

RESUME
Patrick Groves

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Ciencia2007 Fellow/Principal Investigator
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TRAINING / EMPLOYMENT:

School of Biomedical Sciences, University of Ulster, Coleraine, Northern Ireland
Independent RCUK Fellow (01/11/2006-17/12/2007)

Centro de Investigaciones Biologicas, CSIC, Madrid, Spain
EU Marie Curie Training Fellow (01/11/2002-30/10/2004) to Prof. Jesus Jimenez-Barbero
Independent Ramon y Cajal Fellow (16/11/2004-31/10/2006)

Nencki Institute of Experimental Biology, Warsaw, Poland
Assistant and Adjunct to Prof. J. Kuznicki (01/10/1996-31/10/2002)
Sniadeccy Foundation Fellow with Prof. J. Kuznicki (01/10/1996-30/09/1997)

Department Physical Chemistry 2, University of Lund, Lund, Sweden
PostDoc. researcher to Prof. S. Forsén (01/11/1994-30/09/1996)

EDUCATION:

Trinity College, University of Cambridge, UK - Department of Chemistry
specialty - chemistry, graduated 1994 with a Ph.D. (Supervisor Prof. D.H. Williams)
Title: "Recognition of cell-wall analogues by glycopeptide antibiotics".

University of Newcastle-upon-Tyne, UK - Department of Chemistry
specialty - chemistry, graduated 1990 with a B.Sc. (hon.), 1st class

MEMBERSHIP:

Member of the Polish Biochemical Society, 1997-

Publications

Up-to-date citation metrics can be obtained from <http://www.researcherid.com/ViewProfileSearch.action> (my Researcher ID is B-1942-2008)

V. Gaspariunaite, U. Kazlauskaitė, S. Kiseviciute, **P. Groves*** "Polyethylene glycols as universal references for diffusion ordered NMR spectroscopy" in preparation.

P. Groves*, A. Strzelecka-Kiliszek, A. Sekrecka-Belniak, A. Canales, J. Jiménez-Barbero, J. Bendorowicz-Pikula, S. Pikula, F.J. Cañada "Selecting fluorescent nucleotide analogs by transferred NMR methods" in preparation

M. Palczewska, **P. Groves**, B. Mellström, J.R. Naranjo "Identification of DREAM self-oligomerization domains" in preparation

