

## ISI Articles 2023

Year	Publication
2023	Avram Sorin, Liliana Halip, Ramona Curpan, and Tudor I Oprea. "Novel Drug Targets in 2022." NATURE REVIEWS DRUG DISCOVERY; (2023) 22;6;437-437, DOI10.1038/d41573-023-00068-y
2022	Avram, Sorin, and Cristian Neanu. "Large-scale comparison between the diffraction-component precision indexes favors Cruickshanks Rfree function." Journal of the Serbian Chemical Society 87.3 (2022): 321-330. Avram Sorin, Liliana Halip, Ramona Curpan, and Tudor I Oprea. "Novel Drug Targets in 2021." NATURE REVIEWS DRUG DISCOVERY; (2022), 21;5:328-328, DOI10.1038/d41573-022-00057-7
2021	Avram Sorin, Cristian G Bologa, Jayme Holmes, Giovanni Bocci, Thomas B Wilson, Dac-Trung Nguyen, Ramona Curpan, et al. "DrugCentral 2021 Supports Drug Discovery and Repositioning." NUCLEIC ACIDS RESEARCH 49, no. D1 (January 2021): D1160–69. <a href="https://doi.org/10.1093/nar/gkaa997">https://doi.org/10.1093/nar/gkaa997</a> . Halip Liliana, Sorin Avram, and Cristian Neanu. "The B-Factor Index for the Binding Site (BFIs) to Prioritize Crystal Protein Structures for Docking." STRUCTURAL CHEMISTRY 32, no. 4 (August 2021): 1693–99. <a href="https://doi.org/10.1007/s11224-021-01751-9">https://doi.org/10.1007/s11224-021-01751-9</a> . Borota Ana, Liliana Halip, Ramona Curpan, Alina Bora, Sorin Avram, Maria Mracec, and Mircea Mracec. "Structure- and Ligand- Based Studies to Gain Insight into the Pharmacological Implications of Histamine H-3 Receptor." STRUCTURAL CHEMISTRY 32, no. 3 (June 2021): 1141–49. <a href="https://doi.org/10.1007/s11224-020-01711-9">https://doi.org/10.1007/s11224-020-01711-9</a> . Pacureanu Liliana, Avram Sorin and Crisan Luminita, "Comprehensive investigation of selectivity landscape of glycogen synthase kinase-3 inhibitors", JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS 39, no 7 (Apr 2021):2318-2337. <a href="https://doi.org/10.1080/07391102.2020.1747544">https://doi.org/10.1080/07391102.2020.1747544</a> . Avram Sorin, Liliana Halip, Ramona Curpan, and Tudor I Oprea. "Novel Drug Targets in 2019." NATURE REVIEWS DRUG DISCOVERY; (2020) 20;5:333-333, DOI10.1038/d41573-021-00057-z
2020	Avram Sorin, Ramona Curpan, Liliana Halip, Alina Bora, and Tudor Oprea I. "Off-Patent Drug Repositioning." JOURNAL OF CHEMICAL INFORMATION AND MODELING 60, no. 12 (December 2020): 5746–53. <a href="https://doi.org/10.1021/acs.jcim.0c00826">https://doi.org/10.1021/acs.jcim.0c00826</a> . Crisan Luminita, Avram Sorin, Kurunczi Ludovic and Pacureanu, Liliana. "Partial Least Squares Discriminant Analysis and 3D Similarity Perspective Applied to Analyze Comprehensively the Selectivity of Glycogen Synthase Kinase 3 Inhibitors", MOLECULAR INFORMATICS 39, no 6 (January 2020): 1900142. <a href="https://doi.org/10.1002/minf.201900142">https://doi.org/10.1002/minf.201900142</a> Borota Ana, Sorin Avram, Ramona Curpan, Alina Bora, Daniela Varga, Liliana Halip, and Luminita Crisan. "In Silico Studies on Smoothed Human Receptor and Its Antagonists in Search of Anticancer Effects." JOURNAL OF THE SERBIAN CHEMICAL SOCIETY 85, no. 3 (2020): 335–46. <a href="https://doi.org/10.2298/JSC190403085B">https://doi.org/10.2298/JSC190403085B</a> . Avram Sorin, Liliana Halip, Ramona Curpan, and Tudor I Oprea. "Novel Drug Targets in 2019." NATURE REVIEWS DRUG DISCOVERY 20, no. 5 (May 2020): 333. <a href="https://doi.org/10.1038/d41573-021-00057-z">https://doi.org/10.1038/d41573-021-00057-z</a> .
2019	Pacureanu Liliana, Sorin Avram, Alina Bora, Ludovic Kurunczi, and Luminita Crisan. "Portraying the Selectivity of GSK-3 Inhibitors towards CDK-2 by 3D Similarity and Molecular Docking." STRUCTURAL CHEMISTRY 30, no. 3 (June 2019): 911–23. <a href="https://doi.org/10.1007/s11224-018-1224-z">https://doi.org/10.1007/s11224-018-1224-z</a> .
2018	Avram Sorin, Alina Bora, Liliana Halip, and Ramona Curpan. "Modeling Kinase Inhibition Using Highly Confident Data Sets." JOURNAL OF CHEMICAL INFORMATION AND MODELING 58, no. 5 (May 2018): 957–67. <a href="https://doi.org/10.1021/acs.jcim.7b00729">https://doi.org/10.1021/acs.jcim.7b00729</a> . Avram Sorin, Ramona Curpan, Alina Bora, Cristian Neanu, and Liliana Halip. "Enhancing Molecular Promiscuity Evaluation Through Assay Profiles." PHARMACEUTICAL RESEARCH 35, no. 11 (November 2018). <a href="https://doi.org/10.1007/s11095-018-2523-1">https://doi.org/10.1007/s11095-018-2523-1</a> . Mioc Marius, Sorin Avram, Vasile Bercean, Ludovic Kurunczi, Roxana M Ghiulai, Camelia Oprean, Dorina E Coricovac, et al. "Design, Synthesis and Biological Activity Evaluation of S-Substituted 1H-5-Mercapto-1,2,4-Triazole Derivatives as Antiproliferative Agents in Colorectal Cancer." FRONTIERS IN CHEMISTRY 6 (August 2018). <a href="https://doi.org/10.3389/fchem.2018.00373">https://doi.org/10.3389/fchem.2018.00373</a> .

