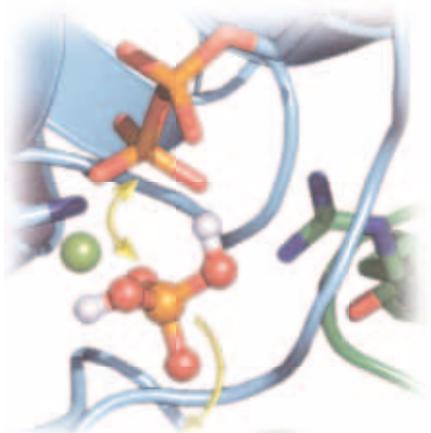




6–10 September 2015

Ruhr-University Bochum • RUB Conference Center



# 16<sup>th</sup> European Conference on the Spectroscopy of Biological Molecules



**PROGRAM**

RUHR  
UNIVERSITÄT  
BOCHUM

**RUB**

RESEARCH DEPARTMENT  
Protein





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Dear Colleagues,

It is my pleasure to welcome you to the 16<sup>th</sup> European Conference on the Spectroscopy of Biological Molecules (ECSBM) to be held from 6<sup>th</sup> September–10<sup>th</sup> September 2015, at Ruhr-University Bochum, Germany.

The European Conference on the Spectroscopy of Biological Molecules (ECSBM) provides a platform for a multidisciplinary community developing a wide range of spectroscopic techniques (IR, Raman, UV-Vis, fluorescence, NMR, EPR) applied to biological molecules. Special topics of the 16<sup>th</sup> ECSBM are molecular reaction mechanisms of proteins and their interactions. In addition novel marker-free imaging techniques for diagnostics in personalized medicine will be presented.

Looking forward to seeing you in Bochum for cutting edge talks, fruitful discussions and a nice come-together.

Klaus Gerwert  
Chairman – ECSBM 2015  
Chair of Biophysics  
Ruhr-University Bochum  
[www.ecsbm2015.de](http://www.ecsbm2015.de)  
[ECSBM2015@bph.rub.de](mailto:ECSBM2015@bph.rub.de)

Venue

Ruhr-University Bochum  
 RUB Conference Center  
 Universitätsstraße 150  
 44801 Bochum, Germany

Date

6<sup>th</sup>–10<sup>th</sup> September 2015

Conference Chair

Prof. Dr. Klaus Gerwert  
 Chair of Biophysics  
 Dept. of Biology and Biotechnology  
 Ruhr-University Bochum  
 Universitätsstraße 150  
 44801 Bochum, Germany

Members of the ECSBM European Committee

Simion Astilean (Babes-Bolyai University, Cluj-Napoca, Romania)  
 Andreas Barth (Stockholm University, Sweden)  
 Luís Batista de Carvalho (University of Coimbra, Portugal)  
 Vladimír Baumruk (Charles University, Prague, Czech Republic)  
 Manuel Dauchez (University of Reims Champagne-Ardenne, France)  
 Roman Efremov (M. M. Shemyakin & Yu. A. Ovchinnikov Institute of Bioorganic Chemistry, Moscow, Russia)  
 Klaus Gerwert (Ruhr-University Bochum, Germany)  
 Karin Hauser (University of Konstanz, Germany)  
 Joachim Heberle (Free University of Berlin, Germany)  
 Belen Hernández (Group of Molecular Biophysics, University of Paris 13, France)  
 Neil Hunt (University of Strathclyde, Glasgow, Great Britain)  
 Nerea Iza (Universidad Complutense de Madrid, Spain)  
 Zoltán Kóta (Biological Research Centre, Szeged, Hungary)  
 Matteo Levantino (University of Palermo, Italy)  
 Maria Paula Marques (University of Coimbra, Portugal)  
 Anthony Parker (Rutherford Appleton Laboratory, Swindon, Great Britain)  
 Eftychia Pinakoulaki (University of Cyprus, Nicosia, Cyprus)  
 Susan Quinn (University College Dublin, Ireland)  
 Maria-Paz Sevilla (Complutense University of Madrid, Spain)  
 Armida Torreggiani (ISOF – CNR, Bologna, Italy)  
 Sander Woutersen (University of Amsterdam, The Netherlands)

### Local Organizing Committee, Ruhr-University Bochum

Klaus Gerwert (Chairman – ECSBM 2015)

Gerd Kock (Chairman Assistance)

Riccarda Aust

Ekaterina Denisova

Samir El-Mashtoly

Frederik Großerüschkamp

Jörn Güldenhaupt

Angela Kallenbach-Thieltges

Carsten Kötting

Mathias Lübben

Axel Martin

Julian Ollesch

Steffen Wolf

### Congress Management

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### ECSBM Previous Meetings

1985 Reims, France

1987 Freiburg, Germany

1989 Rimini, Italy

1991 York, Great Britain

1993 Loutraki, Greece

1995 Lille, France

1997 Madrid, Spain

1999 Enschede, The Netherlands

2001 Prague, Czech Republic

2003 Szeged, Hungary

2005 Aschaffenburg, Germany

2007 Paris, France

2009 Palermo, Italy

2011 Coimbra, Portugal

2013 Oxford, Great Britain

### Design/Layout

Layout

www.krea.tif-design.de

Print

www.siblog.de

Circulation

300

Editorial Deadline

18<sup>th</sup> August 2015



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info@artphotonics.com  
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Founded: 1998  
Employees: 30

### Invited Speakers

Małgorzata Baranska	Jagiellonian University in Krakow, Poland
Hugh Byrne	Dublin Institute of Technology, Ireland
Max Diem	Northeastern University, Massachusetts, USA
Peter Gardner	University of Manchester, Great Britain
Rainer Hillenbrand	IKERBASQUE. Basque Foundation for Science, Spain
Bernhard Lendl	Technical University Vienna, Austria
Ioan Notingher	University of Nottingham, Great Britain
Anthony Parker	STFC Rutherford Appleton Laboratory, Great Britain
Jürgen Popp	University Jena, Germany
Gerwin Puppels	RiverD International, The Netherlands
Markus Sauer	Biocenter of the University Würzburg, Germany
Heinz-Jürgen Steinhoff	University Osnabrück, Germany
Nick Stone	University of Exeter, Great Britain
Anthony Watts	University of Oxford, Great Britain
Peter Wright	The Scripps Research Institute, La Jolla, California, USA
Xiaoliang Sunney Xie	Harvard University, Massachusetts, USA

