ISSUE 2: December 2020

NEWSLETTER

Inside this issue:

Letter from the Editors

Supramolecular chemistry has been one of the most emergent fields in chemistry in the recent years. Latest progress has led to a shift in focus, from understanding the basic concepts of molecular encapsulation to pursuing the controlled uptake and/or release of molecules with the aim to identify and develop new applications in several fields such as drug delivery, catalysis or functional materials.

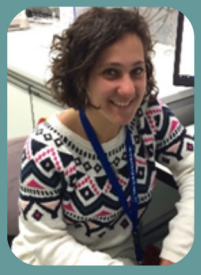
In this second issue the five ESRs not presented in the first issue are introduced (second part of the *Meet our ESRs*). We are also glad to include a written interview to one of the PIs from the project, Prof. Ward (Warwick) in which supramolecular chemistry, relationship between academia and industry and advices for junior researchers are highlighted. We want to thank him for accepting our invitation!

This issue also includes a short history of the Nobel Prizes in Chemistry in the field of supramolecular chemistry (from the first until the latest awarded scientists are included). In this section, the key points on how the field has been evolving are disclosed.

Within this issue you will also read about the experiences of some ESRs in the adventure of their secondments.

Last but not least, what is better than 1.000 words?...**An image!** In this edition we challenge two ESRs to explain their work in one image.

From the Editors of this issue:



Chiara Mirabella
(ESR 10)

Pedro Ferreira
(ESR 1)

Meet our ESRs

In the first NOAH newsletter issue we introduced five of our ESRs. In this edition the last but not least other five ESRs will be presented: Santiago Pons, Daniel Stares, Cristina Mozaceanu, Arturo Llamosí - Fornés, and Dylan Serillon.

University of Neuchâtel

Santiago PONS

Our project is focused on the preparation of coordination-driven arene ruthenium metalla-prisms. These are specially interesting due to their water-solubility, anticancer activity and the ability to deliver "guests" inside their cavities. In specific, functionalization of pyrene moieties to target cancerous tissues will be studied.

I always found scientific research interesting, it is a non-monotonous job where everyday is different!

In my free time I like almost any kind of sportive activity, it is the best way to disconnect from day-to-day work.

Supervisor: Prof. Bruno Therrien

Freie Universität Berlin

Daniel STARES

My role within the NOAH network is to complete characterization of the different containers via mass spectrometry. Mass spectrometry can provide information relating to the size, shape and stability of the containers and can be used to monitor the effect of guest encapsulation upon these properties.

In my spare time, I can occasionally be motivated enough to go running or cycling but will more likely be found in a café/bar around Berlin, reading or playing a board game.

Supervisor: Prof. Dr. Christoph A. Schalley

Cristina MOZACEANU

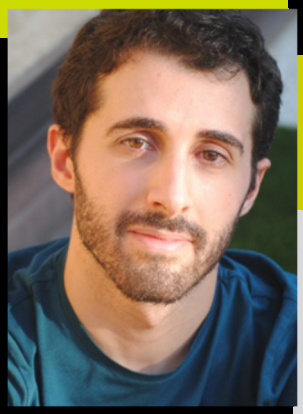
The core of my research project is represented by the study and application of $M^{II}_8L_{12}$ self-assembled coordination cages, which are robust, highly charged (16^+), hollow containers with hydrophobic cavities, capable of encapsulating various small guest molecules. Additionally, these complexes are able to accumulate 'soft' anions, finding applications in host-guest chemistry, supramolecular catalysis, and potentially drug release in artificial skin cells.

Hobbies: Drawing and illustration

Supervisor: Prof. Michael D. Ward

University of Warwick

Arturo LLAMOSÍ



We are looking into expanding the cavity of resorcinarenes to allow accommodation of larger organic guest molecules. Installation of stimuli-sensitive functionality at the upper rim will allow us to introduce switchability and extend the lipophilic cavity. After this, the relationship between structures and properties of the new capsules (e.g. binding selectivity) can be studied. These types of molecular cages are promising candidates for chemoselective and chiral recognition.

Hobbies: Playing basketball, driving and cooking. Someday I would like to have my own brand of beer.

