

Andrey Kovalevsky

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.

116
papers

3,610
citations

33
h-index

56
g-index

206
ext. papers

4,229
ext. citations

6.9
avg, IF

5.32
L-index

#	Paper	IF	Citations
116	Hit Expansion of a Noncovalent SARS-CoV-2 Main Protease Inhibitor.. <i>ACS Pharmacology and Translational Science</i> , 2022 , 5, 255-265	5.9	1
115	Covalent nardlaprevir- and boceprevir-derived hybrid inhibitors of SARS-CoV-2 main protease.. <i>Nature Communications</i> , 2022 , 13, 2268	17.4	10
114	Microgravity crystallization of perdeuterated tryptophan synthase for neutron diffraction.. <i>Npj Microgravity</i> , 2022 , 8, 13	5.3	
113	High-Throughput Virtual Screening and Validation of a SARS-CoV-2 Main Protease Noncovalent Inhibitor. <i>Journal of Chemical Information and Modeling</i> , 2021 ,	6.1	12
112	Michaelis-like complex of SARS-CoV-2 main protease visualized by room-temperature X-ray crystallography. <i>IUCrJ</i> , 2021 , 8, 973-979	4.7	5
111	Structural, Electronic, and Electrostatic Determinants for Inhibitor Binding to Subsites S1 and S2 in SARS-CoV-2 Main Protease. <i>Journal of Medicinal Chemistry</i> , 2021 , 64, 17366-17383	8.3	7
110	Direct Observation of Protonation State Modulation in SARS-CoV-2 Main Protease upon Inhibitor Binding with Neutron Crystallography. <i>Journal of Medicinal Chemistry</i> , 2021 , 64, 4991-5000	8.3	15
109	Capturing the Catalytic Proton of Dihydrofolate Reductase: Implications for General Acid-Base Catalysis. <i>ACS Catalysis</i> , 2021 , 11, 5873-5884	13.1	0
108	Room temperature crystallography of human acetylcholinesterase bound to a substrate analogue 4K-TMA: Towards a neutron structure. <i>Current Research in Structural Biology</i> , 2021 , 3, 206-215	2.8	2
107	Characterization and structural analysis of a thermophilic GH11 xylanase from compost metatranscriptome. <i>Applied Microbiology and Biotechnology</i> , 2021 , 105, 7757-7767	5.7	2
106	Covalent inhibition of hAChE by organophosphates causes homodimer dissociation through long-range allosteric effects. <i>Journal of Biological Chemistry</i> , 2021 , 297, 101007	5.4	2
105	Revertant mutation V48G alters conformational dynamics of highly drug resistant HIV protease PRS17. <i>Journal of Molecular Graphics and Modelling</i> , 2021 , 108, 108005	2.8	0
104	Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease.. <i>Chemical Science</i> , 2021 , 12, 1513-1527	9.4	29
103	Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 5832-5852	6.1	71
102	Visualizing Tetrahedral Oxyanion Bound in HIV-1 Protease Using Neutrons: Implications for the Catalytic Mechanism and Drug Design. <i>ACS Omega</i> , 2020 , 5, 11605-11617	3.9	2
101	Structural plasticity of SARS-CoV-2 3CL M active site cavity revealed by room temperature X-ray crystallography. <i>Nature Communications</i> , 2020 , 11, 3202	17.4	185
100	Protein kinase A in the neutron beam: Insights for catalysis from directly observing protons. <i>Methods in Enzymology</i> , 2020 , 634, 311-331	1.7	

