

# David Goodsell

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/5235054/publications.pdf>

Version: 2024-02-01

254  
papers

47,077  
citations

30047

54  
h-index

1899

208  
g-index

264  
all docs

264  
docs citations

264  
times ranked

48080  
citing authors

| #  | ARTICLE   | IF  | CITATIONS |
|----|---|-----|-----------|
| 1  | Evolution of the SARS-CoV-2 proteome in three dimensions (3D) during the first 6 months of the COVID-19 pandemic. <i>Proteins: Structure, Function and Bioinformatics</i> , 2022, 90, 1054-1080.  | 1.5 | 31        |
| 2  | RCSB Protein Data Bank: Celebrating 50 years of the PDB with new tools for understanding and visualizing biological macromolecules in 3D. <i>Protein Science</i> , 2022, 31, 187-208.   | 3.1 | 84        |
| 3  | PDB-101: Educational resources supporting molecular explorations through biology and medicine. <i>Protein Science</i> , 2022, 31, 129-140.  | 3.1 | 43        |
| 4  | RCSB Protein Data Bank resources for structure-facilitated design of mRNA vaccines for existing and emerging viral pathogens. <i>Structure</i> , 2022, 30, 55-68.e2.  | 1.6 | 10        |
| 5  | Building Structural Models of a Whole Mycoplasma Cell. <i>Journal of Molecular Biology</i> , 2022, 434, 167351.   | 2.0 | 40        |
| 6  | Integrative illustration of a JCVI-syn3A minimal cell. <i>Journal of Integrative Bioinformatics</i> , 2022, 19, .   | 1.0 | 6         |
| 7  | Exploring protein symmetry at the RCSB Protein Data Bank. <i>Emerging Topics in Life Sciences</i> , 2022, 6, 231-243.   | 1.1 | 7         |
| 8  | Modeling in the Time of COVID-19: Statistical and Rule-based Mesoscale Models. <i>IEEE Transactions on Visualization and Computer Graphics</i> , 2021, 27, 722-732.   | 2.9 | 20        |
| 9  | The AutoDock suite at 30. <i>Protein Science</i> , 2021, 30, 31-43.   | 3.1 | 85        |
| 10 | Seeing the PDB. <i>Journal of Biological Chemistry</i> , 2021, 296, 100742.   | 1.6 | 13        |
| 11 | CellPAINT: Turnkey Illustration of Molecular Cell Biology. <i>Frontiers in Bioinformatics</i> , 2021, 1, .  | 1.0 | 20        |
| 12 | Molecular storytelling for online structural biology outreach and education. <i>Structural Dynamics</i> , 2021, 8, 020401.  | 0.9 | 7         |
| 13 | Art as a tool for science. <i>Nature Structural and Molecular Biology</i> , 2021, 28, 402-403.  | 3.6 | 7         |
| 14 | Moltemplate: A Tool for Coarse-Grained Modeling of Complex Biological Matter and Soft Condensed Matter Physics. <i>Journal of Molecular Biology</i> , 2021, 433, 166841.  | 2.0 | 189       |
| 15 | Picturing science: using art and imagination to explore new worlds. <i>Biochemist</i> , 2021, 43, 32-38.  | 0.2 | 1         |
| 16 | RCSB Protein Data Bank: powerful new tools for exploring 3D structures of biological macromolecules for basic and applied research and education in fundamental biology, biomedicine, biotechnology, bioengineering and energy sciences. <i>Nucleic Acids Research</i> , 2021, 49, D437-D451. | 6.5 | 918       |
| 17 | RCSB Protein Data Bank: Enabling biomedical research and drug discovery. <i>Protein Science</i> , 2020, 29, 52-65.  | 3.1 | 223       |
| 18 | RCSB Protein Data Bank tools for 3D structure-guided cancer research: human papillomavirus (HPV) case study. <i>Oncogene</i> , 2020, 39, 6623-6632.   | 2.6 | 6         |

