Peer-reviewed journal articles

1) The fate of branched and linear isomers in the rhodium-catalyzed hydroformylation of 3,4,4-trimethylpent-1-ene
   Giuliano Alagona; Caterina Ghio
   https://dx.doi.org/10.1007/s00214-012-1142-x

2) High linear regioselectivity in the rhodium-catalyzed hydro(deuterio)formylation of 3,4,4-trimethylpent-1-ene: the role of beta-hydride elimination
   Raffaello Lazzaroni; Roberta Settambolo; Giuliano Alagona; Caterina Ghio
   https://dx.doi.org/10.1016/j.molcata.2011.12.021

3) Computational prediction of selectivities in nonreversible and reversible hydroformylation reactions catalysed by unmodified rhodium catalysts
   Giuliano Alagona; Raffaello Lazzaroni; Caterina Ghio
   https://dx.doi.org/10.1007/s00894-010-0864-8

   Raffaello Lazzaroni; Roberta Settambolo; Giuliano Alagona; Caterina Ghio
   *Coordination chemistry reviews (Print)* 255 (2011): 3031-3031.
   https://dx.doi.org/10.1016/j.ccr.2011.06.008

5) Dependence of the Wittig reaction mechanism on the environment and on the substituents at the aldehyde group and at the phosphonium ylide
   Alagona* G.; Ghio C.
   http://www.cnr.it/prodotto/i/40040

6) Free energy landscapes in THF for the Wittig reaction of acetaldehyde and triphenylphosphonium ylide
   Alagona* G.; Ghio* C.
   http://www.cnr.it/prodotto/i/40205

7) The catalytic effect of water on the keto–enol tautomerism. Pyruvate and acetylacetone: a computational challenge
   Alagona* G.; Ghio C.; Nagy P.I.
8) Investigation of alkyl metal intermediates formation in the rhodium-catalyzed hydroformylation: experimental and theoretical approaches
Lazzaroni R.; Settambolo R.; Alagona G.; Ghio C.
*Coordination chemistry reviews (Print)* 254 (2010): 696-706.
https://dx.doi.org/10.1016/j.ccr.2009.09.032

9) Computational Results Provide a Synthetically Unprecedented Explanation for the beta-Regioselectivity in the Rh-catalyzed Hydroformylation of Vinylidenic Substrates
Ghio C.; Lazzaroni R.; Alagona* G.
http://www.cnr.it/prodotto/i/40037

10) Plicatin B Conformational Landscape and Affinity to Copper (I and II) Metal Cations. A DFT Study
Alagona* G.; Ghio C.
http://www.cnr.it/prodotto/i/40038

11) Stepwise vs concerted mechanisms in the Wittig reaction in vacuo and in THF: the case of 2,4-dimethyl-3-pyrrol-1-yl-pentanal and triphenylphosphonium ylide
Alagona* G.; Ghio C.
http://www.cnr.it/prodotto/i/40039

12) Antioxidant properties of pterocarpans through their copper(II) coordination ability. A DFT study in vacuo and in aqueous solution (PCM)
Alagona* G.; Ghio* C.
http://www.cnr.it/prodotto/i/40189

13) Rhodium-catalyzed deuteroformylation of the ketal-masked beta-isophorone: Evidence for a tertiary alkyl rhodium intermediate as a precursor of the main reaction product acetaldehyde derivative
Lazzaroni R.; Settambolo R.; Marchetti M.; Paganelli S.; Alagona G.; Ghio C.
https://dx.doi.org/10.1016/j.ica.2008.07.006

14) Keto-enol tautomerism in linear and cyclic beta-diketones: A DFT study in vacuo and in solution
Alagona* G.; Ghio* C.

http://www.cnr.it/prodotto/i/39934

15)-A test case for time-dependent density functional theory calculations of electronic circular dichroism: 2-chloro-4-methoxy-6-[(R)-1-phenylethlamino]-1,3,5-triazine
Alagona G.; Ghio* C.; Monti* S.
http://www.cnr.it/prodotto/i/39673

