20th International Conference on Chiroptical Spectroscopy

August 25-28, 2025

University of Debrecen, Debrecen, Hungary

Learning Center

Program and Abstracts



https://konferencia.unideb.hu/en/CD2025-debrecen

Contents

General information

- All participants are kindly requested to wear their conference badges during the conference.
- Lunches will be provided at Smart Bistro (Learning Center).
- Refreshments (water, coffee, tea, snacks) will be served during coffee breaks.
- Wi-fi is available in Learning Center for all participants. ID: CD2025, password: Debrecen2025.
- Preferred method of presentation: Projection from your own laptop. Please check the compatibility before begining of the sessions. Alternatively, the presentations can be copied from a pendrive to laptops provided by the organizers, all presentations must be copied and checked in advance during coffee breaks and lunches before begining of the sessions.
- Poster size should be no larger than A0 (1189 mm x 841 mm). All posters can be put up on the poster board in the morning of 26th August (Tuesday) before starting oral presentations or during coffee breaks. Presenters must remove their posters by 10:00 on 28th August.
- Dresscode for Banquet and Excursion: casual wear.
- On the day of the excursion (27th August) please arrive at the parking lot next to Learning Center in time, the buses will leave promptly to Hortobágy.
- If you have any questions or need any help, please feel free to contact the conference staff.

Conference schedule

<table>
<tr><th>Date/Time</th><th>Monday Aug. 25th</th><th>Tuesday Aug. 26th</th><th>Wednesday Aug. 27th</th><th>Thursday Aug. 28th</th></tr>
<tr><td>8:30</td><td rowspan="4">  </td><td rowspan="2">LC 0.14
PL-4 8:30-9:10 N. A. Kotov
IL-1 09:10-9:35 T. Bürgi
IL-2 09:35-9:55 J. Crassous</td><td rowspan="2">LC 0.14
IL-19 8:30-8:55 K. Monde
IL-20 8:55-9:15 S. Matile
IL-21 9:15-9:30 T. Nehira
OC-23 9:30-9:45 M. Sheves
OC-24 9:45-10:00 N. Nesnas</td><td rowspan="2">LC 0.14
IL-27 8:30-8:55 C. Merten
IL-28 8:55-9:15 Y. Phal
IL-29 9:15-9:35 V. P. Nicu
OC-26 9:35-9:50 J. M. Batista Jr.</td></tr>
<tr><td>9:00</td></tr>
<tr><td>9:30</td><td rowspan="2">Coffee Break
9:55-10:25</td><td rowspan="2">Coffee Break
10:00-10:30</td><td rowspan="2">Coffee Break
09:50-10:20</td></tr>
<tr><td>10:00</td></tr>
<tr><td>10:30</td><td rowspan="3">LC 0.14
IL-3 10:25-10:45 K. Matsuo
IL-4 10:45-11:05 J. Olesiak-Bańska
IL-5 11:05-11:25 C. Zhang
OC-1 11:25-11:40 R. Kuroda
OC-2 11:40-11:55 A. Kaczor
OC-3 11:55-12:10 K. Várnagy
OC-4 12:10-12:25 S. H. Pathan</td><td rowspan="3">LC 2.13
IL-6 10:25-10:40 F. Santoro
IL-7 10:40-10:55 M. Górecki
IL-8 10:55-11:10 A. Micsonai
OC-5 11:10-11:25 J. Cheeseman
OC-6 11:25-11:40 M. Pazderková
OC-7 11:40-11:55 N. Kordestani
OC-8 11:55-12:10 E. Machalska
OC-9 12:10-12:25 J. Kessler</td><td rowspan="3">LC 0.14
IL-22 10:30-10:50 G. Pescitelli
IL-23 10:50-11:10 J. Koshoubu
IL-24 11:10-11:30 J. L. A. Gómez
IL-25 11:30-11:50 T. Taniguchi
OC-25 11:50-12:05 G. Mazzeo
IL-26 12:05-12:25 N. Berova</td><td rowspan="2">LC 0.14
IL-30 10:20-10:45 G. Pieters
IL-31 10:45-11:05 P. Bouř
IL-32 11:05-11:25 S. Jähnigen
OC-27 & CD2027 Announcement
11:25-11:45 A. Kartouzian
VOA9 Announcement 11:45-11:55</td></tr>
<tr><td>11:00</td></tr>
<tr><td>11:30</td><td rowspan="2">Closing Remarks
Student Awards
11:55-12:25</td></tr>
<tr><td>12:00</td><td rowspan="3">Registration
(12:00-14:00, Learning Center)</td></tr>
<tr><td>12:30</td><td>Lunch
12:25-13:45</td><td>Lunch
12:25-13:45</td><td>Lunch
12:25-13:45</td></tr>
<tr><td>13:00</td></tr>
<tr><td>13:30</td><td rowspan="3">LC 0.14
IL-9 13:45-14:05 J. Kardos
IL-10 14:05-14:25 B. Wang
IL-11 14:25-14:45 P. L. Polavarapu
OC-10 14:45-15:00 V. Valev
OC-11 15:00-15:15 Y. Chen
OC-12 15:15-15:30 D. Levshov</td><td rowspan="3">LC 2.13
IL-12 13:45-14:00 C. A. Guido
IL-13 14:00-14:15 E. Santoro
OC-13 14:15-14:30 T. Wu
OC-14 14:30-14:45 J. E. Rode
OC-15 14:45-15:00 B. Kovács
OC-16 15:00-15:15 A. F. Perez Mellor
OC-17 15:15-15:30 M. Hałat</td><td rowspan="3"></td><td rowspan="6">PL: Plenary Lecture
IL: Invited Lecture
OC: Oral Contribution

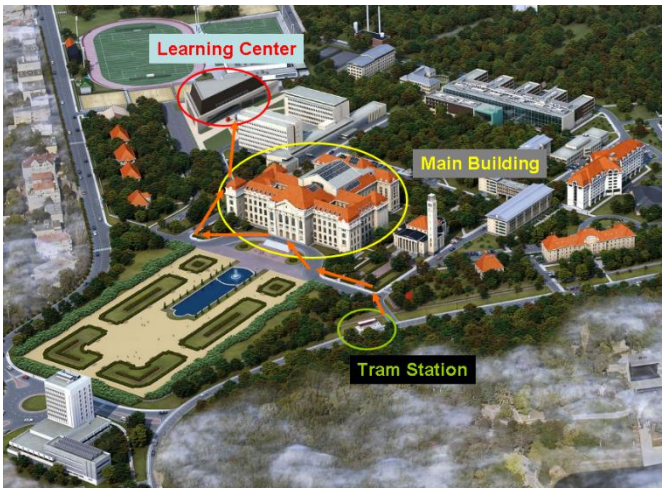
Lectures in Learning Center will take place in rooms LC 0.14 (ground floor) and LC 2.13 (second floor).</td></tr>
<tr><td>14:00</td><td>Opening Ceremony
14:00-14:45</td><td rowspan="5">Registration
(14:00-18:00,
Main Building)</td></tr>
<tr><td>14:30</td></tr>
<tr><td>15:00</td><td rowspan="2">PL-1 14:45-15:45 B. L. Feringa</td><td rowspan="3">14:30
Departure of the Bus to Hortobágy
Excursion (Hortobágy)
Banquet (Hortobágy)</td></tr>
<tr><td>15:30</td><td>Coffee Break
15:30-16:00</td></tr>
<tr><td>16:00</td><td>Coffee Break
15:50-16:20</td><td rowspan="2">LC 0.14
IL-14 16:00-16:20 M. Oppermann
IL-15 16:20-16:40 Y. Liu
IL-16 16:40-16:55 G. Zając
OC-18 16:55-17:15 X. Wan
OC-19 17:15-17:30 T. Beke-Somfai</td><td rowspan="2">LC 2.13
IL-17 16:00-16:20 F. Zinna
IL-18 16:20-16:40 A. Tanatani
OC-20 16:40-16:55 C. Maxim
OC-21 16:55-17:10 V. Andrushchenko
OC-22 17:10-17:25 A. Wajda</td></tr>
<tr><td>16:30</td><td rowspan="2">PL-2 16:20-17:00 Y. Ye
PL-3 17:00-17:40 J. Lacour</td></tr>
<tr><td>17:00</td><td rowspan="2">Poster Session
17:30-18:30</td></tr>
<tr><td>17:30</td><td rowspan="6">Welcome Reception
18:00-21:00</td><td rowspan="5"></td></tr>
<tr><td>18:00</td></tr>
<tr><td>18:30</td></tr>
<tr><td>19:00</td></tr>
<tr><td>19:30</td></tr>
<tr><td>20:00</td></tr>
<tr><td>20:30</td></tr>
</table>

Locations: Learning Center, Main Building, Hortobágy

Maps, venues

- Conference venue: University of Debrecen, Egyetem tér 1., 4032 Debrecen
- Excursion venue: Mátai Ménes, Hortobágy, 4071
- Banquet venue: Hortobágyi Csárda, Hortobágy, Petőfi tér 1., 4071
- Monday, Aug. 25th: Registration at Learning Center* ground floor (12:00-13:30) and Main Building* (14:00-18:00) 2nd floor; plenary lectures (14:00-18:00) at Main Building 2nd floor; welcome reception (18:00-21:00) at Main Building 3rd floor
- Tuesday, Aug. 26th: Oral sessions at Learning Center in LC 0.14 (ground floor) and LC 2.13 (2nd floor) lecture halls (8:30-12:25 and 13:45-17:30); lunch at Learning Center Smart Bistro (12:25-13:45); poster session at Learning Center ground floor (17:30-18:30)
- Wednesday Aug. 27th: Nakanishi sessions at Learning Center in LC 0.14 lecture hall (8:30-12:25); lunch at Learning Center Smart Bistro (12:25-13:45); departure for excursion from the parking lot** next to Learning Center (14:30); excursion and banquet at Hortobágy (14:30-)
- Thursday Aug. 28th: Oral sessions, student awards, closing remarks at Learning Center in LC 0.14 lecture hall (8:30-12:25); deadline of removing posters (10:00); lunch at Learning Center Smart Bistro (12:25-13:45)

***Map of main campus (Egyetem tér)**



****Parking lot of Learning Center**

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Welcome Message

Dear Colleagues and Friends,

We are delighted to welcome you to the 20th International Conference on Chiroptical Spectroscopy (CD2025). This biennial conference is a milestone event, marking the continuation of the rich scientific tradition of chiroptical spectroscopy and celebrating the enduring spirit of innovation and collaboration that has defined our field for decades.

This year is particularly significant as it marks 40 years since the inaugural conference in the field of chiroptical spectroscopy first brought together researchers in Sofia, Bulgaria in 1985. Over the decades, this community has grown into a vibrant and diverse network of researchers, united by a shared passion for understanding molecular chirality and its profound implications for chemistry, biology and materials science. Together, we will celebrate this 40th anniversary of the conference and honour the memory of those who contributed to its success.

We are also honoured to celebrate the centenary of Professor Koji Nakanishi, whose pioneering work has shaped the foundations of chiroptical spectroscopy. His legacy continues to inspire generations of scientists, and we are honoured to pay tribute to his remarkable life and research during this conference.

As we embark on the 20th edition of the conference, we look forward to a dynamic exchange of ideas, the forging of new collaborations, and the continued advancement of chiroptical science. Thank you for being part of this journey.

Warmest regards,

The Organizing Committee

History of the CD Conferences

	Year	City, Country	Conference Chairs
1	1985	Sofia, Bulgaria	G. Snatzke, N. Berova
2	1987	Budapest, Hungary	M. Kajtár
3	1989	Prague, Czech Republic	P. Malon, P. Pancoska
4	1991	Bochum, Germany	H. Klein, G. Snatzke
5	1993	Pingree Park, Colorado, US	R. W. Woody, N. Berova, K. Nakanishi, A.-Young Woody
6	1997	Pisa, Italy	P. Salvadori
7	1999	Mierki, Poland	J. Gawronski, J. Frelek
8	2001	Sendai, Japan	N. Harada
9	2003	Budapest, Hungary	M. Hollósi, S. Antus
10	2005	Sandestin, Florida, US	D. A. Lightner, J.E. Gurst
11	2007	Groningen, The Netherlands	B. L. Feringa, E.W. (Bert) Meijer
12	2009	Brescia, Italy	P. Salvadori, S. Abbate, L. Di Bari
13	2011	Oxford, United Kingdom	G. Siligardi
14	2013	Nashville, Tennessee, US	P. L. Polavarapu
15	2015	Sapporo, Japan	K. Monde, R. Kuroda
16	2017	Rennes, France	J. Crassous, N. Avarvari
17	2019	Pisa, Italy	L. Di Bari, G. Pescitelli, A. Rizzo, F. Santoro
18	2022	New York City, NY, US	B. Kahr, P. Vaccaro, A. Petrovic
19	2023	Hiroshima, Japan	K. Matsuo, T. Nehira

Scientific program

Monday, August 25

Registration (Learning Center)

12:00-13:30

Registration (Main Building)

14:00-18:00

Oral Session 1 (Main Building, Aula, 2nd floor)

Chairperson: András Perczel

14:00-14:45		Opening Ceremony
14:45-15:45	PL-1	B. L. Feringa: Exploring Dynamic Chirality

Coffee Break (Main Building)

15:50-16:20

Oral Session 2 (Main Building, Aula, 2nd floor)

Chairperson: András Perczel

16:20-17:00	PL-2	Y. Ye: Characterization of Novel Sesquiterpenoids from *Artemisia hedinii* and Their Anti-Fibrotic Potential
17:00-17:40	PL-3	J. Lacour: Stereochemical journey among carbocations and precursors

Welcome Reception (Main Building, 3rd floor)

18:00-21:00 dedicated to JASCO Global

Tuesday, August 26

Oral Session 3 (Learning Center, room LC 0.14)

Chairperson: Christian Merten

8:30-9:10	PL-4	N. A. Kotov: Chiral Nanostructures: Next Steps
09:10-9:35	IL-1	T. Bürgi: Atomically Precise Monolayer-Protected Metal Clusters: Chiroptical Properties And Dynamic Nature
09:35-9:55	IL-2	J. Crassous: Exciton Coupling Chirality in Helicene Derivatives

Coffee Break (Learning Center)

9:55-10:25

Oral Session 4 (Learning Center, room LC 0.14)

Chairperson: Jérôme Lacour

10:25-10:45	IL-3	K. Matsuo: Mechanism of Amyloid Fibril Formation of α-Synuclein Interacted with Membrane Analyzed by Vacuum-Ultraviolet Circular Dichroism and Linear Dichroism
10:45-11:05	IL-4	J. Olesiak-Bańska: Probing Chiral Nonlinear Optical Properties in Noble Metal Nanoclusters
11:05-11:25	IL-5	C. Zhang: Discovery and Biosynthesis of Natural Products From Marine Actinomycetes
11:25-11:40	OC-1	R. Kuroda: Chiral Self-assembly of Achiral Metal Porphyrins Studied by Solution and Solid-state CD spectroscopy
11:40-11:55	OC-2	A. Kaczor: Unique Vibrational Circular Dichroism (VCD) of Carbon Dots
11:55-12:10	OC-3	K. Várnagy: Application of CD spectroscopy in characterizing interactions between tau protein fragments and metal ions
12:10-12:25	OC-4	S. H. Pathan: Chiroptical stimuli-responsive behavior of water-soluble chiral polyacetylene polymers

Oral Session 5 (Learning Center, room LC 2.13)

Chairperson: Grégory Pieters

10:25-10:40	IL-6	F. Santoro: ECD Response Symmetric in Cyclic Systems: Comparing the Jahn-Teller and Exciton-Exciton Picture
10:40-10:55	IL-7	M. Górecki: Investigating Solvatomorphism by CD Spectroscopy
10:55-11:10	IL-8	A. Micsonai: Investigation of the topological and spectral diversity of G-quadruplexes by CD spectroscopy
11:10-11:25	OC-5	J. Cheeseman: Simulation of Resonance Raman Optical Activity Spectra for Cobalt Complexes
11:25-11:40	OC-6	M. Pazderková: Stereochemical Analysis of P-chirogenic Compounds using Chiroptical Spectroscopies and Quantum-Chemical Calculations
11:40-11:55	OC-7	N. Kordestani: A Novel Chiroptical Spectroscopy Method Based on X-ray Circular Dichroism
11:55-12:10	OC-8	E. Machalska: CPL, ECD, ROA and VCD of chiral heptazine-based compounds with inverted singlet-triplet states
12:10-12:25	OC-9	J. Kessler: Chirality Detection with Gold Nanowires

Lunch (Learning Center)

12:25-13:45 dedicated to BioTools

Oral Session 6 (Learning Center, room LC 0.14)

Chairperson: Jeanne Crassous

13:45-14:05	IL-9	J. Kardos: Protein CD spectroscopy in the AlphaFold Era
14:05-14:25	IL-10	B. Wang: Structure and stereochemical assignments of various natural products from marine-sourced fungi

14:25-14:45	IL-11	P. L. Polavarapu: How Important are Dimers for Interpreting the Chiroptical Properties of Carboxylic Acids?
14:45-15:00	OC-10	V. Valev: Chiral Light Scattering: Solving a 40-Year-Old Puzzle
15:00-15:15	OC-11	Y. Chen: Directional Crystal Motions Controlled by Chirality
15:15-15:30	OC-12	D. Levshov: Quantifying Enantiomeric Excess of Carbon Nanotube Solutions Using Chiroptical Spectroscopy and Hyperspectral Fluorescence Microscopy

Oral Session 7 (Learning Center, room LC 2.13)

Chairperson: Kenji Monde

13:45-14:00	IL-12	C. A. Guido: Exploring Chiral Electronic Transitions: From Chiroptical Spectroscopies to Electron Beam Probes
14:00-14:15	IL-13	E. Santoro: Inherently Chiral Macrocycles Arenes for Chiral Sensing
14:15-14:30	OC-13	T. Wu: Raman Optical Activity Spectroscopy as a Sensitive Tool for Detecting Lanthanide Optical Activity
14:30-14:45	OC-14	J. E. Rode: UV–vis and ECD Spectroelectrochemistry and MCD spectra of Naphthalenediimides
14:45-15:00	OC-15	B. Kovács: Structural Elucidation of a Cationic Peptide Nanotube: the Peptide Bilayer Model
15:00-15:15	OC-16	A. F. Perez Mellor: A New Frontier in VCD: Fast and Dynamic Chiral Analysis
15:15-15:30	OC-17	M. Hałat: Chirality Transfer in Macro- and Supramolecules: an ROA study

Coffee Break (Learning Center)

15:30-16:00

Oral Session 8 (Learning Center, room LC 0.14)

Chairperson: Prasad L. Polavarapu

16:00-16:20	IL-14	M. Oppermann: Ultrafast chiral spectroscopy for stereocontrolled photochemistry
16:20-16:40	IL-15	Y. Liu: The Acetal Chemistry in Asymmetric Catalysis: Thermodynamic versus Kinetic Control
16:40-16:55	IL-16	G. Zając: From Corrinoids to Heme Proteins: Structural Dynamics of Biochromphores Tracked by Resonance ROA
16:55-17:15	OC-18	X. Wan: π-Hole Bond-Enhanced Enantioselective Discrimination of Helical Polyacetylenes as Chiral Stationary Phases for High-Performance Liquid Chromatography
17:15-17:30	OC-19	T. Beke-Somfai: Assembly Formation of Peptide Supramolecules Tracked by Polarized Light Spectroscopy

Oral Session 9 (Learning Center, room LC 2.13)

Chairperson: Petr Bouř

16:00-16:20	IL-17	F. Zinna: Spectroscopic features of chiral materials enabling chiral photonics and electronics
16:20-16:40	IL-18	A. Tanatani: Chiral Properties of Helical Aromatic Squaramides
16:40-16:55	OC-20	C. Maxim: Tuning the Chiroptical Properties in Zn(II) Amino Acids-helical polymers
16:55-17:10	OC-21	V. Andrushchenko: VCD Beyond Solutions
17:10-17:25	OC-22	A. Wajda: Integrative Analysis of Amyloid Fibrils: Chiral Spectroscopy Meets Nanoscale Morphology

Poster Session (Learning Center, ground floor)

17:30-18:30

Wednesday, August 27

Nakanishi Session 1 (Learning Center, room LC 0.14)

Chairperson: Tohru Taniguchi

8:30-8:55	IL-19	K. Monde: Chiroptical Analysis of the SWIR (Shortwave-infrared) Organic Fluorescent Probes for Deep Tissue Breast Cancer Imaging
8:55-9:15	IL-20	S. Matile: Translational Supramolecular Chemistry
9:15-9:30	IL-21	T. Nehira: Progress in Expanding the Scope and Applications of Circular Dichroism
9:30-9:45	OC-23	M. Sheves: Activation Mechanism of Retinal Proteins: Is Light-Induced Double Bond Isomerization the Initial Step?
9:45-10:00	OC-24	N. Nesnas: Photochemical Release of Bioactive Molecules for Neurological Applications and Beyond

Coffee Break (Learning Center)

10:00-10:30

Nakanishi Session 2 (Learning Center, room LC 0.14)

Chairperson: Stefan Matile

10:30-10:50	IL-22	G. Pesticelli:Walking in the Footsteps of Giants: a Journey in the Scientific Lineage of Koji Nakanishi
10:50-11:10	IL-23	J. Koshoubu: To The Future Guided By Professor Koji Nakanishi
11:10-11:30	IL-24	J. L. A. Gómez: Magic Chirality – Enantiomers Beyond the Mirror
11:30-11:50	IL-25	T. Taniguchi: Exploration and Application of Vibrational Chromophores in the Biomolecularly Transparent Region
11:50-12:05	OC-25	G. Mazzeo: Natural Compounds Studied Through Unusual Spectrocopic/Chiroptical Techniques: MCD and CPL
12:05-12:25	IL-26	N. Berova:Enchanting Life of Koji Nakanishi in the World of Science

Lunch (Learning Center)

12:25-13:45

Departure of the Bus to Hortobágy (Learning Center parking lot)

14:30

Thursday, August 28

Oral Session 10 (Learning Center, room LC 0.14)

Chairperson: Fabrizio Santoro

8:30-8:55	IL-27	C. Merten: Solvent effects on VCD spectra
8:55-9:15	IL-28	Y. Phal: Rapid Quantum Cascade Laser-Based Vibrational Circular Dichroism Spectroscopy Systems for Chirality Sensing
9:15-9:35	IL-29	V. P. Nicu: The Digital Chiroscope from AI-assisted spectral analysis to periodic structure simulations
9:35-9:50	OC-26	J. M. Batista Jr.: Chiroptical properties of “simple” furofuran lignans: structure and solvent effects

Coffee Break (Learning Center)

9:50-10:20

Oral Session 11 (Learning Center, room LC 0.14)

Chairperson: József Kardos

10:20-10:45	IL-30	G. Pieters: BINOL-(tere)phthalonitriles: Versatile Building Blocks for Chiral Emitters Design
10:45-11:05	IL-31	P. Bouř: Theoretical Challenges of Resonance Raman Optical Activity
11:05-11:25	IL-32	S. Jähnigen: Chirality and Vibrational Circular Dichroism in the Solid State
11:25-11:45	OC-27	A. Kartouzian: Nonlinear g-ee Dependence in Chiral Films / CD2027 Announcement
11:45-11:55		VOA9 Announcement
11:55-12:25		Closing Remarks / Student Awards

Lunch (Learning Center)

12:25-13:45

Poster Session

August 26 (Learning Center, ground floor)

PO-1 I. Atirojwanich: Helicenes for and from magnetochiral effect (HEL-MCH)
PO-2 K. Pajor: Exploring the Complexity of Supramolecular Systems by Means of Advanced Chiroptical Methods
PO-3 D. A. Drost: Vibrational Circular Dichroism Spectra of Tartaric Acid in Aqueous Solution
PO-4 M. Feßner: Acetate Binding to Chiral Dithiourea Derivative Studied by VCD Spectroscopy
PO-5 V. Stoianova: Synthesis and VCD spectroscopy of host-guest complexes with chiral azacryptands
PO-6 L. Bednárová: Structural study of β/α-Hybrid Peptide Oligomers
PO-7 P. Mundry: Photochemistry of Chiral Imines Investigated by Matrix Isolation IR/ VCD Spectroscopy
PO-8 M. Cei: CPL Photoscopy: Circularly Polarized Luminescence Detected by Chromaticity Differences
PO-9 R. B. Anastácio: Length-Dependent Nonlinear Chiroptical Signatures in Aromatic Oligoamide Foldamers: From Solutions to Surfaces
PO-10 J. Hudecová: Chiral EDDS-Metal Complexes as Tunable Systems for Resonance and Non-Resonance ROA
PO-11 K. Kwiecień: Flow Reactor Prototype For The Measurement Of Enantiomeric Excess
PO-12 A. Kunnummal: Investigation of The Chiral Properties of Nano Helical Structures by Tuning Their Morphological Characteristics
PO-13 M. Bertuolo: Hierarchical Chirality Transfert in Chiral AIE Material by Silica Nanohelix
PO-14 A. Kołodziejczyk: Chiroptical Investigation of Aggregates Formed by Phenylalanine-based Peptides
PO-15 K. Katkar: Use of Magnetic Circular Dichroism to characterize Biomolecules in Solid-state and Supramolecular Aggregation Conditions
PO-16 H. Shimizu: Enhancing Chiroptical Properties through Hierarchical Architectures of Mesoscopic Chiral Nanostructures
PO-17 R. Aerts: Interpreting peptide ECD signatures for material science applications - an acquired or challenging task?
PO-18 S. Hashimoto: Stepwise Interaction Mechanism between β-Lactoglobulin and SDS Micelles Revealed by Time-Resolved Vacuum-Ultraviolet Circular Dichroism
PO-19 R. Hagen: Arbitrary Angle Raman Optical Activity Detection
PO-20 A. Morice: Identification Of Large Amplitude Motions In Flexible Systems
PO-21 A. Domagała: Resonance Raman Optical Activity Uncovers Chiroptical Features of Cytochrome c
PO-22 S. John: Mueller Matrix Mapping and Electronic Circular Dichroism of 1,1'-Binaphthalene Thin Films
PO-23 K. Hattori: Substitution Effect in Dynamic Structure Conversion of Stimuli–Responsive Helical Co(II) Complexes
PO-24 N. Ahmad: Stereoselective Access to Glycofused Isochromans via Oxa-Pictet–Spengler Cyclization Reaction: Toward Multifunctional Agents Targeting SGLT-2 and Tumor Pathways
PO-25 O. Nedderman: Transferring Chirality From Molecules To Polymer-Based Thin Films
PO-26 N. Murvai: G4SpectraDB: A Comprehensive Database for Spectroscopic and Topological Data of G-Quadruplex Structures
PO-27 A. Kaneta: Development of Circularly Polarized Lumiescence Spectrometer
PO-28 Á. Homolya: Stereoselective Synthesis and Structural Elucidation of Glucose-Isochroman Hybrids
PO-29 I. Cs. Szigyártó: The Fine-tuning Effect of Heterochiral β3-sequences on Structural Motif Associations
PO-30 M. S. P. Kkadan: Raman Optical Activity as a Structural Probe of Polynucleotides in Solution
PO-31 M. Krupova: Tracking of Conformational Dynamics of Vitamin B12 by Chiroptical Spectroscopy

PO-32 R. A. Barta: VCD Analysis of Isochroman Derivatives with Central and Axial Chirality Elements in the Solid State
PO-33 G. M. Fedics: Conformational and Chiroptical Analysis of Biaryl Derivatives Containing Axial and Central Chirality Elements
PO-34 K. Cserepes: STEREOSELECTIVE SYNTHESIS AND STEREOCHEMICAL ANALYSIS OF AXIALLY CHIRAL BIARYL DERIVATIVES
PO-35 Cs. Kállay: The Use of Circular Dichroism in Bioinorganic Chemistry Research
PO-36 Zs. Fazekas: From linear models to neural networks for CD deconvolution
PO-37 I. Jákli: Amyloid or Not? Circular Dichroism Reveals How Sequence Order Drives Aggregation, Structure, and Molecular Evolution
PO-38 A. Perczel: Decoding Functional Amyloids by Chiroptical Fingerprinting: Electronic and Vibrational Circular Dichroism Spectroscopy Sheds Light on Polymorphic Assembly

Oral Presentations

PL-1

Exploring Dynamic Chirality

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Chirality as a " Signature of Life" has many faces and is central to numerous fields. In this lecture the focus is on the dynamic control of chirality based on molecular switches and motors. CD spectroscopy is key to determine the various chiral states and follow the dynamic processes. Various approaches to control chirality along length scales are discussed including supramolecular self-assembly using molecular motors, amplification in liquid crystal materials towards artificial muscle functions and modulation of circular polarized luminescence. Furthermore new multifunctional chiroptical switches will be shown during the lecture.

