

Scientific production (Jan. 2010)

• **Articles:**

1. Horvath, D., Silaghi-Dumitrescu, I., An Interactive Chemical Formula Interpreter, *Studia Univ. Babes-Bolyai; Chemia*, 13, **25** (1989)
2. Horvath, D., Silaghi-Dumitrescu, I., Molecular Mechanics Software for PDP-compatible Microcomputers, *Rev. Rom. Chim.* (1990)
3. Diudea, M.V., Horvath, D., Kacso I.E., Minailiuc O.M., Parv, B., Molecular Topology. 8. Centricities In Molecular Graphs - The Molcen Algorithm, *Journal Of Mathematical Chemistry* 11, **259-270** (1992)
4. Horvath, D., Silaghi-Dumitrescu, I. An Improved First-Order Optimization Method Taking Account of the Molecular Topology, *Studia Univ. Babes-Bolyai; Chemia*, 39, **15-27** (1994)
5. Diudea, M.V. Horvath, D., Bonchev, M., MOLORD Algorithm and Real Number Subgraph Invariants, *Croat. Chem. Acta*, 68, **131** (1995)
6. Diudea, M.V. Horvath, D., Graovac, A. 3D Distance Matrices and Related Topological Indices, *J. Chem. Inf. Comp. Sci.*, 35, **129** (1995)
7. Bourel, L. Willard, X., Pop, I., Baudelle, R., Horvath, D., Deprez, B., Melnyk, P., Tartar, A. Synthèse Combinatoire, *Actualité Chimique* 33 (Dec. 1995)
8. Melnyk, P., Bourel, L., Willard, X., Pop, I., Horvath, D., Deprez, B., Tartar, A. Combinatorial Chemistry: A rational access to molecular diversity, *Act. Chim. Ther.*, 22, **51** (1996)
9. Willard, X., Pop, I., Horvath, D., Baudelle, R., Melnyk,, P., Deprez, B., Tartar, A. Combinatorial Chemistry: A rational approach to chemical diversity, *Eur. J. Med. Chem.*, 31, **87** (1996)
10. Horvath, D., van Belle, D., Lippens, G., Wodak, S.J., Development and Parametrization of Continuum Solvent Models. I. Models based on the Boundary Element Method, *J. Chem. Phys* 104, **6679-6695** (1996)

11. Horvath, D., van Belle, D., Lippens, G., Development and Parametrization of Continuum Solvent Models. II. An Unified Approach to the Solvation Problem, *J. Chem. Phys* 105, **4197** (1996)
12. Baillet, S., Buisine, E., Horvath, D. Maes, L., Bonnet, B., Sergheraert, C. 2-Aminodiphenylsulphides as Inhibitors of Trypanothione Reductase: Modification of the Side Chain, *Biooorg. Med. Chem.*, 6, **891-899** (1996)
13. Horvath, D., A Virtual Screening Approach Applied to the Search of Trypanothione Reductase Inhibitors, *J. Med. Chem.*, 15, **2412-2423** (1997)
14. Horvath, D., Deprez, B., Tartar, A. High Throughput Molecular Modeling Using Fast 3D Descriptors, *Act. Chim. Ther.* 23, **55-67** (1997)
15. Bonnet, B., Soullez, D., Davioud-Charvet, E., Landry, V., Horvath, D., Sergheraert, C., New Spermine and Spermidine Derivatives as Potent Inhibitors of Trypanosoma Cruzi Trypanothione Reductase, *Bioorg. Med. Chem.* 7, **1249-1256** (1997)
16. Girault, S., Baillet, S., Horvath, D., Lucas, V., Davioud-Charvet, E., Tartar, A., Sergheraert, C. New Potent Inhibitors of Trypanothione Reductase from Trypanosoma Cruzi in the 2-Aminodiphenylsulfide Series, *Eur. J. Med. Chem.*, 32, **39-52** (1997)
17. Lippens, G., Wieruszkeski, J.-M., Horvath, D. Talaga, P., Bohin, J.P. Slow Dynamics of the Cyclic Osmoregulated Periplasmic Glucan of *Ralstonia solanacearum* as Revealed by Heteronuclear Relaxation Studies, *J. Am. Chem. Soc.*, 120, **170-177** (1997)
18. Braban, M.; Pop, I.; Willard, X; Horvath, D., Reactivity Prediction Models Applied to the Selection of Novel Candidate Building Blocks for High Throughput Organic Synthesis of Combinatorial Libraries, *J. Chem. Inf. Comp. Sci.*, 39, **1119-1127** (1999)
19. Horvath, D., Jeandenans, C., Molecular similarity and virtual screening. In silico methods to retrieve active analogs in the context of discovering therapeutic compounds, *Actualité Chimique* 9, **64-67** (2000)

