Daniel S Sem

List of Publications by Year
in descending order

82	1,774	304743	289244
papers	citations	22 h-index	40 g-index

86	86	86	2173
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Long-term oral administration of a novel estrogen receptor beta agonist enhances memory and alleviates drug-induced vasodilation in young ovariectomized mice. Hormones and Behavior, 2021, 130, 104948.	2.1	12
2	Synthesis and evaluation of 17Î±-triazolyl and 9Î±-cyano derivatives of estradiol. Bioorganic and Medicinal Chemistry, 2020, 28, 115670.	3.0	3
3	Role of Conserved Histidine and Serine in the HCXXXXXRS Motif of Human Dual-Specificity Phosphatase 5. Journal of Chemical Information and Modeling, 2019, 59, 1563-1574.	5.4	1
4	Discovery and characterization of halogenated xanthene inhibitors of DUSP5 as potential photodynamic therapeutics. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 375, 114-131.	3.9	6
5	Aâ€“C Estrogens as Potent and Selective Estrogen Receptor-Beta Agonists (SERBAs) to Enhance Memory Consolidation under Low-Estrogen Conditions. Journal of Medicinal Chemistry, 2018, 61, 4720-4738.	6.4	16
6	Synthesis and evaluation of 4-cycloheptylphenols as selective Estrogen receptor-Î² agonists (SERBAs). European Journal of Medicinal Chemistry, 2018, 157, 791-804.	5.5	4
7	Serendipitous discovery of light-induced (In Situ) formation of an Azo-bridged dimeric sulfonated naphthol as a potent PTP1B inhibitor. BMC Biochemistry, 2017, 18, 10.	4.4	7
8	Dual Specificity Phosphatase 5â€Substrate Interaction: A Mechanistic Perspective. , 2017, 7, 1449-1461.		16
9	Endocannabinoid Transport Proteins. Methods in Enzymology, 2017, 593, 99-121.	1.0	20
10	Structural Analysis and Antimicrobial Activity of Chromatographically Separated Fractions of Leaves ofSesamum angustifolium(Oliv.) Engl.. Journal of Biologically Active Products From Nature, 2017, 7, 463-474.	0.3	5
11	Docking into Mycobacterium tuberculosis Thioredoxin Reductase Protein Yields Pyrazolone Lead Molecules for Methicillin-Resistant Staphylococcus aureus. Antibiotics, 2017, 6, 4.	3.7	15
12	Critical Role of the Secondary Binding Pocket in Modulating the Enzymatic Activity of DUSP5 toward Phosphorylated ERKs. Biochemistry, 2016, 55, 6187-6195.	2.5	5
13	Generation of Molecular Complexity from Cyclooctatetraene: Preparation of Aminobicyclo[5.1.0]octitols. Chemistry - A European Journal, 2015, 21, 10886-10895.	3.3	6
14	A Novel Scoring Based Distributed Protein Docking Application to Improve Enrichment. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2015, 12, 1464-1469.	3.0	9
15	Novel Uses of In Vitro Data to Develop Quantitative Biological Activity Relationship Models for in Vivo Carcinogenicity Prediction. Molecular Informatics, 2015, 34, 236-245.	2.5	9
16	Identification of inhibitors that target dual-specificity phosphatase 5 provide new insights into the binding requirements for the two phosphate pockets. BMC Biochemistry, 2015, 16, 19.	4.4	8
17	Identification of Polysulfonated Inhibitors that Target Dual Specificity Phosphatase 5 and Provide New Insights into the Binding Requirements for Dualâ€Phosphate Substrate Pockets. FASEB Journal, 2015, 29, 1022.6.	0.5	0
18	Protein expression, characterization and activity comparisons of wild type and mutant DUSP5 proteins. BMC Biochemistry, 2014, 15, 27.	4.4	10

