Andrew Hung

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8889647/publications.pdf

Version: 2024-02-01

103	2,560	186209	223716
papers	citations	28 h-index	46 g-index

103	103	103	2924
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular modeling of lactoferrin for food and nutraceutical applications: insights from in silico techniques. Critical Reviews in Food Science and Nutrition, 2023, 63, 9074-9097.	5.4	2
2	Binding parameters and molecular dynamics of Î²-lactoglobulin-vanillic acid complexation as a function of pH - part B: Neutral pH. Food Chemistry, 2022, 367, 130655.	4.2	11
3	Small molecule interactions with the SARS-CoV-2 main protease: In silico all-atom microsecond MD simulations, PELE Monte Carlo simulations, and determination of in vitro activity inhibition. Journal of Molecular Graphics and Modelling, 2022, 110, 108050.	1.3	5
4	Investigation of small molecule inhibitors of the SARS-CoV-2 papain-like protease by all-atom microsecond modelling, PELE Monte Carlo simulations, and in vitro activity inhibition. Chemical Physics Letters, 2022, 788, 139294.	1.2	10
5	Alpha-lipoic acid analogues in the regulation of redox balance in epilepsy: A molecular docking and simulation study. Journal of Molecular Graphics and Modelling, 2022, 112, 108116.	1.3	5
6	The Effects and Safety of Chinese Herbal Medicine on Blood Lipid Profiles in Placebo-Controlled Weight-Loss Trials: A Systematic Review and Meta-Analysis. Evidence-based Complementary and Alternative Medicine, 2022, 2022, 1-13.	0.5	2
7	Enhancing proline-rich antimicrobial peptide action by homodimerization: influence of bifunctional linker. Chemical Science, 2022, 13, 2226-2237.	3.7	28
8	Systematic comparison of activity and mechanism of antimicrobial peptides against nosocomial pathogens. European Journal of Medicinal Chemistry, 2022, 231, 114135.	2.6	26
9	Identification of novel bioactive compounds from Olea europaea by evaluation of chemical compounds in the OliveNetâ„¢ library: in silico bioactivity and molecular modelling, and in vitro validation of hERG activity. Computers in Biology and Medicine, 2022, 142, 105247.	3.9	5
10	Mechanisms of Action of a Herbal Formula Huangqi Guizhi Wuwu Tang for the Management of Post-Stroke Related Numbness and Weakness: A Computational Molecular Docking Study. Journal of Evidence-based Integrative Medicine, 2022, 27, 2515690X2210829.	1.4	3
11	The SARS-CoV-2 helicase as a target for antiviral therapy: Identification of potential small molecule inhibitors by in silico modelling. Journal of Molecular Graphics and Modelling, 2022, 114, 108193.	1.3	8
12	Interaction of compounds derived from the Chinese medicinal formula Huangqi Guizhi Wuwu Tang with stroke-related numbness and weakness targets: An in-silico docking and molecular dynamics study. Computers in Biology and Medicine, 2022, 146, 105568.	3.9	3
13	How does traditional knowledge of Cassiae semen shed light on weight management? â€“ A classical and modern literature review. Journal of Ethnopharmacology, 2021, 268, 113572.	2.0	12
14	The circadian machinery links metabolic disorders and depression: A review of pathways, proteins and potential pharmacological interventions. Life Sciences, 2021, 265, 118809.	2.0	11
15	Structural and dynamical effects of targeted mutations on Î¼O-Conotoxin MfVIA: Molecular simulation studies. Journal of Molecular Graphics and Modelling, 2021, 102, 107777.	1.3	3
16	Dimeric phosphorylation of glyoxalase I alters its symmetry and substrate binding mechanism: simulation studies. Journal of Biomolecular Structure and Dynamics, 2021, , 1-15.	2.0	0
17	Phytochemistry, pharmacodynamics, and pharmacokinetics of a classic Chinese herbal formula Danggui Beimu Kushen Wan: A review. Phytotherapy Research, 2021, 35, 3673-3689.	2.8	3
18	Herb-target virtual screening and network pharmacology for prediction of molecular mechanism of Danggui Beimu Kushen Wan for prostate cancer. Scientific Reports, 2021, 11, 6656.	1.6	18