| #  | ARTICLE  | IF  | CITATIONS |
|----|--|-----|-----------|
| 19 | Integrative illustration for coronavirus outreach. PLoS Biology, 2020, 18, e3000815.   | 2.6 | 18        |
| 20 | Selective and Effective: Current Progress in Computational Structure-Based Drug Discovery of Targeted Covalent Inhibitors. Trends in Pharmacological Sciences, 2020, 41, 1038-1049.                      | 4.0 | 17        |
| 21 | Art and Science of the Cellular Mesoscale. Trends in Biochemical Sciences, 2020, 45, 472-483.  | 3.7 | 36        |
| 22 | Insights from 20 years of the Molecule of the Month. Biochemistry and Molecular Biology Education, 2020, 48, 350-355.  | 0.5 | 16        |
| 23 | Impact of the Protein Data Bank Across Scientific Disciplines. Data Science Journal, 2020, 19, 25.   | 0.6 | 17        |
| 24 | Molecular storytelling for structural biology outreach and education. Acta Crystallographica Section A: Foundations and Advances, 2020, 76, a9-a9.   | 0.0 | 0         |
| 25 | Insights from 20 Years of the Molecule of the Month and PDB101. FASEB Journal, 2020, 34, 1-1.  | 0.2 | 0         |
| 26 | Late-onset retinal degeneration pathology due to mutations in CTRP5 is mediated through HTRA1. Aging Cell, 2019, 18, e13011.   | 3.0 | 24        |
| 27 | Cuttlefish: Color Mapping for Dynamic Multi-Scale Visualizations. Computer Graphics Forum, 2019, 38, 150-164.  | 1.8 | 11        |
| 28 | Illustrate: Software for Biomolecular Illustration. Structure, 2019, 27, 1716-1720.e1.   | 1.6 | 87        |
| 29 | Integrative modeling of the HIV-1 ribonucleoprotein complex. PLoS Computational Biology, 2019, 15, e1007150.   | 1.5 | 4         |
| 30 | Scientific Delirium Madness 5.0: Gallery. Leonardo, 2019, 52, 220-229.   | 0.2 | 1         |
| 31 | Novel Intersubunit Interaction Critical for HIV-1 Core Assembly Defines a Potentially Targetable Inhibitor Binding Pocket. MBio, 2019, 10, .   | 1.8 | 13        |
| 32 | Parallel Generation and Visualization of Bacterial Genome Structures. Computer Graphics Forum, 2019, 38, 57-68.  | 1.8 | 6         |
| 33 | Protein Data Bank: the single global archive for 3D macromolecular structure data. Nucleic Acids Research, 2019, 47, D520-D528.  | 6.5 | 671       |
| 34 | RCSB Protein Data Bank: biological macromolecular structures enabling research and education in fundamental biology, biomedicine, biotechnology and energy. Nucleic Acids Research, 2019, 47, D464-D474. | 6.5 | 918       |
| 35 | Labels on Levels: Labeling of Multi-Scale Multi-Instance and Crowded 3D Biological Environments. IEEE Transactions on Visualization and Computer Graphics, 2019, 25, 977-986.                            | 2.9 | 16        |
| 36 | Symmetry at the Cellular Mesoscale. Symmetry, 2019, 11, 1170.  | 1.1 | 4         |

| #  | ARTICLE  | IF  | CITATIONS |
|----|--|-----|-----------|
| 37 | Integrative Modeling and Visualization of Exosomes. <i>The Journal of Biocommunication</i> , 2019, 43, .   | 0.1 | 3         |
| 38 | Exploring biology and medicine using 3D biomacromolecules with PDB-101. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2019, 75, a26-a26.                       | 0.0 | 0         |
| 39 | Instant Construction and Visualization of Crowded Biological Environments. <i>IEEE Transactions on Visualization and Computer Graphics</i> , 2018, 24, 862-872.                      | 2.9 | 36        |
| 40 | Lattice Models of Bacterial Nucleoids. <i>Journal of Physical Chemistry B</i> , 2018, 122, 5441-5447.  | 1.2 | 23        |
| 41 | CellPAINT: Interactive Illustration of Dynamic Mesoscale Cellular Environments. <i>IEEE Computer Graphics and Applications</i> , 2018, 38, 51-66.                                    | 1.0 | 33        |
| 42 | Molecular Illustration in Research and Education: Past, Present, and Future. <i>Journal of Molecular Biology</i> , 2018, 430, 3969-3981.   | 2.0 | 52        |
| 43 | From Atoms to Cells: Using Mesoscale Landscapes to Construct Visual Narratives. <i>Journal of Molecular Biology</i> , 2018, 430, 3954-3968.  | 2.0 | 31        |
| 44 | OUP accepted manuscript. <i>Nucleic Acids Research</i> , 2017, 45, D271-D281.  | 6.5 | 619       |
| 45 | A visual review of the human pathogen <i>Streptococcus pneumoniae</i> . <i>FEMS Microbiology Reviews</i> , 2017, 41, 854-879.  | 3.9 | 72        |
| 46 | PDB-101: educational portal for molecular explorations through biology and medicine. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2017, 73, C670-C670.        | 0.0 | 0         |
| 47 | Fragment-Based Analysis of Ligand Dockings Improves Classification of Actives. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1597-1607.                            | 2.5 | 4         |
| 48 | Covalent docking using autodock: Two-point attractor and flexible side chain methods. <i>Protein Science</i> , 2016, 25, 295-301.  | 3.1 | 170       |
| 49 | Computational protein-ligand docking and virtual drug screening with the AutoDock suite. <i>Nature Protocols</i> , 2016, 11, 905-919.  | 5.5 | 1,370     |
| 50 | Visibility Equalizer Cutaway Visualization of Mesoscopic Biological Models. <i>Computer Graphics Forum</i> , 2016, 35, 161-170.  | 1.8 | 13        |
| 51 | Atomic Evidence. , 2016, , .   |     | 11        |
| 52 | RCSB Protein Data Bank: A Resource for Chemical, Biochemical, and Structural Explorations of Large and Small Biomolecules. <i>Journal of Chemical Education</i> , 2016, 93, 569-575. | 1.1 | 66        |
| 53 | Chameleon: Dynamic Color Mapping for Multi-Scale Structural Biology Models. <i>Eurographics Workshop on Visual Computing for Biomedicine</i> , 2016, 2016, .                         | 4.0 | 3         |
| 54 | AutoDockFR: Advances in Protein-Ligand Docking with Explicitly Specified Binding Site Flexibility. <i>PLoS Computational Biology</i> , 2015, 11, e1004586.                           | 1.5 | 287       |

