

1	Authors: A. Arnau, J. Andrés, I. Tuñón, E. Silla Title: HCnN. The Largest Molecules in the Interstellar Medium Reference: J. Chem. Educ., <b>67</b> , 905-906 (1990).	Type: A
2	Authors: A. Arnau, E. Silla, I. Tuñón. Title: The Discovery of a Chemistry among the Stars Reference: J. Chem. Educ., <b>72</b> , 776-781, (1995).	Type: A
3	Authors: I. Tuñón, A. Arnau, E. Silla Title: Aminoácidos en Disolución Acuosa Reference: Mundo Científico, <b>207</b> , 47-51 (2000)	Type: A
4	Authors: A. Arnau, J. Pitarch, E. Silla, I. Tuñón Title: ¿Cómo resisten las bacterias? Reference: Mundo Científico, <b>237</b> , 70-75(2002)	Type: A
5	Authors: E. Silla, I. Tuñón Title: Modelización de Sistemas Químicos en Disolución Acuosa Reference: Anales de Química, <b>Enero</b> , 14-20 (2002)	Type: A
6	Authors: A. Cuñat, I. Tuñón, J. Moratal Title: Química: Una Ciencia para Todos Reference: 'Didáctica de la Física y la Química en los distintos niveles educativos'; ed. G. Pinto, Madrid 2005.	Type: CL
7	Authors: I. Tuñón y E. Silla Title: Química: Una Ciencia para Todos Reference: Editorial Síntesis, Madrid 2008 (ISBN: 978-84-975668-9-9)	Type: L
8	Authors: I. Tuñón, E. Ortí, J. L. Pascual-Ahuir, I. S. Monzó y C. Gómez Title: Química Física Avanzada Reference: Open Course Ware, Universitat de València, 2009	
9	Authors: A. Arnau, I. Tuñón J. Andrés, E. Silla Title: Theoretical Rotational Constants of MeCnN Species Reference: Chem. Phys. Letters., <b>166</b> , 54-56 (1990)	Type: A
10	Authors: E. Silla, I. Tuñón, J. L. Pascual-Ahuir Title: GEPOL: An Improved Description of Molecular Surfaces. II Computing the Molecular Area and Volume Reference: J. Comput. Chem., <b>12</b> , 1077-1088 (1991)	Type: A
11	Authors: I. Tuñón, E. Silla, J. Tomasi Title: Methylamines Basicity Calculations. In Vacuo and in Solution Comparative Analysis Reference: J. Phys. Chem., <b>96</b> , 9043-9048 (1992)	Type: A

12	Authors: J. L. Pascual-Ahuir, E. Silla, I. Tuñón Title: GEPOL/92 (GEometría POLhiedro, 1992) Reference: Quantum Chem. Prog. Exchange Bull., <b>12</b> , 63 (1992)	Type: A
13	Authors: E. Silla, I. Tuñón, F. Villar, J. L. Pascual-Ahuir Title: Molecular Surface Calculations on Organic Compounds Molecular Area-Aqueous Solubility Relationships. Reference: J. Mol. Struc. (Theochem), <b>254</b> , 465-472 (1992)	Type: A
14	Authors: I. Tuñón, E. Silla, J. L. Pascual-Ahuir Title: Molecular Surface Area and Hydrophobic Effect Reference: Protein Eng., <b>5</b> , 715-716 (1992)	Type: A
15	Authors: A. Arnau, E. Silla, I. Tuñón Title: Ab Initio Rotational Constants of Interstellar Species: Cyanoacetylene Hydrogenated Derivatives Reference: Int. J. Quantum Chem., <b>46</b> , 231-238 (1993)	Type: A
16	Authors: I. Tuñón, E. Silla, J. L. Pascual-Ahuir Title: Continuum Uniform Approach Calculations of the Solubility of Hydrocarbons in Water Reference: Chem. Phys. Letters, <b>203</b> , 289-294 (1993)	Type: A
17	Authors: I. Tuñón, E. Silla, J. Bertrán Title: Proton Solvation in Liquid Water. An ab initio Study Using the Continuum Model Reference: J. Phys. Chem., <b>97</b> , 5547-5552 (1993)	Type: A
18	Authors: A. Arnau, E. Silla, I. Tuñón Title: Ab initio Rotational Constants of Isocyanopolyynes Reference: Astrophys. J., <b>415</b> , L151-155 (1993)	Type: A
19	Authors: I. Tuñón, E. Silla, J. L. Pascual-Ahuir Title: A Theoretical Study of the Inversion of the Alcohols Acidity Scale in Aqueous Solution. Towards an Interpretation of the acid-base Behaviour of Organic Compounds in Solution Reference: J. Am. Chem. Soc., <b>115</b> , 2226-2230 (1993)	Type: A
20	Authors: A. Arnau, E. Silla, I. Tuñón Title: Calculated Rotational Constants of Interstellar Species: Hydrogenated Derivatives of HCN and HC <sub>3</sub> N Reference: Astrophys. J. Suppl. S., <b>88</b> , 595-609 (1993).	Type: A
21	Authors: F. R. Tortonda, J. L. Pascual-Ahuir, E. Silla, I. Tuñón Title: Proton Transfer between Water Molecules. A Theoretical Study of	

