

Laboratoire Structure & Dynamique par Résonance Magnétique (LSDRM)
IRAMIS/NIMBE, UMR CEA/CNRS 3685
CEA Saclay
91191 Gif sur Yvette, France

Patents

3. France Patent 17 51895 (March 2017) Cellule de mesure par résonance magnétique nucléaire en milieu liquide, système comprenant une telle cellule et son utilisation.
2. France Patent 14 62890 (2014) A. Causier, P. Berthault, T. Berthelot, "Cellule de mesure de RMN et ensemble de mesure de RMN" ; US Patent 20,160,178,544 (2016) A Causier, P Berthault, T Berthelot, G Carret, "Device and system for measuring nuclear magnetic resonance"
1. France Patent 12 52922 (2012) C. Boutin, P. Berthault, "Procédé de détermination de la résistance cellulaire aux médicaments".

Publications

124. G. Huber, E. Léonce, O. Baydoun, N. De Rycke, T. Brotin, P. Berthault*
"Unsaturated cryptophanes: toward dual PHIP/hyperpolarised xenon sensors"
Accepted in Magnetic Resonance in Chemistry, DOI: [10.1002/mrc.4691](https://doi.org/10.1002/mrc.4691)
123. G. Milanole, B. Gao, A. Paoletti, G. Pieters, C. Dugave, E. Deutsch, S. Rivera, F. Law, J.-L. Perfettini, E. Mari, E. Léonce, C. Boutin, P. Berthault,* H. Volland, F. Fenaille, T. Brotin, B. Rousseau
"Bimodal Fluorescence/¹²⁹Xe NMR Probe for Molecular Imaging and Biological Inhibition of EGFR in Non-Small Cell Lung Cancer"
Bioorganic & Medicinal Chemistry **25** (2017) 6653-6660, DOI: [10.1016/j.bmc.2017.11.002](https://doi.org/10.1016/j.bmc.2017.11.002)
122. G. Milanole, B. Gao, E. Mari, P. Berthault, G. Pieters, B. Rousseau
"A Straightforward Access to Cyclotriveratrylene Analogues with C1-Symmetry: Toward the Synthesis of Monofunctionalizable Cryptophanes"
European Journal of Organic Chemistry (2017) 7091-7100, DOI: [10.1002/ejoc.201701353](https://doi.org/10.1002/ejoc.201701353)
121. E. Mari & P. Berthault
"¹²⁹Xe NMR-based sensors: biological applications and recent methods"
Analyst **142** (2017) 3298-3308. DOI: [10.1039/c7an01088e](https://doi.org/10.1039/c7an01088e)
120. L.-L. Chapellet, J.-P. Dognon, M. Jean, N. Vanthuyne, P. Berthault, T. Buffeteau, T. Brotin
"Experimental and Theoretical Study of the Complexation of Cesium and Thallium Cations by a Water-soluble Cryptophane", ChemistrySelect **2** (2017) 5292 – 5300. DOI: [10.1002/slct.201700979](https://doi.org/10.1002/slct.201700979)
119. P. Berthault, C. Boutin, E. Léonce, E. Jeanneau, T. Brotin
"Role of the Methoxy Groups in Cryptophanes for Complexation of Xenon. Conformational Selection Evidenced by ¹²⁹Xe -1H NMR SPINOE Experiments"
ChemPhysChem **18** (2017) 1561 –1568. DOI: [10.1002/cphc.201700266](https://doi.org/10.1002/cphc.201700266)
118. G. Carret, T. Berthelot, P. Berthault*
"Enhancing NMR of non-relaxing species using a controlled flow motion and a miniaturized circuit"
Analytical Chemistry **89** (2017) 2995–3000, DOI: [10.1021/acs.analchem.6b04488](https://doi.org/10.1021/acs.analchem.6b04488)
117. C. Chauvin, L. Liagre, C. Boutin, E. Mari, E. Léonce, G. Carret, B. Coltrinari, P. Berthault
"Spin-Exchange Optical Pumping in a Van"
Review of Scientific Instruments **87** (2016) 016105, DOI: [10.1063/1.4940928](https://doi.org/10.1063/1.4940928)

