Evans Adei

Department of Chemistry
Kwame Nkrumah University of Science and Technology

ORCID 0000-0003-2544-8883 · Profile knust.peerford.com/staff/d1b0530c-1d1e-4f54-835d-fe0094201605

RESEARCH

Areas: Organic Chemistry · Materials Chemistry · Inorganic Chemistry · Renewable Energy, Sustainability and the Environment · Catalysis · Physical and Theoretical Chemistry

RESEARCH SUMMARY

91	916	18	33	0.60	1%
Publications	Citations	h-index	i10-index	Field-weighted impact	World top 10%

Counted from the 91 publications listed below, 2008–2026. Field-weighted impact is the mean over the 91 works scored for it; 1.00 is the world average for works of the same field, type and year. 1 of the 91 papers scored for it are among the world's most cited tenth for their field, type and year.

POSITIONS

Associate Professor
Chemistry, Kwame Nkrumah University of Science and Technology, Kumasi, Ghana

PUBLICATIONS

Journal articles 90

1. Isaac Ampersand-Kwadwo Akwetey, Joshua Atta-Kumi, Richmond Arhin, Isaac Ofori, Richard Tia, **Evans Adei** (2026). Would the tandem sequential cycloaddition reactions of functionalized acetylene, cyclopentadienyl derivatives, and phenyl azide for the formation of norbornene 1,2,3-triazolines proceed via the [4 + 2]/[3 + 2] or [3 + 2]/[4 + 2] reaction sequences? a DFT mechanistic study. *Journal of Molecular Modeling*. https://doi.org/10.1007/s00894-026-06685-9
2. Mohamed MUTOCHELUH, Charles ANSAH, Kwame Ohene BUABENG, Sampson TWUMASI-ANKRAH, Seth Agyei DOMFEH, Michael OWUSU, Michae OWUSU-ANSAH, Lawrence Sheringha BORQUAYE, **Evans ADEI**, Christiana DUAH, Daniel BOAMAH, Mavis BOAKYE-YIADOM, Kofi Bobi BARIMAH, Ellis OWUSU-DABO (2025). A CRYPTOLEPIS SANGUINOLENTA-BASED PREPARATION REDUCED HOSPITAL STAY AND MORTALITY OF COVID-19 PATIENTS DURING THE PANDEMI. *African Journal of Traditional Complementary and Alternative Medicines*. https://doi.org/10.21010/ajtcamv21i1.1
3. Anthony Tawiah, Gabriel Amankwah, Komla Emmanuel Oyetey, Benjamin Gyedu Akonor, **Evans Adei** (2025). Computational exploration of the (3 + 2) cycloaddition reactions of 3,5-bis-(arylidene)-1-methylpiperidine-4-one with C-substituted-N-phenyl nitrones for the formation of isoxazolidine derivatives. *Journal of Molecular Modeling*. https://doi.org/10.1007/s00894-025-06563-w
4. Anthony Tawiah, Gabriel Amankwah, Benjamin Gyedu Akonor, **Evans Adei** (2025). Deciphering the mechanism and selectivities of the reactions of mesitonitrile oxide with 1,5-Dimethyl-6-methylenetricyclo[3.2.1.02,7]oct-3-en-8-one Derivatives: A computational approach. *Computational and Theoretical Chemistry*. https://doi.org/10.1016/j.comptc.2025.115093
5. Oscar Adjei Boadi Appiah, **Evans Adei**, Richard Tia (2025). Investigating the mechanism of formation of nitro-substituted nicotine analogue via the [3 + 2] cycloaddition reaction of (E)-substituted nitroethene derivatives and (Z)-C-(3-pyridyl)-N-aryl-nitrones: a density functional theory (DFT) study. *Reaction Kinetics Mechanisms and Catalysis*. https://doi.org/10.1007/s11144-025-02800-8
6. Godfred Boakye Adusei, Albert Aniagyei, Elliot Menkah, Caroline R. Kwawu, Gabriel Amankwah,

Richmond Arhin, Hawa Osman, **Evans Adei** (2025). Periselectivity, Chemoselectivity, and Regioselectivity of the Cycloaddition Reaction of Aza-Oxyallyl Cations With Cinnamaldehyde: A Density Functional Theory Study. *Journal of Physical Organic Chemistry*. https://doi.org/10.1002/poc.70003

