Pierre-Alain Carrupt

List of Publications by Year
in descending order

192 papers	11,188 citations	16450 64 h-index	39667 94 g-index
200 all docs	200 docs citations	200 times ranked	10126 citing authors

#	Article	IF	Citations
1	HDM-PAMPA to predict gastrointestinal absorption, binding percentage, equilibrium and kinetics constants with human serum albumin and using 2 end-point measurements. European Journal of Pharmaceutical Sciences, 2017, 97, 143-150.	4.0	16
2	Normal phase HPLC-based activity profiling of non-polar crude plant extracts â€“ acetylcholinesterase inhibiting guttiferones from Montrouziera cauliflora as a case study. Natural Product Research, 2016, 30, 2754-2759.	1.8	3
3	Limits of rapid log P determination methods for highly lipophilic and flexible compounds. Analytica Chimica Acta, 2016, 915, 90-101.	5.4	9
4	Prediction of the Passive Intestinal Absorption of Medicinal Plant Extract Constituents with the Parallel Artificial Membrane Permeability Assay (PAMPA). Planta Medica, 2016, 82, 424-431.	1.3	32
5	Pharmacophoreâ€based discovery of inhibitors of a novel drug/proton antiporter in human brain endothelial hCMEC/D3 cell line. British Journal of Pharmacology, 2015, 172, 4888-4904.	5.4	28
6	Alkaloids from Psychotria Target Sirtuins: In Silico and In Vitro Interaction Studies. Planta Medica, 2015, 81, 517-524.	1.3	8
7	Structure-Based Design and Optimization of Multitarget-Directed 2H-Chromen-2-one Derivatives as Potent Inhibitors of Monoamine Oxidase B and Cholinesterases. Journal of Medicinal Chemistry, 2015, 58, 5561-5578.	6.4	89
8	Modification of a PAMPA model to predict passive gastrointestinal absorption and plasma protein binding. European Journal of Pharmaceutical Sciences, 2015, 77, 273-278.	4.0	12
9	Alkaloids as Inhibitors of Monoamine Oxidases and Their Role in the Central Nervous System. Studies in Natural Products Chemistry, 2014, 43, 123-144.	1.8	10
10	Modeling the Met Form of Human Tyrosinase: A Refined and Hydrated Pocket for Antagonist Design. Chemical Biology and Drug Design, 2014, 84, 206-215.	3.2	23
11	MLP Tools: a PyMOL plugin for using the molecular lipophilicity potential in computer-aided drug design. Journal of Computer-Aided Molecular Design, 2014, 28, 587-596.	2.9	18
12	Retention time prediction for dereplication of natural products (CxHyOz) in LCâ€“MS metabolite profiling. Phytochemistry, 2014, 108, 196-207.	2.9	44
13	Predicting both passive intestinal absorption and the dissociation constant toward albumin using the PAMPA technique. European Journal of Pharmaceutical Sciences, 2014, 63, 36-44.	4.0	19
14	cIEF for rapid pKa determination of small molecules: A proof of concept. European Journal of Pharmaceutical Sciences, 2014, 63, 14-21.	4.0	10
15	Collateral sensitivity of resistant MRP1-overexpressing cells to flavonoids and derivatives through GSH efflux. Biochemical Pharmacology, 2014, 90, 235-245.	4.4	41
16	Study of Leaf Metabolome Modifications Induced by UV-C Radiations in Representative Vitis, Cissus and Cannabis Species by LC-MS Based Metabolomics and Antioxidant Assays. Molecules, 2014, 19, 14004-14021.	3.8	48
17	New high throughput screening method for drug release measurements. European Journal of Pharmaceutics and Biopharmaceutics, 2013, 85, 151-157.	4.3	5
18	High performance affinity chromatography (HPAC) as a high-throughput screening tool in drug discovery to study drugâ€“plasma protein interactions. Journal of Pharmaceutical and Biomedical Analysis, 2013, 74, 205-212.	2.8	36

