

Faculty Profile of Dr.R.Shankar



Dr.R.Shankar
Assistant Professor
Department of Physics

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Research Area

- 2D Materials for Energy and Environmental Applications
- Degradation of Hazardous Atmospheric Reactions
- Biomolecular interactions

Education & Career

Education

Ph. D.

Subject : Physics

Institution : Bharathiar University

Affiliated University : Bharathiar University

Year of Award : 2010

M.Phil.,

Subject : Physics

Institution : Bharathiar University

Affiliated University : Bharathiar University

Year of Award : 2006

M. Sc.,

Subject: Physics

Institution : Sri Ramakrishna Mission Vidyalaya College of Arts and Science

Affiliated University : Bharathiar University

Year of Award : 2004

B. Sc.,

Subject: Physics

Institution: Sri Ramakrishna Mission Vidyalaya College of Arts and Science

Affiliated University: Bharathiar University

Year of Award: 2002

Career**At Bharathiar University (Reverse Order)**

Assistant Professor : Oct- 2013 to till date

Assistant Professor : Feb- 2011 to Oct- 2013

Awards

1. Dr. APJ Abdul Kalam award for Scientific Excellence by MARINA Labs, India in 2016
2. DST Young Scientist Project award by DST, India in 2012
3. DST International Travel Grant (Rs. 95,000) by DST, India in 2011

4. Short Term Visiting by European Science Foundation (ESF-EMBO), Spain in 2011
5. Senior Research Fellow by CSIR, India in 2008
6. Short Term Visiting Fellowship by Gent University, Belgium in 2010
7. European Science Foundation (ESF-EMBO)

Membership

Visits

Country Visited : Spain

Duration of Visit : 2011

Purpose of Visit : Short term visiting

Country Visited : Belgium

Duration of Visit : 2010

Purpose of Visit : Short term visiting

Collaborators

Others

Projects

Funded Projects(National Level)

- [Ongoing - 01](#)
- [Completed - 02](#)

1. UGC-RUSA

Title of the project: Tailoring of new Silicon based electrode materials for the absorption of Na + , SO₂ and CO₂ towards Metal-Air Battery Applications

Funding Agency: UGC-RUSA, Government of India, New Delhi

Amount: Rs. 7.50 Lakhs

Duration: 2019-2020

2. DST

Title of the project: Quantum Chemical and Molecular Dynamics studies on DNA with Intercalators, Partial Intercalators and Groove Binding Molecules

Funding Agency: Department of Science and Technology, Government of India, New Delhi

Amount: Rs. 16.34 Lakhs

Duration: 2012-2016

1. UGC-RUSA

Title of the project : Molecular modeling and investigation of the binding mode of defected human nucleobases to sense tumor cells

Funding Agency : UGC-RUSA, Government of India, New Delhi

Amount : Rs. 21.88 Lakhs

Duration : 2020-2022

Consultancy Projects

- [Ongoing](#)
 - [Completed](#)
-

Research Guidance

- [Post Doc.](#)
- [Ph.D.](#)
- [M.Phil.](#)
- [M.Sc.](#)

Ongoing

Title

Name

Completed

Title

Name

Ongoing

Name of the candidate:

Title of the Thesis :

Date of Submission:

Date of Award:

Completed-03

Dr. S.Vinnarasai

Title of the Thesis : Theoretical investigation of G-Quadruplex DNA with Anti-Cancer Drugs for Targeted Drug Delivery and Two-Dimensional Nanomaterials for DNA Biosensors

Date of submission:

Date of Award: 2020

Dr. R.Akilan

Title of the Thesis : The First principle and Quantum Chemical Modeling of Carbon, Boron, nitrogen and Silicon based Two-Dimensional Adsorbent materials for Energy harvesting Applications

Date of Award: 2020

Dr. V.Saranya

Title of the Thesis : Role of Small molecules and metal ions in the promotion and inhibition mechanism of human Viral proteins-Molecular Dynamics and Quantum Chemical studies

Date of Award: 2020

Ongoing

Name of the candidate:

Title of the Thesis :

Date of Submission:

Date of Award:

Completed-07

S. Mohanapriya

Title of Thesis: Thermodynamic and kinetic studies on degradation of atmospheric isoprene (2-Methyl-1, 3-Butadiene) with chlorine radicals-A theoretical study

Year of Award: 2017

S. Kowsalya

Title of Thesis: Interaction studies of stacked G-tetrads with selected mono and divalent cations- A theoretical study

Year of Award: 2017

N. Venkat Sundaram

Title of Thesis: Kinetics and thermodynamics of reaction between. OH and O₃ with camphene (C₁₀H₁₆) - A theoretical investigation

Year of Award: 2016

M. Malarkodi

Title of Thesis: Electronic properties and surface assimilation of CO₂ and SO₂ gas molecules by defected and boron defected graphene sheets. A theoretical study

Year of Award: 2016

S. Kalaiyarasi

Title of Thesis: Structural and conformational analysis of Cu²⁺ and Zn²⁺ superoxide dismutase (SOD 1) protein – A molecular dynamics and quantum chemical studies

Year of Award: 2015

C. Elakiya

Title of Thesis: A theoretical study on the reaction mechanism and kinetics of allyl alcohol (CH₂CH=CH₂OH) with ozone (O₃) in the atmosphere

Year of Award: 2014

D. Thangamani

Title of Thesis: Mechanism and kinetics of the atmospheric degradation of 2-Formylcinnamaldehyde with ozone (O₃) and hydroxyl OH radicals – A theoretical study

Year of Award: 2012

Ongoing

Sample Data.

Completed-13

T. Vasuki

Title of Thesis: Ethane (C₂H₆) activation by polyatomic molybdenum carbide anion (MoC₃⁻) using computational study

Year of Award: 2019

G. Mohanapriya

Title of Thesis: The interaction between DNA/RNA base pair with double vacancy (5-8-5) and boron doped double vacancy (B-5-8-5): A quantum chemical approach

Year of Award: 2019

S. Monika

Title of Thesis: Theoretical studies on the first principle investigation on electronic and optical properties of structurally remodeled h-BCN sheets

Year of Award: 2019

J. Karthi

Title of Thesis: A theoretical investigation of stone-wales (55-77) defected and B, N doped graphene sheet

Year of Award: 2018

J. Pushpa

Title of Thesis: The surface imbibition of Lithium-ion on Si₂BN sheet: A theoretical exploration

Year of Award: 2018

V. Sowmiya

Title of Thesis: Theoretical studies on interaction of the normal and modified base pairs with pristine graphene sheet and Si-doped graphene sheet

Year of Award: 2017

K. Priyanka

Title of Thesis: Theoretical studies on the interaction of the base pairs (Guanine-Cytosine) with Naphthalimide drugs (Amonafide, Azonafide, 3-Nitro-1,8 Naphthalimide conjugated with nitrogen mustard)

Year of Award: 2017

D. Jamal Rifana

Title of Thesis: Molecular modeling investigation of 6-thio-2'-doxyguanosine with G-tetrad DNA's (SA-AABB and AA) - A theoretical study

Year of Award: 2016

S. Vimale

Title of Thesis: Interaction studies of Favipiravir and Brincidofovir on the N-loop region of Vp40 protein by using Molecular Dynamics Simulation studies

Year of Award: 2016

Farsana Ebrahim

Title of Thesis: A quantum chemical studies on active sites of Ebola virus (VP40) with transition metal ions (Ag²⁺ and Cu²⁺)

Year of Award: 2015

M. Mohanashankari

Title of Thesis: Atmospheric reaction mechanism of allyl alcohol (CH₂=CHCH₂OH) with ozone (O₃) using quantum chemical studies

Year of Award: 2015

T. Kavitha

Title of Thesis: Structural and spectroscopic aspects of 6-mercaptopurine anticancer drug interactions with normal and mismatch base pairs

Year of Award: 2014

M. Sakthivel

Title of Thesis: DFT and TDDFT studies on POLY (3,6 carbazole), poly (indol[3,2-b] carbazole) and their derivatives