7. Komla Emmanuel Oyetey, Albert Aniagyei, Elliot S. Menkah, Caroline R. Kwawu, Collins Obuah, Hawa Osman, **Evans Adei** (2025). [3 + 2] cycloaddition reactions of C, N-diarylnitrone to arylallene and N-aryl-C-carbamoyl nitrones to methyl buta-2, 3-dienoate. A theoretical study of reactivity, site, and regio-selectivity. *Reaction Kinetics Mechanisms and Catalysis*. https://doi.org/10.1007/s11144-025-03027-3
8. Emmanuel Komla Oyetey, Caroline R. Kwawu, Albert Aniagyei, Gabriel Amankwah, Richmond Arhin, **Evans Adei** (2024). A computational study into the mechanism and selectivities of the reaction of 1, 1-diaryl-2-isopropylidene-3-methylenecyclopropane (DIMCP) with C, N-diarylnitrone. *Theoretical Chemistry Accounts*. https://doi.org/10.1007/s00214-024-03121-0
9. Benjamin G. Akonor, Albert Aniagyei, Caroline R. Kwawu, Gabriel Amankwah, Elliot S. Menkah, **Evans Adei** (2024). A quantum mechanistic investigation into the unusual reactions of nitrilimine and nitrile oxide with 2,3,4,5-tetraphenylcyclopentadienone. *Journal of Molecular Modeling*. https://doi.org/10.1007/s00894-024-06074-0
10. Marietjie J. Ungerer, **Evans Adei**, Theopolina Amakali, Cecil H. Botchway, Likius S. Daniel, James Darkwa, Nelson Y. Dzade, Foster Mbaiwa, Mary Mensah, Maipelo Nyepetsi and 11 others (2024). Chem4Energy: a consortium of the Royal Society Africa Capacity-Building Initiative. *Interface Focus*. https://doi.org/10.1098/rsfs.2024.0001
11. Muntaka Is-mail, Albert Aniagyei, Caroline R. Kwawu, Gabriel Amankwah, Elliot Menkah, **Evans Adei** (2024). Exploring the specific chemistries of the cycloaddition reactions of 5-benzoyl-3(2H)-isothiazolone and stable nitrile oxides: Insights from Density Functional Theory analysis. *Journal of Physical Organic Chemistry*. https://doi.org/10.1002/poc.4645
12. Gideon Donkor, Albert Aniagyei, Collins Obuah, Joshua Atta Kumi, **Evans Adei** (2024). Investigating the regio-, chemo- and stereoselectivities of the [3 + 2] cycloaddition reaction of 1-pyrroline-1-oxide and C, N-diphenyl nitrone with a 1, 2-cyclooctadiene carboxylate: a DFT study. *Theoretical Chemistry Accounts*. https://doi.org/10.1007/s00214-024-03148-3
13. Sylvia Adomako, Joshua Atta-Kumi, Cecil H. Botchway, Richard Tia, **Evans Adei**, Albert Aniagyei (2023). A DFT Mechanistic Study of the Regio-, Chemo-, and Stereo- Selectivities of the (3 + 2) Cycloaddition of Diarylnitrone Derivatives with 1-(4-Nitrophenyl)-5H-Pyrrolin-2-One. *Journal of Chemistry*. https://doi.org/10.1155/2023/6375973
14. Gabriel Amankwah, Isaac Ofori, Joshua Atta-Kumi, Caroline R. Kwawu, Richard Tia, **Evans Adei** (2023). A quantum mechanistic insight into the chemo- and regio-selective [3 + 2]-cycloaddition reaction of aryl hetaryl thioketones with diazoalkanes and nitrile oxide derivatives. *Journal of Molecular Graphics and Modelling*. https://doi.org/10.1016/j.jmgm.2023.108418
15. Mary Mensah, Richard Tia, **Evans Adei**, Nora H. de Leeuw (2023). C-H versus C-O Addition: A DFT Study of the Catalytic Cleavage of the β-O-4 Ether Linkage in Lignin by Iridium and Cobalt Pincer Complexes. *Catalysts*. https://doi.org/10.3390/catal13040757
16. Caroline R. Kwawu, Destiny Konadu, Paul Boamah, Kassim Fuwad Mohammed, Isaac Danso Boateng, **Evans Adei** (2023). Catalytic degradation and reforming pathways of guaiacol (lignin monomer) on Ru and Ni modified Cu (111). *MRS Advances*. https://doi.org/10.1557/s43580-023-00579-1
17. Ernest Dumba, Caroline R. Kwawu, Ama Konadu Agyemang, Elliot Menkah, **Evans Adei** (2023). DFT studies of the effect of sulfur impurities on the structural, electronic and magnetic properties of iron (100). *Theoretical Chemistry Accounts*. https://doi.org/10.1007/s00214-022-02945-y
18. Amos Afugu, Caroline R. Kwawu, Elliot Menkah, Richard Tia, **Evans Adei** (2023). Details of CO2 electrochemical reduction reaction (CO2ERR) on Mn–MoS2 monolayer: a DFT study. *Theoretical Chemistry Accounts*. https://doi.org/10.1007/s00214-023-03001-z
19. Richmond Arhin, Isaac Ofori, Anthony Fosu, Richard Tia, **Evans Adei**, Albert Aniagyei (2023). Exploring the peri- and stereo- selectivities of the cycloaddition reaction of 2-(2- dimethylaminovinyl)-1-benzopyran-4-one with N-phenylmaleimide (NPM) and dimethylacetylenedicarboxylate (DMAD) - A DFT study. *Journal*