#	Article	IF	Citations
19	Inhibition of interferon-stimulated gene 15 and lysine 48-linked ubiquitin binding to the SARS-CoV-2 papain-like protease by small molecules: In silico studies. Chemical Physics Letters, 2021, 771, 138468.	1.2	8
20	High-temperature binding parameters and molecular dynamics of 4-hydroxybenzoic acid and Î²-casein complexes, determined via the method of continuous variation and fluorescence spectroscopy. Food Hydrocolloids, 2021, 114, 106567.	5.6	14
21	Interaction of small molecules with the SARS-CoV-2 papain-like protease: In silico studies and inÂvitro validation of protease activity inhibition using an enzymatic inhibition assay. Journal of Molecular Graphics and Modelling, 2021, 104, 107851.	1.3	29
22	Hydrophobins and chaplins: Novel bio-surfactants for food dispersions a review. Trends in Food Science and Technology, 2021, 111, 378-387.	7.8	11
23	In silico investigation of potential small molecule inhibitors of the SARS-CoV-2 nsp10-nsp16 methyltransferase complex. Chemical Physics Letters, 2021, 774, 138618.	1.2	9
24	Biophysical analysis of an HCN1 epilepsy variant suggests a critical role for S5 helix Met-305 in voltage sensor to pore domain coupling. Progress in Biophysics and Molecular Biology, 2021, 166, 156-172.	1.4	16
25	In silico modelling of apo-lactoferrin under simulated gastric conditions: Structural dynamics, binding with Î²-lactoglobulin and Î±-lactalbumin, and functional implications. LWT - Food Science and Technology, 2021, 148, 111726.	2.5	4
26	In silico investigation to identify potential small molecule inhibitors of the RNA-dependent RNA polymerase (RdRp) nidovirus RdRp-associated nucleotidyltransferase domain. Chemical Physics Letters, 2021, 779, 138889.	1.2	4
27	Binding parameters and molecular dynamics of Î²-lactoglobulin-vanillic acid complexation as a function of pH â€“ Part A: Acidic pH. Food Chemistry, 2021, 360, 130059.	4.2	18
28	Computational design of de novo nutraceuticals: Effects of spray drying temperatures on the interaction between apo-lactoferrin whey protein complex and the peptidoglycan layer in lactic acid bacteria. LWT - Food Science and Technology, 2021, 151, 112246.	2.5	3
29	Effects of low temperatures on the conformation of apo-lactoferrin and its interactions with Î±-lactalbumin and Î²-lactoglobulin: Application of in silico approaches. Food Hydrocolloids, 2021, 121, 107055.	5.6	6
30	In silico investigation of DNA minor groove binding bibenzimidazoles in the context of UVA phototherapy. Physical Chemistry Chemical Physics, 2021, 24, 112-121.	1.3	0
31	The cellular and molecular basis of major depressive disorder: towards a unified model for understanding clinical depression. Molecular Biology Reports, 2020, 47, 753-770.	1.0	98
32	Combined spectroscopic and molecular docking study on the pH dependence of molecular interactions between Î²-lactoglobulin and ferulic acid. Food Hydrocolloids, 2020, 101, 105461.	5.6	56
33	Site mapping and small molecule blind docking reveal a possible target site on the SARS-CoV-2 main protease dimer interface. Computational Biology and Chemistry, 2020, 89, 107372.	1.1	30
34	In silico characterisation of olive phenolic compounds as potential cyclooxygenase modulators. Part 1. Journal of Molecular Graphics and Modelling, 2020, 101, 107719.	1.3	3
35	Interactions of the Î±3Î²2 Nicotinic Acetylcholine Receptor Interfaces with Î±-Conotoxin LsIA and its Carboxylated C-terminus Analogue: Molecular Dynamics Simulations. Marine Drugs, 2020, 18, 349.	2.2	4
36	Interaction of small molecules with the SARS-CoV-2 main protease in silico and in vitro validation of potential lead compounds using an enzyme-linked immunosorbent assay. Computational Biology and Chemistry, 2020, 89, 107408.	1.1	52

