

POSTER NUMBERS

(Alphabetical order according to the surname of the presenting author)

Number	Abstract Title	Presenting Author
P1	Intermolecular interactions between mefenamic acid and saccharin	Nursef Acar Selcuki
P2	Modeling of deacetylation reaction mechanism of o-acetylpeptidoglycan esterase with quantum cluster approach	Z. Aksakal
P3	Determination of active organocatalyst using computational methods	Yeşim Çamlısoy, Sezen Alsancak
P4	Resonances in the dielectronic recombination cross section of Ni ¹³⁺	Zikri Altun
P5	Os cation assisted transformation of acetylene to diatomic hydrogen	Zikri Altun
P6	Double fluorescence assay via a β -cyclodextrin containing conjugated polymer as a biomimetic material for cocaine sensing	Mustafa Arslan
P7	Methionine degradation	Busenur Aslanoglu
P8	Mechanistic DFT study on one-pot synthesis of heterocyclic compounds	Müge Atbakar
P9	Selectivity in (4+3) cycloadditions of furfuryl cations	Ö. N. Avcı
P10	Unexpectedly synthesis of copper salen complexes from salicylaldehyde thiosemicarbazone	Elif Avcu
P11	Identification of novel MDM2-p53 protein-protein interaction inhibitors with multidimensional molecular modeling approaches and application of binary QSAR models for prediction of therapeutic activity and toxic effects	Gulsah Aydin
P12	Reactivity descriptors for the prediction of the degradation reactions of sulfonamides	Şeyda Aydoğdu
P13	Cytotoxic activity and synthesis of nickel (II) mixed ligand complex of 4-methoxysalicylaldehyde thiosemicarbazone with N,N-diethylethylenediamine	Tülay Bal-Demirci
P14	A novel methodology to predict plasticization pressures of polymeric membranes	Marcel Balcik
P15	Rationalization of the activity of the lactone form of topotecan towards the DNA/topol complex	Semiha K. Bali
P16	Computational design of small organic molecules as mimics of hydrolase enzymes	İlknur S. Ballica, Emre T. Sarı, Neşe E. Ünsal, Bike Kurter,
P17	Construction of allosteric residue networks in caspase-7 using energy perturbation responses	Elif N. Bingöl
P18	Dye and semiconductor interfaces under scrutiny: cluster versus periodic approach for electron injection and light harvesting	E. B. Boydas
P19	A computational approach to sustainable industrial amines	Esra Boz
P20	Effect of temperature on the molecular dynamics simulations of HLA-A*02 alleles	Asuman Bunsuz
P21	Ab initio study of novel phthalocyanine – based covalent organic frameworks	Yurii Chumakov
P22	Rh-catalyzed [5+1] and [4+1] cycloadditions of 1,4-enynes by CO with concomitant 1,2- versus 1,3-acyloxy migrations: a DFT study	Dilek Coşkun
P23	Theoretical investigation of the degradation mechanism and byproduct assessment of diclofenac	S. Agopcan Çınar
P24	Synthesis, characterization and photoinduced cross-linking of functionalized poly(cyclohexyl methacrylate) copolymer/clay nanocomposite as negative image patterning material	Mustafa Ciftci
P25	Assessing the Ligand-protein Binding Modes with Computational Tools	Gülşah Çıfci
P26	Modeling of homogeneous catalysis reaction of C-H bond activation	Gökçen Alev Çiftçioğlu
P27	A DFT study on electronic and optical properties of BTI-based oligomers	Çisil Alim
P28	Dioxygen activation by [Ni(H)(OH)] ⁺ , an MCSCF study	Yavuz Dede
P29	Computational assessment of iron release from the N- and C-lobes of human serum transferrin	Burcu Dedeoglu
P30	Structure-reactivity relationships in sulfur-centred radical chemistry: a computational study	İsa Degirmenci
P31	Modeling of human GluNR ₁ -GluNR _{2A} NMDA receptor	Ayhan Demir
P32	X-ray diffraction studies of Ni(II) complex derived from 3,4-diaminobenzophenone	Eylem Dilmen

