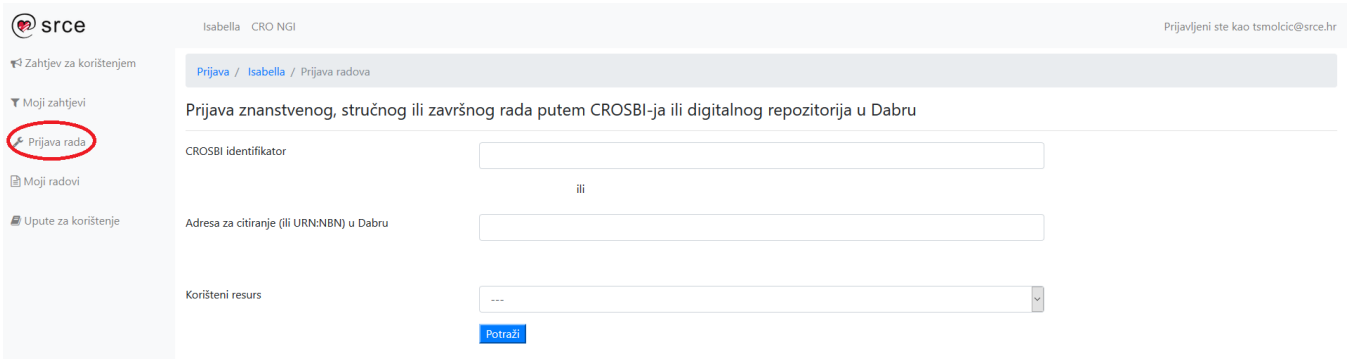
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Mechanistic Study of the Mechanochemical PdII- Catalyzed Bromination of Aromatic C–H bonds by Experimental and Computational methods	Barišić Dajana, Halasz Ivan, Bjelopetrović Alen, Babić Darko, Ćurić Manda	10.1021/acs.organomet.1c00698	0276-7333	2022	Organometallics	41	11	1284-1294
Resistance Coefficient Estimation for a Submarine's Bare Hull Moving in Forward and Transverse Directions	Saghi Hassan, Parunov Joško, Mikulić Antonio	10.3390/app122110953		2022	Applied Sciences	12		-
The structure-activity relationship and computational studies of 1,3-thiazole derivatives as cholinesterase inhibitors with anti-inflammatory activity	Modrić Marina, Božičević Marin, Odak Ilijana, Talić Stanislava, Barić Danijela, Mlakić Milena, Raspudić Anamarija, Škorić Irena	10.5802/crchim.201	1631-0748	2022	Comptes rendus. Chimie	25		267-279
Glucosamine to gold nanoparticles binding studied using Raman spectroscopy	Mohaček Grošev Vlasta, Brljafa Sandro, Škrabić Marko, Marić Ivan, Blažek Bregović Vesna, Amendola Vincenzo, Ropret Polona, Kvaček Blažević Anita	10.1016/j.saa.2021.120326	1386-1425	2022	Spectrochimica acta. Part A, Molecular and biomolecular spectroscopy	264		-
Raman study of water deposited in solid argon matrix	Mohaček Grošev Vlasta, Furić Krešimir, Vujnović Vedran	10.1016/j.saa.2021.120770	1386-1425	2022	Spectrochimica acta. Part A, Molecular and biomolecular spectroscopy	269		-
Pressure-induced and flaring photocatalytic diversity of ZnO particles hallmarked by finely tuned pathways	Vrankić Martina, Šarić Ankica, Nakagawa Takeshi, Ding Yang, Despotović Ines, Kanižaj Lidija, Ishii Hirofumi, Hiraoka Nozomu, Dražić Goran, Lützenkirchen-Hecht Dirk, Peter Robert, Petravić Mladen	10.1016/j.jallcom.2021.162444	0925-8388	2022	Journal of Alloys and Compounds	894		-
Mjerenje performanci platforme Apache Beam u obradi prostorno vremenskih tokova podataka	Aleksandar Novak			2022				-
Synthesis, photochemistry and computational study of novel 1,2,3-triazole heterostilbenes: expressed biological activity of their electrocyclization photoproducts	Mlakić Milena, Faraho Ivan, Odak Ilijana, Talić Stanislava, Vukovinski Ana, Raspudić Anamarija, Bosnar Martina, Zadravec Rahela, Ratković Ana, Lasić Kornelija, Marinić Željko, Barić Danijela, Škorić Irena	10.1016/j.bioorg.2022.105701	0045-2068	2022	Bioorganic chemistry	121		-

COVID-19 infection and neurodegeneration: Computational evidence for interactions between the SARS-CoV-2 spike protein and monoamine oxidase enzymes	Hok Lucija, Rimac Hrvoje, Mavri Janez, Vianello Robert	10.1016/j.csbj.2022.02.020	2001-0370	2022	Computational and Structural Biotechnology Journal	20		1254-1263
Adsorption of a wide variety of antibiotics on graphene-based nanomaterials: A modelling study	Kern Matej, Škulj Sanja, Rožman Marko	10.1016/j.chemosphere.2022.134010	0045-6535	2022	Chemosphere	296		-
Automatic compiler /interpreter generation from programs for Domain-Specific Languages: Code bloat problem and performance improvement	Kovačević Željko, Ravber Miha, Liu Shih-Hsi, Črepinšek Matej	10.1016/j.cola.2022.101105	2665-9182	2022	Journal of Computer Languages	70C		-
Skaliranje energije i širine maločestičnih sustava u 2D	Ivna Baković			2021-09-24				
3D physics-based seismic shaking scenarios for city of Zagreb, Capital of Croatia	Latečki Helena, Molinari Irene, Stipčević Josip	10.1007/s10518-021-01227-5	1570-761X	2021-09-17	Bulletin of Earthquake Engineering	19	12	1-27
Amidino substituted 2-aminophenols: biologically important building blocks for the amidino-functionalization of 2-substituted benzoxazoles	Ptiček Lucija, Hok Lucija, Grbčić Petra, Topić Filip, Cetina Mario, Rissanen Kari, Kraljević Pavelić Sandra, Vianello Robert, Racané Livio	10.1039/d1ob00235j	1477-0520	2021	Organic & biomolecular chemistry	19		2784-2793
N-substituted benzimidazole acrylonitriles as in vitro tubulin polymerization inhibitors: Synthesis, biological activity and computational analysis	Perin Nataša, Hok Lucija, Beč Anja, Persoons Leentje, Vanstreels Els, Daelemans Dirk, Vianello Robert, Hranjec Marijana	10.1016/j.ejmech.2020.113003	0223-5234	2021	European journal of medicinal chemistry	211		-
Selfassembly of cobalt(II) coordination polymers with differently halosubstituted nicotinate ligands and 4,4'bipyridine – the effect of the halosubstituent positions on polymer types	Hok Lucija, Lluch Sanchez Eloi, Vianello Robert, Kukovec Boris-Marko, Popović Zora	10.1002/ejic.202100055	1434-1948	2021	European journal of inorganic chemistry	2021	15	1470-1480

Further investigation of harmicines as novel antiplasmodial agents: synthesis, structure-activity relationship and insight into the mechanism of action	Marinović Marina, Poje Goran, Perković Ivana, Fontinha Diana, Prudêncio Miguel, Held Jana, Pessanha de Carvalho Lais, Tandarić Tana, Vianello Robert, Rajić Zrinka	10.1016/j.ejmech.2021.113687	0223-5234	2021	European journal of medicinal chemistry	224		-
Novel Bis- and Mono-Pyrrolo[2,3-d] pyrimidine and Purine Derivatives: Synthesis, Computational Analysis and Antiproliferative Evaluation	Bistrović Popov Andrea, Vianello Robert, Grbčić Petra, Sedić Mirela, Kraljević Pavelić Sandra, Pavelić Krešimir, Raić-Malić Silvana	10.3390/molecules26113334		2021	Molecules	26	11	-
Direct Metal-Free Transformation of Alkynes to Nitriles: Computational Evidence for the Precise Reaction Mechanism	Hok Lucija, Vianello Robert	10.3390/ijms22063193		2021	International journal of molecular sciences	22	6	-
Understanding the human DPP iii substrate specificity : QM/MM and MD calculations	Tomić Antonija, Tomić Sanja			2021	Math/Chem/Comp 2021 : 32nd MC2 Conference : book of abstracts			42-42
Glycerol as a Substrate and Inactivator of Coenzyme B12 Dependent Diol Dehydratase	Bilić Luka, Barić Danijela, Sandala Gregory M, Smith David M., Kovačević Borislav	10.1002/chem.202100416	0947-6539	2021	Chemistry : a European journal	27	29	7930-7941
Experimental and theoretical (ReaxFF) study of manganese-based catalysts for low-temperature toluene oxidation	Duplančić Marina, Gomzi Vjeran, Pintar Albin, Kurajica Stanislav, Tomašić Vesna	10.1016/j.ceramint.2020.09.147	0272-8842	2021	Ceramics international	47		3108-3121
Error Evaluation and Suitability Assessment of Common Reliability Methods in the Case of Shallow Foundations	Dodigović Filip, Ivandić Krešo, Kovačević Meho Saša, Soldo Božo	10.3390/app11020795		2021	Applied Sciences-Basel	11	2	-
Molecular Dynamics Simulations of Mitochondrial Uncoupling Protein 2	Škulj Sanja, Brkljača Zlatko, Kreiter Jürgen, Pohl Elena E., Vazdar Mario	10.3390/ijms22031214		2021	International journal of molecular sciences	22(3)		-
How Secure Are Two-Way Ping-Pong and LM05 QKD Protocols under a Man-in-the-Middle Attack?	Pavičić Mladen	10.3390/e23020163		2021	Entropy (Basel. Online)	23	2	-
Chemistry and Reactivity of 4-hydroxy-2-nonenal (HNE) in Model Biological Systems	Vazdar Katarina, Škulj Sanja, Bakarić Danijela, Margetić Davor, Vazdar Mario	10.2174/1389557521666210511053838	1389-5575	2021	Mini-reviews in medicinal chemistry	21		1-12

Sulfur molecules in space by X-rays: a computational study	Bilalbegović Goranka, Maksimović Aleksandar, Valencic Lynne Ann, Lehtola Susi	10.1021/acsearthspacechem.0c00238		2021	ACS Earth and Space Chemistry			-
ANT1 Activation and Inhibition Patterns Support the Fatty Acid Cycling Mechanism for Proton Transport	Kreiter Jürgen, Rupprecht Anne, Škulj Sanja, Brkljača Zlatko, Žuna Kristina, Knyazev Denis G., Bardakji Sarah, Vazdar Mario, Pohl Elena E.	10.3390/ijms22052490		2021	International journal of molecular sciences	22(5)		-
Modelling of the adsorption of pharmaceutically active compounds on carbon-based nanomaterials	Ivanković Klaudija, Kern Matej, Rožman Marko	10.1016/j.jhazmat.2021.125554	0304-3894	2021	Journal of hazardous materials	414		-
DFTPCM Study on Solvolytic Behaviour of Nalkyl Xpyridinium Ions	Matić Mirela, Denegri Bernard	10.1002/slct.202004231		2021	ChemistrySelect	6	9	2410-2423
Sensing capabilities of ultrathin BaTiO3 nanostructures toward carbon oxides based on optical signals from the theoretical perspective	Lukačević Igor, Varga Pajtler Maja, Mužević Matko	10.1016/j.matchemphys.2021.124434	0254-0584	2021	Materials chemistry and physics	265		124434-124440
Mechanism of formaldehyde and formic acid formation on (101)-TiO2@Cu4 systems through CO2 hydrogenation	Singh Deobrat, Gupta Sanjeev K., Seriani Nicola, Lukačević Igor, Sonvane Yogesh, Gajjar P. N., Ahuja Rajeev	10.1039/D0SE01587C		2021	Sustainable Energy & Fuels	5	2	564-574
Selective DNA and protein isolation from marine macrophyte surfaces	Korlević Marino, Markovski Marsej, Zhao Zihao, Herndl Gerhard J., Najdek Mirjana	10.3389/fmicb.2021.665999	1664-302X	2021	Frontiers in microbiology	12		-
Synthesis and photochemistry of novel 1,2,3-triazole di-heterostilbenes. An experimental and computational study	Ratković Ana, Mlakić Milena, Dehaen Wim, Opsomer Tomas, Barić Danijela, Škorić Irena	10.1016/j.saa.2021.120056	1386-1425	2021	Spectrochimica acta. Part A, Molecular and biomolecular spectroscopy	261		-
Unravelling the inhibitory zinc ion binding site and the metal exchange mechanism in human DPP III	Tomić Antonija, Brkić Hrvoje, Matić Antonia, Tomić Sanja	10.1039/D1CP01302E	1463-9076	2021	PCCP. Physical chemistry chemical physics	23		13267-13275
Mitochondrial Uncoupling Proteins (UCP1-UCP3) and Adenine Nucleotide Translocase (ANT1) Enhance the Protonophoric Action of 2,4-Dinitrophenol in Mitochondria and Planar Bilayer Membranes	Žuna Kristina, Jovanović Olga, Khailova Ljudmila S., Škulj Sanja, Brkljača Zlatko, Kreiter Jürgen, Kotova Elena A., Vazdar Mario, Antonenko Yuri N. Antonenko, Pohl Elena E.	10.3390/biom11081178		2021	Biomolecules	11		1178-1192
Prediction of the kinetic stability of N-alkyl X-pyridinium ions in dichloromethane	Matić Mirela, Denegri Bernard	10.1002/poc.4248	0894-3230	2021	Journal of physical organic chemistry	34		-

