Curriculum Vitae

Name **Laura Castañar Acedo**
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Plaza de la Ciencias, 28040, Madrid, Spain

EDUCATION

2012 – 2015 **PhD in Chemistry**. Autonomous University of Barcelona, Spain.

2011 – 2012 **MSc in Science and Chemical Technology**. Autonomous University of Barcelona, Spain.

2003 – 2011 **BSc in Chemistry**. Complutense University of Madrid, Spain.

RESEARCH EXPERIENCE

2023 – **Talent Attraction Fellow**. Complutense University of Madrid, Spain.
Project: New NMR methods for the analysis of complex systems

2019 – 2023 **DKO Research Fellow**. University of Manchester, United Kingdom.
Project: New heteronuclear NMR tools for the most complex structural problems

2018 – 2019 **Post-Doctoral Research Associate**. University of Manchester, United Kingdom.
Researcher Co-Investigator, EPSRC grant number EP/R018790/1
Supervisor: Prof Gareth A. Morris
Project: New NMR techniques for mixture analysis of high dynamic range mixtures

2015 – 2017 **Post-Doctoral Research Associate**. University of Manchester, United Kingdom.
EPSRC Grant Number EP/L018500/1
Supervisor: Prof Gareth A. Morris
Project: Improving NMR resolution and sensitivity – Simultaneously?

2012 – 2015 **PhD student**. Autonomous University of Barcelona, Spain.
Supervisors: Drs Teodor Parella and Albert Virgili
Project: Development and application of modern pure shift NMR techniques and improved HSQC/HSQMBC experiments

2012 – 2013 **Visiting researcher**. University of Nantes, France.
Supervisor: Dr Patrick Giraudeau
Project: Ultra-fast NMR

2011 – 2012 **MSc research project**. Autonomous University of Barcelona, Spain.
Supervisors: Dr Teodor Parella and Dr Albert Virgili
Project: Measurement of residual dipolar coupling in organic molecules

2010 – 2011 **BSc research project**. Complutense University of Madrid, Spain.
Supervisors: Dr Antonio Herrera
Project: NMR applications in Chemistry

2009 – 2010 **BSc research project**. Complutense University of Madrid, Spain.
Supervisors: Dr Carlos Otero and Dr David Ávila
Project: Advanced carbon nanomaterials for application as supercapacitors

SUPERVISION EXPERIENCE

Main or co-supervisor at the University of Manchester (from 2019)

PDRA	3 - University of Manchester
PhD students	6 - University of Manchester
MSc students	2 - University of Manchester
UG students	1 - University of Manchester
Academic visitor	1 - University of Rennes, France
PhD visitor	1 - University of Campania, Italy

Assisting in teaching, training and supervision of research students and visitors

Academic visitor	1 - University of Manchester (2018)
PhD students	1 - University of Manchester (2015 – 2018) 2 - Autonomous University of Barcelona (2013 – 2015)
PhD visitor	1 - University of Manchester (2017)
MSc students	1 - University of Manchester (2018) 1 - Autonomous University of Barcelona (2014 – 2015)
MChem students	2 - University of Manchester (2016 – 2018)
Erasmus student	1 - University of Manchester (2018 – 2019)

TEACHING EXPERIENCE

Department of Chemistry, University of Manchester, United Kingdom

2022 – 2023	Magnetic Resonance CHEM63005 (lectures) - MSc Analytical Science	20 h
	Advance NMR CHEM40111 (lectures) – MChem	4 h
	Integrated Spectroscopy and Separations CHEM20611 (lectures, workshops, tutorials)	10 h
	Structure determination by NMR CHEM3011 (workshops) - MChem	4 h
	Introductory Chemistry CHEM10101 (tutorials) - MChem	11h
2021 – 2022	Magnetic Resonance CHEM63005 (lectures) - MSc Analytical Science	10 h
	Integrated Spectroscopy and Separations CHEM20611 (lectures, workshops, tutorials)	10 h
	Structure determination by NMR CHEM3011 (workshops) - MChem	4 h
	Introductory Chemistry CHEM10101 (tutorials) - MChem	11h
	Energy and Change CHEM10212 (tutorials) - MChem	6 h
2020 – 2021	Magnetic Resonance (lectures) - MSc Analytical Science	10 h
	Integrated Spectroscopy and Separations CHEM20611 (lectures, workshops, tutorials)	10 h
	Structure determination by NMR CHEM3011 (workshops) - MChem	4 h
2019 – 2020	Structure determination by NMR CHEM30111 (workshops) - MChem	4 h
	Energy and Change CHEM10212 (tutorials) - MChem	6 h
2017 – 2018	Spectroscopic Techniques CHEM20611 (workshops) - MChem	3 h
	Spectroscopic Techniques CHEM20611 (tutorials) - MChem	3 h
2016 – 2017	NMR for Postgraduate Researchers (lectures)	2 h
2015 – 2016	Integrated Spectroscopy and Separations CHEM20611 (workshops) - MChem	6 h
	Introductory Chemistry CHEM10101 (workshops) - MChem	2 h

