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ENReT: An open-source R-based tool for non-linear modelling specifically implemented for Food Science and Technology applications

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ENReT: An open-source R-based tool for non-linear modelling specifically implemented for Food Science and Technology applications

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Abstract

Food scientists often use nonlinear regression as a common statistical analysis within all those projects whose ultimate goal is to improve food quality. These models have been developed for a wide variety of chemical, microbiological, physical, and biochemical phenomena that occur in food. Fitting these models is not always easy due to a series of theoretical, technical, and usability limitations that can affect researchers. ENReT was created to facilitate this type of analysis and is intended to be used by everyone from university students to researchers or professionals in the field of food science and technology, but not only. The main objective was to obtain an easy-to-use tool without sacrificing statistical formalism and advanced methodologies. This work explains all the reasons why ENReT was created and its possible applications.

1. Introduction

The world of food science, with all its aspects, must deal with complex systems. Classical physics/chemical models fail to correctly predict the changes occurring in food since they strongly deviate from ideal, diluted and/or homogeneous systems. Consequently, over the years, food scientists have developed various specific mathematical models (mechanistic and empirical) to predict complex chemical, microbiological, physical, and biochemical phenomena occurring in foods. This intersection of mathematic and food has as its main objective that of improving the quality of food which can be defined and studied through various intrinsic attributes (i.e. safety, nutritional value, usage proprieties, shelf-life, texture, colour, appearance, and flavour; van Boekel, 2008). These attributes often behave in a nonlinear way, and this required the development of a much more advanced statistic than the linear one, with developments still current. However, this type of mathematical modelling requires a strong mathematical and statistical background that may be less familiar to food science researchers, who typically specialize in different fields.

Understanding how to process the experimental data is important not only for formal accuracy but also to enhance its value. It is currently possible to compute nonlinear regressions either with licensed software or with open-source software, which is often difficult to use because they require coding skills (e.g., R or Python). In recent years, several free modelling apps have been developed, but they often focus on a specific topic and/or do not allow to carry out all the most advanced statistical methods (Liu et al., 2021; Halder et al., 2011). In this context, the software ENReT (Easy Non-linear Regression Tool) was implemented (https://doi.org/10.5281/zenodo.23839619; De Flaviis, 2026), and this paper describes its main features and capabilities. The theoretical basis and statistical vision of ENReT relies on three main scientific books (i.e. van Boekel, 2008; Motulsky, & Christopoulos, 2004; Bates, & Watts, 1988) that were meticulously studied and integrated in the app.

2. Main features of ENReT

There are various motivations behind the development of ENReT, the most important are listed below:

1) Create an easy-to-use and free tool for nonlinear regressions with an intuitive graphical interface accessible to everyone without requiring coding knowledge;

2) Develop an app with a specific theoretical and statistical vision based on internationally renowned authors;

3) Implement advanced statistical methods such as three types of error estimation methods (linear approximation, Monte Carlo simulation, and profile-likelihood), five loss function (mean squared error (MSE), mean absolute error (MAE), Huber loss, log-hyperbolic error, and root mean squared log error (RMSLE)), four optimization algorithm (Levenberg-Marquardt, BFGS, L-BFGS-B, and Nelder-Mead), and four types of weighted least squares regression ($\frac{1}{\hat{y}}$, $\frac{1}{\hat{y}^2}$, $\frac{1}{\hat{y}^\zeta}$, and $\frac{1}{\hat{y}^{2b}}$ from replicates);

4) Gather the most important mathematical functions used in the field of Food Science and Technology in a single app;

5) Develop an advanced module for shelf-life determination based on secondary models (Arrhenius or custom);

6) Possibility of being used in any scientific field that applies nonlinear models, thanks to the possibility of adding custom functions;

7) Implement two types of approaches, one oriented towards analysing different models on the same data (Model comparison module), and one oriented towards analysing different samples with the same model (Batch module);

8) Facilitate successful fitting through a system for visualizing initial guesses, diagnostics plots, loss function trend analysis, and algorithms developed for the Batch module;

9) Develop a tool with a strong educational leaning that can be used in any shelf-life or kinetic modelling course in Food Science and Technology degree (the possibility of generating synthetic data was also implemented for this reason);

10) Implement, with the same features, a web version accessible with one click via any browser and without the need to install any statistical software (https://enret.netlify.app);

11) Customize every plot, as already happens in professional software, and possibility to set output sizes and their digital format (PDF or JPEG) for possible publication purpose;

12) Improve ENReT by continuously testing and validate it with a strong focus on optimizing the user experience and usability.

