# D Horvath

## List of Publications by Year in descending order



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|---|---|---|---|
| 103 papers | 3,291 citations | 147566 31 h-index | 168136 53 g-index |
| 106 all docs | 106 docs citations | 106 times ranked | 2899 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | SynthI: A New Open-Source Tool for Synthon-Based Library Design. Journal of Chemical Information and Modeling, 2022, 62, 2151-2163. | 2.5 | 18 |
| 2 | HIV-1 drug resistance profiling using amino acid sequence space cartography. Bioinformatics, 2022, 38, 2307-2314. | 1.8 | 5 |
| 3 | A Close-up Look at the Chemical Space of Commercially Available Building Blocks for Medicinal Chemistry. Journal of Chemical Information and Modeling, 2022, 62, 2171-2185. | 2.5 | 32 |
| 4 | Chemography: Searching for Hidden Treasures. Journal of Chemical Information and Modeling, 2021, 61, 179-188. | 2.5 | 14 |
| 5 | Discovery of novel chemical reactions by deep generative recurrent neural network. Scientific Reports, 2021, 11, 3178. | 1.6 | 40 |
| 6 | NP Navigator: A New Look at the Natural Product Chemical Space. Molecular Informatics, 2021, 40, e2100068. | 1.4 | 16 |
| 7 | Computer-Aided Design of New Physical Solvents for Hydrogen Sulfide Absorption. Industrial & Engineering Chemistry Research, 2021, 60, 8588-8596. | 1.8 | 9 |
| 8 | Chemoinformatics-Driven Design of New Physical Solvents for Selective CO<sub>2</sub> Absorption. Environmental Science & Technology, 2021, 55, 15542-15553. | 4.6 | 16 |
| 9 | NP Navigator: A New Online Tool for the Exploration of the Natural Products Chemical Space. Medical Sciences Forum, 2021, 7, . | 0.5 | 0 |
| 10 | Diversifying chemical libraries with generative topographic mapping. Journal of Computer-Aided Molecular Design, 2020, 34, 805-815. | 1.3 | 7 |
| 11 | Trustworthiness, the Key to Grid-Based Map-Driven Predictive Model Enhancement and Applicability Domain Control. Journal of Chemical Information and Modeling, 2020, 60, 6020-6032. | 2.5 | 1 |
| 12 | Autoignition temperature: comprehensive data analysis and predictive models. SAR and QSAR in Environmental Research, 2020, 31, 597-613. | 1.0 | 4 |
| 13 | A Chemographic Audit of antiâ€Coronavirus Structureâ€activity Information from Public Databases (ChEMBL). Molecular Informatics, 2020, 39, e2000080. | 1.4 | 16 |
| 14 | â€œBig Dataâ€•Fast Chemoinformatics Model to Predict Generalized Born Radius and Solvent Accessibility as a Function of Geometry. Journal of Chemical Information and Modeling, 2020, 60, 2951-2965. | 2.5 | 1 |
| 15 | Application of the mol2vec Technology to Largeâ€size Data Visualization and Analysis. Molecular Informatics, 2020, 39, e1900170. | 1.4 | 8 |
| 16 | Modelling of ready biodegradability based on combined public and industrial data sources. SAR and QSAR in Environmental Research, 2020, 31, 171-186. | 1.0 | 14 |
| 17 | Parallel Generative Topographic Mapping: An Efficient Approach for Big Data Handling. Molecular Informatics, 2020, 39, 2000009. | 1.4 | 6 |
| 18 | Predictive Models for Kinetic Parameters of Cycloaddition Reactions. Molecular Informatics, 2019, 38, e1800077. | 1.4 | 25 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Consensus models to predict oral rat acute toxicity and validation on a dataset coming from the industrial context. SAR and QSAR in Environmental Research, 2019, 30, 879-897. | 1.0 | 22 |
| 20 | Generative Topographic Mapping of the Docking Conformational Space. Molecules, 2019, 24, 2269. | 1.7 | 4 |
