MEMBERSHIPS AND POSITIONS IN SCIENTIFIC SOCIETIES

1985-	Effective Member of the Physical Chemistry Division - Italian Chemical Society (SCI) Member of the "Gruppo Interdivisionale" of Computational Chemistry of SCI
1987-	Member of the World Association of Theoretical Organic Chemistry (from 1994 "Theoretically Oriented Chemists")
1989-93	Member of the Italian Physical Chemistry Association (AICF)
1990-	Member of the Molecular Graphics and Modelling Society
1999-	Member of the International Society of Quantum Biology and Pharmacology (ISQBP)
2005-2010	**Secretary** of the International Society of Quantum Biology and Pharmacology (ISQBP)
2007-10	**Deputy Representative of the CNR** in the Scientific Council of CECAM (Nov. 1, 2007 - Dec. 31, 2010) – Provv. n. 61, Prot. 6294 – Nov. 2, 2007.

EDUCATION:

1969	*July 18*	University of Pisa -	Doctor in Chemistry (Physical Chemistry branch)

EDUCATION AND SPECIALIZATION (after the degree)

1986	*Oct. 27-30*	Pisa (Italy)	Course of Computer Graphics
1985	*March 28-29*	Pisa (Italy)	Course for the access and the use of the CRAY X-MP12 of the CINECA
1984	*June 20*	Pisa (Italy)	Workshop on the Japanese Supercomputers of Fujitsu (VP100/200)
	April 9-13	Pisa (Italy)	Course on: Efficient FORTRAN Techniques for Vector Processors
1982-1983		San Francisco, CA (USA)	Postdoctoral Fellow at the Dept. of Pharmaceutical Chemistry University of California, San Francisco.
1978	*July 2-15*	Menton (France)	Ecole d'Eté Internationale sur: Surfaces de Potentiel et Realité Moleculaire
1975	*July 16-29*	Menton (France)	Ecole d'Eté sur: Recent Progres de la Theorie Quantique de la Reactivité Chimique
1974	*Sept. 23-Oct. 4*	Brixen (Italy)	14th International Summer Course on: Physical Organic Chemistry
1973	*Sept. 17-29*	Cortona (Italy)	Superior School of Physical Chemistry: III Course: Themes of Quantum Chemistry
1971	*April 13-23*	Pisa (Italy)	School of Theoretical Chemistry
	Sept. 6-18	Ramsau (Germany)	Summer School on: Computational Quantum Chemistry
1970	*Jan. 13-23*	Pisa (Italy)	Course of Algol-60
1969-1970		University of Pisa	Specialization Course in "Automatic Calculus"

COUNSELING ACTIVITIES

1979-1981	Responsible for "Batch and Production" in the General Committee of the CNUCE Users Association.
1985	Member of the examination committee to hire a CTP in ICQEM.
1986-90;1996-2001	Member of the Scientific Committee of ICQEM.
1987	Member of the Performance Evaluation Committee for the PS330 Evans & Sutherland.
1992-2001	Responsible for the ICQEM library from Oct. 1992 to Dec. 31, 2001
1995	Member of examination boards for two fellowships at ICQEM and two fellowships at ICAS.
1995	Member of CNR examination boards for a position of First Researcher and a position of Researcher.
1997	Member of examination boards for 11 positions of Researcher and 3 positions of CTER.
1999	Guest Editor of a Special Issue of *International Journal of Quantum Chemistry,* BQ.
2001	Member of CNR examination boards for a position of Researcher (ICAS), First Researcher (ICM) and for a fellowship (IPCF).
2001	Member of the Scuola Normale Superiore examination board to award a fellowship for the perfectioning course in Molecular Biophysics.
2002	Member of the INFM examination board for a biennial "assegno di ricerca" in "Modeling of Green Fluorescent Proteins with Classical and ab Initio Molecular Dynamics".
2003	Member of the INFM examination board n.766 for a position of Researcher at NEST-SNS in "Computer Modelling of Biomolecules".
2003	Member of the INFM examination board n.767 for a position of Researcher at NEST-SNS in "Physics of Many-body Systems in Crystals of Reduced Dimensionality".
2003	Member of the Scuola Normale Superiore examination board to award two fellowships for the perfectioning course in Molecular Biophysics.

2004	President of the IPCF examination board to award an "assegno di ricerca" in the framework of the FISR Project on Molecular Modelling: "Un nuovo approccio al 'drug-design': Dalla meccanica statistica allo screening di farmaci antivirali" - Bando n. PI/063.000/001 IPCF of Jan. 14, 2004
2004	Member of the Scuola Normale Superiore examination board for a thesis dissertation (perfectioning course in Molecular Biophysics).
2004	Secretary of the IPCF examination board to award a "contratto d'opera" in the framework of the Research Project "Growth and Supra-Organization of Noble and Transition Metal Nanoclusters (Gsomen)" - Contract FP6_2002_NMP-1_STRP_01594"
2007	Member of the IPCF examination board to award a fellowship according to the "Bando n. 126.242.BS.01/2007 of March 12, 2007."
2007-2010	Deputy Representative of the CNR in the Scientific Council of CECAM (Nov. 1, 2007 - Dec. 31, 2010) – Provv. n. 61, Prot. 6294 – Nov. 2, 2007.
2008	Member of the IPCF examination board to award an "assegno di ricerca" in the framework of the FIRB Project BLISS according to the "Bando IPCF-PI/2008/005 of June 23, 2008."
2008	IPCF library and documentation service workgroup coordinator – Prot. 2947, Sept. 11, 2008
2009	Member of the IPCF examination board to award an "assegno di ricerca" in the framework of the SEPON Project
2009	Member of SISSA examination boards for two PhD (Agata Kranjc, Rolando Hong) and one Magister (Zhaleh Ghaemi Bafghii) thesis defenses.

Referee

Journal of the American Chemical Society - Journal of Physical Chemistry
Journal of Chemical Theory and Computation - Journal of Computational Chemistry
International Journal of Quantum Chemistry - Theoretical Chemistry Accounts
Journal of Molecular Structure (THEOCHEM) - Journal of Molecular Structure
Physical Chemistry Chemical Physics - Biophysical Chemistry – Inorganica Chimica Acta
Molecular Physics – Industrial & Engineering Chemistry Research
International Journal of Astrobiology - Cellular and Molecular Biology
Philosophical Transactions of the Royal Society (Series A) - Chemical Physics Letters
Journal of Organic Chemistry - Journal of Molecular Modeling
European Journal of Inorganic Chemistry - Journal of Physical Organic Chemistry
Journal of the Chemical Society, Perkin 2 Trans. - Computers & Chemistry
Acta Chimica Hungarica MODELS IN CHEMISTRY
Gazzetta Chimica Italiana - Third Eurographics Workshop

RESEARCH PLAN RESPONSIBILITIES

1985-1986	Responsible for an Operating Unit of the Strategic Project on "Biotechnologies"
1987	Responsible for the Research Line #3 of ICQEM: "Non covalent interactions in simple and complex systems"
1991,1993	Responsible for the Research Line #3 of ICQEM: "Modelling of Non Covalent Interactions"
1994	Responsible for an Operating Unit of the Biennial Project "Interpretazione e validazione di modelli complessi mediante visualizzazione" Committee #12
1994-1995	Responsible for the Research Line #3 of ICQEM: "Calculation and Modelling of Properties and Reactions in Chemical and Biochemical Complex Systems"
1994-2006	Co-Responsible for Research Contracts with the Guidotti Laboratories, Pisa and Menarini Researches, Pomezia (Rome).
1995	Responsible for the Biennial Project "Interpretazione e validazione di modelli complessi mediante la visualizzazione" Committee #12
1996-1999	Responsible for a Subproject of the Integrated Project "Sviluppo di software parallelo per calcoli QM/MM di sistemi molecolari complessi" Committee #12
1997-1999	Responsible for an Operating Unit of the Strategic Project on "Computational Modelling of Complex Molecular Systems"
1999-2001	Responsible for the Research Line #3 of ICQEM: "Modelling of Properties and Reactions in Chemical and Biochemical Complex Systems"
2001-2003	Responsible for an Operating Unit of the Agenzia 2000 Coordinated Project: "Struttura e proprietà di sistemi chimici complessi e loro perturbazione per effetto del mezzo circostante e di interazioni specifiche"
2002-2004	Responsible for an Operating Unit of the FISR Project on Molecular Modelling: "Un nuovo approccio al 'drug-design': Dalla meccanica statistica allo screening di farmaci antivirali"

