Francesca Spyrakis

List of Publications by Year
in descending order

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94 papers	2,877 citations	172386 29 h-index	206029 48 g-index
98 all docs	98 docs citations	98 times ranked	3480 citing authors

#	Article	IF	Citations
1	Target Flexibility: An Emerging Consideration in Drug Discovery and Design. Journal of Medicinal Chemistry, 2008, 51, 6237-6255.	2.9	280
2	Ten Years with New Delhi Metallo-Î²-lactamase-1 (NDM-1): From Structural Insights to Inhibitor Design. ACS Infectious Diseases, 2019, 5, 9-34.	1.8	123
3	Simple, Intuitive Calculations of Free Energy of Binding for Proteinâ^'Ligand Complexes. 3. The Free Energy Contribution of Structural Water Molecules in HIV-1 Protease Complexes. Journal of Medicinal Chemistry, 2004, 47, 4507-4516.	2.9	112
4	The Roles of Water in the Protein Matrix: A Largely Untapped Resource for Drug Discovery. Journal of Medicinal Chemistry, 2017, 60, 6781-6827.	2.9	111
5	Open challenges in structure-based virtual screening: Receptor modeling, target flexibility consideration and active site water molecules description. Archives of Biochemistry and Biophysics, 2015, 583, 105-119.	1.4	101
6	Robust Classification of â€œRelevantâ€•Water Molecules in Putative Protein Binding Sites. Journal of Medicinal Chemistry, 2008, 51, 1063-1067.	2.9	93
7	Protein Flexibility and Ligand Recognition: Challenges for Molecular Modeling. Current Topics in Medicinal Chemistry, 2011, 11, 192-210.	1.0	86
8	Mapping the Energetics of Waterâ€“Protein and Waterâ€“Ligand Interactions with the â€œNaturalâ€•HINT Forcefield: Predictive Tools for Characterizing the Roles of Water in Biomolecules. Journal of Molecular Biology, 2006, 358, 289-309.	2.0	85
9	Design of O-Acetylserine Sulfhydrylase Inhibitors by Mimicking Nature. Journal of Medicinal Chemistry, 2010, 53, 345-356.	2.9	75
10	A Pipeline To Enhance Ligand Virtual Screening: Integrating Molecular Dynamics and Fingerprints for Ligand and Proteins. Journal of Chemical Information and Modeling, 2015, 55, 2256-2274.	2.5	65
11	The consequences of scoring docked ligand conformations using free energy correlations. European Journal of Medicinal Chemistry, 2007, 42, 921-933.	2.6	58
12	Energetics of the protein-DNA-water interaction. BMC Structural Biology, 2007, 7, 4.	2.3	57
13	Bound Water at Protein-Protein Interfaces: Partners, Roles and Hydrophobic Bubbles as a Conserved Motif. PLoS ONE, 2011, 6, e24712.	1.1	57
14	The Reactivity with CO of AHb1 and AHb2 from Arabidopsis thaliana is Controlled by the Distal HisE7 and Internal Hydrophobic Cavities. Journal of the American Chemical Society, 2007, 129, 2880-2889.	6.6	54
15	Ligand migration through the internal hydrophobic cavities in human neuroglobin. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 18984-18989.	3.3	47
16	Energyâ€based prediction of amino acidâ€nucleotide base recognition. Journal of Computational Chemistry, 2008, 29, 1955-1969.	1.5	44
17	A Blueprint for High Affinity SARS-CoV-2 Mpro Inhibitors from Activity-Based Compound Library Screening Guided by Analysis of Protein Dynamics. ACS Pharmacology and Translational Science, 2021, 4, 1079-1095.	2.5	44
18	Isozyme-Specific Ligands for O-acetylserine sulfhydrylase, a Novel Antibiotic Target. PLoS ONE, 2013, 8, e77558.	1.1	43

