

# Kalyan Das

## List of Publications by Year in descending order

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138  
papers

10,784  
citations

36691

53  
h-index

36203

101  
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146  
all docs

146  
docs citations

146  
times ranked

8722  
citing authors

| #  | ARTICLE  | IF  | CITATIONS |
|----|--|-----|-----------|
| 1  | A systematic approach to identify host targets and rapidly deliver broad-spectrum antivirals. <i>Molecular Therapy</i> , 2022, 30, 1797-1800.  | 3.7 | 5         |
| 2  | Insights into HIV-1 Reverse Transcriptase (RT) Inhibition and Drug Resistance from Thirty Years of Structural Studies. <i>Viruses</i> , 2022, 14, 1027.  | 1.5 | 8         |
| 3  | Cryo-EM Structures Reveal Transcription Initiation Steps by Yeast Mitochondrial RNA Polymerase. <i>Molecular Cell</i> , 2021, 81, 268-280.e5.  | 4.5 | 15        |
| 4  | Assembly and Cryo-EM structure determination of yeast mitochondrial RNA polymerase initiation complex intermediates. <i>STAR Protocols</i> , 2021, 2, 100431.  | 0.5 | 3         |
| 5  | Crystal Structure of a Retroviral Polyprotein: Prototype Foamy Virus Protease-Reverse Transcriptase (PR-RT). <i>Viruses</i> , 2021, 13, 1495.  | 1.5 | 4         |
| 6  | Exploring the dNTP-binding site of HIV-1 reverse transcriptase for inhibitor design. <i>European Journal of Medicinal Chemistry</i> , 2021, 225, 113785.   | 2.6 | 3         |
| 7  | Tenofovir-Amino Acid Conjugates Act as Polymerase Substrates—Implications for Avoiding Cellular Phosphorylation in the Discovery of Nucleotide Analogues. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 782-796. | 2.9 | 2         |
| 8  | HIV-1 gp120 Antagonists Also Inhibit HIV-1 Reverse Transcriptase by Bridging the NNRTI and NRTI Sites. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 16530-16540.  | 2.9 | 4         |
| 9  | Sliding of HIV-1 reverse transcriptase over DNA creates a transient P pocket — targeting P-pocket by fragment screening. <i>Nature Communications</i> , 2021, 12, 7127.  | 5.8 | 6         |
| 10 | Integrative structural biology studies of HIV-1 reverse transcriptase binding to a high-affinity DNA aptamer. <i>Current Research in Structural Biology</i> , 2020, 2, 116-129.                                      | 1.1 | 8         |
| 11 | Development of a Novel SPR Assay to Study CXCR4—Ligand Interactions. <i>Biosensors</i> , 2020, 10, 150.  | 2.3 | 8         |
| 12 | The dynamic landscape of transcription initiation in yeast mitochondria. <i>Nature Communications</i> , 2020, 11, 4281.  | 5.8 | 18        |
| 13 | Structure, mechanism, and regulation of mitochondrial DNA transcription initiation. <i>Journal of Biological Chemistry</i> , 2020, 295, 18406-18425.   | 1.6 | 43        |
| 14 | Structural Basis of HIV-1 Inhibition by Nucleotide-Competing Reverse Transcriptase Inhibitor INDOPY-1. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 9996-10002.   | 2.9 | 20        |
| 15 | Structure of HIV-1 RT/dsRNA initiation complex prior to nucleotide incorporation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 7308-7313.                     | 3.3 | 26        |
| 16 | Structural basis of ECF- $\lambda$ -factor-dependent transcription initiation. <i>Nature Communications</i> , 2019, 10, 710.   | 5.8 | 37        |
| 17 | Alpha-carboxynucleoside phosphonates: direct-acting inhibitors of viral DNA polymerases. <i>Future Medicinal Chemistry</i> , 2019, 11, 137-154.  | 1.1 | 6         |
| 18 | Structure of HIV-1 reverse transcriptase/d4TTP complex: Novel DNA cross-linking site and pH-dependent conformational changes. <i>Protein Science</i> , 2019, 28, 587-597.  | 3.1 | 11        |