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

2014 – 2015	Structure and Reactivity of organic Compounds (laboratory) - BSc Chemistry	50 h
	Organic Chemistry (problems) - BSc Biotechnology	15 h
2013 – 2014	Structure and Reactivity of organic Compounds (laboratory) - BSc Chemistry	48 h
	Organic Chemistry (problems) - BSc Biotechnology	15 h
2012 – 2013	Organic Chemistry (laboratory) - BSc Nanoscience	16 h
	Organic Chemistry (laboratory) - BSc Chemical Engineering	35 h
	Organic Chemistry (problems) - BSc Biotechnology	15 h
2011 – 2012	Integrated Laboratory II (laboratory) - BSc Biotechnology	18 h
	Organic Chemistry (problems) - BSc Biotechnology	15 h

HONOURS AND AWARDS

2023 **Awarded a five-year Talent Attraction Fellowship** at The Complutense University of Madrid.

Awarded a three-year EPSRC grant (EP/X035476/1) as a Researcher Co-Investigator.

Appointed as member of the Editorial Advisory Board of the journal *Magnetic Resonance in Chemistry*.

2022 **Appointed to the Scientific Evaluation Panel of Solid-State UK NMR 2022 and 2023.**

Appointed to the Scientific Committee of PANIC 2022 and 2023 (international conference).

2021 **Appointed to the Scientific Committee of EUROMAR 2022** (international conference).

Appointed as member of the Editorial Advisory Board of the journal *Analytical Science Advances*.

2020 **Appointed to the Organising Committee of EUROMAR 2023** (international conference).

Appointed as member of the Royal Society of Chemistry (RSC) NMR Discussion Group committee.

2019 **Awarded a four-year EPSRC industrial CASE PhD funding** as Academic Supervisor. Industrial partner: Johnson Matthey.

Awarded a five-year Dame Kathleen Ollerenshaw Fellowship at The University of Manchester.

Best poster presentation award at SRUK International Symposium, Liverpool, UK.

2018 **Awarded a three-year EPSRC grant** (EP/R018790/1) as a Researcher Co-Investigator.

Appointed to the Organising Committee of SMASH (international conference).

Appointed Chair of the Associate Editorial Board of the journal *Magnetic Resonance in Chemistry*.

Appointed Director of the Northwest Constituency of the Society of Spanish Researchers in the United Kingdom (SRUK).

2017 **Special prize award for best PhD research** in Chemistry. Awarded by the Autonomous University of Barcelona. Selected by the University Board to give a speech in the Awards Ceremony.

Awarded a Summer Studentship Grant by the Analytical Chemistry Trust Fund to supervise a research project of an undergraduate student with research potential.

Selected by the University of Manchester and the Royal Society, and ratified 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.

2016 **Appointed as member of the Associate Editorial Board** of the journal *Magnetic Resonance in Chemistry*.

2015 **Ritchey award for best PhD research** for contributions to the development and application of advanced NMR techniques. Awarded by the Scientific Committee of the annual Experimental NMR Conference (ENC), USA.

2014 **Lilly award for top 10 PhD students in Spain** in Chemistry. Sponsored by the Lilly European Academic Contacts Committee (EUACC), Lilly Research & Development, Spain.

Prize for best oral communication presented at the Ibero-American NMR Meeting / GERMN Bienal Meeting / Iberian NMR Meeting. Alcalá de Henares, Spain. Sponsored by Janssen.

2012 **PhD research fellowship** for visits to other research institutions. Awarded by the Autonomous University of Barcelona in open competition.

2009 **BSc research fellowship**. Awarded by the Spanish Ministry of Science and Innovation (MICINN) in open national competition.

