Gabriel package: software for education and research

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It is well established that today, personal computers are part of our life either at home, at work or at school. As the computer power increases, the software becomes harder and harder, requiring more time to learn it or to obtain a result. The need of small software using empirical but fast equations becomes urgent in labs as well as at school. Most of this software uses databases patiently collected by the authors. I report here about the use of the three software belonging to the Gabriel package. This software can be obtained free of charge upon request. Today, software for research can be used for education and educational software can be useful for research.

Gabriel Nathalie II (GN2) (actual version: 3.05)

GN2 is usable for calculating the pKa, the chemical shift in ^{31}P NMR of amino phosphonate or the thermodynamics data of bisphosphonate binding to human bones. The equations and the dataset for the pKa and the ^{31}P NMR were found by Piétri *et al.*[1,2] while the thermodynamics dataset were determined by the group of Eric Oldfield[3]. All equations are of the type:

$$\gamma_x = C_0 + \sum C_i.n_i + \varepsilon$$

in which γ_x is the pKa, the chemical shift in ^{31}P NMR or the thermodynamics data, C_0 is a (optional) constant value, a_i is a constant increment depending on the substituent, n_i represents the number of each substituent of type i and ε is an optional nonlinear steric correction. Each calculation has its own screen on GN2 selectable by a tool bar.

Gabriel Calculatrice Savon (GCS) (*Gabriel Soap Calculator*) (actual version: 2.08)

GCS is usable to calculate the amount of alkali needed for making a soap according to the amount and the nature of fat but also the viscosity of some oils at a desired temperature. GCS is now available in several languages (French, English, Spanish and Dutch).
Soaps are salts of fatty acids. Making soap consists in putting together a fat and an alkali and in boiling the mixture for a few hours. The action of the alkali is an hydrolysis of the esters to give glycerol and the salt of fatty acids. It is well known that the quantity of alkali needed for the reaction can be calculated by the Saponification Index that is defined as the number of mg of potassium hydroxide needed to neutralize free fatty acids and to hydrolyze the fatty esters in one gram of fat. What is very important in such software, is the size of the database of saponification index. GCS includes a database with 89 fats.[4] Up to 15 fats can be entered with three zones for unknown fat in the database (the name and especially the saponification index must be given). For each entry of fat, the user can find the saponification index, the iodine index and some properties of soap made with the oil (when they were found). Two screens are devoted to this module, the first one is the input screen, while the second one is for the calculations' results.

The viscosity module has only one screen and uses the equation below, that is the best found by Abramovic.[5]

$$\log \eta = \frac{A}{T} - B$$

where T is the absolute temperature in Kelvin, A and B are correlation constants.

Gabriel Data Analysis (GDA) (actual version: 1.17 Build 1.0b)

In addition to the modules presented last year at the same symposium (Input Module, One Variable Statistic Module, Two Variable Statistic Module, Rheological Module and TVT Analyze Module)[6], other modules have been integrated into GDA such as a module of linear regression with 3 variables (Z = f (X, Y)), a module dedicated to the experimental design in which it is also possible to solve n equations with n unknowns (Experimental Design module), a module for solving quadratic and cubic equations (Resolution x^2, Resolution x^3), a module for finding the parameters of the Arrhenius equation (Arrhenius/Eyring Module)), a complete module for pH analyzing (pH Analyze Module) and finally a complete module for analyzing the curves obtained from a Langmuir-Balance (LFW Analyze Module).