Supervisor: Prof. Agnieszka Szumna

Institute of Organic Chemistry – Polish Academy of Sciences

Dylan SERILLON

I develop computational tools to predict suitable guests for several hosts developed by academic partners. I work mainly on a porphyrin cage, but my tools are supposed to be adapted to any type of molecular structures. The main idea is to predict several physical and chemical properties based on the simulation of the interactions between the host and the guest at the molecular level. Especially the free binding energy which is a numerical value that quantifies the binding affinity of a host -guest complex.
I like computer science, hiking and biking!

***Supervisor*: Prof. Xavi Barril**

University of Barcelona

Interview with the PI

In this section we want to introduce one of the academic PIs of the NOAH consortium, inteviewing him. We invited him to answer to some important key questions that PhD students had asked themselves at least once in their life. With his past own experience as a PhD student with the wish of becoming a researcher in chemistry in the future, Prof. Michael Ward (University of Warwick) shared with us his experience and his point of view on the academic research life. He gives to young researchers some precious tips on the academic research world and on the everyday life of a PhD student.

Prof. Ward can you tell us how you decided to become a scientist, the reason why, the steps you needed to follow and why you became interested in supramolecular chemistry?

I was always interested in science. I never wanted to do anything else. When I was little I had a telescope and looked at the moon and stars form our garden, on cold clear nights, wearing my pyjamas and nearly freezing. I had a chemistry set and made a mess of my bedroom: I made a sodium bicarbonate 'volcano' with vinegar on the carpet, and tried to make gunpowder (not very well). I followed instructions in a magazine to make a crystal radio. I went to university intending to specialise in physics, but decided during my first year that chemistry was more fun (and physics was too hard), so here I am.

What do you like the most about your job and what do you find most challenging in it?

What I like most in research is the satisfaction of seeing a project slowly come together, and then writing a nice paper about it. I really like the writing process: taking a complicated pile of data / results and distilling it into something simple, memorable and completely clear. I also enjoy doing tutorials with undergraduates in groups of 5 - 6: if I have them for an hour I know can send them away understanding more than they did at the start.

Can you share with us one time you "failed", which was your process to overcome the failure and what you learnt from that?

I led on a large grant application (£1M) to get new equipment for my department: NMR, mass spectrometer, X-ray diffractometer. Good departments were asked to apply by EPSRC; they had about £20M to distribute between 20 departments and the implication was that we would all get about £1M. But only 17 were funded (mine was ranked 18th) and we got no feedback why. I and my colleagues were really disappointed as we had thought this was automatic as long as we wrote a good proposal (which we did).

Fortunately, they got some more money the year after and funded the remaining three a year later so we got our equipment eventually! What did I learn? A good grant application is never wasted.

How do you envision the future of supramolecular chemistry?

The integration of structure and function at will. Imagine if we could design a light-harvesting machine that reduced CO_2 to CH_4 and could combine the components (chromophores, electron-transfer species, reaction centres...) with complete certainly about what the structure of the assembly would be – like a virus but with multiple different components whose functions combine as well as their structures. Another analogy would be: mix a large number of electronic

components in a bag, mix them up... and get a working radio or computer.
Wouldn't it be good to be able to do that with molecular components!

How important do you think it is for scientists in academia to collaborate with industry?

Very important but not all-important. Some industry-driven research is short term development and not exciting from a blue-skies-science perspective. On the other hand, much blue-skies-science has little immediate use in the real world and will not feed anyone or make anyone healthier. We need both, of course, and industry funders are part of that.
When I was a new academic I tried to ask someone from Esso (petrochemicals company) for a grant to do some metal coordination chemistry. His reply was: we aren't interested. We don't need to spend money on your research. We make billions by marketing the same products that we did 50 years ago - petrol and lubricants - and we'll do that for the forseeable future.

Fortunately not all industry funders are like that!

PhD students are fascinated by science but in the daily life in the lab the problems are different. We work on one experiment for days to finally find out very little progress. Could you give an advice to young researchers who want to become excellent researchers in their fields keeping enthusiastic with science?

Don't be afraid to spend time trying new or unusual things. You have time to try and fail a few times, it is normal and a useful part of your learning. You can do a PhD in three months... it just takes three years to reach the point where you can do it in three months!

Also - collaborate, collaborate, collaborate. We are mostly highly specialised and can only do one thing (or a few things) well. To do something big requires a combination of skills and outlooks that you are unlikely to have on your own.