PUBLICATIONS

***h*-index** 17 (Web of Science)

Total citations 842 (Web of Science)

Publications

1. M. J. Smith, J. E. Bramham, M. Nilsson, G. A. Morris, A. P. Golovanov, L. Castañar. "Lighting up spin systems: enhancing characteristic ^{1}H signal patterns of fluorinated molecules". *Chem. Commun.*, **2023**
2. C. Mycroft, M. Smith, M. Nilsson, G. A. Morris, L. Castañar. "Pure shift FESTA: An ultra-high resolution NMR tool for the analysis of complex fluorine-containing systems". *Magn. Reson. Chem.*, **2023**
3. C. Mycroft, M. Nilsson, G. A. Morris, L. Castañar. "Rapid measurement of heteronuclear coupling constants in complex NMR spectra". *J. Am. Chem. Soc*., **2023**. DOI: 10.1021/jacs.3c05515
4. D. A. Taylor, P. Kiraly, P. Bowyer, M. Nilsson, L. Castañar, G. A. Morris, R. W. Adams. "Ultra-selective, 1D clean in-phase correlation spectroscopy". *Chem. Commun.*, **2023**, *59*, 6734-6737. DOI: 10.1039/D3CC01333B
5. E. L. Gates, M. J. Smith, J. P. Bradley, M. Johnson, G.Widmalm, M. Nilsson, G. A. Morris, R. W. Adams, L. Castañar. "Ultra-selective, ultra-clean 1D rotating-frame Overhauser effect spectroscopy". *Chem. Commun.*, **2023**, *59*, 5854-5857. DOI: 10.1039/D3CC00550J
6. R. Adams, L. Castañar. "Pure shift 2D NMR spectroscopy". *Fast 2D solution-state NMR: concepts and applications*, chapter 9. Royal Society of Chemistry Ed, **2023**.
7. R. Li, L. Castañar, M. Nilsson, G. A. Morris. "Relaxational signal attenuation during soft refocusing pulses". *J. Magn. Reson*., **2023**, *346*, 107337. DOI:10.1016/j.jmr.2022.107337
8. C. Mycroft, M. Nilsson, G. A. Morris, L. Castañar. "Simultaneous broadband suppression of homonuclear and heteronuclear couplings in ^{1}H NMR spectroscopy". *ChemPhysChem*., **2022**, *23*, e2022004. DOI: 10.1002/cphc.202200495
9. M. J. Smith, L. Castañar, R. W. Adams, G. A. Morris, M. Nilsson. "Giving pure shift NMR spectroscopy a REST - Ultrahigh resolution mixture analysis". *Anal. Chem*., **2022**, *94*, 12757-12761. DOI:10.1021/acs.analchem.2c02411
10. G. Rosseto, P. Kiraly, L. Castañar, G. A. Morris, M. Nilsson. "Improved quantification by NMR spectroscopy of the fatty acid ester composition of extra virgin olive oils". *ACS Food Sci. Technol.*, **2022**, *2*, 1237-1242. DOI: 10.1021/acsfoodscitech.2c00057
11. P. Kiraly, G. Dal Poggetto, L. Castañar, M. Nilsson, A. Deák, G. A. Morris. "Broadband measurement of true transverse relaxation rates in systems with coupled protons: application to the study of conformational exchange". *Chem. Sci.*, **2021**, *12*, 11538–11547. DOI: 10.1039/D1SC03391C
12. Trevorrow, JN Dumez, L. Castañar. "A career in NMR: An interview with Lyndon Emsley". (Perspective) *Magn. Reson. Chem.*, **2021,** *59*, 597-599. DOI:10.1002/mrc.5119
13. T. Barbosa, L. Castañar, P. Moutzouri, M. Nilsson, G. A. Morris, C. Tormena. "Improving the sensitivity of FESTA methods for the analysis of fluorinated mixtures". *Anal. Chem*., **2020**, *92*, 2224-2228. DOI:10.1021/acs.analchem.9b04924
14. L. Castañar, J. Wist. "Tutorials: A powerful source of knowledge transfer and inspiration". (Guest Editorial) *Magn. Reson. Chem.*, **2020,** *58*, 350-351. DOI:10.1002/mrc.5008
15. P. Trevorrow, R. Gil, L. Castañar. "A career in NMR: An interview with Gareth Morris". (Perspective) *Magn. Reson. Chem.*, **2019,** *57*, 915-918. DOI:10.1002/mrc.4901
16. G. Dal Poggetto, L. Castañar, R. W. Adams, G. A. Morris, M. Nilsson. "Dissect and divide: putting NMR spectra of mixtures under the knife". *J. Am. Chem. Soc*., **2019**, 141, 5766-5771. DOI: 10.1021/jacs.8b13290
17. G. Dal Poggetto, L. Castañar, M. Foroozandeh, P. Kiraly, R. W. Adams, G. A. Morris, M. Nilsson. "Unexploited dimension: new software for mixture analysis by 3D diffusion-ordered NMR spectroscopy". *Anal. Chem*., **2018**, *90*, 13695-13701. DOI:10.1021/acs.analchem.8b04093
18. L. Castañar. "Pure shift NMR: past, present, and future". (Guest Editorial) *Magn. Reson. Chem.*, **2018,** *56*, 874-875. DOI:10.1002/mrc.4758

