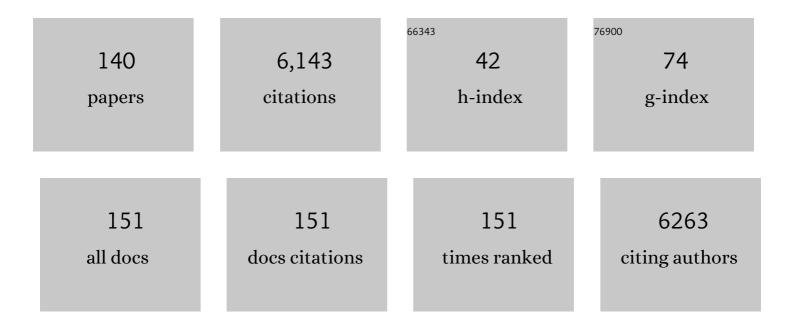
List of Publications by Year in descending order

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| #  | Article   | IF   | CITATIONS |
|----|---|------|-----------|
| 1  | Predicting Amazon customer reviews with deep confidence using deep learning and conformal prediction. Journal of Management Analytics, 2022, 9, 1-16.   | 2.5  | 13        |
| 2  | Identifying Novel Inhibitors for Hepatic Organic Anion Transporting Polypeptides by Machine<br>Learning-Based Virtual Screening. Journal of Chemical Information and Modeling, 2022, 62, 6323-6335.             | 5.4  | 11        |
| 3  | Studying and mitigating the effects of data drifts on ML model performance at the example of chemical toxicity data. Scientific Reports, 2022, 12, 7244.  | 3.3  | 5         |
| 4  | In Silico Identification of Potential Thyroid Hormone System Disruptors among Chemicals in Human<br>Serum and Chemicals with a High Exposure Index. Environmental Science & Technology, 2022, 56,<br>8363-8372. | 10.0 | 5         |
| 5  | Predicting With Confidence: Using Conformal Prediction in Drug Discovery. Journal of Pharmaceutical Sciences, 2021, 110, 42-49.   | 3.3  | 46        |
| 6  | Skin Doctor CP: Conformal Prediction of the Skin Sensitization Potential of Small Organic Molecules.<br>Chemical Research in Toxicology, 2021, 34, 330-344.   | 3.3  | 11        |
| 7  | Combining <i>In Vivo</i> Data with <i>In Silico</i> Predictions for Modeling Hepatic Steatosis by<br>Using Stratified Bagging and Conformal Prediction. Chemical Research in Toxicology, 2021, 34, 656-668.     | 3.3  | 7         |
| 8  | Assessing the calibration in toxicological in vitro models with conformal prediction. Journal of Cheminformatics, 2021, 13, 35.   | 6.1  | 9         |
| 9  | Deep Learning-Based Conformal Prediction of Toxicity. Journal of Chemical Information and Modeling, 2021, 61, 2648-2657.  | 5.4  | 29        |
| 10 | ChemBioSim: Enhancing Conformal Prediction of In Vivo Toxicity by Use of Predicted Bioactivities.<br>Journal of Chemical Information and Modeling, 2021, 61, 3255-3272.   | 5.4  | 13        |
| 11 | Predicting the Skin Sensitization Potential of Small Molecules with Machine Learning Models Trained on Biologically Meaningful Descriptors. Pharmaceuticals, 2021, 14, 790.                                     | 3.8  | 7         |
| 12 | An approach to benchmark fraud detection algorithms in the COVID-19 era. Revista Latinoamericana De<br>EconomÃa Y Sociedad Digital, 2021, , .   | 0.3  | 0         |
| 13 | Un enfoque para hacer benchmark a los algoritmos para la detección de fraude en la era COVID-19.<br>Revista Latinoamericana De EconomÃa Y Sociedad Digital, 2021, , .   | 0.3  | 0         |
| 14 | Synergy conformal prediction applied to large-scale bioactivity datasets and in federated learning.<br>Journal of Cheminformatics, 2021, 13, 77.  | 6.1  | 0         |
| 15 | Associations between clinical signs and pathological findings in toxicity testing. ALTEX: Alternatives To Animal Experimentation, 2021, 38, 198-214.  | 1.5  | 10        |
| 16 | Existing highly accumulating lysosomotropic drugs with potential for repurposing to target COVID-19. Biomedicine and Pharmacotherapy, 2020, 130, 110582.  | 5.6  | 30        |
| 17 | Deep Docking: A Deep Learning Platform for Augmentation of Structure Based Drug Discovery. ACS<br>Central Science, 2020, 6, 939-949.  | 11.3 | 195       |
| 18 | Using Predicted Bioactivity Profiles to Improve Predictive Modeling. Journal of Chemical Information and Modeling, 2020, 60, 2830-2837.   | 5.4  | 14        |

| #  | Article   | IF  | CITATIONS |
|----|---|-----|-----------|
| 19 | CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health<br>Perspectives, 2020, 128, 27002.   | 6.0 | 120       |
