

Dr Laura Castañar Acedo

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EDUCATION

2012 – 15 **PhD in Chemistry**
Faculty of Science, Autonomous University of Barcelona, Barcelona, Spain

2011 - 12 **MSc in Science and Chemical Technology**
Faculty of Science, Autonomous University of Barcelona, Barcelona, Spain

2003 – 11 **BSc in Chemistry**
Faculty of Chemistry, Complutense University of Madrid, Madrid, Spain

RESEARCH EXPERIENCE

2018 – **Post-Doctoral Research Associate**, University of Manchester, UK
Researcher Co-Investigator, EPSRC grant number [EP/R018790/1](#)
Supervisor: Prof Gareth A. Morris
Specialty: Methodology Nuclear Magnetic Resonance (NMR) Spectroscopy
Project: New NMR techniques for mixture analysis of high dynamic range mixtures

2015 – 17 **Post-Doctoral Research Associate**, University of Manchester, UK
EPSRC Grant Number [EP/H024336/1](#)
Supervisor: Prof Gareth A. Morris
Specialty: Methodology Nuclear Magnetic Resonance Spectroscopy
Project: Improving NMR resolution and sensitivity – Simultaneously?

2012 – 15 **PhD student**, Autonomous University of Barcelona, Spain
Supervisors: Dr Teodor Parella and Dr Albert Virgili
Specialty: Methodology Nuclear Magnetic Resonance Spectroscopy
Project: [Pure shift NMR: development and applications](#)
[HSQC&HSQMBC: measurement of scalar and residual dipolar coupling constants](#)

2012 – 13 **Visiting researcher**, University of Nantes, France
(3 months)
Supervisor: Dr Patrick Giraudeau
Specialty: Methodology Nuclear Magnetic Resonance Spectroscopy
Project: Ultra-Fast NMR

2012 **MSc final research project**, Autonomous University of Barcelona, Spain
(6 months)
Supervisors: Dr Teodor Parella and Dr Albert Virgili
Specialty: Methodology Nuclear Magnetic Resonance Spectroscopy
Project: [Measurement of long range RDCs](#)

2010 – 11 **BSc collaboration research project**, Complutense University of Madrid, Spain
Supervisors: Dr Antonio Herrera and Dr Dolores Molero
Specialty: Nuclear Magnetic Resonance Spectroscopy
Project: NMR applications in Chemistry

2009 – 10 **BSc final research project**, Complutense University of Madrid, Spain
 Supervisors: Dr Carlos Otero and Dr David Ávila
 Specialty: Inorganic Solid State Chemistry
 Project: Advanced carbon nanomaterials for application as supercapacitors

TEACHING EXPERIENCE

School of Chemistry, University of Manchester, United Kingdom

2017 – 18	Spectroscopy Techniques CHEM20611 (workshop) - MSc Chemistry	3 h
	Spectroscopy Techniques CHEM20611 (tutorial) - MSc Chemistry	3 h
2016 – 17	NMR for Researchers (lecture)	2 h
2015 – 16	Integrated Spectroscopy and Separations CHEM20611 (workshop) - MSc Chemistry	6 h
	Introductory Chemistry CHEM10101 (workshop) - MSc Chemistry	2 h

Faculty of Science, Chemistry Department, Autonomous University of Barcelona, Spain

2014 – 15	Organic Chemistry (laboratory) - BSc Chemistry	50 h
	Organic Chemistry (problems) - BSc Biotechnology	15 h
2013 – 14	Organic Chemistry (laboratory) - BSc Chemistry	48 h
	Organic Chemistry (problems) - BSc Biotechnology	15 h
2012 – 13	Organic Chemistry (laboratory) - BSc Nanoscience	16 h
	Organic Chemistry (laboratory) – BSc Chemical Engineering	35 h
	Organic Chemistry (problems) - BSc Biotechnology	15 h
2011 – 12	Organic Chemistry (laboratory) - BSc Biotechnology	18 h
	Organic Chemistry (problems) - BSc Biotechnology	15 h

HONORS AND AWARDS

- **Appointed to director of the Northwest constituency** of the Society of Spanish Researchers in the United Kingdom (SRUK). **2018**
- **Appointed to chair of the associate editorial board** of the journal Magnetic Resonance in Chemistry. **2018**
- **Appointed to organising committee of SMASH** (Small molecule NMR conference). **2018**
- **Awarded with an EPSRC Grant** (grant number [EP/R018790/1](#)) as Researcher Co-Investigator. **2018**
- **Special prize award for best PhD research** in Chemistry. Awarded by the Autonomous University of Barcelona, **2017**
- **Awarded with a Summer Studentship Grant by the Analytical Chemistry Trust Fund** to supervise a research project of an undergraduate student with research potential, **2017**
- **Selected by the Royal Society and qualified by the Council for the Lindau Nobel Laureate Meeting** in a global competition among young scientists worldwide to participate in the 67th Lindau Nobel Laureate Meeting dedicated to Chemistry, **2017**
- **Appointed to the associate editorial board** of the journal Magnetic Resonance in Chemistry. **2016**

