

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
THE STATE OF IRON ATOMS AND EXCHANGE INTERACTIONS IN $Bi_3NB_{1-x}Fe_xO_{7-\Delta}$	P4	Nadezhda Zhuk, Nataliya Chezhina, Vladimir Lutoev, Boris Makeev, and Lyba Rychkova	Russia
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. Maserasa,	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, Tomáš 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
A DFT RELATIVISTIC STUDY OF CYANIDE AND ISOCYANIDE CERIUM(III) AND URANIUM(III) COMPLEXES.	P13	Yamina Bouzidi, Lotfi Belkhiri, Michel Ephritikhine, Jean-François Halet, and Abdou Boucekkine	Algeria and France
EXPERIMENTAL AND THEORETICAL INSIGHTS ON $BaW_0.5Mo_0.5O_4$ 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 Matitoo	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 Aragón, 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	<u>P18</u>	<u>Minserk Cheong</u>	<u>Republic of Korea</u>
WATER-GAS SHIFT REACTION COCATALYZED BY K ₃ PM ₁₂ O ₄₀ AND Au(111): THE MAGIC ROLE OF POLYOXOMETALATES	<u>P19</u>	<u>Anna Clotet, Zhongling Lang and Josep M. Poble</u>	<u>Spain</u>
MINIMIZING FALSE-POSITIVE RATES IN HIGH-THROUGHPUT SCREENING: PREDICTORS FOR FLUORESCENT COMPOUNDS	<u>P20</u>	<u>Ramona Curpăn, Sorin Avram, Alina Bora and Liliana Halip</u>	<u>Romania</u>
THE DARK SIDE OF ALUMINUM CHELATION THERAPY: CHARACTERIZATION OF THE AL(III) – LIGAND BINDING FEATURES	<u>P21</u>	<u>Gabriele Dalla Torre, Jon I. Mujika and Xabier Lopez</u>	<u>Spain</u>
THEORETICAL AND SPECTROSCOPIC INVESTIGATION ON CHARGE-TRANSFER COMPLEX BETWEEN N-SULFAMOYLOXAZOLIDINONE AND PICRIC ACID.	<u>P22</u>	<u>Karim DINAR, Mekki KADRI, Achour SERIDI and Mohamed ABDAOUI</u>	<u>Algeria</u>
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ELECTRONIC STRUCTURE ANALYSIS OF KEY ORGANOGOLD TRANSFORMATIONS	<u>P24</u>	<u>Laura Estévez, Maximilian Joost, Ferial Rekhroukh, Abderrahmane Amgoune, Didier Bourissou, Karinne Miqueu</u>	<u>Spain and France</u>
ULTRAFast EXCITED-STATE DECAYS IN [RE(CO) ₃ (N,N)(L)] ^{N+} : NON-ADIABATIC QUANTUM DYNAMICS	<u>P25</u>	<u>Maria Fumanal, Etienne Gindensperger, and Chantal Daniel</u>	<u>France</u>
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CLARIFYING THE MECHANISM OF THE 2-HYDROXYPYRIDINE/2-PYRIDONE PHOTO-TAUTOMERIZATION.	<u>P27</u>	<u>Sara Gil Guerrero and Jose M. Hermida-Ramón</u>	<u>Spain</u>
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Poster Communications - POSTER SESSION 3			
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A COMPUTATIONAL STUDY ON POTENTIAL NEW INHIBITORS OF O-ACETYLPEPTIDOGLYCAN ESTERASE	P70	<u>M.M.Tataroğlu</u> , Z.Aksakal , N.Tüzün, F.A.Sungur	Turkey
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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, <u>Seiji Mori</u>	Japan
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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	<u>Francisco Partal Ureña</u> , M ^a Carmen Ramírez Avi, and Ana África Márquez García	Spain
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THE STATE OF IRON ATOMS AND EXCHANGE INTERACTIONS IN $\text{Bi}_3\text{NB}_{1-x}\text{Fe}_x\text{O}_{7-\Delta}$	P81	<u>Nadezhda Zhuk</u> , 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	<u>Joanna Bednarska</u> , Robert Zaleśny, Wojciech Bartkowiak, Hans Ågren	Poland and Sweden
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