Herman A Schreuder

List of Publications by Year
in descending order

66 papers	3,063 citations	159525 30 h-index	155592 55 g-index
72 all docs	72 docs citations	72 times ranked	3008 citing authors

#	Article	IF	Citations
1	The intact and cleaved human antithrombin III complex as a model for serpinâ€“proteinase interactions. Nature Structural and Molecular Biology, 1994, 1, 48-54.	3.6	275
2	Evidence for Cï£¿Cl/Cï£¿Brâ‹…â‹…â‹…Ï€ Interactions as an Important Contribution to Proteinâ€“Ligand Binding Affinity. Angewandte Chemie - International Edition, 2009, 48, 2911-2916.	7.2	243
3	A new cytokine-receptor binding mode revealed by the crystal structure of the IL-1 receptor with an antagonist. Nature, 1997, 386, 194-200.	13.7	213
4	Crystal structure of the p-hydroxybenzoate hydroxylase-substrate complex refined at 1.9 Ã… resolution. Journal of Molecular Biology, 1989, 208, 679-696.	2.0	210
5	Identification of a novel conserved sequence motif in flavoprotein hydroxylases with a putative dual function in FAD/NAD(P)H binding. Protein Science, 1997, 6, 2454-2458.	3.1	132
6	Crystal Structures of Wild-Type p-Hydroxybenzoate Hydroxylase Complexed with 4-Aminobenzoate, 2,4-Dihydroxybenzoate, and 2-Hydroxy-4-aminobenzoate and of the Tyr222Ala Mutant Complexed with 2-Hydroxy-4-aminobenzoate. Evidence for a Proton Channel and a New Binding Mode of the Flavin Ring. Biochemistry, 1994, 33, 10161-10170.	1.2	119
7	Crystal structure of p-hydroxybenzoate hydroxylase complexed with its reaction product 3,4-dihydroxybenzoate. Journal of Molecular Biology, 1988, 199, 637-648.	2.0	112
8	Probing the Subpockets of Factor Xa Reveals Two Binding Modes for Inhibitors Based on a 2-Carboxyindole Scaffold:Â A Study Combining Structure-Activity Relationship and X-ray Crystallography. Journal of Medicinal Chemistry, 2005, 48, 4511-4525.	2.9	108
9	Quantitative Structureâ^'Activity Relationship of Human Neutrophil Collagenase (MMP-8) Inhibitors Using Comparative Molecular Field Analysis and X-ray Structure Analysis. Journal of Medicinal Chemistry, 1999, 42, 1908-1920.	2.9	85
10	Design and Quantitative Structureâ^'Activity Relationship of 3-Amidinobenzyl-1H-indole-2-carboxamides as Potent, Nonchiral, and Selective Inhibitors of Blood Coagulation Factor Xa. Journal of Medicinal Chemistry, 2002, 45, 2749-2769.	2.9	85
11	Structural Requirements for Factor Xa Inhibition by 3-Oxybenzamides with Neutral P1 Substituents:Â Combining X-ray Crystallography, 3D-QSAR, and Tailored Scoring Functions. Journal of Medicinal Chemistry, 2005, 48, 3290-3312.	2.9	69
12	Analysis of the active site of the flavoprotein p-hydroxybenzoate hydroxylase and some ideas with respect to its reaction mechanism. Biochemistry, 1990, 29, 3101-3108.	1.2	67
13	A small molecule inhibitor of Nicotinamide N-methyltransferase for the treatment of metabolic disorders. Scientific Reports, 2018, 8, 3660.	1.6	64
14	Inhibition of Human Neutrophil Elastase. 4. Design, Synthesis, X-ray Crystallographic Analysis, and Structureâ^'Activity Relationships for a Series of P2-Modified, Orally Active Peptidyl Pentafluoroethyl Ketones. Journal of Medicinal Chemistry, 1998, 41, 2461-2480.	2.9	63
15	Crystal structure of pâ€hydroxybenzoate hydroxylase reconstituted with the modified fad present in alcohol oxidase from methylotrophic yeasts: Evidence for an arabinoflavin. Protein Science, 1994, 3, 2245-2253.	3.1	61
16	Refined Crystal Structure of the Interleukin-1 Receptor Antagonist. Presence of a Disulfide Link and a cis -Proline. FEBS Journal, 1995, 227, 838-847.	0.2	60
17	Switch of coenzyme specificity of p -hydroxybenzoate hydroxylase 1 1Edited by A. R. Fersht. Journal of Molecular Biology, 1999, 292, 87-96.	2.0	55
18	Fragment Deconstruction of Small, Potent Factorâ€…Xa Inhibitors: Exploring the Superadditivity Energetics of Fragment Linking in Proteinâ€“Ligand Complexes. Angewandte Chemie - International Edition, 2012, 51, 905-911.	7.2	54