- Solvent Effects Using the Continuum and the Discrete-Continuum Models
- Reference: J. Phys. Chem., **97**, 11087-11091 (1993) Type: A
- 
- 22  
Authors: J. L. Pascual-Ahuir, E. Silla, I. Tuñón  
Title: GEPOL/93(GEometría POLhiedro, 1993)  
Reference: Quantum Chem. Prog. Exchange Bull., **14**, 63 (1994) Type: A
- 
- 23  
Authors: I. Tuñón, E. Silla, J. L. Pascual-Ahuir  
Title: Evaluation of Transfer Free Energies  
Reference: J. Phys Chem., **98**, 377-379 (1994) Type: A
- 
- 24  
Authors: I. Tuñón, E. Silla, J. Bertrán  
Title: Transition Structures of Friedel Crafts Reaction in Solution  
Reference: J. Chem Soc. Faraday Trans., **90**, 1757-1761 (1994) Type: A
- 
- 25  
Authors: J. Andrés, S. Bohm, V. Moliner, E. Silla, I. Tuñón.  
Title: A Theoretical Study on Stationary Structures for the Addition of Azide Anion to Tetrafuranosides: Modelling the Kinetic and Thermodynamic Controls by Solvent Effects  
Reference: J. Phys. Chem., **98**, 6955-6960, (1994) Type: A
- 
- 26  
Authors: R. Moreno, E. Silla, I. Tuñón, A. Arnau.  
Title: Ab Initio Rotational Constants of the Nitriles Derived from Cyanodiacetylene (HC<sub>4</sub>CN)  
Reference: Astrophys. J., **437**, 532-539 (1994). Type: A
- 
- 27  
Authors: J. L. Pascual-Ahuir, E. Silla, I. Tuñón.  
Title: Gepol: An Improved Description of Molecular Surfaces III. A New Algorithm for the Computation of the Solvent-Excluding Surface  
Reference: J. Comput. Chem., **15**, 1127-1138 (1994). Type: A
- 
- 28  
Authors: I. Tuñón, D. Rinaldi, M. F. Ruiz-López, J. L. Rivail  
Title: Hydroxide Ion in Liquid Water: Structure, Energetics and Proton transfer Using a Mixed Discrete-Continuum ab initio Model  
Reference: J. Phys. Chem., **99**, 3798-3805 (1995) Type: A
- 
- 29  
Authors: F. R. Tortonda, J. L. Pascual-Ahuir, E. Silla, I. Tuñón  
Title: Solvent Effects on the Thermodynamics and Kinetics of the Proton Transfer between Hydronium ion and Ammonia. A Theoretical Study Using the Continuum and the Discrete Models  
Reference: J. Phys. Chem., **99**, 12525-12528 (1995) Type: A
- 
- 30  
Authors: I. Tuñón, M. T. C. Martins-Costa, C. Millot, M. F. Ruiz-López  
Title: Coupled Density Functional/Molecular Mechanics Monte Carlo Simulations of Ions in Water. The Bromide Ion

