Dr. Partha Pratim Roy

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EDUCATIONAL CREDENTIALS

Year	Course	Board/University	Division
2011	**Ph.D**	**Jadavpur University**	**-**
2007	**M.Pharm**	**Jadavpur University**	1st Class
2004	**B.Pharm**	**Jadavpur University**	1st Class with Honours

AREA OF RESEARCH INTEREST

- In silico ADME/T modeling
- Toxicity modeling

Date of Joining: 02/01/2012

RESEARCH EXPERIENCE: 5 years

Post doctoral Fellow (2010-2011): University of Insubria, Varese, Italy.

Title of the project: ***Development and validation of QSAR models on emerging organic pollutants***

DOCTORAL RESEARCH (2007-2010)

TITLE OF THE PROJECT: ***In silico modeling of selected classes of Cytochrome inhibitors using chemometric tools.***

MASTER OF PHARMACY (2005-2007)

TITLE OF THE PROJECT: ***On Some Aspects of Validation of Predictive QSAR Models***

LIST OF PUBLICATIONS:

INTERNATIONAL (20)

1. **Roy PP**, Kovarich S, Gramatica P, QSAR Model Reproducibility and Applicability: A Case Study of Rate Constants of Hydroxyl Radical Reaction Models Applied to Polybrominated Diphenyl Ethers and (Benzo-)Triazoles, *J Comput Chem* **2011**,32: 2386–2396.
2. Pran Kishore D, Balakumar C, Raghuram Rao A, **Roy PP**, Roy K. QSAR of adenosine receptor antagonists: Exploring physicochemical requirements for binding of pyrazolo[4,3-e]-1,2,4-triazolo[1,5-c]pyrimidine derivatives with human adenosine A(3) receptor subtype, *Bioorg Med Chem Lett*, **2011,** 21:818-23.
3. **Roy PP** and Roy K, Molecular docking and QSAR studies of aromatase inhibitor androstenedione derivatives, *J Pharm Pharmacol*, **2010,** 62: 1717-1728.
4. **Roy PP** and Roy K, Pharmacophore mapping, molecular docking and QSAR studies of structurally diverse compounds as CYP2B6 Inhibitors, *Molecular Simulation*, **2010,** 36: 887-905.
5. **Roy PP** and Roy K, Docking and 3-D QSAR studies of diverse classes of human aromatase (CYP19) inhibitors, *Journal of Molecular Modeling* **2010,** 16: 1597–1616.
6. **Roy PP** and Roy K, Classical and 3D-QSAR studies of cytochrome 17 inhibitor imidazole substituted biphenyls, *Molecular Simulation*, **2010,** 36: 311–325.
7. **Roy PP** and Roy K, Exploring QSAR for CYP11B2 binding affinity and CYP11B2/CYP11B1 selectivity of diverse functional compounds, *Journal of enzyme inhibition and medicinal chemistry*, **2010,** 25: 354–369
8. Mitra I, **Roy PP**, Kar S, Ojha P K, Roy K, On further application of r_m^2 as a metric for validation of QSAR models. *Journal of Chemometrics*, **2010**, 24: 22-33.
9. Ray S, **Roy PP**, Sengupta C, Roy K, Exploring QSAR of hydroxyphenylureas as antioxidant using Physicochemical and electrotopological atom parameters, *Molecular Simulation*, **2010**, *36:* 484–492.
10. Roy K and **Roy PP,** QSAR of Cytochrome inhibitors, *Expert opinion on Metabolism and Toxicology*, **2009**, 5: 1245-1266.
11. **Roy PP**, Paul S, Mitra I, Roy K, On Two Novel Parameters for Validation of Predictive QSAR models, *Molecules*, **2009**, 14: 1660-1701.
12. **Roy PP** and Roy K, QSAR Studies of CYP2D6 Inhibitor Aryloxypropanolamine Using 2D and 3D Descriptors, *Chem. Biol drug Des.* **2009**, 73:442-455.
13. Roy K, **Roy PP,** Comparative chemometric modeling of cytochrome 3A4 inhibitory activity of structurally diverse compounds using stepwise MLR, FA-MLR, PLS, GFA, G/PLS and ANN techniques, *European Journal of Medicinal Chemistry* **2009**, 44; 2913-2922.
14. Roy K, **Roy PP**, Exploring QSAR and QAAR for Inhibitors of Cytochrome P450 2A6 and 2A5 Enzymes Using GFA and G/PLS Techniques, *European Journal of Medicinal Chemistry* **2009**, 44: 1941-1951.
15. **Roy PP** & Roy K, On some aspects of variable selection for partial least squares regression models, *QSAR Comb Sci*, **2008:** 27, 302-313.

16. **Roy PP**, Leonard J T & Roy K, Exploring the impact of the size of training sets for the development of predictive QSAR models, *Chemom Intell Lab Sys*, **2008**: 90, 31-42.
17. Roy K, **Roy PP**, Exploring QSARs for binding affinity of azoles with CYP2B and CYP3A enzymes using GFA and G/PLS techniques, *Chem Biol Drug Des.* **2008**, 71: 464-471.
18. Roy K, **Roy PP**, Comparative QSAR studies of CYP1A2 inhibitor flavonoids using 2D and 3D descriptors, *Chem. Biol Drug Des.* **2008**, 72: 370-382.
19. Roy K, Sanyal I and **Roy PP**, QSTR with Extended Topochemical Atom Indices. 9. A QSAR study on the Bioconcentration Factors of Nonionic Organic Compounds in Fish, *SAR QSAR Environ. Res.*, **2006**, 17: 563–582.
20. Ray S, **Roy PP**, A QSAR Study of Biphenyl Analogues of 2-Nitroimidazo-[2,1-b][1,3]-Oxazines as Antitubercular agents using Genetic function Approximation, ***Medicinal Chemistry*** **2102(In press)**

LIST OF PRESENTATIONS IN SEMINARS/CONFERENCES

1. **Roy PP,** Papa E, Gramatica P, QSAR model reproducibility and applicability: Acase Study of Hydroxyl radical rate constants model. **Conferentia Chemometrica**, Sümeg, Hungary, Sept 18-21, 2011.
2. **Roy PP,** Papa E, Gramatica P**,** Exploring the QSARs for OH Tropospheric Degradation of VOCs using freely available online descriptors, **SEATAC Europe**, Milan, 15-19 may, 2011.
3. Roy P P & Roy K, QSAR Studies of CYP2D6 Inhibitor Aryloxypropanolamine Using 2D and 3D Descriptors, **International Conference on Open Source for Computer Aided Drug Discovery (OSCADD)**, March 22-26, 2009, Chandigarh, India.
4. Roy P P & Roy K, Exploring impact of method of selection and size of training sets on the predictability of QSAR models, for three days in **International Conference on Cheminformatics**, 22-24 Jan, 2007, Pune, India.
5. Roy P P & Roy K, Classical and 3D-QSAR studies of cytochrome 17 inhibitor imidazole substituted biphenyls, **National conference of Stem cell research and computational biology and Chemistry**, Chennai, India.
6. Roy K& Roy P P, Comparative QSAR Studies of CYP1A2 Inhibitors using 2D and 3D descriptors, Proceedings of the **"Acharya Prafulla Chandar Ray Memorial Symposium Kolkata**, 01-02 August, 2008.

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