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19	Sterol Carrier Protein-2: Binding Protein for Endocannabinoids. Molecular Neurobiology, 2014, 50, 149-158.	4.0	35
20	Probing the human estrogen receptor-Î± binding requirements for phenolic mono- and di-hydroxyl compounds: A combined synthesis, binding and docking study. Bioorganic and Medicinal Chemistry, 2014, 22, 303-310.	3.0	7
21	Protein structure in context: The molecular landscape of angiogenesis. Biochemistry and Molecular Biology Education, 2013, 41, 213-223.	1.2	6
22	Molecular docking and NMR binding studies to identify novel inhibitors of human phosphomevalonate kinase. Biochemical and Biophysical Research Communications, 2013, 430, 313-319.	2.1	5
23	Solution structures of Mycobacterium tuberculosis thioredoxin C and models of intact thioredoxin system suggest new approaches to inhibitor and drug design. Proteins: Structure, Function and Bioinformatics, 2013, 81, 675-689.	2.6	9
24	The Synthesis, Characterization, and Application of 13C-Methyl Isocyanide as an NMR Probe of Heme Protein Active Sites. Methods in Molecular Biology, 2013, 987, 51-59.	0.9	0
25	Chemical Proteomics-Based Analysis of Off-Target Binding Profiles for Rosiglitazone and Pioglitazone: Clues for Assessing Potential for Cardiotoxicity. Journal of Medicinal Chemistry, 2012, 55, 8260-8271.	6.4	39
26	A Chemical Proteomic Probe for Detecting Dehydrogenases: Catechol Rhodanine. Methods in Molecular Biology, 2012, 803, 55-64.	0.9	0
27	Affinity-Based Profiling of Dehydrogenase Subproteomes. Methods in Molecular Biology, 2012, 803, 157-165.	0.9	0
28	Solution Structures and Models Describing the Thioredoxin System from Mycobacterium tuberculosis. FASEB Journal, 2012, 26, 804.1.	0.5	0
29	Chemical Proteomicsâ€Based Analysis of Offâ€target Binding Profiles for Rosiglitazone and Pioglitazone: Clues for Assessing Potential of Cardiotoxicity. FASEB Journal, 2012, 26, 1127.10.	0.5	0
30	An In Vitro Spectroscopic Analysis to Determine the Chemical Composition of the Precipitate Formed by Mixing Sodium Hypochlorite and Chlorhexidine. Journal of Endodontics, 2011, 37, 983-988.	3.1	48
31	NMR Dynamics Investigation of Ligand-Induced Changes of Main and Side-Chain Arginine Nâ€™Hâ€™s in Human Phosphomevalonate Kinase. Journal of the American Chemical Society, 2010, 132, 2102-2103.	13.7	7
32	An In Vitro Spectroscopic Analysis to Determine Whether Para-Chloroaniline Is Produced from Mixing Sodium Hypochlorite and Chlorhexidine. Journal of Endodontics, 2010, 36, 315-317.	3.1	60
33	Inhibiting Dihydrofolate Reductase as a Treatment for Tuberculosis. FASEB Journal, 2010, 24, lb118.	0.5	1
34	Dabcyl/Fluoresceinâ€based Probes for Detection of Thiols and Disulfides: Proteomic Application to Discovery of Reactive Disulfides in Live Cells. FASEB Journal, 2010, 24, 525.2.	0.5	0
35	13C-Methyl isocyanide as an NMR probe for cytochrome P450 active sites. Journal of Biomolecular NMR, 2009, 43, 171-178.	2.8	7
36	Substrate induced structural and dynamics changes in human phosphomevalonate kinase and implications for mechanism. Proteins: Structure, Function and Bioinformatics, 2009, 75, 127-138.	2.6	7