| 21 | QSPR models for bioconcentration factor (BCF): are they able to predict data of industrial interest?. SAR and QSAR in Environmental Research, 2019, 30, 507-524. | 1.0 | 18 |
| 22 | In silico Design, Virtual Screening and Synthesis of Novel Electrolytic Solvents. Molecular Informatics, 2019, 38, 1900014. | 1.4 | 5 |
| 23 | Crystal structure of a xylulose 5-phosphate phosphoketolase. Insights into the substrate specificity for xylulose 5-phosphate. Journal of Structural Biology, 2019, 207, 85-102. | 1.3 | 8 |
| 24 | Prediction of the Glass-Transition Temperatures of Linear Homo/Heteropolymers and Cross-Linked Epoxy Resins. ACS Applied Polymer Materials, 2019, 1, 1430-1442. | 2.0 | 25 |
| 25 | CovaDOTS: In Silico Chemistry-Driven Tool to Design Covalent Inhibitors Using a Linking Strategy. Journal of Chemical Information and Modeling, 2019, 59, 1472-1485. | 2.5 | 13 |
| 26 | Getting to Know the Neighbours with GTM: The Case of Antiviral Compounds. Molecular Informatics, 2019, 38, 1800166. | 1.4 | 7 |
| 27 | Multi-task generative topographic mapping in virtual screening. Journal of Computer-Aided Molecular Design, 2019, 33, 331-343. | 1.3 | 17 |
| 28 | De Novo Molecular Design by Combining Deep Autoencoder Recurrent Neural Networks with Generative Topographic Mapping. Journal of Chemical Information and Modeling, 2019, 59, 1182-1196. | 2.5 | 93 |
| 29 | Generative topographic mapping in drug design. Drug Discovery Today: Technologies, 2019, 32-33, 99-107. | 4.0 | 19 |
| 30 | Virtual Screening with Generative Topographic Maps: How Many Maps Are Required?. Journal of Chemical Information and Modeling, 2019, 59, 564-572. | 2.5 | 20 |
| 31 | Pros and cons of virtual screening based on public â€œBig Dataâ€: In silico mining for new bromodomain inhibitors. European Journal of Medicinal Chemistry, 2019, 165, 258-272. | 2.6 | 12 |
| 32 | Evolution of commercially available compounds for HTS. Drug Discovery Today, 2019, 24, 390-402. | 3.2 | 53 |
| 33 | Monitoring of the Conformational Space of Dipeptides by Generative Topographic Mapping. Molecular Informatics, 2018, 37, 1700115. | 1.4 | 3 |
| 34 | Transductive Ridge Regression in Structureâ€“activity Modeling. Molecular Informatics, 2018, 37, 1700112. | 1.4 | 3 |
| 35 | Mapping of the Available Chemical Space versus the Chemical Universe of Leadâ€Like Compounds. ChemMedChem, 2018, 13, 540-554. | 1.6 | 33 |
| 36 | Specific Targeting of Plant and Apicomplexa Parasite Tubulin through Differential Screening Using In Silico and Assay-Based Approaches. International Journal of Molecular Sciences, 2018, 19, 3085. | 1.8 | 10 |

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| 37 | Rescoring of docking poses under Occamâ€™s Razor: are there simpler solutions?. Journal of Computer-Aided Molecular Design, 2018, 32, 877-888. | 1.3 | 15 |
| 38 | Visualization and Analysis of Complex Reaction Data: The Case of Tautomeric Equilibria. Molecular Informatics, 2018, 37, e1800056. | 1.4 | 7 |
| 39 | Integrated Strategy for Lead Optimization Based on Fragment Growing: The Diversity-Oriented-Target-Focused-Synthesis Approach. Journal of Medicinal Chemistry, 2018, 61, 5719-5732. | 2.9 | 51 |
| 40 | Generative Topographic Mapping of Conformational Space. Molecular Informatics, 2017, 36, 1700036. | 1.4 | 10 |
| 41 | Privileged Structural Motif Detection and Analysis Using Generative Topographic Maps. Journal of Chemical Information and Modeling, 2017, 57, 1218-1232. | 2.5 | 9 |
