

# Poonam Rawat

## List of Publications by Year in descending order

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47  
papers

793  
citations

535685

17  
h-index

620720

26  
g-index

48  
all docs

48  
docs citations

48  
times ranked

653  
citing authors

#	ARTICLE	IF	CITATIONS
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1	Synthesis, spectral, structural and antimicrobial activities of		
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[Redacted]

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[Redacted]

[Redacted]

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[Redacted]

[Redacted]

#	ARTICLE	IF	CITATIONS
19	Experimental and DFT study on pyrrole tosylhydrazones. Journal of Molecular Structure, 2015, 1081, 543-554.	1.8	9
20	Experimental and DFT study on a newly synthesized ethyl 2-cyano-3-[5-(phenyl-hydrazonomethyl)-1H-pyrrol-2-yl]-acrylate. Journal of Molecular Structure, 2015, 1081, 293-303.	1.8	12
21	Synthesis, conformational, spectroscopic and chemical reactivity analysis of 2-cyano-3-(1H-pyrrol-2-yl)acrylohydrazide using experimental and quantum chemical approaches. Journal of Molecular Structure, 2015, 1082, 118-130.	1.8	13
22	Vibrational spectra, electronic absorption, nonlinear optical properties, evaluation of bonding, chemical reactivity and thermodynamic properties of ethyl 4-(1-(2-(hydrazinecarbonothioyl)hydrazono)ethyl)-3,5-dimethyl-1H-pyrrole-2-carboxylate molecule by ab initio HF and density functional methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 135, 1162-1168.	2.0	16
23	Evaluation of molecular assembly, spectroscopic interpretation, intra-/inter molecular hydrogen bonding and chemical reactivity of two pyrrole precursors. Journal of Molecular Structure, 2014, 1075, 462-470.	1.8	27
24	Quantum chemical study on influence of intermolecular hydrogen bonding on the geometry, the atomic charges and the vibrational dynamics of 2,6-dichlorobenzonitrile. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 121, 464-482.	2.0	35
25	A mixed experimental and DFT study on ethyl 4-[3-(4-dimethylamino-phenyl)-acryloyl]-3,5-dimethyl-1H-pyrrole-2-carboxylate. Journal of Molecular Structure, 2014, 1065-1066, 99-107.	1.8	20
26	Synthesis, characterization and computational study on ethyl 4-(3-Furan-2yl-acryloyl)-3,5-dimethyl-1H-pyrrole-2-carboxylate. Journal of Molecular Structure, 2014, 1076, 437-445.	1.8	16
27	Synthesis, molecular structure, photoluminescence, multiple interaction, chemical reactivity and first hyperpolarizability analysis of ethyl 2-cyano-3-[5-(4-methylbenzenesulfonyl)-hydrazonomethyl]-1H-pyrrol-2-yl]-acrylate: Experimental and quantum chemical approaches. Journal of Molecular Structure, 2014, 1061, 140-149.	1.8	13
28	Synthesis, spectroscopic and structural evaluation of ethyl 2-cyano-3-[5-[(4-nitro-benzoyl)-hydrazonomethyl]-1H-pyrrol-2-yl]-acrylate using experimental and theoretical approaches. Journal of Molecular Structure, 2013, 1049, 419-428.	1.8	17
29	Studies on molecular weaker interactions, spectroscopic analysis and chemical reactivity of synthesized ethyl 3,5-dimethyl-4-[3-(2-nitro-phenyl)-acryloyl]-1H-pyrrole-2-carboxylate through experimental and quantum chemical approaches. Journal of Molecular Structure, 2013, 1037, 338-351.	1.8	20
30	Synthesis, multiple interactions and spectroscopy analysis of ethyl-4-[(benzoyl)-hydrazonomethyl]-3,5-dimethyl-1H-pyrrole-2-carboxylate: Through experimental and quantum chemical approaches. Journal of Molecular Structure, 2013, 1035, 295-306.	1.8	11
31	Spectral analysis, structural elucidation, and evaluation of both nonlinear optical properties and chemical reactivity of a newly synthesized ethyl-3,5-dimethyl-4-[(toluenesulfonyl)-hydrazonomethyl]-1H-pyrrole-2-carboxylate through experimental studies and quantum chemical calculations. Journal of Molecular Structure, 2013, 1054-1055, 65-75.	1.8	25
32	Molecular structure, hydrogen-bonding, chemical reactivity and first hyperpolarizability analysis of a new synthesized 1,9-bis(2-cyano-2-ethoxycarbonylvinyl)-5-(2-nitrophenyl)-dipyrromethane: Experimental and theoretical (DFT and QTAIM) approach. Journal of Molecular Structure, 2013, 1052, 165-176.	1.8	2
33	Studies on molecular structure, spectral analysis, chemical reactivity and first hyperpolarizability of a newly synthesized 1,9-bis[(4-isonicotinoyl)-hydrazonomethyl]-5-phenyl-dipyrromethane using experimental and theoretical approaches. Journal of Molecular Structure, 2013, 1052, 67-75.	1.8	6
34	Study of spectroscopic, reactivity and NLO properties of synthesized dipyrromethane containing cyanovinylhydrazide using experimental and theoretical approaches. Journal of Molecular Structure, 2013, 1048, 448-459.	1.8	3
35	Synthesis, molecular structure, hydrogen-bonding, NBO and chemical reactivity analysis of a novel 1,9-bis(2-cyano-2-ethoxycarbonylvinyl)-5-(4-hydroxyphenyl)-dipyrromethane: A combined experimental and theoretical (DFT and QTAIM) approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 113, 378-385.	2.0	20
36	A combined experimental and quantum chemical (DFT and AIM) study on molecular structure, spectroscopic properties, NBO and multiple interaction analysis in a novel ethyl 4-[2-(carbamoyl)hydrazinylidene]-3,5-dimethyl-1H-pyrrole-2-carboxylate and its dimer. Journal of Molecular Structure, 2013, 1035, 427-440.	1.8	84

