

# Francesca Spyraakis

## 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	A structural homologue of the plant receptor D14 mediates responses to strigolactones in the fungal phytopathogen <i>Cryphonectria parasitica</i> . <i>New Phytologist</i> , 2022, 234, 1003-1017.	3.5	6
2	Cryo-EM structures of staphylococcal IsdB bound to human hemoglobin reveal the process of heme extraction. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, e2116708119.	3.3	6
3	Evaluation of Porcine and <i>Aspergillus oryzae</i> $\alpha$ -Amylases as Possible Model for the Human Enzyme. <i>Processes</i> , 2022, 10, 780.	1.3	4
4	New aldo-keto reductase 1C3 (AKR1C3) inhibitors based on the hydroxytriazole scaffold. <i>European Journal of Medicinal Chemistry</i> , 2022, 237, 114366.	2.6	7
5	The allosteric interplay between S-nitrosylation and glycine binding controls the activity of human serine racemase. <i>FEBS Journal</i> , 2021, 288, 3034-3054.	2.2	8
6	A generator of peroxyxynitrite activatable with red light. <i>Chemical Science</i> , 2021, 12, 4740-4746.	3.7	15
7	A Blueprint for High Affinity SARS-CoV-2 Mpro Inhibitors from Activity-Based Compound Library Screening Guided by Analysis of Protein Dynamics. <i>ACS Pharmacology and Translational Science</i> , 2021, 4, 1079-1095.	2.5	44
8	Binding of Androgen- and Estrogen-Like Flavonoids to Their Cognate (Non)Nuclear Receptors: A Comparison by Computational Prediction. <i>Molecules</i> , 2021, 26, 1613.	1.7	20
9	Folic Acid-peptide Conjugates Combine Selective Cancer Cell Internalization with Thymidylate Synthase Dimer Interface Targeting. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 3204-3221.	2.9	13
10	Chemical Modulation of the 1-(Piperidin-4-yl)-1,3-dihydro-2H-benzo[d]imidazole-2-one Scaffold as a Novel NLRP3 Inhibitor. <i>Molecules</i> , 2021, 26, 3975.	1.7	10
11	Strigolactones, from Plants to Human Health: Achievements and Challenges. <i>Molecules</i> , 2021, 26, 4579.	1.7	18
12	Repurposing the Trypanosomatidic GSK Kinetobox for the Inhibition of Parasitic Pteridine and Dihydrofolate Reductases. <i>Pharmaceuticals</i> , 2021, 14, 1246.	1.7	2
13	A novel small-molecule inhibitor of the human papillomavirus E6-p53 interaction that reactivates p53 function and blocks cancer cells growth. <i>Cancer Letters</i> , 2020, 470, 115-125.	3.2	39
14	Inhibition of the transcriptional repressor LexA: Withstanding drug resistance by inhibiting the bacterial mechanisms of adaptation to antimicrobials. <i>Life Sciences</i> , 2020, 241, 117116.	2.0	16
15	Can We Exploit $\beta$ -Lactamases Intrinsic Dynamics for Designing More Effective Inhibitors?. <i>Antibiotics</i> , 2020, 9, 833.	1.5	6
16	Virtual screening identifies broad-spectrum $\beta$ -lactamase inhibitors with activity on clinically relevant serine- and metallo-carbapenemases. <i>Scientific Reports</i> , 2020, 10, 12763.	1.6	25
17	Rational Design of a User-Friendly Aptamer/Peptide-Based Device for the Detection of <i>Staphylococcus aureus</i> . <i>Sensors</i> , 2020, 20, 4977.	2.1	7
18	NO release regulated by doxorubicin as the green light-harvesting antenna. <i>Chemical Communications</i> , 2020, 56, 6332-6335.	2.2	5

