

**COST**  
Domain Committee  
" **Chemistry and Molecular Sciences and Technologies** "

**COST Action CM1005**  
Start Date 31 March 2011

***Supramolecular Chemistry in water***

**MONITORING  
PROGRESS REPORT**

***Reporting Period: from 21/04/2012 to 15/04/2013***

This Report is presented to the relevant Domain Committee.  
It contains three parts:

***I. Management Report*** prepared by the Grant Holder

***II. Scientific Report*** prepared by the Chair of the Management Committee of the Action

***III. Previous versions of the Scientific Report; i.e., part II of past reporting periods***

The report is a "cumulative" report, i.e. it is updated annually and covers the entire period of the Action.

Confidentiality: the documents will be made available to the public via the COST Action web page except for chapter *II.D. Self evaluation*.

Based on the monitoring results, the COST Office will decide on the following year's budget allocation.

**Executive summary (max.250 words):**

The objective of this COST Action is to develop supramolecular systems that work in water. The Action comprises 22 COST Countries and 79 individual participants. Australia joined the Action this year. During this second year we continued our efforts to achieve the objectives of the Action and we have been quite successfully in doing this. A number of joint and interdisciplinary research programmes has been promoted and carried out thanks to the ample involvement of early-stage researchers. Twelve STMs have been financed.

Two major events have been organized (2<sup>nd</sup> Scientific Meeting and 2<sup>nd</sup> Training School) and also five smaller workshop meetings. This year thirteen publications have resulted from the collaborative work within the Action. (<http://supracheminwater.wordpress.com>)

## **I. Management Report prepared by the Grant Holder**

### **I.A. COST Action Fact Sheet**

- **COST Action** CM1005 – *Supramolecular Chemistry in Water*

- **Domain** CMST

- **Action details:**

**CSO Approval:** 02/12/2010  
**Entry into force:** 17/01/2011

**End date:** 30/03/2015  
**Extension:** (day/month/year)

- **Objectives**

The objective of this COST Action is to develop supramolecular systems that work in water. Such supramolecular systems should allow to (i) monitor environmentally or biologically relevant species in water (ii) control selectivity of reactions in water, and (iii) produce self-assembled organized structures in water which are stimuli responsive and which can be used for programming functions in materials and devices. The Action aims at improving our understanding of the multiple weak non-covalent, but collectively powerful interactions that allow efficient and selective recognition processes to occur in water.

- **Parties (22):**

Belgium (09/03/2011)	Hungary (17/02/2011)	Portugal (07/02/2011)
Bulgaria (01/12/2011)	Ireland (07/02/2011)	Romania (29/08/2011)
Croatia (14/03/2011)	Israel (06/06/2011)	Slovenia (29/11/2011)
Czech Rep. (31/01/2011)	Italy (17/01/2011)	Spain (17/01/2011)
Denmark (08/06/2011)	Malta (30/03/2011)	Switzerland (23/02/2011)
Finland (21/01/2011)	Netherlands (21/01/2011)	Turkey (25/02/2011)
France (17/01/2011)	Poland (17/01/2011)	United Kingdom (17/01/2011)
Germany (20/01/2011)		

- **Intentions to accept:** -

- **Other participants (1):**

Non-COST Institution: The University of Sydney, School of Chemistry (Australia)

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- **Action Web site:** <http://supracheminwater.wordpress.com/>

