Quantitative Structure–Activity Relationship (QSAR) Approximation for Cadmium Oxide (CdO) and Rhodium (III) Oxide (Rh$_2$O$_3$) Nanoparticles as Anti-Cancer Drugs for the Catalytic Formation of Proviral DNA from Viral RNA Using Multiple Linear and Non-Linear Correlation Approach

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Editorial

Human cancer cells are one of the main medical, clinical, biochemical, pharmaceutical, photodynamical and social issues in our era. Cadmium Oxide (CdO) and Rhodium (III) Oxide (Rh$_2$O$_3$) nanoparticles are potent inhibitor of cancer Reverse Transcriptase (RT) which is necessary for the catalytic formation of proviral DNA from viral RNA [1-29,57, 58]. In the current editorial, the three-dimensional (3D) autocorrelation pool was used for encoding structural information of Cadmium Oxide (CdO) and Rhodium (III) Oxide (Rh$_2$O$_3$) nanoparticles analogous and development of linear and non-linear models for prognostication of anti-cancer properties of these nanoparticles [27-60].

Quantitative structure-activity relationship (QSAR) models study has been applied in a series of Cadmium Oxide (CdO) and Rhodium (III) Oxide (Rh$_2$O$_3$) nanoparticles analogous acting as non-nucleoside reverse transcriptase inhibitors (NNRTIs). The molecular information has been encoded in three-dimensional (3D) autocorrelation descriptors, obtained from different weighting designs. Analysis of the linear and non-linear quantitative structure-activity relationship (QSAR) models revealed a correlation coefficient and root mean square error of 0.974 and 0.637, respectively. The predictive ability of the model indicates that this model can be used for virtual library screening of databases for novel potent anti-cancer drugs.

Three spatial autocorrelation vectors were employed for modelling the inhibitory activities: Broto-Moreau’s autocorrelation coefficients (ATS), Moran’s indices (MATS) and Geary’s coefficients (GATS). Autocorrelation vectors were calculated at spatial lags ranging from 1 up to 10. The biochemical, medical, clinical, pharmaceutical, photodynamical and biochemical properties considered in the twenty different weighting plans.

A data set containing 200 Cadmium Oxide (CdO) and Rhodium (III) Oxide (Rh$_2$O$_3$) nanoparticles analogous were used in this editorial. The biological evaluation of these nanoparticles was made by scanning electron microscope (SEM), x-ray diffraction (XRD), attenuated total reflectance fourier transform infrared spectroscopy (ATR-FTIR), transmission electron microscope (TEM), differential thermal analysis-thermal gravim analysis (DTA-TGA), energy-dispersive x-ray spectroscopy (EDX), mass spectroscopy (MS), UV-Vis spectroscopy, FT-Raman spectroscopy, 1HNMR spectroscopy, 13CNMR spectroscopy and 31PNMR spectroscopy, positive logarithm of molar concentration of a drug required to achieve 75% protection of cancer cells against the cytopathic effect of cancer. ESI MS, PMS and DFT studies were used to optimize the three-dimensional (3D) geometry of the molecules.

Using the stepwise multiple regression method, the models were developed for 200 Cadmium Oxide (CdO) and Rhodium (III) Oxide (Rh$_2$O$_3$) nanoparticles analogous. The correlations performed for the whole set provided the optimal equations for different numbers of descriptions in the range of 1 to 10. The robustness of the model and their prediction ability for the anti-cancer activity, were evaluated by leave-one-out cross-validation (LOO-CV) and external validation (EV) procedures. In order to identify novel potent nanoparticles, the developed model considered as good tools for a virtual library screening when the descriptor values, calculated for the molecules belonging to virtual libraries. Virtual screening identified some attractive nanoparticles that have high-quality activities and these deserve further study.
In the present editorial, a quantitative structure-activity relationship (QSAR) approximation using multiple linear and non-linear correlation approach was developed to predict reverse transcriptase inhibition (RTI) of Cadmium Oxide (CdO) and Rhodium (III) Oxide (Rh2O3) nanoparticles analogues acting as non-nucleoside reverse transcriptase inhibitors (NNRTIs).

