

COURSE TITLE**Metodi di Base Computazionali per la Chimica*****Basic Computational Methods for Chemistry****(Laurea triennale in Chimica)*Prof. Fabrizio Lo Celso (e-mail: fabrizio.locelso@unipa.it)

Classroom site: Viale delle Scienze Edificio 17 (Building 17) M. Ruccia Room

Credits (CFU) = 4+2

COURSE PROGRAM**Face-to face lectures (4 CFU, 32 hrs)****Classroom and computer exercises (2 cfu, 24 hrs)**

	Metodi di Base Computazionali per la Chimica
No. Hours	Class Work
6	Error as Uncertainties. Inevitability of Uncertainty. Importance of the Uncertainties. Best estimate plus or minus the Uncertainty. Significant Figures. Discrepancy. Comparison of Measured and Accepted Values. Comparison of two numbers. Checking Relationship with a Graph. Fractional Uncertainties. Significant Figures and Fractional Uncertainties. Multiplying Two Measured Numbers. Sums and Differences; Products and Quotients. Independent Uncertainties. Arbitrary function of One Variable. Propagation Step by Step. General formula for Error Propagation.
6	Random and Systematic Errors. The Mean and Standard Deviation. The Standard Deviation as Uncertainty in a Single Measurement. The Standard Deviation of the Mean. Histograms and Distributions. The Normal Distribution. The Standard Deviation as 68% Confidence Limit. Justification of the Mean as Best Estimate. Justification of Addition in Quadrature. Standard Deviation of the Mean. Acceptability of a Measured Answer.
6	Linear Fitting $Y=Ax+B$. Calculation of the Constants A and B. Uncertainty in the Measurements of Y. Uncertainty in the Constants A and B. Least-Squares Fits to Other Curves. Review of error propagation. Covariance in Error Propagation. Coefficient of Linear Correlation. Quantitative Significance of r .
6	Binomial distribution and Its Properties. Testing of Hypothesis. Poisson Distribution and Its Properties.
4	Introduction of Chi Squared. General definition of Chi squared. Degrees of Freedom and Reduced Chi-Squared. Probabilities from Chi Squared.
4	Gnuplot: software open source for treating experimental data.
	Coursework
24	Numerical exercises on the above cited lectures
Suggested Books	J. R. Taylor. Introduzione all'analisi degli errori. Zanichelli, Bologna, 2006.