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Publisher: Matthias Ernst, ETH Zurich, Switzerland

Editorial

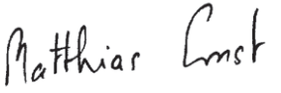
Dear members of the Groupement AMPERE,

after EUROMAR is also before EUROMAR. This is very much reflected in this last issue of the Bulletin AMPERE in 2018. Besides the final report from EUROMAR 2018 in Nantes which was organized by Patrick Giraudeau as the chair, we also have two articles about the Raymond Andrew Prize and the AMPERE Prize which were awarded by the Groupement AMPERE at the EUROMAR 2018.

The next EUROMAR will be jointly organized with ISMAR and be combined with the annual meeting of the Fachgruppe Magnetische Resonanz of the German Chemical Society. You find the first announcement for EUROISMAR 2019 organized by Hartmut Oschkinat in Berlin also in this issue. We hope that many of you can attend this combined meeting which promises to have a very attractive scientific program. This is the second time after Firenze 2010 that EUROMAR and ISMAR organize a combined meeting.
At EUROISMAR 2019 there will again be a Raymond Andrew prize awarded for an outstanding PhD thesis. Please see the announcement in this Bulletin (p. 4) for details and submit your proposals to the prize committee.

In early November, very sad news reached us. Stefano Caldarelli passed away on November 6, 2018 at the age of 55 after a long illness. He was one of the founders of the Alpine Conference in Chamonix and also one of the driving forces in the Groupement AMPERE to organize more schools on different aspects of NMR. We will miss his high spirits, his laughter, and his good humor. You can read more about him and his life in the Obituary on page 34 which was contributed by Lyndon Emsley.

I wish you the very best for the upcoming holiday season and a good start into the year 2019.



Matthias Ernst
Secretary General, Groupement AMPERE

P.S. Remember that the deadline for applying for conference support from AMPERE for conferences in 2019 is January 1st, 2019 (see our webpage for more details).

Portrait: Prof. Anja Böckmann

• why magnetic resonance?
I came to NMR through physical chemistry of solid materials, and opportunities oriented me afterwards towards proteins in solution. After my PhD, I jumped on the emerging combination of both by opting for a post-doc in the group of Prof. Ann McDermott in New York, a pioneer in protein solid-state NMR.

• what is your favorite frequency?
The highest available, hopefully soon 1.2 GHz – enabling many systems where we hit a wall today, like following large molecular machines through different states in their functional cycle, or to observe very small amounts of complex proteins using fast magic-angle spinning.

• what do you still not understand?
Why peaks for certain protein parts are not observed in any NMR experiment we use, and the underlying principles, to derive experimental conditions allowing to recover them.

• luckiest experiment you have ever done.
A 2D solid-state HETCOR which revealed water-protein interactions, and their interpretation as chemical exchange

• what was the worst mistake you have made during your lab time?
I think that there are no real lab mistakes by definition –from most mistakes you learn something.

•most memorable conference story
My first EENC in Oulu, where daylight neared 24h/24h, and the conference never slept.

• with whom (historical person) would you like to meet?
I would love to have coffee with Astrid Lindgren and Peter Høeg, who accompanied my childhood and shape(d) my views on society.

• when do you get your best ideas?
When my mind combines impulses from distant fields.

• if you had just one month time for travelling - where would you go to?
Where beauty lies.

• your idea of happiness.
Family, friends, health - and exciting science.

Position:
Director of Research and PI of the Protein Solid-State NMR group at the Molecular Microbiology and Structural Biochemistry Institute in Lyon at the CNRS/University of Lyon
Awards:
2007 Bronze Medal CNRS; 2014 Prix Pierre Desnuelle of the French Académie des Sciences
Homepage:
http://mmsb.cnrs.fr/en/u/abockmann/

Education:
Diploma (Master) in Chemistry, TU Berlin, Germany; PhD in Chemistry, Université Paris XI Orsay, Paris, France, Habilitation à Diriger des Recherches, Université de Lyon 1, France

Interests:
My research interests lie in the development of methods and approaches to study complex proteins and their assemblies using solid-state NMR. I like to identify systems which need new ideas, and where NMR has unique strengths. I devise their preparation, and let my imagination create goals which push current methods to new limits, and ask for advanced combinations of NMR methods and biochemistry opening new opportunities.

Call for nominations: Raymond Andrew Prize 2019

Dear colleagues,

Call for Nominations for the Raymond Andrew Prize for an outstanding PhD thesis in the field of magnetic resonance

For the Raymond Andrew Prize 2019 the AMPERE Prize Committee is seeking your help in searching for qualified candidates who completed their dissertation during the period of 2017/2018. The prize will be presented during the EUROMAR in Berlin (Germany) from August 25-30.

You are kindly invited to submit nominations by e-mail to
andrewprize@ampere-society.org

Suggestions must be received by **15th February 2019** and should include the following documents:

- Nomination letter
- Curriculum vitae
- List of publications and presentations at conferences
- PhD thesis as a PDF

The thesis should be written in English. In exceptional cases, the thesis may also be submitted in triplicate as a hardcopy to the AMPERE Secretariat. Submissions that arrive too late will automatically be transferred to the next year. The prize committee will reconsider excellent contributions for two years in a row.

For a list of past Andrew Prize winners see:
https://www.ampere-society.org

On the history of the Fourier transform in NMR spectroscopy

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It is well known that significance, prospects and future citations of articles depend on many factors and are often unpredictable. It can be illustrated on the example of two articles which were published 60 years ago (in 1958) and opened the histories of the modern method of recording NMR spectra (Fourier Transform) [1] and of the modern multipulse techniques (rf pulses with different phases) in NMR [2].
The latter article was immediately highly appreciated by the scientific community: more than 3700 citations up to now (Web of Science), 8 in 1959 and 153 in 2018. The fate of the first article turned out to be rather sad although it reported about the first in the world practice real Fourier Transform (FT) of a free induction decay (FID) to obtain a proton NMR spectrum. Note, that the relationship between the spectral and temporal characteristics of the signals has been known in radio engineering for 100 years and, moreover, in the work [3] it was shown "rigorously that, except at very low temperatures, a free-induction decay is the Fourier transform of the corresponding steady-state resonance line shape", but in the work[1] the spectrum of a specific substance was experimentally obtained using FT for the first time (see Figure).

Unfortunately, the work [1] did not attract the attention of contemporaries, because, in the absence of computers, it took a very long time (many days) to calculate one spectrum. As a result, the work [4] is traditionally considered as the „source" of the Fourier NMR spectroscopy (more than 1000 citations up to now, 2 in 1967 and 21 in 2018). In 1983, R.R. Ernst wrote (CC/NUMBER 27, July 4, 1983): "When I joined Varian Associates in fall 1963, my supervisor, Weston Anderson, was already experimenting with a multipole channel spectrometer concept. … In 1964, we tried to find a more practical of this concept. At first an efficient source for the numerous excitation frequencies was required. … This completed the concept of Fourier transform NMR spectroscopy. … Of course many researchers before knew this very basic relationship; however, we seem to have been the first to realize the inherent remarkable gain in sensitivity which is given by the square root of the number of spectral elements.