The employment of three–dimensional (3D) autocorrelation descriptors is extremely useful in modelling the biological activities. We expect this model to be useful in conjunction with computational and experimental methods for filtering likely Cadmium Oxide (CdO) and Rhodium (III) Oxide (Rh2O3) nanoparticles analogous from chemical and physical libraries and virtual chemical databases for identify new potential and selective nanoparticles.
References

1. Heidari A, Brown C (2015) Study of composition and morphology of cadmium oxide (CdO) nanoparticles for eliminating cancer cells, Journal of Nanomedicine Research 2: 20.

2. Yu Z, Mengmeng H, Qiao W, Jun C (2016) Structure-guided unravelling: Phenolic hydroxyls contribute to reduction of acrylamide using multiplex quantitative structure-activity relationship modelling, Food Chemistry 199: 492-501.

3. Alexander P, Ewgenij P, Kai S, Janosch A, Cora W, et al. (2016) Toonenes, Synthetic cannabinoids: In silico prediction of the cannabinoid receptor 1 affinity by a quantitative structure-activity relationship model, Toxicology Letters 245: 1-6.

4. Pedro De-la-Torre, Adriana VT, Margarita G, Horacio P, Jans HA, et al. (2016) Synthesis and in silico analysis of the quantitative structure activity relationship of heteroarylcyclicnitriles as AChE inhibitors, Journal of the Taiwan Institute of Chemical Engineers 59: 45-60.

5. Ammar A, Moustafa Z, Aboul EH (2016) PQSAR: The membrane quantitative structure-activity relationships in cheminformatics, Expert Systems with Applications 54: 219-227.

6. Hwee-Leng S, Chee-Yuen G (2016) Extraction, identification, and structure-activity relationship of antioxidative and α-amylase inhibitory peptides from cumin seeds (Cuminum cyminum), Journal of Functional Foods 22 1-12.

7. Andrea N, Annalisa F, Jose AO, Chiara P, Stefano F, et al. (2016) Potent α-amino-β-lactam carboxylic acid ester as NAAA inhibitors. Synthesis and structure-activity relationship (SAR) studies, European Journal of Medicinal Chemistry 111: 138-159.

8. Lin Z, Yijun Z, Hongzhu D, Guowan S, Mouming Z (2016) Structure-activity relationship of antioxidant dipeptides: Dominant role of Tyr, Trp, Cys and Met residues, Journal of Functional Foods 21: 485-496.

9. Srivinivas D, David R, Peg D, Josephine L, Todd WV, et al. (2016) Design synthesis and structure-activity relationship of 5-substituted (tetrahydrobenzophenanthral-2yl)methyl with N-phenyl-N(piperidin-2-yl) propionamide derivatives as opioid ligands, Bioorganic & Medicinal Chemistry 24: 85-91.

10. Oscar ML (2016) Computational Structure–Activity Relationship Studies of Epigenetic Target Inhibitors, In Epi-Informatics, edited by José L. Medina-Franco, Academic Press 359-384 Boston, USA.

11. Eduardo BM, João PA, Eduardo HM, Márcia MC (2016) A best comprehension about the toxicity of phenylsulfonyl carboxylates in Vibrio fischeri using quantitative structure activity/property relationship methods, Journal of Hazardous Materials 304: 233-241.

12. Sudhir L, Amrita BM, Kavitha N, João N, Venkita S, et al. (2015) Discovery of benzothiazoles as antimycobacterial agents: Synthesis, structure-activity relationships and binding studies with Mycobacterium tuberculosis decaprenylphosphoryl-β-d-ribose 2’-oxidase, Bioorganic & Medicinal Chemistry 23: 7694-7710.

13. Hongmao S (2016) Quantitative Structure–Activity Relationships: Promise, Validations, and Pitfalls, In A Practical Guide to Rational Drug Design, Woodhead Publishing 163-192.