- Reference: Chem. Phys. Letters, **241**, 450-456 (1995) Type: A
- 
- 31  
Authors: I. Tuñón, M. T. C. Martins-Costa, C. Millot, M. F. Ruiz-López  
Title: A Hybrid Density Functional-Classical Molecular Dynamics Simulation Method of a Water Molecule in Liquid Water  
Reference: J. Mol. Model., **1**, 196-201 (1995) Type: A
- 
- 32  
Authors: I. Tuñón, M. T. C. Martins-Costa, C. Millot, M. F. Ruiz-López, J. L. Rivail  
Title: A Coupled Density Functional-Molecular Mechanics Monte Carlo Simulation Method: The Water Molecule in Liquid Water  
Reference: J. Comput. Chem., **17**, 19-29 (1996) Type: A
- 
- 33  
Authors: I. Tuñón, M. F. Ruiz-López, D. Rinaldi, J. Bertrán  
Title: Computation of Hydration Free Energies Using a Parametrized Continuum Model: Study of Equilibrium Geometries and Reactive Processes in Water Solution  
Reference: J. Comput. Chem., **17**, 148-155 (1996) Type: A
- 
- 34  
Authors: V. Moliner, J. Andrés, A. Arnau, E. Silla, I. Tuñón  
Title: Rotational Constants and Dipole Moments of Interstellar Polyynes. A Comparative MP2 and Density Functional (BP86) Study  
Reference: Chem. Phys., **206**, 57-61 (1996) Type: A
- 
- 35  
Authors: J. Pitarch, V. Moliner, J. L. Pascual-Ahuir, E. Silla, I. Tuñón  
Title: Can Hydrophobic Interactions Be Correctly Reproduced by the Continuum Models?  
Reference: J. Phys. Chem., **100**, 9955-9959 (1996) Type: A
- 
- 36  
Authors: I. Tuñón, F. R. Tortonda, J. L. Pascual-Ahuir, E. Silla,  
Title: Correlation Effects in Proton Transfer Reactions in Solution  
Reference: Theochem, **371**, 117-121 (1996) Type: A
- 
- 37  
Authors: F. R. Tortonda, J. L. Pascual-Ahuir, E. Silla, I. Tuñón  
Title: Why is Glycine a zwitterion in aqueous solution? A theoretical Study of Solvent Stabilising Factors  
Reference: Chem. Phys Letters, **260**, 21-26 (1996) Type: A
- 
- 38  
Authors: I. Tuñón, M. T. C. Martins-Costa, C. Millot, M. F. Ruiz-López  
Title: Molecular Dynamics simulations of elementary chemical processes in liquid water using combined Density Functional and Molecular Mechanics potentials. I. Proton transfer in strongly H-bonded complexes  
Reference: J. Chem. Phys., **106**, 3633-3642 (1997) Type: A
-

- 
- 39  
Authors: M. Strnad, M. T. C. Martins-Costa, C. Millot, I. Tuñón, M. F. Ruiz-López, J. L. Rivail  
Title: Molecular Dynamics simulations of elementary chemical processes in liquid water using combined Density Functional and Molecular Mechanics potentials II. Charge separation processes  
Reference: J. Chem. Phys., **106**, 3643-3657 (1997) Type: A
- 
- 40  
Authors: J. Pitarch, M. F. Ruiz-López, J. L. Pascual-Ahuir, E. Silla, I. Tuñón  
Title: Ab Initio Calculations on Neutral and Alkalyne Hydrolysis of  $\beta$ -lactam Antibiotics. A Theoretical Study Including Solvent-Effects  
Reference: J. Phys. Chem, **101**, 3581-3588 (1997) Type: A
- 
- 41  
Authors: V. Moliner, R. Castillo, V. S. Safont, M. Oliva, S. Bohm, I. Tuñón, J. Andrés  
Title: A Theoretical Study of the Favorskii rearrangement. Calculation of the Gas Phase Reaction Paths and Solvation Effects on the Molecular Mechanism for the Transposition of the  $\alpha$ -Chlorocyclobutanone  
Reference: J. Am. Chem. Soc., **119**, 1941-1947 (1997) Type: A
- 
- 42  
Authors: J. Pitarch, M. F. Ruiz-López, E. Silla, J. L. Pascual-Ahuir, I. Tuñón  
Title: Neutral and Alkaline Hydrolyses of Model  $\beta$ -Lactam Antibiotics. An ab Initio Study of Water Catalysis  
Reference: J. Am. Chem. Soc., **120**, 2146-2155 (1998) Type: A
- 
- 43  
Authors: J. L. Pascual-Ahuir, E. Silla, I. Tuñón  
Title: The Solvent-excluding surface as a descriptor of ionic channels: Gramicidin-A  
Reference: Theochem, **426**, 331-338 (1998) Type: A
- 
- 44  
Authors: F. R. Tortonda, J. L. Pascual-Ahuir, E. Silla, I. Tuñón, F. J. Ramírez  
Title: Aminoacid Zwitterions in Solution. Geometric, Energetic and Vibrational Analysis Using Density Functional Theory-Continuum Model Calculations  
Reference: J. Chem. Phys., **109**, 592-602 (1998) Type: A
- 
- 45  
Authors: F. J. Ramírez, I. Tuñón, E. Silla  
Title: Amino Acid Chemistry in Solution. Structural and Vibrational Dynamics of Glutamine in Solution. An ab Initio Reaction Field Model  
Reference: J. Phys. Chem. B, **102**, 6290-6298 (1998). Type: A
- 
- 46  
Authors: M. F. Ruiz-López, A. Oliva, I. Tuñón, J. Bertrán  
Title: Self- Consistent Reaction Field Calculations of Non-equilibrium Solvent Effects on Proton Transfer Processes Through low-barrier Hydrogens-Bonds  
Reference: J. Phys. Chem. A, **102**, 10728-10735 (1998). Type: A
- 
- 47  
Authors: I. Tuñón, E. Silla. M. T. C. Martins-Costa, C. Millot, M. F. Ruiz-López

Title: Intramolecular Proton Transfer of Glycine in Aqueous Solution Using Quantum Mechanics-Molecular Mechanics Simulations  
Reference: J. Phys. Chem. A, **102**, 8673-8678 (1998). Type: A

