

Chimica Analitica

Equilibri in soluzione

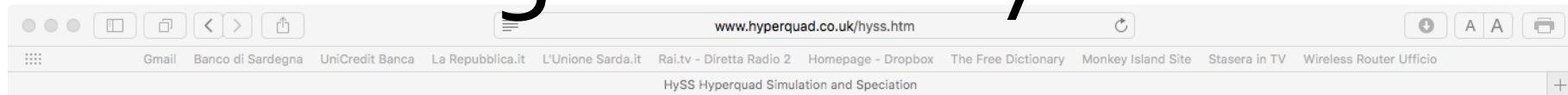
Speciazione

Distribution of an element amongst defined chemical species in a system
(IUPAC recommendation 2003)

Nelle lezioni precedenti abbiamo visto come ricavare la distribuzione delle diverse specie in cui si trova un acido poliprotico in soluzione in funzione del pH.

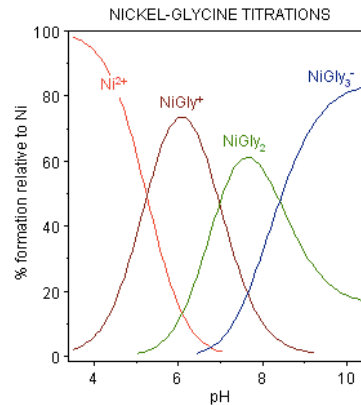
Esistono in letteratura diversi programmi che permettono di calcolare le curve di distribuzione per diversi sistemi a diverse condizioni sperimentali.

Programma HySS



 **HySS2009**

Hyperquad Simulation and Speciation



HySS is a program that can be used to perform 2 distinct functions.

- Titration simulation. A model is specified by defining a set of equilibrium constants
$$b_{pq..} = \frac{[A_p][B_q..]}{([A])^p([B])^q..}$$

A titration is simulated by specifying a set of titration conditions and calculating the concentrations of each complex species as the titration proceeds. The results are shown graphically.
- Calculation of species' concentrations. This requires a model and a set of conditions such as a pH range. Again the result is a plot of concentrations, as above.

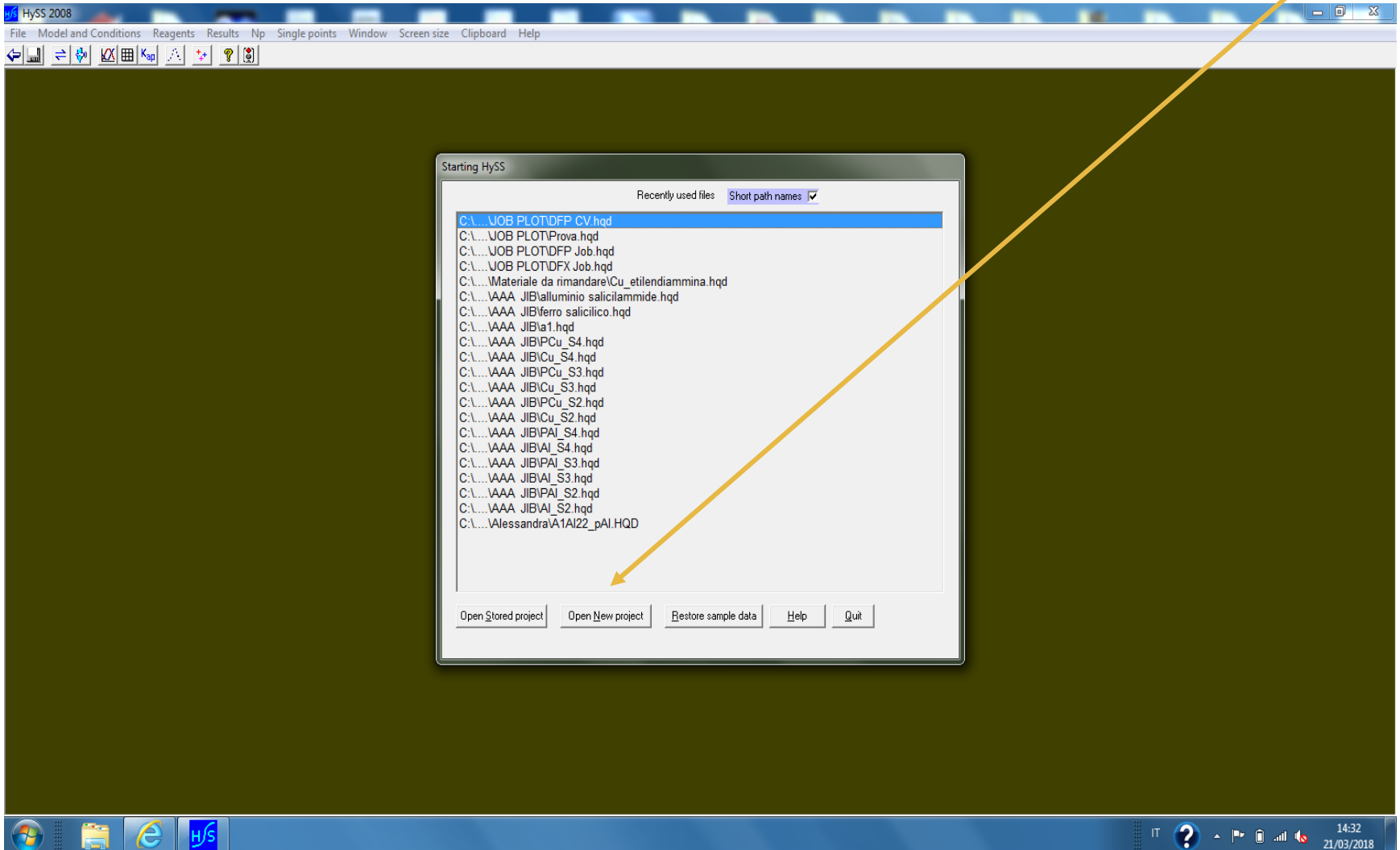
For details concerning the algorithm, etc. see L. Alderighi, P. Gans, A. Ienco, D. Peters, A. Sabatini and A. Vacca, "Hyperquad simulation and speciation (HySS): a utility program for the investigation of equilibria involving soluble and partially soluble species", *Coordination Chemistry Reviews*, **184** (1999) 311-318. [View paper](#) (requires Acrobat reader)

