



European Science Foundation
Standing Committee for Physical and Engineering Sciences (PESC)

ESF PESC EXPLORATORY WORKSHOP

Self-assembly of guanosine derivatives: from quadruplex DNA to biomolecular devices

Scientific Report



Bled, Slovenia, 12 - 15 September 2006

Convened by:

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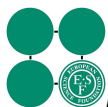
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Co-Sponsored by Slovenian Research Agency





1. Executive summary

1.1 General overview

The ESF Exploratory workshop on Self assembly of guanosine (G) derivatives was held in Bled, Slovenia from September 12-15, 2006. The meeting was convened for 2 ½ days and was attended by 28 leading scientists from the field. 26 contributions presented in the form of oral lectures provided an extensive scientific discussion on the current state-of-the-art as well as on some open problems in the field of the self assembled G-structures. Two round-table discussions pointed out future perspectives in the G research field and open possibilities for cooperation between various research groups involved in the topic.

In addition to usual discussions following the lectures, informal free discussions were also an important part of the meeting. These were made possible by arranging extended periods for meals, which were served for all the participants in the same pleasant place. The »conference dinner«, which was organized at the medieval Bled castle, provided insight into the ethnologic tradition and history of Slovenia.

Before the workshop each participant submitted an one-page abstract describing his/her contribution at the meeting. The abstracts were collected together and electronically distributed to all the participants before the starting. This assured that everybody was informed in advance about the topics that were discussed at the meeting and could envisage coordination with his/her specific research interests. The book of abstracts in printed version was distributed among the participants at the starting of the meeting. Workshop contributions (presentations) were collected in the electronic form and with permissions of the authors they were printed on the CDs, which were sent to all the participants 1 month after the meeting..

1.2 Background of the meeting

Self-assembly of guanosine molecules gained a renewed interest with the recent observation that G-quartets are formed in many sites of the human genome, which indicates the biological relevance of the self-assembly process. This finding triggered an expanding research of the associated structures and phenomena. The importance of G-quadruplex assemblies in vivo (in telomere structure and function) requires development of a comprehensive knowledge of the structural and folding properties of the G-rich DNA regions.

In addition, it was found that Guanosine-based self-assembled structures (G-quartets and G-quadruplexes) possess large potential that connects biological with the technical world. Many recent successful demonstrations of applications of the G-based materials in areas ranging from medical chemistry to molecular nanotechnology and biotechnology require a rapid progress of the interdisciplinary expertise on the topic, which is connecting molecular biology and soft-condensed matter physics with supramolecular chemistry.

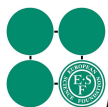
At present the guanosine research field worldwide evolved into various branches and directions. Also in Europe the number of different laboratories and people involved in the field is rapidly increasing and so the field became ripe for exchange of ideas and collaboration. This can be most efficient if a topical meeting in person is organized.

The basic stimulation for organization of the workshop was: (i) to bring together representatives of the important research groups working on self-assembly of the G-quartets, (ii) to establish a link between physicists, chemists and biologists and (iii) to review the current state of knowledge, research activities and future perspectives of the field.

1.3 Content of the meeting

The presentations given at the meeting were divided into the following subtopics:

- Synthesis and supramolecular chemistry of G-assemblies
- Structure analysis by magnetic resonance (NMR) and other techniques
- Chirality and lyotropic liquid crystal polymorphism
- Solution properties
- Surface assembly and surface structures



- G-quadruplex complexes in telomeric DNA
- Atomistic simulations of G4 structures
- Electrical transport and nanotechnical applications

6 participants gave keynote lectures, which took place for 30+10 minutes and were aimed to provide besides the original research results of the speaker also a broad introduction of the specific subtopic and a review of the present state-of-the art in the related subfield. 20 participants described their work in invited lectures, which took place for 15 minutes + 5 minutes for discussion. The details on contributions are given in Section 2.

