

## Scientific Events

- **23<sup>rd</sup> European Symposium on Quantitative Structure-Activity Relationships & Molecular Modelling: EuroQSAR 2022**, 26-30 September, 2022, Heidelberg, Germany
- The 14<sup>th</sup> Edition of the ***New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection***, 20-21 October 2022, Timisoara, Romania
- **IDG Consortium Face-to-Face Meeting**, February 9-11, 2021, Online
- ***Finding Targets for Drug Discovery***, November 15th, 2019, Hinxton, Cambridge, United Kingdom
- New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection, 7-8 October 2021, Timisoara, Romania
- The 12<sup>th</sup> Edition of the ***Symposium New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection***, June 06-07, 2019
- **Summer School on Drug Design**, 15-20 September, 2019, Vienna, Austria
- The 11<sup>th</sup> Edition of the Symposium ***New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection***, June 28-29, 2018
- **11<sup>th</sup> European Conference on Theoretical and Computational Chemistry**, (11 EUCO-TCC), 04-07 September, 2017, Barcelona, Spain
- The 10<sup>th</sup> Edition of ***New Trends and Strategies in the Chemistry of Advanced Materials with Relevance in Biological systems, Technique and Environmental Protection***, 8-9 June 2017, Timisoara, Romania
- **21st EuroQSAR - 21st European Symposium on Quantitative Structure-Activity Relationship - Where Molecular Simulations Meet Drug Discovery** 4-8 September 2016, Verona, Italy

## **Abstracts in the Volumes of Scientific Events**

### **2022**

1. Halip L, **Avram S**, Curpăn R, Bora A, Borota A, Oprea TI, Drug event fingerprints – DEFPs. Book of Abstracts of the 23<sup>rd</sup> European Symposium on Quantitative Structure-Activity Relationships & Molecular Modelling: EuroQSAR 2022, p. 211
2. **Avram S**, Wilson T, Curpăn R, Halip L, Borota A, Bora A, Oprea TI, Veterinary drug extension for DrugCentral database. 23<sup>rd</sup> European Symposium on Quantitative Structure-Activity Relationships & Molecular Modelling: EuroQSAR 2022, p. 214
3. Curpăn R, **Avram S**, Halip L, Borota A, Bora A, Oprea TI, DrugCentral: an open-access drug resource. Book of Abstracts of 23<sup>rd</sup> European Symposium on Quantitative Structure-Activity Relationships & Molecular Modelling: EuroQSAR 2022, p. 216
4. Juncu A, Bora A, Borota A, **Avram S**, Crisan L, Vlaicu O, Sulea S, Petrescu S, Oțelea D, Spiridon L, Pacureanu L, Popescu CI, A New High Throughput Assay For Cis Proteolytic Activity Identifies New Chemical Scaffolds With Inhibitory Activity Against Hepatitis C Virus NS2 Cysteine Protease, Book of Abstracts of *New Trends And Strategies In The Chemistry Of Advanced Materials With Relevance In Biological Systems, Technique And Environmental Protection*, 14th Edition, October 20-21, 2022, Timisoara, ROMANIA, p19.
5. Toma C, **Avram S**, Prioritization Of Kinase Crystal Structures For Docking, Using B-Factor Index For The Binding Site, Book of Abstracts of *New Trends And Strategies In The Chemistry Of Advanced Materials With Relevance In Biological Systems, Technique And Environmental Protection*, 14th Edition, October 20-21, 2022, Timisoara, ROMANIA, p 48
6. Halip L, Curpăn R, Borota A, Bora A, **Avram S**, Drug Repositioning Opportunities In Post-Marketing Adverse Events Data. Book of Abstracts of *New Trends And Strategies In The Chemistry Of Advanced Materials With Relevance In Biological Systems, Technique And Environmental Protection*, 14th Edition, October 20-21, 2022, Timisoara, ROMANIA, p 77
7. Neanu C, Toma C, **Avram S**, New Online Tool For Kinase Crystal Structures Prioritization In Docking Analysis. Book of Abstracts of *New Trends And Strategies In The Chemistry Of Advanced Materials With Relevance In Biological Systems, Technique And Environmental Protection*, 14th Edition, October 20-21, 2022, Timisoara, ROMANIA, p 91