ACTIVITIES OUTSIDE THE CNR

1982-83 Postdoctoral Fellow at the Dept. of Pharmaceutical Chemistry, University of California, San Francisco

1991 Visiting Scientist for three months at the Dept. of Pharmaceutical Chemistry, University of California, San Francisco

THESIS SUPERVISION

1990-91 Andrea Cimino: Degree in Information Sciences - University of Pisa
Development of a Tool for the Molecular Simulation Control in a Visualization-Computation Distributed Environment.

DOCTORAL FELLOW FINAL SEMINARS SUPERVISION

1994 La Pegna

FELLOWSHIP SUPERVISION

1988	Britta Schürmann	NATO Fellowship
1991	Gladys M. Ciuffo	NATO Fellowship
1995-2001	Susanna Monti	Menarini Fellowship (Agreement Menarini-ICQEM)
2002-2003	Silvio Campanile	Menarini Fellowship (Agreement Menarini-ICQEM/IPCF)
2003-2004	Dafne Molin	Menarini Fellowship (Agreement Menarini-IPCF)
2005-2006	Armida Di Fenza	Menarini Fellowship (Agreement Menarini-IPCF)

DOCTORAL FELLOW SUPERVISION

1994-96	Guido Germano	DCCI	University of Pisa
2000-02	Simone Tomasi	DCCI	University of Pisa
2002-04	Silvio Campanile	DCCI	University of Pisa
2007-09	Mwadham Mwombeki Kabanda	Dept. of Chemistry	University of Venda, South Africa

POSTDOCTORAL FELLOW SUPERVISION

2003	Simone Tomasi	IPCF

TEACHING ACTIVITY

1989 *Scuola Nazionale di Scienza delle Proteine - Siena*
1991 *Seminario Nazionale di Chimica Fisica 1991 - Torino*
1992 *II Scuola di Chimica Computazionale 1992 - Siena*
1994 *I Corso di Chimica Computazionale - Siena*
1994 *Ciclo di lezioni per il Corso di Dottorato in Scienze Chimiche - Univ. di Pisa*
1994 *Ciclo di lezioni per il Corso di Chimica Fisica Biologica - Univ. di Pisa*
1995 *Ciclo di lezioni per il Corso di Chimica Fisica Biologica - Univ. di Pisa*
1996 *II Corso di Chimica Computazionale - Siena*
1996 *Scuola dell'Associazione Italiana di Cristallografia - Perugia*
1996 *Ciclo di lezioni per il Corso di Chimica Fisica Biologica - Univ. di Pisa*
1997 *Ciclo di lezioni per il Corso di Chimica Fisica Biologica - Univ. di Pisa*
1998 *Ciclo di lezioni per il Corso di Chimica Fisica Biologica - Univ. di Pisa*
1998 *2nd Iberoamerican School of Computational Chemistry and Molecular Design - University of Havana, Cuba*
1999 *Ciclo di lezioni per il Corso di Chimica Fisica Biologica - Univ. di Pisa*
2000 *Ciclo di lezioni per il Corso di Chimica Fisica Biologica - Univ. di Pisa*
2008 *Winter School of Physical Organic Chemistry – Brixen (Italy)*

AWARDS AND FELLOWSHIPS:

1984 To participate in the course on: Efficient FORTRAN Techniques CNUCE - Pisa (Italy)

1980 To participate in the NATO Advanced Study Institute. Kos (Grecia)

1970-1973 Borsa di Studio e di Addestramento alla Ricerca del Consiglio Nazionale delle Ricerche (15/6/70-15/1/73)

FOREIGN LANGUAGES SPOKEN:

- English.
- Good comprehension of French and Spanish.

RESEARCH INTERESTS AND ACTIVITIES

1) Quantum studies on the solid state, in particular on charge distributions, fields and electric field gradients in ferroelectric crystals and on the interaction of these crystals with a water molecule adsorbed on their various surfaces.
2) Counterpoise corrections of different type to the interaction energy and to its components in dimeric systems.
3) Monte Carlo studies on the solvation of ions and on the solution structure.
4) Conformational properties of molecules in vacuo and in solution.
5) Interpretation of properties of compounds of industrial interest containing double bonds.
6) Development of classical and semiclassical models in theoretical chemistry.
7) Enzyme catalysis studies and evaluation of properties of mutated enzymes.
8) Computer graphics and molecular modelling.
9) Relative stability of various types of H-bonds involving water.
10) Molecular mechanics and development of related force fields.
11) Reaction mechanisms in vacuo and in the field of an enzyme.
12) Effect of internal and external electric fields on molecular properties.
13) Effect of substituents on the properties of a few classes of compounds.
14) Optimization of the molecular geometry in the presence of a continuous solvent.
15) Comparison of various basis sets to determine those minimizing the BSSE (Basis Set Superposition Error).
16) Structure-activity relationships (drug design, protein engineering)
17) Conformational preferences of dehydropeptides.
18) Conducting polymers structures. Models to study their properties.
19) Production and maintenance of theoretical chemistry software.
20) Graphical representation on the molecular surface of various properties, such as electrostatic potential, virtual charge induced on the cavity surface, ΔG of solvatation and solvent transfer energy.

INSTITUTIONS VISITED FOR SEMINARS AND/OR INVOLVED IN COLLABORATIONS

+ Dept. of Pharmaceutical Chemistry, University of California, San Francisco, CA, USA
- College of Pharmacy, University of Toledo, Toledo, OH, USA
- Departamento de Quimica Fisica, Facultat de Quimica de Tarragona, Spain
+ Institute of Chemistry, Technical University of Wrocl aw, Poland
- Dipartimento di Chimica e Chimica Industriale, Università di Pisa, Italy
- Chemical Works of Gedeon Richter Ltd., Budapest, Hungary
- CHINOIN Pharmaceutical and Chemical Works, Budapest, Hungary
- BIONAVION Research and Development Ltd. Budapest, Hungary
- Istituto di Chimica Fisica, Università di Parma, Italy
- Institute Francais du Pétrole, Lyon, France
- Istituto di Chimica Fisica, Università di Padova, Italy
- Dept. of Medicinal Chemistry and Pharmacognosy, University of Illinois, Chicago, IL,U.S.A.
- Dept. of Chemistry and Biochemistry, University of Colorado at Boulder, CO, U.S.A.
- NEST & Scuola Normale Superiore - Pisa, Italy
+ SISSA – Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy
- Dept. of Food Science, Università di Napoli, Portici (Napoli), Italy
- Dept. of Physics, Michigan State University, East Lansing, Michigan, U.S.A.
- Max-Planck-Institut für Polymerforschung, Mainz, Germany
- Dept. of Chemistry, Purdue University, West Lafayette, Indiana, U.S.A.
- City University of New York, Hunter College, New York, N.Y., U.S.A.
- City University of New York, Mount Sinai Hospital, New York, N.Y., U.S.A.
- Max-Planck-Institut für Plasma Physics, Garching, Germany
+ Istituto Superiore di Sanità, Roma, Italy
- Istituto di Chimica Biologica, Università di Ferrara, Italy
- Istituto di Chimica Farmaceutica, Università di Pisa, Italy
- Istituto Donegani - Novara, Italy
- TECNOFARMACI -Pomezia (Roma), Italy
- Centro Internazionale di Chimica Pura ed Applicata - Trieste, Italy
+ Centro di Studi Chimico-Fisici di Macromolecole Sintetiche e Naturali- Genova, Italy
- Laboratori Guidotti S.p.A. Industria Chimica Farmaceutica - Pisa, Italy
- A. Menarini - Industrie Farmaceutiche Riunite s.r.l. - Firenze, Italy
- Menarini Ricerche SpA, Pomezia e Firenze