Two evenings were devoted to 60 min round-table discussions and the following aspects were identified:

a) in relation with future perspectives of the field:

- Guanosine derivatives show great promises for tailored patterning on surfaces and therefore various surface structures should be more explored
- An important open problem is ionic conduction of G4 wires and their analogues
- The materials provide a very rich chemistry which should be further explored, for instance with respect to hydrophobic/hydrophilic modifications
- In future more comparative studies using different experimental techniques should be performed to obtain deeper insight into structural properties.
- More emphasis should be put on protein-G-quadruplex, metal-G-quadruplex complexes and other biologically important issues

b) in relation with future cooperation in the field:

- Similar topical meeting should be organized also in the future
- Informal network of the research groups working on the topic will be established via the web page of G4 researchers initiated by the organizers of the workshop
- Investigations toward medical applications are very promising and closer cooperation with pharmaceutical companies will be envisaged
- Cooperation of the research groups contributing to the workshop will try to be formalised within the calls of the 7th European framework programme

It was agreed that new directions may yield materials which could be exploited for advanced applications as new generation of anticancer drugs, ionophores and synthetic ionic channels, biosensors, and as various elements of molecular electronic devices. They may therefore have impact on a wide range of industrial sectors including pharmaceutical, cosmetics, electronics and various branches of bio and nanotechnology.

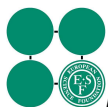
1.4 Output of the meeting

As agreed by the participants, all meeting contributions were collected in the electronic form and printed on the CDs, which provide a wealth of information on the present state-of-the-art in the guanosine research field and will consequently serve as an important knowledge base for younger researchers and newcomers to the field.

As a direct result of the meeting an application for the ESF-FWF Conference (Partnership with LFUI) was submitted on October 2, 2006. If the application is approved, the ESF conference on the topic will take place in Austria in 2008.

There was agreement that possibilities for collaborative research projects would be explored as soon as the first call within the FP7 will be launched at the end of 2006. 13 groups from 6 European countries expressed interest to be actively involved in the proposal preparation for a collaborative project. There was also agreement that other funding routes would be explored in order to exploit the new ideas which are emerging in the field.

In general all the participants found the meeting to be very successful and extremely well organized. The event itself was really enjoyable and very informative. It established strong links between researchers from ESF as well as some non-ESF countries. These links will serve as a platform for much more strengthened Paneuropean and international cooperation in the guanosine research field in future.

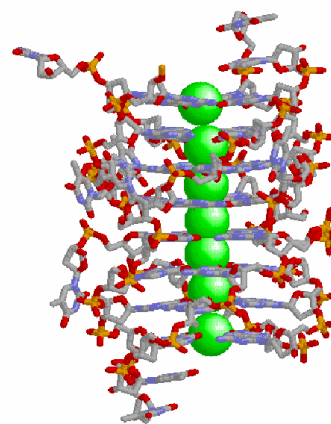


2. Scientific content of the event

In the following we summarize the scientific content of the meeting as divided in 8 thematic subtopics. It is important to note that most of the presentations described the work of larger research teams; the full list of coauthors for a specific contribution is evident from the book of abstracts.

2.1 Synthesis and supramolecular chemistry of G-assemblies

Keynote lecture: J. T. Davis (University of Maryland, USA) addressed the topic of lipophilic G quadruplexes as promising materials for construction of synthetic ionic channels and pores. The emphasis was on possibilities for selective binding of various ions. Recent results on ion transport through liposome membranes were presented. Another focus of the presentation was understanding the interactions in various DNA G-quadruplex systems. Investigations of folding/unfolding processes of some selected G-quadruplex structures were also reviewed.