Year of Award: 2014

Research Publication

- [International](#)
- [National](#)
- [Patents](#)
- [Conferences](#)
- [Books/Chapters](#)
- [Database](#)

Reverse Chronological Order

2021

66. [Epigenetically modified nucleobases \(5hmc, 5fc, and 5caC\) interaction with Boron and Nitrogen doped porous graphene \(B/N-pGr\) as promising materials for biosensing application: A Density Functional Theory calculations,](#)
[S.Vinnarasi R.Akilan,R. Shankar](#)
Environmental Research 197 (2021)

65. [Effect of doping on the opto-electronic properties of hollow spheroid ZnO quantum dots: A theoretical study](#)
S.Gopalakrishnan, R.Shankar, P. Kolandaivel
Materials Science and Engineering: B 270 (2021)
64. [ZnS quantum dots and Bi metals embedded with two dimensional \$\beta\$ -Bi₂O₄ nanosheets for efficient UV-visible light driven photocatalysis](#)
G.Palanisamy, K.Bhuvaneswari, T.Pazhanivel, R.Shankar, Khadijah M.Katubi, N. Alsaiani, M.Ouladsmane
Materials Research Bulletin 142 (2021)
63. [Polyene-metal complexes for use in molecular wire applications: a dft insight, AbhayRamBalakrishnan](#)
R.Shankar, S.Vijayakumar
Computational and Theoretical Chemistry 113328 (2021)
62. [Tuning the reactivity of tri-s-triazine, trinitro-tri-s-triazine and ternary tri-s-triazine graphitic C₃N₄ quantum dots through H-functionalized and B-doped complexes: A density functional study](#)
D.Ravichandran, R.Akilan, S.Vinnarasi, R. Shankar, S.Manickam
Chemosphere 272 (2021)
61. [A comprehensive experimental and computational study of highly efficient organic NLO crystal: Anilinium-L-Tartrate](#)
N. Sudha, R. Mathammal, R. Shankar, G. Sharon Benita
Optics and Laser Technology 137 (2021)
60. [Kinetics and degradation mechanism of atmospheric isoprene \(2-methyl-1, 3-butadiene \(C₅H₈\)\) with chlorine radical and its derivatives-A theoretical study](#)
S.Mohanapriya, R.Akilan, R. Shankar
International journal of Quantum Chemistry 121 (2021)
59. [Kinetics and degradation of camphene with OH radicals and its subsequent fate under atmospheric O₂ and NO radicals - A theoretical study](#)
S.Mohanapriya, S.Vinnarasi, J. Theerthagiri, S. Vijayakumar, T. Pazhanivel, R. Shankar

58. [Functionalized oligoynes: comparison of theoretical parameters with experimental single molecule conductance](#)

AbhayRamBalakrishnan, R. Shankar, S.Vijayakumar
Structural Chemistry 1 (2021)

57. [Enhancing thermoelectric performance of band structure engineered GeSe_{1-x}Te_x alloys](#)

D.Sidharth, AS.AlagarNedunchezian, R.Akilan, A. Srivastava,
B.Srinivasan, P. Immanuel, R.Rajkumar,
N.Yalini Devi, M.Arivanandhan, Chia-Jyi Liu, G.Anbalagan, R. Shankar,
R.Jayavel
Sustainable Energy & Fuels 5 (2021)

56. [Adsorption of H₂ molecules on B/N-doped defected graphene sheets—a DFT study](#)

R. Akilan , S. Vinnarasi, S. Mohanapriya and R. Shankar
Structural Chemistry 21 (2021)

2020

55. [Adsorption of H₂ and Co₂ gas molecules on li/na decorated si₂bn nano-sheet for energy harvesting applications—a density functional study](#)

R.Akilan, D.Ravichandran, S.Vinnarasi, R. Shankar
Materials Letters 279 (2020)

54. [Structural and electronic properties of graphene and its derivatives physisorbed by ionic liquids](#)