| #  | ARTICLE  | IF  | CITATIONS |
|----|--|-----|-----------|
| 55 | Illustrations of the HIV Life Cycle. <i>Current Topics in Microbiology and Immunology</i> , 2015, 389, 243-252.  | 0.7 | 25        |
| 56 | The RCSB PDB "Molecule of the Month" Inspiring a Molecular View of Biology. <i>PLoS Biology</i> , 2015, 13, e1002140.  | 2.6 | 88        |
| 57 | The RCSB Protein Data Bank: views of structural biology for basic and applied research and education. <i>Nucleic Acids Research</i> , 2015, 43, D345-D356.   | 6.5 | 461       |
| 58 | cellPACK: a virtual mesoscope to model and visualize structural systems biology. <i>Nature Methods</i> , 2015, 12, 85-91.  | 9.0 | 130       |
| 59 | 3D molecular models of whole HIV-1 virions generated with cellPACK. <i>Faraday Discussions</i> , 2014, 169, 23-44.   | 1.6 | 52        |
| 60 | Visualising microorganisms from molecules to cells. <i>FEMS Microbiology Letters</i> , 2014, 356, 1-7.   | 0.7 | 0         |
| 61 | Protein structure in context: The molecular landscape of angiogenesis. <i>Biochemistry and Molecular Biology Education</i> , 2013, 41, 213-223.  | 0.5 | 6         |
| 62 | The Effects of the SUN Project on Teacher Knowledge and Self-Efficacy Regarding Biological Energy Transfer Are Significant and Long-Lasting: Results of a Randomized Controlled Trial. <i>CBE Life Sciences Education</i> , 2013, 12, 287-305. | 1.1 | 4         |
| 63 | Revealing structural views of biology. <i>Biopolymers</i> , 2013, 99, 817-824.   | 1.2 | 4         |
| 64 | Protein Structure in Context: The Landscape of Angiogenesis. <i>FASEB Journal</i> , 2013, 27, 1031.10.   | 0.2 | 0         |
| 65 | The RCSB Protein Data Bank: new resources for research and education. <i>Nucleic Acids Research</i> , 2012, 41, D475-D482.   | 6.5 | 418       |
| 66 | Protein Flexibility in Virtual Screening: The BACE-1 Case Study. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 2697-2704.  | 2.5 | 47        |
| 67 | Illustrating the machinery of life: Viruses. <i>Biochemistry and Molecular Biology Education</i> , 2012, 40, 291-296.  | 0.5 | 8         |
| 68 | Putting proteins in context. <i>BioEssays</i> , 2012, 34, 718-720.   | 1.2 | 4         |
| 69 | ePMV Embeds Molecular Modeling into Professional Animation Software Environments. <i>Structure</i> , 2011, 19, 293-303.  | 1.6 | 82        |
| 70 | The evolution of the RCSB Protein Data Bank website. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 782-789.   | 6.2 | 7         |
| 71 | Redox-Based Probes for Protein Tyrosine Phosphatases. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 4423-4427.  | 7.2 | 48        |
| 72 | Eukaryotic cell panorama. <i>Biochemistry and Molecular Biology Education</i> , 2011, 39, 91-101.  | 0.5 | 22        |

| #  | ARTICLE   | IF  | CITATIONS |
|----|---|-----|-----------|
| 73 | Atomic Evidence: The Foundations of Structural Molecular Biology. Science Progress, 2011, 94, 414-430.  | 1.0 | 1         |
| 74 | The RCSB Protein Data Bank: redesigned web site and web services. Nucleic Acids Research, 2011, 39, D392-D401.  | 6.5 | 549       |
| 75 | The RCSB Protein Data Bank: site functionality and bioinformatics use cases. NCI Nature Pathway Interaction Database, 2011, , .   | 0.3 | 2         |
| 76 | Mitochondrion. Biochemistry and Molecular Biology Education, 2010, 38, 134-140.   | 0.5 | 9         |
| 77 | Promoting a structural view of biology for varied audiences: an overview of RCSB PDB resources and experiences. Journal of Applied Crystallography, 2010, 43, 1224-1229.                                | 1.9 | 41        |
| 78 | Visualization of macromolecular structures. Nature Methods, 2010, 7, S42-S55.   | 9.0 | 137       |
| 79 | Visualizing biological data" now and in the future. Nature Methods, 2010, 7, S2-S4.   | 9.0 | 115       |
| 80 | Artophagy: The Art of Autophagy-the Cvt pathway. Autophagy, 2010, 6, 3-6.   | 4.3 | 13        |
| 81 | Virtual screening with AutoDock: theory and practice. Expert Opinion on Drug Discovery, 2010, 5, 597-607.   | 2.5 | 462       |
| 82 | Fact and Fantasy in Nanotech Imagery. Leonardo, 2009, 42, 52-57.  | 0.2 | 9         |
| 83 | AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility. Journal of Computational Chemistry, 2009, 30, 2785-2791.   | 1.5 | 16,850    |
| 84 | Neuromuscular synapse. Biochemistry and Molecular Biology Education, 2009, 37, 204-210.   | 0.5 | 11        |
| 85 | Escherichia coli. Biochemistry and Molecular Biology Education, 2009, 37, 325-332.  | 0.5 | 28        |
| 86 | The Machinery of Life. , 2009, , .  |     | 156       |
| 87 | Computational Docking of Biomolecular Complexes with AutoDock. Cold Spring Harbor Protocols, 2009, 2009, pdb.prot5200.  | 0.2 | 33        |
| 88 | Automated prediction of ligand-binding sites in proteins. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1506-1517.  | 1.5 | 134       |
| 89 | Empirical entropic contributions in computational docking: Evaluation in APS reductase complexes. Journal of Computational Chemistry, 2008, 29, 1753-1761.  | 1.5 | 34        |
| 90 | Structure-Based Virtual Screening and Biological Evaluation of <i>Mycobacterium tuberculosis</i> Adenosine 5'-Phosphosulfate Reductase Inhibitors. Journal of Medicinal Chemistry, 2008, 51, 6627-6630. | 2.9 | 32        |