3. Developing platform and software availability

ENReT is developed in RStudio v2026.6.0.242 (Posit team, 2026) and written in R v4.6.1 (R Core Team, 2026) with the following packages: *shiny* v1.14.0 (Chang et al., 2026), *minpack.lm* v1.2.4 (Elzhov et al., 2023), *bslib* v0.12.0 (Sievert et al., 2026), *writexl* v2.0.1 (Ooms & Denney, 2026), *readxl* v1.5.0 (Wickham & Bryan, 2026), and *zip* v3.0.2 (Csárdi, 2026).

ENReT 1.0.0 consists of 18 source files and 20,116 lines of R code (about 15,000 lines of effective code without comments and blank lines) available on https://github.com/RiccardoDeFlaviis/ENReT under the GNU General Public License v3.0. ENReT 1.0.0 is archived in Zenodo (https://doi.org/10.5281/zenodo.23839619; De Flaviis, 2026).

ENReT can be run locally in R or directly in a web page through Shinylive which permits to launch ENReT in the browser via WebAssembly (https://enret.netlify.app).

4. Outline of ENReT

ENReT is essentially a Graphical User Interface (GUI), and the main screen is shown in Figure 1.

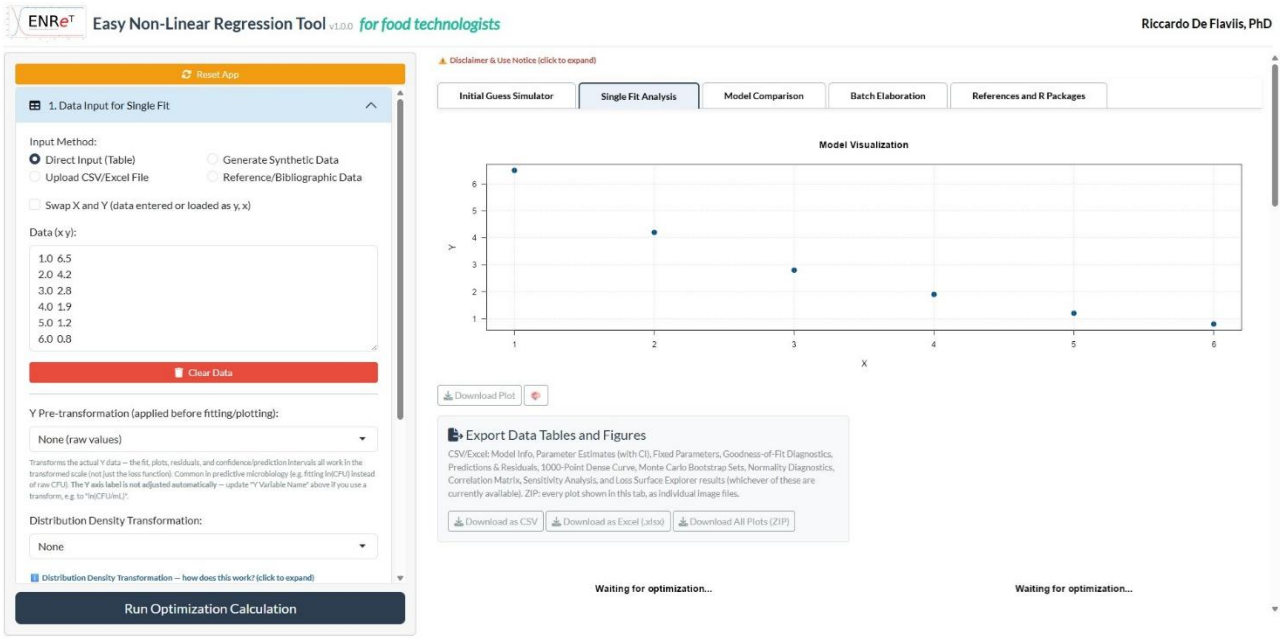


Figure 1. Main screen of ENReT v1.0.0

The core of the app is 4 tabs selectable at the top, namely “Initial Guess Simulator”, “Single Fit Analysis”, “Model Comparison”, and “Batch Elaboration”. In the sidebar, the user can upload the data and choose the mathematical model. With the button “Run Optimization Calculation” located at the bottom left the user can compute the regression. The user can test ENReT even without original data thanks to a synthetic data generator and several public datasets made available and easily usable in the data input section.