1)Pietri, S.; Miollan, M.; Martel, S.; Le Moigne, F.; Blaive, B.; Culcasi, M. *J. Biol. Chem.* **2000**, *275*, 19505-19512.
2)Gosset, G.; Martel, S.; Clement, J.-L.; Blaive, B.; Olive, G.; Culcasi, M.; Rosas, R.; Thevand, A.; Peitri, S. *C. R. Chimie* **2008**, *11*, 541-552.
3)Mukherjee, S.; Huang, C.; Guerra, F.; Wang, K.; Oldfield, E. *J. Am. Chem. Soc.* **2009**, *131*, 8374-8375.
4)Thomaelle *Les lys blancs de Venus (http://lysblancsdevenus.canalblog.com/archives/les_techniques_de_base/index.html)*, 2010.
5)Abramovic, H.; Klofutar, C. *Acta Chim. Slov.* **1998**, *45*, 69-77.
6)Olive, G. *Gabriel Data Analysis (GDA): from data analysis to food analysis*; S. R. C., Ed.: Brussels (Belgium), **2011**, October, 13th, P50.

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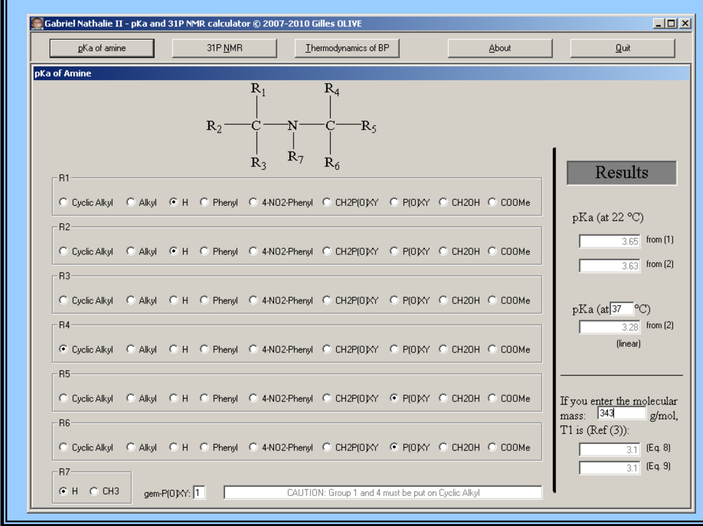