### Contributed Speakers

Huib J. Bakker	FOM Institute AMOLF, Amsterdam, The Netherlands
Andreas Barth	Stockholm University, Sweden
Franz Bartl	Charité – Universitätsmedizin Berlin, Germany
Volker Deckert	University Jena, Germany
Peter Gilch	Heinrich Heine University Düsseldorf, Germany
Erik Goormaghtigh	Université libre de Bruxelles, Belgium
Marie Louise Groot	VU University Amsterdam, The Netherlands
Karin Hauser	University Konstanz, Germany
Joachim Heberle	Free University Berlin, Germany
Petra Hellwig	University of Strasbourg, France
Peter Hildebrandt	Technical University Berlin, Germany
John Kennis	VU University Amsterdam, The Netherlands
Janina Kneipp	Humboldt University Berlin, Germany
Christoph Krafft	University Jena, Germany
Werner Mäntele	Goethe University Frankfurt, Germany
Sebastian Schlücker	University Duisburg-Essen, Germany
Josef Wachtveitl	Goethe University Frankfurt, Germany
Roland Winter	Technical University Dortmund, Germany



# Program Overview

9<sup>th</sup> Sept

Hall 2a	Hall 2b
09:00–10:30	
Vibrational Spectroscopy on Proteins IV <i>Jürgen Popp</i> <i>Hugh Byrne</i> <i>Rainer Hillenbrand</i>	
	p. 18

11:00–12:30
Time-Resolved Fluorescence Spectroscopy and beyond <i>Markus Sauer</i> <i>Anthony Watts</i> <i>Anthony Parker</i>
p. 18

13:00–14:00
Lunch Symposium Agilent Technologies Deutschland
<i>Room: Hall 1</i>
p. 18

14:00–15:00	14:00–15:00
Raman / CARS Imaging	Fluorescence & Bio-Spectroscopy
p. 19	p. 19

From 15:15
Guided Half-day Tour German Mining Museum Bochum (Deutsches Bergbau Museum Bochum)
p. 28

10<sup>th</sup> Sept

Hall 2a	Hall 2b
09:00–10:30	
NMR & ESR Spectroscopy & QCL <i>Heinz-Jürgen Steinhoff</i> <i>Peter Wright</i> <i>Bernhard Lendl</i>	
	p. 21

11:00–12:30
Simulations, SERS & Near Field Spectroscopy
p. 21

14:00–15:15	14:00–15:15
IR Imaging	NMR- & Time-Resolved Raman Spectroscopy
p. 22	p. 22

15:30–16:45	15:30–16:45
Time-Resolved FTIR Spectroscopy I	Biomedical Spectroscopy
p. 23	p. 24

17:00–18:15	17:00–18:15
Time-Resolved FTIR Spectroscopy II	Biomolecular Simulations
p. 24	p. 25

From 18:30
Conference Banquet
p. 28

## Legend

<span style="background-color: #c00000; color: white; padding: 2px;"> </span> Invited Lecture
<span style="background-color: #ff8c00; color: white; padding: 2px;"> </span> Contributed Lecture
<span style="background-color: #90ee90; color: white; padding: 2px;"> </span> Selected Lecture
<span style="background-color: #808080; color: white; padding: 2px;"> </span> Short Poster Presentation
<span style="background-color: #00ff00; color: white; padding: 2px;"> </span> Poster Session
<span style="background-color: #ccccff; color: white; padding: 2px;"> </span> Lunch Symposium
<span style="background-color: #add8e6; color: white; padding: 2px;"> </span> Social Program

15<sup>00</sup>–18<sup>00</sup> Satellite Symposium of Collaborative Research Centre 642 “GTP- and  
Hall 2a/b ATP-dependent membrane processes”  
Guests from ECSBM are cordially welcome

16<sup>00</sup>–19<sup>00</sup> Registration ECSBM  
Foyer

19<sup>00</sup>–21<sup>00</sup> Welcome Reception  
Foyer

Scientific Program • Monday, 7<sup>th</sup> September 2015

09<sup>00</sup>–09<sup>15</sup> Welcome  
Hall 2a/b

09<sup>00</sup> Welcome of conference participants  
Prof. Dr. Dr. h. c. Elmar W. Weiler  
Rector of Ruhr-University Bochum

09<sup>05</sup> Welcome of conference participants  
Prof. Dr. Klaus Gerwert  
Chairman of the 16<sup>th</sup> European Conference on the Spectroscopy of  
Biological Molecules (ECSBM)

09<sup>15</sup>–10<sup>30</sup> Biomedical Imaging I  
Hall 2a/b  
Chair K. Gerwert (Bochum/DE)

09<sup>15</sup> IOS Press Sponsored Lecturer  
Coherent Raman scattering – vibrational imaging for biology and  
medicine  
X. S. Xie (Cambridge, MA/US)

10<sup>00</sup> Towards *in vivo*, realtime Raman measurements of biomolecular  
changes associated with disease  
N. Stone (Exeter/GB)

10<sup>30</sup>–11<sup>00</sup> Break

11<sup>00</sup>–12<sup>30</sup> Biomedical Imaging II

Hall 2a/b

Chair X. S. Xie (Cambridge, MA/US)

11<sup>00</sup> Selective-sampling Raman microscopy – towards fast and objective diagnosis of tumours during cancer surgery  
J. Notinger (Nottingham/GB)

11<sup>30</sup> Bringing Raman spectroscopy into the clinic  
G. Puppels (Rotterdam/NL)

12<sup>00</sup> Recent developments in infrared spectral pathology  
P. Gardner (Manchester/GB)

12<sup>30</sup>–14<sup>00</sup> Lunch Break

13<sup>00</sup>–14<sup>00</sup> Lunch Symposium • HORIBA Jobin Yvon GmbH

Hall 1 Raman in Life Sciences – Innovative Tools for Biomedical Applications

**HORIBA**  
Scientific

13<sup>00</sup> Welcome

13<sup>05</sup> Raman in Life Sciences – innovative tools for biomedical applications  
B. Bleisteiner (Bensheim/DE)

13<sup>25</sup> Beyond spectroscopy – combined techniques for a better understanding of molecular processes  
C. David (Villeneuve d'Ascq/FR)

13<sup>50</sup> Questions/discussion

14<sup>00</sup>–15<sup>00</sup> Short Poster Presentation I

Hall 2a/b

Chair K. Gerwert (Bochum/DE)