- **Ritchey award for best PhD research** for contributions to the development and application of advanced NMR techniques. Awarded by the ENC Scientific Committee. ENC Conference, Asilomar, USA, **2015**
- **Lilly award for top 10 PhD students in Spain** in Chemistry. Awarded by the Lilly European Academic Contacts Committee (EUACC). Lilly Research & Development, Alcobendas, Spain, **2014**
- **Prize for oral communication** presented at the Ibero-American NMR Meeting - GERMN Bienal Meeting – Iberian NMR Meeting. Alcalá de Henares, Spain. Awarded by Janssen, **2014**
- **Research fellowship** to stay in other research institutions. Awarded by the Autonomous University of Barcelona in open competition, **2012**
- **PhD fellowship**. Awarded by the Government of Catalonia in open national competition, **2011**
- **BSc research fellowship**. Awarded by the Spanish Ministry of Science and Innovation (MICINN) in open national competition, **2009**

CONTRIBUTIONS TO SCIENTIFIC MEETINGS AND CONFERENCES

Oral presentations

1. *Pure shift NMR*. **4th NMR Mexican Meeting**, Pachuca del Soto, Mexico, **2018**
2. *Diffusion NMR - A versatile tool for the analysis of mixtures*. **4th NMR Mexican Meeting**, Pachuca del Soto, Mexico, **2018**
3. *Divide and Rule: new NMR methods for the analysis of mixtures*. **EUROMAR Conference**, Nantes, France, **2018**
4. *Pure and simple: understanding pure shift NMR methodology*. **SMASH, Small Molecule NMR Conference**, Baveno, Italy, **2017**
5. *Zangger-Sterk and band-selective methods*. **Workshop on Pure Shift NMR**, Manchester, United Kingdom, **2017**
6. *PSYCHE pure shift NMR: spectral simplification and its applications*. **SMASH, Small Molecule NMR Conference**, La Jolla, USA, **2016**
7. *PSYCHE pure shift NMR: spectral simplification and its applications*. **Postgraduate NMRDG Meeting**, Oxford, UK, **2016**
8. *HOBS: Broadband Homonuclear Decoupled Band-Selective NMR experiments with full sensitivity*. **ENC Conference**, Asilomar, USA, **2015**
9. *Modern NMR methods and their practical applications*. **Merck Co. & Ltd**, Rahway, USA, **2015**
10. *Modern NMR methods for Chemists*. **UAB Postgraduate meeting**, Barcelona, Spain, **2014**
11. *Enantiodifferentiation through frequency-selective pure shift ¹H NMR*. **Ibero-American NMR Meeting- GERMN Bienal Meeting- Iberian NMR Meeting**, Alcalá de Henares, Spain, **2014**

Poster presentations

1. *Simplifying complexity: a new approach for the analysis of fluorine-containing mixtures by NMR*. L. Castañar, P. Moutzouri, T. M. Barbosa, C. F. Tormena, R. Rittner, A. R. Phillips, S. R. Coombes, M. Nilsson, G. A. Morris. **SMASH, Small Molecule NMR Conference**, Baveno, Italy, **2017**