5. Statistical validation

ENReT has been validated using standard datasets and certified fitting parameters provided by NIST (NIST Statistical Reference Datasets, 2003). These data are provided specifically for assessing the accuracy of software. The Nelson dataset was the only one not utilized for validation since it needs to model two x simultaneously. The 26 NIST datasets and models were fitted by Levenberg-Marquardt algorithm (1024 iterations, MSE loss) via ENReT by using two initial guesses provided by the NIST; subsequentially, the parameter estimates, their standard errors, and the residual sum of squares (RSS) were compared with the NIST-certified ones by the log relative error (LRE; McCullough, 1998):

$$\mathrm{LRE} = -\log_{10}\frac{|\theta_{ENReT} - \theta_{NIST}|}{|\theta_{NIST}|}$$

LRE is an indicator that represents the digits of accuracy. Notably, McCullough reported that for nonlinear procedures a value of four or five digits is reasonable for statistical software (McCullough, 1998).

In Table 1, the RSS comparisons are shown. LRE showed always values greater than 10 except for Lanczos1 dataset. This is due to the extremely small RSS certified by NIST (1.4×10^{-25}), a value difficult to be reproduced with precision. The correctness of the fitting can be proved from the value of LRE in the parameter estimation (Figure 2) while as for the errors in the estimated parameters they depend on the RSS and therefore inherit the same problem.

Table 1. LRE computed comparing RSS from ENReT results and certified NIST values

Dataset	Difficulty	Quantity	Start	LRE	Start	LRE
Bennett5	Higher Level of Difficulty	RSS	1	11.1	2	11.2
BoxBOD	Higher Level of Difficulty	RSS	1	10.4	2	10.4
Chwirut1	Lower Level of Difficulty	RSS	1	11.4	2	11.4
Chwirut2	Lower Level of Difficulty	RSS	1	11.2	2	11.2
DanWood	Lower Level of Difficulty	RSS	1	11.7	2	11.7
Eckerle4	Higher Level of Difficulty	RSS	1	10.7	2	10.7
ENSO	Average Level of Difficulty	RSS	1	11.4	2	11.4
Gauss1	Lower Level of Difficulty	RSS	1	11.6	2	11.6
Gauss2	Lower Level of Difficulty	RSS	1	10.6	2	10.6
Gauss3	Average Level of Difficulty	RSS	1	11.0	2	11.0
Hahn1	Average Level of Difficulty	RSS	1	10.6	2	10.6
Kirby2	Average Level of Difficulty	RSS	1	11.6	2	11.6
Lanczos1	Average Level of Difficulty	RSS	1	2.7	2	3.0
Lanczos2	Average Level of Difficulty	RSS	1	10.1	2	10.3
Lanczos3	Lower Level of Difficulty	RSS	1	10.6	2	10.6
MGH09	Higher Level of Difficulty	RSS	1	11.6	2	11.6
MGH10	Higher Level of Difficulty	RSS	1	11.5	2	11.4
MGH17	Average Level of Difficulty	RSS	1	11.5	2	11.5
Misra1a	Lower Level of Difficulty	RSS	1	10.5	2	10.5
Misra1b	Lower Level of Difficulty	RSS	1	11.3	2	11.3
Misra1c	Average Level of Difficulty	RSS	1	11.1	2	11.1
Misra1d	Average Level of Difficulty	RSS	1	11.2	2	11.2
Rat42	Higher Level of Difficulty	RSS	1	11.9	2	11.9
Rat43	Higher Level of Difficulty	RSS	1	11.4	2	11.4
Roszman1	Average Level of Difficulty	RSS	1	12.2	2	12.2
Thurber	Higher Level of Difficulty	RSS	1	11.2	2	11.3

In Figure 2, all the LRE on the estimated parameters and their standard error were reported as a scattergrams plot. Most of the fittings had an LRE > 4 except for Lanczos1 dataset. This validation demonstrates how ENReT is reliable for fitting different nonlinear models without anomalous results.

