Nicolas Moitessier

List of Publications by Year
in descending order

89 papers	3,242 citations	126907 33 h-index	168389 53 g-index
108 all docs	108 docs citations	108 times ranked	3974 citing authors

#	Article	IF	Citations
1	Design, synthesis and inÂvitro evaluation of novel SARS-CoV-2 3CLpro covalent inhibitors. European Journal of Medicinal Chemistry, 2022, 229, 114046.	5.5	41
2	Docking Ligands into Flexible and Solvated Macromolecules. 8. Forming New Bondsâ”€Challenges and Opportunities. Journal of Chemical Information and Modeling, 2022, 62, 1061-1077.	5.4	6
3	Novel Aurora A and Protein Kinase C (Î±, Î²1, Î²2, and Îɣ) Multitarget Inhibitors: Impact of Selenium Atoms on the Potency and Selectivity. Journal of Medicinal Chemistry, 2022, 65, 3134-3150.	6.4	8
4	Modulating the selectivity of inhibitors for prolyl oligopeptidase inhibitors and fibroblast activation protein-Î± for different indications. European Journal of Medicinal Chemistry, 2022, 240, 114543.	5.5	2
5	A cryptic third active site in cyanophycin synthetase creates primers for polymerization. Nature Communications, 2022, 13, .	12.8	12
6	Mutations in Dynamic Structural Elements Alter the Kinetics and Fidelity of the Multifunctional Class II Lanthipeptide Synthetase, HalM2. Biochemistry, 2021, 60, 412-430.	2.5	8
7	Targeting MYC: From understanding its biology to drug discovery. European Journal of Medicinal Chemistry, 2021, 213, 113137.	5.5	17
8	Discovery of covalent prolyl oligopeptidase boronic ester inhibitors. European Journal of Medicinal Chemistry, 2020, 185, 111783.	5.5	11
9	Augmented base pairing networks encode RNA-small molecule binding preferences. Nucleic Acids Research, 2020, 48, 7690-7699.	14.5	30
10	From desktop to benchtop with automated computational workflows for computer-aided design in asymmetric catalysis. Nature Catalysis, 2020, 3, 574-584.	34.4	31
11	Enzyme Kinetics by Isothermal Titration Calorimetry: Allostery, Inhibition, and Dynamics. Frontiers in Molecular Biosciences, 2020, 7, 583826.	3.5	40
12	Use of Extended-HÃ¼ckel Descriptors for Rapid and Accurate Predictions of Conjugated Torsional Energy Barriers. Journal of Chemical Information and Modeling, 2020, 60, 3534-3545.	5.4	5
13	Design and discovery of boronic acid drugs. European Journal of Medicinal Chemistry, 2020, 195, 112270.	5.5	113
14	Integrated Synthetic, Biophysical, and Computational Investigations of Covalent Inhibitors of Prolyl Oligopeptidase and Fibroblast Activation Protein Î±. Journal of Medicinal Chemistry, 2019, 62, 7874-7884.	6.4	9
15	Atom Type Independent Modeling of the Conformational Energy of Benzylic, Allylic, and Other Bonds Adjacent to Conjugated Systems. Journal of Chemical Information and Modeling, 2019, 59, 4750-4763.	5.4	5
16	Torsional Energy Barriers of Biaryls Could Be Predicted by Electron Richness/Deficiency of Aromatic Rings; Advancement of Molecular Mechanics toward Atom-Type Independence. Journal of Chemical Information and Modeling, 2019, 59, 4764-4777.	5.4	11
17	Predicting Positions of Bridging Water Molecules in Nucleic Acidâ€“Ligand Complexes. Journal of Chemical Information and Modeling, 2019, 59, 2941-2951.	5.4	14
18	Automated, customizable and efficient identification of 3D base pair modules with BayesPairing. Nucleic Acids Research, 2019, 47, 3321-3332.	14.5	11