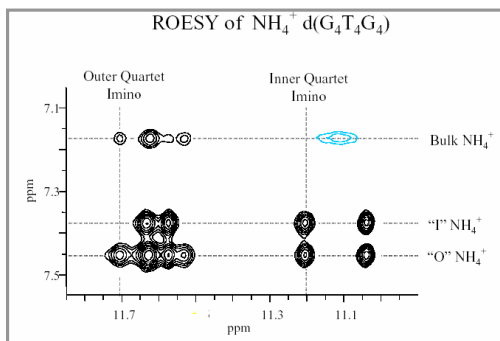


Invited lecture: J. M. Rivera (University of Puerto Rico, USA) reported on advances in supramolecular chemistry based on guanine base. He presented synthesis and studies of the self-assembling properties of a variety of base-modified 8-aryl-guanine derivatives. Part of the lecture considered also the role of metal cations used to template the G-quadruplex formation.

Invited lecture: A. B. Kotlyar (Tel Aviv University, Israel) described the synthesis and characterization of the long guanine-based nanowires. He reported a novel production method of hundreds nanometers long monomolecular G4-structures composed of a single G-strand. These structures are more rigid compared to double stranded DNA and insensitive to disintegration by DNases. Molecular labeling of G4 structures with biotin and avidin was also described.

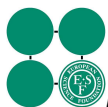
2.2 Structure analysis by magnetic resonance (NMR) and other techniques

Keynote presentation: J. Walmsley (University of Texas at San Antonio, USA) opened the workshop with wide ranging review of historical development and current progress in the field guanosine self-assembly. The emphasis was on structural investigations based on ^1H and ^{31}P NMR spectroscopy. The self-association of several ribonucleotides as a function of cation has also been discussed.



bulk solution and characteristic transport times in the range of milliseconds to seconds were resolved.

Keynote presentation: N. Hud (Georgia Institute of Technology, USA) focused on the quadruplex formed by the oligonucleotide $d(\text{G}_4(\text{T}_4\text{G}_4)_3)$, which contains several telomeric repeats of the protozoa *Oxytricha nova*. NMR experiments revealing the binding properties and mobility of NH_4^+ ions were discussed. The measurements show that these ions exchange amongst the three binding sites within the G-quadruplex and with



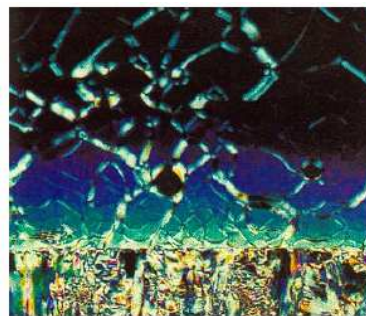
Invited lecture: J. Plavec (National Institute for Chemistry, Slovenia) addressed the problem of ion localization and mobility within dimeric G-quadruplexes. NMR investigations of several thymine residues were reported. Analysis of binding and mobility of Na⁺, K⁺ and NH₄⁺ in different G-quartet folds was reported.

Invited lecture: G. Wu (Queen's University, Kingston, Canada) addresses the quest for direct NMR detection of alkali metal ions in G-quadruplex DNA. He represented a new NMR approach for direct detection of Na⁺, K⁺ and Rb⁺ in G-quadruplex DNA. These studies yielded new information in NMR spectral signatures for alkali metal ions bound to a G-quadruplex, thermodynamic parameters for ion selectivity and ion transport kinetics.

2.3 Chirality and lyotropic liquid crystal polymorphism

Invited lecture: G. P. Spada (University of Bologna, Italy) focused on the similarities and differences between self-assembling properties of hydrophilic and lipophilic guanosine nucleosides. In organic solvents lipophilic derivatives assemble into ribbon-like structures, which form several new lyotropic liquid crystalline phases. Phase sequence of different derivatives was discussed.

Invited lecture: P. Mariani (University of Ancona, Italy) described lyotropic polymorphism, stability and energetics of guanosine four stranded helices. The resume on results of structural investigations by X-ray and neutron scattering techniques was made. The questions related to the preferential hydration, the role of lateral forces and high pressure effects on the structural and energetic properties of GMP helices in the hexagonal phase were also addressed.