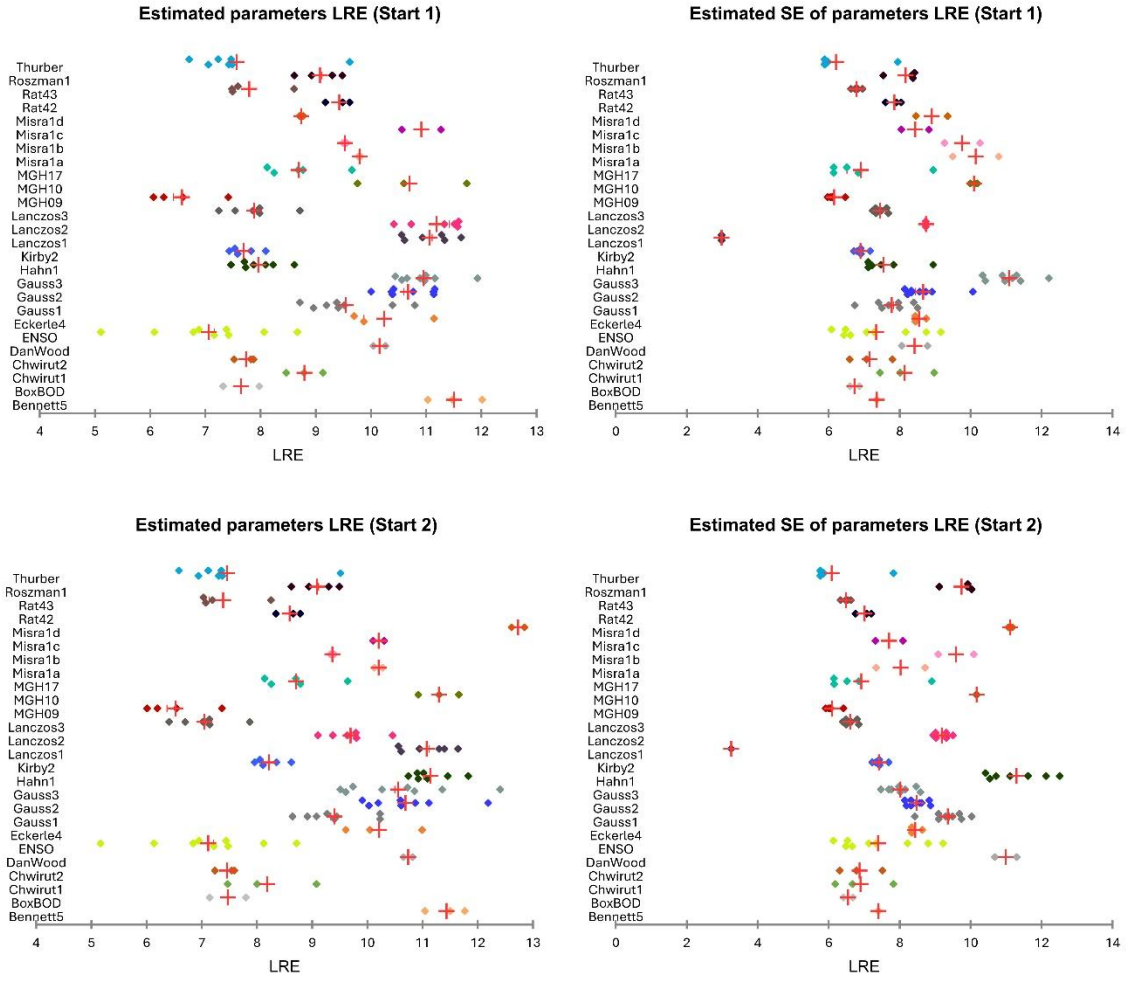


Figure 2. Scattergrams reporting LRE for the estimated parameters and their standard error for start 1 and start 2

6. ENReT applications

Once validated on the software/statistical side, several published datasets were further tested. These datasets were uploaded to ENReT itself for anyone who wanted to test them. In this section two main examples were reported, a microbiological growth dataset obtained from ComBase (https://combase.errc.ars.usda.gov) and a batch analysis of isothermal heating on riboflavin content in spinach (Nisha et al., 2005).

6.1 Microbiological growth

For this application, the dataset of Salmonella spp. growth (Record B092_25) was fitted. ComBase reports the counts of microorganism in $Log_{10,}$ so the data was converted in natural Log (i.e. Ln) in order to be modelled with models which have been developed for this type of mathematical transformation (Zwietering et al., 1990). In ENReT it is possible to convert data from Log_{10} to Ln by a specific selector (i.e. "Y Pre-transformation (applied before fitting/plotting):"). Then, the data were fitted with the reparametrized Gompertz model (Zwietering et al., 1990), leaving all other parameters at default. Once the analysis is performed, ENReT displays the predicted curve (Figure 3), diagnostic graphs, and summary tables of the estimated parameters and goodness-of-fit.