P51–P57 e. Biomolecular Simulation

P58–P62 f. Marker-free Diagnostics

P82–P84 i. NMR Spectroscopy

P92–P118 m. Biomedical Spectroscopy

15<sup>00</sup>–15<sup>15</sup> Break

**15<sup>15</sup>–16<sup>15</sup> Short Poster Presentation II**

Hall 2a/b

- Chair C. Köttling (Bochum/DE)
- P1–P22 a. Time resolved FTIR Spectroscopy
- P23–P30 b. IR Imaging
- P71–P81 h. Fluorescence Spectroscopy

**16<sup>15</sup>–16<sup>30</sup> Break**
**16<sup>30</sup>–17<sup>30</sup> Short Poster Presentation III**

Hall 2a/b

Chair S. El-Mashtoly (Bochum/DE)

- P31–P36 c. Time resolved Raman Spectroscopy
- P37–P50 d. Raman/CARS Imaging
- P63–P70 g. UV-Vis Spectroscopy
- P85–P87 j. Near Field Spectroscopy
- P88–P90 k. ESR Spectroscopy
- P91 l. Super Resolution Imaging of cells

**17<sup>30</sup>–19<sup>30</sup> Poster Session I (see page 36)**

Foyer + Hall 3

**Poster group A**

- |                              |          |
|------------------------------|----------|
| b. IR Imaging                | P23–P30  |
| e. Biomolecular Simulations  | P51–P57  |
| f. Marker-free Diagnostics   | P58–P62  |
| h. Fluorescence Spectroscopy | P71–P81  |
| i. NMR Spectroscopy          | P82–P84  |
| m. Biomedical Spectroscopy   | P92–P118 |

**Poster group B**

- |                                      |         |
|--------------------------------------|---------|
| a. Time resolved FTIR Spectroscopy   | P1–P22  |
| c. Time resolved Raman Spectroscopy  | P31–P36 |
| d. Raman/CARS Imaging                | P37–P50 |
| g. UV-Vis Spectroscopy               | P63–P70 |
| j. Near Field Spectroscopy           | P85–P87 |
| k. ESR Spectroscopy                  | P88–P90 |
| l. Super Resolution Imaging of cells | P91     |

Poster authors of posters in group A are kindly asked to be present at their poster from 17<sup>30</sup>–18<sup>30</sup> for questions and discussions. Poster authors of posters in group B should present on Tuesday.

09<sup>00</sup>–10<sup>30</sup> Biomedical Imaging III

Hall 2a/b

Chair N. Stone (Exeter/GB)

09<sup>00</sup> Accurate, non-morphological classification of cancers by spectral histopathology – What are the limits?

M. Diem (Boston, MA/US)

09<sup>30</sup> Raman-based identification of circulating tumor cells for cancer diagnostics

C. Krafft (Jena/DE)

10<sup>00</sup> Raman imaging of cells and tissues

M. Baranska (Krakow/PL)

10<sup>30</sup>–11<sup>00</sup> Break

11<sup>00</sup>–12<sup>15</sup> Biomedical Imaging IV

Hall 2a/b

Chair M. Baranska (Krakow/PL)

11<sup>00</sup> Will FTIR imaging ever become a tool in the biomedical field?

J. de Meutter, A. Derenne, K.-M. Derfoufi, M. Guilbert, A. Mignolet  
M. Smolina, M. Verdonck, N. Wald, E. Goormaghtigh (Brussels/BE)

11<sup>20</sup> Study of Alzheimer's diseased tissue by Infrared and Raman microspectroscopies

A. Schirer, C. Klein, L. Meyer, C. Patte-Mensah, A. G. Mensah-Nyagan  
P. Hellwig (Strasbourg/FR)

11<sup>40</sup> Higher-harmonic generation microscopy for in-situ brain tumor pathology

M. Groot, N. Kuzmin, P. Wesseling, H. Baayen,  
P. de Witt Hamer (Amsterdam/NL)

12<sup>00</sup> Lung cancer investigation by FTIR-imaging supported proteomic

F. Großerüschkamp, H. Diehl, A. Kallenbach-Thieltges (Bochum/DE)  
D. Theegarten (Essen/DE), B. Sitek, K. Gerwert (Bochum/DE)

12<sup>15</sup>–13<sup>45</sup> Lunch Break

12<sup>45</sup>–13<sup>45</sup> Lunch Symposium • Renishaw GmbH  
Hall 1 Applications for Bio and Transmission Raman



12<sup>45</sup> Raman Spectroscopy in Biology  
M. Richter (Pliezhausen/DE)

13<sup>00</sup> Raman microscopic imaging for chemical and morphological tissue characterization  
C. Krafft (Jena/DE)

13<sup>30</sup> Fast, quantitative analysis of large volume bulk mixtures using transmission raman spectroscopy  
M. Kölbach (Pliezhausen/DE)

13<sup>45</sup>–15<sup>05</sup> Vibrational Spectroscopy on Proteins I

Hall 2a/b

Chair

M. Diem (Boston, MA/US)

13<sup>45</sup> Observation of structured water at anti-freeze protein surfaces using surface sum-frequency generation  
H. Bakker, K. Meister, S. Strazdaite (Amsterdam/NL)

14<sup>05</sup> Proton-coupled electron transfer constitutes the photoactivation mechanism of the plant photoreceptor UVR8  
J. Kennis (Amsterdam/NL)

14<sup>25</sup> Pressure-jump relaxation studies of biomolecular processes and reactions  
R. Winter (Dortmund/DE)

14<sup>45</sup> Modulation of the signal transduction in bathy phytochromes via photo-induced and thermal cofactor isomerisations – a vibrational spectroscopic study  
F. Velázquez Escobar, P. Piwowarski, N. Michael, J. Salevski  
M. Fernandez Lopez, M. A. Mroginski, F. Bartl (Berlin/DE)  
F. Siebert (Berlin, Freiburg/DE), P. Scheerer, P. Hildebrandt (Berlin/DE)

15<sup>05</sup>–15<sup>25</sup> Break

15<sup>25</sup>–16<sup>45</sup> Vibrational Spectroscopy on Proteins II

Hall 2a/b

Chair I. Notingher (Nottingham/GB)

15<sup>25</sup>  $\beta$ -sheet folding and aggregation studied by time-resolved

IR-spectroscopy

A. Popp, B. Heck (Konstanz/DE), L. Wu

T. A. Keiderling (Chicago, IL/US), K. Hauser (Konstanz/DE)

15<sup>45</sup> The mechanism of ion-conducting pore formation and gating in

Channelrhodopsin-2

F. Bartl, J. Kuhne, K. Eisenhauer (Berlin/DE), E. Ritter (Bochum/DE)

P. Hegemann (Berlin/DE), K. Gerwert (Bochum/DE)

16<sup>05</sup> Primary reaction of microbial rhodopsins

J. Wachtveitl, E. Bühl, E. Bamberg, C. Bamann

C. Glaubnitz (Frankfur a. M./DE)

16<sup>25</sup> Symbiosis between density functional theory and vibrational spectroscopy – a study of dephosphorylation of the calcium pump

