

Fidele Ntie-Kang

List of Publications by Year in descending order

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Version: 2024-02-01

96
papers

2,465
citations

218677

26
h-index

223800

46
g-index

112
all docs

112
docs citations

112
times ranked

3014
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular mechanics approaches for rational drug design: forcefields and solvation models. <i>ChemistrySelect</i> , 2023, 8, 457-477.	1.5	2
2	A chemoinformatic analysis of atoms, scaffolds and functional groups in natural products. <i>ChemistrySelect</i> , 2023, 8, 1341-1365.	1.5	1
3	Structural characterization of cassava linamarase-linamarin enzyme complex: an integrated computational approach. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 9270-9278.	3.5	2
4	A Molecular Investigation of the Solvent Influence on Inter- and Intra-Molecular Hydrogen Bond Interaction of Linamarin. <i>Processes</i> , 2022, 10, 352.	2.8	2
5	Fragment-based virtual screening discovers potential new Plasmodium P14KIII ² ligands. <i>BMC Chemistry</i> , 2022, 16, 19.	3.8	3
6	Finding alternatives to 5-fluorouracil: application of ensemble-based virtual screening for drug repositioning against human thymidylate synthase. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, , 1-17.	3.5	3
7	StreptomeDB 3.0: an updated compendium of streptomycetes natural products. <i>Nucleic Acids Research</i> , 2021, 49, D600-D604.	14.5	58
8	Natural products in <i>Cyperus rotundus</i> L. (Cyperaceae): an update of the chemistry and pharmacological activities. <i>RSC Advances</i> , 2021, 11, 15060-15077.	3.6	15
9	Editorial to Special Issue "Structure-Activity Relationships (SAR) of Natural Products". <i>Molecules</i> , 2021, 26, 250.	3.8	2
10	Editorial: Natural Product Epigenetic Modulators and Inhibitors. <i>Frontiers in Pharmacology</i> , 2021, 12, 651395.	3.5	2
11	The use of minimal topological differences to inspire the design of novel tetrahydroisoquinoline analogues with antimalarial activity. <i>Heliyon</i> , 2021, 7, e07032.	3.2	0
12	Rational engineering of specialized metabolites in bacteria and fungi. <i>ChemistrySelect</i> , 2021, 6, 9-26.	1.5	1
13	Editorial: Advanced chemoinformatics applications at the service of natural product discovery. <i>ChemistrySelect</i> , 2021, 6, 217-219.	1.5	0
14	Phytochemical and Ethnopharmacological Perspectives of <i>Ehretia laevis</i> . <i>Molecules</i> , 2021, 26, 3489.	3.8	9
15	Chemical similarity methods for analyzing secondary metabolite structures. <i>ChemistrySelect</i> , 2021, 6, 247-264.	1.5	1
16	A computational multi-targeting approach for drug repositioning for psoriasis treatment. <i>BMC Complementary Medicine and Therapies</i> , 2021, 21, 193.	2.7	7
17	Natural Products as Potential Lead Compounds for Drug Discovery Against SARS-CoV-2. <i>Natural Products and Bioprospecting</i> , 2021, 11, 611-628.	4.3	15
18	Computational Applications in Secondary Metabolite Discovery (CAiSMD): an online workshop. <i>Journal of Cheminformatics</i> , 2021, 13, 64.	6.1	3

