Annexure 1

Research Publications:

1. Synthesis, crystal structure, quantum computational, biological study, molecular docking and molecular dynamic simulations investigations on 2, 2′-((1, 4-phenylenebis … 2025
A Kumar, A Fatima, M Shahid, I Verma, P Sharma, H Arora, S Javed, N Siddiqui*
Journal of Molecular Structure 1319, 139300

2. Structural, Fukui, non-covalent analysis, molecular docking, free energy landscapes, and principle component analysis of biological active 1, 8-naphthalic anhydride 2024
VS Jeba Reeda, JN CheerlinMishma, P Divya, R Suja, A Manikandan, S Javed, N Siddiqui* Spectroscopy Letters, 1-21

3. Multifaceted investigation of Sulfamerazine: Insights from computational methods, experimental techniques, and molecular simulations 2024
S Ahmad, VSJ Reeda, K Aziz, H Arora, M Kumar, K Garima, A Ali, S Javed, N Siddiqui*
Journal of Molecular Structure 1312, 138554

4. Comprehensive Analysis of 2, 5-Dimethyl-1-(Naphthalen-1-yl)-1H-Pyrrole: X-ray Crystal Structure, Spectral, Computational, Molecular Properties, Docking Studies, Molecular … 2024
VSJ Reeda, P Divya, AAJ Ranchani, A Manikandan, S Alvi, R Ali, S. Javed, N Siddiqui*
Journal of Molecular Structure, 140062

5. Spectroscopic, Computational, Molecular Docking and Dynamics Simulations Studies of 4-Amino-3-hydroxyNaphthalene-1-Sulfonic Acid (ANSA) 2024
HK Pathan, A Fatima, P Garg, S Muthu, A Yadav, N Siddiqui, M Ali, S Javed, N Siddiqui* Polycyclic Aromatic Compounds 44 (6), 3787-3806

6. A Comprehensive Investigation of (E)-2, 4-Dimethyl-6-(((2-(Phenylthio) phenyl) imino) methyl) phenol (2PTALD): Synthesis, Crystal Structure, and Computational Insights with … 2024
M Kumar, S Ahmad, VSJ Reeda, H Arora, M Shahid, S Muthu, N Siddiqui, ...
Journal of Molecular Structure, 138761

7. Exploration of Experimental, Theoretical, Molecular Docking, and Electronic Excitation Studies of Carboxylate-Appended (2-Pyridyl)Alkylamine Ligand† 2024
P Kaur, I Verma, G Khanum, A Ali, N Siddiqui, S Javed, H Arora
Polycyclic Aromatic Compounds 44 (4), 2802-2819

8. Exploring role of natural compounds in molecular alterations Associated with Brain Ageing: a perspective towards Nutrition for Ageing Brain 2024
N Siddiqui, A Sharma, A Kesharwani, VK Parihar
Ageing Research Reviews, 102282

9. Quantum computational, spectroscopic investigations on fomepizole (4-Methyl-1H-Pyrazole) by DFT/TD-DFT with different solvents and molecular docking studies 2024
K Pooja, K Garima, S Savita, I Verma, N Siddiqui*, S Javed

10. Synthesis, X-ray diffraction, DFT, and molecular docking studies of 2024

isonicotinohydrazide derivative
A Fatima, N Siddiqui, G Khanum, N Haq, RJ Butcher, SK Srivastava, ...
Zeitschrift für Physikalische Chemie 238 (1), 187-207

11. Synthesis, Characterization and Antibacterial Investigation of Mononuclear Copper (II) Complexes of Amine-phenolate Based Ligands — 2024
A Jindal, S Kapoor, I Verma, A Raju, H Arora, P Tyagi, N Siddiqui*
Polycyclic Aromatic Compounds 44 (1), 162-177

12. Dinuclear Phenoxo-Bridged Nickel (II) and Copper (II) Complexes of Phenolate-Based Tripodal Ligand: Theoretical and Experimental Insights — 2024
P Agarwal, A Kumar, I Verma, G Khanum, N Siddiqui*, ...
Polycyclic Aromatic Compounds 44 (1), 313-332

13. Exploring quantum computational, molecular docking, and molecular dynamics simulation with MMGBSA studies of ethyl-2-amino-4-methyl thiophene-3-carboxylate — 2023
A Fatima, G Khanum, SK Srivastava, P Bhattacharya, A Ali, H Arora, N Siddiqui*
Journal of Biomolecular Structure and Dynamics 41 (20), 10411-10429