| 20 | Conformal Prediction for Ecotoxicology and Implications for Regulatory Decision-Making. Methods in Pharmacology and Toxicology, 2020, , 271-287.  | 0.2 | 2         |
| 21 | LightGBM: An Effective and Scalable Algorithm for Prediction of Chemical Toxicity–Application to the Tox21 and Mutagenicity Data Sets. Journal of Chemical Information and Modeling, 2019, 59, 4150-4158.         | 5.4 | 141       |
| 22 | Multitask Modeling with Confidence Using Matrix Factorization and Conformal Prediction. Journal of Chemical Information and Modeling, 2019, 59, 1598-1604.  | 5.4 | 7         |
| 23 | Towards grouping concepts based on new approach methodologies in chemical hazard assessment:<br>the read-across approach of the EU-ToxRisk project. Archives of Toxicology, 2019, 93, 3643-3667.                  | 4.2 | 82        |
| 24 | QSAR Models for Predicting Five Levels of Cellular Accumulation of Lysosomotropic Macrocycles.<br>International Journal of Molecular Sciences, 2019, 20, 5938.  | 4.1 | 3         |
| 25 | Quantification of Intracellular Accumulation and Retention of Lysosomotropic Macrocyclic<br>Compounds by High-Throughput Imaging of Lysosomal Changes. Journal of Pharmaceutical Sciences,<br>2019, 108, 652-660. | 3.3 | 4         |
| 26 | Predicting Ames Mutagenicity Using Conformal Prediction in the Ames/QSAR International Challenge<br>Project. Mutagenesis, 2019, 34, 33-40.  | 2.6 | 13        |
| 27 | Improvement of quantitative structure–activity relationship (QSAR) tools for predicting Ames<br>mutagenicity: outcomes of the Ames/QSAR International Challenge Project. Mutagenesis, 2019, 34, 3-16.             | 2.6 | 93        |
| 28 | Cheminformatics Explorations of Natural Products. Progress in the Chemistry of Organic Natural Products, 2019, 110, 1-35.   | 1.1 | 14        |
| 29 | Predicting skin sensitizers with confidence — Using conformal prediction to determine applicability domain of GARD. Toxicology in Vitro, 2018, 48, 179-187.   | 2.4 | 22        |
| 30 | Cellular accumulation and lipid binding of perfluorinated alkylated substances (PFASs) – A comparison with lysosomotropic drugs. Chemico-Biological Interactions, 2018, 281, 1-10.                                | 4.0 | 49        |
| 31 | Maximizing gain in high-throughput screening using conformal prediction. Journal of Cheminformatics, 2018, 10, 7.   | 6.1 | 15        |
| 32 | Conformal Regression for Quantitative Structure–Activity Relationship Modeling—Quantifying<br>Prediction Uncertainty. Journal of Chemical Information and Modeling, 2018, 58, 1132-1140.                          | 5.4 | 35        |
| 33 | Creating an efficient screening model for TRPV1 agonists using conformal prediction. Computational Toxicology, 2018, 6, 9-15.   | 3.3 | Ο         |
| 34 | Evaluating parameters for ligand-based modeling with random forest on sparse data sets. Journal of<br>Cheminformatics, 2018, 10, 49.  | 6.1 | 46        |
| 35 | Predicting Aromatic Amine Mutagenicity with Confidence: A Case Study Using Conformal Prediction.<br>Biomolecules, 2018, 8, 85.  | 4.0 | 17        |
| 36 | Fluoxetine Affects Differentiation of Midbrain Dopaminergic Neurons In Vitro. Molecular<br>Pharmacology, 2018, 94, 1220-1231.   | 2.3 | 10        |

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|----|---|------|-----------|
| 37 | Binary classification of imbalanced datasets using conformal prediction. Journal of Molecular<br>Graphics and Modelling, 2017, 72, 256-265.   | 2.4  | 44        |
| 38 | Improving Screening Efficiency through Iterative Screening Using Docking and Conformal Prediction.<br>Journal of Chemical Information and Modeling, 2017, 57, 439-444.  | 5.4  | 42        |
| 39 | Applying Mondrian Cross-Conformal Prediction To Estimate Prediction Confidence on Large<br>Imbalanced Bioactivity Data Sets. Journal of Chemical Information and Modeling, 2017, 57, 1591-1598.                           | 5.4  | 51        |