PL-2

Characterization of Novel Sesquiterpenoids from *Artemisia hedinii* and Their Anti-Fibrotic Potential

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Natural products have long been recognized as a treasure trove of bioactive compounds, playing crucial roles in the development of new drugs and therapies [1]. Accurate structural elucidation, particularly the determination of stereochemistry, is vital for understanding their biological activities and mechanisms of action.

The genus *Artemisia*, with its approximately 1000 species, is renowned for its diverse and bioactive constituents, especially sesquiterpenes. *Artemisia hedinii*, an annual herb traditionally used in folk medicine in China for its heat-clearing, detoxifying, and anti-inflammatory properties, has been the focus of our research. Our previous study revealed the identification of 31 eudesmane-type sesquiterpenes from *A. hedinii*, with some exhibiting anti-inflammatory effects by downregulating IL-2 and TNF-α levels.

Here, we present the isolation and structural elucidation of two new skeleton sesquiterpenoids (**1** and **6**), along with four new iphionane-type sesquiterpenes (**2**-**5**) and six new cyperane-type sesquiterpenes (**7**-**11**) from the title plant. The structures were established through comprehensive spectroscopic analysis, including HR-ESIMS, 1D and 2D NMR spectra. The absolute configurations were determined by ECD spectra, single-crystal X-ray crystallography, TDDFT ECD calculations, DFT NMR calculations, and biomimetic syntheses. All compounds were evaluated for anti-hepatic fibrosis activity in LX-2 cells, with compounds **2**, **8**, and **10** showing significant downregulation of α-SMA expression [2].

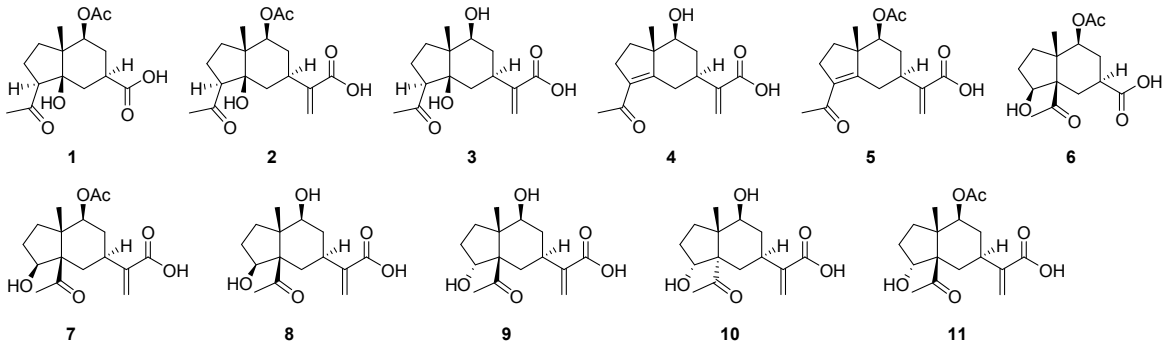

Figure 1. Chemical structures of compounds 1-11 isolated from *A. hedinii*.

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PL-3

Stereochemical journey among carbocations and precursors

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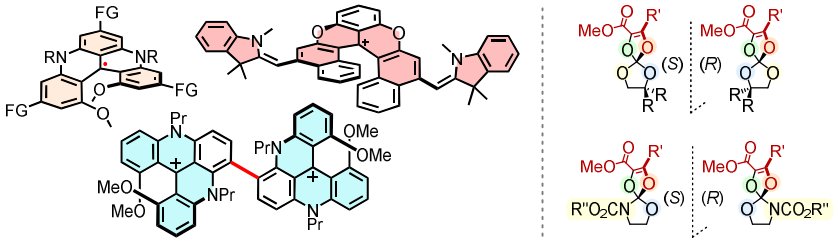
Charged molecules and intermediates display unique reactivity and properties. In this context, studies on original cationic [4] and [6]helicenes will be presented. These compounds display original chemical and electronic properties thanks to the extended delocalization provided by the triarylcarbenium framework.[1] Molecular engineering towards novel reactivities and properties, electronic and chiroptical in particular, will be reported.[2]

Also, a focus will be given on metal-catalyzed decompositions of a-diazocarbonyls – and those involving CpRu complexes [3] particular. An attention will be given to routes affording ylide intermediates and then functionally rich heterocyclic derivatives. Investigations on novel tetra heterosubstituted methanes, *i.e.* tetraoxa and azatrioxa carbon spiro stereocenters, which display remarkable enantiomerization barriers with values up to 34.6 kcal/mol (half-lives >84'000 years at 25 °C), will be detailed during the lecture.



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PL-4

Chiral Nanostructures: Next Steps

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Chiral nanostructures represent a large and rapidly evolving class of mirror-asymmetric compounds that fundamentally change the perception of handedness in chemistry, physics and biology. Unlike typical organic, inorganic or biological molecules, chiral nanostructures display giant ellipticity and multiscale chirality spanning the dimensions from angstroms to micrometers (**Fig. 1**) Furthermore, chiral nanostructures display a continuum of chiral states instead of the binary chirality of, for instance, L- or D-amino acids. Some of the latest developments also include the emergence of terahertz circular dichroism (TCD) displaying exceptionally high amplitudes due to chiral phonons in chiral nanostructures. The size, geometry, and composition of chiral nanostructures can be tuned to resonate with a wide range of photon energies from ultraviolet to terahertz.

The high intensity and sharpness of their circular dichroism peaks facilitated the use of chiral nanostructures in biosensing, which has been widely investigated by many research groups. Based on the current fundamental knowledge about chiral nanostructures, the following academically exciting and technologically impactful research directions can be considered. Chiral nanoparticles are essential for understanding the complexity of biological matter because nanoscale chirality enforces reproducible self-assembly patterns. They can potentially be engineered similarly to proteins to selectively interact with biological counterparts of a similar scale. The strength and selectivity of their interactions can be varied by nanoparticle geometry, surface ligands, and chemical composition, with subsequent utilization in biomedicine and chiral catalysis.

The giant optical activity can be harnessed for detecting and emitting circularly polarized light for emerging information technologies. Thus, future research directions will likely encompass the development of chiroptical materials and devices for extreme conditions, including high temperatures. 6G/7G telecommunications, polarization-based perception systems, and real-time holography should also be considered. These possibilities can be enabled by the intense circularly polarized black body radiation from chiral nanostructures and defect-tolerant manufacturing methods with a high degree of scalability.

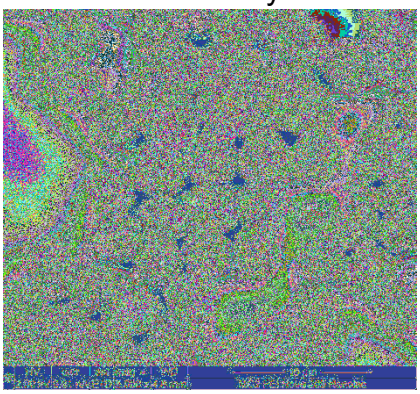

Figure 1. SEM image of self-assembled complex particles with bowtie shape and multiscale chirality.

IL-1

Atomically Precise Monolayer-Protected Metal Clusters: Chiroptical Properties And Dynamic Nature

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Chiral nanomaterials have properties that are of interest for applications in chiral technology but also in materials science. In this contribution we will focus on a special class of materials: Monolayer-protected metal clusters [1,2]. These clusters are atomically precise nanomaterials containing a few to a few hundred metal atoms. They are composed of a metal core surrounded by a layer of protecting ligands. Their properties change drastically with size and composition. The structure of numerous clusters has been determined, which enables detailed studies of their properties as a function of size. The surface layer of the clusters can be engineered to accomplish various tasks. Monolayer-protected metal clusters are excellent model systems to understand surface chemical processes and reactivity and they are attractive for applications in sensing, catalysis [3] and medicine [4].

Many of these clusters turn out to be chiral. The chirality arises at different levels, as will be pointed out. We will discuss the chiroptical properties of such clusters. Vibrational circular dichroism (VCD) provides information on the conformation of ligands adorbed on the cluster surface. Challenges are related to the size of the system, which complicates accurate calculation of VCD spectra.

These clusters, although stable, turn out to be very dynamic. The latter is evidenced for example by the exchange of metal atoms and ligands between clusters in solution. In addition, the clusters show place exchange of ligands on their surface. The dynamic nature of such clusters will be illustrated with several examples.

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IL-2

Exciton Coupling Chirality in Helicene Derivatives

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Circularly polarized luminescence (CPL) emitters have attracted a great deal of research interest due to their promising applications in photonic technologies including optical data storage, optical communication, and stereoscopic 3D imaging systems.[1] In order to design novel chiral organic π-conjugated materials that can emit CPL with both efficient quantum yield of photoluminescence (Φ) and high dissymmetry factors (g_{lum}), we have synthesized new chiral emitters based on an original association between an enantiopure [6]helicene and strong chromophores such as naphthalimides,[2] diketopyrrolopyrroles,[3] or porphyrins.[4] These molecular helical π-conjugated systems show strong Electronic Circular Dichroism (ECD) signal in the visible region, intense red and near-infrared luminescence and corresponding CPL activity arising from efficient Exciton Coupling chirality.

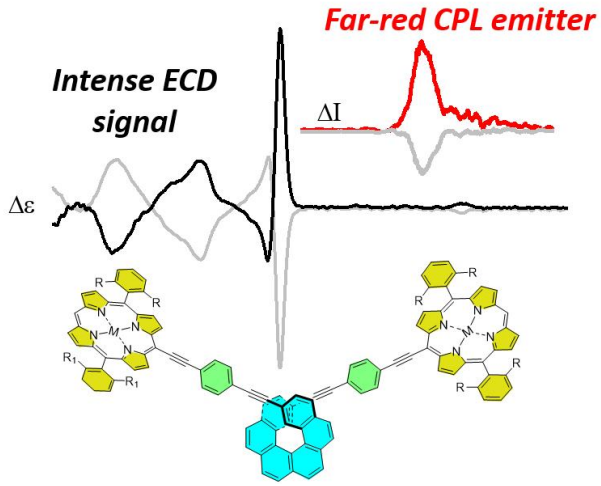

Figure 1: Chemical structure and Chiroptical (ECD and CPL) activities of helicene-porphyrin derivatives.

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IL-3

Mechanism of Amyloid Fibril Formation of α-Synuclein Interacted with Membrane Analyzed by Vacuum-Ultraviolet Circular Dichroism and Linear Dichroism

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Interactions between water-soluble proteins and membranes are the starting point for the expression of various biological functions. Vacumm-ultraviolet circular dichroism (VUVCD) and linear dichroism (LD) spectroscopy using a synchrotron radiation have been used for characterizing the secondary structures (contents, numbers of segments, sequences, and orientations) of membrane-bound proteins under various experimental environments including the presence of membrane [1], allowing us to understand the expression mechanism of the membrane-mediated functions of proteins [2]. α-synuclein (αS), which is composed of N-terminal, non-amyloid-β component (NAC), and C-terminal domains, interacts with synaptic membranes in neuron and transforms into amyloid fibrils only in the presence of salt (NaCl), causing Parkinson's disease. To understand the fibril formation mechanism, the effect of salt on the membrane interaction of αS was characterized at the molecular level [3]. SRCD and LD showed that compared with the absence of NaCl, NaCl reduced the number of helical segments and Tyr residues interacting with the membrane surface and increased the solvent-exposed area. Molecular dynamics (MD) simulations revealed that the N-terminal domain of αS interacted with membranes and formed a helical structure regardless of NaCl, whereas the C-terminal domain formed a random structure with weak membrane interactions, and NaCl inhibited the interaction of the hydrophobic region, suggesting that salt promoted amyloid fibril formations by exposing the hydrophobic C-terminal domain, which can intermolecularly interact with free αS. The fibrils of NAC peptide formed structural polymorphism with two morphologies (thin and thick) in the presence of NaCl but one morphology (thin) in the absence of NaCl [4]. SRCD and LD showed that two helical regions (first and second) formed on the membrane regardless of salt, but the length of the first helix largely shortened in the NaCl present, exposing the hydrophobic area to the solvent. MD simulation disclosed that the exposed region induced two distinct pathways of fibril nucleations. The different pathways mainly affected the β-strand orientation and helical content within the fibril conformations, contributing to the thickness degree, leading to structural polymorphism.

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IL-4

Probing Chiral Nonlinear Optical Properties in Noble Metal Nanoclusters

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Noble metal nanoclusters (NCs) are ultra-small nanomaterials exhibiting optical properties intermediate to those of discrete molecules and bigger nanoparticles [1]. They possess exceptional linear and nonlinear optical characteristics, including tunable photoluminescence (UV-NIR), large Stokes shifts (>0.5 eV), high photostability, and significant two-photon absorption [2]. Importantly, many NCs display chirality, arising from chiral surface ligands, helical core motifs, or inherent kernel asymmetry [3]. These attributes make NCs excellent models for structure-property relationship studies and versatile tools in catalysis, bioimaging, and sensing.

This work investigates the **linear and nonlinear optical properties of NCs** with diverse chirality origins. We synthesized and characterized NCs stabilized by: **1) chiral ligands within primary or secondary ligand shells** (captopril, glutathione, arginin, single stranded DNA), and **2) achiral ligands where chirality was induced by the arrangement of staple motifs**. To quantitatively assess chiral nonlinear optical properties, specifically two-photon circular dichroism (2PCD), we developed and employed two distinct methodologies: z-scan-based two-photon absorption measurements and fluorescence-detected two-photon excited luminescence measurements utilizing circularly polarized light [4, 5]. Our findings reveal that the 2PCD of these NCs is approximately 300 times stronger than their one-photon anisotropy factor. Furthermore, we successfully demonstrated the facile detection of both 2PCD and three-photon circular dichroism (3PCD) in chiral gold NCs [6]. This research provides critical insights into the interplay between chirality and nonlinear optical phenomena in NCs, opening new avenues for their application in advanced photonics and chiroptical technologies.

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IL-5

Discovery and Biosynthesis of Natural Products From Marine Actinomycetes

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Marine-derived actinomycetes are emerging as important sources for novel natural product possessing complicated structures and excellent bioactivities. Herein we present our recent studies on the discovery and biosynthesis of marine actinomycetal natural products and their related bioactivities, including the development of new methods to facilitate the discovery of novel bioactive natural products from marine actinomycetes upon natural isolation and genomic data mining, the elucidation of the biosynthetic pathway of novel marine microbial natural products, the characterization of the unique catalytic mechanisms and structural features of biosynthetic enzymes, the structure-activity relationship of bioactive compounds. Finally, several examples will be presented to highlight the utility of metabolic engineering and synthetic biology strategy to rational design artificial pathways and cell factories for biomanufacturing and yield improvement of marine microbial natural products with potential applications in human health and agriculture.

IL-6

ECD Response Symmetric in Cyclic Systems: Comparing the Jahn-Teller and Exciton-Exciton Picture

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Robust and automatized approaches for vibronic ECD simulations of semirigid systems are avaible in commercial and free codes, but they all work in the hypothesis that each electronic state of the molecule contributes an independent response. However, it has been recently pointed out that the ECD response of typical chiral systems with extended π-conjugation, is modulated by nonadiabatic inter-state couplings involving several excited states and vibrational modes [1,2]. They can be nowadays effectively described with more advanced methods based on quantum dynamical propagations and Hamiltonians parameterized automatically (for instance from DFT/TD-DFT) with effective diabatization techniques [1,2].

Many research groups build up new chiral structures by covalently linking repetitive molecular units, inspired by an exciton-like way of thinking, where the ECD response arises from the interaction of local excitations on each unit. From a different perspective however, this synthetic route leads very often to symmetric cyclic structures characterized by rotational axes of symemtry *Cn* with n>=3, which can undego Jahn-Teller (JT) and/or pseudo- Jahn-Teller (PJT) effects. Here we focus on trigonal systems [3] showing that a proper description of JT and PJT couplings is unavoidable for a fair simulation of their ECD. The new developed techniques also allow to increase our understanding of the chiral response systems of such cyclic molecules through a detailed comparison of the outcomes of alternative with exciton (localized) or JT (delocalized) approaches.

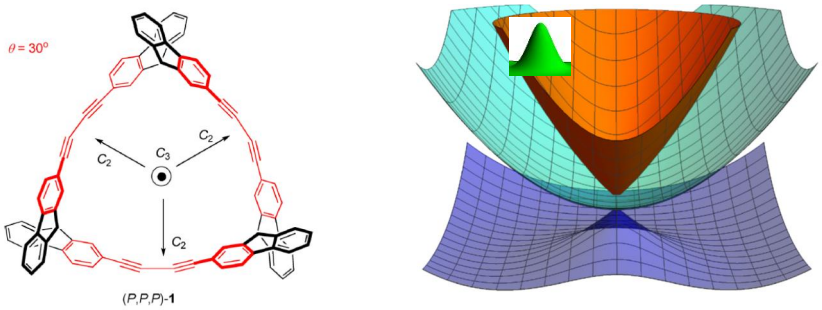

Figure 1. A cartoon of the PES topology responsible for a pseudo JT effect which dominates the ECD response of a cyclic trimer of diethynylspirobifluorenes

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IL-7

Investigating Solvatomorphism by CD Spectroscopy

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Solvatomorphs are different crystalline forms of the same chemical compound that result from crystallization in different solvents. In these forms solvent molecules are incorporated into the crystal structure, which can significantly affect the compound's physical and chemical properties.[1] For chiral compounds, such structural differences also influence their chiroptical properties.

In the context of drug development, solvatomorphs of active pharmaceutical ingredients (APIs) are now routinely obtained through systematic screening. Their significance stems from the fact that different solvatomorphs can exhibit varying solubility, stability, and bioavailability, *i.e.* factors that directly impact the final dosage form and therapeutic efficacy of a drug.

This presentation will highlight the first applications of circular dichroism (CD) spectroscopy in both the vibrational (VCD) [2] and electronic (ECD) regions to study solvatomorphism, using a series of model solvatomorphs of Dutasteride as an example (Figure 1). Emphasis will be placed on solid-state CD measurements, including the use of ECD *imaging* technique, which enables the acquisition of CD anisotropy (CDA) spectra, which are unique and highly characteristic of any chiral system.[3] Finally, the presentation will outline directions for the application of solid-state chiroptical techniques in the structural analysis of non-racemic compounds.

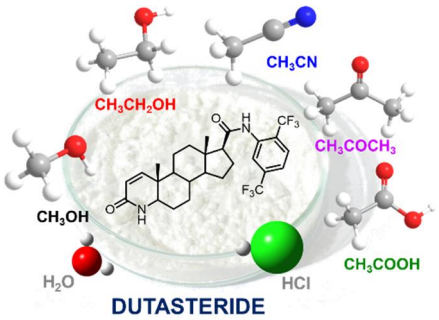

Figure 1. Graphical abstract.

Acknowledgements
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IL-8

Investigation of the topological and spectral diversity of G-quadruplexes by CD spectroscopy

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G-quadruplexes (G4s) are non-canonical nucleic acid structures formed by guanine-rich DNA and RNA sequences. They are frequently found in promoter regions, telomeric sequences, introns, and within 5‘ and 3‘ untranslated regions (UTRs). Due to their roles in maintaining chromosomal stability and regulating gene expression (acting either as oncogenes or tumor suppressors) G4s have become a focal point of diagnostic and therapeutic research in recent years.

G4 structures can be intramolecular or intermolecular and exhibit a variety of topologies, including parallel, antiparallel, or hybrid strand orientations, with diverse loop lengths. These structural variations contribute to significant differences in their stability and interaction profiles.

Determining the topology of G4s is a non-trivial task. Alongside atomic-resolution techniques, circular dichroism (CD) spectroscopy and G4-specific fluorescent dyes have emerged as important tools for structural characterization. CD spectroscopy offers a rapid method to investigate the structural and dynamic properties of G4s under a wide range of conditions. Although several CD-based datasets have been published in recent years, they typically include only a limited number of G4 structures that have been analyzed under comparable conditions using both atomic-resolution methods and CD spectroscopy.

Over the past few years, we have investigated numerous G4 topologies using both conventional and synchrotron radiation CD (SRCD) instruments, and have developed optimized protocols to ensure high-quality and reproducible spectral data acquisition.

Our aim is to establish a comprehensive database that integrates information on G4 topology geometry, spectroscopic characteristics, and interactions with fluorescent probes.

This study was supported by the National Research, Development and Innovation Office of Hungary (grants PD135510, K138937 and 2019-2.1.11-TÉT-2020-00101), Eötvös Loránd University Excellence Fund (EKA 2022/045-P278-1). SRCD measurements were supported by SOLEIL (Proposals 20230777, 20231948, 20240797, and 20241998).

IL-9

Protein CD spectroscopy in the AlphaFold Era

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Proteins are central to nearly all biological functions and constitute key targets in molecular biology, biotechnology, and pharmaceutical research. Elucidating their three-dimensional structures is critical for understanding function, engineering proteins, and addressing biomedical, industrial, and environmental challenges. To expedite structure prediction, AlphaFold was developed as an alternative to labor-intensive experimental methods. While generally accurate, AlphaFold faces challenges accounting for essential factors such as pH, ionic strength, temperature, mutations, and post-translational modifications—that are critical determinants of protein structure and stability. Consequently, experimental validation remains indispensable. Among spectroscopic techniques, CD spectroscopy offers a rapid and informative approach to probing protein secondary structure, stability, and dynamics. The BeStSel method (https://bestsel.elte.hu) enhances CD spectroscopy by enabling precise secondary structure determination and fold prediction from a single spectrum. BeStSel distinguishes eight secondary structure components and uniquely resolves the spectral complexity of β-structures,—including parallel and antiparallel β-sheets with three twist classes—thus outperforming previous approaches in accuracy and structural resolution. Here, we present a robust methodology for protein structure determination and highlight the role of CD spectroscopy in validating bioinformatics predictions using numerous examples on disease-associated proteins.

This work was supported by the National Research, Development and Innovation Office, Hungary (PD135510, K138937, 2019-2.1.11-TÉT-2020-00101), the Hungarian Academy of Sciences (NAP3.0 Program NAP2022-I-3/2022) and Eötvös Loránd University Excellence Fund (EKA 2022/045-P278-1). SRCD measurements were supported by SOLEIL Synchrotron.

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IL-10

Structure and stereochemical assignments of various natural products from marine-sourced fungi

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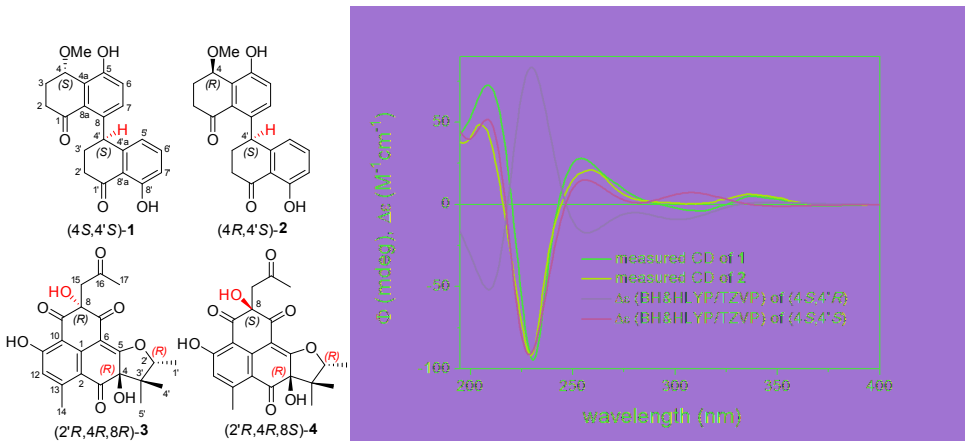
The marine environment has a unique habitat different from that of the terrestrial and is a treasure of biological resources with enormous biomass. Among these, marine-sourced fungi are not only prolific in species diversity, but also in metabolic and functional diversity. On the other hand, marine fungal natural products are commonly possessing unique structures with fused cyclic systems, multi-substitution patterns, and complex stereochemistry. During our research for bioactive natural products from marine-sourced fungi, we obtained a variety of bioactive molecules such as alkaloids, macrolides, peptides, polyketides, and terpenoids. The structures of these molecules are usually determined by spectroscopic methods while the configurations are solved in many cases by DP4+, ECD, OR, RCSA, and RDC and other techniques as well. The related progress will be presented in the presentation.



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IL-11

How Important are Dimers for Interpreting the Chiroptical Properties of Carboxylic Acids?

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Chiroptical spectroscopies are sensitive to the formation of intermolecular interactions for chiral molecules. Experimental Vibrational Circular Dichroism (VCD), Vibrational Raman Optical Activity (ROA) and Optical rotatory dispersion (ORD) data of (–)-[5]-ladderanoic acid in chloroform [1,2], have been analyzed using theoretical predictions for both monomeric and dimeric structures of (*R*)-[5]-ladderanoic acid (Figure 1) to better understand their utility for the interpretation of experimental data. B3LYP, B3PW91 and M06-2X functionals, with and without dispersion corrections, and 6-31+G(2d,p) basis set were used for theoretical predictions. It is found that dimer contributions are important to better reproduce the experimental VCD and associated absorption spectra. However, no significant improvement is evident from dimer contributions to reproduce the experimental ROA and associated Raman spectra. Boltzmann population weighted specific rotations are predicted to be negative both for monomeric and dimeric conformations of (*R*)-[5]-ladderanoic acid and quantitative agreement with experimental ORD of (–)-[5]-ladderanoic acid is obtained with 70:30 mixture of monomers and dimers.

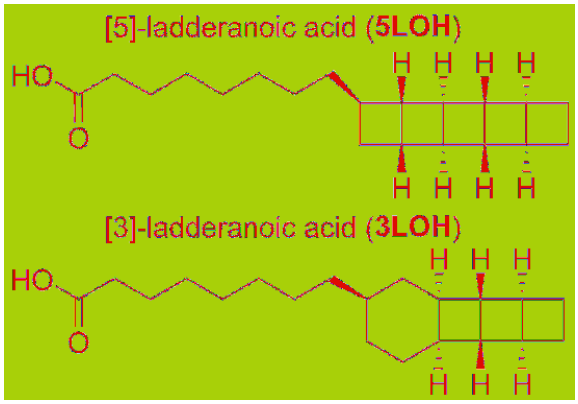

Figure 1. Structures of the (*R*)-ladderanoic acids.

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IL-12

Exploring Chiral Electronic Transitions: From Chiroptical Spectroscopies to Electron Beam Probes

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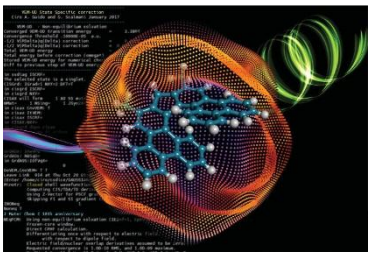

Chiroptical spectroscopies such as electronic circular dichroism (ECD) and circularly polarized luminescence (CPL) remain essential tools for probing the electronic structure of chiral molecules and supramolecular assemblies. In this contribution, we review recent advances in computational methodologies—ranging from time-dependent density functional theory (TDDFT) to multireference approaches—for simulating ECD and CPL spectra, with particular emphasis on the inclusion of environment effects.[1-3]

While these methods have greatly enhanced our understanding of chiral optical responses, a new class of electron-beam spectroscopies is emerging as a powerful alternative. Operating within scanning transmission electron microscopes (STEM), these techniques exploit the inelastic scattering of swift electrons to probe electronic excitations with unprecedented spatial, energy, and temporal resolution. Recent developments in beam shaping and detection, particularly involving electron beams carrying orbital angular momentum (OAM), have opened new avenues for detecting multipolar transitions and chiral electronic signatures beyond the reach of conventional optical probes.[4] We will discuss how these electron-based methods can complement traditional chiroptical spectroscopies, particularly in cases involving dipole-forbidden transitions, spatially inhomogeneous systems, or nanoscale architectures. The potential of combining high-level electronic structure simulations with advanced electron optics represents a promising direction toward a deeper and spatially resolved understanding of molecular chirality.