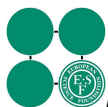
Invited lecture: D.J. Lee (Imperial College, London, UK) reported investigation of helix dependent effects in guanosine assemblies. The short review of the Kornyshev-Leikin theory of interaction between two helical macro-ions was given in the beginning. For the rest the focus was on thermal fluctuations in the azimuthal orientations of G stacks in columnar assemblies. The effect of twisting/stretching fluctuations in the 2-D lattice configuration was also discussed.

Invited lecture: A. Ferrarini (University of Padova, Italy) addressed the relation between the macroscopic chirality of nematic phases of G-quadruplexes with chirality of their molecular structure. The characteristics of the cholesteric phase, i.e. its handedness and pitch, show a subtle and hardly explainable dependence on the molecular structure. Comparison between G-quadruplex structures and B-DNA was made based on the coarse-grained model.

2.4 Solution properties

Invited lecture: H. Jurga-Nowak (A. Mickiewicz University Poznan, Poland) reported investigations of supramolecular structures of Na₂-GMP by means of photon correlation spectroscopy. Two distinctive diffusion processes were resolved, attributed to the diffusion of the stacks of monomeric GMP and to G-quartet stacks. Translational diffusion constant of G-quartet stacks was measured as a function of temperature and decomposition of the stacks was investigated.

Invited lecture: L. Spindler (University of Maribor, Slovenia) presented a study on dynamic properties of G-quartet stacks as a function of ionic concentration. Combined results of ³¹P NMR spectroscopy and dynamic light scattering measurements (DLS)

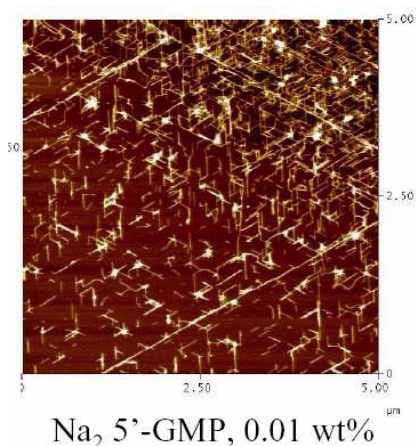


show on a profound polyelectrolyte behavior of the stacks. The observed behavior can be described by the Coupled Mode Theory for polyion solutions taking into account also counterion condensation.

2.5 Surface assembly and surface structures

Keynote presentation: J. Vesenka (University of New England, Biddeford, USA) started his lecture with reviewing investigations of surface structures of guanosine derivatives on different solid substrates. Then he focused on atomic force microscopy (AFM) investigations of G-rich oligonucleotides on the surface of mica. He reported an interesting phenomenon of auto-orientation and manipulation of G-wire DNA networks. The potential for using auto-orientation phenomena in the development of high-density biomolecular nanoelectronic devices was also discussed.

Invited lecture: R. Otero (Autonomous University of Madrid, Spain) reported on self-assembly of Guanine quartet networks and other DNA-base structures on solid surfaces. The emphasis was on surface assemblies formed on Au(111) substrates in high vacuum conditions.



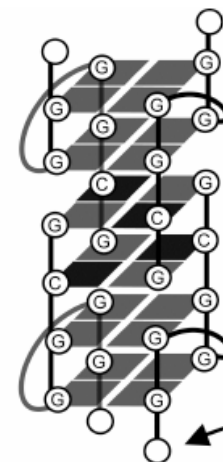
High-resolution variable temperature scanning tunneling microscopy (STM) showed that guanine molecules deposited under such conditions self-assemble into a H-bonded network of g quartets with the same structure as that found in quadruplex telomeric DNA. This finding provides a framework to evaluate the accuracy of different assumptions that are commonly used in MD simulations of nucleic acids.

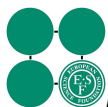
Invited lecture: I. Drevenšek-Olenik (University of Ljubljana, Slovenia) reported on atomic force microscopy (AFM) analysis of surface assemblies of GMP on mica substrates. A comparative study of surface structures deposited from solutions of K, Na and NH₄ GMP salts was made. The results show that cations play a minor role in surface assembly. The formation and orientation of long 1D aggregates (G4 wires) depends mainly on the concentration of the starting solution and on the deposition process.