16)-Caco-2 cell permeability modelling: a neural network coupled genetic algorithm approach
Di Fenza* A.; Alagona G.; Ghio C.; Leonardi R.; Giolitti A.; Madami A.
http://www.cnr.it/prodotto/i/39674

17)-Competitive H-bonds in vacuo and in aqueous solution for N-protonated adrenaline and its monohydrated complexes
Alagona* G.; Ghio* C.
http://www.cnr.it/prodotto/i/39675

18)- Computational prediction of the regio- and diastereoselectivity in a rhodium-catalyzed hydroformylation/cyclization domino process
Alagona* G.; Ghio* C.; Rocchiccioli S.
http://www.cnr.it/prodotto/i/39676

19)-Theoretical Investigation of Tautomeric Equilibria for Isonicotinic Acid, 4-Pyridone, and Acetylacetone in Vacuo and in Solution
Nagy* P.I.; Alagona G.; Ghio* C.
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20)-The Conformational Landscape of (R,R)-Pterocarpans with Biological Activity in Vacuo and in Aqueous Solution (PCM and/or Water Clusters)
Alagona* G.; Ghio C.
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21)-Protonated Serotonin Conformational Landscape in Vacuo and in Aqueous Solution (IEF-PCM): Role of Correlation Effects and Monohydration
Alagona* G.; Ghio C.
22)-Side Chain Dynamics and Alternative Hydrogen Bonding in the Mechanism of Protein Thermostabilization
Khechinashvili* N.N.; Fedorov M.V.; Kabanov A.V.; Monti S.; Ghio C.; Soda K.
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23)-Partially folded states of HIV-1 protease: Molecular dynamics simulations and ligand binding
Cavallari, M; Ghio, C; Monti, S; Ferrario, M; Maritan, A; Carloni, P
http://www.cnr.it/prodotto/i/166877

24)-Structure and dynamics of the hydrogen-bond network around (R,R)-pterocarpans with biological activity in aqueous solution
Alagona* Giuliano; Ghio Caterina; Monti Susanna
http://www.cnr.it/prodotto/i/39349

25)-Alkyl-Rhodium Transition State Stabilities as a Tool to Predict Regio- and Stereoselectivity in the Hydroformylation of Chiral Substrates
Alagona* G.; Ghio C.
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26)-Is the Bias Introduced in an FEP Calculation by Parameterizing a QM Reaction Acceptable? Comparison with Car-Parrinello MD/AMBER Results for the Second Proton Transfer in Triosephosphate Isomerase (TIM)
Alagona G.; Campanile S.; Ghio* C.; Molin D.
729 (2005): 131-139.
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27)-Theoretical Conformational Analysis for Neurotransmitters in the Gas Phase and in Aqueous Solution. Serotonin
Alagona* G.; Ghio C.; Nagy P.I.
http://www.cnr.it/prodotto/i/39368

28)-B3LYP/6-31G* conformational landscape in vacuo of some pterocarpan stereoisomers with biological activity
29) Theoretical Investigation on the Oxazaborolidine-Ketone Interaction in Small Model Systems
Alagona* G.; Ghio C.; Tomasi S.
http://www.cnr.it/prodotto/i/39369

30) Theoretical Studies on the Effects of Methods and Parameterization on the Calculated Free Energy of Hydration for Small Molecules
Alagona* G.; Ghio C.; Nagy P.I.
http://www.cnr.it/prodotto/i/39371

31) Markedly Different Selectivity in the Rhodium Catalyzed Hydroformylation of Vinyl Olefins Containing a Chiral Alkoxy or Alkyl Group: Good Agreement between Theory and Experiment
Alagona G.; Ghio C.; Lazzaroni R.; Settambolo R.
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32) Markedly Different Selectivity in the Rhodium Catalyzed Hydroformylation of Vinyl Olefins Containing a Chiral Alkoxy or Alkyl Group: Good Agreement between Theory and Experiment
Alagona G.; Ghio C.; Lazzaroni R.; Settambolo R.
http://www.cnr.it/prodotto/i/168886