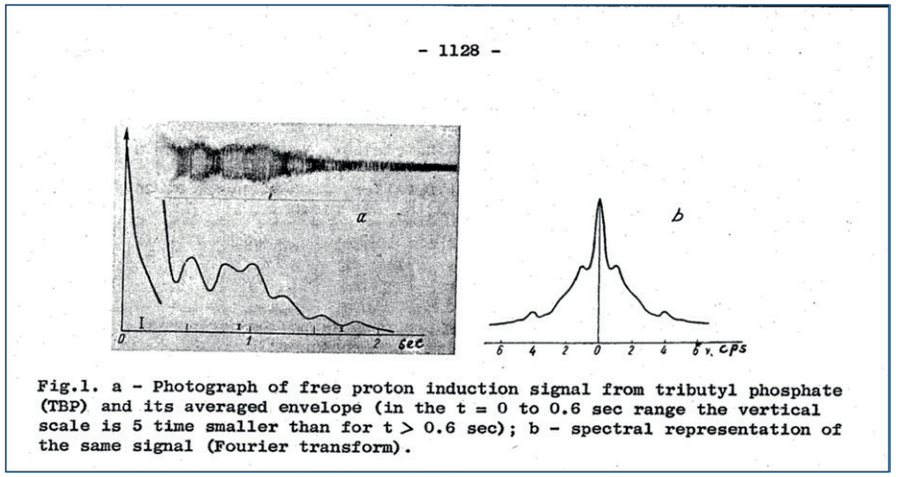

Fig.1. a - Photograph of free proton induction signal from tributyl phosphate (TBP) and its averaged envelope (in the t = 0 to 0.6 sec range the vertical scale is 5 time smaller than for t > 0.6 sec); b - spectral representation of the same signal (Fourier transform).

It was a timely discovery. Laboratory computers just became available and online data processing feasible. Nevertheless, it took several years before the first Fourier transform NMR spectrometer became commercially available". By the way, when in the 70s NMR FT spectrometers began to be widely produced and used, the representatives of the "Varian" company applied against the "Bruker" company in an international court, believing that they owned proper patents. "Bruker" presented namely the Skripov's article [1] and thus rejected the claim.

Without belittling the achievements of the R.R. Ernst, who was awarded the Nobel Prize in 1991 for his contributions towards the development of Fourier Transform nuclear magnetic resonance spectroscopy and the subsequent development of multi-dimensional NMR techniques, I would like to draw the attention of the scientific community to the undeservedly forgotten article [1]. Some of the circumstances surrounding the publication of the work [1] are reflected in the book [5].

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Report: Euromar 2018

EUROMAR 2018, the largest European Congress on Magnetic Resonance, was held in France for the first time since it was created in 2005, in the beautiful western city of Nantes.

The conference, hosted in La Cité Nantes Events Center located in the heart of the city, was a stimulating forum to exchange on the most recent breakthroughs in magnetic resonance, with an impressive scientific programme, a high level selection of invited lectures, promoted oral communications and posters. An impressive number of abstract submissions (522) were received for this edition, which reflects the dynamism of our community.

Committees:

International Scientific Committee:
Patrick GIRAUDEAU, chair, Nantes, Liquid-state, Small molecules
Robert BITTL, Freie Univ. Berlin, EPR
Bernhard BRUTSCHER, IBS Grenoble, Liquid-state NMR, biomolecules
Teresa CARLOMAGNO, Univ. Hannover and HZI Braunschweig, Liquid-state and solid-state NMR, biomolecules
Luisa CIOBANU, CEA Saclay, MRI
Fabien FERRAGE, CNRS Paris, Liquid-state NMR, biomolecules
Sabine HEDIGER, CEA Grenoble, Solid-state NMR and DNP, biomolecules
Olivier LAFON, Univ. Lille, Solid-state (DNP)-NMR, materials
Thomas MEERSMANN, Univ. Nottingham, MRI, hyperpolarized noble gases
Tatyana POLENOVA, Univ. Delaware, Solid-state NMR, biomolecules
Thomas PRISNER, Univ. Frankfurt, EPR Sun UN, CEA Saclay, EPR
Hervé VEZIN, CNRS Lille, EPR

Local Organising Committee:
Patrick GIRAUDEAU, Chair, Univ. Nantes
Olivier LAFON, Vice-Chair, Univ. Lille
Jean-Marie BONNY, INRA Clermont-Ferrand
Catherine DEBORDE, INRA Bordeaux
Fabien FERRAGE, CNRS Paris
Nicolas GIRAUD, Univ. Orsay
Sabine HEDIGER, CEA Grenoble
Gérald REMAUD, Univ. Nantes
Elodie SALAGER, CNRS Orléans
Sophie ZINN-JUSTIN, CEA Saclay

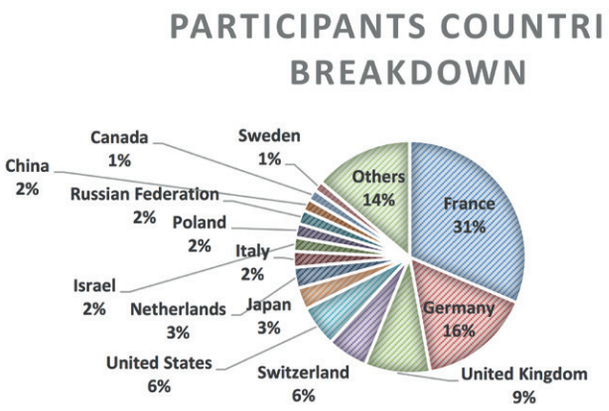
Some figures of Euromar 2018
723 participants from 36 countries
28 exhibiting companies
33 partners (corporate and institutional)

13 invited plenary lectures on the following themes:
- EPR/biomolecules
- Exotica
- Liquid state
- MRI
- NMR methods
- NMR of materials
- EPR/materials
- Hyperpolarization
- NMR/biomolecules
- NMR Metabolomics
- Solid-state NMR/biomolecules
- Solid-state NMR/small molecules

42 invited parallel lectures on the following themes
- Benchtop and low-field
- Biosolids
- EPR
- Hardware
- Liquid-state methods
- MRI and in vivo
- Small Molecules
- Bioliquids
- Computation
- Exotica
- Hyperpolarization
- Materials
- Omics
- Solid-state methods

2 tutorials on DNP (Sami JANNIN & Anne LESAGE from France) and Pure-shift NMR (Gareth MORRIS from UK)
63 abstracts selected for oral communications presented in parallel sessions
405 abstracts selected for poster presentations presented during 3 poster sessions (Monday, Tuesday and Wednesday)
5 workshops organized by Bruker (1), Jeol (2) and Magritek (2)

1 satellite meeting: The GERM (French group for the study of magnetic resonance) celebrated its 30th anniversary on July 6th
31 volunteers



Prizes
Richard R. Ernst Prize in Magnetic Resonance
Laureate: Prof. Claudio Luchinat, University of Florence, Italy

Ampere Prize for Young Investigators
Laureate: Prof. Katja Petzold, Karolinska Institute, Sweden

Raymond Andrew Prize
Laureate: Dr. Giuliana Fusco, University of Cambridge, United Kingdom


Prof. Claudio Luchinat, Prof. Lucia Baci

Dr. Juliana Fusco, Prof. Beat Meier

Recipients of JMR and MRC young scientists' awards, Suraj Manrao Student poster prizes and International EPR society poster prizes as well as Magnetochemistry, FEBS, FRISBI and GERM travel grants were announced during the Closing Ceremony, on Thursday.

Suraj Manrao Student Poster Prizes

Social events & catering
Following the Prizes session, the Welcome Mixer was held in the exhibition area as an ice breaker on Sunday evening, offering a wine & cheese cocktail to participants and exhibitors.

Bruker (the Bruker night) offered an unforgettable moment on Monday evening at the famous Machines de l'Ile where 500 participants could enjoy this unique venue and a dining cocktail.

