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Research Article

Study of stability of structure of organic dye in TiO_2 phtotocatalysis by QSAR

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ABSTRACT

Chemical and organic dyes are compounds that uses in the different industries since this materials according to these structures have some hazards for environment. In any case, one of an important way to decrease the hazards is photocatalyt to degrade in certain wavelength

For providing to do experimental work and decrease the financials, the best way is modeling verses structural and molecule properties for identifying the photocatalyst degradation. According to this work, by modeling of QSAR suitable linear model have been achieved.

Keywords: Organic dye, QSAR, photocatalyst.

INTRODUCTION

(Q)SAR is the study of the correlation between chemical structure and associated biological activity, with the ultimate goal of predicting the activity of untested chemicals based on structurally related compounds with known activity (Cronin, 2010). Structure-activity relationships (SARs) are qualitative relationships, often in the form of structural alerts that incorporate molecular substructures or fragments related to the presence or absence of activity (Dearden *et al*., 2009). Quantitative structure-activity relationships (QSARs) attempt to quantify the relationship between an aspect of chemical structure and an activity or property imparted by that structure. Chemical structure is often described by descriptors (*e.g.*, electrophilicity, hydrogen bonding, molecular fragments) or physical-chemical properties (*e.g.*, Log P) which are then used to develop a mathematical correlation between a group of structures and a defined activity or endpoint. The mathematical correlations usually take the form of statistical algorithms developed through a variety of techniques (*e.g.*, univariate regression, multiple linear regression, partial least squares analysis). The aim of this work is modeling and recognizing the structure stability of phocatalyst behavior. By QSAR modeling can be simulated the properties which affected on photalyst.

PROCEDURE AND RESULTS

For computing some of conformers, we need to get familiar with 3D structure and stable mode of molecule. So, first we must optimize the molecule structure using quantummechanics methods. To do this, first we drew the pigments structure via Gauss View software, then we optimized them through Guassian03 software and B3LYP/6-31G method. Next, to conduct QSAR computations, we entered the optimized structure into DRAGON software and conformers' computations were performed. The selected molecules all are pigments which have several different applications. Also, these structures are classified among unsaturated cyclic compounds with Hetero-atom. All of these molecules are known as hazardous compounds in chemical industry. We assume that cyclicstructure of compoundsis considerably proportionate with their type of color and color wavelength as well as their stability energy. Moreover, when pigments are in the presence of photocatalyst materials and get analyzed, the percentage of damage resulted by photocatalystmaterials can be a function of stability energy (optimized energy of structure).

In order to conduct modeling and gaining the best possible model, we used multiple linear regression

(MLR) and step technique. So, we applied lots of strategies. Firstly, we categorized entireconformers into four groups of topological, electronic, geometrical and physicochemical. Then, we run regression technique for each single block through different Howard orders and step method. During these stages, we obtained several different models. Further, to increase the chance of using more conformers in the model, we employed conformers'elimination method. In this technique, we removed one entered variable in the model,then we run regression. Again, we entered the same variable and removed another variable and run regression. Accordingly, we could obtain greater models with more diverse conformers. In fact, proper models are those which have the highest number of R and F and the lowest number of conformers and standard deviation. So, we select them as appropriate models.

a) photocatalystic properties computed y the model in relation to experimental photocatalystic properties

b) residuals values in relation to experimental photocatalystic properties values

DISCUSSION AND CONCLUSION

Aswe could see, unlike previous works on modeling, in the present study we attempted to consider the overall behavior of molecules in relation to photocatalyst properties. Then, in the process of modeling identical conformers demonstrating different aspects of interactions with photocatalyst properties were provided. Here, we selected conformers as the independent variables and phtocatalyst properties as the dependent variable in form of a mathematical equation. Subsequent to specification of independent and dependent variables using SPSS software and multiple linear regression method, firstly, we opted for a series of good conformers out of entire conformers. Secondly, we created certain linear equations between conformers and photocatalyst properties. Since for computation of some conformers we required to have the 3D structure and stable mode of molecules, before computations we should optimize molecule structure on the basis of quantum mechanics methods.

Table 1
Modeld patterns by MIR technique

Model	R	Adj-R^2	Std.Error	F	N
1	0.948	0.897	0.082	1135	5
2	0.947	0.897	0.083	1893	5
*3	0.959	0.920	0.073	2489	3
4	0.939	0.882	0.088	1614	6
5*	0.957	0.916	0.074	2352	3
6	0.921	0.848	0.099	1460	6
7	0.901	0.810	0.110	1306	5
8	0.953	0.907	0.078	1587	4
*9	0.958	0.918	0.073	2431	3
10	0.889	0.790	0.138	983	6
11	0.956	0.913	0.076	1358	6
*12	0.958	0.918	0.073	2427	3
13	0.905	0.819	0.102	1204	4
14	0.959	0.918	0.073	1829	6
15	0.943	0.888	0.086	1718	5
16	0.945	0.892	0.084	1794	5
17	0.947	0.897	0.082	1893	4
18	0.939	0.882	0.088	1614	3
19	0.899	0.808	0.125	1105	6
20	0.893	0.797	0.131	995	5