33) Theoretical Conformational Analysis for Neurotransmitters in the Gas Phase and in Aqueous Solution. Norepinephrine
Nagy* P.I.; Alagona* G.; Ghio C.; TakÅ¡cs-NovÅ¡k K.
http://www.cnr.it/prodotto/i/39168

34) Quantum Mechanical Study of Stereoselectivity in the Oxazaborolidine-Catalysed Reduction of Acetophenone
Alagona* G.; Ghio C.; Persico M.; Tomasi S.
35)-The Intramolecular Mechanism for the Second Proton Transfer in Triosephosphate Isomerase (TIM): A QM/FE Approach
Alagona G.; Ghio* C.; Kollman P.A.
http://www.cnr.it/prodotto/i/39170

36)-Transferable Group Contributions for a Variety of Chemical Phenomena and Compound
Alagona* G.; Campanile S.; Ghio C.; Giolitti A.; Monti S.
http://www.cnr.it/prodotto/i/39171

37)-Cholic Acid Derivatives Containing both 2-Naphthylcarbamate and 3,5-Dinitrophenylcarbamate Groups: A Combined Circular Dichroism-Molecular Mechanics Approach to the Definition of their Molecular Conformation
Alagona G.; Ghio C.; Iuliano* A.; Monti* S.; Pieraccini I.; Salvadori P.
http://www.cnr.it/prodotto/i/39172

38)-Interplay of Intra- and Intermolecular H-Bonds for the Addition of a Water Molecule to the Neutral and N-Protonated Forms of Noradrenaline
Alagona* G.; Ghio C.
http://www.cnr.it/prodotto/i/39011

39)-5-Fluorouracil Dimers in Aqueous Solution: Molecular Dynamics in Water and Continuum Solvation
Alagona G.; Ghio* C.; Monti S.
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40)-Ab Initio Modelling of Competitive Drug-Drug Interactions: 5-Fluorouracil Dimers in the Gas Phase and in Solution.
Alagona* G.; Ghio C.; Monti S.
http://www.cnr.it/prodotto/i/39680

41)-Reaction mechanisms between methyamine and a few Schiff bases: Ab initio potential energy surfaces of a catalytic step in semicarbazide sensitive amino oxidases (SSAO)
Alagona* G.; Ghio C.
42)-Olefin Insertion into the Rhodium-Hydrogen Bond as the Step Determining the Regioselectivity of Rhodium-Catalyzed Hydroformylation of Vinyl Substrates: Comparison between Theoretical and Experimental Results
Alagona* G.; Ghio C.; Lazzaroni R.; Settambolo R.
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Other publications (journals without peer review, book reviews, etc.)

1)-Antioxidant properties of natural compounds through their copper(II) coordination ability
Alagona G.; Ghio C.
The Intl. Society of Quantum Biology and Pharmacology (ISQBP) PresidentÂ’s Meeting 2010, June 14-16, Cetraro (CS), Italy, 2010
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2)-Theoretical Prediction of Selectivities in Nonreversible and Reversible Hydroformylation Reactions Catalyzed by Unmodified Rh-Carbonyls
Alagona G.; Ghio C.; Lazzaroni R.
Modelling & Design of Molecular Materials, MDMM 2010, July 4-8, Wroclaw (Poland), 2010
http://www.cnr.it/prodotto/i/117110