### **2021**

8. Neanu C, **Avram S**, A Web Tool To Compute The Diffraction Precision Index Of Protein Structures. Book of Abstracts of *New Trends And Strategies In The Chemistry Of Advanced Materials With Relevance In Biological Systems, Technique And Environmental Protection*, 13th Edition, October 07-08, 2021, online, Timisoara, ROMANIA, p44
9. Halip L, Curpăn R, Borota A, Bora A, **Avram S**, Fingerprinting G-Protein Coupled Receptors Superfamily. Book of Abstracts of *New Trends And Strategies In The Chemistry Of Advanced Materials With Relevance In Biological Systems, Technique And Environmental Protection*, 13th Edition, October 07-08, 2021, online, Timisoara, ROMANIA, p67
10. Bora A, Halip L, **Avram S**, Crisan L, Manuka Honey And Its Flavonoid Components – An Affordable Therapeutic Option To Fight Sars-Cov-2 Infections: In Silico Evaluation. Book of Abstracts of *New Trends And Strategies In The Chemistry Of Advanced Materials With Relevance In Biological Systems, Technique And Environmental Protection*, 13th Edition, October 07-08, 2021, online, Timisoara, ROMANIA, p68.
11. **Avram S**, Curpăn R, Halip L, Bora A, A New Landscape For Drug Repurposing. Book of Abstracts of *New Trends And Strategies In The Chemistry Of Advanced Materials With Relevance In Biological*

*Systems, Technique And Environmental Protection*, 13th Edition, October 07-08, 2021, online, Timisoara, ROMANIA, p71

- 12. Avram S**, Bologa CG, Holmes J, Bocci G, Wilson TW, Nguyen DT, Curpăn R, Halip L, Bora A, Yang JJ, Knockel J, Sirimulla S, Ursu O, Oprea TI, Drug Central Demo - from KMC-UNM. *IDG Consortium Face-to-Face Meeting*, February 9-11, 2021, Online

## 2019

- 13.** Halip L, Curpăn R, Borota A, Bora A, **Avram S**. Insights Of GPCRs Binding Site. *The 12th Edition Of The Symposium New Trends And Strategies In The Chemistry Of Advanced Materials With Relevance In Biological Systems, Technique And Environmental Protection*, June 06-07, **2019**, Book Of Abstracts, ISSN: 2065-0760, Pag. 63, P51
- 14.** **Avram S**, Halip S, Curpăn R, Bora A. Fingerprinting The Biological Space Of Kinase Inhibitors. For Drug Discovery *The 12th Edition Of The Symposium New Trends And Strategies In The Chemistry Of Advanced Materials With Relevance In Biological Systems, Technique And Environmental Protection*, June 06-07, **2019**, Book Of Abstracts, ISSN: 2065-0760 Pag. 70, P82
- 15.** Bora A, **Avram S**, Crisan L, Borota A, Halip L, Pacureanu L. Structural, Electronic Properties And Pharmacological Profile Evaluations Of Some Natural Flavonoids. *The 12th Edition Of The Symposium New Trends And Strategies In The Chemistry Of Advanced Materials With Relevance In Biological Systems, Technique And Environmental Protection*, June 06-07, **2019**, Book Of Abstracts, ISSN: 2065-0760, Pag. 85, P97.

## 2018

- 16.** Halip L, Curpăn R, Borota A, Bora A, **Avram S**. GPCRs classification through self-organizing map models. *The 11th Edition of the Symposium New Trends and Strategies in the Chemistry of Advanced Materials with Relevance in Biological Systems, Technique and Environmental Protection*, 08-09 June, **2018**, Timișoara, Romania, Book of abstracts, ISSN: 2065-0760, P11.
- 17.** **Avram S**, Bora A, Curpăn R, Neanu C, Halip L. Defining assay profiles to analyze molecular selectivity. *The 12th Edition Of The Symposium New Trends And Strategies In The Chemistry Of Advanced Materials With Relevance In Biological Systems, Technique And Environmental Protection*, June 06-07, **2019**, Book Of Abstracts, ISSN: 2065-0760, P12.
- 18.** Bora A, **Avram S**, Halip L, Pacureanu L, Curpăn R. Prediction of luciferase inhibitors: a case study. *The 12th Edition Of The Symposium New Trends And Strategies In The Chemistry Of Advanced Materials With Relevance In Biological Systems, Technique And Environmental Protection*, June 06-07, **2019**, Book Of Abstracts, ISSN: 2065-0760P43.

## 2017

- 19.** Curpăn R, **Avram S**, Bora A, Halip L. Minimizing false-positive rates in high-throughput screening: predictors for fluorescent compounds. *11<sup>th</sup> European Conference on Theoretical and Computational Chemistry, EUCCO-TCC*, 4-7 September **2017**, Barcelona, Spain, Book of abstracts, pag. 114, P20.
- 20.** Halip L, **Avram S**, Bora A, Curpăn R. Mapping the chemical space of kinase inhibitors. *11<sup>th</sup> European Conference on Theoretical and Computational Chemistry, EUCCO-TCC*, 4-7 September **2017**, Barcelona, Spain, Book of abstracts, p. 125, P31.
- 21.** Bora A, Halip L, Curpăn R, **Avram S**. Description of PubChemkinina: a comprehensive dataset of kinase inactive compounds *11<sup>th</sup> European Conference on Theoretical and Computational Chemistry, EUCCO-TCC*, 4-7 September **2017**, Barcelona, Spain, Book of abstracts, pag.71, P77.
- 22.** **Avram S**, Bora A, Curpăn R, Halip L, *The 10th Edition of the Symposium New Trends and Strategies in the Chemistry of Advanced Materials with Relevance in Biological Systems, Technique and Environmental Protection*, 08-09 June, **2017**, Timișoara, Romania, Book of abstracts, ISSN: 2065-0760, pag. 95, P44.
- 23.** Bora A, Halip L, Curpăn R, **Avram S**. A survey of electronic properties influence on biological activity of flavonoids. *The 10th Edition of the Symposium New Trends and Strategies in the Chemistry of*

