Curriculum Vitae

Dr. Kunal Roy, PhD

Professor
Drug Theoretics and Cheminformatics Laboratory
& Head, Department of Pharmaceutical Technology, **Jadavpur University**
Kolkata 700 032 (INDIA)
E-mail : kunalroy_in@yahoo.com **,** kroy@pharma.jdvu.ac.in
URL : http://sites.google.com/site/kunalroyindia/ , http://www.jaduniv.edu.in/profile.php?uid=550

Formerly
Marie Curie International Incoming Fellow (2013-2015)
Manchester Institute of Biotechnology (MIB)
University of Manchester
131 Princess Street, Manchester M1 7DN (United Kingdom)

Formerly
Visiting Scientist
IRCCS - Istituto di Ricerche Farmacologiche Mario Negri,
Via La Masa, 19 - 20156 Milano, Italy

Co-Editor-in-Chief, *Molecular Diversity* (Springer) (http://www.springeronline.com/journal/11030/) [Impact Factor 2.013 (2019)]

Editor-in-Chief, *International Journal of Quantitative Structure-Property Relationships (IJQSPR)*, http://www.igi-global.com/journal/international-journal-quantitative-structure-property/126552

Member of the Editorial Advisory Board:
(1) *European Journal of Medicinal Chemistry* (Elsevier, http://www.elsevier.com/locate/ejmech/) [Impact Factor 5.572 (2019)]

(2) *Journal of Molecular Graphics and Modelling* (Elsevier, http://www.journals.elsevier.com/journal-of-molecular-graphics-and-modelling) [Impact factor 2.079 (2019)]

(3) Computational and Structural Biotechnology Journal (Elsevier, https://www.journals.elsevier.com/computational-and-structural-biotechnology-journal) [Impact Factor 6.018 (2019)]

(4) *Chemical Biology and Drug Design* (Wiley, http://onlinelibrary.wiley.com/journal/10.1111/(ISSN)1747-0285) [Impact Factor 2.548 (2019)]

(5) *Expert Opinion on Drug Discovery* (Informa, http://informahealthcare.com/loi/edc) [Impact Factor 4.421 (2018)]

(6) *Letters in Drug Design and Discovery* (Bentham, http://benthamscience.com/journal/index.php?journalID=lddd) [Impact Factor 1.169 (2019)]

(7) Current Computer-Aided Drug Design (Bentham, http://benthamscience.com/journals/current-computer-aided-drug-design/) [Impact Factor 0.935 (2019)]

Recipient of

Marie Curie International Incoming Fellowship (2013),
Commonwealth Academic Staff Fellowship (2007),
AICTE Career Award (2003-04),
DST Fast Track Scheme for Young Scientists (2005)
Bioorganic and Medicinal Chemistry Most Cited Paper 2003-2006, 2004-2007 and 2006-2009 Awards from Elsevier, The Netherlands.
Bioorganic and Medicinal Chemistry Letters Most Cited Paper 2006-2009 Award from Elsevier, The Netherlands.
Professor R. D. Desai 80th Birthday Commemoration Medal & Prize (2017), Indian Chemical Society

Educational Qualifications

B. Pharm (J. U. Gold Medalist) 1993
M.Pharm. (Pharm. Chem.) (J.U. Gold Medalist) 1995
Ph.D. (J.U.) 2000

Specialization : Medicinal and Pharmaceutical Chemistry
(Specific subject area of interest : QSAR and Molecular Modeling)

Medals and Awards

I. Professional life

* **Awarded Marie Curie International Incoming Fellowship (2013-2015)**
* **Awarded one of the 2003 FIP Development Grants by the International Pharmaceutical Federation, The Netherlands**
* **Received Career Award 2003-04 from All India Council for Technical Education, New Delhi, India**
* **Received DST Fast Track Scheme for Young Scientists (2005) (Department of Science and Technology, Govt. of India)**
* **Received Commonwealth Academic Staff Fellowship (2007)**
* **Received Bioorganic and Medicinal Chemistry Most Cited Paper 2003-2006, 2004-2007 and 2006-2009 Awards from Elsevier, The Netherlands.**
* **Received Bioorganic and Medicinal Chemistry Letters Most Cited Paper 2006-2009 Award from Elsevier, The Netherlands.**
* **Professor R. D. Desai 80th Birthday Commemoration Medal & Prize (2017), Indian Chemical Society**

II Academic life

A) Received **UNIVERSITY MEDAL** (Jadavpur University) and other medals for **standing FIRST in order of merit** in B. Pham Exam. 1993 (J. U.)

B) Received **UNIVERSITY MEDAL** (Jadavpur University) for **standing FIRST in order of merit** in M. Pham Exam. 1995 (J. U.)

Fields of Research Interest

1. Exploring QSARs of Ligands acting on Pharmacologically Relevant Targets of Contemporary Interest
2. Exploring QSARs of Antioxidants
3. Modeling of Physicochemical Properties of Organic Compounds
4. Exploring QSTRs of Chemicals and Environmental Pollutants
5. Modeling of Agrochemicals (insecticides, herbicides, plant growth regulators)
6. Exploring QSAR/QSPR/QSTR with Novel Extended Topochemical Atom (ETA) Indices developed in the Drug Theoretics Lab

Keywords: Chemometrics, QSAR, QSPR, QSTR

Publications

ResearcherID: B-1673-2009
ResearchGate: http://www.researchgate.net/profile/Kunal_Roy2/publications/
SCOPUS Author ID: 56962764800
Pubmed:http://www.ncbi.nlm.nih.gov/pubmed?term=(roy%20k%5BAuthor%5D)%20AND%20Jadavpur%5BAffiliation%5D
Mendeley: http://www.mendeley.com/profiles/kunal-roy/
Google scholar citation page: http://scholar.google.com/citations?user=j5iRuhwAAAAJ&hl=en
Publication list: http://publicationslist.org/kunalroy_in
ORCID: http://orcid.org/0000-0003-4486-8074
h index: 44 (SCOPUS)

The Extended Topochemical Atom (ETA) indices developed by the Drug Theoretics and Cheminformatics (DTC) Laboratory, Department of Pharmaceutical Technology, Jadavpur University (https://sites.google.com/site/etaindexingsar/) are now available for computation in PaDEL-Descriptor, an open source software of NUS, Singapore (http://www.yapcwsoft.com/dd/padeldescriptor/).

The DTC Lab has developed several QSAR tools, which are available from http://teqip.jdvu.ac.in/QSAR_Tools/ (Please see https://www.researchgate.net/publication/330383758_Quantitative_structure-activity_relationships_QSARs_A_few_validation_methods_and_software_tools_developed_at_the_DTC_laboratory_J_Indian_Chem_Soc_Vol_95_December_2018_pp_1497-1502)

(International publications are marked with *)

Books

1.* **Roy K**, Kar S, Das RN, Understanding the Basics of QSAR for Applications in Pharmaceutical Sciences and Risk Assessment, Academic Press, 2015, http://books.google.co.uk/books/reader?id=bkFOBQAAQBAJ&printsec=frontcover&output=reader&source=gbs_atb&pg=GBS.PA23 .

2.* **Roy K,** Kar S, Das RN, A Primer on QSAR/QSPR Modeling: Fundamental Concepts (SpringerBriefs in Molecular Science), Springer, 2015, http://www.springer.com/gp/book/9783319172804 .

Edited Books

1.* Roy K (editor), Quantitative Structure-Activity Relationships in Drug Design, Predictive Toxicology, and Risk Assessment, IGI Global, PA, 2015, http://www.igi-global.com/book/quantitative-structure-activity-relationships-drug/120080 .

2.* **Roy K (editor)**, Advances in QSAR Modeling. Applications in Pharmaceutical, Chemical, Food, Agricultural and Environmental Sciences. Springer, 2017, http://www.springer.com/in/book/9783319568492.

3* **Roy K (editor),** Computational Modeling of Drugs Against Alzheimer's Disease. Springer, 2018, http://www.springer.com/in/book/9781493974030

4.* **Roy K (editor),** Multi-Target Drug Design Using Chem-Bioinformatic Approaches, Springer, 2019, https://www.springer.com/us/book/9781493987320

5.* **Roy K (editor),** In Silico Drug Design: Repurposing Techniques and Methodologies, Academic Press, 2019, https://www.elsevier.com/books/in-silico-drug-design/roy/978-0-12-816125-8

6.* **Roy K (editor),** Ecotoxicological QSARs, 2020, https://www.springer.com/gp/book/9781071601495

.

7. **Roy K (editor),** In Silico Modeling of Drugs Against Coronaviruses, Springer 2021, https://www.springer.com/gp/book/9781071613658

1. **8.** **Roy K (editor),** Chemometrics and Cheminformatics in Aquatic Toxicology, Wiley 2021, https://www.wiley.com/en-in/Chemometrics+and+Cheminformatics+in+Aquatic+Toxicology-p-9781119681595

Book Chapters

1.* **Roy K,** Das RN, On Extended Topochemical Atom (ETA) Indices for QSPR Studies. In: Advanced Methods and Applications in Chemoinformatics: Research Progress and New Applications (E A Castro, A K Hagi, Eds.) IGI Global, PA, 2011, pp. 380-411, http://www.igi-global.com/bookstore/chapter.aspx?titleid=56464 .

2.* **Roy K**, Kar S, The r_m^2 Metrics for Validation of QSAR/QSPR Models. In: Chemometrics Applications and Research. QSAR in Medicinal Chemistry (AG Mercader, PR Duchowicz, PM Sivakumar, Eds) Apple Academic Press, New Jersey, USA, 2015 (forthcoming), http://www.appleacademicpress.com/title.php?id=9781771881135 .

