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	186265	223800
papers	citations	28 h-index	46 g-index

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

#	Article	IF	Citations
1	Density functional theory study of the relaxation and energy of iron surfaces. Surface Science, 2002, 513, 389-398.	1.9	154
2	Ordering Surfaces on the Nanoscale: Implications for Protein Adsorption. Journal of the American Chemical Society, 2011, 133, 1438-1450.	13.7	151
3	Density-functional theory studies of pyrite FeS2() and () surfaces. Surface Science, 2002, 513, 511-524.	1.9	144
4	Exploring the Electronic and Mechanical Properties of Protein Using Conducting Atomic Force Microscopy. Journal of the American Chemical Society, 2004, 126, 5601-5609.	13.7	120
5	The cellular and molecular basis of major depressive disorder: towards a unified model for understanding clinical depression. Molecular Biology Reports, 2020, 47, 753-770.	2.3	98
6	Density-functional theory studies of pyrite FeS2 () and () surfaces. Surface Science, 2002, 520, 111-119.	1.9	82
7	OliveNetâ„¢: a comprehensive library of compounds fromOlea europaea. Database: the Journal of Biological Databases and Curation, 2018, 2018, .	3.0	70
8	First-principles studies of the structural and electronic properties of pyriteFeS2. Physical Review B, 2002, 65, .	3.2	64
9	First-principles study of metallic iron interfaces. Surface Science, 2002, 501, 261-269.	1.9	64
10	Dicarba Î±-Conotoxin Vc1.1 Analogues with Differential Selectivity for Nicotinic Acetylcholine and GABA_B Receptors. ACS Chemical Biology, 2013, 8, 1815-1821.	3.4	64
11	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.	2.3	64
12	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.	8.2	60
13	Dicarba Analogues of Î±-Conotoxin RgIA. Structure, Stability, and Activity at Potential Pain Targets. Journal of Medicinal Chemistry, 2014, 57, 9933-9944.	6.4	56
14	Combined spectroscopic and molecular docking study on the pH dependence of molecular interactions between Î²-lactoglobulin and ferulic acid. Food Hydrocolloids, 2020, 101, 105461.	10.7	56
15	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.	2.3	52
16	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.	10.7	50
17	Amphiphilic amino acids: a key to adsorbing proteins to nanopatterned surfaces?. Chemical Science, 2013, 4, 928-937.	7.4	48
18	A Structural Model for Apolipoprotein C-II Amyloid Fibrils: Experimental Characterization and Molecular Dynamics Simulations. Journal of Molecular Biology, 2011, 405, 1246-1266.	4.2	45

#	Article	IF	Citations
19	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.	3.6	45
20	Molecular Dynamics Simulation of the M2 Helices within the Nicotinic Acetylcholine Receptor Transmembrane Domain: Structure and Collective Motions. Biophysical Journal, 2005, 88, 3321-3333.	0.5	43
21	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.	3.4	43
22	Sulfur adsorption on Fe(110): a DFT study. Surface Science, 2003, 540, 420-430.	1.9	42
23	Density-functional theory studies of xanthate adsorption on the pyrite FeS2(110) and (111) surfaces. Journal of Chemical Physics, 2003, 118, 6022-6029.	3.0	42
24	Fritillariae Thunbergii Bulbus: Traditional Uses, Phytochemistry, Pharmacodynamics, Pharmacokinetics and Toxicity. International Journal of Molecular Sciences, 2019, 20, 1667.	4.1	40
25	Alanine Scan of Î±-Conotoxin RegIIA Reveals a Selective Î±3Î²4 Nicotinic Acetylcholine Receptor Antagonist. Journal of Biological Chemistry, 2015, 290, 1039-1048.	3.4	38
26	An ab initio study of structural properties and single vacancy defects in Wurtzite AlN. Journal of Chemical Physics, 2004, 120, 4890-4896.	3.0	31
27	Effects of oxidation, pH and lipids on amyloidogenic peptide structure: implications for fibril formation?. European Biophysics Journal, 2008, 38, 99-110.	2.2	30
28	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.	2.3	30
29	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.	2.4	29
30	Enhancing proline-rich antimicrobial peptide action by homodimerization: influence of bifunctional linker. Chemical Science, 2022, 13, 2226-2237.	7.4	28
31	Systematic comparison of activity and mechanism of antimicrobial peptides against nosocomial pathogens. European Journal of Medicinal Chemistry, 2022, 231, 114135.	5.5	26
32	Gap Junction Hemichannel Interactions with Zwitterionic Lipid, Anionic Lipid, and Cholesterol: Molecular Simulation Studies. Biochemistry, 2011, 50, 1492-1504.	2.5	22
33	Further studies of iron adhesion: () surfaces. Surface Science, 2002, 515, L464-L468.	1.9	19
34	Density-functional theory of xanthate adsorption on the pyrite FeS2(100) surface. Philosophical Magazine Letters, 2004, 84, 175-182.	1.2	19
35	Molecular Basis for Differential Sensitivity of Î±-Conotoxin RegIIA at Rat and Human Neuronal Nicotinic Acetylcholine Receptors. Molecular Pharmacology, 2015, 88, 993-1001.	2.3	19
36	Inhibition of peptide aggregation by lipids: Insights from coarse-grained molecular simulations. Journal of Molecular Graphics and Modelling, 2011, 29, 597-607.	2.4	18

