Edward C Sherer

List of Publications by Year
in descending order

99 papers	3,684 citations	147801 31 h-index	149698 56 g-index
102 all docs	102 docs citations	102 times ranked	4565 citing authors

#	Article	IF	Citations
1	Application of Machine Learning and Reaction Optimization for the Iterative Improvement of Enantioselectivity of Cinchona-Derived Phase Transfer Catalysts. Organic Process Research and Development, 2022, 26, 670-682.	2.7	14
2	Driving to a Better Understanding of Acyl Glucuronide Transformations Using NMR and Molecular Modeling. Chemical Research in Toxicology, 2022, 35, 459-474.	3.3	2
3	Driving Aspirational Process Mass Intensity Using Simple Structure-Based Prediction. Organic Process Research and Development, 2022, 26, 1405-1410.	2.7	8
4	Solution cis-Proline Conformation of IPCs Inhibitor Aureobasidin A Elucidated via NMR-Based Conformational Analysis. Journal of Natural Products, 2022, 85, 1449-1458.	3.0	6
5	Structural revision of a Wnt/Î²-catenin modulator and confirmation of cannabielsoin constitution and configuration. Chemical Communications, 2021, 57, 5658-5661.	4.1	12
6	Identification and characterization of a residual host cell protein hexosaminidase B associated with Nâ€glycan degradation during the stability study of a therapeutic recombinant monoclonal antibody product. Biotechnology Progress, 2021, 37, e3128.	2.6	20
7	Conformational Strain of Macrocyclic Peptides in Ligandâ€“Receptor Complexes Based on Advanced Refinement of Bound-State Conformers. Journal of Medicinal Chemistry, 2021, 64, 3282-3298.	6.4	7
8	Unequivocal structure confirmation of a breitfussin analog by anisotropic NMR measurements. Chemical Science, 2020, 11, 12081-12088.	7.4	9
9	Combination of HDX-MS and in silico modeling to study enzymatic reactivity and stereo-selectivity at different solvent conditions. Journal of Pharmaceutical and Biomedical Analysis, 2020, 182, 113141.	2.8	5
10	Applications of Quantum Chemistry in Pharmaceutical Process Development: Current State and Opportunities. Organic Process Research and Development, 2020, 24, 1496-1507.	2.7	25
11	Analysis of Benzenoid Substitution Patterns in Small Molecule Active Pharmaceutical Ingredients. Journal of Medicinal Chemistry, 2020, 63, 13389-13396.	6.4	51
12	â€œOne-Shotâ€•Measurement of Residual Chemical Shift Anisotropy Using Poly-Î³-benzyl-<scp>l</scp>-glutamate as an Alignment Medium. Organic Letters, 2020, 22, 8850-8854.	4.6	11
13	XGen: Real-Space Fitting of Complex Ligand Conformational Ensembles to X-ray Electron Density Maps. Journal of Medicinal Chemistry, 2020, 63, 10509-10528.	6.4	8
14	Denigrins and Dactylpyrroles, Arylpyrrole Alkaloids from a Dactylia sp. Marine Sponge. Journal of Natural Products, 2020, 83, 3464-3470.	3.0	15
15	Synergism of anisotropic and computational NMR methods reveals the likely configuration of phormidolide A. Chemical Communications, 2020, 56, 7565-7568.	4.1	20
16	Direct regioisomer analysis of crude reaction mixtures via molecular rotational resonance (MRR) spectroscopy. Chemical Science, 2020, 11, 6332-6338.	7.4	18
17	The merger of decatungstate and copper catalysis to enable aliphatic C(sp3)â€“H trifluoromethylation. Nature Chemistry, 2020, 12, 459-467.	13.6	226
18	Synthesis of Fused Oxepane HIV Integrase Inhibitor MK-1376. Synthesis, 2020, 52, 3378-3388.	2.3	3

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19	Deep Dive into Machine Learning Models for Protein Engineering. Journal of Chemical Information and Modeling, 2020, 60, 2773-2790.	5.4	134