116. V. Daniele, F.-X. Legrand, P. Berthault, J.-N. Dumez, G. Huber
"Single-scan multidimensional NMR analysis of mixtures at sub-millimolar concentrations using SABRE hyperpolarization"
ChemPhysChem **16** (2015) 3413–3417, DOI: [10.1002/cphc.201500535](https://doi.org/10.1002/cphc.201500535)
115. N. Kotera, E. Dubost, G. Milanole, E. Doris, E. Gravel, N. Arhel, T. Brotin, J.-P. Dutasta, J. Cochrane, E. Mari, C. Boutin, E. Léonce, P. Berthault, B. Rousseau
"A doubly responsive probe for the detection of Cys4-tagged proteins"
Chemical Communications **51** (2015) 11482-11484 DOI: [10.1039/C5CC04721H](https://doi.org/10.1039/C5CC04721H)
114. L.-L. Chapellet, J. R. Cochrane, E. Mari, C. Boutin, P. Berthault, T. Brotin
"Synthesis of Cryptophanes With Two Different Reaction Sites: Chemical Platforms for Xenon Biosensing"
Journal of Organic Chemistry **80** (2015) 6143-6151 DOI: [10.1021/acs.joc.5b00653](https://doi.org/10.1021/acs.joc.5b00653)
113. A. Causier, G. Carret, C. Boutin, T. Berthelot, P. Berthault
"3D-printed system optimizing dissolution of hyperpolarized gaseous species for micro-sized NMR"
Lab on a Chip **15** (2015) 2049 - 2054 DOI: [10.1039/C5LC00193E](https://doi.org/10.1039/C5LC00193E)
112. P. Berthault, C. Boutin
"Biosensing and Study of Biological Cells using Hyperpolarized ^{129}Xe "
RSC Book Chapter, New Developments in NMR no. 4, Hyperpolarized Xenon-129 Magnetic Resonance: Concepts, Production, Techniques and Applications, Edited by T. Meersmann and E. Brunner (2015)
DOI: [10.1039/9781782628378-00261](https://doi.org/10.1039/9781782628378-00261)
111. A. I. Joseph, G. El-Ayle, C. Boutin, E. Léonce, P. Berthault, K. T. Holman
"Rim-Functionalized Cryptophane-111 Derivatives via Heterocapping, and their Xenon Complexes"
Chemical Communications **50** (2014) 15905-15908. DOI: [10.1039/C4CC08001G](https://doi.org/10.1039/C4CC08001G)
110. E. Dubost, J.-P. Dognon, B. Rousseau, G. Milanole, C. Dugave, Y. Boulard, E. Léonce, C. Boutin, and P. Berthault , "Understanding a Host–Guest Model System through ^{129}Xe NMR Spectroscopic Experiments and Theoretical Studies"
Angewandte Chemie **53** (2014) 9837-9840. DOI: [10.1002/anie.201405349](https://doi.org/10.1002/anie.201405349)
109. N. Tassali, N. Kotera, C. Boutin, E. Léonce, Y. Boulard, B. Rousseau, E. Dubost, F. Taran, T. Brotin, J.-P. Dutasta, P. Berthault
"Smart Detection of Toxic Metal Ions, Pb^{2+} and Cd^{2+} , using a ^{129}Xe NMR-based Sensor"
Analytical Chemistry **86** (2014) 1783–1788. DOI: [10.1021/ac403669p](https://doi.org/10.1021/ac403669p)
108. C. Boutin, E. Léonce, T. Brotin, A. Jerschow, P. Berthault
"Ultrafast Z-Spectroscopy for ^{129}Xe NMR-Based Sensors"
Journal of Physical Chemistry Letters **4** (2013) 4172-4176. DOI : [10.1021/jz402261h](https://doi.org/10.1021/jz402261h)
107. T. Brotin, S. Goncalves, P. Berthault, D. Cavagnat, T. Buffeteau
"Influence of the Cavity Size of Water-Soluble Cryptophanes on Their Binding Properties for Cesium and Thallium Cations", Journal of Physical Chemistry B **117** (2013) 12593-12601. DOI: [10.1021/jp4074009](https://doi.org/10.1021/jp4074009)
106. E. Dubost, N. Kotera, S. Garcia-Argote, Y. Boulard, E. Léonce, C. Boutin, P. Berthault, C. Dugave, B. Rousseau
"Synthesis of a functionalizable water-soluble cryptophane-111"
Organic Letters **15** (2013) 2866-2868 DOI: [10.1021/ol4012019](https://doi.org/10.1021/ol4012019)
105. V. Lewin, J. Rivollier, S. Coudert, D.-A. Buisson, D. Baumann, B. Rousseau, F.-X. Legrand, H. Kouřilová, P. Berthault, J.-P. Dognon, M.-P Heck, G. Huber
"Synthesis of cucurbit[6]uril derivatives and insights into their water solubility"
European Journal of Organic Chemistry (2013) 3857-3865 DOI: [10.1002/ejoc.201300229](https://doi.org/10.1002/ejoc.201300229)
104. L. Delacour, N. Kotera, T. Traoré, S. Garcia-Argote, C. Puente, F. Leteurtre, E. Gravel, N. Tassali, C. Boutin, E. Léonce, Y. Boulard, P. Berthault, B. Rousseau
""Clickable" Hydrosoluble PEGylated Cryptophane as a Universal Platform for ^{129}Xe MRI biosensors"
Chemistry, a European Journal **19** (2013) 6089–6093 DOI: [10.1002/chem.201204218](https://doi.org/10.1002/chem.201204218)

