# Tom Blundell

## List of Publications by Year in Descending Order



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|---|---|---|---|
| 295 papers | 36,152 citations | 86 h-index | 188 g-index |
| 334 ext. papers | 40,151 ext. citations | 11.1 avg, IF | 7.4 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 295 | Structural insights into inhibitor regulation of the DNA repair protein DNA-PKcs.. *Nature*, **2022**, | 50.4 | 5 |
| 294 | Are There Hidden Genes in DNA/RNA Vaccines?. *Frontiers in Immunology*, **2022**, 13, 801915 | 8.4 | 1 |
| 293 | Searching for New Z-DNA/Z-RNA Binding Proteins Based on Structural Similarity to Experimentally Validated ZÐomain.. *International Journal of Molecular Sciences*, **2022**, 23, | 6.3 | 3 |
| 292 | Using Structure-guided Fragment-Based Drug Discovery to Target Infections in Cystic Fibrosis.. *Frontiers in Molecular Biosciences*, **2022**, 9, 857000 | 5.6 | 1 |
| 291 | Can the SARS-CoV-2 Spike Protein Bind Integrins Independent of the RGD Sequence?. *Frontiers in Cellular and Infection Microbiology*, **2021**, 11, 765300 | 5.9 | 1 |
| 290 | PDBe-KB: collaboratively defining the biological context of structural data. *Nucleic Acids Research*, **2021**, | 20.1 | 7 |
| 289 | Three Simple Properties Explain Protein Stability Change upon Mutation. *Journal of Chemical Information and Modeling*, **2021**, 61, 1981-1988 | 6.1 | 5 |
| 288 | Stepwise pathogenic evolution of. *Science*, **2021**, 372, | 33.3 | 23 |
| 287 | Targeting CoaBC through Chemical Inhibition of 4'-Phosphopantothenoyl-l-cysteine Synthetase (CoaB) Activity. *ACS Infectious Diseases*, **2021**, 7, 1666-1679 | 5.5 | 0 |
| 286 | ProtCHOIR: a tool for proteome-scale generation of homo-oligomers. *Briefings in Bioinformatics*, **2021**, 22, | 13.4 | 1 |
| 285 | Utilizing graph machine learning within drug discovery and development. *Briefings in Bioinformatics* , **2021**, 22, | 13.4 | 18 |
| 284 | Structure-Guided Computational Approaches to Unravel Druggable Proteomic Landscape of. *Frontiers in Molecular Biosciences*, **2021**, 8, 663301 | 5.6 | 0 |
| 283 | A small-molecule inhibitor of the BRCA2-RAD51 interaction modulates RAD51 assembly and potentiates DNA damage-induced cell death. *Cell Chemical Biology*, **2021**, 28, 835-847.e5 | 8.2 | 4 |
| 282 | Whole Exome Sequencing reveals NOTCH1 mutations in anaplastic large cell lymphoma and points to Notch both as a key pathway and a potential therapeutic target. *Haematologica*, **2021**, 106, 1693-1704 | 6.6 | 11 |
| 281 | Dimers of DNA-PK create a stage for DNA double-strand break repair. *Nature Structural and Molecular Biology*, **2021**, 28, 13-19 | 17.6 | 30 |
| 280 | SARS-CoV-2 3D database: understanding the coronavirus proteome and evaluating possible drug targets. *Briefings in Bioinformatics*, **2021**, 22, 769-780 | 13.4 | 16 |
| 279 | Deep Learning for Protein-Protein Interaction Site Prediction. *Methods in Molecular Biology*, **2021**, 2361, 263-288 | 1.4 | 3 |

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| 278 | A base measure of precision for protein stability predictors: structural sensitivity. *BMC Bioinformatics*, **2021**, 22, 88 | 3.6 | 8 |
| 277 | SAP domain forms a flexible part of DNA aperture in Ku70/80. *FEBS Journal*, **2021**, 288, 4382-4393 | 5.7 | 1 |
| 276 | Strategies for drug target identification in Mycobacterium leprae. *Drug Discovery Today*, **2021**, 26, 1569-1573 | 8.7 | 1 |
| 275 | Integrated human/SARS-CoV-2 metabolic models present novel treatment strategies against COVID-19. *Life Science Alliance*, **2021**, 4, | 5.8 | 2 |
| 274 | Stages, scaffolds and strings in the spatial organisation of non-homologous end joining: Insights from X-ray diffraction and Cryo-EM. *Progress in Biophysics and Molecular Biology*, **2021**, 163, 60-73 | 4.7 | 2 |