42. M. Kowacz, **P. Groves**, J. Esperança, L.P. Rebelo "On the use of ionic liquids to tune crystallization" *Crystal Growth & Design*, 2011, 11, 684-691.
41. J. Bendorowicz-Pikula, R. Buchet, F.J. Cañada, M. Clémancey, **P. Groves***, J. Jiménez-Barbero, J.-M. Lancelin, O. Marcillat, S. Pikula, A. Sekrecka-Belniak, A. Strzelecka-Kiliszek "Characterization of caged compounds binding to proteins by NMR spectroscopy." *Biochem. Biophys. Res. Commun.*, 2010, 400, 447-451.
40. **P. Groves***, M. Webba da Silva* "Rapid Stoichiometric Analysis of G-Quadruplexes in Solution." *Chem. Eur. J.* 2010, 16, 6451-3.
39. J.P. Ribeiro, M. Palczewska, S. André, F.J. Cañada, H.-J. Gabius, J. Jiménez-Barbero, B. Mellström, J.R. Naranjo, D.J. Scheffers, **P. Groves*** "Diffusion nuclear magnetic resonance spectroscopy detects substoichiometric concentrations of small molecules in protein samples." *Anal. Biochem.* 2010, 396, 117-123.
38. K. Fehér, **P. Groves**, G. Batta, J. Jiménez Barbero, C. Muhle-Goll, K.E. Kövér "Application of isotope edited and filtered STD NMR experiments for ligands with overlapping signals", *J. Am. Chem. Soc.*, 2008, 130, 17148-53.
37. K.E. Kövér, **P. Groves**, J. Jiménez-Barbero and G. Batta "Molecular recognition and screening using STD NMR: ¹⁵N-group selective STD NMR experiment to study intermolecular interactions in heavily overlapped spectra", *J. Am. Chem. Soc.*, 2007, 129, 11579-82.
36. **P. Groves***, K.E. Kövér, S. André, J. Bendorowicz-Pikula, G. Batta, M. Bruix, R. Buchet, A. Canales, F.J. Cañada, H.-J. Gabius, D.V. Laurents, J.R. Naranjo, M. Palczewska, S. Pikula, E. Rial, A. Strzelecka-Kiliszek, and J. Jiménez-Barbero "Effect of temperature in Saturation Transfer Difference NMR experiments", *Magn. Reson. Chem.*, 2007, 45, 745-8.
35. **P. Groves**, A. Canales, M.I. Chavez, M. Palczewska, M.D. Diaz, F.J. Cañada, and J. Jiménez-Barbero "NMR investigations of lectin-carbohydrate interactions", *Lectin Analytical Technologies*, 2007, Elsevier, Amsterdam, 51-73. (book chapter)
34. **P. Groves***, M. Palczewska, and J. Kuźnicki "Calretinin, an EF-hand calcium-binding protein, binds zinc and copper", *Calcium Binding Proteins*, 2006, 1, 156-159.
33. F. Chevalier, J. Lopez-Prados, **P. Groves**, S. Perez, M. Martín-Lomas and P.M. Nieto "Structure and dynamics of the conserved protein GPI anchor core inserted into detergent micelles", *Glycobiol.*, 2006, 16, 969-980.
32. **P. Groves***, A. Strzelecka-Kiliszek, A. Canales, S. Pikula, J. Bendorowicz-Pikula, and Jesus Jimenez-Barbero "NMR Spectroscopy as a tool in annexin research", *Calcium Binding Proteins*, 2006, 1, 20-5. (review)
31. M. Politi, J. Alvaro-Blanco, **P. Groves**, A. Prieto, J.A. Leal, F.J. Cañada and J. Jiménez-Barbero "Screening garlic water extract for binding activity with Cholera Toxin B pentamer by NMR. An old remedy giving a new surprise", *Eur. J. Org. Chem.*, 2006, 2067-73.
30. J. Jiménez-Barbero, F.J. Cañada, J.-L. Asensio, N. Aboitiz, P. Vidal, A. Canales, **P. Groves**, H.-J. Gabius, and H.-C. Siebert "Hevein domains: an attractive model to study carbohydrate-protein interactions at atomic resolution", *Adv. Carbohydr. Chem. Biochem.*, 2006, 60, 303-354. (review)
29. M. Politi, **P. Groves**, M.I. Chávez, F.J. Cañada, and J. Jiménez-Barbero "Useful applications of DOSY experiments for the study of mushroom polysaccharides", *Carbohydrate Res.*, 2006, 341, 84-9.
28. A. Bastida, A. Hidalgo, J.L. Chiara, M. Torrado, F. Corzana, J.M. Cañadillas, **P. Groves**, E. Garcia-Junceda, J. Jimenez-Barbero and J.L. Asensio "Exploring the use of conformationally locked amino-glycosides as a new strategy to overcome bacterial resistance", *J. Am. Chem. Soc.*, 2006, 126, 100-16.
27. M.I. Chavez, C. Andreu, P. Vidal, N. Aboitiz, F. Freire, **P. Groves**, J.-L. Asensio, G. Asensio, M. Muraki, F.J. Cañada, J. Jiménez-Barbero "On the Importance of Carbohydrate-Aromatic Interactions for the Molecular Recognition of Oligosaccharides by Proteins. NMR Studies of the Structure and Binding Affinity of AcAMP2-Like Peptides with non Natural Naphthyl and Fluoroaromatic Residues", *Chem. Eur. J.*, 2005, 11, 7060-74.
26. J.C. Cobas, **P. Groves**, M. Martín-Pastor, A. De Capua "New Applications, Processing methods and Pulse Sequences using Diffusion NMR", *Curr. Anal. Chem.*, 2005, 1, 289-305. (review)
25. M. Palczewska, G. Batta, **P. Groves**, S. Linse, and J. Kuźnicki "Localization of the Ca(2+)- and H(+)-dependent hydrophobic

properties of calretinin", *Protein Sci.*, 2005, 14, 1879-87.