At closing of the conference week, a Gala dinner, sponsored by Jeol, gathered almost 400 participants for a seated dinner with live jazz band and dancing.

Lunches (as a cocktail format) and coffee breaks took place in the exhibition area and were provided to the entire audience.

Exhibition & Sponsoring
The exhibition was in the heart of the congress venue. 28 societies have presented their products in booths from 6 sqm to 100 sqm, depending on their financial support.
A high number of commercial and institutional sponsors supported the event, which gave the possibility to increase the number of student stipends provided by the Organizing Committee
(+ 170 students received 100 €).

Promotion & Communication
A dedicated website, launched in July 2017, mentioned all scientific and practical information for participants. A welcome video from Patrick Giraudeau was put on the landing page.
Tutorials, which were recorded onsite, have been made available in open access on the website immediately after the conference.

EUROMAR 2018 used social media to communicate to the magnetic resonance community and gathered 110 followers on Facebook and 176 followers on Twitter.

8 newsletters were sent to the participant database to promote the event and an app was made available on Google Play and App Store, downloaded by approx. 30% of participants.
EUROMAR signed agreements with the following media partners: Elsevier, MDPI and Wiley.

Ampere Prize for young investigators:
Prof. Dr. Katja Petzold

Prof. Dr. Katja Petzold has received the AMPERE prize for Young Investigators during the EUROMAR conference in Nantes, France. The prize was given "in recognition of her achievements in using solution-state NMR for the study the molecular mechanism of RNA function".

The German biochemist has already in her PhD (Umeå University Sweden, graduated in 2009) worked with dynamics in RNA [(1)] and developed new pulse sequence [(2)], before she moved, after a short stay in South Africa to dip her toes into drug development, for her post-doctoral fellow to the group of Prof. Al-Hashimi to the University of Michigan, USA, from 2010 to 2013. In 2014 she was appointed Assistant Professor at the Karolinska Institute, Stockholm, Sweden, where she was recently promoted to Associate Professor.

Petzold studies structure and dynamics of RNA with focus on RNA based diseases by applying relaxation dispersion NMR. She has been working with a number of biological systems, where she could demonstrate invisible, low populated states that are of relevance to the function of these RNAs, e.g. the dimerization initiation site of the SL1 in HIV [(1)]. She could further show, that dynamics in RNA are not limited to structural changes, but even chemical changes are existing as low-populated states, that can influence translation, in the found keto-enol tautomer present in RNA GU wobble base-pairs [(2)]. She has since established a broad spectrum of RNAs under investigation, from microRNA [(5)], to Hepatitis B virus RNA up to ribosomes, where she uses her expertise in method development to push the limits of current methods [(6)] to discover and understand the importance of these invisible states. In collaboration with several groups from a variety of disciplines, she creates new routes to measure high-resolution dynamical structural ensembles with an NMR informed MD approach. Further, her lab tests structural hypothesis and function of these invisible states in human cell-lines, together with molecular biologists, and even mice to develop a biological relevant structure determination process.

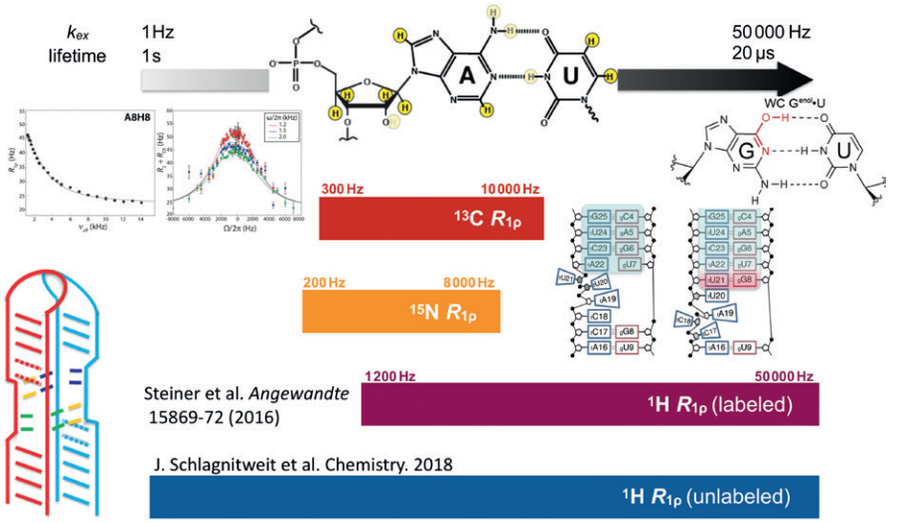


Figure: An overview of methods available to detect invisible states of RNA with examples of these states. Highlighted here is the expansion of the measurement timescale by the use of 1H relaxation dispersion to cover basically the whole µs to ms timescale of chemical exchange. Invisible states visualized are: bottom left: the dimerization initiation site dynamics leading to a zipper like motion, allowing two homo-dimers to perform a strand exchange switching one base-pair at a time. Upper right: the keto-enol tautomer, that converts simple GU wobble base-pairs into Watson-Crick look alikes, increasing the potential for misincorporation during translation. Middle right: the extension of an microRNA seed recognition by a single base-pair switch, that pushes the actor protein, Ago, from the screening mode into the active mode.

In her talk at the EUROMAR in Nantes "Capturing Transient States in RNA", Petzold presented new ^{1}H relaxation dispersion NMR experiments (RD) and invisible states found with the extensive toolbox developed.

The new ^{1}H RD allows to extend the timescale to be probed by NMR from the lower ms to the high-end of the µs timescale and therefore detect many more chemical exchange processes. Additionally, the latest experiment allows to omit the use of expensive heteronuclear labeling, making RD experiments affordable and feasible (samples can be simply bought and one does not require an own RNA production setup) for a large number of people. At the same time the experiment became more sensitive, as the R_2 increase caused by the attached heteronuclei disappears and hindering couplings vanish.

Using these experiments she revealed invisible states in RNA-RNA complexes, specifically on a microRNA (miR) binding its messenger RNA (mRNA) target. MiR finds it target by searching for a 5-8 nucleotide long Watson-Crick complimentary sequence on the mRNA, called seed, binding it in a perfect Watson-Crick base-paired helix. miR-34 binds mRNA of Sirt1, a regulator of P53 by deacetylation, via a 6/7 nucleotide seed, while in an invisible state, this seed gets extended by an additional base-pair stabilizing the previously weak closing base pair to a complete 8 nucleotide seed. We hypothesize that with this conformational change of the RNA, miR-34a bound to mSirt1 overcomes a binding hurdle of the effector protein Argonaut (Ago), causing an induced fit change from a screening state into an active mode, confirmed by an increase of activity of Ago by stabilization of this previously invisible state.

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Raymond Andrew Prize

Giuliana Fusco

Department of Chemistry, University of Cambridge, UK

α-synuclein (αS) is an intrinsically disordered protein that is strongly connected with Parkinson's disease (PD) and a number of other neurodegenerative disorders, including Parkinson's disease with dementia, dementia with Lewy bodies and multiple system amyotrophy. Fibrillar aggregates of αS have been identified as the major constituents of proteinaceous inclusions known as Lewy bodies that form inside the neurons of patients suffering from these conditions. A number of missense mutations, as well as duplications and triplications of the gene encoding αS have also been associated with familial forms of early onset PD. Despite the association between αS aggregation and neurodegeneration is now established, the specific function of αS is still currently unclear, however, a general consensus is forming on its key role in regulating the process of neurotransmitter release, which is associated with the ability of αS to bind a variety of biological membranes. Indeed, in dopaminergic neurons, αS exists in a tightly regulated equilibrium between water-soluble disordered state and membrane-associated forms that are rich in α-helix. Characterising the nature of this binding as well as the structural and functional properties of αS at the surface of biological membranes is currently a top challenge. In particular the intrinsic limitation of current analytical techniques in studying highly heterogeneous protein states in rapid equilibrium between different physical phases demands for novel approaches to be formulated.