- Bora Alina, Sorin Avram, Simona Funar-Timofei, and Liliana Halip. "COMPUTATIONAL ELECTRONIC PROFILE OF THE INSECTICIDE IMIDACLOPRID AND ANALOGUES." *REVUE ROUMAINE DE CHIMIE* 63, no. 9 (September 2018): 861+.
- Crisan Luminita, Daniela Varga, Sorin Avram, and Liliana Pacureanu. "APPLICATION OF 2D AND 3D SIMILARITY METHODS TO GSK-3 BENCHMARKING VALIDATION DATASET INCLUDING SELECTIVE AND NONSELECTIVE INHIBITORS." *REVUE ROUMAINE DE CHIMIE* 63, no. 11 (November 2018): 1083–91.
- Curpan Ramona, Sorin Avram, Alina Bora, Liliana Halip, and Cristian Bologa. "CHEMICAL REACTIVITY IN BIOLOGICAL PROMISCUOUS COMPOUNDS." *REVUE ROUMAINE DE CHIMIE* 63, no. 7–8 (2018): 749+.
- Bora Alina, Sorin Avram, Ana Borota, Ramona Curpan, and Liliana Halip. "THEORETICAL STUDY OF SOME 7,8-DYHYDROXYFLAVONE ANALOGUES AS TROPOMYOSIN-RELATED KINASE B AGONISTS." *REVUE ROUMAINE DE CHIMIE* 63, no. 5–6 (2018): 527–33.
- 2017 Mioc Marius, Codruta Soica, Vasile Bercean, Sorin Avram, Mihaela Balan-Porcarasu, Dorina Coricovac, Roxana Ghiulai, et al. "Design, Synthesis and Pharmaco-Toxicological Assessment of 5-Mercapto-1,2,4-Triazole Derivatives with Antibacterial and Antiproliferative Activity." *INTERNATIONAL JOURNAL OF ONCOLOGY* 50, no. 4 (April 2017): 1175–83. <https://doi.org/10.3892/ijo.2017.3912>.
- Crisan Luminita, Sorin Avram, and Liliana Pacureanu. "Pharmacophore-Based Screening and Drug Repurposing Exemplified on Glycogen Synthase Kinase-3 Inhibitors." *MOLECULAR DIVERSITY* 21, no. 2 (May 2017): 385–405. <https://doi.org/10.1007/s11030-016-9724-5>.
- Mioc Marius, Sorin Avram, Andrei Branco Tomescu, Daniela Veronica Chiriac, Alina Heghes, Mirela Voicu, Adrian Voicu, Cosmin Citu, and Ludovic Kurunczi. "Docking Study of 3-Mercapto-1,2,4-Triazole Derivatives as Inhibitors for VEGFR and EGFR." *REVISTA DE CHIMIE* 68, no. 3 (March 2017): 500–503.
- Mioc Marius, Sorin Avram, Vasile Bercean, Mihaela Balan Porcarasu, Codruta Soica, Razvan Susan, and Ludovic Kurunczi. "Synthesis, Characterization and Antiproliferative Activity Assessment of a Novel 1H-5-Mercapto-1,2,4 Triazole Derivative." *REVISTA DE CHIMIE* 68, no. 4 (April 2017): 745–47.
