Nguyen Thi Ai Nhung

List of Publications by Year
in descending order

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54	742	759233	552781
papers	citations	12 h-index	26 g-index

56	56	56	1058
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A Computational Screening on Inhibitability ofPiper BetleEssential Oil Chemical Structures against Spike Proteins of Mutated SARS-CoV-2-variants D614G, N501Y, and S477N. Smart Science, 2022, 10, 246-263.	3.2	3
2	New insights into the competition between antioxidant activities and pro-oxidant risks of rosmarinic acid. RSC Advances, 2022, 12, 1499-1514.	3.6	11
3	Structural characteristics and chemical reactivity of gold-based clusters Aun (nâ€‰=â€‰16, 17) toward lone pairs. Journal of Molecular Modeling, 2022, 28, 54.	1.8	2
4	A DFT study of the molecular and electronic structures of cis-dioxidomolybdenum (VI) complex of 8-hydroxyquinoline and 4-benzoyl-3-methyl-1-phenyl-2-pyrazolin-5-one with water. Theoretical Chemistry Accounts, 2022, 141, 1.	1.4	1
5	Antimicrobial Properties of Distichochlamys citrea M.F. Newman Rhizome n â€Hexane Extract againstÂ Streptococcus pyogenes : Experimental Evidences and Computational Screening. ChemistrySelect, 2022, 7, .	1.5	2
6	Antioxidant activity and Î±-glucosidase inhibitability of Distichochlamys citrea M.F. Newman rhizome fractionated extracts: in vitro and in silico screenings. Chemical Papers, 2022, 76, 5655-5675.	2.2	5
7	New triterpene sulfates from Vietnamese red alga Tricleocarpa fragilis and their Î±-glucosidase inhibitory activity. Journal of Asian Natural Products Research, 2021, 23, 754-763.	1.4	4
8	Screening for Streptococcus pyogenes antibacterial and Candida albicans antifungal bioactivities of organic compounds in natural essential oils of Piper betle L., Cleistocalyx operculatus L. and Ageratum conyzoides L.. Chemical Papers, 2021, 75, 1507-1519.	2.2	7
9	A molecular docking simulation study on potent inhibitors against Rhizoctonia solani and Magnaporthe oryzae in rice: silver-tetrylene and bis-silver-tetrylene complexes vs. validamycin and tricyclazole pesticides. Structural Chemistry, 2021, 32, 135-148.	2.0	10
10	Isolation, semi-synthesis, docking-based prediction, and bioassay-based activity of Dolichandrone spathacea iridoids: new catalpol derivatives as glucosidase inhibitors. RSC Advances, 2021, 11, 11959-11975.	3.6	21
11	Gold nanoclusters as prospective carriers and detectors of pramipexole. RSC Advances, 2021, 11, 16619-16632.	3.6	20
12	On the Inhibitability of Natural Products Isolated from Tetradium ruticarpum towards Tyrosine Phosphatase 1B (PTP1B) and Î±-Glucosidase (3W37): An In Vitro and In Silico Study. Molecules, 2021, 26, 3691.	3.8	5
13	Styracifoline from the Vietnamese Plant Desmodium styracifolium: A Potential Inhibitor of Diabetes-Related and Thrombosis-Based Proteins. ACS Omega, 2021, 6, 23211-23221.	3.5	5
14	Antioxidant and UV-radiation absorption activity of aaptamine derivatives â€“ potential application for natural organic sunscreens. RSC Advances, 2021, 11, 21433-21446.	3.6	6
15	Theoretical Aspects of Nonconventional Hydrogen Bonds in the Complexes of Aldehydes and Hydrogen Chalcogenides. Journal of Physical Chemistry A, 2021, 125, 10291-10302.	2.5	2
16	Newly synthesised oxime and lactone derivatives from Dipterocarpus alatus dipterocarpol as anti-diabetic inhibitors: experimental bioassay-based evidence and theoretical computation-based prediction. RSC Advances, 2021, 11, 35765-35782.	3.6	11
17	In Silico Inhibitability of Copper Carbenes and Silylenes against Rhizoctonia solani and Magnaporthe oryzae. Journal of Chemistry, 2021, 2021, 1-14.	1.9	1
18	Coumarin-Based Dual Chemosensor for Colorimetric and Fluorescent Detection of Cu²⁺ in Water Media. ACS Omega, 2020, 5, 21241-21249.	3.5	47