VS. Anithaa, R. Shankar, S.Vijayakumar
Diamond and Related Materials 109 (2020)

53. [Exploring the synergistic effect of NixSn₂xS₄x thiospinel with MWCNTs for enhanced performance in dye-sensitized solar cells, the hydrogen evolution reaction, and supercapacitors](#)

T.Saravanakumar, T.Selvaraju, KB.Bhojanaa, M. Ramesh, A.Pandikumar,
R.Akilan, R.Shankar
Dalton Transactions 49 (2020)

52. [Exploring two-dimensional graphene and boron-nitride as potential nanocarriers for cytarabine and clofarabine anti-cancer drugs](#)
S. Vinnarasi, R.Akilan, R.Shankar
Computational Biology and Chemistry 88 (2020)
51. [The hazardous effects of the environmental toxic gases on amyloid beta-peptide aggregation: A theoretical perspective](#)
V. Saranya, P.Violet Mary, S.Vijayakumar, R.Shankar
263 (2020)
50. [In silico studies of the inhibition mechanism of dengue with papain](#)
V.Saranya, R.Radhika, R. Shankar, S.Vijayakumar
Journal of Biomolecular Structure and Dynamics 1 (2020)
49. [Exploring the nature of interaction and stability between dna/rna base pairs and defective & defect-dopant graphene sheets. a possible insights on dna/rna sequencing](#)
S. Vinnarasi, R.Akilan, ,V.Saranya, R.Shankar
International Journals of Biological Macromolecules 146 (2020)
48. [Synthesis of self-assembled micro/nano structured manganese carbonate for high performance, long lifespan asymmetric supercapacitors and investigation of atomic-level intercalation properties of OH- ions via first principle calculation.](#)
M. Karuppaiah, R. Akilan, S Asaithambi, R. Yuvakkumar, R.Shankar, Y.Hayakawa, PN. Sakthive I, G. Ravi
Journal of Energy Storage 27 (2020)
47. [DFT approach on stability and conductance of nine different polyyne and cumulene molecules](#)
AR.Balakrishnan, R. Shankar, S.Vijayakumar
Molecular Physics 118 (2020)
46. [A novel phenyl and thiophenedispiroindenoquinolinepyrrolidine quinolones induced apoptosis via G1/S and G2/M phase cell cycle arrest in MCF-7 Cells](#)
S. Shyamsivappan, R.Vivek, A. Saravanan, T. Suresh, R. Shankar, P.S

.Mohan

New Journal of Chemistry 44 (2020)

45. [Ab initio studies of adsorption of haloarenes on heme group. Rahul Suresh](#)

R. Shankar, S. Vijayakumar

Journal of Molecular Modeling 6 (2020)

44. [Reconnoitring the nature of interaction and effect of electric field on Pd/Pt/Ni decorated 58-5/55-77 defected graphene sheet](#)

R.Akilan, S.Vinnarasi, R.Shankar

International Journal of Hydrogen Energy 45 (2020)

2019-2007

43. [Mechanistic insights into the inhibition mechanism of cysteine cathepsins by chalcone- based inhibitors- A QM cluster model approach](#)

P.V. Mary, R. Shankar, S. Vijayakumar

Structural Chemistry 30 (2019)

42. [Modelling of Si-B-N sheets and derivatives as a potential sorbent materials for absorption of Li⁺ ions and CO₂ gas molecule](#)

R.Akilan, S.Vinnarasi, S.Vijayakumar, R.Shankar

ACS Omega 4 (2019)

41. [Structural exploration of viral matrix protein 40 interaction with the transition metal ions \(Ag⁺ and Cu²⁺\)](#)

V.Sarnya, R. Shankar, S. Vijayakumar

Journal of Biomolecular Structure and Dynamics 37 (2019)

40. [Tetranuclearpalladacycles of 3-acetyl-7-methoxy-2 h -chromen-2-one derived schiff bases: efficient catalysts for suzuki-miyaura coupling in an aqueous medium](#)

