Scientific Publications Summary

Table of Contents

1. Research Articles

2000

1. M. Baaden, P. Granger and A. Strich; "Dependence of isotropic shift averages and nuclear shielding tensors on the internal rotation of the functional group X about the C−X bond in seven simple vinylic derivatives H2C=CH−X.", *Mol. Phys.*, ***98***, 2000, 329−342.
2. B. Lambert, V. Jacques, A. Shivanyuk, S. E. Matthews, A. Tunayar, M. Baaden, G. Wipff, V. Böhmer, J. F. Desreux; "Calix{4}arenes as selective extracting agents. An NMR dynamic and conformational investigation of the lanthanide(III) and thorium(IV) complexes.", *Inorg. Chem.*, ***39***, 2000, 2033−2041.
3. M. Baaden, F. Berny, C. Boehme, N. Muzet, R. Schurhammer and G. Wipff; "Interaction of trivalent lanthanide cations with phosphoryl derivatives, amide, anisole, pyridine and triazine ligands: a quantum mechanics study.", *J. Alloys & Compounds*, ***303−304***, 2000, 104−111.
4. M. Baaden, F. Berny, N. Muzet, L. Troxler, G. Wipff; "Interfacial features of assisted liquid−liquid extraction of uranyl and cesium salts: a molecular dynamics investigation.", in *Calixarenes for Separations*, 2000, edited by G. Lumetta, R. D. Rogers, and A. S. Gopalan (Oxford University Press, New York), ACS Symposium Series 757, pp. 71−85.
5. M. Baaden, G. Wipff, M. R. Yaftian, M. Burgard and D. Matt; "Cation coordination by calix{4}arenes bearing amide and/or phosphine oxide pendant groups: how many arms are needed to bind Li+ vs Na+ ? A combined NMR and molecular dynamics study.", *J. chem. Soc., Perkin Trans. 2.*, 2000, 1315−1321.
6. M. Baaden, F. Berny, G. Wipff and C. Madic; "A molecular dynamics and quantum mechanics study of M3+ lanthanide cation solvation by acetonitrile: the role of cation size, counterions and polarization effects investigated.", *J. Phys. Chem. A*, ***104***, 2000, 7659−7671.
7. M. Baaden, F. Berny, N. Muzet, R. Schurhammer and G. Wipff; "Separation of radioactive cations by liquid−liquid extraction: computer simulations of water / oil solutions of salts and ionophores.", in *Proceedings of the Euradwaste 1999 conference*, 2000, edited by C. Davies (EC, Luxemburg), pp. 390−393.
8. L. Troxler, M. Baaden, V. Böhmer and G. Wipff; "Complexation of M3+ lanthanide cations by calix{4}arene−CMPO ligands: a molecular dynamics study in methanol solution and at a water / chloroform interface.", *Supramol. Chem.*, ***12***, 2000, 27−51.

2001

1. M. Baaden, F. Berny and G. Wipff; "The chloroform / TBP / aqueous nitric acid interfacial system: a molecular dynamics investigation.", *J. Mol. Liq.*, ***90***, 2001, 1−9.
2. M. Baaden, M. Burgard, C. Boehme and G. Wipff; "Lanthanide cation binding to a phosphoryl−calix{4}arene: the importance of solvent and counterions investigated by molecular dynamics and quantum mechanical simulations", *Phys. Chem. Chem. Phys.*, ***3***, 2001, 1317−1325
3. M. Baaden, M. Burgard, and G. Wipff; "TBP at the water − oil interface: the effect of TBP concentration and water acidity investigated by molecular dynamics simulations", *J. Phys. Chem. B*, ***105***, 2001, 11131−11141

2002

1. M. Baaden, R. Schurhammer and G. Wipff; "Molecular dynamics study of the uranyl

extraction by TBP: demixing of water / 'oil' / TBP solutions with a comparison of supercritical CO2 and chloroform.", *J. Phys. Chem. B*, ***106***, 2002, 434−441