| 42 | Virtual screening, synthesis and biological evaluation of DNA intercalating antiviral agents. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 3915-3919. | 1.0 | 15 |
| 43 | QSAR modeling and chemical space analysis of antimalarial compounds. Journal of Computer-Aided Molecular Design, 2017, 31, 441-451. | 1.3 | 13 |
| 44 | From birdâ€™s eye views to molecular communities: two-layered visualization of structureâ€“activity relationships in large compound data sets. Journal of Computer-Aided Molecular Design, 2017, 31, 961-977. | 1.3 | 5 |
| 45 | Neighboring Structure Visualization on a Gridâ€based Layout. Molecular Informatics, 2017, 36, 1700047. | 1.4 | 0 |
| 46 | Generative Topographic Mapping Approach to Chemical Space Analysis. Challenges and Advances in Computational Chemistry and Physics, 2017, , 167-199. | 0.6 | 4 |
| 47 | CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033. | 2.8 | 264 |
| 48 | In Silico Mining for Antimalarial Structure-Activity Knowledge and Discovery of Novel Antimalarial Curcuminoids. Molecules, 2016, 21, 853. | 1.7 | 16 |
| 49 | Prediction of Activity Cliffs Using Condensed Graphs of Reaction Representations, Descriptor Recombination, Support Vector Machine Classification, and Support Vector Regression. Journal of Chemical Information and Modeling, 2016, 56, 1631-1640. | 2.5 | 28 |
| 50 | Predictive Models for the Free Energy of Hydrogen Bonded Complexes with Single and Cooperative Hydrogen Bonds. Molecular Informatics, 2016, 35, 629-638. | 1.4 | 9 |
| 51 | Chemical Space Mapping and Structureâ€“Activity Analysis of the ChEMBL Antiviral Compound Set. Journal of Chemical Information and Modeling, 2016, 56, 1438-1454. | 2.5 | 31 |
| 52 | Redox Polypharmacology as an Emerging Strategy to Combat Malarial Parasites. ChemMedChem, 2016, 11, 1339-1351. | 1.6 | 28 |
| 53 | Predictive Models for Halogenâ€bond Basicity of Binding Sites of Polyfunctional Molecules. Molecular Informatics, 2016, 35, 70-80. | 1.4 | 12 |
| 54 | Kernel Target Alignment Parameter: A New Modelability Measure for Regression Tasks. Journal of Chemical Information and Modeling, 2016, 56, 6-11. | 2.5 | 14 |

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|---|---|---|---|
| 55 | S4MPLEâ€"Sampler for Multiple Protein-Ligand Entities: Methodology and Rigid-Site Docking Benchmarking. Molecules, 2015, 20, 8997-9028. | 1.7 | 25 |
| 56 | Mappability of drug-like space: towards a polypharmacologically competent map of drug-relevant compounds. Journal of Computer-Aided Molecular Design, 2015, 29, 1087-1108. | 1.3 | 52 |
| 57 | Electrochemical Properties of Substituted 2â€Methylâ€1,4â€Naphthoquinones: Redox Behavior Predictions. Chemistry - A European Journal, 2015, 21, 3415-3424. | 1.7 | 35 |
| 58 | Expert System for Predicting Reaction Conditions: The Michael Reaction Case. Journal of Chemical Information and Modeling, 2015, 55, 239-250. | 2.5 | 65 |
| 59 | GTMâ€Based QSAR Models and Their Applicability Domains. Molecular Informatics, 2015, 34, 348-356. | 1.4 | 52 |
| 60 | Stargate GTM: Bridging Descriptor and Activity Spaces. Journal of Chemical Information and Modeling, 2015, 55, 2403-2410. | 2.5 | 28 |
| 61 | Chemical Data Visualization and Analysis with Incremental Generative Topographic Mapping: Big Data Challenge. Journal of Chemical Information and Modeling, 2015, 55, 84-94. | 2.5 | 67 |
| 62 | Prediction of Drug Induced Liver Injury Using Molecular and Biological Descriptors. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 315-322. | 0.6 | 23 |