| 40 | Predicting the Rate of Skin Penetration Using an Aggregated Conformal Prediction Framework.<br>Molecular Pharmaceutics, 2017, 14, 1571-1576.  | 4.6  | 11        |
| 41 | Modelling compound cytotoxicity using conformal prediction and PubChem HTS data. Toxicology Research, 2017, 6, 73-80.   | 2.1  | 45        |
| 42 | Alterations in high-density lipoprotein proteome and function associated with persistent organic pollutants. Environment International, 2017, 98, 204-211.  | 10.0 | 19        |
| 43 | Whole genome microarray analysis of neural progenitor C17.2 cells during differentiation and validation of 30 neural mRNA biomarkers for estimation of developmental neurotoxicity. PLoS ONE, 2017, 12, e0190066.         | 2.5  | 13        |
| 44 | Conformal prediction to define applicability domain – A case study on predicting ER and AR binding.<br>SAR and QSAR in Environmental Research, 2016, 27, 303-316.   | 2.2  | 28        |
| 45 | Conformal Prediction Classification of a Large Data Set of Environmental Chemicals from ToxCast<br>and Tox21 Estrogen Receptor Assays. Chemical Research in Toxicology, 2016, 29, 1003-1010.                              | 3.3  | 43        |
| 46 | Structural and conformational determinants of macrocycle cell permeability. Nature Chemical Biology, 2016, 12, 1065-1074.   | 8.0  | 152       |
| 47 | A proposed framework for the systematic review and integrated assessment (SYRINA) of endocrine disrupting chemicals. Environmental Health, 2016, 15, 74.  | 4.0  | 92        |
| 48 | Conformal Prediction in Spark: Large-Scale Machine Learning with Confidence. , 2015, , .  |      | 5         |
| 49 | Introducing conformal prediction in predictive modeling for regulatory purposes. A transparent and flexible alternative to applicability domain determination. Regulatory Toxicology and Pharmacology, 2015, 71, 279-284. | 2.7  | 24        |
| 50 | The application of conformal prediction to the drug discovery process. Annals of Mathematics and Artificial Intelligence, 2015, 74, 117-132.  | 1.3  | 50        |
| 51 | Evaluation of 309 molecules as inducers of CYP3A4, CYP2B6, CYP1A2, OATP1B1, OCT1, MDR1, MRP2, MRP3 and BCRP in cryopreserved human hepatocytes in sandwich culture. Xenobiotica, 2015, 45, 177-187.                       | 1.1  | 31        |
| 52 | Introducing Conformal Prediction in Predictive Modeling. A Transparent and Flexible Alternative to<br>Applicability Domain Determination. Journal of Chemical Information and Modeling, 2014, 54, 1596-1603.              | 5.4  | 141       |
| 53 | Choosing Feature Selection and Learning Algorithms in QSAR. Journal of Chemical Information and Modeling, 2014, 54, 837-843.  | 5.4  | 83        |
| 54 | Aggregated Conformal Prediction. Lecture Notes in Computer Science, 2014, , 231-240.  | 1.3  | 12        |

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|----|--|------|-----------|
| 55 | QSAR with experimental and predictive distributions: an information theoretic approach for assessing model quality. Journal of Computer-Aided Molecular Design, 2013, 27, 203-219.                               | 2.9  | 31        |
| 56 | Representing descriptors derived from multiple conformations as uncertain features for machine learning. Journal of Molecular Modeling, 2013, 19, 2679-2685.   | 1.8  | 0         |
| 57 | QSAR investigation of NaV1.7 active compounds using the SVM/Signature approach and the Bioclipse<br>Modeling platform. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 261-263.                            | 2.2  | 12        |
| 58 | Comparative analysis of the use of chemoinformatics-based and substructure-based descriptors for quantitative structure-activity relationship (QSAR) modeling. Intelligent Data Analysis, 2013, 17, 327-341.     | 0.9  | 2         |