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19	Challenges and current status of computational methods for docking small molecules to nucleic acids. European Journal of Medicinal Chemistry, 2019, 168, 414-425.	5.5	48
20	Rapid measurement of inhibitor binding kinetics by isothermal titration calorimetry. Nature Communications, 2018, 9, 893.	12.8	43
21	Atom Types Independent Molecular Mechanics Method for Predicting the Conformational Energy of Small Molecules. Journal of Chemical Information and Modeling, 2018, 58, 194-205.	5.4	13
22	Revised Mechanism for a Ruthenium-Catalyzed Coupling of Aldehyde and Terminal Alkyne. ACS Omega, 2018, 3, 3218-3227.	3.5	8
23	Adjusting the Structure of 2â€²-Modified Nucleosides and Oligonucleotides via C4â€²-Î±-F or C4â€²-Î±-OMe Substitution: Synthesis and Conformational Analysis. Journal of Organic Chemistry, 2018, 83, 9839-9849.	3.2	33
24	Complete Kinetic Characterization of Enzyme Inhibition in a Single Isothermal Titration Calorimetric Experiment. Analytical Chemistry, 2018, 90, 8430-8435.	6.5	18
25	Exploring Atypical Fluorineâ€“Hydrogen Bonds and Their Effects on Nucleoside Conformations. Chemistry - A European Journal, 2018, 24, 16432-16439.	3.3	13
26	Customizable Generation of Synthetically Accessible, Local Chemical Subspaces. Journal of Chemical Information and Modeling, 2017, 57, 454-467.	5.4	13
27	Fluoride-Mediated Desulfonylative Intramolecular Cyclization to Fused and Bridged Bicyclic Compounds: A Complex Mechanism. Journal of Organic Chemistry, 2017, 82, 2579-2588.	3.2	3
28	Active Site Crowding of Cytochrome P450 3A4 as a Strategy To Alter Its Selectivity. ChemBioChem, 2017, 18, 248-252.	2.6	13
29	Highly Regioselective Monoacylation of Unprotected Glucopyranoside Using Transient Directingâ€Protecting Groups. European Journal of Organic Chemistry, 2017, 2017, 646-656.	2.4	12
30	Measuring Rapid Time-Scale Reaction Kinetics Using Isothermal Titration Calorimetry. Analytical Chemistry, 2017, 89, 7022-7030.	6.5	30
31	Covalent inhibitors design and discovery. European Journal of Medicinal Chemistry, 2017, 138, 96-114.	5.5	212
32	Accurately Modeling the Conformational Preferences of Nucleosides. Journal of the American Chemical Society, 2017, 139, 13620-13623.	13.7	28
33	4â€²-C-Methoxy-2â€²-deoxy-2â€²-fluoro Modified Ribonucleotides Improve Metabolic Stability and Elicit Efficient RNAi-Mediated Gene Silencing. Journal of the American Chemical Society, 2017, 139, 14542-14555.	13.7	49
34	Elucidating Hyperconjugation from Electronegativity to Predict Drug Conformational Energy in a High Throughput Manner. Journal of Chemical Information and Modeling, 2016, 56, 788-801.	5.4	9
35	Regioselective acylation, alkylation, silylation and glycosylation of monosaccharides. Tetrahedron, 2016, 72, 6283-6319.	1.9	81
36	Medicinal Chemistry Projects Requiring Imaginative Structure-Based Drug Design Methods. Accounts of Chemical Research, 2016, 49, 1646-1657.	15.6	40

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37	3-Oxo-hexahydro-1H-isoindole-4-carboxylic Acid as a Drug Chiral Bicyclic Scaffold: Structure-Based Design and Preparation of Conformationally Constrained Covalent and Noncovalent Prolyl Oligopeptidase Inhibitors. Journal of Medicinal Chemistry, 2016, 59, 4221-4234.	6.4	21
38	Azoâ‹¯phenyl stacking: a persistent self-assembly motif guides the assembly of fluorinated cis-azobenzenes into photo-mechanical needle crystals. Chemical Communications, 2016, 52, 2103-2106.	4.1	35
39	Metabolic Instability of Cyanothiazolidineâ€Based Prolyl Oligopeptidase Inhibitors: a Structural Assignment Challenge and Potential Medicinal Chemistry Implications. ChemMedChem, 2015, 10, 1174-1183.	3.2	9
40	Understanding P450â€mediated Bioâ€transformations into Epoxide and Phenolic Metabolites. Angewandte Chemie - International Edition, 2015, 54, 13743-13747.	13.8	17
41	Single-Point Mutation with a Rotamer Library Toolkit: Toward Protein Engineering. Journal of Chemical Information and Modeling, 2015, 55, 2657-2671.	5.4	6
42	Design, synthesis and evaluation of antiestrogen and histone deacetylase inhibitor molecular hybrids. Bioorganic and Medicinal Chemistry, 2015, 23, 7597-7606.	3.0	28
43	Discovery of novel small-molecule antagonists for GluK2. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 2416-2420.	2.2	1
44	Solvent effect in diastereoselective intramolecular Dielsâ€“Alder reactions. Tetrahedron Letters, 2015, 56, 6852-6856.	1.4	8
45	Docking Ligands into Flexible and Solvated Macromolecules. 7. Impact of Protein Flexibility and Water Molecules on Docking-Based Virtual Screening Accuracy. Journal of Chemical Information and Modeling, 2014, 54, 3198-3210.	5.4	27
46	Docking Ligands into Flexible and Solvated Macromolecules. 6. Development and Application to the Docking of HDACs and other Zinc Metalloenzymes Inhibitors. Journal of Chemical Information and Modeling, 2014, 54, 254-265.	5.4	39
47	Methods for Docking Small Molecules to Macromolecules: A Userâ€™s Perspective. 1. The Theory. Current Pharmaceutical Design, 2014, 20, 3338-3359.	1.9	20
48	Methods for Docking Small Molecules to Macromolecules: A Userâ€™s Perspective. 2. Applications. Current Pharmaceutical Design, 2014, 20, 3360-3372.	1.9	8
49	A Platinum(II) Phenylphenanthroimidazole with an Extended Sideâ€Chain Exhibits Slow Dissociation from a câ€Kit Gâ€Quadruplex Motif. Chemistry - A European Journal, 2013, 19, 17836-17845.	3.3	28
50	Stereo- and Regioselective Synthesis of Polysubstituted Chiral 1,4-Oxazepanes. Journal of Organic Chemistry, 2013, 78, 872-885.	3.2	15
51	Integrating Medicinal Chemistry, Organic/Combinatorial Chemistry, and Computational Chemistry for the Discovery of Selective Estrogen Receptor Modulators with F<scp>orecaster</scp>, a Novel Platform for Drug Discovery. Journal of Chemical Information and Modeling, 2012, 52, 210-224.	5.4	39
52	Development of a Computational Tool to Rival Experts in the Prediction of Sites of Metabolism of Xenobiotics by P450s. Journal of Chemical Information and Modeling, 2012, 52, 2471-2483.	5.4	52
53	Virtual Screening and Computational Optimization for the Discovery of Covalent Prolyl Oligopeptidase Inhibitors with Activity in Human Cells. Journal of Medicinal Chemistry, 2012, 55, 6306-6315.	6.4	47
54	Platinum(II) Phenanthroimidazoles for Targeting Telomeric Gâ€Quadruplexes. ChemMedChem, 2012, 7, 85-94.	3.2	35