2.6 G-quadruplex complexes in telomeric DNA

Invited lecture: J. L. Mergny (National Museum of Natural History, Paris, France) described the role of DNA and RNA quadruplexes in telomeres. Using FRET assay they have identified several series of G4 ligands that exhibit potent and specific anti-telomerase activity. A G-quadruplex interacting agent is able to impair telomere function in a tumor cell line thus providing a basis for the development of new anticancer drugs. These compounds may also target non-human telomeric overhangs, provided that G-rich motif is present.

Invited lecture: S. Haider (The School of Pharmacy, University of London, UK) presented results of molecular dynamics (MD) simulations of G-quadruplex complexes in telomeric DNA. They have carried out MD simulations on two different lengths of telomeric DNA containing 45 and 93 nucleotides. The results revealed extremely stable G-quadruplex structures. They also studied small ligand-quadruplex complexes, which are important to achieve therapeutic selectivity.





Invited lecture: J. Gros (National Museum of Natural History, Paris, France) reported on investigation of kinetics of modified tetramolecular quadruplexes. In order to better understand the formation of TG4T and TG5T quadruplexes they performed kinetic and thermodynamic experiments on variants motifs that involve a single base substitution in which a single guanine was replaced by various natural or modified bases. They demonstrated huge differences in the association and dissociation constants of these quadruplexes.

2.7 Atomistic simulations of G4 structures

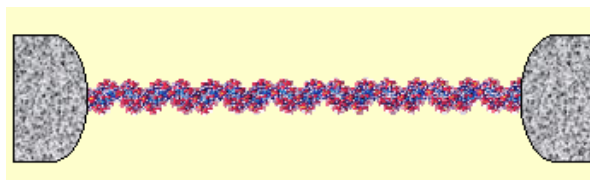
Invited lecture: Keynote presentation: R Di Felice (National Center S3 of INFM-CNR, Modena, Italy) addressed classical and quantum atomistic simulations of G4-wires. The knowledge of the electronic properties and of the conformational regularity of G4-wires is a key ingredient to explore their electrical performance. The DFT calculations show that the band structure is strongly dependent on structural parameters, such as rise and twist, which is in principle the basis for tunneling electronic features with mechanical deformations.

Invited lecture: M. Meyer (Revotar Biopharmaceuticals AG, Henningsdorf, Germany) reported on systematic quantum chemical studies of nucleic acid base structures. He present density functional studies for the analysis of the structure and interaction energies of quartets of different bases (G4, iG4, T4, U4, A4, C4) and their interaction with cations. Except for certain A4 tetrad structures all other tetrads investigated so far have a central cavity with a negative electrostatic potential suitable for cation binding. However, the structure of G4 is most planar, which enables a stacking of several tetrads to form quadruplexes.

Invited lecture: S. Ladame (Cambridge University, UK) reported a dynamic combinatorial approach for targeting G-quadruplex DNA secondary structures. Recently numbers of sequences have been identified in the promoter region of the oncogenes that have been shown to form a quadruplex structure in vitro and suspected to act as regulatory elements for gene expression at the transcriptional level. This generated a necessity for chemists to synthesis quadruplex binding small molecules that can discriminate between different quadruplexes. Dynamic covalent chemistry was employed to identify fragments that recognize specifically different features of a quadruplex.

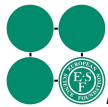
2.8 Electrical transport and nanotechnical applications

Keynote presentation: D. Porath (Hebrew University of Jerusalem, Israel) focused on electrical transport through DNA molecules and their derivatives using conductive AFM and STM. He started with the review of a range of experiments devoted to conductivity of the DNA segments and pointed out a broad diversity and inconsistency of the obtained results. This reveals that it is very difficult to control various side processes, which take



place in such measurements. Then he presented the measurements performed in his research group, which took place using controlled applied force in conductive AFM. He also presented polarizability measurements on G4-DNA wires.