| #   | ARTICLE  | IF   | CITATIONS |
|-----|--|------|-----------|
| 91  | Identification of novel Î²â€secretase inhibitors through the inclusion of protein flexibility in virtual screening calculations. <i>FASEB Journal</i> , 2008, 22, 791.8. | 0.2  | 1         |
| 92  | The Molecular Perspective: Hepatitis B Virus. <i>Oncologist</i> , 2007, 12, 516-517.   | 1.9  | 3         |
| 93  | Filling in the Gaps: Artistic License in Education and Outreach. <i>PLoS Biology</i> , 2007, 5, e308.  | 2.6  | 38        |
| 94  | A semiempirical free energy force field with charge-based desolvation. <i>Journal of Computational Chemistry</i> , 2007, 28, 1145-1152.                                  | 1.5  | 1,854     |
| 95  | Making the step from chemistry to biology and back. <i>Nature Chemical Biology</i> , 2007, 3, 681-684.   | 3.9  | 4         |
| 96  | Active Teaching and Tactile Learning: A Role for Physical Models of Molecular Structures. <i>FASEB Journal</i> , 2007, 21, A297.   | 0.2  | 0         |
| 97  | Seeing the nanoscale. <i>Nano Today</i> , 2006, 1, 44-49.  | 6.2  | 285       |
| 98  | The Molecular Perspective: c-Abl Tyrosine Kinase. <i>Stem Cells</i> , 2006, 24, 209-210.   | 1.4  | 2         |
| 99  | The Molecular Perspective: Cisplatin. <i>Stem Cells</i> , 2006, 24, 514-515.   | 1.4  | 35        |
| 100 | Tactile teaching: Exploring protein structure/function using physical models. <i>Biochemistry and Molecular Biology Education</i> , 2006, 34, 247-254.                   | 0.5  | 77        |
| 101 | Recognition highlights: Toll-like receptors. <i>Journal of Molecular Recognition</i> , 2006, 19, 387-388.  | 1.1  | 0         |
| 102 | The Molecular Perspective: Cisplatin. <i>Oncologist</i> , 2006, 11, 316-317.   | 1.9  | 27        |
| 103 | The Molecular Perspective: Tumor Necrosis Factor. <i>Oncologist</i> , 2006, 11, 83-84.   | 1.9  | 12        |
| 104 | The Molecular Perspective: Tissue Factor. <i>Oncologist</i> , 2006, 11, 849-850.   | 1.9  | 6         |
| 105 | The Molecular Perspective: Alcohol. <i>Oncologist</i> , 2006, 11, 1045-1046.   | 1.9  | 7         |
| 106 | The Molecular Perspective: Estrogen Sulfotransferase. <i>Oncologist</i> , 2006, 11, 418-419.   | 1.9  | 7         |
| 107 | Using physical models of proteins to tell molecular stories of researchâ€based health care. <i>FASEB Journal</i> , 2006, 20, A976.                                       | 0.2  | 0         |
| 108 | Representing Structural Information with RasMol. <i>Current Protocols in Bioinformatics</i> , 2005, 11, Unit 5.4.  | 25.8 | 23        |

| #   | ARTICLE  | IF  | CITATIONS |
|-----|--|-----|-----------|
| 109 | The Molecular Perspective: Morphine. <i>Stem Cells</i> , 2005, 23, 144-145.  | 1.4 | 6         |
| 110 | The Molecular Perspective: Major Histocompatibility Complex. <i>Stem Cells</i> , 2005, 23, 454-455.  | 1.4 | 3         |
| 111 | The Molecular Perspective: L-Asparaginase. <i>Stem Cells</i> , 2005, 23, 710-711.  | 1.4 | 3         |
| 112 | The Molecular Perspective: Double-Stranded DNA Breaks. <i>Stem Cells</i> , 2005, 23, 1021-1022.  | 1.4 | 3         |
| 113 | The Molecular Perspective: RAD51 and BRCA2. <i>Stem Cells</i> , 2005, 23, 1434-1435.   | 1.4 | 1         |
| 114 | Visual Methods from Atoms to Cells. <i>Structure</i> , 2005, 13, 347-354.  | 1.6 | 46        |
| 115 | Recognition in action: flipping pyrimidine dimers. <i>Journal of Molecular Recognition</i> , 2005, 18, 193-195.  | 1.1 | 3         |
| 116 | Recognition in action: DNA mimicry. <i>Journal of Molecular Recognition</i> , 2005, 18, 427-430.   | 1.1 | 4         |
| 117 | 1,2,3-Triazole as a Peptide Surrogate in the Rapid Synthesis of HIV-1 Protease Inhibitors. <i>ChemBioChem</i> , 2005, 6, 1167-1169.                              | 1.3 | 262       |
| 118 | The Molecular Perspective: Double-Stranded DNA Breaks. <i>Oncologist</i> , 2005, 10, 361-362.  | 1.9 | 11        |
| 119 | Identifying Protein Binding Sites and Optimal Ligands. <i>Letters in Drug Design and Discovery</i> , 2005, 2, 483-489.   | 0.4 | 4         |
| 120 | The Molecular Perspective: RAD51 and BRCA2. <i>Oncologist</i> , 2005, 10, 555-556.   | 1.9 | 0         |
| 121 | The Molecular Perspective: c-Abl Tyrosine Kinase. <i>Oncologist</i> , 2005, 10, 758-759.   | 1.9 | 2         |
| 122 | The Molecular Perspective: L-Asparaginase. <i>Oncologist</i> , 2005, 10, 238-239.  | 1.9 | 11        |
| 123 | The cAMP binding domain: An ancient signaling module. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 45-50. | 3.3 | 190       |
| 124 | The Molecular Perspective: Major Histocompatibility Complex. <i>Oncologist</i> , 2005, 10, 80-81.  | 1.9 | 2         |
| 125 | The Molecular Perspective: Cyclins. <i>Oncologist</i> , 2004, 9, 592-593.  | 1.9 | 0         |
| 126 | The Molecular Perspective: Nicotine and Nitrosamines. <i>Oncologist</i> , 2004, 9, 353-354.  | 1.9 | 6         |