3.* Aher RB, Ambure P, **Roy K**, On Some Emerging Concepts in the QSAR Paradigm. In: Current Applications of Chemometrics (M Khanmohammadi, Ed), Nova Science Publishers, USA, 2014, https://www.novapublishers.com/catalog/product_info.php?products_id=51763&osCsid=5e9a553a1b1129fed10cc0ad3598a587

4.* Ambure P, Aher RB, **Roy K**, Recent Advances in the Open Access Cheminformatics Toolkits, Software Tools, Workflow Environments, and Databases. In Methods in Pharmacology and Toxicology, Springer, 2015, http://link.springer.com/protocol/10.1007%2F7653_2014_35#page-1

5.* **Roy K**, Kar S, How to Judge Predictive Quality of Classification and Regression Based QSAR Models? In: Frontiers of Computational Chemistry (Zahir Ul Haq and J Madura, Eds), Bentham, 2015, 71-120, http://ebooks.benthamscience.com/book/9781608059782/chapter/128894/ .

6.* **Roy K**, Kar S, Importance of Applicability Domain of QSAR Models. In: Quantitative Structure-Activity Relationships in Drug Design, Predictive Toxicology, and Risk Assessment (Roy K, Ed), IGI Global, 2015, 180-211, http://dx.doi.org/10.4018/978-1-4666-8136-1.ch005 .

7.* **Roy K**, Das RN, The "ETA" Indices in QSAR/QSPR/QSTR Research. In: Quantitative Structure-Activity Relationships in Drug Design, Predictive Toxicology, and Risk Assessment (Roy K, Ed), IGI Global, 2015, 180-211, http://dx.doi.org/10.4018/978-1-4666-8136-1.ch002 .

8.* Roy PP, Ray S, **Roy K**, Application of GFA-MLR and G/PLS Techniques in QSAR/QSPR Studies with Application in Medicinal Chemistry and Predictive Toxicology. In: Handbook of Genetic Programming Applications (A H Gandomi, A H Alavi, C Ryan, Eds.) Springer, Heidelberg, 2015. pp. 501-529, http://dx.doi.org/10.1007/978-3-319-20883-1_20

9.* Roy K, Kar S, In Silico Models for Ecotoxicity of Pharmaceuticals. In *In Silico Methods for Predicting Drug Toxicity*, Methods in Molecular Biology, Vol. 1425 (Benfenati E, Ed), Springer, 2016, http://dx.doi.org/10.1007/978-1-4939-3609-0_12

10.* Ambure P, Roy K, Scoring Functions in Docking Experiments. In: Methods and Algorithms for Molecular Docking-Based Drug Design and Discovery (Dastmalchi, S., Hamzeh-Mivehroud, M., & Sokouti, B., Eds.) IGI Global, PA, 2016, http://dx.doi.org/10.4018/978-1-5225-0115-2.ch003

11.* Kar S, **Roy K**, Leszczynski J, On Applications of QSARs in Food and Agricultural Sciences: History and Critical Review of Recent Developments. In Advances in QSAR Modeling. Applications in Pharmaceutical, Chemical, Food, Agricultural and Environmental Sciences (Roy K, Ed.), Springer 2017, https://link.springer.com/chapter/10.1007/978-3-319-56850-8_7

12.* Kar S, **Roy K**, Leszczynski J, Applicability Domain: A Step Toward Confident Predictions and Decidability for QSAR Modeling. In Computational Toxicology (Nicolotti E, Ed), Springer, New York, 2018, pp. 141-169, https://link.springer.com/protocol/10.1007/978-1-4939-7899-1_6

13.* Kar S, **Roy K**, Leszczynski J, Impact of Pharmaceuticals on the Environment: Risk Assessment Using QSAR Modeling Approach. In Computational Toxicology (Nicolotti E, Ed), Springer, New York, 2018, pp. 395-443, https://link.springer.com/protocol/10.1007/978-1-4939-7899-1_19

14.* Ambure P, Roy K, Computer-Aided Drug Design for the Identification of Multi-Target Directed Ligands (MTDLs) in Complex Diseases: An Overview. In Pharmaceutical Biocatalysis (P Grunwald, ed.) Pan Stanford, 2019, http://www.panstanford.com/books/9789814800617.html#, https://www.amazon.com/Pharmaceutical-Biocatalysis-Fundamentals-Inhibitors-Diseases/dp/9814800619?ref_=nav_signin&

15.* Krishna JG, Ojha PK, **Roy K**, Chemometric Modeling of Absorption Maxima of Carbazole Dyes Used in Dye-Sensitized Solar Cells. In Challenges and Advances in Computational Chemistry and Physics (Leszczynski J, ed.), 32, 2021, 207–232, http://dx.doi.org/10.1007/978-3-030-69445-6_9

Research Papers and Review Articles (peer reviewed journals)

[http://sites.google.com/site/kunalroyindia/home/krlistofpublications]

1. **Roy K**, Rudra S, De A U & Sengupta C, ***Indian J Pharm Sci***, **60(3)**, 1998, 153.
2. **Roy K**, Rudra S, De A U & Sengupta C, ***Indian J Pharm Sci***, **61(1)**, 1999, 44.
3. **Roy K**, De A U & Sengupta C, ***Indian J Pharm Sci***, **61(2)**, 1999, 76.
4. **Roy K**, Pal D K, De A U & Sengupta C, ***Indian J Chem***, **38B**, 1999, 664.
5. **Roy K**, De A U & Sengupta C, ***Indian J Chem***, **38B**, 1999, 942.

6. **Roy K**, Pal D K, De A U & Sengupta C, ***Indian J Chem***, **38B**, 1999, 1194.
7. **Roy K**, Saha A, Chakraborty S & Sengupta C, ***Indian J Pharm Sci***, **62(1)**, 2000, 46.
8. Saha A, **Roy K**, De K & Sengupta C, ***Indian J Pharm Sci***, **62(2)**, 2000, 115.
9. **Roy K**, De A U & Sengupta C, ***Indian J Exp Biol***, **38**, 2000, 580.
10.* **Roy K**, Pal D K & Sengupta C, ***Drug Design and Discovery***, **17(2)**, 2000, 183.
11. **Roy K**, Pal D K & Sengupta C, ***J Indian Chem Soc***, **77(9)**, 2000, 428.
12. De K, **Roy K**, Saha A & Sengupta C, ***Indian J Pharm Sci***, **62(5)**, 2000, 343.
13.* **Roy K**, Pal D K, De A U & Sengupta C, ***Drug Design and Discovery,* 17(3), 2000**, 199.
14.* **Roy K**, Pal D K & Sengupta C, ***Drug Design and Discovery,* 17(3), 2000**, 207.
15. **Roy K**, Pal D K, De A U & Sengupta C, ***Indian J Chem,* 40B,** 2001, 129.
16.* **Roy K**, Saha A, De K & Sengupta C, ***Acta Polonie Pharmaceutica - Drug Research***, **57(5)**, 2000, 385.
17.* Saha A, **Roy K**, De K & Sengupta C, ***Acta Polonie Pharmaceutica - Drug Research***, **57(6)**, 2000, 441.
18. Saha A, **Roy K**, De K & Sengupta C, ***J Indian Chem Soc***, **78(2)**, 2000,92.
19. **Roy K**, Pal D K, Ghosh C C, De A U & Sengupta C***, Indian J Chem,* 40B, 2001**, 209.
20. **Roy K**, Pal D K, Saha A & Sengupta C, ***Indian J Chem,* 40B,** 2001, 587.
21.* **Roy K**, Pal D K, De A U & Sengupta C, ***Drug Design and Discovery,* 17,** 2001, 315.
22. **Roy K**, ***Indian J Chem,* 40B,** 2001, 688.
23. **Roy K**, Sengupta C & De A U, ***J Sci Ind Res,* 60,** 2001, 699.
24. Saha A, **Roy K**, De K & Sengupta C, ***Indian J Pharm Sci,* 63**, 2001, 317.
25. De K, **Roy K**, Saha A & Sengupta C, ***Indian Pharm Sci,* 63(5),** 2001, 379.
26.* **Roy K**, De A U & Sengupta C, ***Quant. Struct-Act Relat,* 20(4),** 2001, 319**.**
27.* De K, **Roy K**, Saha A & Sengupta C, ***Acta Pol. Pharm. - Drug Res***., **58(5**), 2001, 391.
28.* Saha A, **Roy K**, De K & Sengupta C, ***Acta Pol Pharm - Drug Res***, **59**, 2002, 65.
29. Saha A, Roy K, De K & Sengupta C, ***Indian J Chem,* 41B**, 2002, 1268.
30.* **Roy K**, De A U & Sengupta C, ***Drug Des Discov***, **18**, 2002, 23.
31.* **Roy K**, De A U & Sengupta C, ***Drug Des Discov***, **18**, 2002, 33.
32.* **Roy K**, Saha A, De K & Sengupta C, ***Acta Pol Pharm,* 59**, 2002, 231.
33. De K, **Roy K**, Saha A & Sengupta C, ***J. Indian Chem. Soc.,* 79**, 2002, 513.
34.* Mallick S, **Roy K**, Chakraborty A & Saha S, ***Acta Pol Pharm,* 59**, 2002, 193.
35. Saha A, **Roy K**, De K & Sengupta C, ***Indian J Pharm Sci,* 65**, 2003, 171.
36.* **Roy K** & Saha A, ***Internet Electron J Mol Des,* 2**, 2003, 288, http://www.biochempress.com .
37. **Roy K**, ***Indian J Chem,* 42B**, 2003, 1485.
38. **Roy K**, De A U & Sengupta C, ***Indian J Biochem Biophys***, **40**, 2003, 203.
39.* **Roy K**, *Quant Struct-Act Relat*, **22**, 2003**,** 614..
40.* **Roy K** & Saha A, ***J Mol Model,* 9**, 2003, 259; Epub 20 June 2003, DOI 10.1007/s00894-003-0135-z
41.* **Roy K** & Saha A, ***Internet Electron J Mol Des,* 2**, 2003, 475, http://www.biochempress.com .
42.* **Roy K**, Chakraborty S & Saha A, ***Bioorg Med Chem Lett***, **13**, 2003, 3753-3757.
43.* **Roy K** & Ghosh G, ***Internet Electron J Mol Des,* 2**, 2003, 599, http://www.biochempress.com .
44. **Roy K**, Chakraborty S, Ghosh C C & Saha A, ***J Indian Chem Soc,* 81**, 2004 , 115-125.
45.* Leonard, J T & **Roy K**, ***QSAR Comb Sci***, **23**, 2004, 23-35.
46.* **Roy K** & Leonard J T, ***Bioorg Med Chem***, **12**, 2004, 745-754.
[Received *Bioorganic and Medicinal Chemistry Most Cited Paper 2003-2006 and 2004-2007 Awards from Elsevier, Oxford, UK*]
47.* Toropov A A & **Roy K**, ***J. Chem. Inf. Comput. Sci.***, **44**, 2004, 179-186.
48.* **Roy K** & Ghosh G, ***J. Chem. Inf. Comput. Sci.***, **44**, 2004, 559-567.
49.* **Roy K** & Ghosh G, ***QSAR Comb Sci,,* 23**, 2004, 99-108.
50.* De K, Sengupta C, **Roy K**, ***Bioorg Med Chem* 12**, 2004, 3323-3332.
51.* De K, **Roy K**, Saha A, Sengupta A, ***Acta Pol Pharm,* 61**, 2004, 81.
52.* Sengupta C, Leonard J T, **Roy K**, ***Bioorg Med Chem Lett***, **14**, 2004, 3435-3439.
53.* **Roy K**, Leonard J T, Sengupta C, ***Bioorg Med Chem Lett***, **14**, 2004, 3705-3709.
54.* Chakraborty S, Sengupta C, **Roy K**, ***Bioorg Med Chem Lett***, **14**, 2004, 4665-4670.