| 273 | Cryo-EM of NHEJ supercomplexes provides insights into DNA repair. *Molecular Cell*, **2021**, 81, 3400-3409.e3 | 17.6 | 12 |
| 272 | Using a synthetic switch to regulate insulin receptor activation. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118, | 11.5 | 1 |
| 271 | Using cryo-EM to understand antimycobacterial resistance in the catalase-peroxidase (KatG) from Mycobacterium tuberculosis. *Structure*, **2021**, 29, 899-912.e4 | 5.2 | 7 |
| 270 | The first resolution revolution in protein structure analysis: X-ray diffraction of polypeptide conformations and globular protein folds in 1950s and 1960s. *Progress in Biophysics and Molecular Biology*, **2021**, 167, 32-32 | 4.7 | 0 |
| 269 | Predicted structural mimicry of spike receptor-binding motifs from highly pathogenic human coronaviruses. *Computational and Structural Biotechnology Journal*, **2021**, | 6.8 | 9 |
| 268 | A fragment-based approach to assess the ligandability of ArgB, ArgC, ArgD and ArgF in the L-arginine biosynthetic pathway of. *Computational and Structural Biotechnology Journal*, **2021**, 19, 3491-3506 | 6.8 | 5 |
| 267 | Inhibiting Mycobacterium tuberculosis CoaBC by targeting an allosteric site. *Nature Communications*, **2021**, 12, 143 | 17.4 | 4 |
| 266 | HARP: a database of structural impacts of systematic missense mutations in drug targets of. *Computational and Structural Biotechnology Journal*, **2020**, 18, 3692-3704 | 6.8 | 6 |
| 265 | Common mechanism of thermostability in small □and □proteins studied by molecular dynamics. *Proteins: Structure, Function and Bioinformatics*, **2020**, 88, 1233-1250 | 4.2 | 2 |
| 264 | Computational Deorphaning of Mycobacterium tuberculosis Targets **2020**, | | 1 |
| 263 | Hotspots API: A Python Package for the Detection of Small Molecule Binding Hotspots and Application to Structure-Based Drug Design. *Journal of Chemical Information and Modeling*, **2020**, 60, 1911-1916 | 6.1 | 8 |
| 262 | Fragment-Based Design of InhA Inhibitors. *Journal of Medicinal Chemistry*, **2020**, 63, 4749-4761 | 8.3 | 14 |
| 261 | Using a Fragment-Based Approach to Identify Alternative Chemical Scaffolds Targeting Dihydrofolate Reductase from. *ACS Infectious Diseases*, **2020**, 6, 2192-2201 | 5.5 | 2 |

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| 260 | Fragment-based discovery of a new class of inhibitors targeting mycobacterial tRNA modification. *Nucleic Acids Research*, **2020**, 48, 8099-8112 | 20.1 | 10 |
| 259 | Intrinsic disorder in proteins: Relevance to protein assemblies, drug design and host-pathogen interactions. *Progress in Biophysics and Molecular Biology*, **2020**, 156, 34-42 | 4.7 | 13 |
| 258 | CCDC61/VFL3 Is a Paralog of SAS6 and Promotes Ciliary Functions. *Structure*, **2020**, 28, 674-689.e11 | 5.2 | 12 |
| 257 | Deciphering the enzymatic target of a new family of antischistosomal agents bearing a quinazoline scaffold using complementary computational tools. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2020**, 35, 511-523 | 5.6 | 1 |
| 256 | Computational saturation mutagenesis to predict structural consequences of systematic mutations in the beta subunit of RNA polymerase in. *Computational and Structural Biotechnology Journal*, **2020** , 18, 271-286 | 6.8 | 20 |
| 255 | The Genome3D Consortium for Structural Annotations of Selected Model Organisms. *Methods in Molecular Biology*, **2020**, 2165, 27-67 | 1.4 | 1 |
| 254 | Druggable binding sites in the multicomponent assemblies that characterise DNA double-strand-break repair through non-homologous end joining. *Essays in Biochemistry*, **2020**, 64, 791-806 | 7.6 | 4 |
