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	Design of an in vitro biocatalytic cascade for the manufacture of islatravir. Science, 2019, 366, 1255-1259.	12.6	383
2	The merger of decatungstate and copper catalysis to enable aliphatic C(sp3)â€“H trifluoromethylation. Nature Chemistry, 2020, 12, 459-467.	13.6	226
3	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
4	Deep Dive into Machine Learning Models for Protein Engineering. Journal of Chemical Information and Modeling, 2020, 60, 2773-2790.	5.4	134
5	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
6	Computational prediction of chemical reactions: current status and outlook. Drug Discovery Today, 2018, 23, 1203-1218.	6.4	126
7	Unequivocal determination of complex molecular structures using anisotropic NMR measurements. Science, 2017, 356, .	12.6	124
8	A multifunctional catalyst that stereoselectively assembles prodrugs. Science, 2017, 356, 426-430.	12.6	116
9	Molecular Dynamics Studies of DNA A-Tract Structure and Flexibility. Journal of the American Chemical Society, 1999, 121, 5981-5991.	13.7	101
10	Application of anisotropic NMR parameters to the confirmation of molecular structure. Nature Protocols, 2019, 14, 217-247.	12.0	101
11	Determination of Relative Configuration from Residual Chemical Shift Anisotropy. Journal of the American Chemical Society, 2016, 138, 9548-9556.	13.7	86
12	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
13	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
14	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
15	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
16	Expedited Selection of NMR Chiral Solvating Agents for Determination of Enantiopurity. ACS Central Science, 2016, 2, 332-340.	11.3	58
17	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
18	Capture of Reactive Monophosphine-Ligated Palladium(0) Intermediates by Mass Spectrometry. Journal of the American Chemical Society, 2015, 137, 14035-14038.	13.7	53

#	Article	IF	Citations
19	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
20	Analysis of Benzenoid Substitution Patterns in Small Molecule Active Pharmaceutical Ingredients. Journal of Medicinal Chemistry, 2020, 63, 13389-13396.	6.4	51
21	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
22	Modeling a Crowdsourced Definition of Molecular Complexity. Journal of Chemical Information and Modeling, 2014, 54, 1604-1616.	5.4	48
23	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
24	Systematic Approach to Conformational Sampling for Assigning Absolute Configuration Using Vibrational Circular Dichroism. Journal of Medicinal Chemistry, 2014, 57, 477-494.	6.4	47
25	Imine-based chiroptical sensing for analysis of chiral amines: from method design to synthetic application. Chemical Science, 2014, 5, 2855-2861.	7.4	46
26	A Semiempirical Quantum Model for Hydrogen-Bonded Nucleic Acid Base Pairs. Journal of Chemical Theory and Computation, 2005, 1, 1275-1285.	5.3	45
27	Highly enantioselective synthesis of anti aryl Î²-hydroxy Î±-amino esters via DKR transfer hydrogenation. Tetrahedron Letters, 2011, 52, 1685-1688.	1.4	43
28	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
29	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
30	The PMI Predictor app to enable green-by-design chemical synthesis. Nature Sustainability, 2019, 2, 1034-1040.	23.7	36
31	Biradical and Zwitterionic Cyclizations of Oxy-Substituted Enyne-Allenes. Organic Letters, 2001, 3, 1881-1884.	4.6	34
32	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
33	Enhanced measurement of residual chemical shift anisotropy for small molecule structure elucidation. Chemical Communications, 2018, 54, 4254-4257.	4.1	32
34	Fast approximate methods for calculating nucleic acid base pair interaction energies. Journal of Computational Chemistry, 2003, 24, 57-67.	3.3	30
35	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
36	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

#	Article	IF	Citations
37	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
38	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
39	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
40	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
41	PBLG as a versatile liquid crystalline medium for anisotropic NMR data acquisition. Chemical Communications, 2019, 55, 4327-4330.	4.1	27
42	Applications of Quantum Chemistry in Pharmaceutical Process Development: Current State and Opportunities. Organic Process Research and Development, 2020, 24, 1496-1507.	2.7	25
43	A rational pre-catalyst design for bis-phosphine mono-oxide palladium catalyzed reactions. Chemical Science, 2017, 8, 2841-2851.	7.4	24
44	Antenna Biphenols: Development of Extended Wavelength Chiroptical Reporters. Journal of Organic Chemistry, 2016, 81, 1185-1191.	3.2	23
45	Beyond optical rotation: what's left is not always right in total synthesis. Chemical Science, 2018, 9, 415-424.	7.4	23
46	Using pure shift HSQC to characterize microgram samples of drug metabolites. Tetrahedron Letters, 2014, 55, 5450-5453.	1.4	22
47	Chromatographic Separation and Assignment of Absolute Configuration of Hydroxywarfarin Isomers. Chirality, 2014, 26, 95-101.	2.6	22
48	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
49	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
50	Optical Chirality Sensing with a Stereodynamic Aluminum Biphenolate Probe. Journal of Organic Chemistry, 2019, 84, 4639-4645.	3.2	20
51	Synergism of anisotropic and computational NMR methods reveals the likely configuration of phormidolide A. Chemical Communications, 2020, 56, 7565-7568.	4.1	20
52	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
53	Structural studies on bioactive compounds. Part 29. Bioorganic and Medicinal Chemistry, 2000, 8, 739-750.	3.0	18
54	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