#	Article	IF	Citations
37	In silico characterisation of olive phenolic compounds as potential cyclooxygenase modulators. Part 2. Journal of Molecular Graphics and Modelling, 2020, 101, 107743.	1.3	1
38	Identification of Small Molecule Inhibitors of the Deubiquitinating Activity of the SARS-CoV-2 Papain-Like Protease: in silico Molecular Docking Studies and in vitro Enzymatic Activity Assay. Frontiers in Chemistry, 2020, 8, 623971.	1.8	45
39	Interaction of the prototypical Î±-ketoamide inhibitor with the SARS-CoV-2 main protease active site in silico: Molecular dynamic simulations highlight the stability of the ligand-protein complex. Computational Biology and Chemistry, 2020, 87, 107292.	1.1	64
40	Utilisation of the OliveNetâ„¢ Library to investigate phenolic compounds using molecular modelling studies in the context of Alzheimerâ€™s disease. Computational Biology and Chemistry, 2020, 87, 107271.	1.1	4
41	Investigation of potential anti-pneumococcal effects of l-sulforaphane and metabolites: Insights from synchrotron-FTIR microspectroscopy and molecular docking studies. Journal of Molecular Graphics and Modelling, 2020, 97, 107568.	1.3	4
42	High temperature induced structural changes of apo-lactoferrin and interactions with Î²-lactoglobulin and Î±-lactalbumin for potential encapsulation strategies. Food Hydrocolloids, 2020, 105, 105817.	5.6	15
43	Chromatin modification by olive phenolics: In silico molecular docking studies utilising the phenolic groups categorised in the OliveNetâ„¢ database against lysine specific demethylase enzymes. Journal of Molecular Graphics and Modelling, 2020, 97, 107575.	1.3	3
44	Molecular docking utilising the OliveNetâ„¢ library reveals novel phenolic compounds which may potentially target key proteins associated with major depressive disorder. Computational Biology and Chemistry, 2020, 86, 107234.	1.1	2
45	Inhibitory effect of a weight-loss Chinese herbal formula RCM-107 on pancreatic Î±-amylase activity: Enzymatic and in silico approaches. PLoS ONE, 2020, 15, e0231815.	1.1	9
46	The Effects of a Weight-Loss Herbal Formula RCM-107 and Its Eight Individual Ingredients on Glucagon-Like Peptide-1 Secretionâ€”An In Vitro and In Silico Study. International Journal of Molecular Sciences, 2020, 21, 2854.	1.8	7
47	Screening for a Potential Therapeutic Agent from the Herbal Formula in the 4th Edition of the Chinese National Guidelines for the Initial-Stage Management of COVID-19 via Molecular Docking. Evidence-based Complementary and Alternative Medicine, 2020, 2020, 1-17.	0.5	15
48	Mechanisms of Action of Cassiae Semen for Weight Management: A Computational Molecular Docking Study of Serotonin Receptor 5-HT2C. International Journal of Molecular Sciences, 2020, 21, 1326.	1.8	9
49	A Classic Herbal Formula Guizhi Fuling Wan for Menopausal Hot Flushes: From Experimental Findings to Clinical Applications. Biomedicines, 2019, 7, 60.	1.4	10
50	Herbal formula (Danggui Beimu Kushen Wan) for prostate disorders: a systematic review of classical literature. Integrative Medicine Research, 2019, 8, 240-246.	0.7	8
51	Guizhi Fuling Wan for uterine fibroids: A systematic review of in vivo studies. Journal of Ethnopharmacology, 2019, 245, 112177.	2.0	6
52	Chinese herbal formulae for the treatment of menopausal hot flushes: A systematic review and meta-analysis. PLoS ONE, 2019, 14, e0222383.	1.1	8
53	The inhibitory effects of an eight-herb formula (RCM-107) on pancreatic lipase: enzymatic, HPTLC profiling and in silico approaches. Heliyon, 2019, 5, e02453.	1.4	11
54	Structural effects of divalent calcium cations on the Î±7 nicotinic acetylcholine receptor: A molecular dynamics simulation study. Proteins: Structure, Function and Bioinformatics, 2019, 87, 992-1005.	1.5	3