| 253 | Covalent inactivation of Mycobacterium thermoresistibile inosine-5'-monophosphate dehydrogenase (IMPDH). *Bioorganic and Medicinal Chemistry Letters*, **2020**, 30, 126792 | 2.9 | 2 |
| 252 | Prediction of impacts of mutations on protein structure and interactions: SDM, a statistical approach, and mCSM, using machine learning. *Protein Science*, **2020**, 29, 247-257 | 6.3 | 22 |
| 251 | Structural biology of multicomponent assemblies in DNA double-strand-break repair through non-homologous end joining. *Current Opinion in Structural Biology*, **2020**, 61, 9-16 | 8.1 | 14 |
| 250 | Genome3D: integrating a collaborative data pipeline to expand the depth and breadth of consensus protein structure annotation. *Nucleic Acids Research*, **2020**, 48, D314-D319 | 20.1 | 7 |
| 249 | Genomics, Computational Biology and Drug Discovery for Mycobacterial Infections: Fighting the Emergence of Resistance. *Frontiers in Genetics*, **2020**, 11, 965 | 4.5 | 2 |
| 248 | Mechanism of efficient double-strand break repair by a long non-coding RNA. *Nucleic Acids Research*, **2020**, 48, 10953-10972 | 20.1 | 21 |
| 247 | Systematic Investigation of the Data Set Dependency of Protein Stability Predictors. *Journal of Chemical Information and Modeling*, **2020**, 60, 4772-4784 | 6.1 | 12 |
| 246 | Exploring the structural basis of conformational heterogeneity and autoinhibition of human cGMP-specific protein kinase Iβ through computational modelling and molecular dynamics simulations. *Computational and Structural Biotechnology Journal*, **2020**, 18, 1625-1638 | 6.8 | 6 |
| 245 | A Personal History of Using Crystals and Crystallography to Understand Biology and Advanced Drug Discovery. *Crystals*, **2020**, 10, 676 | 2.3 | 1 |
| 244 | PDBe-KB: a community-driven resource for structural and functional annotations. *Nucleic Acids Research*, **2020**, 48, D344-D353 | 20.1 | 50 |
| 243 | ProCarbDB: a database of carbohydrate-binding proteins. *Nucleic Acids Research*, **2020**, 48, D368-D375 | 20.1 | 9 |

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| 242 | A platform for target prediction of phenotypic screening hit molecules. *Journal of Molecular Graphics and Modelling*, **2020**, 95, 107485 | 2.8 | 1 |
| 241 | Multicomponent assemblies in DNA-double-strand break repair by NHEJ. *Current Opinion in Structural Biology*, **2019**, 55, 154-160 | 8.1 | 13 |
| 240 | Understanding the structure and role of DNA-PK in NHEJ: How X-ray diffraction and cryo-EM contribute in complementary ways. *Progress in Biophysics and Molecular Biology*, **2019**, 147, 26-32 | 4.7 | 7 |
| 239 | Structure-guided fragment-based drug discovery at the synchrotron: screening binding sites and correlations with hotspot mapping. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2019**, 377, 20180422 | 3 | 18 |
| 238 | Synthesis and Structure-Activity relationship of 1-(5-isoquinolinesulfonyl)piperazine analogues as inhibitors of Mycobacterium tuberculosis IMPDH. *European Journal of Medicinal Chemistry*, **2019**, 174, 309-329 | 6.8 | 16 |
| 237 | The Molecular Organization of Human cGMP Specific Phosphodiesterase 6 (PDE6): Structural Implications of Somatic Mutations in Cancer and Retinitis Pigmentosa. *Computational and Structural Biotechnology Journal*, **2019**, 17, 378-389 | 6.8 | 16 |
| 236 | Identification and Characterization of Genetic Determinants of Isoniazid and Rifampicin Resistance in Mycobacterium tuberculosis in Southern India. *Scientific Reports*, **2019**, 9, 10283 | 4.9 | 20 |
| 235 | Structure and dynamics of secretase with presenilin 2 compared to presenilin 1.. *RSC Advances*, **2019**, 9, 20901-20916 | 3.7 | 12 |
