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## Popis radova

| Naslov                                                                                                                                                        | Autori                                                                                                   | DOI                                              | ISSN<br>ili<br>ISBN | Godina | Casopis,<br>knjiga,<br>konferencija | Svezak | Izdanje | Stranice          |
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| Structure prediction of physiological bis (amino acidato) copper(II) species in aqueous solution: The copper(II) compounds with L- glutamine and L- histidine | Ramek, Michael; Sabolović, Jasmina                                                                       | https://doi.org/10.1016/j.jinorgbi o.2023.112430 | 0162-0134           | 2024   | Journal of inorganic biochemistry   | 251    | 2       | str. 112430 /1-18 |
| Structural Determination of the Hexacoordinated [Zn(L)2]2+ Complex Isomer Type Using Solution- State NMR, DFT Calculations and X- ray Crystallography         | Perić Berislav, Pantalon Juraj Natalija, Štefanić Zoran, Kirin Srećko I.                                 | 10.3390/cryst13010016                            |                     | 2023   | Crystals                            | 13     |         | -                 |
| Potential of AMnO3 (A = Ca, Sr, Ba, La) as Active Layer in Inorganic Perovskite Solar Cells                                                                   | Mužević Matko, Lukačević Igor, Kovač Ivan, Gracin Davor, Žužić Andreja, Macan Jelena, Varga Pajtler Maja |                                                  |                     | 2023   | ChemPhysChem                        |        |         | -                 |
| Quantum Contextuality                                                                                                                                         | Pavičić Mladen                                                                                           | 10.22331/q-2023-03-17-953                        |                     | 2023   | Quantum                             | 7      | 953     | 953-1             |

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| High Performance Computing Reinforcement Learning Framework for Power System Control                                                            | Damjanović Ivana, Pavić Ivica, Brčić Mario, Jerčić Roko                                                                                                                                                                                                          | 10.1109/ISGT51731.2023.10066416                                                   |           | 2023 | 2023 IEEE Power & Energy Society Innovative Smart Grid Technologies Conference (ISGT) |     |    | 1-5            |
| Charge carrier dynamics across the metal oxide /BaTiO <sub>3</sub> interfaces toward photovoltaic applications from the theoretical perspective | Kovač Ivan, Mužević Matko, Varga Pajtler Maja, Lukačević Igor                                                                                                                                                                                                    | 10.1016/j.surf.2023.102974                                                        |           | 2023 | Surfaces and interfaces                                                               | 39  |    | 102974-102981  |
| The optical properties of strontium manganite thin films prepared by novel phototreatment technique                                             | Žužić Andreja, Gracin Davor, Zubak Marko, Macan Jelena, Salamon Krešimir, Jurać Krunoslav, Krstulović Nikša, Radičić Rafaela, Lukačević Igor, Mužević Matko, Gajović Andreja                                                                                     | 10.1016/j.jallcom.2023.169972                                                     | 0925-8388 | 2023 | Journal of alloys and compounds                                                       | 951 |    | -              |
| Lithium adsorption on the interface of graphene/boron nitride nanoribbons                                                                       | Pajtler Maja Varga, Lukačević Igor, Dušić Vanja, Mužević Matko                                                                                                                                                                                                   | 10.1007/s10853-023-08292-y                                                        |           | 2023 | Journal of Materials Science                                                          |     |    | -              |
| Synthesis, photochemistry, computational study and potential application of new styryl-thiophene and naphtho-thiophene benzylamines             | Mlakić Milena, Odak Ilijana, Faraho Ivan, Bosnar Martina, Banjanac Mihailo, Lasić Zlata, Marinić Željko, Barić Danijela, Škorić Irena                                                                                                                            | 10.3390/ijms24010610                                                              |           | 2023 | International journal of molecular sciences                                           | 24  | 1  | -              |
| New thienobenzo /naphtho-triazoles as butyrylcholinesterase inhibitors. Design, synthesis and computational study                               | Mlakić Milena, Selec Ida, Čaleta Irena, Odak Ilijana, Barić Danijela, Ratković Ana, Molčanov Krešimir, Škorić Irena                                                                                                                                              | 10.3390/ijms24065879                                                              |           | 2023 | International journal of molecular sciences                                           | 24  | 6  | -              |
| Thieno-thiazolostilbenes, thienobenzo-thiazoles and naphtho-oxazoles: Computational study and cholinesterase inhibitory activity                | Mlakić Milena, Đurčević Ema, Odak Ilijana, Barić Danijela, Juričević Ines, Šagud Ivana, Burčul Franko, Lasić Zlata, Marinić Željko, Škorić Irena                                                                                                                 | 10.3390/molecules28093781                                                         |           | 2023 | Molecules                                                                             | 28  | 9  | -              |
| Plastic and genomic change of a newly established lizard population following a founder event                                                   | Sabolić, Iva; Mira, Óscar; Brandt, Débora Y. C.; Lisicić, Duje; Stapley, Jessica; Novosolov, Maria; Bakarić, Robert; Cizelj, Ivan; Glogoski, Marko; Hudina, Tomislav; Taverne, Maxime; Allentoft, Morten E., Nielsen, Rasmus; Herrel, Anthony; Stambuk, Anamaria | <a href="https://doi.org/10.1111/mec.17255">https://doi.org/10.1111/mec.17255</a> | 0962-1083 | 2023 | Molecular ecology                                                                     |     |    |                |
| Deuteration of Pd-activated C(sp <sup>2</sup> )-H bonds in the solid state                                                                      | Bjelopetrović, Alen; Barišić, Dajana; Juribašić Kulcsar, Marina; Halasz, Ivan; Čurić, Manda; Lukin, Stipe                                                                                                                                                        | 10.1039/D3QI00932G                                                                | 2052-1545 | 2023 | Inorganic chemistry frontiers                                                         | 10  | 20 | str. 6005-6014 |
| Adjustable Pheromone Reinforcement Strategies for Problems with Efficient Heuristic Information                                                 | Ivković, Nikola ; Kudelić, Robert ; Golub, Marin                                                                                                                                                                                                                 | 10.3390/a16050251                                                                 |           | 2023 | Algorithms                                                                            | 16  | 5  | 251, 21        |