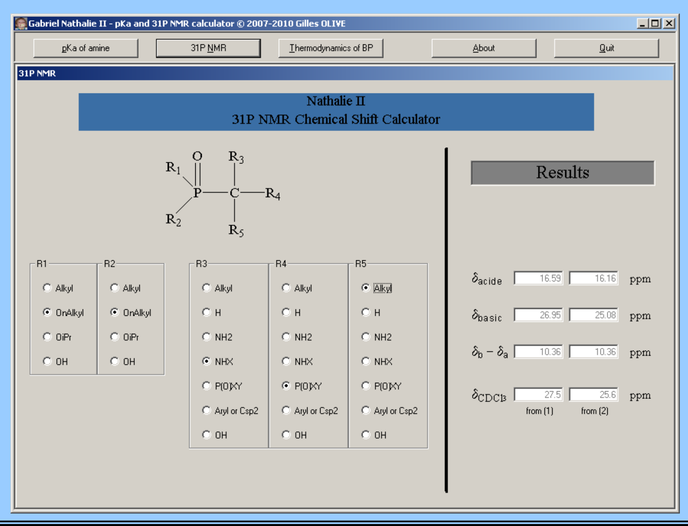

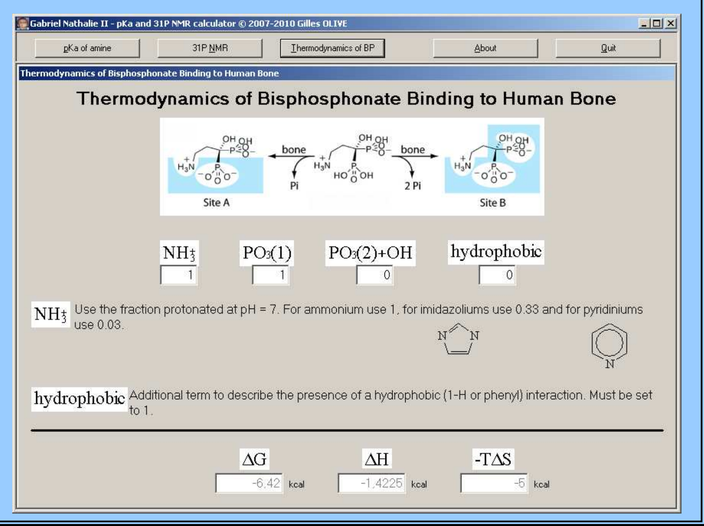

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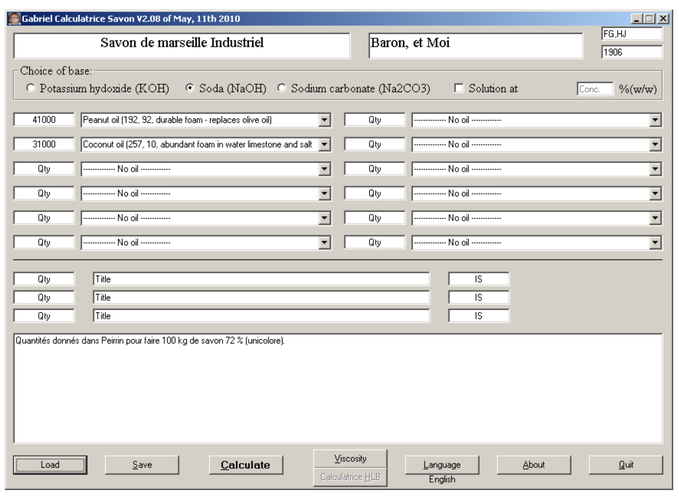
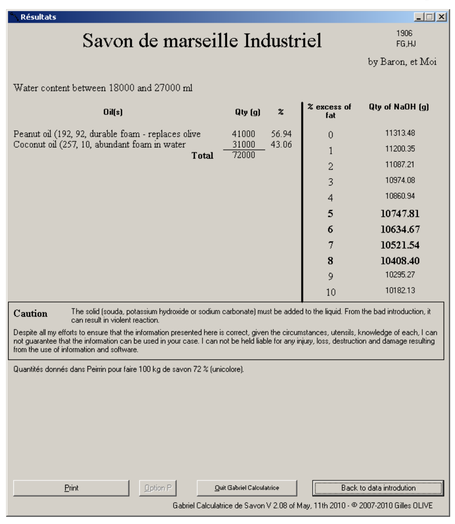
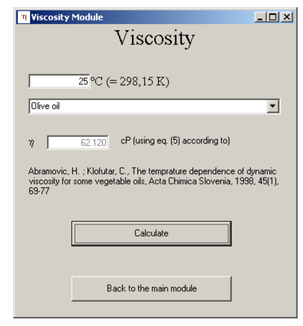
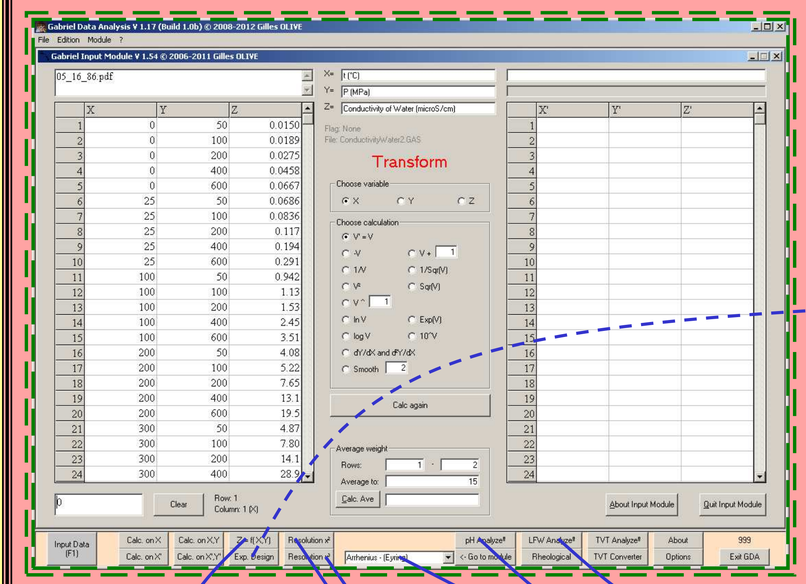