| 234 | Development of Inhibitors against tRNA (mG37) Methyltransferase (TrmD) Using Fragment-Based Approaches. *Journal of Medicinal Chemistry*, **2019**, 62, 7210-7232 | 8.3 | 15 |
| 233 | Understanding the impacts of missense mutations on structures and functions of human cancer-related genes: A preliminary computational analysis of the COSMIC Cancer Gene Census. *PLoS ONE*, **2019**, 14, e0219935 | 3.7 | 6 |
| 232 | SSEThread: Integrative threading of the DNA-PKcs sequence based on data from chemical cross-linking and hydrogen deuterium exchange. *Progress in Biophysics and Molecular Biology*, **2019**, 147, 92-102 | 4.7 | 6 |
| 231 | Mabellini: a genome-wide database for understanding the structural proteome and evaluating prospective antimicrobial targets of the emerging pathogen Mycobacterium abscessus. *Database: the Journal of Biological Databases and Curation*, **2019**, 2019, | 5 | 9 |
| 230 | Structural insights into Escherichia coli phosphopantothenoylcysteine synthetase by native ion mobility-mass spectrometry. *Biochemical Journal*, **2019**, 476, 3125-3139 | 3.8 | 3 |
| 229 | Mycobacterial OtsA Structures Unveil Substrate Preference Mechanism and Allosteric Regulation by 2-Oxoglutarate and 2-Phosphoglycerate. *MBio*, **2019**, 10, | 7.8 | 1 |
| 228 | Mycobacterial genomics and structural bioinformatics: opportunities and challenges in drug discovery. *Emerging Microbes and Infections*, **2019**, 8, 109-118 | 18.9 | 18 |
| 227 | Structural Implications of Mutations Conferring Rifampin Resistance in Mycobacterium leprae. *Scientific Reports*, **2018**, 8, 5016 | 4.9 | 28 |
| 226 | Fragment-Based Approach to Targeting Inosine-5'-monophosphate Dehydrogenase (IMPDH) from Mycobacterium tuberculosis. *Journal of Medicinal Chemistry*, **2018**, 61, 2806-2822 | 8.3 | 32 |
| 225 | Arginine-deprivation-induced oxidative damage sterilizes. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 9779-9784 | 11.5 | 41 |

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| 224 | Identification of new allosteric sites and modulators of AChE through computational and experimental tools. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2018**, 33, 1034-1047 | 5.6 | 21 |
| 223 | The deubiquitylating enzyme UCHL3 regulates Ku80 retention at sites of DNA damage. *Scientific Reports*, **2018**, 8, 17891 | 4.9 | 19 |
| 222 | Dissection of DNA double-strand-break repair using novel single-molecule forceps. *Nature Structural and Molecular Biology*, **2018**, 25, 482-487 | 17.6 | 49 |
| 221 | Mutations at protein-protein interfaces: Small changes over big surfaces have large impacts on human health. *Progress in Biophysics and Molecular Biology*, **2017**, 128, 3-13 | 4.7 | 81 |
| 220 | DNA-PKcs structure suggests an allosteric mechanism modulating DNA double-strand break repair. *Science*, **2017**, 355, 520-524 | 33.3 | 114 |
| 219 | Structural insights into the EthR-DNA interaction using native mass spectrometry. *Chemical Communications*, **2017**, 53, 3527-3530 | 5.8 | 15 |
| 218 | Genomes, structural biology and drug discovery: combating the impacts of mutations in genetic disease and antibiotic resistance. *Biochemical Society Transactions*, **2017**, 45, 303-311 | 5.1 | 26 |
| 217 | Fragment Screening against the EthR-DNA Interaction by Native Mass Spectrometry. *Angewandte Chemie - International Edition*, **2017**, 56, 7488-7491 | 16.4 | 10 |
| 216 | XSuLT: a web server for structural annotation and representation of sequence-structure alignments. *Nucleic Acids Research*, **2017**, 45, W381-W387 | 20.1 | 1 |
| 215 | SDM: a server for predicting effects of mutations on protein stability. *Nucleic Acids Research*, **2017**, 45, W229-W235 | 20.1 | 246 |
