Curriculum Vitae

Professor Speranta Avram
Graduated in Biochemistry and Psychology
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Summary**:** Experience in bioinformatics and computational chemistry, with emphasis on development rational drug design of: small molecules (antiviral inhibitors, anesthetics, ion channels blockers, neuroleptics, antidepressants, antibiotics, antimicrobial peptides antidiabetics), molecular dynamic, quantitative structure-activity relationships (QSAR) focused on 3D-QSAR-CoMFA/CoMSIA/ALMOND on small molecules, peptides and proteins, computational mutagenesis applied in mental disorders and molecular docking. Six years of experiences in psychotherapy and clinical psychology with emphasis on biofeedback and cognitive-behavior therapy.

I have experience in teaching of bioinformatics, biophysics information, molecular modeling, neurochemistry psychopharmacology, physiology and neurofeedback to graduate students. Excellent interpersonal skills.

Education:

March 2013 Habilitation in Biology
February, 2002. Dr. in Biology
2008-2010 M.S. in in Behavioral and Cognitive Psychotherapy
2005-2008 "Titu Maiorescu", University, Faculty of Psychology, B.Sc. Psychology
1997-2001 University of Bucharest, Faculty of Biology, Ph.D. Student
1996-1997 University of Bucharest, Faculty of Biology, M.S. in Neurobiology
1992-1996 University of Bucharest, Faculty of Chemistry, B.Sc in Biochemistry

Professional Positions: 2015-present: Professor in the Anatomy, Animal Physiology and Biophysics Department, Faculty of Biology, University of Bucharest (FB-UB); 2013-2015: Assistant professor at FB-UB; 1997-2013: Lecturer at FB-UB; 1997-2002: PhD in Biology, FB-UB

Doctoral and Postdoctoral fellow: 2011-2013 postdoctoral fellow in Bucharest, Romania, Management of advanced research and forensic psychiatric expertise; 2006 -FEBS fellow at University of Vienna, Theoretical Chemistry Institute, Austria, head of Department Prof. Peter Wolschann; 2003- NATO fellow at the ICS-UNIDO (International Center for Science and High Technology and United Nations Industrial Development Organization), Trieste, Italy; 1997, 1998- TEMPUS fellow at the Computational Chemistry Department, University of Darmstadt, Germany within a Program1997.

Professional skills; Molecular Modeling: Molecular Graphics, Molecular Mechanics, Semiempirical and Ab initio Quantum Mechanics, and Molecular Dynamic. Familiar with software running under UNIX (SYBYL, MOE, Molcad, Insight, Volsurf, Pentacle) and under Windows (HyperChem with ChemPlus and HyperNMR, ChemOffice). Operating systems: MS-DOS; WINDOWS, NT, IRIX 5.2 and 6.2 on SGI Workstations.

PUBLICATIONS LIST-selection

1. Uță G, D Manolescu, S **Avram** - Therapeutic Properties of Several Chemical Compounds from Salvia officinalis L. in Alzheimer's Disease Mini Reviews in Medicinal, Volume 21, Number 12, 2021, pp. 1421-1430(10).
2. **Avram S**, Mernea M, Limban C, Borcan F, Chifiriuc C, Potential Therapeutic Approaches to Alzheimer's Disease by bioinformatics, cheminformatics and predicted ADME-Tox tools. Current Neuropharmacology. 2020, Volume 18, Number 8, pp. 696-719(24)
3. Limban, C, Diţu, L M, Măruţescu L, Missir A V, Chifiriuc M C, Căproiu M T, Morusciag L, Chiriţă C, Udrea A-M, Nuță D C, **Avram S**, Design, Synthesis and Biopharmacological Profile Evaluation of New 2-((4-Chlorophenoxy)Methyl)-N-(Arylcarbamothioyl)Benzamides with Broad Spectrum Antifungal Activity, Current Organic Chemistry, Volume 23, Number 12, 2019, pp. 1365-1377(13).
4. **Avram S,** Milac A, Borcan L-C, Mihailescu D, Borcan F and Castanho M, 2018, Designing of Artificial Peptides for an Improved Antiviral Activity, Current Proteomics, Vol 4, 258-266.
5. **Avram, S**, Mernea M, Bagci, E, Hritcu, L, Borcan L-Cr, Mihailescu Dan F ., 2017, Advanced Structure-activity Relationships Applied to Mentha spicata L. Subsp. spicata Essential Oil Compounds as AChE and NMDA Ligands, in Comparison with Donepezil, Galantamine and Memantine – New Approach in Brain Disorders Pharmacology, CNS & Neurological Disorders - Drug Targets (Formerly Current Drug Targets - CNS & Neurological Disorders), Volume 16, Number 7, pp. 800-811(12)
6. **Avram S**, Alexandrescu I, Puia A, Udrea A M., Mernea M, Mihailescu D F, Borcan L-C, 2017, Aneuploidy-Inducing Mutations in Mitotic Checkpoint Protein hMad1-Carboxi Terminal Domain Analyzed by SAR and Computational Mutagenesis, Current Proteomics, Volume 14, Number 4, , pp. 254-260(7).

