

# Andrey Kovalevsky

## List of Publications by Year in descending order

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127  
papers

5,061  
citations

85707

38  
h-index

106894

65  
g-index

232  
all docs

232  
docs citations

232  
times ranked

6755  
citing authors

| #  | ARTICLE   | IF   | CITATIONS |
|----|---|------|-----------|
| 1  | Visualizing the Active Site Oxyanion Loop Transition Upon Ensitrelvir Binding and Transient Dimerization of SARS-CoV-2 Main Protease. <i>Journal of Molecular Biology</i> , 2024, 436, 168616.                        | 4.3  | 1         |
| 2  | AI-Accelerated Design of Targeted Covalent Inhibitors for SARS-CoV-2. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 1438-1453.  | 5.7  | 7         |
| 3  | Discovering and Designing a Chimeric Hyperthermophilic Chitinase for Crystalline Chitin Degradation. <i>ACS Sustainable Chemistry and Engineering</i> , 2023, 11, 4690-4698.  | 6.9  | 6         |
| 4  | Revealing protonation states and tracking substrate in serine hydroxymethyltransferase with room-temperature X-ray and neutron crystallography. <i>Communications Chemistry</i> , 2023, 6, .                          | 4.9  | 1         |
| 5  | Insights into the mechanism of SARS-CoV-2 main protease autocatalytic maturation from model precursors. <i>Communications Biology</i> , 2023, 6, .  | 4.5  | 6         |
| 6  | Discovery of Novel <i>Rhizoctonia solani</i> DHFR Inhibitors as Fungicides Using Virtual Screening. <i>Journal of Agricultural and Food Chemistry</i> , 2023, 71, 19385-19395.  | 5.3  | 1         |
| 7  | High-Throughput Virtual Screening and Validation of a SARS-CoV-2 Main Protease Noncovalent Inhibitor. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 116-128.  | 5.7  | 64        |
| 8  | Joint neutron/molecular dynamics vibrational spectroscopy reveals softening of HIV-1 protease upon binding of a tight inhibitor. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 3586-3597.                    | 2.9  | 3         |
| 9  | Hit Expansion of a Noncovalent SARS-CoV-2 Main Protease Inhibitor. <i>ACS Pharmacology and Translational Science</i> , 2022, 5, 255-265.  | 4.7  | 18        |
| 10 | Covalent narprevir- and boceprevir-derived hybrid inhibitors of SARS-CoV-2 main protease. <i>Nature Communications</i> , 2022, 13, 2268.  | 13.2 | 77        |
| 11 | Microgravity crystallization of perdeuterated tryptophan synthase for neutron diffraction. <i>Npj Microgravity</i> , 2022, 8, 13.   | 3.8  | 6         |
| 12 | The mechanisms of catalysis and ligand binding for the SARS-CoV-2 NSP3 macrodomain from neutron and x-ray diffraction at room temperature. <i>Science Advances</i> , 2022, 8, .                                       | 10.9 | 30        |
| 13 | EWALD: A macromolecular diffractometer for the second target station. <i>Review of Scientific Instruments</i> , 2022, 93, .   | 1.4  | 4         |
| 14 | An Nâ <sup>-</sup> Hâ <sup>+</sup> N low-barrier hydrogen bond preorganizes the catalytic site of aspartate aminotransferase to facilitate the second half-reaction. <i>Chemical Science</i> , 2022, 13, 10057-10065. | 7.8  | 6         |
| 15 | Structural and functional characterization of NEMO cleavage by SARS-CoV-2 3CLpro. <i>Nature Communications</i> , 2022, 13, .  | 13.2 | 17        |
| 16 | Autoprocessing and oxyanion loop reorganization upon GC373 and nirmatrelvir binding of monomeric SARS-CoV-2 main protease catalytic domain. <i>Communications Biology</i> , 2022, 5, .                                | 4.5  | 14        |
| 17 | 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.                   | 2.3  | 8         |
| 18 | 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.                      | 6.6  | 41        |

