## Program

		Wednesd	ay 21 November	
15:00 - 1	7:50	Registration	(Plaza50)	
18:00 - 1	8:15	Opening	(Room 831)	
18:15 – 1	What hat in the fi	Plenary Lecture as been clarified by Japanese scienti eld of solution chemistry <u>u Nomura</u>	(Room 831) [Chair: Masaru Nakahara] sts and what remains unsolved ahead of us	
19:00 – 2	21:00	Reception	(Cafeteria 2F)	
		Thursda	ty 22 November	
9:00 – 11	:00	General 1	(Room 831) [Chair: Philippe A. Bopp]	
A01L	New Trends in Structural Characterization of Supramolecular Architectures in Solution Phase <u>Gábor Pálinkás</u>			
A02L	On the Solvation of Complexly Shaped Molecules: The Morphometric Approach Roland Roth			
A03T	Towards a Statistical Mechanical Theory for Water: Analytic Theory for a Non-Speculative Reference Model and Its Anomalies <u>Ivo Nezbeda</u>			
A04T	Approach of Rheo-Optical Spectroscopy by Means of Polarization Analysis of a Diffracted Light by a Longitudinal Ultrasound <u>Tatsuro Matsuoka</u> , Junki Miyashita, Shinobu Koda			
A05T	Influence of Diffusion on Bimolecular Reaction Rates: Why Are the Diffusion Coefficients Obtaine from the Transient Effect of Bimolecular Fluorescence Quenching Reaction Smaller than Those Obtaine from Conventional Methods? <u>Toshihiro Tominaga</u> , Sanjay Pant, Hiroyasu Ohtaka-Saiki, Makoto Takezaki, Andrew Scully, Satosh Hiayama			
11:00 - 1	1:30	Coffee Break		
11:30 – 1	3:00	Ionic Liquids 1	(Room 831) [Chair: Renzo Vallauri]	
B01L		Cooperative Dynamics of Mixtures of Ionic Liquids with Polar Solvents <u>Richard Buchner</u>		
B02T	Solution	Corresponding States Analysis and Criticality of the Liquid-Liquid Phase Transition of Ionic Liquids i Solution <u>Wolffram Schröer</u> , Dragos Saracsan, Anna Butka, Vlad Vale		
B03T	1-Ehtyl <u>Kenta F</u>	Molecular and Liquid Structures of Low-viscosity Room Temperature Ionic Liquid 1-Ehtyl-3-methylimidazolium Bis(fluorosulfonyl) Imide <u>Kenta Fujii</u> , Shiro Seki, Shuhei Fukuda, Toshiyuki Takamuku, Shinji Kohara, Yasuo Kameda, Yasuhiro Umebayashi, Shin-ichi Ishiguro		
B04T	<sup>7</sup> Li N N,N-dir		Reaction of Lithium Ion with Cryptand C211 in I)ammonium Bis-(trifluoromethylsulfonyl)imide	

Atsushi Shirai, Yasuhisa Ikeda

13:00 - 14	:30 Lunch			
14:30 - 15	:40 Ionic Liquids 2	(Room 831) [Chair: Shin-ichi Ishiguro]		
B05L	Ionic Liquids as Gas Absorption Media <u>Mitsuhiro Kanakubo</u> , Yasuo Kameda			
B06T	Transport Properties of Ionic Liquids at High Pressure <u>Kenneth R. Harris</u> , Mitsuhiro Kanakubo, Noriaki Tsuchihashi, Kazuyasu Ibuki, Masakatsu Ueno			
B07T	Micro-solvent Cluster Extraction in Mixed Solvents: Ionic Liquids for Separation of Neutral Organic Compounds <u>Masaaki Tabata</u>			
15:40 - 16	:10 Coffee Break			
16:10 – 18	10 Young Scientists	(Room 831) [Chair: Maurizio Musso and Hajime Torii]		
Y01	Self-association Properties of Alkanols: A <u>Francesca Palombo</u> , Marco Paolantoni, Tassaing, Yann Danten, Marcel Besnard	A Vibrational Spectroscopy Study Paola Sassi, Assunta Morresi, Rosario Sergio Cataliotti, Thierry		
Y02	An Integral Equation Theory for Inhomogeneous Molecular Fluids: The Reference Interaction Site Model Approach <u>Ryosuke Ishizuka</u> , Song-Ho Chong, Fumio Hirata			
Y03	Photo-Thermalization Kinetics of Azulene Derivative Solutions Studied by the Transient Grating Spectroscopy <u>H. Fujiwara</u> , T. Miyajima, Y. Matano, M. Terazima, Y. Kimura			
Y04	Ab-Initio Modelling of Structural, Electronic and Magnetic Properties of Free and Supported Prophyrin molecules <u>Pooja M. Panchmatia</u> , Biplab Sanyal, P. M. Oppeneer, O. Erkisson			
Y05	Three-dimensional Solvation Structure around Protein: Theoretical Approach Based on Reference Interaction Site Model <u>Daisuke Yokogawa</u> , Hirofumi Sato, Shigeyoshi Sakaki			
Y06	Coarse-Graining Ions in Colloidal Suspensions for the Study of Transport Properties Vincent Dahirel			
Y07	Molecular Dynamics Simulation of Thermocapillary Convections at Liquid-Liquid Interfaces <u>Holger A. Maier</u> , Philippe A. Bopp, Manfred J. Hampe			
Y08	Self-diffusion and Rotation in Supercritical Water and Benzene and Their Dependencies on the Solvation Shell State and Lifetime <u>Ken Yoshida</u> , Nobuyuki Matubayasi, Masaru Nakahara			
18:10 - 18		(Room 831)		
	Young Scientist Award in Solution Che Theoretical Study on the Ion Pair Dy Electrolyte Solutions <u>Tsuyoshi Yamaguchi</u>	[Chair: Toshihiro Tominaga] namics in the Bulk Relaxation Spectra and Conductivity of		