| #   | ARTICLE  | IF  | CITATIONS |
|-----|--|-----|-----------|
| 127 | The Molecular Perspective: Polycyclic Aromatic Hydrocarbons. <i>Oncologist</i> , 2004, 9, 469-470.   | 1.9 | 1         |
| 128 | Grid-Based Hydrogen Bond Potentials with Improved Directionality. <i>Letters in Drug Design and Discovery</i> , 2004, 1, 178-183.  | 0.4 | 38        |
| 129 | The Molecular Perspective: Morphine. <i>Oncologist</i> , 2004, 9, 717-718.   | 1.9 | 10        |
| 130 | The Molecular Perspective: DNA Polymerase. <i>Oncologist</i> , 2004, 9, 108-109.   | 1.9 | 4         |
| 131 | The Molecular Perspective: Cytochrome c and Apoptosis. <i>Oncologist</i> , 2004, 9, 226-227.   | 1.9 | 27        |
| 132 | The Molecular Perspective: Protein Farnesyltransferase. <i>Stem Cells</i> , 2004, 22, 119-120.   | 1.4 | 2         |
| 133 | The Molecular Perspective: DNA Polymerase. <i>Stem Cells</i> , 2004, 22, 236-237.  | 1.4 | 1         |
| 134 | The Molecular Perspective: Cytochrome c and Apoptosis. <i>Stem Cells</i> , 2004, 22, 428-429.  | 1.4 | 10        |
| 135 | The Molecular Perspective: Nicotine and Nitrosamines. <i>Stem Cells</i> , 2004, 22, 645-646.   | 1.4 | 3         |
| 136 | The Molecular Perspective: Polycyclic Aromatic Hydrocarbons. <i>Stem Cells</i> , 2004, 22, 873-874.  | 1.4 | 3         |
| 137 | The Molecular Perspective: Cyclins. <i>Stem Cells</i> , 2004, 22, 1121-1122.   | 1.4 | 0         |
| 138 | Automated docking of ligands to an artificial active site: augmenting crystallographic analysis with computer modeling. <i>Journal of Computer-Aided Molecular Design</i> , 2003, 17, 525-536. | 1.3 | 81        |
| 139 | The Molecular Perspective: VEGF and Angiogenesis. <i>Stem Cells</i> , 2003, 21, 118-119.   | 1.4 | 37        |
| 140 | The Molecular Perspective: Ubiquitin and the Proteasome. <i>Stem Cells</i> , 2003, 21, 509-510.  | 1.4 | 1         |
| 141 | The Molecular Perspective: Histone Deacetylase. <i>Stem Cells</i> , 2003, 21, 620-621.   | 1.4 | 7         |
| 142 | The Molecular Perspective: Epidermal Growth Factor. <i>Stem Cells</i> , 2003, 21, 702-703.   | 1.4 | 8         |
| 143 | Rapid Diversity-Oriented Synthesis in Microtiter Plates for In Situ Screening of HIV Protease Inhibitors. <i>ChemBioChem</i> , 2003, 4, 1246-1248.   | 1.3 | 134       |
| 144 | Looking at Molecules-An Essay on Art and Science. <i>ChemBioChem</i> , 2003, 4, 1293-1297.   | 1.3 | 6         |

| #   | ARTICLE   | IF  | CITATIONS |
|-----|---|-----|-----------|
| 145 | The Molecular Perspective: Histone Deacetylase. <i>Oncologist</i> , 2003, 8, 389-391.   | 1.9 | 5         |
| 146 | The Molecular Perspective: Epidermal Growth Factor. <i>Oncologist</i> , 2003, 8, 496-497.   | 1.9 | 19        |
| 147 | The Molecular Perspective: Ubiquitin and the Proteasome. <i>Oncologist</i> , 2003, 8, 293-294.  | 1.9 | 2         |
| 148 | The Molecular Perspective: Protein Farnesyltransferase. <i>Oncologist</i> , 2003, 8, 597-598.   | 1.9 | 2         |
| 149 | BioEditor—simplifying macromolecular structure annotation. <i>Bioinformatics</i> , 2003, 19, 897-898.   | 1.8 | 20        |
| 150 | The Molecular Perspective: Restriction Endonucleases. <i>Oncologist</i> , 2002, 7, 82-83.   | 1.9 | 4         |
| 151 | The Molecular Perspective: Cadherin. <i>Oncologist</i> , 2002, 7, 467-468.  | 1.9 | 11        |
| 152 | The Molecular Perspective: Bcl-2 and Apoptosis. <i>Oncologist</i> , 2002, 7, 259-260.   | 1.9 | 14        |
| 153 | The Molecular Perspective: Tamoxifen and the Estrogen Receptor. <i>Oncologist</i> , 2002, 7, 163-164.   | 1.9 | 26        |
| 154 | The Molecular Perspective: DNA Topoisomerases. <i>Oncologist</i> , 2002, 7, 381-382.  | 1.9 | 2         |
| 155 | The Molecular Perspective: VEGF and Angiogenesis. <i>Oncologist</i> , 2002, 7, 569-570.   | 1.9 | 33        |
| 156 | Automated docking to multiple target structures: Incorporation of protein mobility and structural water heterogeneity in AutoDock. <i>Proteins: Structure, Function and Bioinformatics</i> , 2002, 46, 34-40. | 1.5 | 394       |
| 157 | Evolutionary analysis of HIV-1 protease inhibitors: Methods for design of inhibitors that evade resistance. <i>Proteins: Structure, Function and Bioinformatics</i> , 2002, 48, 63-74.                        | 1.5 | 17        |
| 158 | The Molecular Perspective: Antibodies. <i>Stem Cells</i> , 2002, 20, 94-95.   | 1.4 | 1         |
| 159 | The Molecular Perspective: Restriction Endonucleases. <i>Stem Cells</i> , 2002, 20, 190-191.  | 1.4 | 4         |
| 160 | The Molecular Perspective: Tamoxifen and the Estrogen Receptor. <i>Stem Cells</i> , 2002, 20, 267-268.  | 1.4 | 13        |
| 161 | The Molecular Perspective: Bcl-2 and Apoptosis. <i>Stem Cells</i> , 2002, 20, 355-356.  | 1.4 | 28        |
| 162 | The Molecular Perspective: DNA Topoisomerases. <i>Stem Cells</i> , 2002, 20, 470-471.   | 1.4 | 9         |