| 63 | An Evolutionary Optimizer of libsvm Models. Challenges, 2014, 5, 450-472. | 0.9 | 52 |
| 64 | Computational chemogenomics: Is it more than inductive transfer?. Journal of Computer-Aided Molecular Design, 2014, 28, 597-618. | 1.3 | 26 |
| 65 | Individual Hydrogenâ€Bond Strength QSPR Modelling with ISIDA Local Descriptors: a Step Towards Polyfunctional Molecules. Molecular Informatics, 2014, 33, 477-487. | 1.4 | 19 |
| 66 | Design of a Generalâ€Purpose European Compound Screening Library for EUâ€OPENSCREEN. ChemMedChem, 2014, 9, 2309-2326. | 1.6 | 29 |
| 67 | Quantitative Structureâ€"Property Relationship Modeling: A Valuable Support in High-Throughput Screening Quality Control. Analytical Chemistry, 2014, 86, 2510-2520. | 3.2 | 18 |
| 68 | Generative Topographic Mapping-Based Classification Models and Their Applicability Domain: Application to the Biopharmaceutics Drug Disposition Classification System (BDDCS). Journal of Chemical Information and Modeling, 2013, 53, 3318-3325. | 2.5 | 55 |
| 69 | S4MPLE â€" Sampler For Multiple Proteinâ€"Ligand Entities: Simultaneous Docking of Several Entities. Journal of Chemical Information and Modeling, 2013, 53, 88-102. | 2.5 | 26 |
| 70 | Publicly available models to predict normal boiling point of organic compounds. Thermochimica Acta, 2013, 553, 60-67. | 1.2 | 7 |
| 71 | In Silico Fragment-Based Drug Discovery: Setup and Validation of a Fragment-to-Lead Computational Protocol Using S4MPLE. Journal of Chemical Information and Modeling, 2013, 53, 836-851. | 2.5 | 33 |
| 72 | Do Not Hesitate to Use Tverskyâ€"and Other Hints for Successful Active Analogue Searches with Feature Count Descriptors. Journal of Chemical Information and Modeling, 2013, 53, 1543-1562. | 2.5 | 19 |

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| 73 | Models for Identification of Erroneous Atom-to-Atom Mapping of Reactions Performed by Automated Algorithms. Journal of Chemical Information and Modeling, 2012, 52, 3116-3122. | 2.5 | 20 |
| 74 | Mining Chemical Reactions Using Neighborhood Behavior and Condensed Graphs of Reactions Approaches. Journal of Chemical Information and Modeling, 2012, 52, 2325-2338. | 2.5 | 24 |
| 75 | Interpretability of SAR/QSAR Models of any Complexity by Atomic Contributions. Molecular Informatics, 2012, 31, 639-642. | 1.4 | 32 |
| 76 | Generative Topographic Mapping (GTM): Universal Tool for Data Visualization, Structureâ€Activity Modeling and Dataset Comparison. Molecular Informatics, 2012, 31, 301-312. | 1.4 | 107 |
| 77 | Fragment-Based Drug Design: Computational and Experimental State of the Art. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 500-520. | 0.6 | 37 |
| 78 | Pharmacophore-Based Virtual Screening. Methods in Molecular Biology, 2010, 672, 261-298. | 0.4 | 60 |
| 79 | Applicability Domains for Classification Problems: Benchmarking of Distance to Models for Ames Mutagenicity Set. Journal of Chemical Information and Modeling, 2010, 50, 2094-2111. | 2.5 | 202 |
| 80 | ISIDA Propertyâ€Labelled Fragment Descriptors. Molecular Informatics, 2010, 29, 855-868. | 1.4 | 111 |
| 81 | Simplified chain folding models as metaheuristic benchmark for tuning real protein folding algorithms?. , 2010, , . | | 1 |
| 82 | Predicting the Predictability: A Unified Approach to the Applicability Domain Problem of QSAR Models. Journal of Chemical Information and Modeling, 2009, 49, 1762-1776. | 2.5 | 145 |
| 83 | Parallel multi-objective algorithms for the molecular docking problem. , 2008, , . | | 13 |
