POSTER COMMUNICATIONS

Poster Session 1
Monday 4TH September – 17:00 h -18:30 h

Poster Communications - POSTER SESSION 1			
PHOTOTOXICITY OF NON-STEROIDAL ANTI-INFLAMMATORY DRUGS INSIGHT THROUGH IN-SILICO CALCULATIONS	P1	Neus Aguilera-Porta, Giovanni Granucci , Jordi Muñoz-Muriedas and Inés Corral	UK, Spain and Italy
QUANTUM CLUSTER APPROACH TO DEACETYLATION REACTION MECHANISM OF O-ACETYLPEPTIDOGLYCAN ESTERASE	P2	Z.Aksakal, M.M. Tataroğlu, F.A.Sungur, N.Tüzün	Turkey
CONFORMATIONALLY INDUCED PARAMAGNETISM IN ARYL-SUBSTITUTED 2-IMINO THIAZOLE DERIVATIVES	P3	Carlos Heras, Rosendo Valero, Guillermo Albareda, Francisco López-Calahorra, Ibério de P. R. Moreira, and Josep Maria Bofill	Spain
THREE COMPONENT SYSTEM OF DYE, QUANTUM DOT AND GOLD NANOPARTICLE	P4	Anuar Aldongarov, Irina Irgibaeva, Artur Mantel and Mukataev Iskander	Kazakhstan
THE IOCHEM-BD PLATFORM: A BIG DATA SOLUTION FOR COMPUTATIONAL CHEMISTRY	P5	M. Álvarez-Moreno, C. Bo, C. de Graaf, N. López, J. M. Poblet and F. Maseras	Spain
PUBCHEMDFT: A LIVE EXPERIMENT THAT COMPUTES AND TWEETS MOLECULES	P6	Joan González-Fabra, Moises Álvarez-Moreno, Martin Gumbau, Ana Mateo, Enric Petrus, Carles Bo	Spain
INVESTIGATION OF HYDROGEN BOND STABILITY ON N'-(7-CHLORO-4-QUINOLINYL)-N- (CYCLOPROPYLMETHYL)-N-PROPYL-1,3-PROPANEDIAMINE – PFATP6 COMPLEX IN WATER USING MOLECULAR DYNAMICS SIMULATION	P7	Ria Armunanto, Iqmal Tahir, Kurniawan Eka Satrya	Indonesia
DENSITY FUNCTIONAL STUDY OF THE C_{60}-ACETYLENE [2+2+2] CYCLOADDITION PROMOTED BY THE WILKINSON'S CATALYST	P8	A. Artigas, Agustí Lledó, Anna Pla-Quintana, Anna Roglans,Miquel Solà	Spain
DEVELOPMENT OF RELIABLE PREDICTION MODELS FOR THE EFFICIENT PROFILING OF KINASE INHIBITORS	P9	Sorin Avram, Alina Bora, Liliana Halip, Liliana Păcureanu, and Ramona Curpăn	Romania
QUANTUM CHEMICAL DESCRIPTORS OF THE SULFONAMIDES BY DFT	P10	Seyda Aydogdu and Arzu Hatipoglu	Turkey
A COMPARATIVE DFT STUDY OF INTERACTIONS OF AU AND SMALL GOLD CLUSTERS AUN (N = 2 – 4) WITH CH3S AND CH2 RADICALS	P11	Martin Blaško, Tomaš Rajský, and Miroslav Urban	Slovakia
MINIMIZING FALSE-POSITIVE RATES IN HIGH-THROUGHPUT SCREENING (HTS): PREDICTION OF LUCIFERASE INHIBITORS	P12	Alina Bora, Sorin Avram, Liliana Halip, Liliana Păcureanu and Ramona Curpăn	Romania
STRUCTURE- AND FRAGMENT-BASED DESIGN OF NOVEL DIAMINOPYRIMIDINE DERIVATIVES INHIBITORS FOR HUMAN MYT1 KINASE	P13	Abdulkarim Najjar, Charlott Platzer, Matthias Schmidt, Wolfgang Sippl	Germany