A. Barth (Stockholm/SE)

16<sup>45</sup>–17<sup>00</sup> Break

17<sup>00</sup>–18<sup>00</sup> Vibrational Spectroscopy on Proteins III

Hall 2a/b

Chair P. Gardner (Manchester/GB)

17<sup>00</sup> Spectroscopists do it with light – on the development of optical

sensors for medical diagnostics

W. Mäntele (Frankfurt a. M./DE)

17<sup>20</sup> One- and two-photon NIR-excited surface enhanced Raman

scattering to probe complex biological environments

J. Kneipp, T. Büchner, D. Drescher, Z. Heiner, M. Gühlke

F. Madzharova, V. Merk (Berlin/DE)

17<sup>40</sup> Femtosecond spectroscopy of psoralen-DNA-intercalates

S. Fröbel, A. Reiffers, C. Torres Ziegenbein, P. Gilch (Düsseldorf/DE)

18<sup>00</sup>–20<sup>00</sup> Poster Session II (see page 36)

Foyer + Hall 3

**Poster group A**

b. IR Imaging	P23–P30
e. Biomolecular Simulations	P51–P57
f. Marker-free Diagnostics	P58–P62
h. Fluorescence Spectroscopy	P71–P81
i. NMR Spectroscopy	P82–P84
m. Biomedical Spectroscopy	P92–P118

**Poster group B**

a. Time resolved FTIR Spectroscopy	P1–P22
c. Time resolved Raman Spectroscopy	P31–P36
d. Raman/CARS Imaging	P37–P50
g. UV-Vis Spectroscopy	P63–P70
j. Near Field Spectroscopy	P85–P87
k. ESR Spectroscopy	P88–P90
l. Super Resolution Imaging of cells	P91

Poster authors of posters in group B are kindly asked to be present at their poster from 18<sup>00</sup>–19<sup>00</sup> for questions and discussions.

09<sup>00</sup>–10<sup>30</sup> Vibrational Spectroscopy on Proteins IV

Hall 2a/b

Chair A. Watts (Oxford/GB)

09<sup>00</sup> Clinical Raman spectroscopy

J. Popp (Jena/DE)

09<sup>30</sup> Biomedical applications of vibrational spectroscopy: disease diagnostics and beyond

H. Byrne (Dublin/IE)

10<sup>00</sup> Nano-FTIR spectroscopy of individual protein complexes

R. Hillenbrand (Donostia-San Sebastián/ES)

10<sup>30</sup>–11<sup>00</sup> Break

11<sup>00</sup>–12<sup>30</sup> Time-Resolved Fluorescence Spectroscopy and beyond

Hall 2a/b

Chair M. Groot (Amsterdam/NL)

11<sup>00</sup> dSTORM coming of age – from concepts to biological impact

M. Sauer (Würzburg/DE)

11<sup>30</sup> Multiple spectroscopies to unravel the complexities of GPCR-mediated cell signaling

A. Watts (Oxford/GB)

12<sup>00</sup> Spatially offset Raman spectroscopy in the pursuit of transcutaneous detection of bone disease

A. Parker (Oxfordshire/GB)

12<sup>30</sup>–14<sup>00</sup> Lunch Break

12<sup>45</sup>–13<sup>45</sup> Lunch Symposium • Agilent Technologies

Hall 1

Deutschland GmbH

Introducing a Revolutionary Technique to Achieve Highest Spatial Resolution in FTIR Imaging



12<sup>45</sup> Introduction/Short overview Agilent

C. Fiedler (Berlin/DE)

- 13<sup>00</sup> Introducing a revolutionary technique to achieve highest spatial resolution in FTIR imaging  
M. Börger (Bochum/DE)
- 14<sup>00</sup>–15<sup>00</sup> **Raman/CARS Imaging**  
Hall 2a  
Chair C. Krafft (Jena/DE)
- 14<sup>00</sup> *In vitro* evaluation of targeted therapy response in cancer cells by label-free Raman spectral imaging  
S. El-Mashtoly, H. Yosef, L. Mavarani, D. Petersen, C. Kötting  
K. Gerwert (Bochum/DE)
- 14<sup>15</sup> AFM and Raman mapping of neural stem cells before and after differentiation  
F. Sinjab, I. Notingham, R. Boitor (Nottingham/GB)
- 14<sup>30</sup> Theoretical and experimental SERS study of thiocarbonyl compounds adsorbed on metal nanoparticles  
J. L. Castro, J. Roman-Perez, J. C. Otero, M. R. Lopez-Ramirez (Málaga/ES)
- 14<sup>45</sup> Identification of micro-organisms by surface enhanced Raman spectroscopy  
R. Chauvet (Le Mans, Nantes/FR), T. Charrier (Nantes/FR), F. Lagarde  
P. Daniel (Le Mans/FR), G. Thouand (La Roche-sur-Yon/FR)
- 14<sup>00</sup>–15<sup>00</sup> **Fluorescence & Bio-Spectroscopy**  
Hall 2b  
Chair M. Sauer (Würzburg/DE)
- 14<sup>00</sup> Spectroscopic analysis of amyloid  $\beta$  peptide self-association during sedimentation velocity centrifugation  
C. Decker, M. Wolff (Düsseldorf/DE), L. Nagel-Steger  
D. Willbold (Jülich, Düsseldorf/DE)
- 14<sup>15</sup> Time-resolved photoluminescence spectroscopy for the investigation of state transitions in photosynthesis  
I. Bargigia (Milano/IT), M. Ballottari, M. Bressan (Verona/IT), M. Alcocer  
D. Viola, G. Cerullo, C. D'Andrea (Milano/IT), R. Bassi  
L. Dall'Osto (Verona/IT)