2. *PSYCHE pure shift NMR: spectral simplification and its applications*. L. Castañar, M. Foroozandeh, G. Dal Poggetto, M. Nilsson, G. A. Morris. **SMASH, Small Molecule NMR Conference**, La Jolla, USA, **2016**
3. *PSYCHE pure shift NMR: spectral simplification and its applications*. L. Castañar, M. Foroozandeh, G. Dal Poggetto, M. Nilsson, G. A. Morris. **Postgraduate NMRDG Meeting**, Oxford, United Kingdom, **2016**
4. *Ultra-high-resolved pure shift NMR experiments for the analysis of complex mixtures of compounds with near/identical ^1H and ^{13}C NMR spectra*. L. Castañar, R. Roldán, P. Clapés, A. Virgili, T. Parella. **EUROMAR Conference**, Prague, Czech Republic, **2015**
5. *HOBs: Broadband Homonuclear Decoupled Band-Selective NMR experiments with full sensitivity*. L. Castañar, A. Virgili, T. Parella. **ENC Conference**, Asilomar, USA, **2015**
6. *Enantiodifferentiation through frequency-selective pure shift ^1H NMR*. M. Pérez-Trujillo, P. Nolis, E. Monteagudo, A. Virgili, T. Parella. **Ibero-American NMR Meeting- GERMN Bienal Meeting- Iberian NMR Meeting**, Alcalá de Henares, Spain, **2014**
7. *Band-Selective Pure Shift ^1H NMR experiments with full sensitivity*. L. Castañar, P. Nolis, A. Virgili, T. Parella. **EUROMAR Conference**, Zurich, Switzerland, **2014**
8. *Simultaneous multi-slice excitation in spatially encoded NMR experiments*. L. Castañar, P. Nolis, A. Virgili, T. Parella. **SMASH, Small Molecule NMR Conference**, Santiago de Compostela, Spain, **2013**
9. *Slice-selective HSQMBc Experiments*. L. Castañar, P. Nolis, J. Sauri, A. Virgili, T. Parella. **EUROMAR Conference**, Hersonissos, Greece, **2013**
10. *NMR Methods to measure residual long-range proton-carbon dipolar couplings in aligned anisotropic media*. L. Castañar, P. Nolis, A. Virgili, T. Parella. **Ibero-American NMR Meeting- GERMN Bienal Meeting- Iberian NMR Meeting**, Aveiro, Portugal, **2012**

Poster contributions

1. *A new analysis tool for 3D diffusion NMR experiments*. G. Dal Poggetto, L. Castañar, M. Foroozandeh, P. Kiraly, R. W. Adams, G. A. Morris, M. Nilsson. **SMASH, Small Molecule NMR Conference**, Philadelphia, USA, **2018**
2. *A new analysis tool for 3D diffusion NMR experiments*. G. Dal Poggetto, L. Castañar, M. Foroozandeh, P. Kiraly, R. W. Adams, G. A. Morris, M. Nilsson. **EUROMAR**, Nantes, France, **2018**
3. *MODO-FESTA: exploiting fluorine for mixture analysis*. T. M. Barbosa, L. Castañar, P. Moutzouri, M. Nilsson, G. A. Morris, R. Rittner, C. F. Tormena. **Ibero-American NMR Meeting- GERMN Bienal Meeting- Iberian NMR Meeting**, Lisbon, Portugal, **2018**
4. *Analysing highly complex mixtures: combining tailored multilinear relaxation and diffusion experiments with PARAFAC tensor analysis*. G. Dal Poggetto, L. Castañar, R. W. Adams, G. A. Morris, M. Nilsson. **SMASH, Small Molecule NMR Conference**, Baveno, Italy, **2017**
5. *REST and multivariate NMR methods in beer analysis*. G. Dal Poggetto, L. Castañar, R. W. Adams, G. A. Morris, M. Nilsson. **EUROMAR**, Warsaw, Poland, **2017**
6. *A new NMR approach to the analysis of fluorine-containing mixtures*. T. M. Barbosa, C. F. Tormena, R. Rittner, P. Moutzouri, L. Castañar, M. Nilsson, G. A. Morris. **AUREMN**, Angra dos Reis, Brazil, **2017**
7. *Homodecoupled J-resolved HSQC: Direct determination of accurate ^1H - ^{13}C RDCs in a single PMMA compressed gel sample*. L. Castañar, M. García, E. Helleman, P. Nolis, R. R. Gil, T. Parella. **SMASH, Small Molecule NMR Conference**, La Jolla, USA, **2016**

8. *Distinguishing small structural differences with selective pure shift TOCSY.* G. Dal Poggetto, L. Castañar, G. A. Morris, M. Nilsson. **EUROMAR**, Aarhus, Denmark, **2016**
9. *Pure in-phase heteronuclear correlation NMR experiments.* L. Castañar, J. Sauri, R.T. Williamson, A. Virgili, T. Parella. **SMASH, Small Molecule NMR Conference**, Atlanta, USA, **2014**
10. *Fast and efficient enantiodifferentiation through pure shift NMR.* L. Castañar, M. Pérez-Trujillo, E. Monteagudo, L.T. Khun, P. Nolis, A. Virgili, R.T. Williamson, T. Parella. **SMASH, Small Molecule NMR Conference**, Atlanta, USA, **2014**
11. *Perfect-HSQC: Suppression of phase and amplitude J_{HH} modulations.* L. Castañar, E. Sistaré, A. Virgili, R.T. Williamson, T. Parella. **SMASH, Small Molecule NMR Conference**, Atlanta, USA, **2014**
12. *New examples of enantiodifferentiation using ABTE: the case of lamotrigine and colchicine. The application of HOBS sequence.* L. Castañar, A. Virgili, T. Parella, R. Claramunt. **Ibero-American NMR Meeting- GERMN Bienal Meeting- Iberian NMR Meeting**, Alcalá de Henares, Spain, **2014**