14. Mabrouk H, Othmane B, Salah H, Abdelft A, Latifa K, et al. (2016) A Quantitative Structure Activity Relationship for acute oral toxicity of pesticides on rats: Validation, domain of application and prediction, J Hazard Mater 303: 28-40.

15. Sun H (2016) Quantitative Structure-Property Relationships Models for Lipophilicity and Aqueous Solubility, In A Practical Guide to Rational Drug Design. Woodhead Publishing 193-223.

16. Pervez A, Hyunjung WK, Adnan AK, Hatem AA, Youngjoo K, et al. (2016) Design, synthesis, topoisomerase I & II inhibitory activity, antiproliferative activity, and structure-activity relationship study of pyrazoline derivatives: An ATP-competitive human topoisomerase Ila catalytic inhibitor, Bioorganic & Medicinal Chemistry 24: 1898-1908.

17. Sandra Š, Igor O, Mario Z, Dušanka M, Bogdan Š (2016) Quantitative structure retention/activity relationships of biologically relevant 4-amino-7-chloroquinoine based compounds, J Chromatogr A 1013: 144-152.

18. Qing-Song X, Jian X, Dong-Sheng C, Yi-Zeng L (2016) Boosting in block variable subspaces: An approach of additive modeling for structure–activity relationship, Chemometrics and Intelligent Laboratory Systems 152: 134-139.

19. Johan A, Janine N, Huising S, Christian F, Philipp W, et al. (2016) The effect of sodium on the structure–activity relationships of cobalt-modified Cu/ZnO/Al2O3 catalysts applied in the hydrogenation of carbon monoxide to higher alcohols, J Catal 335: 175-186.

20. Dejun Z, Huaming L, Qiong W, Qibing Z (2016) Structure–activity relationship study of anticancer thymidine–quinoxaline conjugates under the low radiation of long wavelength ultraviolet light for photodynamic therapy, Eur J Med Chem 107: 180-191.

21. Andrew GM, Pablo RD (2016) Encoding alternatives for the prediction of polycarboxylates glass transition temperature by quantitative structure–property relationships, Materials Chemistry and Physics 172: 158-164.

22. Jian-Wei Z, Meilan H, Jian-Xiang H, Gui-Xiang H, Yong-Jun J, et al. (2016) Quantitative structure–activity hydrophobicity relationships of molecular fragments and beyond, J Mol Graphics Modell 64: 110-120.

23. Jintao Y, Shuling Y, Ting Z, Xuejie Y, Yunyun C, et al. (2016) QSRR models for predicting generator-column-derived octanol/water and octanol/air partition coefficients of polychlorinated biphenyls, Ecotoxicology and Environmental Safety 128: 171-180.

24. Nikita B, Shikha G, Kunwar PS (2016) Predicting human intestinal absorption of diverse chemicals using ensemble learning based QSAR modeling approaches, Computational Biology and Chemistry 61: 178-196.

25. Josef Seifert (2016) The structural requirements of organophosphorus insecticides (OPI) for reducing chicken embryo NAD+ content in OPI-induced teratogenesis in chickens, Pesticide Biochemistry and Physiology 43-48.

26. Zhiqiang F, Jingwen C, Xuehua L, Ya'nan W, Haiying Y (2016) Comparison of prediction methods for octanol-air partition coefficients of diverse organic compounds, Chemosphere 148: 118-125.

27. Ying W, Xianhai Y, Juining W, Yi C, Jingli M, et al. (2016) A DFT-based toxicity QSAR study of aromatic hydrocarbons to Vibrio fischeri: Consideration of aqueous freely dissolved concentration, J Hazard Mater 308: 149-156.

28. Mikhail SK, Ville V, Pascal MC, Vyatcheslav VI, Dmitry SK, et al. (2016) Quantitative structure–property relationships in propene polymerization by zirconocenes with a rac-SiMe2[Ind]2 based ligand framework, Journal of Molecular Catalysis A: Chemical 412: 39-46.