| 214 | Fragment Screening against the EthR□DNA Interaction by Native Mass Spectrometry. *Angewandte Chemie*, **2017**, 129, 7596-7599 | 3.6 | 1 |
| 213 | Fragment-Sized EthR Inhibitors Exhibit Exceptionally Strong Ethionamide Boosting Effect in Whole-Cell Mycobacterium tuberculosis Assays. *ACS Chemical Biology*, **2017**, 12, 1390-1396 | 4.9 | 17 |
| 212 | Arpeggio: A Web Server for Calculating and Visualising Interatomic Interactions in Protein Structures. *Journal of Molecular Biology*, **2017**, 429, 365-371 | 6.5 | 195 |
| 211 | DNA-PKcs, Allostery, and DNA Double-Strand Break Repair: Defining the Structure and Setting the Stage. *Methods in Enzymology*, **2017**, 592, 145-157 | 1.7 | 5 |
| 210 | Decoding the similarities and differences among mycobacterial species. *PLoS Neglected Tropical Diseases*, **2017**, 11, e0005883 | 4.8 | 24 |
| 209 | Protein crystallography and drug discovery: recollections of knowledge exchange between academia and industry. *IUCrJ*, **2017**, 4, 308-321 | 4.7 | 48 |
| 208 | TIBLE: a web-based, freely accessible resource for small-molecule binding data for mycobacterial species. *Database: the Journal of Biological Databases and Curation*, **2017**, 2017, | 5 | 4 |
| 207 | Book Review on □Molecular Biology of Assemblies and Machines□by Alasdair Steven, Wolfgang Baumeister, Louise Johnson and Richard Perham. Published by Garland Science, Taylor and Francis Group. *FEBS Letters*, **2017**, 591, 3707-3708 | 3.8 | |

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| 206 | Structural Biology and the Design of New Therapeutics: From HIV and Cancer to Mycobacterial Infections: A Paper Dedicated to John Kendrew. *Journal of Molecular Biology*, **2017**, 429, 2677-2693 | 6.5 | 26 |
| 205 | Achieving selectivity in space and time with DNA double-strand-break response and repair: molecular stages and scaffolds come with strings attached. *Structural Chemistry*, **2017**, 28, 161-171 | 1.8 | 9 |
| 204 | The Inosine Monophosphate Dehydrogenase, GuaB2, Is a Vulnerable New Bactericidal Drug Target for Tuberculosis. *ACS Infectious Diseases*, **2017**, 3, 5-17 | 5.5 | 62 |
| 203 | Targeting tuberculosis using structure-guided fragment-based drug design. *Drug Discovery Today*, **2017**, 22, 546-554 | 8.8 | 29 |
| 202 | Essential but Not Vulnerable: Indazole Sulfonamides Targeting Inosine Monophosphate Dehydrogenase as Potential Leads against Mycobacterium tuberculosis. *ACS Infectious Diseases*, **2017**, 3, 18-33 | 5.5 | 62 |
| 201 | Target Identification of Phenotypic Hits Using a Concerted Chemogenomic, Biophysical, and Structural Approach. *Frontiers in Pharmacology*, **2017**, 8, 681 | 5.6 | 14 |
| 200 | Twelve novel HGD gene variants identified in 99 alkaptonuria patients: focus on 'black bone disease' in Italy. *European Journal of Human Genetics*, **2016**, 24, 66-72 | 5.3 | 71 |
| 199 | Different DNA End Configurations Dictate Which NHEJ Components Are Most Important for Joining Efficiency. *Journal of Biological Chemistry*, **2016**, 291, 24377-24389 | 5.4 | 60 |
| 198 | Engineering Archeal Surrogate Systems for the Development of Protein-Protein Interaction Inhibitors against Human RAD51. *Journal of Molecular Biology*, **2016**, 428, 4589-4607 | 6.5 | 6 |
| 197 | Structure-activity relationship of the peptide binding-motif mediating the BRCA2:RAD51 protein-protein interaction. *FEBS Letters*, **2016**, 590, 1094-102 | 3.8 | 6 |
| 196 | Optimization of Inhibitors of Mycobacterium tuberculosis Pantothenate Synthetase Based on Group Efficiency Analysis. *ChemMedChem*, **2016**, 11, 38-42 | 3.7 | 19 |
| 195 | Structure of BRCA1-BRCT/Abraxas Complex Reveals Phosphorylation-Dependent BRCT Dimerization at DNA Damage Sites. *Molecular Cell*, **2016**, 61, 434-448 | 17.6 | 48 |