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- 24.** Halip L, **Avram S**, Bora A, Curpăn R. A Novel Tool for The Chemical Space Mapping of Biological Active Compounds. *The 10th Edition of the Symposium New Trends and Strategies in the Chemistry of Advanced Materials with Relevance in Biological Systems, Technique and Environmental Protection*, 08-09 June, **2017**, Timisoara, Romania, Book of abstracts, ISSN 2065-0760, p. 56, P23, poster.

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- 26.** **Avram S**, Bora A, Halip L, Curpăn R. Measuring the prediction errors for kinase inhibitor models. *21st EuroQSAR - 21st European Symposium on Quantitative Structure-Activity Relationship - Where Molecular Simulations Meet Drug Discovery 4-8 September*, **2016**, Verona, Italia, Book of abstracts, pag.96, P015.
- 27.** Curpăn R, **Avram S**, Halip L, Bora A, Ursu O, Bologa C, Oprea TI. Chemical reactivity in biological promiscuous compounds. *21st EuroQSAR - 21st European Symposium on Quantitative Structure-Activity Relationship - Where Molecular Simulations Meet Drug Discovery 4-8 September*, **2016**, Verona, Italy, Book of Abstracts, p.134, P053.
- 28.** Halip L, **Avram S**, Bora A, Curpăn R, Ursu O, Bologa C, Oprea TI. Virtual biological fingerprints for mining kinase inhibitors. *21st EuroQSAR - 21st European Symposium on Quantitative Structure-Activity Relationship - Where Molecular Simulations Meet Drug Discovery 4-8 September*, **2016**, Verona, Italy, Book of Abstracts, p. 190, P109.
- 29.** Mioc M, Bora A, Curpăn R, Halip L, **Avram S**, Kurunczi L. Modeling the kinase bioactivity space. *The 9th Edition of the Symposium New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection*, 09-10 June, **2016**, Timișoara, Romania, Book of abstracts, ISSN: 2065-0760, pag.96, P47.
- 30.** Dragoș B, Bora A, Curpăn R, Halip L, **Avram S**, Kurunczi L. A kinome-based evaluation of bio-selective flavonoids. *The 9th Edition of the Symposium New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection*, 09-10 June, **2016**, Timișoara, Romania, Book of abstracts, ISSN: 2065-0760, pag.87, P43.
- 31.** **Avram S**, Bora A, Curpăn R, Halip L, Dragos B, Mioc M, Kurunczi L. Versatile biological fingerprints for mining large chemical libraries. *The 9th Edition of the Symposium New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection*, 09-10 June, **2016**, Timișoara, Romania, Book of abstracts, ISSN: 2065-0760, pag. 80, P38.
- 32.** Bora A, Halip L, Curpăn R, Crisan L, Pacureanu L, Kurunczi L, **Avram S**. Electronic feature analysis of some 7,8-dyhydroxyflavone analogues with antidepressant effects. *The 9th Edition of the Symposium New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection*, 09-10 June, **2016**, Timișoara, Romania, Book of abstracts, ISSN: 2065-0760, pag. 78, P35.
- 33.** Bora A, Halip L, Borota A, Curpăn R, **Avram S**. Comprehensive characterization of flavonoids electronic properties using quantum chemical calculations. *The 9th Edition of the Symposium New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection*, 09-10 June, **2016**, Timișoara, Romania, Book of abstracts, ISSN: 2065-0760, pag. 86, P41.
- 34.** Neanu C, Bora A, Halip L, **Avram S**, Curpăn R. The development of a web-based application used to explore and analyze chemical libraries. *The 9th Edition of the Symposium New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique and environmental protection*, 09-10 June, **2016**, Timisoara, Romania, Book of abstracts, ISSN 2065-0760, pag. 73, P57.
- 35.** Curpăn R, Neanu C, **Avram S**, Bora A, Halip L, Kurunczi L, Bologa C. Semiempiric quantum-chemical methods used in the prediction of biological promiscuity. *The 9th Edition of the Symposium New trends and strategies in the chemistry of advanced materials with relevance in biological systems, technique*

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- 37.** **Avram S**, Avram Ş, Bora A, Halip L, Curpăn R. Structure-based virtual screening of novel MEK1 Inhibitors. *The 8<sup>th</sup> Edition of New Trends and Strategies in the Chemistry of Advanced Materials with Relevance in Biological systems, Technique and Environmental Protection*, 4-5 June, **2015**, Timisoara, Book of abstracts, ISSN 2065-0760, p.114, poster49