3)-Selectivities in Hydroformylation Reactions of Variedly Substituted Cyclohexenes and Related Linear Substrates
Alagona G.; Ghio C.
36Â° Congres de Chimistes Theoricien d'Expression Latine, Chitel 2010, Sept. 18-24, Anglet (France), 2010
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4)-Do alkyl-rhodium reactant complex stabilities on each diastereoface account for hydroformylation stereoselectivity?
Alagona G.; Ghio C.
13th Intl. Congress of Quantum Chemistry, June 22-27, Helsinki (Finland), 2009
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5)-Antioxidant properties of natural compounds through their copper(II) chelating ability in vacuo and in aqueous solution (PCM)
Alagona G.; Ghio C.
35Â° Congreso Quimicos Theoricos d'Expression Latina, Quitel 2009, Sept. 18-22, San AndrÃ©s (Colombia), 2009
http://www.cnr.it/prodotto/i/117107
6)-Qual è il rate limiting step nella reazione di Wittig? Studio DFT in vacuo e in soluzione di THF con il PCM
Alagona G.; Ghio C.
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7)-The quest for the identification of the catalyst that favored the diastereoselective annulation reaction
Alagona G.; Ghio C.
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8)-Plicatin B Conformational Landscape and Copper (I) and (II) Chelation Ability. A Comparative DFT Study
Alagona G.; Ghio C.
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9)-Potere antiossidante della plicatina B e sua capacità di chelare il rame (II)
Alagona G.; Ghio C.
34° Congresso Interanzionale Chimici Teorici Espressione Latina, Luglio 3-8, Cetraro (CS), 2008
http://www.cnr.it/prodotto/i/116951

10)-Confronto tra meccanismi sequenziali e concertati nella reazione di Wittig in vacuo e in THF
Alagona G.; Ghio C.
34° Congresso Internazionale Chimici Teorici Espressione Latina, Luglio 3-8, Cetraro (CS), 2008
http://www.cnr.it/prodotto/i/116952

11)-Rhodium-catalyzed Hydroformylation of 3-(Pyrrol-1-yl)Alk-1-enes: Two Examples of High 1,2- and 1,3-Substrate-Induced Diastereoselectivity
Settambolo R.; Alagona G.; Ghio C.; Lazzaroni R.
7th Spanish-Italian Symposium on Organic Chemistry, Sept. 7-10, Oviedo (Spain), 2008
http://www.cnr.it/prodotto/i/116953

12)-Evidence for beta-Elimination Explains the Regioselectivity in the Rh-catalyzed Hydroformylation of Vinylidenic Substrates
Alagona G.; Ghio C.; Lazzaroni R.
13)-Secondary and Tertiary Rh-alkyl Intermediate Competition in the Hydroformylation of 1-methylcyclohexenes and Related Linear Olefins
Alagona G.; Ghio C.
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14)-The agostic interaction in the branched intermediate explains the beta-regioselectivity in the Rh-catalyzed hydroformylation of 1,1-diphenylethene
Alagona G.; Ghio C.
Winter Modeling Á˚08, Dec. 19, 2008, Pisa (Italy), 2008
http://www.cnr.it/prodotto/i/116997

15)-Substrate directed 1,3-asymmetric induction in rhodium-catalyzed hydroformylation of chiral vinyl ethers: the outstanding case of (R)-1-phenyl-2,2-dimethylpropyl vinyl ether
Lazzaroni R.; Settambolo R.; Alagona G.; Ghio C.
International Symposium on Homogeneous Catalysis - ISHC_XVI, July 6-11, Florence (Italy), 2008
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16)-QM/MM methods and applications
Ghio C.
http://www.cnr.it/prodotto/i/137265

17)-Tautomeria Cheto-Enolica in beta-Dichetoni Lineari e Cielici: Studio DFT in Vacuo e in Soluzione Acquosa
Alagona Giuliano; Ghio Caterina
XXXIII CONGRESO DE QUÃMICOS TEÃ“RICOS DE EXPRESIÃ“N LATINA, La Havana (Cuba), 2007
http://www.cnr.it/prodotto/i/116613

18)-Reazione di Wittig tra 2,4-dimetil-3-pirrol-1-il-pentanale e Trifenilmetilenfosforano in Vacuo e in Tetraidrofurano
Alagona Giuliano; Ghio Caterina
XXXIII CONGRESO DE QUÃMICOS TEÃ“RICOS DE EXPRESIÃ“N LATINA, La Havana (Cuba), 2007
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19)-Competing H-Bonds in N-Protonated Adrenaline
20)-Computational Prediction of Regio- and Stereoselectivities in the Hydroformylation of Chiral Olefins
Alagona Giuliano; Ghio Caterina; Lazzaroni Raffaello
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21)-DHAP-GAP Reversible Isomerisation Catalyzed by TIM Revisited using Hybrid Car-Parrinello MD/AMBER Simulations
Alagona Giuliano; Ghio Caterina; Molin Dafne
XII Intl Congress of Quantum Chemistry (ICQC), Kyoto (Japan), 2006
http://www.cnr.it/prodotto/i/116522

