## Thomas R Schneider

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

8,360 88 83 34 h-index g-index citations papers 88 6.03 9,002 10.4 L-index avg, IF ext. citations ext. papers

#	Paper	IF	Citations
83	Ground-state destabilization by electrostatic repulsion is not a driving force in orotidine-5?-monophosphate decarboxylase catalysis. <i>Nature Catalysis</i> , <b>2022</b> , 5, 332-341	36.5	1
82	Profiling cellular diversity in sponges informs animal cell type and nervous system evolution. <i>Science</i> , <b>2021</b> , 374, 717-723	33.3	15
81	Structural insights into the inhibition of glycine reuptake. <i>Nature</i> , <b>2021</b> , 591, 677-681	50.4	18
80	X-ray screening identifies active site and allosteric inhibitors of SARS-CoV-2 main protease. <i>Science</i> , <b>2021</b> , 372, 642-646	33.3	95
79	The structural bases for agonist diversity in an glutamate receptor-like channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2020</b> , 117, 752-760	11.5	37
78	Liquid application method for time-resolved analyses by serial synchrotron crystallography. <i>Nature Methods</i> , <b>2019</b> , 16, 979-982	21.6	41
77	Optical performance and radiation stability of polymer X-ray refractive nano-lenses. <i>Journal of Synchrotron Radiation</i> , <b>2019</b> , 26, 714-719	2.4	6
76	MXCuBE2: the dawn of MXCuBE Collaboration. <i>Journal of Synchrotron Radiation</i> , <b>2019</b> , 26, 393-405	2.4	14
75	Long-wavelength Mesh&Collect native SAD phasing from microcrystals. <i>Acta Crystallographica Section D: Structural Biology</i> , <b>2019</b> , 75, 192-199	5.5	5
74	Visualization of protein crystals by high-energy phase-contrast X-ray imaging. <i>Acta Crystallographica Section D: Structural Biology</i> , <b>2019</b> , 75, 947-958	5.5	11
73	An NAD Phosphorylase Toxin Triggers Mycobacterium tuberculosis Cell Death. <i>Molecular Cell</i> , <b>2019</b> , 73, 1282-1291.e8	17.6	37
72	Clustering of atomic displacement parameters in bovine trypsin reveals a distributed lattice of atoms with shared chemical properties. <i>Scientific Reports</i> , <b>2019</b> , 9, 19281	4.9	4
71	The structure of the N-terminal module of the cell wall hydrolase RipA and its role in regulating catalytic activity. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2018</b> , 86, 912-923	4.2	16
70	Structural and Functional Characterization of the BcsG Subunit of the Cellulose Synthase in Salmonella typhimurium. <i>Journal of Molecular Biology</i> , <b>2018</b> , 430, 3170-3189	6.5	19
69	Microfluidic Chips for In Situ Crystal X-ray Diffraction and In Situ Dynamic Light Scattering for Serial Crystallography. <i>Journal of Visualized Experiments</i> , <b>2018</b> ,	1.6	14
68	Identification of the point of diminishing returns in high-multiplicity data collection for sulfur SAD hasing. <i>Journal of Synchrotron Radiation</i> , <b>2017</b> , 24, 19-28	2.4	4
67	Core Mediator structure at 3.4 lextends model of transcription initiation complex. <i>Nature</i> , <b>2017</b> , 545, 248-251	50.4	74

## (2006-2017)

66	P13, the EMBL macromolecular crystallography beamline at the low-emittance PETRA III ring for[high- and low-energy phasing with variable beam focusing. <i>Journal of Synchrotron Radiation</i> , <b>2017</b> , 24, 323-332	2.4	84
65	Rat ceruloplasmin: a new labile copper binding site and zinc/copper mosaic. <i>Metallomics</i> , <b>2017</b> , 9, 1828-	·1& <del>3</del> 8	13
64	A multicrystal diffraction data-collection approach for studying structural dynamics with millisecond temporal resolution. <i>IUCrJ</i> , <b>2016</b> , 3, 393-401	4.7	14
63	Data collection with a tailored X-ray beam size at 2.69 Iwavelength (4.6 keV): sulfur SAD phasing of Cdc23(Nterm). <i>Acta Crystallographica Section D: Structural Biology</i> , <b>2016</b> , 72, 403-12	5.5	8
62	Advances in experimental phasing. Acta Crystallographica Section D: Structural Biology, 2016, 72, 291-2	5.5	
61	The inhibition mechanism of human 20S proteasomes enables next-generation inhibitor design. <i>Science</i> , <b>2016</b> , 353, 594-8	33.3	123
60	3-Sulfinopropionyl-coenzyme A (3SP-CoA) desulfinase from Advenella mimigardefordensis DPN7(T): crystal structure and function of a desulfinase with an acyl-CoA dehydrogenase fold. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2015</b> , 71, 1360-72		4
59	Terahertz radiation induces non-thermal structural changes associated with Frfilich condensation in a protein crystal. <i>Structural Dynamics</i> , <b>2015</b> , 2, 054702	3.2	37
58	Serial crystallography on in vivo grown microcrystals using synchrotron radiation. <i>IUCrJ</i> , <b>2014</b> , 1, 87-94	4.7	164
57	A novel Fkylosidase structure from Geobacillus thermoglucosidasius: the first crystal structure of a glycoside hydrolase family GH52 enzyme reveals unpredicted similarity to other glycoside hydrolase folds. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2014</b> , 70, 1366-74		14
56	Crystal structure of the gamma-2 herpesvirus LANA DNA binding domain identifies charged surface residues which impact viral latency. <i>PLoS Pathogens</i> , <b>2013</b> , 9, e1003673	7.6	25
55	SCEDS: protein fragments for molecular replacement in Phaser. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2013</b> , 69, 2216-25		12
54	Alignment of protein structures in the presence of domain motions. <i>BMC Bioinformatics</i> , <b>2008</b> , 9, 352	3.6	41
53	RAPIDO: a web server for the alignment of protein structures in the presence of conformational changes. <i>Nucleic Acids Research</i> , <b>2008</b> , 36, W42-6	20.1	91
52	Synchrotron radiation: micrometer-sized x-ray beams as fine tools for macromolecular crystallography. <i>HFSP Journal</i> , <b>2008</b> , 2, 302-6		11
51	Crystal structure of the ubiquitin binding domains of rabex-5 reveals two modes of interaction with ubiquitin. <i>Cell</i> , <b>2006</b> , 124, 1183-95	56.2	233
50	Ultrahigh-resolution study of protein atomic displacement parameters at cryotemperatures obtained with a helium cryostat. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2006</b> , 62, 1535-44		14
49	SITCOM: a program for comparing sites in macromolecular substructures. <i>Journal of Applied Crystallography</i> , <b>2006</b> , 39, 618-619	3.8	9