| 194 | A fragment merging approach towards the development of small molecule inhibitors of Mycobacterium tuberculosis EthR for use as ethionamide boosters. *Organic and Biomolecular Chemistry*, **2016**, 14, 2318-26 | 3.9 | 32 |
| 193 | Developing Antagonists for the Met-HGF/SF Protein-Protein Interaction Using a Fragment-Based Approach. *Molecular Cancer Therapeutics*, **2016**, 15, 3-14 | 6.1 | 7 |
| 192 | In silico functional dissection of saturation mutagenesis: Interpreting the relationship between phenotypes and changes in protein stability, interactions and activity. *Scientific Reports*, **2016**, 6, 19848 | 4.9 | 68 |
| 191 | mCSM-lig: quantifying the effects of mutations on protein-small molecule affinity in genetic disease and emergence of drug resistance. *Scientific Reports*, **2016**, 6, 29575 | 4.9 | 88 |
| 190 | Identifying Interactions that Determine Fragment Binding at Protein Hotspots. *Journal of Medicinal Chemistry*, **2016**, 59, 4314-25 | 8.3 | 64 |
| 189 | Virtual Screening and X-ray Crystallography Identify Non-Substrate Analog Inhibitors of Flavin-Dependent Thymidylate Synthase. *Journal of Medicinal Chemistry*, **2016**, 59, 9269-9275 | 8.3 | 16 |

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| 188 | Structure-guided, target-based drug discovery - exploiting genome information from HIV to mycobacterial infections. *Postepy Biochemii*, **2016**, 62, 262-272 | 0 | 2 |
| 187 | Mutations in the NHEJ component XRCC4 cause primordial dwarfism. *American Journal of Human Genetics*, **2015**, 96, 412-24 | 11 | 59 |
| 186 | Phosphopeptide interactions with BRCA1 BRCT domains: More than just a motif. *Progress in Biophysics and Molecular Biology*, **2015**, 117, 143-148 | 4.7 | 23 |
| 185 | pkCSM: Predicting Small-Molecule Pharmacokinetic and Toxicity Properties Using Graph-Based Signatures. *Journal of Medicinal Chemistry*, **2015**, 58, 4066-72 | 8.3 | 1056 |
| 184 | Achieving high signal-to-noise in cell regulatory systems: Spatial organization of multiprotein transmembrane assemblies of FGFR and MET receptors. *Progress in Biophysics and Molecular Biology*, **2015**, 118, 103-11 | 4.7 | 16 |
| 183 | Platinum: a database of experimentally measured effects of mutations on structurally defined protein-ligand complexes. *Nucleic Acids Research*, **2015**, 43, D387-91 | 20.1 | 58 |
| 182 | Exploring the chemical space of the lysine-binding pocket of the first kringle domain of hepatocyte growth factor/scatter factor (HGF/SF) yields a new class of inhibitors of HGF/SF-MET binding. *Chemical Science*, **2015**, 6, 6147-6157 | 9.4 | 23 |
| 181 | Small-molecule inhibitors that target protein-protein interactions in the RAD51 family of recombinases. *ChemMedChem*, **2015**, 10, 296-303 | 3.7 | 31 |
| 180 | Structure of Mycobacterium thermoresistibile GlgE defines novel conformational states that contribute to the catalytic mechanism. *Scientific Reports*, **2015**, 5, 17144 | 4.9 | 2 |
| 179 | SInCRe-structural interactome computational resource for Mycobacterium tuberculosis. *Database: the Journal of Biological Databases and Curation*, **2015**, 2015, bav060 | 5 | 5 |
| 178 | CHOPIN: a web resource for the structural and functional proteome of Mycobacterium tuberculosis. *Database: the Journal of Biological Databases and Curation*, **2015**, 2015, | 5 | 19 |
| 177 | Protein-Protein Interactions: Structures and Druggability. *NATO Science for Peace and Security Series A: Chemistry and Biology*, **2015**, 141-163 | 0.1 | 4 |
| 176 | Flexibility and small pockets at protein-protein interfaces: New insights into druggability. *Progress in Biophysics and Molecular Biology*, **2015**, 119, 2-9 | 4.7 | 89 |