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|----|---|------|-----------|
| 19 | Developing and Evaluating Inhibitors against the RNase H Active Site of HIV-1 Reverse Transcriptase. <i>Journal of Virology</i> , 2018, 92, .   | 1.5  | 30        |
| 20 | Structural Basis of Transcription Inhibition by Fidaxomicin (Lipiarmycin A3). <i>Molecular Cell</i> , 2018, 70, 60-71.e15.  | 4.5  | 81        |
| 21 | Guanine Î±-carboxy nucleoside phosphonate (G-Î±-CNP) shows a different inhibitory kinetic profile against the DNA polymerases of human immunodeficiency virus (HIV) and herpes viruses. <i>Biochemical Pharmacology</i> , 2017, 136, 51-61. | 2.0  | 9         |
| 22 | Structural Insights into HIV Reverse Transcriptase Mutations Q151M and Q151M Complex That Confer Multinucleoside Drug Resistance. <i>Antimicrobial Agents and Chemotherapy</i> , 2017, 61, .  | 1.4  | 16        |
| 23 | Structural Basis of Mycobacterium tuberculosis Transcription and Transcription Inhibition. <i>Molecular Cell</i> , 2017, 66, 169-179.e8.  | 4.5  | 130       |
| 24 | Conformational States of HIV-1 Reverse Transcriptase for Nucleotide Incorporation vs Pyrophosphorolysisâ€”Binding of Foscarnet. <i>ACS Chemical Biology</i> , 2016, 11, 2158-2164.  | 1.6  | 38        |
| 25 | Structure of HIV reverse transcriptase bound to a novel 38â€mer hairpin templateâ€primer DNA aptamer. <i>Protein Science</i> , 2016, 25, 46-55.   | 3.1  | 33        |
| 26 | Exploring the role of the Î±-carboxyphosphonate moiety in the HIV-RT activity of Î±-carboxy nucleoside phosphonates. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 2454-2465.   | 1.5  | 17        |
| 27 | Alpha-carboxy nucleoside phosphonates as universal nucleoside triphosphate mimics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 3475-3480.   | 3.3  | 29        |
| 28 | Negative-Strand RNA Virus L Proteins: One Machine, Many Activities. <i>Cell</i> , 2015, 162, 239-241.   | 13.5 | 17        |
| 29 | Pronounced Inhibition Shift from HIV Reverse Transcriptase to Herpetic DNA Polymerases by Increasing the Flexibility of Î±-Carboxy Nucleoside Phosphonates. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 8110-8127.                    | 2.9  | 9         |
| 30 | Analysis of the Zidovudine Resistance Mutations T215Y, M41L, and L210W in HIV-1 Reverse Transcriptase. <i>Antimicrobial Agents and Chemotherapy</i> , 2015, 59, 7184-7196.  | 1.4  | 8         |
| 31 | Considerations for Structure-Based Drug Design Targeting HIV-1 Reverse Transcriptase. <i>NATO Science for Peace and Security Series A: Chemistry and Biology</i> , 2015, , 69-81.   | 0.5  | 1         |
| 32 | Drug Resistance in Non-B Subtype HIV-1: Impact of HIV-1 Reverse Transcriptase Inhibitors. <i>Viruses</i> , 2014, 6, 3535-3562.  | 1.5  | 27        |
| 33 | Structures of HIV-1 RT-RNA/DNA ternary complexes with dATP and nevirapine reveal conformational flexibility of RNA/DNA: insights into requirements for RNase H cleavage. <i>Nucleic Acids Research</i> , 2014, 42, 8125-8137.               | 6.5  | 60        |
| 34 | Molecular dynamics study of HIV-1 RT-DNA-nevirapine complexes explains NNRTI inhibition and resistance by connection mutations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 815-829.                                | 1.5  | 15        |
| 35 | Phenyl Substituted 4-Hydroxypyridazin-3(2 <i>H</i> )-ones and 5-Hydroxypyrimidin-4(3 <i>H</i> )-ones: Inhibitors of Influenza A Endonuclease. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 8086-8098.                                  | 2.9  | 50        |
| 36 | Mutations in HIV-1 Reverse Transcriptase Affect the Errors Made in a Single Cycle of Viral Replication. <i>Journal of Virology</i> , 2014, 88, 7589-7601.   | 1.5  | 46        |

