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	Nmr in drug discovery. Nature Reviews Drug Discovery, 2002, 1, 211-219.	46.4	380
2	Fluorescence-based detection of thiols in vitro and in vivo using dithiol probes. Analytical Biochemistry, 2006, 352, 265-273.	2.4	145
3	NMR-based structural characterization of large protein-ligand interactions. Journal of Biomolecular NMR, 2002, 22, 165-173.	2.8	98
4	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
5	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
6	High-resolution solution structure of the retinoid X receptor DNA-binding domain. Journal of Molecular Biology, 1998, 281, 271-284.	4.2	58
7	Mechanistic Studies on the Reductive Half-reaction of NADPH-Cytochrome P450 Oxidoreductase. Journal of Biological Chemistry, 1999, 274, 5391-5398.	3.4	55
8	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
9	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
10	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
11	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
12	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
13	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
14	Sterol Carrier Protein-2: Binding Protein for Endocannabinoids. Molecular Neurobiology, 2014, 50, 149-158.	4.0	35
15	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
16	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
17	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
18	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

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19	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
20	Probing the Nucleotide Binding Domain of the Osmoregulator EnvZ Using Fluorescent Nucleotide Derivatives. Biochemistry, 2002, 41, 13876-13882.	2.5	27
21	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
22	Kinetic Mechanism for the Model Reaction of NADPH-Cytochrome P450 Oxidoreductase with Cytochrome c. Biochemistry, 1994, 33, 12012-12021.	2.5	25
23	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
24	Endocannabinoid Transport Proteins. Methods in Enzymology, 2017, 593, 99-121.	1.0	20
25	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
26	Dual Specificity Phosphatase 5â€Substrate Interaction: A Mechanistic Perspective. , 2017, 7, 1449-1461.		16
27	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
28	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
29	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
30	Docking into Mycobacterium tuberculosis Thioredoxin Reductase Protein Yields Pyrazolone Lead Molecules for Methicillin-Resistant Staphylococcus aureus. Antibiotics, 2017, 6, 4.	3.7	15
31	Application of fluorescence polarization to the steady-state enzyme kinetic analysis of calpain II. FEBS Letters, 1999, 443, 17-19.	2.8	14
32	Systems-Based Design of Bi-Ligand Inhibitors of Oxidoreductases. Chemistry and Biology, 2004, 11, 185-194.	6.0	14
33	A path from primary protein sequence to ligand recognition. Proteins: Structure, Function and Bioinformatics, 2003, 50, 589-599.	2.6	13
34	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
35	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
36	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

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37	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
38	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
39	Systems-Based Design of Bi-Ligand Inhibitors of OxidoreductasesFilling the Chemical Proteomic Toolbox. Chemistry and Biology, 2004, 11, 185-194.	6.0	10
40	Protein expression, characterization and activity comparisons of wild type and mutant DUSP5 proteins. BMC Biochemistry, 2014, 15, 27.	4.4	10
41	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
42	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
43	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
44	Affinity-based chemical proteomic probe for dehydrogenases: Fluorescence and visible binding assays in gels. Analytical Biochemistry, 2007, 370, 171-179.	2.4	8
45	Binding Synergy and Cooperativity in Dihydrodipicolinate Reductase: Implications for Mechanism and the Design of Biligand Inhibitors. Biochemistry, 2008, 47, 9966-9980.	2.5	8
46	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
47	13C-Methyl isocyanide as an NMR probe for cytochrome P450 active sites. Journal of Biomolecular NMR, 2009, 43, 171-178.	2.8	7
48	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
49	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
50	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
51	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
52	Protein structure in context: The molecular landscape of angiogenesis. Biochemistry and Molecular Biology Education, 2013, 41, 213-223.	1.2	6
53	Generation of Molecular Complexity from Cyclooctatetraene: Preparation of Aminobicyclo[5.1.0]octitols. Chemistry - A European Journal, 2015, 21, 10886-10895.	3.3	6
54	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

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55	A Dithio-Coupled Kinase and ATPase Assay. Journal of Biomolecular Screening, 2006, 11, 844-853.	2.6	5
56	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
57	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
58	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
59	Chemical proteomics from a nuclear magnetic resonance spectroscopy perspective. Expert Review of Proteomics, 2004, 1, 165-178.	3.0	4
60	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
61	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
62	Synthesis and evaluation of 17Î±-triazolyl and 9Î±-cyano derivatives of estradiol. Bioorganic and Medicinal Chemistry, 2020, 28, 115670.	3.0	3
63	Triad Therapeutics: integration of NMR structural determinations and smart chemistry to speed drug discovery. Drug Discovery Today, 2002, 7, S35-S38.	6.4	2
64	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
65	Inhibiting Dihydrofolate Reductase as a Treatment for Tuberculosis. FASEB Journal, 2010, 24, lb118.	0.5	1
66	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
67	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
68	A Chemical Proteomic Probe for Detecting Dehydrogenases: Catechol Rhodanine. Methods in Molecular Biology, 2012, 803, 55-64.	0.9	0
69	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
70	Nuclear Magnetic Resonanceâ€“Driven Chemical Proteomics. , 2005, , 467-487.		0
71	Fluorescent probes for thiol quantitation inside cells. FASEB Journal, 2007, 21, A627.	0.5	0
72	Thiol reactive dyes as probes for kinase assays. FASEB Journal, 2007, 21, A263.	0.5	0

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73	NMR characterization of substrate induced changes in structure and dynamics of human phosphomevalonate kinase. FASEB Journal, 2008, 22, 1012.14.	0.5	0
74	Coumarinâ€Fluorescein â€“ Based FRET Probe for Real Time Quantitation of Thiols Redox State. FASEB Journal, 2008, 22, 1059.3.	0.5	0
75	NMR structure and dynamics of the NADH nicotinamide ring bound to dihydrodipicolinate reductase. FASEB Journal, 2008, 22, 1058.2.	0.5	0
76	Drug Discovery and Development: The Senna Plant and Phosphomevalonate Kinase Inhibition. FASEB Journal, 2009, 23, .	0.5	0
77	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
78	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
79	Affinity-Based Profiling of Dehydrogenase Subproteomes. Methods in Molecular Biology, 2012, 803, 157-165.	0.9	0
80	Solution Structures and Models Describing the Thioredoxin System from Mycobacterium tuberculosis. FASEB Journal, 2012, 26, 804.1.	0.5	0
81	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
82	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