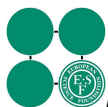
Invited lecture: D. Mihailovič (J. Stefan Institute, Ljubljana, Slovenia) described experiments on photoinduced carrier localization on intercalated dyes and their interaction with vibrational modes of DNA. The main aim of the experiments was to detect possible presence of polarons in these systems. No signs of the polaron excitation



were found, which signifies that change of conformational energy due to photoexcited holes is too small to cause self-trapping at room temperature. Anyway the holes are localized, which is an important finding for biochemistry and electronic device engineering based on DNA materials.

Invited lecture: R. Rinaldi (National nanotechnology laboratory (CNR-INFM), Lecce, Italy) reported investigations towards nano-electronic devices based on modified deoxyguanosines. She discussed the properties of field effect transistor made from (dG(C10)₂) layer interconnecting planar nano-electrodes. The realization of transistor-like device represents a starting point towards the development of planar solid-state bio-molecular electronic devices

Invited lecture: W. Fritsche (Institute for Physical High Technology, Jena, Germany) described perspectives of the G-wires for molecular nanotechnology. Possible G-wire uses in nanotechnology were discussed and experimental results were presented on surface assembling of G-wires. The influence of assembly conditions in order to incorporate gold nanoparticles was addressed.



3. Assessment of the results, contribution to the future direction of the field

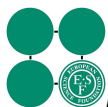
The highly interdisciplinary meeting provided an excellent overview of the current state-of-the-art in the field of self-assembled structures of guanosine derivatives and G-rich oligonucleotides. It resolved links between the experiments and the theory and correlations between the simple model systems and macromolecular assemblies important in biological processes. The **round table discussion devoted to future perspectives of the guanine research field** identified several topics of a broad interest with promising perspectives for medical and technological applications. It is believed that the following aspects will form the basis of the further scientific progress in the field:

- Tailored patterning on surfaces
- Electronic properties and charge transport in G4 wires and their analogues
- G-assemblies in biomimetic systems
- Synthetic ion channels
- Incorporation of gold nanoparticles in G-assemblies
- Further exploration of the rich chemistry of G compounds (for instance with respect to hydrophobic/hydrophilic modifications)
- Protein-G-quadruplex interactions
- Telomerase inhibition with G-structures
- Role of G-assembling in other G-rich segments of the DNA
- Metal-G-quadruplex complexes (with Cs, Ag, ...)
- Tailoring the folding motifs of G-structures
- Structure-properties relationship
- Improved atomistic simulations based on experimental verifications
- Combined experimental approaches (NMR, X-ray scattering, CD, AFM, ...)
- Kinetics versus thermodynamics

These specific “open topics” provide a wealth platform of target problems, which have to be addressed in preparation of proposals for collaborative research projects within the 7th EU framework programme (FP7) and within other frameworks (CIP, EUREKA, ...). Broad future vision on these open problems from the view of various disciplines was generated and several important interdisciplinary correlations were found. An important conclusion was that cooperation of the researchers with very different backgrounds and research expertise (combinatorial chemistry, physics, biology) is vital for rapid future progress of the field and that the ESF workshop at Bled served as a good starting point to realize this aim.

The **round table discussion devoted to open possibilities for future cooperation in the guanine research field** identified that the number of active researchers and research groups involved in the topic has reached a critical mass, which allows for recognition of the G-structures research a specific topic of the modern science. The field is rapidly developing and has become ripe for cooperation. To accelerate the exchange of ideas and build up a platform for formal cooperations the following activities will be initiated:

- The list of G-researchers and research groups will be assembled, based on the list of the participants to the meeting and other researchers which have expressed the interest to be included
- The web page of G-researchers will be established on the basis of the web page of the meeting. It will include links to home-pages of different research groups and provide information on present events and activities important for the field

