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RESEARCH ARTICLE

STUDY OF THE LINEAR CORRELATION BETWEEN THE FIRST OXIDATION POTENTIAL OF A FAMILY OF TETRATHIAFULVALENE MOLECULES AND QUANTUM CHEMICAL DESCRIPTORS

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ABSTRACT

The aim of this work is to link the first oxidation potential of a series of tetrathiafulvalene (TTF) molecules to quantum chemistry descriptors with a view to designing new TTF molecules with more efficient first oxidation potentials. A QSPR (Quantitative Structure-Property Relationships) model has been developed. In this model, the first oxidation potential depends on three (03) parameters, namely the dipole moment (μ_D), the smallest Mulliken partial charge of the molecule (q^-) and the infrared (IR). This model showed very satisfactory statistical and validation parameters. Indeed, $R^2 = 0.9634$;$R^2_{adj} = 0.9451$;$s = 0.0245$; $F = 52.6765$; $Q^2_{LOO} = 0.9200$; $R^2_{ext} = 0.9802$; $Q^2_{ext} = 0.9603$. These statistical and validation parameters reveal that the developed model is validated and performs well in predicting the first oxidation potential of new TTF molecules within its applicability domain. From now on, to design new TTF molecules with desired first oxidation potentials, it will suffice to adjust these three parameters of the developed model.

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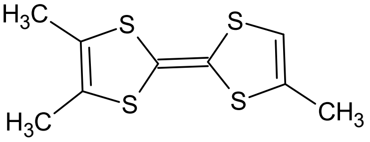
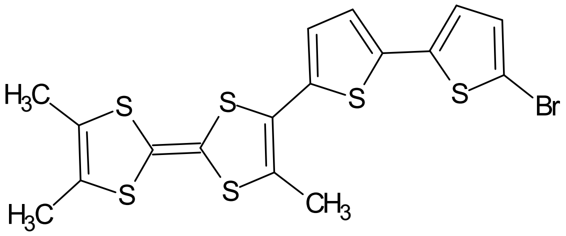
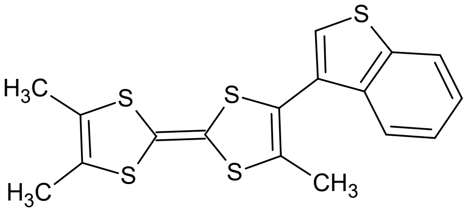
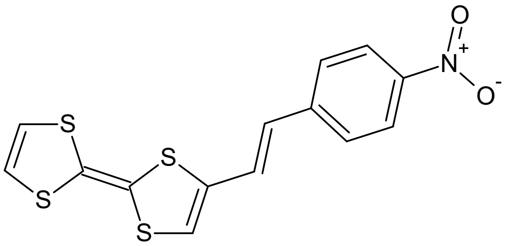
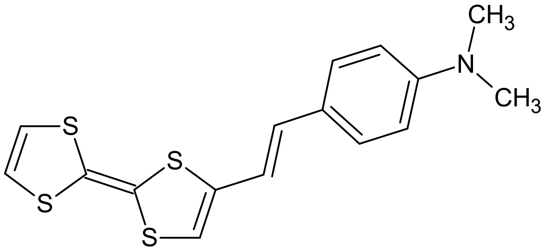
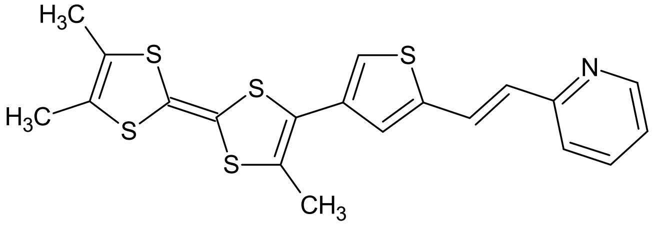
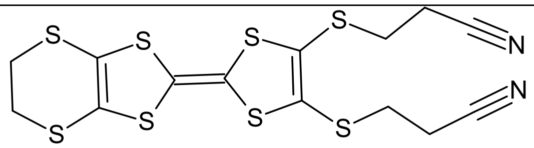
INTRODUCTION