24. **P. Groves**, S. Offermann, M.O. Rasmussen, F.J. Cañada, J.J. Bono, H. Driguez, A. Imberty and J. Jiménez-Barbero "The relative orientation of the lipid and carbohydrate moieties of lipochitooligosaccharides related to nodulation factors depends on lipid chain saturation", *Org. Biomol. Chem.*, 2005, 3, 1381 – 86.
23. N. Aboitiz, M. Vila-Perelló, **P. Groves**, J.L. Asensio, D. Andreu, F.J. Cañada and J. Jiménez-Barbero "NMR and Modeling Studies of Protein-Carbohydrate Interactions: Synthesis, Threedimensional Structure and Recognition Properties of a Minimum Hevein Domain with Binding Affinity for Chitooligosaccharides", *ChemBioChem*, 2004, 5, 1245-55.
22. **P. Groves**, M. Palczewska, M.D. Molero, G. Batta, F.J. Cañada and J. Jiménez-Barbero "Protein Molecular weight standards can compensate systematic errors in Diffusion Ordered Spectroscopy", *Anal. Biochem.*, 2004, 331, 395-7.
21. **P. Groves**, M. O. Rasmussen, M. D. Molero, E. Samain, F. J. Canada, H. Driguez and J. Jimenez-Barbero "Diffusion ordered spectroscopy as a complement to size exclusion chromatography in oligosaccharide analysis", *Glycobiology*, 2004, 14, 451-6.
20. I.A. Ahmad, S.L. Birkby, C.A. Bullen, **P.D. Groves**, T. Lankau, W.H. Lee, H. Maskill, P.C. Miatt, I.D. Menneer and K. Shaw "Hydrolysis of 2-(p-nitrophenoxy)tetrahydropyran: solvent and a-deuterium secondary kinetic isotope effects and relationships with the solvolysis of simple secondary alkyl arenesulfonates and the enzyme-catalyzed hydrolysis of glycosides" *J. Phys. Org. Chem.* 2004, 17: 560–566.
19. M. Palczewska, G. Batta and **P. Groves** "Concanavalin A-agarose removes mannan impurities from an extracellularly expressed *Pichia pastoris* recombinant protein", *Cell Mol. Biol. Lett.* 2003, 8, 783-92.
18. M. Palczewska, **P. Groves**, G. Batta, B. Heise and J. Kuznicki "Calretinin and calbindin D28k have different domain organizations", *Protein Sci.*, 2003, 12, 180-4.
17. M. Palczewska, **P. Groves**, A. Ambrus, A. Kaleta, K. E. Kövér, G. Batta and J. Kuznicki "Structural and biochemical characterization of neuronal calretinin domain I-II (residues 1-100); comparison to homologous calbindin D28k domain I-II (residues 1-93)", *Eur. J. Biochem.*, 2001, 268, 6229-37.
16. **P. Groves** and M. Palczewska "Cation binding properties of calretinin, an EF-hand calcium-binding protein" *Acta Biochim. Polon.*, 2001, 48, 113-9.
15. M. Palczewska, **P. Groves** and J. Kuznicki "Use of *Pichia pastoris* for the expression, purification, and characterization of rat calretinin "EF-hand" domains", *Protein Expr. Purif.*, 1999, 465-76.
14. **P. Groves**, B.E. Finn, J. Kuznicki and S. Forsén "A model for target protein binding to calcium-activated S100 dimers", *FEBS Lett.*, 1998, 421, 175-9.
13. **P. Groves**, S. Linse, E. Thulin and S. Forsén "A calbindin D9k mutant containing a novel structural extension: ¹H nuclear magnetic resonance studies", *Protein Sci.*, 1997, 6, 323-30.

PhD work:

