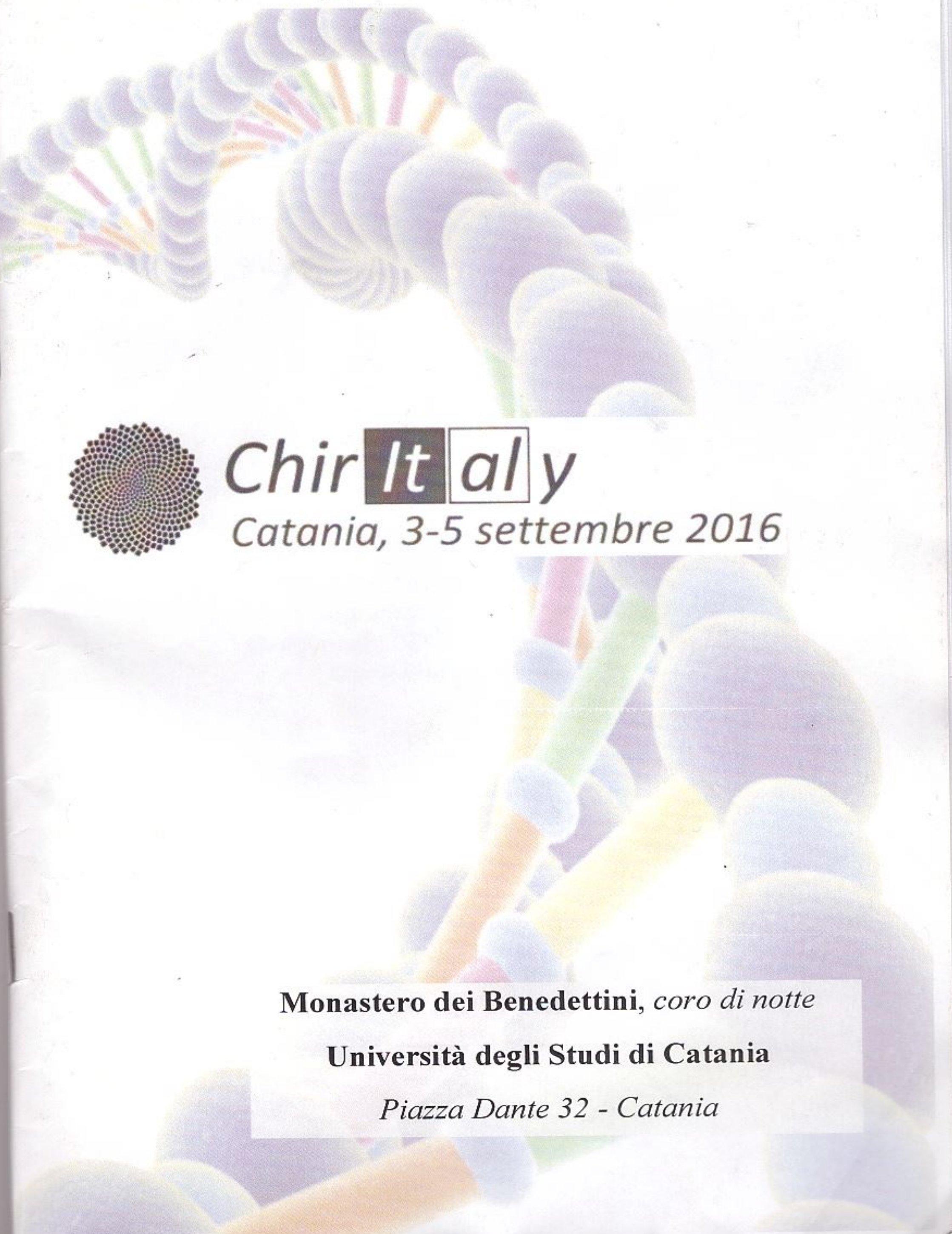

ChirItaly

Catania, 3-5 settembre 2016

Monastero dei Benedettini, *coro di notte*

Università degli Studi di Catania

Piazza Dante 32 - Catania

Domenica 4 Settembre 2016

09:00 – 10:35	**SESSIONE 3** *Chair: Sergio Abbate*
09:00 – 09:45	O-7 **Chiroptical Spectroscopies and metallo-supramolecular architectures** *Giovanna Longhi* **VCD, ECD and ORD spectra of natural products: phytotoxic pyrones and furanones, produced by Diplodia corticola, a cork oak pathogen** *Giuseppe Mazzeo*
09:45 – 10:10	O-8 **Theoretical methods and computational tools to model solvent effects on chiroptical properties and spectroscopies** *Tommaso Giovannini*
10:10 – 10:35	O-9 **Nitrile idratasi-Ammidasi: una possibile soluzione green per la sintesi stereoselettiva di molecole ad elevato valore aggiunto** *Nicola D'Antona*
10:35 – 11:05	*Coffee break*
11:05 – 12:45	**SESSIONE 4** *Chair: Gennaro Pescitelli*
11:05 – 11:30	O-10 **Circular Dichroism of Bilirubin in Presence of Serum Albumin and Anaesthetics and VCD Studies of Chiral Derivatives of Bilirubin** *Simone Ghidinelli*
11:30 – 11:55	O-11 **Allineamento ed orientazione in fasci molecolari supersonici e selezione stereodinamica della chiralità.** *Federico Palazzetti*
11:55 – 12:20	O-12 **Chiral-optical response of s-PS films and of their optically active and inactive guest molecules** *Paola Rizzo*

12:20 – 12:45	O-13 **Chirality in Nature and Art: personal observations** *Salvatore Caccamese*
12:45 – 15:00	*Pranzo* + Sessione Poster
15:00 – 16:00	**Sessione pratica JASCO**
16:00 – 17:40	**SESSIONE DEDICATA A ETTORE CASTIGLIONI** *Chair: Roberto Purrello*
16:00 – 16:20	OE-1 **The Contributions of Ettore Castiglioni to the Group of Chiroptical Spectroscopies in Brescia** *Sergio Abbate*