| 84 | ISIDA - Platform for Virtual Screening Based on Fragment and Pharmacophoric Descriptors. Current Computer-Aided Drug Design, 2008, 4, 191-198. | 0.8 | 173 |
| 85 | Grid-based evolutionary strategies applied to the conformational sampling problem. , 2007, , . | | 3 |
| 86 | Stochastic versus Stepwise Strategies for Quantitative Structureâ^'Activity Relationship GenerationHow Much Effort May the Mining for Successful QSAR Models Take?. Journal of Chemical Information and Modeling, 2007, 47, 927-939. | 2.5 | 32 |
| 87 | A parallel hybrid genetic algorithm for protein structure prediction on the computational grid. Future Generation Computer Systems, 2007, 23, 398-409. | 4.9 | 39 |
| 88 | Optimized Evolutionary Strategies in Conformational Sampling. Soft Computing, 2007, 11, 63-79. | 2.1 | 10 |
| 89 | Molecular Similarity and Property Similarity. Current Topics in Medicinal Chemistry, 2004, 4, 589-600. | 1.0 | 42 |
| 90 | Neighborhood Behavior. Fuzzy Molecular Descriptors and their Influence on the Relationship between Structural Similarity and Property Similarity. QSAR and Combinatorial Science, 2003, 22, 498-509. | 1.5 | 33 |

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| 91 | From Hit to Lead. Analyzing Structureâ^'Profile Relationships. Journal of Medicinal Chemistry, 2001, 44, 3391-3401. | 2.9 | 32 |
| 92 | From Hit to Lead. Combining Two Complementary Methods for Focused Library Design. Application to Î¼ Opiate Ligands. Journal of Medicinal Chemistry, 2001, 44, 3378-3390. | 2.9 | 39 |
| 93 | Recursive Partitioning Analysis of Î¼-Opiate Receptor High Throughput Screening Results. SAR and QSAR in Environmental Research, 2001, 12, 181-212. | 1.0 | 6 |
| 94 | Reactivity Prediction Models Applied to the Selection of Novel Candidate Building Blocks for High-Throughput Organic Synthesis of Combinatorial Libraries. Journal of Chemical Information and Computer Sciences, 1999, 39, 1119-1127. | 2.8 | 9 |
| 95 | Slow Dynamics of the Cyclic Osmoregulated Periplasmic Glucan ofRalstonia solanacearumAs Revealed by Heteronuclear Relaxation Studies. Journal of the American Chemical Society, 1998, 120, 170-177. | 6.6 | 21 |
| 96 | A Virtual Screening Approach Applied to the Search for Trypanothione Reductase Inhibitors. Journal of Medicinal Chemistry, 1997, 40, 2412-2423. | 2.9 | 138 |
| 97 | New spermine and spermidine derivatives as potent inhibitors of Trypanosoma cruzi Trypanothione Reductase. Bioorganic and Medicinal Chemistry, 1997, 5, 1249-1256. | 1.4 | 50 |
| 98 | New potent inhibitors of trypanothione reductase from Trypanosoma cruzi in the 2-aminodiphenylsulfide series. European Journal of Medicinal Chemistry, 1997, 32, 39-52. | 2.6 | 28 |
| 99 | 2-Amino diphenylsulfides as inhibitors of trypanothione reductase: modification of the side chain. Bioorganic and Medicinal Chemistry, 1996, 4, 891-899. | 1.4 | 36 |
| 100 | Combinatorial chemistry: A rational approach to chemical diversity. European Journal of Medicinal Chemistry, 1996, 31, 87-98. | 2.6 | 39 |
| 101 | Development and parametrization of continuum solvent models. I. Models based on the boundary element method. Journal of Chemical Physics, 1996, 104, 6679-6695. | 1.2 | 34 |
| 102 | Development and parametrization of continuum solvent models. II. A unified approach to the solvation problem. Journal of Chemical Physics, 1996, 105, 4197-4210. | 1.2 | 11 |
| 103 | Molecular topology. VIII: Centricities in molecular graphs. The mollen algorithm. Journal of Mathematical Chemistry, 1992, 11, 259-270. | 0.7 | 5 |