103. S. W. Morgan, E. Baudin, G. Huber, P. Berthault, G. Tastevin, M. Goldman, P.-J. Nacher, H. Desvaux
"Multiple echoes due to distant dipolar fields in NMR of hyperpolarized noble gas solutions"
European Physical Journal D **67**:29 (2013)
102. T. Brotin, D. Cavagnat, P. Berthault, R. Montserret, T. Buffeteau
"Water-soluble molecular capsule for the complexation of cesium and thallium cations"
Journal of Physical Chemistry B. 116 (2012) 10905-10914. DOI : 10.1021/jp305110k
101. N. Kotera, N. Tassali, E. Léonce, C. Boutin, P. Berthault, T. Brotin, J.-P. Dutasta, L. Delacour, T. Traoré, D.-A. Buisson, F. Taran, S. Coudert, B. Rousseau
"A Sensitive Zinc-Activated ¹²⁹Xe MRI Probe"
Angewandte Chemie **51** (2012) 4100-4103. DOI: 10.1002/anie.201109194
100. T. Traoré, G. Clavé, L. Delacour, N. Kotera, P.-Y. Renard, A. Romieu, P. Berthault, C. Boutin, N. Tassali, and B. Rousseau
"The first metal-free water-soluble cryptophane-111"
Chemical Communications **47** (2011) 9702-9704. DOI:10.1039/C1CC13378K
99. C. Boutin, A. Stopin, F. Lenda, T. Brotin, J.-P. Dutasta, N. Jamin, A. Sanson, Y. Boulard, F. Leteurtre, G. Huber, A. Bogaert-Buchmann, N. Tassali, H. Desvaux, M. Carrière, and P. Berthault
"Cell uptake of a biosensor detected by hyperpolarized ¹²⁹Xe NMR: the transferrin case"
Bioorganic & Medicinal Chemistry **19** (2011) 4135-4143
98. N. Kotera, L. Delacour, T. Traoré, N. Tassali, P. Berthault, D. Buisson, J. Dognon and B. Rousseau
"Design and Synthesis of New Cryptophanes with Intermediate Cavity Sizes"
Organic Letters **13** (2011) 2153–2155. DOI: 10.1021/ol2005215.
97. G. Huber, F.-X. Legrand, V. Lewin, D. Baumann, M.-P. Heck, and P. Berthault
"Interaction of Xenon with Cucurbit[5]uril in Water"
ChemPhysChem **12** (2011) 1053-1055.
96. C. Boutin, H. Desvaux, M. Carrière, F. Leteurtre, N. Jamin, Y. Boulard and P. Berthault
"Hyperpolarized ¹²⁹Xe NMR signature of living biological cells" NMR in Biomedicine **24** (2011) 1264-1269
DOI: 10.1002/nbm.1686.
95. R. M. Fairchild, A. I. Joseph, K. T. Holman, H. A. Fogarty, T. Brotin, J.-P. Dutasta, C. Boutin, G. Huber and P. Berthault
"A water soluble Xe@cryptophane-111 complex exhibits very high thermodynamic stability and a peculiar ¹²⁹Xe NMR chemical shift"
Journal of the American Chemical Society, **132** (2010) 15505-15507.
94. C. Hocquelet, C. K. Jankowski, A. L. Pelletier, J.-C. Tabet, C. Lamouroux and P. Berthault
"Synthesis and inclusion properties study of some mono 6-amino b-cyclodextrin dimmers bridged by N,N-succinyldiamide linkers"
Journal of Inclusion Phenomena and Macrocyclic Chemistry, **69** (2011) 75-84.
93. P. Berthault, H. Desvaux, T. Wendlinger, M. Gyejacquot, A. Stopin, T. Brotin, J.-P. Dutasta, Y. Boulard
"Effect of pH and Counterions on the Encapsulation Properties of Xenon in Water-Soluble Cryptophanes"
Chemistry, a European Journal, **16** (2010) 12941-12946.