Since the first synthesis of the electron donor, tetrathiafulvalene (TTF) in 1965(1) and the discovery of the electrical conductivity of the first organic charge transfer complexes Tetrathiafulvalene-Tetracyanoquinodimethane (TTF-TCNQ) (2,3), studies of TTF derivatives and their analogues have received a great deal of attention. Since then, the design of new organic conductors has attracted considerable interest. This has led to the discovery of organic superconductors thanks to in-depth research on electron donors (4). It is in this context that various TTF derivatives have been synthesized and their charge transfer complexes with Tetracyanoquinodimethane (TCNQ) and monovalent anions have been prepared (4-7). These compounds exhibit interesting electrical properties such as superconductivity at very low temperatures, conductivity, and semi conductivity (8). Considerable effort has been devoted to understanding and improving the properties of the charge transfer complex (TTF-TCNQ) (9). Since TTF is a strong electron-donating organic molecule, several research groups have focused on synthesizing π-extended TTF derivatives with a view to improving the properties of the materials (12,13). However, these molecules are still very difficult to synthesize and the reagents used are often dangerous (14). Therefore, in the synthesis of TTF-TCNQ charge transfer complexes, organic chemists aim to develop thermodynamically stable radical species. This is no easy task. Under these conditions, the use of alternative methods to experimentation becomes essential. Among these, Quantitative Structure-Property Relationships/Quantitative Structure-Activity Relationships (QSPR/QSAR) are a recommended alternative in the new regulations (15,16). They enable the development of mathematical models linking physicochemical properties and biological activities to molecular structure. These mathematical models explain the origin of properties/activities and predict them for molecules for which experimental data are not available. The application of these methods requires knowledge of the physicochemical properties of the systems studied, known as descriptors. Quantum chemistry, which is based on solving Schrödinger's equation for stationary states, provides access to a large number of descriptors through its various methods.

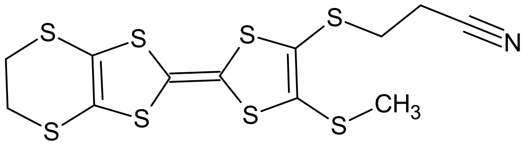
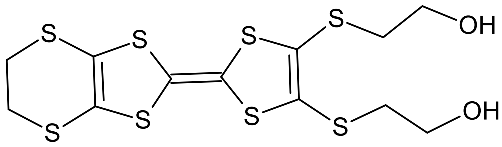
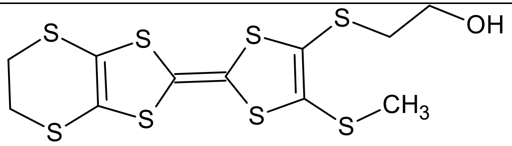
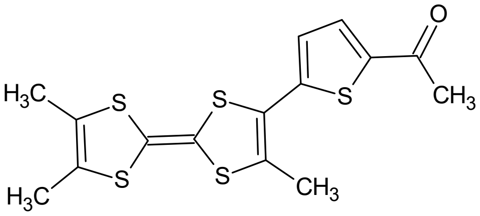
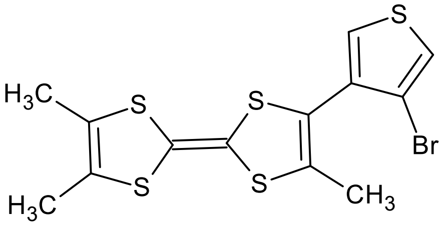
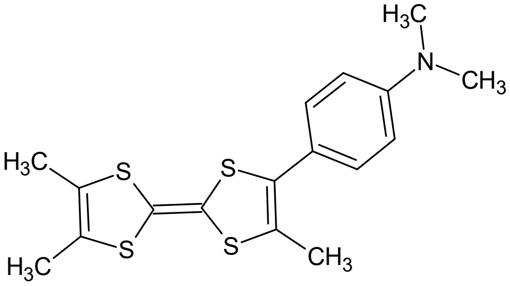
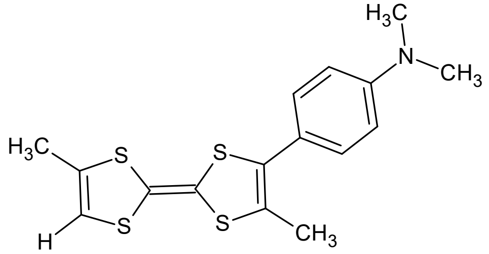
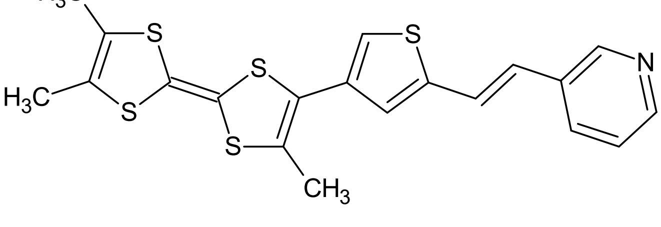
MATERIALS AND METHODS