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19	Structure-based virtual screening and molecular dynamics simulation studies to discover new SARS-CoV-2 main protease inhibitors. <i>Scientific African</i> , 2021, 14, e00970.	1.5	3
20	In search of therapeutic candidates for HIV/AIDS: rational approaches, design strategies, structure-activity relationship and mechanistic insights. <i>RSC Advances</i> , 2021, 11, 17936-17964.	3.6	9
21	Alkaloids with Anti-Onchocercal Activity from <i>Voacanga africana</i> Stapf (Apocynaceae): Identification and Molecular Modeling. <i>Molecules</i> , 2021, 26, 70.	3.8	8
22	Computer-Aided Design of Peptidomimetic Inhibitors of Falcipain-3: QSAR and Pharmacophore Models. <i>Scientia Pharmaceutica</i> , 2021, 89, 44.	2.0	1
23	Anti-psoriatic and immunomodulatory evaluation of <i>psorospermum febrifugum</i> spach and its phytochemicals. <i>Scientific African</i> , 2020, 7, e00229.	1.5	7
24	Natural Products Impacting DNA Methyltransferases and Histone Deacetylases. <i>Frontiers in Pharmacology</i> , 2020, 11, 992.	3.5	28
25	Natural Products as Modulators of Sirtuins. <i>Molecules</i> , 2020, 25, 3287.	3.8	34
26	Pharmacoinformatic Investigation of Medicinal Plants from East Africa. <i>Molecular Informatics</i> , 2020, 39, e2000163.	2.5	28
27	The potential of anti-malarial compounds derived from African medicinal plants: a review of pharmacological evaluations from 2013 to 2019. <i>Malaria Journal</i> , 2020, 19, 183.	2.3	42
28	Structure-Activity-Relationship and Mechanistic Insights for Anti-HIV Natural Products. <i>Molecules</i> , 2020, 25, 2070.	3.8	34
29	Novel Histone Deacetylase Inhibitors and HIV-1 Latency-Reversing Agents Identified by Large-Scale Virtual Screening. <i>Frontiers in Pharmacology</i> , 2020, 11, 905.	3.5	22
30	Antioxidant potential of flavonoid glycosides from <i>Manniophyton fulvum</i> Mill. (Euphorbiaceae): Identification and molecular modeling. <i>Scientific African</i> , 2020, 8, e00423.	1.5	7
31	10. A primer on natural product-based virtual screening. , 2020, , 251-290.		0
32	Virtual Screening Identifies Chebulagic Acid as an Inhibitor of the M2(S31N) Viral Ion Channel and Influenza A Virus. <i>Molecules</i> , 2020, 25, 2903.	3.8	11
33	Case studies on computer-based identification of natural products as lead molecules. <i>ChemistrySelect</i> , 2020, 5, .	1.5	1
34	An enumeration of natural products from microbial, marine and terrestrial sources. <i>Physical Sciences Reviews</i> , 2020, 5, .	0.8	13
35	A computer-based approach for developing linamarase inhibitory agents. <i>ChemistrySelect</i> , 2020, 5, .	1.5	3
36	An overview of tools, software, and methods for natural product fragment and mass spectral analysis. <i>Physical Sciences Reviews</i> , 2019, 4, .	0.8	1

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37	â€œDrug-likenessâ€•properties of natural compounds. <i>Physical Sciences Reviews</i> , 2019, 4, .	0.8	5
38	Fragment-based drug design of nature-inspired compounds. <i>Physical Sciences Reviews</i> , 2019, 4, .	0.8	3
39	Mechanistic role of plant-based bitter principles and bitterness prediction for natural product studies II: prediction tools and case studies. <i>Physical Sciences Reviews</i> , 2019, 4, .	0.8	4
40	A primer on natural product-based virtual screening. <i>Physical Sciences Reviews</i> , 2019, 4, .	0.8	7
41	Mechanistic role of plant-based bitter principles and bitterness prediction for natural product studies I: Database and methods. <i>Physical Sciences Reviews</i> , 2019, 4, .	0.8	2
42	Epigenetic modification, co-culture and genomic methods for natural product discovery. <i>Physical Sciences Reviews</i> , 2019, 4, .	0.8	10
43	Synthesis, Urease Inhibition and Molecular Modelling Studies of Novel Derivatives of the Naturally Occurring Î²-Amyrenone. <i>Natural Products and Bioprospecting</i> , 2019, 9, 49-59.	4.3	1
44	Fundamental physical and chemical concepts behind â€œdrug-likenessâ€•and â€œnatural product-likenessâ€•. <i>Physical Sciences Reviews</i> , 2019, 4, .	0.8	8
45	In silico toxicity profiling of natural product compound libraries from African flora with anti-malarial and anti-HIV properties. <i>Computational Biology and Chemistry</i> , 2018, 72, 136-149.	2.3	20
46	Antitumour, acute toxicity and molecular modeling studies of 4-(pyridin-4-yl)-6-(thiophen-2-yl)pyrimidin-2(1H)-one against Ehrlich ascites carcinoma and sarcoma-180. <i>Heliyon</i> , 2018, 4, e00661.	3.2	10
47	Natural product-derived compounds in HIV suppression, remission, and eradication strategies. <i>Antiviral Research</i> , 2018, 158, 63-77.	4.1	29
48	Identification of Bichalcones as Sirtuin Inhibitors by Virtual Screening and In Vitro Testing. <i>Molecules</i> , 2018, 23, 416.	3.8	20
49	Structurally simple synthetic 1, 4-disubstituted piperidines with high selectivity for resistant <i>Plasmodium falciparum</i> . <i>BMC Pharmacology & Toxicology</i> , 2018, 19, 42.	2.4	7
50	Compounds from African Medicinal Plants with Activities Against Selected Parasitic Diseases: Schistosomiasis, Trypanosomiasis and Leishmaniasis. <i>Natural Products and Bioprospecting</i> , 2018, 8, 151-169.	4.3	34
51	Targeting Cysteine Proteases from <i>Plasmodium falciparum</i> : A General Overview, Rational Drug Design and Computational Approaches for Drug Discovery. <i>Current Drug Targets</i> , 2018, 19, 501-526.	2.1	25
52	Binding of anti-Trypanosoma natural products from African flora against selected drug targets: a docking study. <i>Medicinal Chemistry Research</i> , 2017, 26, 562-579.	2.4	29
53	Antiparasitic Sesquiterpenes from the Cameroonian Spice <i>Scleria striatinux</i> and Preliminary In Vitro and In Silico DMPK Assessment. <i>Natural Products and Bioprospecting</i> , 2017, 7, 235-247.	4.3	3
54	NANPDB: A Resource for Natural Products from Northern African Sources. <i>Journal of Natural Products</i> , 2017, 80, 2067-2076.	3.0	103