92. E. Pouget, N. Fay, E. Dujardin, N. Jamin, P. Berthault, L. Perrin, A. Pandit, T. Rose, C. Valéry, D. Thomas, M. Paternostre and F. Artzner
"Elucidation of the self-assembly pathway of Lanreotide octapeptide into β -sheet nanotubes: role of two stable intermediates"
Journal of the American Chemical Society, **132** (2010) 4230–4241.
91. T. Traore, L. Delacour, S. Garcia-Argotte, P. Berthault, J.-C. Cintrat and B. Rousseau
"Scalable Synthesis of Cryptophane-1.1.1 and its Functionalization"
Organic Letters, **12** (2010) 960-962.
90. A. K.L. Yuen, O. Lafon, T. Charpentier, M. Roy, F. Brunet, P. Berthault, D. Sakellariou, B. Robert, S. Rimsky, F. Pillon, J.-C. Cintrat and B. Rousseau
"Measurement of Long-Range Interatomic Distances by Solid-State Tritium-NMR Spectroscopy"
Journal of the American Chemical Society, **132** (2010) 1734–1735.
89. H. Desvaux, D.J.Y. Marion, G. Huber and P. Berthault
"First nuclear spin-noise spectra of hyperpolarized systems"
Angewandte Chemie, **121** (2009) 4405-4407.
88. D. J.-Y. Marion, P. Berthault and H. Desvaux
"Spectral and temporal features of multiple spontaneous NMR-maser emissions"
European Physical Journal D, **51** (2009) 357-367.
87. P. Berthault, "Petits, mais sensibles ?"
Pour la Science, N° 378 – avril 2009.
86. Y. Michina, D. Carrière, C. Mariet, M. Moskura, P. Berthault, L. Belloni and T. Zemb
"Ripening of catanionic aggregates upon dialysis"
Langmuir, **25** (2009) 698-706.
85. F. Lerouge, O. Melnyk, J.-O. Durand, L. Raehm, P. Berthault, G. Huber, H. Desvaux, A. Constantinesco, P. Choquet, J. Detour and M. Smaïhi
"Towards thrombosis-targeted Zeolite nanoparticles for laser-polarized ^{129}Xe MRI"
Journal of Materials Chemistry, **19** (2009) 379-386.
84. P. Berthault, A. Bogaert-Buchmann, H. Desvaux, G. Huber and Y. Boulard
"Sensitivity and Multiplexing Capabilities of MRI Based on Polarized ^{129}Xe Biosensors"
Journal of the American Chemical Society, **130** (2008) 16456-16457.
83. P. Berthault, G. Huber, H. Desvaux
"Biosensing using laser-polarized xenon NMR/MRI"
Progress in NMR Spectroscopy, **55** (2009) 35-60.
82. G. Huber, L. Beguin, H. Desvaux, T. Brotin, H. A. Fogarty, J.-P. Dutasta and P. Berthault
"Cryptophane-Xenon Complexes in Organic Solvents Observed through NMR Spectroscopy"
Journal of Physical Chemistry A, **112** (2008) 11363–11372.
81. H. Desvaux and P. Berthault
"La RMN, une spectroscopie en constant progrès"
Clefs CEA N°56 - HIVER 2007-2008
80. D. J. Marion, G. Huber, P. Berthault and H. Desvaux
"Observation of noise-triggered chaotic emissions in an NMR-maser."
ChemPhysChem, **10** (2008) 1395-1401.