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19	Indole alkaloids of Psychotria as multifunctional cholinesterases and monoamine oxidases inhibitors. Phytochemistry, 2013, 86, 8-20.	2.9	76
20	Large, chemically diverse dataset of logP measurements for benchmarking studies. European Journal of Pharmaceutical Sciences, 2013, 48, 21-29.	4.0	42
21	Global analytical strategy to measure drugâ€"plasma protein interactions: from high-throughput to in-depth analysis. Drug Discovery Today, 2013, 18, 1030-1034.	6.4	36
22	Methodologies to Assess Drug Permeation Through the Bloodâ€"Brain Barrier for Pharmaceutical Research. Pharmaceutical Research, 2013, 30, 2729-2756.	3.5	36
23	Molecular Docking Using the Molecular Lipophilicity Potential as Hydrophobic Descriptor: Impact on GOLD Docking Performance. Journal of Chemical Information and Modeling, 2012, 52, 1319-1327.	5.4	35
24	High resolution ultra high pressure liquid chromatographyâ€"time-of-flight mass spectrometry dereplication strategy for the metabolite profiling of Brazilian Lippia species. Journal of Chromatography A, 2012, 1259, 167-178.	3.7	63
25	Determination of alkane/water partition coefficients of polar compounds using hydrophilic interaction chromatography. Journal of Chromatography A, 2012, 1260, 164-168.	3.7	9
26	Characterization of drugâ€"protein interactions by capillary electrophoresis hyphenated to mass spectrometry. Electrophoresis, 2012, 33, 3306-3315.	2.4	39
27	Esters of L-Dopa: Structure-hydrolysis Relationships and Ability to Induce Circling Behaviour in an Experimental Model of Hemiparkinsonism. Journal of Pharmacy and Pharmacology, 2011, 47, 861-869.	2.4	20
28	Influence of Lipophilicity and Chirality on the Selectivity of Ligands for Î²1- and Î²2-Adrenoceptors. Journal of Pharmacy and Pharmacology, 2011, 40, 609-612.	2.4	18
29	Ultra High Pressure Liquid Chromatography for Crude Plant Extract Profiling. Journal of AOAC INTERNATIONAL, 2011, 94, 51-70.	1.5	59
30	Evaluation and Prediction of Drug Permeation. Journal of Pharmacy and Pharmacology, 2010, 51, 1339-1357.	2.4	53
31	Drugâ€"protein binding: a critical review of analytical tools. Analytical and Bioanalytical Chemistry, 2010, 398, 53-66.	3.7	326
32	Physicochemical profile and in vitro permeation behavior of a new class of non-steroidal anti-inflammatory drug candidates. European Journal of Pharmaceutical Sciences, 2010, 40, 217-221.	4.0	1
33	Highâ€throughput log P determination by MEEKC coupled with UV and MS detections. Electrophoresis, 2010, 31, 952-964.	2.4	27
34	Improvement of a capillary electrophoresis/frontal analysis (CE/FA) method for determining binding constants: Discussion on relevant parameters. Journal of Pharmaceutical and Biomedical Analysis, 2010, 53, 1288-1297.	2.8	39
35	Standard machine learning algorithms applied to UPLC-TOF/MS metabolic fingerprinting for the discovery of wound biomarkers in Arabidopsis thaliana. Chemometrics and Intelligent Laboratory Systems, 2010, 104, 20-27.	3.5	23
36	Entacapone and Tolcapone, Two Catechol O-Methyltransferase Inhibitors, Block Fibril Formation of Î±-Synuclein and Î²-Amyloid and Protect against Amyloid-induced Toxicity. Journal of Biological Chemistry, 2010, 285, 14941-14954.	3.4	119

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37	Molecular Electrocatalysis for Oxygen Reduction by Cobalt Porphyrins Adsorbed at Liquid/Liquid Interfaces. Journal of the American Chemical Society, 2010, 132, 2655-2662.	13.7	141