of Molecular Graphics and Modelling. https://doi.org/10.1016/j.jmgm.2023.108451

20. Richard Batsa Odonkor, Richard Tia, **Evans Adei** (2023). Investigating the regio-, stereo-, and enantio-selectivities of the [3 + 2] cycloaddition reaction of C, N-diarylnitrone derivatives with N-propadienylindole derivatives. A DFT study. *Computational and Theoretical Chemistry*. https://doi.org/10.1016/j.comptc.2023.114024
21. Harun Abdullah, Ahmed Yusif Abdulai, Richard Tia, **Evans Adei** (2023). Quantum Mechanical Elucidation on [3+2] cycloaddition reaction of aryl nitrile oxide with cyclopentenones. *Journal of Molecular Graphics and Modelling*. https://doi.org/10.1016/j.jmgm.2023.108421
22. Destiny Konadu, Caroline R. Kwawu, Elliot S. Menkah, Richard Tia, **Evans Adei**, Nora de Leeuw (2023). The catalytic hydrogenolysis of compounds derived from guaiacol on the Cu (111) surface: mechanisms from DFT studies. *Physical Chemistry Chemical Physics*. https://doi.org/10.1039/d2cp04352a
23. Michael Anim Safo, Isaac Ofori, **Evans Adei**, Albert Aniagyei (2023). Theoretical insight into the unexpected initial (3 + 2) cycloaddition reaction of mesitonitrile oxide with 1, 4-diazepine derivatives: A computational study. *Journal of Molecular Graphics and Modelling*. https://doi.org/10.1016/j.jmgm.2023.108515
24. Gabriel Amankwah, Caroline R. Kwawu, Elliot S. Menkah, **Evans Adei** (2023). [3 + 2] Cycloaddition reaction of disubstituted-3-benzylidene succinimide with C, N-disubstituted nitrile imines for synthesizing spiro-heterocycles: A computational study. *Computational and Theoretical Chemistry*. https://doi.org/10.1016/j.comptc.2023.114138
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28. Isaac Ofori, George Baffour Pipim, Richard Tia, **Evans Adei** (2021). A DFT study of the double (3 + 2) cycloaddition of nitrile oxides and allenoates for the formation of spirobiisoxazolines. *Journal of Molecular Graphics and Modelling*. https://doi.org/10.1016/j.jmgm.2021.108033
29. Wisdom Kwaku Samba, Richard Tia, **Evans Adei** (2021). A density functional theory study of the reactions of furans with substituted alkynes to form oxanorbornadienes and subsequent [4 + 2] and [2 + 2 + 2] addition reactions. *Journal of Physical Organic Chemistry*. https://doi.org/10.1002/poc.4281
30. Anthony Fosu, George Baffour Pipim, Richard Tia, **Evans Adei** (2021). Does the reaction of nitrone derivatives with allenoates proceed by an initial (3 + 2) cycloaddition or O-Nucleophilic addition? A quantum chemical investigation. *Journal of Molecular Graphics and Modelling*. https://doi.org/10.1016/j.jmgm.2021.108036
31. Anthony Tawiah, George Baffour Pipim, Richard Tia, **Evans Adei** (2021). Exploring the chemo-, regio-, and stereoselectivities of the (3 + 2) cycloaddition reaction of 5,5-dimethyl-3-methylene-2-pyrrolidinone with C,N-diarylnitrones and nitrile oxide derivatives: a DFT study. *Journal of Molecular Modeling*. https://doi.org/10.1007/s00894-021-04911-0
32. Cecil H. Botchway, Richard Tia, **Evans Adei**, Nelson Y. Dzade, Nora H. de Leeuw (2021). H-FER-Catalyzed Conversion of Methanol to Ethanol and Dimethyl Ether: a First-Principles DFT Study. *South African Journal of Chemistry*. https://doi.org/10.17159/0379-4350/2021/v74a6
33. Joshua Atta-Kumi, George Baffour Pipim, Richard Tia, **Evans Adei** (2021). Investigating the site-, regio-, and stereo-selectivities of the reactions between organic azide and 7-heteronorbornadiene: a DFT mechanistic study. *Journal of Molecular Modeling*. https://doi.org/10.1007/s00894-021-04857-3
34. Destiny Konadu, Caroline Rosemyya Kwawu, Richard Tia, **Evans Adei**, Nora Henriette de Leeuw (2021).