79. D. J. Marion, G. Huber, L. Dubois, P. Berthault and H. Desvaux
"Effects on ^1H and ^{129}Xe NMR spectra of large magnetization created by dissolved laser-polarized xenon."
Comptes-Rendus Chimie, **11** (2008) 553-559.
78. H. A. Fogarty, P. Berthault, T. Brotin, G. Huber, H. Desvaux and J.-P. Dutasta
"A cryptophane core optimized for xenon encapsulation."
Journal of the American Chemical Society, **129** (2007) 10332-10333.
77. V. Roy, T. Brotin, J.-P. Dutasta, M.-H. Charles, T. Delair, F. Mallet, G. Huber, H. Desvaux, Y. Boulard and P. Berthault
"A cryptophane biosensor for detection of specific nucleotide targets through xenon-NMR."
ChemPhysChem, **8** (2007) 2082-2085.
76. D. J. Marion, G. Huber, L. Dubois, P. Berthault and H. Desvaux
" ^1H and ^{129}Xe NMR absorption line shapes in the presence of highly polarized and concentrated xenon solutions in high magnetic field."
Journal of Magnetic Resonance, **187** (2007) 78-87.
75. H. Desvaux, D. J. Marion, G. Huber, L. Dubois and P. Berthault
"Direct enhancement of any solution NMR signal using the distant dipolar fields created by highly polarized and highly concentrated nuclear spin systems."
European Physical Journal, Applied-Physics, **36** (2006) 25-34.
74. G. Huber, T. Brotin, L. Dubois, H. Desvaux, J.-P. Dutasta and P. Berthault
"Water soluble cryptophanes showing unprecedented affinity for xenon: candidates as NMR-based biosensors."
Journal of the American Chemical Society, **128** (2006) 6239-6246.
73. P. Berthault, G. Huber, P.-T. Ha, L. Dubois, H. Desvaux and E. Guittet
"Study of the hydrophobic cavity of β -cryptogein through laser-polarized xenon NMR spectroscopy."
ChemBioChem, **7** (2006) 59-64.
72. S. Doussin, N. Birlirakis, D. Georgin, F. Taran and P. Berthault
"Novel Zwitterionic Reverse Micelles for Encapsulation of Proteins in Low-Viscosity Media."
Chemistry - A European Journal, **12** (2006) 4170-4175
71. H. Desvaux, L. Dubois, G. Huber, M.L. Quillin, P. Berthault and B.W. Matthews
"Dynamics of xenon binding inside the hydrophobic cavity of pseudo wild-type bacteriophage T4 lysozyme explored through xenon-based NMR."
Journal of the American Chemical Society, **127** (2005) 11676-11683.
70. P. Berthault and H. Desvaux
"Dissolution of laser-polarized xenon in benzene."
Magnetic Resonance Imaging, **23**, (2005) 315-316.
69. B. D. Allen, J.-C. Cintrat, N. Faucher, P. Berthault, B. Rousseau and D. J. O'Leary
"An isosparteine derivative for stereochemical assignment of stereogenic (chiral) methyl groups using tritium NMR: theory and experiment."
Journal of the American Chemical Society, **127** (2005) 412-420.
68. L. Dubois, P. Da Silva, C. Landon, J.G. Huber, M. Ponchet, F. Vovelle, P. Berthault and H. Desvaux
"Probing the hydrophobic cavity of Lipid Transfer Protein from *Nicotiana tabacum* through Xenon-based NMR."
Journal of the American Chemical Society, **126**, (2004) 15738-15746.
67. J.G. Huber, L. Dubois, H. Desvaux, J.P. Dutasta, T. Brotin and P. Berthault
"NMR study of optically active monosubstituted cryptophanes and their interaction with xenon."
Journal of Physical Chemistry A, **108**, (2004) 9608-9615.

66. L. Dubois, P. Berthault, J.G. Huber and H. Desvaux
"Mapping hydrophobic molecular regions using dissolved laser-polarized xenon NMR."
Comptes Rendus Physique, 5, (2004) 305-313.
65. L. Dubois, S. Parrès, J.G. Huber, P. Berthault and H. Desvaux
"Dynamics of xenon inside hydrophobic cavities as probed by NMR relaxation of dissolved laser-polarized xenon."
Journal of Physical Chemistry B, 108, (2004) 767-773; ibid 15952.
64. F. Alvarez Salgado, P. Berthault, Y. Boulard and H. Desvaux
"Comparison of the solution structures of a DNA dodecamer using nOe and residual dipolar coupling data."
Comptes Rendus Chimie, 7, (2004) 259-263.
63. A. Davidson, P. Berthault and H. Desvaux
"Silicas of unimodal and bimodal porosities probed by ¹²⁹Xe NMR spectroscopy."
Journal of Physical Chemistry B, 107, (2003) 14388-14393.
62. H. Fensterbank, P. Berthault and C. Larpent
"A tunable one-step N,N'-disubstitution of 1,4,11-tetraazacyclotetradecane with acrylamide."
European Journal of Organic Chemistry (2003) 3985-3990.
61. H. Desvaux, J.G. Huber, T. Brotin, J.P. Dutasta and P. Berthault
"Magnetization transfer from laser-polarized xenon to protons with spin-diffusion quenching."
ChemPhysChem, 4, (2003) 383-387.
60. P. Berthault, D. Jeannerat, F. Camerel, F. Alvarez-Salgado, Y. Boulard, J.-C. P. Gabriel, H. Desvaux
"Dilute liquid crystals used to enhance residual dipolar couplings may alter conformational equilibrium in oligosaccharides."
Carbohydrate Research, 338, (2003) 1771-1785.
59. P. Berthault and H. Desvaux
"NMR study of the dissolution of laser-polarized xenon."
European Physical Journal D, 22, (2003) 65-73.
58. N. Faucher, J.-C. Cintrat, P. Berthault and B. Rousseau
"The shortest route to chiral ditosyl methylamine."
Angewandte Chemie International Edition, 41 (2002) 497-498.
57. M. R. de Jong, P. Berthault, A. van Hoek, A. J. W. G. Visser, J. Huskens and D. N. Reinhoudt
"Complexation and sensing behavior of dansyl-appended cyclodextrins and cyclodextrin dimers with bile salts."
Supramolecular Chemistry, 14 (2002) 143-151.
56. C. Landon, P. Berthault, F. Vovelle and H. Desvaux
"Magnetization transfer from laser-polarized xenon to protons located in the hydrophobic cavity of the wheat non-specific lipid transfer protein"
Protein Science, 10 (2001) 762-770.
55. P. Berthault, C. Landon, F. Vovelle and H. Desvaux
"Première détection d'un transfert d'aimantation entre du xénon polarisé par laser et des protons d'une protéine"
Comptes Rendus de l'Académie des Sciences, Série IV, 2 (2001) 327-332.
54. H. Desvaux, J.C. P. Gabriel, P. Berthault and F. Camerel
"First use of a mineral liquid crystal for NMR measurement of residual dipolar couplings of a non-labeled biomolecule."
Angewandte Chemie International Edition, 40 (2001) 373-376.
53. H. Desvaux, T. Gautier, G. Le Goff, M. Pétero and P. Berthault
"Direct evidence of a magnetization transfer between laser-polarized xenon and protons of a cage-molecule"