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37	Drug Discovery and Development: The Senna Plant and Phosphomevalonate Kinase Inhibition. FASEB Journal, 2009, 23, .	0.5	0
38	Toward Understanding the Reaction Kinetics of a Coumarinâ€Fluorescein FRET based Dithio Probe for Quantitation of Cellular Thiols. FASEB Journal, 2009, 23, 534.5.	0.5	0
39	Transferred NOE and Saturation Transfer Difference NMR Studies of Novobiocin Binding to EnvZ Suggest Binding Mode Similar to DNA Gyrase. Chemical Biology and Drug Design, 2008, 71, 28-35.	3.2	3
40	Chemical Proteomics-Based Drug Design: Target and Antitarget Fishing with a Catecholâ^'Rhodanine Privileged Scaffold for NAD(P)(H) Binding Proteins. Journal of Medicinal Chemistry, 2008, 51, 4571-4580.	6.4	33
41	Structural Characterization of the Transmembrane Domain from Subunit e of Yeast F₁F_o-ATP Synthase:â€‰ A Helical GXXXG Motif Located Just under the Micelle Surface. Biochemistry, 2008, 47, 1910-1917.	2.5	11
42	Binding Synergy and Cooperativity in Dihydrodipicolinate Reductase: Implications for Mechanism and the Design of Biligand Inhibitors. Biochemistry, 2008, 47, 9966-9980.	2.5	8
43	NMR characterization of substrate induced changes in structure and dynamics of human phosphomevalonate kinase. FASEB Journal, 2008, 22, 1012.14.	0.5	0
44	Coumarinâ€Fluorescein â€“ Based FRET Probe for Real Time Quantitation of Thiols Redox State. FASEB Journal, 2008, 22, 1059.3.	0.5	0
45	NMR structure and dynamics of the NADH nicotinamide ring bound to dihydrodipicolinate reductase. FASEB Journal, 2008, 22, 1058.2.	0.5	0
46	Conserved amino acids in each subunit of the heteroligomeric tRNA m 1 A58 Mtase from Saccharomyces cerevisiae contribute to tRNA binding. Nucleic Acids Research, 2007, 35, 6808-6819.	14.5	32
47	AmineDB: Large scale docking of amines with CYP2D6 and scoring for druglike propertiesâ€”towards defining the scope of the chemical defense against foreign amines in humans. Xenobiotica, 2007, 37, 221-245.	1.1	11
48	Affinity-based chemical proteomic probe for dehydrogenases: Fluorescence and visible binding assays in gels. Analytical Biochemistry, 2007, 370, 171-179.	2.4	8
49	Structural evidence for a functionally relevant second camphor binding site in P450cam: Model for substrate entry into a P450 active site. Proteins: Structure, Function and Bioinformatics, 2007, 69, 125-138.	2.6	37
50	Fluorescent probes for thiol quantitation inside cells. FASEB Journal, 2007, 21, A627.	0.5	0
51	Thiol reactive dyes as probes for kinase assays. FASEB Journal, 2007, 21, A263.	0.5	0
52	Synergistic Use of Compound Properties and Docking Scores in Neural Network Modeling of CYP2D6 Binding:â€‰ Predicting Affinity and Conformational Sampling. Journal of Chemical Information and Modeling, 2006, 46, 2698-2708.	5.4	41
53	Fluorescence-based detection of thiols in vitro and in vivo using dithiol probes. Analytical Biochemistry, 2006, 352, 265-273.	2.4	145
54	A Dithio-Coupled Kinase and ATPase Assay. Journal of Biomolecular Screening, 2006, 11, 844-853.	2.6	5