99	Rational design, synthesis, and evaluation of uncharged, "smart" bis-oxime antidotes of organophosphate-inhibited human acetylcholinesterase. <i>Journal of Biological Chemistry</i> , 2020 , 295, 40792-4092	5.4	16
98	Pyridoxal 5-phosphate dependent reactions: Analyzing the mechanism of aspartate aminotransferase. <i>Methods in Enzymology</i> , 2020 , 634, 333-359	1.7	3
97	Room-temperature X-ray crystallography reveals the oxidation and reactivity of cysteine residues in SARS-CoV-2 3CL M: insights into enzyme mechanism and drug design. <i>IUCrJ</i> , 2020 , 7,	4.7	27
96	Room-temperature neutron and X-ray data collection of 3CL M from SARS-CoV-2. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2020 , 76, 483-487	1.1	13
95	Studying the Role of a Single Mutation of a Family 11 Glycoside Hydrolase Using High-Resolution X-ray Crystallography. <i>Protein Journal</i> , 2020 , 39, 671-680	3.9	1
94	IMAGINE: The neutron protein crystallography beamline at the high flux isotope reactor. <i>Methods in Enzymology</i> , 2020 , 634, 69-85	1.7	9
93	Proton transfer and drug binding details revealed in neutron diffraction studies of wild-type and drug resistant HIV-1 protease. <i>Methods in Enzymology</i> , 2020 , 634, 257-279	1.7	1
92	Substrate Binding Stiffens Aspartate Aminotransferase by Altering the Enzyme Picosecond Vibrational Dynamics. <i>ACS Omega</i> , 2020 , 5, 18787-18797	3.9	2
91	Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease 2020 ,		2
90	Pressure and Temperature Effects on the Formation of Aminoacrylate Intermediates of Tyrosine Phenol-lyase Demonstrate Reaction Dynamics. <i>ACS Catalysis</i> , 2020 , 10, 1692-1703	13.1	4
89	Unusual zwitterionic catalytic site of SARS-CoV-2 main protease revealed by neutron crystallography. <i>Journal of Biological Chemistry</i> , 2020 , 295, 17365-17373	5.4	50
88	Malleability of the SARS-CoV-2 3CL M Active-Site Cavity Facilitates Binding of Clinical Antivirals. <i>Structure</i> , 2020 , 28, 1313-1320.e3	5.2	61
87	A new crystal form of human acetylcholinesterase for exploratory room-temperature crystallography studies. <i>Chemico-Biological Interactions</i> , 2019 , 309, 108698	5	31
86	Productive reorientation of a bound oxime reactivator revealed in room temperature X-ray structures of native and VX-inhibited human acetylcholinesterase. <i>Journal of Biological Chemistry</i> , 2019 , 294, 10607-10618	5.4	9
85	Zooming in on protons: Neutron structure of protein kinase A trapped in a product complex. <i>Science Advances</i> , 2019 , 5, eaav0482	14.3	15
84	Room-temperature photo-induced martensitic transformation in a protein crystal. <i>IUCrJ</i> , 2019 , 6, 619-629.	4.7	1
83	Neutron Crystallography Detects Differences in Protein Dynamics: Structure of the PKG II Cyclic Nucleotide Binding Domain in Complex with an Activator. <i>Biochemistry</i> , 2018 , 57, 1833-1837	3.2	1
82	"To Be or Not to Be" Protonated: Atomic Details of Human Carbonic Anhydrase-Clinical Drug Complexes by Neutron Crystallography and Simulation. <i>Structure</i> , 2018 , 26, 383-390.e3	5.2	32

81	Understanding the pH-Dependent Reaction Mechanism of a Glycoside Hydrolase Using High-Resolution X-ray and Neutron Crystallography. <i>ACS Catalysis</i> , 2018 , 8, 8058-8069	13.1	7
80	IMAGINE: neutrons reveal enzyme chemistry. <i>Acta Crystallographica Section D: Structural Biology</i> , 2018 , 74, 778-786	5.5	19
79	Hyperconjugation Promotes Catalysis in a Pyridoxal 5'-Phosphate-Dependent Enzyme. <i>ACS Catalysis</i> , 2018 , 8, 6733-6737	13.1	11
78	The Neutron Macromolecular Crystallography Instruments at Oak Ridge National Laboratory: Advances, Challenges, and Opportunities. <i>Crystals</i> , 2018 , 8, 388	2.3	18
77	Neutron scattering in the biological sciences: progress and prospects. <i>Acta Crystallographica Section D: Structural Biology</i> , 2018 , 74, 1129-1168	5.5	31
76	Temperature-Induced Replacement of Phosphate Proton with Metal Ion Captured in Neutron Structures of A-DNA. <i>Structure</i> , 2018 , 26, 1645-1650.e3	5.2	3
75	Room Temperature Neutron Crystallography of Drug Resistant HIV-1 Protease Uncovers Limitations of X-ray Structural Analysis at 100 K. <i>Journal of Medicinal Chemistry</i> , 2017 , 60, 2018-2025	8.3	20
74	Direct evidence that an extended hydrogen-bonding network influences activation of pyridoxal 5'-phosphate in aspartate aminotransferase. <i>Journal of Biological Chemistry</i> , 2017 , 292, 5970-5980	5.4	26
73	Neutron and Atomic Resolution X-ray Structures of a Lytic Polysaccharide Monooxygenase Reveal Copper-Mediated Dioxygen Binding and Evidence for N-Terminal Deprotonation. <i>Biochemistry</i> , 2017 , 56, 2529-2532	3.2	44
72	Direct visualization of critical hydrogen atoms in a pyridoxal 5'-phosphate enzyme. <i>Nature Communications</i> , 2017 , 8, 955	17.4	41
71	Biological Structures. <i>Experimental Methods in the Physical Sciences</i> , 2017 , 49, 1-75	0.4	7
70	Mannobiose Binding Induces Changes in Hydrogen Bonding and Protonation States of Acidic Residues in Concanavalin A As Revealed by Neutron Crystallography. <i>Biochemistry</i> , 2017 , 56, 4747-4750	3.2	21
69	Neutron structures of the <i>Helicobacter pylori</i> 5'-methylthioadenosine nucleosidase highlight proton sharing and protonation states. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016 , 113, 13756-13761	11.5	25
68	Limitations in current acetylcholinesterase structure-based design of oxime antidotes for organophosphate poisoning. <i>Annals of the New York Academy of Sciences</i> , 2016 , 1378, 41-49	6.5	14
67	Visualizing the Bohr effect in hemoglobin: neutron structure of equine cyanomethemoglobin in the R state and comparison with human deoxyhemoglobin in the T state. <i>Acta Crystallographica Section D: Structural Biology</i> , 2016 , 72, 892-903	5.5	6
66	Evolution and characterization of a new reversibly photoswitching chromogenic protein, Dathail. <i>Journal of Molecular Biology</i> , 2016 , 428, 1776-89	6.5	19
65	Long-Range Electrostatics-Induced Two-Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. <i>Angewandte Chemie</i> , 2016 , 128, 5008-5011	3.6	6
64	Long-Range Electrostatics-Induced Two-Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 4924-7	16.4	34