20. Horvath, D., Recursive Partitioning Analysis of μ -Opiate Receptor High Throughput Screening Results, *SAR and QSAR in Environmental Research*, **12**, **181-212**, (2001)
21. Poulain, R.; Horvath, D.; Bonnet, B.; Eckoff, C.; Chapelain, B.; Bodinier, M-C.; Deprez, B. From Hit to Lead. Combining Two Complementary Methods for Focused Library Design Application to μ Opiate Ligands; *J. Med. Chem.*, **44**, **3378-3390**, (2001)
22. Poulain, R.; Horvath, D.; Bonnet, B.; Eckoff, C.; Chapelain, B.; Bodinier, M-C.; Deprez, B. From Hit to Lead. Analyzing Structure-Profile Relationships; *J. Med. Chem.*, **44**, **3391-3401**, (2001).
23. Hamdane, M., Smet, C., Sambo, A.V., Leroy, A., Wieruszeski, J.M., Delobel, P., Maurage, C.A., Ghestem, A., Wintjens, R., Begard, S., Sergeant, N., Delacourte, A., Horvath, D., Landrieu, I., Lippens, G., Buee, L., Pin1: A Therapeutic Target in Alzheimer Neurodegeneration, *J. Mol. Neurosci.*, **19**, **275-288**, (2002).
24. Horvath, D.; Jeandenans, C.; Neighborhood Behavior of In Silico Structural Spaces with respect to In Vitro Activity Spaces – A Novel Understanding of the Molecular Similarity Principle in the Context of Multiple Receptor Binding Profiles., *J. Chem. Inf. Comp. Sci.*, **43**, **680-690**, (2003)
25. Horvath, D.; Jeandenans, C.; Neighborhood Behavior of In Silico Structural Spaces with respect to In Vitro Activity Spaces – A Benchmark for Neighborhood Behavior Assessment of Different In Silico Similarity Metrics., *J. Chem. Inf. Comp. Sci.*, **43**, **691-698**, (2003)
26. Horvath, D., Mao, B. Neighborhood Behavior – Fuzzy Molecular Descriptors and their Influence on the Relationship between Structural Similarity and Property Similarity, *QSAR & Comb. Sci.*, **22**, **498-509**, (2003)
27. Krejsa, CM, Horvath D, Rogalski SL, Penzotti JE, Mao B, Barbosa F, Migeon JC, Predicting ADME properties and side effects: the BioPrint approach, *Curr Opin Drug Discov Devel.* **6**, **470-80**, (2003)
28. Horvath, D.; Barbosa, F., Neighborhood Behavior – the Relation Between

Chemical Similarity and Property Similarity, *Curr. Trends Med. Chem.*, 4, **589-600**, (2004)

29. Gozalbes, R., Rolland C., Nicolaï, E., Paugam M.-F., Coussy L., Horvath D., Barbosa F., Mao B., Revah F., Froloff, N. QSAR strategy and experimental validation for the development of a GPCR focused library, *QSAR & Comb. Sci*, 24, **508-16** (2005)

30. Rolland, C., Gozalbes, R., Nicolai, E., Paugam, M.F., Coussy, L., Barbosa, F., Horvath, D., Revah, F., G-protein-coupled receptor affinity prediction based on the use of a profiling dataset: QSAR design, synthesis, and experimental validation. *J. Med. Chem.*, 48, **6563-74** (2005)