Mechanism of Aurora B activation by INCENP and inhibition by hesperadin. *Molecular Cell*, **2005**, 18, 379-24.6 321 48 Structure of Ecballium elaterium trypsin inhibitor II (EETI-II): a rigid molecular scaffold. Acta 47 33 Crystallographica Section D: Biological Crystallography, 2005, 61, 1255-62 Structural basis for the autoinhibition and STI-571 inhibition of c-Kit tyrosine kinase. Journal of 46 5.4 470 Biological Chemistry, 2004, 279, 31655-63 Subatomic and atomic crystallographic studies of aldose reductase: implications for inhibitor 28 10.3 45 binding. Cellular and Molecular Life Sciences, 2004, 61, 763-73 Ultrahigh resolution drug design. II. Atomic resolution structures of human aldose reductase holoenzyme complexed with Fidarestat and Minalrestat: implications for the binding of cyclic imide 66 4.2 44 inhibitors. Proteins: Structure, Function and Bioinformatics, 2004, 55, 805-13 Ultrahigh resolution drug design I: details of interactions in human aldose reductase-inhibitor 4.2 43 232 complex at 0.66 A. Proteins: Structure, Function and Bioinformatics, 2004, 55, 792-804 The crystallographic structure of the aldose reductase-IDD552 complex shows direct proton 42 25 donation from tyrosine 48. Acta Crystallographica Section D: Biological Crystallography, 2004, 60, 1347-54 Domain identification by iterative analysis of error-scaled difference distance matrices. Acta 41 31 Crystallographica Section D: Biological Crystallography, 2004, 60, 2269-75 HKL2MAP: a graphical user interface for macromolecular phasing withSHELXprograms. Journal of 3.8 40 599 Applied Crystallography, 2004, 37, 843-844 Molecular basis for redox-Bohr and cooperative effects in cytochrome c3 from Desulfovibrio desulfuricans ATCC 27774: crystallographic and modeling studies of oxidized and reduced 39 4.2 17 high-resolution structures at pH 7.6. Proteins: Structure, Function and Bioinformatics, 2004, 54, 135-52 Substrate and metal complexes of 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase from Saccharomyces cerevisiae provide new insights into the catalytic mechanism. Journal of Molecular 38 6.5 37 Biology, 2004, 337, 675-90 Evolution of feedback-inhibited beta /alpha barrel isoenzymes by gene duplication and a single mutation. Proceedings of the National Academy of Sciences of the United States of America, 2003, 11.5 94 37 100, 862-7 36 Automatic solution of heavy-atom substructures. Methods in Enzymology, 2003, 374, 37-83 1.7 31 Stereoselective Synthesis of the Two trans-(16-Hydroxymethyl)-3-methoxy-13\(\text{Estra-1,3,5}(10)\)-trien-17-ol Isomers. Collection of 35 5 Czechoslovak Chemical Communications, 2003, 68, 1141-1148 Use of multiple anomalous dispersion to phase highly merohedrally twinned crystals of 13 34 interleukin-1beta. Acta Crystallographica Section D: Biological Crystallography, 2003, 59, 290-8 Structure of the alpha-amylase inhibitor tendamistat at 0.93 A. Acta Crystallographica Section D: 33 Biological Crystallography, 2003, 59, 1737-43 Optimization of selenium substructures as obtained from SHELXD. Acta Crystallographica Section D: 6 32 Biological Crystallography, 2003, 59, 1987-94 Structural information content at high resolution: MAD versus native. Methods in Enzymology, 2003, 1.7 374, 321-41