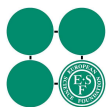


- Topical meetings focused on G-structures will be organized also in the future. Accordingly to this plan an application will be prepared for organization of the ESF-FWF conference on the self-assembly of G-derivatives in 2008.
- Formal cooperation of the research groups contributing to the workshop will try to be established within the 7th European framework programme (FP7). The main target will be collaborative projects. As soon as the first FP7 call will be launched, G-research related priority themes will be identified and related consortia will be assembled, which will immediately start the activities associated with proposal preparation.
- Three possible initiatives for cooperative projects has been identified: (i) new directions in supramolecular chemistry of G-structures (priority theme NMP), (ii) nanotechnical applications of G-structures (priority themes NMP and IST), (iii) the role of G-structures in biological systems (priority theme NMP)
- Cooperation with pharmaceutical companies and other innovative European SMEs will be envisaged in order to stimulate more applied research
- Research toward applications will be focused on generating high added-value products and related processes and technologies

It was agreed that several new directions may yield materials, which could be exploited for advanced applications as new generation of anticancer drugs, synthetic ionic channels, biosensors, and as various elements of molecular electronic devices. They may therefore have impact on a wide range of industrial sectors including pharmaceutical, cosmetics, electronics and various branches of bio and nanotechnology. The link between the fundamental science and applied research in the field is for the moment relatively weak, therefore efforts will be increased to inform the industrial sector about the prospects of the G-materials and to attract interest and investment into research related to G-structures.

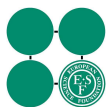


Group photo of the workshop participants.



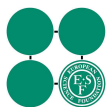
4. Final programme

Wednesday, 13th September		
Chair: I Drevenšek-Olenik		
09:00 – 09:15	Organisers, The Dean of faculty of mathematics and physics, University of Ljubljana, ESF representative	Opening and welcome Presentaion on ESF
09:15 – 10:00	J Walmsley Univ of Texas, US	Structures of guanine mono- and dinucleotides by NMR spectroscopy: the known and unknown
10:00 – 10:20	GP Spada Univ of Bologna, IT	The self-assembly and liquid crystal formation of guanosine derivatives
10:20 – 11:00 Coffee		
Chair : M Čopič		
11:00 – 11:20	P Mariani Univ Politec of Marche, IT	Structural studies on lyotropic polymorphism, stability and energetics of guanosine four-stranded helices
11:20 – 11:40	DJ Lee Imperial College, UK	Helix dependent effects in guanosine assemblies
11:40 – 12:00	A Ferrarini Univ of Padova, IT	Chiral nematic phases of G-quadruplexes: what is the relation with the molecular structure?
12:00 – 14:00 Lunch		
Chair : J Walmsley		
14:00 – 14:40	NV Hud Georgia Inst of Tech, US	Ammonium ion mobility within the d(G ₄ (T ₄ G ₄) ₃) G-quadruplex
14:40 – 15:00	J Plavec National Inst of Chem, SI	Cation localization and mobility within dimeric G-quadruplexes
15:00 – 15:20	G Wu Queen's Univ, Ontario, CA	The quest for direct NMR detection of alkali metal ions in G-quadruplex DNA
15:20 – 16:00 Coffee		
Chair : P Mariani		
16:00 – 16:20	H Jurga-Nowak A. Mickiewicz Univ, PL	Supramolecular disodium guanosine 5'-monophosphate structures investigation by means of photon correlation spectroscopy
16:20 – 16:40	L Spindler Univ of Maribor, SI	Dynamics of self-assembled deoxyguanosine 5'-monophosphate: a pronounced polyelectrolyte behavior
16:45 – 17:30	Round table 1: Perspectives of the Guanine research field: From the past to future Introduction and moderation by P. Mariani	
19:30 Dinner		