This PhD thesis describes major achievements in developing and applying a multidisciplinary approach based on solution-state nuclear magnetic resonance (NMR) and solid-state NMR (ssNMR) and extending to a number of other biophysical techniques, including cryo electron microscopy, super resolution microscopy, FRET and cellular biophysics, which enabled us to elucidate in detail the balance between structural order and disorder associated with the membrane interaction of αS in view of its physiological and pathological roles. Using this approach, we identified the key elements that govern the binding of αS to synaptic vesicles (Fusco et al, 2014, *Nature Communications* 5:3827).

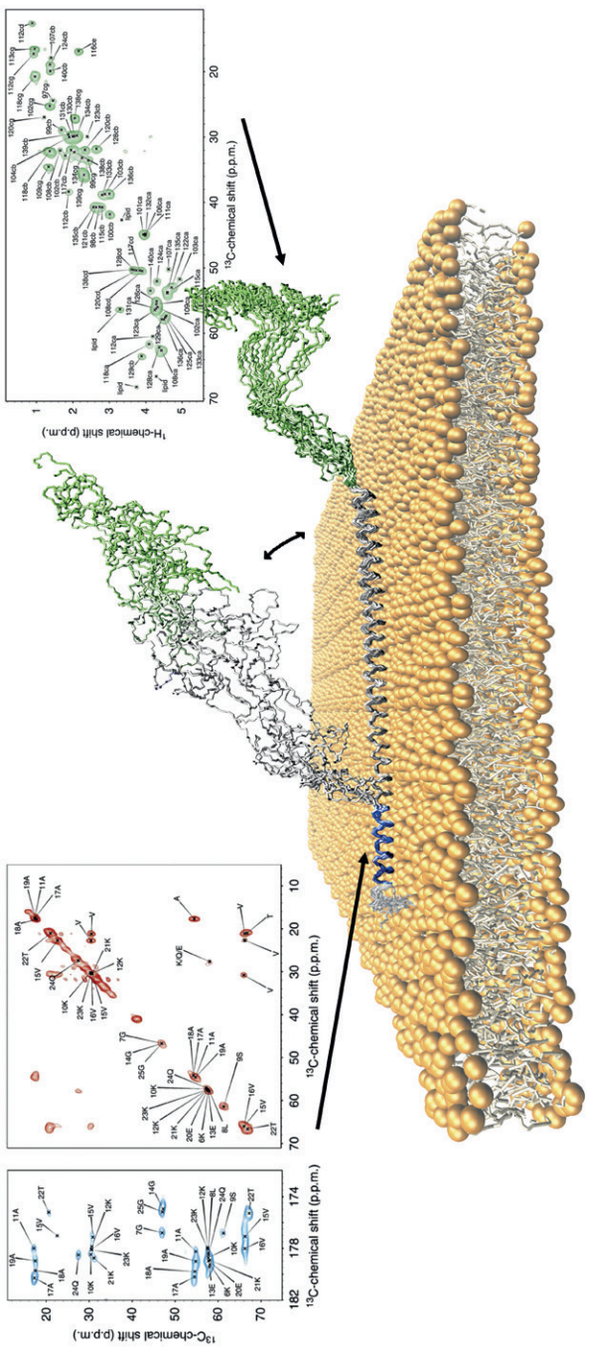


Figure 1. Three regions of αS determine its interaction with lipid bilayers. We identified three different regimes of protein dynamics and membrane affinity in ssNMR experiments.
The N-terminal region (blue) is visible in DARR experiments using magic angle spinning (MAS) ssNMR, indicating that it is rigidly bound and anchored to the membrane. The central region (grey), showing intermediate dynamics is invisible using ssNMR experiments but its binding to lipid bilayers could be indirectly probed using CEST in solution-state NMR, suggesting that this region plays a key role in modulating the affinity of αS for membranes. Finally, a C-terminal fragment (green) was probed using INEPT experiments in MAS ssNMR. This region maintains its unstructured nature and remains essentially uncorrelated with the membrane surface, despite showing weak and transient contacts in PRE ssNMR experiments. Figure adapted from (Fusco et al, 2014, *Nature Communications* 5:3827).

In particular, three regions of αS were shown to possess distinct structural and dynamical properties at the surface of synaptic vesicles, including an N-terminal helical segment having a role of membrane anchor, an unstructured C-terminal region that is weakly associated with the membrane and a central region acting as a sensor of the lipid properties and determining the affinity of αS membrane binding (Figure 1). We refined the structural ensemble of the N-terminal membrane anchor at the surface of synaptic membranes, showing that the partial insertion of this region in the membrane core promotes strong but reversible binding with biological membranes in such a way to enable a fast equilibrium between membrane-bound and cytosolic forms of the protein (Fusco et al, 2016, *Scientific Reports* 6:27125).

Further studies of two mutational variants of αS that are associated to early onset PD, namely A30P and E46K, revealed that two key regions of the protein, namely the N-terminal membrane-anchor (residues 1 to 25) and the central segment of the sequence (residues 65–97, having significant overlap with the non-amyloid β component-NAC-region), have independent membrane-binding properties and therefore are not only able to interact with a single SV, but can also simultaneously bind to two different vesicles thereby promoting their clustering (Fusco et al, 2016, *Nature Communications* 7:12563).
The resulting "double-anchor" mechanism (Figure 2) explains the biological property of αS to promote clusters of synaptic vesicles within the processes of formation of distal pools to the active zone. The double-anchor mechanism reconciles literature data showing that the deletion of the segment 71–82 in the NAC region of αS or the impairment of the membrane affinity of the N-terminal anchor region of the protein severely affect vesicle clustering in vivo. We provided supports for the double anchor mechanism by rationally designing and experimentally testing a swapping mutant of αS, namely αS_{Sw}, engineered to promote stronger interactions between synaptic vesicles (Figure 2).

These data therefore revealed that the NAC region is not only involved in the aggregation of αS, as extensive literature evidence has previously indicated, but also has a specific role in a key molecular mechanism associated with the normal function of αS. The structural characterisation also showed that the active conformations of αS to initiate the double-anchor mechanism are particularly vulnerable to self-association leading to αS aggregation at membrane surfaces, thereby providing a new mechanistic link between functional and pathological roles of αS.