2003

1. M. Baaden, F. Berny, R. Schurhammer, C. Madic and G. Wipff; "Theoretical studies on lanthanide cation extraction by picolinamides: ligand−cation interactions and interfacial behavior.", *Solv. Extr. Ion Exch.*, ***21***, 2003, 199−219
2. J. D. Campbell, P. C. Biggin, M. Baaden and M. S. P. Sansom; "Extending the structure of an ABC transporter to atomic resolution: modelling and simulation studies of Msba.", *Biochemistry*, ***42***, 2003, 3666−3673
3. M. Baaden, C. Meier and M. S. P. Sansom; "A molecular dynamics investigation of mono− and dimeric states of the outer membrane enzyme Ompla.", *J. Mol. Biol.*, ***331***, 2003, 177−189

2004

1. J. D. Faraldo−Gómez, L. R. Forrest, M. Baaden, P. J. Bond, C. Domene, G. Patargias, J. Cuthbertson and M. S. P. Sansom; "Conformational sampling and dynamics of membrane proteins from 10−nanosecond computer simulations.", *Proteins*, ***57***, 2004, 783−791
2. M. Baaden M and M. S. P. Sansom "OMPT: Molecular Dynamics simulations of an outer membrane enzyme.", *Biophys. J.*, ***87***, 2004, 2942−2953

2005

1. R. J. Law, C. Capener, M. Baaden, P. J. Bond, J. Campbell, G. Patargias, Y. Arinaminpathy and M. S. P. Sansom; "Membrane protein structure quality in molecular dynamics simulation.", *J.Mol.Graph.Model.*, ***24*** 2005, 157−165

2007

1. K. Tai, M. Baaden, S. Murdock, B. Wu, M. Hong Ng, S. Johnston, R. Boardman, H. Fangohr, K. Cox, J. W. Essex and M. S. P. Sansom; "Three hydrolases and a transferase: Comparative analysis of active−site dynamics via the BioSimGrid database.", *J.Mol.Graph.Model.*, ***25*** 2007, 896−902

2. Scientific Presentations and Posters

1999

1. M. Baaden, M. Burgard, D. Matt and G. Wipff, *"Selective extraction of lanthanide cations by tetra−phosphineoxide substituted calix{4}arenes: a molecular dynamics study at a water/chloroform interface."*
    - ♦ Meeting of the SFC−Grand Est, Strasbourg, France, January 21−22, 1999.
    - ♦ Annual meeting of the GDR PRACTIS, Avignon, France, Febuary 25th, 1999.
    - ♦ Journée de l'école doctorale de Chimie Physique of Strasbourg, France, April, 1999.
    - ♦ PRACTIS Atelier "Modélisation", Seyssins, France, November 25th 1999.
2. M. Baaden, M. Burgard, D. Matt and G. Wipff, *"Selective extraction of lanthanide cations by tetra−phosphineoxide substituted calix{4}arenes: a molecular dynamics study at a water/chloroform interface."*
    - ♦ Short presentation, Journée de l'école doctorale de Chimie Physique of Strasbourg, France, April, 1999.
3. M. Baaden, *"Solvation of M3+ lanthanide cations in acetonitrile solution"*
    - ♦ Seminar lecture, Strasbourg, France, May, 1999.
4. M. Baaden, L. Troxler and G. Wipff, *"Interfacial aspects in liquid−liquid ion extraction."*
    - ♦ Lecture, 26th International conference on solution chemistry (26ICSC), Fukuoka, Japan, 27 July 1999.
5. A. Strich, M. Baaden and P. Granger, *"Dependence of Isotropic Shift Averages and Nuclear Shielding Tensors on the Internal Rotation of the Functional Group X about the C−X bond in Seven Simple Vinylic Derivatives H2C=CH−X."*
    - ♦ 6ème Ecole d'Eté de Physico−Chimie Théorique, Marly−le Roi, September 6−10, 1999.
    - ♦ 11th European seminar on computational methods in quantum chemistry, Zakopane, Poland, September 23−25, 1999.
    - ♦ 2ème rencontre des Chimistes Théoriciens du Grand Est, Reims, October 15th 1999.