Michael Ward got his PhD in Chemistry at University of Cambridge. After working as post-doc researcher with Jean-Pierre Sauvage in Strasbourg in the field of supramolecular chemistry with the study of catenates, he started his academic career in Bristol in 1990. Then in 2003 he moved to Sheffield and finally in 2017 he moved to the University of Warwick where he is currently Head of Department.

Ward research group investigation is focused on the coordination chemistry of transition metal and lanthanide ions and their multinuclear assemblies. More specifically, its interests are i)self-assembly and host-guest chemistry of hollow metal/ligand cage complexes, and ii) photophysical properties of polynuclear complexes and supramolecular assemblies, with applications in imaging and sensing.

Awards

Corday Morgan medal for 1999
Chemistry of the Transition Metals' award for 2005
Supramolecular Chemistry award for 2016.

Nobel Prizes in Supramolecular Chemistry

By Chiara Mirabella

Between 1901 and 2019, the international awards in Physics, Chemistry, Medicine, Literature, Peace and Economic Sciences founded by Alfred Nobel (Swedish inventor and entrepreneur) called Nobel Prizes and the Prize in Economic Sciences, were awarded each year "*to the person who shall have made the most important discovery or invention within the field…"(Cit. Alfred Nobel).*

But who won (over all this years) the Nobel prize in Chemistry? And how chemistry field has evolved until today?

Starting from the very beginning of the history of Nobel prizes in chemistry,

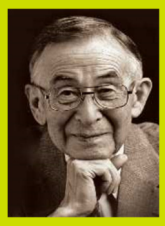
Jacobus Henricus van 't Hoff (1852-1911) was awarded in 1901 for his pioneer contribution to the field of physical chemistry. He was awarded thanks to his discoveries related to the study of the relationship between the heat and the equilibrium condition (later incorporated in the more general and modern Van 't Hoff-Le Chatelier principle) and for the deeper explanation of the already well known fundamental concepts of osmotic pressure.

Since that, many other chemists have been awarded this prestigious prize thanks to discoveries which have changed our daily life.

Meanwhile chemistry has evolved. In the last decades an increasing interest in mimic complex processes which regulate the Nature and the life, has led to the marriage between different fields of chemistry in a unique interdisciplinary area of chemical research. From the fusion between coordination chemistry, organic synthesis, analytical chemistry and bioorganic and bioinorganic chemistry rises the supramolecular chemistry where host guest chemistry is incorporated.

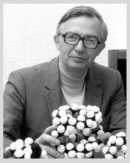
Precisely the two scientists who gave the name to this area of research, **Donald J. Cram** (University of California, Los Angeles, USA) and **Jean-Marie Lehn** (Université Louis Pasteur, Strasbourg, and College de France, Paris, France) together with **Charles J. Pedersen** (Du Pont, Wilmington, Delaware, USA) were jointly awarded with the Nobel prize in 1987 for the development and use of molecules with structure-specific interactions of high selectivity.

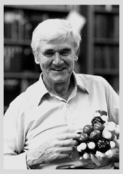
The recognition to this scientists came from their discovery in the synthesis of new type of molecules called "hosts", featuring a hole or a cavity with chemical- physical properties which allow to selectively recognize small anions, cations, and neutral molecules, called "guests". A host and a guest can interact each other via non-covalent interactions, reproducing the ability of molecules involved in biological recognition and regulation processes, to recognize each other forming well-defined complexes.



On one hand to **Pedersen** is given the merits for the design and synthesis of cyclic polyether known as *crown ether*. These molecules contain a circular inner area, in which depending on their dimension, metal ions as Li, Na, K, Rb, Cs, can be selectively discriminated and complexed.

One the other hand, to **Marie Lehn** and **Cram** the merit





was attributed due to the development of organic chemistry for the synthesis of complex molecules containing portals and deep cavities, which can accommodate low molecular weight molecules into their cleft or cavity, named *cavitands* and *criptands*.

From the evolution of this basic "lock and key" concepts, derived the discovery of even more exotic and functional structures which are able to reproduce the function of natural enzymes (i.e. lactasi).

