European Cooperation in Science and Technology
- COST -

Secretariat

Brussels, 16 December 2010

COST 4184/10

MEMORANDUM OF UNDERSTANDING

Subject :	Memorandum of Understanding for the implementation of a European Concerted Research Action designated as COST Action CM1005: Supramolecular Chemistry in Water

Delegations will find attached the Memorandum of Understanding for COST Action CM1005 as approved by the COST Committee of Senior Officials (CSO) at its 180th meeting on 1 December 2010.

MEMORANDUM OF UNDERSTANDING
For the implementation of a European Concerted Research Action designated as

COST Action CM1005
SUPRAMOLECULAR CHEMISTRY IN WATER

The Parties to this Memorandum of Understanding, declaring their common intention to participate in the concerted Action referred to above and described in the technical Annex to the Memorandum, have reached the following understanding:

1. The Action will be carried out in accordance with the provisions of document COST 4159/10 "Rules and Procedures for Implementing COST Actions", or in any new document amending or replacing it, the contents of which the Parties are fully aware of.

2. The main objective of the Action is to develop supramolecular systems that function in water and that can either monitor environmentally or biologically relevant species, control selectivity of reactions, or produce self-assembled organized structures.

3. The economic dimension of the activities carried out under the Action has been estimated, on the basis of information available during the planning of the Action, at 48 Million € in 2010 prices.

4. The Memorandum of Understanding will take effect on being accepted by at least five Parties.

5. The Memorandum of Understanding will remain in force for a period of 4 years, calculated from the date of the first meeting of the Management Committee, unless the duration of the Action is modified according to the provisions of Chapter V of the document referred to in Point 1 above.

A. ABSTRACT AND KEYWORDS

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.

Keywords: molecular recognition in water, supramolecular control of reactivity in water, chemosensors, responsive auto-assembled materials, environmental monitoring and biological diagnostics.

B. BACKGROUND

B.1 General Background

The monitoring in aqueous environments of compounds present at an extremely low concentration is a subject of great current interest. The release of large amount of untreated water deriving from industrial processes and/or from the discharge of urban waste is a problem of great concern. One of the major challenges of this century is the provision of safe drinking water for a growing population. In trying to address this issue, the first need is for water analysis, to determine if a supply is safe.

The analytical detection of compounds present at low concentrations is often difficult and represents a problem not only for environmental monitoring but also in medical diagnostics. A tremendous amount of research needs to be conducted in order to set-up robust new methods for water monitoring. In this context, the development of synthetic receptors or, in general, of synthetic building blocks that can selectively interact in water with a given substrate or self-assemble to yield highly responsive functional materials is a topic of increasing importance. The development of systems that can efficiently and selectively interact with target species in water is intrinsically difficult. Recent developments do however suggest that solutions can be found through a supramolecular approach which takes its inspiration from the natural world. Nature achieves extremely high affinity and selectivity towards targeted substrates in water through multiple weak, non-covalent interactions between the binding partners.

The control of reactions in water (including their regio and stereoselectivity) is also the object of much attention with the growing interest in the development in the chemical industry of environmentally benign processes - water is undoubtedly considered the “greenest” solvent on Earth because of its non-toxicity and abundant natural occurrence. Here too a supramolecular approach should lead to the development of efficient systems able to control reactivity in water.
Why COST? Many European groups are working on recognition in water but a cooperation between these groups would be beneficial for the development of this field of research. Exchange and harmonization of the knowledge already available in the groups should stimulate further developments and breakthroughs. A fruitful cooperation can be guaranteed by a COST Action that offers the best open platform favouring scientific and technological exchange on a large scale. Regular meetings and STSMs prompt the exchange of knowledge and know-how better and with more flexibility than other funding opportunities. A COST Action is the proper tool to “seed” scientific cooperation in Europe. Once closer collaborations have been established between the groups involved in this COST Action, the platform could serve as the ideal starting point to apply for joint project-based funding at the European level.