A - LIST OF PUBLICATIONS (citations from SCI up to Sept. 1996 in bold; total citations from ISI)

1- C. Ghio, J. Tomasi
The Protonation of Three-Membered Ring Molecules: The ab initio SCF versus the Electrostatic Picture of the Proton Approach.
Theoret. Chim. Acta, **30**, 151-158 (1973) from Science Citation Index **58**; 58

2- C. Ghio, E. Scrocco, J. Tomasi
The Effects of the Crystal Lattice on the Electronic Distribution of the Nitrite Ion in the Ferroelectric Phase of $NaNO_2$.
in: ENVIRONMENTAL EFFECTS ON MOLECULAR STRUCTURE AND PROPERTIES, p. 329-342. B. Pullman ed., Dordrecht: Reidel (1975) **17**

3- L. Pasimeni, C. Corvaja, C. Ghio
Cation Migration between Two Unequivalent Sites in 4-CyanoPyridine Alkali Metal Ion Pairs.
Chemical Physics, **31**, 31-37 (1978) **3**; 1

4- C. Ghio, E. Scrocco, J. Tomasi
The Effects of Substitution on the Properties of a Chemical Group. I. An Analysis of the SCF Description of Changes in the C‰N Group in the Monosubstituted Acrylonitriles.
Theoret. Chim. Acta, **50**, 117-134 (1978) **17**; 19

5- R. Ambrosetti, A. Biagi, C. Ghio, C. Guidotti, E. Matteoli
Alcuni Dati Comparativi tra Minicalcolatori.
in: ELABORAZIONE NUMERICA DEI DATI SPERIMENTALI, ed. Ist. Chimica Quantistica Energ. Molecol., p. IV.7.1-IV.7.3, Pisa 1979

6- C. Ghio, E. Scrocco, J. Tomasi
The Effects of Substitution on the Properties of a Chemical Group. II. An Analysis of the SCF Description of Changes in the C=C Group in Monosubstituted Ethylenes and Acrylonitriles.
Theoret. Chim. Acta, **56**, 61-73 (1980) **14**; 14

7- C. Ghio, E. Scrocco, J. Tomasi
The Effects of Substitution on the Properties of a Chemical Group. III. An Analysis of the SCF Description of Changes in the C–H Groups in Monosubstituted Ethylenes and Acrylonitriles.
Theoret. Chim. Acta, **56**, 75-87 (1980) **12**; 14

8- R. Bonaccorsi, C. Ghio, E. Scrocco, J. Tomasi
The Effect of Intramolecular Interactions on the Transferability Properties of Localized Descriptions of Chemical Groups.
Israel J. Chem., **19**, 109-126 (1980) **22**; 24

9- G. Alagona, C. Ghio, J. Tomasi
An Analysis of the Interaction Energy in some SN2 Reactions.
Theoret. Chim. Acta, **60**, 79-87 (1981) **11**; 11

10- R. Bonaccorsi, C. Ghio, J. Tomasi
The Effect of the Solvent on Electronic Transitions and other Properties of Molecular Solutes.
in: "CURRENT ASPECTS OF QUANTUM CHEMISTRY", R. Carbó ed., p. 407-426, Amsterdam: Elsevier Science (1982) **18**

11- C. Ghio
Surface Interactions between a Water Molecule and a Ferroelectric Crystal of $NaNO_2$.
in: "MOLECULAR IONS: GEOMETRIC AND ELECTRONIC STRUCTURES", NATO ASI Series B90, p. 565-568, J. Berkowitz and K.-O. Groeneveld eds., New York: Plenum (1983) **1**

12- G. Alagona, C. Ghio, P.A. Kollman
Bifurcated vs. Linear Hydrogen Bonds: Dimethylphosphate and Formate Anion Interactions with Water.
J. Am. Chem. Soc., **105**, 5226-5230 (1983) **49**; 58

13- S.J. Weiner, P.A. Kollman, D.A. Case, U. Chandra Singh, C. Ghio, G. Alagona, S. Profeta, Jr., and P. Weiner
A New Force Field for Molecular Mechanical Simulation of Nucleic Acids and Proteins.
J. Am. Chem. Soc. **106**, 765-784 (1984) **1777**; 4070
http://pubs.acs.org/action/showMostCitedArticles?topArticlesType=sinceInception&journalCode=jacsat

14- G. Alagona, P. Desmeules, C. Ghio, P.A. Kollman
Quantum Mechanical and Molecular Mechanical Studies on a Model for the Dihydroxy acetone phosphate - Glyceraldehyde phosphate Isomerization Catalyzed by Triose Phosphate Isomerase (TIM).
J. Am. Chem. Soc. **106**, 3623-3632 (1984) **53**; 76

15- R. Bonaccorsi, C. Ghio, J. Tomasi
On a Semiclassical Interpretation of Inter- and Intramolecular Interactions
Int. J. Quantum Chem. **26**, 637-686 (1984) **41**; 45

16- G. Alagona, C. Ghio, P.A. Kollman
Monte Carlo Simulations of the Solvation of the Dimethyl Phosphate Anion.
J. Am. Chem. Soc., **107**, 2229-2239 (1985) **40**; 46

17- G. Alagona, C. Ghio, P.A. Kollman
Monte Carlo Simulation Studies of the Solvation of Ions. 1. Acetate Anion and Methylammonium Cation.
J. Am. Chem. Soc. **108**, 185-191 (1986) **45**; 60

18- G. Alagona, R. Bonaccorsi, C. Ghio, J. Tomasi
Semi-classical Models in Theoretical Chemistry. Some Results and Future Prospects
J. Mol. Struct. (THEOCHEM), Dedicated to Prof. R. S. Mulliken, **135**, 39-66 (1986) **31**

19- C. Ghio, J. Tomasi, J. Weill, B. Sillion
On the Acidic Properties of Compounds with C=C or N=N Electrophilic Double Bonds.
J. Mol. Struct. (THEOCHEM), Dedicated to Prof. R. S. Mulliken, **135**, 299-328 (1986) **11**

20- R. Cammi, C. Ghio, J. Tomasi
Neutral Organic Lewis Acids of π Type.
Int. J. Quantum Chem. **29**, 527-539 (1986) **9**; 13

21- G. Alagona, R. Bonaccorsi, C. Ghio, J. Tomasi
The Influence of the Basis Set on the Evaluation of Conformational Energies for Small Organic Solutes in Aqueous Solutions.
J. Mol. Struct. (THEOCHEM), **137**, 263-277 (1986) **27**

22- G. Alagona, C. Ghio, P.A. Kollman
Simple Model for the Effect of Glu 165 —> Asp 165 Mutation on the Rate of Catalysis in Triose Phosphate Isomerase.
J. Mol. Biology, **191**, 23-27 (1986) **18**; 29

23- G. Alagona, R. Cammi, C. Ghio, J. Tomasi
Interpretation and Modeling of Hydrogen Bonds and other Non Covalent Interactions Using CP Corrected Interaction Energy Contributions
Vestnik Slovenskega Kemijskega Drustva, **34**, 149-174 (1987) **5**