7. Buiu C., Putz M.V., **Avram S,** 2016, Learning the relationship between the primary structure of HIV envelope glycoproteins and neutralization activity of particular antibodies by using artificial neural networks, Int J Mol Sci., in press.
8. Putz MV, Duda-Seiman C, Duda-Seiman D, Putz AM, Alexandrescu I, Mernea M, **Avram S.,**2016, Chemical Structure-Biological Activity Models for Pharmacophores' 3D-Interactions, Int J Mol Sci. Jul 8;17(7). pii: E1087. doi: 10.3390/ijms17071087.
9. Mernea M, Borcan L.C., Borcan F and **Avram S**, 2016, Antipsychotics as Psychosis Drugs and Neuroprotective Promoters Evaluated by Chemical QSAR - in silico and in vivo Studies, *Letter in Drug Design and Discovery* 13(4): 269 – 275.
10. **Avram S**, Mernea M, Borcan F, Mihailescu D. 2016, Evaluation of the Therapeutic Properties of Mastoparan- and Sifuvirtide- Derivative Antimicrobial Peptides Using Chemical Structure-Function Relationship - in vivo and in silico Approaches. *Curr Drug Deliv*. 13(2):202-210.
11. O. Grigore, O. Calborean, G. Cojocaru R. Ungureanu M. Mernea M.P. Dinca**, Avram S.** D.F. Mihailescu T. Dascalu, High-intensity THz pulses application to protein conformational changes, Romanian Reports in Physics, Vol. 67, No. 4, P. 1251–1260, 2015**.**
12. **Avram S**, Borcan F, Borcan LC, Milac AL, Mihailescu D. 2015, QSAR Approaches Applied to Antidepressants Induced Neurogenesis - in vivo and in silico Applications. *Mini Rev Med Chem*. 2016;16(3):230-40.
13. **Avram S**., Mernea M., Mihailescu D., Duda Seiman C., Duda Seiman D., Putz M. 2014, Mitotic checkpoint proteins Mad1 and Mad2 – Structural and functional relationship with implication in genetic diseases. *Current Computer Aided Drug Design*, 10(2), 168-181.
14. **Avram S.**, Shaposhnikov S., Buiu C., Mernea M. 2014, Chondroitin Sulfate Proteoglycans: Structure-Function Relationship with Implication in Neural Development and Brain Disorders,

BioMed Research International, Article ID 642798, 1-11, http://dx.doi.org/10.1155/2014/642798.. Epub 2014 May 14.