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19	Iron Metabolism at the Interface between Host and Pathogen: From Nutritional Immunity to Antibacterial Development. International Journal of Molecular Sciences, 2020, 21, 2145.	1.8	42
20	The multifaceted pyridoxal 5â€²-phosphate-dependent O-acetylserine sulfhydrylase. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2011, 1814, 1497-1510.	1.1	39
21	A novel small-molecule inhibitor of the human papillomavirus E6-p53 interaction that reactivates p53 function and blocks cancer cells growth. Cancer Letters, 2020, 470, 115-125.	3.2	39
22	Structure-Based Virtual Screening for the Discovery of Novel Inhibitors of New Delhi Metallo-Î²-lactamase-1. ACS Medicinal Chemistry Letters, 2018, 9, 45-50.	1.3	38
23	Fine tuning of the active site modulates specificity in the interaction of O-acetylserine sulfhydrylase isozymes with serine acetyltransferase. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2013, 1834, 169-181.	1.1	35
24	Computational and biological profile of boronic acids for the detection of bacterial serine- and metallo-Î²-lactamases. Scientific Reports, 2017, 7, 17716.	1.6	35
25	ComputationalÂTitrationÂAnalysisÂofÂaÂMultiproticÂHIV-1ÂProteaseâ^'LigandÂComplex. Journal of the American Chemical Society, 2004, 126, 11764-11765.	6.6	34
26	Serine racemase: a key player in neuron activity and in neuropathologies. Frontiers in Bioscience - Landmark, 2013, 18, 1112.	3.0	34
27	Getting it right: modeling of pH, solvent and â€œnearlyâ€•everything else in virtual screening of biological targets. Journal of Molecular Graphics and Modelling, 2004, 22, 479-486.	1.3	32
28	Different roles of protein dynamics and ligand migration in non-symbiotic hemoglobins AHb1 and AHb2 from Arabidopsis thaliana. Gene, 2007, 398, 224-233.	1.0	32
29	A novel Bim-BH3-derived Bcl-XL inhibitor: Biochemical characterization, in vitro, in vivo and ex-vivo anti-leukemic activity. Cell Cycle, 2008, 7, 3211-3224.	1.3	32
30	Geminate Rebinding in R-State Hemoglobin:Â Kinetic and Computational Evidence for Multiple Hydrophobic Pockets. Journal of the American Chemical Society, 2005, 127, 17427-17432.	6.6	29
31	From Experiments to a Fast Easy-to-Use Computational Methodology to Predict Human Aldehyde Oxidase Selectivity and Metabolic Reactions. Journal of Medicinal Chemistry, 2018, 61, 360-371.	2.9	29
32	CO Rebinding Kinetics and Molecular Dynamics Simulations Highlight Dynamic Regulation of Internal Cavities in Human Cytoglobin. PLoS ONE, 2013, 8, e49770.	1.1	28
33	Ligand Migration in Nonsymbiotic Hemoglobin AHb1 from Arabidopsis thaliana. Journal of Physical Chemistry B, 2007, 111, 12582-12590.	1.2	27
34	Decoding the Structural Basis For Carbapenem Hydrolysis By Class A Î²-lactamases: Fishing For A Pharmacophore. Current Drug Targets, 2016, 17, 983-1005.	1.0	27
35	Targeting Cystalysin, a Virulence Factor of Treponema denticolaâ€Supported Periodontitis. ChemMedChem, 2014, 9, 1501-1511.	1.6	26
36	Fluorescent Nitric Oxide Photodonors Based on BODIPY and Rhodamine Antennae. Chemistry - A European Journal, 2019, 25, 11080-11084.	1.7	26

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37	Label-free fiber optic optrode for the detection of class C Î²-lactamases expressed by drug resistant bacteria. Biomedical Optics Express, 2017, 8, 5191.	1.5	25
38	Virtual screening identifies broad-spectrum Î²-lactamase inhibitors with activity on clinically relevant serine- and metallo-carbapenemases. Scientific Reports, 2020, 10, 12763.	1.6	25
39	Theoretical Calculations of the Catalytic Triad in Short-Chain Alcohol Dehydrogenases/Reductases. Biophysical Journal, 2008, 94, 1412-1427.	0.2	24
40	The Inhibition of Extended Spectrum β-Lactamases: Hits and Leads. Current Medicinal Chemistry, 2014, 21, 1405-1434.	1.2	23
41	Allosteric communication between alpha and beta subunits of tryptophan synthase: Modelling the open-closed transition of the alpha subunit. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2006, 1764, 1102-1109.	1.1	22
42	Expanding the chemical space of human serine racemase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 4297-4303.	1.0	22
43	Comparing Drug Images and Repurposing Drugs with BioGPS and FLAPdock: The Thymidylate Synthase Case. ChemMedChem, 2016, 11, 1653-1666.	1.6	21
44	Interaction of human hemoglobin and semi-hemoglobins with the Staphylococcus aureus hemophore IsdB: a kinetic and mechanistic insight. Scientific Reports, 2019, 9, 18629.	1.6	21
45	Structural Plasticity and Functional Implications of Internal Cavities in Distal Mutants of Type 1 Non-Symbiotic Hemoglobin AHb1 fromArabidopsis thaliana. Journal of Physical Chemistry B, 2009, 113, 16028-16038.	1.2	20
46	Histidine E7 Dynamics Modulates Ligand Exchange between Distal Pocket and Solvent in AHb1 from Arabidopsis thaliana. Journal of Physical Chemistry B, 2011, 115, 4138-4146.	1.2	20
47	Comparative mapping of on-targets and off-targets for the discovery of anti-trypanosomatid folate pathway inhibitors. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 3215-3230.	1.1	20
48	Structureâ€“activity relationships of strigolactones via a novel, quantitative in planta bioassay. Journal of Experimental Botany, 2018, 69, 2333-2343.	2.4	20
49	Novel peptide-conjugated nanomedicines for brain targeting: In vivo evidence. Nanomedicine: Nanotechnology, Biology, and Medicine, 2020, 28, 102226.	1.7	20
50	Binding of Androgen- and Estrogen-Like Flavonoids to Their Cognate (Non)Nuclear Receptors: A Comparison by Computational Prediction. Molecules, 2021, 26, 1613.	1.7	20
51	Oxygen binding to Arabidopsis thaliana AHb2 nonsymbiotic hemoglobin: evidence for a role in oxygen transport. IUBMB Life, 2011, 63, 355-362.	1.5	19
52	Tools for building a comprehensive modeling system for virtual screening under real biological conditions: The Computational Titration algorithm. Journal of Molecular Graphics and Modelling, 2006, 24, 434-439.	1.3	18
53	Ligand migration through hemeprotein cavities: insights from laser flash photolysis and molecular dynamics simulations. Physical Chemistry Chemical Physics, 2013, 15, 10686.	1.3	18
54	Recent advances in the synthesis of analogues of phytohormones strigolactones with ring-closing metathesis as a key step. Organic and Biomolecular Chemistry, 2017, 15, 8218-8231.	1.5	18

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55	Strigolactones, from Plants to Human Health: Achievements and Challenges. Molecules, 2021, 26, 4579.	1.7	18
56	Oxygen and nitric oxide rebinding kinetics in nonsymbiotic hemoglobin AHb1 from Arabidopsis thaliana. IUBMB Life, 2011, 63, 1094-1100.	1.5	16
57	Inhibition of the transcriptional repressor LexA: Withstanding drug resistance by inhibiting the bacterial mechanisms of adaptation to antimicrobials. Life Sciences, 2020, 241, 117116.	2.0	16
58	How Computational Methods Try to Disclose the Estrogen Receptor Secrecy - Modeling the Flexibility. Current Medicinal Chemistry, 2009, 16, 2987-3027.	1.2	15
59	Ligand migration and hexacoordination in type 1 non-symbiotic rice hemoglobin. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2011, 1814, 1042-1053.	1.1	15
60	A generator of peroxynitrite activatable with red light. Chemical Science, 2021, 12, 4740-4746.	3.7	15
61	Structural analysis in nonsymbiotic hemoglobins: What can we learn from inner cavities?. Plant Science, 2011, 181, 8-13.	1.7	14
62	Unintended consequences? Water molecules at biological and crystallographic proteinâ€“protein interfaces. Computational Biology and Chemistry, 2013, 47, 126-141.	1.1	14
63	FADB: a food additive molecular database forin silicoscreening in food toxicology. Food Additives and Contaminants - Part A Chemistry, Analysis, Control, Exposure and Risk Assessment, 2014, 31, 792-798.	1.1	14
64	4-Amino-1,2,4-triazole-3-thione as a Promising Scaffold for the Inhibition of Serine and Metallo-Î²-Lactamases. Pharmaceuticals, 2020, 13, 52.	1.7	13
65	Folic Acidâ€“Peptide Conjugates Combine Selective Cancer Cell Internalization with Thymidylate Synthase Dimer Interface Targeting. Journal of Medicinal Chemistry, 2021, 64, 3204-3221.	2.9	13
66	Water: How to evaluate its contribution in protein-ligand interactions. International Journal of Quantum Chemistry, 2006, 106, 647-651.	1.0	12
67	Pyridoxal 5â€²-Phosphate-Dependent Enzymes: Catalysis, Conformation, and Genomics. , 2010, , 273-350.		12
68	Chemogenomics of pyridoxal 5â€²-phosphate dependent enzymes. Journal of Enzyme Inhibition and Medicinal Chemistry, 2013, 28, 183-194.	2.5	12
69	BioGPS: The Music for the Chemoâ€•and Bioinformatics Walzer. Molecular Informatics, 2014, 33, 446-453.	1.4	11
70	Complexity in Modeling and Understanding Protonation States: Computational Titration of HIVâ€1â€Proteaseâ€“Inhibitor Complexes. Chemistry and Biodiversity, 2007, 4, 2564-2577.	1.0	10
71	Structural insight into the interaction of Oâ€‹acetylserine sulfhydrylase with competitive, peptidic inhibitors by saturation transfer differenceâ€‹<scp>NMR</scp>. FEBS Letters, 2016, 590, 943-953.	1.3	10
72	Paracetamolâ€“Galactose Conjugate: A Novel Prodrug for an Old Analgesic Drug. Molecular Pharmaceutics, 2019, 16, 4181-4189.	2.3	10

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73	Discovering New Casein Kinase 1d Inhibitors with an Innovative Molecular Dynamics Enabled Virtual Screening Workflow. ACS Medicinal Chemistry Letters, 2019, 10, 487-492.	1.3	10
74	Chemical Modulation of the 1-(Piperidin-4-yl)-1,3-dihydro-2H-benzo[d]imidazole-2-one Scaffold as a Novel NLRP3 Inhibitor. Molecules, 2021, 26, 3975.	1.7	10
75	Tuning the Hydrophobicity of a Mitochondriaâ€Targeted NO Photodonor. ChemMedChem, 2018, 13, 1238-1245.	1.6	9
76	First virtual screening and experimental validation of inhibitors targeting GES-5 carbapenemase. Journal of Computer-Aided Molecular Design, 2019, 33, 295-305.	1.3	9
77	Strigolactone Analogs Are Promising Antiviral Agents for the Treatment of Human Cytomegalovirus Infection. Microorganisms, 2020, 8, 703.	1.6	9
78	Human dopamine transporter: the first implementation of a combined in silico/in vitro approach revealing the substrate and inhibitor specificities. Journal of Biomolecular Structure and Dynamics, 2019, 37, 291-306.	2.0	8
79	The allosteric interplay between Sâ€nitrosylation and glycine binding controls the activity of human serine racemase. FEBS Journal, 2021, 288, 3034-3054.	2.2	8
80	A new approach for investigating protein flexibility based on Constraint Logic Programming. The first application in the case of the estrogen receptor. European Journal of Medicinal Chemistry, 2012, 49, 127-140.	2.6	7
81	Rational Design of a User-Friendly Aptamer/Peptide-Based Device for the Detection of Staphylococcus aureus. Sensors, 2020, 20, 4977.	2.1	7
82	Correct Protonation States and Relevant Waters = Better Computational Simulations?. Current Pharmaceutical Design, 2013, 19, 4291-4309.	0.9	7
83	New aldo-keto reductase 1C3 (AKR1C3) inhibitors based on the hydroxytriazole scaffold. European Journal of Medicinal Chemistry, 2022, 237, 114366.	2.6	7
84	Comparative analysis of inner cavities and ligand migration in non-symbiotic AHb1 and AHb2. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2013, 1834, 1957-1967.	1.1	6
85	Can We Exploit Î²-Lactamases Intrinsic Dynamics for Designing More Effective Inhibitors?. Antibiotics, 2020, 9, 833.	1.5	6
86	A structural homologue of the plant receptor D14 mediates responses to strigolactones in the fungal phytopathogen Cryphonectria parasitica. New Phytologist, 2022, 234, 1003-1017.	3.5	6
87	Cryo-EM structures of staphylococcal IsdB bound to human hemoglobin reveal the process of heme extraction. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2116708119.	3.3	6
88	Modulating Ligand Dissociation through Methyl Isomerism in Accessory Sites: Binding of Retinol to Cellular Carriers. Journal of Physical Chemistry Letters, 2019, 10, 7333-7339.	2.1	5
89	NO release regulated by doxorubicin as the green light-harvesting antenna. Chemical Communications, 2020, 56, 6332-6335.	2.2	5
90	Evaluation of Porcine and Aspergillus oryzae Î±-Amylases as Possible Model for the Human Enzyme. Processes, 2022, 10, 780.	1.3	4

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91	Editorial [Hot topic: Applying Induced Fit in Drug Discovery: Square Pegs and Round Holes? (Guest) Tj ETQq1 1 0.784314 rgBT /Overlock Medicinal Chemistry, 2011, 11, 131-132.	1.0	2
92	Repurposing the Trypanosomatidic GSK Kinetobox for the Inhibition of Parasitic Pteridine and Dihydrofolate Reductases. Pharmaceuticals, 2021, 14, 1246.	1.7	2
93	Applying Computational Scoring Functions to Assess Biomolecular Interactions in Food Science: Applications to the Estrogen Receptors. Nuclear Receptor Research, 2016, 3, .	2.5	1
94	Understanding Water and Its Many Roles in Biological Structure: Ways to Exploit a Resource for Drug Discovery. Methods in Pharmacology and Toxicology, 2015, , 85-110.	0.1	0