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|----|--|-----|-----------|
| 37 | Extension into the entrance channel of HIV-1 reverse transcriptase—Crystallography and enhanced solubility. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013, 23, 5209-5212.   | 1.0 | 33        |
| 38 | Crystallographic Fragment Screening and Structure-Based Optimization Yields a New Class of Influenza Endonuclease Inhibitors. <i>ACS Chemical Biology</i> , 2013, 8, 2501-2508.  | 1.6 | 76        |
| 39 | Phenyl substituted 3-hydroxypyridin-2(1H)-ones: Inhibitors of influenza A endonuclease. <i>Bioorganic and Medicinal Chemistry</i> , 2013, 21, 6435-6446.   | 1.4 | 30        |
| 40 | Snapshot of the equilibrium dynamics of a drug bound to HIV-1 reverse transcriptase. <i>Nature Chemistry</i> , 2013, 5, 174-181.   | 6.6 | 88        |
| 41 | Detecting Allosteric Sites of HIV-1 Reverse Transcriptase by X-ray Crystallographic Fragment Screening. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 2738-2746.   | 2.9 | 78        |
| 42 | HIV-1 reverse transcriptase and antiviral drug resistance. Part 1. <i>Current Opinion in Virology</i> , 2013, 3, 111-118.  | 2.6 | 126       |
| 43 | HIV-1 reverse transcriptase and antiviral drug resistance. Part 2. <i>Current Opinion in Virology</i> , 2013, 3, 119-128.  | 2.6 | 83        |
| 44 | 3-Hydroxyquinolin-2(1 <i>H</i> )-ones As Inhibitors of Influenza A Endonuclease. <i>ACS Medicinal Chemistry Letters</i> , 2013, 4, 547-550.  | 1.3 | 44        |
| 45 | Structural requirements for RNA degradation by HIV-1 reverse transcriptase. <i>Nature Structural and Molecular Biology</i> , 2013, 20, 1341-1342.  | 3.6 | 5         |
| 46 | Nonnucleoside Reverse Transcriptase Inhibitors (NNRTIs)., 2013, , 123-139.   |     | 1         |
| 47 | HIV-1 reverse transcriptase complex with DNA and nevirapine reveals non-nucleoside inhibition mechanism. <i>Nature Structural and Molecular Biology</i> , 2012, 19, 253-259.   | 3.6 | 176       |
| 48 | A comparison of the ability of rilpivirine (TMC278) and selected analogues to inhibit clinically relevant HIV-1 reverse transcriptase mutants. <i>Retrovirology</i> , 2012, 9, 99.   | 0.9 | 29        |
| 49 | Antivirals Targeting Influenza A Virus. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 6263-6277.   | 2.9 | 97        |
| 50 | Crystal Structure of <i>tert</i> -Butyldimethylsilyl-spiroaminoxathioledioxide-thymine (TSAO-T) in Complex with HIV-1 Reverse Transcriptase (RT) Redefines the Elastic Limits of the Non-nucleoside Inhibitor-Binding Pocket. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 2727-2737. | 2.9 | 66        |
| 51 | Structure of the guanylyltransferase domain of human mRNA capping enzyme. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 10104-10108.   | 3.3 | 40        |
| 52 | Structures of influenza A proteins and insights into antiviral drug targets. <i>Nature Structural and Molecular Biology</i> , 2010, 17, 530-538.   | 3.6 | 292       |
| 53 | Structural basis of HIV-1 resistance to AZT by excision. <i>Nature Structural and Molecular Biology</i> , 2010, 17, 1202-1209.   | 3.6 | 115       |
| 54 | Mutations in the Thumb Allow Human Immunodeficiency Virus Type 1 Reverse Transcriptase To Be Cleaved by Protease in Virions. <i>Journal of Virology</i> , 2009, 83, 12336-12344.   | 1.5 | 20        |