Mechanism of Guaiacol Hydrodeoxygenation on Cu (111): Insights from Density Functional Theory Studies. *Catalysts*. https://doi.org/10.3390/catal11040523

35. George Baffour Pipim, Richard Tia, **Evans Adei** (2021). Quantum chemical investigation of the formation of spiroheterocyclic compounds via the (3 + 2) cycloaddition reaction of 1-methyl-3-(2,2,2-trifluoroethylidene) pyrrolidin-2-one with diazomethane and nitrone derivatives. *Tetrahedron*. https://doi.org/10.1016/j.tet.2021.132306
36. Harun Abdullah, Richard Tia, **Evans Adei** (2021). Regio-, stereo-, and site-selectivities of 1,3-dipolar Cycloaddition reaction of benzonitrile oxide with unsymmetrically substituted norbornenes and norbornadienes: A computational study. *Journal of Physical Organic Chemistry*. https://doi.org/10.1002/poc.4259
37. Wisdom Kwaku Samba, Anthony Amoah, Richard Tia, **Evans Adei** (2021). Theoretical investigation of the regio-, enantio-, and stereo-selectivities of the (3 + 2) cycloaddition reactions of N-vinylindoles with nitrones and nitrile oxides. *Theoretical Chemistry Accounts*. https://doi.org/10.1007/s00214-021-02847-5
38. George Baffour Pipim, Richard Tia, **Evans Adei** (2020). (3 + 2) cycloaddition reaction of 7-isopropylidenebenzonorbornadiene and diazomethane derivatives: A theoretical study. *Journal of Molecular Graphics and Modelling*. https://doi.org/10.1016/j.jmgm.2020.107713
39. Daniel Aboagye Akuamoah, Ernest Opoku, Richard Tia, **Evans Adei** (2020). 1,3-Dipolar cycloaddition reaction of indoles with tosyl azide, subsequent dehydroaromatization and ring-opening cascade: a computational study. *Theoretical Chemistry Accounts*. https://doi.org/10.1007/s00214-020-02653-5
40. Caroline R. Kwawu, Albert Aniagyei, Richard Tia, **Evans Adei** (2020). A DFT investigation of the mechanisms of CO2 and CO methanation on Fe (111). *Materials for Renewable and Sustainable Energy*. https://doi.org/10.1007/s40243-020-0164-x
41. Anthony Amoah, Richard Tia, **Evans Adei** (2020). A DFT mechanistic study on [4 + 3] cycloaddition reactions of oxyallyl cations and five-membered cyclopentadiene derivatives. *Tetrahedron*. https://doi.org/10.1016/j.tet.2020.131422
42. George Baffour Pipim, Richard Tia, **Evans Adei** (2020). Computational exploration of the 1,3-dipolar cycloaddition reaction of 7-isopropylidenebenzonorbornadiene with nitrile oxide and cyclic nitrone derivatives. *Journal of Physical Organic Chemistry*. https://doi.org/10.1002/poc.4174
43. Daniel Aboagye Akuamoah, Richard Tia, **Evans Adei** (2020). Computational study on the mechanism of the reaction of benzenesulfonyl azides with oxabicyclic alkenes. *Journal of Molecular Modeling*. https://doi.org/10.1007/s00894-020-04582-3
44. Abdul Rashid Umar, Richard Tia, **Evans Adei** (2020). DFT mechanistic studies on the regio-, stereo-, and enantio-selectivity of 1,3 dipolar cycloadditions of quinolinium imides with olefins, maleimides, and benzynes for the synthesis of fused N,N′-heterocycles. *Journal of Molecular Modeling*. https://doi.org/10.1007/s00894-020-4299-6
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46. George Baffour Pipim, Richard Tia, **Evans Adei** (2020). Investigating the regio-, stereo-, and enantio-selectivities of the 1,3-dipolar cycloaddition reaction of C-cyclopropyl-N-phenylnitrone derivatives and benzylidenecyclopropane derivatives: A DFT study. *Journal of Molecular Graphics and Modelling*. https://doi.org/10.1016/j.jmgm.2020.107672
47. Ernest Opoku, George Baffour Pipim, Richard Tia, **Evans Adei** (2020). Mechanistic study of the tandem intramolecular (4 + 2)/intermolecular (3 + 2) cycloaddition reactions for the formation of polyaza- and polyisoxazolidine-steroids. *Journal of Heterocyclic Chemistry*. https://doi.org/10.1002/jhet.3900
48. George Baffour Pipim, Ernest Opoku, Richard Tia, **Evans Adei** (2020). Peri-, Chemo-, Regio-, Stereo- and Enantio-Selectivities of 1,3-dipolar cycloaddition reaction of C,N-Disubstituted nitrones with disubstituted 4-methylene-1,3-oxazol-5(4H)- one: A quantum mechanical study. *Journal of Molecular Graphics and Modelling*. https://doi.org/10.1016/j.jmgm.2020.107542