---

48  
Authors: P. Scharlin, R. Battino, E. Silla, I. Tuñón, J. L. Pascual-Ahuir  
Title: Solubility of gases in Water: Correlation between solubility and the number of water molecules in the first solvation shell  
Reference: Pure & Appl. Chem., **70**, 1895-1904 (1998) Type: A

---

49  
Authors: J. Pitarch, J. L. Pascual-Ahuir, E. Silla, I. Tuñón, M. F. Ruiz-López, C. Millot, J. Bertrán  
Title: Molecular Dynamics Simulation in Aqueous Solution of N-methylazetidinone as a Model of  $\beta$ -lactam antibiotics  
Reference: Theor. Chem. Acc., **101**, 336-342 (1999) Type: A

---

50  
Authors: J. Pitarch, J. L. Pascual-Ahuir, E. Silla, I. Tuñón, M. F. Ruiz-López  
Title: Modelling  $\beta$ -lactam Interactions in Aqueous Solution Through Combined Quantum Mechanics-Molecular Mechanics Methods  
Reference: J. Comput. Chem., **20**, 1401-1411 (1999) Type: A

---

51  
Authors: J. Pitarch, J. L. Pascual-Ahuir, E. Silla, I. Tuñón, V. Moliner  
Title: Analysis of a Concerted Mechanism in  $\beta$ -lactam Enzymatic Hydrolysis. A Quantum Mechanics/Molecular Mechanics Study  
Reference: J. Chem. Soc. Perkin Trans. 2, 1351-1356 (1999) Type: A

---

52  
Authors: J. A. Collado, I. Tuñón, E. Silla, F. J. Ramírez  
Title: Vibrational Dynamics of Histamine Monocation in Solution: An Experimental (FT-IR, FT-Raman) and Theoretical (SCRF-DFT) Study  
Reference: J. Phys. Chem. A, **104**, 2120-2131 (2000) Type: A

---

53  
Authors: F. R. Tortonda, E. Silla, I. Tuñón, D. Rinaldi, M. F. Ruiz-López  
Title: Intramolecular Proton Transfer of Serine in Aqueous Solution. Mechanism and Energetics  
Reference: Theor. Chem. Acc., **104**, 89-95 (2000) Type: A

---

54  
Authors: J. Pitarch, J. L. Pascual-Ahuir, E. Silla, I. Tuñón  
Title: A Quantum Mechanics/Molecular Mechanics Study of the Acylation Reaction of TEM1  $\beta$ -lactamase and Penicillanate  
Reference: J. Chem. Soc. Perkin Trans. 2, 761-767 (2000) Type: A

---

55  
Authors: I. Tuñón E. Silla, M. F. Ruiz-López  
Title: On the Tautomerization Process of Glycine in Aqueous Solution  
Reference: Chem. Phys. Letters, **321**, 433-437 (2000) Type: A

---

56

Authors: E. Silla, A. Arnau, I. Tuñón  
Title: Solvent Effects on Chemical Systems  
Reference: Handbook of Solvents, ChemTec Publishing,(2000) Type: CL

---

57  
Authors: S.Martí, J. Andrés, V. Moliner, E. Silla, I. Tuñón, J. Bertrán  
Title: A QM/MM Study of the Conformational Equilibria in the Chorismate Mutase Active Site  
Reference: J. Phys. Chem. B, **104**, 11308-11315 (2000) Type: A

---

58  
Authors: S.Martí, J. Andrés, V. Moliner, E. Silla, I. Tuñón, J. Bertrán  
Title: Transition Structure Selectivity in Enzyme catalysis. A QM/MM Study of Chorismate Mutase  
Reference: Theor. Chem. Acc., **105**, 207-212 (2001) Type: A

---

59  
Authors: S.Martí, J. Andrés, V. Moliner, E. Silla, I. Tuñón, J. Bertrán. M. J. Field  
Title: A Hybrid Potential Reaction Path and Free Energy Study of the Chorismate Mutase Reaction  
Reference: J. Am. Chem. Soc., **123**, 1709-1712 (2001) Type: A

---

60  
Authors: R. Castillo, E. Silla, I. Tuñón  
Title: The Role of Protein Flexibility in Enzymatic Catalysis. A QM/MM Study of the Deacylation Reaction in Class A  $\beta$ -Lactamases  
Reference: J. Am. Chem. Soc., **124**, 1809-1816 (2002) Type: A

---

61  
Authors: N. Díaz, D. Suárez, T. L. Sordo, I. Tuñón, E. Silla  
Title: Water-Assited Alakalyne Hydrolysis of Monobactams: A Theoretical Study  
Reference: Chem. Eur. J., **8**, 859-867 (2002) Type: A