PUBLICATIONS

1. G. Dal Poggetto, L. Castañar, M. Foroozandeh, P. Kiraly, R. W. Adams, G. A. Morris, M. Nilsson. "An unexploited dimension: new software for mixture analysis by 3D diffusion-ordered NMR spectroscopy". *Anal. Chem.*, **2018**. DOI: [10.1021/acs.analchem.8b04093](https://doi.org/10.1021/acs.analchem.8b04093).
2. L. Castañar. "Pure shift NMR: Past, present, and future" *Mag. Reson. Chem.*, **2018**, 56, 874-875. DOI: [10.1002/mrc.4758](https://doi.org/10.1002/mrc.4758)
3. L. Castañar, P. Moutzouri, T. Barbosa, C. Tormena, R. Rittner, A. Phillips, S. Coombes, M. Nilsson, G. A. Morris. "FESTA: an efficient NMR approach for the structural analysis of mixtures containing fluorinated species". *Anal. Chem.*, **2018**, 90, 5445-5450. DOI: [10.1021/acs.analchem.8b00753](https://doi.org/10.1021/acs.analchem.8b00753)
4. L. Castañar, G. Dal Poggetto, A. Colbourne, G. A. Morris, M. Nilsson. "The GNAT: A new tool for processing NMR data". *Mag. Reson. Chem.*, **2018**, 56, 546-558. DOI: [10.1002/mrc.4717](https://doi.org/10.1002/mrc.4717)
5. G. Dal Poggetto, L. Castañar, R. W. Adams, G. A. Morris, M. Nilsson. "Relaxation-encoded NMR experiments for mixture analysis: REST and beer". *Chem. Commun*, **2017**, 53, 7461-7464. DOI: [10.1039/C7CC03150E](https://doi.org/10.1039/C7CC03150E)
6. L. Castañar. "Pure shift ^1H NMR: what is next?" *Mag. Reson. Chem.*, **2017**, 55, 47-53. DOI: [10.1002/mrc.4545](https://doi.org/10.1002/mrc.4545)
7. M. Foroozandeh, L. Castañar, L. G. Martins, D. Sinnaeve, G. Dal Poggetto, C. F. Tormena, R. W. Adams, G. A. Morris, M. Nilsson. "Ultrahigh-Resolution Diffusion-Ordered Spectroscopy". *Angew. Chem. Int. Ed.*, **2016**, 55, 15579-15582. DOI: [10.1002/anie.201609676](https://doi.org/10.1002/anie.201609676)
8. G. Dal Poggetto, L. Castañar, G. A. Morris, M. Nilsson. "A new tool for NMR analysis of complex systems: selective pure shift TOCSY". *RSC Adv.*, **2016**, 6, 100063-100066. DOI: [10.1039/C6RA22807K](https://doi.org/10.1039/C6RA22807K)
9. L. Castañar, M. García, E. Hellemann, P. Nolis, R. R. Gil, T. Parella. "One-shot determination of residual dipolar couplings. Application to the structural discrimination of small molecules containing multiple stereocenters". *J. Org. Chem.*, **2016**, 81, 11126-11131. DOI: [10.1021/acs.joc.6b02103](https://doi.org/10.1021/acs.joc.6b02103)
10. L. Castañar, T. Parella. "Broadband ^1H homodecoupled NMR Experiments: Recent developments, methods and applications". *Mag. Reson. Chem.*, **2015**, 53, 399-426. DOI: [10.1002/mrc.4238](https://doi.org/10.1002/mrc.4238)