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19	Crystal structure of recombinant human growth and differentiation factor 5: Evidence for interaction of the type I and type II receptor-binding sites. Biochemical and Biophysical Research Communications, 2005, 329, 1076-1086.	1.0	52
20	Chitinase and Î²-1,3-glucanase in the lutoid-body fraction of Hevea latex. Phytochemistry, 1996, 43, 29-37.	1.4	51
21	Interdomain binding of NADPH in p-Hydroxybenzoate Hydroxylase as Suggested by Kinetic, Crystallographic and Modeling Studies of Histidine 162 and Arginine 269 Variants. Journal of Biological Chemistry, 1998, 273, 21031-21039.	1.6	49
22	Novel Î²-Amino Acid Derivatives as Inhibitors of Cathepsin A. Journal of Medicinal Chemistry, 2012, 55, 7636-7649.	2.9	41
23	Crystal Structures of Mutant Pseudomonas aeruginosa p-Hydroxybenzoate Hydroxylases: The Tyr201Phe, Tyr385Phe, and Asn300Asp Variants. Biochemistry, 1994, 33, 1555-1564.	1.2	40
24	Dual Glucagon-like Peptide 1 (GLP-1)/Glucagon Receptor Agonists Specifically Optimized for Multidose Formulations. Journal of Medicinal Chemistry, 2018, 61, 5580-5593.	2.9	40
25	Custom chemical microarray production and affinity fingerprinting for the S1 pocket of factor VIIa. Analytical Biochemistry, 2004, 335, 50-57.	1.1	34
26	Design, synthesis, and structureâ€“activity relationship of a new class of amidinophenylurea-based factor VIIa inhibitors. Bioorganic and Medicinal Chemistry Letters, 2003, 13, 1463-1467.	1.0	33
27	Novel Small Molecule Inhibitors of Activated Thrombin Activatable Fibrinolysis Inhibitor (TAFIa) from Natural Product Anabaenopeptin. Journal of Medicinal Chemistry, 2015, 58, 4839-4844.	2.9	33
28	Molecular Design and Characterization of an Î±-Thrombin Inhibitor Containing a Novel P1 Moiety. Biochemistry, 1997, 36, 1034-1040.	1.2	32
29	The Crystal Structure of Thrombin-activable Fibrinolysis Inhibitor (TAFI) Provides the Structural Basis for Its Intrinsic Activity and the Short Half-life of TAFIa. Journal of Biological Chemistry, 2008, 283, 29416-29423.	1.6	31
30	Isolation, Co-Crystallization and Structure-Based Characterization of Anabaenopeptins as Highly Potent Inhibitors of Activated Thrombin Activatable Fibrinolysis Inhibitor (TAFIa). Scientific Reports, 2016, 6, 32958.	1.6	30
31	Novel nicotinamide analog as inhibitor of nicotinamide N-methyltransferase. Bioorganic and Medicinal Chemistry Letters, 2018, 28, 922-925.	1.0	30
32	Targeting Dynamic Pockets of HIV-1 Protease by Structure-Based Computational Screening for Allosteric Inhibitors. Journal of Chemical Information and Modeling, 2014, 54, 987-991.	2.5	29
33	Crystal structure of the reduced form of p- hydroxybenzoate hydroxylase refined at 2.3 Ã... resolution. Proteins: Structure, Function and Bioinformatics, 1992, 14, 178-190.	1.5	28
34	Lys42 and Ser42 variants of p-hydroxybenzoate hydroxylase from Pseudomonas fluorescens reveal that Arg42 is essential for NADPH binding. FEBS Journal, 1998, 253, 194-201.	0.2	27
35	The coenzyme analog adenosine 5-diphosphoribose displaces FAD in the active site of p-hydroxybenzoate hydroxylase. An x-ray crystallographic investigation. Biochemistry, 1989, 28, 7199-7205.	1.2	25
36	Modelling of the binding site of the human m1 muscarinic receptor: experimental validation and refinement. Journal of Computer-Aided Molecular Design, 1997, 11, 317-332.	1.3	24