20	Optical Chirality Sensing with a Stereodynamic Aluminum Biphenolate Probe. Journal of Organic Chemistry, 2019, 84, 4639-4645.	3.2	20
21	The PMI Predictor app to enable green-by-design chemical synthesis. Nature Sustainability, 2019, 2, 1034-1040.	23.7	36
22	¹³C NMR-Based Approaches for Solving Challenging Stereochemical Problems. Organic Letters, 2019, 21, 4072-4076.	4.6	16
23	Complex macrocycle exploration: parallel, heuristic, and constraint-based conformer generation using ForceGen. Journal of Computer-Aided Molecular Design, 2019, 33, 531-558.	2.9	29
24	PBLG as a versatile liquid crystalline medium for anisotropic NMR data acquisition. Chemical Communications, 2019, 55, 4327-4330.	4.1	27
25	Design of an in vitro biocatalytic cascade for the manufacture of islatravir. Science, 2019, 366, 1255-1259.	12.6	383
26	Highly Diastereoselective Synthesis of a HCV NS5B Nucleoside Polymerase Inhibitor. Journal of Organic Chemistry, 2019, 84, 4780-4795.	3.2	5
27	Application of anisotropic NMR parameters to the confirmation of molecular structure. Nature Protocols, 2019, 14, 217-247.	12.0	101
28	Computational prediction of chemical reactions: current status and outlook. Drug Discovery Today, 2018, 23, 1203-1218.	6.4	126
29	Enhanced measurement of residual chemical shift anisotropy for small molecule structure elucidation. Chemical Communications, 2018, 54, 4254-4257.	4.1	32
30	Beyond optical rotation: what's left is not always right in total synthesis. Chemical Science, 2018, 9, 415-424.	7.4	23
31	Overcoming Time-Dependent Inhibition (TDI) of Cytochrome P450 3A4 (CYP3A4) Resulting from Bioactivation of a Fluoropyrimidine Moiety. Journal of Medicinal Chemistry, 2018, 61, 10700-10708.	6.4	11
32	Combining traditional 2D and modern physical organic-derived descriptors to predict enhanced enantioselectivity for the key aza-Michael conjugate addition in the synthesis of Prevymisâ„¢ (letermovir). Chemical Science, 2018, 9, 6922-6927.	7.4	22
33	Post-Synthetic Modification of Oligonucleotides via Orthogonal Amidation and Copper Catalyzed Cycloaddition Reactions. Bioconjugate Chemistry, 2018, 29, 1859-1865.	3.6	5
34	A rational pre-catalyst design for bis-phosphine mono-oxide palladium catalyzed reactions. Chemical Science, 2017, 8, 2841-2851.	7.4	24
35	Ruthenium-Catalyzed Dynamic Kinetic Resolution Asymmetric Transfer Hydrogenation of Î²-Chromanones by an Elimination-Induced Racemization Mechanism. ACS Catalysis, 2017, 7, 1446-1451.	11.2	51
36	Microscale High-Throughput Experimentation as an Enabling Technology in Drug Discovery: Application in the Discovery of (Piperidinyl)pyridinyl-1H-benzimidazole Diacylglycerol Acyltransferase 1 Inhibitors. Journal of Medicinal Chemistry, 2017, 60, 3594-3605.	6.4	65

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37	The protecting-group free selective 3â€²-functionalization of nucleosides. Chemical Science, 2017, 8, 2804-2810.	7.4	10
38	Mechanistic Study of the Gas-Phase In-Source Hofmann Elimination of Doubly Quaternized Cinchona-Alkaloid Based Phase-Transfer Catalysts by (+)-Electrospray Ionization/Tandem Mass Spectrometry. Journal of the American Society for Mass Spectrometry, 2017, 28, 452-460.	2.8	7
39	A multifunctional catalyst that stereoselectively assembles prodrugs. Science, 2017, 356, 426-430.	12.6	116