All these important developments constitute a real foundation for the entire field of supramolecular chemistry and put the basis for the design of topologically very challenging structures. In the next years the intriguing idea of build nanoscale machines made by molecules, so small to be only visible by a microscope, was insinuating in scientists mind. Thanks to the realization of this innovative and odd idea in 2016 **Jean-Pierre Sauvage**, **Sir J. Fraser Stoddart** and **Bernard L. Feringa** were awarded with the Nobel Prize for the design and develop of molecular machines.

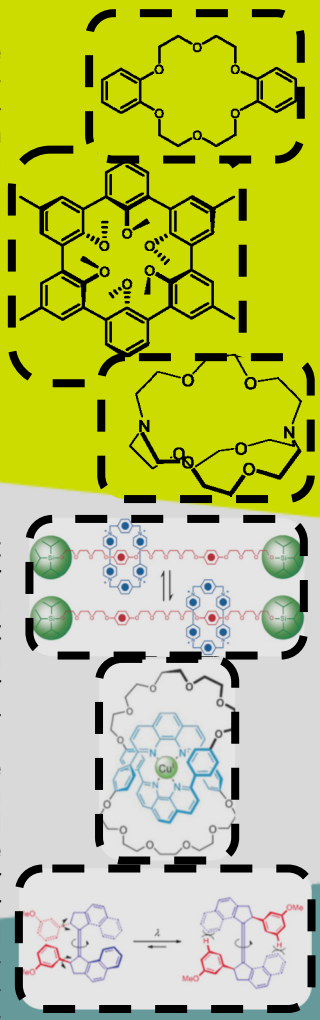
The first step toward the challenging assembly of molecular machines is represent by **Sauvage**'s intuition and realization of molecular rings interlocked between them, called *catenanes*. Under an energy stimulus one of the two rings could rotate around the other.

In addition, **Stoddart** reproduced the movement of a wheel along an axle developing molecules called *rotaxanes,* in which a circular and a linear molecule are mechanically interlocked together. By giving a stimulus (heat) to the system, the wheel can jump forwards and backwards between the two parts of the axle, reproducing a shuttle motion. To Stoddart's research group is also attributed the design of a lift and an artificial muscle, based on rotaxanes.

In 1999, **Feringa** produced the first molecular motor, in which he used a switchable group which under UV light structurally change, provoking the rotation of the all system.

His research group also built a four-wheels drive nanocar in which a molecular skeleton held together four motors that functioned as wheels. When the wheels span, the car moved forward over a surface.

Taken all together, these pioneer works for the design of enzyme like receptors and molecular machines have inspired many supramolecular chemists and still inspire our work as researchers. Making treasure of the previous discoveries in the field of supramolecular chemistry, we fancy to contribute to the further understanding of Nature's forms and functions and participate to relevant realization of smarter and even more advanced supramolecular systems, with our daily creativity in the lab.



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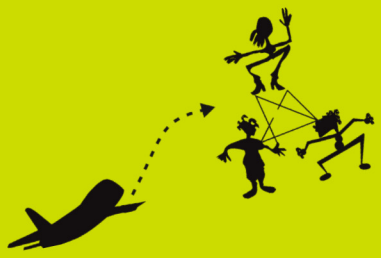


Amy EDO-OSAGIE

I conducted my academic secondment at the University of Warwick, under the supervision of Prof. Mike Ward. Our project aim was to synthesise some new metal-organic cages using Ward-type (pyridyl pyrazolyl) ligands featuring a porphyrin bridge, a motif that is central to my PhD project. As I had previously studied at Warwick, I expected to adjust to my new lab quickly, however I learned that much like snowflakes, no two labs are the same, even at the same university! The secondment allowed me to see and try new, alternative techniques in synthesis and compare the ways in which different universities and departments handle health and safety in the lab. Importantly, it helped me widen my network, and practise communicating my research to other researchers.

Daniel SÁNCHEZ-RESA

My first academic secondment was conducted at the University of Neuchâtel (Switzerland). My project there was about synthesizing new ruthenium based cages. Working in synthesis has been very interesting and challenging to understand the overall project of my PhD and collaborating with another ESR and supervisor has been great to adapt to different environments and network with people with different backgrounds!

Networking within NOAH: Secondments

Secondments are key factors in PhD student's research project once they allow the ESRs to gain knowledge and training in others fields of chemistry. Here we present some testimonies of our colleagues and their experiences.