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|----|--|------|-----------|
| 55 | Crystal Structure and Autoactivation Pathway of the Precursor Form of Human Tripeptidyl-peptidase 1, the Enzyme Deficient in Late Infantile Ceroid Lipofuscinosis. <i>Journal of Biological Chemistry</i> , 2009, 284, 3985-3997.  | 1.6  | 50        |
| 56 | Structural Basis for the Role of the K65R Mutation in HIV-1 Reverse Transcriptase Polymerization, Excision Antagonism, and Tenofovir Resistance. <i>Journal of Biological Chemistry</i> , 2009, 284, 35092-35100.  | 1.6  | 81        |
| 57 | Structures of RNA polymerase-antibiotic complexes. <i>Current Opinion in Structural Biology</i> , 2009, 19, 715-723.   | 2.6  | 132       |
| 58 | Structure of HIV-1 Reverse Transcriptase with the Inhibitor $\hat{2}$ -Thujaplicinol Bound at the RNase H Active Site. <i>Structure</i> , 2009, 17, 1625-1635.   | 1.6  | 135       |
| 59 | Structure and Function of HIV-1 Reverse Transcriptase: Molecular Mechanisms of Polymerization and Inhibition. <i>Journal of Molecular Biology</i> , 2009, 385, 693-713.  | 2.0  | 426       |
| 60 | Crystallographic Study of a Novel Subnanomolar Inhibitor Provides Insight on the Binding Interactions of Alkenyl diaryl methanes with Human Immunodeficiency Virus-1 Reverse Transcriptase. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 6467-6473.   | 2.9  | 11        |
| 61 | Molecular Dynamics Study of Non-nucleoside Reverse Transcriptase Inhibitor 4-[[4-[[4-[[2-Cyanoethenyl]-2,6-dimethylphenyl]amino]-2-pyrimidinyl]amino]benzotrile (TMC278/Rilpivirine) Aggregates: Correlation between Amphiphilic Properties of the Drug and Oral Bioavailability. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 5896-5905. | 2.9  | 17        |
| 62 | Conformational Landscape of the Human Immunodeficiency Virus Type 1 Reverse Transcriptase Non-Nucleoside Inhibitor Binding Pocket: Lessons for Inhibitor Design from a Cluster Analysis of Many Crystal Structures. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 6413-6420.   | 2.9  | 33        |
| 63 | 3D Jigsaw Puzzle in Rotavirus Assembly. <i>Structure</i> , 2008, 16, 1601-1602.  | 1.6  | 1         |
| 64 | High-resolution structures of HIV-1 reverse transcriptase/TMC278 complexes: Strategic flexibility explains potency against resistance mutations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 1466-1471.  | 3.3  | 310       |
| 65 | The RNA Polymerase $\hat{c}$ Switch Region Is a Target for Inhibitors. <i>Cell</i> , 2008, 135, 295-307.   | 13.5 | 234       |
| 66 | Crystal engineering of HIV-1 reverse transcriptase for structure-based drug design. <i>Nucleic Acids Research</i> , 2008, 36, 5083-5092.   | 6.5  | 91        |
| 67 | Structural basis for suppression of a host antiviral response by influenza A virus. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 13093-13098.   | 3.3  | 193       |
| 68 | Two-dimensional infrared spectra reveal relaxation of the nonnucleoside inhibitor TMC278 complexed with HIV-1 reverse transcriptase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 1472-1477.  | 3.3  | 131       |
| 69 | Crystal Structures of Clinically Relevant Lys103Asn/Tyr181Cys Double Mutant HIV-1 Reverse Transcriptase in Complexes with ATP and Non-nucleoside Inhibitor HBY 097. <i>Journal of Molecular Biology</i> , 2007, 365, 77-89.  | 2.0  | 83        |
| 70 | A Conserved Structural Module Regulates Transcriptional Responses to Diverse Stress Signals in Bacteria. <i>Molecular Cell</i> , 2007, 27, 793-805.  | 4.5  | 136       |
| 71 | Synthesis, Biological Activity, and Crystal Structure of Potent Nonnucleoside Inhibitors of HIV-1 Reverse Transcriptase That Retain Activity against Mutant Forms of the Enzyme. <i>Journal of Medicinal Chemistry</i> , 2007, 50, 4003-4015.  | 2.9  | 87        |
| 72 | Linear Interaction Energy (LIE) Models for Ligand Binding in Implicit Solvent: Theory and Application to the Binding of NNRTIs to HIV-1 Reverse Transcriptase. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 256-277.   | 2.3  | 45        |