EXPERIMENTAL AND THEORETICAL INSIGHTS ON BaW0.5Mo0.5O4 SCHEELITE SOLID SOLUTION PREPARED BY CO- PRECIPITATION METHODS	P14	Marisa Carvalho de Oliveira[a], Lourdes Gracia, Içamira Costa Nogueira, Elson Longo and Juan Andres	Brazil and Spain
COMPUTATIONAL MODELING OF VERSATILE PHOTOSENSITIZERS	P15	Irene Casademont, Carla Casadevall, Arnau Call, Julio Lloret, Eloy Ramos-Cordoba, Eduard Matito	Spain and USA
THEORETICAL ESTIMATE OF CHARGE-SEPARATION AND -RECOMBINATION RATE CONSTANTS IN DONOR-ACCEPTOR BUCKYBOWL-BASED SUPRAMOLECULAR COMPLEXES	P16	Jesús Cerdá, Joaquin Calbo, Juan Aragó, Enrique Ortí	Spain
POLAR FLATTENING AND CHARGE TRANSFER CONTRIBUTIONS TO HALOGEN BONDED COMPLEXES	P17	Diego Cesario,Francesca Nunzi, Leonardo Belpassi, and Francesco Tarantelli	Italy
SELECTIVE OXIDATION OF METHANE CATALYZED BY SOLUBLE PLATINUM SPECIES IN OLEUM: DENSITY FUNCTIONAL THEORY STUDY	P18	Minserk Cheong	Republic of Korea
WATER-GAS SHIFT REACTION COCATALYZED BY K3PM12O40 AND AU(111): THE MAGIC ROLE OF POLYOXOMETALATES	P19	Anna Clotet, Zhongling Lang and Josep M. Poblet	Spain

MINIMIZING FALSE-POSITIVE RATES IN HIGH-THROUGHPUT SCREENING: PREDICTORS FOR FLUORESCENT COMPOUNDS	P20	Ramona Curpăn, Sorin Avram, Alina Bora and Liliana Halip	Romania
THE DARK SIDE OF ALUMINUM CHELATION THERAPY: CHARACTERIZATION OF THE AL(III) – LIGAND BINDING FEATURES	P21	Gabriele Dalla Torre, Jon I. Mujika and Xabier Lopez	Spain
THEORETICAL AND SPECTROSCOPIC INVESTIGATION ON CHARGE-TRANSFER COMPLEX BETWEEN N-SULFAMOYLOXAZOLIDINONE AND PICRIC ACID.	P22	Karim DINAR, Mekki KADRI, Achour SERIDI and Mohamed ABDAOUI	Algeria
UNRAVELING THE MECHANISMS OF THE SO-CALLED "PERICYCLIC REACTIONS". A MOLECULAR ELECTRON DENSITY THEORY STUDY	P23	Luis R. Domingo, Mar Ríos-Gutiérrez, and Patricia Pérez	Chile and Spain
ELECTRONIC STRUCTURE ANALYSIS OF KEY ORGANOGOLD TRANSFORMATIONS	P24	Laura Estévez, Maximilian Joost, Feriel Rekhroukh, Abderrahmame Amgoune, Didier Bourissou, Karinne Miqueu	Spain and France
ULTRAFAST EXCITED-STATE DECAYS IN $[RE(CO)_3(N,N)(L)]^{N+}$: NON-ADIABATIC QUANTUM DYNAMICS	P25	Maria Fumanal, Etienne Gindensperger, and Chantal Daniel	France
MODELING OF RING DISTORTION IN HEXOPYRANOSES	P26	Karolina Gaweda, Wojciech Plazinski	Poland
CLARIFYING THE MECHANISM OF THE 2-HYDROXYPYRIDINE/2-PYRIDONE PHOTO-TAUTOMERIZATION.	P27	Sara Gil Guerrero and Jose M. Hermida-Ramón	Spain
