# FEATURED ARTICLE

TRENDS - SOFTWARE FOR REACTION MONITORING WITH TIME-RESOLVED NON-UNIFORM SAMPLING

BY MATEUSZ URBAŃCZYK, ALEXANDRA SHCHUKINA, DARIUSZ GOŁOWICZ AND KRZYSZTOF KAZIMIERCZUK



ALSO IN THIS ISSUE:

REVIEW - TOWARDS PERFECT NMR: SPIN-ECHO VERSUS PERFECT-ECHO BUILDING BLOCKS

BY TEODOR PARELLA



Milehouweipuad could must have hip talk

#### **Editorial Board**

JOURNAL ADMINISTRATOR EDITORIAL BOARD

Dr S. Ryan

**EDITOR IN CHIEF** 

Roberto R. Gil

Garv E. Martin

Patrick Giraudeau,

France

Leonid Krivdin,

Russia

Bozhana P. Mikhova,

Bulgaria

Tadeusz Molinski,

**USA** 

Leonard Mueller,

USA

Teo Parella,

Spain

#### EDITORIAL ADVISORY BOARD

Guiseppe Bifulco,

University of ASalerno

Craig Butts, University of Bristol

Eurico Cabrita, Universidade

Nova de Lisboa

Timothy Claridge, University

of Oxford

Timothy Cross, Florida State

University

Melinda J. Duer, University of Cambridge

Jens Ø Duus, Carlsberg

University

Cees J. Elsevier, Universiteit

van Amsterdam

Ludger Ernst, Technische

Universität Braunschweig

Gerd Gemmecker, Technische

Universität München Steffen J. Glaser, Technische

Universität München-Garching

Christian Griesinger, Max

Planck Institute

Kirk Gustafson, National

Cancer Institute

Poul E. Hansen, Roskilde University

Gerard S. Harbison,

University of Nebraska

Elaine Holmes, Imperial

College London Jozef Kowalewski, Stockholm

University

David Larkin, University of Illinois

Hans-Heinrich Limbach.

Freie Universität Berlin Maili Liu, Chinese

Academy of Sciences

Burkhard Luy, Karlsruher Institut für Technologie

Dominique Massiot, CRMHT-CNRS, France

Eugene P. Mazzola,

University of Maryland

Gareth A. Morris,

University of Manchester

Guillermo Moyna,

Universidad de la República

de Uruguay

Armando Navarro-Vazquez,

Universidade Federal de

Pernambuco, Brazil

Ayyalusamy Ramamoorthy,

University of Michigan

David Russell, Genetec

Andre Simpson, University of Toronto

Yonchao Su, Merck & Co., Inc.

Dean J. Tantillo, UC Davis Claudio Tormena,

Universidade Estadual de

Campinas Antony J. Williams, US

Environmental Protection

R. Thomas Williamson,

University of North Carolina

at Wilmington

ASSOCIATE EDITORIAL BOARD

Anuji Abraham, Bristol-Myers Squibb

Maria Baias, New York

University Abu Dhabi

Laura Castanar (Chair),

University of Manchester Jean-Nicolas Dumez, ICSN-

**CNRS** 

Damien Jeannerat, University

of Geneva

Damodaran Krishnan,

University of Pittsburgh

Manuel Pérez Pacheco,

Mestrelab

Elodie Salager, CNRS

Josep Sauri, Merck & Co., Inc.

Han Sun, FMP

Volker Schmidts, Technische

Universität Darmstadt

Julien Wist, Universidad del

Valle

WILEY EDITOR:

Paul Trevorrow

PUBLISHING ASSISTANT:

Zoe Mills

JOURNAL PRODUCTION MANAGER:

Jim Lilley

PRODUCTION EDITOR: Chona M. Hilferty

E-MAIL:

mrcproofs@wiley.com

PUBLISHER:

Magnetic Resonance in Chemistry

is published by John Wiley & Sons, Ltd.

The Atrium

Southern Gate

Chichester PO19 8SO

United Kingdom

DATA PROTECTION

By submitting a manuscript to or reviewing for this publication, your name, email address, and affiliation, and other contact details the publication might require, will be used for the regular operations of the publication, including, when necessary, sharing with the publisher (Wiley) and partners for production and publication. The publication and the publisher recognize the importance of protecting the personal information collected from users in the operation of these services, and have practices in place to ensure that steps are taken to maintain the security, integrity, and privacy of the personal data collected and processed. You can

learn more at https://authorservices.wiley.com/

statements/data-protection-policy.html. MANUSCRIPT SUBMISSIONS:

http://mc.manuscriptcentral.com/mrc

MARKETING:

Amanda Smith

Email: amasmith@wiley.com

ADVERTISING:

Stephen Parkes

Telephone: +44 (0) 1243 770 367

E-mail: corporatesalesuk@wiley.com

COMMERCIAL REPRINTS:

Email: corporatesaleseurope@wiley.com; corporatesalesusa@wiley.com; or

corporatesalesaustralia@wiley.com

AUTHOR REPRINTS (50-300 COPIES): Order online: http://offprint.

cosprinters.com/blackwell Email: offprint@cosprinters.com

COPYRIGHT PERMISSIONS:

permissionsuk@wiley.com PUBLICATION:

12 issues in 2019

© 2019 John Wiley & Sons, Ltd.

Chichester, UK

#### **Identification Statement**

MAGNETIC RESONANCE IN CHEMISTRY, (Print ISSN 0749-1581; Online ISSN 1097-458X), is published monthly. US mailing agent: Mercury Media Processing, LLC, 1850 Elizabeth Avenue, Suite #C, Rahway, NJ 07065 USA. Periodical postage paid at Rahway, NJ. Postmaster: Send all address changes to MAGNETIC RESONANCE IN CHEMISTRY, John Wiley & Sons Inc., C/O The Sheridan Press, PO Box 465, Hanover, PA 17331 USA.

MRC

Volume 57 Number 1 January 2019

#### Aims & scope

*MRC* is devoted to the rapid publication of papers which are concerned with the development of magnetic resonance techniques, or in which the application of such techniques plays a pivotal part. Contributions from scientists working in all areas of NMR, ESR and NQR are invited, and papers describing applications in all branches of chemistry, structural biology and materials chemistry are published.

The journal is of particular interest not only to scientists working in academic research, but also those working in commercial organisations who need to keep up-to-date with the latest practical applications of magnetic resonance techniques.

### **Featured Article**

Time-resolved non-uniform sampling (TR-NUS) allows for reaction monitoring using multidimensional experiments. Here, we present TReNDS - the program for convenient setup and processing of TR-NUS measurement. The software performs spectral reconstruction and analysis including peak-peaking and tracking.



TReNDS—Software for reaction monitoring with time-resolved non-uniform sampling

4\_1′

M. Urbańczyk, A. Shchukina, D. Gołowicz and K. Kazimierczuk

## **Review**

The concept of "perfect NMR" includes the design of robust pulse sequences that allow obtaining undistorted pure in-phase signals, with pure absorption lineshapes and free of phase anomalies derived from undesired *J* modulations. Here, alternative NMR building blocks to spin-echo which are based on a general double SE module, known as perfectecho, are reviewed. Several implementations to minimize/remove unwanted dispersive contributions in homonuclear and heteronuclear NMR experiments are described and illustrated with some examples of broad interest for small molecules.

Perfect NMR

Spin-Echo

Perfect Echo

Perfect CPMG DOSY

Tz

Perfect HSQC

NMR

Perfect selective excitation

Perfect DISPT

Tz

Perfect BIRD

Perfect

Perfect Perfect Satellite-Free Selective excitation

Perfect DOSY

Reasurement Tz

Perfect DISPT

Perfect DIS

Towards perfect NMR: spin-echo versus perfect-echo building blocks 13-29

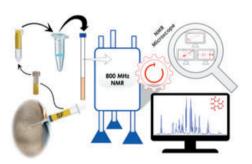
T. Parella



# **Research Article**

#### Contents continued

The NMR assignment of normal and ultra-filtered synovial fluid (SF) samples have been reported as a guide for future SF-based metabolomics studies. Ultra-filtration allowed identification of 64 metabolites in SF compared with 48 metabolites identified in normal (unfiltered) SF.



Metabolite assignment of ultrafiltered synovial fluid extracted from knee joints of reactive arthritis patients using high resolution NMR spectroscopy 30-43

D. Dubey, S. Chaurasia, A. Guleria, S. Kumar, D. R. Modi, R. Misra and D. Kumar

# Letter - application note

Monitoring of hydrogenation by benchtop nmr with parahydrogen-induced polarization

44-48

K. Jeong, S. Min, H. Chae and S. K. Namgoong

# Letter - spectral assignments

A new asymmetric diketopiperazine dimer from the sponge-associated fungus  $Aspergillus\ versicolor\ 16F-11$ 

49-54

B.-B. Gu, Y.-H. Gui, L. Liu, Z.-Y. Su, W.-h. Jiao, L. Li, F. Sun, S.-P. Wang, F. Yang and H.-W. Lin

 $^1H$  and  $^{13}C$  NMR assignments for (N-Methyl)-(–)-( $\alpha$ ) isosparteinium iodide and (N-Methyl)-(–)-sparteinium iodide

55-64

K. Kolahdouzan, O. M. Ogba and D. J. O'Leary

# MRC

#### Information for subscribers

MRC is published in 12 issues per year. Institutional subscription prices for 2019 are: Print & Online: US\$15905 (US and Rest of World), €10263 (Europe), £8118 (UK). Prices are exclusive of tax. Asia-Pacific GST, Canadian GST/HST and European VAT will be applied at the appropriate rates. For more information on current tax rates, please go to www.wileyonlinelibrary.com/tax-vat. The price includes online access to the current and all online back files to January 1st 2015, where available. For other pricing options, including access information and terms and conditions, please visit https://onlinelibrary.wiley.com/library-info/products/price-lists.

#### **Delivery terms and legal title**

Where the subscription price includes print issues and delivery is to the recipient's address, delivery terms are Delivered at Place (DAP); the recipient is responsible for paying any import duty or taxes. Title to all issues transfers FOB our shipping point, freight prepaid. We will endeavour to fulfil claims for missing or damaged copies within six months of publication, within our reasonable discretion and subject to availability.

#### **PSC**

**Back issues:** Single issues from current and recent volumes are available at the current single issue price from cs-journals@wiley.com. Earlier issues may be obtained from Periodicals Service Company, 351 Fairview Avenue – Ste 300, Hudson, NY 12534, USA. Tel: +1 518 822-9300, Fax: +1 518 822-9305, Email: psc@periodicals.com

#### Contact details

**Journal Customer Services:** For ordering information, claims and any enquiry concerning your journal subscription please go to https://hub.wiley.com/community/support/onlinelibrary or contact your nearest office.

**Americas:** Email: cs-journals@wiley.com; Tel: +1 781 388 8598 or +1 800 835 6770 (toll free in the USA & Canada).

**Europe, Middle East and Africa:** Email: cs-journals@wiley.com; Tel: +44 (0) 1865 778315.

Asia Pacific: Email: cs-journals@wiley.com; Tel: +65 6511 8000. Japan: For Japanese speaking support, Email: cs-japan@wiley.com;

**Visit our Online Customer Help** available in 7 languages at https://hub.wiley.com/community/support/onlinelibrary

**Production Editor:** Chona M. Hilferty (MRCProofs@wiley.com)

#### **Copyright and copying (in any format)**

Copyright © 2019 John Wiley & Sons, Ltd. All rights reserved. No part of this publication may be reproduced, stored or transmitted in any form or by any means without the prior permission in writing from the copyright holder. Authorization to photocopy items for internal and personal use is granted by the copyright holder for libraries and other users registered with their local Reproduction Rights Organisation (RRO), e.g. Copyright Clearance Center (CCC), 222 Rosewood Drive, Danvers, MA 01923, USA (www.copyright.com), provided the appropriate fee is paid directly to the RRO. This consent does not extend to other kinds of copying such as copying for general distribution, for advertising and promotional purposes, for republication, for creating new collective works or for resale. Permissions for such reuse can be obtained using the RightsLink "Request Permission" link on Wiley Online Library. Special requests should be addressed to: permissions@wiley.com