2000

1. M. Baaden, F. Berny, N. Muzet, R. Schurhammer and G. Wipff, "Computer Modeling of liquid − liquid ion extraction."
    - ♦ Euradwaste '99, Luxembourg, November 15−18, 1999.
    - ♦ PRACTIS Atelier "Modélisation", Seyssins, France, November 25th 1999.
    - ♦ 2nd COST D11 workshop on supramolecular chemistry, Strasbourg, France, December 10−12, 1999.
    - ♦ Journées PRACTIS, Villeneuve−lès−Avignon, February 17−18, 2000.
2. M. Baaden, *"Etudes de molécules extractantes en solution: aspects structuraux et mécanistiques des effets de synergie"*
    - ♦ Doctoriales d'Alsace 1999, Mittelwihr, France, November 1999.
    - ♦ Journées PRACTIS, Villeneuve−lès−Avignon, February 17−18, 2000.
3. M. Baaden, L. Troxler and G. Wipff, *"Interfacial aspects in liquid−liquid ion extraction."*
    - ♦ Seminar lecture, Oxford, England, 9 June 2000.
4. M. Baaden, *"Energy profiles for interface crossing in liquid−liquid ion extraction."*
    - ♦ Seminar lecture, Zurich, Switzerland, 24 May 2000.
5. M. Baaden, *"Energy profiles for interface crossing in liquid−liquid ion extraction."*

- ♦ CECAM workshop on challenges in Free energy calculations, Lyon, France, 22 June 2000.

2001

1. M. Baaden, M. S. P. Sansom, *"Barrels & corks in a computer, modelling bacterial iron transport systems."*
   - ♦ Poster presentation at the Biochemical Society Meeting, University of York, 17−19 December 2001. (*Biochemical Soc. Trans. Part 1*, ***30***, 2002, A44)
2. M. Baaden, *"Modelling the ligand−gated protein channel and ferric enterobactin receptor FepA."*
   - ♦ Seminar, Mathematical Biology Division, National Institute for Medical Research, London, 4 December 2001.
3. M. Baaden, *"Modélisation de la protéine membranaire FepA, transporteur bactérien du fer."*
   - ♦ Seminar, Laboratoire de Biochimie Théorique, Institut de Biologie Physico−Chimique, Paris, 18 October 2001.
4. M. Baaden, M. S. P. Sansom, *"Modelling the FepA protein, a bacterial iron transporter in the outer membrane."*
   - ♦ Lecture, Biophysical Chemistry 2001 Conference, Imperial College, London, 21 September 2001.
5. M. Baaden, various seminar lectures, Oxford, England.

2002

1. M. Baaden, M. S. P. Sansom, *"Barrels & corks in a computer, modelling bacterial iron transport systems."*
   - ♦ Poster presentation at the Kollman Memorial Symposium, UCSF, San Francisco, 21−22 February 2002.
   - ♦ Poster presentation at the 46th Annual Meeting of the Biophysical Society, San Francisco, 23−27 February 2002. (*Biophys. J. Part 2*, ***82***, 2002, 2610)
   - ♦ Poster presentation at the 6èmes Journées Francophones des Jeunes Physico−Chimistes, Marseille, 3−5 July 2002.
2. M. Baaden, *"Modelling the ligand−gated protein channel and ferric enterobactin receptor FepA."*
   - ♦ Seminar, Laboratory of Molecular Biophysics, Oxford, 5 February 2002
3. M. Baaden, M. S. P. Sansom, *"Understanding bacterial iron transport."*
   - ♦ Lecture, SFC Eurochem Conference, Toulouse, France, 8 July 2002.

2003

1. M. Baaden, C. Meier and M. S. P. Sansom; "Molecular dynamics simulations of outer membrane phospholipase A."
   - ♦ Poster presentation at the EURESCO Conference 2003−192 Bionanotechnology: "Euroconference on Biomolecular Devices", Granada, Spain, 9−14 July, 2003.
2. M. Baaden, *"La dynamique moléculaire in silico."*
   - ♦ Course and tutorial, Ecole Thématique du CNRS, Outils pour étudier la structure et la dynamique des peptides et des protéines, Arcachon, 18−24 Mai 2003.
3. M. Baaden, M. S. P. Sansom, *"Les protéines membranaires Ompla et Fepa."*
   - ♦ Lecture, GGMM bi−annual conference, Cabourg, France, 7 Mai 2003.