- 2016 Bora Alina, Sorin Avram, Ionel Ciucanu, Marius Raica, and Stefana Avram. "Predictive Models for Fast and Effective Profiling of Kinase Inhibitors." *JOURNAL OF CHEMICAL INFORMATION AND MODELING* 56, no. 5 (May 2016): 895–905. <https://doi.org/10.1021/acs.jcim.5b00646>.
- Avram Stefana, Corina Danciu, Ioana Zinuca Pavel, Raluca Amalia Ceausu, Sorin Avram, Cristina Dehelean, and Marius Raica. "Polyphenols, Antioxidant Activity and Anti-Angiogenic Potential of Red and White Grapes." *REVISTA DE CHIMIE* 67, no. 2 (February 2016): 382–85.
- Avram Sorin, Stefana Avram, and Cristina Dehelean. "Effective Predictor of Human Mast Cell Tryptase Inhibitors." *REVISTA DE CHIMIE* 67, no. 1 (January 2016): 119–22.
- 2015 Avram Sorin, Stefana Avram, Luminita Crisan, Liliana Pacureanu, Ludovic Kurunczi, and Alina Bora. "SELF-ORGANIZING MAP CLASSIFICATION MODEL FOR THE PREDICTION OF MEK1 INHIBITORS." *REVUE ROUMAINE DE CHIMIE* 60, no. 2–3 (2015): 167–73.
- Bora Alina, Sorin Avram, Luminita Crisan, Liliana Halip, Ramona Curpan, Liliana Pacureanu, and Ionel Ciucanu. "THEORETICAL INVESTIGATIONS OF QUERCETIN AND ITS ANALOGUES AS ANTICANCER AGENTS." *REVUE ROUMAINE DE CHIMIE* 60, no. 2–3 (2015): 175–81.
- Crisan Luminita, Sorin Avram, Alina Bora, Ludovic Kurunczi, and Liliana Pacureanu. "3D-QSAR STUDY OF MALEIMIDE ANALOGUES AS GLYCOGEN SYNTHASE KINASE-3 (GSK-3) INHIBITORS USING CoMSIA APPROACH." *REVUE ROUMAINE DE CHIMIE* 60, no. 2–3 (2015): 183–88.
- Curpan Ramona, Sorin Avram, Liliana Halip, and Cristian Bologa. "BIOLOGICAL PROMISCUITY OF HTS HITS EVALUATED VIA CHEMICAL REACTIVITY DESCRIPTORS." *REVUE ROUMAINE DE CHIMIE* 60, no. 2–3 (2015): 205–11.
- 2014 Avram Sorin, Simona Funar-Timofei, Ana Borota, Sridhar Rao Chennamaneni, Anil Kumar Manchala, and Sorel Muresan. "Quantitative Estimation of Pesticide-Likeness for Agrochemical Discovery." *JOURNAL OF CHEMINFORMATICS* 6 (September 2014). <https://doi.org/10.1186/s13321-014-0042-6>.
- Avram Sorin I, Liliana M Pacureanu, Alina Bora, Luminita Crisan, Stefana Avram, and Ludovic Kurunczi. "ColBioS-FlavRC: A Collection of Bioselective Flavonoids and Related Compounds Filtered from High-Throughput Screening Outcomes." *JOURNAL OF*