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55	The value of pyrans as anticancer scaffolds in medicinal chemistry. <i>RSC Advances</i> , 2017, 7, 36977-36999.	3.6	157
56	Application of Computer Modeling to Drug Discovery: Case Study of PRK1 Kinase Inhibitors as Potential Drugs in Prostate Cancer Treatment. , 2017, , .		0
57	Pharmacophore modeling and in silico toxicity assessment of potential anticancer agents from African medicinal plants. <i>Drug Design, Development and Therapy</i> , 2016, Volume 10, 2137-2154.	4.3	25
58	4-arylpiperidines and 4-(\pm -hydroxyphenyl)piperidines as selective sigma-1 receptor ligands: synthesis, preliminary pharmacological evaluation and computational studies. <i>Chemistry Central Journal</i> , 2016, 10, 53.	2.6	2
59	11th German Conference on Chemoinformatics (GCC 2015). <i>Journal of Cheminformatics</i> , 2016, 8, 18.	6.1	1
60	The Chemistry and Biological Activities of Natural Products from Northern African Plant Families: From Taccaceae to Zygophyllaceae. <i>Natural Products and Bioprospecting</i> , 2016, 6, 63-96.	4.3	16
61	Screening of the Pan-African Natural Product Library Identifies Ixoratannin A-2 and Boldine as Novel HIV-1 Inhibitors. <i>PLoS ONE</i> , 2015, 10, e0121099.	2.5	38
62	Exploring Cancer Therapeutics with Natural Products from African Medicinal Plants, Part II: Alkaloids, Terpenoids and Flavonoids. <i>Anti-Cancer Agents in Medicinal Chemistry</i> , 2015, 16, 108-127.	1.7	43
63	The chemistry and biological activities of natural products from Northern African plant families: from Ebenaceae to Solanaceae. <i>RSC Advances</i> , 2015, 5, 26580-26595.	3.6	8
64	Virtually Designed Triclosan-Based Inhibitors of Enoyl Acyl Carrier Protein Reductase of <i>Mycobacterium tuberculosis</i> and of <i>Plasmodium falciparum</i> . <i>Molecular Informatics</i> , 2015, 34, 292-307.	2.5	8
65	Protease-inhibiting, molecular modeling and antimicrobial activities of extracts and constituents from <i>Helichrysum foetidum</i> and <i>Helichrysum mechowianum</i> (compositae). <i>Chemistry Central Journal</i> , 2015, 9, 32.	2.6	9
66	The chemistry and bioactivity of Southern African flora II: flavonoids, quinones and minor compound classes. <i>RSC Advances</i> , 2015, 5, 57704-57720.	3.6	9
67	The chemistry and bioactivity of Southern African flora I: a bioactivity versus ethnobotanical survey of alkaloid and terpenoid classes. <i>RSC Advances</i> , 2015, 5, 43242-43267.	3.6	5
68	Anti-Trypanosomal Activity of Nigerian Plants and Their Constituents. <i>Molecules</i> , 2015, 20, 7750-7771.	3.8	44
69	Molecular modeling of plant metabolites with anti-Onchocerca activity. <i>Medicinal Chemistry Research</i> , 2015, 24, 2127-2141.	2.4	2
70	Exploring Cancer Therapeutics with Natural Products from African Medicinal Plants, Part I: Xanthenes, Quinones, Steroids, Coumarins, Phenolics and other Classes of Compounds. <i>Anti-Cancer Agents in Medicinal Chemistry</i> , 2015, 15, 1092-1111.	1.7	18
71	Virtualizing the p-ANAPL Library: A Step towards Drug Discovery from African Medicinal Plants. <i>PLoS ONE</i> , 2014, 9, e90655.	2.5	51
72	The potential of anti-malarial compounds derived from African medicinal plants, part III: an in silico evaluation of drug metabolism and pharmacokinetics profiling. <i>Organic and Medicinal Chemistry Letters</i> , 2014, 4, 6.	2.0	39