S. DharaniGiriraj , K. Kalaiarasi, D.Sindhuja, R.Shankar,R. Karvembu, R.Prabhakaran

Inorganic Chemistry 58 (2019)

39. [Theoretical insights into the metal chelating and antimicrobial properties of the chalcone based Schiff bases](#)
P.V. Mary, S. Vijayakumar, R. Shankar
Molecular Simulation 45 (2019)
38. [Coumarin based hydrazone as an ICT -based fluorescence chemosensor for the detection of Cu²⁺ ions and the application in HeLa cells](#)
K.Saravana Mani, R.Rajamanikandan, B.Murugesapandian, R. Shankar, G.Sivaraman, M.Ilancheelian, S.P.Rajendran
Spectrochimica Acta Part A 214 (2019)
37. [Insights into structural and inhibitory mechanisms of low pH-induced conformational change of influenza HA2 protein: a computational approach](#)
S. Kannan, R. Shankar, P. Kolandaivel
Journal of Molecular Modeling 99 (2019)
37. [Structural insights into the anti-cancer activity of quercetin on G-tetrad, mixed G-tetrad, and G-quadruplex DNA using quantum chemical and molecular dynamics simulations](#)
S.Vinnarasi, R.Radhika, S.Vijayakumar, R. Shankar
38 (2019)
36. [Inhibition mechanism of cathepsin B by curcumin molecule: a DFT study](#)
C Pitchumani Violet Mary, S.Vijayakumar, R. Shankar
Theoretical Chemistry Accounts 138 (2019)
35. [Synthesis and x-ray study of dispiro 8-nitroquinolone analogues and their cytotoxic properties against human cervical cancer cells](#)
S. Shyamsivappan, R.Vivek, A. Saravanan, T. Arasakumar, G. Subashini, T. Suresh, R. Shankar, P.S. Mohan
Med ChemComm 10 (2019)
34. [Modeling of 2-D hydrogen-edge capped defected & boron-doped defected graphene sheets for the adsorption of CO₂, SO₂ towards energy harvesting applications](#)
R.Akilan, M.Malarkodi, S.Vijayakumar, S.Gopalakrishnan, R. Shankar
Applied Surface Science 463 (2019)

33. [Reduced bond length alternation and helical molecular orbitals in Donor and Acceptor substituted linear carbon chains](#)
B. Abhayram, S.Vijayakumar, R. Shankar
Journal of Theoretical and Computational Chemistry 17 (2018)
32. [DFT/TD-DFT study on halogen doping and solvent contributions to the structural and optoelectronic properties of poly \[3, 6-carbazole\] and poly \[indolo \(3, 2-b\)-carbazole\]](#)
S.Gopalakrishnan, S.Vijayakumar, R .Shankar
Structural Chemistry 29 (2018)
31. [A versatile “on-off-on” quinolinepyrazoline hybrid for sequential detection of Cu²⁺ and S²⁻ ions towards bio imaging and tannery effluent monitoring](#)
G.Subashini, A.Saravanan, S.Shyamsivappan, T.Arasakumar, V. Mahalingam, R.Shankar, P.S.Mohan
Inorganic Chimica Acta 483 (2018)
30. [D-A-D structured bis-acylhydrazone exhibiting aggregation induced emission, mechanochromic luminescence and al\(iii\) detection](#)
K. Santhiya, S. Sen, R. Natarajan, R. Shankar, B. Murugesapandian
Journal of Organic Chemistry 83 (2018)
29. [Role of 6-Mercaptopurine in the potential therapeutic targets DNA base pairs and G- quadruplex DNA: insights from Quantum chemical and Molecular dynamics simulations](#)
R.Radhika, R. Shankar, S .Vijayakumar, P.Kolandaivel
Journal of Bimolecular Structure and Dynamics 36 (2018)
28. [DFT/TD-DFT study on the electronic and spectroscopic properties of hollow cubic and hollow spherical \(ZnO\)_n quantum dots interacting with CO, NO₂ and SO₃ molecules](#)
S. Gopalakrishnan, R. Shankar, P. Kolandaivel
Applied Physics A 124 (2018)
27. [Theoretical studies on the interaction between the nitrile-based inhibitors and the catalytic triad of cathepsin](#)
K. P.V. Mary, R .Shankar, S.Vijayakumar
Journal of Bimolecular Structure and Dynamics 36 (2018)