Presentation of the series of tetrathiafulvalene molecules studied: In this work, a series of fifteen (15) molecules derived from tetrathiafulvalene, coded TTF were studied. These molecules were synthesized by two groups of researchers, namely Tahar Abbaz et al. (14,17) and Jean-Pierre Legros et al (18). These molecules were chosen because of the availability of experimental values for their first oxidation potential $E^1_{1/2}$, all determined by cyclic voltammetry. They formed our experimental database. Of these, ten (10), or two-thirds of the database, were used for the training set, and five (05), or one-third of the database, were used for the test set. These molecules are presented in Table 1 with their different experimental first oxidation potentials expressed in volts (V).

Tableau 1. Series of studied TTF molecules

	Training set		
CODE	STRUCTURE	$E^1_{1/2}$(V)	REFERENCE
TTF_1		+0.327	[17]
TTF_2		+0.371	[17]
TTF_3		+0.355	[17]
TTF_4		+0.500	[14]
TTF_5		+0.460	[14]
TTF_6		+0.332	[18]
TTF_7		+0.600	[18]

Continue ….

TTF_8		**+0.560**	**[18]**
TTF_9		**+0.540**	**[18]**
TTF_10		**+0.550**	**[18]**
	Test set		
TTF_11		**+0.408**	**[17]**
TTF_12		**+0.352**	**[17]**
TTF_13		**+0.460**	**[14]**
TTF_14		**+0.480**	**[14]**
TTF_15		**+0.329**	**[17]**

In what follows, the first oxidation potential will be denoted **E**.

Software used and level of used theory: After representing the 3D structures using the gaussView 05 graphical interface, optimization and frequency calculations were performed with Gaussian 09 (19) at the B3LYP/6-31G (d, p) level of theory. Next, physicochemical quantities called molecular descriptors were calculated using the output file from the Gaussian calculation. Finally, EXCEL (20) and XLSTAT (21) software were used to calculate the statistical parameters and establish the QSPR model obtained.

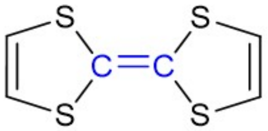
Calculated molecular descriptors: A series of five (05) molecular descriptors was calculated in this work. These descriptors are described as follows:

- **Dipole moment μ_D:** This highlights the polar or nonpolar nature of a molecule. When the dipole moment is not zero, the molecule is said to be polar. It is said to be nonpolar if the opposite is true (dipole moment is zero). It is frequently used in quantitative structure-property/activity studies. Its value is provided by the Gaussian 09 software.

- **Smallest Mulliken partial charge q^- of the molecule:** The smallest Mulliken partial charge of a molecule is generally negative. It is given by the Gaussian 09 software.

- **Infrared corresponding to the vibration frequency of the carbon double bond C=C of the TTF nucleus.**

This is a spectroscopic descriptor. It is obtained by calculating the frequency using Gaussian 09 software.



•**Electron-acceptor power** ω^+ **:** This approach was formulated by Gazquez et al.(22). It measures a molecule's ability to accept electrons. Its value is calculated according to equation (1).

$$\omega^+ = \frac{(IE+3EA)^2}{16(IE-EA)} \quad (1)$$

With IE being the ionization energy and EA being the electron affinity

• **Electron-donating power** ω^- **:** This approach was also formulated by Gazquez et al.(22). Unlike ω^+, it measures a molecule's ability to donate electrons. Its value is calculated using formula (2).

$$\omega^- = \frac{(3IE+EA)^2}{16(IE-EA)} \quad (2)$$

Multiple Linear Regression (MLR)

The generalized form of the multiple linear regression (MLR) equation (23) is as follows:

$$Y = a_0 + a_1X_1 + a_2X_2 + \cdots + a_nX_n \quad (3)$$

In this expression, Y is the response or dependent variable, $X_1, X_2, \ldots, X_n$ are descriptors (characteristics or independent variables) present in the model with the corresponding regression coefficients $a_1, a_2, \ldots, a_n$, respectively, and a_0 is the constant term of the model.