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|----|---|-----|-----------|
| 73 | Structures of Wild-Type and AZT-Resistant HIV-1 Reverse Transcriptase Complexed with AZTppppA Yield Insights into the Nucleotide Excision Mechanism. <i>FASEB Journal</i> , 2007, 21, A640.   | 0.2 | 0         |
| 74 | Spectroscopic Studies of Rilpivirine (TMC278/R278474) in Complex with HIV-1 Reverse Transcriptase. <i>FASEB Journal</i> , 2007, 21, A630.   | 0.2 | 0         |
| 75 | Crystallography and the design of anti-AIDS drugs: conformational flexibility and positional adaptability are important in the design of non-nucleoside HIV-1 reverse transcriptase inhibitors. <i>Progress in Biophysics and Molecular Biology</i> , 2005, 88, 209-231.  | 1.4 | 210       |
| 76 | The 2.35 Å structure of the TenA homolog from <i>Pyrococcus furiosus</i> supports an enzymatic function in thiamine metabolism. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2005, 61, 589-598.  | 2.5 | 12        |
| 77 | Synthesis of Novel Diarylpyrimidine Analogues and Their Antiviral Activity against Human Immunodeficiency Virus Type 1. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 2072-2079.  | 2.9 | 118       |
| 78 | Crystal Structures for HIV-1 Reverse Transcriptase in Complexes with Three Pyridinone Derivatives: A New Class of Non-Nucleoside Inhibitors Effective against a Broad Range of Drug-Resistant Strains. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 7582-7591.   | 2.9 | 132       |
| 79 | Concentration and pH Dependent Aggregation of Hydrophobic Drug Molecules and Relevance to Oral Bioavailability. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 1974-1983.  | 2.9 | 119       |
| 80 | Design, Synthesis, and SAR of a Novel Pyrazinone Series with Non-Nucleoside HIV-1 Reverse Transcriptase Inhibitory Activity. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 1910-1918.   | 2.9 | 49        |
| 81 | 4-Benzyl and 4-Benzoyl-3-dimethylaminopyridin-2(1H)-ones: In Vitro Evaluation of New C-3-Amino-Substituted and C-5,6-Alkyl-Substituted Analogues against Clinically Important HIV Mutant Strains. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 1948-1964.  | 2.9 | 38        |
| 82 | In Search of a Novel Anti-HIV Drug: A Multidisciplinary Coordination in the Discovery of 4-[[4-[[4-[(1E)-2-Cyanoethenyl]-2,6-dimethylphenyl]amino]-2-pyrimidinyl]amino]benzotrile (R278474,) <i>TJ ETQ0290 rgBT / Overlock 1</i>  | 2.9 | 120       |
| 83 | Crystal structure of RlmA: Implications for understanding the 23S rRNA G745/G748-methylation at the macrolide antibiotic-binding site. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004, 101, 4041-4046.   | 3.3 | 31        |
| 84 | Crystal Structures of Arginine Deiminase with Covalent Reaction Intermediates. <i>Structure</i> , 2004, 12, 657-667.  | 1.6 | 90        |
| 85 | Taking aim at a moving target: designing drugs to inhibit drug-resistant HIV-1 reverse transcriptases. <i>Current Opinion in Structural Biology</i> , 2004, 14, 716-730.  | 2.6 | 130       |
| 86 | Correlations between Factors Determining the Pharmacokinetics and Antiviral Activity of HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitors of the Diaryltriazine and Diarylpyrimidine Classes of Compounds. <i>Drugs in R and D</i> , 2004, 5, 245-257.  | 1.1 | 19        |
| 87 | HIV-1 Reverse Transcriptase Structure. , 2004, , 388-392.   |     | 0         |
| 88 | Roles of Conformational and Positional Adaptability in Structure-Based Design of TMC125-R165335 (Etravirine) and Related Non-nucleoside Reverse Transcriptase Inhibitors That Are Highly Potent and Effective against Wild-Type and Drug-Resistant HIV-1 Variants. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 2550-2560. | 2.9 | 507       |
| 89 | 382 In vitro characterization and molecular modeling analysis of a novel adefovir resistance mutation RTN236T in the HBV polymerase. <i>Journal of Hepatology</i> , 2004, 40, 114.  | 1.8 | 18        |
| 90 | On the detection of multiple-binding modes of ligands to proteins, from biological, structural, and modeling data. <i>Journal of Computer-Aided Molecular Design</i> , 2003, 17, 129-134.   | 1.3 | 42        |