| #   | ARTICLE  | IF  | CITATIONS |
|-----|--|-----|-----------|
| 163 | The Molecular Perspective: Cadherin. Stem Cells, 2002, 20, 583-584.  | 1.4 | 9         |
| 164 | A hierarchical model of HIV-1 protease drug resistance. Applied Bioinformatics, 2002, 1, 3-12.   | 1.7 | 2         |
| 165 | The Molecular Perspective: The Ribosome. Stem Cells, 2001, 19, 92-93.  | 1.4 | 0         |
| 166 | Recognition templates for predicting adenylate-binding sites in proteins. Journal of Molecular Biology, 2001, 314, 1245-1255.  | 2.0 | 16        |
| 167 | Analysis of a data set of paired uncomplexed protein structures: New metrics for side-chain flexibility and model evaluation. Proteins: Structure, Function and Bioinformatics, 2001, 43, 271-279. | 1.5 | 50        |
| 168 | The Molecular Perspective: Targeted Toxins. Stem Cells, 2001, 19, 161-162.   | 1.4 | 0         |
| 169 | The Molecular Perspective: Cytochrome P450. Stem Cells, 2001, 19, 263-264.   | 1.4 | 1         |
| 170 | The Molecular Perspective: Ultraviolet Light and Pyrimidine Dimers. Stem Cells, 2001, 19, 348-349.   | 1.4 | 35        |
| 171 | The Molecular Perspective: Interferons. Stem Cells, 2001, 19, 467-468.   | 1.4 | 0         |
| 172 | The Molecular Perspective: The src Oncogene. Stem Cells, 2001, 19, 553-555.  | 1.4 | 1         |
| 173 | The Molecular Perspective: Cytochrome P450. Oncologist, 2001, 6, 205-206.  | 1.9 | 4         |
| 174 | The Molecular Perspective: Interferons. Oncologist, 2001, 6, 374-375.  | 1.9 | 2         |
| 175 | The Molecular Perspective: Ultraviolet Light and Pyrimidine Dimers. Oncologist, 2001, 6, 298-299.  | 1.9 | 70        |
| 176 | The Molecular Perspective: The src Oncogene. Oncologist, 2001, 6, 474-476.   | 1.9 | 2         |
| 177 | The Molecular Perspective: Targeted Toxins. Oncologist, 2001, 6, 110-111.  | 1.9 | 0         |
| 178 | The Molecular Perspective: Antibodies. Oncologist, 2001, 6, 547-548.   | 1.9 | 4         |
| 179 | Sequence Recognition of DNA by Lexitropsins. Current Medicinal Chemistry, 2001, 8, 509-516.  | 1.2 | 21        |
| 180 | A Study on Docking Mode of HIV Protease and Their Inhibitors.. Journal of Chemical Software, 2001, 7, 103-114.   | 0.2 | 9         |