12. M.S. Searle, G.J. Sharman, **P. Groves**, B. Benhamu, D.A. Beauregard, M.S. Westwell, R.J. Dancer, A.J. Maguire, A.C. Try and D.H. Williams, "Enthalpic (electrostatic) contribution to the chelate effect: a correlation between ligand binding constant and a specific hydrogen bond strength in complexes of glycopeptide antibiotics with cell wall analogues", *J. Chem. Soc., Perkin Trans. I*, 1996, 2781-6.
11. Y.R. Cho, A.J. Maguire, A.C. Try, M.S. Westwell, **P. Groves** and D.H. Williams, "Cooperativity and anti-cooperativity between ligand binding and the dimerization of ristocetin A: Asymmetry of a homodimer complex and implications for signal transduction", *Chem. Biol.*, 1996, 3, 207-15.
10. M.S. Searle, M.S. Westwell, **P. Groves**, G.J. Sharman and D.H. Williams "Enhancement of electrostatic binding through cooperative interactions: Enthalpy entropy compensation and peptide - Peptide recognition", *NATO Adv. Sci. Inst. Se.*, 1995, 473, 151-9. (review)
9. G.J. Sharman, M.S. Searle, B. Benhamu, **P. Groves** and D.H. Williams, "Burial of Hydrocarbon Causes Cooperative Enhancement of Electrostatic Binding", *Angew. Chem. Int. Ed. Engl.*, 1995, 34, 1483-5.
8. **P. Groves**, M.S. Searle, J.P. Waltho and D.H. Williams, "Asymmetry in the structure of Glycopeptide Antibiotic Dimers: NMR Studies of the Ristocetin A Complex with a Cell-Wall Analogue", *J. Am. Chem. Soc.*, 1995, 117, 7958-64.
7. D.H. Williams, M.S. Searle, M.S. Westwell, J.P. Mackay, **P. Groves** and D.A. Beauregard, "The Role of Weak Interactions, Dimerization and Cooperativity in Antibiotic Action and Biological Signalling", *Chemtracts*, 1994, 7, 133-59. (review)
6. M.S. Searle, **P. Groves** and D.H. Williams, "Rationally designed ligands as models for bacterial cell-wall recognition by vancomycin-group antibiotics", *Proc. Indian Acad. Sci.*, 1994, 106, 937-54.
5. D.H. Williams, M.S. Searle, **P. Groves**, J.P. Mackay, M.S. Westwell, D.A. Beauregard and M.F. Cristofaro, "Functional Roles of Natural Products: The Involvement of Extended Arrays of Weak Interactions in Cooperative Binding Phenomena", *Pure and Applied Chem.*, 1994, 66, 1975-82. (review)
4. **P. Groves**, M.S. Searle, J.P. Mackay and D.H. Williams, "The Structure of an Asymmetric Dimer Relevant to the Mode of Action of the Glycopeptide Antibiotics", *Structure*, 1994, 2, 747-54.
3. **P. Groves**, M.S. Searle, M.S. Westwell and D.H. Williams, "Expression of Electrostatic Binding Cooperativity in the Recognition of Cell-Wall Peptide Analogues by Vancomycin Group Antibiotics", *J. Chem. Soc., Chem Commun.*, 1994, 1519-20.
2. **P. Groves**, M.S. Searle, I. Chicarelli-Robinson and D.H. Williams, "Recognition of the Cell-Wall Binding Site of Vancomycin-Group Antibiotics by Unnatural Structural Motifs: ¹H NMR Studies of the Effects of Ligand Binding on Antibiotic Dimerisation", *J. Chem. Soc. Perkin Trans. I*, 1994, 659-65.

1. S.E. Holroyd, **P. Groves**, M.S. Searle, U. Gerhard and D.H. Williams, "Rational design and binding of modified cell-wall peptides to vancomycin-group antibiotics: Factorising free energy contributions to binding", ***Tetrahedron***, 1993, 49, 9171-82.

PARTICIPATION IN RESEARCH PROJECTS

PROJECT TITLE: Structure- function analysis of calretinin - a neuronal calcium binding protein
FINANCIAL ENTITY: *International Center for Genetic Engineering and Biotechnology*
LENGTH **FROM:** 01/01/1998 **TO:** 31/12/2000
RESPONSIBLE RESEARCHER: Jacek Kuznicki (Warsaw, Poland) y Gyula Batta (Debrecen, Hungary)

PROJECT TITLE: Solving the Baseline Problems on the Lodz 500 MHz NMR Spectrometer
FINANCIAL ENTITY: *small Network grant from the Molecular Cell Biology Network of UNESCO*
LENGTH **FROM:** 01/01/1998 **TO:** 31/12/1998
RESPONSIBLE RESEARCHER: **Patrick Groves** (Warsaw, Poland)

PROJECT TITLE: Functional and structural aspects of various metal cations binding to calretinin
FINANCIAL ENTITY: *Polish State Committee for Scientific Research (KBN)*
LENGTH **FROM:** 01/07/1998 **TO:** 30/09/2001
RESPONSIBLE RESEARCHER: **Patrick Groves** (Warsaw, Poland)

PROJECT TITLE: *Towards a structure of calretininI-II*
FINANCIAL ENTITY: *European Union V Framework (Mobility grant for access to equipment)*
LENGTH **FROM:** 01/01/2001 **TO:** 31/12/2001
RESPONSIBLE RESEARCHER: Jacek Kuznicki (Warsaw, Poland), Patrick Groves (Warsaw, Poland) and Gyula Batta (Debrecen, Hungary)