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19	Novel peptide-conjugated nanomedicines for brain targeting: In vivo evidence. <i>Nanomedicine: Nanotechnology, Biology, and Medicine</i> , 2020, 28, 102226.	1.7	20
20	Strigolactone Analogs Are Promising Antiviral Agents for the Treatment of Human Cytomegalovirus Infection. <i>Microorganisms</i> , 2020, 8, 703.	1.6	9
21	Iron Metabolism at the Interface between Host and Pathogen: From Nutritional Immunity to Antibacterial Development. <i>International Journal of Molecular Sciences</i> , 2020, 21, 2145.	1.8	42
22	4-Amino-1,2,4-triazole-3-thione as a Promising Scaffold for the Inhibition of Serine and Metallo- $\beta$ -Lactamases. <i>Pharmaceutics</i> , 2020, 13, 52.	1.7	13
23	Modulating Ligand Dissociation through Methyl Isomerism in Accessory Sites: Binding of Retinol to Cellular Carriers. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 7333-7339.	2.1	5
24	Paracetamol-Galactose Conjugate: A Novel Prodrug for an Old Analgesic Drug. <i>Molecular Pharmaceutics</i> , 2019, 16, 4181-4189.	2.3	10
25	Fluorescent Nitric Oxide Photodors Based on BODIPY and Rhodamine Antennae. <i>Chemistry - A European Journal</i> , 2019, 25, 11080-11084.	1.7	26
26	Interaction of human hemoglobin and semi-hemoglobins with the Staphylococcus aureus hemophore IsdB: a kinetic and mechanistic insight. <i>Scientific Reports</i> , 2019, 9, 18629.	1.6	21
27	First virtual screening and experimental validation of inhibitors targeting GES-5 carbapenemase. <i>Journal of Computer-Aided Molecular Design</i> , 2019, 33, 295-305.	1.3	9
28	Ten Years with New Delhi Metallo- $\beta$ -lactamase-1 (NDM-1): From Structural Insights to Inhibitor Design. <i>ACS Infectious Diseases</i> , 2019, 5, 9-34.	1.8	123
29	Discovering New Casein Kinase 1d Inhibitors with an Innovative Molecular Dynamics Enabled Virtual Screening Workflow. <i>ACS Medicinal Chemistry Letters</i> , 2019, 10, 487-492.	1.3	10
30	Human dopamine transporter: the first implementation of a combined in silico/in vitro approach revealing the substrate and inhibitor specificities. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 291-306.	2.0	8
31	Tuning the Hydrophobicity of a Mitochondria-Targeted NO Photodonor. <i>ChemMedChem</i> , 2018, 13, 1238-1245.	1.6	9
32	Structure-activity relationships of strigolactones via a novel, quantitative in planta bioassay. <i>Journal of Experimental Botany</i> , 2018, 69, 2333-2343.	2.4	20
33	Structure-Based Virtual Screening for the Discovery of Novel Inhibitors of New Delhi Metallo- $\beta$ -lactamase-1. <i>ACS Medicinal Chemistry Letters</i> , 2018, 9, 45-50.	1.3	38
34	From Experiments to a Fast Easy-to-Use Computational Methodology to Predict Human Aldehyde Oxidase Selectivity and Metabolic Reactions. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 360-371.	2.9	29
35	The Roles of Water in the Protein Matrix: A Largely Untapped Resource for Drug Discovery. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 6781-6827.	2.9	111
36	Recent advances in the synthesis of analogues of phytohormones strigolactones with ring-closing metathesis as a key step. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 8218-8231.	1.5	18