| 59 | Beyond the Scope of Free-Wilson Analysis: Building Interpretable QSAR Models with Machine Learning Algorithms. Journal of Chemical Information and Modeling, 2013, 53, 1324-1336.                                | 5.4  | 37        |
| 60 | <i>In Silico</i> Categorization of <i>in Vivo</i> Intrinsic Clearance Using Machine Learning.<br>Molecular Pharmaceutics, 2013, 10, 1318-1321.   | 4.6  | 11        |
| 61 | A Pragmatic Approach Using First-Principle Methods to Address Site of Metabolism with Implications for Reactive Metabolite Formation. Journal of Chemical Information and Modeling, 2012, 52, 686-695.           | 5.4  | 7         |
| 62 | Classification of Inhibitors of Hepatic Organic Anion Transporting Polypeptides (OATPs): Influence of<br>Protein Expression on Drug–Drug Interactions. Journal of Medicinal Chemistry, 2012, 55, 4740-4763.      | 6.4  | 299       |
| 63 | Introducing Uncertainty in Predictive Modeling—Friend or Foe?. Journal of Chemical Information and Modeling, 2012, 52, 2815-2822.  | 5.4  | 3         |
| 64 | Two personal perspectives on a key issue in contemporary 3D QSAR. Wiley Interdisciplinary Reviews:<br>Computational Molecular Science, 2012, 2, 108-113.   | 14.6 | 7         |
| 65 | Benchmarking Variable Selection in QSAR. Molecular Informatics, 2012, 31, 173-179.   | 2.5  | 21        |
| 66 | Application of Conformal Prediction in QSAR. International Federation for Information Processing, 2012, , 166-175.   | 0.4  | 14        |
| 67 | Crystallographic, theoretical and molecular modelling studies on the conformations of the salicylamide, raclopride, a selective dopamine-D2 antagonist. Journal of Pharmacy and Pharmacology, 2011, 39, 787-796. | 2.4  | 16        |
| 68 | Structural Features Determining the Intestinal Epithelial Permeability and Efflux of Novel HIV-1<br>Protease Inhibitors. Journal of Pharmaceutical Sciences, 2011, 100, 3763-3772.                               | 3.3  | 12        |
| 69 | Automated QSAR with a Hierarchy of Global and Local Models. Molecular Informatics, 2011, 30, 960-972.  | 2.5  | 36        |
| 70 | Trade-off between accuracy and interpretability for predictive <i>in silico</i> modeling. Future<br>Medicinal Chemistry, 2011, 3, 647-663.   | 2.3  | 59        |
| 71 | Pin-pointing concept descriptions. , 2010, , .   |      | 2         |
| 72 | Evaluation of Quantitative Structureâ^'Activity Relationship Modeling Strategies: Local and Global<br>Models. Journal of Chemical Information and Modeling, 2010, 50, 677-689.                                   | 5.4  | 25        |

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|----|--|------|-----------|
| 73 | Pre-Processing Structured Data for Standard Machine Learning Algorithms by Supervised Graph<br>Propositionalization - A Case Study with Medicinal Chemistry Datasets. , 2010, , .                                      |      | 7         |
| 74 | Using Feature Selection with Bagging and Rule Extraction in Drug Discovery. Smart Innovation, Systems and Technologies, 2010, , 413-422.   | 0.6  | 2         |
| 75 | Identification of Novel Specific and General Inhibitors of the Three Major Human ATP-Binding Cassette<br>Transporters P-gp, BCRP and MRP2 Among Registered Drugs. Pharmaceutical Research, 2009, 26,<br>1816-1831.     | 3.5  | 276       |
| 76 | Age related changes in brain metabolites observed by 1H MRS in APP/PS1 mice. Neurobiology of Aging, 2008, 29, 1423-1433.   | 3.1  | 97        |
| 77 | Prediction and Identification of Drug Interactions with the Human ATP-Binding Cassette Transporter<br>Multidrug-Resistance Associated Protein 2 (MRP2; ABCC2). Journal of Medicinal Chemistry, 2008, 51,<br>3275-3287. | 6.4  | 119       |