31. Parent, B., Kökösy, A., Horvath, D., Optimized Evolutionary Strategies in Conformational Sampling. *Soft Computing*, 11, **63-79** (2007)

32. Tantar, A.-A., Melab, N., Talbi E.-G., Parent, B., Horvath, D., A parallel hybrid genetic algorithm for protein structure prediction on the computational grid, *Future Generation Computer Systems*, 23, **398-409** (2007)

33. Bonachéra, F., Parent, B., Barbosa, F., Froloff, N., Horvath, D., Fuzzy Tricentric Pharmacophore Fingerprints. 1 - Topological Fuzzy Pharmacophore Triplets and adapted Molecular Similarity Scoring Schemes, *J. Chem. Inf. Mod.*, 46, **2457-2477** (2006)

34. Horvath, D., Bonachera, F., Solov'ev, V., Gaudin, C, Varnek, A., Stochastic versus Stepwise Strategies for Quantitative Structure-Activity Relationship Generation-How Much Effort May the Mining for Successful QSAR Models Take?, *J. Chem. Inf. Mod.*, 47, **927-939** (2007)

35. Hanouille, X., Melchior, A., Sibille, N., Parent, B., Denys, A., Wieruszeski, J.-M., Horvath, D., Allain, F., Lippens, G., Landrieu, I., Structural and Functional Characterization of the Interaction between Cyclophilin B and a Heparin-derived Oligosaccharide, *J. Biol. Chem.*, 282, **34148-34158** (2007)

36. Bonachera, F.; Horvath, D., Fuzzy Tricentric Pharmacophore Fingerprints. 2. Application of Topological Fuzzy Pharmacophore Triplets in Quantitative Structure-

Activity Relationships. *J. Chem. Inf. Model.*, 48, **409-425** (2008)

37. Varnek, A.; Fourches, D.; Horvath, D.; Klimchuk, O.; Gaudin, C.; Vayer, P.; Solov'ev, V.; Hoonakker, F.; Tetko, I. V.; Marcou, G., ISIDA - Platform for virtual screening based on fragment and pharmacophoric descriptors. *Current Computer-Aided Drug Design*, 4 (3), **191-198** (2008)

38. Parent, B.; Tantar, A.; Melab, N.; Talbi, E. G.; Horvath, D., GRID-BASED CONFORMATIONAL SAMPLING. *Stud. Univ. Babes-Bolyai Chem.*, 53 (2), 43-48 (2008)

39. Tantar, A.-A., Conilleau, S., Parent, B., Melab, N., Brillet, L., Roy, S., Talbi, E.-G., Horvath, D., Docking and Biomolecular Simulations on Computer Grids: Status and Trends. *Current Computer-Aided Drug Design*, 4 (3), **235-249** (2008)

40. Gozalbes, R. F. B., Nicolaï, E., Horvath, D., Froloff, N. Development and Validation of a Pharmacophore-Based QSAR Model for the Prediction of CNS Activity. *ChemMedChem*, 4 (2), **204-209** (2009).

41. Horvath, D.; Marcou, G.; Varnek, A., Predicting the Predictability: A Unified Approach to the Applicability Domain Problem of QSAR Models. *Journal of Chemical Information and Modeling*, 49 (7), 1762-1776 (2009).

42. Horvath, D., THE PHARMACOPHORE APPROACH IN CHEMOINFORMATICS. *Rev. Roum. Chim.*, 54 (6), 441-453 (2009)

• **Published Conference Proceedings:**

43. Migeon, J. C.; Rogalski, S. L.; Krejsa, C. M.; Horvath, D.; Mao, B.; Barbosa, F.; Merrick, S. E.; Mersberg, M.; Lakehal, F., Using large in vitro ADME data sets to predict in vivo properties. In *Drug Metab. Rev.*, Marcel Dekker Inc: Providence, Rhode Island, 2003; Vol. 3, p 168

44. Parent, B., Tantar, A., Melab, N., Talbi, E.-G., Horvath, D. In *Grid-based Evolutionary Strategies Applied to the Conformational Sampling Problem.*, IEEE Congress on Evolutionary Computation, CEC 2007, Singapore, Singapore, 2007; pp 291-296

45. Horvath, D.; Brillet, L.; Roy, S.; Conilleau, S.; Tantar, A.-A.; Boisson, J.-C.; Melab, N.; Talbi, E.-G., Local vs. global search strategies in evolutionary GRID-based conformational sampling & docking. In *IEEE Congress on Evolutionary Computation CEC 09*, IEEE: Trondheim, Norway, 2009; pp 247-254.