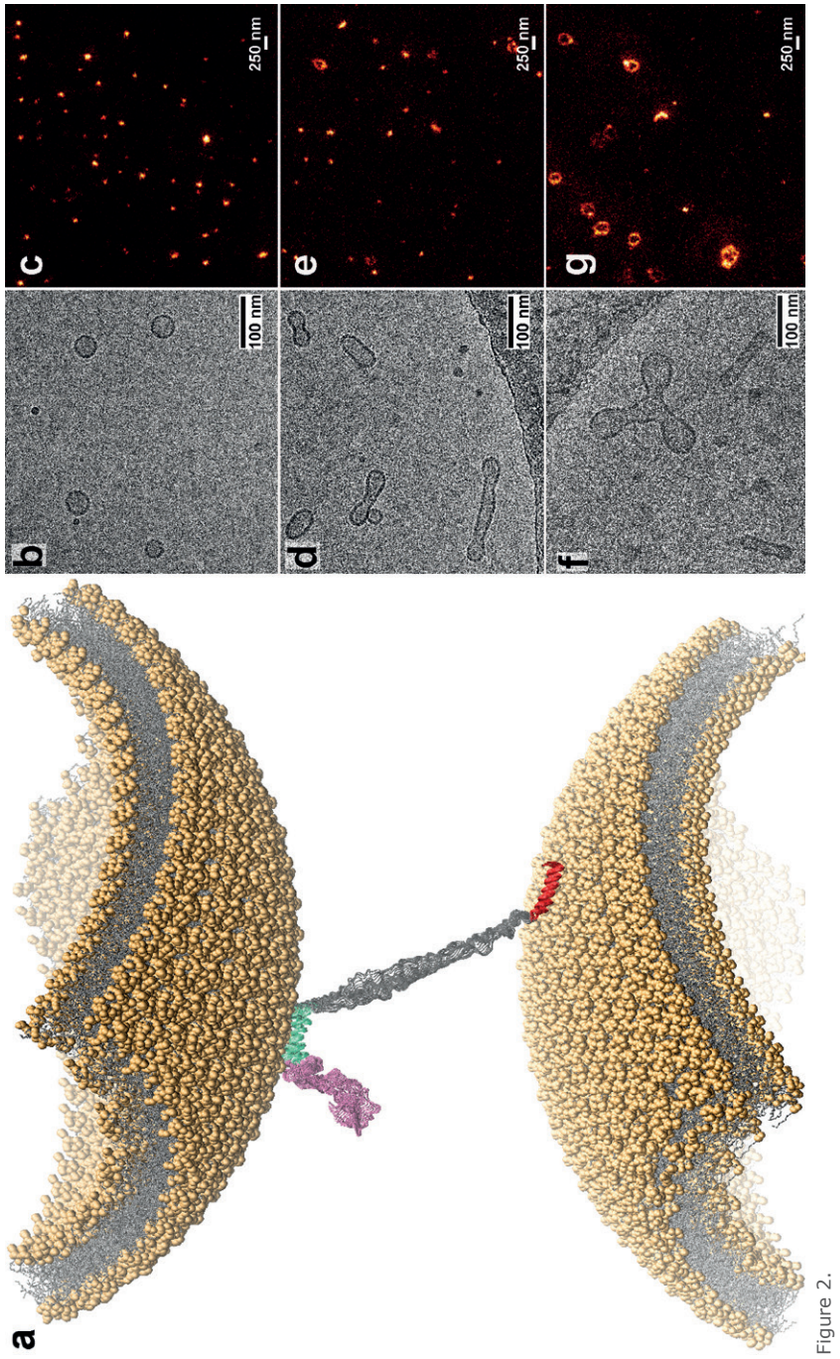


Figure 2.

Figure 2. Vesicle assembly induced by αS. (a) Molecular details of the double-anchor mechanism described in this PhD thesis. αS was modelled with the N-terminal anchor in an amphipathic α-helical conformation (red) and bound to the lower vesicle. The region 65 to 97 (cyan) of αS was modelled in an amphipathic α-helical conformation bound to the upper vesicle. The C-terminal fragment (residues 98 to 140) and the linker region 26 to 59 are shown in pink and grey colours, respectively. With this topology the modelling reveals that a single αS molecule could simultaneously bind two vesicles that are up to 150 Å apart. (b-c) Cryo-EM (b) and super resolution microscopy (c) images acquired on SUVs at a concentration of 0.6 mg/ml. (d-e) Cryo-EM (d) and super resolution microscopy (e) images measured on SUVs following a 12 h incubation with 200 μM αS_{WT} (f-g) Cryo-EM (f) and super resolution microscopy (g) images acquired on SUVs following a 12 h incubation with 200 μM αS_{Sw}. Figure adapted from (Fusco et al, 2016, *Nature Communications* 7:12563).

In addition to studying the physiological membrane interactions by αS, we characterised the fundamental mechanism of membrane disruption by αS oligomers resulting in the generation of neuronal toxicity in PD (Fusco et al, 2017, *Science*, 358:1440-3). Indeed, while fibrillar aggregates of αS represent the major histopathological hallmarks of PD, small oligomeric assemblies of this protein are believed to play a crucial role in neuronal impairment. We obtained a detailed structural characterisation of toxic αS oligomers and compared these results to the study of non-toxic oligomeric species. The results reveal the fundamental structural characteristics driving the toxicity of αS oligomers, including a highly lipophilic element that promotes strong interactions with biological membranes and a structured region that inserts into lipid bilayers and disrupts their integrity (Figure 3). We obtained additional support for these conclusions by showing that mutations targeting the region of αS promoting such interactions with the membrane dramatically suppress the toxicity of αS aggregates in neuroblastoma cells and primary cortical neurons.

Taken together our studies enabled the characterisation of a series of structural properties of the membrane-bound states of αS in both its monomeric and oligomeric forms. The results revealed the nature of the fine balance between functional and pathological membrane interactions of αS and delineated how subtle perturbations of this equilibrium can lead to the rapid evolution of processes that trigger pathological mechanisms.

Understanding this balance is a top challenge for advancing the research in PD and requires innovation across different disciplines to overcome current limitations in probing the conformational transitions of this disordered and metamorphic neuronal protein.

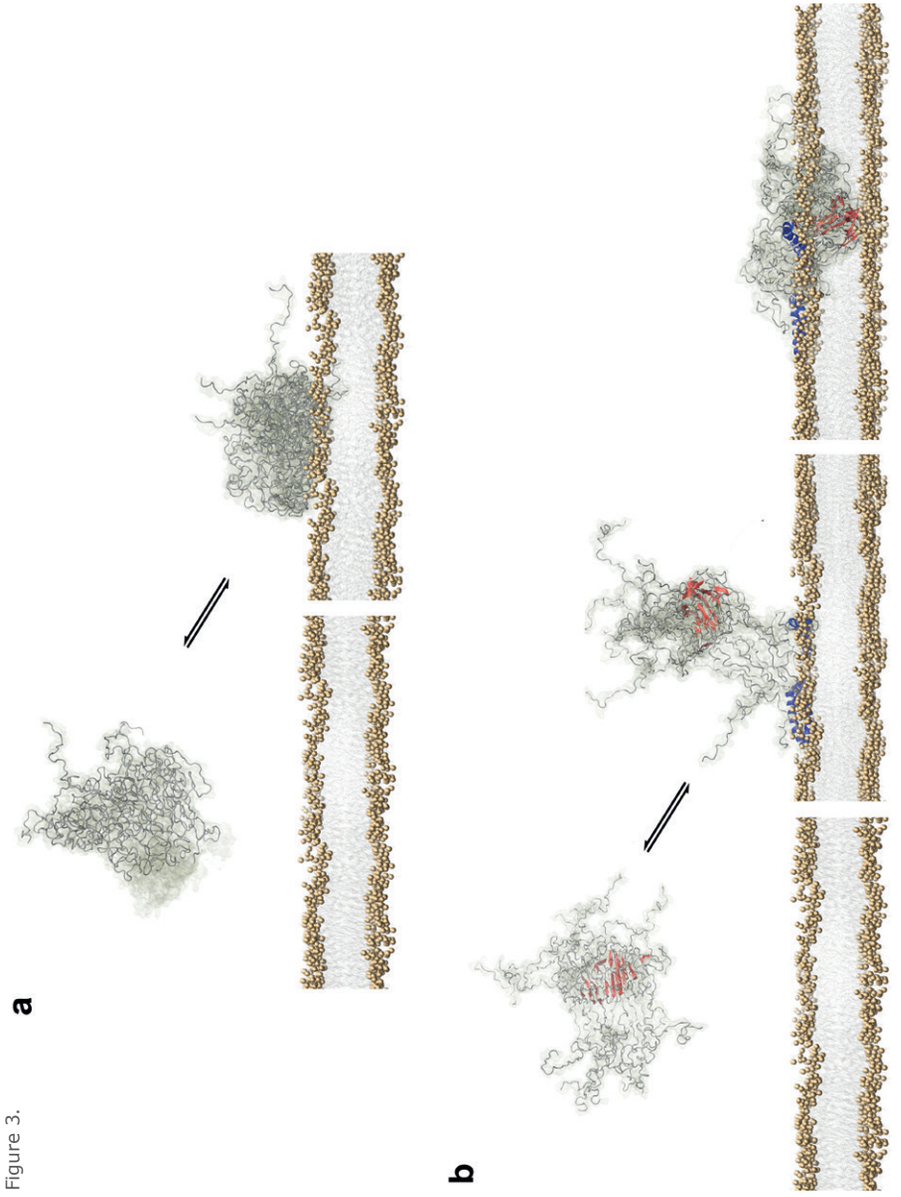
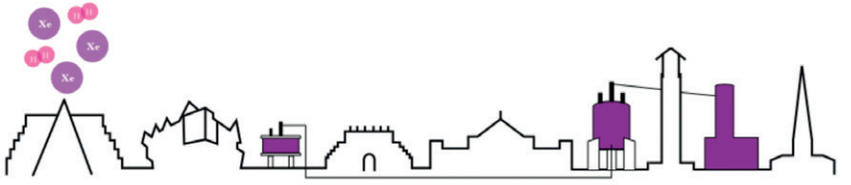