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|-----|--|-----|-----------|
| 91  | Trapping HIV-1 Reverse Transcriptase Before and After Translocation on DNA. <i>Journal of Biological Chemistry</i> , 2003, 278, 16280-16288.   | 1.6 | 79        |
| 92  | The Hepatitis B Virus Polymerase Mutation rtV173L Is Selected during Lamivudine Therapy and Enhances Viral Replication In Vitro. <i>Journal of Virology</i> , 2003, 77, 11833-11841.   | 1.5 | 531       |
| 93  | Structural basis of BLYS receptor recognition. <i>Nature Structural Biology</i> , 2002, 9, 288-292.  | 9.7 | 76        |
| 94  | Structures of HIV-1 reverse transcriptase with pre- and post-translocation AZTMP-terminated DNA. <i>EMBO Journal</i> , 2002, 21, 6614-6624.  | 3.5 | 185       |
| 95  | HIV-1 Reverse Transcriptase Mutations Found in a Drug-Experienced Patient Confer Reduced Susceptibility to Multiple Nucleoside Reverse Transcriptase Inhibitors. <i>Antiviral Therapy</i> , 2002, 6, 231-238.  | 0.6 | 1         |
| 96  | The Lys103Asn mutation of HIV-1 RT: a novel mechanism of drug resistance. <i>Journal of Molecular Biology</i> , 2001, 309, 437-445.  | 2.0 | 175       |
| 97  | Evolution of Anti-HIV Drug Candidates Part 2: Diaryl triazine (DATA) Analogues. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2001, 11, 2229-2234.   | 1.0 | 119       |
| 98  | Evolution of anti-HIV drug candidates. Part 3: diaryl pyrimidine (DAPY) analogues. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2001, 11, 2235-2239.  | 1.0 | 183       |
| 99  | X-ray crystal structure of MTH938 from <i>Methanobacterium thermoautotrophicum</i> at 2.2 Å... resolution reveals a novel tertiary protein fold. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001, 45, 486-488.  | 1.5 | 5         |
| 100 | Crystal structure of HIV-1 reverse transcriptase in complex with a polypurine tract RNA:DNA. <i>EMBO Journal</i> , 2001, 20, 1449-1461.  | 3.5 | 388       |
| 101 | Molecular Modeling and Biochemical Characterization Reveal the Mechanism of Hepatitis B Virus Polymerase Resistance to Lamivudine (3TC) and Emtricitabine (FTC). <i>Journal of Virology</i> , 2001, 75, 4771-4779.   | 1.5 | 263       |
| 102 | A Mutation in Human Immunodeficiency Virus Type 1 Protease, N88S, That Causes In Vitro Hypersensitivity to Amprenavir. <i>Journal of Virology</i> , 2000, 74, 4414-4419.   | 1.5 | 85        |
| 103 | Lamivudine (3TC) resistance in HIV-1 reverse transcriptase involves steric hindrance with beta-branched amino acids. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1999, 96, 10027-10032.   | 3.3 | 288       |
| 104 | Touching the heart of HIV-1 drug resistance: the fingers close down on the dNTP at the polymerase active site. <i>Chemistry and Biology</i> , 1999, 6, R137-R146.  | 6.2 | 107       |
| 105 | Structure-based design of inhibitors of HIV-1 reverse transcriptase: a potential class of bidentate nonnucleoside inhibitors. <i>Computational and Theoretical Chemistry</i> , 1998, 423, 101-111.   | 1.5 | 4         |
| 106 | Dithiaheterocycle-annelated tetrathiafulvalene $\pi$ -donors: a structure-property correlation study. <i>Journal of the Chemical Society Perkin Transactions 1</i> , 1998, , 1769-1778.  | 0.9 | 10        |
| 107 | Structures of Tyr188Leu mutant and wild-type HIV-1 reverse transcriptase complexed with the non-nucleoside inhibitor HBV 097: inhibitor flexibility is a useful design feature for reducing drug resistance 1 Edited by J. Karn. <i>Journal of Molecular Biology</i> , 1998, 284, 313-323. | 2.0 | 135       |
| 108 | Structure and functional implications of the polymerase active site region in a complex of HIV-1 RT with a double-stranded DNA template-primer and an antibody fab fragment at 2.8 Å... resolution. <i>Journal of Molecular Biology</i> , 1998, 284, 1095-1111.                            | 2.0 | 317       |