19. 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
20. L. Castañar, G. Dal Poggetto, A. Colbourne, G. A. Morris, M. Nilsson. "The GNAT: a new tool for processing NMR data". *Magn. Reson. Chem.*, **2018**, *56*, 546-558. DOI:10.1002/mrc.4717
21. 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
22. L. Castañar. "Pure shift ^{1}H NMR: what is next?". *Magn. Reson. Chem.*, **2017**, *55*, 47-53. DOI:10.1002/mrc.4545
23. 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
24. 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
25. 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
26. L. Castañar, T. Parella. "Broadband ^{1}H homodecoupled NMR Experiments: recent developments, methods and applications". *Magn. Reson. Chem.*, **2015**, *53*, 399-426. DOI:10.1002/mrc.4238
27. L. Castañar, R. Roldan, P. Clapés, A. Virgili, T. Parella. "Disentangling complex mixtures of compounds with near-identical ^{1}H and ^{13}C NMR spectra using pure shift NMR spectroscopy". *Chem. Eur. J.*, **2015**, *21*, 7682-7685. DOI:10.1002/chem.201500521
28. 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
29. 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
30. M. Pérez-Trujillo, L. Castañar, E. Monteagudo, L. T. Khun, P. Nolis, A. Virgili, R. T. Williamson, T. Parella, "Simultaneous ^{1}H and ^{13}C NMR enantiodifferentiation from highly-resolved pure shift HSQC spectra". *Chem. Commun*, **2014**, *50*, 10214-10217. DOI:10.1039/C4CC04077E
31. 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
32. L. Castañar, P. Nolis, A. Virgili, T. Parella, "Measurement of T_1/T_2 relaxation times in overlapped regions from homodecoupled ^{1}H singlet signals". *J. Magn. Reson*., **2014**, *244*, 30-35. DOI:10.1016/j.jmr.2014.04.003
33. L. Castañar, M. Pérez-Trujillo, P. Nolis, E. Monteagudo, A. Virgili, T. Parella, "Enantiodifferentiation through frequency-selective pure shift ^{1}H Nuclear Magnetic Resonance Spectroscopy". *ChemPhysChem*, **2014**, *15*, 854-857. DOI: 10.1002/cphc.201301130
34. J. Saurí, L. Castañar, P. Nolis, A. Virgili, T. Parella, "Straightforward measurement of individual $^{1}J_{CH}$ and $^{2}J_{HH}$ in diastereotopic CH_2 groups". *J. Magn. Reson*., **2014**, *242*, 33-40. DOI:10.1016/j.jmr.2014.02.003
35. 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
36. 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
37. 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
38. 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

RESEARCH FUNDING

Research grants

Multiple independent NMR dimensions: smart experiments for complicated problems

Role	Co-Investigator
Period	September 2023 - August 2026
Amount	£588,705. Funded by EPSRC (Grant: EP/X035476/1)

New NMR methods for the analysis of complex systems

Role	Principal Researcher
Period	March 2023 - February 2028
Amount	181,150€. Funded by the Comunidad de Madrid (Grant: 2022-T1/BMD-24030)

Clearing the undergrowth: new NMR techniques for high dynamic range mixtures

Role	Researcher (PDRA Jan 2018 – Mar 2019) and Co-Investigator (Apr 2019 – Sep 2021)
Period	January 2018 - September 2021
Amount	£623,173. Funded by EPSRC (Grant: EP/R018790/1)

Improving NMR resolution and sensitivity – Simultaneously?

Role	Researcher (PDRA Oct 2015– Dec 2017)
Period	March 2014 - December 2017
Amount	£340,726. Funded by EPSRC (Grant: EP/L018500/1)

New methods in Nuclear Magnetic Resonance (IV)

Role	Researcher (PhD student)
Period	February 2013 - January 2016
Amount	85,750€. Funded by FEDER (Grant: CTQ2012-32436)

Nanometallomics applied to soybean cultivation for studying the effects of metal-related nanoparticles

Role	International collaborator
Period	October 2019 - September 2014
Amount	R$ 603,688. Funded by FAPESP (Grant: 2018/25207-0)

Other grants

Advanced NMR Methods for Complex Mixture Analysis Driven by Industrial Challenges

Role	Principal investigator (Academic supervisor)
Industrial partner	Johnson Matthey
Period	October 2020 - September 2024
Amount	£116,928. Funded by EPSRC Industrial CASE

Purchase of Specject-II and VAMP-III

Role	Co-Investigator
Period	August 2020 - March 2020
£61,440	Funded by EPSRC Early Career Capital Award

Pure shift NMR training (ERASMUS+ Staff Training Mobility)