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|----|--|------|-----------|
| 19 | Capturing the Catalytic Proton of Dihydrofolate Reductase: Implications for General Acid-Base Catalysis. <i>ACS Catalysis</i> , 2021, 11, 5873-5884.   | 11.7 | 8         |
| 20 | Characterization and structural analysis of a thermophilic GH11 xylanase from compost metatranscriptome. <i>Applied Microbiology and Biotechnology</i> , 2021, 105, 7757-7767.                                     | 3.7  | 10        |
| 21 | Covalent inhibition of hAChE by organophosphates causes homodimer dissociation through long-range allosteric effects. <i>Journal of Biological Chemistry</i> , 2021, 297, 101007.                                  | 3.5  | 8         |
| 22 | Revertant mutation V48G alters conformational dynamics of highly drug resistant HIV protease PRS17. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 108, 108005.  | 2.5  | 1         |
| 23 | Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease. <i>Chemical Science</i> , 2021, 12, 1513-1527.  | 7.8  | 51        |
| 24 | Michaelis-like complex of SARS-CoV-2 main protease visualized by room-temperature X-ray crystallography. <i>IUCr</i> , 2021, 8, 973-979.   | 2.3  | 28        |
| 25 | 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.                     | 6.6  | 35        |
| 26 | 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.                               | 11.7 | 8         |
| 27 | Unusual zwitterionic catalytic site of SARS-CoV-2 main protease revealed by neutron crystallography. <i>Journal of Biological Chemistry</i> , 2020, 295, 17365-17373.  | 3.5  | 104       |
| 28 | Malleability of the SARS-CoV-2 3CL Mpro Active-Site Cavity Facilitates Binding of Clinical Antivirals. <i>Structure</i> , 2020, 28, 1313-1320.e3.  | 3.4  | 115       |
| 29 | Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5832-5852.  | 5.7  | 144       |
| 30 | Visualizing Tetrahedral Oxanion Bound in HIV-1 Protease Using Neutrons: Implications for the Catalytic Mechanism and Drug Design. <i>ACS Omega</i> , 2020, 5, 11605-11617.   | 3.6  | 7         |
| 31 | Structural plasticity of SARS-CoV-2 3CL Mpro active site cavity revealed by room temperature X-ray crystallography. <i>Nature Communications</i> , 2020, 11, 3202.   | 13.2 | 368       |
| 32 | 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  | 0         |
| 33 | Rational design, synthesis, and evaluation of uncharged, <i>smart</i> -bis-oxime antidotes of organophosphate-inhibited human acetylcholinesterase. <i>Journal of Biological Chemistry</i> , 2020, 295, 4079-4092. | 3.5  | 27        |
| 34 | Pyridoxal 5-phosphate dependent reactions: Analyzing the mechanism of aspartate aminotransferase. <i>Methods in Enzymology</i> , 2020, 634, 333-359.   | 1.7  | 13        |
| 35 | 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.   | 1.6  | 3         |
| 36 | IMAGINE: The neutron protein crystallography beamline at the high flux isotope reactor. <i>Methods in Enzymology</i> , 2020, 634, 69-85.   | 1.7  | 21        |

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|----|---|------|-----------|
| 37 | 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  | 4         |
| 38 | Substrate Binding Stiffens Aspartate Aminotransferase by Altering the Enzyme Picosecond Vibrational Dynamics. <i>ACS Omega</i> , 2020, 5, 18787-18797.  | 3.6  | 7         |
| 39 | Room-temperature X-ray crystallography reveals the oxidation and reactivity of cysteine residues in SARS-CoV-2 3CL M <sup>pro</sup> : insights into enzyme mechanism and drug design. <i>IUCr</i> , 2020, 7, 1028-1035.     | 2.3  | 54        |
| 40 | Room-temperature neutron and X-ray data collection of 3CL M <sup>pro</sup> from SARS-CoV-2. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2020, 76, 483-487.                                 | 0.9  | 21        |
| 41 | A new crystal form of human acetylcholinesterase for exploratory room-temperature crystallography studies. <i>Chemico-Biological Interactions</i> , 2019, 309, 108698.  | 4.2  | 97        |
| 42 | 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. | 3.5  | 13        |
| 43 | Zooming in on protons: Neutron structure of protein kinase A trapped in a product complex. <i>Science Advances</i> , 2019, 5, eaav0482.   | 10.9 | 33        |
| 44 | Room-temperature photo-induced martensitic transformation in a protein crystal. <i>IUCr</i> , 2019, 6, 619-629.   | 2.3  | 2         |
| 45 | 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.                          | 2.6  | 1         |
| 46 | "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.                                     | 3.4  | 41        |
| 47 | The Neutron Macromolecular Crystallography Instruments at Oak Ridge National Laboratory: Advances, Challenges, and Opportunities. <i>Crystals</i> , 2018, 8, 388.   | 2.3  | 26        |
| 48 | Neutron scattering in the biological sciences: progress and prospects. <i>Acta Crystallographica Section D: Structural Biology</i> , 2018, 74, 1129-1168.   | 2.4  | 49        |
| 49 | Temperature-Induced Replacement of Phosphate Proton with Metal Ion Captured in Neutron Structures of A-DNA. <i>Structure</i> , 2018, 26, 1645-1650.e3.  | 3.4  | 4         |
| 50 | 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.  | 11.7 | 17        |
| 51 | IMAGINE: neutrons reveal enzyme chemistry. <i>Acta Crystallographica Section D: Structural Biology</i> , 2018, 74, 778-786.   | 2.4  | 25        |
| 52 | Hyperconjugation Promotes Catalysis in a Pyridoxal 5 $\alpha$ -Phosphate-Dependent Enzyme. <i>ACS Catalysis</i> , 2018, 8, 6733-6737.   | 11.7 | 16        |
| 53 | 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.                          | 6.6  | 25        |
| 54 | Direct evidence that an extended hydrogen-bonding network influences activation of pyridoxal 5 $\alpha$ -phosphate in aspartate aminotransferase. <i>Journal of Biological Chemistry</i> , 2017, 292, 5970-5980.            | 3.5  | 42        |

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|----|--|------|-----------|
| 55 | 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.   | 2.6  | 55        |
| 56 | Direct visualization of critical hydrogen atoms in a pyridoxal 5â€²-phosphate enzyme. <i>Nature Communications</i> , 2017, 8, 955.   | 13.2 | 59        |
| 57 | 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.  | 2.6  | 25        |
| 58 | Biological Structures. <i>Experimental Methods in the Physical Sciences</i> , 2017, 49, 1-75.  | 0.1  | 10        |
| 59 | Direct observation of protonation states in a PLP-dependent enzyme by neutron crystallography. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2017, 73, a26-a26.  | 0.1  | 1         |
| 60 | Longâ€Range Electrostaticsâ€Induced Twoâ€Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. <i>Angewandte Chemie</i> , 2016, 128, 5008-5011.  | 2.1  | 6         |
| 61 | Longâ€Range Electrostaticsâ€Induced Twoâ€Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 4924-4927.   | 14.8 | 43        |
| 62 | Neutron structure of human carbonic anhydrase II in complex with methazolamide: mapping the solvent and hydrogen-bonding patterns of an effective clinical drug. <i>IUCr</i> , 2016, 3, 319-325.   | 2.3  | 29        |
| 63 | Neutron structures of the <i>Helicobacter pylori</i> 5â€²-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.             | 7.6  | 31        |
| 64 | 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.                      | 2.4  | 8         |
| 65 | Evolution and characterization of a new reversibly photoswitching chromogenic protein, Dathail. <i>Journal of Molecular Biology</i> , 2016, 428, 1776-1789.  | 4.3  | 20        |
| 66 | 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, 5673-5678. | 7.6  | 39        |
| 67 | Phosphoryl Transfer Reaction Snapshots in Crystals. <i>Journal of Biological Chemistry</i> , 2015, 290, 15538-15548.   | 3.5  | 25        |
| 68 | 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, 1448-1452.   | 0.9  | 8         |
| 69 | 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, 12384-12389.                 | 7.6  | 37        |
| 70 | Protein Kinase A Catalytic Subunit Primed for Action: Time-Lapse Crystallography of Michaelis Complex Formation. <i>Structure</i> , 2015, 23, 2331-2340.   | 3.4  | 22        |
| 71 | Novel complex MAD phasing and RNase H structural insights using selenium oligonucleotides. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 354-361.  | 2.4  | 17        |
| 72 | 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, 18225-18230.                       | 7.6  | 76        |