14. Evaluation of experimental, computational, molecular docking and dynamic simulation of flucytosine — 2023
N Agarwal, A Fatima, P Bhattacharya, S Muthu, H Arora, N Siddiqui, ...
Journal of Biomolecular Structure and Dynamics 41 (20), 10430-10449

15. Study of L-tryptophan (a neurotransmitter precursor): spectral, Hirshfeld surface, molecular docking and dynamics simulations — 2023
A Fatima, A Kumar, AKA Saral, S Muthu, M Afzal, N Haq, I Nazar, N Siddiqui*
Zeitschrift für Physikalische Chemie

16. Synthesis, crystal structure, DFT, Hirshfeld surface, 3D energy frameworks analysis and Molecular Docking of pyrimidine derivative: a theoretical and experimental approach — 2023
A Fatima, G Khanum, N Siddiqui, S Muthu, M Afzal, RJ Butcher, ...
Chemical Physics Impact 7, 100345

17. Quantum computational, spectroscopic characterization, Hirshfeld analysis & molecular docking studies on p-toluenesulfonic acid (p-TSA) or tosylic acid — 2023
HK Pathan, G Khanum, R Javed, N Siddiqui, S Selvakumari, S Muthu, ...
Chemical Physics Impact 7, 100320

18. Synthesis, Crystal Structure, DFT Studies on Tetramethyl-(p-Tolyl)-Hexahydro-1H-Xanthene-1, 8 (2H)-Dione — 2023
A Fatima, G Khanum, A Sharma, N Siddiqui, RJ Butcher, SK Srivastava, ...
Polycyclic Aromatic Compounds 43 (10), 9210-9232

19. Synthesis, Spectroscopic, Quantum Chemical, and Molecular Docking Studies of 2-Cyano-*N*-Cyclopropylacetamide and 2-Cyano-*N*-(1-Phenylethyl)Acetamide — 2023
G Khanum, A Fatima, RA Rather, N Siddiqui, S Muthu, SK Srivastava, ...
Polycyclic Aromatic Compounds 43 (10), 9047-9073

20. Experimental Spectroscopic, DFT, Molecular Docking, and Molecular Dynamics — 2023

Simulation Investigations on m-Phenylenediamine (Monomer and Trimer)
A Fatima, A Ali, R Rajan, I Verma, S Muthu, N Siddiqui, P Garg, S Javed
Polycyclic Aromatic Compounds 43 (10), 8599-8631

21. Quantum Computational, Spectroscopic, Hirshfeld Surface Analysis of 3-Picoline (Monomer and Dimer) by DFT/TD-DFT with Different Solvents, Molecular Docking, and Molecular … 2023
K Garima, A Fatima, K Pooja, S Savita, M Sharma, M Kumar, S Muthu, N Siddiqui*
Polycyclic Aromatic Compounds 43 (9), 7828-7852

22. Synthesis, X-Ray Diffraction, DFT and Hirshfeld Surface Studies of 9-(4-Hydroxyphenyl-Tetramethyl-Hexahydro-1H-Xanthene-1, 8 (2H)-Dione 2023
A Fatima, G Khanum, A Sharma, N Siddiqui, RJ Butcher, SK Srivastava, ...
Polycyclic Aromatic Compounds 43 (8), 6953-6976

23. Experimental Spectroscopic (FT-IR, ^{1}H and ^{13}C NMR, ESI-MS, UV) Analysis, Single Crystal X-Ray, Computational, Hirshfeld Analysis, and Molecular Docking of 2-Amino … 2023
G Khanum, A Fatima, N Siddiqui, RJ Butcher, NS Alsaiari, SK Srivastava, ...
Polycyclic Aromatic Compounds 43 (8), 7127-7151

24. Synthesis, single crystal, TD-DFT, molecular dynamics simulation and DNA binding studies of carbothioamide analog 2023
M Rana, S Ahmedi, A Fatima, S Ahmad, N Siddiqui, K Raza, N Manzoor, ...
Journal of Molecular Structure 1287, 135701

25. Experimental spectroscopic, quantum chemical, molecular docking, and molecular dynamic simulation studies on hydantoin (monomer and dimer) 2023
S Sharma, A Fatima, FM Manhas, N Agarwal, M Singh, S Muthu, N Siddiqui*
Polycyclic Aromatic Compounds 43 (7), 6627-6653

26. Carbothioamide Based Pyrazoline Derivative: Synthesis, Single Crystal Structure, DFT/TD-DFT, Hirshfeld Surface Analysis and Biological Studies 2023
M Rana, A Fatima, N Siddiqui, S Ahmedi, SH Dar, N Manzoor, S Javed, ...
Polycyclic Aromatic Compounds 43 (7), 6181-6201