in water."

European Physical Journal D, **12** (2000) 289-296.

52. P. C. Leverd, P. Berthault, M. Lance and M. Nierlich

"Successive inclusion of water, $[H_3NCH_2CH_2NH_3]^{2+}$ and $[H_3NCH_2CH_2NH_2]^+$ in the aromatic cavity of (p-Sulfonato)calix[4]arene."

European Journal of Organic Chemistry (2000) 133-139.

51. Y.-M. Zhang, B. Dausse, P. Sinaÿ, M. Afsahi, P. Berthault and H. Desvaux

"Synthesis and NMR study of a heptasaccharide, epitope of the stage specific antigen-1 (SSEA-1)."

Carbohydrate Research, **324** (2000) 231-234.

50. P. Berthault and N. Birlirakis

"Folding of a beta-cyclodextrin monosubstituted at its secondary face, revealed by NMR study of local structural variations."

Tetrahedron: Asymmetry, **11** (2000) 2463-2469.

49. M. Hamang, V. Forge, L. Liagre, A. Sanson and P. Berthault

"Fast mixing device inside a standard NMR magnet: a tool for observing early steps in protein folding."

Review of Scientific Instruments, **71** (2000) 2180-2183.

48. M. Guenneugues, P. Berthault, H. Desvaux and M. Goldman

"Direct determination of the heteronuclear T_1/T_2 ratio by off-resonance steady-state magnetization measurement: Investigation of the possible application to fast exchange characterization of ^{15}N -labeled proteins."

Journal of Biomolecular NMR, **15** (1999) 295-307.

47. P. Berthault, H. Desvaux, G. Le Goff and M. Pétro

"A simple way to properly invert intense nuclear magnetization: application to laser-polarized xenon."

Chemical Physics Letters, **314** (1999) 52-56.

46. B. Henry, H. Desvaux, M. Prischepa, P. Berthault, Y.-M. Zhang, J.-M. Mallet, J. Esnault and P. Sinaÿ

"NMR study of a Lewis^X pentasaccharide derivative: solution structure and interaction with cations."

Carbohydrate Research, **315** (1999) 48-62.

45. H. Desvaux and P. Berthault

"Study of dynamic processes in liquids using off-resonance rf irradiation."

Progress in NMR Spectroscopy, **35** (1999) 295-340.

44. M. Guenneugues, P. Berthault and H. Desvaux

"A method for determining B_1 field inhomogeneity. Are the biases assumed in heteronuclear relaxation experiments usually underestimated?"

Journal of Magnetic Resonance, **136** (1999) 118-126.

43. B. Hamelin, L. Jullien, C. Derouet, C. Hervé du Penhoat and P. Berthault

"Self-assembly of a molecular capsule driven by electrostatic interaction in aqueous solution."

Journal of the American Chemical Society, **120** (1998) 8438-8447.

42. F. Venema, H. F. M. Nelissen, P. Berthault, N. Birlirakis, A. E. Rowan, M. C. Feiters and R. J. M. Nolte

"Synthesis, conformation, and binding properties of cyclodextrin homo- and heterodimers connected through their secondary sides."

Chemistry - A European Journal, **4** (1998) 2237-2250.

41. P. C. Leverd, P. Berthault, M. Lance and M. Nierlich

"Caesium control of the coordination chemistry of tBu-calix[6]arene towards uranyl."

European Journal of Inorganic Chemistry (1998) 1859-1862.

40. P. Brocca, P. Berthault and S. Sonnino

"Conformation of the oligosaccharide chain of GM1 ganglioside in a carbohydrate-enriched surface."

Biophysical Journal, **74** (1998) 309-318.