16:20 – 16:40	OE-2 *Paolo Albertini*
16:40 – 17:00	OE-3 **Insights into stereocontrolled complexation and ECD response of chiral dimeric zinc-poprhyrin host with achiral diamine guests:Induction of two-step inversion of interporphyrin helicity upon host-guest complexation** *Nina Berova*
17:00 – 17:20	OE-4 **Electronic Circular Dichroism spectra of chiral conjugated polymers in their aggregated phases: experimental and theoretical investigations** *Gennaro Pescitelli*
17:20 – 17:40	OE-5 **Extraordinary chiroptical properties of metal complexes** *Lorenzo Di Bari*
20:00	*Cena Sociale* ***(Trattoria da Peppino - via Empedocle 35)***

Lunedì 5 Settembre 2016

09:15 – 10:25	**SESSIONE 5** *Chair: Angela Patti*
09:15 – 10:00	O-14 **Chiroptical Sensor for Determination of Enantiomeric Excess of Amino Acids**

O-7/1

Chiroptical Spectroscopies and metallo-supramolecular architectures

Giovanna Longhi,[1] *Giuseppe Mazzeo*[1], *Sergio Abbate*[1]
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In recent years there has been a growing interest towards chirality manifestations connected to coordination between organic molecules and metals. We recently had the opportunity to use the whole set of most common chiroptical spectroscopies (ECD, VCD and CPL) in the study of two categories of systems for which the role of the metal is crucial to determine chiral properties: organic foldamers triggered by Ag ion coordination and chiral organometallic complexes.

Within the first category, π-conjugated scaffolds of *o*-phenylethynylene oligomers acquire different folding due to Ag^+ - alkyne interaction: the on/off switching can be easily followed with chiroptical spectroscopies. The project has been conducted in collaboration with the group of Prof. Cuerva in Granada, Spain[1].