27. Synthesis, spectroscopic, crystal structure, DFT, hirshfeld surface and molecular docking analysis of hexahydroquinoline derivative (HQ) 2023
A Fatima, G Khanum, DD Agrawal, SK Srivastava, RJ Butcher, S Muthu, N Siddiqui*
Polycyclic Aromatic Compounds 43 (5), 4242-4270

28. Experimental spectroscopic, structural (monomer and dimer), molecular docking, molecular dynamics simulation and hirshfeld surface analysis of 2-amino-6-methylpyridine 2023
A Fatima, M Singh, KM Abualnaja, K Althubeiti, S Muthu, N Siddiqui, N Siddiqui*
Polycyclic Aromatic Compounds 43 (5), 3910-3940

29. Molecular docking, dynamic simulation and DFT approach to noble “2-hydrazinobenzothiazole” compound 2023
A Sharma, A Fatima, MA Malla, G Khanum, A Kumar, M Singh, N Siddiqui*
Polycyclic Aromatic Compounds 43 (5), 4271-4298

30. Copper (II) monomer bearing phenolate-based ligand: theoretical and experimental visions — 2023
A Jindal, P Agarwal, I Verma, G Khanum, K Althubeiti, N Siddiqui, S Javed, ...
Polycyclic Aromatic Compounds 43 (4), 3489-3501

31. Experimental spectroscopic, quantum computational, hirshfeld surface, molecular docking, and electronic excitation studies on an antibiotic agent: SDZ — 2023
M Kumar, A Fatima, M Singh, I Verma, G Khanum, S Muthu, K Althubeiti, N Siddiqui*
Polycyclic Aromatic Compounds 43 (4), 3122-3146

32. Dimeric ZnII complex of carboxylate-appended (2-pyridyl) alkylamine ligand and exploration of experimental, theoretical, molecular docking and electronic excitation studies of … — 2023
P Kaur, I Verma, G Khanum, N Siddiqui, S Javed, H Arora
Journal of Molecular Structure 1276, 134715

33. Quantum Computational, Spectroscopic (FT-IR, FT-Raman, NMR, and UV–Vis) Hirshfeld Surface and Molecular Docking-Dynamics Studies on 5-Hydroxymethyluracil (Monomer and Trimer) — 2023
M Kumar, G Jaiswar, M Afzal, M Muddassir, A Alarifi, A Fatima, N Siddiqui, N Siddiqui* Molecules 28 (5), 2116

34. Synthesis, characterization, crystal structure, Hirshfeld surface, electronic Excitation, molecular Docking, and DFT studies on 2-amino thiophene derivative — 2023
A Fatima, G Khanum, I Verma, RJ Butcher, N Siddiqui, SK Srivastava, N Siddiqui*
Polycyclic Aromatic Compounds 43 (2), 1644-1675

35. Experimental spectroscopic, computational, hirshfeld surface, molecular docking investigations on 1H-Indole-3-Carbaldehyde — 2023
A Fatima, G Khanum, A Sharma, I Verma, H Arora, N Siddiqui, S Javed
Polycyclic Aromatic Compounds 43 (2), 1263-1287

36. DFT, molecular docking, molecular dynamics simulation, MMGBSA calculation and hirshfeld surface analysis of 5-sulfosalicylic acid — 2023
A Fatima, H Arora, P Bhattacharya, N Siddiqui, KM Abualnaja, P Garg, ...
Journal of Molecular Structure 1273, 134242

37. Synthesis, single crystal X-ray, DFT, Hirshfeld surface and molecular docking studies of 9-(2, 4-dichlorophenyl)-4a-hydroxy-tetramethyl-octahydro-1H-xanthene-1, 8 (2H)-dione — 2022
A Fatima, G Khanum, A Sharma, N Siddiqui, S Muthu, RJ Butcher, ...
Journal of Molecular Structure 1268, 133613

38. Quantum computational, spectroscopic (FT-IR, NMR and UV–Vis) profiling, Hirshfeld surface, molecular docking and dynamics simulation studies on pyridine-2, 6-dicarbonyl dichloride — 2022
FM Manhas, A Fatima, I Verma, N Siddiqui, S Muthu, HS AlSalem, ...
Journal of Molecular Structure 1265, 133374

39. Density functional studies and spectroscopic analysis (FT-IR, FT-Raman, UV–visible, — 2022

and NMR) with molecular docking approach on an anticancer and antifungal drug 4-hydroxy-3 …
G Khanum, A Kumar, M Singh, A Fatima, S Muthu, KM Abualnaja, N Siddiqui*
Journal of Molecular Structure 1264, 133134