55.* Leonard J T, **Roy K,** ***QSAR Comb Sci,*** **23**, 2004, 387-398.

56. **Roy K** & Saha A, ***Indian J Chem***, **43A**, 2004, 1369-1376.

57.* Leonard J T & **Roy K**, ***Drug Des Dicov***, 18, **2003**, 165-180.

58.* Ray S, Sengupta C & **Roy K**, ***Acta Pol Pharm,*** **62**, 2005, 145-152.

59.* Chakraborty S, Dev Bhuti P, Ray S, Sengupta C & **Roy K**, ***Acta Pol Pharm,*** **62**, 2005, 141-143.

60.* **Roy K** & Ghosh G, ***QSAR Comb Sci,*** **23,** 2004, 387-398.526-535.

61.* **Roy K** & Toropov A A, ***J Mol Model,*** 2005, 89-96. http://dx.doi.org/10.1007/s00894-004-0224-7

62.* **Roy K** & Ghosh G, ***Bioorg Med Chem*** **13**, 2004, 1185-1194. http://dx.doi.org/10.1016/j.bmc.2004.11.014

63.* Bhattacharya P, Leonard J T & **Roy K**, ***Bioorg Med. Chem.*** **13**, 2004, 1159-1165. http://dx.doi.org/10.1016/j.bmc.2004.11.022

64.* **Roy K**, (Guest Editorial). ***Mol Divers***, **8**, 2004, 321-323. http://dx.doi.org/10.1023/B:MODI.0000047519.35591.b7

65.* Bhattacharya P, Leonard J T & **Roy K**, ***J Mol Model*** **11,** 2005**,** 516-524. http://dx.doi.org/10.1007/s00894-005-0273-6

66.* Mukherjee S, Saha A & **Roy K**, ***Bioorg Med. Chem. Letters,*** **15,** 2005, 957-961. http://dx.doi.org/10.1016/j.bmcl.2004.12.048

67.* **Roy K** & Leonard J T, QSAR by LFER Model of Cytotoxicity Data of Anti-HIV 5-phenyl-1-phenylamino-1*H*-imidazole Derivatives Using Principal Component Factor Analysis and Genetic Function Approximation. ***Bioorg Med Chem*** **13**, 2005, 2967-2973. doi:10.1016/j.bmc.2005.02.003

68.* **Roy K**, Leonard J T, ***QSAR Comb Sci*** **24,** 2005, 579-592**,** http://dx.doi.org/10.1002/qsar.200430901

69. Chakraborty S, Sengupta C & **Roy K,** ***Indian J Biochem Biophys*** **42**, 2005, 106-112.

70.* Bhattacharya P & **Roy K**, ***Bioorg Med. Chem Lett.,*** **15,** 2005**,** 3737-3743, http://dx.doi.org/10.1016/j.bmcl.2005.05.051

71.* **Roy K** & Lenard J T, ***J Chem Inf Model,*** **45**, 2005, 1352-1368, http://dx.doi.org/10.1021/ci050205x

72.* Leonard J T & **Roy K**, ***Bioorg Med Chem,*****14,** 2005, 1039-1046, http://dx.doi.org/10.1016/j.bmc.2005.09.022 ***[Bioorganic and Medicinal Chemistry Most Cited Paper 2006-2009 Award from Elsevier, The Netherlands]***

73. **Roy K** & Saha A, ***Indian J Chem,*** **44B**, 2005, 1693-1707, http://nopr.niscair.res.in/bitstream/123456789/9155/1/IJCB%2044B%288%29%201693-1707.pdf

74.* Leonard J T and **Roy K**, ***QSAR Comb Sci,*** **25**, 2006, 235-251, http://dx.doi.org/10.1002/qsar.200510161 .

75.* **Roy K** and Ghosh G, ***J. Mol. Model, 12,*** 2006, 306-316, http://dx.doi.org/10.1007/s00894-005-0033-7 .

76.* **Roy K** and Sanyal I., ***QSAR Comb Sci,*** **25**, 2006, 359-371, http://dx.doi.org/10.1002/qsar.200530172 .

77.* Leonard J T and **Roy K**, ***Curr Med Chem,*** **13,** 2006, 911-934. http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?cmd=Retrieve&db=pubmed&dopt=Abstract&list_uids=16611075&query_hl=6&itool=pubmed_docsum

78. **Roy K** & Leonard J T, ***Indian J Chem,*** **45A,** 2006, 126-137.

79. **Roy K** & Saha A, ***J Indian Chem Soc,*** **83,** 2006**,** 351-355**.**

80.* **Roy K** & Ghosh G, ***QSAR Comb Sci,*** **25**, 2006, 846-859. http://dx.doi.org/10.1002/qsar.200510211 .

81.* De K, **Roy K**, Sengupta C, ***Acta Pol Pharm,*** **62**, 2005, 257-264.

82. Dalai M K, Leonard J T & **Roy K**, ***Indian J Biochem Biophys***, **43**, 2006, 105-118.

83. Ray S, **Roy K** & Sengupta C, ***Indian J Pharm Sci,*** **68**, 2006, 199-204. http://www.ijpsonline.com/article.asp?issn=0250-474X;year=2006;volume=68;issue=2;spage=199;epage=204;aulast=Ray;type=0

84.* Leonard J T & **Roy K**, ***Bioorg Med Chem Lett***, **16**, 2006, 4467-4474 doi:10.1016/j.bmcl.2006.06.031 . ***[Bioorganic and Medicinal Chemistry Letters Most Cited Paper 2006-2009 Award from Elsevier, The Netherlands]***

85.* **Roy K**, ***Mol Divers,*** **10,** 2006, 93-94. http://dx.doi.org/10.1007/s11030-006-9025-5 .

86.* **Roy K**, Toropov A and Raska I Jr, ***QSAR Comb Sci,*** **26**, 2007, 460-468, http://dx.doi.org/10.1002/qsar.200630072.

87.* **Roy K**, Sanyal I and Roy P P, ***SAR QSAR Environ Res,*** **17**, 2006, 563-582. http://dx.doi.org/10.1080/10629360601033499.

88.* **Roy K**, Sanyal I and Ghosh G, ***QSAR Comb Sci,*** **26**, 2007, 629-646, http://dx.doi.org/10.1002/qsar.200610112

89. Dalai M K, Leonard J T and **Roy K**, ***Indian J Chem,*** **45B,** 2006, 2497-2505.

90.* Leonard J T and **Roy K**, ***Eur J Med Chem***, **43**, 2008, 81-92**,** http://dx.doi.org/10.1016/j.ejmech.2007.02.021 .

91.* Leonard J T and **Roy K**, ***QSAR Comb Sci*****, 26**, 2007**,** 980-990, http://dx.doi.org/10.1002/qsar.200630140.

92. **Roy K** and Dalai M K, ***Indian J Biochem Biophys*****, 44,** 2007, 114-121. http://www.niscair.res.in/ScienceCommunication/ResearchJournals/rejour/ijbb/ijbb2k7/ijbb_april07.asp#a8

93. Chakraborty S, Sengupta C & **Roy K**, ***Indian J Biochem Biophys,* 44**, 2007, 169-175.

94.* Roy P P & **Roy K**, ***QSAR Comb Sci*****, 27,** 2008, 302-313**,** http://dx.doi.org/10.1002/qsar.200710043 .

95.* Chakraborty S, **Roy K** & Sengupta C, ***Acta Pol Pharm*****, 64**, 2007, 211-216.

96.* De K, **Roy K** & Sengupta C, ***Acta Pol Pharm*****, 64**, 2007, 201-210.