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55	Directing/protecting groups mediate highly regioselective glycosylation of monoprotected acceptors. Tetrahedron, 2011, 67, 8411-8420.	1.9	26
56	Toward a computational tool predicting the stereochemical outcome of asymmetric reactions: Development of the molecular mechanicsâ€based program ACE and application to asymmetric epoxidation reactions. Journal of Computational Chemistry, 2011, 32, 2878-2889.	3.3	31
57	Theory and application of medium to high throughput prediction method techniques for asymmetric catalyst designâ˜†. Journal of Molecular Catalysis A, 2010, 324, 146-155.	4.8	20
58	Expedient synthesis of novel bicyclic peptidomimetic scaffolds. Tetrahedron Letters, 2010, 51, 2820-2823.	1.4	8
59	Inhibitors of Prolyl Oligopeptidases for the Therapy of Human Diseases: Defining Diseases and Inhibitors. Journal of Medicinal Chemistry, 2010, 53, 3423-3438.	6.4	80
60	Modeling Reality for Optimal Docking of Small Molecules to Biological Targets. Current Computer-Aided Drug Design, 2009, 5, 241-263.	1.2	13
61	Functional Characterization and In Silico Docking of Full and Partial GluK2 Kainate Receptor Agonists. Molecular Pharmacology, 2009, 75, 1096-1107.	2.3	19
62	Docking Ligands into Flexible and Solvated Macromolecules. 5. Force-Field-Based Prediction of Binding Affinities of Ligands to Proteins. Journal of Chemical Information and Modeling, 2009, 49, 2564-2571.	5.4	36
63	Constrained Peptidomimetics Reveal Detailed Geometric Requirements of Covalent Prolyl Oligopeptidase Inhibitors. Journal of Medicinal Chemistry, 2009, 52, 6672-6684.	6.4	47
64	Docking Ligands into Flexible and Solvated Macromolecules. 4. Are Popular Scoring Functions Accurate for this Class of Proteins?. Journal of Chemical Information and Modeling, 2009, 49, 1568-1580.	5.4	77
65	Docking Ligands into Flexible and Solvated Macromolecules. 3. Impact of Input Ligand Conformation, Protein Flexibility, and Water Molecules on the Accuracy of Docking Programs. Journal of Chemical Information and Modeling, 2009, 49, 997-1009.	5.4	101
66	Platinum Phenanthroimidazole Complexes as Gâ€Quadruplex DNA Selective Binders. Chemistry - A European Journal, 2008, 14, 1145-1154.	3.3	113
67	Toward a Computational Tool Predicting the Stereochemical Outcome of Asymmetric Reactions: Development and Application of a Rapid and Accurate Program Based on Organic Principles. Angewandte Chemie - International Edition, 2008, 47, 2635-2638.	13.8	37
68	Docking Ligands into Flexible and Solvated Macromolecules. 2. Development and Application of Fitted 1.5 to the Virtual Screening of Potential HCV Polymerase Inhibitors. Journal of Chemical Information and Modeling, 2008, 48, 902-909.	5.4	60
69	A Platinum Supramolecular Square as an Effective G-Quadruplex Binder and Telomerase Inhibitor. Journal of the American Chemical Society, 2008, 130, 10040-10041.	13.7	200
70	Docking Ligands into Flexible and Solvated Macromolecules. 1. Development and Validation of FITTED 1.0. Journal of Chemical Information and Modeling, 2007, 47, 435-449.	5.4	182
71	Evaluation of docking programs for predicting binding of Golgi Î±-mannosidase II inhibitors: A comparison with crystallography. Proteins: Structure, Function and Bioinformatics, 2007, 69, 160-176.	2.6	55
72	A Method for Induced-Fit Docking, Scoring, and Ranking of Flexible Ligands. Application to Peptidic and Pseudopeptidic Î²-secretase (BACE 1) Inhibitors. Journal of Medicinal Chemistry, 2006, 49, 5885-5894.	6.4	60