#	Article	IF	Citations
55	Direct regioisomer analysis of crude reaction mixtures via molecular rotational resonance (MRR) spectroscopy. Chemical Science, 2020, 11, 6332-6338.	7.4	18
56	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
57	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
58	Sustainable Practices in Medicinal Chemistry Part 2: Green by Design. Journal of Medicinal Chemistry, 2017, 60, 5955-5968.	6.4	17
59	Quantum chemical characterization of the cytosine: 2-Aminopurine base pair. Journal of Computational Chemistry, 2001, 22, 1167-1179.	3.3	16
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	Development of a novel tricyclic class of potent and selective FIXa inhibitors. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 5437-5443.	2.2	16
62	¹³C NMR-Based Approaches for Solving Challenging Stereochemical Problems. Organic Letters, 2019, 21, 4072-4076.	4.6	16
63	Further Quantum Mechanical Evidence that Difluorotoluene Does Not Hydrogen Bond. Journal of Physical Chemistry B, 2001, 105, 8445-8451.	2.6	15
64	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
65	Denigrins and Dactylpyrroles, Arylpyrrole Alkaloids from a Dactylia sp. Marine Sponge. Journal of Natural Products, 2020, 83, 3464-3470.	3.0	15
66	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
67	Rapid development of two factor IXa inhibitors from hit to lead. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 2321-2325.	2.2	14
68	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
69	Asymmetric Formal Synthesis of the Long-Acting DPP-4 Inhibitor Omarigliptin. Journal of Organic Chemistry, 2017, 82, 9023-9029.	3.2	13
70	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
71	Structural revision of a Wnt/Î²-catenin modulator and confirmation of cannabielsoin constitution and configuration. Chemical Communications, 2021, 57, 5658-5661.	4.1	12
72	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

#	Article	IF	Citations
73	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
74	The protecting-group free selective 3â€²-functionalization of nucleosides. Chemical Science, 2017, 8, 2804-2810.	7.4	10
75	Absolute configuration of remisporines A & B. Organic and Biomolecular Chemistry, 2015, 13, 4169-4173.	2.8	9
76	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
77	Unequivocal structure confirmation of a breitfussin analog by anisotropic NMR measurements. Chemical Science, 2020, 11, 12081-12088.	7.4	9
78	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
79	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
80	Absolute configuration assignment of (+)â€fluralaner using vibrational circular dichroism. Chirality, 2017, 29, 854-864.	2.6	8
81	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
82	Driving Aspirational Process Mass Intensity Using Simple Structure-Based Prediction. Organic Process Research and Development, 2022, 26, 1405-1410.	2.7	8
83	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
84	Mining Chromatographic Enantioseparation Data Using Matched Molecular Pair Analysis. Molecules, 2016, 21, 1297.	3.8	7
85	Systematic chemical modifications of single stranded siRNAs significantly improved CTNNB1 mRNA silencing. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 4513-4517.	2.2	7
86	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
87	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
88	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
89	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
90	Heterocyclic Regioisomer Enumeration (HREMS): A Cheminformatics Design Tool. Journal of Chemical Information and Modeling, 2015, 55, 1130-1135.	5.4	5

#	Article	IF	Citations
91	Post-Synthetic Modification of Oligonucleotides via Orthogonal Amidation and Copper Catalyzed Cycloaddition Reactions. Bioconjugate Chemistry, 2018, 29, 1859-1865.	3.6	5
92	Highly Diastereoselective Synthesis of a HCV NS5B Nucleoside Polymerase Inhibitor. Journal of Organic Chemistry, 2019, 84, 4780-4795.	3.2	5
93	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
94	Antibiotics Targeting the Ribosome: Structure-Based Design and the Nobel Prize. Annual Reports in Computational Chemistry, 2010, 6, 139-166.	1.7	4
95	Selective Formation of Functionalized Î±-Quaternary Malononitriles toward 5,5-Disubstituted Pyrrolopyrimidinones. Organic Letters, 2017, 19, 4448-4451.	4.6	4
96	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
97	Synthesis of Fused Oxepane HIV Integrase Inhibitor MK-1376. Synthesis, 2020, 52, 3378-3388.	2.3	3
98	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
99	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