30	A genetic algorithm for the identification of conformationally invariant regions in protein molecules. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2002</b> , 58, 195-208		113
29	Substructure solution with SHELXD. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2002</b> , 58, 1772-9		1408
28	3-Methoxy-1?-phenyl-4?ြ5-dihydro-1H-pyrazolo[4?,3?:16,17]estra-1,3,5(10)-triene. <i>Acta Crystallographica Section E: Structure Reports Online</i> , <b>2002</b> , 58, o810-o811		2
27	Stereoselective synthesis of some novel heterocyclic estrone derivatives by intramolecular 1,3-dipolar cycloaddition. <i>Tetrahedron</i> , <b>2002</b> , 58, 6843-6849	2.4	34
26	Crystal structure of the endosomal SNARE complex reveals common structural principles of all SNAREs. <i>Nature Structural Biology</i> , <b>2002</b> , 9, 107-11		207
25	Silylhydrazine und dimere N,N?-Dilithium-N,N?-bis(silyl)hydrazide <b>(</b> Synthesen, Reaktionen, Isomerisierungen. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2001</b> , 627, 2581-2588	1.3	12
24	X-ray snapshots of serine protease catalysis reveal a tetrahedral intermediate. <i>Nature Structural Biology</i> , <b>2001</b> , 8, 689-94		89
23	The First Structurally Characterized Aluminum Compounds with Terminal Acetylide Groups This work was supported by the Deutsche Forschungsgemeinschaft. N.C.MZ. thanks the Schweizerischer Nationalfonds for a fellowship. <i>Angewandte Chemie - International Edition</i> , <b>2000</b> ,	16.4	31
22	Alumoxane Hydride and Aluminum Chalcogenide Hydride Compounds with Pyrazolato Ligands. Angewandte Chemie - International Edition, <b>2000</b> , 39, 4276-4279	16.4	32
21	A steroidal phenyldihydro-1,3-oxazine derivative. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , <b>2000</b> , 56, e363-e364		6
20	Ab initio structure determination of the lantibiotic mersacidin. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2000</b> , 56, 705-13		25
19	Objective comparison of protein structures: error-scaled difference distance matrices. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2000</b> , 56, 714-21		74
18	Protein-protein recognition, hydride transfer and proton pumping in the transhydrogenase complex. <i>Structure</i> , <b>2000</b> , 8, 809-15	5.2	53
17	Asymmetric Tris- and Cyclic Silylhydroxylamines from Trimeric and Tetrameric Lithium N,N-Bis(silyl)hydroxylamides. <i>Organometallics</i> , <b>2000</b> , 19, 5376-5383	3.8	25
16	1.7 A structure of the stabilized REIv mutant T39K. Application of local NCS restraints. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>1999</b> , 55, 1158-67		25
15	Crystallization and preliminary X-ray analysis of 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase (tyrosine inhibitable) from Saccharomyces cerevisiae. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>1999</b> , 55, 1586-8		2
14	Structure of catalase HPII from Escherichia coli at 1.9 A resolution. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>1999</b> , 34, 155-66	4.2	51
13	Influence of internal dynamics on accuracy of protein NMR structures: derivation of realistic model distance data from a long molecular dynamics trajectory. <i>Journal of Molecular Biology</i> , <b>1999</b> , 285, 727-40	6.5	33

12	Structure of balhimycin and its complex with solvent molecules. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>1998</b> , 54, 175-83		17
11	Refinement of triclinic hen egg-white lysozyme at atomic resolution. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>1998</b> , 54, 522-46		85
10	Loop closure and intersubunit communication in tryptophan synthase. <i>Biochemistry</i> , <b>1998</b> , 37, 5394-406	3.2	135
9	[16] SHELXL: High-resolution refinement. <i>Methods in Enzymology</i> , <b>1997</b> , 319-343	1.7	1940
8	X-ray crystallography reveals stringent conservation of protein fold after removal of the only disulfide bridge from a stabilized immunoglobulin variable domain. <i>Folding &amp; Design</i> , <b>1997</b> , 2, 357-61		18
7	Macromolecular Cryocrystallography. <i>Journal of Applied Crystallography</i> , <b>1997</b> , 30, 211-237	3.8	220
6	X-ray structure determination of a metastable state of carbonmonoxy myoglobin after photodissociation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>1996</b> , 93, 7013-6	11.5	131
5	Crystal structure of vancomycin. <i>Structure</i> , <b>1996</b> , 4, 1509-15	5.2	150
4	Contribution of the intramolecular disulfide bridge to the folding stability of REIv, the variable domain of a human immunoglobulin kappa light chain. <i>Folding &amp; Design</i> , <b>1996</b> , 1, 431-40		59
3	Comparison of different X-ray data-collection systems using the crystal structure of octreotide. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>1995</b> , 51, 60-8		3
2	Crystal structure of domain A of Thermus flavus 5S rRNA and the contribution of water molecules to its structure. <i>FEBS Letters</i> , <b>1994</b> , 351, 159-64	3.8	53
1	Structural insights into glycine reuptake inhibition		1