Seasonal dynamics of epiphytic microbial communities on marine macrophyte surfaces	Korlević Marino, Markovski Marsej, Zhao Zihao, Herndl Gerhard J., Najdek Mirjana	10.3389/fmicb.2021.671342	1664-302X	2021	Frontiers in microbiology	12		-
Differential enrichment of H3K9me3 at annotated satellite DNA repeats in human cell lines and during fetal development in mouse	Vojvoda Zeljko Tanja, Ugarković Đurđica, Pezer Željka	10.1186/s13072-021-00423-6		2021	Epigenetics & Chromatin	14	1	47-16
Molecular and evolutionary basis for survival, its failure, and virulence factors of the zoonotic nematode Anisakis pegreffii	Trumbić Željka, Hrabar Jerko, Palevich Nikola, Carbone Vincenzo, Mladineo Ivona	10.1016/j.ygeno.2021.06.032	0888-7543	2021	Genomics	113	5	2891-2905
Understanding the conformational, electronic and vibrational properties of Tetrahydrocannabinol (THC) and Cannabidiol (CBD). Pharmacophoric similarities and differences	Baranović Goran	10.1016/j.molstruc.2021.130945	0022-2860	2021	Journal of molecular structure	1244		-
Role of substituents in the Hofmann–Löffler–Freytag reaction. A quantum-chemical case study on nicotine synthesis	Shkunnikova Sofia, Zipse Hendrik, Šakić Davor	10.1039/d0ob02187c	1477-0520	2021	Organic & biomolecular chemistry	19		854-865
Low-pressure chromatographic separation and UV/Vis spectrophotometric characterization of the native and desialylated human apo-transferrin	Friganović Tomislav, Tomašić Antonela, Šeba Tino, Biruš Ivan, Kerep Robert, Borko Valentina, Šakić Davor, Gabričević Mario, Weitner Tin	10.1016/j.heliyon.2021.e08030	2405-8440	2021	Heliyon	7	9	-
Towards the Well-Tempered Chloroplast DNA Sequences	Turudić Ante, Liber Zlatko, Grdiša Martina, Jakše Jernej, Varga Filip, Šatović Zlatko	10.3390/plants10071360	2223-7747	2021	Plants	10	7	-
Combining Raman spectroscopy, DFT calculations and atomic force microscopy in the study of clinker materials	Mohaček Grošev Vlasta, Đuroković Marija, Maksimović Aleksandar	10.3390/ma14133648		2021	Materials	14	13	-
Uncovering the ElectronPhonon Interplay and Dynamical Energy Dissipation Mechanisms of Hot Carriers in Hybrid Lead Halide Perovskites	Chan Christopher C. S., Fan Kezhou, Wang Han, Huang Zhanfeng, Novko Dino, Yan Keyou, Xu Jianbin, Choy Wallace C. H., Lončarić Ivor, Wong Kam Sing	10.1002/aenm.202003071	1614-6832	2021	Advanced Energy Materials	11	9	-

Microbiome of the Successful Freshwater Invader, the Signal Crayfish, and Its Changes along the Invasion Range	Dragičević Paula, Bielen Ana, Petrić Ines, Vuk Marija, Žučko Jurica, Hudina Sandra	10.1128/Spectrum.00389-21		2021	Microbiology Spectrum	9	2	-
Combined NMR and Computational Study of Cysteine Oxidation during Nucleation of Metallic Clusters in Biological Systems	Pem Barbara, Toma Mateja, Vrček Valerije	10.1021/acs.inorgchem.1c00321	0020-1669	2021	Inorganic chemistry	60	6	4144-4161
Photocatalytic degradation of imidacloprid in the flat-plate photoreactor under UVA and simulated solar irradiance conditions—The influence of operating conditions, kinetics and degradation pathway	Babić Kristina, Tomašić Vesna, Gilja Vanja, Le Cunff Jerome, Gomzi Vjeran, Pintar Albin, Žerjav Gregor, Kurajica Stanislav, Duplančić Marina, Zelić Ivana Elizabeta, Pavičić Tomislava Vukušić, Grčić Ivana	10.1016/j.jece.2021.105611	2213-3437	2021	Journal of Environmental Chemical Engineering	9	4	-
ReaxFF force field development and application for toluene adsorption on MnMOx (M=Cu, Fe, Ni) catalysts	Gomzi Vjeran, Movre-Šapić Iva, Vidak Andrej			2021				41-41
Photodegradation of neonicotinoids on a TiO2-based photocatalysts - efficiency of reactive oxygen species	Duplančić Marina, Zelić Ivana Elizabeta, Gomzi Vjeran, Tomašić Vesna, Carić Dejana, Žilić Dijana			2021	27th Croatian Meeting of Chemists and Chemical Engineers: Book of abstracts			295-295
Grass pea natural variation reveals oligogenic resistance to Fusarium oxysporum f. sp. pisi	Sampaio Ana Margarida, Alves Mara Lisa, Pereira Priscila, Valiollahi Ehsan, Santos Carmen, Šatović Zlatko, Rubiales Diego, de Sousa Araújo Susana, van Eeuwijk Fred, Vaz Patto Maria Carlota	10.1002/tpg2.20154	1940-3372	2021	Plant Genome	2021		-
Accessing Ancestral Origin and Diversity Evolution by Net Divergence of an Ongoing Domestication Mediterranean Olive Tree Variety	Sales Hélia, Šatović Zlatko, Alves Mara Lisa, Fevereiro Pedro, Nunes João, Vaz Patto Maria Carlota	10.3389/fpls.2021.688214		2021	Frontiers in plant science	12		-
Genetic diversity and structure analysis of Croatian garlic collection assessed by SSR markers	Poljuha Danijela, Franić Mario, Kralj Ines, Weber Tim, Šatović Zlatko, Ban Dean, Toth Nina, Dumičić Gvozden, Kereša Snježana, Pinto da Cunha Camila, Goreta Ban Smiljana	10.2478/fhort-2021-0011	0867-1761	2021	Folia Horticulturae	33	1	1-15
High Genetic Diversity and Low Population Differentiation in Wild Hop (Humulus lupulus L.) from Croatia	Grdiša Martina, Šatović Zlatko, Liber Zlatko, Jakše Jernej, Varga Filip, Erhatić Renata, Srečec Siniša	10.3390/app11146484		2021	Applied Sciences-Basel	21	14	1-14
Genome-Wide Association Studies of Mineral Content in Common Bean	Gunjača Jerko, Carović-Stanko Klaudija, Lazarević Boris, Vidak Monika, Petek Marko, Liber Zlatko, Šatović Zlatko	10.3389/fpls.2021.636484		2021	Frontiers in plant science	12		-

Assessment of the Origin and Diversity of Croatian Common Bean Germplasm Using Phaseolin Type, SSR and SNP Markers and Morphological Traits	Vidak Monika, Šatović Zlatko, Liber Zlatko, Grdiša Martina, Gunjača Jerko, Kilian Andrzej, Carović-Stanko Klaudija	10.3390/plants10040665	2223-7747	2021	Plants	10	4	-
Seismic shaking scenarios for city of Zagreb, Croatia	Latečki Helena, Stipčević Josip, Molinari Irene	10.5194/egusphere-egu21-8781		2021	Book of Abstracts EGU General Assembly 2021			8781-8781
Triarylborane Dyes as a Novel Non Covalent and Non Inhibitive Fluorimetric Markers for DPP III Enzyme	Ban Željka, Karačić Zrinka, Tomić Sanja, Amini Hashem, Marder Todd B., Piantanida Ivo	10.3390/molecules26164816		2021	Molecules	26		-
SHH-N non-canonically sustains androgen receptor activity in androgen-independent prostate cancer cells	Trnski Diana, Sabol Maja, Tomić Sanja, Štefanac Ivan, Mrčela Milanka, Musani Vesna, Rinčić Nikolina, Kurtović Matea, Petrić Tina, Levanat Sonja, Ozretić Petar	10.1038/s41598-021-93971-6		2021	Scientific reports	11	1	-
Aryl-diyne linkers in bis-triarylborane cations control fluorimetric and Raman sensing of various DNA and RNA	Ferger Matthias, Ban Željka, Krošl Ivona, Tomić Sanja, Dietrich Lena, Lorenzen Sabine, Rauch Florian, Sieh Daniel, Friedrich Alexandra, Griesbeck Stefaine, Kenđel Adriana, Miljanić Snežana, Piantanida Ivo, Marder Todd B.	10.1002/chem.202005141	0947-6539	2021	Chemistry : a European journal	27		5142-5159
Importance of protein intrinsic conformational dynamics and transient nature of non-covalent interactions in ligand binding affinity	Kekez Mario, Zanki Vladimir, Antičević Ivan, Rokov-Plavec Jasmina, Maršavelski Aleksandra	10.1016/j.ijbiomac.2021.10.045	0141-8130	2021	International journal of biological macromolecules	192		692-700
Mannosylated adamantane-containing desmuramyl peptide recognition by the NOD2 receptor: a molecular dynamics study	Maršavelski Aleksandra, Paurević Marija, Ribić Rosana	10.1039/D1OB00679G	1477-0520	2021	Organic & biomolecular chemistry	19		7001-7012
A ferrocene-based pseudopeptide chiroptical switch	Opačak Saša, Babić Darko, Perić Berislav, Marinić Željko, Smrečki Vilko, Pem Barbara, Vinković Vrček Ivana, Kirin Srećko I.	10.1039/D1DT00508A	1477-9226	2021	Dalton transactions	13		4504-4511
Aluminum in dental implants: how to reduce a potential risk to patient´s health?	Petrović Željka, Šarić Ankica, Despotović Ines, Katić Jozefina, Petković Marin	10.3390/CMDWC2021-09933		2021	Materials Proceedings			-
Priprava novih indenskih heteropolicikličkih sustava	Znika Monika			2021				-
A crystallographic and solid-state NMR study of 1,4-disubstituted 2,5-diketopiperazines	Perić Berislav, Pantalon Juraj Natalija, Szalontai Gábor, Veličković Suzana R., Veljković Filip M., Vikić-Topić Dražen, Kirin Srećko I.	10.1016/j.molstruc.2021.130157	0022-2860	2021	Journal of molecular structure	1234		-

Search for Novel Lead Inhibitors of Yeast Cytochrome bc1, from Drugbank and COCONUT	Jović Ozren, Šmuc Tomislav	10.3390/molecules26144323		2021	Molecules	26		4323-4343
Coumarin derivatives act as novel inhibitors of human dipeptidyl peptidase III: Combined in vitro and in silico study	Agić Dejan, Karnaš Maja, Šubarić Domagoj, Lončarić Melita, Tomić Sanja, Karačić Zrinka, Bešlo Drago, Rastija Vesna, Molnar Maja, Popović Boris M., Lisjak Miroslav	10.3390/ph14060540		2021	Pharmaceuticals	14	6	-
Structure prediction of neutral physiological copper(II) compounds with L-cysteine and L-histidine	Ramek Michael, Pejić Jelena, Sabolović Jasmina	10.1016/j.jinorgbio.2021.111536	0162-0134	2021	Journal of inorganic biochemistry	223		-
Largescale mitogenome sequencing reveals consecutive expansions of domestic taurine cattle and supports sporadic aurochs introgression	CubricCurik Vlatka, Novosel Dinko, Brajkovic Vladimir, Rota Stabelli Omar, Krebs Stefan, Sölkner Johann, Šalamon Dragica, Ristov Strahil, Berger Beate, Trivizaki Stamatina, Bizelis Iosif, Ferenčaković Maja, Rothammer Sophie, Kunz Elisabeth, Simčič Mojca, Dovč Peter, Bunevski Gojko, Bytyqi Hysen, Marković Božidarka, Brka Muhamed, Kume Kristaq, Stojanović Srđan, Nikolov Vasil, Zinovieva Natalia, Schönherz Anna Amanda, Guldbrandtsen Bernt, Čačić Mato, Radović Siniša, Miracle Preston, Vernesi Cristiano, Curik Ino, Medugorac Ivica	10.1111/eva.13315	1752-4571	2021	Evolutionary Applications	00		1-16
Benchmarking Apache Beam for IoT Applications	Žaja Mateo, Lipić Tomislav, Čavrak Igor			2021	44rd MIPRO 2021 International Convention - Proceedings			298-303
Intra-domain and cross-domain transfer learning for time series data – How transferable are the features?	Otović Erik, Njirjak Marko, Jozinović Dario, Mauša Goran, Michelini Alberto, Stajduhar Ivan	10.1016/j.knosys.2021.107976	0950-7051	2021	Knowledge-Based Systems	239		-
Investigation of the newly characterized baimantuoluoamide A and baimantuoluoamide B alkaloids as potential cyclin-dependent kinase 4 (CDK4) inhibitors using molecular docking and molecular dynamics simulations	Gurushankar Krishnamurti, Rimac Hrvoje, Potemkin Vladimir, Grishina Maria	10.1016/j.molstruc.2021.129925	0022-2860	2021	Journal of molecular structure	1230		-
Complementarity principle in terms of electron density for the study of EGFR complexes	Kandagalla Shivananda, Rimac Hrvoje, Potemkin Vladimir A, Grishina Maria A	10.4155/fmc-2020-0265	1756-8919	2021	Future Medicinal Chemistry	13	10	863-875
Proposition of a new allosteric binding site for potential SARS-CoV-2 3CL protease inhibitors by utilizing molecular dynamics simulations and ensemble docking	Novak Jurica, Rimac Hrvoje, Kandagalla Shivananda, Pathak Prateek, Naumovich Vladislav, Grishina Maria, Potemkin Vladimir	10.1080/07391102.2021.1927845	0739-1102	2021	Journal of biomolecular structure & dynamics	1		1-14