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IL-13

Inherently Chiral Macrocycles Arenes for Chiral Sensing

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Chiral sensing has gained great interest in the recent years, due to its application in several fields, such as medicinal chemistry, environmental control, and natural products. Among the most promising molecular structures for chiral sensing and recognition are the so-called stereodynamic chiroptical probes [1]. To this family belong polyaromatic host macrocycles having planar chirality, able provide host-guest complexes with chiral guests in which the host exhibits a preferred chiral conformation that correlates with the absolute configuration (AC) of the guest. In 2020 a novel class of macrocyclic hosts named prism[n]arenes have been reported by Gaeta and coworkers [2]. Prismarenes are constituted by 1,5-methylene bridged 2,6-dialkoxynaphthalene units and exhibit a deep π-electron rich aromatic cavity, thus being able to form endo-cavity complexes with ammonium guests stabilized by secondary interactions such as cation···π, C–H···π, van der Waals, and hydrophobic effect. For these macrocycles, the changes in the chiral conformations of the probe can be easily detected and interpreted by means of Electronic Circular Dichroism (ECD) spectroscopy due to its ability to discriminate between enantiomers (Figure 1) [3]. Additionally, Vibrational CD (VCD), provides useful insight on local interaction and conformational stability of the Host-Guest system [4]. In this work, we report the study of the chiral induction and host/guest interactions among different chiral guests and Prism[n]arenes hosts supported by ECD and VCD measurements and their DFT simulation.

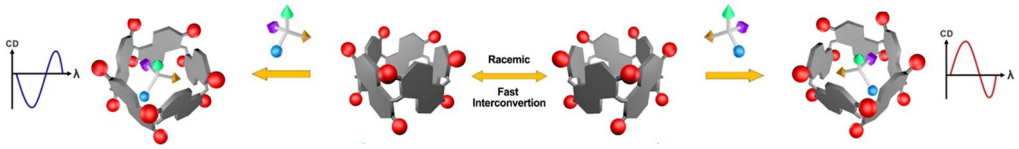

Figure 1. Host-Guest complex mechanism of action.

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IL-14

Ultrafast chiral spectroscopy for stereocontrolled photochemistry

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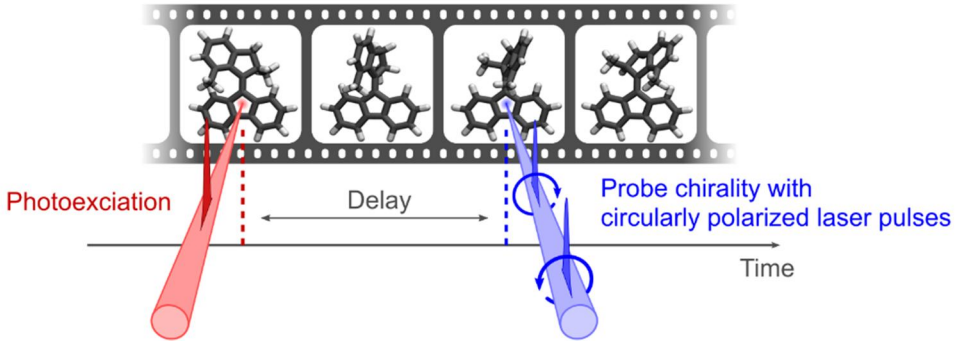

The incorporation of chiral structures into photochemical systems is a powerful strategy to control their functions [1]. For example, uni-directional molecular motors, chiral metal nanostructures, and chiral luminescent molecules with circularly-polarized luminescence (CPL) have achieved exceptional levels of stereocontrol over mechanical motion, electric charge-carriers, and light-emission on the nanoscale. However, the direct characterization of the underlying chiral photoexcited states remains a formidable experimental challenge, due to a lack of analytical techniques that combine high chiral sensitivity in solution with ultrafast time resolution [2].

To address this challenge, we have developed an ultrafast circular dichroism technique that measures the absorption difference of left- and right-circularly polarized laser pulses in photoexcited chiral molecules [3,4]. On this basis, we can now resolve the chiral features of electronic excited states and track their evolution with sub-picosecond time resolution. In this talk, I will show how this approach can be used to resolve the stereochemistry of CPL-active emissive states, and present a recent study on the intramolecular energy transfer and accompanying chiral structural dynamics of a prototypical lanthanide-based CPL complex [5].

Finally, I will briefly present our recent development of a novel fiber-based femtosecond laser source to deliver ultra-broadband deep ultraviolet laser pulses and extend time-resolved circular dichroism to the far ultraviolet spectral regime.

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IL-15

The Acetal Chemistry in Asymmetric Catalysis: Thermodynamic *versus* Kinetic Control

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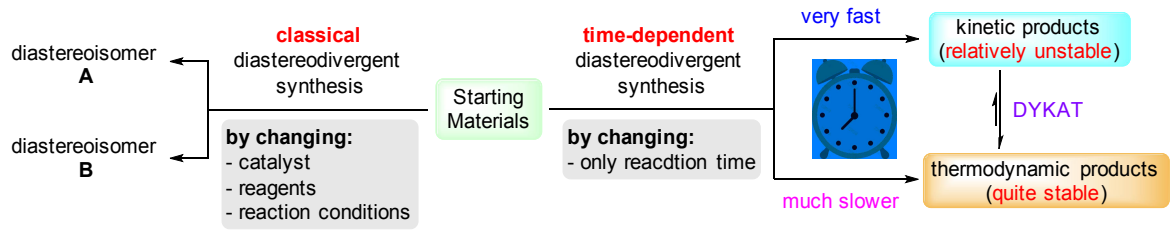
Stereodivergent synthesis is a key challenge in asymmetric synthesis, enabling access to multiple diastereomers with high enantiopurity from the same starting materials. While catalyst and reaction condition optimization are commonly employed to achieve stereodivergence, reaction time remains an underexplored parameter. We report a novel time-dependent stereodivergent synthesis mediated by an asymmetric S_N1 reaction. The strategy hinges on kinetic vs. thermodynamic control of a chiral tertiary carbocation intermediate, generated via acid-catalyzed deracemization of racemic tertiary alcohols. Subsequent enantio- and diastereocontrolled cascade S_N1 cyclization leads to divergent outcomes. This work demonstrates reaction time as a critical variable in stereodivergent synthesis, offering a versatile approach to accessing structurally diverse stereoisomers from a single substrate.



Scheme 1. Time-dependent stereodivergent synthesis.

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IL-16

From Corrinoids to Heme Proteins: Structural Dynamics of Biochromphores Tracked by Resonance ROA

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Raman optical activity (ROA) is a powerful chiroptical technique that enables the structural characterization of biomolecules through differences in circularly polarized Raman scattering. However, due to its inherently low signal intensity, typically 3-4 orders of magnitude weaker than conventional Raman scattering, ROA requires high sample concentrations and extended acquisition times. Resonance ROA (RROA) offers a solution by enhancing the chiral signal when the excitation wavelength coincides with an electronic transition of the chromophore. This allows for the study of biochromophores at lower concentrations, yet it introduces new challenges in measurement and spectral analysis like ECD-Raman effect. [1-2]

We present a RROA investigation of vitamin B12 derivatives and cytochrome c, two structurally distinct yet analogous systems centered around a metal ion coordinated by a macrocyclic ligand (corrin or porphyrin). For cobalamins, our recent results have shown that RROA spectra sensitively detect pH-induced transitions between “base-on” and “base-off” states, reflecting conformational switching in the axial coordination of the cobalt ion. In the case of cytochrome c, we report the RROA spectra for both reduced and oxidized forms, demonstrating how the iron oxidation state modulates resonance enhancement and induced chirality of the heme group. These results shed light on how the oxidation state of the iron center influences the electronic structure and chiral properties of cytochrome c, factors that are closely linked to its diverse biological functions. In addition, important aspects regarding the RROA measurements and ECD-Raman correction of experimental RROA are discussed. Furthermore, quantum chemical calculations of RROA on studied systems were performed to rationalize experimental results.

This work was supported by the National Science Centre in Poland (Grant No. 2019/35/B/ST4/04161). We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Center: ACK Cyfronet AGH) for providing computer facilities and support within computational grant no. PLG/2024/017686.

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IL-17

Spectroscopic features of chiral materials enabling chiral photonics and electronics

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Chiral conjugated organic materials find nowadays applications in photonics and electronics devices, where they are used as thin films. Their supramolecular aggregation may unlock very peculiar properties, such as intense chiroptical properties or the so-called non-reciprocal chiroptical behaviour. Despite this interest, the precise structure of such supramolecular materials is often unknow, severely limiting the progress of the field.

Recently, we have shown that magnetic circular dichroism, paired with more common techniques, can give important information about the molecular packing of chiral conjugated organic compounds.[1]

We have used NIR-emitting supramolecular organic chiral materials to achieve NIR CP-OLEDs, whose polarization strongly depends on the device architecture, and we have shown how to model the polarization outcoupling of the device.[2]

Finally, we have investigated chiral materials displaying non-reciprocal (i.e. opposite from the two faces of the film) ECD and CPL, and used them in resonant cavities generating circularly polarized light.[3],[4]

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IL-18

Chiral Properties of Helical Aromatic Squaramides

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Squaramide is a squaric acid derivative with two amino groups on the four-membered ring, and is used as key functional group of various functional molecules such as molecular recognition and organocatalysts for asymmetric synthesis (Fig. 1a). In this study, we applied the conformational properties of aromatic squaramides to construct unique helical structures, and analyzed their chiral properties.

N,N'-Diphenylurea without *N*-alkyl group generally exist in (trans, trans) structure, and can form network structure with linear head-to-tail type hydrogen bonds. we found that many *N,N'*-bis(*ortho*-substituted phenyl)squaramides afforded chiral crystals by simple recrystallization [1]. In the crystal, helical network structure of (trans, trans) form of the squaramides were formed, and the high frequency of spontaneous resolution with one-handed helix are very interesting from viewpoints of molecular chirality.

N,N'-Dimethyl-*N,N'*-diphenylsquaramide has the (cis, cis) structure in the crystal, in which the two phenyl groups located at the face-to-face position [2]. The bissquaramides that consisted of three benzene rings linked by *N,N'*-dialkylsquaramide bonds at the meta position showed the aromatic layered structures with the helical conformation [3]. Introduction of chiral *N*-substituents biased the one-handed helical structure, and the absolute structure was determined by X-ray crystallographic study, and experimental and theoretical studies of CD spectra in solution [4].

Thus, squaramide is key linking group for helical molecules with unique chiral property.

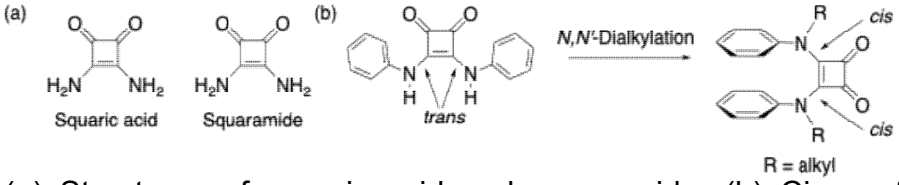

Figure 1. (a) Structures of squaric acid and squaramide. (b) Cis conformational preference of aromatic squaramide caused by *N,N'*-dimethyllation

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IL-19

Chiroptical Analysis of the SWIR (Shortwave-infrared) Organic Fluorescent Probes for Deep Tissue Breast Cancer Imaging

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The development of organic fluorophores emitting in the ShortWave-InfraRed (SWIR, 900–1400 nm) region is an emerging approach to advance clinical optical diagnostics. Fluorescence imaging in the SWIR region enables deeper tissue penetration due to reduced light absorption, scattering, and negligible autofluorescence compared to the conventional near-infrared (NIR, 700–900 nm) window. For biomedical applications, the creation of highly biocompatible organic fluorophores is critical. Although several SWIR-emitting organic probes have been reported, developing clinically applicable fluorophores remains a significant challenge. Indocyanine green (ICG), the only FDA-approved NIR dye, is widely used in clinical settings. Herein, we report the synthesis of π-conjugation-extended ICG analogues (ex. ICG-C11) and their conjugation to monoclonal antibodies, yielding SWIR-emitting molecular probes for targeted imaging.[1)-3)]

Covalent conjugation between the developed dyes and antibodies was carried out to enable specific biomolecular recognition. Also surprisingly, we observed aromatic ring modified ICG derivatives tend to accumulate to the cancer tissue without antibodies due to Enhanced Permeability and Retention (EPR) effect. Using CD spectra, we conducted experiments on the binding of albumin and the pigments, which is thought to be the cause of the EPR effect, and will summarize the results here.

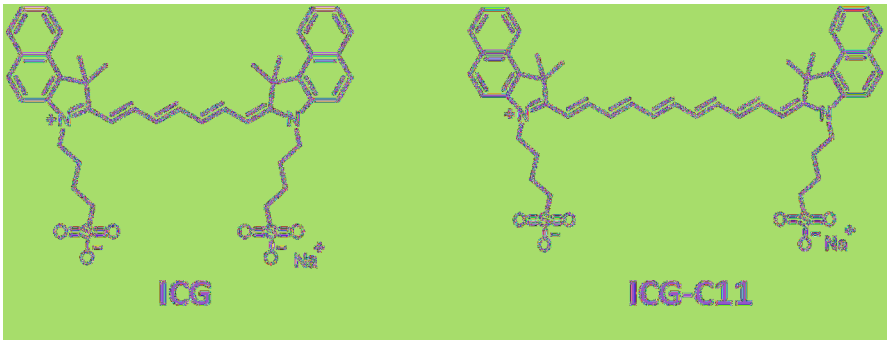

Figure 1. Structures of ICG and ICG-C11.

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IL-20

Translational Supramolecular Chemistry

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The unifying theme in our research group is to integrate underrecognized, at best new principles from supramolecular chemistry into functional systems, because we expect that offering new ways to get into contact on the molecular level will allow us to approach the big questions from new directions. In honor of his 100 anniversary, this lecture will outline how inspiration from Koji Nakanishi during a wonderful two-year postdoc in New York can be found throughout the different topics covered in this spirit. Highlights will include unorthodox systems to catalyze epoxide polyether cascade cyclizations, at best violating the Baldwin rules as in the Nakanishi hypothesis for the biosynthesis of brevetoxin B [1]. Besides pnictogen-bonding and the most recent microfluidic electric-field catalysis [2], this will include functional anion-π interactions as in the origin of color vision. The full concept of the opsin shift, a combination of chromophore planarization and polarization, will be translated into mechanosensitive fluorescent probes that change color like lobsters during cooking and image physical forces in living systems [3].

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IL-21

Progress in Expanding the Scope and Applications of Circular Dichroism

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The CD exciton chirality method is extremely useful for determining the absolute stereochemistry of a diverse array of organic molecules [1]. The method relies on the correlation between the sign pattern of the bisignate CD signal and the absolute spatial orientation of interacting chromophores. The mechanism has been explained quantum-mechanically, eliminating the need for external standards or references in applications, which makes the method both useful and robust. After some controversies in the early 1970s, a general consensus has been widely shared that conclusions drawn from this method should always be consistent with those from the X-ray Bijvoet method, another important non-empirical technique. The method has long been one of the primary choices for determining the stereochemistry of newly isolated or synthesized compounds.

The interpretability of CD spectra has improved, regardless of whether exciton coupling is clearly observed. Complexity in molecular structure can complicate the direct interpretation of exciton chirality. The absolute stereochemistry of the natural atropisomer biflavone was determined by total synthesis, following a series of twists and turns in its publication history [2]. In cases like this, theoretical calculations of CD can help interpret experimental CD spectra. Recent advances in both computer hardware and software now allow even experimental researchers to perform sophisticated calculations independently.

The observable range of CD has also been extended. Vacuum Ultraviolet CD (VUVCD) increases the range of chromophores that can be studied. We have successfully applied VUVCD to observe characteristic CD patterns of chiral allenes near 180 nm. With the help of CD calculations, the stereochemistry of allenes can be analyzed even in more complex molecules containing multiple chiral centers [3]. Fluorescence-detected CD (FDCD) can provide CD spectra exclusively for fluorescent molecules in mixed solutions. Using an ellipsoidal-mirror FDCD attachment that we developed [4], which is completely free from artifacts, we have been investigating exciton-coupling CD spectra of various chromophoric patterns.

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IL-22

Walking in the Footsteps of Giants:
a Journey in the Scientific Lineage of Koji Nakanishi

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Koji Nakanishi's legacy in the scientific community is reflected not only in his seminal contributions to multiple fields of chemistry but also in the lasting inspiration he has provided to his students, collaborators, and peers.

This lecture will summarize some applications of chiroptical spectroscopies to different stereochemical problems which have been inspired by Koji Nakanishi and prompted by the collaboration with the research group at Columbia University in the past 25 years:

1) Structural elucidation of natural products [1,2].
2) Development and applications of exciton chirality method [3].
3) Use of porphyrins as ECD probes [4,5].
4) Interpretation of the chiroptical signature of rhodopsin and related proteins Figure 1) [6,7].

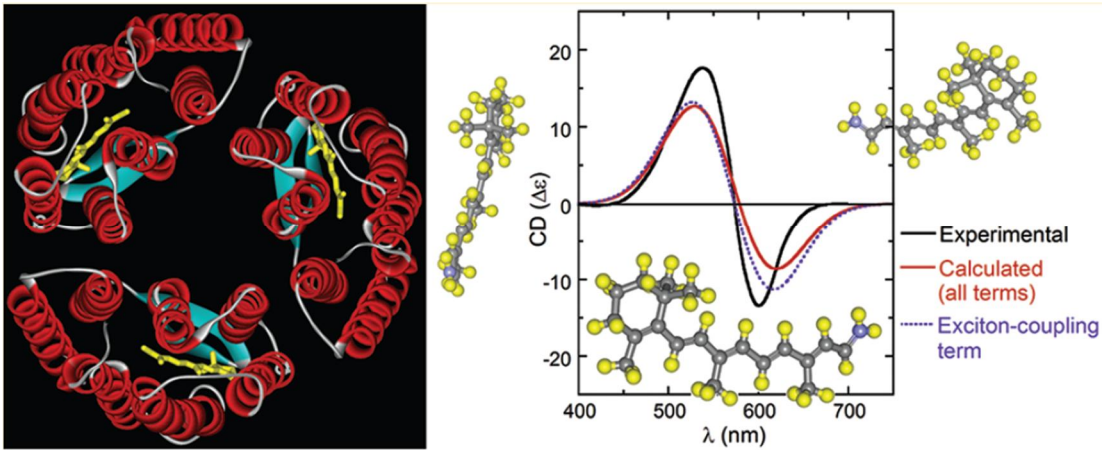

Figure 1. Exciton-coupled ECD spectrum of bacteriorhodopsin [7].

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IL-23

To The Future Guided By Professor Koji Nakanishi

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We are deeply honored for inviting to the session dedicated for 100-year anniversary of the birth of Prof. Koji Nakanishi. We would like to take this opportunity to express to our gratitude to Prof. Koji Nakanishi for his guidance and support over the years since the early days of our company. Here, we introduce some episodes related to Prof. Koji Nakanishi and our company.

JASCO Corporation was established at Tokyo in 1958 to commercialize the results of research and development of infrared spectrometers at the institute of Optics of Tokyo University of Education, which later became Tsukuba University. At the same time, Prof. Koji Nakanishi was transferred from Nagoya University to Tokyo University of Education as a professor, and due to the relationship with our company, in which he frequently use infrared spectrometers in his research, we began to receive various instructions and teachings from Prof. Koji Nakanishi.

Prof. Koji Nakanishi asked us to exhibit our infrared spectrometer at the International Symposium of the International Union of Pure and Applied Chemistry (IUPAC) held in Singapore in April 1961. This was the first oppotunity for us to exhibit our products overseas. This exhibition led to the first export of our infrared spectrometer to the National University of Singapore.

The second export was also based on information provided through Prof. Koji Nakanishi. It was the International Conference on Natural Products and Polymers held in Hong Kong in September 1961. At that time, our colleagues who went to Hong Kong were able to make acquaintance with Prof. Carl Djerassi of Stanford University through the arrangement of Prof. Koji Nakanishi. The encounter with Prof. Carl Djerassi, who was a prominent researcher in the application of the optical rotatory dispersion to stereochemistry[1], led to the decision to install our Polarimeter, which was under development, at Stanford University. We also learned from Prof. Carl Djerassi that circular dichroism is an important analysis method for stereochemistry. As a result ,this encounter and guidance by Prof. Koji Nakanishi became the starting point for the development of our circular dichroism spectrophotometer.

In this report, we will introduce the development and latest results[2-4] of our products based on chiroptical spectroscopy.

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IL-24

Magic Chirality – Enantiomers Beyond the Mirror

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In achiral environments, enantiomeric systems are typically expected to exhibit responses that are equal in magnitude but opposite in sign. However, a growing body of evidence reveals that enantiomeric pairs can display marked differences in response amplitude—even in achiral settings—including phenomena such as oxygen evolution [1] and reduction[2] reactions, and spin polarization.[3] However, the origin of these disparities remains unclear.

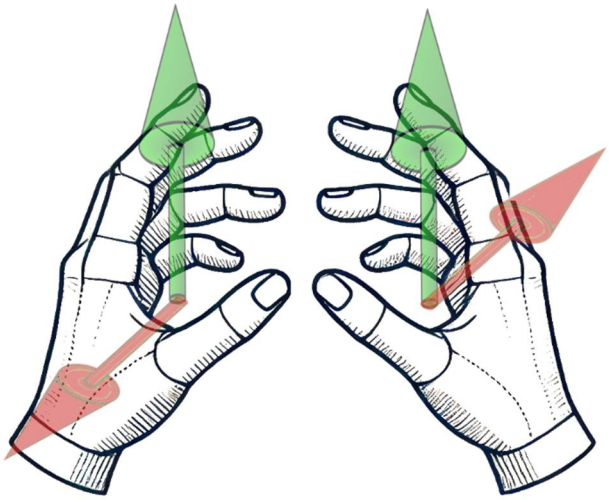

Figure 1. Schematic representation of electric transition dipole moment (ETDM, green) and magnetic transition dipole moment (MTDM, red) vectors in opposite enantiomers represented by hands.

Unraveling the mechanisms behind such enantioselective effects is essential for understanding how molecular handedness can dictate catalytic, electronic, and energy-conversion performance. In this presentation, we propose a stereoelectronic explanation based on our recent findings involving chiral spirobifluorene macrocycles in electrocatalytic oxygen evolution reaction, offering a new perspective on how chirality may shape reactivity beyond structural asymmetry.

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IL-25

Exploration and Application of Vibrational Chromophores in the Biomolecularly Transparent Region

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After my stay in Koji's group in 2005-2006 and 2007-2008 [1-3] and Dan Kahne's group in 2008-2010, I started a new career at Hokkaido University. My first paper as a faculty member is about structural analysis based on C=O stretching VCD signals [4]. This analysis method is referred to as the VCD exciton chirality method for its similarity to the ECD exciton chirality method invented by Koji and Harada-sensei. While the caution for the VCD exciton chirality method was pointed out [5,6], it has shown successes for relatively small molecules [7]. This approach was found useful also for augmenting VCD signal intensity. However, its application to larger (bio)molecules with multiple C=O groups was difficult due to severe signal overlap. Inspired by studies of the ECD exciton chirality method to use longer-wavelength chromophores (e.g., porphyrin) to observe a CD couplet in a spectrally silent region, we thought of using the 2400-1900 cm^{-1} region for the VCD exciton chirality method.

When Koji and I talked about a possible development of the VCD exciton chirality method at CD2013 in Nashville, he liked the idea of testing cyano group as a vibrational chromophore. In addition to a dicyano molecule (**1**), we synthesized diisocyano (**2**), dialkynyl (**3**), and diazido (**4**) molecules and measured their VCD [8]. In this talk, I discuss the VCD (and some ROA) properties of **1**-**4** and other molecules such as deuterated molecules [9] in the 2400-1900 cm^{-1} region.

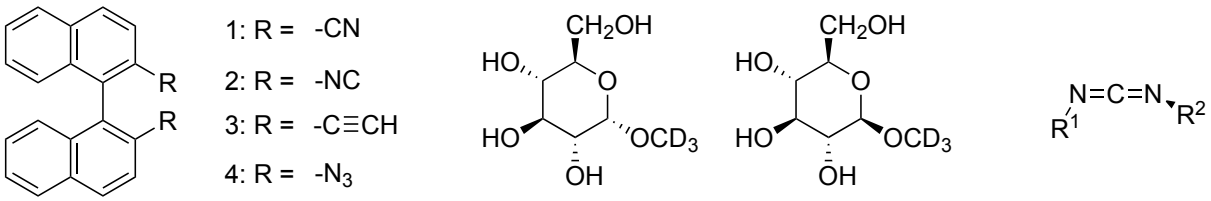

Figure 1. Molecules with chromophores in the 2400-1900 cm^{-1} region studied here.

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IL-26

Enchanting Life of Koji Nakanishi in the World of Science

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We will now conclude the Centennial Session dedicated to the 100th birthday of Koji Nakanishi, a world-renowned leader in the fields of the chemistry of bioactive natural products and bioorganic science, with some brief remarks. He and his team succeeded in isolating and determining the structure of more than 200 new natural products. The biological activity and mechanism of action of some of these natural products, such as brevetoxin B and ginkgolides, have also been investigated. Other studies by his team led to the establishment of a widely applicable nonempirical CD methodology for determining the absolute configuration of structurally diverse chiral compounds. Among the many achievements of his prolific 60-year research career are the long-term studies that clarified the mechanism of vision. His group prepared over 100 retinal analogues that were incorporated into rhodopsin, and the visual process was traced using the photoaffinity labelling method. Studies on the chemistry of the visual transduction process are part of modern photobiology. They form part of his most valuable legacy.

IL-27

Solvent effects on VCD spectra

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Correctly treating solute-solvent interactions is a key challenge of computational spectroscopy and in particular for VCD spectrscopy.[1, 2] Solute-solvent hydrogen bonding interactions are known to affect conformational equilibria and VCD band shapes making chloroform the solvent of choice for determinations of absolute configurations. Its interactions with solutes are typically so weak, that they do not need be considered explicitly in the spectra calculations, allowing VCD calculations to proceed along an established and robust workflow[3] consisting of a conformational search and subsequent spectra calculations within a continuum solvation model. If hydrogen bonding solvents cannot be avoided, for instance due to solubility issues, they often require the explict consideration through a micro-solvation approach and beyond.

In this contribution, we discuss some recent examples from our work, in which solvent effects played a key structure-determining role. Following a short introduction, it will be demonstrated that not only the „typical suspects“ such as DMSO and ACN are prone to show solvent effects. In particular, we will discuss examples in which solvation in general, *i.e.*, the presence of any solvent, has effects on conformational equlibria, that can clearly be characterizde by means of VCD spectroscopy.[4, 5] Furthermore, we will discuss cases in which the solvation shell structure itself determines the VCD signature.[6]

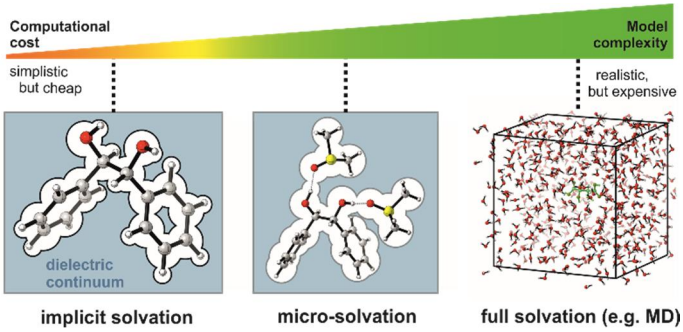

Figure 1. Treating solvation for the simulation of solute-solvent interactions in VCD.