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| FTIR spectroscopy and molecular level insight of diluted aqueous solutions of acetic acid                                                                                  | Pem, Barbara; Brkljača, Zlatko; Philippe, Alan; Schaumann, Gabriele E.; Vazdar, Mario; Bakarić, Danijela                                                               | 10.1016/j.saa.2023.123135      | 1386-1425 | 2023 | Spectrochimica acta. Part A, Molecular and biomolecular spectroscopy | 302  |    | 123135, 10             |
| Cucurbit[8]uril Forms Tight Complexes with Cationic Triamantanes                                                                                                           | King, David ; Šumanovac, Tatjana ; Murkli, Steven ; Schreiner, R. Peter ; Šekutor, Marina ; Isaacs, Lyle                                                               | 10.1039/d3nj00156c             | 1144-0546 | 2023 | New journal of chemistry                                             | 47   |    | str. 5338-5346         |
| Diamondoid ether clusters in helium nanodroplets                                                                                                                           | Alić, Jasna ; Messner, Roman ; Alešković, Marija ; Küstner, Florian ; Rubčić, Mirta ; Lackner, Florian ; Wolfgang, E. Ernest ; Šekutor, Marina                         | 10.1039/D3CP00489A             | 1463-9076 | 2023 | PCCP. Physical chemistry chemical physics                            | 25   |    | str. 11951-11958       |
| Nanostructured supramolecular networks from selfassembled diamondoid molecules at ultracold conditions                                                                     | Alešković, Marija ; Küstner, Florian ; Messner, Roman ; Lackner, Florian ; Ernst, E. Wolfgang ; Šekutor, Marina                                                        | 10.1039/D3CP02367B             | 1463-9076 | 2023 | PCCP. Physical chemistry chemical physics                            | 25   |    | str. 17869-17876       |
| Increasing complexity in adamantyl thioethers characterized by rotational spectroscopy                                                                                     | Pinacho, Pablo; Loru, Donatella; Šumanovac Ramljak, Tatjana; Šekutor, Marina; Schnell, Melanie;                                                                        | 10.1002/cphc.202300561         | 1439-4235 | 2023 | ChemPhysChem                                                         | 24   | 23 | str. e2023005-e2023005 |
| Hosting of diamantane alcohols in water and hydrogen-bonded organic solvents: the (non-) classical hydrophobic effect                                                      | Usenik, Andrea; Alešković, Marija; Roca, Sunčica; Mrkuš, Iva; Šekutor, Marina; Požar, Josip                                                                            | 10.1039/d3nj03097k             | 1144-0546 | 2023 | New journal of chemistry                                             | 2023 | 47 | str. 18745-18755       |
| Copper–zinc /chitosan complex hydrogels: Rheological, degradation and biological properties                                                                                | Lončarević, Andrea; Malbaša, Zoran; Kovačić, Marin; Ostojić, Karla; Angaš, Ange; Skoko, Željko; Szpunar, Joanna; Urić, Inga; Gallego Ferrer, Gloria; Rogina, Anamarija | 10.1016/j.ijbiomac.2023.126373 | 0141-8130 | 2023 | International journal of biological macromolecules                   | 251  |    | 126373, 10             |
| Proton affinity and gas phase basicity of diamondoid molecules: diamantane to C131H116                                                                                     | Camacho-Mojica Dulce C., Ha Jong-Kwon, Min Seung Kyu, Vianello Robert, Ruoff Rodney S.                                                                                 | 10.1039/d1cp04177k             | 1463-9076 | 2022 | PCCP. Physical chemistry chemical physics                            | 24   |    | 3470-3477              |
| Spectroscopic and Computational Study of the Protonation Equilibria of Amino-Substituted benzo [b]thieno[2,3-b] pyrido[1,2-a] benzimidazoles as Novel pH-Sensing Materials | Perin Nataša, Babić Darko, Kassal Petar, Čikoš Ana, Hranjec Marijana, Vianello Robert                                                                                  | 10.3390/chemosensors10010021   |           | 2022 | Chemosensors                                                         | 10   | 1  | -                      |
| Compositional stability of sediment microbial communities during a seagrass meadow decline                                                                                 | Markovski Marsej, Najdek Mirjana, Herndl Gerhard J., Korlević Marino                                                                                                   | 10.3389/fmars.2022.966070      |           | 2022 | Frontiers in Marine Science                                          | 9    |    | -                      |