A triterpene glochidon from Phyllanthus debilis: Isolation, computational studies, and antidiabetic activity evaluation	Verma Amita, Pathak Prateek, Rimac Hrvoje, Khalilullah Habibullah, Kumar Vikas, Grishina Maria, Potemkin Vladimir, Ahmed Bahar	10.1016/j.bcab.2021.102138	1878-8181	2021	Biocatalysis and Agricultural Biotechnology	36		-
Potentiometric Surfactant Sensor Based on 1,3-Dihexadecyl-1H-benzo[d]imidazol-3-ium for Anionic Surfactants in Detergents and Household Care Products	Sakač Nikola, Madunić-Čačić Dubravka, Marković Dean, Hok Lucija, Vianello Robert, Šarkanj Bojan, Đurin Bojan, Hajdek Krunoslav, Smoljan Božo, Milardović Stjepan, Matasović Brunislav, Jozanović Marija	10.3390/molecules26123627		2021	Molecules	26	12	-
Disocijacijska duljina raspršenja atomskog trimera u osnovnome stanju	Leon Ćatipović			2020-07-02				
Effect of source-code preprocessing techniques on plagiarism detection accuracy in student programming assignments	Matija Novak			2020-02-02				
Modeling and synthesis of novel oxime derivatives as potential cholinesterase inhibitors	Ratković Ana, Pavlović Kristina, Barić Danijela, Marinić Željko, Grgičević Ivan, Škorić Irena	10.1016/j.molstruc.2019.127149	0022-2860	2020	Journal of molecular structure	1200		127149-127149
From Grammar Inference to Semantic Inference—An Evolutionary Approach	Kovačević Željko, Mernik Marjan, Ravber Miha, Črepinšek Matej	10.3390/math8050816		2020	Mathematics	8	5	1-24
Molecular Dynamics Simulations of the Elusive Matrixopen State of Mitochondrial ADP/ATP Carrier	Škulj Sanja, Brkljača Zlatko, Vazdar Mario	10.1002/ijch.202000011		2020	Israel journal of chemistry			-
Chloride-Assisted Peptide Macrocyclization	Vidović Nikolina, Horvat Gordan, Riva Davide, Rinkovec Tamara, Cindro Nikola, Tomišić Vladislav, Speranza Giovanna	10.1021/acs.orglett.0c00036	1523-7060	2020	Organic letters	22	6	2129-2134
Synthesis, photochemistry and photophysics of new butadiene derivatives: influence of the fluoro, dimethylamino and nitro substituents on the molecular structure and photoinduced behavior	Grgičević Ana, Fodor Lajos, Barić Danijela, Poje Margareta, Marinić Željko, Horváth Ottó, Škorić Irena	10.1016/j.jphotochem.2020.112690	1010-6030	2020	Journal of photochemistry and photobiology. A, Chemistry	400		112690-112690
Učenje prijenosom znanja iz vremenskih serija - u kojoj su mjeri značajke prenosive?	Otović Erik			2020				-

Novel radial distribution function approach in the study of point mutations: the HIV-1 protease case study	Novak Jurica, Grishina Maria A., Potemkin Vladimir A.	10.4155/fmc-2020-0042	1756-8919	2020	Future Medicinal Chemistry	12	11	1025-1036
Benzobicyclo[3.2.1] octene derivatives as a new class of cholinesterase inhibitors	Čadež Tena, Grgičević Ana, Ahmetović Ramiza, Barić Danijela, Maček Hrvat Nikolina, Kovarik Zrinka, Škorić Irena	10.3390/molecules25214872		2020	Molecules	25	21	-
Inferring Absolutely Non-Circular Attribute Grammars with a Memetic Algorithm	Ravber Miha, Kovačević Željko, Črepinšek Matej, Mernik Marjan	10.1016/j.asoc.2020.106956	1568-4946	2020	Applied Soft Computing	100		-
Implicit Hari–Zimmermann algorithm for the generalized SVD on the GPUs	Novaković Vedran, Singer Sanja	10.1177/10943420209772		2020	International journal of high performance computing applications			-
Coordination polymers of paramagnetic bis (leucinato)copper (II) diastereomers: experimental and computational study of the stereoisomerism and conformations	Vušak Darko, Pejić Jelena, Jurković Mia, Szalontai Gábor, Sabolović Jasmina	10.1039/D0CE00585A		2020	CrystEngComm	22	34	5587-5600
Symmetry breaking in the solid state of 9,10- anthracene amino acid conjugates as seen by X-ray diffraction and NMR spectroscopy	Perić Berislav, Szalontai Gabor, Borovina Mladen, Vikić-Topić Dražen, Srećko Kirin	10.1016/j.molstruc.2020.128834	0022-2860	2020	Journal of molecular structure	1221		-
A Detailed Kinetico-Mechanistic Investigation on the Palladium C–H Bond Activation in Azobenzenes and Their Monopalladated Derivatives	Bjelopetrović Alen, Barišić Dajana, Duvnjak Zrinka, Džajić Ivan, Juribašić Kulcsar Marina, Halasz Ivan, Martinez Manuel, Budimir Ana, Babić Darko, Ćurić Manda	10.1021/acs.inorgchem.0c02418	0020-1669	2020	Inorganic chemistry	59	23	17123-17133
Structural characterization of β-glycolaldehyde dimer	Mohaček Grošev Vlasta, Prugovečki Biserka, Prugovečki Stjepan	10.5562/cca3606	0011-1643	2020	Croatica chemica acta	93	1	P1-P8
Kinetic Isotope Effects and Hydrogen Tunnelling in PCET Oxidations of Ascorbate: New Insights into Aqueous Chemistry?	Ana Karković Marković Cvijeta Jakobušić Brala	10.3390/molecules25061443		2020	Molecules	25	6	-
Vibrational dynamics of 1, 3-propanediol in liquid, polycrystalline and glassy states: a Raman spectroscopic study	Mohaček Grošev Vlasta, Baran Nikola	10.1016/j.saa.2019.117567	1386-1425	2020	Spectrochimica acta. Part A, Molecular and biomolecular spectroscopy	226		-
Phase control for quasi-2D blue emitters by spacer cation engineering	Tam Ho Won, Leung Tik Lun, Sun Wenting, Liu Fangzhou, Ma Chao, Kam Chun Sing, Lončarić Ivor, Grisanti Luca, Ovčar Juraj, Skoko Željko, Popović Jasminka, Đurisic Aleksandra	10.1039/d0tc01631d	2050-7526	2020	Journal of Materials Chemistry C	8		11052-11060

Mono Phosphazenyl Phosphines (R 2 N) 3 P=N–P(NR 2) 2 – Strong P Bases, PDonors, and PNucleophiles for the Construction of Chelates	Kögel Julius F., Ullrich Sebastian, Kovačević Borislav, Wagner Sebastian, Sundermeyer Jörg	10.1002/zaac.202000108	0044-2313	2020	Zeitschrift für anorganische und allgemeine Chemie	646	13	923-932
The role of non-covalent intermolecular interactions on the diversity of crystal packing in supramolecular dihalopyridine–silver(I) nitrate complexes	Roca Sunčica, Hok Lucija, Vianello Robert, Borovina Mladen, Đaković Marijana, Karanović Ljiljana, Vikić-Topić Dražen, Popović Zora	10.1039/d0ce01257b		2020	Crystengcomm	22		7962-7974
Drug screening with the Autodock Vina on a set of kinases without experimentally established structures	Tomić Draško, Davidović Davor, Janđel Vladimir, Mesarić Josip, Skala Karolj, Lipić Tomislav	10.23919/mipro48935.2020.9245440		2020	MIPRO 2020 43rd International Convention			395-401
Phylogeography of Campanula fenestrellata s.l. (Campanulaceae) in the northern Adriatic	Rešetnik Ivana, Temunović Martina, Liber Zlatko, Satovic Zlatko, Bogdanovic Sandro	10.1007/s00606-020-01668-6	0378-2697	2020	Plant systematics and evolution	306		-
Spatial distribution, niche ecology and conservation genetics of Degenia velebitica (Brassicaceae), a narrow endemic species of the north-western Dinaric Alps	Liber Zlatko, Surina Boštjan, Nikolić Toni, Škrtić Danijel, Šatović Zlatko	10.1007/s00606-020-01695-3	0378-2697	2020	Plant systematics and evolution	306	4	-
Salvia officinalis survived in situ Pleistocene glaciation in ‘refugia within refugia’ as inferred from AFLP markers	JugDujaković Marija , Ninčević Tonka , Liber Zlatko , Grdiša Martina , Šatović Zlatko	10.1007/s00606-020-01665-9	0378-2697	2020	Plant systematics and evolution	306		-
Binding of dipeptidyl peptidase III to the oxidative stress cell sensor Kelch-like ECH-associated protein 1 is a two-step process	Matić Sara, Kekez Ivana, Tomin Marko, Bogár Ferenc, Šupljika Filip, Kazazić Saša, Hanić Maja, Jha Shalinee, Brkić Hrvoje, Bourgeois Benjamin, Madl Tobias, Gruber Karl, Macheroux Peter, Matković-Čalogović Dubravka, Matovina Mihaela, Tomić Sanja	10.1080/07391102.2020.1804455		2020	Journal of biomolecular structure & dynamics			-
The substrate selectivity of the two homologous SGNH hydrolases from Streptomyces bacteria: Molecular dynamics and experimental study	Maršavelski Aleksandra, Sabljić Igor, Sugimori Daisuke, Kojić-Prodić Biserka	10.1016/j.ijbiomac.2020.04.198	0141-8130	2020	International journal of biological macromolecules	158		222-230
Nanosized zeolite beta - determining the safety of usage by zebrafish Danio rerio embryos	Palčić Ana, Babić Sanja, Maršavelski Aleksandra, Galić Maja, Topić Popović Natalija, Strunjak Perović Ivančica, Čož-Rakovac Rozelindra, Bronić Josip, Valtchev Valentin	10.1016/j.micromeso.2020.110103		2020	Microporous and mesoporous materials			-

Can natural products stop the SARS-CoV-2 virus? A docking and molecular dynamics study of a natural product database	Novak Jurica, Rimac Hrvoje, Kandagalla Shivananda, Grishina Maria A., Potemkin Vladimir A.			2020	Future Medicinal Chemistry			-
Attenuation of hepatic and breast cancer cells by Polygonatum verticillatum embedded silver nanoparticles	Pathak Manish, Pathak Prateek, Rimac Hrvoje, Grishina Maria, Bagale Uday, Kumar Vikas, Majee Rahul, Potemkin Vladimir, Verma Amita	10.1016/j.bcab.2020.101863	1878-8181	2020	Biocatalysis and Agricultural Biotechnology	30		-
Design, synthesis, and computational study of hybrid quinazoline-1,3,5-triazines as epidermal growth factor receptor (EGFR) inhibitors with anticancer activity	Pathak Prateek, Rimac Hrvoje, Grishina Maria, Verma Amita, Potemkin Vladimir	10.1002/cmdc.202000646		2020	ChemMedChem			-
Pathway enrichment analysis of virus-host interactome and prioritization of novel compounds targeting the spike glycoprotein receptor binding domain-human angiotensin-converting enzyme 2 interface to combat SARSCoV-2	Pavan Gollapalli, Sharath Belenahalli Shekarappa, Rimac Hrvoje, Patil Prakash, Kumari Nalilu Suchetha, Kandagalla Shivanandha, Shetty Praveenkumar	10.1080/07391102.2020.1841681		2020	Journal of biomolecular structure & dynamics			-
Computational insights into the binding mode of curcumin analogues against EP300 HAT domain as potent acetyltransferase inhibitors	Kandagalla Shivananda, Belenahalli Shekarappa Sharath, Rimac Hrvoje, Grishina Maria A., Potemkin Vladimir A., Hanumanthappa Manjunatha	10.1016/j.jmgm.2020.107756	1093-3263	2020	Journal of molecular graphics & modelling	101		-
Indomethacin increases quercetin affinity for human serum albumin: a combined experimental and computational study and its broader implications	Rimac Hrvoje, Tandarić Tana, Vianello Robert, Bojić Mirza	10.3390/ijms21165740		2020	International journal of molecular sciences	21	16	-
Novel Harmicines with Improved Potency against Plasmodium	Marinović Marina, Perković Ivana, Fontinha Diana, Prudêncio Miguel, Held Jana, Pessanha de Carvalho Lais, Tandarić Tana, Vianello Robert, Zorc Branka, Rajić Zrinka	10.3390/molecules25194376		2020	Molecules	25	19	-
Photophysical properties and immobilisation of fluorescent pH responsive aminated benzimidazo[1, 2-a] quinoline-6-carbonitriles	Horak Ema, Babić Darko, Vianello Robert, Perin Nataša, Hranjec Marijana, Steinberg Ivana	10.1016/j.saa.2019.117588	1386-1425	2020	Spectrochimica acta. Part A, Molecular and biomolecular spectroscopy	227		-