• **Grant Holder Representative:**

Prof. Kristin BARTIK, Université libre de Bruxelles, kbartik@ulb.ac.be

• **Working Groups (3)**

<b>WG1 : Supramolecular recognition and sensing in Water (40)</b>	
Kristin BARTIK	Belgium
Wim DEHAEN	Belgium
Ivan JABIN	Belgium
Mathieu SURIN	Belgium
Johan WOUTERS	Belgium
Petko IVANOV	Bulgaria
Tomas KRAUS	Czech Republic
Michael PITTELKOW	Denmark
Brigitte BIBAL	France
Jean-Claude CHAMBRON	France
Benoit COLASSON	France
Ivan HUC	France
Alexandre MARTINEZ	France
Evgeny KATAEV	Germany
Stefan KUBIK (WG Leader)	Germany
Werner NAU	Germany
Rita SKODA-FOLDES	Hungary
Alessandro CASNATI	Italy
Antonella DALLA CORT	Italy
David MAGRI	Malta
Jerzy RADECKI	Poland
Joao Carlos LIMA	Portugal
Fernando PINA	Portugal
Pablo BALLESTER	Spain
Enrique GARCIA-ESPANA	Spain
Jose Miguel LLINARES	Spain
Juan C. MORALES	Spain
Uwe PISCHEL	Spain
Roberto QUESADA	Spain
Laura RODRIGUEZ	Spain
Bruno THERRIEN	Switzerland
Felix ZELDER	Switzerland
Ilke GUROL	Turkey
Mustafa Selman YAVUZ	Turkey
Mustafa YILMAZ	Turkey
Anthony DAVIS	United Kingdom
Philip GALE	United Kingdom
Zoe PIKRAMENOU	United Kingdom
Ramon VILAR	United Kingdom
Kate JOLLIFFE	Australia

<b>WG2 : Supramolecular control of reactivity in water (12)</b>	
Svetlana SIMOVA	Bulgaria
Kari RISSANEN	Finland
Yves LE MEST	France
Olivia REINAUD	France
Bart Jan RAVOO	Germany
Gonen ASHKENASY	Israel
Giulia LICINI	Italy
Miriam MBA BLAZQUEZ	Italy
F. Matthias BICKELHAUPT	Netherlands
Beatriu ESCUDER (WG Leader)	Spain
Thomas R. WARD	Switzerland
Donus TUNCEL	Turkey

<b>WG3 : Self-assembly in water (22)</b>	
Gilles BRUYLANTS	Belgium
Richard HOOGENBOOM	Belgium
Marina ILAKOVAC KVEDER	Croatia
Ivo PIANTANIDA	Croatia
Pol BESENIUS	Germany
Luisa DE COLA	Germany
Carsten SCHMUCK	Germany
Thorri GUNNLAUGSSON (WG leader)	Ireland
Andrea MELE	Italy
Roberto PURELLO	Italy
Sylvestre BONNET	Netherlands
Alexander KROS	Netherlands
Sijbren OTTO	Netherlands
Rint SIJBESMA	Netherlands
Aurica CHIRIAC	Romania
Loredana NITA	Romania
Damjan MAKUC	Slovenia
Janez PLAVEC	Slovenia
Patrick SHAHGALDIAN	Switzerland
Mustafa O. GULER	Turkey
David K. SMITH	United Kingdom
Salvador TOMAS	United Kingdom

### ***I.B. Management Committee member list (38)***

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Philip GALE	UK	philip.gale@soton.ac.uk

Non-COST participants:

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## I.C. Overview activities and expenditure

### Budget Grant period I (02/06/2012-01/06/2013)

**Total Action Budget: 146 000.00 EUR**

**Remaining Action Commitment:**

#### Meetings

Meeting Type	Date	Place	Forecast	Cost	Total
Core Group	28-29/09/2012	Brussels, BE		2 575.37	
MC + WG + Conf.	16-20/11/2012	Lisbon, PT		31 914.86	
Core Group	27/01/2013	Bressanone, IT		0	
Workshop	21-23/03/2013	Brussels, BE	3 690.00		
Workshop	02-03/05/2013	Leuven, BE	3 890.00		
Workshop	03-04/05/2013	Jyväskylä, FI	1 910.00		
Workshop	10-12/05/2013	Rome, IT	7 520.00		
Workshop	17-18/05/2013	Barcelona, ES	3 800.00		
			20 810.00	34 490.23	<b>(55 300.23)</b>