97. Ray S, **Roy K** & Sengupta C, ***Indian J Pharm Sci***, **69**, 2007, 190-196. http://www.ijpsonline.com/article.asp?issn=0250-474X;year=2007;volume=69;issue=2;spage=190;epage=196;aulast=Ray;type=0

98.* **Roy K** & Ghosh G, ***Chemosphere*****, 70,** 2007, 1-12. http://dx.doi.org/10.1016/j.chemosphere.2007.07.037

99. Ray S, **Roy K** & Sengupta C, ***Indian J Pharm Sci,* 69**, 2007, 378-383, http://www.ijpsonline.com/article.asp?issn=0250-474X;year=2007;volume=69;issue=3;spage=378;epage=383;aulast=Ray;type=0

100.* Roy P P, Leonard J T & **Roy K**, ***Chemom Intell Lab Sys,* 90,** 2008, 31-42, http://dx.doi.org/10.1016/j.chemolab.2007.07.004.

101.* Ray S, Sengupta C, **Roy K**, ***Central Eur J Chem***, **5**, 2007 1094-1113, http://dx.doi.org/10.2478/s11532-007-0047-3 .

102* **Roy K**, ***Expert Opin Drug Discov*****, 2**, 2007, 1567-1577, http://dx.doi.org/10.1517/17460441.2.12.1567 .

103.***** **Roy K,** Mandal A S, ***J Enz Inh Med Chem***, **23**, 2008, 980-995, http://dx.doi.org/10.1080/14756360701811379 .

104.* Ray S, Sengupta C & **Roy K**, ***Central Eur J Chem*****, 6**, 2008**,** 267-276, http://dx.doi.org/10.2478/s11532-008-0014-7 .

105.* **Roy K** & Mandal A S, ***J Enz Inh Med Chem,* 24,** 2009, 205-223, http://dx.doi.org/10.1080/14756360802051297 .

106.* **Roy K** & Roy P P, ***Chem Biol Drug Des,* 71,** 2008, 464-473, http://dx.doi.org/10.1111/j.1747-0285.2008.00658.x .

107.* **Roy K** & Popelier P L A, ***Bioorg Med Chem Lett,* 18**,2008, 2604–2609, http://dx.doi.org/10.1016/j.bmcl.2008.03.035 .

108.* **Roy K** & Popelier P L A, ***QSAR Comb Sci***, **27**, 2008, 1006-1012, http://dx.doi.org/10.1002/qsar.200810028 .

109. Ray S, De K, Sengupta C & **Roy K**, ***Indian J Biochem Biophys*****, 45,** 2008, 198-205.

110.* Mandal A S & **Roy K**,. ***Eur J Med Chem,* 44,** 2009, 1509-1524, http://dx.doi.org/10.1016/j.ejmech.2008.07.020 .

111.* **Roy K** & Popelier P, ***J Phys Org Chem*****, 22,** 2009, 186-196, http://dx.doi.org/10.1002/poc.1447.

112.* **Roy K** & Ghosh G, ***Chem Biol Drug Des*****, 72,** 2008, 383-394, http://dx.doi.org/10.1111/j.1747-0285.2008.00712.x .

113.* **Roy K** & Roy PP, ***Chem Biol Drug Des*****, 72,** 2008, 370-382, http://dx.doi.org/10.1111/j.1747-0285.2008.00717.x .

114.* **Roy K** & Roy PP, ***Eur J Med Chem*****, 44,** 2009, 1941-1951, http://dx.doi.org/10.1016/j.ejmech.2008.11.010 .

115.* **Roy K**, Paul S, ***QSAR Comb Sci*****, 28**, 2009, 406-425, http://dx.doi.org/10.1002/qsar.200810130 .

116.* **Roy K** & Roy PP, ***Eur J Med Chem*****, 44,** 2009, 2913-2922, http://dx.doi.org/10.1016/j.ejmech.2008.12.004 .

117.* **Roy K**, Ghosh G, ***Molecular Simulation,* 35,** 2009, 648-659, http://dx.doi.org/10.1080/08927020902744664 .

118.* Roy P P & **Roy K**, ***Chem Biol Drug Des,* 73,** 2009, 442-455, http://dx.doi.org/10.1111/j.1747-0285.2009.00791.x**.**

119.* Mitra I, Saha A, **Roy K**, ***Chem Biol Drug Des,* 73,** 2009, 526-536, http://dx.doi.org/10.1111/j.1747-0285.2009.00801.x**.**

120.* Mitra I, **Roy K**, Saha A, ***J Comput Chem***, **30**, 2009, 2712-2722, http://dx.doi.org/10.1002/jcc.21298

121.* Roy PP, Paul S, Mitra I, **Roy K**, ***Molecules,* 14,** 2009, 1660-1701, http://dx.doi.org/10.3390/molecules14051660.
This publication is freely downloadable from http://www.mdpi.com/1420-3049/14/5/1660 .

122.* **Roy K**, Ghosh G, ***Molecular Simulation,* 15,** 2009, 1256-1268, http://dx.doi.org/10.1080/08927020903015379 .

123.* **Roy K**, Paul S, ***J Mol Model*, 16,** 2010, 137-153, http://dx.doi.org/10.1007/s00894-009-0528-8 .
124.* Roy PP, **Roy K**, ***J Enz Inhib Med Chem*, 25,** 2010, 354-369, http://dx.doi.org/10.3109/14756360903179476**.**
125.* **Roy K**, Roy PP, ***Expert Opin Drug Metabol Toxicol*, 5,** 2009, 1245-1266, http://dx.doi.org/10.1517/17425250903158940 .
126.* **Roy K**, Ghosh G, ***Chemosphere*, 77,** 2009, 999-1009**,** http://dx.doi.org/10.1016/j.chemosphere.2009.07.072.
127.* **Roy K**, Mitra I, Saha A, ***Chem Biol Drug Des*, 74,** 2009, 507-516, http://dx.doi.org/10.1111/j.1747-0285.2009.00888.x **.**
128.* **Roy K**, Mitra I, ***Expert Opin Drug Discov*, 4,** 2009, 1157 – 1175, http://dx.doi.org/10.1517/17460440903307409 .
129.* **Roy K**, Paul S, ***J Mol Model*, . *J Mol Model*, 16,** 2010, 951-964, http://dx.doi.org/10.1007/s00894-009-0596-9 **.**
130.* Mitra I, Roy PP, Kar S, Ojha P, **Roy K, *J Chemometrics*, 24,** 2010, 22-33, http://dx.doi.org/10.1002/cem.1268
131.* Roy PP, **Roy K**, ***Molecular Simulation*, 36,** 2010, 311-325 http://dx.doi.org/10.1080/08927020903426493 .
132.* Kar S, **Roy K**, ***J Hazard Mater*, 177,** 2010, 344-351**,** http://dx.doi.org/10.1016/j.jhazmat.2009.12.038.
133.* Kar S, Harding AP, **Roy K**, Popelier P, ***SAR QSAR Environ Res*, 21**, 2010, 149 - 168**,** http://www.informaworld.com/10.1080/10629360903568697 .
134.* Begum NA, Roy N, Laskar RA, **Roy K**, ***Med Chem Res*, 20,** 2011, 184-191, http://dx.doi.org/10.1007/s00044-010-9305-6 .
135.* Mitra I, Saha A, **Roy K**, . ***J Mol Model*, 16,** 2010, 1585-1596, http://dx.doi.org/10.1007/s00894-010-0661-4 .
136.* Roy PP, **Roy K**, ***J Mol Model*, 16,** 2010, 1597-1616, http://dx.doi.org/10.1007/s00894-010-0667-y .
137.* Ray S, Roy PP, Sengupta C, **Roy K**, ***Molecular Simulation*, 36**, 2010, 484–492**,** http://dx.doi.org/10.1080/08927021003664058**.**
138.* Roy PP, **Roy K**, ***Molecular Simulation*, 36,** 2010, 887-905, http://dx.doi.org/10.1080/08927022.2010.492834 **.**
139.* Ojha PK, **Roy K**, ***Molecular Simulation*, 36,** 2010, 939-952, http://dx.doi.org/10.1080/08927022.2010.492835 **.**
140.* Roy PP, **Roy K**, ***J Pharm Pharmacol*, 62,** 2010, 1717-1728, http://dx.doi.org/10.1111/j.2042-7158.2010.01154.x.
141.* **Roy K**, Ojha PK, ***Expert Opin Drug Discov Expert Opin Drug Discov* 5,** 2010, 751-778, http://dx.doi.org/10.1517/17460441.2010.497812
142.* Mitra I, Saha A, **Roy K**, ***Molecular Simulation* 36,** 2010, 1067-1079, http://dx.doi.org/10.1080/08927022.2010.503326 .
143.* **Roy K**, Ghosh G, ***Current Pharm Des*, 16,** 2010, 2625-2639**,** http://www.bentham.org/cpd/contabs/cpd16-24.html, http://www.benthamdirect.org/pages/b_viewarticle.php?3161953 .
144.* **Roy K**, Kar S, ***Chemosphere*, 81,** 2010, 738-747, http://dx.doi.org/10.1016/j.chemosphere.2010.07.019 .
145.* Ojha PK, **Roy K**, ***Eur J Med Chem* 45**, 2010, 4645-4656, http://dx.doi.org/10.1016/j.ejmech.2010.07.034 .
146.* **Roy K**, Das RN, ***J Hazard Mater* 183**, 2010, 913-922, http://dx.doi.org/10.1016/j.jhazmat.2010.07.116
147.* Mitra I, Saha A, **Roy K**, ***Eur J Med Chem* 45,** 2010, 5071-5079, http://dx.doi.org/10.1016/j.ejmech.2010.08.016 .
148.* Prankishore D, Balakumar C, Raghuram Rao A, Roy PP, **Roy K**, ***Bioorg Med Chem Lett* 21,** 2011, 930-935, http://dx.doi.org/10.1016/j.bmcl.2010.11.094.
149.* Mitra I, Saha A, **Roy K**, ***Molecular Simulation* 37,** 2011, 394-413**,** http://dx.doi.org/10.1080/08927022.2010.543980 .
150.* Mitra I, Saha A, **Roy K**, ***Scientia Pharmaceutica* 79,** 2011, 31-57, http://dx.doi.org/10.3797/scipharm.1011-02 .
151.* Ojha P K, **Roy K**, ***Molecular Simulation* 37,** 2011, 779-803, http://dx.doi.org/10.1080/08927022.2010.548384
152.* **Roy K**, Das R N, ***SAR QSAR Environ Res* 22,** 2011, 451-472, http://dx.doi.org/10.1080/1062936X.2011.569900
153. Kar S, **Roy K**, ***J Indian Chem Soc* 87,** 2010, 1455-1515, http://indianchemsoc.org/journals/dec10.pdf .
154. Kar S, **Roy K**, ***Indian J Biochem Biophys* 48,** 2011, 111-122, http://nopr.niscair.res.in/bitstream/123456789/11614/1/IJBB%2048%282%29%20111-122.pdf .
155.* Ojha PK, Mitra I, Das R, **Roy K**, ***Chemom Intell Lab Syst* 107,** 2011, 194-205, http://dx.doi.org/10.1016/j.chemolab.2011.03.011