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37	Comparative mapping of on-targets and off-targets for the discovery of anti-trypanosomatid folate pathway inhibitors. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2017, 1861, 3215-3230.	1.1	20
38	Computational and biological profile of boronic acids for the detection of bacterial serine- and metallo- $\beta$ -lactamases. <i>Scientific Reports</i> , 2017, 7, 17716.	1.6	35
39	Label-free fiber optic optrode for the detection of class C $\beta$ -lactamases expressed by drug resistant bacteria. <i>Biomedical Optics Express</i> , 2017, 8, 5191.	1.5	25
40	Structural insight into the interaction of <i>O</i> -acetylserine sulfhydrylase with competitive, peptidic inhibitors by saturation transfer difference NMR. <i>FEBS Letters</i> , 2016, 590, 943-953.	1.3	10
41	Comparing Drug Images and Repurposing Drugs with BioGPS and FLAPdock: The Thymidylate Synthase Case. <i>ChemMedChem</i> , 2016, 11, 1653-1666.	1.6	21
42	Decoding the Structural Basis For Carbapenem Hydrolysis By Class A $\beta$ -lactamases: Fishing For A Pharmacophore. <i>Current Drug Targets</i> , 2016, 17, 983-1005.	1.0	27
43	Applying Computational Scoring Functions to Assess Biomolecular Interactions in Food Science: Applications to the Estrogen Receptors. <i>Nuclear Receptor Research</i> , 2016, 3, .	2.5	1
44	Understanding Water and Its Many Roles in Biological Structure: Ways to Exploit a Resource for Drug Discovery. <i>Methods in Pharmacology and Toxicology</i> , 2015, , 85-110.	0.1	0
45	Open challenges in structure-based virtual screening: Receptor modeling, target flexibility consideration and active site water molecules description. <i>Archives of Biochemistry and Biophysics</i> , 2015, 583, 105-119.	1.4	101
46	A Pipeline To Enhance Ligand Virtual Screening: Integrating Molecular Dynamics and Fingerprints for Ligand and Proteins. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 2256-2274.	2.5	65
47	Expanding the chemical space of human serine racemase inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2015, 25, 4297-4303.	1.0	22
48	FADB: a food additive molecular database for <i>in silico</i> screening in food toxicology. <i>Food Additives and Contaminants - Part A Chemistry, Analysis, Control, Exposure and Risk Assessment</i> , 2014, 31, 792-798.	1.1	14
49	BioGPS: The Music for the Chemo- and Bioinformatics Walzer. <i>Molecular Informatics</i> , 2014, 33, 446-453.	1.4	11
50	Targeting Cystalyisin, a Virulence Factor of <i>Treponema denticola</i> Supported Periodontitis. <i>ChemMedChem</i> , 2014, 9, 1501-1511.	1.6	26
51	The Inhibition of Extended Spectrum $\beta$ -Lactamases: Hits and Leads. <i>Current Medicinal Chemistry</i> , 2014, 21, 1405-1434.	1.2	23
52	Unintended consequences? Water molecules at biological and crystallographic protein-protein interfaces. <i>Computational Biology and Chemistry</i> , 2013, 47, 126-141.	1.1	14
53	Ligand migration through hemeprotein cavities: insights from laser flash photolysis and molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 10686.	1.3	18
54	Fine tuning of the active site modulates specificity in the interaction of <i>O</i> -acetylserine sulfhydrylase isozymes with serine acetyltransferase. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2013, 1834, 169-181.	1.1	35

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55	Comparative analysis of inner cavities and ligand migration in non-symbiotic AHb1 and AHb2. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2013, 1834, 1957-1967.	1.1	6
56	Chemogenomics of pyridoxal 5â€²-phosphate dependent enzymes. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2013, 28, 183-194.	2.5	12
57	Serine racemase: a key player in neuron activity and in neuropathologies. <i>Frontiers in Bioscience - Landmark</i> , 2013, 18, 1112.	3.0	34
58	CO Rebinding Kinetics and Molecular Dynamics Simulations Highlight Dynamic Regulation of Internal Cavities in Human Cytoglobin. <i>PLoS ONE</i> , 2013, 8, e49770.	1.1	28
59	Isozyme-Specific Ligands for O-acetylserine sulfhydrylase, a Novel Antibiotic Target. <i>PLoS ONE</i> , 2013, 8, e77558.	1.1	43
60	Correct Protonation States and Relevant Waters = Better Computational Simulations?. <i>Current Pharmaceutical Design</i> , 2013, 19, 4291-4309.	0.9	7
61	A new approach for investigating protein flexibility based on Constraint Logic Programming. The first application in the case of the estrogen receptor. <i>European Journal of Medicinal Chemistry</i> , 2012, 49, 127-140.	2.6	7
62	Histidine E7 Dynamics Modulates Ligand Exchange between Distal Pocket and Solvent in AHb1 from <i>Arabidopsis thaliana</i> . <i>Journal of Physical Chemistry B</i> , 2011, 115, 4138-4146.	1.2	20
63	The multifaceted pyridoxal 5â€²-phosphate-dependent O-acetylserine sulfhydrylase. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2011, 1814, 1497-1510.	1.1	39
64	Structural analysis in nonsymbiotic hemoglobins: What can we learn from inner cavities?. <i>Plant Science</i> , 2011, 181, 8-13.	1.7	14
65	Editorial [Hot topic: Applying Induced Fit in Drug Discovery: Square Pegs and Round Holes? (Guest) Tj ETQq1 1 0.784314 rgBT /Overlo <i>Medicinal Chemistry</i> , 2011, 11, 131-132.	1.0	2
66	Oxygen binding to <i>Arabidopsis thaliana</i> AHb2 nonsymbiotic hemoglobin: evidence for a role in oxygen transport. <i>IUBMB Life</i> , 2011, 63, 355-362.	1.5	19
67	Oxygen and nitric oxide rebinding kinetics in nonsymbiotic hemoglobin AHb1 from <i>Arabidopsis thaliana</i> . <i>IUBMB Life</i> , 2011, 63, 1094-1100.	1.5	16
68	Ligand migration and hexacoordination in type 1 non-symbiotic rice hemoglobin. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2011, 1814, 1042-1053.	1.1	15
69	Protein Flexibility and Ligand Recognition: Challenges for Molecular Modeling. <i>Current Topics in Medicinal Chemistry</i> , 2011, 11, 192-210.	1.0	86
70	Bound Water at Protein-Protein Interfaces: Partners, Roles and Hydrophobic Bubbles as a Conserved Motif. <i>PLoS ONE</i> , 2011, 6, e24712.	1.1	57
71	Pyridoxal 5â€²-Phosphate-Dependent Enzymes: Catalysis, Conformation, and Genomics. , 2010, , 273-350.		12
72	Design of <i>O</i> -Acetylserine Sulfhydrylase Inhibitors by Mimicking Nature. <i>Journal of Medicinal Chemistry</i> , 2010, 53, 345-356.	2.9	75