The plots produced by HySS are designed to be suitable for publication. Corresponding to the plots there is also the possibility of producing tables of concentrations that can be used, for example, in a program like Excel or Origin to produce customized plots.

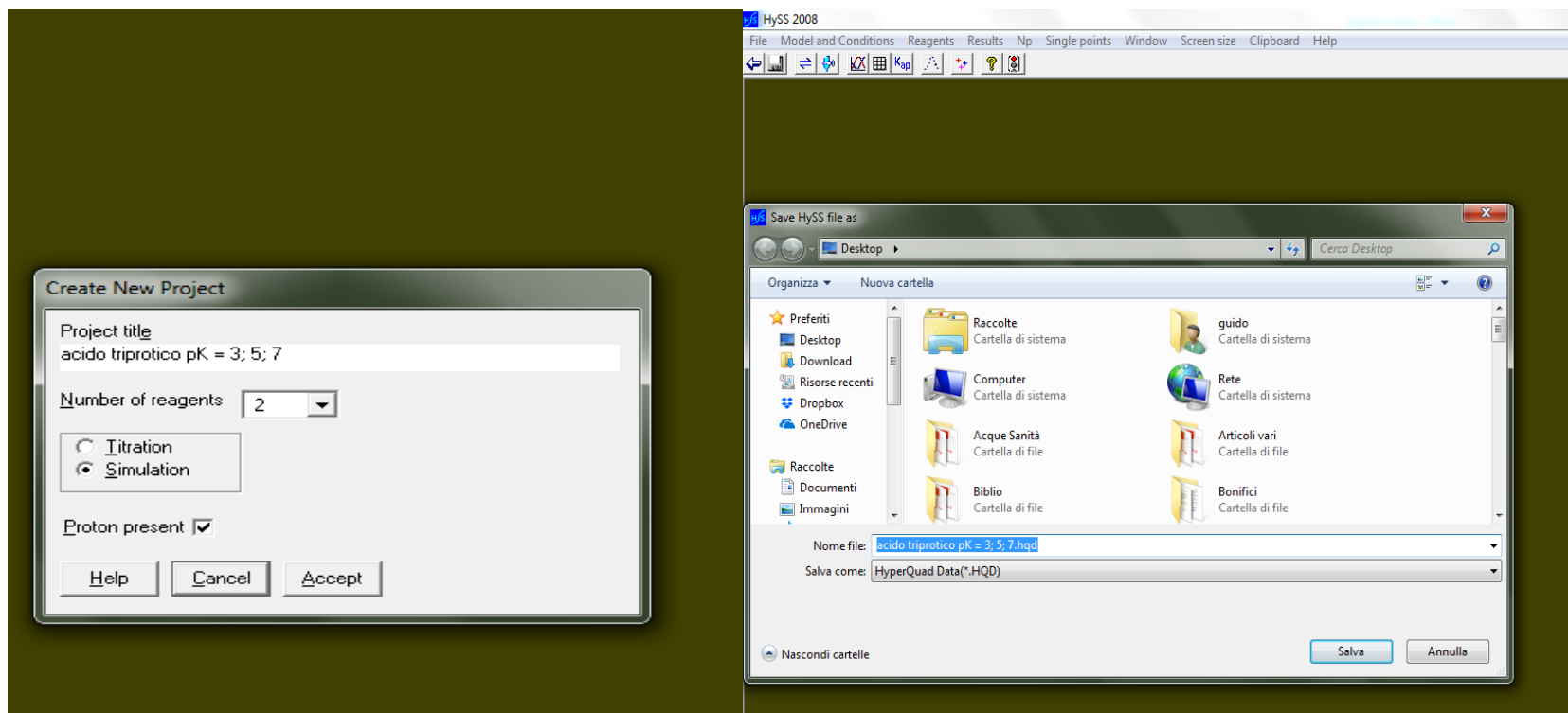


2009. The program may be downloaded, free of charge. Download and save the HySS2009 installation file (8.2MB) [Install HySS2009.EXE](#). Run it to install the software.

Programma HySS



Progetto



Modello

The screenshot displays the HySS2009 software interface. The main window title is "HySS2009: C:\Users\guido\Desktop\acido triprotico pK = 3; 5; 7.hqd". The menu bar includes "File", "Model and Conditions", "Reagents", "Results", "Np", "Single points", "Window", "Screen size", "Clipboard", and "Help". The toolbar contains various icons for navigation and analysis.

A "Model" window is open, showing the configuration for "acido triprotico pK = 3; 5; 7". The window has tabs for "Model", "Conditions", and "Solids". The "Model" tab is active, displaying a table of chemical species and their parameters.

Formula	Log Beta	A	H	
AH	0,0	1	1	constant
H ₋₁	-13,77	0	-1	constant

The Windows taskbar at the bottom shows the Start button, taskbar icons for Internet Explorer, Microsoft Word, and HySS, and the system tray with the date and time: 14:55, 21/03/2018.

HySS