Role	Supervisor
Period	September 2018 (1 week)
600€	Funded by Complutense University of Madrid and European Union

Pure shift NMR: an analytical tool for mixture analysis (Analytical Chemistry Summer Studentship)

Role	Principal investigator (Academic supervisor)
Period	June 2017 - August 2017
£1,440	Funded by Analytical Chemistry Trust Fund

Ultra-fast NMR

Role	Visiting Researcher (PhD student)
Period	November 2012 - January 2013
2,500€	Funded by Autonomous University of Barcelona

Advanced carbon nanomaterials for application as supercapacitors

Role	Researcher (BSc student)
Period	October 2009 - June 2010
2,500€	Funded by Spanish Ministry of Science and Innovation (MICINN)

Travel grants

EUROMAR Conference, Czech Republic, 2015.
250€ Funded by GERMN
300€ Funded by EUROMAR

ENC Conference, USA, 2015.
250€ Funded by GERMN
$1000 Ritchey travel award
$250 Funded by ENC

Ibero-American NMR Meeting / GERMN Bienal Meeting / Iberian NMR Meeting, Spain, 2014.
200€ Funded by Autonomous University of Barcelona
250€ Funded by GERMN

EUROMAR Conference, Switzerland, 2014.
250€ Funded by GERMN
250€ Funded by EUROMAR

*SMASH, Small Molecule NMR Conference, Spain, 2013***.**
$500 Funded by SMASH

EUROMAR Conference, Greece, 2013.
200€ Funded by Autonomous University of Barcelona
250€ Funded by GERMN
250€ Funded by EUROMAR

Ibero-American NMR Meeting / GERMN Bienal Meeting / Iberian NMR Meeting, Portugal, 2012.
250€ Funded by GERMN

GERMN Scientific Meeting, Spain, 2011.
100€ Funded by GERMN

CONTRIBUTIONS TO SCIENTIFIC MEETINGS

Invited talks

1. *Cutting-edge NMR methods for the analysis of fluorinated systems.* SMASH, Small Molecule NMR Conference, Baveno, Italy, **2023**.
2. *Novel NMR methods: the art of simplifying complexity.* Bruker User Meeting, Barcelona, Spain, **2023**.
3. *2D Heteronuclear NMR spectroscopy*. XVI Manuel Rico NMR School, Jaca, Spain, **2023.**
4. *New NMR tools for the study complex systems*. Blas Cabrera Seminar, IQF-CSIC Madrid, Spain, **2023.**
5. *Understanding Pure Shift NMR*. Global NMR Discussion Meetings, **2023**. (Online)
6. *Cutting-edge NMR methods: tales from a mnacNMR methodologist.* An NMR testimonial Symposium, Manchester, UK, **2023**.
7. *Cutting-edge NMR methods for the analysis of complex systems.* Integrative Resonance Meeting, Barcelona, Spain, **2023**.
8. II Symposium GERMN-junior, Madrid, Spain, **2023**.
9. *Seeking simplicity in spectral complexity? Cutting-edge NMR methods at your disposal*. 11th GERMN Bienal Meeting, Almería, Spain, **2022**.
10. *New NMR tools for complex structural problems.* Spanish Royal Society of Chemistry (RSEQ) biennial meeting, Granada, Spain, **2022**.
11. *New NMR tools for getting the most out of your spectra*. New advances in Chemistry Seminar, IIQ-CSIC Seville, Spain, **2022.**
12. *New NMR tools for analysis of carbohydrates.* 1st GlycoNMR Summit, USA, **2022**. (Online)
13. *Pure shift NMR spectroscopy*. XV Manuel Rico NMR School, Jaca, Spain, **2022**.