Synthesis and Basicity Studies of Quinolino[7,8h] quinoline Derivatives	Rowlands Gareth J., Severinsen Rebecca J., Buchanan Jenna K., Shaffer Karl J., Jameson Heather T., Thennakoon Nishani, Leito Ivo, Lõkov Maïrt, Kütt Agnes, Vianello Robert, Despotović Ines, Radić Nena, Plieger Paul G.	10.1021/acs.joc.0c01428	0022-3263	2020	Journal of organic chemistry	85		11297-11308
The Effect of Deuteration on the H2 Receptor Histamine Binding Profile: A Computational Insight into Modified Hydrogen Bonding Interactions	Hok Lucija, Mavri Janez, Vianello Robert	10.3390/molecules25246017		2020	Molecules	25	24	-
Evolutionary operators for the Hamiltonian completion problem	Puljić Krunoslav, Manger Robert	10.1007/s00500-020-05063-8	1432-7643	2020	Soft computing	24	23	18073-18088
Fluorinated twist-bend nematogens: the role of intermolecular interaction	Knežević Anamarija, Dokli Irena, Novak Jurica, Kontrec Darko, Lesac Andreja	10.1080/02678292.2020.1817585		2020	Liquid crystals			-
QMC study of trapped Bose-Bose mixtures at finite temperature	Dželalija Krešimir, Cikojević Viktor, Boronat Jordi, Vranješ Markić Leandra			2020	Exploring Quantum Many Body Physics with Ultracold Atoms and Molecules-Booklet with abstracts			105-105
Trapped Bose-Bose mixtures at finite temperature: A quantum Monte Carlo approach	Dželalija Krešimir, Cikojević Viktor, Boronat Jordi, Vranješ Markić Leandra	10.1103/physreva.102.063304	2469-9926	2020	Physical Review A	102	6	063304-1
Quantum Monte Carlo study of strongly interacting bosonic one-dimensional systems in periodic potentials	Dželalija K., Markić L. Vranješ	10.1103/physreva.101.013626	2469-9926	2020	Physical review. A	101	1	-
Crossover from one to two dimensions in liquid 4He in a nanopore	Vranješ Markić Leandra, Dželalija Krešimir	10.1103/PhysRevB.101.104505	2469-9950	2020	Physical review. B.	101		104505-1
Ferrocene-Fused Acenequinones: Synthesis, Structure and Reaction Chemistry	Mahrholdt Julia, Kovalski Eduard, Korb Marcus, Hildebrandt Alexander, Vrček Valerije, Lang Heinrich	10.1002/ejic.202000956		2020	European journal of inorganic chemistry			-
Ionization Energy and Reduction Potential in Ferrocene Derivatives. Comparison of Hybrid and Pure DFT Functionals	Toma Mateja, Kuvek Tea, Vrček Valerije	10.1021/acs.jpca.0c06663	1089-5639	2020	The journal of physical chemistry. A, Molecules, spectroscopy, kinetics, environment, & general theory	124	39	8029-8039
Uloga mitohondrijskih proteina rasprezanja u mehanizmu prijenosa protona kroz unutrašnju mitohondrijsku membranu	Škulj Sanja			2020				-

Toluene oxidation on metal-oxide catalysts: Theoretical modeling	Gomzi Vjeran			2020				1-1
Optimizacija parametara reakcijskog polja sila i teorijsko istraživanje katalitičkih svojstava MnFeO3	Gomzi Vjeran, Duplančić Marina, Tomašić Vesna			2020	18th Ružička days Book of abstracts			142-142
Toluene oxidation on metal-oxide catalysts: Theoretical modeling	Gomzi Vjeran			2020				1-1
A quadrupolar bis triarylborane chromophore as a fluorimetric and chirooptic probe for simultaneous and selective sensing of DNA, RNA and proteins	Ban Željka, Griesbeck Stefanie, Tomić Sanja, Nitsch Jörn, Marder Todd, Piantanida Ivo	10.1002/chem.201903936	0947-6539	2020	Chemistry : a European journal	26		2195-2203
The guanidiniocarbonyl pyrrole - fluorophore conjugates as theragnostic tools for DPP III monitoring and inhibition	Ćehić Mirsada, Suć Sajko Josipa, Karačić Zrinka, Piotrowski Patryciusz, Šmidlehner Tamara, Jerić Ivanka, Schmuck Carsten, Piantanida Ivo, Tomić Sanja	10.1080/07391102.2019.1664936	0739-1102	2020	Journal of biomolecular structure & dynamics	38	13	3790-3800
On the metal ion selectivity of PNP-lariat ether—an insight from density functional theory calculations	Despotović Ines	10.1007/s11224-020-01542-8	1040-0400	2020	Structural chemistry	31	5	1801-1819
A New Insight into Coating's Formation Mechanism Between TiO2 and Alendronate on Titanium Dental Implant	Petrović Željka, Šarić Ankica, Despotović Ines, Katić Jozefina, Peter Robert, Petravić Mladen, Petković Marin	10.3390/ma13143220		2020	Materials	13	14	-
Influence of Biocompatible Coating on Titanium Surface Characteristics	Petrović Željka, Katić Jozefina, Šarić Ankica, Despotović Ines, Matijaković Nives, Leskovac Mirela, Kralj Damir, Petković Marin	10.2174/2352094910999200407095723	2352-0949	2020	Innovations in Corrosion and Materials Science	10	1	37-46
Functional Coatings for Titanium Dental Implants: Differences and Similarities	Petrović Željka, Šarić Ankica, Despotović Ines, Katić Jozefina, Petković Marin	10.3390/PCMS-08941		2020	First Poster Competition on Materials Science			-
Funkcionalizacija površine titanijeva dentalnog implantata bioaktivnim prevlakama	Varzić Katarina, Katić Jozefina, Šarić Ankica, Despotović Ines, Leskovac Mirela, Petković Marin, Petrović Željka			2020	XIII. susret mladih kemijskih inženjera, SMLKI, Knjiga sažetaka			146-146
Functionalization of Titanium Surface by Innovative Anticorrosion Coating	Katić Jozefina, Šarić Ankica, Despotović Ines, Petković Marin, Petrović Željka			2020	71st Annual Meeting ISE, Book of Abstracts			1211-1211

Reaktivnost i efekti stabilizacije difenil-fosfinata	Ivana Tarandek			2019-06-14				
Covalent modification of phosphatidylethanolamine by 4-hydroxy-2-nonenal increases sodium permeability across phospholipid bilayer membranes	Jovanović Olga, Škulj Sanja, Pohl Elena E., Vazdar Mario	10.1016/j.freeradbiomed.2019.08.027	0891-5849	2019	Free radical biology & medicine	143		433-440
Utilizing the Azaazulene Scaffolds in the Design of New Organic Superbases	Barić Danijela	10.1021/acsomega.9b02087		2019	ACS Omega	4	12	15197-15207
Inquisitive Geometric Sites in h-BN Monolayer for Alkali Earth Metal Ion Batteries	Kansara Shivam, Gupta Sanjeev K., Sonvane Yogesh, Varga Pajtler Maja, Ahuja Rajeev	10.1021/acs.jpcc.9b04498	1932-7447	2019	The Journal of Physical Chemistry C	123	32	19340-19346
Prospects for experimental realization of two-dimensional aluminium allotropes	Lukačević Igor, Varga Pajtler Maja, Mužević Matko, Gupta Sanjeev K.	10.1039/C8TC04718A	2050-7526	2019	Journal of Materials Chemistry C	7	9	2666-2675
Hypergraph Contextuality	Pavičić Mladen	10.3390/e21111107	1099-4300	2019	Entropy (Basel. Online)	21	11	1107-1
New zinc ion parameters suitable for classical MD simulations of zinc metallo-peptidases	Tomić Antonija, Horvat Gordan, Ramek Michael, Agić Dejan, Brkić Hrvoje, Tomić Sanja	10.1021/acs.jcim.9b00235	1549-9596	2019	Journal of chemical information and modeling	59	8	3437-3453
A Computational Insight into Reaction Between Different Amino Acids with Reactive Aldehydes 4-hydroxy-2-nonenal and 4-oxo-2-nonenal	Škulj Sanja, Vazdar Mario			2019	Croatica chemica acta			-
Effect of electric field on optoelectronic properties of indiene monolayer for photoelectric nanodevices	Singh Deobrat, Gupta Sanjeev K., Lukacevic Igor, Muzevic Matko, Sonvane Yogesh, Ahuja Rajeev	10.1038/s41598-019-53631-2		2019	Scientific reports	9		-
Conformational Analyses of Physiological Binary and Ternary Copper(II) Complexes with L Asparagine and L Histidine ; Study of Tridentate Binding of Copper(II) in Aqueous Solution	Ramek Michael, Marković Marijana, Mutapčić Ilina, Pejić Jelena, Kelterer Anne-Marie, Sabolović Jasmina	10.1002/open.201900159	2191-1363	2019	ChemistryOpen	8		852-868
Facile Mechanochemical Anion Substitution in Cyclopalladated Azo-benzenes	Bjelopetrović Alen, Robić , Marko Halasz, Babić Darko, Juribašić Kulcsar Marina, Ćurić Manda	10.1021/acs.organomet.9b00626	0276-7333	2019	Organometallics	38	22	4479-4484

Mixed Spacer Cation Stabilization of BlueEmitting n = 2 Ruddlesden–Popper Organic–Inorganic Halide Perovskite Films	Leung Tik Lun, Tam Ho Won, Liu Fangzhou, Lin Jingyang, Ng Alan Man Ching, Chan Wai Kin, Chen Wei, He Zhubing, Lončarić Ivor, Grisanti Luca, Ma Chao, Wong Kam Sing, Lau Ying Suet, Zhu Furong, Skoko Željko, Popović Jasminka, Djurišić Aleksandra B.	10.1002/adom.201901679		2019	Advanced optical materials	8	4	-
Modeliranje nekovalentnih interakcija u procesima solvatacije kvercetina i reorganizacije konformacije fragmenta U6 snRNA	Mihaljević Frano			2019				-
Metalo-biomolekulski polimeri s aminokiselinama: eksperimentalna i komputacijska studija polimernih L- piroglutamato Cu (II)kompleksa	Popović Zora, Pilepić Viktor, Matković- Čalogović Dubravka			2019	XXVI konferencija Srpskog kristalografskog društva : izvodi radova = XXVI Conference of the Serbian Crystallographic Society : Abstracts			50-51
Computational Study of Glycerol Binding within the Active Site of Coenzyme B12-Dependent Diol Dehydratase	Bilić Luka, Barić Danijela, Banhatti Radha Dilip, Smith David M., Kovačević Borislav	10.1021/acs.jpcb.9b04071	1520-6106	2019	The journal of physical chemistry. B, Condensed matter, materials, surfaces, interfaces & biophysical	123	29	6178-6187
Racemization of oxazepam and chiral 1, 4-benzodiazepines. DFT study of the reaction mechanism in aqueous solution	Hok Lucija, Božičević Lucija, Sremec Helena, Šakić Davor, Vrček Valerije	10.1039/C8OB02991A	1477-0520	2019	Organic & biomolecular chemistry	17		1471-1479
Experimental and Computational Study of the Antioxidative Potential of Novel Nitro and Amino Substituted Benzimidazole /Benzothiazole- 2-Carboxamides with Antiproliferative Activity	Cindrić Maja, Sović Irena, Mioč Marija, Hok Lucija, Boček Ida, Roškarić Petra, Butković Kristina, Martin-Kleiner Irena, Starčević Kristina, Vianello Robert, Kralj Marijeta, Hranjec Marijana	10.3390/antiox8100477		2019	Antioxidants	8	10	-
From Hydrogen Peroxide-Responsive Boronated Nucleosides Towards Antisense Therapeutics – A Computational Mechanistic Study	Tandarić Tana, Hok Lucija, Vianello Robert	10.5562/cca3592	0011-1643	2019	Croatica chemica acta	92	2	287-295
Divergent selection and genetic structure of Sideritis scardica populations from southern Balkan Peninsula as revealed by AFLP fingerprinting	Grdiša Martina, Radosavljević Ivan, Liber Zlatko, Stefkov Gjoshe, Ralli Parthenopi, Chatzopoulou Paschalina S., Carović-Stanko Klaudija, Šatović Zlatko	10.1038/s41598-019-49097-x	2045-2322	2019	Scientific Reports	9		-

Genetic and morphological data reveal new insights into the taxonomy of Campanula versicolor s.l. (Campanulaceae)	Janković Ivana, Šatović Zlatko, Liber Zlatko, Kuzmanović Nevena, Di Pietro Romeao, Radosavljević Ivan, Nikolov Zoran, Lakušić Dmitar	10.1002/tax.12050	0040-0262	2019	Taxon	68	2	340-369
Genetic diversity and structure of Fusarium oxysporum f.sp. lentis isolates from Iran, Syria and Algeria	Pouralibaba Hamid R., Šatović Zlatko, Cobos Maria Jose, Rubiales Diego, Fondevilla Sara	10.1007/s10658-018-01617-7	0929-1873	2019	European journal of plant pathology	153	4	1019-1029
Morphological, genetic and epigenetic aspects of homoploid hybridization between Salvia officinalis L. and Salvia fruticosa Mill.	Radosavljević Ivan, Bogdanović Sandro, Celep Ferhat, Filipović Maja, Satovic Zlatko, Surina Boštjan, Liber Zlatko	10.1038/s41598-019-40080-0	2045-2322	2019	Scientific Reports	9	1	1-13
Electrochemical oxidation of flavonoids: PM6 and DFT for elucidating electronic changes and modelling oxidation potential	Miličević Ante, Miletić Goran I., Novak Jovanović Ivana	10.1016/j.molliq.2019.04.128	0167-7322	2019	Journal of molecular liquids	285		551-556
Electrochemical oxidation of flavonoids: PM6 and DFT for elucidating electronic changes and modelling oxidation potential (part II)	Miličević Ante, Miletić Goran I., Novak Jovanović Ivana	10.1016/j.molliq.2019.111730	0167-7322	2019	Journal of molecular liquids	295		-
Transacylation in Ferrocenoyl-Purines. NMR and Computational Study of the Isomerization Mechanism	Toma Mateja, Božičević Lucija, Lapić Jasmina, Djaković Senka, Šakić Davor, Tandarić Tana, Vianello Robert, Vrček Valerije	10.1021/acs.joc.9b01944	0022-3263	2019	Journal of organic chemistry	84	19	12471-12480
Computational Insight into the Mechanism of the Irreversible Inhibition of Monoamine Oxidase Enzymes by the Antiparkinsonian Propargylamine Inhibitors Rasagiline and Selegiline	Tandarić Tana, Vianello Robert	10.1021/acschemneuro.9b00147	1948-7193	2019	ACS Chemical Neuroscience	10	8	3532-3542
DNA/RNA recognition controlled by the glycine linker and the guanidine moiety of phenanthridine peptides	Matić Josipa, Šupljika Filip, Tandarić Tana, Dukši Marko, Piotrowski Patryciusz, Vianello Robert, Brozović Anamaria, Piantanida Ivo, Schmuck Carsten, Radić Stojković Marijana	10.1016/j.ijbiomac.2019	0141-8130	2019	International journal of biological macromolecules	134		422-434
Luminescent pyrenyl–GNA nucleosides: synthesis, photophysics and confocal microscopy studies in cancer HeLa cells	Kowalski Konrad, Skiba Joanna, Kowalczyk Aleksandra, Fik Marta Anna, Gapińska Magdalena, Trzybiński Damian, Wozniak Krzysztof, Vrček Valerije, Czerwieniec Rafał	10.1039/C9PP00271E	1474-905X	2019	Photochemical & photobiological sciences	18		2449-2460

