

SUNDAY 1ST JULY

This session will be held at the Municipal Theatre of Faro,
known as Teatro das Figuras

- 14:00h **Registration**
- 16:00h **Opening Ceremony**
Introductory Remarks
- 17:00h Plenary Session 1a. Chair: **Artur Silva**
PL1 – **BERNARD FERINGA**
DYNAMIC MOLECULAR SYSTEMS
- 18:00h Plenary Session 1b. Chair: **Ian Williams**
PL2 – **FRANCES ARNOLD**
INNOVATION BY EVOLUTION: BRINGING NEW CHEMISTRY TO LIFE
- 19:00 h **Welcome Reception**

MONDAY 2ND JULY

- 9:00 h Plenary/Keynote Session 2. Chair: **Manabu Abe**
PL3 – **PETER CHEN**
BOND STRENGTHS IN THE GAS PHASE, IN SOLUTION, AND IN SILICO:
- 9:50 h **DISPERSION EFFECTS AND BIG MOLECULES**
KN1 – **PETER SCHREINER**
CARBOHYDRATE FORMATION IN THE ABSENCE OF BIOSYNTHESIS
- 10:20 h **Coffee Break**
- 11:00 h Plenary/Keynote Session 3. Chair: **Jason Harper**
PL4 – **JINPEI CHENG**
REVITALIZE BOND ENERGETICS FOR UNDERSTANDING IONIC LIQUID CHEMISTRY
- 11:50 h KN2 – **LUÍS GARCIA-RIO**
COMPETITIVE AND COOPERATIVE COUNTERION EFFECTS ON SUPRAMOLECULAR RECOGNITION
- 12:20 h **Lunch**

PARALLEL SESSIONS

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|---------|----------------------------|-----------------------------|-----------------------------|
| | Session 1a | Session 2a | Session 3a |
| | Chair: S. Fornarini | Chair: P. Schreiner | Chair: U. Pischel |
| 14:00 h | IL1-H. OTTOSSON | IL2-H. MAYR | IL3-S. HIRAOKA |
| 14:30 h | O1- ITOH | O10- PAGE | O19- SATO |
| 14:50 h | O2- BUCHER | O11- ALABUGIN | O20- BROTIN |
| 15:10 h | O3- JONES | O12- LI | O21- VANČIK |
| 15:30 h | O4- G.-PORANNE | O13- HUMERES | O22- NEKIPELOVA |
| 15:50 h | Coffee Break | | |
| | Session 1b | Session 2b | Session 3b |
| | Chair: U. Wille | Chair: A. O'Donoghue | Chair: L. Garcia-Rio |
| 16:20 h | O5- MILO | O14- UGGERUD | O23- LAINÉ |
| 16:40 h | O6- PERRIN | O15- KANENO | O24- BASÍLIO |
| 17:00 h | O7- CRUZEIRO | O16- FARIA | O25- SALONEN |
| 17:20 h | O8- MARDYUKOV | O17- IGNATCHENKO | O26- GUIEU |
| 17:40 h | O9- NAKATA | O18- BUURMA | O27- REANY |

TUESDAY 3RD JULY

- 9:00 h Plenary/Keynote Session 4. Chair: **Rui Fausto**
PL5 – **STEFAN GRIMME**
**DEVELOPMENT AND APPLICATION
OF LOW-COST QUANTUM CHEMISTRY METHODS**
- 9:50 h KN3 – **RAGHAVAN SUNOJ**
**ASYMMETRIC DUAL CHIRAL CATALYSIS: MECHANISM AND
CHIRAL INDUCTION**
- 10:20 h **Coffee Break**
- 10:50 h Plenary/Keynote Session 5. Chair: **Carlos Afonso**
PL6 – **JANINE COSSY**
**CHEMISTRY AND PHYSICS:
SYNTHESIS AND VECTORIZATION OF DRUGS TOWARDS THE TUMORS**
- 11:40 h KN4 – **JASON HARPER**
SOLVENT CONTROL OF REACTION OUTCOME USING IONIC LIQUIDS
- 12:10 h KN5 – **RUI LOUREIRO**
USE OF MODELLING IN PHARMACEUTICAL PROCESS DEVELOPMENT
- 12:40 h **Lunch**