40. Synthesis, single crystal structure, DNA binding and antioxidant properties of 5-(4-(dimethylamino) phenyl)-3-(thiophen-2-yl)-pyrazoline-1-carbothioamide — 2022
M Rana, A Fatima, N Siddiqui, SH Dar, S Javed
Journal of Molecular Structure 1261, 132950

41. Synthesis, crystal structure, characterization, Hirshfeld analysis, molecular docking and DFT calculations of 5-Phenylamino-isophthalic acid: A good NLO material — 2022
A Fatima, A Ali, S Shabbir, M Khan, M Mehkoom, SM Afzal, M Ahmad, N Siddiqui*
Journal of Molecular Structure 1261, 132791

42. Conformational stability, quantum computational, spectroscopic, molecular docking and molecular dynamic simulation study of 2-hydroxy-1-naphthaldehyde — 2022
A Sharma, G Khanum, A Kumar, A Fatima, M Singh, KM Abualnaja, N Siddiqui*
Journal of Molecular Structure 1259, 132755

43. Experimental, theoretical, hirschfeld surface, electronic excitation and molecular docking studies on fomepizole (4-Methyl-1H-pyrazole) — 2022
K Pooja, A Fatima, A Sharma, K Garima, S Savita, M Kumar, I Verma, N Siddiqui*
Journal of Molecular Structure 1256, 132549

44. Nanocomposites: A Boon To Material Sciences — 2022
S Saxena, N Siddiqui, M Srivastava
Nanocomposite Materials for Sensor, 15

45. Quantum chemical, spectroscopic, hirshfeld surface and molecular docking studies on 2-aminobenzothiazole — 2022
M Kumar, M Singh, G Jaiswar, RSK Lalji, BK Singh, A Sharma, G Khanum, N Siddiqui*
Journal of Molecular Structure 1253, 132254

46. Exploration of experimental, theoretical, Hirshfeld surface, molecular docking and electronic excitation studies of Menadione: A potent anti-cancer agent — 2022
N Singh, A Fatima, M Singh, I Verma, S Muthu, N Siddiqui, S Javed
Journal of Molecular Liquids 351, 118670

47. Vibrational Spectroscopy, Quantum Computational and Molecular Docking Studies on 2-[(1H-benzimidazol-1-yl)-methyl] benzoic acid — 2022
G Khanum, A Ali, S Shabbir, A Fatima, N Alsaiari, Y Fatima, M Ahmad, N Siddiqui*
Crystals 12 (3), 337

48. Synthesis, single crystal, characterization and computational study of 2-amino-N-cyclopropyl-5-ethyl-thiophene-3-carboxamide — 2022
G Khanum, A Fatima, N Siddiqui, DD Agarwal, RJ Butcher, SK Srivastava, ...
Journal of Molecular Structure 1250, 131890

49. Computational, spectroscopic, Hirshfeld surface, electronic state and molecular — 2022

docking studies on phthalic anhydride
A Fatima, G Khanum, A Sharma, K Garima, S Savita, I Verma, N Siddiqui, ...
Journal of Molecular Structure 1249, 131571

50. Quantum computational, spectroscopic, Hirshfeld surface, electronic state and molecular docking studies on sulfanilic acid: An anti-bacterial drug — 2022
A Fatima, G Khanum, S Savita, K Pooja, I Verma, N Siddiqui, S Javed
Journal of Molecular Liquids 346, 117150

51. Quantum Chemical, experimental spectroscopic, Hirshfeld surface and molecular docking studies of the anti-microbial drug Sulfathiazole — 2021
A Fatima, K Pooja, S Savita, M Singh, I Verma, N Siddiqui, S Javed
Journal of Molecular Structure 1245, 131118

52. Experimental spectroscopic and quantum computational analysis of pyridine-2, 6-dicarboxalic acid with molecular docking studies — 2021
N Agarwal, I Verma, N Siddiqui, S Javed
Journal of Molecular Structure 1245, 131046

53. Synthesis, computational, spectroscopic, hirshfeld surface, electronic state and molecular docking studies on diethyl-5-amino-3-methylthiophene-2, 4-dicarboxylate — 2021
A Fatima, G Khanum, SK Srivastava, I Verma, N Siddiqui, S Javed
Chemical Physics Letters 784, 139103

54. Spectroscopic, molecular structure, electronic, Hirshfeld surface, molecular docking, and thermodynamic investigations of trans-4-hydroxy-L-proline by DFT method — 2021
A Fatima, M Singh, N Agarwal, I Verma, RJ Butcher, N Siddiqui, S Javed
Journal of Molecular Liquids 343, 117549