63	Neutron structure of human carbonic anhydrase II in complex with methazolamide: mapping the solvent and hydrogen-bonding patterns of an effective clinical drug. <i>IUCrJ</i> , 2016 , 3, 319-325	4.7	24
62	Phosphoryl Transfer Reaction Snapshots in Crystals: INSIGHTS INTO THE MECHANISM OF PROTEIN KINASE A CATALYTIC SUBUNIT. <i>Journal of Biological Chemistry</i> , 2015 , 290, 15538-15548	5.4	18
61	Neutron and high-resolution room-temperature X-ray data collection from crystallized lytic polysaccharide monooxygenase. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2015 , 71, 1448-52	1.1	8
60	Direct determination of protonation states and visualization of hydrogen bonding in a glycoside hydrolase with neutron crystallography. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015 , 112, 12384-9	11.5	26
59	Protein Kinase A Catalytic Subunit Primed for Action: Time-Lapse Crystallography of Michaelis Complex Formation. <i>Structure</i> , 2015 , 23, 2331-2340	5.2	16
58	Joint neutron crystallographic and NMR solution studies of Tyr residue ionization and hydrogen bonding: Implications for enzyme-mediated proton transfer. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015 , 112, 5673-8	11.5	30
57	Neutron diffraction reveals hydrogen bonds critical for cGMP-selective activation: insights for cGMP-dependent protein kinase agonist design. <i>Biochemistry</i> , 2014 , 53, 6725-7	3.2	25
56	L-Arabinose binding, isomerization, and epimerization by D-xylose isomerase: X-ray/neutron crystallographic and molecular simulation study. <i>Structure</i> , 2014 , 22, 1287-1300	5.2	19
55	Metal-free cAMP-dependent protein kinase can catalyze phosphoryl transfer. <i>Biochemistry</i> , 2014 , 53, 3179-86	3.2	17
54	Engineering acidic <i>Streptomyces rubiginosus</i> D-xylose isomerase by rational enzyme design. <i>Protein Engineering, Design and Selection</i> , 2014 , 27, 59-64	1.9	15
53	X-ray crystallographic studies of family 11 xylanase Michaelis and product complexes: implications for the catalytic mechanism. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014 , 70, 11-23		29
52	Novel complex MAD phasing and RNase H structural insights using selenium oligonucleotides. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014 , 70, 354-61		10
51	Toward resolving the catalytic mechanism of dihydrofolate reductase using neutron and ultrahigh-resolution X-ray crystallography. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014 , 111, 18225-30	11.5	58
50	Preliminary joint X-ray and neutron protein crystallographic studies of ecDHFR complexed with folate and NADP+. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2014 , 70, 814-8	1.1	7
49	The IMAGINE instrument: first neutron protein structure and new capabilities for neutron macromolecular crystallography. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013 , 69, 2157-60		60
48	Insights into the phosphoryl transfer catalyzed by cAMP-dependent protein kinase: an X-ray crystallographic study of complexes with various metals and peptide substrate SP20. <i>Biochemistry</i> , 2013 , 52, 3721-7	3.2	22
47	Neutron protein crystallography reveals unique details of clinical drug binding to a human target enzyme. <i>Neutron News</i> , 2013 , 24, 20-23	0.4	
46	Joint X-ray/neutron crystallographic study of HIV-1 protease with clinical inhibitor amprenavir: insights for drug design. <i>Journal of Medicinal Chemistry</i> , 2013 , 56, 5631-5	8.3	51