11. L. Castañar, R. Roldan, P. Clapés, A. Virgili, T. Parella. "Disentangling complex mixtures of compounds with near-identical ^1H and ^{13}C NMR spectra using pure shift NMR spectroscopy". *Chem. Eur. J.*, **2015**, 21, 7682-7685. DOI: [10.1002/chem.201500521](https://doi.org/10.1002/chem.201500521)
12. L. Castañar, T. Parella. "Recent advances in small molecule NMR: improved HSQC and HSQMBC experiments". *Annu. Rep. NMR Spectrosc.*, **2015**, 84, 163-232. DOI: [10.1016/bs.arnmr.2014.10.004](https://doi.org/10.1016/bs.arnmr.2014.10.004)
13. L. Castañar, E. Sistaré, A. Virgili, R. T. Williamson, T. Parella, "Suppression of phase and amplitude J_{HH} modulations in HSQC experiments". *Magn. Reson. Chem.*, **2014**, 53, 115-119. DOI: [10.1002/mrc.4149](https://doi.org/10.1002/mrc.4149)
14. M. Pérez-Trujillo, L. Castañar, E. Monteagudo, L. T. Khun, P. Nolis, A. Virgili, R. T. Williamson, T. Parella, "Simultaneous ^1H and ^{13}C NMR enantiodifferentiation from highly-resolved pure shift HSQC spectra". *Chem. Commun.*, **2014**, 50, 10214-10217. DOI: [10.1039/C4CC04077E](https://doi.org/10.1039/C4CC04077E)
15. L. Castañar, J. Saurí, R. T. Williamson, A. Virgili, T. Parella, "Pure in-phase heteronuclear correlation NMR experiments". *Angew. Chem. Int. Ed.*, **2014**, 53, 8379-8382. DOI: [10.1002/anie.201404136](https://doi.org/10.1002/anie.201404136)
16. L. Castañar, P. Nolis, A. Virgili, T. Parella, "Measurement of T_1/T_2 relaxation times in overlapped regions from homodecoupled ^1H singlet signals". *J. Magn. Reson.*, **2014**, 244, 30-35. DOI: [10.1016/j.jmr.2014.04.003](https://doi.org/10.1016/j.jmr.2014.04.003)
17. L. Castañar, M. Pérez-Trujillo, P. Nolis, E. Monteagudo, A. Virgili, T. Parella, "Enantiodifferentiation through frequency-selective pure shift ^1H Nuclear Magnetic Resonance Spectroscopy". *ChemPhysChem*, **2014**, 15, 854-857. DOI: [10.1002/cphc.201301130](https://doi.org/10.1002/cphc.201301130)
18. J. Saurí, L. Castañar, P. Nolis, A. Virgili, T. Parella, "Straightforward measurement of individual $^1J_{\text{CH}}$ and $^2J_{\text{HH}}$ in diastereotopic CH_2 groups". *J. Magn. Reson.*, **2014**, 242, 33-40. DOI: [10.1016/j.jmr.2014.02.003](https://doi.org/10.1016/j.jmr.2014.02.003)
19. L. Castañar, J. Saurí, P. Nolis, A. Virgili, T. Parella, "Implementing homo- and heterodecoupling in region-selective HSQMBC experiments". *J. Magn. Reson.*, **2014**, 238, 63-69. DOI: [10.1016/j.jmr.2013.10.022](https://doi.org/10.1016/j.jmr.2013.10.022)
20. L. Castañar, P. Nolis, A. Virgili, T. Parella, "Full sensitivity and enhanced resolution in homodecoupled band-selective NMR experiments". *Chem. Eur. J.*, **2013**, 19, 17283-17286. DOI: [10.1002/chem.201303235](https://doi.org/10.1002/chem.201303235)
21. L. Castañar, P. Nolis, A. Virgili, T. Parella, "Simultaneous multi-slice excitation in spatially encoded NMR experiments". *Chem. Eur. J.*, **2013**, 19, 15472-15475. DOI: [10.1002/chem.201303272](https://doi.org/10.1002/chem.201303272)
22. J. Saurí, L. Castañar, P. Nolis, A. Virgili, T. Parella, "P.E. HSQMBC: Simultaneous measurement of proton-proton and proton-carbon coupling constants". *J. Magn. Reson.*, **2012**, 224, 101-106. DOI: [10.1016/j.jmr.2012.09.007](https://doi.org/10.1016/j.jmr.2012.09.007)

COURSES AND SCIENTIFIC EVENTS

- **67th Lindau Nobel Laureate Meeting.** Lindau, Germany, **2017**
- **NMR Discussion Group Christmas Meeting.** London ,United Kingdom, **2016**
- **NMR Discussion Group Christmas Meeting.** London ,United Kingdom, **2015**
- **Ultrafast 2D NMR Symposium.** Santiago de Compostela, Spain, **2013**
- **GERMN Scientific Meeting.** Santiago de Compostela, Spain, **2013**
- **GERMN Scientific Meeting.** Madrid, Spain, **2011**
- **IX Advance course in Nuclear Magnetic Resonance.** Jaca, Spain, **2011**

MEMBERSHIP

- Society of Spanish Researchers in the United Kingdom (SRUK)
- Spanish Young Chemistry Research Society (JIQ)
- Spanish Nuclear Magnetic Resonance Society (GERMN)
- Spanish Royal Society Chemistry (RSEQ)