

AIC – Akaike Information Criterion and Enzyme Inhibition

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This program allows the calculation of parameters of the *Akaike Information Criterion* (Akaike, 2003) for the statistical discrimination between nonlinear models.

1 Equation:

$$AIC = n \cdot \ln! \left(\frac{SSE}{n} \right) + 2k + \left[\frac{2k(k+1)}{n-k-1} \right]$$

Where:

- $k = p + 1$ (with p being the number of model parameters);
- SSE = sum of squared residuals from the fit.

$$probab.B = \frac{e^{-0.5 \cdot \Delta AIC}}{1 + e^{-0.5 \cdot \Delta AIC}}$$

Where:

- $probab. B$ = probability that model B is better than model A (range 0–1);
- ΔAIC = difference $AIC_B - AIC_A$.

2 Files

- Program;
- Source code;
- This tutorial

3 Usage:

To run the program, the following data must be entered sequentially into the stack:

```
# Data input

1. After selecting "AIC", the program requests the following values (INPUT):
   n, kA, kB, ssA, ssB
2. After ENTER, the program computes:
   "AIC_A, AIC_B, delta, prob.B"
```

4 Example

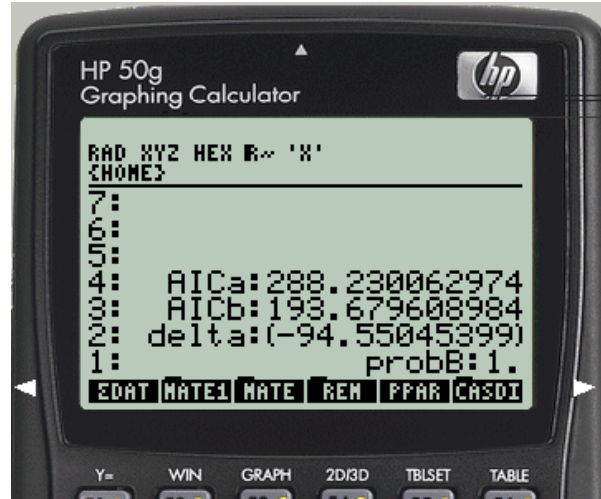
The table and figures below refer, respectively, to enzyme inhibition data reported by Bezerra *et al.* (2013), and to the data input and output obtained for a pair of competing models.

Table 1 – Experimental enzyme inhibition data ($n = 105$). Source: Bezerra et al., 2013.

Type	Control	Competitive	Pure non-competitive	Mixed non-competitive	Uncompetitive
SSE	1540.1	613.1	1122.7	613.2	1436.4
p	2	3	3	4	3



(a) Input of values for comparison between control and competitive models.



(b) Comparison results obtained.

Figure 1: Execution of the program for comparison between control and competitive models of enzyme inhibition.

By running the *AIC* program, the following comparison results were obtained for selected pairs of models:

Table 2 — Results of model comparison using the *AIC* criterion.

Model A / B	AIC_A	AIC_B	Δ	Probab. B
Control / Competitive	288.2	193.7	-94.6	1.0
Control / Mixed NComp.	288.2	195.9	-92.3	1.0
Competitive / Mixed NComp.	193.7	195.9	2.2	0.25

Based on these results, the probability associated with model B supports the selection of the competitive enzyme inhibition model, with a 75% likelihood over the mixed non-competitive model, in agreement with the conclusions reported by the authors.

References

1. Akaike, Hirotugu. *A new look at the statistical model identification*. IEEE Transactions on Automatic Control, 19(6), 716–723, 2003.
2. Bezerra, Rui M. F., Irene Fraga, and Albino A. Dias. *Utilization of integrated Michaelis–Menten equations for enzyme inhibition diagnosis and determination of kinetic constants using the Solver supplement of Microsoft Office Excel*. Computer Methods and Programs in Biomedicine, 109(1), 26–31, 2013.

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