40	Sustainable Practices in Medicinal Chemistry Part 2: Green by Design. Journal of Medicinal Chemistry, 2017, 60, 5955-5968.	6.4	17
41	Unequivocal determination of complex molecular structures using anisotropic NMR measurements. Science, 2017, 356, .	12.6	124
42	Discovery of selective, orally bioavailable, N -linked arylsulfonamide Na v 1.7 inhibitors with pain efficacy in mice. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 2087-2093.	2.2	38
43	Absolute configuration assignment of (+)â€fluralaner using vibrational circular dichroism. Chirality, 2017, 29, 854-864.	2.6	8
44	Model for the Enantioselectivity of Asymmetric Intramolecular Alkylations by Bis-Quaternized Cinchona Alkaloid-Derived Catalysts. Journal of Organic Chemistry, 2017, 82, 8645-8650.	3.2	29
45	Selective Formation of Functionalized Î±-Quaternary Malononitriles toward 5,5-Disubstituted Pyrrolopyrimidinones. Organic Letters, 2017, 19, 4448-4451.	4.6	4
46	Asymmetric Formal Synthesis of the Long-Acting DPP-4 Inhibitor Omarigliptin. Journal of Organic Chemistry, 2017, 82, 9023-9029.	3.2	13
47	Mining Chromatographic Enantioseparation Data Using Matched Molecular Pair Analysis. Molecules, 2016, 21, 1297.	3.8	7
48	Discovery and development of benzo-[1,2,4]-triazolo-[1,4]-oxazepine GPR142 agonists for the treatment of diabetes. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 2947-2951.	2.2	15
49	Toward structure-based predictive tools for the selection of chiral stationary phases for the chromatographic separation of enantiomers. Journal of Chromatography A, 2016, 1467, 206-213.	3.7	29
50	Expedited Selection of NMR Chiral Solvating Agents for Determination of Enantiopurity. ACS Central Science, 2016, 2, 332-340.	11.3	58
51	Discovery and Optimization of a Novel Triazole Series of GPR142 Agonists for the Treatment of Type 2 Diabetes. ACS Medicinal Chemistry Letters, 2016, 7, 1107-1111.	2.8	12
52	Systematic chemical modifications of single stranded siRNAs significantly improved CTNNB1 mRNA silencing. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 4513-4517.	2.2	7
53	Discovery of N-[Bis(4-methoxyphenyl)methyl]-4-hydroxy-2-(pyridazin-3-yl)pyrimidine-5-carboxamide (MK-8617), an Orally Active Pan-Inhibitor of Hypoxia-Inducible Factor Prolyl Hydroxylase 1â€“3 (HIF PHD1â€“3) for the Treatment of Anemia. Journal of Medicinal Chemistry, 2016, 59, 11039-11049.	6.4	37
54	Determination of Relative Configuration from Residual Chemical Shift Anisotropy. Journal of the American Chemical Society, 2016, 138, 9548-9556.	13.7	86

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55	Optimization of Novel Aza-benzimidazolone mGluR2 PAMs with Respect to LLE and PK Properties and Mitigation of CYP TDI. ACS Medicinal Chemistry Letters, 2016, 7, 312-317.	2.8	8
56	Definitive Metabolite Identification Coupled with Automated Ligand Identification System (ALIS) Technology: A Novel Approach to Uncover Structureâ€"Activity Relationships and Guide Drug Design in a Factor IXa Inhibitor Program. Journal of Medicinal Chemistry, 2016, 59, 1818-1829.	6.4	17
57	SAR exploration at the C-3 position of tetrahydro-Î²-carboline sstr3 antagonists. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 1529-1535.	2.2	8
58	Antenna Biphenols: Development of Extended Wavelength Chiroptical Reporters. Journal of Organic Chemistry, 2016, 81, 1185-1191.	3.2	23
59	Homodecoupled 1,1â€•and 1,nâ€ADEQUATE: Pivotal NMR Experiments for the Structure Revision of Cryptospirolepine. Angewandte Chemie - International Edition, 2015, 54, 10160-10164.	13.8	49