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| New insight in the 2-flavor Schwinger model based on lattice simulations                                                                                  | Nieto Castellanos Jaime Fabián, Bietenholz Wolfgang, Hip Ivan                                                                                                                               | 10.31349/supprevmexfis.3.020707 |           | 2022 | Joint Proceedings of the XXXV Annual Meeting DPyC-SMF & XIX Mexican School on Particles and Fields           |           |    | -         |
| Finite temperature and delta-regime in the 2-flavor Schwinger model                                                                                       | Hip Ivan, Nieto Castellanos Jaime Fabián, Bietenholz Wolfgang                                                                                                                               | 10.22323/1.396.0279             |           | 2022 | Proceedings of Science - Volume 396 - The 38th International Symposium on Lattice Field Theory (LATTICE2021) |           |    | -         |
| Deep Reinforcement Learning-Based Approach for Autonomous Power Flow Control Using Only Topology Changes                                                  | Damjanović Ivana, Pavić Ivica, Puljiz Mate, Brcic Mario                                                                                                                                     | 10.3390/en15196920              |           | 2022 | Energies                                                                                                     | 15        | 19 | -         |
| On Comprehension of Genetic Programming Solutions: A Controlled Experiment on Semantic Inference                                                          | Slivnik Boštjan, Kovačević Željko, Mernik Marjan, Kosar Tomaž                                                                                                                               | 10.3390/math10183386            |           | 2022 | Mathematics                                                                                                  | 10        | 18 | -         |
| Surface Functionalisation of Dental Implants with a Composite Coating of Alendronate and Hydrolysed Collagen: DFT and EIS Studies                         | Petrović Željka, Šarić Ankica, Despotović Ines, Katić Jozefina, Peter Robert, Petravić Mladen, Ivanda Mile, Petković Marin                                                                  | 10.3390/ma15155127              | 1996-1944 | 2022 | Materials                                                                                                    | 15        | 15 | -         |
| Insight into the Growth Mechanism and Photocatalytic Behavior of Tubular Hierarchical ZnO Structures: An Integrated Experimental and Theoretical Approach | Šarić Ankica, Vrankić Martina, Lützenkirchen- Hecht Dirk, Despotović Ines, Petrović Željka, Dražić Goran, Eckelt Franz                                                                      | 10.1021/acs.inorgchem.1c03905   | 0020-1669 | 2022 | Inorganic chemistry                                                                                          | 61        | 6  | 2962-2979 |
| Experimental and computation study of thermal transformations of thienyl and furyl o-divinylbenzenes in acidic media                                      | Lovrinčević Vilma, Vuk Dragana, Despotović Ines                                                                                                                                             |                                 |           | 2022 |                                                                                                              |           |    | 81-81     |
| Streptomyces coelicolor macromodomain hydrolase SCO6735 cleaves thymidine-linked ADP-ribosylation of DNA                                                  | Hloušek-Kasun Andrea, Mikolčević Petra, Matthias Rack Johannes Gregor, Tromans-Coia Callum, Schuller Marion, Jankevicius Gytis, Matković Marija, Bertoša Branimir, Ahel Ivan, Mikoč Andreja | 10.1016/j.csbj.2022.08.002      | 4337-4350 | 2022 | Computational and Structural Biotechnology Journal                                                           | Volume 20 |    | 4337-4350 |
| Ferrocenoyl-adenines: substituent effects on regioselective acylation                                                                                     | Toma Mateja, Zubčić Gabrijel, Lapić Jasmina, Djaković Senka, Šakić Davor, Vrček Valerije                                                                                                    | 10.3762/bjoc.18.133             | 2195-951X | 2022 | Beilstein journal of organic chemistry                                                                       | 18        |    | 1270-1277 |