24- G. Alagona, C. Ghio, R. Cammi, J. Tomasi
The Effect of "Full" and "Limited" Counterpoise Corrections with Different Basis sets on the Energy and the Equilibrium Distance of Hydrogen Bonded Dimers.
Int. J. Quantum Chem., **32**, 207-226 (1987) **37**; 48

25- G. Alagona, C. Ghio, R. Cammi, J. Tomasi
The Decomposition of the SCF Interaction Energy in Hydrogen Bonded Dimers Corrected for Basis Set Superposition Errors: an Examination of the Basis Set Dependence.
Int. J. Quantum Chem., **32**, 227-248 (1987) **23**; 30

26- J. Tomasi, G. Alagona, R. Bonaccorsi, C. Ghio
A Theoretical Model for Solvation - some Applications to Biological Systems
in: MODELLING OF STRUCTURE AND PROPERTIES OF MOLECULES, Cap. 20, p.330-355, Z. B. Maksic ed., Chichester: Horwood (1987). **42**

27- G. Alagona, C. Ghio, P.A. Kollman
Computational Approaches to the Study of Protein-Ligand Interactions.
in: "MACROMOLECULAR BIORECOGNITION", I. Chaiken, E. Chiancone, A. Fontana and P. Neri eds., p.13-28, Clifton: Humana Press (1988).

28- G. Alagona, R. Bonaccorsi, C. Ghio, R. Montagnani, J. Tomasi
Towards a Unified View of the Description of Internal and External Fields Acting on Chemical Functional Groups.
Pure and Appl. Chem. **60**, 231-244 (1988) **19**

29- G. Alagona, C. Ghio, P.A. Kollman
Monte Carlo Simulation Studies of the Solvation of Ions. 2. Glycine Zwitterion.
J. Mol. Structure (THEOCHEM) **166**, 385-392 (1988) **14**

30- G. Alagona, C. Ghio, R. Cammi, J. Tomasi
A Reappraisal of the Hydrogen Bonding Interaction Obtained by Combining Energy Decomposition Analyses and Counterpoise Corrections.
in: "MOLECULES IN PHYSICS, CHEMISTRY AND BIOLOGY", Vol. 2, J. Maruani ed., Topics in Molecular Organization and Engineering, p.507-559, Dordrecht: Kluwer (1988) **28**

31- J. Tomasi, G. Alagona, R. Bonaccorsi, C. Ghio
A Theoretical Model for Solvation with some Applications to Organic and Biological Systems.
WATOC Annual Yearbook (1987)

32- G. Alagona, R. Bonaccorsi, C. Ghio, J. Tomasi
Elaborazione di Modelli Teorici per lo Studio di Problemi in Soluzione.
F.C.T.L. **15**, 175-184 (1987)

33- G. Alagona, R. Cammi, C. Ghio, J. Tomasi
Non Covalent Interactions of Medium Strength. A Revised Interpretation and Examples of its Applications.
Int. J. Quantum Chemistry **35**, 223-239 (1989) **6**; 13

34- G. Alagona, C. Ghio, J. Igual, J. Tomasi
Appraisal of Solvation Effects on Chemical Functional Groups: Amides and Esters in Terms of Transferable Subgroup Contributions.
J. Am. Chem. Soc. **111**, 3417-3421 (1989) **19**; 39

35- G. Alagona, C. Ghio, P. Nagy
Theoretical Calculations on the 1:1 Complexes of N-aromatics with Water.
J. Mol. Structure (THEOCHEM) **187**, 219-232 (1989) **9**

36- G. Alagona, C. Ghio, J. Tomasi
Effect of Counterpoise Corrections on the Components of the Interaction Energy in the Formate-, Acetate-, and Phosphate-Water Dimers. A Study of Basis Set Effects.
J. Phys. Chem. **93**, 5401-5410 (1989) **20**; 29

37- G. Alagona, C. Ghio
Theoretical Calculations on an Enzyme Catalyzed Reaction Mechanism
in: NATO-ASI "THE ENZYME CATALYSIS PROCESS: ENERGETICS, MECHANISM AND DYNAMICS", A. Cooper, J. L. Houben and L. C. Chien eds., p. 345-355, Series A, Vol. 178, New York: Plenum (1989) **2**

38- G. Alagona, C. Ghio, J. Igual, J. Tomasi
An Appraisal of Solvation Effects on Chemical Functional Groups: the Amidic and the Esteric Linkages.
J. Mol. Structure (Theochem) **204**, 253-283 (1990) **40**

39- G. Alagona, C. Ghio, Z. Latajka, J. Tomasi
Basis Set Superposition Error and Counterpoise Corrections for some Basis Sets Evaluated for a Few $X^-\cdots M$ Dimers.
J. Phys. Chem. **94**, 2267-2273 (1990) **12;** 19

40- G. Alagona, C. Ghio
The Effect of Diffuse Functions on Minimal Basis Set Superposition Errors for H-bonded Dimers.
J. Comput. Chem. **11**, 930-942 (1990) **9**; 21

41- G. Alagona, C. Ghio, P. Nagy, K. Simon, G. Náray-Szabó
Comparative Study of Imidazole Hydration: Ab Initio and Electrostatic Calculations vs. Cambridge Structural Database Analysis.
J. Comput. Chem. **11**, 1038-1046 (1990) **9**; 12

42- J. Tomasi, G. Alagona, R. Bonaccorsi, C. Ghio, R. Cammi
Noncovalent Interactions in Bimolecular up to Mesoscopic Systems.
J. Mol. Structure (Theochem) **210**, 311-322 (1990) **1**

43- G. Alagona, C. Ghio
Monte Carlo Simulation Studies of the Solvation of Ions. 3. The nonintramolecularly H-bonded Form of Glycine Zwitterion.
J. Mol. Liquids **47**, 139-160 (1990) **7**; 23

44- C. Ghio, P. Palamidese
Aspetti di Grafica Molecolare
PIXEL n. 1/2, 7-12 (1991)

45- G. Alagona, C. Ghio, A. Cimino, P. Palamidese
Visualization Techniques for Theoretical Chemistry Problems
Proceedings of the Second Eurographics Workshop on Visualization in Scientific Computing, F.H. Post and A.J.S. Hin eds., p. 79-109, Delft University (1991) **1**

46- W.J. Dunn III, P.I. Nagy, E.R. Collantes, W.G. Glen, G. Alagona, C. Ghio
Log P and Solute Structure.
in: "QSAR: RATIONAL APPROACHES TO THE DESIGN OF BIOACTIVE COMPOUNDS" C. Silipo and A. Vittoria eds., p. 59-65, Elsevier, Amsterdam (1991) **1**

47- J. Tomasi, G. Alagona, R. Bonaccorsi, C. Ghio, R. Cammi
Semiclassical Interpretation of Intramolecular Interactions.
in: THEORETICAL MODELS OF CHEMICAL BONDING, Z. B. Maksic, Ed., Part 3, p. 545-614, Berlin: Springer (1991). **2 3**

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PROFESSIONAL ACTIVITIES:

Legenda: **IS** = Invited Speaker, **IP** = Invited Poster, **I** = Invited Participant, **R** = Referee, **O** = Organizer,
***** = Active Participant, **C**=Chairperson, **SC**=Member of the Scientific Committee