60	Development of a novel class of potent and selective FIXa inhibitors. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 4945-4949.	2.2	16
61	Heterocyclic Regioisomer Enumeration (HREMS): A Cheminformatics Design Tool. Journal of Chemical Information and Modeling, 2015, 55, 1130-1135.	5.4	5
62	Discovery of substituted (4-phenyl-1H-imidazol-2-yl)methanamine as potent somatostatin receptor 3 agonists. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 3520-3525.	2.2	2
63	Discovery of MK-1421, a Potent, Selective sstr3 Antagonist, as a Development Candidate for Type 2 Diabetes. ACS Medicinal Chemistry Letters, 2015, 6, 513-517.	2.8	20
64	Tricyclic 1,5-naphthyridinone oxabicyclooctane-linked novel bacterial topoisomerase inhibitors as broad-spectrum antibacterial agents-SAR of left-hand-side moiety (Part-2). Bioorganic and Medicinal Chemistry Letters, 2015, 25, 1831-1835.	2.2	32
65	Absolute configuration of remisporines A & B. Organic and Biomolecular Chemistry, 2015, 13, 4169-4173.	2.8	9
66	Rapid development of two factor IXa inhibitors from hit to lead. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 2321-2325.	2.2	14
67	Capture of Reactive Monophosphine-Ligated Palladium(0) Intermediates by Mass Spectrometry. Journal of the American Chemical Society, 2015, 137, 14035-14038.	13.7	53
68	Development of a novel tricyclic class of potent and selective FIXa inhibitors. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 5437-5443.	2.2	16
69	Carbon Multiplicity Editing in Long-Range Heteronuclear Correlation NMR Experiments: A Valuable Tool for the Structure Elucidation of Natural Products. Journal of Natural Products, 2015, 78, 2236-2241.	3.0	9
70	LR-HSQMBC: A Sensitive NMR Technique To Probe Very Long-Range Heteronuclear Coupling Pathways. Journal of Organic Chemistry, 2014, 79, 3887-3894.	3.2	132
71	Systematic Approach to Conformational Sampling for Assigning Absolute Configuration Using Vibrational Circular Dichroism. Journal of Medicinal Chemistry, 2014, 57, 477-494.	6.4	47
72	Imine-based chiroptical sensing for analysis of chiral amines: from method design to synthetic application. Chemical Science, 2014, 5, 2855-2861.	7.4	46

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73	Diamine Derivatives as Novel Small-Molecule, Potent, and Subtype-Selective Somatostatin SST3 Receptor Agonists. ACS Medicinal Chemistry Letters, 2014, 5, 690-695.	2.8	3
74	Using pure shift HSQC to characterize microgram samples of drug metabolites. Tetrahedron Letters, 2014, 55, 5450-5453.	1.4	22
75	Chromatographic Separation and Assignment of Absolute Configuration of Hydroxywarfarin Isomers. Chirality, 2014, 26, 95-101.	2.6	22
76	Modeling a Crowdsourced Definition of Molecular Complexity. Journal of Chemical Information and Modeling, 2014, 54, 1604-1616.	5.4	48
77	1,3,8-Triazaspiro[4.5]decane-2,4-diones as Efficacious Pan-Inhibitors of Hypoxia-Inducible Factor Prolyl Hydroxylase 1â€“3 (HIF PHD1â€“3) for the Treatment of Anemia. Journal of Medicinal Chemistry, 2012, 55, 2945-2959.	6.4	57
78	QSAR Prediction of Passive Permeability in the LLCâ€PK1 Cell Line: Trends in Molecular Properties and Crossâ€Prediction of Cacoâ€2 Permeabilities. Molecular Informatics, 2012, 31, 231-245.	2.5	27
79	Highly enantioselective synthesis of anti aryl Î²-hydroxy Î±-amino esters via DKR transfer hydrogenation. Tetrahedron Letters, 2011, 52, 1685-1688.	1.4	43