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| Zn(II) halide coordination compounds with imidazole and 2-methylimidazole. Structural and computational characterization of intermolecular interactions and disorder                          | Tašner Marina, Vušak Darko, Ivana Kekez, Gabud Andrea, Pilepić Viktor, Mrvoš-Sermek Draginja, Matković-Čalogović Dubravka                                                                                            | 10.1016/j.heliyon.2022.e11100 | 2405-8440 | 2022 | Heliyon                                 | 8   |      | -         |
| Design and synthesis of harmiquins, harmine and chloroquine hybrids as potent antiparasitic agents                                                                                            | Poje Goran, Pessanha de Carvalho Lais, Held Jana, Moita Diana, Prudêncio Miguel, Perković Ivana, Tandarić Tana, Vianello Robert, Rajić Zrinka                                                                        | 10.1016/j.ejmech.2022.114408  | 0223-5234 | 2022 | European journal of medicinal chemistry | 238 |      | -         |
| A series of nickel (II) thiocyanate complexes comprising various molar contents of isonicotinamide and water as ligands or co-crystallized moieties – an experimental and computational study | Hok Lucija, Vianello Robert, Matković-Čalogović Dubravka, Karanović Ljiljana, Roca Sunčica, Jaźwiński Jarosław, Tašner Marina, Vušak Darko, Đaković Marijana, Popović Zora                                           | 10.1039/d2ce00847e            |           | 2022 | CrystEngComm                            | 24  | 37   | 6564-6578 |
| Imidazo[4,5-b]pyridine derived tubulin polymerization inhibitors: Design, synthesis, biological activity in vitro and computational analysis                                                  | Boček Ida, Hok Lucija, Persoons Leentje, Daelemans Dirk, Vianello Robert, Hranjec Marijana                                                                                                                           | 10.1016/j.bioorg.2022.106032  | 0045-2068 | 2022 | Bioorganic chemistry                    | 127 |      | -         |
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| Effect of Functionalized Benzene Derivatives as Potential Hole Scavengers for BiVO <sub>4</sub> and rGO-BiVO <sub>4</sub> Photoelectrocatalytic Hydrogen Evolution                            | Sharifi Tayebbeh, Kovačić Marin, Belec Monika, Perović Klara, Popović Marin, Radić Gabrijela, Žener Boštjan, Pulitika Anamarija, Kraljić Roković Marijana, Lavrenčić Štangar Urška, Lončarić Božić Ana, Kušić Hrvoje | 10.3390/molecules27227806     |           | 2022 | Molecules                               | 27  | 22   | -         |
| Amphiphilic Silver Nanoparticles for Inkjet-Printable Conductive Inks                                                                                                                         | Ivanišević Irena, Kovačić Marin, Zubak Marko, Ressler Antonia, Krivačić Sara, Katančić Zvonimir, Gudan Pavlović Iva, Kassal Petar                                                                                    | 10.3390/nano12234252          |           | 2022 | Nanomaterials                           | 12  | 23   | -         |

