

Nicholas K Sauter

List of Publications by Year in descending order

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72
papers

11,164
citations

109321

35
h-index

85541

71
g-index

75
all docs

75
docs citations

75
times ranked

14866
citing authors

#	ARTICLE	IF	CITATIONS
1	Chemical crystallography by serial femtosecond X-ray diffraction. <i>Nature</i> , 2022, 601, 360-365.	27.8	33
2	XFEL serial crystallography reveals the room temperature structure of methyl-coenzyme M reductase. <i>Journal of Inorganic Biochemistry</i> , 2022, 230, 111768.	3.5	6
3	Challenges in solving structures from radiation-damaged tomograms of protein nanocrystals assessed by simulation. <i>Acta Crystallographica Section D: Structural Biology</i> , 2021, 77, 572-586.	2.3	0
4	Reply to Wang et al.: Clear evidence of binding of O ₂ to the oxygen-evolving complex of photosystem II is best observed in the omit map. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, e2102342118.	7.1	7
5	An on-demand, drop-on-drop method for studying enzyme catalysis by serial crystallography. <i>Nature Communications</i> , 2021, 12, 4461.	12.8	34
6	X-ray free-electron laser studies reveal correlated motion during isopenicillin N synthase catalysis. <i>Science Advances</i> , 2021, 7, .	10.3	23
7	Room temperature XFEL crystallography reveals asymmetry in the vicinity of the two phylloquinones in photosystem I. <i>Scientific Reports</i> , 2021, 11, 21787.	3.3	11
8	Structural dynamics in the water and proton channels of photosystem II during the S ₂ to S ₃ transition. <i>Nature Communications</i> , 2021, 12, 6531.	12.8	73
9	Photoreversible interconversion of a phytochrome photosensory module in the crystalline state. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 300-307.	7.1	19
10	High-Resolution XFEL Structure of the Soluble Methane Monooxygenase Hydroxylase Complex with its Regulatory Component at Ambient Temperature in Two Oxidation States. <i>Journal of the American Chemical Society</i> , 2020, 142, 14249-14266.	13.7	41
11	Serial femtosecond crystallography on in vivo-grown crystals drives elucidation of mosquitoicidal Cyt1Aa bioactivation cascade. <i>Nature Communications</i> , 2020, 11, 1153.	12.8	31
12	Transactions from the 69th Annual Meeting of the American Crystallographic Association: Data best practices—current state and future needs. <i>Structural Dynamics</i> , 2020, 7, 021301.	2.3	1
13	Best practices for high data-rate macromolecular crystallography (HDRMX). <i>Structural Dynamics</i> , 2020, 7, 014302.	2.3	10
14	Artificial Iron Proteins: Modeling the Active Sites in Non-Heme Dioxygenases. <i>Inorganic Chemistry</i> , 2020, 59, 6000-6009.	4.0	10
15	Untangling the sequence of events during the S ₂ → S ₃ transition in photosystem II and implications for the water oxidation mechanism. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 12624-12635.	7.1	149
16	Comparing serial X-ray crystallography and microcrystal electron diffraction (MicroED) as methods for routine structure determination from small macromolecular crystals. <i>IUCr</i> , 2020, 7, 306-323.	2.2	32
17	Towards the spatial resolution of metalloprotein charge states by detailed modeling of XFEL crystallographic diffraction. <i>Acta Crystallographica Section D: Structural Biology</i> , 2020, 76, 176-192.	2.3	14
18	Beyond integration: modeling every pixel to obtain better structure factors from stills. <i>IUCr</i> , 2020, 7, 1151-1167.	2.2	8