| 78 | Comprehensible Models for Predicting Molecular Interaction with Heart-Regulating Genes. , 2008, , .  |      | 2         |
| 79 | Structural Requirements for Drug Inhibition of the Liver Specific Human Organic Cation Transport<br>Protein 1. Journal of Medicinal Chemistry, 2008, 51, 5932-5942.  | 6.4  | 175       |
| 80 | A Global Drug Inhibition Pattern for the Human ATP-Binding Cassette Transporter Breast Cancer<br>Resistance Protein (ABCG2). Journal of Pharmacology and Experimental Therapeutics, 2007, 323, 19-30.                  | 2.5  | 115       |
| 81 | Discrimination between modes of toxic action of phenols using rule based methods. Molecular<br>Diversity, 2006, 10, 207-212.   | 3.9  | 17        |
| 82 | Prediction of ADMET Properties. ChemMedChem, 2006, 1, 920-937.   | 3.2  | 194       |
| 83 | Exploring the Role of Different Drug Transport Routes in Permeability Screening. Journal of Medicinal Chemistry, 2005, 48, 604-613.  | 6.4  | 134       |
| 84 | Global and Local Computational Models for Aqueous Solubility Prediction of Drug-Like Molecules<br>ChemInform, 2004, 35, no.  | 0.0  | 0         |
| 85 | Global and Local Computational Models for Aqueous Solubility Prediction of Drug-Like Molecules.<br>Journal of Chemical Information and Computer Sciences, 2004, 44, 1477-1488.   | 2.8  | 101       |
| 86 | Support vector machine models in drug design: applications to drug transport processes and QSAR using simplex optimisations and variable selection. Neurocomputing, 2003, 55, 337-346.                                 | 5.9  | 83        |
| 87 | Molecular Descriptors Influencing Melting Point and Their Role in Classification of Solid Drugs<br>ChemInform, 2003, 34, no.   | 0.0  | 0         |
| 88 | Molecular Descriptors Influencing Melting Point and Their Role in Classification of Solid Drugs.<br>Journal of Chemical Information and Computer Sciences, 2003, 43, 1177-1185.  | 2.8  | 96        |
| 89 | Improving Structure-Based Virtual Screening by Multivariate Analysis of Scoring Data. Journal of<br>Medicinal Chemistry, 2003, 46, 5781-5789.  | 6.4  | 134       |
| 90 | Computational approaches to the prediction of the blood–brain distribution. Advanced Drug Delivery<br>Reviews, 2002, 54, 291-313.  | 13.7 | 281       |

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| 91  | Experimental and computational screening models for prediction of aqueous drug solubility.<br>Pharmaceutical Research, 2002, 19, 182-188.   | 3.5 | 153       |
| 92  | Experimental and Computational Screening Models for the Prediction of Intestinal Drug Absorption.<br>Journal of Medicinal Chemistry, 2001, 44, 1927-1937.   | 6.4 | 238       |
| 93  | Theoretical calculation and prediction of drug transport processes using simple parameters and partial least squares projections to latent structures (PLS) statistics. The use of electrotopological state indices. Journal of Pharmaceutical Sciences, 2001, 90, 1076-1085. | 3.3 | 51        |
| 94  | Title is missing!. Journal of Chemical Crystallography, 2001, 31, 321-328.  | 1.1 | 5         |
| 95  | Prediction of drug transport processes using simple parameters and PLS statistics The use of ACD/logP and ACD/ChemSketch descriptors. European Journal of Pharmaceutical Sciences, 2001, 12, 327-337.   | 4.0 | 73        |
| 96  | Theoretical calculation and prediction of P-glycoprotein-interacting drugs using MolSurf parametrization and PLS statistics. European Journal of Pharmaceutical Sciences, 2000, 10, 295-303.  | 4.0 | 82        |
| 97  | Refinement of Catalyst hypotheses using simplex optimisation. , 2000, 14, 545-557.  |     | 16        |
| 98  | Title is missing!. , 2000, 19, 1-18.  |     | 18        |
| 99  | Prediction of Polar Surface Area and Drug Transport Processes Using Simple Parameters and PLS Statistics. Journal of Chemical Information and Computer Sciences, 2000, 40, 1408-1411.   | 2.8 | 94        |