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|-----|--|-----|-----------|
| 109 | Synthesis and Reactivity of Chiral Tellurium Azomethines: Pseudopolymorphism of [o-(((1S,2R)-2-Hydroxy-2-phenyl-1-methylethyl)amino)methinyl]phenyl]tellurium(IV) Bromide. <i>Organometallics</i> , 1997, 16, 563-571.   | 1.1 | 40        |
| 110 | Synthesis of some functionalised isomeric bis(ethylenedithio)tetrathiafulvalene (BEDT-TTF) and dithiophenetetrathiafulvalene (DTTTF) $\pi$ -donors. <i>Tetrahedron</i> , 1997, 53, 11627-11644.  | 1.0 | 19        |
| 111 | Conformation, Protein-Carbohydrate Interactions and a Novel Subunit Association in the Refined Structure of Peanut Lectin-Lactose Complex. <i>Journal of Molecular Biology</i> , 1996, 259, 281-296.   | 2.0 | 174       |
| 112 | Crystal Structures of 8-Cl and 9-Cl TIBO Complexed with Wild-type HIV-1 RT and 8-Cl TIBO Complexed with the Tyr181Cys HIV-1 RT Drug-resistant Mutant. <i>Journal of Molecular Biology</i> , 1996, 264, 1085-1100.  | 2.0 | 214       |
| 113 | Structure of unliganded HIV-1 reverse transcriptase at 2.7 Å resolution: implications of conformational changes for polymerization and inhibition mechanisms. <i>Structure</i> , 1996, 4, 853-860.   | 1.6 | 286       |
| 114 | Electron density averaging using multiple crystal forms or diffraction datasets in structure determination of protein at moderate resolution. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 1996, 52, C81-C81.   | 0.3 | 0         |
| 115 | Refined structure of HIV-1 reverse transcriptase complexed with a double-stranded DNA and an antibody Fab fragment at 2.8 Å resolution. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 1996, 52, C155-C155.   | 0.3 | 0         |
| 116 | Non-nucleoside RT inhibitors give HIV-1 RT a crooked back. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 1996, 52, C234-C235.  | 0.3 | 0         |
| 117 | Structure of HIV-1 reverse transcriptase in a complex with the non-nucleoside inhibitor $\hat{\pm}$ -APA R 95845 at 2.8 Å resolution. <i>Structure</i> , 1995, 3, 365-379.   | 1.6 | 225       |
| 118 | Molecular modeling studies of HIV reverse transcriptase nonnucleoside inhibitors: Total energy of complexation as a predictor of drug placement and activity. <i>Protein Science</i> , 1995, 4, 2203-2222.   | 3.1 | 66        |
| 119 | Structure of HIV-1 RT/TIBO R 86183 complex reveals similarity in the binding of diverse nonnucleoside inhibitors. <i>Nature Structural and Molecular Biology</i> , 1995, 2, 407-415.   | 3.6 | 296       |
| 120 | 1-O-(2-Iodophenyl)- $\hat{1}$ -D-galactopyranose. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 1994, 50, 1726-1728.   | 0.4 | 1         |
| 121 | Crystal structure of peanut lectin, a protein with an unusual quaternary structure.. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1994, 91, 227-231.   | 3.3 | 122       |
| 122 | Acetylenic derivatives of [Fe <sub>2</sub> (CO) <sub>6</sub> ( $\mu$ -Se <sub>2</sub> )]: acetylenic bond reduction on a selenium-stabilised Fe <sub>2</sub> Pt mixed-metal complex. <i>Journal of the Chemical Society Chemical Communications</i> , 1993, , 46-48.                                   | 2.0 | 27        |
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