38	Advances in LC platforms for drug discovery. Expert Opinion on Drug Discovery, 2010, 5, 475-489.	5.0	20
39	A fast screening strategy for characterizing peptide delivery by transdermal iontophoresis. Journal of Controlled Release, 2009, 137, 123-129.	9.9	12
40	Analytical tools for the physicochemical profiling of drug candidates to predict absorption/distribution. Analytical and Bioanalytical Chemistry, 2009, 394, 707-729.	3.7	68
41	Fast log P determination by ultra-high-pressure liquid chromatography coupled with UV and mass spectrometry detections. Analytical and Bioanalytical Chemistry, 2009, 394, 1919-1930.	3.7	41
42	Metabolite profiling of plant extracts by ultra-high-pressure liquid chromatography at elevated temperature coupled to time-of-flight mass spectrometry. Journal of Chromatography A, 2009, 1216, 5660-5668.	3.7	61
43	Lipophilicity of Basic Drugs Measured by Hydrophilic Interaction Chromatography. Journal of Medicinal Chemistry, 2009, 52, 3416-3419.	6.4	28
44	Monoamine oxidase inhibition by Rhodiola rosea L. roots. Journal of Ethnopharmacology, 2009, 122, 397-401.	4.1	158
45	Antioxidant Phenylethanoid Glycosides and a Neolignan from Jacaranda caucana. Journal of Natural Products, 2009, 72, 852-856.	3.0	23
46	UPLCâ€“TOF-MS for plant metabolomics: A sequential approach for wound marker analysis in Arabidopsis thaliana. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2008, 871, 261-270.	2.3	96
47	Structure-Antioxidant Activity Relationships in a Series of NO-Donor Phenols. ChemMedChem, 2008, 3, 1443-1448.	3.2	6
48	Physicochemical Profiling of Sartans: A Detailed Study of Ionization Constants and Distribution Coefficients. Helvetica Chimica Acta, 2008, 91, 468-482.	1.6	51
49	Optimized liquid chromatographyâ€“mass spectrometry approach for the isolation of minor stress biomarkers in plant extracts and their identification by capillary nuclear magnetic resonance. Journal of Chromatography A, 2008, 1180, 90-98.	3.7	97
50	High-Throughput logâ€‰P Determination by Ultraperformance Liquid Chromatography: A Convenient Tool for Medicinal Chemists. Journal of Medicinal Chemistry, 2008, 51, 396-399.	6.4	34
51	In vitro screening assays to identify natural or synthetic acetylcholinesterase inhibitors: Thin layer chromatography versus microplate methods. European Journal of Pharmaceutical Sciences, 2008, 33, 109-119.	4.0	110
52	High throughput UV method for the estimation of thermodynamic solubility and the determination of the solubility in biorelevant media. European Journal of Pharmaceutical Sciences, 2008, 33, 230-240.	4.0	85
53	The PAMPA technique as a HTS tool for partition coefficients determination in different solvent/water systems. European Journal of Pharmaceutical Sciences, 2008, 35, 68-75.	4.0	16
54	Antioxidant C-Glucosylxanthones from the Leaves of Arrabidaea patellifera. Journal of Natural Products, 2008, 71, 1887-1890.	3.0	34

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55	Ferulenol specifically inhibits succinate ubiquinone reductase at the level of the ubiquinone cycle. Biochemical and Biophysical Research Communications, 2007, 355, 252-257.	2.1	27
56	Computational Approaches to Lipophilicity: Methods and Applications. Reviews in Computational Chemistry, 2007, , 241-315.	1.5	45
57	In Silico and In Vitro Filters for the Fast Estimation of Skin Permeation and Distribution of New Chemical Entities. Journal of Medicinal Chemistry, 2007, 50, 742-748.	6.4	33