Figure 3.

Figure 3. Structural basis of membrane binding of αS oligomers. (a) Non-toxic αS oligomers are represented in disordered conformations using grey ribbons. ssNMR experiments show that non-toxic αS oligomers bind to the surface of acidic lipid bilayers via various lysine rich segments randomly exposed to the surface of the oligomer and without inserting into the core of the bilayer. (b) Toxic αS oligomers feature both structured (red) and disordered (grey) regions and bind the surfaces of the lipid bilayers via the exposed N-terminal regions of αS molecules in the oligomer, which fold into amphipathic α-helices (blue) upon membrane binding. In contrast to non-toxic oligomers, rigid regions of toxic oligomers were shown to insert into the lipid bilayers thereby promoting membrane disruption. Figure adapted from (Fusco et al, 2017, *Science*, 358:1440-3).

Report: HYP18



HYP18

An International Conference on Nuclear Hyperpolarization, Sep 2-5 2018

The HYP18 international conference on nuclear hyperpolarization was held from the 2nd to the 5th September 2018 in Southampton UK, with 195 attendees.
This conference follows a series of more closely focussed symposia on Dynamic Nuclear Polarization, which were held in Nottingham, UK (2007), Königstein, Germany (2009), Lausanne, Switzerland (2011), Copenhagen, Denmark (2013), and Egmond aan Zee, The Netherlands (2015). The HYP18 meeting had a broader scope, covering a range of hyperpolarization methodologies including optical pumping and parahydrogen, as well as DNP. A representative set of applications of hyperpolarization, ranging from clinical medicine to materials science and even cosmology, were also covered. The HYP18 meeting was an activity of the Hyperpolarization subdivision of Ampère.

The chair of HYP18 was Malcolm Levitt, and the local organizer was Giuseppe Pileio, both from the University of Southampton.

The scientific committee was as follows:
Malcolm Levitt, Southampton, UK (Chair)
Jan Henrik Ardenkjaer-Larsen, Copenhagen, Denmark
Marc Baldus, Utrecht, The Netherlands
John Blanchard, Mainz, Germany
Konstantin Ivanov, Novosibirsk, Russia
Thomas Meersman, Nottingham, UK

The meeting attracted 195 attendees from the following countries: Belgium, China, Denmark, Finland, France, Germany, Greece, Iceland, India, Israel, Italy, Japan, Poland, Russia, Slovenia, South Korea, Sweden, Switzerland, The Netherlands, United Kingdom, United States.

The following topics were covered in 45 oral presentations and 126 posters:
Parahydrogen-Induced Polarization;
Chemically Induced Dynamic Nuclear Polarization;
Spin-Isomer Conversion and Quantum-Rotor-Induced Polarization;
Brute Force Hyperpolarization;
DNP-Enhanced Solid-State NMR;
Dissolution-DNP; Triplet DNP;
Spin Dynamics far from Equilibrium;
Advances in Magic-Angle-Spinning DNP Technology;
Optical Pumping and Noble Gas DNP;
Ultrasensitive Magnetic Resonance using Diamond Magnetometry;
Novel Hyperpolarization Methods using Photodissociation, Infrared Light, and Plasmas;
Magic-Angle-Spinning DNP-Enhanced NMR of Surfaces;
Applications of Hyperpolarized NMR to Nonlinear Physics,
Chemical Reaction Kinetics, Clinical and In Vivo Spectroscopy and Imaging;
Searching for Dark Matter Using Hyperpolarized NMR.

The oral presentations were given by:
John Kurhanewicz, University of San Francisco, USA
Mor Mishkovsky, EPFL, Switzerland
Eleonora Cavallari, University of Torino, Italy
Mathilde Lerche, Technical University of Denmark
Kevin Brindle, University of Cambridge, UK
Thomas Theis, Duke University, USA
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Wing Chow, FMP-Berlin, Germany
Sami Jannin, University of Lyon, France
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Marek Pruski, Ames Laboratory, Iowa, USA
Tomas Orlando, MPI-Göttingen, Germany
Alessandra Lucini Paioni, Utrecht University, The Netherlands
Bob Griffin, MIT, Cambridge, USA

The conference concluded with an evening dinner.
It was announced that the next conference in the series, which will be called HYP20, will be held in Lyon, France, in August/September 2020. It will be organized by Anne Lesage and Sami Jannin.

Report: MR Food 2018

14th International Conference on the
Applications of Magnetic Resonance in Food Science (MRFOOD2018)

Scientific Advisory Board
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Local Organizing Committee (IRSTEA Rennes, France)
Asma Allée, Sylvain Challois, Guylaine Collewet, Brigitte Marchix, Maja Musse, Corinne Rondeau-Mouro (chair)

For the fourth time the International Conference on the Applications of Magnetic Resonance in Food Science (MRFOOD) was organized under the auspices of the Groupement AMPERE. The conference series has built a long tradition in presenting the latest innovations in magnetic resonance and in particular new applications to understanding the functionality of foods, their processing and stability and their impact on health and sensorial perception. The 14th edition of the conference was held from 17th to 21st September 2018 in France and was organized by researchers of the National Research Institute of Science and Technology for Environment and Agriculture (IRSTEA). This year, the conference took place at Rennes in the new congress center "Le Couvent des Jacobins" founded in 1369 by the Order of Preachers (Dominicans) and the property of Rennes Métropole since 2002. The conference attracted 122 participants (among whom 37 students) from 18 countries from Europe, Asia, Oceania, and the Americas. With this steady and broad representation of scientists the MRFOOD conference has firmly established itself as an AMPERE subdivision.