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37	5-Chlorothiophene-2-carboxylic Acid [(S)-2-[2-Methyl-3-(2-oxopyrrolidin-1-yl)benzenesulfonylamino]-3-(4-methylpiperazin-1-yl)-3-oxopropyl]amide (SAR107375), a Selective and Potent Orally Active Dual Thrombin and Factor Xa Inhibitor. Journal of Medicinal Chemistry, 2013, 56, 9441-9456.	2.9	23
38	Chemical modification of tyrosine-38 in P-Hydroxybenzoate hydroxylase from Pseudomonas fluorescens by 5'-P-fluorosulfonylbenzoyladenosine: A probe for the elucidation of the NADPH binding site?. Involvement in cataysis, assignment in sequence and fitting to the tertiary structure. FEBS Journal, 1988, 176, 449-459.	0.2	21
39	Phe161and Arg166variants ofp-hydroxybenzoate hydroxylase. FEBS Letters, 1999, 443, 251-255.	1.3	20
40	Structure-based design of amidinophenylurea-derivatives for factor VIIa inhibition. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 3715-3720.	1.0	20
41	Structure and Function of Mutant Arg44Lys of 4-Hydroxybenzoate Hydroxylase. Implications for NADPH Binding. FEBS Journal, 1995, 231, 157-165.	0.2	19
42	Novel factor Xa inhibitors based on a benzoic acid scaffold and incorporating a neutral P1 ligand. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 2801-2805.	1.0	18
43	Factor Xa inhibitors based on a 2-carboxyindole scaffold: SAR of neutral P1 substituents. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 4191-4195.	1.0	18
44	Inhibition of CatA: an emerging strategy for the treatment of heart failure. Future Medicinal Chemistry, 2013, 5, 399-409.	1.1	18
45	A Combination of Spin Diffusion Methods for the Determination of Proteinâ€“Ligand Complex Structural Ensembles. Angewandte Chemie - International Edition, 2015, 54, 6511-6515.	7.2	18
46	Novel Inhibitors of Nicotinamide-N-Methyltransferase for the Treatment of Metabolic Disorders. Molecules, 2021, 26, 991.	1.7	17
47	Novel factor Xa inhibitors based on a 2-carboxyindole scaffold: SAR of P4 substituents in combination with a neutral P1 ligand. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 4197-4201.	1.0	15
48	Structureâ€based prediction of modifications in glutarylamidase to allow singleâ€step enzymatic production of 7â€aminocephalosporanic acid from cephalosporin C. Protein Science, 2002, 11, 92-103.	3.1	12
49	Fractal Dimensions of Macromolecular Structures. Molecular Informatics, 2014, 33, 588-596.	1.4	12
50	Crystallization and Preliminary Crystallographic Analysis of Antistasin, a Leech-derived Inhibitor of Blood Coagulation Factor Xa. Journal of Molecular Biology, 1993, 231, 1137-1138.	2.0	10
51	Crystal structure of cathepsin A, a novel target for the treatment of cardiovascular diseases. Biochemical and Biophysical Research Communications, 2014, 445, 451-456.	1.0	10
52	Crystallization and Preliminary X-ray Analysis of Human Antithrombin III. Journal of Molecular Biology, 1993, 229, 249-250.	2.0	9
53	Sulfamide as Zinc Binding Motif in Small Molecule Inhibitors of Activated Thrombin Activatable Fibrinolysis Inhibitor (TAFIa). Journal of Medicinal Chemistry, 2016, 59, 9567-9573.	2.9	9
54	Poly(ADP-Ribose) Polymerase-1 (PARP-1) Inhibitors Based on a Tetrahydro-1(2H)-isoquinolinone Scaffold: Synthesis, Biological Evaluation and X-ray Crystal Structure. Synthesis, 2005, 2005, 1550-1554.	1.2	8

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55	Crystal structures of monkey and mouse nicotinamide N-methyltransferase (NNMT) bound with end product, 1-methyl nicotinamide. Biochemical and Biophysical Research Communications, 2017, 491, 416-422.	1.0	8
56	Determination of Î²-galactosidase activity in the intestinal tract of mice by ion-exchange high-performance liquid chromatography using Ïµ-N-1-(1-deoxylactulosyl)-L-lysine as substrate. Biomedical Applications, 1983, 278, 275-282.	1.7	6
57	Crystals of soluble interleukin-1 receptor complexed with its natural antagonist reveal a 1:1 receptor-ligand complex. FEBS Letters, 1995, 373, 39-40.	1.3	6
58	Refined Crystal Structure of the Interleukinâ€1 Receptor Antagonist. FEBS Journal, 1995, 227, 838-847.	0.2	3
59	Protein Crystallography and Drug Discovery. , 2008, , 605-634.		3
60	Protein Crystallography and Drug Discovery. , 2015, , 511-537.		3
61	Application of conformationally restricted peptidomimetics to modeling the bound conformation of peptide antagonists with the IL-1 receptor. International Journal of Peptide Research and Therapeutics, 1998, 5, 93-100.	0.1	2
62	Design, Synthesis, and Structureâ€"Activity Relationship of a New Class of Amidinophenylurea-Based Factor VIIa Inhibitors.. ChemInform, 2003, 34, no.	0.1	0
63	PROTEIN CRYSTALLOGRAPHY AND DRUG DISCOVERY. , 2003, , 417-443.		0
64	InnenrÃ¼cktitelbild: Fragment Deconstruction of Small, Potent Factorâ€…Xa Inhibitors: Exploring the Superadditivity Energetics of Fragment Linking in Protein-Ligand Complexes (Angew. Chem. 4/2012). Angewandte Chemie, 2012, 124, 1103-1103.	1.6	0
65	Inside Back Cover: Fragment Deconstruction of Small, Potent Factorâ€…Xa Inhibitors: Exploring the Superadditivity Energetics of Fragment Linking in Protein-Ligand Complexes (Angew. Chem. Int. Ed.) Tj ETQq1 1 0.784314 rgBT /Over		
66	IL-1 antagonist discovery. , 2000, , 205-222.		0