P33	Exo-Selective inverse-electron-demand hetero Diels–Alder reactions of norbornene with 5-benzylidene-2-arylimino-3-aryl-thiazolidine-4-thiones	Ilknur Dogan
P34	Crystallographic studies of dioxomolybdenum(VI) complex	Songül Eğlence
P35	Virtual screening of approved drugs for pyruvate kinase inhibition of antibiotic-resistant bacteria	Cagla Ergun
P36	Synthesis of stable tetrahedral intermediates (hemiaminals) and kinetics of their conversion to thiazol-2-imines	Sule Erol Gunal
P37	Theoretical investigation of thiol-ene click reactions: a DFT perspective	Volkan Fındık
P38	Catalytic activity of Au(210) surface for sodium and lithium borohydride hydrolysis reaction: a DFT study	A. E. Genç
P39	Mutations affecting communication of residues disclose residues of evolutionary relevance	T.F. Guclu
P40	Discovery of cryptochrome destabilizer small molecules enhancing the apoptosis	Şeref Gül
P41	Computational study of N-acetylneuraminic acid tryptophan interactions	Ersin Gündeğer
P42	3-Bromo-5-chloro-2-hydroxyacetophenone-N4-butyl-thiosemicarbazidato triphenylphosphine palladium(II) complex	Şükriye Güveli
P43	Nickel(II) complex based on thiosemicarbazone: crystallographic, spectroscopic and DFT calculations	Şükriye Güveli
P44	Nano-hemoglobin film based sextet state biomemory device by cross-linked photosensitive hapten monomer	Remziye Güzel
P45	Elucidation of atroposelective synthesis of axially chiral thiohydantoin derivatives	Z. P. Haşlak
P46	Mechanistic aspects of catalytic asymmetric 6-π electrocyclization: a DFT study	B. Horoz
P47	Predicting self-assembly of nanoparticles for targeted drug delivery	Mehtap Işık
P48	Developing doxycycline imprinted hydrogels using computational and experimental approaches	Tugce Inan
P49	A computational study on the formation of keteniminium salts	Ulfet Karadeniz
P50	X-ray crystallographic studies of bithiocarbohydrazone ligand derived from 2-hydroxy-4-methoxybenzophenone	Yeliz Kaya
P51	Square pyramidal iron(III) complex of an N2O2-chelating thiosemicarbazone with azide co-ligands	Büşra Kaya
P52	The effect of cation doping on the electronic structure of TiO ₂	Serap Kırıcı
P53	Computational assessment of allosteric mutations on the dynamics of pdz domains	Nazlı Kocatuğ
P54	Design of donor-acceptor copolymers for organic photovoltaic materials: a computational study	O. Kucur, HT. Turan, B. Kahraman
P55	A study of rolling mechanism of single molecule on metal surface: DFT and molecular dynamic simulations	Melihat Madran
P56	On the development of molecular mechanics force field parameters	Antoine Marion
P57	Molecular dynamics and docking studies on the interactions of DNA with quaternary metallo phthalocyanines	Lalehan Özalp
P58	The efficient cyclopolymerization of silyl-tethered styrenic difunctional monomers	Beste Ozaydin
P59	Oncogenic mutations on Rac1 regulate Rac1-PAK1 binding by shifting the binding state through global mode perturbations	Saliha E. Acuner-Ozbabacan
P60	Towards “synthetic metals” with acceptor-donor type conducting polymers	Alimet Sema Ozen
P61	Computational investigation of the KMO catalysed reaction mechanism between L-Kyn and FAD	Yılmaz Özkılıç
P62	Allosteric control of the DNA-RNA translocation in telomerase	Aydın Özmaldar
P63	Action of nicc enzyme on nicotinate: a model DFT study	Neriman E. Pehlivanoğlu
P64	¹ H and ¹³ C NMR studies of 1,2,4,5-oxadiazaborole derivatives	Meryem Pir
P65	Mechanistic dft study on the function of homoboroproline as asymmetric catalyst in enantioselective aldol reactions	Safiye Sağ Erdem
P66	Molecular docking of arylcoumarins to carbapenemase enzyme	Safiye Sağ Erdem
P67	Unusual disproportionative condensation of indoles with cyclohexanone: an experimental and computational study	Nurullah Saracoglu

P68	A combined experimental and theoretical study for the formation of indolizine, pyrrolo[1,2,a]pyrazine, pyrrolo[1,2-a]pyrazinone	Ozlem Sari
P69	Gels confined to narrow capillaries	Ozan S. Sariyer
P70	Intermolecular interactions between protoporphyrine and hydroxypyrene	Cenk Selçuki
P71	Singlet oxygen generation aptitude of thiophene-derivatives	Ozlem Sengul
P72	A software tool for parallel computation and characterization of residue interaction energies from molecular dynamics simulations	Onur Serçinoğlu
P73	Molecular modeling of metal organic frameworks for the controlled release of topical steroids	F. Aylin Sungur
P74	A Mechanistic study on the catalytic mechanism of protein arginine deiminase 2	Fethiye Aylin Sungur
P75	Michael addition reaction of cyclobuteniminium salts and various nucleophiles - a DFT study	Gamze Tanriver
P76	A computational insight into cyclopropanone activated dehydration reaction of alcohols	M. M. Tataroğlu
P77	ZnO and TiO ₂ loaded MnO ₂ nanocomposites and photoactivity investigation	Duygu Tuncel
P78	Understanding the impact of thiophene/furan substitution to intrinsic charge-carrier mobility	H. T. Turan
P79	Photocatalytic decolorization of reactive Blue 221 on TiO ₂ : prediction of mechanism via conceptual DFT	Nazlı Türkten
80	The binuclear CuAAC mechanism in the light of new experiments	Nurcan Ş. Tüzün
P81	the inhibitory effect of quinone derivatives on oacetylpeptidoglucan esterase enzyme	N. Ş. Tüzün
P82	Dynamical origin of room-temperature charge-transport in organic crystal	I. Yavuz
P83	Investigation of allosteric pathways on the bacterial ribosome	Hatice Zeynep Yildirim
P84	Investigating self-assembly behaviour of lipid-like structures in dual solvents	Aygul Zengin