80	Antibiotics Targeting the Ribosome: Structure-Based Design and the Nobel Prize. Annual Reports in Computational Chemistry, 2010, 6, 139-166.	1.7	4
81	Efficient and Accurate Characterization of the Bergman Cyclization for Several Enediynes Including an Expanded Substructure of Esperamicin A1. Journal of Physical Chemistry B, 2008, 112, 16917-16934.	2.6	18
82	Benchmark RI-MP2 database of nucleic acid base trimers: performance of different density functional models for prediction of structures and binding energies. Physical Chemistry Chemical Physics, 2007, 9, 5000.	2.8	64
83	DNA Base Trimers: Empirical and Quantum Chemical Ab Initio Calculations versus Experiment in Vacuo. Chemistry - A European Journal, 2007, 13, 2067-2077.	3.3	28
84	A Semiempirical Quantum Model for Hydrogen-Bonded Nucleic Acid Base Pairs. Journal of Chemical Theory and Computation, 2005, 1, 1275-1285.	5.3	45
85	Structural and dynamic variations in DNA hexamers containing T-T and F-F single and tandem internal mispairs. Theoretical Chemistry Accounts, 2004, 111, 311-327.	1.4	5
86	Fast approximate methods for calculating nucleic acid base pair interaction energies. Journal of Computational Chemistry, 2003, 24, 57-67.	3.3	30
87	Quantum Chemical Characterization of Methane Metathesis in L2MCH3(L = H, Cl, Cp, Cp*; M = Sc, Y, Lu). Organometallics, 2003, 22, 1682-1689.	2.3	47
88	Internal Loopâ^'Helix Coupling in the Dynamics of the RNA Duplex (GC*C*AGUUCGCUGGC)2. Journal of Physical Chemistry B, 2002, 106, 5075-5085.	2.6	7
89	Absolute Configurational Assignments of Secondary Amines by CD-Sensitive Dimeric Zinc Porphyrin Host. Journal of the American Chemical Society, 2002, 124, 10320-10335.	13.7	152
90	Further Quantum Mechanical Evidence that Difluorotoluene Does Not Hydrogen Bond. Journal of Physical Chemistry B, 2001, 105, 8445-8451.	2.6	15

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91	Biradical and Zwitterionic Cyclizations of Oxy-Substituted Enyne-Allenes. Organic Letters, 2001, 3, 1881-1884.	4.6	34
92	Quantum chemical characterization of the cytosine: 2-Aminopurine base pair. Journal of Computational Chemistry, 2001, 22, 1167-1179.	3.3	16
93	Structural studies on bioactive compounds. Part 29. Bioorganic and Medicinal Chemistry, 2000, 8, 739-750.	3.0	18
94	Molecular Dynamics Simulations of PNAÂ·DNA and PNAÂ·RNA Duplexes in Aqueous Solution. Journal of the American Chemical Society, 2000, 122, 5997-6008.	13.7	67
95	Observation of Spontaneous Base Pair Breathing Events in the Molecular Dynamics Simulation of a Difluorotoluene-Containing DNA Oligonucleotide. Journal of the American Chemical Society, 1999, 121, 8653-8654.	13.7	59
96	Molecular Dynamics Studies of DNA A-Tract Structure and Flexibility. Journal of the American Chemical Society, 1999, 121, 5981-5991.	13.7	101
97	Comparison of Experimental and Theoretical Structures of a Transition State Analogue Used for the Induction of Anti-Cocaine Catalytic Antibodies. Journal of Physical Chemistry A, 1997, 101, 8526-8529.	2.5	28
98	Investigation of the potential energy surface for the first step in the alkaline hydrolysis of methyl acetate. International Journal of Quantum Chemistry, 1995, 56, 83-93.	2.0	17
99	A computationally efficient procedure for modeling the first step in the alkaline hydrolysis of esters. International Journal of Quantum Chemistry, 1995, 56, 103-112.	2.0	14