The screenshot displays the HySS software interface. The main window title is "HySS2009: C:\Users\guido\Desktop\acido tripotico pK = 3; 5; 7.hqd". The menu bar includes "File", "Model and Conditions", "Reagents", "Results", "Np", "Single points", "Window", "Screen size", "Clipboard", and "Help". The "Model" window is open, showing the model name "acido tripotico pK = 3; 5; 7" and tabs for "Model", "Conditions", and "Solids". The "Model" tab is active, displaying a table of species and their properties. A yellow arrow points from the "Log Beta" column in the software window to a larger, highlighted version of the same table.

Formula	Log Beta	AH3	H	
(AH ₃)H ₋₁	-3,0	1	-1	constant
(AH ₃)H ₋₂	-10,0	1	-2	constant
(AH ₃)H ₋₃	-17,0	1	-3	constant
H ₋₁	-13,77	0	-1	constant

Condizioni

In Conditions si sceglie il campo di pH. Nel caso di una acido le curve di distribuzione sono indipendenti dalla concentrazione dell'acido.

The screenshot shows the HySS2009 software interface. The main window title is "HySS2009: C:\Users\guido\Desktop\acido triprotico pK = 3; 5; 7.hqd". The menu bar includes "File", "Model and Conditions", "Reagents", "Results", "Np", "Single points", "Window", "Screen size", "Clipboard", and "Help". The toolbar contains various icons for navigation and simulation control. The "Model" window is open, showing the "Conditions" tab. The "Conditions" section has two radio buttons: "Titration simulation" (unselected) and "Species Distribution" (selected). Below this is a table with the following data:

Reagent	initial concentration	final concentration	start pH	final pH
AH ₃	0,2	0,2		
H ⁺			1,0	10

The Windows taskbar at the bottom shows the Start button, several application icons (File Explorer, Internet Explorer, Word, HySS), and the system tray with the time 15:16 and date 21/03/2018.

Grafici