#	Article	IF	Citations
37	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.	2.4	18
38	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.	2.4	18
39	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.	3.3	18
40	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.	8.2	18
41	Lipids Enhance Apolipoprotein C-II-Derived Amyloidogenic Peptide Oligomerization but Inhibit Fibril Formation. Journal of Physical Chemistry B, 2009, 113, 9447-9453.	2.6	17
42	Solidâ€state NMR and simulation studies of equinatoxin II Nâ€terminus interaction with lipid bilayers. Proteins: Structure, Function and Bioinformatics, 2010, 78, 858-872.	2.6	17
43	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.	4.2	16
44	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.	2.6	16
45	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.	2.9	16
46	Effects of mutation on the amyloidogenic propensity of apolipoprotein C-II60â€“70 peptide. Physical Chemistry Chemical Physics, 2010, 12, 14762.	2.8	15
47	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.	10.7	15
48	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.	1.2	15
49	Modelling the interactions between animal venom peptides and membrane proteins. Neuropharmacology, 2017, 127, 20-31.	4.1	14
50	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.	10.7	14
51	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.	2.6	13
52	"Janus" Cyclic Peptides: A New Approach to Amyloid Fibril Inhibition?. PLoS ONE, 2013, 8, e57437.	2.5	13
53	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.	4.1	12
54	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.	2.1	12

#	Article	IF	Citations
55	Lipid Concentration Effects on the Amyloidogenic apoC-II60â^'70 Peptide: A Computational Study. Journal of Physical Chemistry B, 2010, 114, 7974-7982.	2.6	11
56	The inhibitory effects of an eight-herb formula (RCM-107) on pancreatic lipase: enzymatic, HPTLC profiling and in silico approaches. Heliyon, 2019, 5, e02453.	3.2	11
57	The circadian machinery links metabolic disorders and depression: A review of pathways, proteins and potential pharmacological interventions. Life Sciences, 2021, 265, 118809.	4.3	11
58	Hydrophobins and chaplins: Novel bio-surfactants for food dispersions a review. Trends in Food Science and Technology, 2021, 111, 378-387.	15.1	11
59	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.	8.2	11
60	A Classic Herbal Formula Guizhi Fuling Wan for Menopausal Hot Flushes: From Experimental Findings to Clinical Applications. Biomedicines, 2019, 7, 60.	3.2	10
61	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.	2.6	10
62	Iron Surfaces: Pathways to Interfaces. Surface Review and Letters, 2003, 10, 169-174.	1.1	9
63	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.	5.4	9
64	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.	1.2	9
65	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.	2.5	9
66	In silico investigation of potential small molecule inhibitors of the SARS-CoV-2 nsp10-nsp16 methyltransferase complex. Chemical Physics Letters, 2021, 774, 138618.	2.6	9
67	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.	4.1	9
68	The pH-dependent assembly of Chaplin E from Streptomyces coelicolor. Journal of Structural Biology, 2017, 198, 82-91.	2.8	8
69	Herbal formula (Danggui Beimu Kushen Wan) for prostate disorders: a systematic review of classical literature. Integrative Medicine Research, 2019, 8, 240-246.	1.8	8
70	Chinese herbal formulae for the treatment of menopausal hot flushes: A systematic review and meta-analysis. PLoS ONE, 2019, 14, e0222383.	2.5	8
71	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.	4.6	8
72	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.	2.6	8

#	Article	IF	Citations
73	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.	2.4	8
74	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.	4.1	7
75	Guizhi Fuling Wan for uterine fibroids: A systematic review of in vivo studies. Journal of Ethnopharmacology, 2019, 245, 112177.	4.1	6
76	Temperature-induced structural changes of apo-lactoferrin and their functional implications: a molecular dynamics simulation study. Molecular Simulation, 2019, 45, 533-548.	2.0	6
77	pH-induced structural changes of apo-lactoferrin and implications for its function: a molecular dynamics simulation study. Molecular Simulation, 2019, 45, 87-103.	2.0	6
78	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.	10.7	6
79	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.	2.4	5
80	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.	2.4	5
81	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.	7.0	5
82	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.	4.6	4
83	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.	2.3	4
84	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.	2.4	4
85	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.	5.2	4
86	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.	2.6	4
87	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.	2.6	3
88	In silico characterisation of olive phenolic compounds as potential cyclooxygenase modulators. Part 1. Journal of Molecular Graphics and Modelling, 2020, 101, 107719.	2.4	3
89	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.	2.4	3
90	Structural and dynamical effects of targeted mutations on Î¼O-Conotoxin MfVIA: Molecular simulation studies. Journal of Molecular Graphics and Modelling, 2021, 102, 107777.	2.4	3

#	Article	IF	Citations
91	Phytochemistry, pharmacodynamics, and pharmacokinetics of a classic Chinese herbal formula Danggui Beimu Kushen Wan: A review. Phytotherapy Research, 2021, 35, 3673-3689.	5.8	3
92	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.	5.2	3
93	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.	2.6	3
94	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.	7.0	3
95	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.	2.3	2
96	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.	1.2	2
97	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.	10.3	2
98	Effects of interfaces on aggregates of peptides derived from pancreatic islet amyloid polypeptide. Molecular Simulation, 2016, 42, 580-595.	2.0	1
99	pH-Induced interfacial properties of Chaplin E from Streptomyces coelicolor. Colloids and Surfaces B: Biointerfaces, 2017, 160, 589-597.	5.0	1
100	Structure-Dependent Interfacial Properties of Chaplin F from Streptomyces coelicolor. Biomolecules, 2017, 7, 68.	4.0	1
101	In silico characterisation of olive phenolic compounds as potential cyclooxygenase modulators. Part 2. Journal of Molecular Graphics and Modelling, 2020, 101, 107743.	2.4	1
102	Dimeric phosphorylation of glyoxalase I alters its symmetry and substrate binding mechanism: simulation studies. Journal of Biomolecular Structure and Dynamics, 2021, , 1-15.	3.5	0
103	In silico investigation of DNA minor groove binding bibenzimidazoles in the context of UVA phototherapy. Physical Chemistry Chemical Physics, 2021, 24, 112-121.	2.8	0