#	Article	IF	Citations
55	Effects of C-Terminal Carboxylation on Î±-Conotoxin LsIA Interactions with Human Î±7 Nicotinic Acetylcholine Receptor: Molecular Simulation Studies. Marine Drugs, 2019, 17, 206.	2.2	8
56	Fritillariae Thunbergii Bulbus: Traditional Uses, Phytochemistry, Pharmacodynamics, Pharmacokinetics and Toxicity. International Journal of Molecular Sciences, 2019, 20, 1667.	1.8	40
57	Temperature-induced structural changes of apo-lactoferrin and their functional implications: a molecular dynamics simulation study. Molecular Simulation, 2019, 45, 533-548.	0.9	6
58	Combined spectroscopic, molecular docking and quantum mechanics study of Î²-casein and ferulic acid interactions following UHT-like treatment. Food Hydrocolloids, 2019, 89, 351-359.	5.6	50
59	pH-induced structural changes of apo-lactoferrin and implications for its function: a molecular dynamics simulation study. Molecular Simulation, 2019, 45, 87-103.	0.9	6
60	Do the Natural Chemical Compounds Interact with the Same Targets of Current Pharmacotherapy for Weight Management?-A Review. Current Drug Targets, 2019, 20, 399-411.	1.0	12
61	Combined spectroscopic, molecular docking and quantum mechanics study of Î²-casein and p-coumaric acid interactions following thermal treatment. Food Chemistry, 2018, 252, 163-170.	4.2	60
62	A Classic Herbal Formula Danggui Beimu Kushen Wan for Chronic Prostatitis: From Traditional Knowledge to Scientific Exploration. Evidence-based Complementary and Alternative Medicine, 2018, 2018, 1-11.	0.5	9
63	OliveNetâ„¢: a comprehensive library of compounds fromOlea europaea. Database: the Journal of Biological Databases and Curation, 2018, 2018, .	1.4	70
64	The pH-dependent assembly of Chaplin E from Streptomyces coelicolor. Journal of Structural Biology, 2017, 198, 82-91.	1.3	8
65	pH-Induced interfacial properties of Chaplin E from Streptomyces coelicolor. Colloids and Surfaces B: Biointerfaces, 2017, 160, 589-597.	2.5	1
66	Modelling the interactions between animal venom peptides and membrane proteins. Neuropharmacology, 2017, 127, 20-31.	2.0	14
67	Structure-Dependent Interfacial Properties of Chaplin F from Streptomyces coelicolor. Biomolecules, 2017, 7, 68.	1.8	1
68	Molecular simulation study of the unbinding of Î±-conotoxin [Ï'4E]GID at the Î±7 and Î±4Î²2 neuronal nicotinic acetylcholine receptors. Journal of Molecular Graphics and Modelling, 2016, 70, 109-121.	1.3	18
69	Effects of interfaces on aggregates of peptides derived from pancreatic islet amyloid polypeptide. Molecular Simulation, 2016, 42, 580-595.	0.9	1
70	Alanine Scan of Î±-Conotoxin RegIIA Reveals a Selective Î±3Î²4 Nicotinic Acetylcholine Receptor Antagonist. Journal of Biological Chemistry, 2015, 290, 1039-1048.	1.6	38
71	Molecular Basis for Differential Sensitivity of Î±-Conotoxin RegIIA at Rat and Human Neuronal Nicotinic Acetylcholine Receptors. Molecular Pharmacology, 2015, 88, 993-1001.	1.0	19
72	The Implication of Cancer Progenitor Cells and the Role of Epigenetics in the Development of Novel Therapeutic Strategies for Chronic Myeloid Leukemia. Antioxidants and Redox Signaling, 2015, 22, 1425-1462.	2.5	9