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| A mononuclear iron (III) complex with unusual changes of color and magneto-structural properties with temperature: synthesis, structure, magnetization, multi-frequency ESR and DFT study | Garg Nitish Kumar, Goriya Yogesh, Manojveer Seetharaman, Muratović Senada, Pajić Damir, Cetina Mario, Petreska Irina, Krupskaya Yulia, Kataev Vladislav, Johnson Magnus T., Wendt Ola F., Žilić Dijana                                                       | 10.1039/D1DT03751J             | 1477-9226 | 2022 | Dalton transactions                                                                                                           | 51  | 6  | 2338-2345   |
| Unusual magnetism and thermochromism of mononuclear iron (III) complex                                                                                                                    | Garg Nitish Kumar, Goriya Yogesh, Manojveer Seetharaman, Muratović Senada, Pajić Damir, Cetina Mario, Petreska Irina, Krupskaya Yulia, Kataev Vladislav, Johnson Magnus T., Wendt Ola F., Žilić Dijana                                                       |                                |           | 2022 | CPSM 2022 Book of Abstracts                                                                                                   |     |    | 9-9         |
| Neuropeptides, substrates and inhibitors of human dipeptidyl peptidase III, experimental and computational study — A new substrate identified                                             | Karačić Zrinka, Šupljika Filip, Tomić Antonija, Brkljačić Lidija, Tomašić Paić Ana, Čehić Mirsada, Tomić Sanja                                                                                                                                               | 10.1016/j.ijbiomac.2022.09.119 | 0141-8130 | 2022 | International journal of biological macromolecules                                                                            | 220 |    | 1390-1401   |
| Demystifying DPP III Catalyzed Peptide Hydrolysis—Computational Study of the Complete Catalytic Cycle of Human DPP III Catalyzed Tynorphin Hydrolysis                                     | Tomić Antonija, Tomić Sanja                                                                                                                                                                                                                                  | 10.3390/ijms23031858           |           | 2022 | International journal of molecular sciences                                                                                   | 23  | 3  | -           |
| Computational modelling an aid to understand binding and hydrolysis of neuropeptides in the active site of human DPP III                                                                  | Tomić Antonija, Karačić Zrinka, Šupljika Filip, Tomić Sanja                                                                                                                                                                                                  |                                |           | 2022 | Book of abstracts of the 1st Central and Eastern European Conference on Physical Chemistry and Materials Science (CEEC-PCMS1) |     |    | 196-196     |
| Computational study of the human DPP III catalyzed peptide hydrolysis - difference between „good“ and „slow“ substrate                                                                    | Tomić Antonija, Tomić Sanja                                                                                                                                                                                                                                  |                                |           | 2022 | Math/Chem /Comp 2022 and 33rd MC2 Conference : Book of Abstracts                                                              |     |    | 24-24       |
| Gaussian field-based 3D-QSAR and molecular simulation studies to design potent pyrimidine–sulfonamide hybrids as selective BRAFV600E inhibitors                                           | Singh Ankit Kumar, Novak Jurica, Kumar Adarsh, Singh Harshwardhan, Thareja Suresh, Pathak Prateek, Grishina Maria, Verma Amita, Yadav Jagat Pal, Khalilullah Habibullah, Pathania Vikas, Nandanwar Hemraj, Jaremko Mariusz, Emwas Abdul-Hamid, Kumar Pradeep | 10.1039/d2ra05751d             |           | 2022 | RSC Advances                                                                                                                  | 12  | 46 | 30181-30200 |
| Withasomniferol C, a new potential SARS-CoV-2 main protease inhibitor from the Withania somnifera plant proposed by in silico approaches                                                  | Kandagalla Shivananada, Rimac Hrvoje, Krishnamoorthy Gurushankar, Novak Jurica, Grishina Maria, Potemkin Vladimir                                                                                                                                            | 10.7717/peerj.13374            |           | 2022 | PeerJ                                                                                                                         | 10  |    | -           |