• **Books & Book Chapters:**

46. Horvath, D. Silaghi-Dumitrescu, I. 'Mecanica Moleculara', *Ed. Univ. Cluj-Napoca, Romania* (1996).

47. Horvath, D. ComPharm: Automated Comparative Analysis of Pharmacophoric Patterns and Derived QSAR Approaches, Novel Tools in High Throughput Drug Discovery. A Proof of Concept Study Applied to Farnesyl Protein Transferase Inhibitor Design, pp. **395-439**; in 'QSPR / QSAR Studies by Molecular Descriptors', Diudea, M., Editor, Nova Science Publishers, Inc., New York (2001)

48. Horvath, D., High Throughput Conformational Sampling & Fuzzy Similarity Metrics: A Novel Approach to Similarity Searching and Focused Combinatorial Library Design and its Role in the Drug Discovery Laboratory, pp **429-472**, in 'Combinatorial Library Design and Evaluation: Principles, Software Tools and Applications', Ghose, A. & Viswanadhan, V. Eds., Marcel Dekker, Inc., New York (2001)

49. Horvath, D. , Mao, B., Gozalbes, R., Barbosa, F., Rogalski, S., Strenght and Limitations of Pharmacophore-Based Virtual Screening, in 'Cheminformatics in Drug Discovery'. Oprea, T.I. Ed., WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim (2004)

50. Gozalbes, R., Barbosa, F., Froloff, N., Horvath, D., The BioPrint Approach for the Evaluation of ADME-T Properties: Application to the Prediction of Cytochrome P450 2D6 Inhibition., in 'Pharmacokinetic Profiling in Drug Research: Biological, Physicochemical, and Computational Strategies', Testa, B., Krämer, S.D., Wunderli-Allenspach, H., Folkers, G. Eds., , VHCA, Zrich, WILEY-VCH, Weinheim, pp. **395-415** (2006)

51. Horvath, D., L'annotation et la classification de l'espace chimique pour la chemogénomique, in 'CHEMOGÉNOMIQUE : Des petites molécules pour explorer

le vivant.' Edited by E. Marchal, S. Roy and L. Lafanechère. Grenoble Sciences (2007)

52. Horvath, D., Topological Pharmacophores. In *Chemoinformatics Approaches to Virtual Screening*, Varnek, A.; Tropsha, A., Eds. RCS Publishing: Cambridge, UK, pp 44-72 (2008)

• **International Conference Participations**

53. *ECCC1- Computational Chemistry*, Nancy(France), May 1994 (**poster**)

54. *Workshop on Protein-Ligand Interactions*, Heidelberg (BRD), Avril 1995 (**oral presentation**)

55. *BSP Trypanosomiasis and Leishmaniasis Seminar*, Glasgow (UK), 3-6 Sept. 1995 (**poster**).

56. *Rhône-Poulenc-Rorer Combinatorial Chemistry Round Table*, Vineuil Saint Firmin (France), Juin 1996, (**oral presentation**)

57. *Gordon Research Conference on Magnetic Resonance in Biology and Medicine*, Ventura, California (USA), Jan./Feb. 1997 (**poster**)

58. *Keystone Symposia on Molecular & Cellular Biology - Frontiers of NMR in Molecular Biology*, Taos, New Mexico (USA), Feb. 1996 (**poster**)

59. *Second European Workshop on Drug Design*, Certosa di Pontignano/Siena, Italy, Mai 1998 (**poster**); *Third European Workshop on Drug Design*, Certosa di Pontignano/Siena, Italy, Juin 2001 (**poster**);

60. *Gordon Research Conference on Computational Chemistry*: New Hampton, New Hampshire (USA), Jul. 1996 (**poster**); Tilton School, New Hampshire (USA), Jul. 1998 (**poster**), Queen's College, Oxford (UK), Jul. 2000 (**oral presentation+poster**), Les Diablerets (CH) Oct. 2006, (**poster**)

61. *MSI Combinatorial Chemistry Consortium Meetings*, Del Mar, CA , February 1997; La Jolla, CA, February 1998, Palm Springs, CA, February 1999, Ermenonville, France, September 1999 (**oral presentations**).

