

## **Publications de travaux de recherche scientifiques**

Mots-clefs : Chimie analytique & physique, RMN, milieux orientés, méthodologie RMN, chiralité, développement d'outils analytiques pour la chimie organique, analyse conformationnelle, modélisation d'interactions soluté/solvant, relaxation de spin et diffusion, augmentation de sensibilité RMN

### **Articles de recherche publiés dans des revues internationales à comités de lecture**

A29-"Cyclobishelices: shape-persistent figure-eight aromatic molecules with promising chiroptical properties".

A. Robert, G. Naulet, H. Bock, N. Vanthuyne, M. Jean, M. Giorgi, Y. Carissan, C. Aroulanda, F. Durola, Y. Coquerel, accepté à *Chem: A Eur. J.* (2019), publié en ligne.

A28- " The Use of Residual Dipolar Couplings for Conformational Analysis of Non-Steroidal Anti-Inflammatory Drugs Dissolved in Weakly Ordering Media".

M. E. Di Pietro, G. Celebre, R. Salvino, C. Aroulanda, D. Merlet, G. De Luca, *Liq Cryst*, (2018), 45(13-15), 2033-2047.

A27- " Assessing the stable conformations of Ibuprofen in solution by means of Residual Dipolar Couplings"

M. E. Di Pietro, G. Celebre, C. Aroulanda, D. Merlet, G. De Luca, *European Journal of Pharmaceutical Sciences*, (2017), 116, 113.

A26- " Investigation of Solute-Fiber Affinity and Orientational Ordering of Norbornadiene Interacting with Two-polypeptide Chiral Liquid Crystalline Solvents by NAD NMR"

Z. Serhan, C. Aroulanda, P. Lesot, *J. Phys. Chem. A*, (2016), 120, 6076.

A25- " The conformational behaviour of naproxen and flurbiprofen in solution by NMR spectroscopy"

M. E. Di Pietro, C. Aroulanda, G. Celebre, D. Merlet, G. De Luca, *New J. Chem.*, (2015), 39, 9086.

A24- " On the Content of Conformational and Orientational Information from Dipolar Couplings in two Anisotropic Media with a Very Different Degree of Ordering : Thermotropic versus Lyotropic Liquid Crystals "

M. E. Di Pietro, G. De Luca, G. Celebre, D. Merlet, C. Aroulanda, *Mol. Cryst. Liq. Cryst.* (2015), 614, 39.

A23- " Conformational investigation in solution of a fluorinated anti-inflammatory drug by NMR spectroscopy in weakly ordering"

M. E. Di Pietro, C. Aroulanda, D. Merlet, G. Celebre, G. De Luca, *J. Phys. Chem. B* (2014), 118, 9007.

A22- "GET-SERF, a new gradient encoded SERF experiment for the trivial edition of  $^1\text{H}$ - $^{19}\text{F}$  couplings"

M. E. Di Pietro, C. Aroulanda, D. Merlet, *J. Magn. Reson.*, (2013), 234, 101.

A21- "Analytical contribution of NAD 2D-NMR spectroscopy in polypeptide mesophases to the investigation of triglycerides"

P. Lesot, Z. Serhan, C. Aroulanda, I. Billault, *Magn. Reson. Chem.* (2012), 50, S2.

A20- "Conformation and Dynamics of 18-Membered Hexathia-Metacyclophanes: A Two Steps Racemization as Studied by Deuterium NMR in Chiral Lyotropic Liquid Crystals"

P. Lesot, C. Aroulanda, P. Berdagué, H. Zimmermann, Z Luz, *J. Phys. Chem. B* (2011), 115, 11793.

A19- "Enantiotopic Discrimination in the Deuterium NMR Spectrum of Solutes with  $S_4$  Symmetry in Chiral Liquid Crystals"

C. Aroulanda, H. Zimmermann, Z. Luz, P. Lesot, *J. Chem. Phys.* (2011), 134, 134502.

A18- " Evolution of the Saupe Order Parameters of Enantiomers from a Racemic to a non-Racemic Liquid Crystal Solvent: an Original Light on the Absolute Configuration Determination Problem"

J. Courtieu, C. Aroulanda, P. Lesot, A. Meddour, D. Merlet, *Liq. Cryst.* (2010), 37 (6-7), 903.

A17- "Analysis of enantiotopic discrimination in the NMR spectra of prochiral solutes in chiral liquid crystals by symmetry factorization of the Saupe ordering matrix"

P. Lesot, C. Aroulanda, Z. Luz, *J. Chem. Phys.* (2009), 131, 104501.

A16- "Enantiodiscrimination of Flexible Cyclic Solutes Using NMR Spectroscopy in Polypeptide Chiral Mesophases: Investigation of *cis*-decalin and THF"