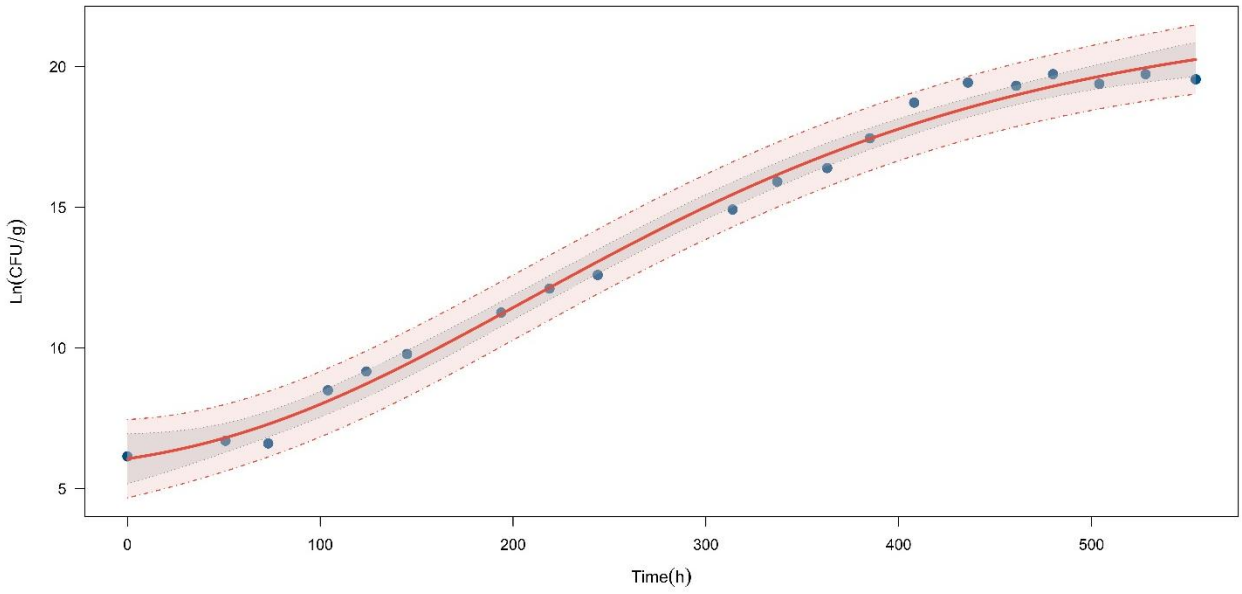


Figure 3. Predicted Salmonella spp. growth curve (ComBase data: Record B092_25) obtained with the reparametrized Gompertz model. Confidence and prediction bands at 95% level are shown. The figure is generated by ENReT v1.0.0

Subsequently, the reparametrized logistics (Zwietering et al., 1990) and the reparametrized Baranyi & Roberts model (Baranyi & Roberts, 1994) were tested with the same dataset. In model comparison tab, the models were compared as shown in Figure 4.