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IL-28

Rapid Quantum Cascade Laser-Based Vibrational Circular Dichroism Spectroscopy Systems for Chirality Sensing

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Vibrational Circular Dichroism (VCD) spectroscopy is a progressive technique capable of enantiomeric distinction through the exploitation of chiroptical effects, which manifest from the differential absorption of circularly polarized light. The implementation of a rapid VCD system has traditionally faced challenges due to low signal-to-noise ratios (SNR) and prolonged data collection times inherent in Fourier Transform Infrared (FT-IR) VCD spectrometers. By harnessing the high spectral density and tunability of Quantum Cascade Laser (QCL) sources, our study demonstrates a swift measurement approach that concurrently conducts VCD and infrared absorption analysis. This talk will discuss the integration of QCLs and the challenges it presents, offering potential solutions for enhancing VCD systems. These advancements pave the way for significant research into minute chiroptical activities essential for enantiomeric studies and have the potential to revolutionize drug delivery systems with improved diagnostic capabilities, thereby aiding the development of molecular therapeutics.

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IL-29

The Digital Chiroscope

from AI-assisted spectral analysis to periodic structure simulations

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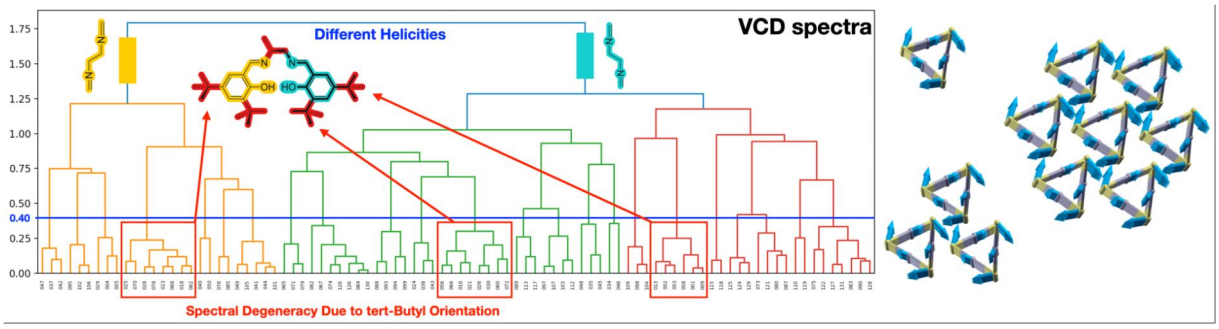
While DFT calculations are indispensable for absolute configuration (AC) assignments and the interpretation of chiroptical spectra, one important aspect has received little explicit attention so far: whether the performed calculations provide sufficient structural resolution to support a reliable AC assignment. Most often, it is implicitly assumed—without systematic verification—that the comparison between experimental and Boltzmann-averaged spectra is meaningful.

To identify and quantify the structural resolution of various chiroptical spectroscopic techniques, we introduce a spectral dendrogram analysis [1], which performs hierarchical clustering of the spectra computed for the low-energy conformers. This AI-based approach is intuitive, visually interpretable, and requires no specialized expertise. Through a few illustrative examples, we show that this approach transforms the widely used chiroptical protocol for AC assignment from a "yes/no/maybe" comparison into a high-resolution digital chiroscope—serving both as an early warning system for problematic AC assignments and as a tool for revealing which structural features a spectroscopic technique can reliably detect, and which it cannot distinguish.

The second part of the talk presents a simple yet effective computational protocol for calculating accurate vibrational spectra of large periodic structures using DFT. This protocol is applied to investigate the origin of the remarkably enhanced vibrational circular dichroism (VCD) signals observed in experimental terahertz VCD spectra measured for Cinnabar helical nanostructures.



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IL-30

BINOL-(tere)phthalonitriles: Versatile Building Blocks for Chiral Emitters Design

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During this lecture, we will highlight the versatility of **BINOL-(tere)phthalonitrile** (**BN(T)PN**) units as central building blocks for the design of a diverse class of chiral emitters. In the first part of the talk, the molecular design and property optimization of circularly polarized thermally activated delayed fluorescence (CP-TADF) emitters based on **BN(T)PN** cores will be briefly summarized.[1-2] We will then discuss how the **BNPN** unit can be used to easily access CPL-active single-benzene fluorophores and the impact of the nature of the cyclic alkylamine moiety on their photophysical and chiroptical properties.[3] Finally, we will present the design of chiral twisted donor–acceptor (D–A) fluorophores, in which the dynamic chirality of the D–A system is controlled by the BN unit of the **BNTPN** subunit.[4]

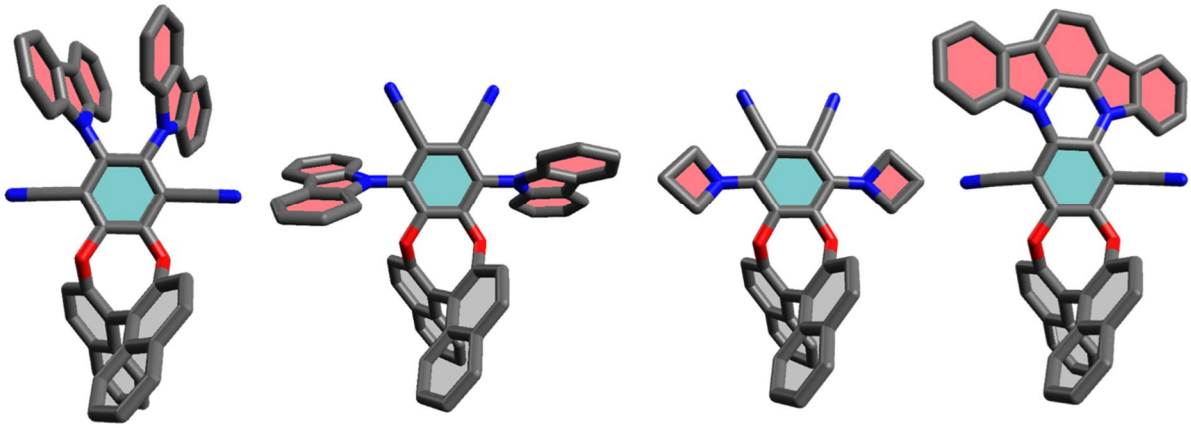

Figure 1. Examples of chiral emitters based on **BN(T)PN** subunits

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IL-31

Theoretical Challenges of Resonance Raman Optical Activity

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Resonance Raman optical activity (RROA) has been pursued for a long time, as a mean to increase the notoriously weak Raman and even weaker non-resonance ROA signals. However, it was as late as 2020 when a formula to subtract the signal from the ECD-Raman effect was found and RROA could be reliably measured [1]. Contemporary quantum chemical technologies provide basic understanding of resonance Raman and ROA intensities (**Figure 1**). They are based on the sum over state formulae [2], time-dependent methodology [3], or the effective bandwidth Ansatz [4].

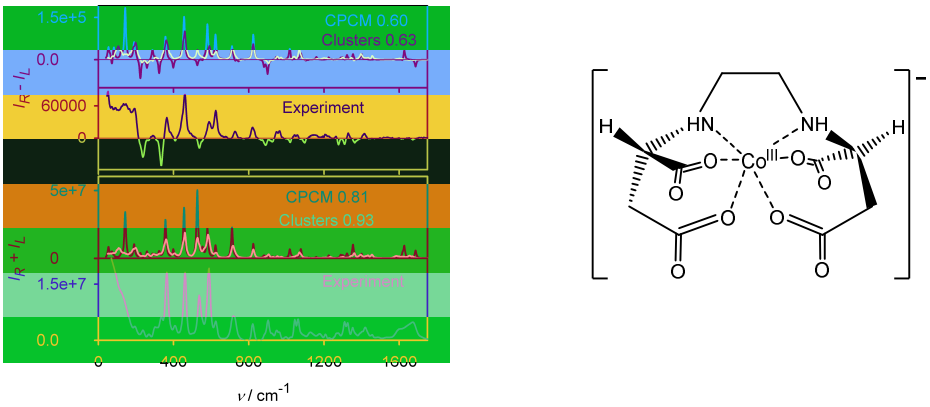

Figure 1. A cobalt complex resonating at 532 nm, and ROA and Raman spectra calculated with the CPCM and cluster models of the aqueous environment (similarities to experiment are indicated, unpublished).

Yet many aspects appear unexplored, such as the role of the Born-Oppenheimer and Placzek approximations, which does not appear quite suitable for the resonance case [5-6].

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IL-32

Chirality and Vibrational Circular Dichroism in the Solid State

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In recent years, VCD measurements of solid samples have become increasingly popular. Regardless of molecular chirality, crystals of specific space groups invariably exhibit chirality and are thus amenable to VCD analysis. Within a crystal, molecules assume fixed conformations and show reduced mobility. Consequently, VCD spectra of crystalline samples showcase narrower and more intense peaks compared to solutions, as they are no longer broadened or obscured by conformational dynamics.[1,2] Moreover, stable supramolecular connections facilitate delocalized vibrations within the non-covalent chiral network, which leads to novel non-local VCD signatures. Thus, the sensitivity of VCD to crystal enantiomorphism extends its applicability beyond merely determining absolute configurations to distinguishing polymorphic forms and discerning induced chirality. [3-5]

The increased complexity of the experimental data obtained from a solid sample renders their interpretation more challenging, as local terms arising from molecular chirality appear together with non-local terms from crystal chirality. In addition, the computational model should account for the periodicity of the crystal structure as well as the shallow potential energy surface of non-covalent interactions. [6] Under such conditions, normal mode analysis, typically used for determining vibrational modes and frequencies, becomes unreliable. Similarly, Magnetic Field Perturbation Theory (MFPT) encounters difficulties due to periodic boundary conditions.

However, with modifications to the conventional computational protocol such calculations become feasible: While molecular dynamics effectively sample the vibrational dynamics in the solid, the VCD response can be computed using its alternative formulation within Nuclear Velocity Perturbation Theory (NVPT). [7]

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OC-1

Chiral Self-assembly of Achiral Metal Porphyrins Studied by Solution and Solid-state CD spectroscopy

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Porphyrins exhibit strong and characteristic absorption in the Soret band region, and the induced circular dichroism (iCD) enables sensitive detection of intermolecular interactions in chiral environments. We showed that metalloporphyrins exhibit high sequence preference depending on the central metal on interaction with DNA. The CD spectra, which changed greatly depending on the porphyrin to DNA base-pair molar ratio, were deconvoluted to three independent component binding modes [1,2]. We discovered zinc porphyrin generate helical aggregates upon interaction with chiral amines in the solid state [3, 4]. In this study, we characterize self-assembly of zinc and magnesium porphyrins with chiral cyclohexanohemicucurbit[*n*]urils, (cycHC[*n*] (n= 6,8), where the chirality of cycHCs is imprinted onto achiral porphyrins in both solution and the solid phase. Diverse coordination environments, influenced by solvents and porphyrin substituents, led to discrete complexes, 1D-, helical 1D, and 2D-square-grid coordination polymers, all with metal-urea coordination centers. Binding strengths, ECD (Electronic), and VCD (vibrational) will be discussed [5].

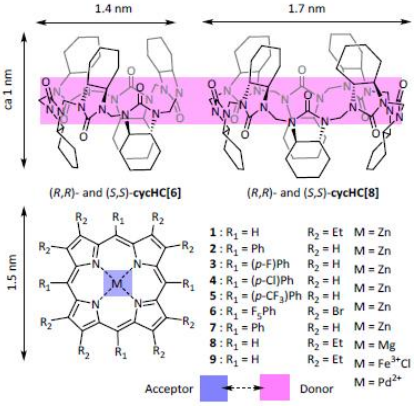

Figure 1. Structures of hemicucurbiturils and metalloporphyrins studied.

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OC-2

Unique Vibrational Circular Dichroism (VCD) of Carbon Dots

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In Chiroptical Spectrocopy Group JU we have been analyzing various supramolecular systems providing intense Vibrational Optical Activity (VOA). Examples of such systems are amyloid fibrils, providing very intense VCD and Raman Optical Activity (ROA) or carotenoid aggregates that generate quite exceptional ROA. [1,2] These studies deepend our understanding on mechanisms of VOA enhancement and show new capabilities of these spectroscopies.

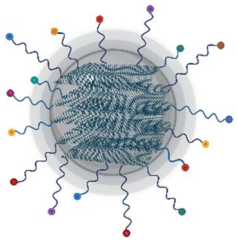

Figure 1. A schematic representation of the carbon dot structure showing the carbon core and functional groups – the colors denote various possible groups such as -C=O, -OH, -NH_2, -COOH, -SH, -SO_3H, -PO_4^{3-}, etc.

Driven by the quest for novel systems with such properties, we turned our attention to chiral carbon dots. Carbon dots are zero-dimensional nanostructures composed of the carbon core connected with diverse organic functional groups. Their characteristic features are tunable fluorescence and rich surface chemistry. [1] In our recent study, we prepared carbon dots from *L*- and *D*-cysteine [3] and characterized them using VCD and Electronic Circular Dichroism (ECD) spectroscopy, as well as high-resolution microscopy. We show that these nanostructures exhibit unique chiroptical properties, including the remarkably intense VCD, and enable chiral recognition of cysteine enantiomers.

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OC-3

Application of CD spectroscopy in characterizing interactions between tau protein fragments and metal ions

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More than two decades ago, our research group began investigating the interactions between proteins and metal ions involved in neurodegenerative diseases. Recently, we have been studying metal complexes of tau protein fragments that play a role in tauopathies.

Neurodegenerative taupathies are characterized by extracellular protein deposits of amyloid-β and intracellular aggregates of hyperphosphorylated tau in the brain. Great number of publications supports that otherwise essential metal ions (such as zinc and copper) play an important role in the development of neurodegeneration. The histidine imidazole nitrogen and cysteine thiolate sulphur donor atoms are frequent metal binding sites in proteins and the tau protein is relatively rich in this moiety. The 12 histidyl and 2 cysteinyl residues of the protein are well-separated and can be found in different chemical environment, hence we can assume that their metal binding properties – at least slightly – differ [1-3].

In order to understand the role of metal ions in metal ion-protein interactions, we synthesised peptides containing the potential metal ion binding sites of the tau protein and studied the complex formation and hydrolytic processes involving metal ions [4-7].

In this presentation, it will be demonstrated how circular dichroism studies can help in following complex formation and hydrolytic processes, identifying metal ion binding sites, and estimating the distribution of metal ions at different binding sites through the investigation of metal complexes of tau proteins.

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OC-4

Chiroptical stimuli-responsive behavior of water-soluble chiral polyacetylene polymers

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Helical polymers are promising materials with wide-ranging applications in asymmetric catalysis, chiral recognition, sensing, optoelectronic devices, and biological systems. [1] Among them, poly(phenylacetylene)s (PPAs) are dynamic helical polymers capable of tuning their P/M helical sense and compression/elongation in response to external stimuli such as pH, temperature, solvent polarity, chiral additives, and metal ions. [1,2] The helical backbone is not rigid but dynamic, allowing external stimuli to influence not only the induced helical sense of the polymer but also the stretching or compression of the helical scaffold. Thus, chiral amplification toward a specific helical sense or helical inversion between P and M helices can be accompanied by the elongation or compression of the helical structure. The functional groups present in the pendant will be oriented in a specific position towards the helix. [2,3] The spatial arrangement of pendant functional groups along the polymer backbone plays a critical role in controlling these transitions, enabling helical inversion, screw-sense amplification, and helical structural modulation through supramolecular interactions and cooperative effects. [2,3] While polyacetylene containing aromatic phenyl groups as PPA's have been extensively explored, their aliphatic-unsaturated counterparts remain relatively underexplored. To address this gap, we introduce a novel class of water-soluble unsaturated chiral polyacetylene polymers in both homo and copolymer forms. Their chiroptical properties are demonstrated to exhibit reversible ON/OFF switching behavior and compression-elongation of helical screws in response to external stimuli, including the formation of chiral complexes. These findings contribute to the fundamental understanding of dynamic helical polymers and pave the way for their potential applications in smart materials and responsive molecular systems.

Keywords: Chiral, dynamic helical polymer, polyacetylene, and stimuli-response.

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OC-5

Simulation of Resonance Raman Optical Activity Spectra for Cobalt Complexes

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One approach for computing Resonance Raman Optical Activity, the difference in Raman scattering intensity for left and right circularly polarized light, is the finite-lifetime or damped linear response method. In this approach, an imaginary empirical damping parameter, corresponding to an effective inverse lifetime of the excited states, is added to the incident frequency. The various complex transition polarizabilities needed to simulate the spectra are then computed at this incident frequency. Within this approximation, the frequency of the outgoing radiation is neglected. In this work, we introduce an approximate method for including the effects of the outgoing radiation through a modification of the polarizability expressions to include a dependence on the vibrational frequencies. For model cobalt complexes, this vibrational frequency-adapted formulation leads to a significantly better agreement with respect to the measured spectra.

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OC-6

Stereochemical Analysis of P-chirogenic Compounds using Chiroptical Spectroscopies and Quantum-Chemical Calculations

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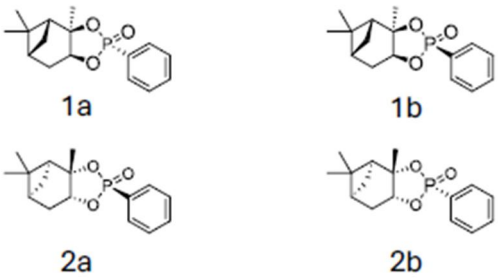
Phosphorus is an important element in both nature and modern organic chemistry. However, stereochemical analysis of P-containing compounds can be sometimes rather challenging. It has been already shown that molecules with a stereogenic center on the phosphorus atom (P-chirogenic compounds) can be advantageously studied by the advanced methods of nuclear magnetic resonance (NMR) [1]. Here we demonstrate that the stereochemical information provided by NMR can be significantly enhanced through the application of chiroptical spectroscopy (electronic and vibrational circular dichroism and Raman optical activity). We employed rigid model molecules – phosphorylated derivatives of isopinocampheol (Scheme 1). The experimental results were systematically correlated with ab initio quantum-chemical calculations [2].



Scheme 1. Phosphorylated derivatives of isopinocampheol.

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OC-7

A Novel Chiroptical Spectroscopy Method Based on X-ray Circular Dichroism

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X-ray Natural Circular Dichroism (XNCD) offers several distinctive and potent analytical capabilities. Due to its inherent element specificity, XNCD serves as a powerful tool for determining the absolute configuration of chiral centres, though its detection is limited to oriented systems, such as single crystals [1]. In addition, XNCD experiments require synchrotron radiation, and have been performed most often at the ESRF ID12 beamline, which supports measurements at the K-edge of light transition metals [2], as well as the L-edge of heavier elements [3].
Our research focuses on advancing X-ray optical activity techniques for studying optically active single crystals of coordination compounds. We have employed both XNCD and, for the first time, RIXS-NCD (Resonant Inelastic X-ray Scattering-NCD), to explore these systems. We will present our recent results including the detection of XNCD in optically active but non-chiral systems, as well as the first experimental evidence of RIXS-NCD.

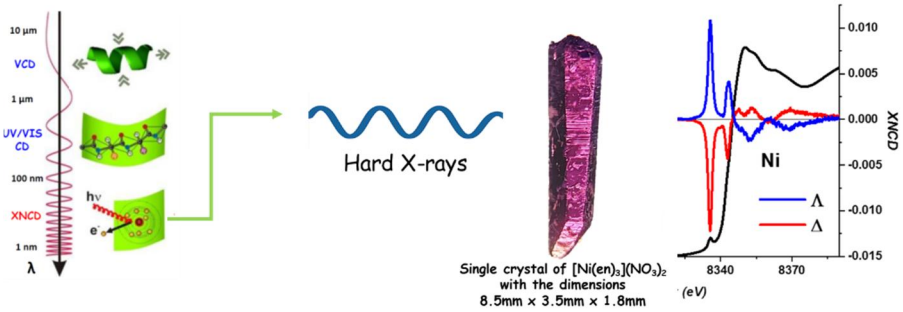

Figure 1. XNCD and XANES (black line) spectra for $[Ni(en)_3](NO_3)_2$

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OC-8

CPL, ECD, ROA and VCD of chiral heptazine-based compounds with inverted singlet-triplet states

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Chiral materials can absorb, emit, or scatter circularly polarised light, enabling the measurement of vibrational circular dichroism (VCD), circularly polarised luminescence (CPL), and Raman optical activity (ROA), respectively. While non-resonant ROA and VCD focus on molecular vibrations within a molecule's electronic ground state, providing insights into chirality transfer phenomena, absolute configuration, and structural or conformational aspects, CPL offers information on the electronic excited state of chiral luminescent systems.

Chiral circularly polarised emitters have been extensively studied due to their applications in optical communication, bioimaging, 3D displays, and encrypted transport. Increasing external quantum efficiency involves synthesising molecules with singlet-triplet gap inversion, thereby accelerating the re-population of the (singlet) emissive state from the (triplet) harvesting state.[1] In this instance, no single-molecule emission from a chiral dye with an inverted gap has been reported, and only one case shows such emission from a supramolecular structure.[2]

In this contribution, we report successful examples of chiral heptazine compounds. To introduce chirality into the studied heptazine analogues, the optically active ligand, i.e., (+)-Bis[(*S*)-1-phenylethyl]amine, was incorporated into the achiral core. All synthesised analogues produce notable CPL, ECD, ROA, and VCD signals due to chiral transfer from ligands to the achiral heptazine core (**Figure 1**). For the first time, we have shown experimentally and using advanced theoretical modelling that individual chiral heptazine-based molecules give rise to delayed emission and CPL from inverted singlet and triplet excited states.

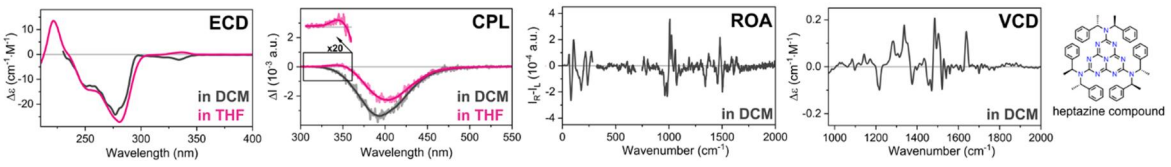

Figure 1. ECD, CPL, ROA and VCD spectra of the studied heptazine-based compound.

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OC-9

Chirality Detection with Gold Nanowires

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Optical activity calculations offer valuable insight into chiral properties of molecular systems. Chiral colloidal and nanostructure assemblies can probe the chirality of surface-bound molecules, induced particle asymmetry, and organize chiral complexes in solution.

As an example, we investigated chiral gold nanowires that exhibit exceptionally strong chiral anisotropy in surface-enhanced Raman scattering. We developed a robust computational model that elucidates key mechanisms relevant to analyte interaction and the enantiomeric discrimination. Combining molecular dynamics and quantum chemical calculations, the simulations revealed that self-polarization of the gold produces static electric field that reflects the chirality of the nanowires. The assymetry is further enhanced by the resonance scattering. While the computational modeling is constrained by system size, it remains amenable to future refinement. The understanding strengthens the potential of the method as a powerful analytical tool for chirality detection across chemical, biological, and environmental applications.

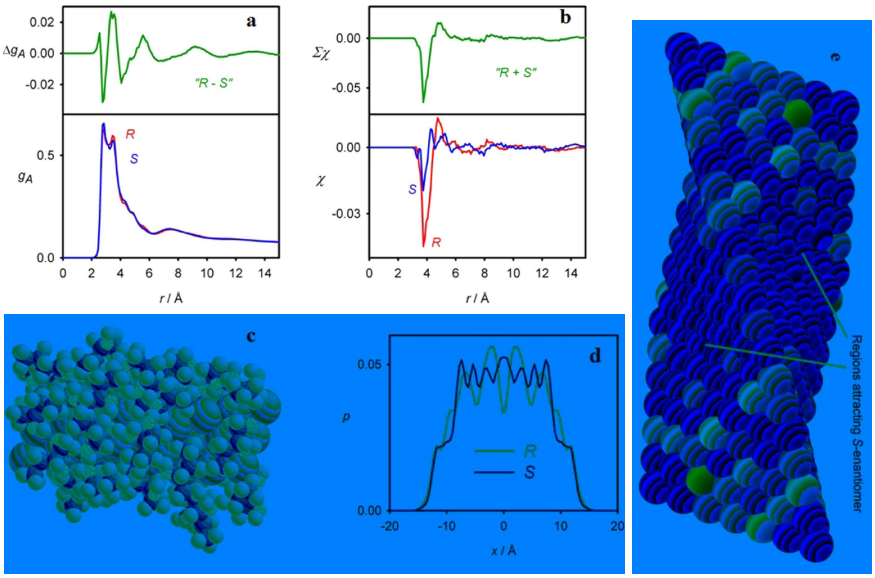

Figure 1. Mechanical preference for enantiomers of R and S butanediols. (a) Solvent distribution functions and (b) chirality indices dependent on the distance from the gold surface, (c) first solvation sphere strucure, (d) average probability distribution of the R- and S-analyte, (e) model of the gold wire, the color relative indicates difference in the chiral affinities.

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OC-10

Chiral Light Scattering: Solving a 40-Year-Old Puzzle

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Back in 1979, it was predicted that shining circularly polarized light on chiral molecules would cause them to scatter light at harmonic frequencies in a way that reveals their chirality [1]. The associated physical effects are *chiroptical harmonic scattering* and *hyper-Raman optical activity*, but for decades no one was able to observe them clearly. That has now changed, as we demonstrated in chiral inorganic nanoparticles.

The chiroptical harmonic scattering effects come in three types, depending on particle size with respect to the wavelength of light: *hyper-Rayleigh* (small particles), *hyper-Mie* (large particles), and *hyper-Tyndall* (intermediate). In each case, incident light produces light scattered at a harmonic frequency, and the scattering depends on the chirality of the material. Because these are nonlinear optical processes, they involve higher-order responses of the material, known as hyperpolarizabilities; hence, the names of these effects.

In 2019, we observed *hyper-Rayleigh optical activity* using silver nanohelices [2]. In 2022, we showed *hyper-Mie optical activity* with CdTe nanohelices [3]. Last year, we completed the picture by demonstrating *hyper-Tyndall optical activity* using silicon nanohelices [4].

We also recently reported *hyper-Raman optical activity*, which is different because it involves inelastic scattering, where light loses energy as it interacts with molecules. Surprisingly, we saw this effect in achiral dye molecules (crystal violet) placed near gold nanohelices [5]. The chiral nanostructures made the molecules behave as if they were chiral. Earlier attempts had failed due to technical issues, like overheating and polarization artifacts [6].

These results bring a long-standing theoretical prediction into the lab and open new ways to study chirality using light. Here, we will present several important updates, including additional confirmation of the *hyper-Raman optical activity* effect, comparing forward and backward chiroptical harmonics scattering, and nonlinear chiroptical photochemistry.

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OC-11

Directional Crystal Motions Controlled by Chirality

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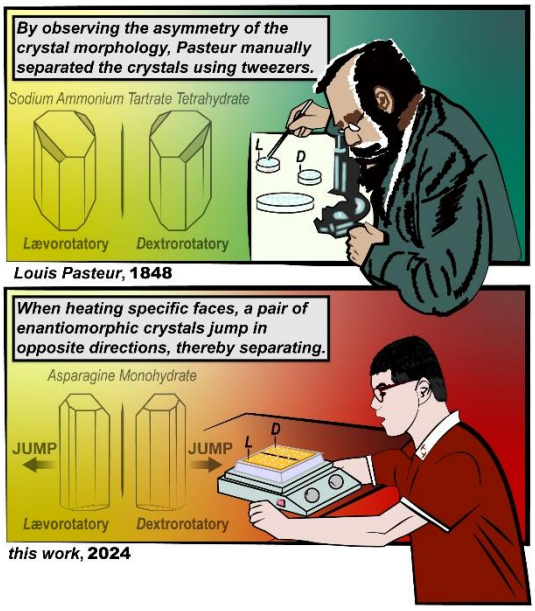
Jumping crystals of racemic mixtures of asparagine monohydrate have been presented in this contribution to emphasize the key role of molecular chirality in governing the direction of macroscopic motions. When heated at the specific faces of the single crystals, a pair of enantiomorphs jump in opposite directions, which are further utilized for chiral resolution. The hydrogen-bonded networks between asparagine molecules in a specific direction provide oriented channels for the escape of water molecules during the dehydration, serving as a foundation for the directional crystal jumping. Our findings not only lay the foundation for the future creation of directed actuation systems based on dynamic crystals but shall also guide the efforts to reveal the correlation between chirality and motion across diverse realms of knowledge.[1] We acknowledge the National Natural Science Foundation of China (52333008, 22405011) for financial support. Y. C. acknowledges the funding of Boya Postdoctoral Fellowship at Peking University and BMS Junior Fellow Program.