2010			**CHITEL 2010** XXXVI Congrès de Chimie Théorique d'Expression Latine Anglet (France)	Sept. 19-24	
	IS-C	*	Modeling and Design of Molecular Materials 2010 Wroclaw (Poland)	July 4-8	(Plenary lecture)
	IS	*	ISQBP President's Meeting 2010: *Folding and Recognition: Similarities and Differences* Cetraro (CS), Italy	June 14-16	(Invited Lecture)
		*	*Frontiers in Atomic Physics* (On the occasion of the 60th birthday of Massimo Inguscio) Florence (Italy)	April 9-10	
2009	SC	*	**QUITEL'09** XXXV Congreso de Químicos Teóricos de Expresión Latina San Andrés (Colombia)	Sept. 18-22	(2 Posters)
		*	*13th International Congress of Quantum Chemistry* Helsinki (Finland)	June 22-27	(Poster)
		*	**ProSurf'09** Sestri Levante (GE), Italy	June 4-6	
2008		*	*Winter Modeling '08* Pisa (Italy)	Dec. 19	(Poster)
		*	**WATOC 2008** Sydney (Australia)	Sept. 14-19	(2 Posters)
			SISOC-7 7th Spanish-Italian Symposium on Organic Chemistry Oviedo (Spain)	Sept. 7-10	(Poster)
			ISHC XIV International Symposium on Homogeneous Catalysis Florence (Italy)	July 6-11	(Poster)
		*	**CHITEL08** XXXIV Congresso dei Chimici Teorici di Espressione Latina Cetraro (CS), Italy	July 3-8	(Poster + Comm)
		*	ISQBP President's Meeting 2008: *Pushing the Boundaries of Biomolecular Simulations* Ascona (Switzerland)	June 8-13	(Poster)
		*	*Giornata scientifica in ricordo del Prof. Oriano Salvetti* Pisa (Italy)	March 28	
		*	*XXXVII Congresso Nazionale di Chimica Fisica* Camogli (GE), Italy	Feb. 24-29	(Poster)
	IS	*	Winter School on Physical Organic Chemistry Brixen (Italy)	Jan. 27 - Feb. 1	(Lecture)
2007	IS	*	XXXIII Congreso de Químicos Teóricos de Expresión Latina **QUITEL 2007** La Havana (Cuba)	Sept. 17-21	(Plenary lecture & Poster)
2006	IS-C	*	*Modelling and Design of Molecular Materials 2006* Wroclaw (Poland)	Sept. 10-15	(Plenary lecture)
			1st Annual National Congress of the Italian Proteomic Association *Proteomics: deciphering the phenotype* Pisa (Italy)	July 2-4	(Poster)

	C	*	*ISQBP President's Meeting 2006* Strasbourg (France)	June 24-27	(Poster)
		*	*XIIth International Congress of Quantum Chemistry* Kyoto (Japan)	May 21-26	(2 Posters)
2005		*	XXXI Congreso de Químicos Teóricos de Expresión Latina **QUITEL 2005** Isla de Margarita (Venezuela)	Oct. 2-6	(2 Posters)
		*	IUPAC Workshop: *Hydrogen Bonding and Other Molecular Interactions* San Giuliano Terme (Italy)	Sept. 5-9	
		*	**WATOC 2005:** *Modelling Structure and Reactivity* Cape Town (South Africa)	Jan. 16-21	(Comm. & Poster)
2004			**QUITEL 2004** Porto (Portugal)	Sept. 8-12	(2 Comm.)
	O SC	*	*μ-TheoChem: Modelling and Understanding in Theoretical Chemistry* Lucca (Italy)	Aug. 1-4	(2 Posters)
			14th *International Symposium on Homogeneous Catalysis* Munich, Germany	July 5-9	(Poster)
			INFMeeting 2004 Genova (Italy)	June 8-10	(Poster)
	C	*	*ISQBP President's Meeting* Como (Italy)	June 5-8	(Poster)
2003		*	V Congresso del Gruppo Interdivisionale di Chimica Computazionale: *dal Calcolo della Struttura Elettronica alla Bioinformatica* Certosa di Pontignano, Siena (Italy)	Dec. 18-19	(Comm.)
		*	**CAPI 2003**, *Modellistica Molecolare – Biochimica e Farmaceutica* Assolombarda Milano (Italy)	Nov. 14	
		*	**CHITEL 03**: *29ème Congrès des Chimistes Théoriciens d'Expression Latine* Marrakech (Maroc)	Sept. 7-12	(Poster)
		*	*XIth International Congress of Quantum Chemistry* Bonn (Germany)	July 20-26	(2 Posters)
			Modelling chemical reactivity: from gas-phase to solution and enzymes. An international conference in honor of Professor Jean-Louis Rivail Nancy (France)	July 16-18	(Poster)
	IS-C	*	VI Convegno su**:** *Complex systems: structure, properties, reactivity and dynamics* Bologna (Italy)	June 10-13	(Lecture)
			Scuola Nazionale in: *Simulazioni Computazionali Multiscala Applicate alle Scienze dei Materiali* Modena (Italy)	Feb. 17-21	(2 Posters)
2002	I	*	**IRCAW'02** Italian-Russian Coordinated research Activity Workshop Mosca (Russia)	Sept. 26-28	
	IS SC	*	**QUITEL 02** *XXVIII Congreso de Químicos Teóricos de Expresión Latina* Montevideo (Uruguay)	Sept. 1-8	(Comm.-Poster)

		*	**WATOC '02** *Sixth World Congress of Theoretically Oriented Chemists* Lugano (Switzerland) Aug. 4-9 (Comm.-Poster)
	C	*	UCSF/Biophysical Society Symposium Honoring Peter A. Kollman "*Molecular Simulations in Structural Biology and Drug Discovery*" San Francisco (USA) Feb. 21-22 (2 Posters)
2001	IS	*	**CAPI 2001**, *Supercalcolo in Biotecnologia, Bioinformatica e Bioingegneria* Università Cattolica del Sacro Cuore Milano (Italy) Oct. 17 (Lecture)
	IP-C	*	**CHITEL 2001** *27ème Congrès des Chimistes Théoriciens d'Expression Latine* Toulouse (France) Sept. 3-7 (2 Posters)
			9h Brazilian Meeting on Organic Synthesis Curitiba, Paraná, Brazil Aug. 20-24 (Poster)
		*	*XXXI Congresso Nazionale di Chimica Fisica* Padova (Italy) June 19-23 (Poster)
2000	C-R	*	*Zerner Conference* - ISQBP 2000 New Orleans, Louisiana (USA) Aug. 17-19 (Poster)
	IS	*	*Xth International Congress of Quantum Chemistry* Menton (France) June 5-10 (Lecture & Poster)
			CCT 6th Annual Seminar&Meeting: *Drug Delivery Systems* Faenza (Italy) Mar. 9-11 (Poster)
1999	C	*	*Riunione Scientifica Sezione Toscana della SCI* Pisa (Italy) Dec. 10 (Comm.)
		*	*XXX Congresso Nazionale di Chimica Fisica* Firenze (Italy) Sept. 26- Oct. 1 (Poster)
		*	**CHITEL '99** *XXV Congresso Internazionale dei Chimici Teorici di Espressione Latina* Napoli (Italy) Sept. 13-18 (Poster)
	C	*	**WATOC '99** *Fifth World Congress of Theoretically Oriented Chemists* London (UK) Aug. 1-6 (Poster)
	IS-R-C	*	5th International Conference: *Computers in Chemistry '99* and Workshop: *New Trends in Computational Methods for Large Molecular Systems* Szklarska Poreba Srednia (Poland) July 1-6 (Lecture and Poster)
			TUMA '99, XVIII Convegno Interregionale Toscano Umbro Marchigiano Abruzzese Perugia (Italy) June 3-5 (Comm. and Poster)
			XXXII Midwest Theoretical Chemistry Conference Universisty of Notre Dame in South Bend, IN (USA) May 20-22 (Comm.)
			MM/QM Methods and Applications Southampton (UK) April 14-16 (Poster)
1998	R	*	QUITEL98 *XXIV Congreso Internacional de Químicos Teóricos de Expresión Latina* Puebla (Mexico) Sept. 20-25 (3 Posters)
	O SC	*	ISQBP President's Meeting: *Molecular Structure and Dynamics in Biology* La Biodola, Elba (Italy) Sept. 8-11 (2 Posters)
	R	*	*European Conference: Computational Chemistry and the Living World: from Sequence to Functions*