## Friday 23 November

9:00 - 11:00		General 2	(Room A201) [Chair: Masao Takayanagi]		
C01L	Theoretical Multidimensional Spectroscopy of Water Shinji Saito				
C02T	Low-Frequency Spectra of Polar Solute Molecules in Non-Polar Solvents by Terahertz Time-Domain Spectroscopy <u>Partha Dutta</u> , Keisuke Tominaga				
C03L	The Effect of Microscopic Inhomogeneities in Binary Liquid Mixtures Observed through the Raman Spectroscopic Noncoincidence Effect <u>Maurizio Musso</u> , Maria Grazia Giorgini, Hajime Torii				
C04T	Solvation Behavior of Diol Molecule in Alcohol-Water Mixtures <u>Toshiyuki Takamuku</u> , Miho Tanaka, Takunosuke Sako, Kenta Fujii, Munetaka Takeuchi				
C05T	Models of Internal Parameters for Studying Supramolecular Ordering in Liquids in Nanoscale of Intermolecular Distances <u>Vladimir A. Durov</u>				
11:00 - 1	1:30	Coffee Break			
11:30 – 13	3:00	Liquids in Confined Geometry and at Inte	e <b>rface</b> (Room A201) [Chair: Marie-Claire Bellissent-Funel]		
D01L	Water Surface Is Acidic <u>Pavel Jungwirth</u> , Victoria Buch, Anne Milet, Robert Vácha, J. Paul Devlin				
D02L	Surfactant Self-Assembly in Silica Nanopores <u>Gerhard Findenegg</u>				
D03L	03L New Aspects in the Theory of Electrical Double Layer <u>Myroslav Holovko</u> , Jean-Pierre Badiali, Dung di Caprio				
13:00 – 14:30 Lunch					
14:30 - 16:40		Micelles and Macromolecular Solutions	(Room A201) [Chair: Susumu Okazaki]		
E01L		ulsions as Models <u>ennerström</u>			
E02L	Interactions between cholesterol and phospholipids in lipid bilayers: Insights from detailed molecular simulations <u>Max L. Berkowitz</u>				
E03L	Phase Transitions of Polymers under Complex Conditions Se'verine Boyer				
E04T	Solution Behavior of Poly(L-lysine)-Surfactant Complexes Laszlo Almasy, Sirkku Hanski, Susanna Junnila, Janne Ruokolainen, Olli Ikkala				
E05T	E05T Combination of Molecular Dynamics Method and 3d-RISM Theory for Conformational Sampling of Flexible Molecules in Solution <u>Tatsuhiko Miyata</u> , Fumio Hirata				
16:40 – 1	7:10	Coffee Break			
17:10 - 19:10		Poster 1 - Odd Number	(Oasis)		