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|----|--|------|-----------|
| 73 | Preliminary joint X-ray and neutron protein crystallographic studies of ecDHFR complexed with folate and NADP <sup>+</sup> . Acta Crystallographica Section F, Structural Biology Communications, 2014, 70, 814-818.               | 0.9  | 7         |
| 74 | Neutron Diffraction Reveals Hydrogen Bonds Critical for cGMP-Selective Activation: Insights for cGMP-Dependent Protein Kinase Agonist Design. Biochemistry, 2014, 53, 6725-6727.   | 2.6  | 34        |
| 75 | L-Arabinose Binding, Isomerization, and Epimerization by D-Xylose Isomerase: X-Ray/Neutron Crystallographic and Molecular Simulation Study. Structure, 2014, 22, 1287-1300.  | 3.4  | 25        |
| 76 | Metal-Free cAMP-Dependent Protein Kinase Can Catalyze Phosphoryl Transfer. Biochemistry, 2014, 53, 3179-3186.  | 2.6  | 18        |
| 77 | Engineering acidic Streptomyces rubiginosus D-xylose isomerase by rational enzyme design. Protein Engineering, Design and Selection, 2014, 27, 59-64.  | 2.4  | 19        |
| 78 | X-ray crystallographic studies of family 11 xylanase Michaelis and product complexes: implications for the catalytic mechanism. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 11-23.                     | 2.4  | 38        |
| 79 | The IMAGINE instrument: first neutron protein structure and new capabilities for neutron macromolecular crystallography. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 2157-2160.                        | 2.4  | 76        |
| 80 | 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. Biochemistry, 2013, 52, 3721-3727.                  | 2.6  | 24        |
| 81 | Neutron protein crystallography reveals unique details of clinical drug binding to a human target enzyme. Neutron News, 2013, 24, 20-23.   | 0.2  | 0         |
| 82 | Joint X-ray/Neutron Crystallographic Study of HIV-1 Protease with Clinical Inhibitor Amprenavir: Insights for Drug Design. Journal of Medicinal Chemistry, 2013, 56, 5631-5635.  | 6.6  | 62        |
| 83 | Heterologous expression, purification, crystallization and preliminary X-ray analysis of Trichoderma reesei xylanase II and four variants. Acta Crystallographica Section F: Structural Biology Communications, 2013, 69, 320-323. | 0.7  | 2         |
| 84 | Direct observation of hydrogen atom dynamics and interactions by ultrahigh resolution neutron protein crystallography. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 15301-15306.    | 7.6  | 52        |
| 85 | Inhibition of D-xylose isomerase by polyols: atomic details by joint X-ray/neutron crystallography. Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 1201-1206.   | 2.4  | 18        |
| 86 | Capturing the Reaction Pathway in Near-Atomic-Resolution Crystal Structures of HIV-1 Protease. Biochemistry, 2012, 51, 7726-7732.  | 2.6  | 14        |
| 87 | Neutron Diffraction of Acetazolamide-Bound Human Carbonic Anhydrase II Reveals Atomic Details of Drug Binding. Journal of the American Chemical Society, 2012, 134, 14726-14729.   | 14.6 | 100       |
| 88 | Inorganic pyrophosphatase crystals from Thermococcus thio-reducens for X-ray and neutron diffraction. Acta Crystallographica Section F: Structural Biology Communications, 2012, 68, 1482-1487.                                    | 0.7  | 21        |
| 89 | Room-temperature ultrahigh-resolution time-of-flight neutron and X-ray diffraction studies of H/D-exchanged crambin. Acta Crystallographica Section F: Structural Biology Communications, 2012, 68, 119-123.                       | 0.7  | 9         |
| 90 | Low- and room-temperature X-ray structures of protein kinase A ternary complexes shed new light on its activity. Acta Crystallographica Section D: Biological Crystallography, 2012, 68, 854-860.                                  | 2.4  | 26        |