58	Development of a twoâ€step screening ESIâ€TOFâ€MS method for rapid determination of significant stressâ€induced metabolome modifications in plant leaf extracts: The wound response in Arabidopsis thaliana as a case study. Journal of Separation Science, 2007, 30, 2268-2278.	2.5	46
59	Novel screening assay for antioxidant protection against peroxyl radicalâ€induced loss of protein function. Journal of Pharmaceutical Sciences, 2007, 96, 2931-2944.	3.3	23
60	Multivariate data analysis of rapid LC-TOF/MS experiments from Arabidopsis thaliana stressed by wounding. Chemometrics and Intelligent Laboratory Systems, 2007, 86, 189-197.	3.5	35
61	NO-donor melatonin derivatives: synthesis and in vitro pharmacological characterization. Journal of Pineal Research, 2007, 42, 371-385.	7.4	13
62	Rapid determination of pK a values of 20 amino acids by CZE with UV and capacitively coupled contactless conductivity detections. Analytical and Bioanalytical Chemistry, 2007, 389, 1869-1878.	3.7	58
63	Impact of Species-Dependent Differences on Screening, Design, and Development of MAO B Inhibitors. Journal of Medicinal Chemistry, 2006, 49, 6264-6272.	6.4	79
64	Parallel Artificial Membrane Permeability Assay:â€‰ A New Membrane for the Fast Prediction of Passive Human Skin Permeability. Journal of Medicinal Chemistry, 2006, 49, 3948-3954.	6.4	160
65	Immobilized pH Gradient Gel Cell To Study the pH Dependence of Drug Lipophilicity. Analytical Chemistry, 2006, 78, 1503-1508.	6.5	25
66	Development of an in Vitro Rat Intestine Segmental Perfusion Model to Investigate Permeability and Predict Oral Fraction Absorbed. Pharmaceutical Research, 2006, 23, 1543-1553.	3.5	7
67	Structureâ€"permeation relationships for the non-invasive transdermal delivery of cationic peptides by iontophoresis. European Journal of Pharmaceutical Sciences, 2006, 29, 53-59.	4.0	26
68	The Lipophilicity Behavior of Three Catechol-O-methyltransferase (COMT) Inhibitors and Simple Analogues. Helvetica Chimica Acta, 2006, 89, 144-152.	1.6	13
69	Identification of Novel Multifunctional Compounds for the Treatment of Some Aging Related Neurodegenerative Diseases. Chimia, 2005, 59, 315-320.	0.6	8
70	Experimental and Virtual Physicochemical and Pharmacokinetic Profiling of New Chemical Entities. Chimia, 2005, 59, 308-314.	0.6	13
71	Human recombinant monoamine oxidase B as reliable and efficient enzyme source for inhibitor screening. Bioorganic and Medicinal Chemistry, 2005, 13, 6212-6217.	3.0	121
72	Numerical simulation of two-phase partition chromatography in microchannels for moderated logP measurements. Journal of Chromatography A, 2005, 1063, 89-97.	3.7	3

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73	Novel RPLC stationary phases for lipophilicity measurement: Solvatochromic analysis of retention mechanisms for neutral and basic compounds. Journal of Separation Science, 2005, 28, 2350-2362.	2.5	28
74	Determination of pKa values by capillary zone electrophoresis with a dynamic coating procedure. Journal of Separation Science, 2005, 28, 2374-2380.	2.5	81
75	Imidazole H3-antagonists: relationship between structure and ex vivo binding to rat brain H3-receptors. European Journal of Pharmaceutical Sciences, 2004, 23, 89-98.	4.0	13
76	Quantitative Structure-Permeation Relationships (QSPeRs) to Predict Skin Permeation: A Critical Evaluation. Pharmaceutical Research, 2004, 21, 83-92.	3.5	134
77	Screening of Non-Alkaloidal Natural Compounds as Acetylcholinesterase Inhibitors. Chemistry and Biodiversity, 2004, 1, 819-829.	2.1	69