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| On the propensity of formation of cyclobutane dimers in face-to-face and face-to-back uracil stacks in solution                                         | Milovanović Branislav, Novak Jurica, Etinski Mihajlo, Domcke Wolfgang, Došlić Nada                                                                                                                                                          | 10.1039/d2cp00495j              | 1463-9076 | 2022 | PCCP. Physical chemistry chemical physics   | 24  | 24  | 14836-14845   |
| Mixed Halide Ordering as a Tool for the Stabilization of Ruddlesden–Popper Structures                                                                   | Ovčar Juraj, Leung Tik Lun, Grisanti Luca, Skoko Željko, Vrankić Martina, Low Kam-Hung, Wang Shixun, You Pei-Ying, Ahn Hyeyoung, Lončarić Ivor, Djurišić Aleksandra B., Popović Jasminka                                                    | 10.1021/acs.chemmater.1c03815   | 0897-4756 | 2022 | Chemistry of materials                      | 34  | 10  | 4286-4297     |
| Preparation and Characterization of Non-Aromatic Ether Self-Assemblies on a HOPG Surface                                                                | Alić Jasna, Biljan Ivana, Štefanić Zoran, Šekutor Marina                                                                                                                                                                                    | 10.1088/1361-6528/ac6e72        | 0957-4484 | 2022 | Nanotechnology                              | 33  | 35  | -             |
| Unravelling Binding Effects in Cyclodextrin Inclusion Complexes with Diamondoid Ammonium Salt Guests                                                    | Alešković Marija, Roca Sunčica, Jozepović Ruža, Bregović Nikola, Šekutor Marina                                                                                                                                                             | 10.1039/D2NJ00938B              | 1144-0546 | 2022 | New journal of chemistry                    | 46  |     | 13406-13414   |
| Reference-Guided De Novo Genome Assembly of the Flour Beetle <i>Tribolium freemani</i>                                                                  | Volarić Marin, Despot-Slade Evelin, Veseljak Damira, Meštrović Nevenka, Mravinac Brankica                                                                                                                                                   | 10.3390/jms23115869             |           | 2022 | International journal of molecular sciences | 23  | 11  | -             |
| Phylogeographic structure of common sage ( <i>Salvia officinalis</i> L.) reveals microrefugia throughout the Balkans and colonizations of the Apennines | Radosavljević Ivan, Satović Zlatko, di Pietro Romeo, Jug Dujaković Marija, Varga Filip, Škrtić Danijel, Liber Zlatko                                                                                                                        | 10.1038/s41598-022-20055-4      |           | 2022 | Scientific Reports                          | 12  |     | -             |
| Gene flow between wild trees and cultivated varieties shapes the genetic structure of sweet chestnut ( <i>Castanea sativa</i> Mill.) populations        | Tumpa Katarina, Šatović Zlatko, Liber Zlatko, Vidaković Antonio, Idžojić Marilena, Ježić Marin, Čurković-Perica Mirna, Poljak Igor                                                                                                          | 10.1038/s41598-022-17635-9      |           | 2022 | Scientific reports                          | 12  |     | -             |
| Intra- and Inter-Cultivar Variability of Lavandin ( <i>Lavandula × intermedia</i> Emeric ex Loisel.) Landraces from the Island of Hvar, Croatia         | Jug-Dujaković Marija, Ninčević Runjić Tonka, Grdiša Martina, Liber Zlatko, Šatović Zlatko                                                                                                                                                   | 10.3390/agronomy12081864        |           | 2022 | Agronomy                                    | 12  | (8) | -             |
| Utility of EST-SNP Markers for Improving Management and Use of Olive Genetic Resources: A Case Study at the Worldwide Olive Germplasm Bank of Córdoba   | Belaj Angelina, Ninot Antònia, Gómez-Gálvez Francisco J., El Riachy Milad, Gurbuz-Veral Melek, Torres Mariela, Lazaj Adhurim, Klepo Tatjana, Paz Sergio, Ugarte Javier, Baldoni Luciana, Lorite Ignacio J., Šatović Zlatko, de la Rosa Raúl | 10.3390/plants11070921          |           | 2022 | Plants                                      | 11  | 7   | -             |
| Quantum capacitance of multi-layered δ-6 borophene: A DFT study                                                                                         | Kolavada Himalay, Singh Shilpa, Lukačević Igor, Gajjar P. N., Gupta Sanjeev K.                                                                                                                                                              | 10.1016/j.electacta.2022.141589 | 0013-4686 | 2022 | Electrochimica acta                         | 439 |     | 141589-141595 |