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19	Selling reduction versus Niggli reduction for crystallographic lattices. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, 115-120.	0.1	14
20	The crystal structure of dGTPase reveals the molecular basis of dGTP selectivity. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 9333-9339.	7.1	12
21	Mix-and-inject XFEL crystallography reveals gated conformational dynamics during enzyme catalysis. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 25634-25640.	7.1	56
22	A space for lattice representation and clustering. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, 593-599.	0.1	7
23	SAD phasing of XFEL data depends critically on the error model. Acta Crystallographica Section D: Structural Biology, 2019, 75, 959-968.	2.3	15
24	Towards in cellulose virus crystallography. Scientific Reports, 2018, 8, 3771.	3.3	11
25	Structures of the intermediates of Kokâ€™s photosynthetic water oxidation clock. Nature, 2018, 563, 421-425.	27.8	386
26	Improving signal strength in serial crystallography with <i>DIALS</i> geometry refinement. Acta Crystallographica Section D: Structural Biology, 2018, 74, 877-894.	2.3	49
27	A convolutional neural network-based screening tool for X-ray serial crystallography. Journal of Synchrotron Radiation, 2018, 25, 655-670.	2.4	41
28	<i>DIALS</i> : implementation and evaluation of a new integration package. Acta Crystallographica Section D: Structural Biology, 2018, 74, 85-97.	2.3	811
29	Free-electron laser data for multiple-particle fluctuation scattering analysis. Scientific Data, 2018, 5, 180201.	5.3	6
30	Drop-on-demand sample delivery for studying biocatalysts in action at X-ray free-electron lasers. Nature Methods, 2017, 14, 443-449.	19.0	150
31	High-speed fixed-target serial virus crystallography. Nature Methods, 2017, 14, 805-810.	19.0	106
32	Responses to 'Atomic resolution': a badly abused term in structural biology. Acta Crystallographica Section D: Structural Biology, 2017, 73, 381-383.	2.3	7
33	XFEL structures of the influenza M2 proton channel: Room temperature water networks and insights into proton conduction. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 13357-13362.	7.1	64
34	<i>TakeTwo</i> : an indexing algorithm suited to still images with known crystal parameters. Acta Crystallographica Section D: Structural Biology, 2016, 72, 956-965.	2.3	35
35	Measuring and modeling diffuse scattering in protein X-ray crystallography. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 4069-4074.	7.1	48
36	No observable conformational changes in PSII. Nature, 2016, 533, E1-E2.	27.8	40

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37	De novo phasing with X-ray laser reveals mosquito larvicide BinAB structure. <i>Nature</i> , 2016, 539, 43-47.	27.8	98
38	Structure of photosystem II and substrate binding at room temperature. <i>Nature</i> , 2016, 540, 453-457.	27.8	323
39	IOTA: integration optimization, triage and analysis tool for the processing of XFEL diffraction images. <i>Journal of Applied Crystallography</i> , 2016, 49, 1057-1064.	4.5	17
40	On the release of <i>cppxfel</i> for processing X-ray free-electron laser images. <i>Journal of Applied Crystallography</i> , 2016, 49, 1065-1072.	4.5	28
41	Diffraction-geometry refinement in the <i>DIALS</i> framework. <i>Acta Crystallographica Section D: Structural Biology</i> , 2016, 72, 558-575.	2.3	158
42	Advances in X-ray free electron laser (XFEL) diffraction data processing applied to the crystal structure of the synaptotagmin-1 / SNARE complex. <i>ELife</i> , 2016, 5, .	6.0	28
43	Structure of CPV17 polyhedrin determined by the improved analysis of serial femtosecond crystallographic data. <i>Nature Communications</i> , 2015, 6, 6435.	12.8	56
44	A revised partiality model and post-refinement algorithm for X-ray free-electron laser data. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2015, 71, 1400-1410.	2.5	60
45	XFEL diffraction: developing processing methods to optimize data quality. <i>Journal of Synchrotron Radiation</i> , 2015, 22, 239-248.	2.4	85
46	<i>Data Exploration Toolkit</i> for serial diffraction experiments. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2015, 71, 352-356.	2.5	28
47	Indexing amyloid peptide diffraction from serial femtosecond crystallography: new algorithms for sparse patterns. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2015, 71, 357-366.	2.5	18
48	Architecture of the synaptotagmin SNARE machinery for neuronal exocytosis. <i>Nature</i> , 2015, 525, 62-67.	27.8	268
49	Structure of the toxic core of α -synuclein from invisible crystals. <i>Nature</i> , 2015, 525, 486-490.	27.8	528
50	Enabling X-ray free electron laser crystallography for challenging biological systems from a limited number of crystals. <i>ELife</i> , 2015, 4, .	6.0	106
51	Tightly integrated single- and multi-crystal data collection strategy calculation and parallelized data processing in <i>JBLuce</i> beamline control system. <i>Journal of Applied Crystallography</i> , 2014, 47, 1992-1999.	4.5	12
52	<i>dxtbx</i> : the diffraction experiment toolbox. <i>Journal of Applied Crystallography</i> , 2014, 47, 1459-1465.	4.5	29
53	Methods development for diffraction and spectroscopy studies of metalloenzymes at X-ray free-electron lasers. <i>Philosophical Transactions of the Royal Society B: Biological Sciences</i> , 2014, 369, 20130590.	4.0	23
54	Improved crystal orientation and physical properties from single-shot XFEL stills. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 3299-3309.	2.5	38