39. N. Birlirakis, B. Henry, P. Berthault, F. Venema and R. J. M. Nolte
"High resolution ^1H -NMR study of self-complexation phenomena in cyclodextrin dimers."
Tetrahedron, **54** (1998) 3513-3522.
38. S. Zinn-Justin, P. Berthault, M. Guenneuges and H. Desvaux
"Off-resonance rf fields in heteronuclear NMR Application to the study of slow motions"
J. Biomol. NMR, **10** (1997) 363-372.
37. G. Rubinstenn, P. Sinaÿ and P. Berthault
"Evidence of conformational heterogeneity for carbohydrate mimetics. NMR study of methyl- β -C-lactoside in aqueous solution"
J. Phys. Chem. A, **101** (1997) 2536-2540.
36. S. Zinn-Justin, M. Guenneuges, P. Drevet, P. Berthault, B. Gilquin and A. Menez
"Dynamics of the uniformly ^{15}N labelled toxin α "
Toxicon, **34** (1996) 1097.
35. H. Desvaux and P. Berthault
"Apports des champs rf hors r sonance aux  tudes structurales et dynamiques en solution par RMN"
J. Chim. Phys. **93** (1996) 403-426 (Review paper).
34. N. Birlirakis, P. Berthault, H. Desvaux, M. Goldman, T.E. Malliavin and M. Piotto
"Off-resonance ROESY: a new ^1H -NMR method for the simultaneous study of molecular structure and dynamics"
Bruker Reports, **142** (1996) 34-38.
33. P. Berthault, N. Birlirakis, G. Rubinstenn, P. Sinaÿ and H. Desvaux
"Solution structure of a Lewis x analogue by off-resonance ^1H NMR spectroscopy without use of internal distance reference"
J. Biomol. NMR, **8** (1996) 23-35.
32. H. Desvaux, C. Wary, N. Birlirakis and P. Berthault
"Study of slow molecular motions in solution using off-resonance irradiation in homonuclear NMR Part I: Long dipolar correlation times"
Mol. Phys. **86** (1995) 1048-1058.
31. H. Desvaux, N. Birlirakis, C. Wary and P. Berthault
"Study of slow molecular motions in solution using off-resonance irradiation in homonuclear NMR Part II: Fast chemical exchange processes"
Mol. Phys. **86** (1995) 1059-1073.
30. H. Desvaux, P. Berthault, N. Birlirakis, M. Goldman and M. Piotto
"Improved versions of off-resonance ROESY"
Journal of Magnetic Resonance, Series A, **113** (1995) 47-52.
29. H. Desvaux, P. Berthault and N. Birlirakis
"Dipolar spectral densities from off-resonance ^1H -NMR relaxation measurements"
Chem. Phys. Lett. **233** (1995) 545-549.
28. A. Bondon, P. Berthault, I. Segalas, B. Perly and H. Wroblewski
"Solution structure determination by NMR spectroscopy of a synthetic peptide corresponding to a putative amphipathic α helix of spiralin: resonance assignment, distance geometry and simulated annealing."
Biochimica et Biophysica acta, **1235** (1995) 169-177.
27. P. Berthault, D. Duchesne, H. Desvaux and B. Gilquin
"A self-included cyclomaltoheptaose derivative studied by NMR and molecular modeling"
Carbohydrate Research, **276** (1995) 267-287.
26. H. Desvaux, P. Berthault, N. Birlirakis and M. Goldman
"Off-resonance ROESY for the study of dynamics processes"
Journal of Magnetic Resonance, Series A, **108** (1994) 219-229.
25. H. Desvaux, P. Berthault, N. Birlirakis and M. Goldman