Cristina MOZACEANU

This year I had the opportunity to go on my first secondment, at Freie Universität Berlin, Germany, where for five months I undertook activities within Prof. Christoph A. Schalley's group. Throughout this placement, I have gained a significant expertise in mass spectrometry on supramolecular complexes, covering various aspects, ranging from background information in mass spectrometry to sample preparation, data acquisition and analysis, as well as technical aspects. Additionally, I managed to integrate myself within a new city and expand my research network by collaborating with Daniel Stares (ESR3) and other researchers in this field. This period was marked by the COVID-19 global pandemic, leading to a significant impact, allowing me to engage in self-development both professionally and personally.

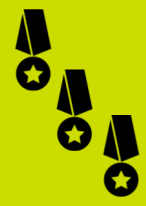
During this event questions were answered and knowledge was exchanged. Out of it, three where awarded for the best **poster presentation**.

This year during the 2ºNOAH School there was a high creative level from the ESRs.

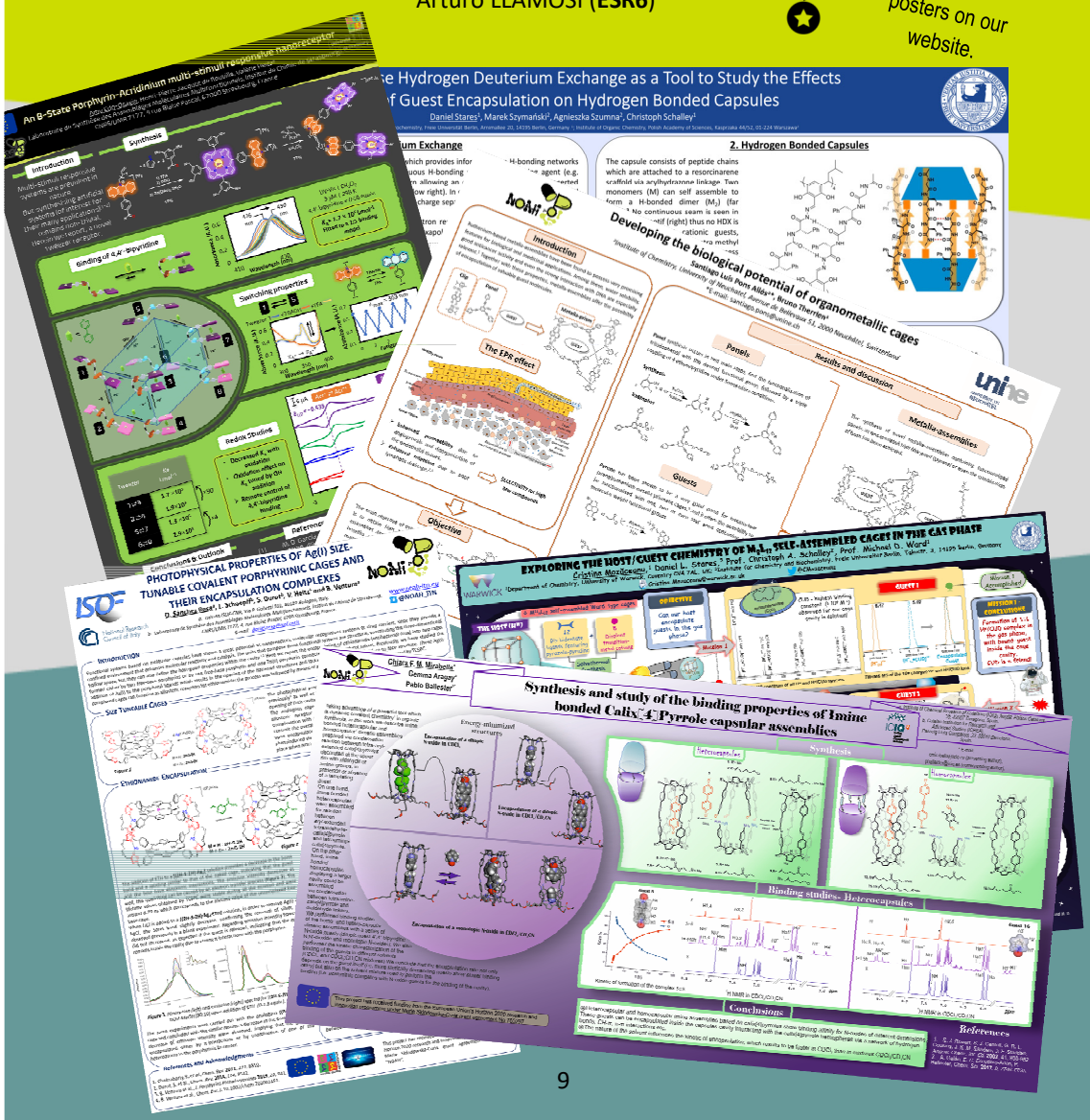
Chiara Mirabella (**ESR10**)