14. *Getting the most out of your NMR spectra: Novel NMR tools.* Tokyo Institute of Technology Seminar, **2021**. (Online)
15. *Tales from an NMR spectroscopist.* University Complutense of Madrid, **2021**. (Online)
16. *Divide and Rule. 1st Symposium GERMN-junior*, **2021**. (Online)
17. *Ultra-high NMR: Pure shift NMR.* Mexico, **2020**. (Online)
18. *Separating the wheat from the chaff.* India, **2020**. (Online)
19. *Defeating Complexity: New NMR methods for mixture analysis.* Magnetic Resonance Meet the Future of Biophysics, **2020**. (Online)
20. *Pure shift NMR spectroscopy*. Mexico, **2020**. (Online)
21. *Defeating Complexity: New NMR methods for mixture analysis.* ENC Conference, Baltimore, USA, **2020**.
22. *New NMR tools for getting the most out of your spectra.* SMASH, Small Molecule NMR Conference, Porto, Portugal, **2019**.
23. *Dame Kathleen Ollerenshaw Fellowship*. PDRA Fellowship advice session organized by the University of Manchester, UK, **2019**.
24. *Pure shift NMR spectroscopy*. XIV Manuel Rico NMR School, Jaca, Spain, **2019**.
25. *Simplifying the analysis of mixtures: new NMR methods and software.* PANIC, South Carolina, USA, **2019**.
26. *Pure shift NMR.* Mexican NMR Meeting, Pachuca del Soto, Mexico, **2018**.
27. *Diffusion NMR - A versatile tool for the analysis of mixtures*. Mexican NMR Meeting, Pachuca del Soto, Mexico, **2018**.
28. *Divide and rule: new NMR methods for the analysis of mixtures*. EUROMAR Conference, Nantes, France, **2018**.
29. *Pure and simple: understanding pure shift NMR methodology*. SMASH, Small Molecule NMR Conference, Baveno, Italy, **2017**. (Workshop)
30. *HOBS: broadband homonuclear decoupled band-selective NMR experiments with full sensitivity*. ENC Conference, Asilomar, USA, **2015**.
31. *Modern NMR methods and their practical applications.* Merck Co. & Ltd, Rahway, USA, **2015**.

Other oral presentations

32. *Zangger-Sterk and band-selective methods*. Workshop on Pure Shift NMR, Manchester, UK, **2017**. (Co-organiser/speaker)
33. *PSYCHE pure shift NMR: spectral simplification and its applications.* SMASH, Small Molecule NMR Conference, La Jolla, USA, **2016**.
34. *PSYCHE pure shift NMR: spectral simplification and its applications.* Postgraduate NMRDG Meeting, Oxford, UK, **2016**.
35. *Modern NMR methods for Chemists*. UAB Postgraduate meeting, Barcelona, Spain, **2014**.
36. *Enantiodifferentiation through frequency-selective pure shift ^{1}H NMR.* Ibero-American NMR Meeting / GERMN Bienal Meeting / Iberian NMR Meeting, Alcalá de Henares, Spain, **2014**.

Poster presentations

1. *New NMR tools for getting ultra-high resolution spectra: Pure shift NMR.* L. Castañar. SRUK International Symposium, Liverpool, UK, **2019**.
2. *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**.
3. *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**.

4. *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, UK, **2016**.
5. *Ultrahigh-resolved pure shift NMR experiments for the analysis of complex mixtures of compounds with near/identical ^{1}H and ^{13}C NMR spectra.* L. Castañar, R. Roldán, P. Clapés, A. Virgili, T. Parella. EUROMAR Conference, Prague, Czech Republic, **2015**.
6. *HOBS: broadband homonuclear decoupled band-selective NMR experiments with full sensitivity.* L. Castañar, A. Virgili, T. Parella. ENC Conference, Asilomar, USA, **2015**.
7. *Enantiodifferentiation through frequency-selective pure shift ^{1}H NMR.* L. Castañar, 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**.
8. *Band-selective pure shift ^{1}H NMR experiments with full sensitivity*. L. Castañar, P. Nolis, A. Virgili, T. Parella. EUROMAR Conference, Zurich, Switzerland, **2014**.
9. *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**.
10. *Slice-selective HSQMBC experiments.* L. Castañar, P. Nolis, J. Sauri, A. Virgili, T. Parella. EUROMAR Conference, Hersonissos, Greece, **2013**.
11. *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**.