MECHANISTIC INVESTIGATION PD CATALYZED C-N CROSS-COUPLING USING AMMONIA.	P28	Pablo Gómez-Orellana , Agustí Lledós, Gregori Ujaque	Spain
ANALYSIS OF TITANIUM DIOXIDE SURFACES IN THE WATER SPLITTING PROCESS	P29	Amanda Fernandes Gouveia, Mateus Meneghetti Ferrer, Júlio Ricardo Sambrano, Elson Longo[a] and Juan Andrés	Spain and Brazil
THE CATALYTIC ROLE OF WATER CLUSTERS IN THE FORMATION OF ACID RAIN[1]	P30	José Manuel Guevara-Vela, Eduardo Romero-Montalvo, Wilmer Esteban Vallejo Narváez, Aurora Costales, Ángel Martín Pendás, Marcos Hernández-Rodríguez and Tomás Rocha-Rinza	Spain and Mexico
MOLECULAR MODELING OF CARBORANE-CONTAINING DRUG MOLECULES	RT1	Menyhárt-Botond Sárosi	Germany
Wittig olefination, An OLD REACTION WITH NEW PERSPECTIVES	RT2	Mauro Fianchini, Maria Besora, and Feliu Maseras	Spain
COMPUTATIONAL INSIGHTS INTO REACTIVITY OF THE PHILLIPS CrOx/SiO2 CATALYST – ROLE OF AMORPHOUS SILICA MODEL	RT3	Maciej Gierada, Jarosław Handzlik	Poland
MOLECULAR DYNAMICS-BASED STRUCTURE-ACTIVITY RELATIONSHIPS FOR THE AFFINITY OF POLYOXOMETALATES TOWARDS PROTEINS	RT4	Albert Solé-Daura, Josep M. Poblet, and Jorge J. Carbó	Spain

Poster Session 2
Tuesday 5th September – 17:00 h -18:30 h

Poster Communications - POSTER SESSION 2			
MAPPING THE CHEMICAL SPACE OF KINASE INHIBITORS	P31	Liliana Halip, Sorin Avram, Alina Bora, and Ramona Curpăn	Romania
ASSESSMENT OF DFT METHODS FOR STUDYING OLEFIN METATHESIS CATALYSED BY MOLYBDENUM AND TUNGSTEN SYSTEMS	P32	Jarosław Handzlik, Maciej Gierada	Poland
ELECTRONIC STRUCTURES OF THE HALOGENATED ORGANOPHOSPHORUS COMPOUNDS: A DFT STUDY	P33	Arzu Hatipoğlu and Didem Civan	Turkey
NUCLEAR QUANTUM EFFECT ON HYDROGEN FLUORIDE TRIMER STUDIED BY *AB INITIO* PATH INTEGRAL MOLECULAR DYNAMICS SIMULATION	P34	Aiko Hayashi, Yuki Oba,Tsutomu Kawatsu,and Masanori Tachikawa	Japan
DFT COMPUTATIONS ON THE MECHANISM OF FLAVIN OXIDATIVE HALF-REACTION	P35	Safiye Sağ Erdem and İlke Demir	Turkey
COMBINED PLANE WAVE AND LOCALIZED ORBITAL ELECTRONIC STRUCTURE CALCULATION	P36	Takayoshi Ishimoto, Hiroaki Honda, and Hiroyuki Kai	Japan
PALLADIUM CATALYSED CONVERSION OF CYCLIC VINYL CARBONATES TO ALLYLIC AMINES: A DFT STUDY	P37	Rositha Kuniyil, Feliu Maseras,	Spain
ELECTRONIC EXCITED STATES EQUILIBRIUM GEOMETRIES OF MOLECULES PRESENTING AN EXCITED STATE PROTON TRANSFER	P38	Orian Louant, Benoît Champagne, Vincent Liégeois	*Belgium*