55. Investigations on experimental, theoretical spectroscopic, electronic excitations, molecular docking of Sulfaguanidine (SG): An antibiotic drug — 2021
A Fatima, M Singh, N Singh, S Savita, I Verma, N Siddiqui, S Javed
Chemical Physics Letters 783, 139049

56. Experimental spectroscopic, Quantum computational, Hirshfeld surface and molecular docking studies on 3-Pyridinepropionic acid — 2021
S Savita, A Fatima, K Garima, K Pooja, I Verma, N Siddiqui, S Javed
Journal of Molecular Structure 1243, 130932

57. N-[4-(phenyl telluro) butyl] phthalimide: Synthesis, spectral characterization, DFT studies and its complexes with mercury salts — 2021
A Chopra, A Fatima, SK Srivastava, N Siddiqui, S Javed
Journal of Molecular Structure 1243, 130902

58. Exploration of experimental and theoretical properties of 5, 5-dimethyl 3-amino-cyclohex-2-en-1-one (AMINE DIMEDONE) by DFT/TD-DFT with ethanol and DMSO as solvents and … — 2021
A Fatima, J Bhadoria, SK Srivastava, I Verma, N Siddiqui, S Javed
Journal of Molecular Liquids 338, 116551

59. Linagliptin, a DPP-4 inhibitor, ameliorates Aβ (1− 42) peptides induced neurodegeneration and brain insulin resistance (BIR) via insulin receptor substrate-1 (IRS-1) in rat … 2021
N Siddiqui, J Ali, S Parvez, S Zameer, AK Najmi, M Akhtar
Neuropharmacology 195, 108662

60. Identification of potential inhibitors of SARS-CoV-2 from Artemisia annua compounds by In silico evaluation and their density functional theory (DFT) 2021
E Abdirahman, AS Mohamed, N Siddiqui, S AL JAWAD, M Nour, ...
Journal of Drug Delivery and Therapeutics 11 (1-s), 71-82

61. Quantum computational, spectroscopic investigations on ampyra (4-aminopyridine) by dft/td-dft with different solvents and molecular docking studies 2021
N Siddiqui, S Javed
Journal of Molecular Structure 1224, 129021

62. Spectroscopic, molecular structure, electronic, Hirshfeld surface, molecular docking, and thermodynamic investigations of trans-4-hydroxy-L-proline by DFT method 2021
N Siddiqui, S Javed
J. Mol. Struct. 1224, 1-13

63. Quantum Mechanical Conformational Analysis of β-Alaninemide Dipeptide 2020
S. Javed, N. Siddiqui
Lambert Publication, 1-190

64. Tuning Thin Film Properties by Structural Modulations in Red Fluorescent Protein Chromophore Analogues 2019
A Singh, R Gupta, N Siddiqui, SS Kumar Iyer, G Ramanathan
ChemistrySelect 4 (45), 13320-13326

65. Trans-Bis {2-[bis (1H-pyrazol-1-yl) methyl]-1-methyl-1H-benzimidazole} iron (II) bis (perchlorate) acetonitrile disolvate 2019
A Kumar, MSH Faizi, S Javed, N Siddiqui, T Iskenderov
IUCrData 4 (1), x190050

66. 2-Amino-5-chlorobenzophenone
S Javed, MSH Faizi, N. Siddiqui, T Iskenderov 1 2018
IUCrData 3 (10), x181444

67. Spin-Transition in FeIIN6 Complexes: Effect of Counter-Anions on Spin-Transtion of FeII Complexes 2017
S.Javed, N Siddiqui
Lamber Publication, 1-128

68. TRANSFER COMPLEX FORMED BETWEEN 6, 6-DIMETHYL-222 2017
N SIDDIQUI, S KANT, AKS JAVED
Dr. Bhimrao Ambedkar University, Agra (UP) 1 (3), 23-28

69. Quantum Mechanical Conformational Analysis of Inositols 2017
N Siddiqui, S Javed

Lambert Publication, 1-228

70. Crystal structure of N1, N1-diethyl-N4-[(quinolin-2-yl) methylidene] benzene-1, 4-diamine
MSH Faizi, N Siddiqui, S Javed
Acta Crystallographica Section E: Crystallographic Communications 71 (1 … 2015

71. Structures, stability and hydrogen bonding in inositol conformers
N Siddiqui, V Singh, MM Deshmukh, R Gurunath
Physical Chemistry Chemical Physics 17 (28), 18514-18523 2015