The conference was preceded by tutorials on the hardware (Prof. H. Saint-Jalmes), technical aspects and applications (Dr. Florence Franconi) of MRI in food science and measurement uncertainties in the context of quantitative MRI studies (Dr. Guylaine Collewet).
The scientific part of the conference opened with a session on advanced method developments with inspirational presentations on future food applications. Petrik Galvosas from the Victoria University of Wellington (New-Zealand) has been invited for this session to foster AMPERE cross-division interactions (Magnetic Resonance in Porous Media). The following session dealt with signal processing of MRI and NMR data. Three sessions were dedicated to applications of Low Field NMR, MRI and Diffusion in Food physics, for Postharvest and Food technologies. The last session, shared in two mornings, were dedicated to NMR applications in FoodOmics.
The programme included 7 invited speakers and 28 oral presentations selected from submitted abstracts. The conference is indebted to Petrik Galvosas (Victoria University of Wellington), Saïd Moussaoui (Ecole Centrale Nantes), Shingo Matsukawa (Tokyo University), Henk Van As (Wageningen University), Luiz A. Colnago (Embrapa), Roberto Consonni (CNR) and Patrick Giraudeau (University of Nantes) for providing excellent keynote and invited presentations.
The poster session comprised 42 presentations; Mrs. Kathryn Williamson from the Ohio State University was awarded with a prize for the quality of her poster (p. 28).
25 submitted abstracts (oral presentations mainly) have been selected for publication into a special issue of the prestigious Magnetic Resonance in Chemistry journal (Wiley) after the standard peer-reviewing process.

During the meeting the General Meeting of the MRFOOD Division approved its bylaws, and welcomed Roberto Consonni (ISMAC, Milan, Italy) as a new member of the Scientific Advisory Board. Manfred Spraul (Bruker, Germany) resigned and is gratefully acknowledged for his long service in the board.

For an afternoon in the week, participants have had the opportunity to visit the UNESCO-classed site of the Mont Saint-Michel before the Gala dinner which took place at the Convent of Jacobins.

This conference was sponsored by NMR suppliers (Bruker, JEOL, Niumag, Oxford, Magritek), agro-food industries (Roullier, DianaPetFood), the Rennes metropolis, the Brittany region and the University of Bretagne-Loire (UBL). AMPERE provided financial support for the cross-divisional speaker. Without the generous support of these sponsors this conference would not have been able to offer such an attractive programme at low fees especially for students.

The 15th edition of this conference will be held in 2020 in Aarhus (Denmark) and will be organized by Hanne Christine Bertram. We expect to welcome (even) more participants and see many new developments in the applications of magnetic resonance in food science.

Poster Award: Kathryn Williamson

Application of magnetic resonance for the analysis and assessment of the lipid fraction of green and roasted *Coffea Arabica* beans

Kathryn Williamson, Emmanuel Hatzakis
Department of Food Science and Technology, The Ohio State University

Approximately 15% of the mass of an Arabica coffee bean, *Coffea Arabica*, consists of lipids. This lipid fraction has a number of applications in the food, cosmetic, and pharmaceutical industries, and the effect of roasting on this important lipid fraction is not yet fully understood. The objective of this study is to employ multinuclear and multidimensional NMR spectroscopy as a rapid and reliable method for the quantitative analysis and evaluation of the non-polar, including unsaponifiable, fraction of *Coffea Arabica*, as well as employ MRI to visualize the coffee roasting process. Our results suggest that NMR can be a valuable tool for the determination of many compounds in coffee oil and can be used for quantifying the impact of the coffee roasting process. Green and roasted coffee beans, as well as spent coffee grounds, were analyzed for their lipid components. A number of gradient-selected two-dimensional NMR techniques were applied for a systematic two-dimensional analysis of the various components in coffee oil, including FA, terpenes, oxidation and hydrolysis products, caffeine, and sterols. Quantification was achieved by integration of the appropriate diagnostic signals in the NMR spectra using 2,6-Di-tert-butyl-4-methylphenol (BHT) as an internal standard (IS), as well as the PULCON method, which offers several advantages compared to IS. Bland-Altman analysis showed that PULCON and IS approaches are in a good agreement.

Overall, it was found that the major fatty acids in coffee oil are linoleic, oleic, linolenic and saturated fatty acids. Targeted analysis showed that, with the exception of linolenic acid, only minor changes occur in the fatty acid profile during roasting. A statistically significant increase occurs in secondary oxidation products and free fatty acids after roasting. Additionally, 1,3-diacylglycerides significantly decrease with roasting due to their instability to hydrolysis. Untargeted analyses, namely PCA and OPLS-DA, revealed differences between green and roasted samples. MRI indicated significant morphological changes in coffee beans due to roasting, which may be responsible for these compositional variations. Finally, lipids extracted from spent coffee grounds can be successfully used as precursors for the production of bioplastics. Overall, NMR and MRI are effective tools to help monitor the coffee roasting process and quantify the changes that occur in coffee lipids during roasting.

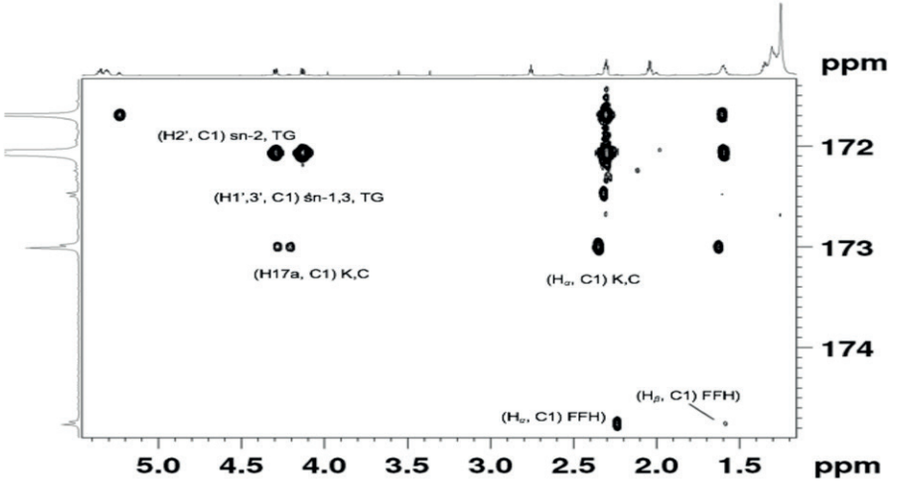

Figure 1. Band selective HMBC spectrum of a green coffee oil sample acquired over a 3 ppm spectral width, in $CDCl_3$:DMSO-*d6* solution.

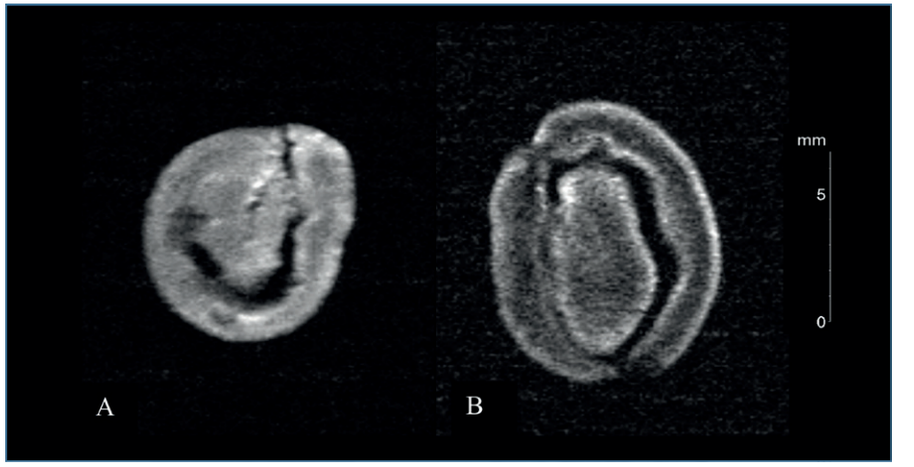

Figure 2. Proton Density Image of a green coffee bean (A) and roasted coffee bean (B).