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73	Docking of Aminoglycosides to Hydrated and Flexible RNA. Journal of Medicinal Chemistry, 2006, 49, 1023-1033.	6.4	93
74	Orthogonally protected carbohydrate-based scaffolds. Tetrahedron Letters, 2005, 46, 6191-6194.	1.4	13
75	Directing-protecting groups for carbohydrates. Design, conformational study, synthesis and application to regioselective functionalization. Tetrahedron, 2005, 61, 6839-6853.	1.9	48
76	Combining Pharmacophore Search, Automated Docking, and Molecular Dynamics Simulations as a Novel Strategy for Flexible Docking. Proof of Concept:Â Docking of Argincineâ^'Glycineâ^'Aspartic Acid-like Compounds into the Î±vÎ²3Binding Site. Journal of Medicinal Chemistry, 2004, 47, 4178-4187.	6.4	53
77	Modulation of the relative reactivities of carbohydrate secondary hydroxyl groups. Modification of the hydrogen bond network. Tetrahedron Letters, 2003, 44, 1731-1735.	1.4	26
78	On the Origin of the Facial Selectivity of the Sharpless Asymmetric Dihydroxylation of Styrene Derivatives. Journal of Carbohydrate Chemistry, 2003, 22, 25-34.	1.1	8
79	Vitronectin Receptor -αVβ3 Integrin- Antagonists: Chemical and Structural Requirements for Activity and Selectivity. Mini-Reviews in Medicinal Chemistry, 2002, 2, 531-542.	2.4	27
80	Toward a Computational Tool Predicting the Stereochemical Outcome of Asymmetric Reactions. 1. Application to Sharpless Asymmetric Dihydroxylation. Journal of Organic Chemistry, 2002, 67, 7275-7282.	3.2	39
81	d-myo-Inositol-1,4,5-trisphosphate and Adenophostin Mimics: Importance of the Spatial Orientation of a Phosphate Group on the Biological Activity. Bioorganic and Medicinal Chemistry, 2002, 10, 759-768.	3.0	16
82	Design and Synthesis of Matrix Metalloproteinase Inhibitors Guided by Molecular Modeling. Picking the S1Pocket Using Conformationally Constrained Inhibitors. Journal of Medicinal Chemistry, 2001, 44, 3074-3082.	6.4	51
83	N-Aryl Sulfonyl Homocysteine Hydroxamate Inhibitors of Matrix Metalloproteinases:Â Further Probing of the S1, S1â€˜, and S2â€˜ Pockets. Journal of Medicinal Chemistry, 2001, 44, 3066-3073.	6.4	45
84	Design, modeling and synthesis of functionalized paromamine analogs. Tetrahedron, 2001, 57, 3255-3265.	1.9	38
85	Design, synthesis and preliminary biological evaluation of a focused combinatorial library of stereodiverse carbohydrate-scaffold-based peptidomimetics. Bioorganic and Medicinal Chemistry, 2001, 9, 511-523.	3.0	50
86	A comparative docking study and the design of potentially selective MMP inhibitors. Journal of Computer-Aided Molecular Design, 2001, 15, 873-881.	2.9	27
87	Molecular Dynamics-Based Models Explain the Unexpected Diastereoselectivity of the Sharpless Asymmetric Dihydroxylation of Allyl D-Xylosides. European Journal of Organic Chemistry, 2000, 2000, 995-1005.	2.4	31
88	Elucidation of a common structure of selective fibrinogen receptor antagonists. Journal of Computer-Aided Molecular Design, 1998, 12, 533-542.	2.9	6
89	Asymmetric dihydroxylation of d-xylose-derived allyl ethers. Tetrahedron: Asymmetry, 1997, 8, 2889-2892.	1.8	16