- 14<sup>30</sup> Advanced fluorescence based approaches to study proteins in cell-like environments  
J. Fitter (Aachen, Jülich/DE)
- 14<sup>45</sup> An artificial membrane system tailored for the surface-enhanced infrared spectroscopic investigation of membrane proteins  
J. Kozuch, S. Wiebalck, C. C. Tzschucke (Berlin/DE)  
L. J. C. Jeuken (Leeds/GB), P. Hildebrandt (Berlin/DE)
- 16<sup>00</sup>–19<sup>00</sup> Guided Half-day Tour (see page 28)  
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- 09<sup>00</sup>–10<sup>30</sup> NMR-, ESR-Spectroscopy & QCL  
Hall 2a/b  
Chair R. Hillenbrand (Donostia-San Sebastián/ES)
- 09<sup>00</sup> EPR and DEER Spectroscopy reveal conformational heterogeneity and dynamics of membrane protein complexes  
H.-J. Steinhoff (Osnabrück/DE)
- 09<sup>30</sup> Characterization of protein dynamics and excited states by NMR relaxation  
P. Wright (La Jolla, CA/US)
- 10<sup>00</sup> New opportunities for studying biomolecules using mid-IR quantum cascade lasers  
B. Lendl (Vienna/AT)
- 10<sup>30</sup>–11<sup>00</sup> Break
- 11<sup>00</sup>–12<sup>30</sup> Simulations, SERS & Near Field Spectroscopy  
Hall 2a/b  
Chair W. Mäntele (Frankfurt a. M./DE)
- 11<sup>00</sup> Immuno-SERS microscopy for protein localization in tissue biopsies  
S. Schlücker, Y. Zhang (Essen/DE)
- 11<sup>30</sup> Modeling peptide vibrations with dynamic change in structure: Local and extended contributions  
T. Keiderling (Chicago, IL/US), J. Kubelka (Laramie, WY/US)  
P. Bouř (Prague/CZ), Y. Wei, F. Vazquez (Chicago, IL/US)
- 11<sup>50</sup> Insulin fibrillation monitored by tip-enhanced Raman scattering (TERS)  
T. Deckert-Gaudig, I. Götz, S. Trautmann, L. Langelüddecke  
V. Deckert (Jena/DE)
- 12<sup>10</sup> Novel time-resolved, surface-enhanced and near-field IR spectroscopies to probe folding and functionality of membrane proteins  
J. Heberle, K. Ataka, B. Süss, B.-J. Schultz, R. Schlesinger (Berlin/DE)
- 12<sup>30</sup>–14<sup>00</sup> Lunch Break

14<sup>00</sup>–15<sup>15</sup> IR Imaging

Hall 2a

Chair B. Lendl (Vienna/AT)

14<sup>00</sup> Fourier-transform infrared imaging and clustering – toward an automated histology of normal colon

T. N. Q. Nguyen, P. Jeannesson (Reims/FR), A. Groh

D. Guenot (Strasbourg/FR), C. Gobinet (Reims/FR)

14<sup>15</sup> Optimal spectral histology of human normal colon by genetic algorithm

J. Farah, T. N. Q. Nguyen, A. Groh, D. Guenot, P. Jeannesson

C. Gobinet (Reims/FR)

14<sup>30</sup> Nano-chemical imaging of protein nanoribbons involved in dental enamel formation using s-SNOM

M. Wagner (Santa Barbara, CA/US), K. Carneiro

S. Habelitz (San Francisco, CA/US), T. Mueller (Santa Barbara, CA/US)

14<sup>45</sup> An ATR-FTIR sensor for the analysis of Abeta peptide secondary structure present in complex fluids

A. Nabers, J. Ollesch, J. Schartner, C. Kötting, K. Gerwert (Bochum/DE)

15<sup>00</sup> Detecting fixation damage by correlating hydrated Synchrotron-FTIR with super resolution dSTORM imaging at the single cell level

D. Whelan, T. Bell (Clayton/AU)

14<sup>00</sup>–15<sup>15</sup> NMR- & Time-Resolved Raman Spectroscopy

Hall 2b

Chair P. Wright (La Jolla, CA/US)

14<sup>00</sup> Bisphenol A analogues bind to Ras proteins and compete with guanine nucleotide exchange

R. Stoll, M. Schöpel (Bochum/DE)

14<sup>15</sup> Soft independent modeling based non-linear NMF for classification of 1H-magnetic resonance spectroscopy of brain glioma

M. Khanmohammadi, K. Ghasemi, H. Saligheh Rad (Qazvin/IR)

14<sup>30</sup> Raman microspectroscopy and dynamic vapour sorption highlights age-related changes of collagen-bound water in dermal tissue

C. Eklouh-Molinier, M. Pernes, M. Essendoubi, J. Beaugrand

M. Manfait, O. Piot (Reims/FR)

- 14<sup>45</sup> Transient stimulated Raman spectroscopy in channelrhodopsin  
Y. Hontani (Amsterdam/NL), K. Stehfest (Berlin/DE), T. Mathes  
M. Kloz (Amsterdam/NL), P. Hegemann (Berlin/DE)  
J. T. M. Kennis (Amsterdam/NL)
- 15<sup>00</sup> Resonance Raman spectroscopy as new tool to gain structural  
insights into catalytic intermediates and reactions of hydrogenases  
I. Zebger (Berlin/DE)
- 15<sup>15</sup>–15<sup>30</sup> Break
- 15<sup>30</sup>–16<sup>45</sup> Time-Resolved FTIR Spectroscopy I  
Hall 2a  
Chair H. Byrne (Dublin/IE)
- 15<sup>30</sup> Isotope-edited FTIR reveals distinct structural features of Amyloid  $\beta$   
peptide  
G. Goldblatt, J. Matos, J. Gornto, L. Puentes, A. Docobo J. Williams  
R. Ratajczak, S. Tatulian (Orlando, FL/US)
- 15<sup>45</sup> What vibrations tell us about GTPases  
C. Kötting, K. Gerwert (Bochum/DE)
- 16<sup>00</sup> Probing the dynamics of the signal transducer protein HemAT-Bs by  
time-resolved step-scan FTIR spectroscopy  
A. Pavlou (Nicosia/CY), H. Yoshimura, S. Aono (Okazaki/JP)  
E. Pinakoulaki (Nicosia/CY)
- 16<sup>15</sup> Monitoring one-electron photo-oxidation of guanine in DNA crystals  
using ultrafast infrared spectroscopy  
J. Hall (Reading/GB), F. Poynton, P. Keane (Dublin/IE), S. Gurung  
J. Brazier, D. Cardin (Reading/GB), G. Winter (Didcot/GB)  
T. Gunnlaugsson (Dublin/IE), I. Sazanovich, M. Towrie (Didcot/GB)  
C. Cardin (Reading/GB), J. Kelly, S. Quinn (Dublin/IE)
- 16<sup>30</sup> Time-resolved UV/Vis spectroscopy on the blue light sensor plant  
cryptochrome complementing time-resolved FT-IR difference  
experiments  
S. Oldemeyer, C. Thöing, T. Kottke (Bielefeld/DE)