29. Dominic A, Clarence MO, Chan YW, Alan SC, Michael KD (2016) Bioprocess challenges to the isolation and purification of bioactive peptides, Food and Bioproducts Processing 98: 244-256.

30. Nicholas VC, Paul FD (2016) Receptor binding profiles and quantitative structure–affinity relationships of some 5-substituted-N,N-diallyltryptamines, Bioorganic & Medicinal Chemistry Letters 26: 959-964.
31. Paola G, Stefano C, Alessandro S (2016) Are some “safer alternatives” hazardous as PBTs? The case study of new flame retardants, J Hazard Mater 306: 237-246.

32. Xianchao P, Hu M, Sujun Q, Shuheng H, Jiaying S, et al. (2016) Prediction and characterization of P-glycoprotein substrates potentially bound to different sites by emerging chemical pattern and hierarchical cluster analysis, Int J Pharm 502: 61-69.

33. Naga ST, Mohammed AA (2016) Pharmacophore modeling, 3D-QSAR and docking study of 2-phenylpyrimidine analogues as selective PDE4B inhibitors, J Theor Biol 394: 117-126.

34. Francesca G, Viviana C, Marco V, Sara V, Roberto T (2016) Investigating the mechanisms of bioconcentration through QSAR classification trees. Environment International 88: 198-205.

35. Alessandra P, Stefan B, Mark AH, Ragas MJ, Karin V, et al. (2016) QSARs for estimating intrinsic hepatic clearance of organic chemicals in humans, Environmental Toxicology and Pharmacology 42: 190-197.

36. Koji O, Satoshi T, Tomohiko E, Akihiko K, Kuzuhiko L, et al. (2012) Phosphodiesterase inhibitors. Part 3: Design, synthesis and structure–activity relationships of dual PDE3/4-inhibitory fused bicyclic heteroaromatic-dihydropyridazinones with anti-inflammatory and bronchodilatory activity. Bioorganic & Medicinal Chemistry 20: 1644-1658.

37. Sanna PN, Elangovan M, Sanna R, Juhani H, Olli TP (2016) Identification of estrogen receptor α ligands with virtual screening techniques, J Mol Graphics Modell 64: 30-39.

38. Tomas L, Rotimi EA, Dilip KR, Paula OC, Maria H (2016) Identification of bioactive peptides from a papain hydrolysate of bovine serum albumin and assessment of an antihypertensive effect in spontaneously hypertensive rats, Food Research International 81: 99-111.

39. Fabiola P, Anna L, Marc B, Alberto M, Emilie B (2016) A new integrated in silico strategy for the assessment and prioritization of persistence of chemicals under REACH. Environment International 88: 250-260.

40. Liang S, Dongsheng C, Qingsong X, Xin H, Nan X, Yizeng L (2016) A novel local manifold-ranking based K-NN for modeling the regression between bioactivity and molecular descriptors, Chemometrics and Intelligent Laboratory Systems 151: 71-77.

41. Jing C, Miao Z, Qing M, Dongdong Q, Liping Z, et al. (2016) QSAR study of pyrazol(1,5-α)pyrimidine derivative inhibitors of Chk1, Chemometrics and Intelligent Laboratory Systems. 150: 23-28.

42. Snezana AK, David M (2016) Chapter 9 - Data Mining in Drug Discovery and Design, In Artificial Neural Network for Drug Design, Delivery and Disposition, edited by Munish Purtyashwant PathakVijay Kumar SutariyaSrinivas TippurajuWilfrido Moreno, Academic Press 283: 544-552.

43. Saw S, Rickard M, Daniel A, Hao L, Chuleeporn P, et al. (2016) Unraveling the origin of splice switching activity of hemoglobin B-globin gene modulators via QSAR modeling, Chemometrics and Intelligent Laboratory Systems 151: 51-60.