Saturday 24 November				
9:00 - 10	:50	Biomolecular Solutions 1 [Cha	(Room A201) ir: Masahide Terazima]	
F01L		n and Volumetric Properties of Unfolded Polypeptides <u>Chalikian</u>		
F02T	Hydrogen-Bonding Strengths of the Water in Aqueous Solutions of Polypeptides Probed by v(O-D) in IR and $\delta_{H2O}$ in NMR <u>Kazuko Mizuno</u>			
F03T	Effects of Complex Sugar and Salt Solutions on Biopolymers: An in Silico Study Maxim V Fedorov, Jonathan M Goodman, Stephan Schumm			
F04T	Heat Capacity of Protein and Hydration Entropy Hitomi Kitazato, <u>Masayuki Irisa</u>			
F05T	Evidence of Hyper-Mobile Water: Enhanced Proton Diffusion Coefficients in F-Actin Solutions with Bound Myosin S1 by PFG-SE NMR <u>Makoto Suzuki</u> , Xinying Gan, Tetsuichi Wazawa, Takashi Miyazaki			
10:50 - 1	1:20	Coffee Break		
11:20 – 1	2:50	Biomolecular Solutions 2 [Cha	(Room A201) ir: Tigran V. Chalikian]	
F06L	Role of C <u>P. L. Cha</u>	Cell Membrane in General Anaesthetic Action		
F07T	F07T Protein-Protein Interaction and Its Implication in Medical Application of Artificial Blood Substitutes <u>Takaaki Sato</u> , Hiromi Sakai, Keitaro Sou, Teruyuki Komatsu, Akito Nakagawa, Otto Glatter, Richard Buchner, Eishun Tsuchida			
F08T	8T Conformational Dynamics of Mg:ADP/Mg:ATP and Mg <sup>2+</sup> Coordination Dynamics in F1-ATPase and Other Molecular Motors <u>Alexe Bojovschi</u> , Ming S. Liu, Richard Sadus			
F09T	Time-resolved Thermodynamics and Diffusion for Detecting Conformation Changes during Functions of Biological Proteins Yusuke Nakasone, Takeshi Eitoku, Daisuke Matsuoka, Satoru Tokutomi, <u>Masahide Terazima</u>			
12:50 - 1	4:00	Lunch		
14:00 - 1	6:00	Poster 2 – Even Number	(Oasis)	
16:00 - 1	6:30	Coffee		
16:30 – 17:30 Award Lecture (Room A201) Distinguished Research Award in Solution Chemistry				
[Chair: Fumio Hirata] Spectroscopic Study on Solvation, Reaction and Molecular Dynamics in Supercritical Fluids Yoshifumi Kimura				
	Spectros	Chemistry of Supercritical Water through De copy and Solution Theory <u>ci Matubayasi</u>	velopment of High-Temperature NMR	
17:30 – 1	8:10	Assembly SSCJ30	(Room A201)	
18:10 – 1	8:50	Assembly EMLG/JMLG	(Room A201)	
19:00 – 2	21:00	Banquet	(Restaurant 16F)	

## Sunday 25 November

		Sunaay 25 Noven	nver	
9:00 - 10	:50	General 3	(Room A201) [Chair: Gábor Pálinkás]	
G01L	Molecular Dynamics Simulations of Aqueous LiCl Solutions: Concentration and Model Dependence Kazuyasu Ibuki, <u>Philippe A. Bopp</u>			
G02T	The Structure of Aqueous Rb and Cs Halide Solutions from Reverse Monte Carlo Modelling of Diffraction Data Laszlo Pusztai			
G03T	The Nature of Chemical Bond in Solvated Systems: An Analysis Based on the New Resonance Theory <u>Atsushi Ikeda</u> , Hirofumi Sato, Shigeyoshi Sakaki			
G04T	Comparison of the Application of Specific Ion Interaction and Debye-Hückel Theories for the Tungsten(VI) Complexes with EDDA and NTA <u>Kavosh Majlesi</u>			
G05T	Stability and Structure of the Ternary Complexes of La(III) with Beta-Diketone and Polyethers in Solution Gene Frederick Gagabe, Keiichi Satoh, Kiyoshi Sawada			
10:50 – 1	1:20	Coffee Break		
11:20 – 13:00 Liquids under Extreme Conditions 1 (Room A201)   [Chair: Pavel Jungwirth]				
H01L	Peculiar Structural and Dynamic Properties of Hydration Water. A Liquid-Liquid Transition <u>MC. Bellissent-Funel</u>			
H02L	Nature of Liquid-Liquid Transition in Single-Component Molecular Liquids <u>Hajime Tanaka</u>			
H03T	Coupling/Decoupling between Translational and Rotational Motions in Supercooled Molecular Liquid <u>Song-Ho Chong</u> , Walter Kob			
H04T	Structure of Supercooled Water <u>Haruhiko Yokoyama</u> , Miyoko Kannami, Hitoshi Kanno			
13:00 - 14:20		Lunch	(Cafeteria 1F)	
14:20 - 1	5:50	Liquids under Extreme Conditions 2	(Room A201) [Chair: Nobuyuki Matubayasi]	
H05L	New Insight on Aqueous Solution by Spectroscopy Analysis: Raman, XAS, IXS, SAXS and WAXS Jean-Louis Hazemann			
H06T	Polarized and Depolarized Raman Scattering Spectra of Supercritical Water Yasunori Tominaga, Mika Murai, Yuko Amo			
H07T	Neutron Diffraction with Isotope Substitution of Supercritical Methanol-Water Mixture <u>Koji Yoshida</u> , Yu Sakai, Shigeru Ishida, Daniel Bowron, Toshio Yamaguchi			
H08T	New Acoustic and Fibre Optic Approaches to Probing of High-Pressure and High-Temperature Media <u>Vladimir K. Popov</u> , Victor N. Bagratashvili, Yuri E. Gorbaty, Alexey N. Konovalov, Toshio Yamaguchi			
15:50 – 16:00 Closing				