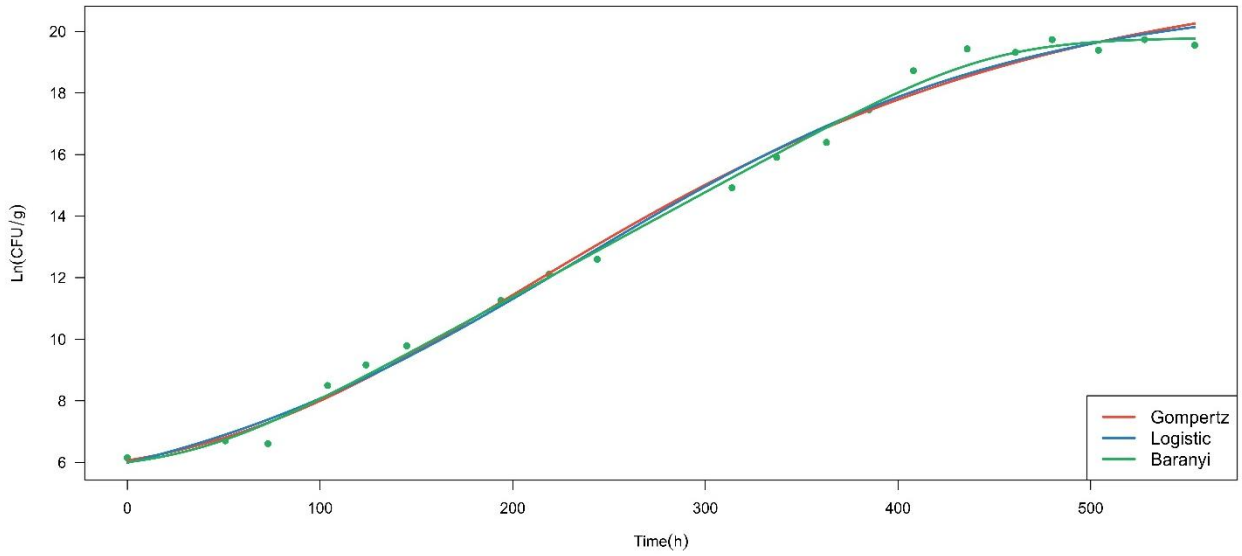


Figure 4. Predicted Salmonella spp. growth curve (ComBase data: Record B092_25) obtained with three different models. The figure is generated by ENReT v1.0.0

Table 2 reports the goodness-of-fit statistics, and the Baranyi model resulted the best model considering the AICc index.

Table 2. Goodness-of-fit statistics of the three models tested on Salmonella spp. growth (ComBase data: Record B092_25). The table is generated by ENReT v1.0.0 via "Copy to Clipboard" button. RMSE: Root Mean Square Errors; AIC: Akaike Information Criterion; BIC: Bayesian Information Criterion

Model	Converged	N Param	RMSE	R^2	R^2 Adj	AIC	AICc	BIC
Baranyi	Yes	4	0.345	0.996	0.995	-36.975	-32.690	-31.997
Logistic	Yes	4	0.478	0.992	0.991	-23.957	-19.671	-18.978
Gompertz	Yes	4	0.503	0.992	0.990	-21.929	-17.643	-16.950

Table 3 summaries all the estimated parameters demonstrating that no big differences were present among the models. This is also confirmed by the "Post-Hoc Comparison (3+ Models):" module showing no statistical differences within the same parameters (all the parameters were labelled "a" in the post-hoc analysis).

Table 3. Estimated parameters of the three models tested on Salmonella spp. growth (ComBase data: Record B092_25). The table is generated by ENReT v1.0.0 via "Copy to Clipboard" button

Model	Parameter	Estimate	St. Error	CI 95 Lower	CI 95 Upper
Gompertz	N_0	5.604	0.764	3.984	7.225
Gompertz	A	16.446	1.489	13.289	19.602
Gompertz	μ_{max}	0.037	0.002	0.033	0.042
Gompertz	λ	44.464	29.192	-17.420	106.348
Logistic	N_0	4.032	1.151	1.592	6.473
Logistic	A	17.099	1.683	13.530	20.668
Logistic	μ_{max}	0.037	0.002	0.033	0.042
Logistic	λ	5.239	43.140	-86.214	96.693
Baranyi	N_0	6.005	0.315	5.338	6.672
Baranyi	A	13.786	0.377	12.988	14.585
Baranyi	μ_{max}	0.034	0.001	0.032	0.036
Baranyi	λ	42.781	12.967	15.293	70.269

6.2 Isothermal heating on riboflavin content in spinach

For a batch application, data of isothermal heating (seven different temperatures) on riboflavin content in spinach (Nisha et al., 2005) were fitted by using a first-order kinetic model. ENReT will automatically fit, one after the other, all the isothermal decays with the chosen model. Once the analysis is performed, ENReT displays the predicted curves (Figure 5), and summary tables of the estimated parameters and goodness-of-fit statistics.