Criteria for selecting molecular descriptors for a model: The selection of descriptors is a crucial step in any QSPR/QSAR modeling. In this study, descriptors were selected based on two fundamental criteria described as follows:

Selection criterion 1: There must be a linear relationship between the first oxidation potential and the descriptors. Under these conditions, $|R| \geq 0.50$ (24). Where R is the linear correlation coefficient of the equation $\text{Propriété} = f(\text{Descripteur}_i)$.

Selection criterion 2: The descriptors must be independent of each other in pairs. To achieve this, the partial correlation coefficient a_{ij} between descriptors i and j must be less than 0.70 ($a_{ij} < 0.70$) (24). a_{ij} is simply the slope of the line $\text{Descripteur}_i = f(\text{Descripteur}_j)$ obtained using XLSTAT software.

Statistical and validation parameters of the model

Analysis of variance table (ANOVA table)

The analysis of variance is based on various sums of squares defined as follows:

- TSS (Total Sum of Squares): This is the sum of the squares of the deviations from the mean. It is given by the following relationship:

$$\mathrm{TSS} = \sum(y_i - \overline{Y}_{exp})^2 = \sum(y_{i,exp} - \overline{Y}_{exp})^2 \qquad (4)$$

- ESS (Extended Sum of Squares):

$$\mathrm{ESS} = \sum(\hat{y}_i - \overline{Y}_{exp})^2 = \sum(y_{i,cal} - \overline{Y}_{exp})^2 \qquad (5)$$

RSS (Residual Sum of Squares):

$$\mathrm{RSS} = \sum(y_i - \hat{y}_i)^2 = \sum(Y_{i,exp} - Y_{i,cal})^2 \qquad (6)$$

These different formulas help reduce rounding errors and are the easiest to use when performing a manual analysis of variance. It is common and practical to display the results of an analysis of variance in a table called an analysis of variance table or ANOVA table (25), as shown below:

Table 2. General ANOVA table

Source	DF	SS	MS	F
Model	p	ESS	$\frac{\mathrm{ESS}}{p}$	$\frac{\mathrm{ESS}}{p}\frac{n-p-1}{\mathrm{RSS}}$
Error	$n-p-1$	RSS	$\frac{\mathrm{RSS}}{n-p-1}$	
Total	$n-1$	TSS		

DF: Degrees of Freedom, SS: Sum of Squares MS: Mean of Squares, F: Fisher's Test

Quality of linear regression: The quality of a linear relationship between Y and X_i is verified by several coefficients:

Coefficient of determination R^2(26)**:** This is used to assess the accuracy with which the dependency found describes the variance of the dependent variable, i.e., the quality of the statistical fit. The coefficient of determination is given by relation 7.

$$\mathbf{R^2 = \frac{RSS}{TSS} = 1 - \frac{ESS}{TSS}} \qquad (7)$$

Adjusted coefficient of determination R^2_{adj} (27)

This coefficient is used in multiple regression because it takes into account the number of parameters (descriptors) in the model.

$$\mathbf{R^2_{adj} = 1 - \frac{(n-intercept)(1-R^2)}{n-p-1}} \qquad (8)$$

Fisher-Snedecor test (28)**:** This test is useful in the context of multiple regression, i.e., with p regressors X_1, X_2,.... X_p. It allows us to determine the overall contribution of all variables X_1, ...X_p to the determination of Y. We test the null hypothesis: H_0: β_1=...... βp= 0 against H_1: there is at least one β_j among β_1...βp that is not equal to 0. A regression equation is considered statistically significant if the observed value of F is greater than a tabulated value for the chosen significance level (typically 95%) and the corresponding degrees of freedom of F. The degrees of freedom of F are equal to p and n-p-1. If p-value $\leq\alpha$, then the null hypothesis is rejected. The F statistic is related to the coefficient of determination by the following relationship:

$$\mathbf{F = \frac{R^2}{1-R^2}\frac{n-p-1}{p}} \qquad (9)$$

Model validation

Internal validation: Internal validation of a QSPR/QSAR model only concerns molecules in the training set. It involves predicting the properties/activities of the molecules studied, followed by an estimation of parameters that enable the accuracy of the predictions to be detected.