26. [Metal chelating ability and antioxidant properties of Curcumin-metal complexes – A DFT approach](#)
P.V. Mary, R. Shankar, S.Vijayakumar
Journal of Molecular Graphics and Modeling 79 (2018)
25. [Theoretical investigation on hydrogen bond investigation of Diketo /Keto-enol form Uracil and Thymine](#)
[Tautomer's with Intercalators](#)
V.S Anithaa, R. Shankar, S.Vijayakumar
Journal of Molecular Modeling 23 (2017)
24. [DFT-based investigation on adsorption of methane on pristine and defected grapheme](#)
V.S.Anithaa, R. Shankar, S. Vijayakumar
Structural Chemistry 28 (2017)
23. [New pyrazolo-quinoline scaffold as a reversible colorimetric fluorescent probe for selective detection of](#)
[Zn²⁺ions and its imaging in live cells](#)
K. Gayathri, K. Velmurugan, R. Nandhakumar, P.S. Mohan, R.Shankar
Journal of Photochemistry and Photobiology A: Chemistry 341 (2017)
22. [Quinoline appended pyrazoline based Ni sensor and its application towards live cell Imaging and](#)
[environmental monitoring](#)
G. Subashini, R. Shankar, T. Arasakumar, PS Mohan
Sensors and Actuators B: Chemical 243 (2017)
21. [Comparative theoretical and experimental study on novel tri-quinoline system and its Anti-cancer studies](#)
K. Gayathri, R. Radhika, R. Shankar, M. Malathi, K. Savithiri, HA. Sparkes
Journal foMolecularstructure 1134 (2017)
20. [Theoretical study on the reaction mechanism and kinetics of Allyl alcohol \(CH₂=CHCH₂OH\) with ozone \(O₃\)](#)
[in the atmosphere](#)
C. Elakiya R. Shankar, S.Vijayakumar and P.Kolandaivel
Molecular Physics 115 (2017)
19. [Adsorption of Mn atom on pristine and defected graphene: a density](#)

[functional theory study](#)

V.S Anithaa, R. Shankar, S.Vijayakumar
Journal of Molecular Modelling 23 (2017)

18. [Growth and spectral analysis of piperazinium I-tartrate salt: A combined experimental and theoretical approach](#)

R. Mathammal, N. Sudha, R. Shankar, M. Rajaboopathi, S. Janagi
Journal of Molecular Structure, 1131,(2017),

17. [Synthesis of first ever 4-quinolone-3-carboxylic acid-appended spirooxindole-pyrrolidine derivatives and their biological applications](#)

T. Arasakumar, S.Mathusalini, Athar Ata, R. Shankar, G. Subashini K. Lakshmi, P. Sakthivel, P. S.Mohan
Molecular diversity, 21,(2017),

16. [Unpredicted formation of copper \(II\) complexes containing 2-thiophen-2-yl-1-thiophen-2-ylmethyl-1h-benzimidazole and most promising in vitro cytotoxicity in MCF-7 and HeLa cell lines over Cisplatin](#)

P. Naveen, Ruchi Jain, P. Kalaivani, R. Shankar, F. Dallemer and R. Prabhakaran
New Journal of Chemistry 41 (2017)

15. [Novel Synthetic and Mechanistic Approach of TFA Catalysed Friedländer Synthesis of 2-Acylquinolines from Symmetrical and Unsymmetrical 1, 2-Diketones with o-Aminoarylketones.](#)

R. Satheeshkumar, R. Shankar, W. Kaminsky, K.J. Rajendra Prasad
Chemistry Select 21 (2016)

14. [Mechanism and kinetics of the atmospheric degradation of 2-formylcinnamaldehyde with O₃ and hydroxyl OH radicals - a theoretical study](#)DThangamani