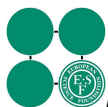
Thursday, 14th September

Chair : GP Spada		
09:00 – 09:40	J Vesenka Univ of New England, US	Auto-orientation and manipulation of G-wire DNA networks
09:40 – 10:00	R Otero, Univ Autonoma Madrid, ES	Self-assembly of guanine quartet networks and other DNA-base structures on solid surfaces
10:00 – 10:20	I Drevenšek-Olenik Univ of Ljubljana, SI	Self-assembly of guanosine 5'-monophosphate on mica substrates
10:20 – 11:00 Coffee		
Chair : J Davis		
11:00 – 11:20	JL Mergny Museum National d'Histoire Naturelle, Paris, FR	DNA and RNA quadruplexes: implications for telomeres
11:20 – 11:40	J Gros Mus Nat d'Hist Natur, FR	Guanines are a quartet's best friend. Kinetics of modified tetramolecular quadruplexes
11:40 – 12:00	S Haider Univ of London, UK	MD simulation of G-quadruplex complexes in telomeric DNA
12:00 – 14:00 Lunch		
Chair : W Fritzsche		
14:00 – 14:20	S Ladame Cambridge Univ, UK	A dynamic combinatorial approach for targeting G-quadruplex DNA secondary structures
14:20 – 14:40	M Meyer Revotar Biopharm AG, Hennigsdorf, DE	Systematic quantum chemical studies of nucleic acid base structures: From quartets to sandwich complexes with alkali ions
14:40 – 15:20	R Di Felice INFN-CNR, Modena, IT	Classical and quantum atomistic simulations of G4-wires
15:20 – 16:00 Coffee		
Chair : A Kotlyar		
16:00 – 16:40	D Porath Hebrew Univ of Jerusalem, IL	Electrical transport, polarizability and spectroscopy measurements through DNA molecules and derivatives using conductive AFM and STM
16:40 – 17:00	D Mihailovič J Stefan Inst, Ljubljana, SI	Optical investigations of electronic states in DNA
17:15 – 18:00	Round table 2: Open possibilities for future cooperation in the Guanine research field Introduction and moderation by I Drevenšek-Olenik	
19:30	Dinner at the Bled castle	



Friday, 15th September

Friday, 15th September		
Chair: JL Mergny		
09:00 – 09:40	JT Davis Univ of Maryland, US	The supramolecular chemistry of lipophilic G-quadruplexes
09:40 – 10:00	JM Rivera Univ of Puerto Rico, US	Modulating the supramolecular structure and properties of quadruplexes by using 8-aryl-guanine derivatives
10:00 – 10:20	R Rinaldi Univ of Lecce, IT	Nano-electronic devices based on modified deoxyguanosines
10:20 – 11:00	Coffee	
Chair : L Spindler		
11:00 – 11:20	AB Kotlyar Tel Aviv Univ, IL	Synthesis of long guanine-based nanowires
11:20 – 11:40	W Fritzsche IPHT, Jena, DE	G-wires for molecular nanotechnology
11:40 – 12:00	Organisers	Closing summary and discussion
12:00 – 14:00	Lunch	



5. Statistical information on participants

There were 29 participants at the meeting: **28 researchers** + 1 ESF representative. 24 researchers received ESF support for lodging and meals. 4 participants received ESF support for travelling. The remaining delegates (5 participants from non-ESF countries) attended the meeting at full cost or were supported from the Co-sponsor (ARRS).

Age profile

Ph.D. students	1
Young scientists	11
Senior Scientists	16

In this table Young scientists include scientists in the early stage of their research career, which received their Ph.D. degree less than 10 years ago. Senior scientists are defined as researchers with more than 10 years research experience.

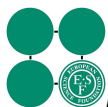
Gender profile

Female	7
Male	21

Country of origin

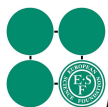
Canada (CA)	1
France (FR)	2
Germany (DE)	2
Israel (IL)	2
Italy (IT)	5
Poland (PL)	1
Slovenia (SI)	6
Spain (ES)	1
UK	3
USA	5

1 of the participants from Slovenia was a Ph.D. student, who helped in organization of the meeting.

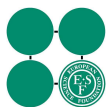


6. The final list of participants

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