44. Teng A, Li Q, Jiaxu X, Robert JG, Liqiang C (2016) Design and synthesis of an activity-based protein profiling probe derived from cinnamic hydroxamic acid, Bioorganic & Medicinal Chemistry. 24: 686-692.

45. Arnab C, Sam M, Tahir C (2016) Chapter 9 - Application of Modeling for Industrial Hygiene and Toxicological Issues, In Multiscale Modeling for Process Safety Applications, Butterworth-Heinemann 397-406, Boston, USA.

46. Agnieszka AK, Ewelina R, Damian B, Katarzyna MT, Dariusz M, et al. (2016) Chapter 17 - Computational methods for studying G protein-coupled receptors (GPCRs). Methods in Cell Biology 132: 359-399.

47. Meihang C, Pei L, Deyu H, Song Z, Tianxian L, et al. (2016) Synthesis, antiviral activity, 3D-QSAR, and interaction mechanisms study of novel malonate derivatives containing quinazolin-4(3H)-one moiety, Bioorganic & Medicinal Chemistry Letters 26: 168-173.

48. Saloni P, Bhumiaka P, Hardik B (2016) 3D-QSAR studies on 5-hydrox-6-oxo-1,6-dihydropyrimidine-4-carboxamide derivatives as HIV-1 integrase inhibitors. J Taiwan Inst Chem Eng 59: 61-68.

49. Daniel AV (2016) Chapter 8 - Biotechnological Implications: A Systems Approach, In Environmental Biotechnology (Second Edition), Academic Press, 359-405, Boston, USA.

50. Pan W, Li D, Bao-Ting Z (2016) Use of computational modeling approaches in studying the binding interactions of compounds with human estrogen receptors, Steroids. 105: 26-41.

51. Carlos AL, Marcelo LW, Ewelina B, Christoł L, Eno LM, et al. (2016) Degradation of cyclophosphamide and 5-fluourouracil by UV and simulated sunlight treatments: Assessment of the enhancement of the biodegradability and toxicity. Environmental Pollution 208: 467-476.

52. Daniel AV (2016) Chapter 5 - Environmental Risks of Biotechnologies, In Environmental Biotechnology (2ndedn), Academic Press, 209-247, Boston, USA.

53. Joren B, Christophe W, Katriijn VH, Herman VL (2016) Determination of the gas-to-liquid partitioning coefficients using a new dynamic absorption method (DynAb method), Chemical Engineering Journal 283: 544-552.

54. Michael HA, Joelie MR, Enrique CM (2016) An assessment of air quality reflecting the chemosensory irritation impact of mixtures of volatile organic compounds. Environment International 86: 84-91.

55. Sahil S, Jagjeet S, Ritu O, Haribinder S, Manpreet K, et al. (2016) Design strategies, structure activity relationship and mechanistic insights for purines as kinase inhibitors. European Journal of Medicinal Chemistry 112: 298-346.

56. Alejandro S (2016) Drug self-assembly: A phenomenon at the nanometer scale with major impact in the structure–biological properties relationship and the treatment of disease, Progress in Materials Science 82: 39-82.

57. Heidari A, Brown C (2015) Study of surface morphological, physiochemical and structural characteristics of rhodium (lll) oxide (Rh2O3) nanoparticles", International Journal of Pharmacology, Phytochemistry and Ethnomedicine 1: 15–19.

58. Heidari A (2012) A Thesis submitted to the Faculty of the Chemistry, California South University (CSU), Irvine, California, The United States of America (USA) in Fulfillment of the Requirements for the Degree of Doctor of Philosophy (PhD) in Chemistry.

59. Fernández M, Caballero J (2007) QSAR modeling of matrix metalloproteinase inhibition by N-hydroxy-α-phenylsulfonylacetamide derivatives, Bioorganic & Medicinal Chemistry 15: 6298-6310.

60. Shovanlal G, Bikash D, Soma S, Tarun J (2004) QSAR study on some anti-HIV HEPT analogues using physicochemical and topological parameters, Bioorganic & Medicinal Chemistry 12: 1493-1503.