15. **Avram S.,** Milac A., Mernea M., Mihailescu D., Putz M.V., Buiu C. 2014, Structure-biological function relationship extended to mitotic arrest-deficient 2-like protein mad2 native and mutants-new opportunity for genetic disorder control. *Int. J. Mol. Sci***.** 15(11), 21381-21400.
16. **Avram S.,** Buiu C., Milac A., Duda Seiman D., Duda Seiman C., Pacureanu L., Borcan F. 2014, More Effective DPP4 Inhibitors as Antidiabetics Based on Sitagliptin Applied QSAR and Clinical Methods, *Current Computer Aided Drug Design*, 10(3), ISSN 1875-6697 .
17. Crisan L. E., Pacureanu L., Avram S. I., Bora A. M., **Avram S**., Kurunczi L. 2014, PLS and shape-based similarity analysis of maleimides - GSK-3 inhibitors. *Journal Of Enzyme Inhibition And Medicinal Chemistry*, 29(4), 599-610.
18. **Avram S.,** Milac A., Carta F., Supuran C. T. 2013. More effective dithiocarbamates derivatives inhibiting carbonic anhydrases, generated by QSAR and computational design. *Journal Of Enzyme Inhibition And Medicinal Chemistry*, 28(2), 350-359.
19. **Avram S.,** Mernea M., Mihailescu D., Duda Seiman D., Duda Seiman C. 2013. Advanced QSAR methods evaluated polycyclic aromatic compounds duality as drugs and inductors in psychiatric disorders. *Current Organic Chemistry*, 17(23), 2880-2890.
20. Calborean O., Mernea M., **Avram S.,** Mihailescu D. F., 2013. Pharmacological descriptors related to the binding of gp120 to CD4 corresponding to 60 representative HIV-1 Strains. *Journal Of Enzyme Inhibition And Medicinal Chemistry*, 28(5), 1015-1025.
21. **Avram S.,** Mihailescu D., Milac A.L., 2012. 3D-QSAR study indicates an enhancing effect of membrane ions on psychiatric drugs targeting serotonin receptor 5-HT1A. *Molecular Biosystems*, 8 (5), 1418 – 1425.
22. **Avram S.,** Mihailescu D., Borcan F., Milac A.L. 2012. Prediction of improved antimicrobial mastoparan derivatives by 3D-QSARCoMSIA/CoMFA and computational mutagenesis. *Monthly Chemistry*, 143 (4), 535-543.
23. **Avram S.,** Buiu C., Borcan F., Milac A., 2012. More effective antimicrobial mastoparan derivatives, generated by 3D-QSAR-Almond and computational mutagenesis. *Molecular Biosystems*, , 8 (2), 587–594.
24. **Avram S.,** Buiu C., Duda-Seiman D., Borcan F., Duda-Seiman C., Mihailescu D. 2012. Evaluation of the pharmacological descriptors related to the induction of antidepressant activity and its prediction by QSAR/QRAR methods. *Mini Reviews in Medicinal Chemistry***,** 12(6), 467-476.
25. Petrescu L. , Cinteza O., Voiculescu A.-M., Rosu T. Enculescu I., Matei E., Georgescu S., Birjega R., **Avram S.,** Mihailescu D. 2012. Interaction of $NaYF_4$:Er:Yb nanoparticles with phospholipid monolayers as models of biological membranes. *Rev. Chim. (Bucharest),* , 63 (9), 956-961.
26. **Avram S.,** Duda-Seiman D., Borcan F., Radu B., Duda-Seiman C., Mihailescu D. 2011. Evaluation of antimicrobial activity of new mastoparan derivatives using QSAR and computational mutagenesis, *International Journal of Peptide Research and Therapeutics*, 17(1), 7-17.
27. Lazlo T., **Avram S.,** Mihailescu D., 2011. QSAR study on biochemical activity of some escitalopram derivatives with possible antidepressant activity. *Rev. Chim. (Bucharest),* 62 (4), 371-375.
28. **Avram S.,** Duda-Seiman D., Borcan F., Wolschann P. 2011. QSAR-CoMSIA applied to antipsychotic drugs with their dopamine D2 and serotonine 5HT2A membrane receptors. *Journal of the Serbian Chemical Society*, 76 (2), 263-281.
29. Duda-Seiman D, **Avram S.,** Mancaş S., Careja V., Duda-Seiman C., Putz M. V., Ciubotariu D. 2011. MTD-CoMSIA Modelling of HMG-CoA Reductase Inhibitors. *Journal of the Serbian Chemical Society*, 76 (1), 85-99.