B.2 Current State of Knowledge

The reviews by Reinhoudt and Oshovsky entitled "Supramolecular Chemistry in water" (*Angew. Chem., Int. Ed.* 2007, *46*, 2366-2393) and by Zayed *et al* entitled "Chemical complexity – supramolecular self-assembly of synthetic and biological building blocks in water" (*Chem. Soc. Rev.* 2010, *39*, 2806-2816) present an overview of the most recent advances in the area of water-soluble synthetic receptors and of self-assembly and molecular recognition in water. These reviews can be considered as an extensive description of the state of the art in the field of this proposal. In the conclusions of Reinhoudt's review one can read: "*However, the role of the unique properties of water in molecular recognition and self assembly is not completely understood, and good receptors for many organic guests have not yet been found. Therefore, a substantial growth of research in the area of supramolecular chemistry in water is expected*". In 2007 an Exploratory Workshop on Biosupramolecular Chemistry supported by the European Science Foundation (ESF) was held in Bristol, U.K. Participants were asked to define priorities and the task that received top priority was related to non-covalent interactions between polar units in water because "*this aspect of molecular recognition is still poorly understood, and a concerted effort to solve the problems would be very timely*". This COST Action aims at fulfilling this vision.

The need for the monitoring of important, biologically relevant species or pollutants in aqueous environments, the development of synthetic receptors or, in general, of synthetic building blocks that can selectively interact in water with a given substrate or self-assemble to yield highly responsive functional materials, require thoughtful investigations and rigorous answers. The complexity of the problem and the broadness of possible applications (medical diagnostics, analysis of biological systems, environmental monitoring etc.) definitely call for this COST Action.
A number of research groups in COST countries are currently studying how to construct water-soluble receptors, but there is a lack of coordination in these efforts and there is no unified European network devoted to this important field. COST is undoubtedly the appropriate system to help unify these ideas, strengthen the necessary trans-national research and innovation capacities and develop the potentialities and future applications of the proposed objectives.

The present project will advance the state of the art by:

- coordinating the efforts of the participating groups
- integrating different expertises
- enhancing collaboration and the exchange of ideas
- providing an open architecture that supports data exchange among the participants.

The basic innovative contribution of this project consists in a supramolecular approach to selective, highly efficient recognition in water and to its related applications that have not been pursued till now in a systematic way by a network of coordinated and deeply interacting laboratories, like in this Action. Human potential in research and technology in Europe will be strengthened, both quantitatively and qualitatively.

B.3 Reasons for the Action

The main purpose of the research that will be undertaken in the framework of this COST Action is to develop supramolecular systems that allow efficient and selective recognition processes to occur in water, to learn how to control the reactivity of such systems in aqueous medium and to achieve "smart" self assembling organized systems. The Action aims at boosting the application of such systems to encounter practical societal needs while providing scientific and technological advances. The reason for launching this Action is to help overcome the lack of interaction between the different groups working on topics related to the field of supramolecular recognition in water and to bring together knowledge that is currently disseminated in different groups. There is excellent research occurring in Europe and the interaction among the groups involved in this Action will bring the fundamental research already performed in this field to an even higher level, promoting scientific excellence and competitiveness.

B.4 Complementarity with other Research Programmes

Interest in the objectives addressed by this Action is witnessed by different projects undertaken within Europe, although they vary with respect to the way the problems are addressed:

- The importance to have efficient tools for detecting pollutants present in water is evidenced by COST Action 636 “Xenobiotics in the Urban Water Cycle” (end March 2009) and Action 637 “Metals and Related Substances in Drinking Water” (end November 2010). Theses Actions had as objective to set up strategies for minimizing the impact of water pollutants on humans and ecosystems. In the recent July 2010 FP7 call one can furthermore find the call "NMP.2011.1.2-3 Active nanomembranes/-filters/-adsorbents for efficient water treatment with stable or regenerable low-fouling surfaces" which is described as “nanotechnology for benefiting environment, energy and health”.
- The design of sensing devices for analytes of biological importance (medical diagnostics) is addressed in the July 2010 FP7 call “HEALTH.2011.2.3.1-4: Development of multi-analyte diagnostic tests” and also in the “NMP-2009-4.0: Development of nanotechnology-based systems for molecular diagnostics and imaging” and the “NMP.2010.4.0-1 Development of nanotechnology-based systems for detection, diagnosis and therapy for cancer”.
- Self-assembly in water of synthetic building blocks promoted by the environment and/or the presence of specific analytes can lead to the formation of fascinating structures that contribute to progress in the science and technology of sustainable and functional materials. Also in this field, several separate initiatives within Europe confirm the interest of the scientific community. For example, in the November 2008 FP7 call *Nanosciences, Nanotechnologies, Materials and new Production Technologies* the following theme is presented “NMP-2009-2.3-1 Biomimetic gels and polymers for tissue repair”.