The second study has regarded metal complexes with different coordination structures, all of them exhibiting chirality at the Metal. These compounds may have interesting applications in material science and bio-related fields. Among the systems studied: octahedral Ru(II)-carbonyl complexes [2], octahedral Ir(III) complexes[3,4] .

Chiroptical spectroscopies permit to distinguish the role of chirality at the metal from that of other possible stereogenic centers. In particular, we have identified characteristic VCD features and have studied, when possible, emission chiroptical response. This research is the result of fruitful collaborations with the group of Prof Cesarotti, Unimi [2,3] and Dr. Cannazza, Unimore[4].

References

[1] SP Morcillo, D Miguel, LÁ de Cienfuegos, J Justicia, S Abbate, E Castiglioni, C Bour, M Ribagorda, DJ Cárdenas, JM Paredes, L Crovetto, D Choquesillo-Lazarte, AJ Mota, MC Carreño, G Longhi, JM Cuerva Chem. Sci., 2016, DOI: 10.1039/c6sc01808d

[2]M Fusè, G Mazzeo, G Longhi, S Abbate, D Zerla, I Rimoldi, A Contini, E Cesarotti, *Chem.Comm.*, 51, 2015, 9385-9387

[3] G Mazzeo, M Fusè, G Longhi, I Rimoldi, E Cesarotti, A. Crispini, S. Abbate, *Dalton Transactions*, 45, 2016 , 992-999

[4] C Citti, UM Battisti, G Ciccarella, V Maiorano, G Gigli, S Abbate, G Mazzeo, E Castiglioni, G Longhi, G Cannazza – *J. of Chromatography* A, 2016, doi:10.1016/j.chroma.2016.05.059

O-7/2

VCD, ECD and ORD spectra of natural products: phytotoxic pyrones and furanones, produced by *Diplodia corticola*, a cork oak pathogen

Giuseppe Mazzeo,[1] *Giovanna Longhi*[1], *Sergio Abbate*[1], *Alessio Cimmino*[2], *Marco Masi*[2], *Lucia Maddau*[3], *Antonio Evidente*[2]
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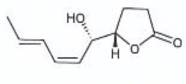
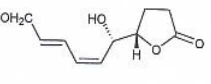
α-Pyrones and α-furanones are a class of phytotoxic metabolites produced by *Diplodia corticola* one of the main pathogens responsible of cork oak decline in Sardinia, which determine heavy losses to the island economy. Among this class of phytotoxins the absolute configuration (AC), linked to biological activity, was assigned only for diplopyrone, together with structure determination. The AC of sapinofuranones B and C, diplofuranone A as well diplobifruranylones A-C instead remains still to be investigated. [1,2] These compounds were studied by a full set of chiroptical spectroscopies namely vibrational and electronic circular dichroism (VCD and ECD respectively) and optical rotatory dispersion (ORD). [3]

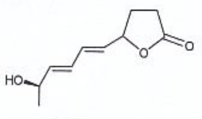
By means of Density Functional Theory (DFT) and Time-dependent DFT (TD-DFT), AC assignment and interesting spectroscopic and conformational aspects, strictly correlated to γ-lactone core, were analysed and interpreted. The latter chemical motif exhibits indeed common spectroscopic features to the various members of the two chemical families in which we partitioned the compounds. (Please notice that the first family is endowed with two stereogenic centers and the second one with four; previous studies [1,2] have reduced the unknown AC determination to 2 and 4 diastereomers respectively).



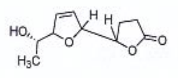
1, *S,S*-sapinofuranone B



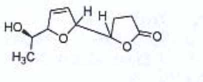
2, Sapinofuranone C



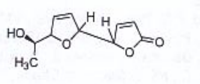
3, Diplofuranone A



4, Diplobifuranylone A



5, Diplobiduranylone B



6, Diplobifuranylone C

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