PROJECT TITLE: The Oligosaccharide Signalling in Plants Network (SACC-SIG-NET)
FINANCIAL ENTITY: *European Union V Framework (Training and Mobility)*
LENGTH **FROM:** 01/07/2002 **TO:** 30/06/2006
RESPONSIBLE RESEARCHER: Julie Cullimore (Toulouse, France – Coordinator) plus group leaders in six other research centres, including the CIB, CSIC in Madrid, Spain (Jesús Jiménez-Barbero)

PROJECT TITLE: Una aproximación pluridisciplinar a la química y reconocimiento molecular de hidratos de carbono. Estudios sobre la síntesis, estructura y conformación de carbohidratos y análogos y de sus interacciones a escala molecular con otras biomoléculas.
FINANCIAL ENTITY: *MCyT-DGI BQU2003-03550-C03-01*
LENGTH **FROM:** 11/2003 **TO:** 10/2006
RESPONSIBLE RESEARCHER: Jesús Jiménez-Barbero (Madrid, Spain)

PROJECT TITLE: Interaction of nucleotides with human annexin A6 studied by NMR.
FINANCIAL ENTITY: *CSIC & Polish Academy of Sciences bilateral agreement*
LENGTH **FROM:** 01/2005 **TO:** 12/2006
RESPONSIBLE RESEARCHER: Jesús Jiménez-Barbero (Madrid, Spain) with Slawomir Pikula (Nencki Institute, Warsaw)

PROJECT TITLE: Development of new NMR methods to study intermolecular interactions.
FINANCIAL ENTITY: *bilateral agreement* **FROM:** 11/2003 **TO:** 10/2006
RESPONSIBLE RESEARCHER: Jesús Jiménez-Barbero (Madrid, Spain) with Gyula Batta

(Debrecen University, Hungary)

PROJECT TITLE: Ligand-bound structures for drug design: vesicle associated annexin as a target
FINANCIAL ENTITY: bilateral agreement FROM:01/2006 TO: 12/2007
RESPONSIBLE RESEARCHER: F. Javier Cañada (Madrid, Spain) with Rene Buchet (Lyon University)

PROJECT TITLE: Development of NMR screening methods
FINANCIAL ENTITY: bilateral agreement FROM:01/2009 TO: 12/2010
RESPONSIBLE RESEARCHER: **Patrick Groves** with Jesus Jimenez-Barbero (CIB, Madrid)

PROJECT TITLE: COST Action MP802: Self-assembled Guanosine Structures for Molecular Electronic Devices
FINANCIAL ENTITY: EU FROM:07/2008 TO: 06/2012
RESPONSIBLE RESEARCHER: **Patrick Groves** is one of two Portuguese Management Committee members

PROJECT TITLE: Molecular mechanism of the interaction of human annexin A6 with various ligands
FINANCIAL ENTITY: bilateral agreement FROM:01/2009 TO: 12/2012
RESPONSIBLE RESEARCHER: **Patrick Groves** with Slawomir Pikula (Nencki Institute, Warsaw)

PROJECT TITLE: Structural and functional investigation of type II NADH:quinone oxidoreductases
FINANCIAL ENTITY: FCT (Portugal) FROM:01/2010 TO: 12/2012
RESPONSIBLE RESEARCHER: Manuela Pereira. PG provides 8% support to the project

PROJECT TITLE: Engineering mini Superoxide Dismutases with tunable redox properties
FINANCIAL ENTITY: FCT (Portugal) FROM:01/2010 TO: 12/2012
RESPONSIBLE RESEARCHER: Olga Iranzo. PG provides 5% support to the project

PROJECT TITLE: MTBSS: Mycobacterium Tuberculosis: bioinformatic and structural strategies towards treatment
FINANCIAL ENTITY: EU ERANET (NewIndigo) project FROM:09/2010 TO: 08/2012
RESPONSIBLE RESEARCHER: **Patrick Groves** (EU coordinator) with Pedro Fernandes (IGC, Portugal), Antonio Pineda-Lucena (CIPF, Spain) and Shekhar Mande (CDFS, India)

PROJECT TITLE: Identification of plant extracts with protective action against bacterial enterotoxins belonging to AB5 group: cholera toxin, heat labile toxin from Escherichia coli and shiga toxin (dysentery)
FINANCIAL ENTITY: FCT (Portugal) FROM:01/2011 TO: 12/2013
RESPONSIBLE RESEARCHER: Patrick Groves with Malgorzata Palczewska