---

62  
Authors: A. Soriano, E. Silla, I. Tuñón  
Title: Quantum Mechanics-Molecular Mechanics Study of Dissociative Electron Transfer: The Methylchloride Radical Anion in Aqueous Solution  
Reference: J. Chem. Phys. **116**, 6102-6110 (2002) Type: A

---

63  
Authors: R. Castillo, M. Oliva, S. Martí, V. Moliner, I. Tuñón, J. Andrés  
Title: Hybrid QM/MM Studies on Chemical Reactivity  
Reference: Recent Res. Devel. Quantum Chem., **3**, 51-74(2002) Type:CL

---

64  
Authors: S. Martí, J. Andrés, V. Moliner, E. Silla, I. Tuñón, J. Bertrán  
Title: Preorganization and Reorganization as Related Factors in Enzyme Catalysis: The Chorismate Mutase Case  
Reference: Chem. Eur. J., **9**, 984-991 (2003) Type:A

---

65  
Authors: F. J. Ramírez, I. Tuñón, J. A. Collado, E. Silla

Title: Structural and Vibrational Study of the Tautomerism of Histamine Free Base in Solution  
Reference: J. Am. Chem. Soc., **125**, 2328-2340 (2003) Type: A

---

66  
Authors: F. R. Tortonda, J. L. Pascual-Ahuir, E. Silla, I. Tuñón  
Title: A Theoretical Study of Solvent Effects on the Conformational Equilibria of Neutral Glycine in Aqueous Solution  
Reference: TheoChem, **623**, 203-210 (2003) Type: A

---

67  
Authors: M. Roca, S. Martí, J. Andrés, V. Moliner, I. Tuñón, J. Bertrán, I. H. Williams  
Title: Theoretical Modelling of Enzyme Catalytic Power: Analysis of Cratic and Electrostatic Factors in Cathecol O-MethylTransferase  
Reference: J. Am. Chem. Soc., **125**, 7726-7737 (2003) Type: A

---

68  
Authors: S. Martí, J. Andrés, V. Moliner, E. Silla, I. Tuñón, J. Bertrán  
Title: Conformational Equilibrium of Chorismate. A QM/MM theoretical Study Combining Statistical Simulations and Geometry Optimisations in Gas Phase and in Aqueous Solution  
Reference: TheoChem, **632**, 197-206 (2003) Type: A

---

69  
Authors: S. Martí, V. Moliner, I. Tuñón, I. H. Williams  
Title: QM/MM Calculations of Kinetic isotopic Effects in the Chorismate Mutase Active Site  
Reference: Org. Biomol. Chem., **1**, 483-487 (2003) Type: A

---

70  
Authors: S. Ferrer, E. Silla, I. Tuñón, S. Martí, V. Moliner  
Title: Catalytic Mechanism of Dihydrofolate Reductase Enzyme. A Combined Quantum-Mechanical/Molecular-Mechanical Characterization of the N5 Protonation Step  
Reference: J. Phys. Chem. B., **107**, 14036-14041 (2003) Type: A

---

71  
Authors: A. Soriano, E. Silla, I. Tuñón  
Title: Internal Rotation of 1,2-dichloroethane in haloalkane Dehalogenase. A Test Case for Analyzing Electrostatic Effects in Enzymes  
Reference: J. Phys. Chem. B, **107**, 6234-6238 (2003) Type: A

---

72  
Authors: S. Martí, J. Andrés, V. Moliner, E. Silla, I. Tuñón, J. Bertrán  
Title: A Comparative Study of Claisen and Cope Rearrangements Catalyzed by Chorismate Mutase. An Insight into Enzymatic Efficiency: Transition State Stabilization or Substrate Preorganization?  
Reference: J. Am. Chem. Soc, **126**, 311-319 (2004) Type: A

---

73  
Authors: S. Martí, M. Roca, J. Andrés, V. Moliner, E. Silla, I. Tuñón, J. Bertrán  
Title: Theoretical Insights in Enzyme Catalysis



Reference: Chem. Soc. Rev., **33**, 98-107 (2004) Type: R

---

74

Authors: J. J. Ruiz-Pernía, E. Silla, I. Tuñón, S. Martí, V. Moliner  
Title: Hybrid QM/MM Potentials of mean Force with Interpolated Corrections  
Reference: J. Phys. Chem. B, **108**, 8427-8433 (2004) Type: A

---

75

Authors: F. J. Ramirez, I. Tuñón, E. Silla  
Title: Aminoacid Chemistry in Solution: Structural Properties and Vibrational Dynamics of Serine Using Density Functional Theory and a Continuum Solvent Model  
Reference: Chem. Phys., **303**, 85-96 (2004) Type: A