156.* Ojha PK, **Roy K**, ***Medicinal Chemistry*, 7,** 2011, 173-199, http://www.benthamdirect.org/pages/content.php?MC/2011/00000007/00000003/D0004C.SGM

157.* **Roy K,** Mitra I, ***Comb Chem High Throughput Screen*, 14,** 2011, 450-474, [Invited Review Article], http://www.ncbi.nlm.nih.gov/pubmed/21521150, http://www.benthamdirect.org/pages/content.php?CCHTS/2011/00000014/00000006/0003A.SGM

158.* Mitra I, Saha A, **Roy K,** ***J Mol Model* 18,** 2012, 1819-1840, http://dx.doi.org/10.1007/s00894-011-1198-x .

159.* Ojha PK, **Roy K**, ***Chemom Intell Lab Sys*, 109,** 2011, 146-161, http://dx.doi.org/10.1016/j.chemolab.2011.08.007 .

160.* **Roy K**, Das RN, ***SAR QSAR Environ Res* 23,** 2012, 125-140, http://dx.doi.org/10.1080/1062936X.2011.645872 **.**

161.* Kar S, **Roy K**, ***Expert Opin Drug Saf* 11,** 2012, 235-274, http://dx.doi.org/10.1517/14740338.2012.644272 **.**

162.* Kar S, **Roy K**, ***Chemosphere*, 87,** 2012, 339-355, http://dx.doi.org/10.1016/j.chemosphere.2011.12.019.

163.* **Roy K**, Mitra I, Kar S, Ojha PK, Das RN, Kabir H, ***J Chem Inf Model*, 52,** 2012, 396-408, http://pubs.acs.org/doi/abs/10.1021/ci200520g .

164.* **Roy K**, Kabir H, ***Chem Engg Sci* 73,** 2012, 86-98, http://dx.doi.org/10.1016/j.ces.2012.01.005 .

165.* Mitra I, Saha A, **Roy K**, ***J Mol Model* 18,** 2012, 3951-3967, http://dx.doi.org/10.1007/s00894-012-1392-5 .

166.* Mitra I, **Roy K**, ***Mini Rev Med Chem* 12,** 2012, 491-504, http://www.benthamdirect.org/pages/content.php?MRMC/2012/00000012/00000006/0006N.SGM .

167.* Mitra I, **Roy K**, ***Curr Comp Aid Drug Des* 8,** 2012, 135-158, http://www.benthamdirect.org/pages/content.php?CAD/2012/00000008/00000002/D0007AD.SGM .

168.* Kar S, Deeb O**, Roy K**, ***Ecotox Environ Saf* 82,** 2012, 85-95, http://dx.doi.org/10.1016/j.ecoenv.2012.05.013

169.* **Roy K**, Das RN, ***Struc Chem* 24,** 2013, 303-331, http://dx.doi.org/10.1007/s11224-012-0080-5 .

170.* **Roy K**, Mitra I, Ojha PK, Kar S, Das RN, Kabir H, **118,** 2012, 200-210, http://dx.doi.org/10.1016/j.chemolab.2012.06.004 .

171.* Das RN, **Roy K**, ***Toxicol Res* 1,** 2012, 186-195, http://dx.doi.org/10.1039/C2TX20020A .

172.* **Roy K**, Kabir H, ***Chemical Engineering Science*, 81,** 2012, 169-178, http://dx.doi.org/10.1016/j.ces.2012.07.008 .

173.* Kar S, **Roy K**, ***Expert Opin Drug Discov*, 2012,** 7, 877-902, http://dx.doi.org/10.1517/17460441.2012.716420 .

174.* Ojha PK, Mitra I, Kar S, Das RN, **Roy K**, ***Mol Inform* 31,** 2012, 711-718, http://dx.doi.org/10.1002/minf.201200045**.**

175.* Ojha PK, **Roy K**, ***Comb Chem High Throughput Screen*, 16,** 2013, 7-21, http://www.ncbi.nlm.nih.gov/pubmed/22963325 .

176.* Mitra I, Saha A, **Roy K**, ***Sci Pharm* 81,** 2013, 57-80, http://dx.doi.org/10.3797/scipharm.1208-01

177.* **Roy K**, Kabir H, ***Chem Engg Sci* 87,** 2013, 141-151, http://dx.doi.org/10.1016/j.ces.2012.10.002.

178.* Nandy A, Kar S, **Roy K**, ***Molecular Simulation*, 39,** 2013, 432-441, http://dx.doi.org/10.1080/08927022.2012.738421 .

179.* Saha A, **Roy K**, (Editorial). ***Current Drug Safety*, 7,** 2012, 255-256, http://www.benthamdirect.org/pages/article/1/3183046/editorial-hot-topic-in-silico-modeling-for-prediction-of-drug-induced-adverse-reactions-and-environmental-hazards-using-qsar-tools.html .

180.* Kar S, **Roy K**, ***Toxicol in vitro*, 27,** 2013, 597-608, http://dx.doi.org/10.1016/j.tiv.2012.10.015 .

181.* Pal P, Mitra I, **Roy K**, ***Flavour Frag J*, 28,** 2013, 102-117, http://dx.doi.org/10.1002/ffj.3135 .

182.* Kar S, **Roy K**, ***Mol Inform* 31,** 2012, 879-894, http://dx.doi.org/10.1002/minf.201200039 **.**

183.* Das RN, Sanderson H, Mwambo AE, **Roy K**, ***Bull Env Contam Toxicol* 90,** 2013, 375-381, http://dx.doi.org/10.1007/s00128-012-0921-3

184.* Das RN**, Roy K**, ***Mol Divers* 17,** 2013, 151-196, http://dx.doi.org/10.1007/s11030-012-9413-y

185.* Mitra I, Saha A, **Roy K**, ***Future Med Chem*, 5,** 2013, 261-280, http://dx.doi.org/10.4155/FMC.12.207/

186.* **Roy K**, Chakraborty P, Mitra I, Ojha PK, Kar S, Das RN, ***J Comput Chem* 34,** 2013, 1071-1082, http://dx.doi.org/10.1002/jcc.23231 **.**

187.* Kar S, **Roy K**, ***Expert Opin Drg Discov*, 8,** 2013, 245-261, http://dx.doi.org/10.1517/17460441.2013.761204 .

188.* Mitra I, Saha A, **Roy K**, ***Canadian J Chem* 91,** 2013, 428-441, http://dx.doi.org/10.1139/cjc-2012-0527

189.* Das RN, **Roy K**, ***J Hazard Mater* 254-255,** 2013, 166-178, http://dx.doi.org/10.1016/j.jhazmat.2013.03.023 .

190.* Pramanik S, **Roy K,** ***Chemosphere*** **92,** 2013, 600-607, http://10.1016/j.chemosphere.2013.03.065

191.* Kar S, **Roy K**, ***Mol Inform*** **32,** 2013, 693-705, http://dx.doi.org/10.1002/minf.201300018

192.* Nandy A, Kar S, **Roy K**, ***Mol Simul*** **40,** 2014, 261-274, http://dx.doi.org/10.1080/08927022.2013.801076

193.* Nandy A, Kar S, **Roy K**, ***SAR QSAR Environ Res*** **24,** 2013, 1009-1023, http://dx.doi.org/10.1080/1062936X.2013.821422 **.**

194.* Ojha PK, **Roy K**, ***Comb Chem High Throughput Screen,*** **16,** 2013, 739-757, http://www.ncbi.nlm.nih.gov/pubmed/23701009 .

195.* Ojha PK, **Roy K**, ***Curr Comput Aid Drug Des*** **9,** 2013, 336-349, http://www.ncbi.nlm.nih.gov/pubmed/24010932

196.* Ojha PK**, Roy K**, ***Biosystems*** **113**, 2013, 177-195, http://dx.doi.org/10.1016/j.biosystems.2013.07.005

197.* Ray S, **Roy K**, ***Chem Engg Sci*** **104**, 2013, 427-438, http://dx.doi.org/10.1016/j.ces.2013.09.018

198.* Mridha P, Pal P, **Roy K**, ***Mol Simul*** **40,** 2014, 1218-1235, http://dx.doi.org/10.1080/08927022.2013.854897 **.**

199.* Pramanik S, **Roy K**, ***Environ Sci Pollut Res*****, 2013**, http://dx.doi.org/10.1007/s11356-013-2247-z .

200.* Das RN, **Roy K**, ***Chemosphere*****, 104,** 2014, 170-176, http://dx.doi.org/10.1016/j.chemosphere.2013.11.002.