This non-exhaustive list of examples helps to prove the significance of the problems that will be addressed as well as the interest of the scientific community towards them. This COST Action aims to coordinate the different efforts in this area with a supramolecular approach, which has not yet been undertaken. Thus this Action is unique in the sense that it will give the opportunity to create a European network focusing on different aspects of supramolecular chemistry in water. The aim is ultimately to provide answers to practical problems related to water pollution, to the sensing of biologically relevant species and to the development of new materials with potential applications in regenerative medicine and tissue engineering. The attention that will be devoted to the practical applications of the research will also intensify the dialogue between science and society in Europe.

C. OBJECTIVES AND BENEFITS

C.1 Main/primary Objectives

The main scientific objective of this COST Action is to develop supramolecular systems that function in water. Through the investigation and control of the multiple weak reversible non-covalent, but collectively powerful, interactions that allow efficient and selective recognition processes to occur in water, it will be possible to boost the application of such systems towards the achievement of several major goals: (i) the 'de novo' design of receptors able to monitor biologically and environmentally relevant species in an aqueous environment with high selectivity and affinity; (ii) the control of supramolecular reactivity in water by biomimetically inspired systems; (iii) the production in water of self assembled organized structures which are stimuli responsive and which can be used for programming functions in materials and devices.

C.2 Secondary Objectives

It is important to consider the main objective mentioned above within the context of the following long-term scientific goals that will be carried out during the whole Action:

- To gain insight into the nature of weak interactions that enable recognition at the molecular level to occur in water with high selectivity,
- To apply the principles of supramolecular chemistry to the design of systems which can mimic the catalytic action of enzymes.
- To obtain self-assembly in water.

The secondary objectives of this action include:

- Focusing on high affinity/high sensitivity for a chosen analyte
- Investigating multiple, instead of isolated, non covalent interactions that enhance binding affinity as well as selectivity.
- Obtaining rationally designed synthetic building blocks that can selectively interact in water with a given substrate.
- Developing chemical sensors for monitoring biologically and environmentally relevant species.
- Designing scaffolds able to self-assemble to yield highly responsive functional materials.

C.3 How will the objectives be achieved?

The objectives of this Action will be reached through the creation of a network of leading European groups who have expertise and knowledge in the field of supramolecular chemistry. The participation in this Action of researchers with sound and documented experience in supramolecular chemistry and who have methodological complementarities will provide the appropriate manpower necessary to pursue the tasks outlined in the project. A good coordination of the different expertises and a close collaboration among the groups represent the key to success. The participation of young researchers will add new creative and original contributions and for these researchers, being part of such a large community will enable them to broaden their scientific and generic skills. The establishment of an international network will provide a central point for those who wish to join the Action in a subsequent period.

C.4 Benefits of the Action

The benefits of the Action for the European society will be:

- To learn how to master self assembly in water via specific interactions occurring between simple building blocks.
- The design of simple systems able to mimic and compete with the catalytic action of enzymes.
- The development of “smart systems” (synthetic receptors, auto-assembled responsive materials) that can monitor biologically relevant species and dangerous xenobiotics in water.
- An enhancement in the knowledge related to weak, multiple interactions working in water. This will help to develop artificial systems inspired by Nature.
- The strengthening, through coordination, of international research with a view to reap all the advantages deriving from the exchange of expertises and knowledge among the groups and the benefits of internationalisation, such as the mobility of young researchers.
- The “creation” of human resources, i.e. young specialists with good knowledge in a topical, high performance field.