CHYMOTRYPSIN-LIKE ACTIVITY INHIBITION MODEL OF HUMAN 20S PROTEASOME	P39	Emilia A. Lubecka	Poland
***AB INITIO* MOLECULAR DYNAMICS STUDIES OF HYDRATED MAGNESIUM, CALCIUM AND STRONTIUM HYDROXIDES**	P40	Olivia Lynesa, Jonathan Austin, Andy Kerridge	UK
Theoretical investigation of CO catalytic oxidation by Fe-$PtSe_2$ monolayer	P41	P. Lyu, J. He, P. Nachtigall	Czech Republic
PHENYLACETYLENE AND STYRENE ADSORPTION ON Pd(111): A RELATIVISTIC DFT STUDY	P42	Ravshan Shamsiev, Filipp Danilov	Russian Federation
ENANTIO- AND REGIOSELECTIVITY OF ARYLATION REACTIONS WITH SULFOXIDES: COMPUTATIONAL STUDIES SHED THE LIGHT ON THE MECHANISM	P43	Boris Maryasin, Leticia González, and Nuno Maulide	Austria
ON THE ROLE OF THE BASE IN THE NICKEL-CATALYZED BORYLATION REACTION OF ARYL FLUORIDES: A COMPUTATIONAL AND MICROKINETIC STUDY	P44	Ana Mateo and Carles Bo	Spain
PHOTOELECTRON SPECTRA FROM OPTIMALLY TUNED TDDFT AND DYSON ORBITAL FORMALISM	P45	Tobias Möhle , Sergey I. Bokarev , Olga S. Bokareva , Gilbert Grell , Oliver Kühn	Germany
DEVELOPMENT OF INTERACTION POTENTIALS FOR DESIGNING NEW HETEROCYCLE-CONTAINING MOLECULAR RINGS FOR CARBON CAPTURE AND STORAGE	P46	Ángel Vidal-Vidal, Carlos Silva López,and Olalla Nieto Faza	Spain
TUNING ELECTRONIC FACTORS CONTROLLING OXIDATIVE ADDITION OF AMMONIA N-H BOND TO IR(I) PXP PINCER COMPLEXES	P47	Julen Munarriz, Victor Polo	Spain
CHEMICAL AND STRUCTURAL EFECTS OF INHIBITOR MOLECULES ON INFLUENZA A VIRUS M2 PROTEIN CHANNEL	P48	Mehmet Özbil	Turkey
PYRANOSE RING PUCKERING IN ALDOPENTOSES, KETOHEXOSES AND DEOXYALDOHEXOSES. A MOLECULAR DYNAMICS STUDY	P49	Karina Panczyk, Wojciech Plazinski	Poland
PEPTIDE BOND FORMATION CATALYSED BY TiO_2 (101) ANATASE SURFACE	P50	Stefano Pantaleone, Albert Rimola, Mariona Sodupe	Spain
A DFT STUDY ON THE ELECTRONIC CONFIGURATION AND OPTICAL PROPERTIES OF APIGENIN AND ITS Cu2+ COORDINATION COMPLEX	P51	Francisco Partal Ureña, Mª Carmen Ramírez Avi, Eulogio J. Llorent-Martínez, and Ana África Márquez García	Spain

		Sukuba and Michael Probst	Slovakia
DFT STUDY ON THE STRUCTURE OF COBALT(II)/(III)-CITRATE-WATER COORDINATION COMPLEXES	P53	Mª Carmen Ramírez Avi, Ana África Márquez García and Francisco Partal Ureña	Spain
HOW DOES THE GLOBAL ELECTRON DENSITY TRANSFER DIMINISH $DE^{\neq}$ IN POLAR CYCLOADDITION REACTIONS? AN MEDT STUDY	P54	Mar Ríos-Gutiérrez, Luis R. Domingo,and Patricia Pérez	Spain