15<sup>30</sup>–16<sup>45</sup> Biomedical Spectroscopy

Hall 2b

Chair A. Parker (Didcot/GB)

15<sup>30</sup> Raman spectroscopy of protein conformational changes induced by disulphide bond breaking  
N. Brandt, A. Chikishev, V. Kruzhilin (Moscow/RU)

15<sup>45</sup> Spectral signature of drug action – from the bench to the cell  
M. P. Marques (Coimbra/PT), D. Gianolio, G. Cinque  
C. Kelley (Didcot/GB), P. Gardner, M. Pilling (Manchester/GB)  
J. Doherty (Didcot, Manchester/GB), L. Batista de Carvalho (Coimbra/PT)

16<sup>00</sup> Synchrotron radiation spectro-microscopy study on  $\alpha$ -synuclein neuronal regulation of cellular manganese and calcium content  
T. Ducic (Barcelona/ES), B. Lai (Argonne, IL/US), S. Chen (Argonne/US)  
L. Barski, P. Lingor (Göttingen/DE)

16<sup>15</sup> Raman confocal micro-probe for cosmetic and pharmaceutical applications  
C. David, V. Larat, R. Lewandowska, E. Froignuex (Villeneuve d'Ascq/FR)

16<sup>30</sup> Cancer detection using combined molecular methods with the focus on miniaturized probes  
F. Schulte, V. Artyushenko, I. Usenov, U. Zabarylo, T. Saeb-Gilani  
T. Sakharova (Berlin/DE)

16<sup>45</sup>–17<sup>00</sup> Break

17<sup>00</sup>–18<sup>15</sup> Time-Resolved FTIR Spectroscopy II

Hall 2a

Chair S. Schlücker (Essen/DE)

17<sup>00</sup> Thermal denaturation of DNA studied by ultrafast 2D-IR spectroscopy  
N. Hunt, G. Hithell (Glasgow/GB), G. Greetham, M. Towrie  
A. Parker (Didcot/GB), G. Burley, M. Baker (Glasgow/GB)

17<sup>15</sup> Time-resolved step-scan FTIR studies of heme-based oxygen sensor proteins  
A. Pavlou (Nicosia, Uppsala/SE), E. Pinakoulaki (Nicosia/CY)

- 17<sup>30</sup> Static and time-resolved differential FTIR applied to photosynthesis: from the investigation of proton transfer, electron transfer, internal water molecule displacement, conformational changes in isolated proteins under controlled hydration, to the real-time study of the mechanism of photoinduced biochemical reactions *in vivo*  
A. Mezzetti (Gif-sur-Yvette/FR)
- 17<sup>45</sup> Amyloidogenic self-assembly of polyglutamic acid chains – Is length an issue?  
W. Dzwolak (Warsaw/PL)
- 18<sup>00</sup> Time resolved infrared and UV/VIS spectroscopy on Channelrhodopsins is used to monitor their activation mechanism  
J. Kuhne, M.-A. Dreier, K. Eisenhauer (Bochum/DE), E. Ritter P. Hegemann, F. Bartl (Berlin/DE), K. Gerwert (Bochum/DE)
- 17<sup>00</sup>–18<sup>15</sup> **Biomolecular Simulations**  
Hall 2b  
Chair H.-J. Steinhoff (Osnabrück/DE)
- 17<sup>00</sup> Tracking proton wires and storage sites consisting out of water molecules within membrane proteins  
S. Wolf, E. Freier, K. Gerwert (Bochum/DE)
- 17<sup>15</sup> Exploring GTPase catalysis at atomic structure level by combining biomolecular simulations with FTIR spectroscopy  
T. Rudack (Urbana, IL/US)
- 17<sup>30</sup> Multi-level modeling of vibrational spectra of the phosphate group  
V. Andrushchenko, P. Bouř (Prague/CZ)
- 17<sup>45</sup> Chiroptical properties of the antimicrobial peptide Lasiocepsin and of its analogs  
V. Baumruk, M. Pazderková, P. Maloň, V. Profant, L. Bednářová (Prague/CZ)
- 18<sup>00</sup> Nonlinear vibrational spectroscopy and molecular modeling for the structural investigation of biomolecular adsorption  
S. Roy, T. Jarisz, P. Covert, D. Hore (Victoria, BC/CA)
- 18<sup>30</sup>–23<sup>00</sup> **Conference Banquet**  
Mensa

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7 <sup>th</sup> –8 <sup>th</sup>	1	AHF analysentechnik AG (Tübingen/DE)
7 <sup>th</sup> –10 <sup>th</sup>	12	A • P • E GmbH Angewandte Physik & Elektronik GmbH (Berlin/DE)
7 <sup>th</sup> –10 <sup>th</sup>	15	art photonics GmbH (Berlin/DE)
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### Welcome Reception

The Welcome Reception will take place after opening of the registration for the conference on Sunday, 6<sup>th</sup> September 2015. We welcome all participants of 16<sup>th</sup> ECSBM and invite you to enjoy an evening with snacks and drinks in the foyer of the RUB Conference Center. Meet colleagues and friends, have a first look at the poster exhibition and visit the industrial exhibition.



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Date	Sunday, 6 <sup>th</sup> September 2015
Time	19 <sup>00</sup> –21 <sup>00</sup>
Place	Foyer RUB Conference Center
Fee	Included in conference fee

### Guided Half-day Tour

#### German Mining Museum Bochum/Deutsches Bergbaumuseum Bochum

Come and visit the world of mining close-up! During the guided tour, participants will visit the visitor mine 20m below the museum. After the tour you can take a ride up our head frame and enjoy the view of the whole Ruhr area. Dress warmly! The average temperature in the visitor mine is only 12 °C. Therefore please bring an extra jacket.



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Date	Wednesday, 9 <sup>th</sup> September 2015
Time	16 <sup>00</sup> –19 <sup>00</sup>
Place	Europaplatz • 44791 Bochum, Germany
Fee	15 EUR/person

### Conference Banquet

We welcome you to enjoy a wonderful evening including a dinner buffet and beverages! You can continue scientific discussions aside from the session program and exchange with your colleagues in a relaxed atmosphere. Mr. Gregor Stennecken will accompany this evening with a combination of DJ activity and saxophone live performance, drawing you to the dance floor. We wish you a pleasant evening!