Leave-One-Out (LOO) cross-validation coefficient: For LOO (Leave-One-Out) cross-validation, the training set is mainly modified by removing one compound from the training set. The QSPR/QSAR model is then rebuilt based on the molecules remaining in the training set using the combination of descriptors originally selected, and the property/activity of the removed compound is calculated based on the resulting QSPR/QSAR model. This cycle is repeated until all molecules in the training set have been removed once and the predicted property/activity data has been obtained for the entire training set. The predicted property/activity values of the compounds are used to calculate various internal validation parameters. The predictive power of the model is evaluated using the Predicted Residual Sum (PRESS) and the cross-validation coefficient (Q^2_{LOO}) (29).

External validation: External validation must be applied to any QSPR/QSAR model in order to generalize it to new compounds that should fall within its applicability domain. The model must be tested on a sufficiently large number of compounds not used during model development; as mentioned above, at least 20% of the database is recommended.

External validation coefficient Q^2_{ext}(30)

It measures the accuracy of the prediction on the test set data.

$$Q^2_{ext} = 1 - \frac{n}{n_{ext}} \frac{PRESS(test)}{TSS} \quad (10)$$

Golbraikh and Tropsha criteria

According to Golbraikh and Tropsha (31), models are considered acceptable if they meet the following five (05) criteria:

- Criterion 1: $R^2_{ext} > 0.70$ (11)
- Criterion 2 : $Q^2_{ext} > 0.60$ (12)
- Criterion 3: $\frac{|R^2_{ext} - R^2_0|}{R^2_{ext}} < 0.1$ and 0.85<k<1.15 (13)
- Criterion 4: $\frac{|R^2_{ext} - R'^2_0|}{R^2_{ext}} < 0.1$ and 0.85<k'<1.15 (14)
- Criterion 5: $|R^2_{ext} - R^2_0| < 0.3$ (15)

R^2_{ext}: Coefficient of determination for molecules in the test series and Q^2_{ext}: external validation coefficient. These criteria are known as "external validation criteria" or "Tropsha criteria."

Applicability Domain of a Model: The usefulness of a QSPR/QSAR model lies in its predictive power for new chemical compounds. Thus, once the QSPR/QSAR model has been constructed, its Applicability Domain (AD) must be defined. A model is considered valid only within its applicability domain, and only predictions for new compounds within this domain can be considered reliable and not an extrapolation of the model. The most common method for defining the AD is based on determining the leverage value of each compound (32). The Williams plot (plot of standardized residuals R as a function of leverage values h_i) is used in this study to visualize the AD of the QSPR models developed. A leverage is a kind of distance to the barycenter of the points in the space of explanatory variables. It identifies observations that are abnormally distant from the others. For an observation i, the leverage is expressed as follows:

$$h_i = x_i (X^T X)^{-1} x_i^T \quad (16)$$

where xi is the descriptor vector of the compound under consideration, X is the descriptor matrix derived from the descriptor values of the training set, the threshold is defined as follows:

$$h^* = \frac{3\,(p+1)}{n} \quad (17)$$

where n is the number of compounds in the training set, p is the number of descriptors in the proposed model.

RESULTS AND DISCUSSION

Values of calculated molecular descriptors: In this QSPR study, five (05) molecular descriptors were calculated. These are: dipole moment (μ_D), smallest Mulliken charge of the molecule (q-), infrared (IR) corresponding to the vibration of the carbon-carbon double bond, electron-accepting power (ω^+), and electron-donating power (ω^-). The values of these descriptors are recorded in Table 3.

Table 3. Values of calculated descriptors

CODE	μ_D	q-	IR	ω^+	ω^-
Training set					
TTF_1	1.1150	-0.3627	0.2740	0.7926	3.3955
TTF_2	3.3474	-0.3586	19.7642	2.1138	5.2566
TTF_3	1.0877	-0.3858	1.9723	1.1275	3.9051
TTF_4	6.5033	-0.4150	7.1812	4.4633	8.0887
TTF_5	4.0947	-0.4678	7.9052	0.7280	3.1756
TTF_6	2.0482	-0.5201	69.8755	1.8773	4.9338
TTF_7	7.9252	-0.4455	0.8016	1.2523	4.3766
TTF_8	4.7433	-0.4687	1.7830	1.3331	4.4447
TTF_9	5.0860	-0.5303	7.8175	1.1794	4.0774
TTF_10	5.2755	-0.5288	3.0309	1.2453	4.1809
Test set					
TTF_11	4.8330	-0.3965	31.7942	2.6903	6.0166
TTF_12	2.1991	-0.3564	1.7358	1.1485	3.9434
TTF_13	3.2379	-0.4693	0.9608	1.2020	3.9719
TTF_14	3.9137	-0.4693	3.9287	0.7200	3.2034
TTF_15	3.0391	-0.4423	55.0046	1.9588	5.0810