CHEMICAL INFORMATION AND MODELING 54, no. 8 (August 2014): 2360–70.  
<https://doi.org/10.1021/ci5002668>.

Curpan Ramona, Sorin Avram, Robert Vianello, and Cristian Bologna. "Exploring the Biological Promiscuity of High-Throughput Screening Hits through DFT Calculations." BIOORGANIC & MEDICINAL CHEMISTRY 22, no. 8 (April 2014): 2461–68.  
<https://doi.org/10.1016/j.bmc.2014.02.055>.

Crisan Luminita, Liliana Pacureanu, Sorin Avram, Alina Bora, Speranta Avram, and Ludovic Kurunczi. "PLS and Shape-Based Similarity Analysis of Maleimides - GSK-3 Inhibitors." JOURNAL OF ENZYME INHIBITION AND MEDICINAL CHEMISTRY 29, no. 4 (August 2014): 599–610. <https://doi.org/10.3109/14756366.2013.833196>.

2013

Goodarzi Mohammad, Alina Bora, Ana Borota, Simona Funar-Timofei, Sorin Avram, and Yvan Vander Heyden. "Modeling of 2-Pyridin-3-Yl-Benzo[*d*][1,3]Oxazin-4-One Derivatives by Several Conformational Searching Tools and Molecular Docking." CURRENT PHARMACEUTICAL DESIGN 19, no. 12 (April 2013): 2194–2203.  
<https://doi.org/10.2174/1381612811319120007>.

Avram Sorin I, Luminita Crisan, Alina Bora, Liliana M Pacureanu, Stefana Avram, and Ludovic Kurunczi. "Retrospective Group Fusion Similarity Search Based on EROCE Evaluation Metric." BIOORGANIC & MEDICINAL CHEMISTRY 21, no. 5 (March 2013): 1268–78. <https://doi.org/10.1016/j.bmc.2012.12.041>.

Crisan Luminita, Liliana Pacureanu, Alina Bora, Sorin Avram, Ludovic Kurunczi, and Zeno Simon. "QSAR Study and Molecular Docking on Indirubin Inhibitors of Glycogen Synthase Kinase-3." CENTRAL EUROPEAN JOURNAL OF CHEMISTRY 11, no. 1 (January 2013): 63–77. <https://doi.org/10.2478/s11532-012-0133-z>.

Crisan Luminita, Liliana Pacureanu, Sorin Avram, Alina Bora, and Ludovic Kurunczi. "Implementation of PLS Discriminant Analysis to Rank Indirubin Derivatives against Decoys." CENTRAL EUROPEAN JOURNAL OF CHEMISTRY 11, no. 10 (October 2013): 1644–56. <https://doi.org/10.2478/s11532-013-0300-x>.

Avram Sorin I, Luminita Crisan, Liliana M Pacureanu, Alina Bora, Edward Seclaman, Monica Balint, and Ludovic G Kurunczi. "Challenges in Docking 2'-Hydroxy and 2',4'-Dihydroxychalcones into the Binding Site of ALR2." MEDICINAL CHEMISTRY RESEARCH 22, no. 8 (August 2013): 3589–3605. <https://doi.org/10.1007/s00044-012-0367-5>.

2012

Pacureanu Liliana, Luminita Crisan, Alina Bora, Sorin Avram, and Ludovic Kurunczi. "In Silico Classification and Virtual Screening of Maleimide Derivatives Using Projection to Latent Structures Discriminant Analysis (PLS-DA) and Hybrid Docking." MONATSHFTE FUR CHEMIE 143, no. 11 (November 2012): 1559–73. <https://doi.org/10.1007/s00706-012-0816-3>.

Crisan Luminita, Alina Bora, Liliana Pacureanu, Sorin Avram, and Ludovic Kurunczi. "PLS (Partial Least Square) Study for GSK-3 (Glycogen Synthase Kinase-3) Inhibition by Indirubin Derivatives." REVISTA DE CHIMIE 63, no. 5 (May 2012): 481–88.

2011

Avram Sorin, Liliana M Pacureanu, Edward Seclaman, Alina Bora, and Ludovic Kurunczi. "PLS-DA - Docking Optimized Combined Energetic Terms (PLSDA-DOCET) Protocol: A Brief Evaluation." JOURNAL OF CHEMICAL INFORMATION AND MODELING 51, no. 12 (December 2011): 3169–79. <https://doi.org/10.1021/ci2002268>.

Seclaman Edward, Alina Bora, Sorin Avram, Zeno Simon, and Ludovic Kurunczi. "MTD-PLS and Docking Study for a Series of Substituted 2-Phenylindole Derivatives with Oestrogenic Activity." CHEMICAL PAPERS 65, no. 4 (August 2011): 566–76.  
<https://doi.org/10.2478/s11696-011-0040-3>.