201.* Pramanik S, **Roy K**, ***Toxicol in vitro*****, 28,** 2013, 265-272, http://dx.doi.org/10.1016/j.tiv.2013.11.002.

202.* Pal P, Mitra I, **Roy K**, ***Flavour Frag J*****, 29,** 2014, 157-165, http://dx.doi.org/10.1002/ffj.3191.

203.* Kar S, **Roy K**, ***Ind Engg Chem Res*****, 52,** 2013, 17648−17657 http://dx.doi.org/10.1021/ie402803h

204.* Ambure P, Kar S, **Roy K**, ***Biosystems*****, 116,** 2014, 10-20, http://dx.doi.org/10.1016/j.biosystems.2013.12.002.

205.* Aher RB, **Roy K**, ***Comb Chem High Throughput Screen*****, 17,** 2014, 396-406, http://www.ncbi.nlm.nih.gov/pubmed/24372050.

206.* Pal P, Mitra I, **Roy K**, ***Croat Chem Acta*****, 87,** 2014, 29-37, http://dx.doi.org/10.5562/cca2284

207.* Pramanik S, **Roy K**, ***Ecotox Environ Saf,*** **101,** 2014, 184-190, http://dx.doi.org/10.1016/j.ecoenv.2013.12.030.

208.* Kar S, Gajewicz A, Puzyn T, **Roy K**, ***Toxicol in vitro,*** **28,** 2014, 600-606, http://dx.doi.org/10.1016/j.tiv.2013.12.018

209.* Ambure P, **Roy K**, ***RSC Advances*****, 4,** 2014, 6702-6709, http://dx.doi.org/10.1039/C3RA46861E .

210.* Das RN, **Roy K**, ***Ind Engg Chem Res*****, 53,** 2014, 1020-1032, http://dx.doi.org/10.1021/ie403636q

211.* Kar S, **Roy K**, ***Mol Simul*****, 2014,** http://dx.doi.org/10.1080/08927022.2014.888718

212.* Kar S, **Roy K**, ***Computer Biol Med*****, 48,** 2014, 102-108, http://dx.doi.org/10.1016/j.compbiomed.2014.02.014

213.* Aher RB, **Roy K**, ***Med Chem Res*** **23**, 2014, 4238-4249, http://dx.doi.org/10.1007/s00044-014-0997-x

214.* Bhayye S, Saha A, **Roy K**, ***Med Chem Res*** **23,** 2014, 3705-3713, http://dx.doi.org/10.1007/s00044-014-0955-7

215.* **Roy K**, Das R N, Popelier PLA, ***Chemosphere*****, 112**, 2014, 120-127, http://dx.doi.org/10.1016/j.chemosphere.2014.04.002

216.* Ambure P, **Roy K**, ***Expert Opin Drug Discov*****, 9**, 2014, 697-723, http://dx.doi.org/10.1517/17460441.2014.909404

217.* **Roy K**, Kar S, ***Eur J Pharm Sci*****, 62,** 2014, 111-114, http://dx.doi.org/10.1016/j.ejps.2014.05.019

218.* Kar S, Gajewicz A, Puzyn T, **Roy K**, Leszczynski J. ***Ecotox Environ Saf*****, 107,** 2014, 162-169, http://dx.doi.org/10.1016/j.ecoenv.2014.05.026

219.* Aher RB, **Roy K**, ***Comb Chem High Throughput Screen*****, 17,** 2014, 745-755, http://dx.doi.org/10.2174/13862073176661408281239 20.

220.* **Roy K**, Das RN, ***Current Drug Metabol*****, 15,** 2014, 346-379, http://dx.doi.org/10.2174/13892002156661409081022 30.

221.* Das S, Mitra I, Batuta S, Alam MN, **Roy K**, ***Bioorg Med Chem Lett,*** **24,** 2014, 5050-5054, http://dx.doi.org/10.1016/j.bmcl.2014.09.028 .

222.* **Roy K**, Popelier PLA, ***J Mol Liq*****, 200,** 2014**,** 223-228, http://dx.doi.org/10.1016/j.molliq.2014.10.018 .

223.* Bubalo MC, Radošević K, Srček VG, Das RN, Popelier P, **Roy K**, ***Ecotox Environ Saf*, 112,** 2015, 22-28, http://dx.doi.org/10.1016/j.ecoenv.2014.10.029**.**

224.* **Roy K**, Das R N, Popelier PLA, ***Environ Sci Pollut Res*, 22**, 2015, 6634-6641, http://dx.doi.org/10.1007/s11356-014-3845-0 .

225.* Ojha PK, **Roy K**, ***Comb Chem High Throuput Screen*, 18,** 2015, 91- 128, http://benthamscience.com/journal/abstracts.php?journalID=cchts&articleID=127214

226.* Aher RB, **Roy K**, ***Comb Chem High Throuput Screen*, 18,** 2015, 217-226, http://benthamscience.com/journal/abstracts.php?journalID=cchts&articleID=127211 **.**

227.* Ambure P, **Roy K**, ***Comb Chem High Throughput Screen*, 18,** 2015, 411-419, http://benthamscience.com/journal/abstracts.php?journalID=cchts&articleID=129184

228.* **Roy K**, Kar S, Ambure P, ***Chemom Intell Lab Sys*, 145,** 2015, 22-29, http://dx.doi.org/10.1016/j.chemolab.2015.04.013 .

229.* Nandy A, **Roy K**, Saha A, ***SAR QSAR Environ Res*, 26,** 2015, 363-382, http://dx.doi.org/10.1080/1062936X.2015.1039576

230.* Brahmachari G, Choo C, Ambure P, **Roy K** ***Bioorg Med Chem*, 23,** 2015, 4567-4575, http://dx.doi.org/10.1016/j.bmc.2015.06.005

231.* Das RN, **Roy K**, Popelier P, ***Chemosphere*, 139,** 2015, 163-173, http://dx.doi.org/10.1016/j.chemosphere.2015.06.022

232.* Ambure P, Aher R, Gajewicz A, Puzyn T, **Roy K**, ***Chemom Intell Lab Sys*, 147,** 2015, 1-13, http://dx.doi.org/10.1016/j.chemolab.2015.07.007

233.* Aher RA**, Roy K,** ***SAR QSAR Environ Res*** **26,** 2015, 959-976**,** http://dx.doi.org/10.1080/1062936X.2015.1104518 **.**

234.* Das RN, **Roy K**, Popelier K, ***Ecotox Environ Saf*, 122,** 2015, 497-520, http://dx.doi.org/10.1016/j.ecoenv.2015.09.014

235.* Aher RB, **Roy K,** ***Letters Drug Des Discov*, 13,** 2015, 129-134, http://benthamscience.com/journals/letters-in-drug-design-and-discovery/volume/13/issue/2/page/129/

236.* Ambure P, **Roy K**, ***Curr Drug Targets*, 2015 (In press),** http://benthamscience.com/journals/current-drug-targets/article/134722/

237.* **Roy K**, Das RN, Ambure P, Aher RB, ***Chemom Intell Lab Sys*, 152**, 2016, 18-33, http://dx.doi.org/10.1016/j.chemolab.2016.01.008**.**

238.* Kar S, Gajewicz A, **Roy K**, Leszczynski J, Puzyn T, ***Ecotox Environ Saf*, 126,** 2016, 238-244, http://dx.doi.org/10.1016/j.ecoenv.2015.12.033 **.**

239.* Das RN, **Roy K**, ***J Mol Liq*, 216,** 2016, 754-763, http://dx.doi.org/10.1016/j.molliq.2016.02.013 .

240.* Kar S, Das RN, **Roy K**, Leszcznyski, J, ***Int J Quant Struct-Prop Relat*, 1(2),** 2016, 23-51, http://dx.doi.org/10.4018/IJQSPR.2016070102

241.* Ambure P, **Roy K**, ***RSC Advances*, 6,** 2016, 28171-28186, http://dx.doi.org/10.1039/C6RA04104C

242.* Aher RB, **Roy K**, . ***RSC Advances*, 6, 2016,** 51957–51982, http://dx.doi.org/10.1039/C6RA05692J

243.* Das RN, Sintra T, Coutinho J, Ventura S, **Roy K**, Popelier, P, ***Toxicol Res*, 5,** 2016, 1388-1399 http://dx.doi.org/10.1039/C6TX00180G **.**

244.* **Roy K**, Ambure P, ***Chemom Intell Lab Sys*, 159,** 2016, 108-126, http://dx.doi.org/10.1016/j.chemolab.2016.10.009

245.* González-Durruthy M, Castro M, Nunes SM, Ventura-Lima J, Alberici LC, Naal Z, Atique-Sawazaki DT, Curti C, Ruas CP, Gelesky MA, **Roy K**, González-Díaz H, Monserrat JM, ***Carbon, 115,*** 2017, 312-330, http://dx.doi.org/10.1016/j.carbon.2017.01.002

246.* **Roy K**, Ambure P, Aher R, How important is to detect systematic error in predictions and understand statistical applicability domain of QSAR models? ***Chemom Intell Lab Sys,* 162,** 2017, 44-54, https://authors.elsevier.com/a/1UOpFcc6LvBdv

247.* Ojha PK, **Roy K**, ***Food and Chemical Toxicology,* 112,** 2018, 551-562, http://www.sciencedirect.com/science/article/pii/S0278691517301394

248.* Aher RB, **Roy K,**. ***SAR QSAR Environ Res*, 28,** 2017, 390-414, https://doi.org/10.1080/1062936X.2017.1326401

249.* Das S, Ojha PK, **Roy K**, ***J Mol Liq*, 240,** 2017, 454-467, http://dx.doi.org/10.1016/j.molliq.2017.05.113

250.* Kar S, Sepúlveda MS, **Roy K**, Leszczynski J, ***Chemosphere*, 184**, 2017, 514-523, http://dx.doi.org/10.1016/j.chemosphere.2017.06.024