DESIGN OF NEW BIOENGINEERED GLYCOSIDASES FOR THE SYNTHESIS OF OLIGOSACCHARIDES. INSIGHTS FROM COMPUTATIONAL CALCULATIONS.	P55	Sonia Romero Téllez, Àngels González-Lafont, and Laura Masgrau	Spain
SUBSTITUENT EFFECT ON THE REDUCTION TENDENCY AND CONFORMATION OF FLAVIN RING: A DFT STUDY	P56	Safiye Sağ Erdem and Arzu Topal	Turkey
INVESTIGATION OF RUBIDIUM(I) ION SOLVATION IN LIQUID AMMONIA USING QMCF-MD SIMULATION AND NBO ANALYSIS OF FIRST SOLVATION SHELL STRUCTURE	P57	Yuniawan Hidayat, Ria Armunanto and Harno Dwi Pranowo	Indonesia
PREFERENTIAL SOLVATION AND DYNAMICAL PROPERTIES OF Cu^{+} ION IN 18.6% AQUEOUS AMMONIA SOLUTION: AB INITIO QUANTUM MECHANICAL CHARGE FIELD (QMCF) MOLECULAR DYNAMICS STUDY	P59	Wahyu Dita Saputri, Karna Wijaya, Ria Armunanto	Indonesia
ON THE WAY TO FINDING NOVEL PHOTOINITIATED DRUGS: REVEALING RELAXATION MECHANISMS OF MODIFIED NUCLEOBASES	P60	Serra Arslancan, Lara Martínez-Fernández, Giovanni Granucci, Maurizio Persico and Inés Corral	Spain and Italy
SPLITTING THE COULOMB HOLE INTO ITS DYNAMIC AND NONDYNAMIC PARTS	RT5	Mireia Via-Nadala, Mauricio Rodriguez-Mayorga Eloy Ramos-Cordoba and Eduard Matito	Spain and USA
TOWARD AN ACCURATE ESTIMATE OF THE EXFOLIATION ENERGY OF BLACK PHOSPHORUS	RT6	Sansone	Italy
TOWARDS NEXT-GENERATION SEMIEMPIRICAL QM METHODS AND RELIABLE MACHINE LEARNING-BASED TECHNIQUES	RT7	Pavlo Dral and Walter Thiel	Germany
QM/MM STUDY OF ATOM TUNNELING IN THE HYDROXYLATION PROCESS OF TAURINE/ α-KETOGLUTARATE DIOXYGENASE (TauD)	RT8	Sonia Álvarez Barcia and Johannes Kästner	Germany
MAGNETIC FINGERPRINT OF DITHIAZOLYL-BASED MOLECULE MAGNETS	RT9	Tommaso Francese, Mercè Deumal, Jordi Ribas-Arino and Juan J. Novoa	Spain
MOLECULAR DYNAMIC SIMULATIONS OF OIL-WATER WETTING ON MINERAL SURFACES	RT10	Gerard Alonso, Pablo Gamallo, Cristina Rincón and Ramón Sayós	Spain

Poster Session 3
Wednesday 6th September – 17:00 h -18:30 h

Poster Communications - POSTER SESSION 3			
INFLUENCE ON ANTIOXIDANT PROPERTIES OF HYDROXYL GROUP SUBSTITUTION IN FLAVONE SCAFFOLD: A DFT INSIGHT	P61	Ana África Márquez García, Mª Carmen Ramírez Avi, and Francisco Partal Ureña	Spain
EFFECT OF CENTRAL METAL ION ON THE PHOTOPHYSICAL PROPERTIES OF METALLOPHTHALOCYANINES: A DFT/TDDFT STUDY	P62	Ravshan Shamsiev	Russian Federation