- "A new NMR method for studying the dynamics of the molecule: Off-resonance ROESY"
J. Chim. Phys. **91** (1994) 646-652.
24. H. Desvaux, P. Berthault, N. Birlirakis and M. Goldman
"ROESY hors résonance: Une nouvelle méthode d'étude de la relaxation par R M N"
C. R. Acad. Sci. **317 Série II** (1993) 19-25.
23. P. Berthault and B. Perly
Investigation of inclusion phenomena using ultra-high resolution NMR"
Supramol. Chem. **2** (1993) 225-231.
22. P. Berthault, H. Desvaux and B. Perly
"Simple solutions to resolve extreme NMR spectral overcrowding using shaped pulses"
Magn. Reson. Chem. **31** (1993) 259-265.
21. P. Berthault, F. Djedaïni-Pilard and B. Perly
"2D NMR principles, processing and analysis, in *Textbook of Magnetic Resonance Spectroscopy in Biology and Medicine* (Ed.: W.M.M.J.B. J.D. de Certaines, F. Podo), Pergamon Press, Oxford, **1992**, pp. 59-76.
20. A. Aumelas, L. Chiche, E. Brun, E. Mahé, D.L. Nguyen, P. Sizun, P. Berthault and B. Perly
"Vasoactive intestinal contractor peptide structure in solution as determined by proton NMR"
J. Chim. Phys. **89** (1992) 175-181.
19. B. Perly, F. Djedaïni and P. Berthault
"Novel one and two-dimensional Nuclear Magnetic Resonance techniques for ultra-high resolution analysis of cyclodextrin derivatives, in *New trends in cyclodextrins and derivatives* (Ed.: D. Duchêne), Editions de Santé, Paris, **1991**, pp. 179-216.
18. P. Berthault, F. Djedaïni and B. Perly
"High accuracy measurement of proton chemical shifts and coupling constants in substituted cyclic oligosaccharides using phase-sensitive two-dimensional soft experiments."
J. Magn. Reson. **91** (1991) 102-112.
17. P. Berthault and H. Desvaux
"RMN par détection inverse"
Rapport CEA-R-5547, **R-5547** (1991) 1-72.
16. A. Aumelas, L. Chiche, E. Mahe, D. Le-Nguyen, P. Sizun, F. Né, P. Berthault and B. Perly
"H-1-NMR structures of endothelin family peptides", in *Peptides 1990, Twenty-first European Peptide Symposium* (Eds.: E. Giralt, D. Andreu), ESCOM Science Publishers B. V. **1991**, pp. 553-554.
15. A. Aumelas, L. Chiche, E. Mahé, D. Le-Nguyen, P. Sizun, P. Berthault and B. Perly
"1H NMR study of the solution structure Sarafotoxin-S6b"
Neurochem. Int. **18** (1991) 471-475.
14. A. Aumelas, L. Chiche, E. Mahe, D. Le-Nguyen, P. Sizun, P. Berthault and B. Perly
"Determination of the structure of [Nle7]-Endothelin by 1H NMR"
International Journal of Peptide and Protein Research, **37** (1991) 315-324
13. P. Berthault, B. Perly and M. Petitou
"Selective excitation techniques in 13C NMR. Part II : new sequences for fast heteronuclear correlation "
Magn. Reson. Chem. **28** (1990) 696-701
12. V. Bossennec, P. Firmin, B. Perly and P. Berthault
"Use of selective excitation techniques for the rapid analysis of 13C NMR data for enriched carbohydrates"
Magn. Reson. Chem. **28** (1990) 149-155.
11. P. Berthault, V. Bossennec and B. Perly
"Strategy for structural and conformational analysis of biomolecules by 1H NMR"
Analisis, **18** (1990) i84-i94.
10. B. Perly, P. Berthault and P. Sizun, in *Colloque INSERM, Vol. 174* (Eds.: A. Aubry, M. Marraud, B. Vitoux), John Libbey Eurotext Ltd. Nancy, **1989**, pp. 411-414.

9. P. Berthault and B. Perly
"A novel solution to relayed double quantum correlation : The DREAM sequence"
J. Magn. Reson. **81** (1989) 631-634.
8. M. Petitou, J.C. Lormeau, B. Perly, P. Berthault, V. Bossennec, P. Sié and J. Choay
"Is there a unique sequence in heparin for interaction with heparin cofactor II ?"
J. Biol. Chem. **263** (1988) 8685-8690.
7. B. Perly, P. Berthault, L. Vidaud and J.F. Labarre
"Two-dimensional ³¹P NMR approaches in the cyclophosphazenic series"
J. Mol. Struct. **172** (1988) 345-353.
6. B. Perly, P. Berthault, L.J.P. Bonnet and J.F. Labarre
"The case of unsymmetrical cyclophosphazenic BINO structures"
J. Mol. Struct. **176** (1988) 285-294.
5. P. Berthault and B. Perly
"Applications de la Résonance Magnétique Nucléaire à une et deux dimensions à l'étude structurale et conformationnelle des oligosaccharides. Conception et mise au point de nouvelles techniques"
Rapport CEA-R-5452, (1988).
4. B. Perly, V. Bossennec, P. Berthault and M. Petitou
"New tools for proton NMR analysis : one-dimensional multiple relay magnetization transfers. Application to oligosaccharides"
Tetrahedron Letters, **28** (1987) 3331-3334.
3. B. Perly, P. Berthault, L. Vidaud, G. Guerch, J.F. Labarre and F. Sournies
"Conformational analysis in cyclophosphazenic series"
J. Mol. Struct. **162** (1987) 87-95.
2. B. Perly, P. Berthault, L. Vidaud, J.P. Bonnet and J.F. Labarre
"The challenge of the spiro phosphazenic series"
J. Mol. Struct. **161** (1987) 175-180.
1. P. Berthault, B. Perly, L. Vidaud and J.F. Labarre
"Application of selective excitation pulse transfer for identification of correlations (ASEPTIC) to cyclophosphazenes"
J. Mol. Struct. **162** (1987) 97-100.