C. Aroulanda\*, O. Lafon, P. Lesot, *J. Phys. Chem. B* (2009), 113, 10628.

- A15-"<sup>2</sup>H NMR Studies on Two-Homopolypeptide Lyotropic Enantiodiscriminating Mesophases : Experimental Quantification of Solute-Fiber Affinities"  
P. Lesot, O. Lafon, C. Aroulanda, R. Y. Dong, *Chem. Eur. J.* (2008), 14, 4082.
- A14-"Longitudinal Nuclear Spin Relaxation of *Ortho*- and *Para*-Hydrogen Dissolved in Organic Solvents"  
C. Aroulanda, L. Starovoytova, D. Canet, *J. Phys. Chem. A* (2007), 111, 10615.
- A13-"About Long-Lived Nuclear Spin States Involved in *Para*-Hydrogenated Molecules"  
D. Canet, S. Bouquet-Bonnet, C. Aroulanda, F. Reineri, *J. Am. Chem. Soc.* (2007), 129, 1445.
- A12-"*Para*-Hydrogen Enrichment and Hyperpolarization"  
D. Canet, C. Aroulanda, P. Mutzenhardt, S. Aime, R. Gobetto, F. Reineri, *Concepts in Magn. Reson. A.* (2006), 28, 321.
- A11-"Molecular Ordering and Structure of Quasi-spherical Solutes by Liquid Crystal NMR and Monte Carlo Simulations: the Case of Norbornadiene"  
C. Aroulanda, C. Celebre, G. De Luca, M. Longer, *J. Phys. Chem. B.* (2006), 110, 10485.
- A10-"First Stereoselective Synthesis of Potassium Aeshynomate and its no-natural Stereoisomers"  
S. Claudel, T. K. Olszewski, P. Mutzenhardt, C. Aroulanda, P. Coutrot, C. Grison, *Tetrahedron* (2006), 62, 1787.
- A9-"Exploring the Analytical Potential of NMR in Chiral Anisotropic Media for the Study of the Natural Abundance Deuterium Distribution in Organic Molecules"  
P. Lesot\*, C. Aroulanda, I. Billault\*, *Anal. Chem.* (2004), 76, 2827.
- A8-"Structural Ambiguities in Two Bridged Ring Systems Exhibiting Enantiotopic Elements Revisited using Natural Abundance Deuterium NMR in Chiral Liquid Crystals"  
C. Aroulanda, P. Lesot\*, D. Merlet, J. Courtieu, *J. Phys. Chem. A.* (2003), 107, 10911.
- A7-"Weakly Oriented Liquid Crystal NMR Solvent as a General Tool to Determine Relative Configurations"  
C. Aroulanda, V. Boucard, F. Guibé, J. Courtieu, D. Merlet\*, *Chem. Eur. J.* (2003), 9, 4536.
- A6-"Efficient Enantiodiscrimination of Chiral Monophosphine Oxides and Boranes by Phosphorus coupled Carbon-13 NMR Spectroscopy in the Presence of Chiral Ordering Agents"  
M. Rivard, F. Guillen, J. C. Fiaud, C. Aroulanda, P. Lesot, *Tetrahedron : Asym.* (2003), 14, 1141.
- A5-"Investigation of SmI<sub>2</sub> mediated Cyclisation Process of δ-iodo- and δ-bromo-α,β-Unsaturated Esters by Deuterium 2D NMR in Oriented Solvents"  
H. Villar, F. Guibé\*, C. Aroulanda, P. Lesot\*, *Tetrahedron : Asym.* (2002), 13, 1465.
- A4-"Routine Use of Natural Abundance Deuterium in a Polypeptidic Chiral Oriented Solvent for the Determination of the Enantiomeric Composition of Chiral Building Blocks"  
A. Parenty, J. M. Campagne\*, C. Aroulanda, P. Lesot, *Org. Lett.* (2002), 4, 1663.
- A3-"NMR Experimental Evidence of the Differentiation of Enantiotopic Directions in C<sub>s</sub> and C<sub>2v</sub> Molecules Using Partially Oriented, Chiral Media"  
C. Aroulanda, D. Merlet, J. Courtieu, P. Lesot, *J. Am. Chem. Soc.* (2001), 123, 12059.
- A2-"Investigation of the Enantioselectivity of three Polypeptide Liquid Crystal Solvents Using NMR Spectroscopy"  
C. Aroulanda, M. Sarfati, J. Courtieu, P. Lesot, *Enantiomer* (2001), 6, 281.
- A1-"Enantiomeric Recognition of Chiral Invertomers through NMR in Chiral Oriented Phases: a Study of *cis*-decalin"  
M. Sarfati, C. Aroulanda, J. Courtieu, P. Lesot, *Tetrahedron : Asym.* (2001), 12, 737.

### Articles de revue publiés dans des revues internationales à comités de lecture

- R2-"Enantiotopic Discrimination in the NMR Spectrum of Prochiral Solutes in Chiral Liquid Crystals"  
P. Lesot, C. Aroulanda, H. Zimmermann, Z. Luz, *Chem. Soc. Rev.* (2015), 44, 2330.
- R1-"NMR Discrimination in Non-Rigid Prochiral Solutes Dissolved in Chiral Liquid Crystals: Symmetry Considerations"  
P. Lesot, Z. Luz, C. Aroulanda, H. Zimmermann, *Magn. Reson. Chem.* (2014), 52, 581.

#### Articles publiés dans des ouvrages spécialisés

## OS2-"Analytical Potentials of Natural Abundance Deuterium NMR Spectroscopy in Achiral Thermotropics and Polypeptide Chiral Oriented Solvents"

P. Lesot, C. Aroulanda, *NMR in Liquids Crystals, Chapter 2, pages 37-78, 2010, éditeur : R. Y. Dong, Elsevier.*

## OS1—"Chiral Liquid Crystal NMR : A Tool for Enantiomeric Analysis"

J. Courtieu, P. Lesot, A. Meddour, D. Merlet, C. Aroulanda, *Encyclopedia of NMR*, volume 9, pages 497-505, 2002, éditeurs : D. M Grant et R. K. Harris, Wiley.