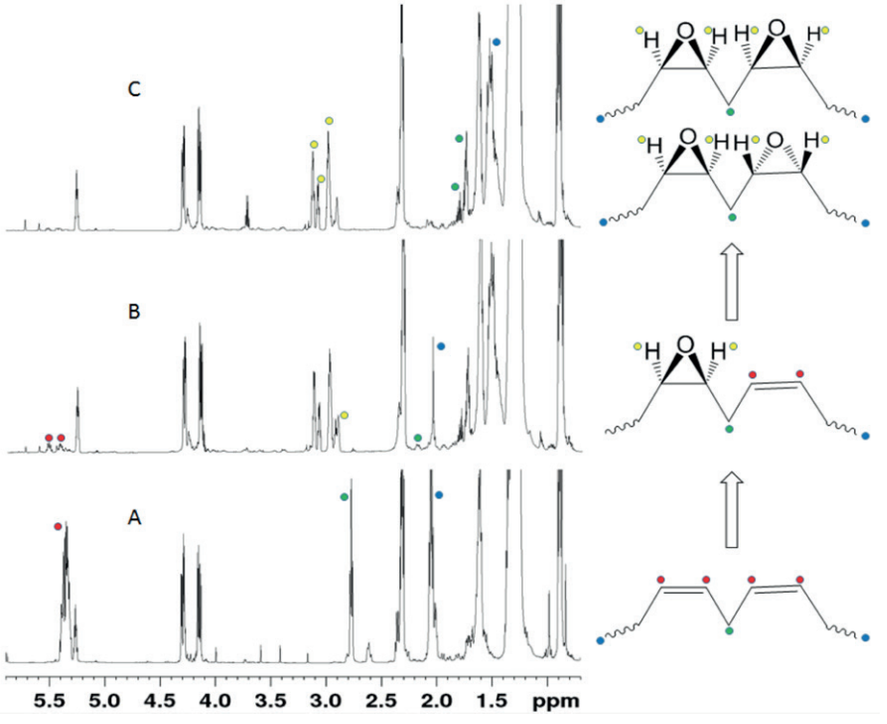

Figure 3. Epoxidation scheme of (A) spent coffee ground lipids, (B) partially epoxidized lipids, (C) fully epoxidized lipids ^{1}H NMR spectra

References

Farah, A. (2012). Coffee: Emerging Health Effects and Disease Prevention. (Yi-Fang Chu, Ed.) (1st ed.). Blackwell Publishing Ltd.

First Announcement

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Our Solution

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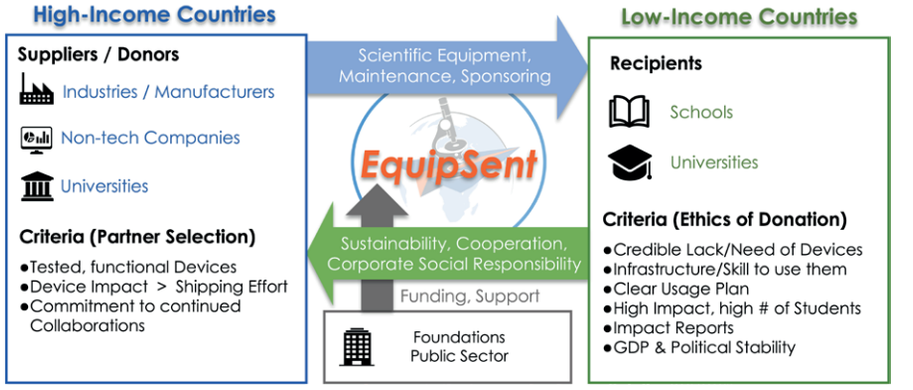
Target Impact

- Access to Education. Students around the world will be granted access to hands-on training and education, rather than theory only.
- Collaboration and Development. The matched donor, sponsor and recipient of equipment are encouraged to collaborate on a long-term basis, which offers learning opportunities on all sides.
- Resource Efficiency & Waste Minimization. The equipment donor profits by reducing costs for space, waste and personnel, while benefitting from a positive image generated through sustainable use.

Founded by a group of ETH students, *EquipSent* is giving a second life to devices, promotes sustainable use and offers access to education and research to more people.



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CGI U COMMITMENT-MAKER 2016

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Obituary

Stefano Caldarelli

*November 24th 1962
†November 6th 2018

photo by Ichrak Toumi

My friend and colleague Stefano Caldarelli, who has died aged 55, a professor of chemistry at Aix-Marseille University, was known throughout the NMR community. He made very diverse disruptive contributions to our field over the last 30 years, reflecting his broad-minded approach and creativity. Stefano is today perhaps best known for his work on developing methods to study complex mixtures by NMR.

He completed his PhD in physical chemistry at Pisa in 1992 under the supervision of Carlo Alberto Veracini. During this time probing the nature of liquid crystals he developed an interest for NMR spectroscopy that he would pursue for the rest of his career. I first met him when he came to spend the final year of his PhD in Alex Pines' lab at the University of California, Berkeley. Like many others I benefited from his academic breadth and intellectual incisiveness. He will also be remembered for the singular way in which he was always looking for alternative approaches to think about challenging problems in science, and for his personal warmth and humour.

Stefano was born in Spoleto, Italy. His father died while he was still a child and he was raised and guided in his education by his mother, who survives him.

In 1993 he took up a staff position at the Université de Lausanne before moving to join my brand new lab at the Ecole normale supérieure in Lyon in 1996, where he was my first post-doc. Not only did he develop landmark solid-state correlation experiments, but he defined many of the traits that are still present in the group today. He then moved on to a position at the CNRS in Lyon, where he developed NMR methods to study catalytic materials.
In 2001 he took up a Professorship at Aix-Marseille University and established an independent group focusing his work on the emerging problem of how to study complex mixtures, materials and foodstuffs by NMR. Not only did he contribute major scientific discoveries, but he mentored many students and post-docs who have gone on to independent academic careers in France and abroad.

He was a curious sharp-minded scholar and phenomenal epicurean, and he retained passions for music, martial arts, and cultures around the world all his life. He had a large vision of science and society, and he was actively involved in promoting NMR across the globe, from Europe to South America, notably through his contribution to founding the Alpine Conference on Solid-state NMR.
He became ill in 2015, and died on 6 November 2018 after a valiant fight.

Lyndon Emsley
EPFL Lausanne

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Future conferences

Ampere Events 2019

16th International Youth School Conference „Magnetic resonance and its applications - Spinus 2019“	Saint Petersburg (Russia)	March 31 to April 1 2019
Ampere NMR School 2019	Zakopane (Poland)	June 23-29 2019
15th ICMRM	Paris (France)	August 18-22 2019
ISMAR / Euromar 2019	Berlin (Germany)	August 25-30 2019
11th Alpine Conference on Solid-State NMR	Chamonix	September 15-19 2019

Ampere Events 2020

Euromar 2020	Bilbao (Spain)	July 2020
‚HYP20‘ Hyperpolarized Magnetic Resonance 2020	Lyon (France)	August 30 to September 2 2020