Gold-Induced Desulfurization in a Bis(ferrocenyl) Alkane Dithiol	Pensa Evangelina, Karpowicz Rafal, Jabłoński Artur, Trzybiński Damian, Woźniak Krzysztof, Šakić Davor, Vrček Valerije, Long Nicholas J., Albrecht Tim, Kowalski Konrad	10.1021/acs.organomet.9b00175	0276-7333	2019	Organometallics	38	9	2227-2232
Quinoline and ferrocene conjugates: Synthesis, computational study and biological evaluations	Maračić Silvija, Lapić Jasmina, Djaković Senka, Opačak-Bernardi Teuta, Glavaš-Obrovac Ljubica, Vrček Valerije, Raić-Malić Silvana	10.1002/aoc.4628	0268-2605	2019	Applied organometallic chemistry	33	1	e4628-e4628
Isotope Labeling Reveals Fast Atomic and Molecular Exchange in Mechanochemical Milling Reactions	Lukin Stipe, Tireli Martina, Stolar Tomislav, Barišić Dajana, Blanco Maria Valeria, di Michiel Marco, Užarević Krunoslav, Halasz Ivan	10.1021/jacs.8b12149	0002-7863	2019	Journal of the American Chemical Society	141	3	1212-1216
Raširenost infektivne ličinke oblića Anisakis pegreffii (Nematoda, Anisakidae) u parateničnom domaćinu (Sardina pilchardus) i molekularna karakterizacija odgovora modelnog slučajnog domaćina (Rattus norvegicus)	Bušelić Garber Ivana			2019				-
The conformational equilibrium and vibrational properties of chalcone	Bakarić Danijela, Baranović Goran	10.1016/j.molstruc.2019.06.098	0022-2860	2019	Journal of molecular structure	1196		429-438
Surface modification of Ti dental implant by bioactive coatings: experimental and theoretical studies	Katić Jozefina, Šarić Ankica, Despotović Ines, Petković Marin, Varzić Katarina, Leskovac Mirela, Petrović Željka			2019	7th Regional Symposium on Electrochemistry – South East Europe & 8th Kurt Schwabe Symposium : Book of Abstract			143-143
Alcoholic Solvent Influence on ZnO Synthesis: A Joint Experimental and Theoretical Study	Šarić Ankica, Despotović Ines, Štefanić Goran	10.1021/acs.jpcc.9b07411	1932-7447	2019	Journal of physical chemistry. C	123		29394-29407
Solvothermal synthesis of zinc oxide nanoparticles: A combined experimental and theoretical study	Šarić Ankica, Despotović Ines, Štefanić Goran	10.1016/j.molstruc.2018.10.025	0022-2860	2019	Journal of molecular structure	1178		251-260
Aprotinin interacts with substrate-binding site of human dipeptidyl peptidase III	Agić Dejan, Brkić Hrvoje, Kazazić Saša, Tomić Antonija, Abramić Marija	10.1080/07391102.2018.1521343	0739-1102	2019	Journal of Biomolecular Structure and Dynamics	37	14	3596-3606

Vector generation of contextual sets	Pavičić Mladen, Megill Norman D.			2019	EPJ Web of Conferences Volume 198 (2019) Quantum Technology International Conference 2018 (QTech 2018)			-
Modulation Of Optical Properties With Multilayer Thickness In Antimonene And Indiene	Mužević Matko, Varga Pajtler Maja, Gupta Sanjeev Kumar, Lukačević Igor	10.5185/amlett.2019.2220	0976-397X	2019	Advanced Materials Letters	10	4	270-274
Universality of size-energy ratio in four-body systems	Stipanović Petar, Vranješ Markić Leandra, Gudyma Andrii, Boronat Jordi	10.1038/s41598-019-42312-9	2045-2322	2019	Scientific Reports	9	1	6289(1)-6289(8)
Automated generation of Kochen-Specker sets	Pavičić Mladen, Waegell Mordecai, Megill Norman D., Aravind P. K.	10.1038/s41598-019-43009-9	2045-2322	2019	Scientific Reports	9	1	-
Calculation of Apparent pKa Values of Saturated Fatty Acids with Different Lengths in DOPC Phospholipid Bilayers	Škulj Sanja, Vazdar Mario	10.1039/C9CP01204D	1463-9076	2019	PCCP. Physical chemistry chemical physics	21	19	10052-10060
Revisited Mechanism of Reaction between a Model Lysine Amino Acid Side Chain and 4-Hydroxynonenal in Different Solvent Environments	Škulj Sanja, Vazdar Katarina, Margetić Davor, Vazdar Mario	10.1021/acs.joc.8b02231	0022-3263	2019	Journal of organic chemistry	84	2	526-535
Improving electron transport in the hybrid perovskite solar cells using CaMnO3-based buffer layer	Pandey Kavita, Singh Deobrat, Gupta Sanjeev Kumar, Yadav Pankaj, Sonvane Yogesh, Lukačević Igor, Kumar Manjeet, Kumar Manoj, Ahuja Rajeev	10.1016/j.nanoen.2018.01.009	2211-2855	2018	Nano Energy	45		287-297
2 H magic-angle spinning NMR and powder diffraction study of deuterated paramagnetic copper(II) glycinato complexes. Information on crystallographic symmetries, stereo-isomerism, and molecular mobility available from ssNMR spectra	Szalontai Gábor, Csonka Róbert, Kaizer József, Bombicz Petra, Sabolović Jasmina	10.1016/j.ica.2017.05.071	0020-1693	2018	Inorganica chimica acta	472		320-329
The average local ionization energy and Fukui function of quercetine	Fabijanić Ivana, Pilepić Viktor			2018				-
The non-covalent interaction plots of U6 internal stem-loop domain	Mihaljević Frano, Pilepić Viktor			2018				-

Computational Tale of Two Enzymes: Glycerol Dehydration With or Without B12	Kovačević Borislav, Barić Danijela, Babić Darko, Bilić Luka, Hanževački Marko, Sandala Gregory M., Radom Leo, Smith David M.	10.1021/jacs.8b03109	0002-7863	2018	Journal of the American Chemical Society	140	27	8487-8496
Chlorination of 5-fluorouracil: Reaction mechanism and ecotoxicity assessment of chlorinated products	Hok Lucija, Ulm Lea, Tandarić Tana, Krivohlavek Adela, Šakić Davor, Vrček Valerije	10.1016/j.chemosphere.2018.05.140	0045-6535	2018	Chemosphere	207	18	612-619
Empirical Valence Bond Simulations Suggest a Direct Hydride Transfer Mechanism for Human Diamine Oxidase	Maršavelski Aleksandra, Petrović Dušan, Bauer Paul, Vianello Robert, Kamerlin Shina Caroline Lynn	10.1021/acsomega.8b00346		2018	ACS Omega	3	4	3665-3674
Calibration of Source-Code Similarity Detection Tools for Objective Comparisons	Novak Matija, Kermek Dragutin, Joy Mike	10.23919/MIPRO.2018.8400147		2018	MIPRO 2018 - 41st International Convention			794-799
Infrared spectroscopy of flavones and flavonols. Reexamination of the hydroxyl and carbonyl vibrations in relation to the interactions of flavonoids with membrane lipids	Baranović Goran, Šegota Suzana	10.1016/j.saa.2017.11.057	1386-1425	2018	Spectrochimica acta. Part A, Molecular and biomolecular spectroscopy	192		473-486
Hydrogen attachment and release in Fe(H)2(H2)(PEtPh2)3. Theoretical predictions.	Gomzi Vjeran			2018	8 th Regional Biophysics Conference Book of Abstracts			-
Design of Exceptionally Strong Organic Superbases Based on Aromatic Pnictogen Oxides: Computational DFT Analysis of the Oxygen Basicity in the Gas Phase and Acetonitrile Solution	Tandarić Tana, Vianello Robert	10.1021/acs.jpca.7b11945	1089-5639	2018	The journal of physical chemistry. A, Molecules, spectroscopy, kinetics, environment, & general theory	122	5	1464-1471
A DFT/PCM-based methodology for predicting solvolytic reactivities of organic carbonates	Matić Mirela, Denegri Bernard	10.1039/C8OB00917A	1477-0520	2018	Organic & biomolecular chemistry	16	25	4665-4674
Mechanism of Mechanochemical C–H Bond Activation in an Azobenzene Substrate by Pd(II) Catalysts	Bjelopetrović Alen, Lukin Stipe, Halasz Ivan, Užarević Krunoslav, Đilović Ivica, Barišić Dajana, Budimir Ana, Juribašić Kulcsar Marina, Ćurić Manda	10.1002/chem.201802403	0947-6539	2018	Chemistry : a European journal	24	42	10672-10682
Benzoylguanidines as the Anion Responsive Systems	Glasovac Zoran, Barešić Luka, Antol Ivana, Margetić Davor			2018	ChemPlusChem			-
Basicity of Some Pyridinophanes in Gas Phase and Acetonitrile – a DFT Study	Despotović Ines	10.1002/slct.201801449	2365-6549	2018	ChemistrySelect	3	27	7718-7731

Ferrocenyl GNA nucleosides: a bridge between organic and organometallic xeno-nucleic acids	Kowalski Konrad, Skiba Joanna , Yuan Qing, Hildebrandt Alexander, Trzybinski Damian, Wozniak Krzystof, Balogh Ria, Gyurcsik Bela, Vrček Valerije	10.1002/cplu.201700551	2192-6506	2018	ChemPlusChem	83	2	77-86
Disorder at the Chiral Cα Center and Room-Temperature Solid-State cis–trans Isomerization ; Synthesis and Structural Characterization of Copper(II) Complexes with D-allo, L-Isoleucine	Pejić Jelena, Vušak Darko, Szalontai Gábor, Prugovečki Biserka, Mrvoš-Sermek Draginja, Matković-Čalogović Dubravka, Sabolović Jasmina	https://pubs.acs.org/doi/10.1021/acs.cgd.8b00589	1528-7483	2018	Crystal Growth & Design	18	9	5138-5154
Harmonically trapped Bose-Bose mixtures: a quantum Monte Carlo study	V. Cikojević , L. Markic Vranješ , J. Boronat	10.1088/1367-2630/aad6cc	1367-2630	2018	New journal of physics	20	085002	-
Ultradilute quantum liquid drops	Cikojević Viktor, Dželalija Krešimir, Stipanović Petar, Vranješ Markić Leandra, Boronat Jordi	10.1103/physrevb.97.140502	2469-9950	2018	Physical Review B	97	14	-
Vector Generation of Quantum Contextual Sets in Even Dimensional Hilbert Spaces	Pavičić Mladen, Megill Norman D.	10.3390/e20120928	1099-4300	2018	Entropy (Basel. Online)	20	12	-
Tetrahedral hydrocarbon nanoparticles in space: X-ray spectra	Bilalbegović Goranka, Maksimović Aleksandar, Valencic Lynne	10.1093/mnras/sty607	0035-8711	2018	Monthly notices of the Royal Astronomical Society	476	4	5358-5364
Structure of Helium–Alkali Pentamers	Stipanović Petar, Vranješ Markić Leandra	10.1007/s00601-018-1367-x	0177-7963	2018	Few-body systems	59	3	-
Ground-state characteristics of helium–alkali tetramers	Stipanović Petar, Vranješ Markić Leandra	10.1088/1361-6455/aacb45	0953-4075	2018	Journal of Physics B: Atomic, Molecular and Optical Physics	51	15	-
Structural and computational analysis of intermolecular interactions in a new 2- thiouracil polymorph	Fabijanić Ivana, Matković-Čalogović Dubravka, Pilepić Viktor, Sanković Krešimir	10.1107/s2053229617001542x	2053-2296	2017	Acta Crystallographica Section C-Structural Chemistry	73	12	1078-1086
New investigations of the guanine trichloro cuprate(II) complex crystal	Fabijanić Ivana, Matković-Čalogović Dubravka, Pilepić Viktor, Ivanišević Irena, Mohaček- Grošev Vlasta, Sanković Krešimir	10.1016/j.molstruc.2016.08.069	0022-2860	2017	Journal of molecular structure	1128		317-324
Spin-dependent electron transport in C and Ge doped BN monolayers	Gupta Sanjeev K., He Haiying, Lukačević Igor, Pandey Ravindra	10.1039/C7CP05596J	1463-9076	2017	PCCP. Physical chemistry chemical physics	19	45	30370-30380
Genetic Diversity of Croatian Common Bean Landraces	Carović-Stanko Klaudija, Liber Zlatko, Vidak Monika, Barešić Ana, Grdiša Martina, Lazarević Boris, Šatović Zlatko	10.3389/fpls.2017.00604	1664-462X	2017	Frontiers in Plant Science	8		604-1