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|-----|--|------|-----------|
| 91  | Neutron Structure of Human Carbonic Anhydrase II: A Hydrogen-Bonded Water Network Observed between pH 7.8 and 10.0. <i>Biochemistry</i> , 2011, 50, 9421-9423.   | 2.6  | 53        |
| 92  | High-resolution neutron crystallographic studies of the hydration of the coenzyme cob(II)alamin. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011, 67, 584-591.  | 2.4  | 30        |
| 93  | 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, 283-286.             | 0.7  | 6         |
| 94  | 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, 258-262.                             | 0.7  | 4         |
| 95  | Time-of-flight neutron diffraction study of bovine $\beta$ -chymotrypsin at the Protein Crystallography Station. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2011, 67, 587-590.   | 0.7  | 1         |
| 96  | 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.   | 2.1  | 8         |
| 97  | 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, 7520-7523.  | 14.8 | 62        |
| 98  | 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, 688-699.   | 3.4  | 143       |
| 99  | 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, 1144-1152.                             | 2.4  | 8         |
| 100 | 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, 1249-1256.                     | 2.4  | 1         |
| 101 | Macromolecular neutron crystallography at the Protein Crystallography Station (PCS). <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 1206-1212.  | 2.4  | 11        |
| 102 | Using neutron protein crystallography to understand enzyme mechanisms. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 1257-1261.  | 2.4  | 5         |
| 103 | Neutron Structure of Human Carbonic Anhydrase II: Implications for Proton Transfer. <i>Biochemistry</i> , 2010, 49, 415-421.   | 2.6  | 82        |
| 104 | Direct Determination of Protonation States of Histidine Residues in a 2.2 Å Neutron Structure of Deoxy-Human Normal Adult Hemoglobin and Implications for the Bohr Effect. <i>Journal of Molecular Biology</i> , 2010, 398, 276-291.                     | 4.3  | 37        |
| 105 | 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, 7689-7705. | 6.6  | 41        |
| 106 | The Catalytic Mechanism of an Aspartic Proteinase Explored with Neutron and X-ray Diffraction. <i>Journal of the American Chemical Society</i> , 2008, 130, 7235-7237.   | 14.6 | 108       |
| 107 | Effect of Flap Mutations on Structure of HIV-1 Protease and Inhibition by Saquinavir and Darunavir. <i>Journal of Molecular Biology</i> , 2008, 381, 102-115.  | 4.3  | 81        |
| 108 | Structural Evidence for Effectiveness of Darunavir and Two Related Antiviral Inhibitors against HIV-2 Protease. <i>Journal of Molecular Biology</i> , 2008, 384, 178-192.  | 4.3  | 44        |



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|-----|---|------|-----------|
| 109 | 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.   | 2.9  | 17        |
| 110 | Solution Kinetics Measurements Suggest HIV-1 Protease Has Two Binding Sites for Darunavir and Amprenavir. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 6599-6603.  | 6.6  | 30        |
| 111 | Hydrogen Location in Stages of an Enzyme-Catalyzed Reaction: Time-of-Flight Neutron Structure of <i>scpd</i> -Xylose Isomerase with Bound <i>scpd</i> -Xylulose. <i>Biochemistry</i> , 2008, 47, 7595-7597.   | 2.6  | 44        |
| 112 | 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, 14854-14864.   | 2.6  | 44        |
| 113 | Anion Chain Structure Controlled Behavior of Phase Transition in Quasi-Two-Dimensional Organic Metal (EDT-TTF) <sub>4</sub> [Hg <sub>3</sub> I <sub>8</sub> ]·x. <i>Crystal Growth and Design</i> , 2007, 7, 2768-2773.   | 3.2  | 7         |
| 114 | Atomic resolution crystal structures of HIV-1 protease and mutants V82A and I84V with saquinavir. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 67, 232-242.  | 3.2  | 86        |
| 115 | Structural aspects of two-stage dimerization in an ionic C <sub>60</sub> complex with bis(benzene)chromium: Cr(C <sub>6</sub> H <sub>6</sub> ) <sub>2</sub> ·C <sub>60</sub> ·C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub> . <i>Dalton Transactions</i> , 2006, , 3716-3720.   | 3.4  | 37        |
| 116 | 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, 1191-1199.   | 4.3  | 48        |
| 117 | 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, 161-173.   | 4.3  | 137       |
| 118 | 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-m32.   | 0.4  | 0         |
| 119 | Synthesis, Crystal Structures, Magnetic Properties and Photoconductivity of C <sub>60</sub> and C <sub>70</sub> Complexes with Metal Dialkylthiocarbamates M(R <sub>2</sub> dtc) <sub>x</sub> , 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. | 2.2  | 44        |
| 120 | Synthesis, crystal structure and photoconductivity of the first [60]fullerene complex with metal diethylthiocarbamate: {CuI(dedtc) <sub>2</sub> } <sub>2</sub> ·C <sub>60</sub> . <i>Dalton Transactions</i> , 2005, , 1821.  | 3.4  | 20        |
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