C.5 Target groups/end users

The target audience of this COST Action who should benefit from the disseminated results is University and Research laboratories operating in the field of supramolecular chemistry within Europe. The end users of the generated knowledge will be mainly the research scientists but also SME´s (Small/Medium Enterprise), start-up and spin-off companies.

D. SCIENTIFIC PROGRAMME

D.1 Scientific focus

All the projects carried out by the participating scientists and laboratories will be driven by the need to fulfil the primary objective of this COST Action: the development of supramolecular systems that work in water. This action is flexible enough to incorporate a variety of projects ranging from fundamental research to the design of devices and materials that can be used for various applications. It is open to host the large variety of existing research related to the problem of supramolecular recognition in water. The scientific program is securely based on the extensively documented knowledge already present in the interested laboratories which are furthermore well equipped to undertake the research.

The main lines of research which will be adopted and on which work will focus within this Action can be summarized as follows:

i) The design and synthesis of receptors that present both high affinity and high selectivity in water for selected guests. Natural systems provide inspiration for the design of artificial receptors and should be used to gain some understanding pertaining to the binding forces that contribute to the formation of complexes. Biology shows us that remarkable feats can be achieved by highly structured molecules through non-covalent interactions. The highest level of sophistication of supramolecular chemistry is found in living systems where elegant supramolecular assemblies of bio-organic molecules make up the machinery which enables and supports life functions. For example enzymes, which are macromolecular protein hosts, catalyze important reactions with non-covalently bound guest organic molecules. The recognition of the guest molecule among all others present in the surrounding aqueous environment and the transport of this guest to the active site involves a sequence of steps starting with the recognition of the substrate by the exterior of the global supramolecular assembly followed by the binding of the guest to the external surface of the enzyme. The guest is then shuttled from the external surface through to the enzyme’s internal structure until it reaches the active site to which it binds.

When comparing the affinity of biological receptors for their target molecule vs. that of known synthetic ones, one can observe that there is a difference of at least 6 orders of magnitude. Much effort still needs to be made in order to fill this gap. A better knowledge and understanding of the principles of supramolecular chemistry in water will enable the design of simple models of biomolecules that can mimic the natural recognition process and also in certain cases their catalytic action.

ii) The supramolecular control of reactivity in water is a relatively new and exciting area of research which represents a very stimulating challenge. The use of non-covalent interactions to maintain and orient reactants during a bond-forming reaction is an appealing objective. This can be achieved, for example, by using a supramolecular host to simultaneously bind the reactants while controlling the regioselectivity or stereoselectivity of the reaction between them. Other challenging aspects of supramolecular assisted synthesis will also be addressed. One is supramolecular assistance to the synthesis of molecular compounds, in which either a recyclable template dictates the outcome of a reaction to give a product that would not be made as efficiently without the template, or in which a permanently entrapped template leads to the formation of an interlocked molecule, e.g., a catenane or a rotaxane. Furthermore it should be possible to obtain (i) small discrete supermolecules, such as molecular capsules or (ii) large supramolecular arrays (grids, helicates). Achieving these goals in an aqueous environment will bring research a step closer to functional systems that imitate biological processes and have the potential to even participate in them.