78	Liposome/water lipophilicity: Methods, information content, and pharmaceutical applications. Medicinal Research Reviews, 2004, 24, 299-324.	10.5	100
79	Liposome/Water Lipophilicity: Methods, Information Content, and Pharmaceutical Applications. ChemInform, 2004, 35, no.	0.0	0
80	A Comparison of the Solvation Properties of 2-Nitrophenyloctyl Ether, Nitrobenzene, andn-Octanol as Assessed by Ion Transfer Experiments. Journal of Physical Chemistry B, 2004, 108, 4565-4572.	2.6	73
81	Fluoride curcumin derivatives: new mitochondrial uncoupling agents. FEBS Letters, 2004, 569, 37-42.	2.8	37
82	Water-oil partition profiling of ionized drug molecules using cyclic voltammetry and a 96-well microfilter plate system. Pharmaceutical Research, 2003, 20, 1317-1322.	3.5	42
83	Partition Coefficients of Ionizable Compounds ino-Nitrophenyl Octyl Ether/Water Measured by the Potentiometric Method. Analytical Chemistry, 2003, 75, 7036-7039.	6.5	22
84	Solvatochromic Analysis of Partition Coefficients in theo-Nitrophenyl Octyl Ether (o-NPOE)/Water System. Helvetica Chimica Acta, 2003, 86, 3533-3547.	1.6	26
85	Immobilized Artificial Membrane HPLC in Drug Research. ChemInform, 2003, 34, no.	0.0	0
86	Immobilized Artificial Membrane HPLC in Drug Research. Journal of Medicinal Chemistry, 2003, 46, 655-665.	6.4	128
87	Standard partition coefficients of anionic drugs in the n-octanol/water system determined by voltammetry at three-phase electrodes. Physical Chemistry Chemical Physics, 2003, 5, 3748-3751.	2.8	85
88	Exploration of the Pharmacophore of 3-Alkyl-5-Arylimidazolidinediones as New CB1Cannabinoid Receptor Ligands and Potential Antagonists: Synthesis, Lipophilicity, Affinity, and Molecular Modeling. Journal of Medicinal Chemistry, 2002, 45, 1748-1756.	6.4	46
89	A simple model to predict bloodâ€"brain barrier permeation from 3D molecular fields. Biochimica Et Biophysica Acta - Molecular Basis of Disease, 2002, 1587, 118-125.	3.8	63
90	Recognition forces involved in mitochondrial binding to a low-affinity trimetazidine binding site related to anti-ischemic activity. Biochemical Pharmacology, 2002, 63, 1691-1697.	4.4	20

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91	The relative partitioning of neutral and ionised compounds in sodium dodecyl sulfate micelles measured by micellar electrokinetic capillary chromatography. European Journal of Pharmaceutical Sciences, 2002, 15, 225-234.	4.0	23
92	Lipophilicity and Solvation of Anionic Drugs. Chemistry - A European Journal, 2002, 8, 3478.	3.3	87
93	Structural Properties Governing Retention Mechanisms on Immobilized Artificial Membrane (IAM) HPLC Columns. Helvetica Chimica Acta, 2002, 85, 519-532.	1.6	40
94	Natural and synthetic geiparvarins are strong and selective MAO-B inhibitors. synthesis and SAR studies. Bioorganic and Medicinal Chemistry Letters, 2002, 12, 3551-3555.	2.2	87
95	Immobilized artificial membrane liquid chromatography: proposed guidelines for technical optimization of retention measurements. Journal of Chromatography A, 2002, 953, 39-53.	3.7	42
96	Cyclic voltammetry of highly hydrophilic ions at a supported liquid membrane. Journal of Electroanalytical Chemistry, 2002, 530, 10-15.	3.8	54
97	Molecular factors influencing retention on immobilized artifical membranes (IAM) compared to partitioning in liposomes and n-octanol. Pharmaceutical Research, 2002, 19, 729-737.	3.5	85
98	Theoretical and experimental exploration of the lipophilicity of zwitterionic drugs in the 1,2-dichloroethane/water system. Pharmaceutical Research, 2002, 19, 1150-1159.	3.5	37