| 100 | Theoretical calculation and prediction of intestinal absorption of drugs in humans using MolSurf parametrization and PLS statistics. European Journal of Pharmaceutical Sciences, 1999, 8, 49-56.   | 4.0 | 101       |
| 101 | Theoretical Calculation and Prediction of Brain–Blood Partitioning of Organic Solutes Using<br>MolSurf Parametrization and PLS Statistics. Journal of Pharmaceutical Sciences, 1998, 87, 952-959.   | 3.3 | 119       |
| 102 | Descriptors for amino acids using MolSurf parametrization. Journal of Computational Chemistry, 1998, 19, 51-59.   | 3.3 | 8         |
| 103 | Recent Progress in CoMFA Methodology and Related Techniques. , 1998, , 25-39.   |     | 7         |
| 104 | A 3D-QSAR Study of Analogs of (Z)-5-Decenyl Acetate, A Pheromone Component of the Turnip Moth,<br>Agrotis segetum. Journal of Chemical Ecology, 1997, 23, 2917-2934.  | 1.8 | 15        |
| 105 | Theoretical calculation and prediction of Caco-2 cell permeability using MolSurf parametrization and PLS statistics. Pharmaceutical Research, 1997, 14, 1786-1791.  | 3.5 | 95        |
| 106 | A quantitative structureâ€activity relationship study of some substance Pâ€related peptides A multivariate<br>approach using PLS and variable selection. Chemical Biology and Drug Design, 1997, 49, 155-162.   | 1.1 | 21        |
| 107 | Single and domain mode variable selection in 3D QSAR applications. Journal of Chemometrics, 1996, 10, 95-105.   | 1.3 | 75        |
| 108 | Quantitative Structure-Property Relationships of Azurin Mutants fromPseudomonas Aeruginosa.<br>QSAR and Combinatorial Science, 1996, 15, 475-479.   | 1.2 | 2         |

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| 109 | A PLS quantitative structure-activity relationship study of some monoamine oxidase inhibitors of the phenyl alkylamine type. European Journal of Medicinal Chemistry, 1994, 29, 191-195.   | 5.5  | 12        |
| 110 | Theoretical Descriptors of Nucleic Acid Bases. Application to DNA Promoter Sequences. QSAR and Combinatorial Science, 1994, 13, 295-301.   | 1.2  | 3         |
| 111 | A PLS QSAR analysis using 3D generated aromatic descriptors of principal property type: Application to some dopamine D2 benzamide antagonists. Journal of Computer-Aided Molecular Design, 1993, 7, 671-682.   | 2.9  | 11        |
| 112 | Multivariate Free-Wilson Analysis of Some N-Alkylmorphinan-6-one Opioids Using PLS. QSAR and Combinatorial Science, 1993, 12, 119-123.   | 1.2  | 5         |
| 113 | Analysis of reversed-phase liquid chromatographic separations using the data-reduction methods PCR and PLS. Analytica Chimica Acta, 1992, 259, 105-108.  | 5.4  | 9         |
| 114 | PLS-Based Quantitative Structure–Activity Relationship for Substituted Benzamides of Clebopride Type.<br>Application of Experimental Design in Drug Design Acta Chemica Scandinavica, 1992, 46, 363-366.   | 0.7  | 11        |
| 115 | Theoretical amino acid descriptors. Application to bradykinin potentiating peptides. Peptides, 1991, 12, 1223-1227.  | 2.4  | 37        |
| 116 | QSAR on Substituted Salicylamides Using with Implementation of 3D MEP Descriptors. QSAR and Combinatorial Science, 1991, 10, 1-5.  | 1.2  | 5         |
| 117 | Chiral separation ofN-aminoalkylsuccinimides on an ?1 - acid glycoprotein column: A quantitative structure?enantioselectivity relationship study. Chirality, 1991, 3, 422-426.   | 2.6  | 18        |
| 118 | 3-D QSAR analysis of steroid/protein interactions: The use of difference maps. Journal of<br>Computer-Aided Molecular Design, 1991, 5, 419-426.  | 2.9  | 17        |
| 119 | Experimental design based 3-D QSAR analysis of steroid-protein interactions: Application to human CBG complexes. Journal of Computer-Aided Molecular Design, 1990, 4, 381-389.   | 2.9  | 34        |