251.* Khan K, **Roy K**, ***SAR QSAR Environ Res*, 28,** 2017, 567-594, http://dx.doi.org/10.1080/1062936X.2017.1352621

252.* Bhayye S, **Roy K**, Saha A, ***Struct Chem***, **29,** 2018, 657-666, http://dx.doi.org/10.1007/s11224-017-1059-z

253.* **Roy K**, Ambure P, Kar S, Ojha PK, ***J Chemom* 32,** 2018, e2992, http://dx.doi.org/10.1002/cem.2992

254.* Ojha PK, **Roy K**, ***RSC Adv*, 8**, 2018, 4750–4760, http://dx.doi.org/10.1039/c7ra12295k

255.* Ojha PK, **Roy K**, ***RSC Adv*, 8**, 2018, 2293-2304, http://dx.doi.org/10.1039/c7ra12914a

256.* De P, Aher RB, **Roy K**, ***RSC Adv*, 8**, 2018, 4662–4670, http://dx.doi.org/10.1039/c7ra13159c

257.* De P, **Roy K, *SAR QSAR Environ Res, 29,*** 2018, 319-337, http://dx.doi.org/10.1080/1062936X.2018.1436086

258.* Ambure P, Bhat J, Puzyn T, **Roy K**, ***J Biomol Str Dyn*, 37,** 2019, 1282-1306, https://doi.org/10.1080/07391102.2018.1456975

259.* Hossain KA, **Roy K**, ***Ecotox Environ Saf*, 166,** 2018, 92-101, https://doi.org/10.1016/j.ecoenv.2018.09.068

260.* **Roy K**, Ambue P, Kar S,. ***ACS Omega*, 3,** 2018, 11392-11406, http://dx.doi.org/10.1021/acsomega.8b01647

261.* Khan PM, Rasulev B, **Roy K, *ACS Omega* 3,** 2018, 13374−13386, http://dx.doi.org/10.1021/acsomega.8b01834

262.* Khan PM, **Roy K**, ***SAR QSAR Environ Res* 29,** 2018, 935-956, http://dx.doi.org/10.1080/1062936X.2018.1536078

263.* Khan PM, **Roy K**, ***Expert Opin Drug Discov*, 13,** 2018, 1075-1089, http://dx.doi.org/10.1080/17460441.2018.1542428

264.* Khan K, Benfenati E, **Roy K**, ***Ecotox Environ Saf* 168**, 2019, 287-297, https://doi.org/10.1016/j.ecoenv.2018.10.060

265.* Aher RB, **Roy K**, ***J Biomol Str Dyn* 37, 2019**, 3660-3673, https://doi.org./10.1080/07391102.2018.1524333

266.* Ojha PK, Kar S, **Roy K**, Leszczynski J, ***Nanotoxicology*, , 13,** 2019, 14-34, https://doi.org/10.1080/17435390.2018.1529836

267.* De P, Kar S, **Roy K**, Leszczynski J, ***Environ Sci Nano*, 5,** 2018, 2742-2760, http://dx.doi.org/10.1039/c8en00809d

268.* Roy J, Ghosh S, Ojha PK, **Roy K**, ***Environ Sci Nano*, 6,** 2019, 224-247, http://dx.doi.org/10.1039/C8EN01059E

269.* Khan K, Kar S, Sanderson H, **Roy K**, Leszczynski J, ***Mol Inform*, 38,** 2019, article 1800078, http://dx.doi.org/10.1002/minf.201800078

270.* Khan K, **Roy K**, Benfenati E, ***J Hazard Mater* 369C,** 2019, 707-718, https://www.sciencedirect.com/science/article/pii/S0304389419301499

271.* Khan PM, **Roy K**, Benfenati E, ***Chemosphere* 224C,** 2019, 470-479**,** https://doi.org/10.1016/j.chemosphere.2019.02.147

272.* Roy J, Ojha PK, **Roy K**, ***Nanotoxicology***, **13**, 2019, 701-716, http://dx.doi.org/10.1080/17435390.2019.1593543

273.* Karmakar A, Ambure P, Mallick T, Das S, **Roy K**, Begum NA, ***Med Chem Res*****, 28,** 2019, 723-741, http://dx.doi.org/10.1007/s00044-019-02330-8

274.* Bhayye SS, Brahmachari G, Nayek N, Roy S, **Roy K**, ***J Biomol Str Dyn*****, 38,** 2020, 1415-1424,https://doi.org/10.1080/07391102.2019.1606735

275.* Ghosh S, Ojha PK, **Roy K**, ***Chemosphere***, **228**, 2019, 545-555, https://doi.org/10.1016/j.chemosphere.2019.04.124

276.* Khan K, Khan PM, Lavado G, Valsecchi C, Pasqualini J, Baderna D, Marzo M, Lombardo A, **Roy K**, Benfenati E, ***Chemosphere*****, 229,** 2019, 8-17, https://doi.org/10.1016/j.chemosphere.2019.04.204

277.* Khan K, Baderna D, Cappelli C, Toma C, Lombardo A, **Roy K,** Benfenati E, ***Aquat Toxicol*****, 212,** 2019, 162-174, https://doi.org/10.1016/j.aquatox.2019.05.011

278.* Khan PM & **Roy K**, ***SAR QSAR Environ Res*****, 30**, 2019, 363-382, https://doi.org/10.1080/1062936X.2019.1607549

279.* De P, Bhattacharyya D, **Roy K**, ***Struct Chem*****,** 30, **2019**, 2429-2445,http://dx.doi.org/10.1007/s11224-019-01376-z

280.* Khan K, **Roy K**,. ***SAR QSAR Environ Res,*** **30,** 2019, 665-681, https://doi.org/10.1080/1062936X.2019.1648315

281.* Khan PM, Baderna D, Lombardo A, **Roy K**, Benfenati E, ***J Hazard Mater*** **2019**, http://dx.doi.org/10.1016/j.jhazmat.2019.121035

282.* Aher RB, **Roy K**, ***Curr Comp Aid Drug Des*****, 15**, 2019, 369-383, http://dx.doi.org/10.2174/1573409915666190130153214

283.* Ambure P, Gajewicz-Skretna, Cordeiro MNDS, **Roy K**, ***J Chem Inf Model*** **59,** 2019, 4070-4076, https://doi.org/10.1021/acs.jcim.9b00476

284.* Kumar V, Ojha PK, Saha A, **Roy K**, ***SAR QSAR Env Res*****, 31,** 2020, 87-133, http://dx.doi.org/10.1080/1062936X.2019.1695226

285.* Roy J, Ojha PK, Carnesecchi E, Lombardo A, **Roy K**, Benfenati E, ***J Hazard Mater*****, 386,** 2020, Article 121660, https://doi.org/10.1016/j.jhazmat.2019.121660

286.* Ghosh S, Ojha PK, Carnesecchi E, Lombardo A, **Roy K**, Benfenati E, ***Ecotox Environ Saf*** **190**, 2020, Article 110067, https://doi.org/10.1016/j.ecoenv.2019.110067

287.* De P, Bhattacharyya D, **Roy K**, ***Struct Chem***, **31**, 2020, 1043-1055, http://dx.doi.org/10.1007/s11224-019-01481-z

288.* Kumar V, Ojha P, De P, Saha A, **Roy K**, ***Curr Topics Med Chem*****, 20**, 2020, 1601-1627, http://dx.doi.org/10.2174/1568026620666200616142753

289.* Krishna JG, Ojha PK, Kar S, **Roy K**, Leszczynski J, ***Nano Energy*****, 70**, 2020, Article 104537, http://dx.doi.org/10.1016/j.nanoen.2020.104537

290.* Kar S, Sanderson H, **Roy K**, Benfenati E, Leszczynski J, ***Green Chem*****, 22,** 2020, 1458-1516, http://dx.doi.org/10.1039/C9GC03265G

291.* Kumar V, Ojha PK, Saha A, **Roy K**, ***Computers in Biology and Medicine***, **118**, 2020, article 103658, http://dx.doi.org/10.1016/j.compbiomed.2020.103658

292.* Jillela GK, Khan K, **Roy K**, ***Toxicol in vitro*****, 65**, 2020, Article 104768, https://doi.org/10.1016/j.tiv.2020.104768 .

293.* Khan PM, **Roy K**, ***Mol Inform*****, 2020**, https://dx.doi.org/10.1002/minf.202000030

294.* Kumar V, **Roy K**, ***SAR QSAR Environ Res*****, 31**, 2020, 511-526, https://doi.org/10.1080/1062936X.2020.1776388

295.* De P, Bhayye S, Kumar V, **Roy K**, ***J Biomol Str Dyn*****, 2020**, http://dx.doi.org/10.1080/07391102.2020.1821779

296.* Khan PM, Kumar V, **Roy K**, ***Comb Chem High Throughput Screen*** **2020**, http://dx.doi.org/10.2174/1386207323666200914094712