Chambéry, French Alps (France) Apr. 20-24 (Poster)

IS * *2nd Iberoamerican School of Computational Chemistry and Molecular Design*
La Havana (Cuba) Jan. 5-16 (2 lectures)

1997 C * *V Convegno Nazionale della Divisione di Chimica dei Sistemi e dei Processi Biologici della SCI*
Parma (Italy) Dec. 15-17 (Poster)

CD '97 - 6th International Conference on Circular Dichroism: Molecular Chirality in Chemistry and Life Sciences
Pisa (Italy) Sept. 21-24 (Poster)

Model(l)ing '97
Erlangen (Germany) Sept. 2-5 (Poster)

R * *9th International Congress of Quantum Chemistry*
Atlanta, Georgia (USA) June 9-14 (Poster)

IS * *Satellite Symposium: Theoretical Chemistry in Biology: from Molecular Structure to Functional Mechanisms*
Savannah, Georgia (USA) June 3-7 (Lecture+2 Posters)

* *Forum/INFM - SNS 1997 Workshop: Computer Simulations of Systems of Biological Interest*
Pisa (Italy) May 12-14 (Commun.)

III Convegno Nazionale di Informatica Chimica (2 Posters)
Napoli (Italy) Feb. 27-Mar. 1

* *XXVIII Congresso Nazionale di Chimica Fisica*
Pisa (Italy) Feb. 10-14 (2 Posters)

* *La Ricerca Chimica verso il 2000: attività ed iniziative del Comitato Scienze Chimiche*
Rome (Italy) Jan. 9-10

1996 R * **QTEL96** *XXIII Congreso Internacional de Químicos Teóricos de Expresión Latina*
Cáceres (Spain) Sept. 16-20 (3 Posters)

IS * *Scuola dell'Associazione Italiana di Cristallografia "Cristallografia strutturale e riconoscimento di specie molecolari e ioniche"* (2 Lectures)
Villa "La Colombella", Perugia (Italy) Sept. 9-13

* **WATOC '96** *Fourth World Congress of Theoretically Oriented Chemists*
Jerusalem (Israel) July 7-12 (3 Posters)

XIX Congresso Nazionale della SCI (Poster)
Riccione (Italy) June 10-15

IS * *II Corso di Chimica Computazionale "Impiego combinato di dati sperimentali e modeling nello studio di macromolecole biologiche"* (Lecture)
Certosa di Pontignano, Siena (Italy) June 9-15

1995 R * **QUITEL95** *XXII Congreso Internacional de Químicos Teóricos de Expresión Latina*
Pucón (Chile) Sept. 25-29 (2 Posters)

Giornate Mediterranee CAT '95
Cagliari (Italy) Sept. 12-16 (Poster)

* *Giornata di Coordinamento Ist. Naz. Chimica Sistemi Biologici*
Rome (Italy) June 30 (Poster)

Convegno "*Verso la Complessità Molecolare: Modelli per la Dinamica e per i Processi Reattivi*"
Monselice, Padova (Italy) June 14-17 (Comm.)

IS * *Convegno "Nuove Applicazioni di Telecomunicazione al Servizio del Mondo del Lavoro"*
Pisa (Italy) May 24 (Demo)

IP * *V Symposium "Peptide Conformation and Protein Structure"*
Karpacz (Poland) April 29-May 2 (Poster)

1994

* *Symposium of Theoretical Chemistry in Honour of Roy McWeeny and Oriano Salvetti*
Pisa (Italy) Sept. 26

* *XXVII Congresso Nazionale di Chimica Fisica*
Montepaone Lido, Catanzaro (Italy) Sept. 18-22 (2 Posters)

IS * Workshop on "*Multidimensional Data Representation*" (Round table)
Rome (Italy) July 6-8

IS 3rd Conference "*Computers in Chemistry '94*", including workshop
* "*Computational Methods for Large Molecular Systems*" (Lecture)
Wroclaw (Poland) June 24-26 (Poster)

* *8th International Congress of Quantum Chemistry*
Prague (Czeck Republic) June 19-23 (Poster)

* *P. Pino - E. Scrocco e*
Lo sviluppo delle Scienze Chimiche a Pisa dagli anni '50 ad oggi
Pisa (Italy) June 9

IS * *I Corso di Chimica Computazionale "Studio dell'Interazione Macromolecola-Ligando"*
Certosa di Pontignano, Siena (Italy) May 29-June 4 (Lecture)

1994 E-MRS Spring Conference "Symposium D on Organic Materials for Electronics: Polymer Interfaces with Metals and Semiconductors" (Poster)
Strasbourg (France) May 24-27

XXVII Midwest Theoretical Chemistry Conference (Commun.)
Columbia, Missouri (USA) May 19-21

* *II Convegno Nazionale di Informatica Chimica* (Poster)
Bologna (Italy) Feb. 16-18

IS * Workshop "*Metodologie Computazionali nella Ricerca Farmaceutica Industriale: Strumenti e Applicazioni*" (Lecture)
Bologna (Italy) Feb. 14-15

1993

* *Seminario Italo-Britannico sui Finanziamenti alla Ricerca*
Pisa (Italy) Dec. 7

* *XXVI Congresso Nazionale di Chimica Fisica* (2 Posters)
Rimini, Forlì (Italy) Sept. 27-30

R * **CHI-TEL XXI** (2 Posters)
Grenoble (France) Sept. 20-24

IS-IP * *Third World Congress on Theoretical Organic Chemistry - WATOC 93*
Toyohashi, Aichi (Japan) Jul. 18-24 (Commun-Poster)

* Workshop: *Modelli ed algoritmi per lo studio teorico di processi reattivi in sistemi isolati, in soluzione ed alle interfasi* (Comm.)
Pisa (Italy) May 31-June 3

* Pisa-Workshop: *Materiali Avanzati: Scienza e Prospettive Tecnologiche*

			Pisa (Italy)	Feb. 4-5	
1992		*	**JANUACHEM 92** Genova (Italy)	Oct. 25-29	(Poster)
	R	*	**QUITEL XX** Mérida, Venezuela	Oct. 12-17	(2 Posters)
	IS	*	*II Scuola di Chimica Computazionale 1992* Certosa di Pontignano, Siena (Italy) July 19-25		(Lecture)
	IS	*	*Ruolo della Chimica nelle Moderne Biotecnologie* Bologna (Italy)	July 2	(Comm.)
		*	*Convegno "Capitale Umano e Mobilità"* Genova (Italy)	Apr. 29	
		*	*Workshop "Calcolo Avanzato in Chimica"* Montelibretti, Roma (Italy)	Feb. 27-28	
1991		*	*UCSF, Dept. of Pharmaceutical Chemistry Retreat 1991* Asilomar, CA (U.S.A.)	Dec. 8-10	(2 Posters)
		*	*Conference on Future Methodologies* San Francisco, CA (U.S.A.)	Nov. 22	
	IS	*	*Seminario Nazionale di Chimica Fisica 1991* Villa Gualino, Torino (Italy)	Sept. 1-6	(2 Lectures)
		*	*VII International Congress of Quantum Chemistry* Menton (France)	July 2-5	(Poster)
		*	*International Symposium: Computer Simulation of Biomolecular Systems and Mechanisms* Menton (France)	June 27-29	(Poster)
		*	*XXV Congresso Nazionale di Chimica Fisica* Chia, Cagliari (Italy)	June 17-21	(2 Posters)
	I	*	*NATO ARW "The Role of Computational Models and Theories in Biotechnology"* Sant Feliu de Guixols (Spain)	June 13-19	(2 Posters)
			II Eurographics Workshop on Visualization in Scientific Computing Delft (Netherlands)	April 22-24	(Paper)
		*	*I Convegno Nazionale di Informatica Chimica* Venezia (Italy)	March 3-6	(2 Posters)
1990		*	*Incontro LUG Toscano DECUS* Pisa (Italy)	Oct. 19	
		*	*XXIV Congresso Nazionale di Chimica Fisica* Potenza (Italy) Oct. 8 and Maratea (Italy), Oct. 9-12		(Poster)
	IS	*	*CECAM Workshop on "Quantum Chemistry and Chemical Reactions in Solution"* Orsay (France)	Oct. 1-5	(Lecture)
		*	*International Conference: The Industrial Applications of Natural, Modified and Artificial Enzymes* Pisa (Italy)	Sept. 23-29	(Poster)
		*	**XIX CICTPEL** *Congresso Internazionale dei Chimici Teorici dei Paesi di Espressione Latina* Rome (Italy)	Sept. 10-14	(Poster)