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73	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
74	Structural Plasticity and Functional Implications of Internal Cavities in Distal Mutants of Type 1 Non-Symbiotic Hemoglobin AHb1 from <i>Arabidopsis thaliana</i> . Journal of Physical Chemistry B, 2009, 113, 16028-16038.	1.2	20
75	How Computational Methods Try to Disclose the Estrogen Receptor Secrecy - Modeling the Flexibility. Current Medicinal Chemistry, 2009, 16, 2987-3027.	1.2	15
76	Energy-based prediction of amino acid-nucleotide base recognition. Journal of Computational Chemistry, 2008, 29, 1955-1969.	1.5	44
77	Theoretical Calculations of the Catalytic Triad in Short-Chain Alcohol Dehydrogenases/Reductases. Biophysical Journal, 2008, 94, 1412-1427.	0.2	24
78	Target Flexibility: An Emerging Consideration in Drug Discovery and Design. Journal of Medicinal Chemistry, 2008, 51, 6237-6255.	2.9	280
79	Robust Classification of "Relevant" Water Molecules in Putative Protein Binding Sites. Journal of Medicinal Chemistry, 2008, 51, 1063-1067.	2.9	93
80	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
81	Different roles of protein dynamics and ligand migration in non-symbiotic hemoglobins AHb1 and AHb2 from <i>Arabidopsis thaliana</i> . Gene, 2007, 398, 224-233.	1.0	32
82	The Reactivity with CO of AHb1 and AHb2 from <i>Arabidopsis thaliana</i> is Controlled by the Distal HisE7 and Internal Hydrophobic Cavities. Journal of the American Chemical Society, 2007, 129, 2880-2889.	6.6	54
83	Ligand Migration in Nonsymbiotic Hemoglobin AHb1 from <i>Arabidopsis thaliana</i> . Journal of Physical Chemistry B, 2007, 111, 12582-12590.	1.2	27
84	Complexity in Modeling and Understanding Protonation States: Computational Titration of HIV-1 Protease Inhibitor Complexes. Chemistry and Biodiversity, 2007, 4, 2564-2577.	1.0	10
85	The consequences of scoring docked ligand conformations using free energy correlations. European Journal of Medicinal Chemistry, 2007, 42, 921-933.	2.6	58
86	Energetics of the protein-DNA-water interaction. BMC Structural Biology, 2007, 7, 4.	2.3	57
87	Mapping the Energetics of Water-Protein and Water-Ligand Interactions with the "Natural" HINT Forcefield: Predictive Tools for Characterizing the Roles of Water in Biomolecules. Journal of Molecular Biology, 2006, 358, 289-309.	2.0	85
88	Water: How to evaluate its contribution in protein-ligand interactions. International Journal of Quantum Chemistry, 2006, 106, 647-651.	1.0	12
89	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
90	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

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91	Geminate Rebinding in R-State Hemoglobin: Kinetic and Computational Evidence for Multiple Hydrophobic Pockets. <i>Journal of the American Chemical Society</i> , 2005, 127, 17427-17432.	6.6	29
92	Getting it right: modeling of pH, solvent and <i>“nearly”</i> everything else in virtual screening of biological targets. <i>Journal of Molecular Graphics and Modelling</i> , 2004, 22, 479-486.	1.3	32
93	Computational Titration Analysis of Multiprotic HIV-1 Protease Ligand Complex. <i>Journal of the American Chemical Society</i> , 2004, 126, 11764-11765.	6.6	34
94	Simple, Intuitive Calculations of Free Energy of Binding for Protein-Ligand Complexes. 3. The Free Energy Contribution of Structural Water Molecules in HIV-1 Protease Complexes. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 4507-4516.	2.9	112