297.* De P, Roy J, Bhattacharyya D, **Roy K**, ***Struct Chem*, 31,** 2020, 1969-1981, http://dx.doi.org/10.1007/s11224-020-01560-6
298.* Ojha PK, Kar S, Krishna JG, **Roy K**, Leszczynski, ***Mol Divers* 25,** 2021, 625-659, http://dx.doi.org/10.1007/s11030-020-10134-x
299.* Pandey S, Ojha P, **Roy K**, ***Chemosphere*, 252,** 2020, article 126508, http://dx.doi.org/10.1016/j.chemosphere.2020.126508
300.* Seth A, Ojha P, **Roy K**, ***Journal of Hazardous Materials*, 394**, 2020, article 122498, http://dx.doi.org/10.1016/j.jhazmat.2020.122498
301.* Pandey S, **Roy K**, ***Ecotoxicology and Environmental Safety*, 208,** 2021, article 111411, http://dx.doi.org/10.1016/j.ecoenv.2020.111411
302.* Seth A, **Roy K**, ***Aquatic Toxicology*, 228**, 2020, article 105627, http://dx.doi.org/10.1016/j.aquatox.2020.105627
303.* Ojha PK, Kumar V, Roy J, **Roy K**, ***Expert Opin Drug Discov*, 16,** 2021, 659 – 695, https://doi.org/10.1080/17460441.2021.1866535
304.* De P, **Roy K**, ***Theoretical Chemistry Accounts*, 139,** 2020, 176, https://doi.org/10.1007/s00214-020-02687-9
305.* Kumar V, Saha A, **Roy K**, ***Computational Biology and Chemistry*, 88,** 2020, 107355, https://doi.org/10.1016/j.compbiolchem.2020.107355
306.* Khan PM, Kumar V, **Roy K, *Comb Chem High Throughput Screen*, 2020**, http://dx.doi.org/10.2174/1386207323666200914094712 .
307.* Khan PM, Lombardo A, Benfenati E, **Roy K**, ***Environmental Science and Pollution Research*, 28, 2021,** 1627–1642, https://doi.org/10.1007/s11356-020-10500-0
308.* De P, **Roy K, *Struct Chem*, 32**, 2021, 631-642, https://doi.org/10.1007/s11224-021-01734-w
309.* Chatterjee M, **Roy K**, ***Journal of Hazardous Materials*, 408**, 2021, 124936, https://doi.org/10.1016/j.jhazmat.2020.124936
310.* Lavado GJ Baderna D, Gadaleta D, Ultre M, **Roy K**, Benfenati E, ***Chemosphere*, 280**, 2021, 130652, https://doi.org/10.1016/j.chemosphere.2021.130652

Teaching Experience

Total teaching experience till date is of about **25 years**.

1. **Lecturer** (October 1995 – January 2002)
2. **Sr. Lecturer** (January 2002 - January 2007).
3. **Reader** (January 2007 – January 2010).
4. **Associate Professor** (January 2010 – January 2013)
5. **Professor** (January 2013 – till date)

PhD theses guided

1. **J. Thomas Leonard**
   Thesis Title: QSAR Modeling of Selected Classes of Anti-HIV Compounds (Awarded 2007)
2. **Supratim Ray**
   Thesis Title: Approaches to Improvement of Drug Action: Antioxidant Cotherapy, Rational Design and Pharmacophore Mapping of Anticancer Drugs (Co-Guide: Prof. C. Sengupta) (Awarded 2008)
3. **Santanu Chakraborty**
   Thesis Title: Studies on Correlation of Biological Activity of NSAIDs with Structural, Physicochemical and Biological Parameters (Co-Guide: Prof. C. Sengupta) (Awarded 2008)
4. **Gopinath Ghosh**
   Thesis Title: Exploring Quantitative Structure-Toxicity Relationships (QSTRs) with Extended Topochemical Atom Indices (Awarded 2010)

5. **Partha Pratim Roy**
   Thesis Title: IN SILICO MODELING OF SELECTED CLASSES OF CYTOCHROME INHIBITORS USING CHEMOMETRIC TOOLS (Awarded 2011)
6. **Indrani Mitra**
   Thesis Title: QUANTITATIVE STRUCTURE-ACTIVITY RELATIONSHIPS OF ANTIOXIDANTS OF BIOLOGICAL SIGNIFICANCE USING CHEMOMETRIC TOOLS (Awarded 2014)
7. **Probir Kumar Ojha**
   Thesis Title: Exploring quantitative structure-activity relationships (QSARs) of selected classes of antimalarial compounds (Awarded 2014)
8. **Supratik Kar**
   Thesis Title: Exploring Quantitative Structure-Toxicity Relationships (QSTRs) Using Chemometric Tools for Development of Robust and Predictive Models (2015)
9. **Rudra Narayan Das**
   Thesis Title: "ETA" Indices for Effective Encoding of Chemical Information in Modeling Different Toxicity Endpoints of Ionic Liquids (2016)
10. **Pravin Sundarao Ambure**
    Thesis Title: MOLECULAR MODELING AND QSAR STUDIES OF POTENTIAL ANTI-ALZHEIMER'S AGENTS (Awarded 2017)
11. **Rahul Balasaheb Aher**
    Thesis Title: IN SILICO MODELING OF POTENTIAL ANTIMALARIAL AGENTS ACTING ON SELECTED TARGETS (Awarded 2018)

Projects completed

1. Potential Pharmacological Targets and Cheminformatics: Exploring Selectivity Requirements of Novel Ligands for Binding with Specific Receptor Subtypes (AICTE, 2004-2007, 10.5 lakhs)
2. In silico Design and Modeling of HIV-1 Reverse Transcriptase, Protease, Integrase and Entry Inhibitors (DST, 2005-2008, 8.16 lakhs)
3. In silico ADME/Tox prediction using chemometric tools (UGC, 2007-2010, 7.48 lakhs)
4. Predictive In Silico Modeling of Different Classes of Antioxidants of Biological and Medicinal Significance Using Cheminformatics Tools (ICMR, 2009-2012, 11. 05 lakhs)
5. Exploring Quantitative Structure-Activity Relationships (QSARs) of Selected Classes of Antimalarial Compounds for Development of Predictive Models (UGC, 2011-2014, 8 lakhs)
6. In silico modeling of ecotoxicological hazards of chemicals using advanced chemometric tools (CSIR, 2012-2014, 11.12 lakhs)
7. Development of AChE-inhibitor for Alzheimer s Disease- Screening Designing Synthesis and Biological validation using Chemical Library & North-East Indian Plants (DBT, 2012-2015, 14.43 lakhs)
8. In silico modeling of property/toxicity/activity of nanomaterials using chemometric tools (CSIR, 2017, ~7 lakhs)
9. Application of QSARs for the design of PET and SPECT imaging agents (DAE-BRNS, 2018, ~28 lakhs)

Project ongoing

1. Development of a novel work□ow of Quantitative Read-Across (QRA) analysis for application as a non-testing method in regulatory toxicology (DST SERB MATRICS, 2020, 6.6 lakhs)

Other Professional Activities

Reviewer of QSAR papers of different Journals: *Bioorganic and Medicinal Chemistry Letters* (Elsevier), *Journal of Molecular Modeling* (Springer), *European Journal of Medicinal Chemistry* (Elsevier), *Journal of Chemical Information and Modeling* (ACS), *Chemical Biology and Drug Design* (Blackwell-Wiley), *Molecular Informatics* (Wiley), *SAR and QSAR in Environmental Research* (Taylor and Francis) etc.

Co-Editor-in-Chief, *Molecular Diversity* (Springer) (http://www.springeronline.com/journal/11030/) [Impact Factor 2.013 (2019)]

Editor-in-Chief, *International Journal of Quantitative Structure-Property Relationships (IJQSPR)*, http://www.igi-global.com/journal/international-journal-quantitative-structure-property/126552

Member of the Editorial Advisory Board:
(1) *European Journal of Medicinal Chemistry* (Elsevier, http://www.elsevier.com/locate/ejmech/) [Impact Factor 5.572 (2019)]

(2) *Journal of Molecular Graphics and Modelling* (Elsevier, http://www.journals.elsevier.com/journal-of-molecular-graphics-and-modelling) [Impact factor 2.079 (2019)]

(3) Computational and Structural Biotechnology Journal (Elsevier, https://www.journals.elsevier.com/computational-and-structural-biotechnology-journal) [Impact Factor 6.018 (2019)]

(4) *Chemical Biology and Drug Design* (Wiley, http://onlinelibrary.wiley.com/journal/10.1111/(ISSN)1747-0285) [Impact Factor 2.548 (2019)]

(5) *Expert Opinion on Drug Discovery* (Informa, http://informahealthcare.com/loi/edc) [Impact Factor 4.421 (2018)]

(6) *Letters in Drug Design and Discovery* (Bentham, http://benthamscience.com/journal/index.php?journalID=lddd) [Impact Factor 1.169 (2019)]

(7) Current Computer-Aided Drug Design (Bentham, http://benthamscience.com/journals/current-computer-aided-drug-design/) [Impact Factor 0.935 (2019)]
Guest Editor, Special Issue of *Molecular Diversity* (http://www.springeronline.com/journal/11030/) on "Topological Descriptors in Drug Design and Modeling Studies" [Vol. 8, No. 4, 2004]

Guest Editor, Special Issue of *Molecular Diversity* (http://www.springeronline.com/journal/11030/) on "Ecotoxicological Modeling and Risk Assessment Using Chemometric Tools" [Vol. 10, No. 2, 2006]

Co-Guest Editor, Special issue of *Current Drug Safety* (http://www.benthamscience.com/cds/) on "*In Silico* Modeling for Prediction of Drug-Induced Adverse Reactions and Environmental Hazards Using QSAR Tools" [Vol 7, No. 4, 2012]

Guest Editor, Special issue of Current Topics in Medicinal Chemistry (http://www.benthamscience.com/ctmc/) on "**Pharmacophore Mapping and High Throughput Screening in Drug Discovery" [Vol 13, No. 9, 2013]**

Guest Editor, Special Issue of Combinatorial Chemistry and High Throughput Screening (https://www.eurekaselect.com/128495/article) on "Application of Chemometrics and Cheminformatics in Antimalarial Drug Research" [Vol. 18, No. 2, 2015]

Memberships

1. Indian Association for the Cultivation of Science, Kolkata 700 032
2. Indian Chemical Society, Calcutta 700 009
3. Indian Science Congress Association, Kolkata 700 017
4. Indian Pharmaceutical Association, Mumbai 400 098
5. Indian Society for Technical Education, New Delhi
6. The Cheminformatics and QSAR Society

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Mail me to kunalroy_in@yahoo.com

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