemistry, 298(10), 102402.

Kuznetsova AA, et al. (2022) Insight into the mechanism of DNA synthesis by human terminal deoxynucleotidyltransferase. Life science alliance, 5(12).

Senchurova SI, et al. (2022) The mechanism of damage recognition by apurinic/apyrimidinic endonuclease Nfo from Escherichia coli. Biochimica et biophysica acta. General subjects, 1866(11), 130216.

Bhujbalrao R, et al. (2022) Identification of allosteric hotspots regulating the ribosomal RNA binding by antibiotic resistance-conferring Erm methyltransferases. The Journal of biological chemistry, 298(8), 102208.