Bridge virtual meeting

June 7, 2021

WAITING FOR

20th International CYCLODEXTRIN Symposium

BOOK OF ABSTRACTS

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Bridge virtual meeting

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Final Program
STARTING 13:00 PM CEST TIME - June, 7 2021

10' **OPENING WELCOME**
Antonino MAZZAGLIA, Conference Chair, CNR-ISMN - Messina, Italy
Michele MUCCINI, CNR-ISMN Director

OPENING SESSION
Chair: Hidetoshi ARIMA, Past President of Japanese CD Society, Daiichi University of Pharmacy - Fukuoka, Japan

20' **Cyclodextrins against SARS-CoV-2: a tool or a weapon?**
KN1 - Tamás SOHAJDA, *Cyclolab Ltd - Budapest, Hungary*

20' **Cyclodextrin vesicles as templates for the self-assembly of versatile polymer nanocontainers**
KN2 - Bart Jan RAVOO, *University of Münster - Münster, Germany*

20' **Biomedical application of iron(II)porphyrin-cyclodextrin supramolecular complexes working as artificial hemoglobin in vivo**
KN3 - Hiroaki KITAGISHI, *Doshisha University - Kyoto, Japan*

12' **DISCUSSION (live)**

YOUNG SCHOLARS SESSION I
Chair: Carmen ALVAREZ-LORENZO, University of Santiago de Compostela - Spain

15' **Chemical and biological advancements of graphene family materials functionalized with cyclodextrins**
SKN - Angela SCALA, *University of Messina - Messina, Italy*

6' **Molecular dynamics of a-CD/PEG polyrotaxane in solution**
SP1 - Yusuke YASUDA, *The University of Tokyo - Kashiwa-City, Japan*

6' **Determination of the crosslinking density of β-cyclodextrin-based nanosponges**
SP2 - Gjylije HOTI, *University of Turin - Turin, Italy*

6' **Nanocomposites based on cyclodextrins and clay minerals and their applications**
SP3 - Marina MASSARO, *University of Palermo - Palermo, Italy*

6' **Calculating the complexation constant of oxyresveratrol/cyclodextrin based nanosponges complexes**
SP4 - Adrián MATENCIO DURÁN, *University of Turin - Turin, Italy*

6' **Investigation of the cellular effects of β-cyclodextrin derivatives**
SP5 - Ágnes RUSZNYÁK, *Debreceni Egyetem - Debrecen, Hungary*

10' **BREAK (questions in chat)**

KN=Invited keynote speaker; **SKN**=Invited short keynote speaker; **SP**=Invited short presentation

YOUNG SCHOLARS SESSION II

Chair: Milo MALANGA, Cyclolab Budapest - Hungary

6' Mechanochemical synthesis and functionalization of crosslinked cyclodextrin polymers
SP6 - Alberto Rubin PEDRAZZO, *University of Turin - Turin, Italy*

6' Cyclodextrins as supramolecular materials in the design of smart and longer lifespan Li-S batteries
SP7 - Fanny BÉTERMIER, *Université d'Évry - Evry, France*

6' FFC-NMR techniques for assessing the texture features of nanosponges
SP8 - Samuele TERRANOVA, *University of Palermo - Palermo, Italy*

6' Hydrophilic and hydrophobic cyclodextrins as excipients in quick/slow release bilayer tablets
SP9 - Jaime CONCEIÇÃO, *University of Porto- Port, Portugal*

6' Inclusion mode of eriocitrin into β-CD and HP-β-CD: an NMR and molecular dynamics investigation
SP10 - Andrea CESARI, *University of Pisa - Pisa, Italy*

6' Stability, characterization, and kinetics of difluprednate in cyclodextrin solution
SP11 - Manisha PRAJAPATI, *University of Iceland - Reykjiavik, Iceland*

6' Physicochemical characterization of levofloxacin-loaded chitosan/cyclodextrin nanospheres and antibacterial activity evaluation
SP12 - Federica DE GAETANO, *University of Messina - Messina, Italy*

6' Synthesis and characterization of cyclodextrin-based carriers to target the central nervous system
SP13 - Eszter KALYDI, *Cyclolab Ltd - Budapest, Hungary*