Genetic diversity of the sweet chestnut (Castanea sativa Mill.) in central Europe and the western part of the Balkan Peninsula, and evidence of marron genotype introgression into wild populations	Poljak Igor, Idžojtić Marilena, Šatović Zlatko, Ježić Marin, Ćurković Perica Mirna, Simovski Bojan, Acevski Jane, Liber Zlatko	10.1007/s11295-017-1107-2	1614-2942	2017	Tree Genetics and Genomes		1	13-1
Establishing the Bases for Introducing the Unexplored Portuguese Common Bean Germplasm into the Breeding World	Leitão Susana T., Dinis Marco, Veloso Maria M., Šatović Zlatko, Vaz Patto Maria C.	10.3389/fpls.2017.01296	1664-462X	2017	Frontiers in Plant Science	8		1296-1
New investigations of the guanine trichloro cuprate(II) complex crystal	Ivana Fabijanic, Dubravka Matkovic-Calogovic, Viktor Pilepic , Irena Ivanisevic, Vlasta Mohacek-Grosev, Kresimir Sankovic	10.1016/j.molstruc.2016.08.069		2017	Journal of Molecular Structure	1128		317-324
1, 1'-Bis(thymine) ferrocene Nucleoside : Synthesis and Study of Its Stereoselective Formation	Kowalski Konrad, Anisimov Iurii, Salomon Sebastian, Hildebrandt Alexander, Lang Heinrich, Trzybinski Damian, Wozniak Krzysztof, Šakić Davor, Vrček Valerije	10.1002/cplu.201700215	2192-6506	2017	ChemPlusChem	82	6	859-866
Fluorescent benzimidazo[1, 2-a] quinolines: Synthesis, spectroscopic and computational studies of protonation equilibria and metal ion sensitivity	Hranjec Marijana, Horak Ema, Babić Darko, Plavljanin Sanela, Srdović Zrinka, Murković Steinberg Ivana, Vianello Robert, Perin Nataša	10.1039/C6NJ02268E	1144-0546	2017	New journal of chemistry	41	1	358-371
Novel pyrimidine-2, 4-dione-1, 2, 3-triazole and furo[2, 3-d]pyrimidine-2-one-1, 2, 3-triazole hybrids as potential anti-cancer agents: Synthesis, computational and X-ray analysis and biological evaluation	Gregorić Tomislav, Sedić Mirela, Grbčić Petra, Tomljenović Paravić Andrea, Kraljević Pavelić Sandra, Cetina Mario, Vianello Robert, Raić-Malić Silvana	10.1016/j.ejmech.2016.11.028	0223-5234	2017	European journal of medicinal chemistry	125		1247-1267
What a difference a methyl group makes - the selectivity of monoamine oxidase B towards histamine and N-methylhistamine	Maršavelski Aleksandra, Vianello Robert	10.1002/chem.201605430	0947-6539	2017	Chemistry : a European journal	23	12	2915-2925
Arbitrarily exhaustive hypergraph generation of 4-, 6-, 8-, 16-, and 32-dimensional quantum contextual sets	Pavičić Mladen	10.1103/PhysRevA.95.062121	2469-9934	2017	Physical Review A	95	6	-
Reversible Gas−Solid Ammonia N−H Bond Activation Mediated by an Organopalladium Complex	Juribašić Kulcsar Marina, Halasz Ivan, Budimir Ana, Užarević Krunoslav, Lukin Stipe, Monas Andrea, Emmerling Franziska, Plavec Janez, Ćurić Manda	10.1021/acs.inorgchem.7b00422	0020-1669	2017	Inorganic chemistry	56	9	5342-5351

Solvolytic Behavior of Aryl and Alkyl Carbonates. Impact of the Intrinsic Barrier on Relative Reactivities of Leaving Groups	Matić Mirela, Katić Matija, Denegri Bernard, Kronja Olga	10.1021/acs.joc.7b00885	0022-3263	2017	Journal of organic chemistry	82	15	7820-7831
New Classes of Kochen-Specker Contextual Sets	Megill Norman D., Pavičić Mladen			2017	Proceedings of The 40th International Convention on Information and Communication Technology, Electronics, and Microelectronics, May 22-26, 2017			195-200
Calculating the geometry and Raman spectrum of physiological bis (L-histidinato) copper(II): an assessment of DFT functionals for aqueous and isolated systems	Sabolović Jasmina, Ramek Michael, Marković Marijana	10.1007/s00894-017-3448-z	1610-2940	2017	Journal of molecular modeling	23		290-1
Pronounced conformational flexibility of physiological (L-histidinato)(L-threoninato)copper (II) in aqueous solution disclosed by a quantum chemical study	Ramek Michael, Marković Marijana, Loher Caludia, Sabolović Jasmina	10.1016/j.poly.2017.06.041	0277-5387	2017	Polyhedron	135		121-133
Localization improvement of deuterium uptake in hydrogen /deuterium exchange in proteins	Babić Darko, Smith David M.	10.1002/cem.2876	0886-9383	2017	Journal of chemometrics	31	3	e2876-1
Reduction Potential of Ferrocenoyl-Substituted Nucleobases. Experimental and Computational Study	Havaić Valentina, Djaković Senka, Lapić Jasmina, Weitner Tin, Šakić Davor, Vrček Valerije	10.5562/cca3229	0011-1643	2017	Croatica chemica acta	90	4	589-594
Validation of flavonoids as potential dipeptidyl peptidase III inhibitors: experimental and computational approach	Agić Dejan, Brkić Hrvoje, Tomić Sanja, Karačić Zrinka, Špoljarević Marija, Lisjak Miroslav, Bešlo Drago, Abramić Marija	10.1111/cbdd.12887	1747-0277	2017	Chemical biology & drug design	89	4	619-627
Missing Fe: hydrogenated iron nanoparticles	Bilalbegović Goranka, Maksimović Aleksandar, Mohaček-Grošev Vlasta	10.1093/mnrasl/slw226	1745-3925	2017	Monthly Notices of the Royal Astronomical Society	466	1	L14-L18
Structure of Halo and Quasi-halo Helium–Helium–Alkali Trimers	Stipanović Petar, Vranješ Markić Leandra, Boronat Jordi	10.1007/s00601-017-1288-0	0177-7963	2017	Few-body systems	58		123-1

Quantum Halo States in Helium Tetramers	Stipanović Petar, Vranješ Markić Leandra, Boronat Jordi	10.1021/acs.jpca.6b10656	1089-5639	2017	Journal of Physical Chemistry A	121	1	308-314
Ground-state properties of weakly bound helium- alkali trimers	Stipanović Petar, Vranješ Markić Leandra, Zarić Darko, Boronat Jordi	10.1063/1.4973381	0021-9606	2017	The Journal of chemical physics	146		014305-1
A novel antimicrobial target—expanded and revisited mode of action of pantothenamides	Maršavelski Aleksandra	10.1039/C6RA07430H	2046-2069	2016	RSC Advances	6		44888-44895
Genetic diversity and morphological variability in the Balkan endemic Campanula secundiflora s.l. (Campanulaceae)	Janković Ivana, Šatović Zlatko, Liber Zlatko, Kuzmanović Nevena, Radosavljević Ivan, Lakušić Dmitar	10.1111/boj.12359	0024-4074	2016	Botanical Journal of the Linnean Society	180	1	64-88
Characterizing Croatian Wheat Germplasm Diversity and Structure in a European Context by DArT Markers	Novoselović Dario, Bentley Alison R., Šimek Ruđer, Dvojković Krešimir, Sorrells Mark E., Gosman Nicolas, Horsnell Richard, Drezner Georg, Šatović Zlatko	10.3389/fpls.2016.00184	1664-462X	2016	Frontiers in Plant Science	7		184-1
Synthesis and characterization of ML and ML2 metal complexes with amino acid substituted bis(2-picolyl)amine ligands	Škalamera Đani, Sanders Ernest, Vianello Robert, Maršavelski Aleksandra, Pevec Andrej, Turel Iztok, Kirin Srećko I.	10.1039/C5DT03387J	1477-9226	2016	Dalton transactions	45	7	2845-2858
The Quantum Nature of Drug-Receptor Interactions: Deuteration Changes Binding Affinities for Histamine Receptor Ligands	Kržan Mojca, Vianello Robert, Maršavelski Aleksandra, Repič Matej, Zakšek Maja, Kotnik Kristina, Fijan Estera, Mavri Janez	10.1371/journal.pone.0154002	1932-6203	2016	PLoS One	11		e0154002-e0154002
15N NMR Spectroscopy, X-ray and Neutron Diffraction, Quantum-Chemical Calculations, and UV/vis-Spectrophotometric Titrations as Complementary Techniques for the Analysis of Pyridine-Supported Bicyclic Guanidine Superbases	Schwamm Ryan J., Vianello Robert, Maršavelski Aleksandra, García M. Ángeles, Claramunt Rosa M., Alkorta Ibon, Saame Jaan, Leito Ivo, Fitchett Christopher M., Edwards Alison J., Coles Martyn P.	10.1021/acs.joc.6b01330	0022-3263	2016	Journal of organic chemistry	81	17	7612-7625
Quantum Chemical Study of HOCl-Induced Transformations of Carbamazepine	Tandarić Tana, Vrček Valerije, Šakić Davor	10.1039/C6OB02166B	1477-0520	2016	Organic & biomolecular chemistry	14		10866-10874
Tuning Ag29 nanocluster light emission from red to blue with one and two-photon excitation	Russier-Antoine, Isabelle; Bertorelle, Franck; Hamouda, Ramzi.; Rayane, Driss; Dugourd, Philippe; Sanader, Željka; Bonačić-Koutecký, Vlasta; Brevet, Pierre-Francois; Antoine, Rodolphe	10.1039/C5NR08122J		2016	Nanoscale	8		2892-2898

Two-photon absorption of ligand-protected Ag15 nanoclusters. Towards a new class of nonlinear optics nanomaterials	Sanader, Zeljka; Krstic, Marjan; Russier-Antoine, Isabelle; Bertorelle, Franck; Dugourd, Philippe; Brevet, Pierre-François; Antoine, Rodolphe; Bonačić-Koutecký, Vlasta	10.1039/C6CP00207B		2016	Physical Chemistry Chemical Physics	18		12404-12408
The Use of Multiscale Molecular Simulations in Understanding a Relationship between the Structure and Function of Biological Systems of the Brain: The Application to Monoamine Oxidase Enzymes	Vianello Robert, Domene Carmen, Mavri Janez	10.3389/fnins.2016.00327	1662-453X	2016	Frontiers in Neuroscience	10		-
Vapour-induced solid-state C–H bond activation for the clean synthesis of an organopalladium biothiol sensor	Monas Andrea, Užarević Krunoslav, Halasz Ivan, Juribašić Kulcsar Marina, Ćurić Manda	10.1039/c6cc06062e	1359-7345	2016	Chemical communications	52	88	12960-12963
The role of negative hyperconjugation in decomposition of bicarbonate and organic carbonate anions	Denegri Bernard, Matić Mirela, Kronja Olga	10.1002/slct.201601357	2365-6549	2016	ChemistrySelect	1	16	5250-5259
Classical Logic and Quantum Logic with Multiple and Common Lattice Models	Pavičić Mladen	10.1155/2016/6830685	1687-9120	2016	Advances in Mathematical Physics	2016		6830685-1
Massive Generation of Contextual Quantum Sets	Pavičić Mladen.			2016	EMN Meeting on Quantum Communication and Quantum Imaging-2016 Program & Abstracts			28-29
The Important Role of the Hydroxyl Group on the Conformational Adaptability in Bis (L-threoninato) copper(II) Compared to Bis(L-allo-threoninato) copper(II): Quantum Chemical Study	Marković Marijana, Ramek Michael, Loher Claudia, Sabolović Jasmina	10.1021/acs.inorgchem.6b01157	0020-1669	2016	Inorganic chemistry	55	15	7694-7708
Elusive structure of helium trimers	Stipanović Petar, Vranješ Markić Leandra, Boronat Jordi	10.1088/0953-4075/49/18/185101	0953-4075	2016	Journal of physics. B, Atomic molecular and optical physics	49	18	185101-1
Structural and electronic determinants of flavonoid binding to human serum albumin: An extensive ligand-based study	Rimac Hrvoje, Debeljak Željko, Šakić Davor, Weitner Tin, Gabričević Mario, Vrček Valerije, Zorc Branka, Bojić Mirza	10.1039/c6ra17796d	2046-2069	2016	RSC Advances	6	79	75014-75022

Solidification of He-4 clusters adsorbed on graphene	Vranješ Markić Leandra, Stipanović Petar, Bešlić Ivana, Zillich Robert E.	10.1103/PhysRevB.94.045428	2469-9950	2016	Physical Review B	94	4	045428-1
The DFT local reactivity descriptors of alpha-tocopherol	Fabijanić Ivana, Jakobušić Brala Cvijeta, Pilepić Viktor	10.1007/s00894-015-2644-y	1610-2940	2015	Journal of molecular modeling	21		99-1
Human 3-hydroxyanthranilate 3, 4-dioxygenase (3HAO) dynamics and reaction, a multilevel computational study	Brkić, Hrvoje; Kovačević, Borislav; Tomić, Sanja			2015	Molecular biosystems	11		898-907
Causes and consequences of contrasting genetic structure in sympatrically growing and closely related species	Radosavljević Ivan, Šatović Zlatko, Liber Zlatko	10.1093/aobpla/plv106	2041-2851	2015	AoB Plants	7		plv106-1
The origin of specificity and insight into recognition between an aminoacyl carrier protein and its partner ligase	Maršavelski Aleksandra, Močibob Marko, Gruić- Sovulj Ita, Vianello Robert	10.1039/C5CP03066H	1463-9076	2015	Physical Chemistry Chemical Physics	17	29	19030-19038
Supramolecular Ionic-Liquid Gels with High Ionic Conductivity	Maršavelski Aleksandra, Smrečki Vilko, Vianello Robert, Žinić Mladen, Moguš-Milanković Andrea, Šantić Ana	10.1002/chem.201500887	0947-6539	2015	Chemistry : a European journal	21	34	12121-12128
Experimental and theoretical study of the cation binding properties of macrocyclic dehydrodibenzopyrido[15]annulenes	Zimmermann Boris, Baranović Goran, Gembarovski Dubravka	10.1016/j.saa.2014.08.076	1386-1425	2015	Spectrochimica acta. Part A, Molecular and biomolecular spectroscopy	137		730-739
Mechanochemical reactions studied by in situ Raman spectroscopy : base catalysis in liquid-assisted grinding	Tireli Martina, Juribašić Kulcsar Marina, Cindro Nikola, Gracin Davor, Biliškov Nikola, Borovina Mladen, Ćurić Manda, Halasz Ivan, Užarević Krunoslav	10.1039/c5cc01915j	1359-7345	2015	Chemical communications	51	38	8058-8061
A comparison of force fields for ethanol-water mixtures	Mijaković M., Polok K., Kežić B., Sokolić F., Perera A., Zoranić L.		0892-7022	2014	Molecular Simulation			1029-0435
A New Ant Colony Optimization Algorithm: Three Bound Ant System	Ivkovic N., Golub M.		0302-9743	2014	9th International Conference, ANTS 2014, Brussels, Belgium, September 10-12, 2014. Proceedings Series: Lecture Notes in Computer Science	8667		280-281

