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Chem Sci Trans., 2012, 1(3), 572-581 578 The third set of QSAR models have been developed with the help of DFT based results

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James Devillers, Centre de Traitement de l'Information Scientifique, France

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Summary As the 21st century approaches, there is little doubt that the tools and resources are available to unlock all the secrets of Quantitative Structure-Activity

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Synthesis, pharmacological activity and

European Journal of Medicinal Chemistry 2010-05-01 Synthesis, pharmacological activity and comparative QSAR modeling of 1,5-N,N'-substituted-2-(substituted

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1. Crit Rev Toxicol. 1995;25(1):67-89. Comparative QSAR in toxicology: examples from teratology and cancer chemotherapy of aniline mustards.

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Cyclo-oxygenase 2 (COX2) inhibiting drugs were subjected to comparative quantitative structure activity relationship (QSAR) analysis with an attempt to derive and to

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Comparative QSAR and the Radical Toxicity of Various Functional Groups Cynthia D. Selassie,* Rajni Garg, Sanjay Kapur, Alka Kurup, Rajeshwar P. Verma, Suresh Babu

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Author: James Devillers, Title: Comparative Qsar (Hardcover), Publisher: CRC Press, Category: Books, ISBN: 9781560327165, Price: \$319.00, Release_date: 1998-03-03

Quantitative structure activity relationship -

Quantitative structure activity relationship models (QSAR models) are regression or classification models used in the chemical and biological sciences and engineering.

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Abstract. A number of binary QSAR models have been developed using methods of artificial neural networks, k-nearest neighbors, linear discriminative analysis, and

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