Amy Edo-Osagie (**ESR7**)

Arturo LLAMOSÍ (**ESR6**)



Check all posters on our website.

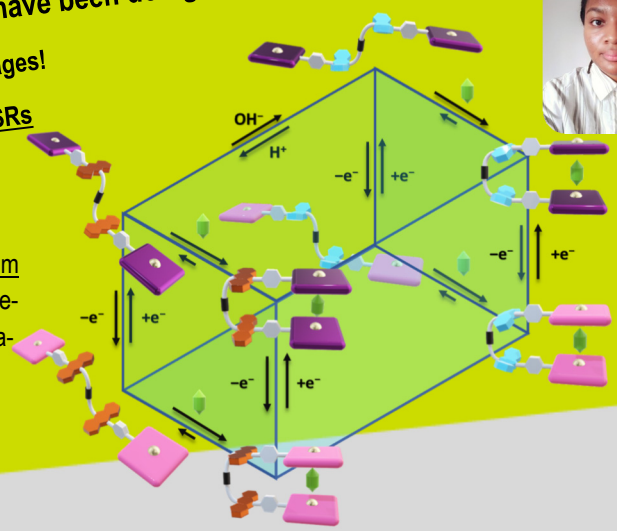


Here you can find what we have been doing so far,

Not with words but with nice images!

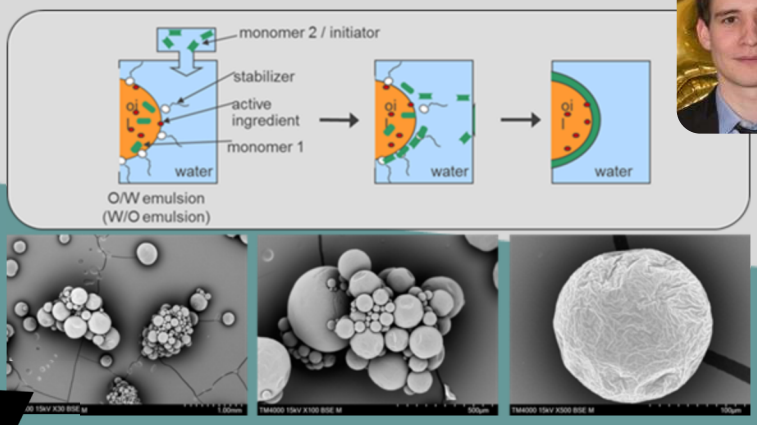
Graphical Abstracts form the ESRs

Amy



An 8-state Porphyrin-Acridinium tweezer: Cubic illustrative scheme displaying the different states the tweezer can reach through multiple stimuli (chemical and redox)

Quentin



This process involves the reaction of two monomers at the interface of an oil-in-water emulsion, in which the isocyanate monomer and the amine monomer are soluble in the oil phase and in the water phase respectively. This reaction allows the formation of a strong polymeric wall around the emulsion droplets, leading to microcapsules after drying.

SEM picture of polyurea microcapsules filled with up to 70%w of a liquid hexamethylene diisocyanate (HDI) trimer derivative.

Attended conferences /workshops

⇒ Elixir course: train the trainer, Paris-France, Feb. 2020

⇒ 2nd French-Israeli workshop on chemoinformatics, Strasbourg-France, Feb. 2020

⇒ Virtual conference on Molecular capsules: from design to applications (NIST), online conference, March 2020

⇒ 2nd NOAH School, online event, Nov. 2020

2nd NOAH School (Virtual edition)

Upcoming events

3rd NOAH School	August/September	2021
SupraBio 2021 International Symposium on SupraBiomolecular Systems, 7th edition	May	2021
International Conferences on Noncovalent Interactions	July	2021
International Symposium of Macrocyclic and Supramolecular Chemistry	August	2021

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