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| Density functional theory demonstrates orientation effects in the Raman spectra of hydroxy- and carbonated apatite                                                  | Gemer Dejan, Živković Aleksandar, Lukačević Igor, Bahmann Hilke, King Helen E.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | 10.1002/jrs.6465                |           | 2022 | Journal of Raman Spectroscopy                |     |        | -         |
| Resveratrol-maltol and resveratrol-thiophene hybrids as cholinesterase inhibitors and antioxidants: Synthesis, bio-metal chelating capability and crystal structure | Mrakić Milena, Fodor Lajos, Odak Ilijana, Horváth Ottó, Lovrić Marija Jelena, Barić Danijela, Milašinović Valentina, Molčanov Krešimir, Marinić Željko, Lasić Zlata, Škorić Irena                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | 10.3390/molecules27196379       |           | 2022 | Molecules                                    | 27  | 19     | -         |
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| Why monoamine oxidase B preferably metabolizes N-methylhistamine over histamine: evidence from the multiscale simulation of the rate-limiting step                  | Maršavelski Aleksandra, Mavri Janez, Vianello Robert, Stare Jernej                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 10.3390/ijms23031910            |           | 2022 | International journal of molecular sciences  | 23  | 3      | -         |
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| Biocatalytic approach to chiral fluoroaromatic scaffolds                                                                                                            | Dokli Irena, Brkljača Zlatko, Švaco Petra, Tang Lixia, Stepanić Višnja, Majerić Elenkov Maja                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 10.1039/D2OB01955H              | 1477-0520 | 2022 | Organic & biomolecular chemistry             | 20  |        | 9734-9741 |
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| Inhibitory effect of DMSO on halohydrin dehalogenase: Experimental and computational insights into the influence of an organic co-solvent on the structural and catalytic properties of a biocatalyst | Milčić Nevena, Štepanić Višnja, Črnolatac Ivo, Findrik Blažević Zvezdana, Brkljača Zlatko, Majerić Elenkov Maja                                                                                             | 10.1002/chem.202201923        | 0947-6539 | 2022 | Chemistry : a European journal                                       | 28  | 56 | -         |
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| Resistance Coefficient Estimation for a Submarine's Bare Hull Moving in Forward and Transverse Directions                                                                                             | Saghi Hassan, Parunov Joško, Mikulić Antonio                                                                                                                                                                | 10.3390/app12110953           |           | 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   |
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| 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 |                                                                      |     |    | -         |
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| 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  |    | -         |
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| 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  |    | -         |
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| 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) |    | -         |
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| 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   |   | -             |
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| 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/forth-2021-0011       | 0867-1761 | 2021 | Folia Horticulturae                                                         | 33   | 1  | 1-15      |
| High Genetic Diversity and Low Population Differentiation in Wild Hop ( <i>Humulus lupulus</i> L.) from Croatia                                                                                       | Grdiša Martina, Šatović Zlatko, Liber Zlatko, Jakše Jernej, Varga Filip, Erhatic 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   |    | -         |

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| 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 Stefanie, Kendel 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 desmursamyl 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 heteropolicičkih sustava                                                                                           | Znika Monika                                                                                                                                                                                                                 |                                |           | 2021 |                                                    |      |   | -         |
| A crystallographic and solid-state NMR study of 1,4-disubstituted 2,5-diketopiperazines                                                     | Perić Berislav, Pantalun 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 |   | -         |

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| 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.jinorgbioc.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, Brajković Vladimir, Rota Stabelli Omar, Krebs Stefan, Sölkner Johann, Šalamon Dragica, Ristov Strahil, Berger Beate, Trivizaki Stamatina, Bizelis Iosif, Ferenčaković Maja, Rothammer Sophie, Kunz Elisabeth, Simčić 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 baimantuoluamide A and baimantuoluamide 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      |