| 120 | Cis-trans photoisomerization of a p-styrylstilbene, a one- and twofold adiabatic process. Journal of<br>the American Chemical Society, 1990, 112, 3082-3086.   | 13.7 | 84        |
| 121 | Structural factors of importance for 5-hydroxytryptaminergic activity. Conformational preferences and electrostatic potentials of 8-hydroxy-2-(di-n-propylamino)tetralin (8-OH-DPAT) and some related agents. Journal of Medicinal Chemistry, 1988, 31, 212-221. | 6.4  | 23        |
| 122 | StructureStability Relationships in Vinyl Sulfides. IV. Evaluation of the ppi Conjugation Energies in<br>Vinyl Sulfides and Vinyl Ethers Acta Chemica Scandinavica, 1988, 42b, 592-595.  | 0.7  | 4         |
| 123 | A Note on Further use of Computer Aided Chemistry to Predict Chiral Separations in Liquid Chromatography: Selecting the Most Appropriate Derivative. , 1988, , 127-130.  |      | 0         |
| 124 | Theoretical Investigation of Benzylideneaniline and Salicylideneanile: An AM1 Study. Molecular<br>Crystals and Liquid Crystals, 1987, 149, 195-201.  | 0.8  | 2         |
| 125 | The Use of Computer Aided Chemistry to Predict Chiral Separation in Liquid Chromatography. Journal of Liquid Chromatography and Related Technologies, 1987, 10, 2825-2844.   | 1.0  | 28        |
| 126 | Intermolecular Energy Calculations on Benzylideneaniline, Salicylideneaniline, MMBA and MMSA.<br>Molecular Crystals and Liquid Crystals, 1987, 147, 149-162.   | 0.8  | 6         |

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| 127 | Conformational analysis of 3-methylene-1,4-pentadiene using molecular mechanics and quantum mechanical calculations. Computational and Theoretical Chemistry, 1987, 150, 85-91.     | 1.5  | 10        |
| 128 | A theoretical reinvestigation of the nucleic bases adenine, guanine, cytosine, thymine and uracil using AM1. Computational and Theoretical Chemistry, 1987, 151, 259-269.           | 1.5  | 94        |
| 129 | The dianion of [2.2.2]paracyclophene; a 20 π-perimeter species?. Tetrahedron, 1986, 42, 4499-4502.  | 1.9  | 24        |
| 130 | A sixfold triplet-sensitized Z/E isomerization of a π-perimeter macrocycle. Tetrahedron Letters, 1986,<br>27, 1063-1066.  | 1.4  | 8         |
| 131 | On the Relation between the Frontier Orbitals in Small Rings, Macrocyclic Compounds, and Linear<br>Polymers with Extended pi Systems Acta Chemica Scandinavica, 1986, 40b, 328-336. | 0.7  | 4         |
| 132 | Force field calculations on cyclophanes with unsaturated bridges. The Journal of Physical Chemistry, 1985, 89, 3233-3237.   | 2.9  | 8         |
| 133 | 1,6:9,14-bismethano[16]annulene - a new bridged [4n]annulene. Tetrahedron Letters, 1985, 26, 3087-3090.   | 1.4  | 11        |
| 134 | Hückel theory applied to large linear and cyclic conjugated π-systems. Tetrahedron, 1985, 41, 713-726.  | 1.9  | 10        |
| 135 | Macrocyclic π-systems with 2-symmetry as the sum of π-systems with hückel and möbius topology.<br>Tetrahedron Letters, 1984, 25, 1397-1400.   | 1.4  | 9         |
| 136 | Correlated flipping of four benzene rings in substituted [2.2.2.2]Paracyclophanetetraenes.<br>Tetrahedron Letters, 1984, 25, 4787-4790.   | 1.4  | 2         |
| 137 | Diatropic cyclophane dianions. Journal of the American Chemical Society, 1984, 106, 7514-7522.  | 13.7 | 51        |
| 138 | [26]paracyclophanehexaenes. Tetrahedron Letters, 1983, 24, 5411-5414.   | 1.4  | 10        |
| 139 | Resonance Energies of Unsaturated Cyclophanes with 4N and (4N + 2) Perimeters Acta Chemica<br>Scandinavica, 1983, 37a, 431-436.   | 0.7  | 0         |
| 140 | Correlation of Hückel Calculations and Reduction Potentials for Some Conjugated Cyclophanes<br>Acta Chemica Scandinavica, 1981, 35b, 403-406.                                       | 0.7  | 4         |