22)-Docking of protonated ethylamine neurotransmitters in rhodopsin-based receptor models
Alagona Giuliano; Ghio Caterina; Nagy Peter I.
Intl Society of Quantum Biology & Pharmacology (ISQBP) President's Meeting, Strasbourg, France, 2006
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23)-Human Oral Absorption Models Using a Neural Network Coupled Genetic Algorithm
Di Fenza Armida; Alagona Giuliano; Ghio Caterina; Leonardi Riccardo; Giolitti Alessandro; Madami Andrea
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24)-Can Computational Methods Explain and Even Predict Diastereoselectivity in the Rh-catalyzed Annulation of a Chiral Aldehyde?
Alagona Giuliano; Ghio Caterina; Lazzaroni Raffaello
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25)-Conformational Analysis for Protonated Serotonin in Vacuo and in Aqueous Solution. Docking into a 5-HT2A Receptor Model
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26)-Effects of the Computational Description on Alkyl-Rhodium Transition States in Chiral Olefin Hydroformylation
   Alagona Giuliano; Ghio Caterina
   WATOC 2005 - Modelling Structure and Reactivity, Cape Town (South Africa), 2005
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27)-Solvent Effects on two Pterocarpans with Biological Activity: Continuum vs Discrete Approaches
   Alagona Giuliano; Ghio Caterina
   WATOC 2005 - Modelling Structure and Reactivity, Cape Town (South Africa), 2005
   http://www.cnr.it/prodotto/i/116618

28)-Effects of the Computational Description on Alkyl-Rhodium Intermediates in Chiral Olefin Hydroformylation
   Alagona G.; Ghio C.
   XXX CONGRESSO INTERNACIONAL DE QUÃMICOS TEÃ‘RICOS DE EXPRESSAO LATINA, Porto (Portugal), 2004
   http://www.cnr.it/prodotto/i/116619

29)-Is the Bias Introduced in an FEP Calculation by Reparameterizing a Chemical Reaction Acceptable?
   Alagona G.; Ghio C.; Laino T.; Molin D.
   XXX CONGRESSO INTERNACIONAL DE QUÃMICOS TEÃ‘RICOS DE EXPRESSAO LATINA, Porto (Portugal), 2004
   http://www.cnr.it/prodotto/i/116620

30)-Oxazaborolidine-Catalysed Reductions of Prochiral ketones: Quantum Mechanical Study of the Mechanism in Solution and in the Gas Phase
   Alagona G.; Ghio C.; Tomasi S.
   Modelling and Understanding in Theoretical Chemistry, Lucca (Italy), 2004
   http://www.cnr.it/prodotto/i/116621

31)-Solvent Effects at the B3LYP/6-31G* Level on the Most Stable Diastereomer of Two Pterocarpans with Biological Activity
   Alagona G.; Ghio C.
   Modelling and Understanding in Theoretical Chemistry, Lucca (Italy), 2004
   http://www.cnr.it/prodotto/i/116622