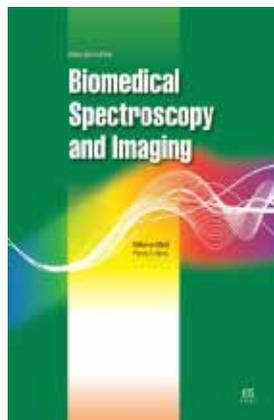


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Date	Thursday, 10 <sup>th</sup> September 2015
Time	From 18 <sup>30</sup>
Place	Mensa of the Ruhr-University Bochum
Fee	Included in conference fee 50 EUR for accompanying person

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## Aims and Scope

*Biomedical Spectroscopy and Imaging* (BSI) is a multidisciplinary journal devoted to the timely publication of basic and applied research that uses spectroscopic and imaging techniques in different areas of life science including biology, biochemistry, biotechnology, bionanotechnology, environmental science, food science, pharmaceutical science, physiology and medicine. Scientists are encouraged to submit their work for publication in the form of original articles, brief communications, rapid communications, reviews and mini-reviews.

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Opening Hours	Sunday	Monday	Tuesday	Wednesday	Thursday
Exhibition		09 <sup>00</sup> –20 <sup>00</sup>	09 <sup>00</sup> –20 <sup>00</sup>	09 <sup>00</sup> –15 <sup>00</sup>	09 <sup>00</sup> –16 <sup>45</sup>
Check-In desk	16 <sup>00</sup> –19 <sup>00</sup>	08 <sup>30</sup> –19 <sup>00</sup>	08 <sup>30</sup> –19 <sup>00</sup>	08 <sup>30</sup> –14 <sup>30</sup>	08 <sup>30</sup> –17 <sup>00</sup>

### Cloakroom

An unmanned cloakroom is located next to the Check-In desk in the foyer of the RUB Conference Center.

### WIFI Access

WIFI is available for free throughout the whole conference area. Please ask at the Check-In desk for the login data.

### Ticket for Local Public Transportation

On the backside of your name badge you have a ticket for the local public transportation (BOGESTRA) within the city of Bochum that is valid from 6<sup>th</sup>–11<sup>th</sup> September 2015. Please note that this ticket is not transferable. Please carry a photo identification with you when using the ticket.

### Catering

During morning and afternoon breaks, snacks, coffee and beverages will be provided in the foyer of the RUB Conference Center. Lunch is available in the Mensa close to the conference venue, but not included in the conference fee. During lunch symposia companies will provide lunch boxes at no charge. To have dinner at the area of the university, please visit the restaurant Q-West (<http://q-we.st>). Here you can have dinner until 22<sup>00</sup>.



### Information for Speakers

Speakers are asked to prepare their presentations either in MS PowerPoint 2010 format or as a PDF file. The use of personal notebooks is possible upon agreement. However, it may interrupt the flow of the programme in the lecture hall. Please provide an adapter for VGA if necessary and contact the technical staff in the lecture hall. All technical equipment required for the presentation will be available. For video and audio files please provide AVI, WMV and MPG files only as a separate file. Your presentation and any additional files should be uploaded at least one hour before the start of the session.

Please note: If you use a USB flash drive to save your files, do not file protect it.

### Information for Poster Presenters

The poster number can be found in this program brochure. All poster authors are asked to hang up their posters on Monday, 7<sup>th</sup> September 2015 until 11<sup>00</sup> and remove them before Thursday, 10<sup>th</sup> September 2015, 18<sup>00</sup>.

Thumb tacks can be found on the poster walls, which will be marked with the poster numbers.

### Publication of Abstracts

All abstracts will be published in an abstract book on an USB flash drive that you are welcome to get at the check-in desk. The abstract book is also available for download on the conference website [www.ecsbm2015.de](http://www.ecsbm2015.de).

### Publication of Proceedings

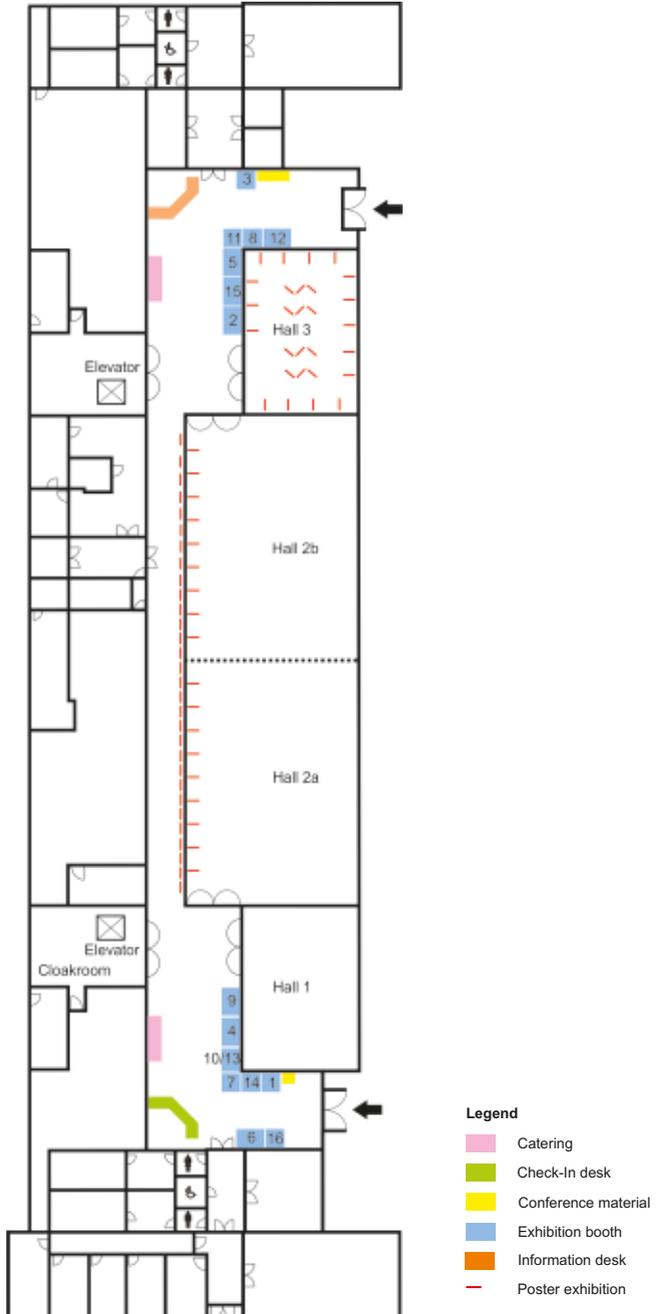
The proceedings of the 16<sup>th</sup> ECSBM will be published in "Biomedical Spectroscopy and Imaging" (IOS Press, NL). Authors are requested to submit their manuscript electronically to journal's editorial management system until 30<sup>th</sup> September 2015. For further information, please visit [www.ecsbm2015.de](http://www.ecsbm2015.de).