| 175 | Genome3D: exploiting structure to help users understand their sequences. *Nucleic Acids Research*, **2015**, 43, D382-6 | 20.1 | 33 |
| 174 | Germline Mutations in the CDKN2B Tumor Suppressor Gene Predispose to Renal Cell Carcinoma. *Cancer Discovery*, **2015**, 5, 723-9 | 24.4 | 61 |
| 173 | Lst4, the yeast Fnip1/2 orthologue, is a DENN-family protein. *Open Biology*, **2015**, 5, 150174 | 7 | 23 |
| 172 | Enriching the annotation of Mycobacterium tuberculosis H37Rv proteome using remote homology detection approaches: insights into structure and function. *Tuberculosis*, **2015**, 95, 14-25 | 2.6 | 8 |
| 171 | DNA repair. PAXX, a paralog of XRCC4 and XLF, interacts with Ku to promote DNA double-strand break repair. *Science*, **2015**, 347, 185-188 | 33.3 | 202 |

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| 170 | Analysis of HGD Gene Mutations in Patients with Alkaptonuria from the United Kingdom: Identification of Novel Mutations. *JIMD Reports*, **2015**, 24, 3-11 | 1.9 | 36 |
| 169 | The spatial organization of non-homologous end joining: from bridging to end joining. *DNA Repair*, **2014**, 17, 98-109 | 4.3 | 55 |
| 168 | Mycobacterium tuberculosis dihydrofolate reductase reveals two conformational states and a possible low affinity mechanism to antifolate drugs. *Structure*, **2014**, 22, 94-103 | 5.2 | 20 |
| 167 | Innate immunity. A Spaetzle-like role for nerve growth factor in vertebrate immunity to Staphylococcus aureus. *Science*, **2014**, 346, 641-646 | 33.3 | 55 |
| 166 | Respiratory flexibility in response to inhibition of cytochrome C oxidase in Mycobacterium tuberculosis. *Antimicrobial Agents and Chemotherapy*, **2014**, 58, 6962-5 | 5.9 | 89 |
| 165 | Pantothenic acid biosynthesis in the parasite Toxoplasma gondii: a target for chemotherapy. *Antimicrobial Agents and Chemotherapy*, **2014**, 58, 6345-53 | 5.9 | 11 |
| 164 | A structure-guided fragment-based approach for the discovery of allosteric inhibitors targeting the lipophilic binding site of transcription factor EthR. *Biochemical Journal*, **2014**, 458, 387-94 | 3.8 | 27 |
| 163 | mCSM: predicting the effects of mutations in proteins using graph-based signatures. *Bioinformatics*, **2014**, 30, 335-42 | 7.2 | 505 |
| 162 | An integrated computational approach can classify VHL missense mutations according to risk of clear cell renal carcinoma. *Human Molecular Genetics*, **2014**, 23, 5976-88 | 5.6 | 19 |
| 161 | DUET: a server for predicting effects of mutations on protein stability using an integrated computational approach. *Nucleic Acids Research*, **2014**, 42, W314-9 | 20.1 | 437 |
| 160 | Threonine 57 is required for the post-translational activation of Escherichia coli aspartate decarboxylase. *Acta Crystallographica Section D: Biological Crystallography*, **2014**, 70, 1166-72 | | 5 |
| 159 | Structure of the catalytic region of DNA ligase IV in complex with an Artemis fragment sheds light on double-strand break repair. *Structure*, **2013**, 21, 672-9 | 5.2 | 44 |
| 158 | Using a fragment-based approach to target protein-protein interactions. *ChemBioChem*, **2013**, 14, 332-42 | 3.8 | 99 |
| 157 | Cooperative heparin-mediated oligomerization of fibroblast growth factor-1 (FGF1) precedes recruitment of FGFR2 to ternary complexes. *Biophysical Journal*, **2013**, 104, 1720-30 | 2.9 | 40 |
| 156 | Molecular mechanism of SSR128129E, an extracellularly acting, small-molecule, allosteric inhibitor of FGF receptor signaling. *Cancer Cell*, **2013**, 23, 489-501 | 24.3 | 99 |
| 155 | CREDO: a structural interactomics database for drug discovery. *Database: the Journal of Biological Databases and Curation*, **2013**, 2013, bat049 | 5 | 30 |