32)-Markedly Different Selectivity in the Rhodium Catalyzed Hydroformylation of Vinyl Olefins Containing a Chiral Alkoxy or Alkyl Group
   Lazzaroni R.; Rocchiccioli S.; Guazzelli G.; Settambolo R.; Alagona G.; Ghio C.
   I4th International Symposium on Homogeneous Catalysis, Munich (Germany), 2004
33)-Hybrid Car-Parrinello Molecular Dynamics/Molecular Mechanics Simulations on the Second Proton Transfer in Triosephosphate Isomerase
Molin D.; Laino T.; Ghio C.; Alagona G.
INFMeeting 2004, Genova (Italy), 2004
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34)-Comparison between QM/MM Approaches in an Enzyme Catalyzed Reaction Mechanism
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ISQBP President's Meeting, Como (Italy), 2004
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35)-Quantum Mechanical Study of Stereoselectivity in the Oxazaborolidine-Catalysed Reduction of Acetophenone
Alagona G.; Ghio C.; Persico M.; Tomasi S.
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36)-A Combined ab initio and Free Energy Approach for Studying Enzyme Catalyzed Reaction Mechanisms
Alagona G.; Campanile S.; Ghio C.; Kollman P.A.
VI Convegno su: Complex systems: structure, properties, reactivity and dynamics - 10-13 giugno, Bologna, 2003
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37)-A Combined Circular Dichroism-Molecular Mechanics Approach to Define the Molecular Conformation of Cholic Acid Derivatives
Alagona G.; Ghio C.; Iuliano A.; Monti S.
XIIth International Congress of Quantum Chemistry, July 20-26, Bonn (Germany), 2003
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38)-Conformational Preferences of R-norepinephrine in the Gas Phase and in Aqueous Solution
Alagona G.; Ghio C.; Nagy P.I.
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39)-QM/FE Comparison between the through-Enediolate and through-Enediol Pathways in TIM
Alagona G.; Campanile S.; Ghio C.
40)-B3LYP/6-31G* vs MMFF94 Conformational Landscapes of all the Possible Stereoisomers of a few Pterocarpans with Biological Activity
Alagona G.; Ghio C.; Monti S.
29ème Congrès International des Chimistes Théoriciens d'Expression Latine (ChiTEL 2003), Sept. 7-12, Marrakech (Morocco), 2003
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41)-Analysis of the Interaction Energy for Various Oxazaborolidine-Ketone Adducts and Related Systems
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42)-B3LYP/6-31G* Conformational Preferences in Vacuo of Natural Isoflavonoid Pterocarpans with Antitumoral Activity
Alagona G.; Ghio C.; Monti S.
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43)-Quantum Mechanical Study of Stereoselectivity in the Oxazaborolidine-catalysed Reduction of Acetophenone
Alagona G.; Ghio C.; Persico M.; Tomasi S.
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44)-Transferable Group Contributions for a Variety of Chemical Phenomena and Compounds
Alagona G.; Campanile S.; Ghio C.; Giolitti A.; Monti S.
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45)-Ab Initio Theoretical Methods for Studying Intermolecular Forces
Alagona G.; Ghio C.
46)-Ab Initio Evaluation of the Strength of Hydrogen Bonding and Stacking Interactions
Alagona G.; Ghio C.
2003
http://www.cnr.it/prodotto/i/137199

47)-Valutazione del ruolo del legame a idrogeno nella biodisponibilitÃ  di farmaci
Campanile Silvio; Alagona Giuliano; Ghio Caterina
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48)-Transferable Group Contributions for a Variety of Chemical Phenomena and Compounds
Alagona G.; Campanile S.; Ghio C.; Monti S.
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49)-BSSE Study of the Oxazaborolidine-Ketone Interaction in a Model System
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50)-Continuum Solvation of Stable Conformers of Neutral and Protonated Noradrenaline in Vacuo and in the Presence of a Water Molecule
Alagona G.; Ghio C.
WATOC 2002, Lugano (Switzerland), 2002
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51)-Is the Second Proton Transfer in Triosephosphate Isomerase Intramolecular or His 95 Assisted?
Alagona G.; Ghio C.; Kollman P.A.
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Alagona G.; Ghio C.; Kollman P.A.
*Molecular Simulations in Structural Biology and Drug Discovery, San Francisco, CA, USA, 2002*
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54)-Drug Delivery by Biodegradable Poly(Ester-Ether-Ester)s: a Tentative Theoretical Evaluation of the Interactions between Drug and Macromolecular Matrix
Alagona G.(1); Ghio C.(1); Monti S.(1); Guerra G.D.(2); Maltinti S.(3)
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