| #   | ARTICLE  | IF   | CITATIONS |
|-----|--|------|-----------|
| 181 | Structural Symmetry and Protein Function. Annual Review of Biophysics and Biomolecular Structure, 2000, 29, 105-153.   | 18.3 | 806       |
| 182 | The Molecular Perspective: Cyclooxygenase-2. Stem Cells, 2000, 18, 227-229.  | 1.4  | 6         |
| 183 | The Molecular Perspective: The Ribosome. Oncologist, 2000, 5, 508-509.   | 1.9  | 0         |
| 184 | The Molecular Perspective: Caspases. Oncologist, 2000, 5, 435-436.   | 1.9  | 11        |
| 185 | The Molecular Perspective: DNA. Oncologist, 2000, 5, 81-82.  | 1.9  | 0         |
| 186 | The Molecular Perspective: Microtubules and the Taxanes. Oncologist, 2000, 5, 345-346.   | 1.9  | 7         |
| 187 | The Molecular Perspective: Simian Virus 40. Oncologist, 2000, 5, 260-262.  | 1.9  | 2         |
| 188 | The Molecular Perspective: Cyclooxygenase-2. Oncologist, 2000, 5, 169-171.   | 1.9  | 16        |
| 189 | The Molecular Perspective: Matrix Metalloproteinase 2. Stem Cells, 2000, 18, 73-75.  | 1.4  | 3         |
| 190 | The Molecular Perspective: DNA. Stem Cells, 2000, 18, 148-149.   | 1.4  | 5         |
| 191 | The Molecular Perspective: Simian Virus 40. Stem Cells, 2000, 18, 301-303.   | 1.4  | 2         |
| 192 | The Molecular Perspective: Microtubules and the Taxanes. Stem Cells, 2000, 18, 382-383.  | 1.4  | 4         |
| 193 | The Molecular Perspective: Caspases. Stem Cells, 2000, 18, 457-458.  | 1.4  | 11        |
| 194 | The art of molecular graphics. Journal of Molecular Graphics and Modelling, 2000, 18, 173.   | 1.3  | 0         |
| 195 | The Molecular Perspective: Methotrexate. Oncologist, 1999, 4, 340-341.   | 1.9  | 43        |
| 196 | Coevolutionary analysis of resistance-evading peptidomimetic inhibitors of HIV-1 protease. Proceedings of the National Academy of Sciences of the United States of America, 1999, 96, 1369-1374. | 3.3  | 14        |
| 197 | The Molecular Perspective: p53 Tumor Suppressor. Stem Cells, 1999, 17, 189-190.  | 1.4  | 7         |
| 198 | The Molecular Perspective: The <i>ras</i> Oncogene. Stem Cells, 1999, 17, 235-236.   | 1.4  | 49        |

| #   | ARTICLE   | IF  | CITATIONS |
|-----|---|-----|-----------|
| 199 | The Molecular Perspective: Methotrexate. <i>Stem Cells</i> , 1999, 17, 314-315.   | 1.4 | 29        |
| 200 | Docking of 4-oxalocrotonate tautomerase substrates: Implications for the catalytic mechanism. , 1999, 50, 319-328.  |     | 26        |
| 201 | Coevolution and subsite decomposition for the design of resistance-evading HIV-1 protease inhibitors 1 Edited by F. E. Cohen. <i>Journal of Molecular Biology</i> , 1999, 287, 77-92. | 2.0 | 13        |
| 202 | Atomistic vs. Continuous Representations in Molecular Biology. , 1999, , 146-155.   |     | 4         |
| 203 | The Molecular Perspective: p53 Tumor Suppressor. <i>Oncologist</i> , 1999, 4, 138-139.  | 1.9 | 11        |
| 204 | The Molecular Perspective: The <i>ras</i> Oncogene. <i>Oncologist</i> , 1999, 4, 263-264.   | 1.9 | 91        |
| 205 | The Molecular Perspective: The Multidrug Transporter. <i>Oncologist</i> , 1999, 4, 428-429.   | 1.9 | 2         |
| 206 | The Molecular Perspective: Matrix Metalloproteinase 2. <i>Oncologist</i> , 1999, 4, 509-511.  | 1.9 | 3         |
| 207 | The molecular perspective: p53 tumor suppressor. <i>Oncologist</i> , 1999, 4, 138-9.  | 1.9 | 7         |
| 208 | The molecular perspective: the ras oncogene. <i>Oncologist</i> , 1999, 4, 263-4.  | 1.9 | 45        |
| 209 | The molecular perspective: methotrexate. <i>Oncologist</i> , 1999, 4, 340-1.  | 1.9 | 21        |
| 210 | The molecular perspective: the multidrug transporter. <i>Oncologist</i> , 1999, 4, 428-9.   | 1.9 | 0         |
| 211 | The molecular perspective: matrix metalloproteinase 2. <i>Oncologist</i> , 1999, 4, 509-11.   | 1.9 | 0         |
| 212 | Morphology of protein-protein interfaces. <i>Structure</i> , 1998, 6, 421-427.  | 1.6 | 218       |
| 213 | Automated docking using a Lamarckian genetic algorithm and an empirical binding free energy function. <i>Journal of Computational Chemistry</i> , 1998, 19, 1639-1662.                | 1.5 | 8,897     |
| 214 | Interactive modeling of supramolecular assemblies. <i>Journal of Molecular Graphics and Modelling</i> , 1998, 16, 115-120.  | 1.3 | 7         |
| 215 | Automated Docking and the Search for HIV Protease Inhibitors. <i>SAR and QSAR in Environmental Research</i> , 1998, 8, 273-285.   | 1.0 | 24        |
| 216 | An Analysis of a Class of DNA Sequence Reading Molecules. <i>Journal of Computational Biology</i> , 1998, 5, 571-583.   | 0.8 | 1         |