| 154 | Integrated biophysical approach to fragment screening and validation for fragment-based lead discovery. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 12984-9 | 11.5 | 83 |
| 153 | Genome3D: a UK collaborative project to annotate genomic sequences with predicted 3D structures based on SCOP and CATH domains. *Nucleic Acids Research*, **2013**, 41, D499-507 | 20.1 | 48 |

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| 152 | Structural insights into the role of domain flexibility in human DNA ligase IV. *Structure*, **2012**, 20, 1212-22 | 5.2 | 34 |
| 151 | Crystal structure of folliculin reveals a hidDENN function in genetically inherited renal cancer. *Open Biology*, **2012**, 2, 120071 | 7 | 84 |
| 150 | What can we learn from the evolution of protein-ligand interactions to aid the design of new therapeutics?. *PLoS ONE*, **2012**, 7, e51742 | 3.7 | 20 |
| 149 | Spatial and temporal organization of multi-protein assemblies: achieving sensitive control in information-rich cell-regulatory systems. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2012**, 370, 3023-39 | 3 | 22 |
| 148 | Structural biology and drug discovery for protein-protein interactions. *Trends in Pharmacological Sciences*, **2012**, 33, 241-8 | 13.2 | 130 |
| 147 | Structural biology and drug discovery of difficult targets: the limits of ligandability. *Chemistry and Biology*, **2012**, 19, 42-50 | | 159 |
| 146 | Biophysical and computational fragment-based approaches to targeting protein-protein interactions: applications in structure-guided drug discovery. *Quarterly Reviews of Biophysics*, **2012**, 45, 383-426 | 7 | 74 |
| 145 | Structural investigation of inhibitor designs targeting 3-dehydroquinate dehydratase from the shikimate pathway of Mycobacterium tuberculosis. *Biochemical Journal*, **2011**, 436, 729-39 | 3.8 | 33 |
| 144 | Non-homologous end-joining partners in a helical dance: structural studies of XLF-XRCC4 interactions. *Biochemical Society Transactions*, **2011**, 39, 1387-92, suppl 2 p following 1392 | 5.1 | 59 |
| 143 | Comprehensive, atomic-level characterization of structurally characterized protein-protein interactions: the PICCOLO database. *BMC Bioinformatics*, **2011**, 12, 313 | 3.6 | 44 |
| 142 | SDM--a server for predicting effects of mutations on protein stability and malfunction. *Nucleic Acids Research*, **2011**, 39, W215-22 | 20.1 | 343 |
| 141 | Crystal structure of DNA-PKcs reveals a large open-ring cradle comprised of HEAT repeats. *Nature*, **2010**, 463, 118-21 | 50.4 | 165 |
| 140 | Structural biology of DNA repair: spatial organisation of the multicomponent complexes of nonhomologous end joining. *Journal of Nucleic Acids*, **2010**, 2010, | 2.3 | 23 |
| 139 | Structural biology in fragment-based drug design. *Current Opinion in Structural Biology*, **2010**, 20, 497-507 | 8.1 | 173 |
| 138 | Structural and functional restraints on the occurrence of single amino acid variations in human proteins. *PLoS ONE*, **2010**, 5, e9186 | 3.7 | 29 |
| 137 | BIPA: a database for protein-nucleic acid interaction in 3D structures. *Bioinformatics*, **2009**, 25, 1559-60 | 7.2 | 42 |
| 136 | Application of fragment growing and fragment linking to the discovery of inhibitors of Mycobacterium tuberculosis pantothenate synthetase. *Angewandte Chemie - International Edition*, **2009**, 48, 8452-6 | 16.4 | 120 |
| 135 | Structural bioinformatics mutation analysis reveals genotype-phenotype correlations in von Hippel-Lindau disease and suggests molecular mechanisms of tumorigenesis. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77, 84-96 | 4.2 | 50 |

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