R Shankar, S Vijayakumar, P Kolandaivel
Molecular Physics 114 (2016)

13. [Interaction studies of human prion protein \(HuPrP109-111: methionine-lysine-histidine\) tripeptide model with](#)

transition metal cations

C Pitchumani Violet Mary, R Shankar, S Vijayakumar, P Kolandaivel
Journal of Molecular Graphics and Modelling 69 (2016)

12. Theoretical and experimental investigations on molecular structure of 7-Chloro-9- phenyl-2,3-

dihydroacridin-4 (1H)-one with cytotoxic studies

R Satheeshkumar, R Shankar, W .Kaminsky, S.Kalaiselvi, VV Padma
Journal of Molecular Structure 1109 (2016)

11. Synthesis of bisbenzimidazoquinoline fluorescent receptor for Fe²⁺ion in theAqueous medium–

An experimental and theoretical approach

M Mahalingam, M Irulappan, G Kasirajan, R.Shankar
Journal of Molecular Structure 1099 (2015)

10. Theoretical studies on interaction of anticancer drugs (dacarbazine, procarbazine and triethylenemelamine)

with normal (AT and GC) and mismatch (GG, CC, AA and TT) base pairs

R. Shankar, R.Radhika, D.Thangamani, L.Senthil Kumar, P.Kolandaivel
Molecular
Simulation 41 (2015)c

9. A strategic approach to the synthesis of novel class of dispiroheterocyclic derivatives through 1, 3 dipolar

cycloaddition of azomethineylide with (E)-3-arylidene-2, 3- dihydro-8-nitro-4-quinolone

K.Chandraprakash, M.Sankaran, C.Uvarani, R.Shankar, Athar. Ata, F.Dallemer, P. S. Mohan
Tetrahedron Letters 54 (2013)

8. Coordination and binding properties of zwitterionic metal cations glutathione with transition metal cations

R. Shankar, P. Kolandaivel, L. Senthil Kumar
InorganicaChimicaActa, 387,(2012)

7. A theoretical study on decomposition and rearrangement reaction mechanism of trichloroacetyl chloride

(CCl₃COCl)

R. Shankar, P .Kolandaivel, K.Senthilkumar

6. [Interaction of Cysteine with Li⁺, Na⁺, K⁺, Be²⁺, Mg²⁺ and Ca²⁺ Metal Cation Complexes](#)
R. Shankar, P. Kolandaivel and K. Senthilkumar
Journal of physical Organic Chemistry 24 (2011)
5. [Experimental and theoretical evaluation of dimerization mechanism in the synthesis of 7H-6, 8-dichloro-7-methylpyrano \[3, 2-b: 3', 2'-b'\] diquinoline](#)
M.MalathiR.Shankar, R.J Butcher, P,S. Mohan, P.Kolandaivel
Journal of Molecular Structure 979 (2010)
4. [Reaction mechanism of cystein proteases model compound HSH with diketone inhibitor PhCOCOCH₃-n X_n, \(X= F, Cl, n= 0, 1, 2\)](#)
R. Shankar, P. Kolandaivel and K. Senthilkumar
International Journal of Quantum Chemistry 110 (2010)
3. [Calculation of ionization potential and chemical hardness: a comparative study of different methods](#)
R. Shankar, K. Senthilkumar, P. Kolandaivel
International Journal of Quantum Chemistry 109 (2009)
2. [Reaction mechanism of O-acylhydroximate with cysteine proteases](#)
R.Shankar and P.Kolandaivel
Journal of Chemical Sciences 119 (2007)
1. [Molecular Interaction of H₂, N₂, and HF Molecules with the Silicon Carbide \(SiC\)_n= 5– 9 Clusters: A Theoretical Study](#)
R Shankar, P Kolandaivel, V.Nirmala, SK.Narayandass
Journal of Computational and Theoretical Nanoscience 4 (2007)

Reverse Chronological Order

2021

2020-2013

National Publications - Reverse Chronological Order

Patent Info

Conference Info

Books & Chapters Related Info

Database Related Info

Alumini Reflections: