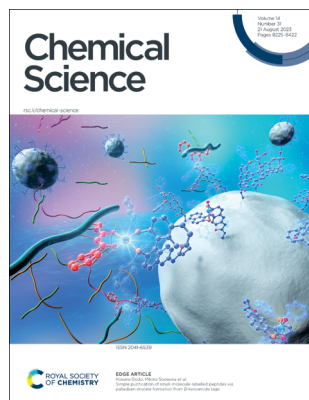


IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(31) 8225–8422 (2023)



Cover

See Kosuke Dodo, Mikiko Sodeoka *et al.*, pp. 8249–8254.
Image reproduced by permission of Kosuke Dodo and Mikiko Sodeoka from *Chem. Sci.*, 2023, 14, 8249.



Inside cover

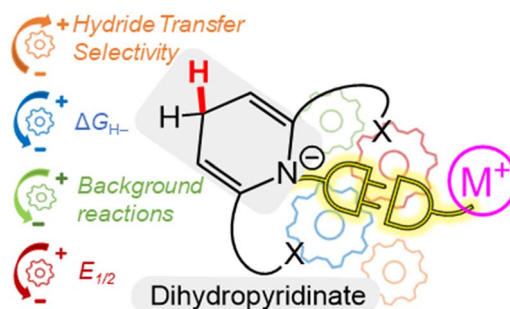
See Bina Fu, Xueming Yang, Kaijun Yuan *et al.*, pp. 8255–8261.
Image reproduced by permission of Kaijun Yuan from *Chem. Sci.*, 2023, 14, 8255.

PERSPECTIVE

8234

Metallated dihydropyridinates: prospects in hydride transfer and (electro)catalysis

Leo W. T. Parsons and Louise A. Berben*

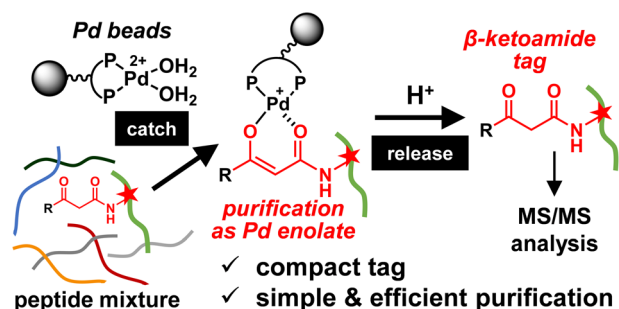


EDGE ARTICLES

8249

Simple purification of small-molecule-labelled peptides via palladium enolate formation from β -ketoamide tags

Kenji Hayamizu, Kota Koike, Kosuke Dodo,*
Miwako Asanuma, Hiromichi Egami and Mikiko Sodeoka*



Editorial Staff

Executive Editor

May Copsey

Deputy Editor

Samantha Apps

Senior Editor

James Moore

Scientific Editors

Ellis Crawford, Jingtao Huang, Esther Johnston, Sophie Orchard, Richard Thompson and Amy Welch

Editorial Assistant

Karina Webster

Publishing Assistant

David Bishop

For queries about submitted articles please contact James Moore, Senior Editor, in the first instance. E-mail chemicalscience@rsc.org

For pre-submission queries please contact May Copsey, Executive Editor. E-mail chemicalscience-rsc@rsc.org

Chemical Science (electronic: ISSN 2041-6539) is published 48 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK.

Chemical Science is a Gold Open Access journal and all articles from 2015 onwards are free to read.

Please email orders@rsc.org to register your interest or contact Royal Society of Chemistry Order Department, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK

Tel +44 (0)1223 432398; E-mail orders@rsc.org

Whilst this material has been produced with all due care, the Royal Society of Chemistry cannot be held responsible or liable for its accuracy and completeness, nor for any consequences arising from any errors or the use of the information contained in this publication. The publication of advertisements does not constitute any endorsement by the Royal Society of Chemistry or Authors of any products advertised. The views and opinions advanced by contributors do not necessarily reflect those of the Royal Society of Chemistry which shall not be liable for any resulting loss or damage arising as a result of reliance upon this material. The Royal Society of Chemistry is a charity, registered in England and Wales, Number 207890, and a company incorporated in England by Royal Charter (Registered No. RC000524), registered office: Burlington House, Piccadilly, London W1J 0BA, UK, Telephone: +44 (0) 207 4378 6556.

Advertisement sales:

Tel +44 (0) 1223 432246; Fax +44 (0) 1223 426017;

E-mail advertising@rsc.org

For marketing opportunities relating to this journal, contact marketing@rsc.org

Chemical Science

rsc.li/chemical-science

Editorial Board

Editor-in-Chief

Andrew Cooper, University of Liverpool

Associate Editors

Vincent Artero, CEA-Grenoble
Luis M. Campos, Columbia University
Michelle Chang, University of California, Berkeley
Lin X. Chen, Northwestern University
Graeme Day, University of Southampton
Serena DeBeer, Max Planck Institute for Chemical Energy Conversion

Mircea Dincă, MIT

François Gabbai, Texas A&M University
Subi George, JNCASR
Ryan Gilmour, WWU Münster
Jinlong Gong, Tianjin University
Stephen Goldup, University of Birmingham
Zaiping Guo, University of Adelaide
Christopher A. Hunter, University of Cambridge
Malika Jefferies-EL, Boston University
Ning Jiao, Peking University
Tanja Junkers, Monash University

Hemamala Karunadasa, Stanford University
Maja Köhn, University of Freiburg
Yi-Tao Long, Nanjing University
Gabriel Merino, CINVESTAV Merida
James K. McCusker, Michigan State University
Thomas Meade, Northwestern University
Paolo Melchiorre, University of Bologna
Carsten Schultz, Oregon Health & Science University
Dmitri Talapin, The University of Chicago
Toshiharu Teranishi, Kyoto University
Andrei Yudin, University of Toronto

Advisory Board

Dave Adams, University of Glasgow
Ayyappanpillai Ajayaghosh, NIIST
Ulf-Peter Apfel, Ruhr-University Bochum
Polly Arnold, University of California, Berkeley
Xinhe Bao, Dalian Institute of Chemical Physics
Zhenan Bao, Stanford University
Gonçalo Bernardes, University of Cambridge
Frank Biedermann, Karlsruhe Institute of Technology
Donna Blackmond, Scripps Research Institute
Jeffrey Bode, ETH Zurich
Jennifer S. Brodbelt, University of Texas at Austin, USA
Christopher Chang, University of California, Berkeley
Chi-Ming Che, University of Hong Kong
Jun Chen, Nankai University
R. Graham Cooks, Purdue University
Christophe Copéret, ETH Zurich
Eugenio Coronado, University of Valencia
Leroy Cronin, University of Glasgow
James Crowley, University of Otago
Christopher C. Cummins, Massachusetts Institute of Technology
Ben Davis, University of Oxford
Jillian Dempsey, University of North Carolina at Chapel Hill
Kazunari Domen, University of Tokyo
James Durrant, Imperial College London
Xinlang Feng, TU Dresden
Ben Feringa, University of Groningen
Makoto Fujita, University of Tokyo
Phillip Gale, University of Technology Sydney
Song Gao, Peking University
Jeremiah Gassensmith, University of Texas at Dallas
Elizabeth Gibson, Newcastle University
Hubert Girault, EPFL
Frank Glorius, WWU Münster
Leticia González, University of Vienna
Duncan Graham, University of Strathclyde

Vicki Grassian, University of California, San Diego
Alexis Grimaud, Boston College
Christian Hackenberger, FMP Berlin
Buxing Han, Chinese Academy of Sciences
Christy Haynes, University of Minnesota
Patrick Holland, Yale University
Kim Jelfs, Imperial College London
Yousung Jung, KAIST
Stephanie Kath-Schorr, University of Cologne
Takashi Kato, University of Tokyo
Christopher Kelly, Janssen Research & Development
Jérôme Lacour, University of Geneva
Ai-Lan Lee, Heriot-Watt University
Daniele Leonori, RWTH Aachen University
Chao-Jun Li, McGill University
Yi Li, Jilin University
Mi Hee Lim, KAIST
Wenbin Lin, University of Chicago
Kopin Liu, Academia Sinica
Watson Loh, UNICAMP
Bettina Lotsch, Max Planck Institute
Xiong Wen (David) Lou, Nanyang Technological University
Kazuhiko Maeda, Tokyo Institute of Technology
Satoshi Maeda, Hokkaido University
Swadhin Mandal, IISER Kolkata
Ellen Matson, University of Rochester
Scott Miller, Yale University
Daniel Mindiola, University of Pennsylvania
Wonwoo Nam, Ewha Womans University
Jonathan Nitschke, University of Cambridge
Allie Obermeyer, Columbia University
Martin Oestreich, Technical University of Berlin
Takashi Ooi, Nagoya University
Rachel O'Reilly, University of Birmingham
Oleg Ozerov, Texas A&M University
Xiulian Pan, Dalian Institute of Chemical Physics
Nicolas Plummer, Technical University of Munich
Rasmita Raval, University of Liverpool
Erwin Reisner, University of Cambridge
Andrea Rentmeister, WWU Münster
Jeffrey Rinehart, University of California, San Diego
Stuart Rowan, University of Chicago
Richmond Sarpong, University of California, Berkeley
Danielle Schultz, Merck
Dwight Seferos, University of Toronto
Oliver Seitz, Humboldt University of Berlin
Roberta Sessoli, University of Florence
Kay Severin, Federal Polytechnic School of Lausanne
Mikiko Sodeoka, RIKEN
Galo Soler-Illia, Universidad Nacional de San Martin
David Spring, University of Cambridge
Brian Stoltz, California Institute of Technology
Brent Sumerlin, University of Florida
Raghavan B. Sunoj, IIT Bombay
Yogesh Surendranath, MIT
Mizuki Tada, Nagoya University
Ben Zhong Tang, The Chinese University of Hong Kong
Zhiyong Tang, National Center for Nanoscience and Nanotechnology
Christine Thomas, Ohio State University
He Tian, East China University of Science & Technology
Zhong-Qun Tian, Xiamen University
F. Dean Toste, University of California, Berkeley
Takashi Uemura, University of Tokyo
Jan van Hest, Radboud University
Latha Venkataraman, Columbia University
Chu Wang, Peking University
Julia Weinstein, University of Sheffield
Tom Welton, Imperial College London
Charlotte Williams, University of Oxford
Vivian Yam, University of Hong Kong
Qi-Lin Zhou, Nankai University
Jenny Zhang, University of Cambridge

Information for Authors

Full details on how to submit material for publication in Chemical Science are given in the Instructions for Authors (available from <http://www.rsc.org/authors>). Submissions should be made via the journal's homepage: rsc.li/chemical-science

Authors may reproduce/republish portions of their published contribution without seeking permission from the Royal Society of Chemistry, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation)–Reproduced by permission of the Royal Society of Chemistry.

This journal is © The Royal Society of Chemistry 2023.

Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

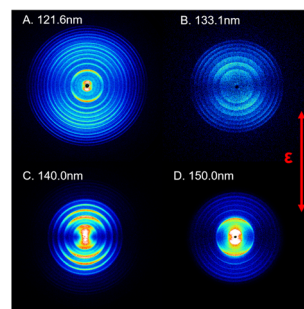
Registered charity number: 207890



8255

Vacuum ultraviolet photodissociation of sulfur dioxide and its implications for oxygen production in the early Earth's atmosphere

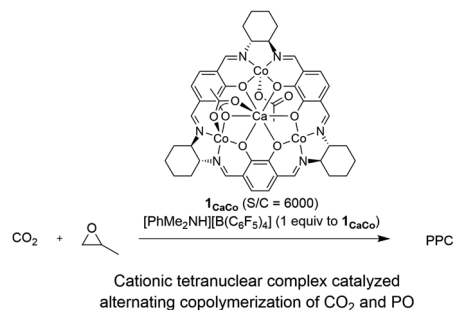
Yao Chang, Yanlin Fu, Zhichao Chen, Zijie Luo, Yarui Zhao, Zhenxing Li, Weiqing Zhang, Guorong Wu, Bina Fu,^{*} Dong H. Zhang, Michael N. R. Ashfold, Xueming Yang^{*} and Kaijun Yuan^{*}



8262

Cationic tetranuclear macrocyclic CaCo_3 complexes as highly active catalysts for alternating copolymerization of propylene oxide and carbon dioxide

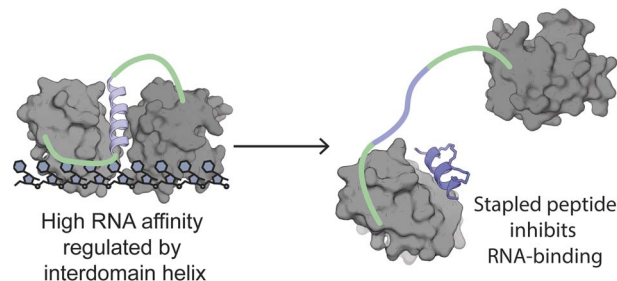
Haruki Nagae, Saki Matsushiro, Jun Okuda^{*} and Kazushi Mashima^{*}



8269

Rationally designed stapled peptides allosterically inhibit PTBP1–RNA-binding

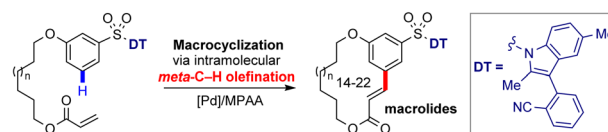
Stefan Schmeing, Gulshan Amrahova, Katrin Bigler, Jen-Yao Chang, Joseph Openy, Sunit Pal, Laura Posada, Raphael Gasper and Peter 't Hart^{*}



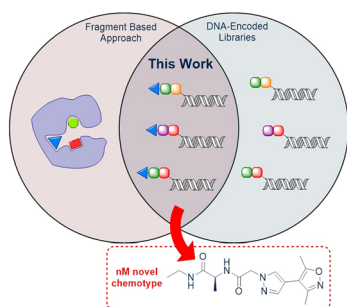
8279

Macrocyclization via remote *meta*-selective C–H olefination using a practical indolyl template

Pengfei Zhang, Zhiwei Jiang, Zhoulong Fan, Guoshuai Li, Qingxue Ma, Jun Huang, Jinghong Tang, Xiaohua Xu,^{*} Jin-Quan Yu^{*} and Zhong Jin^{*}



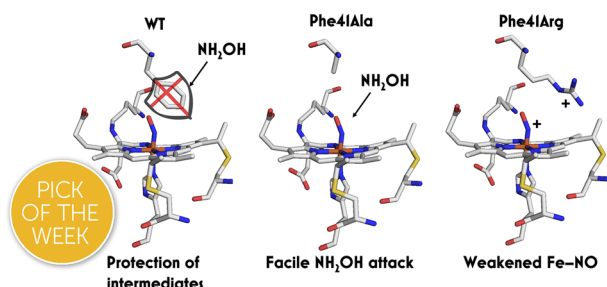
8288



Fragment expansion with NUDELs – poised DNA-encoded libraries

Catherine L. A. Salvini, Benoit Darlot, Jack Davison, Mathew P. Martin, Susan J. Tudhope, Shannon Turberville, Akane Kawamura, Martin E. M. Noble, Stephen R. Wedge, James J. Crawford and Michael J. Waring*

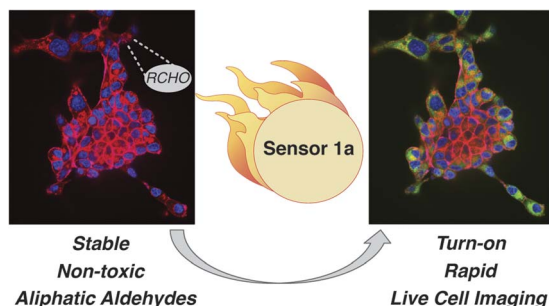
8295



Outer coordination sphere influences on cofactor maturation and substrate oxidation by cytochrome P460

Melissa M. Bollmeyer, Sean H. Majer, Rachael E. Coleman and Kyle M. Lancaster*

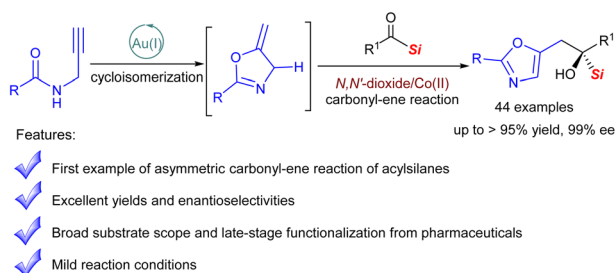
8305



Chemical sensors for imaging total cellular aliphatic aldehydes in live cells

Rachel Wills, Jonathan Farhi, Patrick Czabala, Sophia Shahin, Jennifer M. Spangle and Monika Raj*

8315



Bimetallic tandem catalysis-enabled enantioselective cycloisomerization/carbonyl-ene reaction for construction of 5-oxazoylmethyl α -silyl alcohol

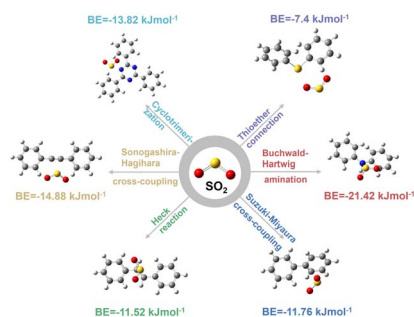
Xinpeng Sang, Yuhao Mo, Shiya Li, Xiaohua Liu, Weidi Cao* and Xiaoming Feng*



8321

Feasible bottom-up development of conjugated microporous polymers (CMPs) for boosting the deep removal of sulfur dioxide

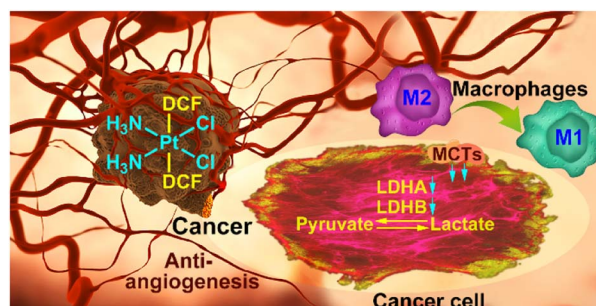
He Li, Hanqian Pan, Yijian Li, Shuaishuai Shang, Shihui Huang, Xili Cui,* Jun Hu* and Honglai Liu



8327

Regulating tumor glycometabolism and the immune microenvironment by inhibiting lactate dehydrogenase with platinum(IV) complexes

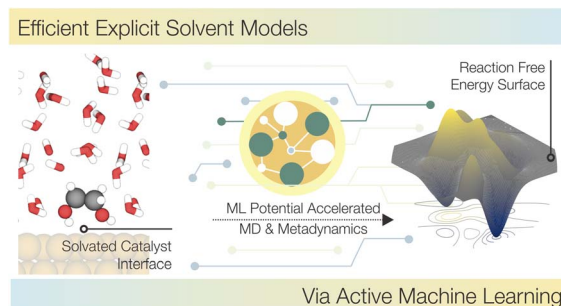
Suxing Jin, Enmao Yin, Chenyao Feng, Yuewen Sun, Tao Yang, Hao Yuan, Zijian Guo and Xiaoyong Wang*



8338

Accelerating explicit solvent models of heterogeneous catalysts with machine learning interatomic potentials

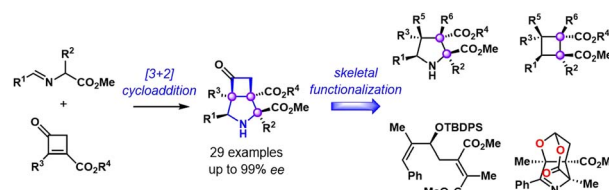
Benjamin W. J. Chen,* Xinglong Zhang* and Jia Zhang



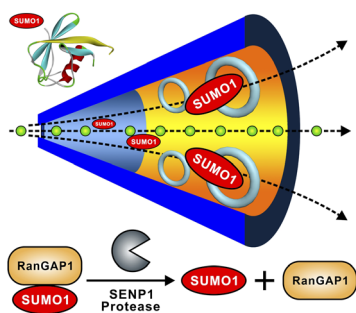
8355

Enantioselective [3+2]-cycloaddition of 2,3-disubstituted cyclobutenones: vicinal quaternary stereocenters construction and skeletal functionalization

Licheng Lu and Ping Lu*



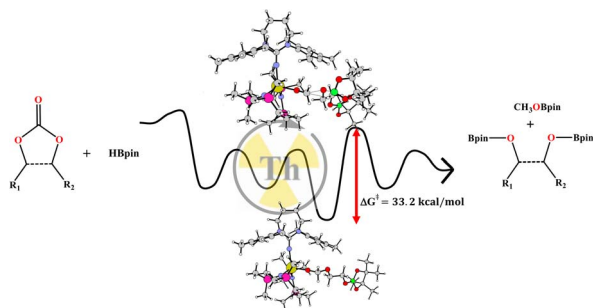
8360



A highly sensitive nanochannel device for the detection of SUMO1 peptides

Yue Qin, Xiaoyu Zhang, Yanling Song, Bowen Zhong, Lu Liu, Dongdong Wang, Yahui Zhang, Wenqi Lu, Xinjia Zhao, Zhiqi Jia, Minmin Li, Lihua Zhang* and Guangyan Qing*

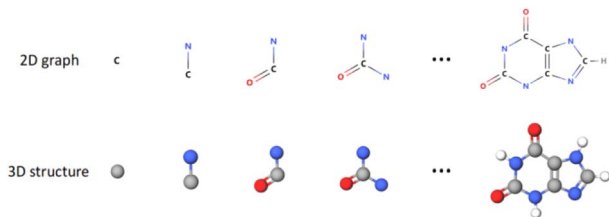
8369



Catalytic regeneration of metal-hydrides from their corresponding metal-alkoxides via the hydroboration of carbonates to obtain methanol and diols

Hemanta Deka, Ida Ritacco, Natalia Fridman, Lucia Caporaso* and Moris S. Eisen*

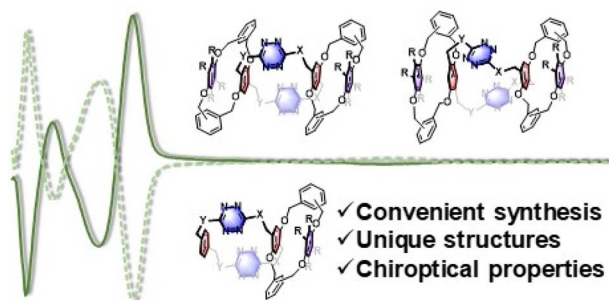
8380



An equivariant generative framework for molecular graph-structure Co-design

Zaixi Zhang, Qi Liu,* Chee-Kong Lee, Chang-Yu Hsieh and Enhong Chen

8393



Tetrahomo corona[4]arene-based spirophanes: synthesis, structure, and properties

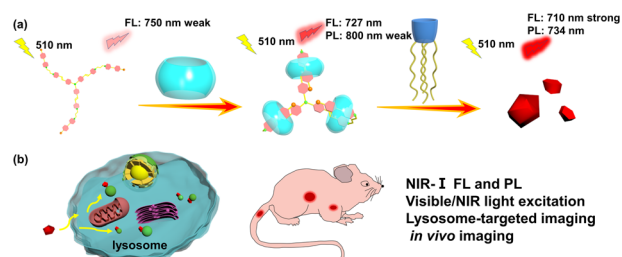
Shen-Yi Guo, Zhuo-Ang Zhang, Shuo Tong,* Qing-Hui Guo, Ruimao Hua and Mei-Xiang Wang*



8401

Conformationally confined three-armed supramolecular folding for boosting near-infrared biological imaging

Hui-Juan Wang, Meng-Meng Zheng, Wen-Wen Xing, Yong-Xue Li, Yao-Yao Wang, Hongjie Zhu, Ying-Ming Zhang,* Qilin Yu* and Yu Liu*



8408

The H-NOX protein structure adapts to different mechanisms in sensors interacting with nitric oxide

Byung-Kuk Yoo, Sergei G. Kruglik, Jean-Christophe Lambry, Isabelle Lamarre, C. S. Raman, Pierre Nioche and Michel Negrerie*

