

# Sonam Shakya

## List of Publications by Year in descending order

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papers

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times ranked

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#	ARTICLE	IF	CITATIONS
1	Exploring Colorimetric Real-Time Sensing Behavior of a Newly Designed CT Complex toward Nitrobenzene and Co <sup>2+</sup> : Spectrophotometric, DFT/TD-DFT, and Mechanistic Insights. ACS Omega, 2019, 4, 9983-9995.	3.5	66
2	Preparation, single-crystal investigation and spectrophotometric studies of proton transfer complex of 2,6-diaminopyridine with oxalic acid in various polar solvents. Journal of Molecular Liquids, 2018, 250, 150-161.	4.9	62
3	Charge transfer complex based real-time colorimetric chemosensor for rapid recognition of dinitrobenzene and discriminative detection of Fe <sup>2+</sup> ions in aqueous media and human hemoglobin. Journal of Photochemistry and Photobiology A: Chemistry, 2020, 392, 112402.	3.9	54
4	Charge transfer complexes: Emerging and promising colorimetric real-time chemosensors for hazardous materials. Journal of Hazardous Materials, 2021, 403, 123537.	12.4	54
5	Synthesis, characterization, antimicrobial and DNA binding properties of an organic charge transfer complex obtained from pyrazole and chloranilic acid. Bioorganic Chemistry, 2020, 99, 103779.	4.1	45
6	Novel thiophene Chalcones-Coumarin as acetylcholinesterase inhibitors: Design, synthesis, biological evaluation, molecular docking, ADMET prediction and molecular dynamics simulation. Bioorganic Chemistry, 2022, 119, 105572.	4.1	40
7	Exploring interaction dynamics of designed organic cocrystal charge transfer complex of 2-hydroxypyridine and oxalic acid with human serum albumin: Single crystal, spectrophotometric, theoretical and antimicrobial studies. Bioorganic Chemistry, 2020, 100, 103872.	4.1	39
8	Synthesis and spectrophotometric studies of CT complex between 1,2-dimethylimidazole and picric acid in different polar solvents: exploring antimicrobial activities and molecular (DNA) docking. Physics and Chemistry of Liquids, 2021, 59, 753-769.	1.2	32
9	Low concentrated phosphorus sorption in aqueous medium on aragonite synthesized by carbonation of seashells: Optimization, kinetics, and mechanism study. Journal of Environmental Management, 2021, 280, 111652.	7.8	31
10	Multispectroscopic and Computational Analysis Insight into the Interaction of Cationic Diester-Bonded Gemini Surfactants with Serine Protease I $\pm$ -Chymotrypsin. ACS Omega, 2020, 5, 3624-3637.	3.5	30
11	Synthesis, spectroscopic characterization, antimicrobial activity, molecular docking and DFT studies of proton transfer (H-bonded) complex of 8-aminoquinoline (donor) with chloranilic acid (acceptor). Journal of Biomolecular Structure and Dynamics, 2022, 40, 12194-12208.	3.5	25
12	Solvatochromic Absorbance and Fluorescence Probe Behavior within Ionic Liquid + $\gamma$ -Butyrolactone Mixture. Journal of Chemical & Engineering Data, 2019, 64, 4169-4180.	1.9	23
13	Molecular engineering of complexation between RNA and biodegradable cationic gemini surfactants: role of the hydrophobic chain length. Molecular Systems Design and Engineering, 2022, 7, 487-506.	3.4	22
14	Synthesis, DFT and <i>In Silico</i> Anti-COVID Evaluation of Novel Tetrazole Analogues. Polycyclic Aromatic Compounds, 2023, 43, 1941-1956.	2.6	22
15	Crystal Structure, Topology, DFT and Hirshfeld Surface Analysis of a Novel Charge Transfer Complex (L3) of Anthraquinone and 4-[(anthracen-9-yl)methyl] amino-benzoic Acid (L2) Exhibiting Photocatalytic Properties: An Experimental and Theoretical Approach. Molecules, 2022, 27, 1724.	3.8	22
16	Enhancing the Antipsychotic Effect of Risperidone by Increasing Its Binding Affinity to Serotonin Receptor via Picric Acid: A Molecular Dynamics Simulation. Pharmaceuticals, 2022, 15, 285.	3.8	21
17	Synthesis and spectroscopic characterizations of nanostructured charge transfer complexes associated between moxifloxacin drug donor and metal chloride acceptors as a catalytic agent in a recycling of wastewater. Journal of Molecular Liquids, 2022, 349, 118121.	4.9	20
18	Effect of geraniol against arecoline induced toxicity in the third instar larvae of transgenic Drosophila melanogaster (hsp70-lacZ) Bg9. Toxicology Mechanisms and Methods, 2019, 29, 187-202.	2.7	19

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19	Thermodynamic and structural studies of newly prepared CT complex between pyrazole as a donor and salicylic acid as acceptor at various temperatures in ethanol. Journal of Molecular Structure, 2020, 1206, 127758.	3.6	19
20	In silico discovery of multi-targeting inhibitors for the COVID-19 treatment by molecular docking, molecular dynamics simulation studies, and ADMET predictions. Structural Chemistry, 2022, 33, 1645-1665.	2.0	19
21	Supramolecular charge-transfer complex generated by the interaction between tin(II) 2,3-naphthalocyanine as a donor with DDQ as an acceptor: Spectroscopic studies in solution state and theoretical calculations. Journal of Molecular Liquids, 2022, 362, 119757.	4.9	19
22	Enhancement of Haloperidol Binding Affinity to Dopamine Receptor via Forming a Charge-Transfer Complex with Picric Acid and 7,7,8,8-Tetracyanoquinodimethane for Improvement of the Antipsychotic Efficacy. Molecules, 2022, 27, 3295.	3.8	11
23	Increasing the Efficacy of Seproxetine as an Antidepressant Using Charge-Transfer Complexes. Molecules, 2022, 27, 3290.	3.8	11
24	Exploring microstructural, optical, electrical, and DFT/TD-DFT studies of boron subphthalocyanine chloride for renewable energy applications. Optik, 2022, 263, 169367.	2.9	10
25	Water Environment Policy and Climate Change: A Comparative Study of India and South Korea. Sustainability, 2019, 11, 3284.	3.2	9
26	Impedance spectroscopy and DFT/TD-DFT studies of diyttrium trioxide for optoelectronic fields. Journal of Rare Earths, 2023, 41, 605-612.	4.8	6
27	Spectroscopic and Molecular Docking Studies of Cu(II), Ni(II), Co(II), and Mn(II) Complexes with Anticonvulsant Therapeutic Agent Gabapentin. Molecules, 2022, 27, 4311.	3.8	5
28	Biochemical and histopathological analysis after sub-chronic administration of oxyresveratrol in Wistar rats. Drug and Chemical Toxicology, 2023, 46, 166-175.	2.3	3
29	Synthesis, experimental and theoretical analyses of bis(2-ethylphenyl)phosphorodithioates of nickel(II). Journal of Molecular Structure, 2022, 1263, 133166.	3.6	3
30	Intermolecular charge-transfer complexes between chlorothiazide antihypertensive drug against iodine sigma and picric acid pi acceptors: DFT and molecular docking interaction study with Covid-19 protease. Journal of the Indian Chemical Society, 2022, 99, 100605.	2.8	1