Sociedad Española de Química Terapéutica
SEQT

VIII SYMPOSIUM OF MEDICINAL CHEMISTRY YOUNG RESEARCHERS

VIII SYMPOSIUM OF MEDICINAL CHEMISTRY YOUNG RESEARCHERS

JULY 22nd 2022
Barcelona

VIII SYMPOSIUM
SEQT
OF MEDICINAL CHEMISTRY YOUNG RESEARCHERS

Sociedad Española de Química Terapéutica
SEQT

VIII SYMPOSIUM OF MEDICINAL CHEMISTRY YOUNG RESEARCHERS

SCIENTIFIC PROGRAMME

8:45-9:30	**REGISTRATION**	
9:30-9:45	**OPENING CEREMONY**	
9:45-10:30	**JUSTE PLENARY LECTURE L1: Prof. Maria Laura Bolognesi**	
10:30-11:15	**ORAL COMMUNICATIONS – SESSION 1**	
	10:30-10:45	Oral 1: Greg Kettley
	10:45-11:00	Oral 2: Pau Nadal
	11:00-11:15	Oral 3: Anna Clua
11:15-11:45	**FLASH POSTER PRESENTATIONS – SESSION 1: Odd Numbers**	
11:45-12:15	**COFFEE BREAK & POSTER SESSION**	
12:15-13:00	**ORAL COMMUNICATIONS – SESSION 2**	
	12:15-12:30	Oral 4: Anna Duran
	12:30-12:45	Oral 5: James Eills
	12:45-13:00	Oral 6: Iván Sánchez
13:00-13:45	**MOLECULES PLENARY LECTURE L2: Dr. Olalla Vázquez**	
13:45-14:15	**FLASH POSTER PRESENTATIONS – SESSION 2: Even Numbers**	
14:15-16:00	**LUNCH & POSTER SESSION**	
16:00-17:30	**WORKSHOP – COACHING: Antonio Bonilla**	
17:30-18:15	**ORAL COMMUNICATIONS – SESSION 3**	
	17:30-17:45	Oral 7: Mercedes Rubio
	17:45-18:00	Oral 8: Ramona Santini
	18:00-18:15	Oral 9: Craig Steven
18:15-18:45	**CLOSING REMARKS AND AWARDS**	
18:45-21:00	**NETWORKING**	

ORGANIZING COMMITTEE

Sara Preciado - *Board SEQT member (Enantia S.L.)*

Carles Galdeano - *Board SEQT member (Universidad de Barcelona)*

Laia Josa-Culleré - *Instituto de Química Avanzada de Cataluña (IQAC-CSIC)*

Carolina Izquierdo García - *Instituto de Química Médica (IQM-CSIC)*

Pau Nadal Rodríguez - *Facultad de Farmacia y Ciencias de la Alimentación (Universidad de Barcelona)*

Ainoa Sánchez Arfelis - *Facultad de Farmacia y Ciencias de la Alimentación (Universidad de Barcelona)*

Hadrián Álvarez Fernández - *Instituto de Química Médica (IQM-CSIC)*

Andreea Larisa Turcu - *Biopharma Synergies S.L*

Laura Márquez Cantudo - *Facultad de Farmacia (Universidad CEU San Pablo)*

Darío Miranda Pastoriza - *CiQUS-Facultad de Farmacia (Universidad de Santiago de Compostela)*

Andrea Bertran Mostazo - *Facultad de Farmacia y Ciencias de la Alimentación (Universidad de Barcelona)*

SPONSORS

Spanish Society of Medicinal Chemistry (seqt.org/)

Enantia (enantia.com/)

Molecules (mdpi.com/journal/molecules)

Grupo Juste (grupojuste.com/)

Minoryx Therapeutics (minoryx.com/)

European Federation of Medicinal Chemistry (EFMC) (efmc.info/)

Faes Farma (faesfarma.com)

BioPharma Synergies (bpsynergies.com)

ORAL COMMUNICATIONS

O8 DRUG LOADING STRATEGIES FOR DISCOTIC AMPHIPHILE SUPRAMOLECULAR POLYMERS IN WATER

R. Santini[1,2], E. Fuentes[1], G. Malieieva[1], C. Matera[1,3,4], F. Riefolo[1], L. Albertazzi[1,5], P. Gorostiza[1,4,6], S. Pujals[1,7]

[1] IBEC, Barcelona, Spain; [2] Erasmus+ Unipharma-Graduates Programme, University of Bologna, Italy; [3] DISFARM, University of Milan, Italy; [4] CIBER-BBN, Madrid, Spain; [5] ICMS, Eindhoven University of Technology, The Netherlands; [6] ICREA, Barcelona, Spain; [7] IQAC, Barcelona, Spain; spujals@ibecbarcelona.eu (S.P.), pau@icrea.cat (P.G.)

Keywords: *supramolecular polymers, photopharmacology, drug delivery, transmission electron microscopy*

BTA-based supramolecular polymers are interesting systems for medical applications because of their high dynamicity and stimuli responsiveness in water[1]. Recently, IBEC developed a new class of BTA-based supramolecular polymers which showed responsiveness to temperature, salt concentration, pH, and light[2]. This versatility makes this new class of self-assembled fibers appealing for drug delivery purposes.

In this work, we explored two strategies to incorporate different biologically active ligands into these polymers and demonstrate their employability as **light-driven drug delivery systems**.

In the first strategy, we used a **co-assembly approach** in which two **new discotic BTA-azo-monomers** assemble forming the final helicoidal supramolecular fibers. In the second one, we decided to cage **Photoiperoxo**[3], a potent photoswitchable derivative of the mAChR agonist Iperoxo[3]. Here, the interaction is based on the **stacking** between the azobenzene units of the ligand and the monomers. From the first approach, we obtained satisfying co-assemby results which were evaluated by transmission electron microscopy.

Remarkably, the second system showed light-dependent biological effects in calcium imaging experiments on cells overexpressing M1 mAChRs. While caged Photoiperoxo did not evoke significant changes, UV pre-illuminated fibers caused an increase in intracellular calcium levels because of the activation of M1 mAChRs by the uncaged ligand. These results suggest that the new class of BTA-based supramolecular polymers[2] can potentially be used as light-driven drug delivery system for small, planar and amphiphilic drugs.

References

[1] Kantekin, S.; de Greef, T.F.A.; Palmans, A.R.A. Chemical Society Reviews. 2012, 41, 6125-6137.
[2] Fuentes E.; Gerth M.; Berrocal J.A.; Matera C.; Gorostiza P.; Voets I.K.; Pujals S.; Albertazzi L. J Am Chem Soc. 2020, 142, 10069-10078.
[3] Agnetta, L.; Bermudez, M.; Riefolo, F.; Matera, C.; Claro, E.; Messerer, R.; Littmann, T.; Wolber, G.; Holzgrabe, U.; Decker, M. Journal of Medicinal Chemistry. 2019, 62, 3009-3020.