Scheme 1. Schematic representations of Louis Pasteur's manual separation experiment in 1848 and the finding about directional crystal jumping controlled by chirality in the present work.

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OC-12

Quantifying Enantiomeric Excess of Carbon Nanotube Solutions Using Chiroptical Spectroscopy and Hyperspectral Fluorescence Microscopy

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Recent advances in sorting techniques have enabled the enantiomeric separation of single-walled carbon nanotubes (SWCNTs) [1], opening new avenues for chiral molecule sensing and separation in chemistry and biology, as well as circularly polarized light emission and detection in optoelectronics. However, accurately determining the enantiomeric excess (*ee*) of these SWCNT samples remains a significant challenge. In this study, we combine electronic circular dichroism (ECD) and Raman optical activity (ROA) with hyperspectral fluorescence microscopy [2] to analyze (6,5) SWCNT enantiomers obtained from various synthesis and processing methods. By leveraging fluorescence peak shifts in hyperspectral data [2], we quantify the *ee* of SWCNTs and calibrate the corresponding ECD and ROA signals. We show that accurate *ee* determination using chiroptical methods requires careful control of SWCNT concentration, as optical artifacts, such as the ECD-Raman effect, can significantly influence the measurements. Our results establish a robust framework for *ee* quantification of SWCNTs using chiroptical spectroscopy, paving the way for systematic studies of chirality-dependent properties and applications.

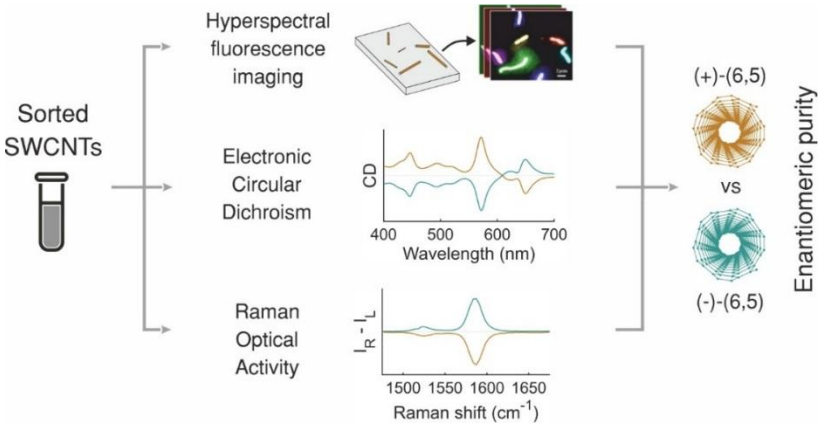

Figure 1. Principle of enantiomer-sorted SWCNT sample characterization.

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OC-13

Raman Optical Activity Spectroscopy as a Sensitive Tool for Detecting Lanthanide Optical Activity

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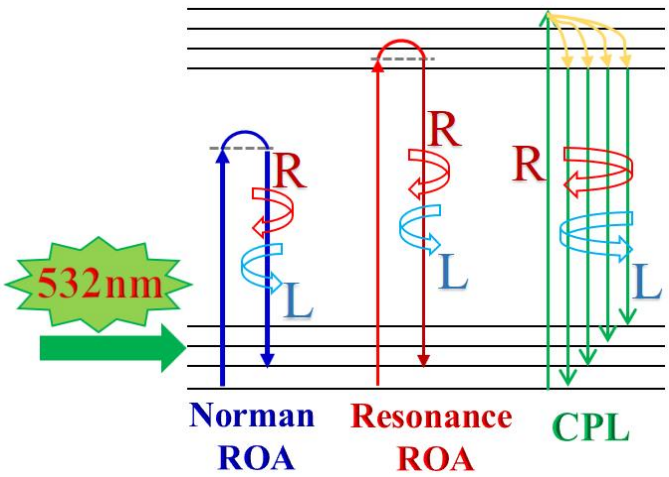
Recent studies have demonstrated that Raman optical activity (ROA) spectroscopy, commonly with green-light (532 nm) excitation, is a convenient method for detecting circularly polarized luminescence (CPL) [1–2]. This approach enables the observation of weak luminescence signals from lanthanide complexes, including their circular polarization characteristics.

When using near-infrared (785 nm) laser excitation, the genuine Raman scattering from lanthanide complexes otherwise obscured by CPL under 532 nm excitation can be effectively resolved [3]. CPL spectroscopy offers a powerful approach for probing biomolecular structures, with lanthanide complexes serving as sensitive molecular probes. Laser-excited CPL detection provides notable advantages, including lower required analyte concentrations and reduced acquisition times compared to conventional ROA methods.

Induced lanthanide CPL is especially valuable for studying systems that lack suitable UV-absorbing chromophores (antenna ligands), making it a versatile tool for structural investigations of peptides,[4] proteins, and other biomolecules.[2]



Scheme 1. Simplified Energy diagram of the ROA-CPL detection scheme.

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OC-14

UV–vis and ECD Spectroelectrochemistry and MCD spectra of Naphthalenediimides

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Naphthalenediimides (NDIs) are remarkable molecules with many exceptional properties and applications [1,2]. Here, we show chiral NDIs (Fig. 1a), cyclic voltammetry (Fig. 1b), UV-Vis spectra (Fig. 1c), electronic circular dichroism spectro-electrochemistry (ECD SEC, Fig. 1d), and magnetic circular dichroism (MCD). NDIs undergo two-step, reversible electrochemical reduction in which the generated radical anion transforms into a spinless dianion [3]. At the same time, the oxidation process leads to radical cation localized at the BINAM part (Fig. 1b). Formation of NDI radicals manifests by a series of new UV-Vis absorption bands (Fig. 1c). In that range, the ECD spectra varied with the electrode potential change more than the absorption ones. For the first time, an isosbestic point (at 455 nm of ECD SEC) was found for the NDI-NH_2 radical-cation in equilibrium with its neutral form (Fig. 1d). Interestingly, the ECD and oxidation ECD SEC signals originate from the BINAM unit of NDI-NH_2, while MCD and reduction ECD SEC signals from the sole NDI core.
The calculations using the hybrid (*explicit* combined with *implicit*) solvation model fairly well reproduced the ECD SEC and MCD spectra of the NDIB-NH_2 molecule.

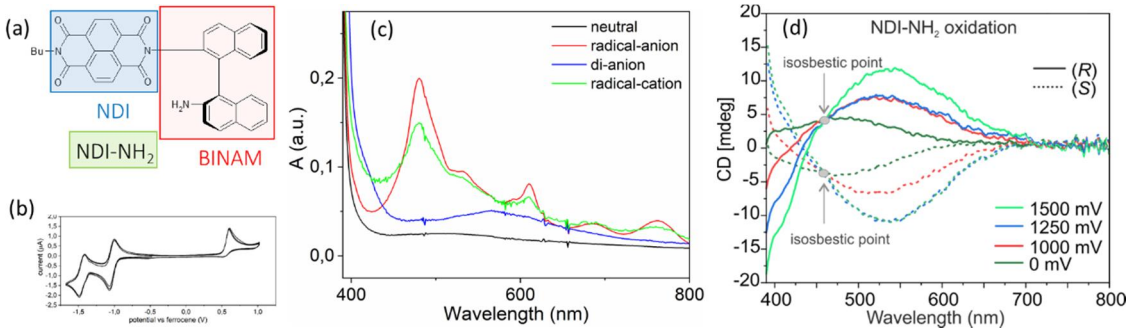

Figure 1. (a) structure, (b) cyclic voltammetry curve, (c) UV-Vis absorption spectra, and (d) oxidation process in the ECD SEC spectra of NDI-NH_2.

Acknowledgments
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OC-15

Structural Elucidation of a Cationic Peptide Nanotube: the Peptide Bilayer Model

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Supramolecular assemblies of peptides have been heavily studied due to their potential as functional materials in biomedicine and bionanotechnology. [1] We developed synthetically modified tetrapeptide analogues which self-assemble to form nanoparticles with characteristic morphologies. [2] These feature a common GLF amino acid sequence that is coupled to a spyropiran (SP) chromophor at the N-terminus and extended by a C-terminal amino acid with ionizable side-chain. Strikingly, the SP-GLFK sequence assemble into hollow cationic nanotubes which display antibacterial properties. The membrane disrupting mechanism of the SP-GLFK nanotubes was captured recently in-situ using electron microscopy which showed that the nanotubes are able to pierce through the bacterial membrane through their edges. Molecular level understanding of the structure of such self-assembled systems opens up the possibility to design and fine tune their properties and functions. We propose that the self-assembly process of SP-GLFK follows the formation of a peptide bilayer with the hydrophobic SP-GLF core which is covered by the charged lysine residues on both sides. In this study we aim to refine this bilayer model using chiroptical spectroscopy as well as computational methods which were extended to SP-GLFK stereoisomers. In monomeric form SP-GLFK shows no circular dichroism (CD) signals, however, in self-assembled state induced CD (ICD) signals of the SP chromophore emerge in a shape of exciton couplets which suggests the chiral packing of the SP moieites. The expected SP-SP contacts were identified based on the comparison of the experimental and computed electronic CD (ECD) spectra. Further insights into the arrangement of the oligopeptide backbone and the stabilizing intermolecular interactions were gained using infrared spectroscopy (IR), vibrational CD (VCD) and molecular dynamics (MD) simulations. The SP-GLFK bilayer model was corroborated by observing chirality transfer between the tetrapeptide chain and the SP packing. That is, switching the backbone stereochemistry of the inner L and F residues from L- to D-configuration results in a flip in SP ICD signal sign in self-assembled state which also comes with the loss of the nanotubular morphology.

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OC-16

A New Frontier in VCD: Fast and Dynamic Chiral Analysis

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Chirality is a fundamental property in the molecular sciences[1], describing entities that are non-superimposable on their mirror images, akin to left and right hands. This property is crucial in understanding the stereochemistry of organic molecules in biological systems[2]. Traditionally, determining the absolute configuration of chiral molecules has relied on techniques such as Vibrational Circular Dichroism (VCD)[3], which measures the differential absorption of circularly polarized light by chiral substances in solution. However, VCD's application has been limited by its need for prolonged data accumulation, typically requiring six to eight hours[4] to achieve a reliable signal due to the minimal absorption differences (10^{-5} to 10^{-4}).

In a significant advancement, our research group has developed an innovative method that drastically reduces the data accumulation time to approximately two minutes. Our approach exploits the enhanced VCD signals found in solid-state materials, allowing for rapid and dynamic monitoring of molecular processes. This enhancement not only improves the efficiency of VCD but also extends its practical applications beyond steady-state measurements, facilitating real-time insights into the dynamic stereochemical landscapes of organic molecules.

The method monitors the growth of crystalline alanine films produced by physical vapor deposition and their phase transition upon moisture exposure. Ex situ morphological techniques, including atomic force microscopy and surface X-ray powder diffraction, are used for further characterization.

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OC-17

Chirality Transfer in Macro- and Supramolecules: an ROA study

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Chiral molecules can spontaneously assemble into larger complexes or aggregates, which may radically change their biological activity. A key role in this phenomenon is played by weak non-covalent forces, that stabilize macro- and supramolecular structures and mediate chirality transfer/induction processes. Recent experiments show that Raman Optical Activity (ROA) is not only suitable for isolated chiral molecules, but also for mixtures of chiral and/or achiral components, such as achiral solutes dissolved in a chiral solvent.[1] We present results of an ROA study of various macro- and supramolecular systems exhibiting chirality transfer phenomena. The first of them is the Cas9 protein and its ribonucleoprotein complex (RNP), used in the CRISPR/Cas genome editing. We demonstrate that ROA combined with CPL (circularly polarized luminescence) can be used to identify the active form of RNP capable of cleaving DNA, as a result of chirality transfer between the nuclease and an appropriate Eu(III)-based probe.[2] As another example, we present chirality induction in the achiral carotenoid canthaxanthin (CAX), upon mixing with chiral polysaccharides (heparin, hyaluronic acid). A strong optical activity is visible in the electronic circular dichroism (ECD) and resonance ROA spectra.[3] Finally, we show enhanced ROA spectra recorded for polypeptides upon aggregation with achiral TPPS porphyrin or due to the presence of Cu^{2+} cations. Their ROA signals result from chirality transfer and the SPIF (Substituted Peptide Inhibitor of Folding) reaction.

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OC-18

π-Hole Bond-Enhanced Enantioselective Discrimination of Helical Polyacetylenes as Chiral Stationary Phases for High-Performance Liquid Chromatography

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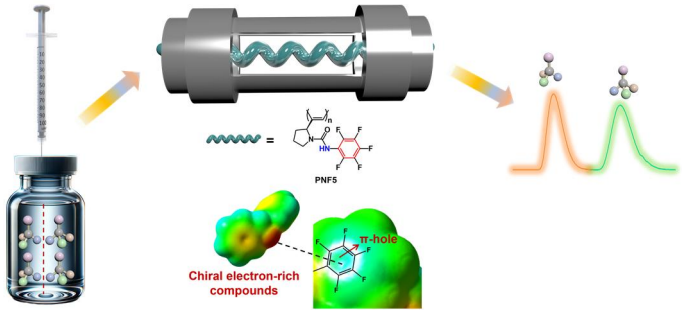
The enantioselective efficacy of chiral stationary phases (CSPs) is fundamentally governed by stereospecific interactions with target analytes. This study pioneers the development of π-hole donating CSPs through the synthesis of poly[(*S*)-2-ethynyl pyrrolidine] derivatives functionalized with pentafluorophenyl groups - the first reported application of directional π-hole bonding interactions in CSP design. The resulting polymers demonstrated exceptional helical stereoregularity and remarkable optical activity, enabling unprecedented chiral discrimination capabilities. The fabricated CSPs exhibited superior separation performance, successfully resolving 8 out of 9 challenging racemates (including baseline separation for 2 compounds) with excellent reproducibility. Through systematic control experiments and computational studies, we established that π-hole bonding serves as the dominant interaction mechanism for *trans*-1,2-diphenylethylene oxide recognition and molecular docking revealed a cooperative interplay between π-hole bonding and hydrogen bonding in the chiral recognition process. This work was financially supported by the National Natural Science Foundation of China (Grant Nos. 52273002 and 52333008).



Scheme 1. Schematic Illustration of Enantioseparation for Electron-Rich Compounds via π-Hole Bond Interaction with Helical Polyacetylene Chiral Stationary Phases.

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OC-19

Assembly Formation of Peptide Supramolecules Tracked by Polarized Light Spectroscopy

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Self- and co-assembled peptide nanostructures can be formed spontaneously *in vivo* with various biological small molecules, but could also be designed and studied also as promising novel functional materials. Supramolecular constructs that can interact with lipid membranes in a controllable way could be used both for membrane engineering and, upon toxic membrane effect, also to provide supramolecular antimicrobial agents. Here we present examples on peptide assemblies with membrane activity. [1-4]. Mapping the interactions can readily be done monitoring conformational or orientational changes of individual peptides, or peptide assemlies via polarized light spectroscopy techniques such as circular or linear dichroism (CD, LD) supported by imaging methods.
Here we present a selected collection of characteristic CD/LD features of AMP interaction systems at the molecular and supramolecular chirality level. Results demonstrate the flexibility and versatility of the AMP structures, ranging from self-assemly, through induced folding, to co-assembly. Illustrated on numerous examples, we aim to show where CD/LD analysis provided useful adds, however, difficulties and limitations are also indicated.
It is hoped that these controllable assemblies will result further applications in membrane manipulation and as higher order antimicrobial systems.

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OC-20

Tuning the Chiroptical Properties in Zn(II) Amino Acids-helical polymers

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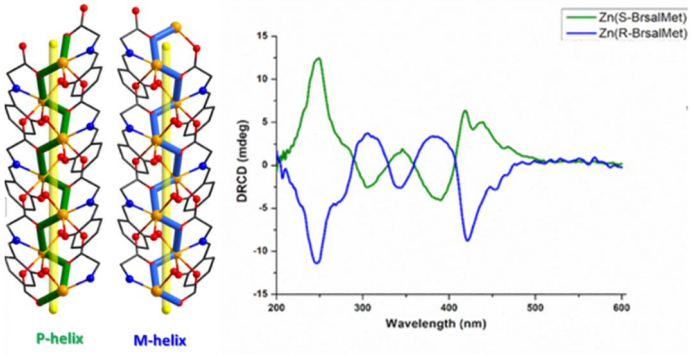
Chirality plays a decisive, albeit low-profile role in various scientific disciplines, including chemistry, biology, and materials science. Tuning the chiroptical properties is achieved by altering the optical activity of the involved chiral molecules through external stimuli such as light, temperature, electric/magnetic fields, and chemical environment.[1] This manipulation can lead to changes in the magnitude and/or direction of chiroptical responses and consequently offers new opportunities for controlling molecular chirality and designing functional materials with tunable optical properties. The most reliable strategy for introducing the chiral information into a metal ion-based network consists in employing an enantiomerically pure ligand. In this respect, the usage of natural amino acids is a straightforward and effective alternative.[2] The study to be presented focuses on a set of tridentate salicylaldimine-type ligands containing different halogen substituents of the aromatic ring. As highlights, we mention: (i) the supramolecular architectures of simple organic chiral Schiff base, (ii) the Zn(II) helices assembled by exploiting these organic compounds as ligands, (iii) their optical properties (UV-Vis, PL, CD, and CPL spectra).



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OC-21

VCD Beyond Solutions

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Vibrational circular dichroism (VCD) spectroscopy has been successfully used to study a wide variety of samples in solution. However, the application of this method to solid-state samples has been limited due to experimental difficulties (orientational artifacts, anisotropic contributions, scattering, etc.) as well as the absence of a reliable theoretical framework for rationalizing the observed spectra. This is unfortunate because, similar to solid-state IR spectroscopy, solid-state VCD experiments could provide a wealth of new information and, in principle, be more straightforward due to the absence of a solvent. Furthermore, a direct correlation between observed spectral features and those calculated based on X-ray structures could facilitate computational analysis.

Recent advances in instrumentation, methodology, and computations have boosted non-solution VCD applications. In this talk, I will present a brief overview of the main directions in solid-state VCD (Figure 1). I will also discuss the primary advantages and obstacles of these applications, provide general recommendations for overcoming such challenges, and offer a glimpse into available and developing theoretical approaches. For an in-depth look at the state-of-the-art in VCD spectroscopy of non-solution samples, see our recently published review [1].

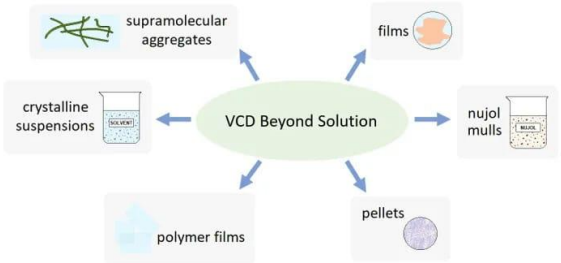

Figure 1. Main directions of the VCD applications for non-solution samples.

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OC-22

Integrative Analysis of Amyloid Fibrils: Chiral Spectroscopy Meets Nanoscale Morphology

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This study explores the chiral and structural properties of amyloid fibrils using a combined spectroscopic and microscopic approach, the latter focusing on Electronic Circular Dichroism (ECD), Vibrational Circular Dichroism (VCD), and Raman Optical Activity (ROA). These techniques provide insight into the chiral architecture of fibrils formed from lysozyme and insulin, proteins known to exhibit pronounced polymorphism. Various fibril polymorphs are prepared under carefully controlled conditions to investigate how structural differences affect the intensity and shape of VCD and ROA signals. In addition, polymorphic variants generated via seeding protocols were examined, with particular attention given to the role of secondary nucleation processes in modulating fibril morphology and their corresponding chiroptical signatures.

To correlate spectroscopic features with nanoscale morphology, atomic force microscopy (AFM) and transmission electron microscopy (TEM) are employed. High-resolution AFM imaging is critical for identifying fibril handedness and for verifying the supramolecular organization suspected to influence chiroptical activity. Through this multidisciplinary analysis, the study aims to deepen understanding of the chiral hierarchy of amyloid fibrils and to provide a more complete picture of the origin of their VCD and ROA responses.

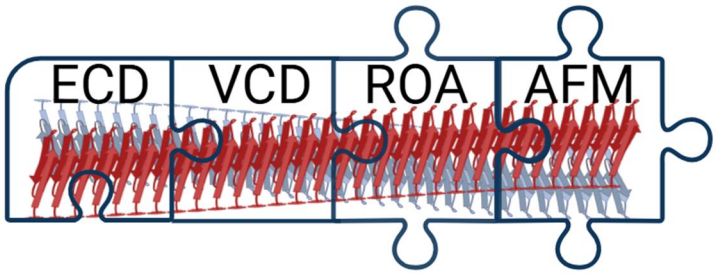

Figure 1. Fitting the puzzle together: complementary tools to decode amyloid fibril structure and chirality.

Acknowledgement
This work was supported by the National Science Centre Poland (NCN, OPUS19, project no. 2020/37/B/ST4/01168 and OPUS25, project no. 2023/49/B/ST4/01785). The research has been supported by a grant from the Faculty of Chemistry under the Strategic Programme Excellence Initiative at Jagiellonian University ("Young Laboratories" Program Edition 4 and 5).

OC-23

Activation Mechanism of Retinal Proteins: Is Light-Induced Double Bond Isomerization the Initial Step?

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The biological activity of retinal proteins is triggered by the absorption of light by the retinal chromophore, which initiates a photocycle leading to protein activation. However, the exact mechanism by which light excitation of retinal induces a conformational response in the protein remains incompletely understood.

To investigate whether protein conformational changes can occur without light-induced isomerization of the retinal C13=C14 double bond, we employed the hydroxylamine reaction. This reaction cleaves the protonated Schiff base linkage through which the retinal chromophore is covalently bound to the protein. The hydroxylamine reaction is light-catalyzed and can serve as an indicator of protein conformational alterations.

Our results show that in retinal proteins, the hydroxylamine reaction proceeds under light even in artificial pigments derived from synthetic retinal analogs in which the critical C13=C14 double bond is constrained and cannot isomerize. These findings suggest that light-induced charge redistribution in the retinal excited state is sufficient to polarize the protein and trigger conformational changes, independent of double bond isomerization.

This mechanism may have broader implications, extending to other photoreceptor proteins containing retinal or non-retinal chromophores, where light excitation alone could influence protein conformation.

OC-24

Photochemical Release of Bioactive Molecules for Neurological Applications and Beyond

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It is a great honor to speak in celebration of Professor Koji Nakanishi's 100th birthday. Koji is fondly remembered for his prolific scientific contributions—from isolating and characterizing hundreds of natural products to pioneering chiroptical methods for stereochemical analysis and elucidating the molecular basis of vision. His charisma and insight profoundly influenced my career, especially in harnessing light to control neural pathways.

This talk will follow a path from studying insect vision to developing light-responsive molecular tools for neuroscience. The human brain, with its 86 billion neurons and trillions of synapses, presents a formidable challenge for mapping function. Neural circuits are not only complex but also highly dynamic. To address this, molecular tools that selectively activate defined neuron populations have proven powerful.

Optogenetics revolutionized neuroscience by enabling light-mediated control of genetically defined neurons with exceptional spatial and temporal precision. Complementing this, photoprotecting groups (PPGs), or photocages, allow for light-triggered release of neurotransmitters or agonists [1]. Our early work focused on UV-activatable systems and improved synthetic methods, demonstrated by the controlled release of glutamate, the primary excitatory neurotransmitter [2]. We later developed systems responsive to blue and green light with quantum yields up to 0.65 [3]. These advances extended to applications such as photoinitiated organocatalysis [4] and light-activated calcium ion uptake [5].

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OC-25

Natural Compounds Studied Through Unusual Spectrocopic/Chiroptical Techniques: MCD and CPL

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Chiroptical spectroscopies played a crucial role in stereochemical characterization of natural compounds. Powerful techniques, such as Electronic (ECD) and Vibrational (VCD) Circular Dichroism, Raman Optical Activity (ROA), Optical Rotatory (OR) and Optical Rotatory Dispersion (ORD), have been indispensable tools to determine the absolute configuration and the conformational aspects of natural bioactive compounds.[1,2] In this work we explore whether less conventional techniques making use of circularly polarized radiation can be employed in the field of natural products.

Some chiral Amryllidaceae alkaloids, isocoumarines and achiral bioactive napho- and anthra-quinones were investigated via Circularly Polarized Luminescence (CPL) and Magnetic Circular Dichroism (MCD). CPL has been found to provide useful information on excited state phenomena, like the ESIPT (excited state intramolecular proton transfer, see Figure 1) mechanism, which appears as a widely recurrent phenomenon in natural products.[3-5] MCD appears instead a necessary tool for the class of the numerous non-chiral natural products: for them, minimally, MCD provides a unique means to resolve congested UV bands. Furthermore we investigated whether MCD spectra of non-chiral compounds bear similarities to MCD spectra of chemicallly similar chiral compounds and why. [6]

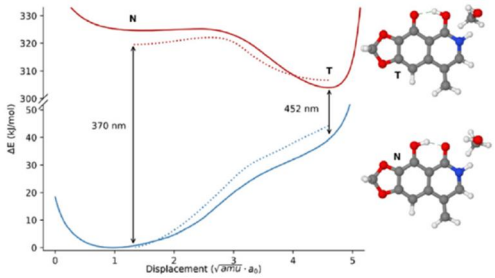

Figure 1. Description of the ESIPT mechanism in Narciclasine, as per DFT calculations in ref. [3].

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OC-26

Chiroptical properties of “simple” furofuran lignans: structure and solvent effects

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Recently, we demonstrated that a key VCD spectral feature of the natural furofuran lignans phillygenin, epieudesmin and eudesmin was reproduced only by means of an MD-QM/MM protocol [1]. This was valid even for molecules devoid of H-bond donor groups in acetonitrile and chloroform solutions. Interestingly, this spectral feature was less pronounced in fargesin [2], which differs from phillygenin and epieudesmin by the aromatic ring substitution pattern (Figure 1).

Herein, experimental and theoretical investigations of the furofuran lignans sesamin, episesamin and kobusin were performed to further probe the impact of both molecular symmetry and the flexibility of the aromatic ring substituents for their VCD properties in different solvents. Preliminary results indicate that the inclusion of explicit solvation becomes necessary for VCD simulations as molecular symmetry and flexibility increase. The effects on ORD and ECD properties seem to be less evident. A rationale for the observables as well as a possible structural hierarchy for the effects will be discussed.

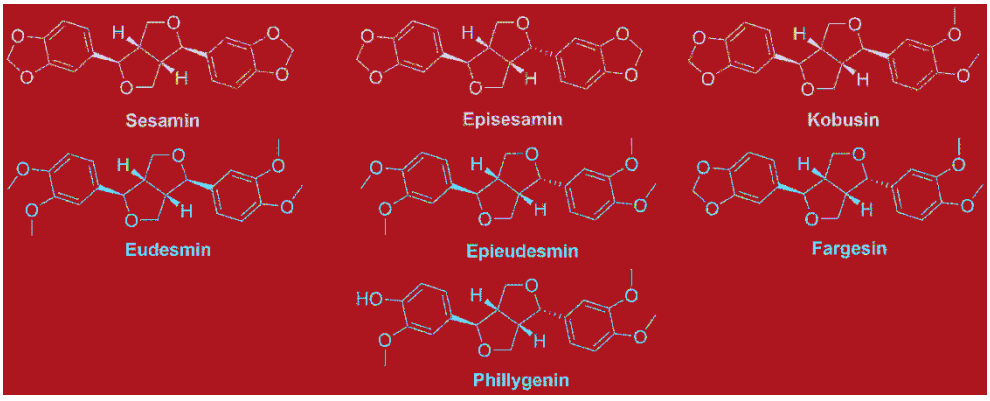

Figure 1. Structures and relative configurations of the furofuran lignans investigated.