99	Quantitative structure-permeation relationships for solute transport across silicone membranes. Pharmaceutical Research, 2002, 19, 1622-1629.	3.5	55
100	Coumarins Derivatives as Dual Inhibitors of Acetylcholinesterase and Monoamine Oxidase. Journal of Medicinal Chemistry, 2001, 44, 3195-3198.	6.4	267
101	Generalization of Ionic Partition Diagrams to Lipophilic Compounds and to Biphasic Systems with Variable Phase Volume Ratios. Journal of the American Chemical Society, 2001, 123, 10684-10690.	13.7	65
102	Development of molecular hydrogen-bonding potentials (MHBPs) and their application to structureâ€"permeation relations. Journal of Molecular Graphics and Modelling, 2001, 19, 521-535.	2.4	31
103	Ionic Partition Diagram of the Zwitterionic Antihistamine Cetirizine. Helvetica Chimica Acta, 2001, 84, 375-387.	1.6	31
104	Natural and Synthetic Xanthones as Monoamine Oxidase Inhibitors: Biological Assay and 3D-QSAR. Helvetica Chimica Acta, 2001, 84, 552-570.	1.6	72
105	Structural damage to proteins caused by free radicals: asessment, protection by antioxidants, and influence of protein binding11Abbreviations: AAPH, 2,2â€²-azobis(2-amidinopropane) 2 HCl; and HSA, human serum albumin.. Biochemical Pharmacology, 2001, 61, 1237-1242.	4.4	96
106	Physicochemical Characterization of Sildenafil: Ionization, Lipophilicity Behavior, and Ionic-Partition Diagram Studied by Two-Phase Titration and Electrochemistry. Helvetica Chimica Acta, 2000, 83, 1465-1474.	1.6	62
107	The influence of lipophilicity on the pharmacokinetic behavior of drugs: Concepts and examples. Journal of Computer - Aided Molecular Design, 2000, 19, 179-211.	1.0	190
108	Predicting Bloodâ˜'Brain Barrier Permeation from Three-Dimensional Molecular Structure. Journal of Medicinal Chemistry, 2000, 43, 2204-2216.	6.4	428

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109	Inhibition of Monoamine Oxidases by Functionalized Coumarin Derivatives:Â Biological Activities, QSARs, and 3D-QSARs. Journal of Medicinal Chemistry, 2000, 43, 4747-4758.	6.4	248
110	Reversible Inhibition of MAO-A and B by Diazoheterocyclic Compounds: Development of QSAR/CoMFA Models. , 2000, , 353-354.		0
111	Ionic partition diagrams of ionisable drugs: pH-lipophilicity profiles, transfer mechanisms and charge effects on solvation. Journal of Electroanalytical Chemistry, 1999, 462, 235-250.	3.8	113
112	Production and characterization of 22 monoclonal antibodies directed against S 20499, a new potent 5-HT1A chiral agonist: influence of the hapten structure on specificity and stereorecognition. Pharmaceutical Research, 1999, 16, 725-735.	3.5	1
113	The pH-partition profile of the anti-ischemic drug trimetazidine may explain its reduction of intracellular acidosis. Pharmaceutical Research, 1999, 16, 616-624.	3.5	29
114	Effects of Charge and Intramolecular Structure on the Lipophilicity of Nitrophenols. Journal of the American Chemical Society, 1999, 121, 1743-1747.	13.7	58
115	Combined molecular lipophilicity descriptors and their role in understanding intramolecular effects. Pharmaceutical Science & Technology Today, 1999, 2, 327-335.	0.7	65
116	Development of a Capillary Electrophoresis Method to Monitor Protein Oxidation and Antioxidant Protection. Helvetica Chimica Acta, 1999, 82, 870-878.	1.6	10
117	Structure-Lipophilicity Relationships of Neutral and ProtonatedÎ²-Blockers, Part I, Intra- and Intermolecular Effects in Isotropic Solvent Systems. Helvetica Chimica Acta, 1999, 82, 1211-1222.	1.6	91