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37	Investigation of spectroscopic, structural and non-linear optical properties of ethyl 3,5-dimethyl-4-[(benzenesulfonyl)-hydrazonoethyl]-1H-pyrrol-2-carboxylate. <i>Journal of Molecular Structure</i> , 2013, 1054-1055, 123-133.	1.8	18
38	A combined experimental and quantum chemical studies on molecular structure, spectral properties, intra and intermolecular interactions and first hyperpolarizability of 4-(benzyloxy)benzaldehyde thiosemicarbazone and its dimer. <i>Journal of Molecular Structure</i> , 2013, 1034, 374-385.	1.8	4
39	A combined experimental and theoretical (DFT and AIM) studies on synthesis, molecular structure, spectroscopic properties and multiple interactions analysis in a novel Ethyl-4-[2-(thiocarbamoyl)hydrazinylidene]-3,5-dimethyl-1H-pyrrole-2-carboxylate and its dimer. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 112, 182-190.	2.0	62
40	Synthesis, molecular structure, multiple interactions and chemical reactivity analysis of a novel ethyl 2-cyano-3-[5-(hydrazinooxalylidene)hydrazonomethyl]-1H-pyrrol-2-yl]-acrylate and its dimer: A combined experimental and theoretical (DFT and QTAIM) approach. <i>Journal of Molecular Structure</i> , 2013, 1037, 420-430.	1.8	11
41	Synthesis, molecular structure, hydrogen-bonding and chemical reactivity analysis of 1,9-bis(2-cyano-2-ethoxycarbonylvinyl)-5-(2-chlorophenyl)-dipyrromethane: A combined experimental and theoretical approach. <i>Journal of Molecular Structure</i> , 2013, 1047, 169-178.	1.8	6
42	Synthesis, molecular structure, and spectral analyses of ethyl-4-[(2,4-dinitrophenyl)-hydrazonomethyl]-3,5-dimethyl-1H-pyrrole-2-carboxylate. <i>Structural Chemistry</i> , 2013, 24, 713-724.	1.0	21
43	Formation of 2-imino-malononitrile and diaminomaleonitrile in nitrile rich environments: A quantum chemical study. <i>Computational and Theoretical Chemistry</i> , 2012, 983, 7-15.	1.1	12
44	A computational study on conformational geometries, chemical reactivity and inhibitor property of an alkaloid bicuculline with [ $\beta$ ]-aminobutyric acid (GABA) by DFT. <i>Computational and Theoretical Chemistry</i> , 2012, 993, 80-89.	1.1	41
45	Molecular structure, heteronuclear resonance assisted hydrogen bond analysis, chemical reactivity and first hyperpolarizability of a novel ethyl-4-[(2,4-dinitrophenyl)-hydrazono]-ethyl]-3,5-dimethyl-1H-pyrrole-2-carboxylate: A combined DFT and AIM approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 92, 285-301.	2.0	32
46	Molecular structure, spectral studies, intra and intermolecular interactions analyses in a novel ethyl 4-[3-(2-chloro-phenyl)-acryloyl]-3,5-dimethyl-1H-pyrrole-2-carboxylate and its dimer: A combined DFT and AIM approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 94, 288-301.	2.0	27
47	Synthesis, molecular structure and spectral analysis of ethyl 4-formyl-3,5-dimethyl-1H-pyrrole-2-carboxylate thiosemicarbazone: A combined DFT and AIM approach. <i>Journal of Molecular Structure</i> , 2012, 1016, 97-108.	1.8	29