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OC-27

Nonlinear g-*ee* Dependence in Chiral Films

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In non-interacting systems such as dilute solutions [1] or the gas phase [2], the enantiomeric excess (*ee*) of chiral materials typically exhibits a linear correlation with their chiroptical activity, characterized by the anisotropy factor (g). In condensed phases – dense liquids and solid films – however, this relationship can deviate significantly from linearity due to enhanced intermolecular interactions among chiral units [3, 4]. While this nonlinear g-*ee* dependence remains underappreciated, we previously reported a striking example in polycrystalline films of BINOL, where a pronounced negative nonlinearity was observed [5]. Here, we present additional cases across a diverse set of chiral samples, reinforcing that such nonlinear behavior may be more widespread than commonly assumed. These findings underscore the need to incorporate *ee*-dependent chiroptical measurements as a routine component in the study of chiral materials in the condensed phase.

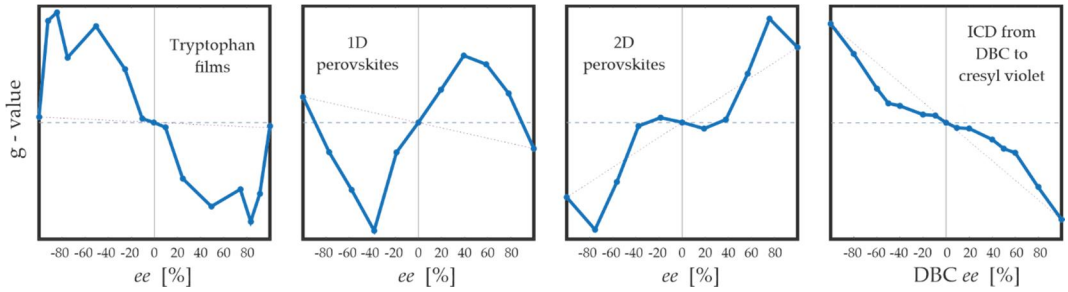

Figure 1. Nonlinear g-ee dependence in diverse samples. From left to right: Films of tryptophan evaporated under vacuum; 1D hybrid organic-inorganic perovskites; 2D hybrid organic-inorganic perovskites; colored gels: N',N'-dibenzyol-cystine, dyed with cresyl violet perchlorate.

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Poster Presentations

PO-1

Helicenes for and from magnetochiral effect (HEL-MCH)

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Preparing chiral compound with higher enantiopure excess is still an exciting goal for scientist and key challenge for widely application such as pharmaceutical, material science and also the homochirality[1] in Nature. Since 1848, Louis Pasteur tried to generate an excess of one enantiomer under magnetic field, which failed by lacking of the chiral force[2]. Thus, the technique was discovered in the modern year from his inspiration, by using light propagating collinear to the applied magnetic field, which it called magnetochiral effect (MCh).[3] Indeed, Rikken and Raupach demonstrated in the 2000s that it was possible to generate a small enantiomeric excess by means of a magnetochiral field (enantioselective magnetochiral photochemistry) on chiral chromium trioxalate type complexes.[4] Our group and collaborators reported the strong magnetochiral dichroism (MChD) from ytterbium(III) based helicene ligand.[5] Currently, we are studying the MChD of Erbium enantiomers (Figure (a)). In parallel, we will be preparing the olefin ligand coordination with lanthanide complex ($Ln(hfac)_3$ Ln= Yb, Dy) and we will attempt to create an enantiomeric excess under a MChD field (Figure (b)).

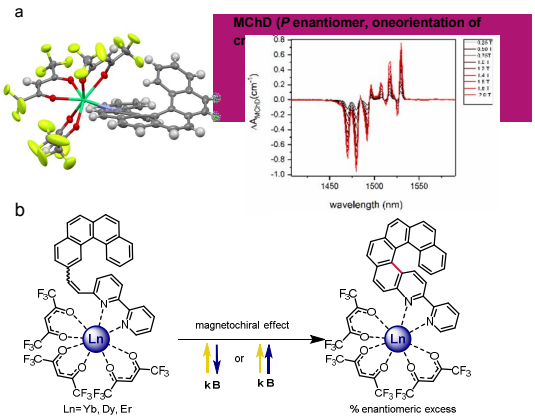

Figure 1. (a) MChD of Er(III) complex, (b) olefin-lanthanide complex studying enantiomeric excess under MChD field.

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PO-2

Exploring the Complexity of Supramolecular Systems by Means of Advanced Chiroptical Methods

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Chirality is a fundamental property of nature. It may be generated at the supramolecular level as a result of non-covalent interactions between molecules. Compounds such as carotenoids, porphyrins, or polyene antibiotics can spontaneously aggregate in solution or biological membranes under various conditions.[1,2,3] Different environmental factors, i.e., pH value, concentration, or solvent type, can significantly influence the structural, biological, and therapeutic properties of selected molecules. Recently, novel therapies targeting the staphyloxanthin, a carotenoid naturally found in the membranes of Staphylococcus aureus, have been proposed.[4] At the same time, AmB-ion complexes can reduce the drug's toxicity, while porphyrin supramolecular systems are used to formulate new drug carriers. Here, we applied chiroptical spectroscopic techniques, including electronic circular dichroism (ECD) and Raman optical activity (ROA), to study the chirality at the supramolecular level. We have observed a strong dependency between the aggregate types formed under several experimental conditions. Moreover, the observed supramolecular organization resulted in a substantial enhancement of the chiral signal. Using both vibrational and electronic optical activity methods turned out to be crucial for obtaining a complete characterization of chiral self-organized systems and their component molecules. Our work leads to the conclusion that the spectroscopic methods used are an excellent tool for investigating the nature of supramolecular aggregates.

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PO-3

Vibrational Circular Dichroism Spectra of Tartaric Acid in Aqueous Solution

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Vibrational Circular Dichroism (VCD) Spectroscopy in aqueous solution presents a powerful technique to investigate chiral molecules in different protonation states but it also poses multiple challenges regarding both, the experiment and calculations. Due to the strong IR absorbance of water, short pathlength of 6-8 µm are required to acquire good quality IR and VCD spectra.[1] As demonstrated in our work on proline in aqueous solution,[2] the implicit and micro-solvation approaches are not sufficient to represent the experimental spectra well. We introduced the solvent-shell approach, which is based on MD simulations, from which solute-solvent clusters with ~1.5 solvent shells are extracted and optimized for the calculation of the IR and VCD spectra on DFT level.
Compared to proline, tartaric acid is a rather flexible molecule that we investigated in two protonation states: neutral and dianionic. We used two different semi-empirics during the MD simulation for the description of tartaric acid and compared their influence on the final spectra. We found that the neutral tartaric acid is described well by both AM1 and PM6, while there are large differences between the methods for the dianionic species. Further investigations revealed that the spectral changes are a result of different dihedral distributions obtained from the semi-empiric levels.

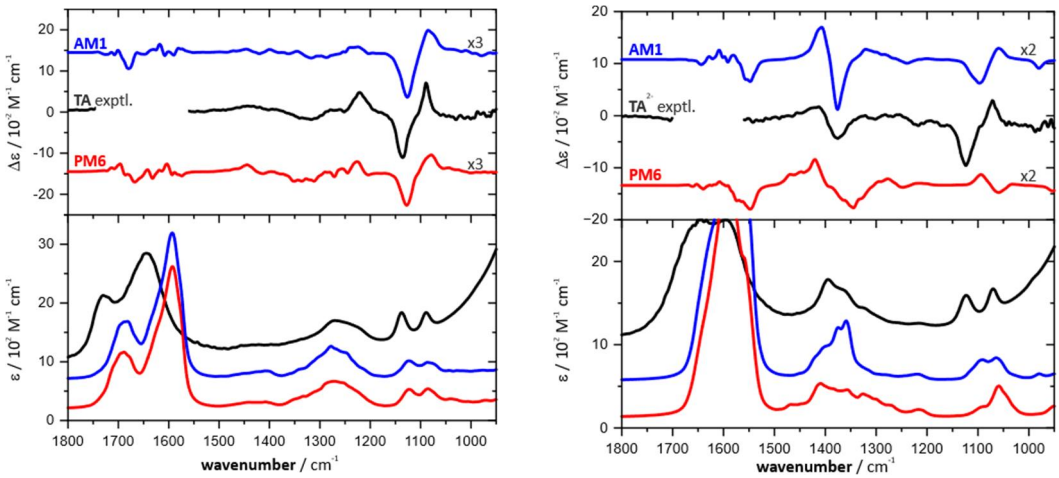

Figure 1. Comparison of (black) experimental and computed IR and VCD spectra for (left) neutral and (right) dianionic tartaric acid. The MD simulations were performed with (blue) AM1 and (red) PM6 as a semi-empiric and B3LYP/def2-TZVP/CPCM (water) level of theory for the optimization and frequency calculation.

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PO-4

Acetate Binding to Chiral Dithiourea Derivative Studied by VCD Spectroscopy

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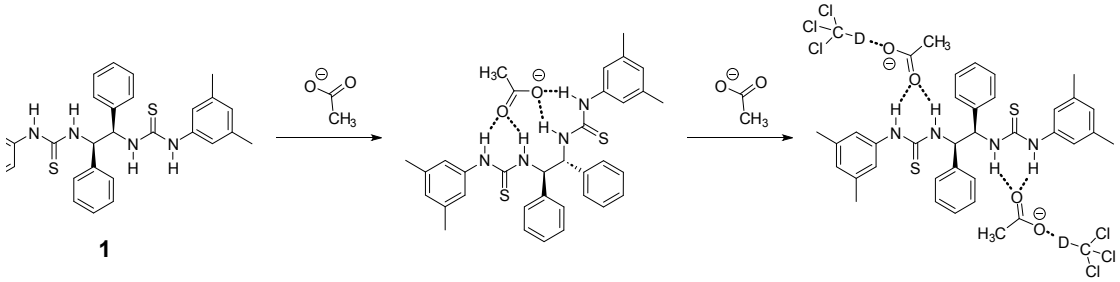
The ability of chiral thioureas to form double hydrogen bonding interactions is ideal to stabilize anions and electrophiles in a chiral environment, therefore they frequently find application in molecular recognition [1] and stereoselective organocatalysis.[2] Using vibrational circular dichroism (VCD) spectroscopy, our group has previously shown that the structure of the thiourea-substrate complexes are not always as initially expected.[3,4] For the interaction of a thiourea with an acetate ion, for example, it was found that instead of the typical interaction of both oxygen atoms with the thiourea NH protons, only one oxygen is interacting with the thiourea while the other one is binding to the solvent.[4]

In the present study, we investigate a chiral bifunctional thiourea (**1**) and its interaction with acetate ions. Comparing the experimental spectra of **1** itself in solution phase to DFT-based calculations shows a stretched-out conformation of the thiourea groups to be preferred. Upon addition of one equivalent of the acetate, **1** adopts a twisted structure with both thiourea moieties interacting with one oxygen of the acetate each. By adding a second equivalent, the structure stretches out again and shows two independent interactions of the thiourea groups. In contrast to the expected interaction of each oxygen with one thiourea proton, as show previously, it was found that one oxygen atom interactions with the thiourea moiety and the other one shows a solute-solvent interaction with the $CDCl_3$.



1

Scheme 1. Illustration of the conformational change upon adding more equivalents of tetrabutylammonium acetate to the diphenyl-dithiourea derivative (**1**).

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PO-5

Synthesis and VCD spectroscopy of host-guest complexes with chiral azacryptands

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Octaazacryptands are well-studied achiral polycyclic amines that act as hydrogen bond donors for the encapsulation of both charged and neutral particles. [1] However, only a few examples of chiral cryptands containing polyamine units have been investigated for guest encapsulation. [2, 3]
Recently, we introduced chiral TREN-based (tris[2-aminoethyl]amine) octaazacryptands. [4] It was shown that these macromolecules tend to reduce their inner cavity volume, which is initially too small to accommodate a solvent molecule.
In the present study, our azacryptands are used as receptors for simple dipodal and tripodal anions. To this end, titration experiments and CD spectra were recorded. Initial results indicate that the encapsulation of small oxyanions is feasible. We also discuss challenges related to solubility and to determining the protonation state of the cages, which is essential for accurate CD calculations. [5]

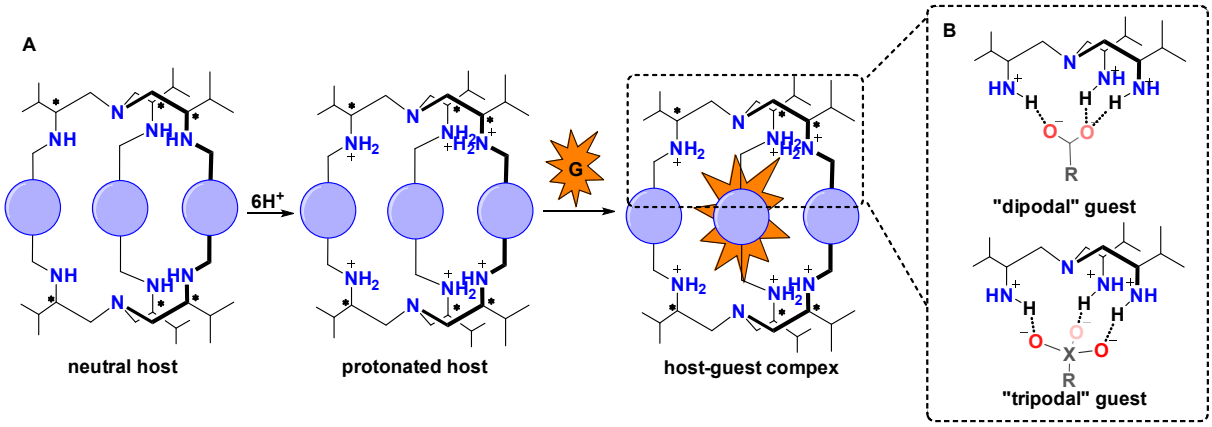

Figure 1. Research target. **A:** schematic representation of the host-guest complexes synthesis starting from a neutral host molecule [4]; **B:** suggested binding mode of the guests within the cage cavity.

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PO-6

Structural study of β/α-Hybrid Peptide Oligomers

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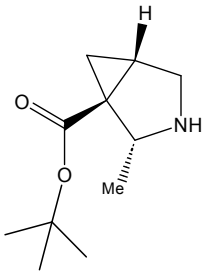
Precise control of the three-dimensional structure and proper ordering of molecules is a major goal of modern medicinal chemistry. Among numerous scaffolds used for the design of bioactive compounds, peptides and their analogues are widely explored. Their major advantage is their biocompatibility and their synthetic accessibility, but, the development of effective drugs based on α-peptides is limited due to their high conformational freedom of short fragments and low proteolytic stability in vivo. To overcome these drawbacks, modifications of native α-peptides have been developed, including variations of both the backbone and side chains.[1,2]

Here we report a study of secondary structure of peptide-like foldamers consisting of alternating 3,4-Methano-β-Proline (Scheme 1) and amino acids glycine and L- /D-alanine utilizing a combination of circular dichroism (both vibrational and electronic) and NMR spectroscopies. The experimental results are further supported by Quantum-mechanical calculations and molecular dynamics simulations.



Scheme 1. 3,4-Methano-β-Proline - a building block for β/α foldamers

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PO-7

Photochemistry of Chiral Imines Investigated by Matrix Isolation IR/ VCD Spectroscopy

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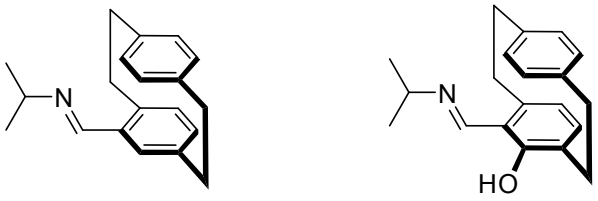
Photoswitches are molecules that can switch between different isomers upon irradiation with light. Introducing them into materials can provide a wide variety of different controllable properties.[1] One example for photo switching is the E/Z isomerization of imines. Tuning their properties has become an important goal in the last few years.[2] Of particular interest are salicylimine derivatives which not only show E/Z isomerization, but are also known to perform excited-state intramolecular proton transfers (ESIPTs) making them a valuable tool as chemosensors and for biological imaging.[3] Upon excitation the hydroxy proton is transferred to the imine to form a ketone and a secondary amine while also loosing aromaticity.[4,5]

Our group previously studied the photochemistry of a salicylimine derivative using matrix isolation IR spectroscopy and ultrafast spectroscopy.[5] In this study, we characterise the chiral imines **1** and **2** in solution phase using IR and VCD spectroscopy. Since it is not possible to investigate the photochemistry in solution phase, we perform these measurements under matrix isolation conditions, measuring IR and VCD at cryogenic temperatures (5-20 K) in a solid inert environment (pH_2 or Ar) and compare them to DFT-based calculations. For **1,** the focus is solely on the switchable E/Z isomerization, for **2**, we also aim to investigate a possible ESIPT.



1 **2**

Scheme 1. Illustration of the investigated compounds, a chiral imine (**1**) and a chiral salicylimine derivative (**2**).

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PO-8

CPL Photoscopy: Circularly Polarized Luminescence Detected by Chromaticity Differences

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Circularly polarized luminescence (CPL) is attracting growing interest for a wide range of applications,[1] spanning from materials with advanced optical properties[2,3] to innovative imaging techniques.[4] The traditional approach to CPL consists of measuring the emission intensity difference between the left and right polarizations of light and usually requires spectral separation through colour filters or a monochromator. However, in the last few years many efforts were undertaken to make CPL detection cheaper and easier.[5,6]

In this work, we show the possibility of extracting CPL information from the chromaticity values of a couple of snapshots of the emitted light taken under different polarizations when a CPL spectrum contains at least two bands with different polarizations. This concept paves the way for a novel approach to CPL measurements, based on chromaticity difference rather than intensity difference. This technique requires cheap instrumentation, as it can be performed with an entry-level camera, offers complementary features with respect to the traditional methods and could potentially be applied to CPL imaging.

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PO-9

Length-Dependent Nonlinear Chiroptical Signatures in Aromatic Oligoamide Foldamers: From Solutions to Surfaces

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The link between chirality and optical activity in nonlinear scattering processes was long predicted but has only recently been confirmed experimentally.[1,2] These processes offer a promising alternative to conventional linear techniques like circular dichroism (CD) or optical rotatory dispersion (ORD) for probing chirality in solution and on surfaces. In a recent study, we investigated the nonlinear optical response of aromatic oligoamide foldamers (AOFs) – helical molecules with tunable length and handedness – in solution using Hyper-Rayleigh Scattering (HRS). With linearly polarized excitation, we observed a non-monotonic chiral response, unlike the linear trend typical of CD or ORD, suggesting sensitivity to additional structural and symmetry-related factors.[3] We are now extending this approach to surfaces by introducing thiol groups on the foldamers for immobilization on gold substrates and adapting the optical setup for interface-sensitive measurements.

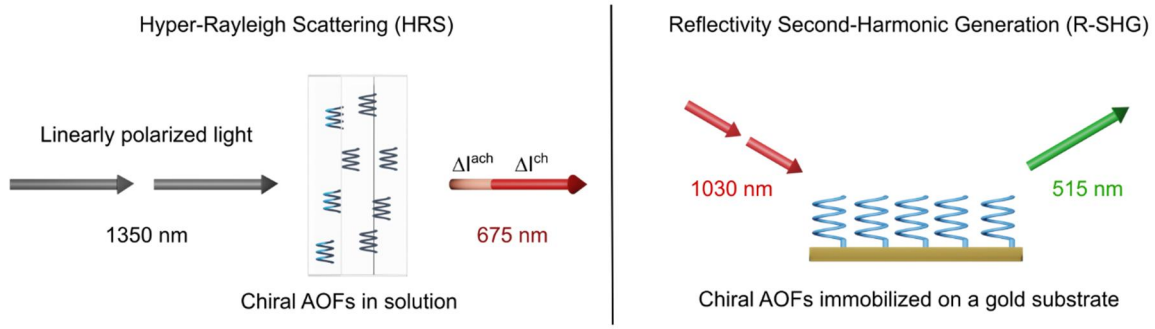

Figure 1. Detection of chirality in AOFs using nonlinear optics in solution (left) and on surfaces (right).

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PO-10

Chiral EDDS-Metal Complexes as Tunable Systems for Resonance and Non-Resonance ROA

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EDDS (ethylenediamine-N,N′-disuccinic acid) is a biodegradable, water-soluble chelating agent that forms stable, chiral octahedral complexes with various metals. Some of them, in particular with metals supplying *d–d* electronic transitions, exhibit strong resonance Raman optical activity (**Figure**). [1]

To systematically explore the resonance behavior, several complexes were prepared, typically by mixing EDDS with metal chlorides. pH titrations were performed to determine optimal stability conditions. NaCl mimicking the ionic strength of the sample proved useful as Raman baseline, rather than pure water. [2] For reliable resonance spectra, possible heating of the absorbing sample had to be considered, and the ECD-Raman signal [3] subtracted.

It appeared that EDDS-metal complexes form a modular system helping us to understand the interplay of coordination geometry, oxidation state and electronic structure with the vibrational and electronic spectra.

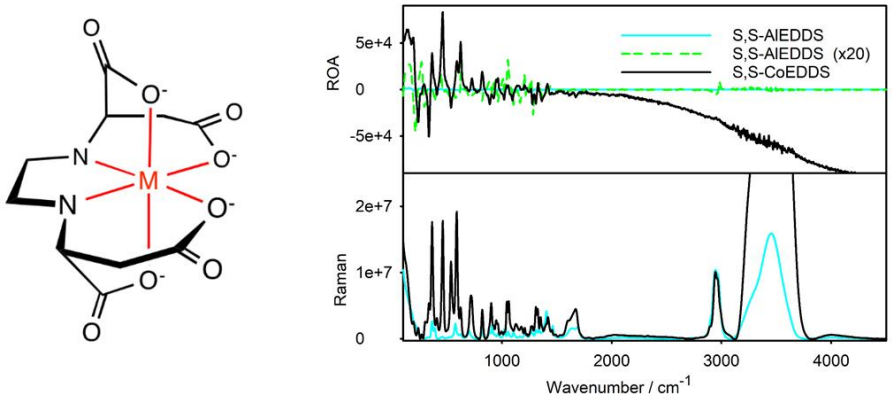

Figure. Structure of the metal EDDS complexes, and example of resonance ROA and Raman enhancement for Co^{3+} vs. Al^{3+}. [1]

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PO-11

Flow Reactor Prototype For The Measurement Of Enantiomeric Excess

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The increasing demands of the pharmaceutical industry regarding quality control of chiral compounds create the need to develop methods that enable fast and precise monitoring of chemical reactions and assessment of enantiomeric purity without the need for physical separation of enantiomers. This is particularly important because enantiomers of the same molecule can exhibit different biological, pharmacokinetic or toxicological properties. Despite this awareness, racemic mixtures are still widely used, mainly due to the high cost of obtaining enantiomerically pure compounds.[1,2] In this context, vibrational optical activity (VOA) methods offer a promising alternative to traditional techniques for enantiomer separation. Their application in real-time monitoring of stereoselective processes enhances control over synthesis and improves the efficiency of analyses.[3,4]

In response to these challenges, we have developed a flow reactor opening the possibility for real-time analysis of the optical purity of samples using Raman Optical Activity (ROA) and Electronic Circular Dichroism (ECD).[5] This approach not only shortens analysis time and reduces material consumption but also provides greater control over the course of stereoselective reactions. This is especially important in the synthesis and characterization of chiral active pharmaceutical ingredients (APIs), including those carried out in aqueous solutions.

The optimized reactor was used to determine the enantiomeric excess of several monoterpenes, such as limonene and pinene. The obtained values were consistent with reference results, obtained using standard cells, confirming the effectiveness of the proposed solution. Additionally, partial least squares (PLS) analysis demonstrated very good agreement between the calibration models and the actual measurements, further confirming the high precision and analytical potential of the developed system.

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PO-12

Investigation of The Chiral Properties of Nano Helical Structures by Tuning Their Morphological Characteristics

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Chirality is a fascinating material property with broad applications in fields such as optoelectronics, sensing, and catalysis. Self-assembled chiral structures arise from the spontaneous organization of molecules via non-covalent interactions like hydrogen bonding and π–π stacking. In our group, we have been developing self-assembling systems of cationic surfactant, 16-2-16 gemini tartrate having C16 hydrocarbon chains, to form mesoscopic chiral helical structures[1] with around 60 nm pitches. These organic helices can then be transformed into inorganic silica helices via sol-gel transcription[2]. These silica helices serve as platforms to impart chirality to a wide variety of molecules and nanoparticles[3,4].
The objective of this work is to tune the chiral characteristics of these mesoscopic chiral structures simply by modifying their morphological features. Specifically, we aim to vary the length of the hydrocarbon chains, thereby adjusting the helical pitch of the resulting structures, and to investigate how these changes affect their chiral properties without introducing any additional chiral additives. These organic helices are then transcribed into silica helices, and we systematically study how their pitch affects the chiroptical response induced in grafted molecules and nanoparticles.

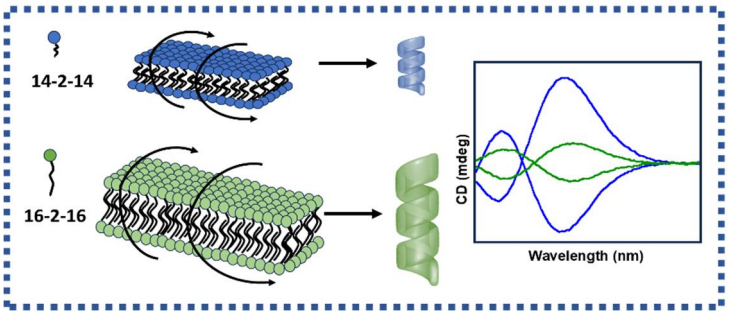

Figure 1. The schematic representation of the morphological changes and the corresponding changes of the chiral properties.

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PO-13

Hierarchical Chirality Transfert in Chiral AIE Material by Silica Nanohelix

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AIE materials (aggregation-induced emission) have received growing attention for their outstanding emissive properties, making them particularly promising for optoelectronic applications. The self-assembly process, driven by intermolecular interactions, enables the formation of ordered supramolecular structures capable of promoting effective light–matter interaction. When these molecules possess chirality, their hierarchical organization allows the transfer of chirality from individual molecular units to mesoscopic and macroscopic structures. This results in pronounced chiroptical properties, especially in the discrimination of circularly polarized light [1].

Chirality transfer can occur not only between the same object but also between different species. A significant example is the induction of chirality by chiral structures or templates onto originally achiral molecules, thereby modifying their properties. In this context, silica nanohelices have proven to be promising chiral inducers for organic [2], and inorganic chromophores [3] as well as nanomaterials [4], showing significant results.

This work aims to take a step further by investigating chirality transfer between two chiral species across two distinct hierarchical levels. The goal is to guide the aggregation of AIE materials at the molecular scale through their interaction with silica helices, characterized by nanometric dimensions, thereby enhancing the overall CD and CPL responses.

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PO-14

Chiroptical Investigation of Aggregates Formed by Phenylalanine-based Peptides

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In recent years peptide nanostructures have been gaining attention due to their biocompatibility and vast potential use in nanotechnology. Studies show that peptides comprising as few as one to seven residues are able to self-assembly into ordered nanostructures with diverse architectures, including nanotubes, fibrils and nanovesicles. [1]

Among others, aggregation of short peptides consisting of phenylalanine (Phe, F) building block is of particular interest. Most studies have focused on diphenylalanine (FF) - a key recognition motif of the β-amyloid that plays an important role in formation of amyloid fibrils in Alzheimer's disease. It was shown that FF forms well-ordered nanotubes in aqueous solution. [2] Research onto self-assembly of longer F-peptides (especially tri- and tetra-peptides) were also conducted, revealing that they can form various nanoassemblies (e.g. nanorods, nanospheres, nanoplates). [3] Extremely interesting is also Phe by itself, that can self-organize into fibrils with amyloid-like characteristics. [4]

Chiroptical spectroscopies, especially Vibrational Circular Dichroism (VCD), have emerged as valuable tools for studying amyloid fibrils [5] as well as other chiral supramolecular structures. However, these methods were scarcely used in studies of Phe aggregates. In our work we characterized nanoassemblies formed by short peptides of L- or D-Phe using VCD in tandem with electronic circular dichroism and cryo-electron microscopy. Acquired spectra show an intense chiroptical signal that suggests formation of highly ordered structures. Obtained results can give new insight into the process of self-assembly of peptide-based nanostructures.