118	Charge and Delocalisation Effects on the Lipophilicity of Protonable Drugs. Chemistry - A European Journal, 1999, 5, 39-47.	3.3	78
119	Monoamine oxidase inhibitory properties of some benzazoles: Structure-; Activity relationships. AAPS PharmSci, 1999, 1, 1-4.	1.3	65
120	Mechanism and dynamics of methyl and ethyl orange transfer across the water/1,2-dichloroethane interface. Electrochimica Acta, 1998, 44, 3-13.	5.2	45
121	Mechanisms of liposomes/water partitioning of (p-methylbenzyl)alkylamines. Pharmaceutical Research, 1998, 15, 1407-1413.	3.5	38
122	Inhibition of Monoamine Oxidase-B by Condensed Pyridazines and Pyrimidines:Â Effects of Lipophilicity and Structureâ˜Activity Relationships. Journal of Medicinal Chemistry, 1998, 41, 3812-3820.	6.4	84
123	Evidence for the existence of [3 H]-trimetazidine binding sites involved in the regulation of the mitochondrial permeability transition pore. British Journal of Pharmacology, 1998, 123, 1385-1394.	5.4	46
124	Facilitated ion transfer reactions across oil|water interfaces. Journal of Electroanalytical Chemistry, 1998, 451, 59-76.	3.8	108
125	Facilitated ion transfer reactions across oil|water interfaces. Part I. Algebraic development and calculation of cyclic voltammetry experiments for successive complex formation. Journal of Electroanalytical Chemistry, 1998, 449, 49-65.	3.8	82
126	Isoquinoline derivatives as endogenous neurotoxins in the aetiology of Parkinsonâ€™s disease. Biochemical Pharmacology, 1998, 56, 921-933.	4.4	120

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127	Structureâ€"Property Relationships of Trimetazidine Derivatives and Model Compounds as Potential Antioxidants. Free Radical Biology and Medicine, 1998, 25, 113-120.	2.9	165
128	Theoretical Parameters to Characterize Antioxidants. Part 2. The cases of melatonin and carvedilol. Helvetica Chimica Acta, 1998, 81, 1337-1348.	1.6	17
129	Molecular Properties and Pharmacokinetic Behavior of Cetirizine, a Zwitterionic H₁-Receptor Antagonist. Journal of Medicinal Chemistry, 1998, 41, 853-863.	6.4	122
130	Chiral Inversion and Hydrolysis of Thalidomide:Â Mechanisms and Catalysis by Bases and Serum Albumin, and Chiral Stability of Teratogenic Metabolites. Chemical Research in Toxicology, 1998, 11, 1521-1528.	3.3	121
131	Ligand Specificity of the Genetic Variants of Human Î±₁-Acid Glycoprotein: Generation of a Three-Dimensional Quantitative Structure-Activity Relationship Model for Drug Binding to the A Variant. Molecular Pharmacology, 1998, 54, 129-138.	2.3	103
132	Intermolecular forces expressed in 1,2-dichloroethaneâ€"water partition coefficients. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 401-406.	1.7	74
133	Solvatochromic analysis of di-n-butyl ether/water partition coefficients as compared to other solvent systems. Journal of the Chemical Society Perkin Transactions II, 1997, , 2639-2644.	0.9	24
134	Lipophilicity Profiles of Ampholytes. Chemical Reviews, 1997, 97, 3385-3400.	47.7	139
135	Cyclic voltammetry for the transfer of multiple charged ions at large ITIES: general computational methodology and application to simple and facilitated ion transfer reactions. Journal of Electroanalytical Chemistry, 1997, 424, 121-139.	3.8	41
136	Blood-to-brain transfer of various oxicams: effects of plasma binding on their brain delivery. Pharmaceutical Research, 1997, 14, 650-656.	3.5	47
137	Pharmacokinetics of Î²-adrenoceptor blockers in obese and normal volunteers. British Journal of Clinical Pharmacology, 1997, 43, 563-570.	2.4	74