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19	Coordination complexes of slight tetrylene with platinum(II)-8-hydroxyquinolines: Structure and bonding analysis. Vietnam Journal of Chemistry, 2020, 58, 364-371.	0.8	0
20	A density functional theory study on silver and bis-silver complexes with lighter tetrylene: are silver and bis-silver carbenes candidates for SARS-CoV-2 inhibition? Insight from molecular docking simulation. RSC Advances, 2020, 10, 30961-30974.	3.6	18
21	Evaluation of the Inhibitory Activities of COVIDâ€19 of Melaleuca cajuputi Oil Using Docking Simulation. ChemistrySelect, 2020, 5, 6312-6320.	1.5	33
22	Growth Pattern, Stability, and Properties of Complexes of C₂H₅OH and nCO₂ (n = 1â€“5) Molecules: A Theoretical Study. ACS Omega, 2020, 5, 14408-14416.	3.5	2
23	Iron ions chelation-based antioxidant potential vs. pro-oxidant risk of ferulic acid: A DFT study in aqueous phase. Computational and Theoretical Chemistry, 2020, 1185, 112905.	2.5	26
24	Insight prediction of receptor binding activity of a set of benzamide derivatives using hybrid QSAR models: GA-MLR and GA-SVR. Vietnam Journal of Chemistry, 2020, 58, 191-200.	0.8	0
25	Calculation of thermodynamic properties of vaporâ€“liquid equilibria using ab initio intermolecular potential energy surfaces for dimer O₂â€“O₂. Molecular Physics, 2020, 118, .	1.7	3
26	Diagram of vapor-liquid equilibria for n -pentane using hybrid Gibbs ensemble Monte Carlo simulation. Vietnam Journal of Chemistry, 2020, 58, 101-107.	0.8	0
27	Investigation into SARS-CoV-2 Resistance of Compounds in Garlic Essential Oil. ACS Omega, 2020, 5, 8312-8320.	3.5	213
28	In-Depth Investigation of a Donorâ€“Acceptor Interaction on the Heavy-Group-14@Group-13-Diyls in Transition-Metal Tetrylone Complexes: Structure, Bonding, and Property. ACS Omega, 2020, 5, 21271-21287.	3.5	11
29	A theoretical study of structure, bonding and property of platinum(II)-8-hydroxyquinolines complexes with carbene and heavier homologues. Hue University Journal of Science: Natural Science, 2020, 129, 41-48.	0.1	0
30	Novel QSPR modeling of stability constants of metal-thiosemicarbazone complexes by hybrid multivariate technique: GA-MLR, GA-SVR and GA-ANN. Journal of Molecular Structure, 2019, 1195, 95-109.	3.6	16
31	Theoretical assessment of donorâ€“acceptor complexes [X(PPh3)2â€‰â†’â€‰AlH2]+ (Xâ€‰=â€‰Câ€“Pb): structures and bonding. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	1
32	Theoretical exploitation of donor-acceptor ability in low-valent group-14 elements complexes [E(PPh3) Tj ETQq0 0 0 rgBT /Overlock 10 T 418-424.	0.8	0
33	Roles of H2 O to hydrogen bonds, structure and strength of complexes of CH3 CHS and H2 O. Vietnam Journal of Chemistry, 2019, 57, 425-432.	0.8	2
34	An insight QSPR-based prediction model for stability constants of metal-thiosemicarbazone complexes using MLR and ANN methods. Vietnam Journal of Chemistry, 2019, 57, 500-506.	0.8	3
35	Theoretically predicted divalent silicon(0) compounds: Structures and chemical bonding of silylone in molybdenum pentacarbonyl complexes [Mo(CO)5-Si(XCpâ^—)2] (Xâ€¯=â€¯Bâ€“Tl). Computational and Theoretical Chemistry, 2018, 1131, 13-24.	2.5	5
36	Structure and property of complexes of group 13 diyl containing subvalent silylone using energy decomposition analysis with natural orbitals for chemical valence. Vietnam Journal of Chemistry, 2018, 56, 742-750.	0.8	1

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37	Bonding Situation of Bis-gold Chloride Complexes with N-heterocyclic Carbene-Analogues [(AuCl)₂-NHE_{Me}] (E=C â€“ Pb) based on DFT Calculations. Zeitschrift Fur Physikalische Chemie, 2017, 231, 1467-1487.	2.8	5
38	Can Tetrylone Act in a Similar Fashion to Tetrylene in Ni(CO)₂ Complexes? A Theoretical Study based on a Comparison using DFT Calculations. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2017, 643, 826-838.	1.2	5
39	A Benzothiazolium-derived Colorimetric and Fluorescent Chemosensor for Detection of Hg²⁺ Ions. Chemistry Letters, 2017, 46, 135-138.	1.3	8
40	A quantum chemical computation insight into the donor-acceptor bond interaction of silver complexes with tetrylene. Vietnam Journal of Chemistry, 2017, 55, .	0.8	0
41	Structures and Bonding Situation of Iron Complexes of Groupâ€13 Halfâ€Sandwich ECp* (E =) Tj ETQq1 1 0.784314 rgBT 609-617.	1.2	4
42	A hemicyanine complex for the detection of thiol biomolecules by fluorescence. Dyes and Pigments, 2016, 131, 301-306.	3.7	14
43	A Comparison of Donor-acceptor Interactions in Borane Complexes of Divalent Tetrylenes(II) and Divalent Tetrylones(0) using Energy Decomposition Analysis Method with Natural Orbital for Chemical Valence Theory. Smart Science, 2016, 4, 28-37.	3.2	1
44	Prediction of anticancer activities of cynaroside and quercetin in leaf of plants Cynara scolymus L and Artocarpus incisa L using structureâ€“activity relationship. Cogent Chemistry, 2016, 2, 1212452.	2.5	6
45	An insight into C_{sp}â€“Hâ‹¯Ï€ hydrogen bonds and stability of complexes formed by acetylene and its substituted derivatives with benzene and borazine. RSC Advances, 2016, 6, 106662-106670.	3.6	8
46	Density function theory study of water gas shift reaction on 2Cu/ZnO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:mo		