#### Disclaimer

The Publisher and Editors cannot be held responsible for errors or any consequences arising from the use of information contained in this journal; the views and opinions expressed do not necessarily reflect those of the Publisher

the views and opinions expressed do not necessarily reflect those of the Publisher and Editors, neither does the publication of advertisements constitute any endorsement by the Publisher and Editors of the products advertised.

#### **Abstracting and indexing services**

The Journal is indexed by Academic OneFile (GALE Cengage), Advanced Polymers Abstracts (ProQuest), Aerospace & High Technology Database (ProQuest), ANTE: Abstracts in New Technologies & Engineering (ProQuest), CAS: Chemical Abstracts Service (ACS), Ceramic Abstracts/World Ceramic Abstracts (ProQuest), ChemWeb (ChemIndustry.com), Computer & Information Systems Abstracts (ProQuest), CrossFire Beilstein (Elsevier), CSA Civil Engineering Abstracts (ProQuest), CSA Corrosion Abstracts (ProQuest), CSA Engineering Research Database (ProQuest), CSA Materials Business File (ProQuest), CSA Materials Research Database with METADEX (ProQuest), CSA Mechanical & Transportation Engineering Abstracts (ProQuest), CSA Technology Research Database (ProQuest), Current Contents: Physical, Chemical & Earth Sciences (Thomson Reuters), Earthquake Engineering Abstracts (ProQuest), Electronics & Communications Abstracts (ProQuest) Health Reference Center Academic (GALE Cengage), Index Medicus/ MEDLINE (NLM), InfoTrac, INSPEC (IET), MEDLINE/PubMed (NLM), METADEX (ProQuest), Natural Products Update (RSC), ProQuest Central (ProQuest), ProQuest Central: Professional Edition (ProQuest), ProQuest Health & Medical Complete (ProQuest), ProQuest SciTech Collection (ProOuest), Science Citation Index (Thomson Reuters), Science Citation Index Expanded (Thomson Reuters), SCOPUS (Elsevier), SIIC Databases (Sociedad Iberoamericana de Informacion Cientifica), VINITI (All-Russian Institute of Science & Technological Information).

#### **Online Open**

*MRC* accepts articles for Open Access publication. Please visit https://authorservices.wiley.com/author-resources/Journal-Authors/open-access/onlineopen.html for further information about OnlineOpen.

#### Manuscript submission

For submission instructions, subscription and all other information visit: wileyonlinelibrary.com/journal/mrc

#### Wiley's corporate citizenship initiative statement

Wiley's Corporate Citizenship initiative seeks to address the environmental, social, economic, and ethical challenges faced in our business and which are important to our diverse stakeholder groups. Since launching the initiative, we have focused on sharing our content with those in need, enhancing community philanthropy, reducing our carbon impact, creating global guidelines and best practices for paper use, establishing a vendor code of ethics, and engaging our colleagues and other stakeholders in our efforts.

Follow our progress at www.wiley.com/go/citizenship

#### **Statement on Research4Life**

Wiley is a founding member of the UN-backed HINARI, AGORA, and OARE initiatives. They are now collectively known as Research4Life, making online scientific content available free or at nominal cost to researchers in developing countries. Please visit Wiley's Content Access – Corporate Citizenship site: http://www.wiley.com/WileyCDA/Section/id-390082.html

#### **Note to NIH grantees**

Pursuant to NIH mandate, Wiley Blackwell will post the accepted version of contributions authored by NIH grant-holders to PubMed Central upon acceptance. This accepted version will be made publicly available 12 months after publication. For further information, see www.wiley.com/go/nihmandate.

#### **Printer detail**

Printed in the UK by Hobbs.