TUNING THE STRENGTH OF THE RESONANCE-ASSISTED HYDROGEN BOND IN O-HYDROXYBENZALDEHYDE BY SUBSTITUTION IN THE AROMATIC RING	P63	Gerard Pareras Marcin Palusiak, Miquel Solà, Miquel Duran, and Sílvia Simon	Spain and Poland
IN SILICO BINDING ANALYSIS OF PGC-1α INTERACTION WITH PEROXISOME PROLIFERATOR-ACTIVATED RECPTORα MODULALTORS	P64	Vladimir Sladek, Yuta Yamamoto, Kenta Takei, Yoshimi Nakagawa, Hitoshi Shimano, Hiroaki Tokiwa	Slovakia and Japan
EFFECT OF STACKING INTERACTIONS AND CONFORMATION CHANGES ON POLYMER POLARIZABILITY	P65	Krzysztof Moorthi and Shintaro Maekawa	Japan
MECHANISTIC ASPECTS OF THE PALLADIUM-CATALYZED STEREOSELECTIVE SYNTHESIS OF METHYLENE OXINDOLES	P66	Theresa Sperger, Christine M. Le, Mark Lautens, and Franziska Schoenebeck	Germany and Canada
PROPERTIES OF SIGMA-HOLE	P67	Denisa Suchá, Michal H. Kolář, Michal Pitoňák[a]	Slovakia and Germany
INCREASING REACTIVITY OF ALUMINUM Al_{13}^- CLUSTERS TOWARDS WATER BY DOPING WITH TRANSITION METAL ELEMENTS	P68	Martin Šulka, and Andrej Antušek	Slovakia
PATH INTEGRAL SIMULATION ON THE HYPERFINE COUPLING CONSTANTS OF THE MUONIATED AND HYDROGENATED ACETONE RADICALS	P69	Yuki Oba, Tsutomu Kawatsu, and Masanori Tachikawa	Japan
A COMPUTATIONAL STUDY ON POTENTIAL NEW INHIBITORS OF O-ACETYLPEPTIDOGLYCAN ESTERASE	P70	M.M.Tataroğlu, Z.Aksakal , N.Tüzün, F.A.Sungur	Turkey
AB INITIO CALCULATIONS ON POLYMONONUCLEOTIDE AND POLYDINUCLEOTIDES AS MODEL OF B-TYPE DNA POLYMERS	P71	Hiroyuki Teramae and Yuriko Aoki	Japan
NOVEL COMPUTATIONAL WORKFLOW TO THE RATIONAL DESIGN OF PPI INHIBITORS. THE CHALLENGE OF INHIBITING E-CADHERIN/N-CADHERIN INTERACTIONS.	P72	Ignacio Viciano, Anna Labernardie, Xavier Trepat, Alfons Nonell-Canals and Melchor Sanchez-Martinez	Spain
EXPERIMENTAL AND COMPUTATIONAL INVESTIGATIONS ON THE CU(I)-CATALYSED ENANTIOSELECTIVE ALKYNYLATION OF α-KETOESTERS	P73	Martin C. Schwarzer, Akane Fujioka, Takaoki Ishii, Hirohisa Ohmiya,Masaya Sawamura, Seiji Mori	Japan
BINDING OF POTENTIAL LEAD COMPOUNDS TO *Plasmodium falciparum* GLUCOSE-6-PHOSPHATE DEHYDROGENASE	P74	Antonio Viayna, David Vílchez, Diego Muñoz-Torrero, F. Javier Luque	Spain
CONFORMATIONAL DISTRIBUTIONS OF LINEAR ALCOHOLS FROM *AB INITIO* CALCULATIONS	P75	Peng Wang, Knut J. Børve, and Leif J. Sæthre	Norway
***IN SILICO* BINDING ANALYSIS OF NOVEL SEECTIVE PEROXISOME PROLIFERATOR-ACTIVATED RECPTORα MODULALTORS (SPPARMα)**	P76	Yuta Yamamoto, Vladimir Sladek, Kenta Takei, Yoshimi Nakagawa, Hitoshi Shimano, Hiroaki Tokiwa	Japan and Slovakia
DESCRIPTION OF PUBCHEMKININA: A COMPREHENSIVE DATASET OF KINASE INACTIVE COMPOUNDS	P77	Alina Bora, Sorin Avram, Liliana Halip, and Ramona Curpăn	Romania