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PO-15

Use of Magnetic Circular Dichroism to characterize Biomolecules in Solid-state and Supramolecular Aggregation Conditions

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Magnetic Circular Dichroism is a spectroscopic technique helping uncover detailed electronic and structural information that are difficult to obtain with other spectroscopic techniques; it has been widely used in the past and recently it found novel interest.

Despite it has often been used for studying non chiral molecules, it is not unusual to apply it to chiral material analysis as well.

In this study, we explore the application of MCD to two distinct classes of Porphyrin: biological heme containing Myoglobin and synthetic chiral Zinc Porphyrin supramolecular polymer.

J-1500 versatile layout allow to easily and successfully record MCD in both liquid and solid samples: a wide spectroscopic analysis has been performed on heme protein, namely Myoglobin from Equine skeletal muscle. MCD spectra of myoglobin has been recorded in a wide spectral range in liquid samples as well as drop-casted films, highlighting technique's applicability beyond solution phase measurements[1].

In the second part, we report a modified MCD setup optimized for temperature variable measurements on chiral Zn porphyrin supramolecular polymer[2]. MCD signal collected over a range of temperature reveal distinct signals that correlated with monomeric and aggregated states of porphyrin supramolecular polymer.

These temperature-resolved MCD approach can enable detailed transitions of supramolecular structures. Overall, our work highlights the versality of MCD spectroscopy in studying both biological hemoproteins and synthetic supramolecular systems.

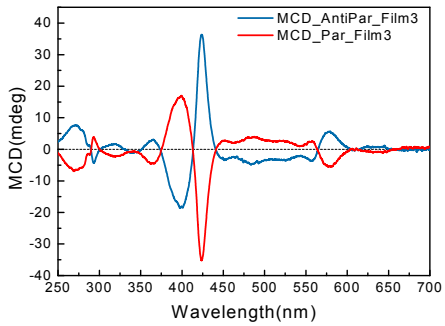

Figure 1: MCD spectra of Myoglobin film in the Magnetic field parallel and antiparallel to the direction of light.

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PO-16

Enhancing Chiroptical Properties through Hierarchical Architectures of Mesoscopic Chiral Nanostructures

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Chirality is a fundamental property of objects observed across scales from biomolecules to metamaterials. It plays a crucial role in determining the physical and optical behavior of materials[1]. Mesoscopic silica helices can be used to helically organize quantum size luminophores, such as quantum dots[2] or carbon dots (C-dots)[3] which can exhibit induced CD (circular dichroism) and CPL (circularly polarized luminescence) signals. Therefore, chirality can be hierarchically enhanced stepwise from small luminescent units to larger chiral structures[4,5]. In order to build this type of hierarchical structures, it is crucial to control their alignment.

In this study, we synthesized mesoscopic silica helices made from surfactant self-assembly, which were thereafter templated to silica structures through sol-gel transcription (Scheme 1). These silica helices were then mixed with EVA polymer solution. The mixture was casted into films, subsequently aligned using shear stress during the stretching of polymer films. TEM observations revealed clear alignment of silica helices within the polymer matrix (Figure 1). Fine control of both the film thickness and the ratio between helices and polymer were crucial to obtain this film. After aligning helices, these aligned silica helices can be further organized, for example by stacking them with a given angle between them, to obtain cholesteric structure.

Scheme 1. Schematic illastration of inorganic transcription.

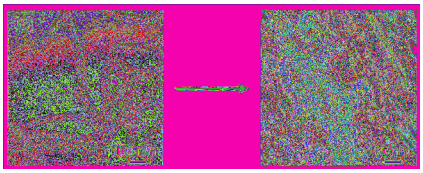

Figure 1. TEM observation of silca helices (a) without and (b) with stretched in polymer

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PO-17

Interpreting peptide ECD signatures for material science applications - an acquired or challenging task?

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Peptides are encountered on numerous occasions as valuable materials in various application areas, ranging from medicinal chemistry to water treatment. To explain or *a priori* predict the effectiveness of peptide systems in their application, a thorough insight into their three-dimensional structural behavior is required. Through electronic circular dichroism (ECD) spectroscopy such an analysis can be performed.

As our lab specializes in chiroptical spectroscopy for the conformational characterization of biomolecules, non-expert research groups frequently request an analysis of their compounds through our platform. As such, we have recently been involved in the characterization of phenylglycine-phenylalanine derived peptide hydrogels [1] and peptides that collect microalgea present in water systems [2]. In the former study, we analyzed hdyrogels with varying amino acid contents, exhibiting strongly deviating ECD patterns. A direct extraction of the underlying peptide structure, however, proofed to be challenging. Then, for the second study, the structural assignment turned out unexpectedly tricky, as different conclusions could be drawn depending on the analysis strategy. After a literature dive and the addition of Raman and Raman optical activity (ROA) spectral analyses, there are indications of the presence of 3_{10}-helical and PPII structure.

These two investigations are illustrations of how deploying ECD spectroscopy for peptide characterization is powerful, but remain delicate. This is partially attributable to the heterogenity of ECD patterns manifested by peptides. We witnessed that protein rules do not consequently apply either, which is a common way of analyzing peptide spectra (especially among non-experts). Indeed, there does not seem to be a collection of reference work yet that allows unequivocal assignments. This makes us conclude that, in the context of both recent and future ECD inquiries, there is still room for systematic ECD-peptide work aimed at increasing the reliability of the structural assignment of peptides.

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PO-18

Stepwise Interaction Mechanism between β-Lactoglobulin and SDS Micelles Revealed by Time-Resolved Vacuum-Ultraviolet Circular Dichroism

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Water-soluble proteins often undergo structural transitions upon interaction with membranes, expressing biological functions such as drug transport and amyloid fibril formation [1,2]. Surfactants have been widely used as membrane mimics and adapted as a practical model for studying these interactions. In this study, we investigated the interaction between β-lactoglobulin (bLG), a model membrane-binding protein, and sodium dodecyl sulfate (SDS), an anionic surfactant, using time-resolved vacuum-ultraviolet circular dichroism (TR-VUVCD) to elucidate the structural transition mechanism from the native (N-) to micelle-bound (M-) state [3,4].

TR-VUVCD spectra of bLG were recorded in the 0.2–120 s range with 0.2 s resolution, revealing a transition from β-strand–rich to α-helix–rich structures (corresponding to N- and M-states, respectively) (Figure.A). Kinetic analysis identified two intermediates (I_1 and I_2), showing a stepwise increase in helical content (Figure.B). Molecular dynamics (MD) simulations based on these data further clarified the interaction mechanism, where initial electrostatic attraction facilitates approach to the micelle surface, followed by hydrophobic stabilization. These findings enabled us to propose a model for SDS micelle wrapping by bLG.

Our study demonstrates that combining TR-VUVCD and MD simulation is a powerful approach for probing protein–surfactant interactions and membrane-associated protein dynamics.

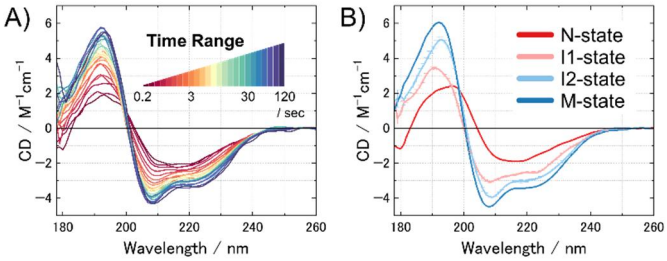

Figure. (A) TR-VUVCD spectra of bLG during the interaction with SDS micelles, measured from 0.2 to 120 s. (B) Representative spectra of four states (N-, I_1-, I_2-, and M-states) obtained through the kinetic analysis of TR-VUVCD data.

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PO-19

Arbitrary Angle Raman Optical Activity Detection

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In Raman optical activity (ROA), the relevant experimental observable is the circular intensity differential (CID) between left- and right-circularly polarized scattered light. The general expression for CID depends on the scattering angle [1], with standard formulations typically tabulated for scattering geometries of 0 °, 90 ° and 180 ° [2,3]. To date, all ROA spectrometers have used one of these [4,5,6] or a magic scattering angle configuration [7]. Here we present a novel instrument concept for ROA detection at arbitrary scattering angles. This approach can help to better isolate the different contributions of the optical activity tensor to the spectra across multiple scattering geometries, thus supporting a more comprehensive study of chiral molecules.

The design builds on the ROA detection scheme with high-frequency polarization modulation developed by Lightner et al. [6]. A linearly polarized 532 nm laser beam from a compact diode-pumped continuous-wave laser passes through a polarization scrambler and is focused onto a cylindrical sample cell. The scattered light is collimated and passes through a photoelastic modulator (PEM) followed by a polarizer, which converts the left- and right-circular polarization states into an intensity-modulated signal. A detector based on the Zurich Imaging Polarimeter (ZIMPOL) design, is synchronized with the PEM, and detects the CID by demodulating this time-varying intensity signal.

To enable detection at variable angles, either the excitation or the scattered light collection path must rotate freely around the sample. Given the compact form factor of the laser, we propose to mount the excitation optics on a rotating arm while the detection path remains stationary. The rotation axis of the arm is in the centre of the sample, which is placed in a cylindrical vial to make sure that both the incident and scattered beams are always perpendicular to the walls of the vial. This should help to ensure uniform scattering conditions at all angles and allow for quantitative comparison.

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PO-20

Identification Of Large Amplitude Motions In Flexible Systems

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Vibrational analysis plays a crucial role in the investigation of molecular systems and to interpret increasingly refined experimental spectra successfully, accurate simulation are necessary. To this end, the combination of density functional theory (DFT) and second-order vibrational perturbation theory (VPT2) can provide the necessary accuracy, provided that the computational protocol is carefully established. Including an anharmonic treatment is essential to compare experiments while avoiding any empirical scaling factors directly and is mandatory in particular regions of the spectrum. However, it is often still considered a specialized task. The reason can be sought in two main challenges encountered in VTP2 calculations. First, resonances must be carefully identified and treated. Second, large amplitude motions (LAMs), frequently found in flexible molecules, are generally poorly described at the VPT2 level[1,2]. It is therefore necessary to properly identify vibrations associated with these motions. Defining LAMs is not a straightforward task, and comprehensive protocols are currently lacking. Indeed, LAMs identification is often based on either chemical intuition or empirical parameters, which can be problematic when dealing with larger or more complex systems.

In this contribution, we will present several metrics developed to identify LAMs, to build a black-box, automated protocol to identify them with minimal or no input from the users. The devised protocol combines topological analysis, such as the hindered rotation analysis[3], and numerical analysis based on anharmonic constants and VPT2 core quantities. The impact of these criteria on the definition of the LAMs will be illustrated through the simulation of IR and VCD spectra of narciclasine and a ruthenium complex. Paths toward a full protocol to compute VPT2 spectra in the presence of LAMs will also be sketched.

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PO-21

Resonance Raman Optical Activity Uncovers Chiroptical Features of Cytochrome c

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Cytochrome c (CytC) is a compact heme protein with three α-helices and two axial ligands, histidine (His18) and methionine (Met80), that coordinate the central iron ion. It primarily facilitates electron transfer between the cytochrome bc1 complex and cytochrome c oxidase in mitochondria, but also participates in apoptosis through cardiolipin oxidation and acts as a reactive oxygen species (ROS) scavenger.[1] While its structure has been well studied using techniques such as resonance Raman spectroscopy, its chiroptical properties and the mechanisms behind resonance enhancement remain unclear.

To explore these aspects, we applied Resonance Raman Optical Activity (ROA) in combination with Electronic Circular Dichroism (ECD). These chiroptical techniques measure the differences in the interaction of circularly polarized light with chiral molecules, offering enhanced structural sensitivity compared to conventional methods. When the excitation wavelength matches electronic transition energies, resonance conditions amplify the ROA signal, known as Resonance ROA (RROA).[2] However, RROA spectra may be distorted by the ECD-Raman effect, particularly in colored, chiral samples. Advances in data correction now allow for accurate extraction of true RROA spectra.[3,4]

Here, we present the first true RROA spectra of both reduced and oxidized CytC. These results deepen our understanding of its chiroptical structure, explaining the mechanism underlying the induced heme chirality, and demonstrate how the iron oxidation state affects resonance enhancement in ROA.

This work is supported by the National Science Centre in Poland (Grant No. 2019/35/B/ST4/04161 to GZ) and the Polish National Agency for Academic Exchange (to AD).

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PO-22

Mueller Matrix Mapping and Electronic Circular Dichroism of 1,1'-Binaphthalene Thin Films

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1,1'-Binaphthalene is an axially chiral molecule whose thin film crystallization into a chiral phase from racemic powder can be induced under controlled conditions introduced in this study. This study also explores the deracemization of binaphthalene through the influence of a chiral additive, 1,1'Bi-2-naphthol. Spatially resolved Mueller Matrix Polarimetry (MMP), an effective technique for probing chirality in thin films, was employed to map localized circular dichroism in binaphthalene films. Crystallization behavior was investigated using both fully racemized and non-racemized solutions to evaluate the influence of molecular configuration on chiroptical properties. In the solid state, binaphthalene adopts two conformers: cis for the racemate and trans for the enantiomers, with respective dihedral angles of 68° and 103°.[1,2] The crystallization kinetics are strongly surface-dependent. For racemized solutions, selective adsorption of the trans conformer at the substrate interface promotes full crystallization into the chiral phase. In contrast, films from non-racemized solutions often crystallize as the racemate, initiated by cis conformer nucleation at the air–liquid interface. Furthermore, enantioselective crystallization can be guided by the use of tailored chiral additives, achieving spatially resolved chiral purity. These results are confirmed through solid-state electronic circular dichroism and synchrotron-based Mueller Matrix Polarimetry mapping.

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PO-23

Substitution Effect in Dynamic Structure Conversion of Stimuli–Responsive Helical Co(II) Complexes

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Stimuli–responsive molecules, that change their structure and optical properties upon external stimuli such as heat, light and solvent, are expected to be applied to sensing materials, security device, and so on. We previously reported reversible helicity inversion of extended left–handed Co(II) complex (ext–Λ H_2**L1**–Co(II) complex) upon NO_3^- stimulus and elastic motion between extended form (ext–Λ H_2**L1**–Co(II) complex) and contracted form (cont–Λ **L1**–Co(II) complex) upon base/acid stimuli (**Figure 1**). Moreover, the contracted structure was frozen by oxidation of Λ **L1**–Co(II) complex [1]. Herein, we discuss structure conversion of helical Co(II) complexes accomodated with chiral ligands H_2**L2**–H_2**L8**, which have substitution group at 3–position of 2–methoxyphenylamide terminals.

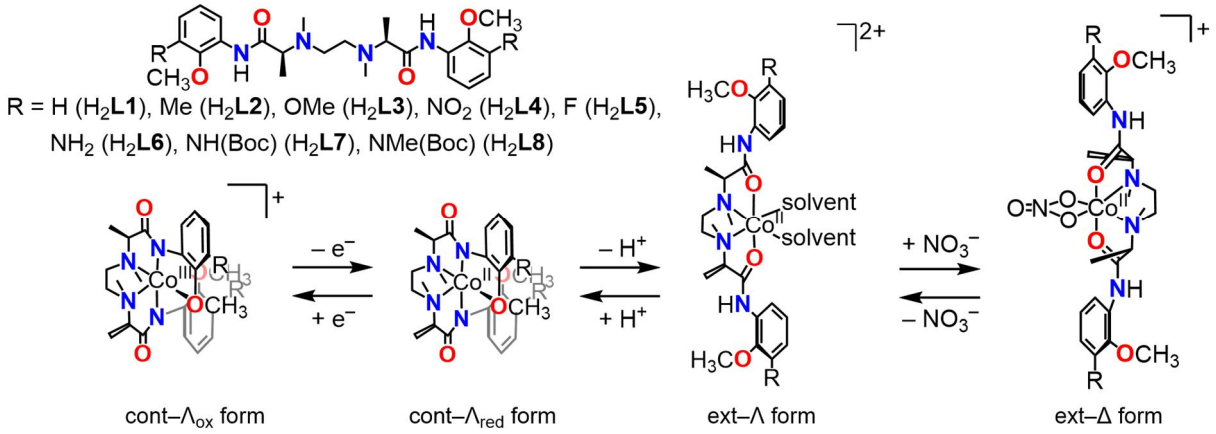

Figure 1 Structure conversion of Co(II) complexes in response to NO_3^- and base/acid, and structure freezing upon oxidation of Co(II) center.

We synthesized chiral ligands H_2**L2**–H_2**L8** in 6–9 steps from *N*–*tert*–butoxycarbonyl–(*S*)–alanine for H_2**L2**–H_2**L5** and *N*–benzyloxycarbonyl–(*S*)–alanine for H_2**L6**–H_2**L8**. The ext–Λ H_2**L**–Co(II) complexes were prepared by mixing corresonding ligand and an equimolar $Co(ClO_4)_2 \cdot 6H_2O$ in CH_3CN, which exhibited helicity inversion and structure contraction in response to NO_3^- and base, respectively. We report on the effect of a substitution group at the 3–position of 2–methoxyphenylamide terminals.

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PO-24

Stereoselective Access to Glycofused Isochromans via Oxa-Pictet–Spengler Cyclization Reaction: Toward Multifunctional Agents Targeting SGLT-2 and Tumor Pathways

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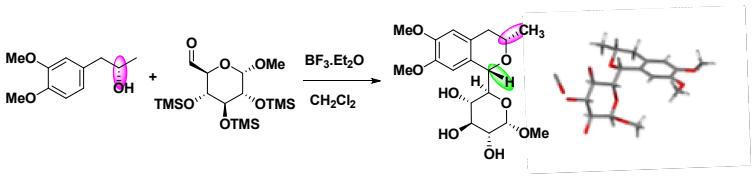
Diabetes and cancer continue to pose major health challenges worldwide, underscoring the urgent need for innovative therapeutic approaches. Recent studies highlight the dual potential of C-aryl glycoside-based SGLT2 inhibitors and their structurally related scaffolds, in simultaneously addressing glucose regulation and tumor progression. Bridging diabetes and cancer therapeutics, we engineered glycofused isochromans, combining the versatile bioactivity of the isochroman with the pharmacological functionality of glycoside moieties, establishing a versatile platform for multifunctional therapeutic development [1,2]. This study reports the stereoselective synthesis of novel glycofused isochromans hybrids via oxa-Pictet-Spengler cyclization reaction of chiral alcohols with sugar aldehyde derivatives (**Scheme 1**) [3]. Reaction conditions, including protecting groups manipulation, the configuration of the starting materials, and importantly, the applied acid amount, were optimized to enable control over yield and stereochemistry, with structures elucidated by NMR, X-ray, and VCD analyses. Preliminary data demonstrate moderate glycogen phosphorylase inhibition and considerable antitumor activity in our synthesized adducts, with SGLT-2 inhibition under evaluation, offering a strategic approach to multifunctional drug development.



Scheme 1. Synthesis of an isochroman-sugar hybrid with silyl protecting groups

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PO-25

Transferring Chirality From Molecules To Polymer-Based Thin Films

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Poly(9,9-dioctylfluorene-alt-benzothiadiazole), commonly known as F8BT, is an emissive polymer extensively used in the OPV field.[1] Chiral dopants have been employed to induce dissymmetry in the ground and excited states of F8BT.[2] Cyclobisbiphenylenecarbonyl (CBBC) compounds exhibit optical activity and can be functionalised to produce a donor–acceptor-type emitters.[3]

Here we show that the figure-eight molecules (CBBC) induce strong chirality in F8BT thin films. We have observed how the meta- and para-substituted derivatives interact differently with F8BT resulting in a large discrepancy in the resulting CD signal intensity. These chiral thin films have also been shown to emit chiral light in the form of circularly polarised luminescence (CPL) which is of great interest for optoelectronic technologies.

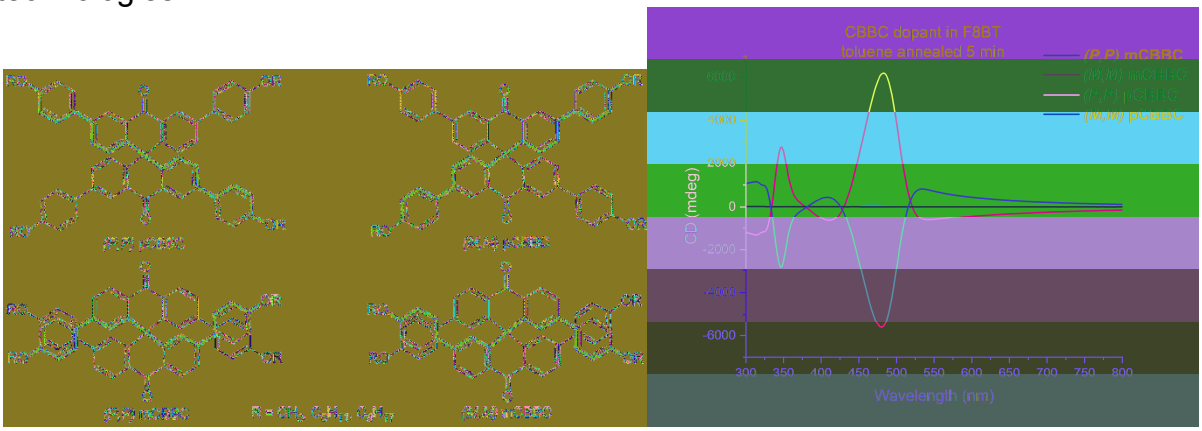

Figure 1. Strcutures of CBBC compounds (left). CD spectrum of F8BT based thin films doped with 10% CBBC compounds (right).

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PO-26

G4SpectraDB: A Comprehensive Database for Spectroscopic and Topological Data of G-Quadruplex Structures

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G-quadruplexes (G4s) are non-canonical nucleic acid secondary structures formed by guanine-rich sequences capable of stacking planar G-tetrads stabilized by Hoogsteen hydrogen bonding and monovalent cations. These structures are implicated in key biological processes such as gene regulation, genome stability, and telomere maintenance, and are increasingly recognized as promising targets in therapeutic and diagnostic applications.

G4s exhibit a remarkable topological diversity, usually grouped as parallel, antiparallel, and hybrid forms, and spectroscopic comparisons have been limited to these three divisions. da Silva and colleagues have developed a quadruplex topology system that includes 26 possible groups [1]. These topologies also can be effectively characterized by spectroscopic techniques—especially circular dichroism (CD) spectroscopy.

Additionally, fluorescent small molecules are widely used for *in vitro* and *in vivo* detection of G4s, often described as G4-specific; however, no systematic comparison has been conducted across all known G4 topologies. In this project, we developed G4SpectraDB, a curated database integrating synchrotron radiation and conventional CD spectra, absorbance and fluorescence data, thermal denaturation profil along with detailed topological annotations. This resource enables the exploration of topology-resolved spectroscopic fingerprints and supports the development of novel structure-specific G4 detection strategies.

This study was supported by the National Research, Development and Innovation Office of Hungary (grants PD135510, K138937 and 2019-2.1.11-TÉT-2020-00101), Eötvös Loránd University Excellence Fund (EKA 2022/045-P278-1). SRCD measurements were supported by SOLEIL (Proposals 20230777, 20231948, 20240797, and 20241998).

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PO-27

Development of Circularly Polarized Lumiescence Spectrometer

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Circularly polarized luminescence (CPL) spectroscopy can be used to analyze the molecular structure of excited states of chiral molecules, and is therefore used in the research and development of CPL materials [1,2]. In recent years, CPL materials are expected to be applied to three-dimensional displays as well as next-generation optical information technologies such as quantum computers and cryptographic communications.

Biomolecules usually have small luminescence asymmetry factor (glum), so that CPL spectrometers are required to have high sensitivity, high accuracy, and minimal artifacts caused by linear anisotropy. To achieve high sensitivity, JASCO CPL-300 spectrometer is equipped with a double prism monochromator that minimizes stray light without linear polarization effects caused by diffraction gratings. In addition, the emission optics with a collection angle of 0° eliminates artifacts caused by fluorescence anisotropy.

There are increasing interests in the CPL materials that emit light in the near infrared wavelength region and under the external perturbations such as magnetic field. In this study, we will demonstrate accessories for the CPL-300 and their measurement results.

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PO-28

Stereoselective Synthesis and Structural Elucidation of Glucose-Isochroman Hybrids

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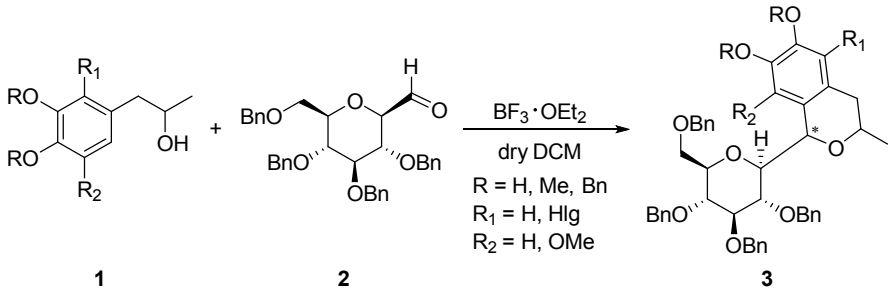
Gliflozins are β-*C*-aryl-glucosides bearing aryl or heteroaryl aglycon moiety. Some members of this family have been approved as hypoglycemic agents for the treatment of type 2 diabetes mellitus. The aglycon part of these molecules is usually made up of two aryl/heteroaryl units connected to each other by a methylene linker [1].

Our research aims to synthesize novel gliflozin analogue C-glucosides starting from β-*C*-glucopyranosyl aldehyde. To build the isochroman part of the compounds oxa-Pictet-Spengler cyclization was carried out using versatile substituted enantiopure phenethyl alcohol derivatives (Scheme 1).



Scheme 1. Synthesis of glucose-isochroman hybrids by oxa-Pictet-Spengler reaction

The effect of the starting alcohol was investigated on the yield and stereochemical outcome of the cyclization. The reactions showed high selectivity in most cases, regardless of the configuration of the alcohol. The configuration of the newly formed chiral centers was determined by NMR and CD techniques. Having a halogen in position R1 gives the opportunity to transform these compounds in Pd-catalyzed cross-coupling reactions to present further aromatic units on the molecules.

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PO-29

The Fine-tuning Effect of Heterochiral β³-sequences on Structural Motif Associations

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Peptide assemblies composed of non-natural β-amino acids have gained increasing attention in different areas, due to their programmable and diverse secondary structures, high metabolic stability, and strong self-association propensity. Inspired by the alternating side-chain chirality pattern of natural peptides we have designed short, acyclic β³-sequences [1,2] with lamellar morphological structures. These sequences with positively charged side chains are capable of incising the cell envelope of Gram-negative bacteria and thus showing antibacterial activity. The formation of supramolecular assemblies triggered by lipopolysaccharides or adenosine phosphates could be exploited in diverse areas, however identifying oligomerisation stages, and more importantly, controlling the spontaneous process at different levels is still lacking. Starting from the basic scaffold But-$L^RL^RE^SL^RK^SL^R$-NH_2, we have performed systematic, small variations in the sequences, *i.e.* single point mutation or N-terminal modification in order to understand how these will influence the resulting assemblies and to allow the control of these morphologies. Combined cryo-EM and negative staining TEM with molecular dynamics simulation and spectroscopic analysis enable the identification and differentiation of morphological stages throughout the entire multi-step process (Figure 1). Depending on the position of sequence modifications, the self-assembled structures formed either small oligomers, individual protofibrils, flat lamellae, bundles or macroscopic clusters. These results outline how the self-assembly process can be qualitatively fine-tuned by sequence modifications, which contribute to understanding the general peptide assembly processes for fibrillar morphologies.