PARALLEL SESSIONS

- | | Session 1c | Session 2c | Session 3c |
|---------|---------------------------------|----------------------------|-------------------------|
| | chair: S. Kozuch | Chair: M. P. Muñoz | Chair: R. Herges |
| 14:30 h | IL4– R. MCMAHON | IL5– H. SZATYLOWICZ | IL6– S. LUO |
| 15:00 h | O28– WILLIAMS | O33– ZIPSE | O38– SEKIYA |
| 15:20 h | O29– WALLIS | O34– CHECHIK | O39– AURAS |
| 15:40 h | O30– VÁÑA | O35– THAMATTOOR | O40– KURTH |
| 16:00 h | O31– DUARTE | O36– CANLE | O41– MCCONNELL |
| 16:20 h | O32– REVA | O37– VIEGAS | O42– MEDRONHO |
| 16:40 h | Poster Session and Refreshments | | |

WEDNESDAY 4TH JULY

- 9:00 h Plenary/Keynote Session 6. Chair: **Hugh Burrows**
PL7 – **TITO SCAIANO**
**ORGANIC PHOTOCATALYSIS WITH METAL-DECORATED
TITANIUM DIOXIDE**
- 9:50 h KN6 – **RAINER HERGES**
**MOLECULAR ASSEMBLERS, MOLECULAR MACHINES
PERFORMING SYNTHESIS**
- 10:20 h **Coffee Break**
- 10:50 h Plenary/Keynote Session 7. Chair: **Igor Alabugin**
PL8 – **DAVID COLLUM**
**STRUCTURE-REACTIVITY-SELECTIVITY RELATIONSHIPS
IN ALKALI METAL CHEMISTRY**
- 11:40 h KN7 – **MARIA JOÃO RAMOS**
UNDERSTANDING HOW ENZYMES WORK
- 12:10 h IL7 – **MASATAKA NAGAOKA**
**TOWARD COMPUTATIONAL MOLECULAR TECHNOLOGY OF COMPLEX
CHEMICAL REACTION SYSTEMS: APPLICATIONS OF RED
MOON METHODOLOGY**
- 12:40 h **Lunch**
- 14:00 h **Excursion**

THURSDAY 5TH JULY

- 9:00 h Plenary/Keynote Session 8. Chair: **Einar Uggerud**
PL9 – **GUY LLOYD-JONES**
EXPLORING CATALYTIC LANDSCAPES: DON'T BE INHIBITED
- 9:50 h KN8 – **ANNMARIE O'DONOGHUE**
**UNDERSTANDING CHEMOSELECTIVITY IN UMPOLUNG
ACYL ANION CATALYSIS**
by Carbenes
- 10:20 h **Coffee Break**
- 10:50 h Plenary/Keynote Session 9. Chair: **Henrik Ottosson**
PL10 – **CARLOS AFONSO**
DIVERSE REACTIVITY OF FURAN BASED BIORENEWABLE RESOURCES
- 11:40 h KN9 – **SEBASTIAN KOZUCH**
**QUANTUM TUNNELING: COMPUTATIONAL PREDICTIONS
IN EXOTHERMIC AND ISOTHERMIC REACTIONS**
- 12:10 h KN10 – **SIMONETTA FORNARINI**
BINDING MOTIFS OF CISPLATIN WITH AMINO ACID TARGETS PROBED
by IR Spectroscopy of Isolated Species
- 12:40 h **Lunch**

PARALLEL SESSIONS

	Session 1d	Session 2d	Session 3d	Session 3e
	Chair: E. Humeres	Chair: M. Ludwig	Chair: H. Vancik	Chair: M. Canle
14:30 h	IL8– U. WILLE	IL9– M. MUÑOZ IL	10– A. GEROLA	IL11– S. HOZ
15:00 h	043– SHAINYAN	047– USUI	051– SETAKA	055– LIMA
15:20 h	044– SIEHL	048– FRIJA	052– PISCHEL	056– SIMÕES
15:40 h	045– MAGUIRE	049– BRANCO	053– RYAN	057– AURELIANO
16:00 h	046– KHMELINSKII	050– SOUZA	054– BALEIZÃO	058– OSTOS

Conference Dinner

FRIDAY 6TH JULY

- 9:20 h Plenary/Keynote Session 10: Chair: **José Gaspar Martinho**
PL11 – **JOÃO ROCHA**
**ORGANIC AND ORGANIC–INORGANIC HYBRID MATERIALS
FOR LIGHT EMISSION AND SENSING**
- 10:10 h KN11 – **HERMENIGILDO GARCIA**
**DEFECTIVE GRAPHENES FROM BIOMASS AS PHOTOCATALYSTS
FOR SOLAR FUELS PRODUCTION**
- 10:40 h **Coffee Break**
- 11:10 h Plenary/Keynote Session 11. Chair: **Hans-Ullrich Siehl**
PL12 – **MANABU ABE**
**IS Π SINGLE-BONDING (C– Π –C) POSSIBLE?
A CHALLENGE IN ORGANIC CHEMISTRY**
- 12:00 h Concluding Remarks
- Lunch**