#### STSM

Beneficiary	Date		Place		Cost	Total
	From	To	From	To		
N. BUSSCHAERT	23/07/12	05/08/12	Southampton, UK	Ljubljana, SI	907.00	
A. SCHALY	16/09/12	26/09/12	Kaiserslautern, DE	Valencia, ES	500.00	
C. GLIONNA	14/06/12	09/11/12	Rome, IT	Beer Sheva, IL	2 500.00	
L. KARAGIANNIDIS	02/12/12	15/12/12	Southampton, UK	Ljubljana, SI	1 420.00	
A. BAHREMAN	28/01/13	09/02/13	Leiden, NL	Brussels, BE	1 080.00	
G. FORTE	06/03/13	30/03/13	Rome, IT	Kaiserslautern, DE	2 500.00	
E. AGUILO	11/03/13	12/04/13	Barcelona, ES	Lisbon, PT	1 250.00	
F. KEYMEULEN	08/05/13	22/05/13	Brussels, BE	Rome, IT	1 500.00	
P. FEZZARDI	01/03/13	31/05/13	Parma, IT	Strasbourg, FR	2 500.00	
G. DE LEENER	08/04/13	31/05/13	Brussels, BE	Paris, FR	2 100.00	
L. DAVIN CARDONA	15/04/13	31/05/13	Barcelona, ES	Rome, IT	2 500.00	
E. AGUILO	01/05/13	31/05/13	Barcelona, ES	Jyväskylä, FI	1 500.00	
						<b>20 257.00</b>

#### Schools

Title	Date	Place	Forecast	Cost	Total
Training School 2	27/01-01/02/2013	Bressanone, IT		46 786.49	
					<b>46 786.49</b>

#### Dissemination

Title	Date	Place	Forecast	Total
Website management	-/04/13	<a href="http://supracheminwater.wordpress.com">http://supracheminwater.wordpress.com</a>	800.00	
				<b>800.00</b>

**Others**

					<b>0</b>

			<b>Action Total :</b>	<b>(123 143.72)</b>
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**Budget Grant period I (01/05/2011-01/06/2012)****Total Action Budget: 112 600.00 EUR****Remaining Action Commitment:****Meetings**

Meeting Type	Date	Place	Cost	Total
Core Group	2-3/07/2011	Brighton, UK	4 308.23	
MC + WG + Conf.	19-21/11/2011	Frascati, IT	39 690.35	
Core Group	23/03/2012	Venice, IT	1 922.94	
				<b>45 921.52</b>

**STSM**

Beneficiary	Date		Place		Cost	Total
	From	To	From	To		
F. KEYMEULEN	18/11/11	26/11/11	Brussels, BE	Rome, IT	1 110.00	
G. FORTE	08/01/12	21/01/12	Rome, IT	Neuchatel, CH	1 500.00	
I. GIANNICCHI	08/01/12	17/02/12	Rome, IT	Barcelona, ES	1 800.00	
R. GAVARA	01/02/12	15/03/12	Lisbona, PT	Barcelona, ES	1 500.00	
A. INTASOT	01/02/12	06/04/12	Brussels, BE	Paris, FR	2 500.00	
M. BRUSCHINI	01/03/12	30/04/12	Rome, IT	Southampton, UK	2 500.00	
A. JARGILO	01/03/12	31/05/12	Olsztyn, PL	Leuven, BE	2 500.00	
S. MOERKERKE	02/04/12	20/04/12	Brussels, BE	Jyvaskyla, FI	1 200.00	
L. RODRIGUEZ	10/04/12	04/05/12	Barcelona, ES	Lisbona, PT	1 500.00	
C. GLIONNA	12/04/12	31/05/12	Rome, IT	Beer Sheva, IL	2 000.00	
F. SCARAMUZZO	01/05/12	31/05/12	Padova, IT	Jyvaskyla, FI	2 000.00	
G. ASHKENASY	06/05/12	12/05/12	Beer Sheva, IL	Castello, ES	1 270.00	
S. BARTOCCI	14/05/12	31/05/12	Rome, IT	Brussels, BE	1 500.00	
P. DE BERNARDIN	17/05/12	25/05/12	Rome, IT	Brussels, BE	900.00	
						<b>23 780.00</b>

**Schools**

Title	Date	Place	Forecast	Cost	Total
First Training School	16-19/04/2012	Riccione, IT	22 550.00		
					(22 550.00)

**Dissemination**

Title	Date	Place	Cost	Total
Website creation	30/08/11	<a href="http://supracheminwater.wordpress.com">http://supracheminwater.wordpress.com</a>	2 000.00	
				<b>2 000.00</b>

**Others**

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			<b>Action Total :</b>	<b>(91 851.52)</b>	

## **II. Scientific Report**

### **II.A. Innovative networking**

Innovative knowledge has been generated from networking through the Action and from the organization of a series of events.

