

## 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, analyse métabolomique par RMN, développement de nouveaux solvants orientés eco-compatibles.

- **30 Articles de recherche** (et 1 en préparation), **4 Articles de revue** publiés dans des revues internationales à comités de lecture.
- **2 Articles publiés dans des ouvrages spécialisés.**
- **3 Conférences internationales** (2010-2020) présentées en anglais ou en italien.
- **17 Communications orales** dont 9 internationales, et 11 présentées en personne.
- **10 Séminaires** dont 7 internationaux.
- **29 Communications par affiche** dont 7 présentées en personne et 2 prix de la meilleure affiche.

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

A30-"Metabolic Composition and Authenticity Evaluation of Bergamot Essential Oil Assessed by Nuclear Magnetic Resonance Spectroscopy".

R. A. Salvino, C. Aroulanda, G. De Filpo, G. Celebre, G. De Luca, *Analytical and Bioanalytical Chemistry* (2022), 414, 2297–2313. DOI : 10.1007/s00216-021-03869-5

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

A. Robert, G. Naulet, H. Bock, N. Vanthuynne, M. Jean, M. Giorgi, Y. Carissan, C. Aroulanda, F. Durola, Y. Coquerel, *Chem: A Eur. J.* (2019), 25, 14364-14369. DOI 10.1002/chem.201902637

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. DOI: 10.1080/02678292.2018.1499975

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, *Eur. J. Pharm.Sc.*, (2017), 116, 113. DOI:10.1016/j.ejps.2017.05.029

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. DOI: 10.1021/acs.jpca.6b04254

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. DOI : 10.1039/C5NJ01753J

A24-" Conformational and Orientational Determination from Dipolar Couplings in a Weakly Ordering Organic-Based Lyotropic and a Strongly Ordering Thermotropic Liquid Crystal"

M. E. Di Pietro, G. De Luca, G. Celebre, D. Merlet, C. Aroulanda, *Mol. Cryst. Liq. Cryst.* (2015), 614, 39. DOI: 10.1080/15421406.2015.1049907

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

M. E. Di Pietro, C. Aroulanda, D. Merlet, G. Celebre, G. De Luca, *J. Phys. Chem. B* (2014), 118, 9007. DOI : 10.1021/jp505084g

A22-"GET-SERF, a new gradient encoded SERF experiment for the trivial edition of <sup>1</sup>H-<sup>19</sup>F couplings"

M. E. Di Pietro, C. Aroulanda, D. Merlet, *J. Magn. Reson.*, (2013), 234, 101. DOI: 10.1016/j.jmr.2013.06.011

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. C. Aroulanda, I. Billault, *Magn. Reson. Chem.* (2012), 50, S2. DOI

- 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. DOI: 10.1021/jp205958k
- A19- "Enantiotopic Discrimination in the Deuterium NMR Spectrum of Solutes with S<sub>4</sub> Symmetry in Chiral Liquid Crystals"  
C. Aroulanda, H. Zimmermann, Z. Luz, P. Lesot, *J. Chem. Phys.* (2011), 134, 134502. DOI: 10.1063/1.3554640
- A18-" Evolution of the Sauepe 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. DOI: 10.1080/02678291003784164; HAL Id : hal-02311001, version 1
- A17-"Analysis of enantiotopic discrimination in the NMR spectra of prochiral solutes in chiral liquid crystals by symmetry factorization of the Sauepe ordering matrix"  
P. Lesot, C. Aroulanda, Z. Luz, *J. Chem. Phys.* (2009), 131, 104501. DOI: 10.1063/1.3197853; HAL Id : hal-02310983, version 1
- 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. DOI: 10.1021/jp902233m
- 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. DOI: 10.1002/chem.200701543
- 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. DOI: 10.1021/jp073162r
- A13-"About Long-Lived Nuclear Spin States Involved in *Para*-Hydrogenated Molecules"  
D. Canet, S. Bouguet-Bonnet, C. Aroulanda, F. Reineri, *J. Am. Chem. Soc.* (2007), 129, 1445. DOI: 10.1021/ja066313x
- 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. DOI : 10.1002/cmra.20065
- 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. Longeri, *J. Phys. Chem. B.* (2006), 110, 10485. DOI: 10.1021/jp061345s
- A10-"First Stereoselective Synthesis of Potassium Aeshynomate and its no-natural Stereomers"  
S. Claudel, T. K. Olszewski, P. Mutzenhardt, C. Aroulanda, P. Coutrot, C. Grison, *Tetrahedron* (2006), 62, 1787. DOI: 10.1016/j.tet.2005.11.051; HAL Id : hal-00125069, version 1
- 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. DOI: 10.1021/ac030385e
- 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. DOI: 10.1021/jp030137m
- 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. DOI: 10.1002/chem.200204701

- 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.  
DOI: 10.1016/S0957-4166(03)00202-7; HAL Id : hal-02310631, version 1
- A5-"Investigation of Sml<sub>2</sub> mediated Cyclisation Process of  $\delta$ -iodo-  $\alpha$ ,  $\beta$ - unsaturated Esters by Deuterium 2D NMR in Oriented Solvents"  
H. Villar, F. Guibé, C. Aroulanda, P. Lesot\*, *Tetrahedron : Asym.* (2002), 13, 1465.  
DOI: 10.1016/S0957-4166(02)00259-8; HAL Id : hal-02310609, version 1
- 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.  
DOI: 10.1021/ol20038b; HAL Id : hal-00165644, version 1
- 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.  
DOI: 10.1021/ja011685l
- 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.  
DOI: 10.1016/S0957-4166(01)00103-3; HAL Id : hal-02309129, version 1

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

- R4-"Molecular Enantiodiscrimination by NMR Spectroscopy in Chiral Oriented Systems: Concept, Tools and Applications"  
C. Aroulanda, P. Lesot, *Chirality*, (2022), 34(2), 182-244. DOI:10.1002/chir.23386
- R3-"Multinuclear NMR in Polypeptide Lyotropic Liquid Crystals: Three Fertile Decades of Methodological Developments and Analytical Challenges"  
P. Lesot, C. Aroulanda, P. Berdagué, A. Meddour, D. Merlet, J. Farjon, N. Giraud, O. Lafon, *Progress in NMR*, (2020), 116, 85. DOI: 10.1016/j.pnmrs.2019.10.001
- 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.  
DOI: 10.1039/C4CS00260A
- 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.  
DOI: 10.1002/mrc.4110; HAL Id : hal-02314350, version 1

#### 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.*