---

76

Authors: A. Soriano, E. Silla, I. Tuñón, S. Martí, V. Moliner, J. Bertrán  
Title: Electrostatic Effects in Enzyme Catalysis: A Quantum Mechanics/Molecular Mechanics Study of the Nucleophilic Substitution Reaction in Haloalkane Dehalogenase  
Reference: Theor. Chem Acc., **112**, 327-334 (2004) Type: A

---

77

Authors: G. D. Ruggiero, I. H. Williams, M. Roca, V. Moliner, I. Tuñón  
Title: QM/MM Determination of Kinetic isotope Effects for COMT-catalysed methyl transfer does not Support Compression Hypothesis  
Reference: J. Am. Chem. Soc., **126**, 8634-8635 (2004) Type: A

---

78

Authors: A. Soriano, E. Silla, I. Tuñón, M. F. Ruiz-López  
Title: Dynamic and Electrostatic Effects in Enzymatic Processes. An Analysis of the Nucleophilic Substitution Reaction in Haloalkane Dehalogenase  
Reference: J. Am. Chem. Soc., **127**, 1946-1957 (2005) Type: A

---

79

Authors: S. Martí, J. Andrés, V. Moliner, E. Silla, I. Tuñón, J. Bertrán  
Title: Towards a rational Design of Antibody Catalysts through Computational Chemistry  
Reference: Angew. Chem.Int Ed. Eng., **44**, 904-909 (2005) Type: A

---

80

Authors: S. Martí, V. Moliner, I. Tuñón, I. H. Williams  
Title: Computing Kinetic Isotopic Effects for Chorismate Mutase with High Accuracy. A New DFT/MM Strategy  
Reference: J. Phys. Chem. B, **109**, 3707-3710 (2005) Type: A

---

81

Authors: S. Ferrer, J. J. Ruiz-Pernía, I. Tuñón, V. Moliner, M. García-Viloca, A. Gonzalez-Lafont, J. M. Lluch  
Title: A QM/MM Exploration of the Potential Energy Surface of the Pyruvate to Lactate Transformation Catalyzed by LDH. Improving the Accuracy of Semiempirical Descriptions

- Reference: J. Chem. Theor. Comput., **1**, 750-761 (2005) Type: A
- 
- 82  
Authors: S. Martí, V. Moliner, I. Tuñón  
Title: Improving the QM/MM Description of Chemical Processes: A Dual Level Strategy to Explore the Potential Energy Surface in Very Large Systems  
Reference: J. Chem. Theor. Comput., **1**, 1008-1016 (2005) Type: A
- 
- 83  
Authors: M. Roca, J. Andrés, V. Moliner, I. Tuñón, J. Bertrán  
Title: On the Nature of the Transition State in Catechol O-Methyltransferase. A Complementary Study Based on Molecular Dynamics and Potential Energy Surface Explorations  
Reference: J. Am. Chem. Soc., **127**, 10648-10655 (2005) Type: A
- 
- 84  
Authors: L. Gorb, A. Asensio, I. Tuñón, M. F. Ruiz-López  
Title: The Mechanism of Formamide Hydrolysis in Water from ab initio Calculations and Simulations  
Reference: Chem. Eur. J., **11**, 6743-6753 (2005) Type: A
- 
- 85  
Authors: S. Ferrer, E. Silla, I. Tuñón, M. Oliva, V. Moliner, I. H. Williams  
Title: Dependence of Enzyme Reaction Mechanism on Protonation State of Titratable Residues and QM level Description: Lactate Dehydrogenase  
Reference: Chem. Comm., 5873-5875 (2005) Type: A
- 
- 86  
Authors: M. Roca, V. Moliner, J. J. Ruiz-Pernía, E. Silla, I. Tuñón  
Title: Activation Free Energy of Catechol O-Methyltransferase. Corrections to the Potential of Mean Force.  
Reference: J. Phys. Chem. A, **110**, 593-509 (2006) Type: A
- 
- 87  
Authors: S. Martí, J. Andrés, V. Moliner, E. Silla, I. Tuñón, J. Bertrán  
Title: Stereoselectivity Behavior of the AZ28 Antibody Catalyzed Oxy-Cope Rearrangement  
Reference: J. Phys. Chem. A, **110**, 726-730 (2006) Type: A
- 
- 88  
Authors: S. Martí, J. Andrés, V. Moliner, E. Silla, I. Tuñón, J. Bertrán  
Title: Improving catalytic antibodies by means of computational techniques  
Reference: "Modelling Molecular Structure and Reactivity in Biological Systems" Special Royal Society of Chemistry Volume. Editores: K. J. Naidoo, J. Brady, M. J. Field, J. Gao, M. Hann. RSC Publishing, pp 261-268. Type: CL
- 
- 89  
Authors: A. J. Ruiz-Chica, A. Soriano, I. Tuñón, F. M. Sánchez-Jiménez, E. Silla, F. J. Ramírez  
Title: FT-Raman and QM/MM Study of the Interaction between Histamine and DNA  
Reference: Chem. Phys., **324**, 579-590 (2006) Type: A