10' BREAK (questions in chat)

CLOSING SESSION

Chair: Sophie FOURMENTIN, President of French CD Society, University of Littoral-Côte d'Opale - France

20' Enabling technologies in cyclodextrin synthesis
KN4 - Giancarlo CRAVOTTO, *University of Turin - Turin, Italy*

5' DISCUSSION (live)

10' CLOSING REMARKS
Francesco TROTTA, President of Italian CD Society, University of Torino - Italy
Antonino MAZZAGLIA, Conference Chair, ISMN-CNR - Messina, Italy

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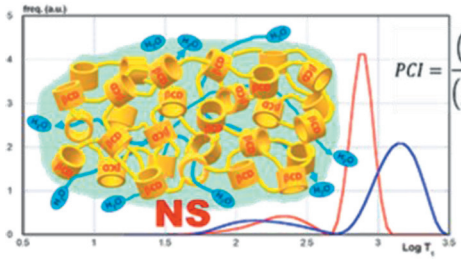
FFC-NMR techniques for assessing the texture features of nanosponges

Paolo Lo Meo[a], Samuele Terranova[a], Antonella Di Vincenzo[a], Delia Chillura Martino[a], Pellegrino Conte[b]

[a] Dept. of Biological, Chemical and Pharmaceutical Sciences and Technologies (STEBICEF), University of Palermo; V.le delle Scienze ed. 17, 90128 Palermo, Italy.
[b] Dept. of Agricoltural, Food and Forest Sciences (SAAF), University of Palermo; V.le delle Scienze ed. 4, 90128 Palermo, Italy.
paolo.lomeo@unipa.it , pellegrino.conte@unipa.it

Nanosponges (NSs), i.e. hyper-cross-linked polymeric materials obtained by reticulating cyclodextrin units with suitable linker units, constitute an emerging class of functional materials, due to their easy synthesis and chemical modification, and to their tunable absorption and controlled release abilities as well. NSs are supposed to possess a thick network of nanochannels in their highly disordered structure. However, their textural features (average pore size, specific surface and specific pore volume) are quite difficult to estimate, and classical evaluation methodologies (N_2 absorption isotherms analyzed by BET or BJH methods, or dye absorption isotherms[1]) have afforded questionable results. Indeed, partly due to their fair swellability, the concept itself of specific area seems quite elusive to define for these materials. In this communication we present the results of a Fast-Field-Cycling (FFC) NMR relaxometric investigation on a set of suitably selected NSs, aimed at providing a viable method to evaluate their texture properties. A suitable heuristic analysis of the NMRD dispersion curves enables to individuate the dynamic domains which can be led back to the structural motifs present in the materials structures. Moreover, The FFC relaxometric technique is able to afford valuable information on the mobility of water molecules inside the nanochannels of the swellable NS structure, providing indirect information on pore size distribution.[1] Inspired by results gained in soil science,[2] we propose to extend to nanosponge materials the concept of "connectivity", by defining a "Pore Connectivity Index" (PCI)[3,4] based on T_1 realxation times distribution functions, which may constitute a valuable alternative to quantify the functional permeability of NSs.



$$PCI = \frac{\left(\int_{T_{A,fast}}^{T_{B,fast}} P(T_{fast}) T_{fast} dT_{fast}\right)^{-1} - R_w}{\left(\int_{T_{A,slow}}^{T_{B,slow}} P(T_{slow}) T_{slow} dT_{slow}\right)^{-1} - R_w}$$

REFERENCES

1. Wilson L. D.; Mohamed M. H.; Headley J. V., *J. Colloid Interf. Sci.*, **2011**, 357, 215-222.
2. Conte, P.; Lo Meo, P., *Agronomy,* **2020,** 10*,* 1040.
3. Lo Meo, P.; Mundo, F.; Terranova, S.; Conte, P.; Chillura Martino, D., *J. Phys. Chem. B* **2020,** 124, 1847-1857.
4. Cataldo S.; Lo Meo P.; Conte P.; Di Vincenzo A.; Milea D.; Pettignano A., *Carbohyd. Polym.* **2021**, 118151.