8th European Symposium on QSAR
Sorrento (Italy) Sept. 9-13 (Lecture)

IS-IP * *Second World Congress on Theoretical Organic Chemistry*
Toronto, Ontario (Canada) Jul. 8-14 (Commun-Poster)

* *International Symposium on Applied Theoretical Chemistry*
La Habana (Cuba) Jul. 2-6 (Poster)

XXIII Midwest Theoretical Chemistry Conference
Madison, Wisconsin (USA) May 17-21 (Commun.)

Symposium on Classical and Quantal Simulations for Reactive and Solvation Dynamics and Their Critical Experimental Tests. A.C.S. National Meeting
Boston, Massachussets (USA) Apr. 23-27 (Poster)

* *XI Simposio Nazionale DECUS*
Montecatini Terme (Italy) Apr. 4-6

1989 O * *Workshop on "Aspects of Molecular Graphics"* (Org.Comm., Scient.Comm.)
Pisa (Italy) Dec. 4-6 (Lect., Poster)

IS * *Scuola Nazionale di Scienza delle Proteine. Società Italiana di Biochimica. Tema: "L'uso dell'elaboratore nella chimica delle proteine"*
Siena (Italy) Oct.29-Nov. 3 (Lecture, Exerc.)

IS * **CISCI89** (Conference)
XXIII Congresso Nazionale di Chimica Fisica
Perugia (Italy) Oct. 7-11 (2 Posters)

* **XVIII CQTEL**
La Plata (Argentina) Sept. 23-29 (2 Posters)

R * **TOC at MUN'89**: *Theory of Environmental Effects on Molecular Structure and Chemical Reactivity*
St. John's, Newfoundland (Canada) Jun. 25-Jul. 1
R = Referee of the J. Mol. Struct. (THEOCHEM) (Poster)

IS * *International Workshop: "From Molecular Modeling and Dynamics to Protein Structures and Drug Interactions"*
San Miniato, Pisa (Italy) Jun. 19-20 (Lecture)

IS * *Giornate di lavoro Unità Operativa PF "Sistemi Informatici e Calcolo Parallelo", SP1 - Tema 3.2*
Roma (Italy) May 25-26 (Lecture)

* *8th Annual Conference of Molecular Graphics Society*
St. Andrews (Scotland) Mar. 29-31 (Poster)

1988 * *X Convegno Nazionale AICAT*
Pisa (Italy) Dec. 11-14 (Poster)

* *XVI Congresso Nazionale della Societa' Chimica Italiana*
Bologna (Italy) Oct. 9-14 (Poster)

* *Primo Convegno Nazionale di Chimica Fisica Ambientale*
Venezia (Italy) Oct. 2-4

* *Control Data "Transparent Computing Environment" EXPO*
Wien, (Ofterreich), Sept. 14

International Symposium "Molecular Recognition: Its Role in Chemistry and Biochemistry"

Sopron (Hungary), Aug. 24-27 (Poster)

IS * *NATO-ASI "The Enzyme Catalysis Process: Energetics, Structure and Dynamics"*
Il Ciocco, Barga (Italy) July 10-23 (Lecture)

1987 * *XXII Congresso Nazionale di Chimica Fisica*
Villa Olmo, Como (Italy) Oct. 20-23 (2 Posters)

IS * *Round Table "The EEC Project for BIOTECHNOLOGY: Proteins and their Effectors. The Relationship between the Biological Activity of Polypeptides and the Dynamical Behavior of their Structures"*
IFAM, Pisa (Italy) Oct. 8 (Lecture)

* *Colloque on "The Scientific Dimension of Cultural Development", Academie Europeenne and UNESCO*
Accademia dei Lincei, Roma (Italy) Sept. 30-Oct. 2

R * **XVII CQTEL**
Peñiscola (Spain) Sept. 20-25 (2 Posters)
R = Referee of the Journal of Molecular Structure (THEOCHEM)

R * **WATOC '87** *World Congress*
Budapest (Hungary) Aug. 12-19 (Poster)
R = Referee of the Journal of Molecular Structure (THEOCHEM)

* *Satellite Symposium:*
"Structure and Mechanisms in Molecular and Quantum Pharmacology"
Tatranska Lomnica (Czecoslov.) Aug. 23-28 (Poster)

* *Convegno "Chimica: Obiettivi 2000"*
Roma (Italy) Jan. 28-29

1986 * *Congresso Nazionale dell'A.I.C.F.*
Siena (Italy) Oct. 6-9 (2 Posters)

IS * *Conferenza Nazionale su: Meccanismi del Riconoscimento in Macromolecole Biologiche. Aspetti Molecolari ed Applicazioni Biotecnologiche.*
Siena (Italy) Sept. 4-6 (Lecture)

* **XVI Congres CTEL**
Lyon (France) Jul. 7-11 (Poster)

* *International Symposium "Molecules in Physics, Chemistry and Biology"*
Paris (France) Jun. 16-21 (Poster)

* *Round Table: Theory of Molecular Interactions: Problems and Prospects*
Pisa (Italy) Apr. 23

1985 * *XX Congresso Nazionale dell'A.I.C.F.*
Torino (Italy) Oct. 21-24 (2 Posters)

* *Second European Seminar and Exhibition on Computer-Aided Molecular Design*
Basel (Switzerland) Oct. 17-18

R * *5th International Congress on Quantum Chemistry*
Montreal, Quebec (Canada) Aug. 18-24 (3 Posters)
R = Referee of the International Journal of Quantum Chemistry.

IP * *Satellite Symposium on Quantum Chemistry of Biological Systems*
New York, NY (U.S.A.) Aug. 15-16 (Invited Poster)

* *Satellite Symposium on Molecular Structure and Reactivity*
Toronto, Ontario (Canada) Aug. 25-28 (Poster)

1984 O * *XIX Congresso dell'Associazione Italiana di Chimica Fisica*
Pisa (Italy) Oct. 15-19 (Poster)

O = Participation in the organization

* **XV QUI/CHI T E L** *Portugal '84*
Viana do Castelo (Portugal) Sept. 3-6 (2 Posters)

1983 * *XVIII Congresso Nazionale di Chimica Fisica*
Bari (Italy) Oct. 17-21 (Poster)

1982 * *Conference on*
Structure and Dynamics of Nucleic Acids and Proteins
La Jolla, CA (U.S.A.) Sept. 5-9 (2 Posters)

1981 *VII Convegno Nazionale di Fotochimica*
Gargnano sul Garda (Italy) Oct. 22-23 (Poster)

XII Congres dels Quimics Teorics d'Expressio Llatina
Barcelona (Spain) Sept. 28 - Oct. 1 (Commun.)