138	Theoretical Parameters to Characterize Antioxidants. Part 1. The case of vitamin E and analogs. Helvetica Chimica Acta, 1997, 80, 1613-1626.	1.6	71
139	A systems approach to molecular structure, intermolecular recognition, and emergence-dissolvence in medicinal research. , 1997, 17, 303-326.		39
140	Toxicity to PC12 cells of isoquinoline derivatives structurally related to 1-methyl-4-phenyl-1,2,3,6-tetrahydropyridine. Neuroscience Letters, 1996, 206, 37-40.	2.1	31
141	Effects of isoquinoline derivatives structurally related to 1-methyl-4-phenyl-1,2,3,6-tetrahydropyridine (MPTP) on mitochondrial respiration. Biochemical Pharmacology, 1996, 51, 1503-1511.	4.4	44
142	Inhibition of [3H]dopamine uptake into striatal synaptosomes by isoquinoline derivatives structurally related to 1-methyl-4-phenyl-1,2,3,6-tetrahydropyridine. Biochemical Pharmacology, 1996, 52, 29-34.	4.4	36
143	Binding of Arylpiperazines, (Aryloxy)propanolamines, and Tetrahydropyridylindoles to the 5-HT1AReceptor:Â Contribution of the Molecular Lipophilicity Potential to Three-Dimensional Quantitative Structureâ^'Affinity Relationship Models. Journal of Medicinal Chemistry, 1996, 39, 126-134.	6.4	53
144	Nigral Cell Loss Produced by Infusion of Isoquinoline Derivatives Structurally Related to 1-Methyl-4-Phenyl-1,2,3,6-Tetrahydropyridine. Experimental Neurology, 1996, 5, 265-274.	1.7	25

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145	Ionic Partition Diagrams:Â A Potentialâ˜pH Representation. Journal of the American Chemical Society, 1996, 118, 11951-11957.	13.7	116
146	Lipophilicity in molecular modeling. Pharmaceutical Research, 1996, 13, 335-343.	3.5	145
147	Insight into the lipophilicity of the aromatic N-oxide moiety. Pharmaceutical Research, 1996, 13, 1186-1190.	3.5	19
148	Mechanism of Transfer of a Basic Drug across the Water/1,2-Dichloroethane Interface: The case of quinidine. Helvetica Chimica Acta, 1996, 79, 101-117.	1.6	66
149	Kinetics and Mechanisms of Racemization: 5-Substituted Hydantoins (= Imidazolidine-2,4-diones) as Models of Chiral Drugs. Helvetica Chimica Acta, 1996, 79, 767-778.	1.6	25
150	Electrochemical Behaviour and Antioxidant Activity of Some Natural Polyphenols. Helvetica Chimica Acta, 1996, 79, 1147-1158.	1.6	91
151	How do antibodies and lectins recognize histo-blood group antigens? A 3D-QSAR study by comparative molecular field analysis (CoMFA). Bioorganic and Medicinal Chemistry, 1996, 4, 1979-1988.	3.0	18
152	Knowledge-based modeling of a legume lectin and docking of the carbohydrate ligand: The Ulex europaeus lectin I and its interaction with fucose. Journal of Molecular Graphics, 1996, 14, 322-327.	1.1	20
153	Inhibition of Î±-Ketoglutarate dehydrogenase by isoquinoline derivatives structurally related to 1 -methyl-4-phenyl-1,2,3,6-tetrahydropyridine (MPTP). NeuroReport, 1995, 6, 1105-1108.	1.2	45
154	Racemization, enantiomerization, diastereomerization, and epimerization: Their meaning and pharmacological significance. Chirality, 1995, 7, 396-400.	2.6	149
155	Low configurational stability of amfepramone and cathinone: Mechanism and kinetics of chiral inversion. Chirality, 1995, 7, 469-473.	2.6	21
156	Structure-Lipophilicity and Structure-Polarity relationships of amino acids and peptides. Helvetica Chimica Acta, 1995, 78, 471-485.	1.6	30
157	Microscopic Protonation/Deprotonation Equilibria of the Anti-Inflammatory Agent Piroxicam. Helvetica Chimica Acta, 1995, 78, 553-562.	1.6	46
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