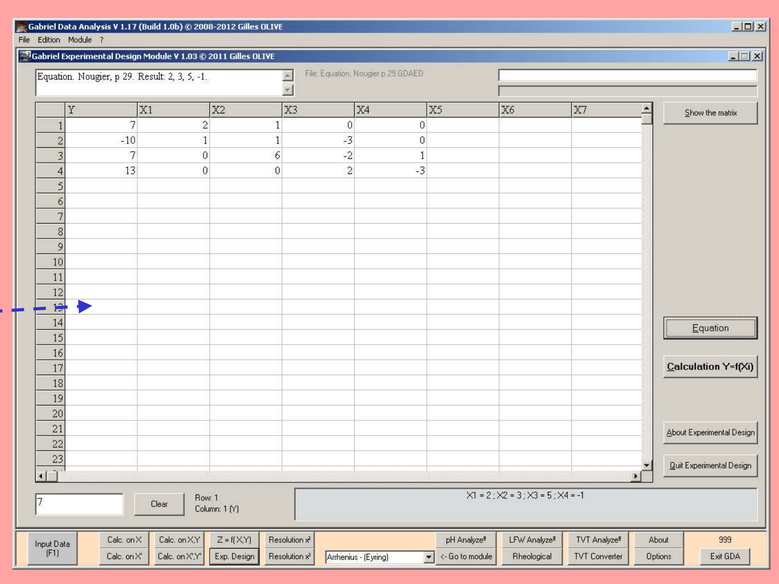


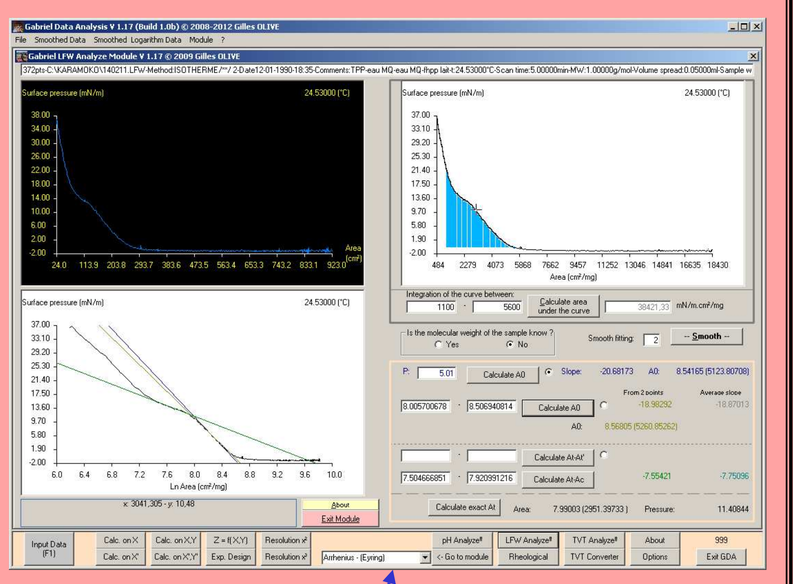


Gabriel Data Analysis (GDA) (actual version: 1.17 Build 1.0b)

GDA is a software devoted to data analysis. GDA is built around modules. In addition to the modules presented last year at the same symposium (Input Module, One Variable Statistic Module, Two Variable Statistic Module, Rheological Module and TVT Analyze Module), other modules have been integrated into GDA as can been seen in the images below. The most important one is always the Input Module, in which data are entered, directly or from an apparatus before processing.







The other modules can be found at Olive, G. *Gabriel Data Analysis (GDA): from data analysis to food analysis*; S. R. C., Ed.: Brussels (Belgium), **2011**, October, 13th, P50