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55	Homology-Modeled Ligand-Binding Domains of Zebrafish Estrogen Receptors Î±, Î²1, and Î²2: From in Silico to in Vivo Studies of Estrogen Interactions in Danio rerio as a Model System. Molecular Endocrinology, 2005, 19, 2979-2990.	3.7	27
56	Cofactor fingerprinting with STD NMR to characterize proteins of unknown function: identification of a rare cCMP cofactor preference. FEBS Letters, 2005, 579, 661-666.	2.8	11
57	Nuclear Magnetic Resonanceâ€“Driven Chemical Proteomics. , 2005, , 467-487.		0
58	Chemical Proteomic Tool for Ligand Mapping of CYP Antitargets: An NMR-Compatible 3D QSAR Descriptor in the Heme-Based Coordinate System.. ChemInform, 2004, 35, no.	0.0	0
59	Systems-Based Design of Bi-Ligand Inhibitors of Oxidoreductases. Chemistry and Biology, 2004, 11, 185-194.	6.0	14
60	Chemical proteomics from a nuclear magnetic resonance spectroscopy perspective. Expert Review of Proteomics, 2004, 1, 165-178.	3.0	4
61	Chemical Proteomic Tool for Ligand Mapping of CYP Antitargets:â€‰ An NMR-Compatible 3D QSAR Descriptor in the Heme-Based Coordinate System. Journal of Chemical Information and Computer Sciences, 2004, 44, 1456-1465.	2.8	12
62	Systems-Based Design of Bi-Ligand Inhibitors of OxidoreductasesFilling the Chemical Proteomic Toolbox. Chemistry and Biology, 2004, 11, 185-194.	6.0	10
63	A path from primary protein sequence to ligand recognition. Proteins: Structure, Function and Bioinformatics, 2003, 50, 589-599.	2.6	13
64	Probing the Nucleotide Binding Domain of the Osmoregulator EnvZ Using Fluorescent Nucleotide Derivatives. Biochemistry, 2002, 41, 13876-13882.	2.5	27
65	Elucidation of Protein Structural and Pharmacophore Features Based on Sequence Clustering by Common Neighbor Comparisons. Scientific World Journal, The, 2002, 2, 17-18.	2.1	0
66	Triad Therapeutics: integration of NMR structural determinations and smart chemistry to speed drug discovery. Drug Discovery Today, 2002, 7, S35-S38.	6.4	2
67	Nmr in drug discovery. Nature Reviews Drug Discovery, 2002, 1, 211-219.	46.4	380
68	NMR-based structural characterization of large protein-ligand interactions. Journal of Biomolecular NMR, 2002, 22, 165-173.	2.8	98
69	SEA-TROSY (Solvent Exposed Amides with TROSY):Â A Method to Resolve the Problem of Spectral Overlap in Very Large Proteins. Journal of the American Chemical Society, 2001, 123, 4633-4634.	13.7	45
70	Object-oriented approach to drug design enabled by NMR SOLVE: First real-time structural tool for characterizing protein-ligand interactions. Journal of Cellular Biochemistry, 2001, 84, 99-105.	2.6	15
71	Mechanistic Studies on the Reductive Half-reaction of NADPH-Cytochrome P450 Oxidoreductase. Journal of Biological Chemistry, 1999, 274, 5391-5398.	3.4	55
72	Application of fluorescence polarization to the steady-state enzyme kinetic analysis of calpain II. FEBS Letters, 1999, 443, 17-19.	2.8	14

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73	Antibody Affinities and Relative Titers in Polyclonal Populations: Surface Plasmon Resonance Analysis of anti-DNA Antibodies. Archives of Biochemistry and Biophysics, 1999, 372, 62-68.	3.0	22
74	Structural Characterization and Optimization of Antibody-Selected Phage Library Mimotopes of an Antigen Associated with Autoimmune Recurrent Thrombosis. Biochemistry, 1998, 37, 16069-16081.	2.5	18
75	High-resolution solution structure of the retinoid X receptor DNA-binding domain. Journal of Molecular Biology, 1998, 281, 271-284.	4.2	58
76	NMR Spectroscopic Studies of the DNA-binding Domain of the Monomer-binding Nuclear Orphan Receptor, Human Estrogen Related Receptor-2. Journal of Biological Chemistry, 1997, 272, 18038-18043.	3.4	31
77	Effect of Ionic Strength on the Kinetic Mechanism and Relative Rate Limitation of Steps in the Model NADPH-Cytochrome P450 Oxidoreductase Reaction with Cytochrome c. Biochemistry, 1995, 34, 12768-12774.	2.5	37
78	NMR Assignments and Secondary Structure of the Retinoid X Receptor alpha DNA-binding Domain. Evidence for the Novel C-terminal Helix. FEBS Journal, 1994, 224, 639-650.	0.2	15
79	Kinetic Mechanism for the Model Reaction of NADPH-Cytochrome P450 Oxidoreductase with Cytochrome c. Biochemistry, 1994, 33, 12012-12021.	2.5	25
80	Enzyme-substrate binding interactions of NADPH-cytochrome P-450 oxidoreductase characterized with pH and alternate substrate/inhibitor studies. Biochemistry, 1993, 32, 11539-11547.	2.5	31
81	Interaction with arginine 597 of NADPH-cytochrome P-450 oxidoreductase is a primary source of the uniform binding energy used to discriminate between NADPH and NADH. Biochemistry, 1993, 32, 11548-11558.	2.5	61
82	Geometric relationship between the nicotinamide and isoalloxazine rings in NADPH-cytochrome P-450 oxidoreductase: implications for the classification of evolutionarily and functionally related flavoproteins. Biochemistry, 1992, 31, 3391-3398.	2.5	31