30. **Avram S.,** Duda-Seiman D., Duda-Seiman C., Borcan F., Mihailescu D., 2010. Predicted binding rate of new cephalosporin antibiotics by 3D-QSAR- method – new approach. *Monthly Chemistry*, 141(5), 589-597.
31. **Avram S**., Buiu C., Duda-Seiman D., Duda-Seiman C., Mihailescu D. 2010. Design of new escitalopram derivatives for the treatment of major depressive disorder by 3D-QSAR. *Sci Pharm.*, 78(2), 233–248.
32. **Avram S.,** Duda-Seiman D., Svab I., Mancas S., Duda-Seiman C., Mihailescu D. 2009. Aspirin and Other Non-Steroidal Anti-Inflammatory Drugs as Cyclooxygenase Inhibitors: State of the Art, Barriers and Perspectives, *Current Computer-Aided Drug Design*, 5(1), 1-12.
33. **Avram S.**, Berner H., Milac A.L., Wolschann P. 2008. Quantitative structure – activity relationship studies on membrane receptors inhibition by antipsychotic drugs. Application to schizophrenia treatment. *Monthly Chemistry*, 139 (4), 407-426.
34. Milac A.L., **Avram S.**, Petrescu A.J. 2006, Evaluation of a neural networks QSAR method based on ligand representation using substituent descriptors. Application to HIV-1 protease inhibitors, *Journal of Molecular Graphics and Modelling*, , 25(1), 37-45.
35. **Avram S.**, Bologa C., Flonta M.L. 2005, Quantitative structure-activity relationship by CoMFA for cyclic urea and nonpeptidecyclic cyanoguanidine derivatives on the wild type and mutants HIV-1 protease. *J .Mol .Modeling*, 11(2), 105-115.
36. **Avram S.**, Milac A.L., Flonta M.L. 2005, Computer-aided drug design for typical and atypical antipsychotic drugs. A review of application of QSAR and combinatorial chemistry methods-tools for new antipsychotics design. *Current Computer-Aided Drug Design*,1(4), 347-364.
37. **Avram S.**, Svab I., Bologa C., Flonta M.L., 2003, Correlation between the predicted and the observed biological activity of the symmetric and nonsymmetric cyclic urea derivatives used as HIV-1 protease inhibitors by 3D-QSAR-CoMFA method – a tool for new antiviral drugs design, *Journal of Cellular and Molecular Medicine*, 7(3), 287-296.
38. **Avram S.**, Movileanu L., Mihailescu D., Flonta M.L., 2002, Comparative study of some energetic and steric parameters of the wild type and mutants HIV-1 protease: a way to explain the viral resistance, *Journal of Cellular and Molecular Medicine*, 6 (2), 251-260.

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1. Duda-Seiman, Daniel; Duda-Seiman, Corina; Borcan, Florin; Borcan, Livia-Cristina; Mancas, Silvia; **Avram S**, 2015, Calcium Channel Blockers–Benefits Upon Vascular Biology in Hypertensive Patients, Cardiovascular & Hematological Agents in Medicinal Chemistry (Formerly Current Medicinal Chemistry - Cardiovascular & Hematological Agents), Volume 13, Number 1, April 2015, pp. 54-62(9).

2. **Avram S**., Duda-Seiman D., Duda-Seiman C., Borcan F., Pacureanu L., 2014, Evaluation of calcium channel blocker activity of new dihydropyridine derivatives using 2D-QSAR and three-dimensional similarity. *International Journal of Pharmacy and Therapeutics***,** 5(1), 56-68.

3. Duda-Seiman C., Isvoran A., Grigorie C., Duda-Seiman D., **Avram S.**, Puscas C., Bolcu C., Mancas S., Cinca R., Ciubotaru D. 2012, QSAR study (quantitative relations-structure-biological activity) within calcium channel blockers, dihydropyridines type, *Medicine in evolution*, 2(3), 274-281.

4. **Avram S**., Dimitriu O. 2012, Multiple family group therapy – behavioral cognitive aproach for the depressive pathology. *Rev. Psih*.,58(2), 133–140.

5. Nastase S., Avram S., Mihailescu A,.2012, A non-invasive treatment of depression in young adults – neurofeedback, *Romanian Journal of Psychiatry,* 14, (3), 103-106.

6. **Avram S**., Milac A.L., Dabu A., Flonta M. L. 2006, *Computer-aided drug design applied to beta and gamma secretase inhibitors – perspectives for new Alzheimer disease therapy-review*, *Current Enzyme Inhibition*, 2 (4), 311-328.

7. Milac A, **Avram S,** Petrescu A, *Bioinformatic tools in biochemistry. (i) a new neural network method for predicting biological activity of chemical compounds*, *Rom. J. Biochem.*, 2003, 40, 1-2: 35-45.
8. Amuzescu B., Ion S., Popescu D., L. Movileanu, **Avram S.,** Macri B, Flonta M.L. 2002, Thermal group motion creates stochastic pores in plane phosphatidylcholine bilayers, *Romanian. J. Biophys.*,12(1–2), 37–52.
9. **Avram S.,** Bologa C, Banda M, Flonta M.L., 2001, A quantitative structure-activity relationship study used to predict the biological activity of the HIV-1 protease cyclic urea inhibitors, *Romanian. J. Biophys.*, 11:1-2, 11–24.
10. Popescu D., Movileanu L., Pluteanu F., **Avram S.,** Marinescu D., Flonta M.-L., 2001, The elastic waves induce the appearance of pores in a lipid bilayer membrane (II), *Romanian J. Biophys*. 11(3-4), 163-17.