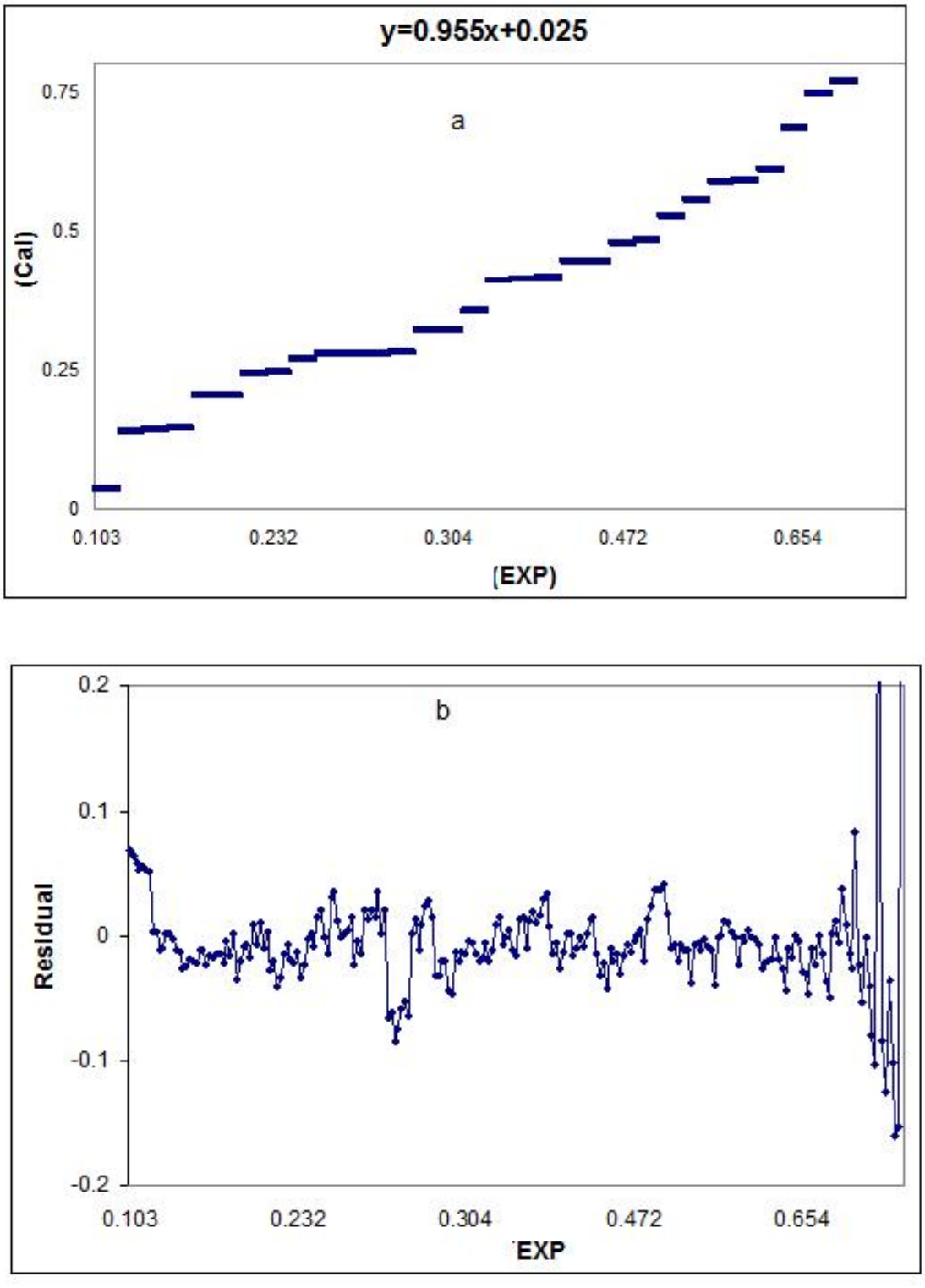

Fig.1
Values of selected model evaluation for percentage of pigment damage

Moreover, because we needed to optimize and use the most stable conformers of each category in its gaseous form, for different conformers of each compound we computed enthalpy of formation. Next, according to the numerical value of enthalpy of formation (heat of formation) of structure, the most negative enthalpy of formation was selected as the best conformer. For all molecules of the data series, the stable conformer is similarly computed. Following to molecules optimization, we applied DRAGON software to compute conformers. To this end, we entered data relevant to existingcompounds in reference series and predicting series into DRAGON software separately and 1497 conformers were computed for each category. Along with computations, we excluded those conformers without statisticallysignificant value, i.e. zero or constant values or r>0.95.

Of the total conformers, 418 had constant or zero values, and 783 conformers had r>0.95 all were removed.

For modeling process and gaining the best possible model, we employed multiple linear regression (MLR) method as well as step technique. Accordingly, we utilized numerous strategies. First, we categorized whole conformers into four topological, electronic, geometrical and physicochemical classes. Then, we run step regression technique for each single block. During these stages, we obtained 24 (4!) models. Further, to increase the chance of using more conformers in the model, we employed conformer elimination method. In this technique, we removed one entered variable in the model,then we run regression. Again, we entered the same variable and removed another variable and run regression. Therefore, we could obtain greater models with more diverse conformers.

Table 1 illustrates statistical features of a number of these models for the reference series. As it is seen, among these models, models 3, 5, 9 and 12 have the highest F and R and the lowest number of conformers and standard deviation. So, they are selected as appropriate models.

Fig.1 presents computed photocatalyst properties in relation to values of experimental photocatalyst properties for molecules of the predicting series. So, we performed this procedure only for evaluation of the linear model.

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