45	Heterologous expression, purification, crystallization and preliminary X-ray analysis of <i>Trichoderma reesei</i> xylanase II and four variants. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2013 , 69, 320-3		2
44	Low- and room-temperature X-ray structures of protein kinase A ternary complexes shed new light on its activity. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 854-60		20
43	Inhibition of D-xylose isomerase by polyols: atomic details by joint X-ray/neutron crystallography. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012 , 68, 1201-6		14
42	Capturing the reaction pathway in near-atomic-resolution crystal structures of HIV-1 protease. <i>Biochemistry</i> , 2012 , 51, 7726-32	3.2	10
41	Neutron diffraction of acetazolamide-bound human carbonic anhydrase II reveals atomic details of drug binding. <i>Journal of the American Chemical Society</i> , 2012 , 134, 14726-9	16.4	84
40	Inorganic pyrophosphatase crystals from <i>Thermococcus thioreducens</i> for X-ray and neutron diffraction. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2012 , 68, 1482-7		14
39	Room-temperature ultrahigh-resolution time-of-flight neutron and X-ray diffraction studies of H/D-exchanged crambin. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2012 , 68, 119-23		8
38	Direct observation of hydrogen atom dynamics and interactions by ultrahigh resolution neutron protein crystallography. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012 , 109, 15301-6	11.5	48
37	High-resolution neutron crystallographic studies of the hydration of the coenzyme cob(II)alamin. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011 , 67, 584-91		27
36	Preliminary joint X-ray and neutron protein crystallographic studies of endoxylanase II from the fungus <i>Trichoderma longibrachiatum</i> . <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2011 , 67, 283-6		5
35	Preliminary joint neutron time-of-flight and X-ray crystallographic study of human ABO(H) blood group A glycosyltransferase. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2011 , 67, 258-62		3
34	Time-of-flight neutron diffraction study of bovine Ecthyotrypsin at the Protein Crystallography Station. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2011 , 67, 587-90		1
33	Identification of the Elusive Hydronium Ion Exchanging Roles with a Proton in an Enzyme at Lower pH Values. <i>Angewandte Chemie</i> , 2011 , 123, 7662-7665	3.6	8
32	Identification of the elusive hydronium ion exchanging roles with a proton in an enzyme at lower pH values. <i>Angewandte Chemie - International Edition</i> , 2011 , 50, 7520-3	16.4	60
31	Neutron structure of human carbonic anhydrase II: a hydrogen-bonded water network "switch" is observed between pH 7.8 and 10.0. <i>Biochemistry</i> , 2011 , 50, 9421-3	3.2	48
30	Amprenavir complexes with HIV-1 protease and its drug-resistant mutants altering hydrophobic clusters. <i>FEBS Journal</i> , 2010 , 277, 3699-714	5.7	100
29	Neutron structure of human carbonic anhydrase II: implications for proton transfer. <i>Biochemistry</i> , 2010 , 49, 415-21	3.2	77
28	Direct determination of protonation states of histidine residues in a 2 Å neutron structure of deoxy-human normal adult hemoglobin and implications for the Bohr effect. <i>Journal of Molecular Biology</i> , 2010 , 398, 276-91	6.5	33