The 2<sup>nd</sup> Scientific Meeting of the Action was held in Lisbon, Costa da Caparica (PT), on 16-20 November 2012. It was organized and promoted by Prof. Fernando Pina (Universidade Nova de Lisboa). The meeting has been attended by 60 persons, 39 supported by the Action.

The scientific program (see **Annex 1**) consisted in 5 plenary lectures of which one was delivered by an invited expert (who subsequently asked to join the Action), 20 oral communications (20 min) and 9 flash communications (10 min) centred on the topics of the Action. It is worth mentioning that about 33 % of the participants were early stage researchers, and 33 % were women scientists.

During the meeting, the 3 WGs also held meetings in parallel. Every WG members had the opportunity to describe their individual research interests and to establish new collaborations with colleagues involved in the Action.

From January 27 to February 1, 2013, the 2<sup>nd</sup> Training School of the Action took place. It was organized by Prof. Giulia Licini (Università di Padova) in Bressanone (IT). The school was attended by 133 persons including 106 students (47 supported by the Action), 8 senior participants, 13 lecturers (all supported by the Action). Most of the trainees presented posters. (Program in **Annex 2**)

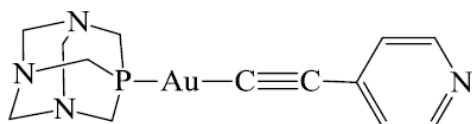
A driving principle of our Action is to encourage and enable collaborations between all the participants. We consequently decided to provide opportunity to organize a number of small workshop meetings meant to represent the perfect ground for nurturing these collaborations and to enable knowledge and skill transfer. 5 such small workshops have been programmed this year involving in total 16 labs of the Action.

The list of publications (see **Annex 3**) derived from collaborations born within the frame of the Action is the best sign of innovative networking. The high impact factor and the quality of the journals in which these papers have been published highlight this point. This year 13 joint publications were accepted. Clearly some of the results of the research carried within the Action can find applications in the field of diagnosis and detection of water pollutants leading to important social implications. Moreover the network established thanks to the Action favoured interactions and promoted applications for funding at national and European level. (See Part

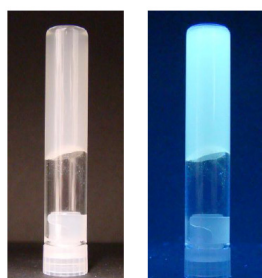
## II.B.)

The following examples of joint results obtained during this year are worth mentioning:

i. Concerning self-assembly in water, a luminescent gel, the [(PTA)Au(4-pyridylethynyl)] molecule, **1**, was obtained for the first time. It is characterized by a simple structure that through subtle modifications (for example the position of the pyridil unit) can induce unexpected and interesting rheological properties in water. As far as we know this is the first example of formation of a luminescent organometallic gold(I) hydrogelator obtained from a discrete molecule (R. Gavara, J. Llorca, J. Carlos Lima and L. Rodriguez *Chem. Commun.*, **2013**, 49, 72-74, Working Group 1).

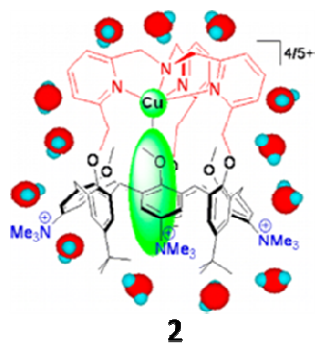


**1**



Gel texture of **1** in water under visible (left) and UV light (right)

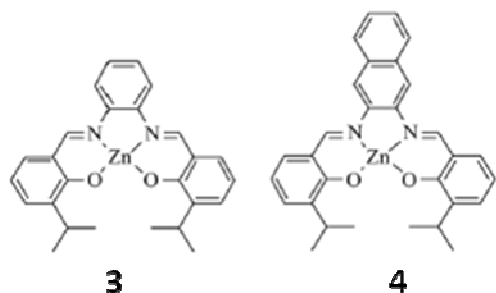
ii. The Action objective focused on the control of supramolecular reactivity in water by biomimetically inspired systems has implied the study of model systems. In this context the construction of artificial metallo-enzymes aims at reproducing structural and functional



**2**

properties of natural systems. To implement the model compounds generally used for this type of investigations, considering that the enzymatic pocket plays a key role for substrate selective binding, a possible approach consists in associating a metal complex to a hydrophobic cavity. The other key point is to the water-solubilization of promising artificial systems. The fruitful collaboration between two groups belonging to different WGs (1 and 2) lead to the preparation of a water-soluble calix-[6]TPMA (TPMA = tris(2-pyridylmethyl)amine) ligand and to the corresponding Cu(I)/Cu(II) complexes, **2**, that have been studied in pure water. These represent a very rare example (if not the first) of an artificial structure capable of stabilizing in pure water a copper ion featuring a coordinative unsaturation in both +I and +II oxidation states (G. Thiabaud, A. Brugnara, M. Carboni, N. Le Poul, B. Colasson, Y. Le Mest, O. Renaud *Org. Lett.*, **2012**, 14, 2500-2503).





iii. With the aim of developing chemical sensors for monitoring biologically and environmentally relevant species, we started to investigate the biological activity *in vitro* and *in vivo* of some of the artificial receptors we are developing by testing their potentialities as fluorescence markers in cells.

Two fluorescent Zn(II)-salophen derivatives have been evaluated. It was observed that these compounds enter the cells and the cellular uptake occurs without damaging the DNA strands. Preliminary studies carried out with living cells have shown IC<sub>50</sub> values in a millimolar range, indicative of a non-cytotoxic behaviour. These data indeed encourage their use as fluorescence markers in cells. (R. Brissos, D. Ramos, J. C. Lima, F. Yafteh Mihan, M. Borràs, J. de Lapuente, A. Dalla Cort, L. Rodríguez *NewJ. Chem.* **2013**, 37, 1046-1055).

iv. One of the main objectives of this Action is the design of receptors able to monitor biologically and environmentally relevant species in an aqueous environment with high selectivity and affinity. The detection of unbound metal ions such as Zn<sup>2+</sup> (or Cu<sup>2+</sup>) in neutral tissues is a very important task due to the clinical relevance of these ions in neurodegenerative diseases such as Alzheimer's disease. It has been found that coordination of zinc dichloride turns the water-insoluble bapbpy (6,6'-bis(2-aminopyridyl)-2,2'-bipyridine) ligand into a water-soluble, highly fluorescent complex. This can be used to measure biologically relevant concentrations of zinc in vitro (E. Molenbroek, N. Straathof, S. Duck, Z. Rashid, J. H. van Lenthe, M. Lutz, A. Gandubert, R. J. M. Klein Gebbink, L. De Cola, S. Bonnet, *Dalton Trans.*, **2013**, 42, 2973-2984).

## **II.B. Inter-disciplinary networking**

Inter-disciplinarity is one of the main concerns of this Action. Researchers involved belong to different disciplines (synthetic organic chemistry, inorganic and physical chemistry, physics etc.) and this makes the networking really stimulating and fruitful: many researchers working together under the wide "umbrella" of supramolecular chemistry. For example the choice of having a single conference where the 3 WGs meet was decided in order to promote the interactions, to encourage the dissemination of knowledge. As a result a number of new collaborations between WG members have been initiated. A list of collaborations (new ones and already on-going) is in **Annex 4**.

The following members were able to obtain funding for research projects related to the overall topic of this Action through national funding agencies during this funding period.

- A. CASNATI received a grant from the Italian Ministry of Education and University, PRIN 2010JMAZML for an Italian network for the development of multivalent nanosystems MULTINANOITA.
- As mentioned in the previous progress report, A. DAVIS and P. GALE had submitted a joint

application to the British funding agency EPSRC to receive funding for research on the development and characterization of new carrier molecules for anions across lipid membranes. In the meantime, this application was granted allowing both groups to collaborate on this subject.

- A. DALLA CORT received a grant from Ministero dell' Università e Ricerca for the PRIN Project "Integrated supramolecular technologies for chemical information processing: advanced molecular devices and materials" (INFOCHEM). K. BARTIK, L. RODRIGUEZ, G. LICINI, K. RISSANEN, J. LIMA, B. THERRIEN are also involved in this project.
- Z. PIKRAMENOU received EPSRC funds for 3 months postdoc placements on probe-nanoparticle assembly in water and a Leverhulme Trust-research fellowship for the development of nanoparticles in biomedical applications.
- M. PITTELKOW has qualified for the interview stage of an ERC starting grant, with a project called 'wetchem' that is about dynamic combinatorial chemistry in water. The interview will take place in April 2013.
- S. OTTO received fundings within the EU: Marie Curie Initial Training Network READ Replication and adaptation in molecular networks (as coordinator).
- G. BRUYLANTS received funding from the "Fonds National de la Recherche Scientifique – FRS" for his research devoted to the interaction between biomolecules and nanoparticles.

### ***II.C. New networking***

During this second year new members joined the Action. In total we had 10 new entries and in particular we welcomed Professor Kate Jolliffe, University of Sidney, Australia, a non-COST country. She attended the meeting in Lisbon and delivered a lecture "Peptide Based Receptors for Selective Anion Recognition in Water". A collaboration with Prof Gale has already established. The status of the Action is: currently 22 COST countries + 1 non-COST country, 79 members (among them one from industry), 71 research groups from 62 different institutions.

Dr Susana Fernandez Prieto from Procter&Gamble joined the Action and her company sponsored a national conference on Supramolecular Chemistry (SupraChem 2013) which was organized in Münster by J. B. Ravoo and P. Besenius.

Among the Action members 21 team leaders are women and 13 women scientists are in the MC. There are 14 ESR (< PhD +8) which are members of the Action. As reported in the Management Report part, 12 Short Term Scientific Missions have been accomplished. Interesting results have been obtained that will be the objective of joint publications (13 papers co-authored by members of at least two different research groups). In addition, 3 publications are currently submitted or at the revision stage. As mentioned before 7 groups belonging to the Action have been funded by National and European Agencies.

### **III. Previous scientific report**

Part II of the first reporting period is here.

#### **II.A. Innovative networking**

The 1<sup>st</sup> Scientific Meeting of the Action has been held in Frascati, Villa Tuscolana on the 19-21 November 2011. It was organized and promoted by the Chair of the Action, A. Dalla Cort. The meeting has been attended by 77 persons, 42 of them have been supported by the Action.

The scientific program, Annex 1, consisted in 5 plenary lectures delivered by the invited experts, 20 oral communications (20 min) and ten flash communications (10 min) centered on the topics of the Action. It is worth of mention that about 30 percent of the participants were early stage researchers, and 30 percent were women scientists.

During this first scientific meeting, we had also the three WGs meetings in common and parallel sessions. Every WG member gave a short presentation describing the individual research interests to stimulate new collaborations between the groups.

In April 2012, the 1<sup>st</sup> Training School of the Action took place. It was organized by A. Dalla Cort in Riccione (IT) from April 16 to 19. The participants were 46 (7 senior scientists) and 39 young researchers. The scientific program, Annex 2, consisted in **5** lessons delivered by the senior participants, and 32 oral communications (20 min) delivered by the young researchers. A large amount of time was dedicated to discussions coordinated by the senior participants. Dr Robert Eagling, Editor of the Chemical Science Journal, delivered a lecture on publishing on high IF journals and on the editorial policy of RSC.

The Action has a dedicated website, <http://supracheminwater.wordpress.com>, that represents its foremost mean of dissemination.

Innovative knowledge has been already generated resulting from COST networking through the Action. A driving principle is to encourage and seek to enable collaboration in relevant research among all the participants. The products of our work are better collaborative research, knowledge and skills transfer.

#### **II.B. Inter-disciplinary networking**

Inter-disciplinarity is at the heart of this Action, and the organization of a common event like the Frascati meeting, without specialist sessions, and the choice of having the three WG's meeting held together at the same time were meant to promote the dissemination of knowledge. As a result, mainly of the meeting and partially of the recent Training School, a number of new collaborations between WG members were initiated. Some of these collaborations are still at a relatively early stage. Other collaborations instead are well established and have already yielded publications. As a matter of fact, several of these collaborations involve members of different WGs and this represents the result of the good integration among the participants and of the good level of inter-disciplinary networking. Here is reported a list of collaborations having place within the Action frame at the present this stage:

- BIBAL/QUESADA: Collaboration planned concerning anion transport and organocatalysis in water.
- CASNATI/DE COLA: CASNATI collaborates with L. DE COLA to functionalize zeolite nanocrystals with *p*-guanidinocalixarenes and study the interactions of these systems with cells and bacteria. Another collaborative project between these groups involves the use of carbohydrates as recognition elements to achieve selective cell-entry and as key feature for the construction of new organic-inorganic hybrid materials.

- CASNATI/RAVOO: A. CASNATI collaborates with B. J. RAVOO to study self-aggregation processes in water.
- CASNATI/NAU: A. CASNATI collaborates with W. NAU to use polycationic calixarenes for the detection of anions of biological interest.
- COLASSON/NAU: Water-soluble fluorescent probes synthesized in the NAU group were used for displacement binding assays with metal-coordination based receptors.
- COLASSON/LE MEST: Samples of calix[6]arene based receptors synthesized in the COLASSON group have been sent to the group of Y. LE MEST for electrochemical studies.
- DALLA CORT/BARTIK: collaborate on the topic concerning anion recognition in water through the use of uranyl-salophen complexes/micelle systems.
- DALLA CORT/RODRIGUEZ: newly synthesized Zn-salophen derivatives are studied as receptors for biological relevant anions ( $\text{AMP}^{2-}$ ,  $\text{ADP}^{3-}$  and  $\text{ATP}^{4-}$ )
- DALLA CORT/THERRIEN: collaborative work, addressing the possibility of solubilising in water metal-salophen complexes through the use of arene-ruthenium cages
- DALLA CORT/ASHKENASY: research program focused on the incorporation of hydrophobic metal ion complexes into the  $\beta$ -sheet assemblies, made of amphiphilic peptides in water, and study of their properties as anion binders.
- GALE/KUBIK: Samples were sent from the GALE group to the KUBIK group for calorimetric measurements.
- DEHAEN/RADECKI: Dipyrromethene and corrole derivatives synthesized in the DEHAEN group have been applied for the preparation of different types of electro-active monolayers. The characterization of the SAMs under study has been done by cyclic voltammetry (CV), Osteryoung square-wave voltammetry (OSVW), electrochemical impedance spectroscopy (EIS) along with scanning tunneling microscopy (STM).
- ESCUDE/ASHKENASY: A new collaboration directed at finding supramolecular peptide catalysts has been established between the Universitat Jaume I. It will be focused on the synthesis and structural characterization of these systems.
- GUROL/NAU: I. GUROL now collaborates with the NAU group to use cucurbiturils as sensitive coatings for QCM chemical sensors. In this context, cucurbiturils CB6 and CB7 have already been sent to the GUROL group. Quartz crystal microbalance (QCM) transducers were coated with the CBs in a self-assembly process and the materials were then characterized in their sensing performance both in gas and liquid media. A publication about the results of this work is currently being prepared.
- GARCÍA-ESPAÑA/PINA: Collaborative work between the GARCÍA-ESPAÑA and the PINA group addressed molecular reorganisation within a polytopic ligand composed of a macrocyclic compound appended with a phenanthroline unit. Also within this collaboration, work detection and discriminative of nucleotides and phosphate anions by double scorpion-like polyazamacrocycles has been carried out.
- GARCÍA-ESPAÑA/PIANTANIDA: In this context, interactions of polycyclophanes with nucleic acids were investigated.
- HUC/O'SHEA: The HUC group has started collaborating with Donal O'SHEA dealing with cell penetration using helical foldamers.
- JABIN/REINAUD/COLASSON: One PhD student (Alex Inthasot) is co-supervised by I. JABIN and B. COLASSON.
- JABIN/WOUTERS: One undergraduate student (Roy Lavendomme) from the JABIN group is currently working on the characterization by XRD analysis of calix[6]arene-based receptors in collaboration with the WOUTERS group.
- JABIN/BARTIK/BRUYLANTS: Two PhD students (Jean-François Picron and Damien Cornut) from the JABIN group are currently studying the host-guest properties of calix[6]arene based receptors in collaboration with the group of K. BARTIK.
- JABIN/LE MEST: Samples of calix[6]arene based receptors synthesized in Belgium have been sent to the group of Y. Le MEST for electrochemical studies.
- KUBIK/KRAUS: The KUBIK and the KRAUS group are planning to develop water-soluble conjugates from cyclodextrins and cyclopeptides as anion receptors.
- KUBIK/GALE: Samples were sent from the KUBIK group to the RISSANEN group for x-ray crystallography
- KUBIK/GALE/DAVIS: The KUBIK group is currently preparing samples to be sent to the DAVIS and GALE group for the evaluation of membrane transport studies.

- LICINI/RISSANEN: characterisation of triphenolamines and tris(2-pyridylmethyl)amines and the corresponding metal complexes via X-ray diffraction techniques.
- MAGRI/GALE: The MAGRI group has started collaborating with the group of P. A. GALE to study the fluorescence properties of anion sensors.
- NAU/HARBECK: A new line of collaborative research was established between the NAU group and the one of M. HARBECK involving the use of cucurbiturils for the surface modification of gold on QCM sensors, with interesting initial experimental results already available.
- NAU/PISCHEL: Research efforts in this collaboration address photophysical effects of water-soluble macrocycles, particularly cucurbiturils, on fluorescent dyes. One example involves complexation of the Hoechst 33258 dye by cucurbit[7]uril and release of the guest by a photo-induced pH jump.
- QUESADA/OTTO: R. QUESADA and S. OTTO have started a collaboration focussing on the exploration of the different factors involved in the translocation of ions through membranes mediated by synthetic receptors, in order to provide insights into the rational design of such systems.
- SKODA-FOLDES/LE MEST: The SKODA-FOLDES group has discussions with Yves LE MEST about possible collaboration in the field of electrochemical sensors.
- WOUTERS/GALE: Collaboration planned to apply high-resolution crystallography for charge density studies on cyclodextrin complexes.

It is perhaps too early to report whether socio-economic impacts can be observed within this first year of the Action.

### **II.C New networking**

This Action comprises 22 Countries and 63 individual participants. Among the participants 15 team leaders are women and 12 women scientists are in the MC. Early stage researchers represent the 35% of the participants. During the 2<sup>nd</sup> Management Committee Meeting that took place within the frame of the 1<sup>st</sup> Scientific Conference, 16 new applications to join the Action were accepted, 8 new members for WG1, 1 for WG 2, and 7 for WG3.

A new member joined the Action during the year, after the Frascati meeting, i.e. Dr Felix Zender (Switzerland) and another request of joining has been received from Australia from Prof. Kate Jolliffe. Both the applications have been approved by MC Members (e-vote). The application of Prof Jolliffe has now to be sent for approval to DC.

As reported in the Management Report part, 14 Short Term Missions have been accomplished during this first year (12 runned by young early stage researchers, mainly PhDs and Postdocs, and 2 by researchers). A series of interesting results have been obtained that will be the objective of joint publications. Concerning this, 20 papers co-authored by members of at least two different research groups collaborating within the Action were published since funding began, Annex 3.

Some members of this Action were able to obtain funding for research projects related to the overall topic of this Action through national funding agencies. Some of them are instead still awaiting the results of their applications.

- The PITTELKOW group has received funding for a project entitled "Dynamic Combinatorial Chemistry - Supramolecular Chemistry in Water". The funding is from the Lundbeck foundation, a private Danish foundation and amounts to 1.3 Million Euros.
- The KRAUS group received a grant from the Czech Ministry of Education for the project titled "Dynamic Libraries of Cyclodextrin Duplexes as a Source of High Affinity Hosts for Complexation of Organic Molecules in Aqueous Environment".
- The GARCÍA-ESPAÑA group receives funding from the Spanish Ministry of Economy and Innovation (MINECO) for two projects related to the topic of the Action: Consolider Ingenio CSD-2010-0065 and CTQ2009-14288-CO4-O1 In the first one the group

coordinates the work of eight research groups belonging to seven different Spanish Institutions.

- A. CASNATI has just submitted a proposal to the Italian Ministry of Research, which addresses anion detection in water and involves collaborating with the NAU group to use guanidinium-substituted calixarenes for the monitoring of biocatalytic reactions.
- A. DAVIS and P. GALE submitted a joint application to the British funding agency EPSRC.
- In the area of transmembrane anion transport A. DAVIS, P. GALE and R. QUESADA are involved in an EC FP7 training network application.
- A. DALLA CORT, K. BARTIK, L. RODRIGUEZ, G. LICINI, K. RISSANEN, J. LIMA, B. THERRIEN have submitted to the Italian Ministry of Research a proposal named "Integrated supramolecular technologies for chemical information processing: advanced molecular devices and materials (InfoChem)" still pending.