#	Article	IF	Citations
73	Dicarba Analogues of Î±-Conotoxin RgIA. Structure, Stability, and Activity at Potential Pain Targets. Journal of Medicinal Chemistry, 2014, 57, 9933-9944.	2.9	56
74	Dicarba Î±-Conotoxin Vc1.1 Analogues with Differential Selectivity for Nicotinic Acetylcholine and GABA_B Receptors. ACS Chemical Biology, 2013, 8, 1815-1821.	1.6	64
75	Amphiphilic amino acids: a key to adsorbing proteins to nanopatterned surfaces?. Chemical Science, 2013, 4, 928-937.	3.7	48
76	Identifying Key Amino Acid Residues That Affect Î±-Conotoxin AuIB Inhibition of Î±3Î²4 Nicotinic Acetylcholine Receptors. Journal of Biological Chemistry, 2013, 288, 34428-34442.	1.6	43
77	"Janus" Cyclic Peptides: A New Approach to Amyloid Fibril Inhibition?. PLoS ONE, 2013, 8, e57437.	1.1	13
78	Use of a Short Peptide as a Building Block in the Layer-by-Layer Assembly of Biomolecules on Polymeric Surfaces. Journal of Physical Chemistry B, 2012, 116, 1120-1133.	1.2	13
79	A Cyclic Peptide Inhibitor of ApoC-II Peptide Fibril Formation: Mechanistic Insight from NMR and Molecular Dynamics Analysis. Journal of Molecular Biology, 2012, 416, 642-655.	2.0	16
80	Analysis of Fasciola cathepsin L5 by S2 subsite substitutions and determination of the P1â€“P4 specificity reveals an unusual preference. Biochimie, 2012, 94, 1119-1127.	1.3	16
81	Investigation of a predicted N-terminal amphipathic Î±-helix using atomistic molecular dynamics simulation of a complete prototype poliovirus virion. Journal of Molecular Graphics and Modelling, 2012, 38, 165-173.	1.3	18
82	Ordering Surfaces on the Nanoscale: Implications for Protein Adsorption. Journal of the American Chemical Society, 2011, 133, 1438-1450.	6.6	151
83	A Structural Model for Apolipoprotein C-II Amyloid Fibrils: Experimental Characterization and Molecular Dynamics Simulations. Journal of Molecular Biology, 2011, 405, 1246-1266.	2.0	45
84	Gap Junction Hemichannel Interactions with Zwitterionic Lipid, Anionic Lipid, and Cholesterol: Molecular Simulation Studies. Biochemistry, 2011, 50, 1492-1504.	1.2	22
85	Inhibition of peptide aggregation by lipids: Insights from coarse-grained molecular simulations. Journal of Molecular Graphics and Modelling, 2011, 29, 597-607.	1.3	18
86	Solidâ€state NMR and simulation studies of equinatoxin II Nâ€terminus interaction with lipid bilayers. Proteins: Structure, Function and Bioinformatics, 2010, 78, 858-872.	1.5	17
87	Effects of mutation on the amyloidogenic propensity of apolipoprotein C-II60â€“70 peptide. Physical Chemistry Chemical Physics, 2010, 12, 14762.	1.3	15
88	Lipid Concentration Effects on the Amyloidogenic apoC-II60â^'70 Peptide: A Computational Study. Journal of Physical Chemistry B, 2010, 114, 7974-7982.	1.2	11
89	Lipids Enhance Apolipoprotein C-II-Derived Amyloidogenic Peptide Oligomerization but Inhibit Fibril Formation. Journal of Physical Chemistry B, 2009, 113, 9447-9453.	1.2	17
90	Effects of oxidation, pH and lipids on amyloidogenic peptide structure: implications for fibril formation?. European Biophysics Journal, 2008, 38, 99-110.	1.2	30

#	Article	IF	Citations
91	Molecular Dynamics Simulation of the M2 Helices within the Nicotinic Acetylcholine Receptor Transmembrane Domain: Structure and Collective Motions. Biophysical Journal, 2005, 88, 3321-3333.	0.2	43
92	Exploring the Electronic and Mechanical Properties of Protein Using Conducting Atomic Force Microscopy. Journal of the American Chemical Society, 2004, 126, 5601-5609.	6.6	120
93	Density-functional theory of xanthate adsorption on the pyrite FeS2(100) surface. Philosophical Magazine Letters, 2004, 84, 175-182.	0.5	19
94	An ab initio study of structural properties and single vacancy defects in Wurtzite AlN. Journal of Chemical Physics, 2004, 120, 4890-4896.	1.2	31
95	Sulfur adsorption on Fe(110): a DFT study. Surface Science, 2003, 540, 420-430.	0.8	42
96	Density-functional theory studies of xanthate adsorption on the pyrite FeS2(110) and (111) surfaces. Journal of Chemical Physics, 2003, 118, 6022-6029.	1.2	42
97	Iron Surfaces: Pathways to Interfaces. Surface Review and Letters, 2003, 10, 169-174.	0.5	9
98	First-principles studies of the structural and electronic properties of pyriteFeS2. Physical Review B, 2002, 65, .	1.1	64
99	First-principles study of metallic iron interfaces. Surface Science, 2002, 501, 261-269.	0.8	64
100	Density functional theory study of the relaxation and energy of iron surfaces. Surface Science, 2002, 513, 389-398.	0.8	154
101	Density-functional theory studies of pyrite FeS2() and () surfaces. Surface Science, 2002, 513, 511-524.	0.8	144
102	Further studies of iron adhesion: () surfaces. Surface Science, 2002, 515, L464-L468.	0.8	19
103	Density-functional theory studies of pyrite FeS2 () and () surfaces. Surface Science, 2002, 520, 111-119.	0.8	82