

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, *Bioorg. 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)
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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**), *EurQSAR 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