Other contributions

1. *Solvent signal suppression in pure shift NMR.* E. Gates, J. Bradley, M. Johnson, G. A. Morris, R. W. Adams, L. Castañar. SMASH, Small Molecule NMR Conference, Baveno, Italy, **2023**. (Talk)
2. *How to stop convection ruining pure shift NMR experiments*. E. Caytan, H. Foster, L. Castañar, R. W. Adams, M. Nilsson, G. A. Morris. EUROMAR Conference, Glasgow, UK, **2023**. (Talk)
3. *Investigation of exhaled breath condensate by NMR based metabolomics*. H. Wang, L. Castañar, S. Fowler, M. Nilsson. EUROMAR Conference, Glasgow, UK, **2023**.
4. *Solvent signal suppression in pure shift NMR.* E. Gates, J. Bradley, M. Johnson, G. A. Morris, R. W. Adams, L. Castañar. EUROMAR Conference, Glasgow, UK, **2023**.
5. *Ultra-high resolution fluorine and phosphorus NMR Spectroscopy.* C. Mycroft, B. Ijzendoorn, M. Mehta, M. Nilsson, G. A. Morris, L. Castañar. EUROMAR Conference, Glasgow, UK, **2023**.
6. *Ultra-selective, 1D clean in-phase correlation spectroscopy.* D. A. Taylor, P. Kiraly, P. Bowyer, M. Nilsson, L. Castañar, G. A. Morris, R. W. Adams. EUROMAR Conference, Glasgow, UK, **2023**.
7. *Ultra-high resolution NMR analysis of fluorine-containing systems.* C. Mycroft, G. A. Morris, M. Nilsson, L. Castañar. SMASH Conference, La Jolla, USA, **2022**.
8. *GEMSTONE-ROESY: Ultra-selective, ultra-clean 1D rotating-frame Overhauser spectrocopy.* E. Gates, J. Montgomery, M. J. Smith, J. Bradley, M. Johnson, G. Widmalm, M. Nilsson, G. A. Morris, R. W. Adams, L. Castañar. SMASH Conference, La Jolla, USA, **2022**.
9. *New NMR methods for structural and conformational analysis of fluorinated systems.* C. Mycroft, G. A. Morris, M. Nilsson, L. Castañar. EUROMAR Conference, Utrecht, Netherlands, **2022**. (Talk)
10. *GEMSTONE: ultra-selective NMR methods for complex spectra.* E. Gates, J. Montgomery, M. J. Smith, J. Bradley, M. Johnson, G. Widmalm, M. Nilsson, G. A. Morris, R. W. Adams, L. Castañar. EUROMAR Conference, Utrecht, Netherlands, **2022**. (Talk)
11. *Relaxational signal attenuation during selective pulse.* R. Li, L. Castañar, M. Nilsson, G. A. Morris. EUROMAR Conference, Utrecht, Netherlands, **2022**.
12. *Putting heteronuclei on the chopping block – extracting component spectra from complex mixtures.* M. J. Smith, G. Dal Poggetto, C. F. Tormena, L. Castañar, R. W. Adams, G. A. Morris, M. Nilsson. EUROMAR Conference, Utrecht, Netherlands, **2022**.

13. *Pure shift relaxation-encoded selective TOCSY.* M. J. Smith, L. Castañar, R. W. Adams, G. A. Morris, M. Nilsson. SMASH, Small Molecule NMR Conference, **2021**.
14. *Broadband suppression of heteronuclear and homonuclear couplings in ^{1}H NMR.* C. Mycroft**,** M. Nilsson, G. A. Morris, L. Castañar. SMASH, Small Molecule NMR Conference, **2021**.
15. *Efficient, free and open-source tools to process NMR data: GNAT and MAGNATE.* L. Castañar, G. Dal Poggetto, R. W. Adams, G. A. Morris, M. Nilsson. ENC Conference, Asilomar, USA, **2019**.
16. *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**.
17. *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 Conference, Nantes, France, **2018**.
18. *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**.
19. *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**.
20. *REST and multivariate NMR methods in beer analysis.* G. Dal Poggetto, L. Castañar, R. W. Adams, G. A. Morris, M. Nilsson. EUROMAR Conference, Warsaw, Poland, **2017**.
21. *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**.
22. *Homodecoupled J-resolved HSQC: direct determination of accurate ^{1}H-^{13}C RDCs in a single PMMA compressed gel sample*. L. Castañar, M. García, E. Hellemann, P. Nolis, R. R. Gil, T. Parella. SMASH, Small Molecule NMR Conference, La Jolla, USA, **2016**.
23. *Distinguishing small structural differences with selective pure shift TOCSY.* G. Dal Poggetto, L. Castañar, G. A. Morris, M. Nilsson. EUROMAR Conference, Aarhus, Denmark, **2016**.
24. *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**.
25. *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**.
26. *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**.
27. *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**.

ORGANIZATION OF SCIENTIFIC EVENTS

2023 *EUROMAR 2023*. Member of scientific committee.

SMASH, Small Molecule NMR Conference. Member of organising committee.

Symposium: An NMR testimonial, University of Manchester, Manchester, UK. Member of organising committee.

2022 *PANIC 2022*. Member of scientific committee.

EUROMAR 2022. Member of scientific committee and session Chair.

NMR Discussion Group Postgraduate Meeting, University of Manchester, Manchester, UK. Member of organising committee

SMASH, Small Molecule NMR Conference. Member of organising committee.

Postgraduate Research Meeting, University of Manchester, Manchester, UK. Member of organising committee.

Research Seminars, Department of Chemistry, University of Manchester, Manchester, UK. Member of organising committee.

2021 *SMASH, Small Molecule NMR Conference*, online. Member of organising committee.

Research Seminars, Department of Chemistry, University of Manchester, Manchester, UK. Member of organising committee.

2020 *SMASH, Small Molecule NMR Conference*, La Jolla, USA. Member of organising committee.