iii) The study of the principles that govern self-assembly in water is a very challenging part of the project and developments in this area can lead to highly responsive self-assembled materials with fascinating properties. The history of human civilization is divided into ages according to the materials that dominated in the society. We entered the “modern materials age”, the plastic age and the silicon age in the 20th century. When looking at the types of materials that lie ahead, they can be designated as “designed materials”. One way to achieve these new materials is through molecular self-assembly. Self-assembly is ubiquitous in Nature at both the macroscopic and microscopic scales and describes the spontaneous association and organization, without external instructions, of numerous individual entities into coherent and well-defined structures. Molecular self-assembly is by definition the spontaneous organization of molecules under thermodynamic equilibrium into structurally well-defined and rather stable arrangements. The stability is the result of a number of non-covalent interactions which are individually weak, but their large numbers will dominate the structural and conformational behaviour of the assembly. The key elements in molecular self-assembly are the complementarity and structural compatibility of chemical functional group. The achievement of self-assembly in water, starting from simple synthetic building blocks, will lead to supramolecular materials that are instructed, dynamic, combinatorial and which can behave as adaptive materials. Potentially important applications of such derivatives can be envisioned for example in regenerative medicine and tissue engineering. There is also an interest in the controlled self-assembly from complex mixtures of different building blocks with the aim of building systems with multiple components, capable of orthogonal molecular recognition and hence of self-sorting different molecular-scale and nanoscale components. This may, in the longer term, allow 'smart' (programmed) self-assembly to lead to hybrid multi-component materials in which different building blocks assemble into different nanostructures that endow the material with different properties. Materials with new properties are keys to the future competitiveness of European industry and the basis for technical progress in many areas.

D.2 Scientific work plan methods and means

Based on the lines of the scientific research described above, the Action will be divided into three Working Groups (WG). It is however important to point out that the three lines of research are deeply interconnected and derive from the common starting point of gaining insight into the nature of weak interactions that allow recognition at the molecular level in water.

Working Group 1: Supramolecular Recognition and Supramolecular Sensing in water.
Experimental studies as well as theoretical and modelling studies will be undertaken on different systems in order to shed light on the fundamental processes of molecular recognition in water with the aim to achieve a full thermodynamic understanding of the structure-activity effects which underpin binding:
The design and building of water-soluble supramolecular structures that can act as hosts in molecular recognition processes and accommodate guest molecules by means of weak intermolecular interactions will be undertaken. A variety of systems will be investigated by the different research groups who have different synthetic expertise: non-natural cyclopeptides, metallosupramolecular complexes, multivalent dendritic structures, abiotic guanidinium based hosts, cyclodextrin, calixarene and cucurbituril based systems. Systems will be systematically varied in order to turn on or off interactions so as to understand how multiples interactions are influencing each other and how interactions need to be combined to achieve stable and selective substrate binding in an aqueous environment.

The binding of different species of interest, such as neurotransmitters, amino acids, drugs, carbohydrates, protein surfaces, physiologically important anions and pollutants, will be monitored. These receptors should eventually serve as molecular sensors to detect biologically and environmentally relevant species. The affinity, selectivity and stereoselectivity will be examined using different techniques: isothermal titration calorimetry, spectroscopic methods, electrochemical methods, modelling.
The structure of the systems will also be studied using the different methods (NMR, Xray crystallography, modelling…) with which the different laboratories are equipped.

Working Group 2: Supramolecular Control of Reactivity in Water.

Supramolecular control of reactivity in water represents a challenge and a real innovative task of this proposal. One of the aspects of reactivity that will be explored within this WG is catalysis, which is a longstanding proposed application of supramolecular chemistry. Work will be done in this context to make use of weak, non-covalent interactions as tools for the development of more active and more selective catalytic systems working in water. Nature is of course a good guide and a source of inspiration for the design of these systems. With this perspective molecular receptors will be designed and synthesised in which a catalytic site is placed close to a binding site that has been designed to interact selectively with the reactant and also molecular receptors that promote the reaction of two simultaneously complexed reactants, kept together reversibly in a ternary complex. Many of the systems already handled by the research teams involved in this Action will be tested in this context and new ones will be prepared *ad hoc*, taking into account that these have to be, or become, water soluble. Among the most appealing systems for this kind of study supramolecular gels will also be considered. In these materials molecular information is precisely translated from the molecular level into the supramolecular one. Thus gelators will be designed and synthesised with active groups on their periphery in which changes of activity are observed upon aggregation into fibrillar gels. This will lead to the development of self-supported reusable catalysts for organic transformations.

Through the investigation of the weak interactions surviving in water the possibility of performing supramolecular assisted synthesis in this medium will also be studied. The guiding principles for the development of this point are molecular recognition and self-assembly. The control can be either kinetic or thermodynamic or a mixture thereof.

Workgroup 3: Self-Assembly in Water.

Work will be undertaken in order to contribute to the fundamental understanding of the factors which control self-assembly and in order to try to highlight how changes at the molecular level affect the properties of the assembled structure at the nanometre scale. Different tasks will be undertaken.

Synthesis of different classes of self-assembling units: zwitterionic based units with different linker sizes and flexibility, dendrimers, metallosupramolecular polymers, fibrillar networks.
Study of the self-assembly process and its possible control by external stimuli such as pH or the presence of competing ions. The combination of different synthetic fragments will also be envisaged in order to assemble multi-component systems in aqueous solution.
The structure and the properties of the obtained soft materials will be characterized using the techniques available in the different groups.

E. ORGANISATION

E.1 Coordination and organisation

"Ice-Breaking" stage of the Action. This COST Action will represent an open and flexible framework running for 4 years. To be successful, the Action will need both a large creative input from European scientists and a high level of coordination between the participants. The participation to the COST Action during the first stage will be promoted by actively advertising it in relevant conferences, journals, webpages and via mailing lists.
The Management Committee will be the top-level supervisory body of the COST Action and will coordinate the Action's activities according to the "Rules and procedures for implementing COST Actions". The constitutional MC meeting will take place in the first months and the Action's chairpersons and Working Group Leaders will be appointed. They will form the Steering Group, which will examine and decide, on behalf of the MC, WG participation. Decisions will be based on meritocratic principles and intrinsic research quality, taking into account thematic complementarity, pertinence of the application, the participation of early-stage researchers as well as gender issues.
After the recruitment step (6 months), the Action will have its kick-off meeting. On this occasion the MC will elect (i) a STSM (Short Term Scientific Missions) manager and (ii) a Dissemination manager. During this kick-off meeting, the local organizer for the first annual meeting will be chosen.

The WGs will have their constitutional meetings up to 3 months after the kick-off meeting.
At the end of the constitution phase the Action will have the following management structure:

- A Management Committee in accordance with the COST rules working in good agreement with the COST Science Officer and the Domain Committee.
- A Steering Group elected among the MC members and including: Action Chair, Action Vice, WG Leaders, STSM Manager, Dissemination Manager.

Operation Stage. The MC will meet at least every six months and its main responsibilities will be to plan and design the activities of the Action, supervise their implementation, monitor progress, allocate resources and reconcile eventual conflicting viewpoints. The MC will monitor the effective and correct development of the COST Action through its regular meetings. The first annual meeting is scheduled for month 18 after the start of the Action. The Action Chair will present the structure and the objectives of the Action. Workplan lectures for each WG will be delivered by the WG leaders. Before the scientific programme, the Steering Group will meet briefly to discuss organizational issues. A number of contributions by invited external experts will favour brainstorming discussions helpful for the development of the Action. A MC meeting will be scheduled at the end of the event. Other meetings will follow according to the schedule established by the MC.

Research in this COST Action will be addressed in the WGs with a strong emphasis on horizontal contacts so as to be able to exchange research directions, information and expertise. Each WG will have meetings on a regular basis and these will be open to the researchers of the other WGs.
The establishment of a broader network and the attraction of new scientists to the research area promoted by this COST action will be achieved through the planned annual conference, the regular update of the COST Action website and periodical e-mail newsletters. The Action will promote and support the launch of National and EU research activities in the field of supramolecular chemistry in wate,. The Steering Group will work out the annual budgeting, distributing funding for the annual meetings of the Action, the meetings of the WG and STSMs.
Training Schools on topics relevant to a large number of Action members will also be organized and funded.

The progress of the different activities (especially of the STSM involving early-stage researchers) will be recorded in an annual Progress Report. The MC will also confirm and adjust the planning of the action in order to increase the value of its achievements and to correct or update deviations from the original plans.

Expected milestones include:

- A substantial number of high-level papers from participants [throughout the 4 year period].
- The attainment of a strong European network [till the midterm evaluation].
- The boosting of the application of the research towards the achievement of the major goals addressed by this Action [from midterm evaluation till the end].
- The launching of joint applications to research funding programmes [after the first year, till the end of the Action].

E.2 Working Groups

In this COST Action, three WG will be formed, responsible for the fulfilment of the scientific goals of the presented Research Project. The limited number of the WGs proposed will guarantee a high level of horizontal contacts and coordination.

WG coordinators will lead the scientific discussions, coordinate the activities of the sub-projects, monitor the milestones and provide the Chair with brief yearly reports which will be disseminated on the WG webpage linked to the Action's webpage. WG coordinators will coordinate the activities in their own research areas, but also in areas resulting from ideas sparked by the dialogue that will be created and sustained between the three research communities.

Each WG is expected to meet at least once a year.

The three working groups planned at this moment cover the following subjects:

- Supramolecular Recognition and Supramolecular Sensing in Water
- Supramolecular Control of Reactivity in Water
- Self-Assembly in Water

E.3 Liaison and interaction with other research programmes

The Action includes topics, which might be interesting and constitute points of potential contacts for ongoing research in the following European initiatives:

- CMST COST Action CM 0703 “Systems Chemistry” (End date: April 2012).
- CMST COST Action CM 0701 “Cascade Chemoenzymatic Processes – New Synergies Between Chemistry and Biochemistry” (End date: April 2012)
- CMST COST Action TD 1003: “Bio-inspired nanotechnologies: from concepts to applications” (End date: May 2014)
- ESF Research Networking Programme in Medical Sciences “Regenerative Medicine (REMEDIC)” (End date 2013)
- Research programmes supported by FP7 and dealing with the theme “Nanosciences, Nanotechnologies, Materials and New Production Technologies”
- The EUROCORES (**Euro**pean **Co**llaborative **Res**earch) programme "Synthetic Biology: Engineering Complex Biological Systems (EuroSYNBIO)" of the ESF

Frequent contacts with other COST Actions and with coordinators of Projects and Networks under FP7 and ESF will ensure complementarity with this Action and will provide a list of scientists who could be potentially invited to participate in the Action’s activities.

The Action will have an impact on the worldwide forum notably by (i) participation in international conferences; (ii) creation of associate memberships for active research groups in the field outside Europe and bordering Europe; (iii) representation in global organisations.

E.4 Gender balance and involvement of early-stage researchers

This COST Action will respect an appropriate gender balance in all its activities and will also be committed to considerably involve early-stage researchers which will be one of the hallmarks of the Action. These items will be placed as standard items on all MC agendas.
An effort will be made to maintain a good gender balance in the elected members of the COST Action and maintain national diversity in all teams.
The development and the management of the relationships between the research groups are very important. STSMs will be employed as a managerial means to achieve this, especially with the aim of creating novel, unexpected links between disciplines and providing individuals with the understanding, skills and access to information, knowledge and training that enables them to perform effectively. The different research groups will provide significant scope for Short Term Scientific Missions, with priority given to early stage researchers (MS, PhD students and young postdoctoral scientists). This will promote the involvement and also the career of the early-stage researchers too. Short training courses will be announced during the WG meetings to help the PhD students/early-stage researchers to access information necessary for their cultural enrichment.
The COST Action is committed to the goals of the Helsinki Group on Women and Science and will encourage a strong participation of young women researchers. The participation of women early in their careers is seen as a way to fortify their involvement in the field, increasing the possibility of achieving a better gender balance in the future.

F. TIMETABLE

Year 1	
Month (M) 1-2	First MC meeting bundled with Steering Group meeting
M3	Website Publication
M6	Kick-off meeting bundled with Steering Group meeting and MC meeting
M7-M12	WG meetings
M9-M12	STSMs
Year 2	
M4	Annual meeting bundled with Steering Group and MC meeting
M5	Training School
M8-12	WG meetings
M1-M12	STSMs
Year 3	
M4	Midterm evaluation meeting bundled with Steering Group and MC meeting
M8-12	WG meetings
M1-M12	STSMs
Year 4	
M3	Steering Committee Meeting and MC meeting for Action closing conference and for final evaluation preparation.
M4-10	WG meetings
M5-M7	Training School
M11-M12	Closing conference and MC meeting for final report
M1-M10	STSMs

G. ECONOMIC DIMENSION

The following COST countries have actively participated in the preparation of the Action or otherwise indicated their interest: BE, CZ, DE, ES, FI, FR, IE, IT, NL, PL, PT, UK. On the basis of national estimates, the economic dimension of the activities to be carried out under the Action has been estimated at 48 Million € for the total duration of the Action. This estimate is valid under the assumption that all the countries mentioned above but no other countries will participate in the Action. Any departure from this will change the total cost accordingly.

H. DISSEMINATION PLAN

H.1 Who?

This Action will disseminate its research results with the aim of promoting the leadership of the European supramolecular community in order to counterbalance the increasingly severe competition from Asian, American, and other non-European countries. Research institutes, universities, industrial laboratories, and national scientific societies will be informed of the work undertaken by the Action's members, thereby promoting supramolecular chemistry in water and its related applications. Although the Action itself is primarily academic in nature, the fundamental research produced by it should have a significant impact in the industrial sector. The main target audiences for the dissemination of the results of the Action will be:

Target A: Researchers in (bio)chemistry, physics, computing science from academia or industry.

Target B: European Union policy makers in charge of planning.

Target C: The general public and particularly high school students by promoting interest in this area of chemistry, encouraging them to choose science as a path for their future career.

H.2 What?

The results of this Action will be disseminated within the research community by established scientific communication channels, such as publications, web sites, oral and poster presentations at conferences, and seminars. Short Term Scientific Missions between the COST participants will allow dissemination of knowledge between the adhering groups. The two Training Schools planned by this Action will promote the dissemination of research activities to a wider scientific community by attracting young researchers. Support from funding agencies will be asked for in order to provide a large number of grants to enable early-stage researchers to participate in the Training Schools. The annual reports will be made available by electronic means to all potentially interested in the work undertaken. The final report will be printed and distributed widely to scientists and researchers in both academia and European companies with an interest in the field.
All target audiences will have access to the Action's web page. It will contain:

- a searchable description of the project together with results,
- news and announcements to the members of the Action and to the general public,
- a web based mailing lists and an archived discussion forum.
- databases of articles, data and other information compiled for knowledge transfer,
- update the schedule of meetings and STSMs.

The webpage will be partly password secured and allow upload of data, findings, draft reports and unpublished material. Activity reports, publications and news will be published on the free-access part of the web page.

Target A will be addressed through publications in leading scientific journals,. Joint publications involving researchers from more than one group will be strongly encouraged. The scientific community at large will benefit from review articles published in journals and on web sites, including the annual reports and the final report of the Action, by, invited or contributed lectures at (inter)national conferences and workshops, and also by talks delivered at institute seminars.

Target B will be reached by research proposals, individual or joint ones at the EU level.

Target C will be addressed by public media. Preparation of articles directed to a more general audience and published in non-specialised journals will be used to expand the public knowledge of this Action. The contents of selected conferences and the material presented at the training schools could be the subject of specific books and of interactive CD/DVD supports. Contributions to educational TV science shows will also be considered.

H.3 How?

- Each Action participant will be obliged to acknowledge COST funding if a peer-reviewed paper is published in the broad context of supramolecular chemistry in water.
- Each Action member will mention and briefly describe the Action if he gives a lecture or a talk anywhere outside the Action.
- The COST and Action's logo will routinely appear on the acknowledgement slide of talks and on conference posters.
- Scientists belonging to Target A will be informed about the Action's annual and Working Group meetings via electronic mail and by the dissemination of fliers announcing the event.
- A number of leading scientists from outside the Action will be invited to present keynote or invited lectures at the different meetings of the WG or at the annual meetings.
- Each Action member who is invited to contribute to a TV or radio interview, or to a general overview article in a journal addressing the general public will announce that his or her work is embedded in a COST Action on supramolecular chemistry in water.
- The Action will proactively contact the press, once a breakthrough result has been freshly published in a high-level journal.
- The refinement of the Action's objectives as a result of self-evaluation and external evaluation (midterm) will be published on the Action's website.