Acetamide as the Model of the Peptide Bond: Nonadiabatic Photodynamical Simulations in the Gas Phase and in the Argon Matrix	Eckert-Maksić M., Antol I., Vazdar M.	10.1016/j.comptc.2014.02.025		2014	Computational and Theoretical Chemistry	1040-1041		136-143
Aging and Ball Milling as Low-Energy and Environmentally-Friendly Methods for the Synthesis of Pd(II) Photosensitizers	Juribašić M., Halasz I., Babić D., Cinčić D., Plavec J., Ćurić M.			2014	Journal: Organometallics; Conference: Hot Topics in Contemporary Crystallography 2014, HTCC2014, Šibenik, Hrvatska, 10. -15.5.2014.	33	5	1227-1234
Chlorination of N-Methylacetamide and Amide-Containing Pharmaceuticals. Quantum-Chemical Study of the Reaction Mechanism	Šakić D., Šonjić P., Tandarić T., Vrček V.			2014	The journal of physical chemistry A.	118	12	2367-2376
Computational study of the IRES subdomain IIa structural plasticity and the ligand binding affinity	M. Grabar Branilović, S. Tomić			2014	Chemistry towards Biology 7th Central European Conference - Book of Abstracts / Jarzembek, Krystyna (ur.) (ur.). Katowice, Poljska (poster, međunarodna recenzija, sažetak, znanstveni)			P10-P10
Computational study of the structural plasticity and the ligand binding affinity of the IRES subdomain IIa	M. Grabar Branilović, S. Tomić	10.1039/c4mb00469h	1742-206X	2014	Molecular biosystems	10	12	3272-3279
Constrained-Geometry Bisphosphazides Derived from 1, 8-Diazidonaphthalene: Synthesis, Spectroscopic Characteristics, Structural Features, and Theoretical Investigations	J.F. Kögel, N.C. Abacılar, F. Weber, B. Oelkers, K. Harms, B. Kovačević, J. Sundermeyer			2014	Chemistry - A European Journal	20	20	5994-6009
Cyclopropenimine as a hydrogen bond acceptor—towards the strongest non-phosphorus superbases	D. Barić, I. Dragičević, B. Kovačević			2014	Tetrahedron	70	25	8571-8576
Decay Mechanisms of Protonated 4-Quinolone Antibiotics After Electrospray Ionization and Ion Activation	B. Kovačević, P. Schorr, Y. Qi, D.A. Volmer			2014	Journal of The American Society for Mass Spectrometry	25	11	1974-1986

Do cement nanoparticles exist in space?	G. Bilalbegović, A. Maksimović, V. Mohaček-Grošev	10.1093/mnras/stu869	0035-8711	2014	Monthly Notices of the Royal Astronomical Society	442		1319-1325
Effect of Intramolecular Hydrogen Bonds on the Gas-phase Basicity of Guanidines	Glasovac, Z., Eckert-Maksić M.	10.1071/CH14182	0004-9425	2014	Australian journal of chemistry	67	7	1056-1062
Eksperimentalno utemeljeno modeliranje interakcija nukleinskih kiselina i malih molekula	M. Grabar Branilović			2014	PhD Thesis			
The average local ionization energy and Fukui function of L-ascorbate, the local reactivity descriptors of antioxidant reactivity	Jakobušić Brala Cvijeta, Fabijanić Ivana, Karković Marković Ana, Pilepić Viktor	10.1016/j.comptc.2014.09.008	2210-271X	2014	Computational and theoretical chemistry	1049		1-6
Guanidine and guanidinium cation in the excited state—theoretical investigation	Antol I., Glasovac Z., Crespo-Otero R., Barbatti M.	10.1063/1.4892569	0021-9606	2014	The journal of chemical physics	141	7	074307-1-10
Mechanochemical C–H Bond Activation: Rapid and Regioselective Double Cyclopalladation Monitored by in situ Raman Spectroscopy	Juribašić M., Užarević K., Gracin D., Ćurić M.,			2014	Chemical communications	50	71	10287-10290
Memory of chirality in the phthalimide photocyclization of adamantane dipeptides	Šumanovac Ramljak T., Sohora M., Antol I., Kontrec D., Basarić N., Mlinarić-Majerski K.	10.1016/j.tetlet.2014.05.118		2014	Tetrahedron letters	55		4078-4081
A single amino acid substitution affects the substrate specificity of the seryl-tRNA synthetase homologue	Maršavelski Aleksandra, Lesjak Sonja, Močibob Marko, Weygand-Đurašević Ivana, Tomić Sanja	10.1039/C4MB00416G	1742-206X	2014	Molecular biosystems	10	12	3207-3216
Solid-State NMR Characterization of Paramagnetic Bis (L-valinato)copper (II) Stereoisomers – Effect of Conformational Disorder and Molecular Mobility on 13C and 2H Fast Magic-Angle Spinning Spectra	Szalontai G., Sabolović J., Marković M., Balogh S.	10.1002/ejic.201300746	1099-0682	2014	European journal of inorganic chemistry	2014		3330-3340
Structure, defects, and strain in silicon-silicon oxide interfaces	Kovacevic G., Pivac B.	10.1063/1.4862809		2014	Journal of Applied Physics	115	4	
Sulfur-bearing species in molecular clouds	G. Bilalbegović, G. Baranović	10.1093/mnras/stu2313	0035-8711	2014	Monthly Notices of the Royal Astronomical Society (MNRAS)	446	3	3118-3129

Superbasic Alkyl-Substituted Bisphosphazene Proton Sponges: Synthesis, Structural Features, Thermodynamic and Kinetic Basicity, Nucleophilicity and Coordination Chemistry	J.F. Kögel, X. Xie, E. Baal, D. Gesevičius, B. Oelkers, B. Kovačević, J. Sundermeyer			2014	Chemistry - A European Journal	20	25	7670-7685
Supramolecular stabilization of metastable tautomers in solution and solid state.	Juribašić M., Bregović N., Stilinović V., Tomišić V., Cindrić M., Šket P., Plavec J., Rubčić M., Užarević K.	10.1002/chem.201403543		2014	Chemistry : a European journal.			
The average local ionization energy and Fukui function of L-ascorbate, the local reactivity descriptors of antioxidant reactivity	C. Jakobušić Brala, I. Fabijanić, A. Karković Marković, V. Pilepić	10.1016/j.comptc.2014.09.008		2014	Computational and Theoretical Chemistry	1049		01.lip
The Stability of Nitrogen-Centered Radicals, Organic & biomolecular chemistry	Hioe J., Šakić D., Vrček V., Zipse H.			2014		1	1	01.sij
Universality in molecular halo clusters	Stipanović, Petar; Vranješ Markić, Leandra; Bešlić, Ivana; Boronat, Jordi	10.1103/PhysRevLett.113.253401		2014	Physical Review Letters	113	25	253401 - 253405
Vibrational Analysis of 3-Glycidoxypropyltrimethoxysilane Polymer	Movre Šapić I., Bistričić L., Volovšek V., Dananić V.	10.1002/masy.201300145	1521-3900	2014	Macromolecular Symposia	339	1	122-129
Why does the coordination mode of physiological bis (L-histidinato) copper(II) differ in the gas phase, crystal lattice and aqueous solutions? A quantum chemical study	Marković, M., Ramek M., Sabolović J.	10.1002/ejic.201300746	1099-0682	2014	European journal of inorganic chemistry	2014	1	198-212
A DFT-based model for calculating solvolytic reactivity. The nucleofugality of aliphatic carboxylates in terms of Nf parameters	Denegri Bernard, Matić Mirela, Kronja Olga	10.1039/C4OB00563E	1477-0520	2014	Organic & biomolecular chemistry	12	30	5698-5709
Obtaining massive data sets for contextual experiments in quantum information	Pavičić Mladen			2014	Information and Communication Technology, Electronics and Microelectronics (MIPRO), 2014 37th International Convention on.			332-335

4He clusters adsorbed on graphene	Vranješ Markić, Leandra; Stipanović, Petar; Bešlić, Ivana; Zillich, Robert E.	10.1103/PhysRevB.88.125416		2013	Physical Review B	88	12	125416-1 - 125416-13
A New Synthetic Pathway to the Second and Third Generation of Superbasic Bisphosphazene Proton Sponges: The Run for the Best Chelating Ligand for a Proton	Kögel J.F., Oelkers B., Kovačević B., Sundermeyer J.			2013	Journal of the American Chemical Society	35	47	17768-17774
Atropisomerism in 1-(2-Adamantyl) naphthalene Derivatives	Veljković J., Antol I., Basarić N., Smrečki V., Molčanov K., Müller N., Mlinarić-Majerski K.	10.1016/j.molstruc.2013.04.027		2013	Journal of molecular structure	1046		101-109
Quantum-chemical approach to determining the high potency of clorgyline as an irreversible acetylenic monoamine oxidase inhibitor	Pavlin Matic, Mavri Janez, Repič Matej, Vianello Robert	10.1007/s00702-013-1016-y	0300-9564	2013	Journal of neural transmission	120	6	875-882
Design of Superbasic Guanidines: The Role of Multiple Intramolecular Hydrogen Bonds	Barić D., Dragičević I., Kovačević B.			2013	Journal of organic chemistry	78	8	4075-4082
Dibenzotetraaza [14]annulene – adenine conjugate recognizes complementary poly dT among ss-DNA / ss-RNA sequences	M. Radić Stojković, M. Škugor, S. Tomić, M. Grabar, V. Smrečki, L. Dudek, J. Grolik, J. Eilmes, Julita, I. Piantanida	10.1039/c3ob40519b	1477-0520	2013	Organic & biomolecular chemistry	11	24	4077-4085
Glycolaldehyde dimer in the stable crystal phase has axial OH groups: Raman, infrared and X-ray data analysis	V. Mohaček-Grošev , B. Prugovečki, S. Prugoveč, N. Strukan	10.1016/j.molstruc.2013.05.006	0022-2860	2013	Journal of Molecular Structure	1047		209-215
Mechanisms and reaction-path dynamics of hydroxyl radical reactions with aromatic hydrocarbons: The case of chlorobenzene	Kovacevic G., Sabljic A.	10.1016/j.chemosphere.2013.04.041	0045-6535	2013	Chemosphere	92	7	851–856
Neighboring Effect in Fragmentation Pathways of Cage 2 Guanylhydrazones in the Gas Phase	Šekutor M., Glasovac Z., Mlinarić-Majerski K.	10.1021/jp311049f	1089-5639	2013	Journal of physical chemistry. A.	117	10	2242-2252
Non-heme iron dependent enzymes – understanding transport of iron cation in acetylacetone dioxygenase from Acinetobacter johnsoii	Tomić S., Brkić H., Straganz G., Buongiorno D.		0175-7571	2013	European Biophys. J.	42	1	814

Observed bands in Raman and infrared spectra of 1,3-dioxolane and their assignments	V. Mohaček-Grošv, K. Furić, H. Ivanković	10.1016/j.vibspec.2012.11.007	0924-2031	2013	Vibrational Spectroscopy	64		101-107
Photodeactivation paths in norbornadiene	Antol I.	10.1002/jcc.23270		2013	Journal of computational chemistry	34	17	1439-1445
Proteini i nukleinske kiseline u vremenu i prostoru	S. Tomić, H. Brkić, M. Grabar Branilović, A. Tomić, B. Bertoša, M. Šikić			2013	Bioinformatics and biological physics: proceedings of the scientific meeting/ V. Paar (ur.); Zagreb, Hrvatska akademija znanosti i umjetnosti (pozvano predavanje, domaća recenzija, objavljeni rad)			149-157
Quantum-chemical approach to determining the high potency of clorgyline as an irreversible acetylenic monoamine oxidase inhibitor	M. Pavlin, J. Mavri, M. Repič, R. Vianello			2013	Journal of Neural Transmission	120		875–882
Study of lipophilicity and membrane partition of 4-hydroxycoumarins by HPLC and PCA	Ilijaš M., Malnar I., Gabelica Marković V., Stepanić V.			2013	J. Pharm. Biomed. Anal.	76		104-111
The bis-phenanthridinium system flexibility and position of covalently bound uracil finely tunes the interaction with polynucleotides	M. Grabar Branilović, S. Tomić, L.-M. Tumir, I. Piantanida	10.1039/C3MB25578F	1742-206X	2013	Molecular biosystems	9	8	2051-2062
The chemical fate of paroxetine metabolites. Dehydration of radicals derived from 4-(4-fluorophenyl)-3-(hydroxymethyl) piperidine	Achrainer F., Šakić D., Vrček V., Zipse H.			2013	Organic & biomolecular chemistry	11	25	4232-4239
Theoretical study on the mechanism and kinetics of addition of hydroxyl radicals to fluorobenzene	Kovacevic G., Sabljic A.	10.1002/jcc.23175	1096-987X	2013	Journal of Computational Chemistry	34	8	646–655
Toward Extension of the Gas-Phase Basicity Scale by Novel Pyridine Containing Guanidines	Glasovac Z., Pavošević F., Štrukil V., Eckert-Maksić M., Schlangen M., Kretschmer R.	10.1016/j.ijms.2013.06.012	1387-3806	2013	International journal of mass spectrometry	354/355		113-122
Universality of atomic quantum halo clusters	Stipanović, Petar; Vranješ Markić, Leandra; Bešlić, Ivana; Boronat, Jordi			2013	MBT17 XVII. International conference on recent progress in many-body theories			56