### Poster Prize

Poster prizes (two to graduate students and one to PostDocs) will be awarded by a jury consisting of the members of the ECSBM European Committee. The jury judges the posters according to the following criteria:

- Logic of structure (is the structure of the content logically presented)
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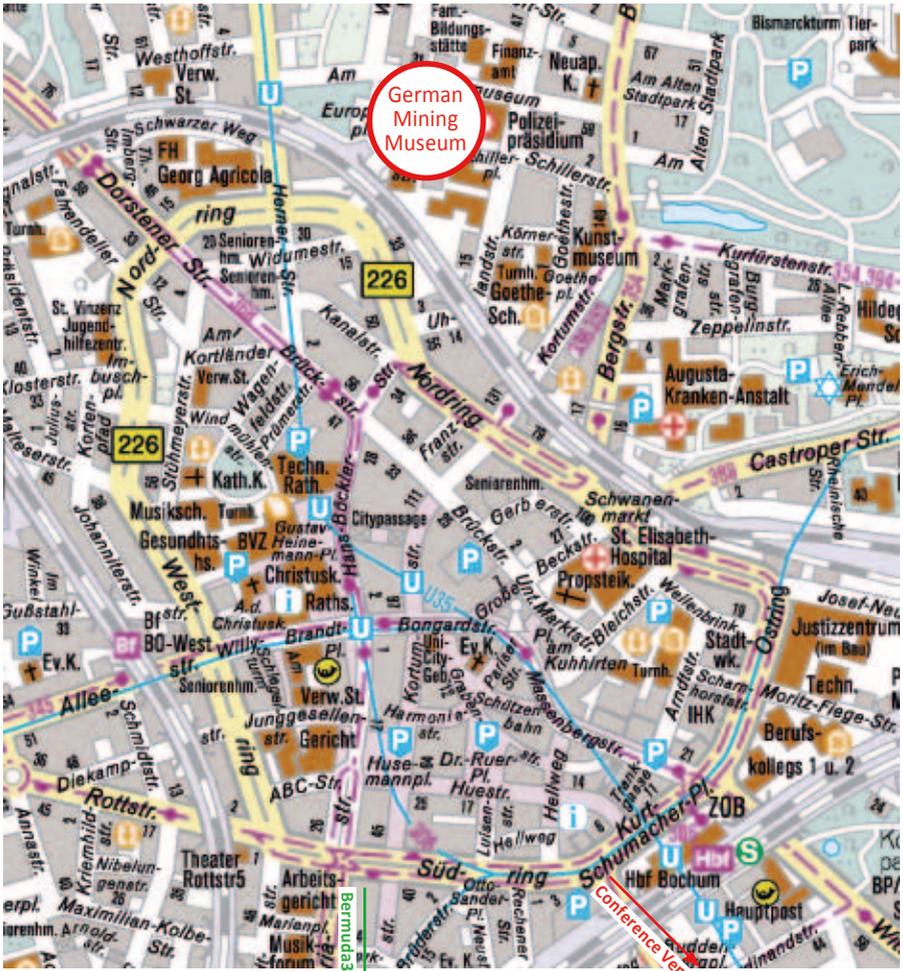
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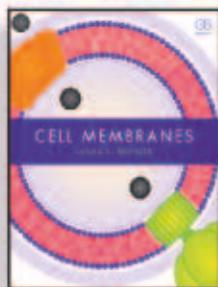
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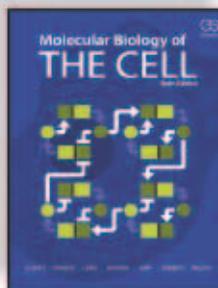
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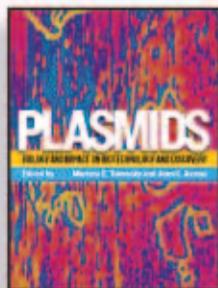
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- P2 Monitoring the composition of short chain fructo-oligosaccharides produced during transfructosylation reactions by means of infrared spectroscopy  
 N. Romano, M. Santos, P. Mobili (La Plata/AR)  
 M. E. Zuñiga-Hansen (Valparaiso/CL), A. Gomez-Zavaglia (La Plata/AR)
- P3 Time-resolved FTIR spectroscopy to monitor the influence of the lipid environment on retinal proteins  
M. Jawurek, S. Schmidt (Konstanz/DE), C. Glaubitz (Frankfurt a. M./DE)  
 K. Hauser (Konstanz/DE)
- P4 Devising alkanethiol self-assembled-monolayers for time-resolved surface enhanced infrared absorption of poly-L-lysine  
M. A. Fallah (Konstanz/DE), C. Stanglmair, C. Pacholski (Stuttgart/DE)  
 K. Hauser (Konstanz/DE)
- P5 Complete proton transfer cycle in GFP and its T203V and S205V mutants  
S. P. Laptенок (Norwich/GB), A. Lukacs (Norwich/GB, Pécs/HU)  
 A. Gil, R. Brust (Stony Brook, NY/US), I. V. Sazanovich  
 G. M. Greetham (Stony Brook, NY/US, Didcot/GB)  
 P. J. Tonge (Pécs/HU), S. R. Meech (Norwich/GB)
- P6 Synchrotron based single-shot mid infrared spectrometer  
E. Ritter, U. Schade, L. Puskar, F. Bartl, E. F. Aziz, P. Hegemann (Berlin/DE)
- P7 Germanium catches proteins in action  
J. Schartner, J. Güldenhaupt, A. Nabers, N. Hoeck, K. Gerwert  
 C. Kötting (Bochum/DE)
- P8 Infrared band assignments of catalytical residues in Gai1  
C. Teuber, D. Mann (Bochum/DE), K. Gerwert (Bochum/DE, Shanghai/CN)  
 C. Kötting (Bochum/DE)
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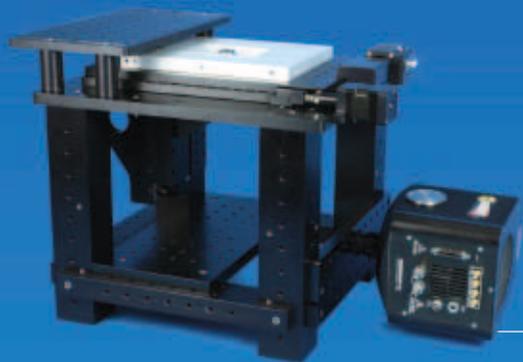
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