* *American Conference on Theoretical Chemistry*
Boulder, CO (U.S.A.) Jun. 22-26 (Poster)

* *Meeting on Calculation of Stationary States of Atoms and Molecules*
Pisa (Italy) Jun. 3-5

1980 * *Nato ASI: Conference on Molecular Ions: Geometric and Electronic Structure*
Kos (Greece) Sept. 29-Oct. 10 (Commun.)

* *XI Colloque des Chimistes Theoriciens d'Expression Latine*
Pau (France) Sept. 8-11 (Software exchange)

* *Colloquium on the Nature of Binding in Molecular Associations, Atom Clusters, and Surface Phases*
Sorrento (Italy) May 12-16

* *European Conference on the Dynamics of Excited States*
Pisa (Italy) Apr. 14-16

1979 * *XIV Congresso Nazionale A.I.C.F.*
Firenze (Italy) Oct. 24-26

* *X Congres des Chimistes Theoriciens d'Expression Latine*
Geneva (Switzerland) Sept. 25-27 (Commun.)

* *Metodologie Avanzate per lo Studio di Sistemi Paramagnetici*
Pisa (Italy) Feb. 26-28

1978 * *XIII Congresso Nazionale A.I.C.F.*
Catania (Italy) Oct. 10-13

* *IX Congresso Chimici Teorici di Espressione Latina*
Stresa (Italy) Sept. 3-8

Round Table:
Elaborazione Numerica Dati Sperimentali
Pisa (Italy) Jun. 15-16 (Commun.)

1977 * *VIII Coloquio Internacional de los Quimicos Cuantico de Expresion Latina*
Salamanca (Spain) Sept. 20-23 (Commun.)

* *Meeting in Honour of Prof. R.S. Mulliken*
Novara (Italy) Jul. 11

1976 * *A-76. Exploring the Chemical Bond, New developments - European Physical Society (Chemical Physics Section)*
Amsterdam (Netherlands) Aug. 30 - Sept. 1 (Commun.)

* *VII Colloque International des Chimistes Theoriciens d'Expression Latine*
Wepion (Belgium) Aug. 24-27 (Commun.)

1975 * *X Congresso Nazionale A.I.C.F.*
Padova (Italy) Oct. 20-24

* *VI Colloque International des Chimistes Theoriciens d'Expression Latine*
Arles (France) Sept. 2-5 (Commun.)

VIII Jerusalem Symposium on Quantum Chemistry and Biochemistry
Jerusalem (Israel) Apr. 7-11 (Commun.)

1974 * *IX Congresso Nazionale A.I.C.F.*
Napoli (Italy) Nov. 5-9

1973 * *II International Symposium on Nuclear Quadrupole Resonance Spectroscopy*
Viareggio, Lucca (Italy) Sept. 3-6

1971 * *VI Congresso Nazionale A.I.C.F.*
Siena (Italy) Dec. 16-18

1970 *V Congresso Nazionale dell'Associazione Italiana di Chimica Fisica*
Milano (Italy) Dec. 16-18 (Commun.)

II Colloque International des Chimistes Theoriciens d'Expression Latine
Paris (France) Sept. 23-26 (Commun.)

1969 * *I Colloquio Internazionale Chimici Teorici di Lingua Latina*
Modena (Italy) Sept. 9-12

INVITED LECTURES FOR CONGRESSES, SCHOOLS AND ROUND TABLES

(1) - G. Alagona, C. Ghio, P.A. Kollman
Computational Approaches to the Study of Protein-Ligand Interactions
Conferenza Nazionale su: "Meccanismi del Riconoscimento in Macromolecole Biologiche. Aspetti Molecolari ed Applicazioni Biotecnologiche"
Siena (Italy) Sept. 4-6, 1986

(2) - G. Alagona, C. Ghio
Towards Computer-aided Site-specific Mutagenesis
Round Table on The EEC Project for BIOTECHNOLOGY: "Proteins and their Effectors. The Relationship between the Biological Activity of Polypeptides and the Dynamical Behavior of their Structures"
IFAM, Pisa Oct. 8, 1987

(3) - G. Alagona, C. Ghio
Theoretical Calculations on an Enzyme Catalyzed Reaction Mechanism.
NATO-ASI "The Enzyme Catalysis Process: Energetics, Structure and Dynamics"
Il Ciocco, Barga (Italy) July 11-23, 1988

(4) - C. Ghio, P. Palamidese
Visualizzazioni per Problemi di Grafica Molecolare.
IAC, Roma May 25-26, 1989

(5) - G. Alagona, C. Ghio, C. Pratesi
Conformational Preferences of a Dehydrophenylalanine Containing Peptide
International Workshop "From Molecular Modeling and Dynamics to Protein Structures and Drug Interactions"
San Miniato, Pisa (Italy) June 19-20, 1989

(6) - G. Alagona, C. Ghio
"Model Building" and Energy Functions: Useful Tools to Understand Molecular Structure and Interactions
Minisimposio "Molecular Graphics", CISCI89
Perugia (Italy) Oct. 7-11, 1989

(7) - C. Ghio
Un "force field" per la simulazione di meccanica molecolare delle proteine. Esempi di modellistica molecolare.
Scuola Nazionale di Scienza delle Proteine - Soc. Italiana di Biochimica.
Siena (Italy) Oct. 29-Nov. 3, 1989

(8) - G. Alagona, C. Ghio
The Hydration of Ethanediol with the Continuum in Comparison with Recent Monte Carlo Results.
Second World Congress on Theoretical Organic Chemistry.
Toronto (Canada) July 8-14, 1990

(9) - G. Alagona, C. Ghio
The Continuum Model vs. Monte Carlo Results for the Hydration of Ethylene Glycol.
CECAM Workshop on Quantum Chemistry and Chemical Reactions in Solution.
Orsay (Francia) Oct. 1-5, 1990

(10) - C. Ghio
"Force fields" per Simulazioni di Meccanica Molecolare.
Seminario Nazionale di Chimica Fisica 1991- AICF, Soc. Chimica Italiana.
Villa Gualino, Torino (Italy) Sept. 1-6, 1991

(11) - C. Ghio
Applicazioni di Grafica Molecolare.
Seminario Nazionale di Chimica Fisica 1991- AICF, Soc. Chimica Italiana.
Villa Gualino, Torino (Italy) Sept. 1-6, 1991

(12) - G. Alagona, C. Ghio
Meccanismi di Reazioni Catalizzate da Enzimi Naturali e Modificati.
Ruolo della Chimica nelle Moderne Biotecnologie.
Bologna (Italy) July 2, 1992

(13) - C. Ghio
Osservabili SCF: potenziale elettrostatico molecolare (scelta del set di base).
Scuola di Chimica Computazionale 1992- Soc. Chimica Italiana.
Certosa di Pontignano, Siena (Italy) July 19-25, 1992

(14) - G. Alagona, C. Ghio
Razionalizzazione della Relazione Struttura Attività per Oligopeptidi Contenenti Deidrofenilalanina.
Workshop "*Metodologie Computazionali nella Ricerca Farmaceutica Industriale: Strumenti e Applicazioni*"
Bologna (Italy) Feb. 14-15, 1994

(15) - C. Ghio
Studi ab initio di interazioni molecolari complesse
I Corso di Chimica Computazionale "*Studio dell'Interazione Macromolecola-Ligando*"
Siena (Italy) May 29-June 4, 1994

(16) - G. Alagona, C. Ghio
Successes and drawbacks in the computer modelling of enzyme catalyzed reaction mechanisms.
Workshop "*Computational Methods for Large Molecular Systems*"
Wrocl aw (Poland) June 24-26, 1994

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