Research Seminars, Department of Chemistry, University of Manchester, Manchester, UK. Member of organising committee.

Postgraduate Research Meeting, Department of Chemistry, University of Manchester, Manchester, UK. Member of organising committee.

2019 *SMASH, Small Molecule NMR Conference*, Lisbon, Portugal. Member of organising committee and session chair

SMASH, Small Molecule NMR Conference, Lisbon, Portugal. Session Chair.

Research Seminars, Department of Chemistry, University of Manchester, Manchester, UK. Member of organising committee.

Staff Symposium, Department of Chemistry, University of Manchester, Manchester, UK. Chair.

2018 *SMASH, Small Molecule NMR Conference*, Philadelphia, USA. Member of organising committee.

2017 *Pure shift workshop*, University of Manchester, UK. Co-organiser.

Pure shift workshop, SMASH, Small Molecule NMR Conference, Baveno, Italy. Co-organiser.

SCIENCE OUTREACH ACTIVITIES

2023 *International Women's day event*. Invited speaker. (Online)

On Resonance initiative at SMASH conference, Baveno, Italy. Member of organising committee.

2022 *Woman in STEM Conference*. University of Manchester, Manchester, UK. Invited speaker and session chair.

Women in Science 8M event. Invited speaker. (Online)

On Resonance initiative at SMASH conference, La Jolla, USA. Member of organising committee.

2021 *Research Photography Competition "Investigación en Foco"*. Member of organising committee.

2020 *Research Photography Competition "Investigación en Foco"*. Member of organising committee.

11F *CineScience*, Manchester, UK. Member of organising committee.

2019 *On Resonance* initiative at SMASH conference, La Jolla, USA. Member of organising committee.

Symposium on Neuroscience, Manchester, UK. Member of organising committee.

Schools' Analyst Competition: Northwest heat, Department of Chemistry, University of Manchester, Manchester, UK.

Scientific Walking Tour, Manchester, UK. Member of organising committee.

Pint of Knowledge, Liverpool, UK. Member of organising committee.

CineScience, Manchester, UK. Member of organising committee.

2018 *Sustainability and Climate Change Seminar*, Manchester, UK. Chair and member of organising committee.

Science-me a Story Contest. Member of organising committee.

Pint of Knowledge, Liverpool, UK. Member of organising committee.

SCIENTIFIC EVALUATIONS PANELS

2023 Member of the Scientific Evaluation Panel of the UK High-Field Solid-State NMR National Research Facility.

Grant evaluator of the French National Research Agency (ANR).

Member of the Scientific Evaluation Panel of the Global NMR Twitter Conference.

Member of the PhD evaluation panel of Dr Xi Chen
Université Paris Cité, France.
Thesis title: *Fully tailored ultrahigh-resolution pulse sequences for the analysis of complex mixtures*.

2022 Member of the Scientific Evaluation Panel of the UK High-Field Solid-State NMR National Research Facility.

2021 Member of the PhD evaluation panel of Dr Kumar Motiram Corral
Autonomous University of Barcelona, Spain.
Thesis title: *Advances in NMR spectroscopic methodology and applications: time-efficient methods, ultra-long-range heteronuclear correlation experiments and enantiospecific analysis of complex mixtures*.

2020 Member of the PhD evaluation panel of Dr Corentin Jacquemmoz
University of Nantes, France.
Thesis title: *Ultra-fast Multidimensional NMR for the monitoring of chemical reactions.*

Member of the MRes evaluation panel of Arika Hisatsune
University of Manchester, United Kingdom.
Dissertation title: *Development of novel 2D NMR techniques for mixture analysis*.

2018 Member of the MSc evaluation panel of Christian Felipe Pantoja
University of Valle, Colombia.
Thesis title: *Cooperative diffusion in mixture analysis by NMR.*

OTHER MEETINGS ATTENDED

2018 NMR Discussion Group Christmas Meeting. London, UK.

2017 67th Lindau Nobel Laureate Meeting. Lindau, Germany.

2016 NMR Discussion Group Christmas Meeting. London, UK.

2015 NMR Discussion Group Christmas Meeting. London, UK.

2013 Ultrafast 2D NMR Symposium. Santiago de Compostela, Spain.
GERMN Scientific Meeting. Santiago de Compostela, Spain.

2012 GERMN Scientific Meeting. Madrid, Spain.

MEMBERSHIP

RSC Royal Society of Chemistry

SRUK Society of Spanish Researchers in the United Kingdom

JIQ Spanish Young Chemistry Research Society

GERMN Spanish Nuclear Magnetic Resonance Society

RSEQ Spanish Royal Society for Chemistry