62. **Conférencier invité** aux séminaires MSI à Rome & Paris, 17/18 Juin 1999. **Co-organisateur du Cerius2 User Group Meeting**, Rueil-Malmaison, Mai 2001

63. *Euroforum "Chimie Combinatoire – Quelle stratégie adopter pour la recherche de nouveaux produits? "*, Paris, Feb. 2001 (**invited lecturer**).
64. *Drug Discovery Technology Europe*, Stuttgart, Apr. 2001 (**invited lecturer**)
65. *SBS (Society for Biomolecular Screening) Meeting*, Den Haag, Sept. 2002 (**invited lecturer**)
66. *EuroQSAR 2002*, Bournemouth, UK (**poster**) , *EuroQSAR 2004*, Istanbul, TR (**oral presentation**), *EuroQSAR 2008* Uppsala, Sweden (**poster**)
67. *CMPTI 2005*, Shanghai, China (**oral presentation**)
68. *European Workshop on Chemoinformatics*, Obernai, Alsace, Mai 2006 (**oral presentation, posters**)
69. *ChemAxon User Group Meeting*, Budapest, June 2006 & June 2007 (**oral presentations, member of organizing committee**)
70. *Topomol 2006*, Cluj (Romania), Sept. 2006 (**oral presentation**)
71. *MolMod 2007*, Arcalia (Romaina) July 2007 (**oral presentation**)
72. IEEE Congress on Evolutionary Computation, Singapore, Sept. 2007 and Trondheim, Norway 2009 (**oral presentations**)
73. Conference on Metaheuristics *META 08*, Hammamet, Tunisia, 2008 (**oral presentation**)
74. German Conference on Chemoinformatics, 3rd edition Nov. 2007 (**poster**) and 5th edition Nov. 2009 (**oral presentation**)

- **Patents:**

75. Horvath, D., Method of Virtual Retrieval of Analogs of Lead Compounds by Constituting Potential Libraries. **Patent# 97402620.5-2201**, European Patent Office (Feb. 1999).
76. Horvath, D. Method of predicting biological activity profiles based on the neighborhood behavior of *in silico* similarity metrics calibrated with respect to activity spaces. **Patent# 01402656.1-2212**, European Patent Office (Dec. 2001)

- **Participation in collaborative research projects:**

- Projet International de Collaboration Scientifique (PICS) France-Japon (Univ. Tsukuba) – Roumanie (Univ. Cluj) – Molecular Overlay Algorithms (2004-2006)
- ACCAMBA Data Mining Project 'Analyse de Chimiothèques et Construction Automatique de Modèles de Bio-Activité' (2003-2007, ACI IMPBIO <http://accamba.imag.fr/>)
- ANR [Docking@Grid](#) (ongoing since 2006): in partnership with the 'Laboratoire d'Informatique Fondamentale de Lille' (Prof. Talbi, coordinator) and CEA Grenoble (Sylvaine Roy)
- Groupe de Service 'Chimiothèque Nationale' (<http://chimiotheque-nationale.enscm.fr/>)
- ANR BACTARGET (started 2009) in partnership with CBPS – UMR 5263 Montpellier
- Several ongoing collaborations with pharmaceutical industry

UMinho contributed 9% to the Portuguese scientific production in Scopus and 8% in ISI WoS, registering a growth average of around 15%, above the national average of 11%. A growing percentage of scientific production can be found in the RepositoriUM, most of it available in open access. RepositoriUM. Reports.Â Scientific Production of the University of Minho indexed in Web of Science and Scopus 2010-2014 (available in April 2016). ĩ»¿ UMinho.