Univerzalnost atomskih kvantnih halo klastera	Stipanović, Petar; Vranješ Markić, Leandra; Bešlić, Ivana; Boronat, Jordi		978-953-7178-15-4	2013	8. znanstveni sastanak HFD-a			121
Dicyclopalladated Complexes of Asymmetrically Substituted Azobenzenes: Synthesis, Kinetics and Mechanisms	Juribašić Marina, Budimir Ana, Kazazić Snježana, Ćurić Manda	10.1021/ic402017v	0020-1669	2013	Inorganic chemistry	52	21	12749-12757
Adsorption of 4HeN and 4HeN3He Clusters on Cesium	Stipanović, Petar; Vranješ Markić, Leandra; Bešlić, Ivana; Martinić, Tea	10.1007/s10909-011-0406-5	0022-2291 (print) / 1573-7357 (online)	2012	Journal of low temperature physics	166	01.vlj	68-79
Computational Study of Radical Derived from Hydroxyurea and Its Methylated Analogues	Vinković Vrček I., Šakić D., Vrček V., Zipse H., Biruš M.			2012	Organic & biomolecular chemistry	10	6	1196-1206
Ring Strain and Other Factors Governing the Basicity of Nitrogen Heterocycles - An Interpretation by Triadic Analysis	Radić Nena, Despotović Ines, Vianello Robert	10.5562/cca2121	0011-1643	2012	Croatica chemica acta	85	4	495-504
Dke1 – Structure, Dynamics and Function, A Theoretical and Experimental Study Elucidated the Role of the Binding Site Shape and the H-Bonding Network in Catalysis	H. Brkić, D. Buongiorno, M. Ramek, G. Straganz, S. Tomić	10.1007/s00775-012-0898-8	0949-8257	2012	Journal of biological inorganic chemistry	17	5	801-815
Interplay of crystallography and modelling in studying biological macromolecules	Tomić S., Abramić M., Brkić H., Tomić A.		978-953-154-157-2	2012	Conference: Kristalografija u Hrvatskoj			129 - 137
Kinetic differentiation between homo- and alternating AT-DNA by sterically restricted phosphonium dyes	L.-M. Tumir, I. Crnolatac, T. Deligeorgiev, A. Vasilev, S. Kaloyanova, M. Grabar Branilović, S. Tomić, I. Piantanida	10.1002/chem.201102968	0947-6539	2012	Chemistry : a European journal	18	13	3859-3864
Liquid and solid 4He clusters adsorbed on graphene	Vranješ Markić, Leandra; Bešlić, Ivana; Stipanović, Petar; Zillich, Robert E.			2012	International Conference on Quantum Fluids and Solids 2012			P4.33
Method for Estimating SN1 Rate Constants: Solvolytic Reactivity of Benzoates	Matić M., Denegri B., Kronja O.			2012	J. Org. Chem.	77		8986−8998

Molecular modeling of nucleic acid - small molecule interactions	S. Tomić, M. Grabar Branilović, I. Piantanida			2012	Book of Abstracts Regional Biophysical Conference 2012 / Zakrzewska, Joanna, Živić, Miroslav, Andjus, Pavle (ur.). Beograd, Srbija : Društvo biofizičara Srbije (pozvano predavanje, međunarodna recenzija, saţetak, znanstveni)			13-13
Molecular Modelling Of Copper(II) Complexes With Amino Acids In Vacuum, Crystal, And In Aqueous Solution	Marković M.			2012	PhD Thesis			
Prereactive complexes in chlorination of benzene, triazine, and tetrazine. A quantum chemical study	Šakić D., Vrček V.			2012	Journal of physical chemistry A.	116	4	1298-1306
QM/MM nonadiabatic decay dynamics of formamide in polar and nonpolar solvents	Antol I., Eckert-Maksić M., Vazdar M., Ruckenbauer M., Lischka H.	10.1039/C2CP41830D		2012	Physical Chemistry Chemical Physics	14	38	13262-13272
Ring strain and other factors governing the basicity of nitrogen heterocycles – an interpretation by triadic analysis	N. Radić, I. Despotović, R. Vianello			2012	Croatica Chemica Acta	85		495–504
Structural effects responsible for stability and solvolytic reactivity of sulfonium ions	Jurić S., Denegri B., Kronja O.			2012	J. Phys. Org. Chem.	25		147−152
Tebrophen - an old polyphenol drug with anticancer potential	Rubelj, I., Stepanić, V., Jelić, D., Vidaček, N.Š., Kalajžić, A.Ć., Ivanković, M., Nujić, K., Matijašić, M., Verbanac, D.			2012	Molecules	17		7864-7886
New Algorithms for Generating Arbitrary Kochen-Specker Sets	Megill Norman D., Pavičić Mladen			2012	Bulletin of the American Physical Society, APS March Meeting 2012, Volume 57, Number 1			Z30.00011-Z30.00011
4He clusters adsorbed on graphene	Vranješ Markić, Leandra; Bešlić, Ivana; Stipanović, Petar; Zillich, Robert			2011	The 26th International Conference on Low Temperature Physics (LT26)			349

A Pheromone Trails Model for MAX-MIN Ant System	Ivković N., Golub M., Maleković M.		978-2-9539267-1-2	2011	10th Biennal International Conference on Artificial Evolution, Angers, Francuska, October 24-26, 2011			35-46
Adsorpcija klastera 4HeN i 4HeN3He na površini cezija	Stipanović, Petar; Vranješ Markić, Leandra; Bešlić, Ivana; Martinić, Tea		978-953-7178-20-8	2011	7. znanstveni sastanak HFD-a			109
Adsorption of 4HeN and 4HeN3He clusters on cesium	Stipanović, Petar; Vranješ Markić, Leandra; Bešlić, Ivana; Martinic, Tea			2011	The 26th International Conference on Low Temperature Physics (LT26)			346
Adsorption of helium clusters on graphene	Vranješ Markić, Leandra; Bešlić, Ivana; Stipanović, Petar; Zillich, Robert E			2011	Adsorption at the Nanoscale: A New Frontier in Fundamental Science and Applications			12
Base-catalyzed reactions of environmentally relevant N-chloro-piperidines. A quantum-chemical study	Šakić D., Zipse H., Vrček V.			2011	Organic & biomolecular chemistry.	9	11	4336-4346
Extended Trail Reinforcement Strategies for Ant Colony Optimization	Ivković N., Maleković M., Golub M.	10.1007/978-3-642-27172-4_78	0302-9743	2011	Second International Conference, SEMCCO 2011, Visakhapatnam, Andhra Pradesh, India, December 19-21, 2011, Proceedings, Part I, Lecture Notes in Computer Science	7076	1	662-669
Ground state of small mixed helium and spin-polarized tritium clusters : A quantum Monte Carlo study	Stipanović, Petar; Vranješ Markić, Leandra; Boronat, Jordi; Kezić, Bernarda	10.1063/1.3530837		2011	The Journal of chemical physics	134	5	054509-1 - 054509-8
Guanidiniocarbonyl-pyrrole-aryl conjugates as nucleic acid sensors: switch of binding mode and spectroscopic responses by introducing additional binding sites into the linker	K. Groger, D. Baretić, I. Piantanida, M. Marjanović, M. Kralj, M. Grabar, S. Tomić, C. Schmuck	10.1039/C0OB00103A	1477-0520	2011	Organic & biomolecular chemistry	9	1	198-209
Intriguing Differences in the Gas-Phase Dissociation Behavior of Protonated and Deprotonated Gonyautoxin Epimers	Dörr F.A., Kovačević B., Maksić Z.B., Pinto E., Volmer D.A.			2011	Journal of the American Society for Mass Spectrometry	22	11	2011-2020

Kinetics and Mechanism of Oxidation of Hydroxyurea Derivatives with Hexacyanoferrate (III) in Aqueous Solution	Budimir A., Weitner T., Kos I., Šakić D., Gabričević M., Bešić E., Biruš M.			2011	Croatica chemica acta.	84	2	133-147
Molecular modeling of new permanently charged phenanthridinium-nucleobase conjugates in complexes with double stranded polynucleotides	M. Grabar, S. Tomić, L.-M. Tumir, I. Piantanida			2011	Ninth Triennial Congress of the World Association ot Theoretical and Computational Chemists - Book of Abstracts / Yáñez, Manuel ; Mó, Otilia (ur.). Santiago de Compostela (poster, međunarodna, recenzija, sažetak, znanstveni)			PII 017
Osnovno stanje klastera 4He adsorbiranih na grafenu	Vranješ Markić, Leandra; Bešlić, Ivana; Stipanović, Petar; Zillich, E. Robert		978-953-7178-20-8	2011	7. znanstveni sastanak HFD-a			90
Photoinduced rearrangement of aromatic N-chloroamides to chloroaromatic amides in the solid state. Inverted PI_N—SIGMA_N occupational stability of amidyl radicals	Naumov P., Topcu Y., Eckert-Maksić M., Glasovac Z., Pavošević F., Manoj K., Hara H.	10.1021/jp203771c	1089-5639	2011	Journal of Physical Chemistry	115	26	7834-7848
Vibrational analysis of 1-methyl-pyridinium-2-aldoxime and 1-methyl-pyridinium-4-aldoxime cations	V. Mohaček Grošev, B. Foretić, O. Gamulin	10.1016/j.saa.2011.01.012	1386-1425	2011	Spectrochimica Acta A Molecular and Biomolecular Spectroscopy	78		1376-1379
New Insight into Solid-State Molecular Dynamics: Mechanochemical Synthesis of Azobenzene /Triphenylphosphine Palladacycles	Cinčić Dominik, Juribašić Marina, Babić Darko, Molčanov Krešimir, Šket Primož, Plavec Janez, Ćurić Manda	10.1039/c1cc15377c	1359-7345	2011	Chemical communications	47	41	11543-11545
Probabilistic Generation of Quantum Contextual Sets	Megill Norman D., Fresl Krešimir, Waegell Mordecai, Aravind P.K., Pavičić Mladen	10.1016/j.physleta.2011.07.050	0375-9601	2011	Physics letters. A	375	39	3419-3424
Kochen-Specker Sets and Generalized Orthoarguesian Equations	Megill Norman D., Pavičić Mladen	10.1007/s00023-011-0109-0	1424-0637	2011	Annales henri poincare	12	7	1417-1429
New Class of 4-Dim Kochen-Specker Sets	Pavičić Mladen, Megill Norman. D., Aravind Padmanabhan K., Waegell Mordecai	10.1063/1.3549586	0022-2488	2011	Journal of mathematical physics	52	2	022104-1
Parity proofs of the Bell-Kochen-Specker theorem based on the 600-cell	Waegell Mordecai, Aravind P.K., Megill Norman D., Pavičić Mladen	10.1007/s10701-011-9534-7	0015-9018	2011	Foundations of physics	41	5	883-904

Proofs of the Kochen-Specker theorem based on the 600-cell	Aravind P.K., Waegell Mordecai, Megill Norman, Pavičić Mladen			2011	Bulletin of the American Physical Society, APS March Meeting 2011 Volume 56, Number 2 Monday–Friday, March 21–25, 2011 ; Dallas, Texas			J29.00002-J29.00002
Polycyano Derivatives of some Organic Tri- and Hexacyclic Molecules are Powerful Super- and Hyperacids in the Gas-Phase and DMSO - Computational Study by DFT Approach	Vianello Robert, Maksić Zvonimir	10.1021/jo101581a	0022-3263	2010	Journal of organic chemistry	75	22	7670-7681
Experimental and DFT study of 2-ferrocenylpropan-2-ol cyclodimerization products	Lapić J., Cetina M., Šakić D., Djaković S., Vrček V., Rapić V.			2010	Arkivoc.	11	9	257-268
Formamide as the Model Compound for Photodissociation Studies of the Peptide Bond, Kinetics and Dynamics	Eckert-Maksić M., Antol I., Vazdar M., Barbatti M., Lischka H.		978-90-481-3033-7	2010	Kinetics and Dynamics: From Nano- to Bio-Scale / Paneth, P.; Dybala-Defratyka, A. (ur.). Netherlands : Springer			77-107
Ground-state properties of small mixed helium and spin-polarized tritium clusters	Stipanović, Petar; Vranješ Markić, Leandra; Boronat, Jordi			2010	QFS2010 : International Symposium on Quantum Fluids and Solids			112
Interaction of phosphonium cyanine dyes with DNA	M. Grabar, S. Tomić, L.-M. Tumir, I. Piantanida, I. Crnolatac, T. Deligeorgiev, A. Vasilev, S. Kaloyanova			2010	Abstracts of the Fourth Humboldt Conference on Computational Chemistry / Petrova, P. Galina ; Vayssilov, N. Georgie (ur.). Sofia (poster, međunarodna recenzija, sažetak, znanstveni)			62
Molecular modelling of phosphonium cyanine dyes in complex with DNA	M. Grabar, S. Tomić, L.-M. Tumir, I. Piantanida, I. Crnolatac			2010	Book of Abstracts of the The 5th Central European Conference - Chemistry towards Biology; Zagreb, IRB (poster, međunarodna recenzija, sažetak, znanstveni)			85
Nuclear Magnetic Resonance Parameters of Water Hexamers	Bilalbegović G.			2010	J. Phys. Chem. A	114	2	715-720

Optical spectrum of proflavine and its ions	Bonaca A., Bilalbegović G.			2010	Chemical physics letters			
Polycyano derivatives of some organic tri– and hexacyclic molecules are powerful super– and hyperacids in the gas phase and DMSO: computational study by DFT approach	R. Vianello, Z. B. Maksić			2010	Journal of Organic Chemistry	22		7670–7681
Unusual azobenzene /bipyridine palladacycles: structural, dynamical, photophysical and theoretical studies	Juribašić Marina, Ćurić Manda, Molčanov Krešimir, Matković-Čalogović Dubravka, Babić Darko	10.1039/C0DT00018C	1477-9226	2010	Dalton transactions	39	37	8769-8778
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