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73	Control of malaria and other vector-borne protozoan diseases in the tropics: enduring challenges despite considerable progress and achievements. <i>Infectious Diseases of Poverty</i> , 2014, 3, 1.	3.7	88
74	A Bioactivity Versus Ethnobotanical Survey of Medicinal Plants from Nigeria, West Africa. <i>Natural Products and Bioprospecting</i> , 2014, 4, 1-19.	4.3	54
75	How "drug-like" are naturally occurring anti-cancer compounds?. <i>Journal of Molecular Modeling</i> , 2014, 20, 2069.	1.8	13
76	Binding of pyrazole-based inhibitors to Mycobacterium tuberculosis pantothenate synthetase: docking and MM-GB(PB)SA analysis. <i>Molecular BioSystems</i> , 2014, 10, 223-239.	2.9	30
77	The chemistry and biological activities of natural products from Northern African plant families: from Aloaceae to Cupressaceae. <i>RSC Advances</i> , 2014, 4, 61975-61991.	3.6	12
78	1-Aryl-1,2,3,4-tetrahydroisoquinolines as potential antimalarials: synthesis, in vitro antiplasmodial activity and in silico pharmacokinetics evaluation. <i>RSC Advances</i> , 2014, 4, 22856-22865.	3.6	22
79	Molecular Modeling of Potential Anticancer Agents from African Medicinal Plants. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 2433-2450.	5.4	70
80	The uniqueness and therapeutic value of natural products from West African medicinal plants, part III: least abundant compound classes. <i>RSC Advances</i> , 2014, 4, 40095-40110.	3.6	11
81	The uniqueness and therapeutic value of natural products from West African medicinal plants, part II: terpenoids, geographical distribution and drug discovery. <i>RSC Advances</i> , 2014, 4, 35348-35370.	3.6	16
82	Anti-onchocerca Metabolites from <i>Cyperus articulatus</i> : Isolation, In Vitro Activity and In Silico "Drug-Likeness"™. <i>Natural Products and Bioprospecting</i> , 2014, 4, 243-249.	4.3	12
83	The potential of anti-malarial compounds derived from African medicinal plants, part II: a pharmacological evaluation of non-alkaloids and non-terpenoids. <i>Malaria Journal</i> , 2014, 13, 81.	2.3	92
84	The uniqueness and therapeutic value of natural products from West African medicinal plants. Part I: uniqueness and chemotaxonomy. <i>RSC Advances</i> , 2014, 4, 28728-28755.	3.6	23
85	ConMedNP: a natural product library from Central African medicinal plants for drug discovery. <i>RSC Advances</i> , 2014, 4, 409-419.	3.6	50
86	Perspectives on Tuberculosis Pathogenesis and Discovery of Anti-Tubercular Drugs. <i>Current Medicinal Chemistry</i> , 2014, 21, 3466-3477.	2.4	6
87	Potential Natural Antimycobacterial Metabolites from Some Sub-Saharan Medicinal Plants. <i>Anti-Infective Agents</i> , 2014, 12, 178-190.	0.4	9
88	Cameroonian medicinal plants: a bioactivity versus ethnobotanical survey and chemotaxonomic classification. <i>BMC Complementary and Alternative Medicine</i> , 2013, 13, 147.	3.7	63
89	CamMedNP: Building the Cameroonian 3D structural natural products database for virtual screening. <i>BMC Complementary and Alternative Medicine</i> , 2013, 13, 88.	3.7	65
90	Assessing the pharmacokinetic profile of the CamMedNP natural products database: an in silico approach. <i>Organic and Medicinal Chemistry Letters</i> , 2013, 3, 10.	2.0	31

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91	In silico drug metabolism and pharmacokinetic profiles of natural products from medicinal plants in the Congo basin. <i>In Silico Pharmacology</i> , 2013, 1, 12.	3.3	79
92	An in silico evaluation of the ADMET profile of the StreptomeDB database. <i>SpringerPlus</i> , 2013, 2, 353.	1.2	117
93	The potential of anti-malarial compounds derived from African medicinal plants. Part I: A pharmacological evaluation of alkaloids and terpenoids. <i>Malaria Journal</i> , 2013, 12, 449.	2.3	146
94	Bioactive natural products derived from the Central African flora against neglected tropical diseases and HIV. <i>Natural Product Reports</i> , 2013, 30, 1098.	10.3	73
95	AfroDb: A Select Highly Potent and Diverse Natural Product Library from African Medicinal Plants. <i>PLoS ONE</i> , 2013, 8, e78085.	2.5	176
96	New Antimalarial Hits from <i>Dacryodes edulis</i> (Burseraceae) - Part I: Isolation, In Vitro Activity, In Silico "drug-likeness" and Pharmacokinetic Profiles. <i>PLoS ONE</i> , 2013, 8, e79544.	2.5	27