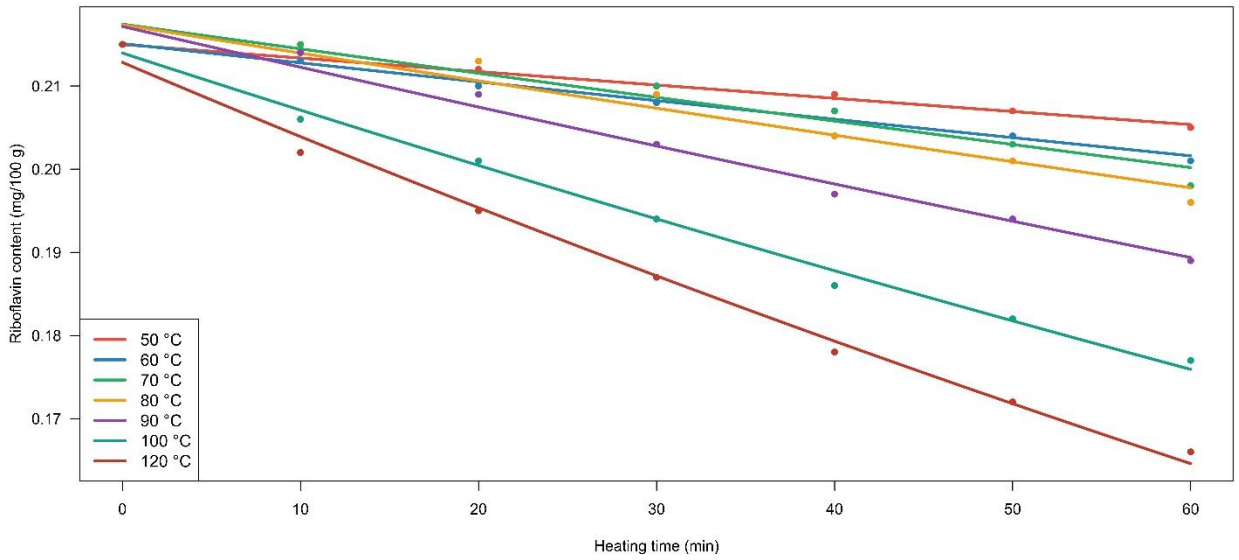


Figure 5. Predicted riboflavin content in spinach with seven different temperatures. The figure is generated by ENReT v1.0.0

Table 4 shows the estimated parameters with the letters computed by the "Post-Hoc Comparison (3+ Models):" module (Holm correction). differences were present among the models. A_0, the parameter indicating the initial decay value, is statistically non-different between temperatures. The parameter k, which represents the decay rate, shows many statistically significant differences with a linear increase as the temperature increases.

Table 4. Estimated parameters of the first-order kinetic model for riboflavin content in spinach datasets. Different letters within the same parameters indicate significantly differences ($p < 0.05$). The table is generated by ENReT v1.0.0 via "Copy to Clipboard" button, letters were added

Sample	Converged	A_0 Estimate	A_0 St. Err.	k Estimate	k St. Err.
50 °C	Yes	0.21499 a	0.00023	0.00076 a	0.00003
60 °C	Yes	0.21509 a	0.00041	0.00108 b	0.00005
70 °C	Yes	0.21744 a	0.00126	0.00138 bc	0.00016
80 °C	Yes	0.21736 a	0.00128	0.00158 c	0.00017
90 °C	Yes	0.21716 a	0.00107	0.00228 d	0.00014
100 °C	Yes	0.21397 a	0.00084	0.00326 e	0.00012
120 °C	Yes	0.21284 a	0.00112	0.00428 f	0.00016

7. Limitations and future implementations

ENReT has several limitations, some of these could be improved in future versions (some implementations are not possible for the online version). The most important are:

1) Possibility to fit systems of equations;

2) Possibility to fit differential equations;

3) Analyse non-isotherms for models other than kinetic models;

4) Reduce analysis time by improving code, especially for bootstrap analysis;

5) Fitting equations with two *x* (e.g. time and temperature) at the same time;

6) Possibility to model equations by Bayesian approach (MCMC method).

8. Conclusions

ENReT may represent an effective tool for food technologists who encounter dozens of mathematical models throughout their careers, from university studies to the different professional roles hold in companies and research centres. Despite all the statistical software available on the market (licensed or open), the combination of usability, statistical robustness, ease of use, diagnostic systems and a strong educational orientation make ENReT an extremely useful alternative.

Conflicts of Interest Statement

The authors certify that they have no affiliations with or involvement in any organization or entity with any financial interest, or non-financial interest in the subject matter or materials discussed in this manuscript.

Generative AI disclosure statement

During the preparation of this manuscript, the authors did not use any AI tool. Conversely, ENReT was developed with the aid of AI, specifically Gemini (Gemini Pro 3.1, Google) and Claude (Sonnet 5 and subsequently Opus 5.5, Anthropic) mainly to write the R code. The authors independently validated and reviewed ENReT and take full responsibility for the content of the publication and the app.

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