27	Metal ion roles and the movement of hydrogen during reaction catalyzed by D-xylose isomerase: a joint x-ray and neutron diffraction study. <i>Structure</i> , 2010 , 18, 688-99	5.2	128
26	Protonation states of histidine and other key residues in deoxy normal human adult hemoglobin by neutron protein crystallography. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010 , 66, 1144-52		5
25	Hemoglobin redux: combining neutron and X-ray diffraction with mass spectrometry to analyse the quaternary state of oxidized hemoglobins. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010 , 66, 1249-56		1
24	Macromolecular neutron crystallography at the Protein Crystallography Station (PCS). <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010 , 66, 1206-12		11
23	Using neutron protein crystallography to understand enzyme mechanisms. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010 , 66, 1257-61		5
22	Design, synthesis, protein-ligand X-ray structure, and biological evaluation of a series of novel macrocyclic human immunodeficiency virus-1 protease inhibitors to combat drug resistance. <i>Journal of Medicinal Chemistry</i> , 2009 , 52, 7689-705	8.3	37
21	The catalytic mechanism of an aspartic proteinase explored with neutron and X-ray diffraction. <i>Journal of the American Chemical Society</i> , 2008 , 130, 7235-7	16.4	99
20	Effect of flap mutations on structure of HIV-1 protease and inhibition by saquinavir and darunavir. <i>Journal of Molecular Biology</i> , 2008 , 381, 102-15	6.5	69
19	Structural evidence for effectiveness of darunavir and two related antiviral inhibitors against HIV-2 protease. <i>Journal of Molecular Biology</i> , 2008 , 384, 178-92	6.5	40
18	Potent HIV-1 protease inhibitors incorporating meso-bicyclic urethanes as P2-ligands: structure-based design, synthesis, biological evaluation and protein-ligand X-ray studies. <i>Organic and Biomolecular Chemistry</i> , 2008 , 6, 3703-13	3.9	14
17	Solution kinetics measurements suggest HIV-1 protease has two binding sites for darunavir and amprenavir. <i>Journal of Medicinal Chemistry</i> , 2008 , 51, 6599-603	8.3	27
16	Hydrogen location in stages of an enzyme-catalyzed reaction: time-of-flight neutron structure of D-xylose isomerase with bound D-xylulose. <i>Biochemistry</i> , 2008 , 47, 7595-7	3.2	41
15	Caught in the Act: the 1.5 Å resolution crystal structures of the HIV-1 protease and the I54V mutant reveal a tetrahedral reaction intermediate. <i>Biochemistry</i> , 2007 , 46, 14854-64	3.2	40
14	Anion Chain Structure Controlled Behavior of Phase Transition in Quasi-Two-Dimensional Organic Metal (EDT-TTF) ₄ [Hg ₃ I ₈]1 $\frac{1}{2}$. <i>Crystal Growth and Design</i> , 2007 , 7, 2768-2773	3.5	6
13	Atomic resolution crystal structures of HIV-1 protease and mutants V82A and I84V with saquinavir. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007 , 67, 232-42	4.2	74
12	Synthesis, Crystal Structures, Magnetic Properties and Photoconductivity of C ₆₀ and C ₇₀ Complexes with Metal Dialkyldithiocarbamates M(R ₂ dtc) _x , where M = CuI, CuI, AgI, ZnII, CdII, HgII, MnII, NiII, and PtII; R = Me, Et, and nPr. <i>European Journal of Inorganic Chemistry</i> , 2006 , 2006, 1881-1895	2.3	40
11	Structural aspects of two-stage dimerization in an ionic C ₆₀ complex with bis(benzene)chromium: Cr(C ₆ H ₆) ₂ .C ₆₀ .C ₆ H ₄ Cl ₂ . <i>Dalton Transactions</i> , 2006 , 3716-20	4.3	36
10	Mechanism of drug resistance revealed by the crystal structure of the unliganded HIV-1 protease with F53L mutation. <i>Journal of Molecular Biology</i> , 2006 , 358, 1191-9	6.5	45

9	Ultra-high resolution crystal structure of HIV-1 protease mutant reveals two binding sites for clinical inhibitor TMC114. <i>Journal of Molecular Biology</i> , 2006 , 363, 161-73	6.5	117
8	Bis[bis(3-phenylpyrazol-1-yl)(pyrazol-1-yl)methane]copper(II) bis(perchlorate) acetonitrile disolvate. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2006 , 62, m30-2		
7	Synthesis, crystal structure and photoconductivity of the first [60]fullerene complex with metal diethyldithiocarbamate: {CuII(dedtc)2}2.C60. <i>Dalton Transactions</i> , 2005 , 1821-5	4.3	18
6	Physical and kinetic analysis of the cooperative role of metal ions in catalysis of phosphodiester cleavage by a dinuclear Zn(II) complex. <i>Journal of the American Chemical Society</i> , 2003 , 125, 1988-93	16.4	207
5	Creating nanocavities of tunable sizes: hollow helices. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002 , 99, 11583-8	11.5	130
4	Photoinduced linkage isomers of transition-metal nitrosyl compounds and related complexes. <i>Chemical Reviews</i> , 2002 , 102, 861-84	68.1	372
3	First Observation of Photoinduced Nitrosyl Linkage Isomers of Iron Nitrosyl Porphyrins. <i>Journal of the American Chemical Society</i> , 2000 , 122, 7142-7143	16.4	66
2	Protonation states in SARS-CoV-2 main protease mapped by neutron crystallography		1
1	High Throughput Virtual Screening and Validation of a SARS-CoV-2 Main Protease Non-Covalent Inhibitor		9