4. M. Baaden, *"Protéines membranaires à repliement 'tonneau béta' − modélisation et dynamique moléculaire de l'enzyme OmplA et du transporteur bactérien du fer FepA."*
    - ♦ Seminar, Institut Européen de Chimie et Biologie, Bordeaux, 4 April 2003.
5. M. S. P. Sansom, P.Bond, M. Baaden, J.D. Faraldo−Gómez, S. Deol, C. Meier, K. Cox, "Simulation of Outer Membrane Proteins."
    - ♦ Poster presentation at the Gordon Research Conference "Protons & Membrane Reactions", Ventura, CA, United States, 23−28 February 2003.
    - ♦ 47th Annual Meeting of the Biophysical Society, San Antonio, United States, 1−5 March 2003.

2004

1. M. Baaden, C. Meier and M. S. P. Sansom; "Molecular dynamics simulations of outer membrane phospholipase A."
    - ♦ Poster presentation at the 48th Annual Meeting of the Biophysical Society, Baltimore, United States, 14−18 February 2004.
2. M. Baaden, "Molecular dynamics simulations of outer membrane phospholipase A."
    - ♦ Seminar, Woolf lab, Johns−Hopkins University School of Medicine, Baltimore, 20 February 2004.
    - ♦ Seminar, Osman lab, Mount Sinai School of Medicine, New York, 23 February 2004.
    - ♦ Seminar, Roux lab, Weill Medical College of Cornell University, New York, 26 February 2004.
3. M. Baaden, *"Dynamique moléculaire de OmplA, une phospholipase de la membrane externe bactérienne."*
    - ♦ Seminar, Huitièmes Entretiens de l'IBPC, Paris, France, 6 April 2004.
4. M. Baaden, M. S. P. Sansom, "La protéine membranaire Ompla."
    - ♦ Seminar, Ben Msik Sciences Faculty, Casablanca, Morocco, 16 June 2004.

2005

1. M. Baaden, M. S. P. Sansom; "Molecular Dynamics Simulations of an Outer Membrane Enzyme."
    - ♦ Platform presentation at the 49th Annual Meeting of the Biophysical Society, Long Beach, United States, 12−16 February 2005.
2. J. D. Faraldo−Gómez, L. R. Forrest, M. Baaden, P. J. Bond, C. Domene, G. Patargias, J. Cuthbertson, M. S. P. Sansom; "On the convergence of the conformational sampling in molecular dynamics simulations of membrane proteins."
    - ♦ Poster presentation at the 49th Annual Meeting of the Biophysical Society, Long Beach, United States, 12−16 February 2005.
3. M. S. P. Sansom, K. Tai, B. Wu, S. Khalid, M. Baaden; *"BioSimGRID: Application to Analysis of Membrane Protein Simulations."*
    - ♦ 49th Annual Meeting of the Biophysical Society, Long Beach, United States, 12−16 February 2005.
4. M. Baaden; *"Utilisation de VMD et OpenDX."*
    - ♦ Presentation at the Journée Visualisation Scientifique, IDRIS, Orsay, France, 8 March 2005.
5. M. Baaden; *"Le système SHAMAN: Système HAptique pour MAnipulation Nanoscopique."*
    - ♦ Seminar, CEA/DIF Centre DAM−Île de France Bruyères−le−Chatel, 14 April 2005.
6. R. Chater, D. Perahia, K. A. Chihab, S. Moussamih, A. Adlouni, M. Baaden, K. Zakrzewska, R. Lavery, M. El Messal, A. Kettani; *"Modélisation moléculaire des mutations du récepteur*

des lipoprotéines de faible densité impliquées dans l'hypercholesterolémie familiale au Maroc"

- Poster presentation at the Xème Symposium ICSN, Gif−sur−Yvette, France, 1−3 June 2005.