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| A triterpene<br>glochidon from<br>Phyllanthus debilis:<br>Isolation,<br>computational<br>studies, and<br>antidiabetic activity<br>evaluation                                                                                    | Verma Amita, Pathak Prateek, Rimac Hrvoje, Khalilullah Habibullah, Kumar Vikas, Grishina Maria, Potemkin Vladimir, Ahmed Bahar                                                                          | 10.101<br>6/j.<br>bcab.<br>2021.1<br>02138           | 1878-<br>8181 | 2021           | Biocatalysis<br>and<br>Agricultural<br>Biotechnology                 | 36   |    | -                 |
| Potentiometric<br>Surfactant Sensor<br>Based on 1,3-<br>Dihexadecyl-1H-<br>benzo[d]imidazol-3-<br>ium for Anionic<br>Surfactants in<br>Detergents and<br>Household Care<br>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 | 10.339<br>0<br>/molec<br>ules26<br>123627            |               | 2021           | Molecules                                                            | 26   | 12 | -                 |
| Disocijacijska<br>duljina raspršenja<br>atomskeg trimera u<br>osnovnome stanju                                                                                                                                                  | Leon Čatipović                                                                                                                                                                                          |                                                      |               | 2020-07-<br>02 |                                                                      |      |    |                   |
| Effect of source-<br>code<br>preprocessing<br>techniques on<br>plagiarism<br>detection accuracy<br>in student<br>programming<br>assignments                                                                                     | Matija Novak                                                                                                                                                                                            |                                                      |               | 2020-02-<br>02 |                                                                      |      |    |                   |
| Modeling and<br>synthesis of novel<br>oxime derivatives<br>as potential<br>cholinesterase<br>inhibitors                                                                                                                         | Ratković Ana, Pavlović Kristina, Barić Danijela, Marinić Željko, Grgičević Ivan, Škorić Irena                                                                                                           | 10.101<br>6/j.<br>molstru<br>c.<br>2019.1<br>27149   | 0022-<br>2860 | 2020           | Journal of<br>molecular<br>structure                                 | 1200 |    | 127149-<br>127149 |
| From Grammar<br>Inference to<br>Semantic<br>Inference—An<br>Evolutionary<br>Approach                                                                                                                                            | Kovačević Željko, Mernik Marjan, Ravber Miha, Črepinšek Matej                                                                                                                                           | 10.339<br>0<br>/math8<br>050816                      |               | 2020           | Mathematics                                                          | 8    | 5  | 1-24              |
| Molecular<br>Dynamics<br>Simulations of the<br>Elusive Matrixopen<br>State of<br>Mitochondrial ADP<br>/ATP Carrier                                                                                                              | Škulj Sanja, Brkljača Zlatko, Vazdar Mario                                                                                                                                                              | 10.100<br>2/ijch.<br>202000<br>011                   |               | 2020           | Israel journal<br>of chemistry                                       |      |    | -                 |
| Chloride-Assisted<br>Peptide<br>Macrocyclization                                                                                                                                                                                | Vidović Nikolina, Horvat Gordan, Riva Davide, Rinkovec Tamara, Cindro Nikola, Tomišić Vladislav, Speranza Giovanna                                                                                      | 10.102<br>1/acs.<br>orglett.<br>0c00036              | 1523-<br>7060 | 2020           | Organic letters                                                      | 22   | 6  | 2129-2134         |
| Synthesis,<br>photochemistry<br>and photophysics<br>of new butadiene<br>derivatives:<br>influence of the<br>fluoro,<br>dimethylamino and<br>nitro substituents<br>on the molecular<br>structure and<br>photoinduced<br>behavior | Grgičević Ana, Fodor Lajos, Barić Danijela, Poje Margareta, Marinić Željko, Horváth Ottó, Škorić Irena                                                                                                  | 10.101<br>6/j.<br>jphotoc<br>hem.<br>2020.1<br>12690 | 1010-<br>6030 | 2020           | Journal of<br>photochemistry<br>and<br>photobiology.<br>A, Chemistry | 400  |    | 112690-<br>112690 |
| Učenje prijenosom<br>znanja iz<br>vremenskih serija -<br>u kojoj su mjeri<br>značajke<br>prenosive?                                                                                                                             | Otović Erik                                                                                                                                                                                             |                                                      |               | 2020           |                                                                      |      |    | -                 |

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| 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                                                                                                                                              | 10.1177/1094342020972772       |           | 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, Srečko Kirin                                                                                          | 10.1016/j.molstruc.2020.128834 | 0022-2860 | 2020 | Journal of molecular structure                                       | 1221 |    | -           |
| A Detailed Kinetic-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, Čurić 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 Jakobišić 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, Đurisić Aleksandra | 10.1039/d0tc01631d             | 2050-7526 | 2020 | Journal of Materials Chemistry C                                     | 8    |    | 11052-11060 |

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| Mono Phosphazeny Phosphines (R <sub>2</sub> N) <sub>3</sub> P=N-P(NR <sub>2</sub> ) <sub>2</sub> – 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, Jandel Vladimir, Mesarić Josip, Skala Karolj, Lipić Tomislav                                                                                                                                                         | 10.23919/mipro48935.2020.9245440 |           | 2020 | MIPRO 2020 43rd International Convention           |     |    | 395-401   |
| Phylogeography of <i>Campanula fenestrellata</i> 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 <i>Degenia velebitica</i> (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  | -         |
| <i>Salvia officinalis</i> 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 <i>Streptomyces</i> bacteria: Molecular dynamics and experimental study                                   | Maršavelski Aleksandra, Sabljic 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 <i>Danio rerio</i> 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               |     |    | -         |

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| 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 |    | - |

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| 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  | -           |
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| 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   |
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| 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       |
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| 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                                                                 | Varžić 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 |

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| 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 Iliana, Pejić Jelena, Kelterer Anne-Marie, Sabolović Jasmina | 10.1002/open.201900159              | 2191-1363 | 2019       | ChemistryOpen                                | 8   |    | 852-868     |
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| 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     |
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| Genetic diversity of the sweet chestnut ( <i>Castanea sativa</i> Mill.) in central Europe and the western part of the Balkan Peninsula, and evidence of marron genotype introgression into wild populations   | Poljak Igor, Idžojić Marilena, Šatović Zlatko, Ježić Marin, Čurković Perica Mirna, Simovski Bojan, Acevski Jane, Liber Zlatko                               | 10.1007/s11295-017-1107-2      | 1614-2942 | 2017 | Tree Genetics and Genomes               |      | 1  | 13-1      |
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