- 
- 90  
Authors: J. J. Ruiz-Pernía, E. Silla, I. Tuñón, S. Martí  
Title: Hybrid Quantum Mechanics/Molecular Mechanics Simulations with two-dimensional Interpolated Corrections: Application to Enzymatic Processes  
Reference: J. Phys. Chem. B, **110**, 17663-17670 (2006) Type: A
- 
- 91  
Authors: J. J. Ruiz-Pernía, E. Silla, I. Tuñón  
Title: Comparative Computational Analysis of Different Active Site Conformations and Substrates in a Chalcone Isomerase Catalyzed Reaction  
Reference: J. Phys. Chem. B, **110**, 20686-20692 (2006) Type: A
- 
- 92  
Authors: M. Roca, V. Moliner, I. Tuñón, J. T. Hynes  
Title: Coupling Between Protein and Reaction Dynamics in Enzymatic Processes: Application of Grote-Hynes Theory to Catechol O-Methyl Transferase  
Reference: J. Am. Chem. Soc., **128**, 6186-6193 (2006) Type: A
- 
- 93  
Authors: A. Soriano, R. Castillo, C. Christov, J. Andrés, V. Moliner, I. Tuñón  
Title: Catalysis in Glycine N-Methyltransferase: Testing the Electrostatic Stabilization and Compression Hypothesis  
Reference: Biochemistry, **45**, 14917-14925 (2006) Type: A
- 
- 94  
Authors: S. Ferrer, I. Tuñón, S. Martí, V. Moliner, M. García-Viloca, A. González-Safont, J. M. Lluch  
Title: A Theoretical Analysis of Rate Constants and Kinetic Isotope Effects Corresponding to Different Reaction Valleys in Lactate Dehydrogenase  
Reference: J. Am. Chem. Soc., **128**, 16851-16863 (2006) Type: A
- 
- 95  
Authors: S. Martí, J. Andrés, V. Moliner, E. Silla, I. Tuñón, J. Bertrán  
Title: Computer Aided rational Design of Catalytic Antibodies: The 1F7 Case  
Reference: Angew. Chem. Int. Ed., **46**, 286-290 (2006) Type: A
- 
- 96  
Authors: J. H. Alzate-Morales, R. Contreras, A. Soriano, I. Tuñón, E. Silla  
Title: A Computational Study of the Protein-Ligan Interactions in CDK2 Inhibitors: Using QM/MM Interaction Energy as a Predictor of Biological Activity  
Reference: Biophysical J., **92**, 430-439 (2007) Type: A
- 
- 97  
Authors: C. N. Alves, S. Martí, R. Castillo, J. Andrés, V. Moliner, I. Tuñón, E. Silla  
Title: Calculation of binding energy using BLYP/MM for the HIV-1 integrase complexed with the S-1360 and two analogues  
Reference: Bioorg. Med. Chem. **15**, 3818-3824 (2007) Type: A

- 
- 98  
Authors: C. N. Alves, S. Martí, R. Castillo, J. Andrés, V. Moliner, I. Tuñón, E. Silla  
Title: A Quantum Mechanics/Molecular Mechanics Study of the Protein–Ligand Interaction for Inhibitors of HIV-1 Integrase  
Reference: Chem. Eur. J. **13**, 7715-7724 (2007) Type: A
- 
- 99  
Authors: J. J. Ruiz-Pernía, E. Silla, I. Tuñón  
Title: Enzymatic Effects on Reactant and Transition States. The Case of Chalcone Isomerase  
Reference: J. Am. Chem. Soc. **129**, 9117-9124 (2007) Type: A
- 
- 100  
Authors: S. Martí, J. Andrés, V. Moliner, E. Silla, I. Tuñón, J. Bertrán  
Title: Theoretical Study of Catalytic Efficiency of a Diels-Alderase Catalytic Antibody: An Indirect Effect Produced During the Maturation Process  
Reference: Chem. Eur. J. **14**, 596-602 (2008) Type: A
- 
- 101  
Authors: C. N. Alves, S. Martí, R. Castillo, J. Andrés, V. Moliner, I. Tuñón, E. Silla  
Title: A Quantum Mechanic/Molecular Mechanic Study of the Wild-type and N155S Mutant HIV-1 Integrase Complexed with Diketo Acid  
Reference: Biophys. J. **94**, 2443-2451 (2008) Type: A
- 
- 102  
Authors: J. J. Ruiz-Pernía, I. Tuñón, V. Moliner, J. T. Hynes, M. Roca  
Title: Dynamic Effects on Reaction Rates in a Michael Addition Catalyzed by Chalcone Isomerase. Beyond the Frozen Environment Approach  
Reference: J. Am. Chem. Soc. **130**, 7477-7488 (2008) Type: A
- 
- 103  
Authors: S. Martí, J. Andrés, V. Moliner, E. Silla, I. Tuñón, J. Bertrán  
Title: Predicting an Improvement of the Secondary Catalytic Activity of Promiscuous Pyruvate Lyase by Computational Design  
Reference: J. Am. Chem. Soc. **130**, 2894-2895 (2008) Type: A
- 
- 104  
Authors: A. A. Moya-García, J. J. Ruiz-Pernía, S. Martí, F. Sánchez-Jiménez, I. Tuñón  
Title: Analysis of the Decarboxylation Step in Mammalian Histidine Decarboxylase. A Computational Study  
Reference: J. Biol. Chem. **283**, 12393-12401 (2008) Type: A
- 
- 105  
Authors: R. Castillo, M. Roca, A. Soriano, V. Moliner, I. Tuñón  
Title: Using Grote-Hynes Theory to Quantify Dynamical Effects on the Reaction Rate of Enzymatic Processes. The Case of Methyltransferases  
Reference: J. Phys. Chem. B **112**, 529-534 (2008) Type: A
- 
- 106