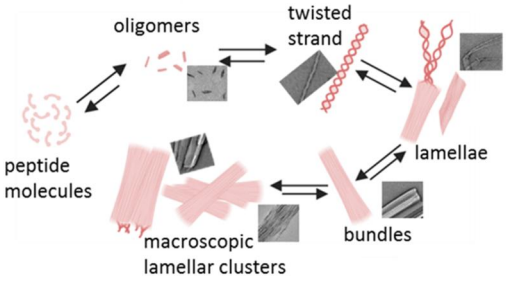

Figure 1. Schematic representation of assemblies formation process.

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PO-30

Raman Optical Activity as a Structural Probe of Polynucleotides in Solution

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Understanding the solution-phase structures of nucleic acids is essential for elucidating their function and reactivity. Raman optical activity (ROA) spectroscopy, which measures differential scattering of right and left circularly polarized light, offers high sensitivity to molecular conformation and stereochemistry. However, its application to nucleic acids has been limited due to the structural complexity and challenges associated with spectral interpretation [1,2].

In this study, we combine experimental Raman and ROA spectroscopy with advanced computational modeling to investigate structure-spectra relationships in the polynucleotides. Spectral simulations are performed using molecular dynamics (MD) simulations and density functional theory (DFT) calculations, with the aid of the fragment-based Cartesian Coordinate Tensor Transfer (CCT) approach [3], which enables efficient treatment of large nucleic acid systems. Our results demonstrate that the ROA spectra reliably reflect conformational features and temperature-induced structural changes. Furthermore, experimental spectral intensities can serve as effective benchmarks for evaluating and refining MD force fields.

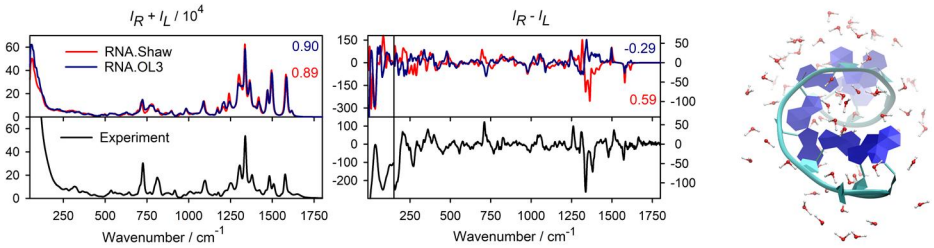

Figure 1. Raman and ROA spectra of PolyA calculated with the RNA.OL3 and RNA.Shaw force fields, and the experiment at 20 °C.

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PO-31

Tracking of Conformational Dynamics of Vitamin B12 by Chiroptical Spectroscopy

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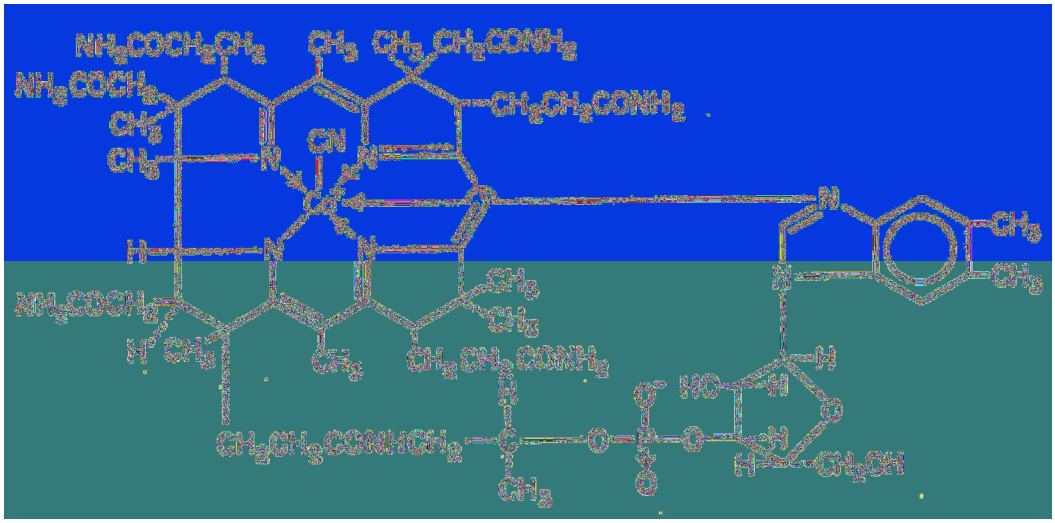
Vitamin B12, also known as cobalamin, is an essential water-soluble vitamin crucial for DNA synthesis, formation of red blood cells, or neurological function. Its structure is characterized by a cobalt(I) ion at the center of a corrin ring, which is similar to a porphyrin, and a side chain that features a nitrogenous base (Scheme 1). The ability of the base to coordinate with the cobalt ion (designated as "base on") is crucial for the biological activity of vitamin B12, while an unbound state ("base off") can also exist depending on various factors, such as pH.

In this study, we employed Resonance Raman Optical Activity (RROA) technique to investigate the dynamics of the base on and base off states of vitamin B12. Our findings demonstrate that alterations in pH lead to switching between the base on and base off states, and these changes can be tracked using the RROA spectroscopy. Moreover, significant changes in the Degree of Circularity (DOC) were observed for various conformational states of B12, which can be linked to different polarization of light when interacting with two conformations of B12.

These results suggest a straightforward and effective methodology for tracking the base on vs. base off transition of vitamin B12, facilitating deeper insights into its biochemical behavior and structural dynamics. Furthermore, our experimental observations are supported by Density Functional Theory (DFT) calculations based on the sum-of-states methodology and Time-Dependent DFT (TDDFT).



Scheme 1. Chemical formula of vitamin B12.

PO-32

VCD Analysis of Isochroman Derivatives with Central and Axial Chirality Elements in the Solid State

Roland Albert Barta,[1] András Vaskó,[1] Zoltán Czenke,[1] Tibor Kurtán,[1] Attila Mándi[1]

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ECD measurements in the solid state is considered routine [1], often relying on a single molecular geometry, which may be derived from single crystal X-ray analysis. Unlike the standardized workflows of ECD, VCD protocols still often lack consistency, especially when dealing with complex crystalline environments.

The limited number of high-quality solid-state VCD studies in the literature reflects this difficulty [2]. Even if solid-state VCD typically demands only a small amount of sample, its experimental and computational reproducibility remains a significant challenge [3-5].

Unlike ECD, VCD often requires consideration of intermolecular interactions within the crystal lattice, since neighboring molecules can significantly affect vibrational coupling and signal intensity. An accurate approach needs to consider dimers, tetramers, or larger aggregates to better reflect these interactions [6].

Additionally, selecting the appropriate DFT functional is not trivial; different functionals can yield different results, and systematic testing is often required to identify the best match with experimental data [4].

Computational challenges are demonstrated through examples of calculations for optically active *ortho*-trisubstituted 5,5′-linked heterodimeric *bis*-isochromans containing both central and axial chirality elements [7]. Single crystal X-ray diffraction structures were used for calculations at different levels of theory as well as for the generation of dimeric and tetrameric structures.

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PO-33

Conformational and Chiroptical Analysis of Biaryl Derivatives Containing Axial and Central Chirality Elements

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Knowledge of stereochemistry is crucial in the design of potentially bioactive drug derivatives, since the bioactivity often depends on the relative and absolute configuration of the stereogenic elements. Many naturally occurring biaryl compounds with beneficial bioactivity possess both axial and central chirality the parallel determination of which is not trivial. [1-3] In addition to single crystal X-ray diffraction and NMR spectroscopy, the combination of chiroptical techniques can also be employed for stereochemical structural elucidation. [4]

I have studied the parallel assignment of central and axial chirality elements of synthetic *bis*-isochromans [5-6], using experimental and computational ECD and VCD to distinguish stereoisomers. Characteristic VCD transitions were identified to report both the axial and central chirality, while ECD spectra surprisingly could not be used to determine the axial chirality. In addition to conventional solution conformational and chiroptical approaches, I evaluated the performance of three conformational search programs and several force-field models on the studied stereoisomers.

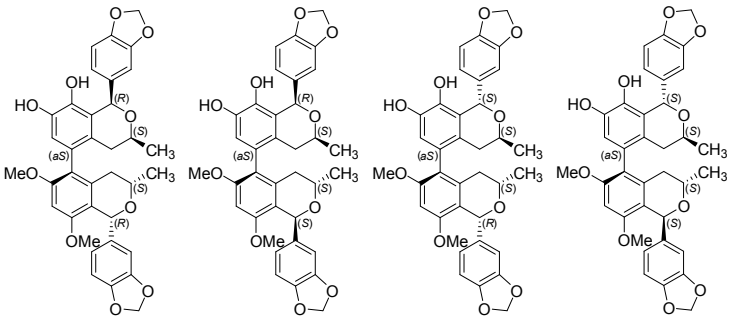

Figure 1. Structure of the four stereoisomers of the investigated compound

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PO-34

STEREOSELECTIVE SYNTHESIS AND STEREOCHEMICAL ANALYSIS OF AXIALLY CHIRAL BIARYL DERIVATIVES

Krisztián Cserepes[1], Attila Mándi[1], Tibor Kurtán[1]

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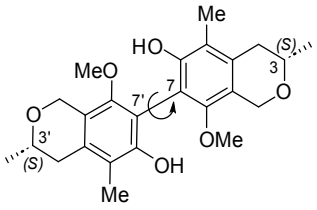
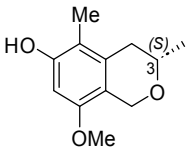
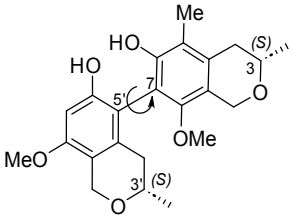
Naturally occurring axially chiral *bis*-isochromans have been only described in two publications [1], and their total synthesis has not been accomplished yet. We have synthesized analogous heterodimeric *bis*-isochromans, and we identified antibacterial activity against methicillin-resistant *Staphylococcus aureus* for some of them [2].



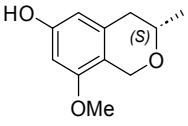
penicisteckin C (a*R*,3*S*,3'*S*) **1**
penicisteckin D (a*S*,3*S*,3'*S*) **2**



3 (3*S*)



penicisteckin A (a*R*,3*S*,3'*S*) **4**
penicisteckin B (a*S*,3*S*,3'*S*) **5**



6 (3*S*)

We have achieved the stereoselective synthesis of homodimeric natural penicisteckins C/D (**1**,**2**) in ten steps, with the stereogenic tetrasubstituted biaryl axis established by a radical dimerization using *di*-*tert*-butyl peroxide. In the *oxa*-Pictet–Spengler cyclization reactions of optically active 1-arylpropan-2-ols, we produced the monomeric units (**3**,**6**) of natural penicistectin A–D (**1**,**2**,**4**,**5**). VCD and ECD analysis of our sytnethic penicisteckins and their ischroman monomers were recorded and computed to confirm the absolute configurations of the central and axial chirality elements. We also synthesized methylene-linked dimers of isochromans, analogues of natural *bis*-isochromans, by treating isochromans with methoxymethyl-chloride. Their VCD and ECD spectra were recorded and computed to check the effect of the two isochroman units on the chiroptical properties.

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PO-35

The Use of Circular Dichroism in Bioinorganic Chemistry Research

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The interaction of various transition metal ions with oligopeptides has been studied in the Bioinorganic Chemistry Research Group at the University of Debrecen for several decades. The study of peptides relevant to neurodegenerative diseases is now a major focus of our research.

The stoichiometry of the formed complexes is determined by pH potentiometry. The structure of the complexes is investigated using various spectroscopic methods, including UV-Vis spectrophotometry, circular dichroism (CD), electron spin resonance (ESR), and ^{1}H NMR spectroscopy.

This work will summarize the role of circular dichroism spectroscopy in these studies. This method has been used to

- determine the type of coordinating donor atoms
- identify binding sites
- confirm the proposed complex structures
- establish the order of binding preferences at different donor atoms for different metal ions
- determine the ratio of various coordination isomers
- prove the rearrangement of metal ions around binding sites in the presence of other metal ions.

Several examples will be presented using studied model systems that mimic the active site of copper-zinc superoxide dismutase, as well as peptide fragments of the human prion protein and amyloid beta.

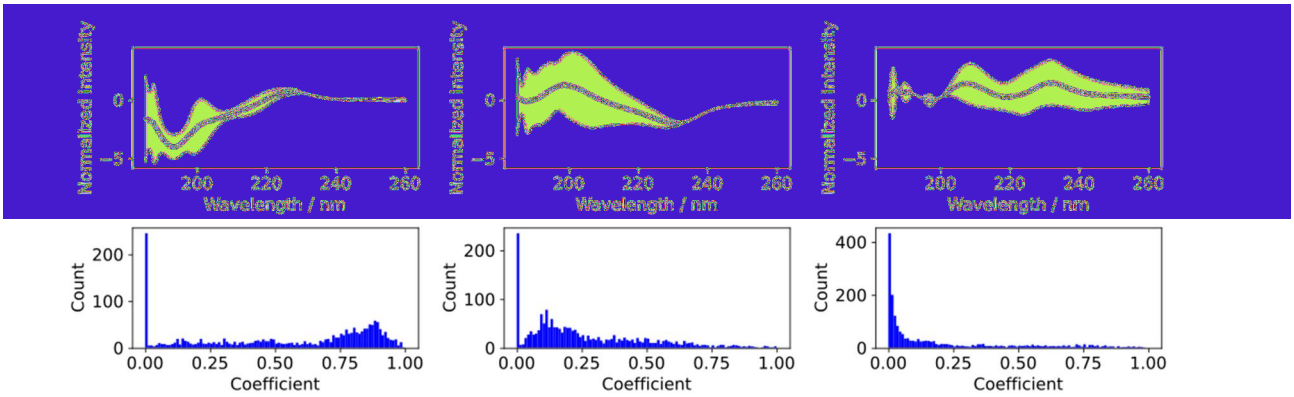
Acknowledgement
This research was supported by the University of Debrecen Program for Scientific Publication.
I would like to express my gratitude to all current and former members of the bioinorganic chemistry research group who contributed to this work, with special mention of Prof. Dr. Imre Sóvágó and Prof. Dr. Katalin Várnagy, who supervised these studies.

PO-36

From linear models to neural networks for CD deconvolution

Zsolt Fazekas

Here, we present an in-house curated circular dichroism spectrum database of various hexapeptides in various conditions, containing more than 1800 measurements for 41 peptides. These spectra, along with their metadata, were analyzed through both conventional and newly developed methods, highlighting the biases and limitations present in the database and suggesting directions for improvement. Additionally, we reimplemented the CCA+ algorithm for spectrum deconvolution using a neural-network-like architecture and supplemented the resulting basis spectra with wavelength-dependent variance estimations.



PO-37

Amyloid or Not? Circular Dichroism Reveals How Sequence Order Drives Aggregation, Structure, and Molecular Evolution

*Fruzsina Bencs[1], Imre Jákli[1,2], Nóra Taricska[2], Viktor Farkas[1,2], András Perczel[1,2]**

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Short amyloidogenic oligopeptides are suggested to be the earliest macromolecular building blocks under prebiotic Earth conditions. These peptides were believed to be capable of forming phase-separated, solvent-excluded nanosystems. Here, we present experimental evidence showing that the aggregation-prone peptide APR-A can be converted into APR-B via mutational pathways consisting entirely of either insoluble, amyloid-forming sequences or soluble, non-aggregating ones. These parallel pro- and anti-amyloid trajectories exhibit distinct physicochemical properties governed solely by the order of point mutations. Sequences along the pro-amyloid pathway undergo heterogeneous phase separation, yielding nanocrystalline amyloid assemblies. Several of these assemblies were structurally resolved, including rare polymorphs with class 3 topology. Circular dichroism spectroscopy during aggregation revealed dynamic spectral evolution, enabling AI-assisted analysis of shape and packing transitions in growing amyloids. Reconstructing these evolutionary trajectories demonstrates how mutational tuning of amyloidogenicity could have enabled the emergence of both water-soluble miniproteins and insoluble structural scaffolds. This duality provides a framework for understanding the mechanistic basis of early macromolecular self-organization and sheds light on how medically relevant peptides may be directed toward or away from pathogenic aggregation.

PO-38

Decoding Functional Amyloids by Chiroptical Fingerprinting: Electronic and Vibrational Circular Dichroism Spectroscopy Sheds Light on Polymorphic Assembly

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Amyloid fibrils are usually linked to harmful clumps, but many hormone-like polypeptides in the human body (like glucagon, GLP-1, and β-endorphin) naturally take on amyloid shapes while being stored and change back into their active forms when they're released. The structural determinants of such reversible aggregation and polymorphism were investigated to be understood. The amyloid-forming behavior of the GNNQQNY heptapeptide from the Sup35 prion protein was examined, as well as two mutants in which glutamine was substituted with norleucine at positions 4 or 5. These substitutions, which were designed with rationality, selectively removed hydrogen bonding capacity while preserving hydrophobicity. This allowed us to dissect side-chain contributions to stability.

Our findings reveal a stepwise aggregation process. Early β-sheet alignment is followed by π-π interactions among Tyr residues. This leads to hydrophobic zipper formation and partial solvent exclusion. These interactions promote hierarchical assembly and encode twist and chirality into growing protofilaments. Notably, the structural context of tyrosine "ladders" directs the emergence of distinct polymorphs: chiral fibrils or achiral nanocrystals. This highlights the structural adaptability of amyloids. These insights provide a structural basis for understanding both pathogenic and functional amyloids and inform the design of stable, depot-forming peptide therapeutics, in which aggregation is a useful tool rather than a risk.

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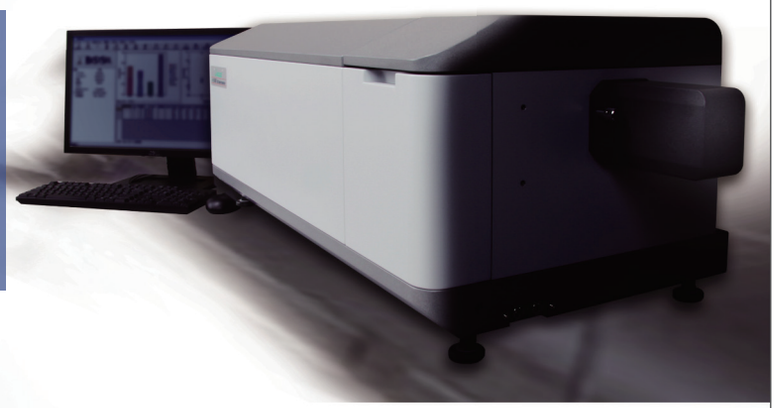

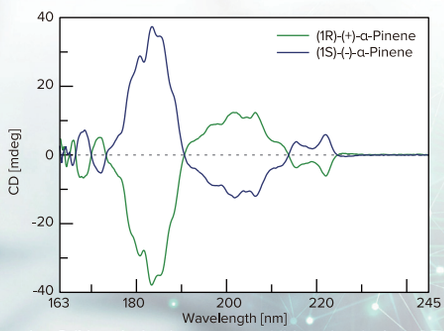

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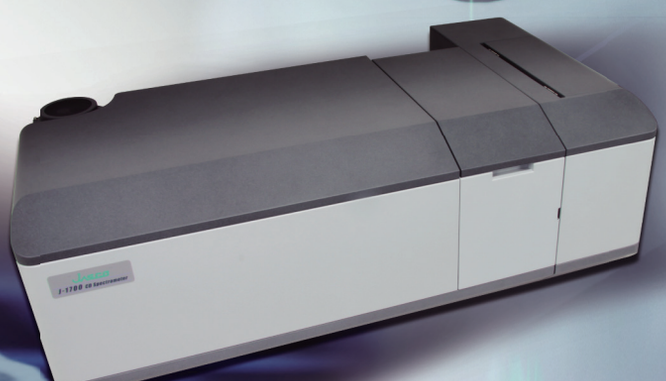

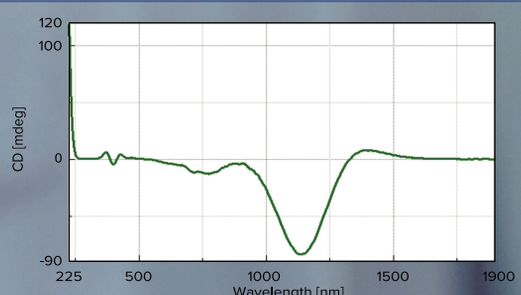

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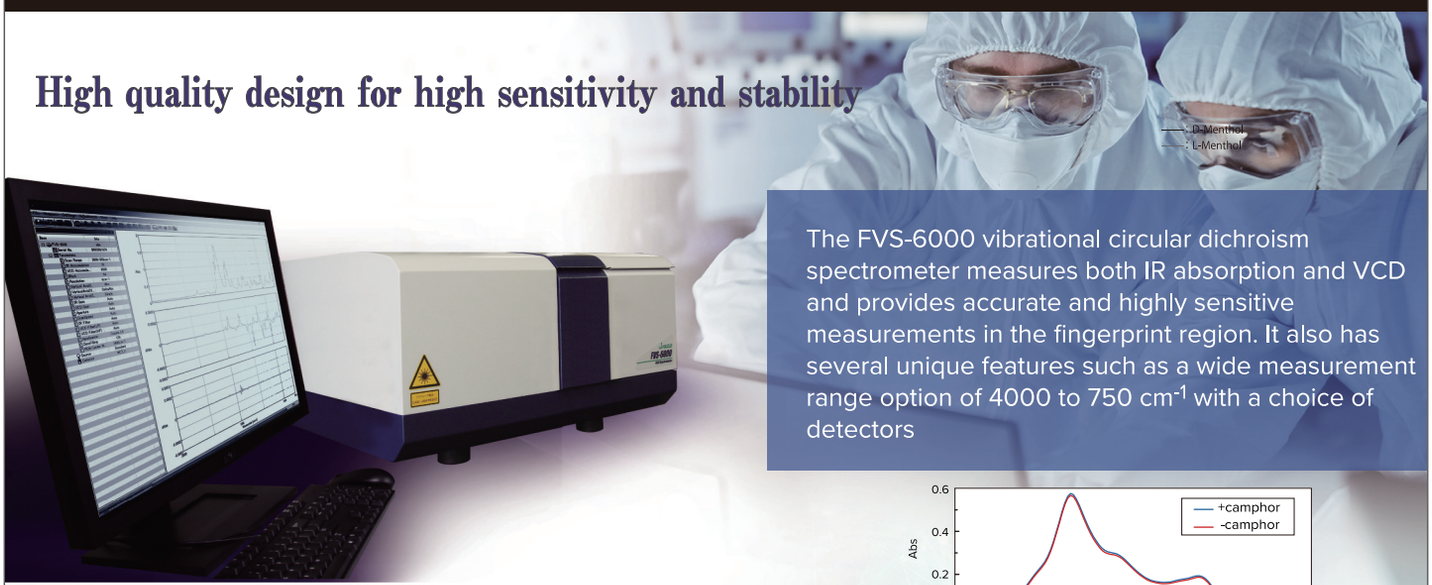
JASCO Not only Circular Dichroism but also other Chiroptical spectroscopy

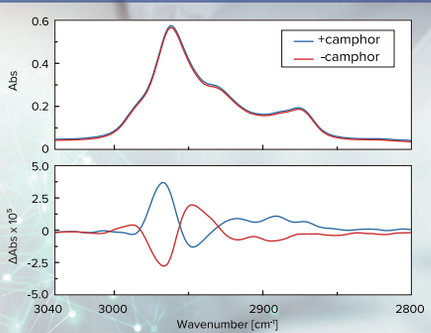
High quality design for high sensitivity and stability



The FVS-6000 vibrational circular dichroism spectrometer measures both IR absorption and VCD and provides accurate and highly sensitive measurements in the fingerprint region. It also has several unique features such as a wide measurement range option of 4000 to 750 cm^{-1} with a choice of detectors

Virational Circular Dichroism Spectrometer

FVS-6000



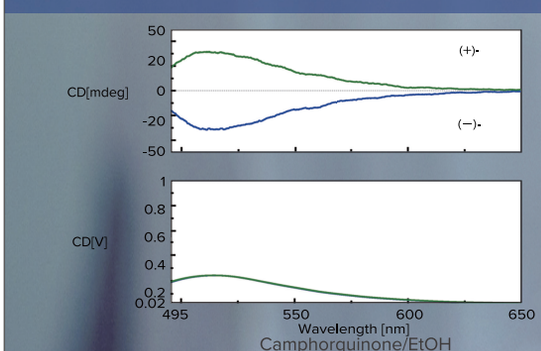
VCD and IR spectra of camphor(narrow band mode)

Chiroptical Spectroscopy Solutions

CPL-300

Circularly polarized luminescence measurement system

The CPL-300 is designed with two monochromators: an excitation monochromator generates monochromatic depolarized light which excites a chiral sample and an emission monochromator collects the fluorescence light emitted by the sample.



Camphorquinone/EtOH

JASCO Web: https://www.jasco-global.com/

Products described herein are designed and manufactured by ISO-9001 and ISO-14001 certified JASCO Corporation

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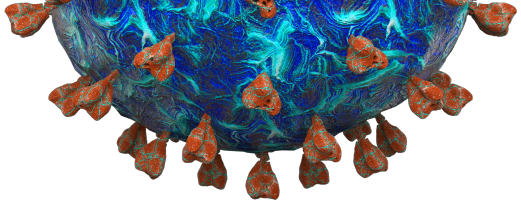
Characterization Experts: Chirality & Biologics



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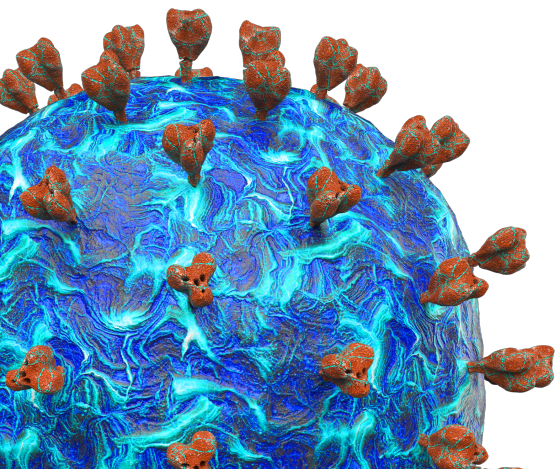
ChiralRAMAN-2X™

- MEASURING ALL 4 FORMS OF ROA - ICP, SCP, DCP1 & DCP2
- NEW VERSION INCLUDES PROTACAL SOFTWARE



info@biotools.us
http://biotools.us
5730 Corporate Way, Ste. 220, West Palm Beach, FL 33407
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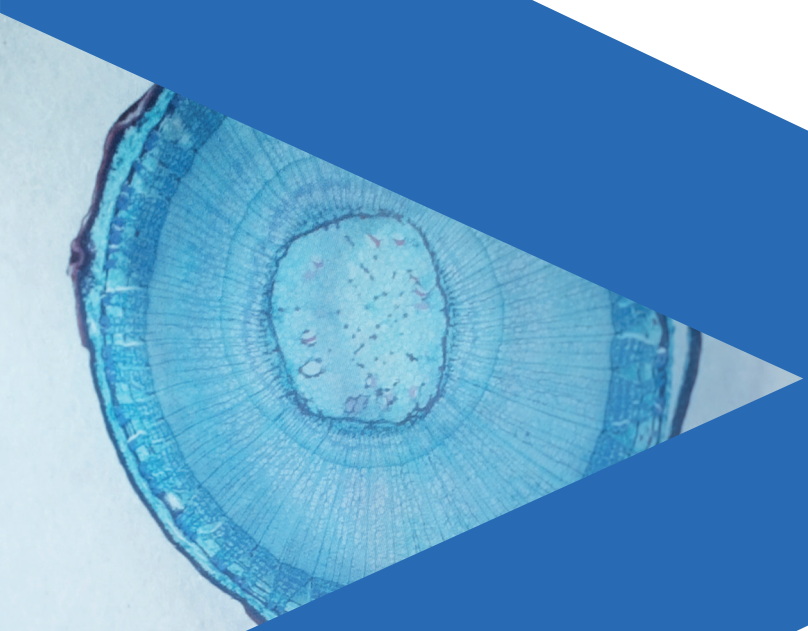

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Acknowledgement

We thank to our sponsors for the support.

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