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50. Wisdom Kwaku Samba, Richard Tia, **Evans Adei** (2020). Regio-, enantio-, peri-, and stereo-selectivities of the reactions of five-membered cyclodiene derivatives with itaconic anhydride toward the formation of norbornene lactones. *Journal of Physical Organic Chemistry*. https://doi.org/10.1002/poc.4132

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53. Grace Arhin, Anita Houston Adams, Ernest Opoku, Richard Tia, **Evans Adei** (2019). 1, 3-Dipolar cycloaddition reactions of selected 1,3-dipoles with 7-isopropylidenenorbornadiene and follow-up thermolytic cleavage: A computational study. *Journal of Molecular Graphics and Modelling*. https://doi.org/10.1016/j.jmgm.2019.08.004

54. Ernest Opoku, Richard Tia, **Evans Adei** (2019). Computational studies on [4 + 2] / [3 + 2] tandem sequential cycloaddition reactions of functionalized acetylenes with cyclopentadiene and diazoalkane for the formation of norbornene pyrazolines. *Journal of Molecular Modeling*. https://doi.org/10.1007/s00894-019-4056-x

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56. Elliot S. Menkah, Nelson Y. Dzade, Richard Tia, **Evans Adei**, Nora H. de Leeuw (2019). Hydrazine adsorption on perfect and defective fcc nickel (100), (110) and (111) surfaces: A dispersion corrected DFT-D2 study. *Applied Surface Science*. https://doi.org/10.1016/j.apsusc.2019.02.128

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58. Ernest Opoku, Richard Tia, **Evans Adei** (2019). Quantum chemical studies on the mechanistic aspects of tandem sequential cycloaddition reactions of cyclooctatetraene with ester and nitrones. *Journal of Molecular Graphics and Modelling*. https://doi.org/10.1016/j.jmgm.2019.06.019

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