

# Programme

## Sunday 1<sup>st</sup> 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	<b>Plenary Session 1a</b> PL1 - Bernard Feringa Dynamic Molecular Systems
18:00h	<b>Plenary Session 1b</b> PL2- Frances Arnold Innovation by Evolution: Bringing New Chemistry to Life
19:00 h	Welcome Reception

# Monday 2<sup>nd</sup> July

## 9:00 h **Plenary/Keynote Session 2**

PL3 - Peter Chen

Bond Strengths in the Gas Phase, in Solution, and In Silico:  
Dispersion Effects and Big Molecules

## 9:50 h **KN1 - Peter Schreiner**

Carbohydrate Formation in the Absence of Biosynthesis

## 10:20 h **Coffee Break**

## 11:00 h **Plenary/Keynote Session 3**

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**

#### **Session 1a**

#### **Session 2a**

#### **Session 3a**

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**

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 3<sup>rd</sup> July

## 9:00 h **Plenary/Keynote Session 4**

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**

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**

14:30 h	IL4-R. McMahon	IL5-H. Szatyłowicz	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-Váňa	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 4<sup>th</sup> July

9:00 h **Plenary/Keynote Session 6**

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**

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 5<sup>th</sup> July

## 9:00 h **Plenary/Keynote Session 8**

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**

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**

14:30 h	IL8-U. Wille	IL9-M. Muñoz	IL10-A. Gerola	IL11-S. Hoz
15:00 h	O43-Shainyan	O47-Usui	O51-Setaka	O55-Lima
15:20 h	O44-Siehl	O48-Frija	O52-Pischel	O56-Simões
15:40 h	O45-Maguire	O49-Branco	O53-Ryan	O57-Aureliano
16:00 h	O46-Khmelinskii	O50-Souza	O54-Baleizão	O58-Ostos

## Conference Dinner

# Friday 6<sup>th</sup> July

9:20 h **Plenary/Keynote Session 10**

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**

PL12 - Manabu Abe

Is  $\pi$  Single-Bonding (C- $\pi$ -C) Possible?  
A Challenge in Organic Chemistry

12:00 h

Concluding Remarks

Lunch