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55	New methods for indexing multi-lattice diffraction data. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 2652-2666.	2.5	56
56	Accurate macromolecular structures using minimal measurements from X-ray free-electron lasers. <i>Nature Methods</i> , 2014, 11, 545-548.	19.0	140
57	Protein crystal structure obtained at 2.9 Å... resolution from injecting bacterial cells into an X-ray free-electron laser beam. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 12769-12774.	7.1	111
58	Taking snapshots of photosynthetic water oxidation using femtosecond X-ray diffraction and spectroscopy. <i>Nature Communications</i> , 2014, 5, 4371.	12.8	206
59	The Mn ₄ Ca photosynthetic water-oxidation catalyst studied by simultaneous X-ray spectroscopy and crystallography using an X-ray free-electron laser. <i>Philosophical Transactions of the Royal Society B: Biological Sciences</i> , 2014, 369, 20130324.	4.0	17
60	Simultaneous Femtosecond X-ray Spectroscopy and Diffraction of Photosystem II at Room Temperature. <i>Science</i> , 2013, 340, 491-495.	12.6	378
61	New Python-based methods for data processing. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013, 69, 1274-1282.	2.5	95
62	Nanoflow electrospinning serial femtosecond crystallography. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012, 68, 1584-1587.	2.5	167
63	Room temperature femtosecond X-ray diffraction of photosystem II microcrystals. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 9721-9726.	7.1	144
64	Autoindexing with outlier rejection and identification of superimposed lattices. <i>Journal of Applied Crystallography</i> , 2010, 43, 611-616.	4.5	24
65	Detection and correction of underassigned rotational symmetry prior to structure deposition. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 503-513.	2.5	13
66	Autoindexing the diffraction patterns from crystals with a pseudotranslation. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2009, 65, 553-559.	2.5	13
67	Automated diffraction image analysis and spot searching for high-throughput crystal screening. <i>Journal of Applied Crystallography</i> , 2006, 39, 112-119.	4.5	106
68	Improved statistics for determining the Patterson symmetry from unmerged diffraction intensities. <i>Journal of Applied Crystallography</i> , 2006, 39, 158-168.	4.5	20
69	Robust indexing for automatic data collection. <i>Journal of Applied Crystallography</i> , 2004, 37, 399-409.	4.5	149
70	The Computational Crystallography Toolbox: crystallographic algorithms in a reusable software framework. <i>Journal of Applied Crystallography</i> , 2002, 35, 126-136.	4.5	262
71	PHENIX: building new software for automated crystallographic structure determination. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2002, 58, 1948-1954.	2.5	3,979
72	Blu-Ice and the Distributed Control System: software for data acquisition and instrument control at macromolecular crystallography beamlines. <i>Journal of Synchrotron Radiation</i> , 2002, 9, 401-406.	2.4	1,018