- Authors: M. Roca, L. De Maria, S. J. Wodak, V. Moliner, I. Tuñón, J. Giraldo  
Title: Coupling of the Guanosine Glycosidic Bond Conformation and the Ribonucleotide Cleavage Reaction: Implications for Barnase Catalysis  
Reference: *Proteins*, **70**, 415-428 (2008) Type: A
- 
- 107  
Authors: J. Lameria, C. N. Alves, V. Moliner, S. Martí, N. Kanaan, I. Tuñón  
Title: A Quantum Mechanics/Molecular Mechanics Study of the Protein-Ligand Interaction of two Potent Inhibitors of Human O-GlcNAcase: PUGNAc and NAG\_Thiazoline  
Reference: *J. Phys. Chem. B* **112**, 14260-14266 (2008) Type: A
- 
- 108  
Authors: S. Martí, J. Andrés, V. Moliner, E. Silla, I. Tuñón, J. Bertrán  
Title: Computational Design of Biological Catalysts  
Reference: *Chem. Soc. Rev.* **37**, 2634-2643 (2008) Type: A
- 
- 109  
Authors: S. Ferrer, I. Tuñón, V. Moliner, I. H. Williams  
Title: Theoretical site-directed Mutagenesis: Asp168Ala Mutant of Lactate Dehydrogenase  
Reference: *J. R. Soc. Interface.* **5**, S217-S224 (2008) Type: A
- 
- 110  
Authors: J. J. Ruiz-Pernía, C. N. Alves, V. Moliner, E. Silla, I. Tuñón  
Title: A QM/MM Study of the Reaction Mechanism for the 3'-processing Step Catalyzed by HIV-1 Integrase  
Reference: *Theochem*, **898**, 115-120 (2009) Type: A
- 
- 111  
Authors: V. López, S. Martí, J. Bertrán, V. Moliner, I. Tuñón  
Title: Theoretical Modeling of the Reaction Mechanism of Phosphate Monoester Hydrolysis in Alkaline Phosphatase  
Reference: *J. Phys. Chem. B*, **113**, 7816-7824 (2009) Type: A
- 
- 112  
Authors: V. López, J. J. Ruiz-Pernía, I. Tuñón, S. Ferrer, V. Moliner  
Title: Theoretical Modeling on the Reaction Mechanism of p-Nitrophenylmethylphosphate Alkaline Hydrolysis and its Kinetic Isotopic Effects.  
Reference: *J. Chem. Theory Comput.*, **5**, 439-442 (2009) Type: A
- 
- 113  
Authors: S. Martí, J. Andrés, V. Moliner, E. Silla, I. Tuñón, J. Bertrán  
Title: Mechanism and Plasticity of Isochorismate Pyruvate Lyase: A Computational Study  
Reference: *J. Am. Chem. Soc.*, **131**, 16156-16161 (2009) Type: A
- 
- 114  
Authors: J. J. Ruiz-Pernía, M. Garcia-Viloca, S. Bhattacharyya, J. Gao, D. G. Truhlar, I. Tuñón  
Title: Critical Role of Substrate Conformational Change in the Proton Transfer Process Catalyzed by 4-Oxalocrotonate Tautomerase  
Reference: *J. Am. Chem. Soc.*, **131**, 2687-2698 (2009) Type: A

---

115

Authors: P. Pérez-Bermúdez, A. A. Moya-García, I. Tuñón, I. Gavidia

Title: Digitalis Purpurea P5 $\beta$ R2 Encoding Steroid 5 $\beta$ -reductase is a Novel Defense-related Gene Involved in Cardenolide Biosynthesis

Reference: New Phytologist, **185**, 687-700 (2010)

Type: A