A DFT STUDY ON THE ELECTRONIC STRUCTURE AND ANTI- / PROOXIDANT PROPERTIES OF FLAVONOIDS: 3,5-DIHYDROXYFLAVONE AND ITS Cu^+, Cu^{2+} AND Zn^{2+} COORDINATION COMPLEXES	P78	Francisco Partal Ureña, Mª Carmen Ramírez Avi, and Ana África Márquez García	Spain
MOLECULAR DYNAMICS STUDIES OF A COMPLEX SYSTEM TO	P79		Spain

DISORDERED PROTEIN.		Crehuet	
A PROGRAM TO SEARCH FOR ADSORPTION SITES IN MOFS	P80	Pavel N. Zolotarev, Vladislav A. Blatov, Davide M. Proserpio	Russia and Italy
THE STATE OF IRON ATOMS AND EXCHANGE INTERACTIONS IN $BI_3NB_{1-X}FE_XO_{7-\Delta}$	P81	Nadezhda Zhuk, Nataliya Chezhina, Vladimir Lutoev, Boris Makeev, and Lyba Rychkova	Russia
PINPOINTING DFT PERFORMANCE IN THE SIMULATIONS OF TWO-PHOTON ABSORPTION SPECTRA OF ORGANIC CHROMOPHORES	P82	Joanna Bednarska, Robert Zaleśny, Wojciech Bartkowiak, Hans Ågren	Poland and Sweden
THE BEST COMPUTATIONAL INDICES FOR INTRAMOLECULAR HYDROGEN BOND STUDYING, CONFIRMED BY EXPERIMENTAL OBSERVATION	P83	A-Reza Nekoei, Sahar Jamshidpanah	Iran
SMALL MOLECULE BINDING PATHWAY AND KINETICS WITH HTMD	P84	João M. Damas, Nathaniel Stanley, Matt J. Harvey, Stefan Doerr and Gianni De Fabritiis	Spain
SELECTIVE CYCLIC CARBONATE FORMATION FROM CO_2 AND EPOXY-ALCOHOLS: MECHANISTIC ELUCIDATION VIA DFT ANALYSIS	RT11	Joan González-Fabra, Jeroen Rintjema, Nuno A. G. Bandeira, Arjan W. Kleij and Carles Bo	Spain
CARBON DIOXIDE REDUCTION ON SODIUM AND POTASSIUM HYDROXIDE ACTIVATED GRAPHITIC CARBON NITRIDE	RT12	Julia M. T. A. Fischer, Marlies Hankel, and Debra J. Searles	Australia
MOFS DECOMPOSITION AND THE DATABASE OF SECONDARY BUILDING UNITS	RT13	Andrey A. Golov, Vladislav A. Blatov, Davide M. Proserpio	Russia and Italy
MULTI-LEVEL STRATEGY FOR ANALYSIS OF BIOACTIVE DRUG CONFORMATIONS	RT14	Sanja Zivanovic, Adam Hospital, Modesto Orozco	Spain
POTENTIAL ENERGY LANDSCAPE AND SPECTROSCOPICAL CHARACTERIZATION OF AZA-NANOHOOPS: PROMISING STRUCTURES FOR GAS CAPTURE	RT15	Ángel Vida-Vidal, Olalla Nieto Faza, and Carlos Silva López	Spain
UNDERSTANDING THE SYNTHESIS OF PROSTAGLANDIN G2 FROM ARACHIDONIC ACID CATALYZED BY CYCLOOXYGENASE-2: A MOLECULAR DYNAMICS/QM/MM APPROACH	RT16	Anna Cebrián, Àngels González-Lafont and José María Lluch	Spain