| #   | ARTICLE   | IF  | CITATIONS |
|-----|---|-----|-----------|
| 217 | The theoretical limits of DNA sequence discrimination by linked polyamides. Proceedings of the National Academy of Sciences of the United States of America, 1998, 95, 4315-4320.           | 3.3 | 7         |
| 218 | Estimation of the DNA sequence discriminatory ability of hairpin-linked lexitropsins. Proceedings of the National Academy of Sciences of the United States of America, 1997, 94, 5634-5639. | 3.3 | 21        |
| 219 | Defining GC-specificity in the minor groove: side-by-side binding of the di-imidazole lexitropsin to C-A-T-G-G-C-C-A-T-G. Structure, 1997, 5, 1033-1046.                                    | 1.6 | 109       |
| 220 | Design of stapled DNA-minor-groove-binding molecules with a mutable atom simulated annealing method. Journal of Computer-Aided Molecular Design, 1997, 11, 539-546.                         | 1.3 | 3         |
| 221 | The art of molecular graphics Irving Geis: Dean of molecular illustration. Journal of Molecular Graphics and Modelling, 1997, 15, 57-59.  | 1.3 | 3         |
| 222 | Progress in the design of DNA sequence-specific lexitropsins. , 1997, 44, 323-334.  |     | 28        |
| 223 | Chapter 7 Molecules in living cells. Principles of Medical Biology, 1996, , 173-180.  | 0.1 | 0         |
| 224 | Automated docking of flexible ligands: Applications of autodock. Journal of Molecular Recognition, 1996, 9, 1-5.  | 1.1 | 1,284     |
| 225 | Distributed automated docking of flexible ligands to proteins: Parallel applications of AutoDock 2.4. Journal of Computer-Aided Molecular Design, 1996, 10, 293-304.                        | 1.3 | 907       |
| 226 | Automated docking of flexible ligands: Applications of autodock. , 1996, 9, 1.  |     | 7         |
| 227 | Design of B-DNA cross-linking and sequence-reading molecules. Biopolymers, 1995, 35, 543-553.   | 1.2 | 15        |
| 228 | Crystal Structure of C-T-C-T-C-G-A-G-A-G. Implications for the Structure of the Holliday Junction. Biochemistry, 1995, 34, 1022-1029.   | 1.2 | 62        |
| 229 | Structure of a dicationic monoimidazole lexitropsin bound to DNA. Biochemistry, 1995, 34, 16654-16661.  | 1.2 | 31        |
| 230 | Refinement of Netropsin Bound to DNA: Bias and Feedback in Electron Density Map Interpretation. Biochemistry, 1995, 34, 4983-4993.  | 1.2 | 86        |
| 231 | Crystal Structure of a Covalent DNA-Drug Adduct: Anthramycin Bound to C-C-A-A-C-G-T-T-G-G and a Molecular Explanation of Specificity. Biochemistry, 1994, 33, 13593-13610.                  | 1.2 | 115       |
| 232 | The Crystal Structure of C-C-A-T-T-A-A-T-G-G. Journal of Molecular Biology, 1994, 239, 79-96.   | 2.0 | 149       |
| 233 | Bending and curvature calculations in B-DNA. Nucleic Acids Research, 1994, 22, 5497-5503.   | 6.5 | 284       |
| 234 | Automated docking in crystallography: Analysis of the substrates of aconitase. Proteins: Structure, Function and Bioinformatics, 1993, 17, 1-10.  | 1.5 | 84        |

| #   | ARTICLE   | IF  | CITATIONS |
|-----|---|-----|-----------|
| 235 | Soluble proteins: Size, shape and function. Trends in Biochemical Sciences, 1993, 18, 65-68.  | 3.7 | 92        |
| 236 | Crystallographic analysis of C-C-A-A-G-C-T-T-G-G and its implications for bending in B-DNA. Biochemistry, 1993, 32, 8923-8931.  | 1.2 | 76        |
| 237 | Crystal structure of CATGGCCATG and its implications for A-tract bending models.. Proceedings of the National Academy of Sciences of the United States of America, 1993, 90, 2930-2934. | 3.3 | 158       |
| 238 | Macromolecular graphics. Current Opinion in Structural Biology, 1992, 2, 193-201.   | 2.6 | 9         |
| 239 | Visualizing Biological Molecules. Scientific American, 1992, 267, 76-81.  | 1.0 | 31        |
| 240 | Molecular illustration in black and white. Journal of Molecular Graphics, 1992, 10, 235-240.  | 1.7 | 17        |
| 241 | Inside a living cell. Trends in Biochemical Sciences, 1991, 16, 203-206.  | 3.7 | 315       |
| 242 | Automated docking of substrates to proteins by simulated annealing. Proteins: Structure, Function and Bioinformatics, 1990, 8, 195-202.   | 1.5 | 1,109     |
| 243 | Rendering volumetric data in molecular systems. Journal of Molecular Graphics, 1989, 7, 41-47.  | 1.7 | 55        |
| 244 | RMS: programs for generating raster molecular surfaces. Journal of Molecular Graphics, 1988, 6, 41-44.  | 1.7 | 10        |
| 245 | The Effect of Crystal Packing on Oligonucleotide Double Helix Structure. Journal of Biomolecular Structure and Dynamics, 1987, 5, 557-579.  | 2.0 | 126       |
| 246 | Isohelical analysis of DNA groove-binding drugs. Journal of Medicinal Chemistry, 1986, 29, 727-733.   | 2.9 | 162       |
| 247 | Binding of an antitumor drug to DNA. Journal of Molecular Biology, 1985, 183, 553-563.  | 2.0 | 424       |
| 248 | Bionanotechnology Today. , 0, , 227-294.  |     | 1         |
| 249 | Bionanomachines in Action. , 0, , 9-41.   |     | 1         |
| 250 | Structural Principles of Bionanotechnology. , 0, , 75-134.  |     | 0         |
| 251 | The Quest for Nanotechnology. , 0, , 1-8.   |     | 4         |
| 252 | Functional Principles of Bionanotechnology. , 0, , 135-226.   |     | 0         |

| #   | ARTICLE  | IF | CITATIONS |
|-----|--|----|-----------|
| 253 | The Future of Bionanotechnology. , 0, , 295-311.     |    | 0         |
| 254 | Biomolecular Design and Biotechnology. , 0, , 43-74. |    | 1         |