Submission of calculated molecular descriptors to selection criteria

Table 4. Selection of descriptors according to criterion 1

Equation	Correlation coefficient |R|	Descriptor rejected if |R| < 0.50
$E_{exp} = f(\mu_D)$	0.9034	Selected
$E_{exp} = f(q^-)$	0.4939	Selected
$E_{exp} = f(IR)$	0.4727	Selected
$E_{exp} = f(\omega^+)$	0.0537	Rejected
$E_{exp} = f(\omega^-)$	0.1195	Rejected

Selection criterion 1: Analysis of the data in **Table 4** shows that there is a linear relationship between the first oxidation potential and $\mu_D$because $|R| > 0.50$. This descriptor will therefore be subject to criterion 2. With regard to the q^- charge and IR infrared, we note that |R| are 0.4939 and 0.4727, respectively. However, as these values are very close to 0.50, we can say that there is indeed a linear dependence relationship between the first oxidation potential and these two descriptors. Like μ_D, these descriptors will immediately be subject to criterion 2.

Critère de sélection 2

The three descriptors selected are subject to selection criterion 2. Analysis of the data in **Table 5** shows that all partial correlation coefficients are less than 0.70. It is therefore clear that the descriptors (μ_D, q^- and IR) are independent of each other and can be used in the same model. They can therefore coexist in the same model.

Table 5. Selection of descriptors according to criterion 2

Correlation	Coefficient a_{ij}	Independent descriptors if $a_{ij} < 0.70$
μ_D and q^-	-11.671	Independent
μ_D and IR	-0.0336	Independent
q^- and IR	-0.001	Independent

Model study: $E_{theo} = f(\mu_D, q^-$ and IR)

Table 6. Regression coefficient values for the model

	coefficient	**Standard deviation**	**Test t**	**p-value**
Constant	0.0795	0.0586	1.3564	0.2238
μ_D	0.0299	0.0044	6.8336	0.0005
q^-	-0.6254	0.1487	-4.2049	0.0057
IR	-0.0020	0.0005	-4.2226	0.0055

According to **Table 6** given by the XLSTAT software, the equation of the regression line of the model is written:

$$E_{theo} = 0.0795 + 0.0299 * \boldsymbol{\mu_D} - 0.6254 * \mathbf{q}^- - 0.0020 * \mathbf{IR}$$

The regression equation shows through the signs of the coefficients of each variable that the first oxidation potential evolves inversely with q^- and IR while it evolves in the same direction as μ_D. Starting from the absolute values of the Student t Test, the importance of the descriptors is in the following decreasing order: μ_D > IR > q-. The dipole moment therefore makes the strongest contribution in the prediction of the first oxidation potential of the series of molecules studied: It is the priority descriptor. As for IR, the contribution is approximately equal to that of q^-. These different contributions are elucidated by the diagram in **Figure 1**.

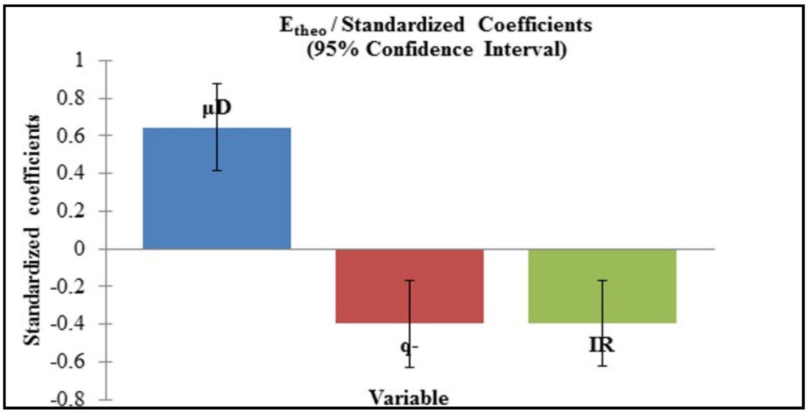


Figure 1. Contribution of model descriptors

Table 7. ANOVA table of the model

	DF	SS	MS	F	p-value
Model	3	0.0951	0.0317	52.6765	0.0001
Error	6	0.0036	0.0006		
Corrected total	9	0.0987			

Analysis of the data in the ANOVA table (**Table 7**) shows that the p-value is less than α=0.05 (5% threshold). Consequently, the model's regression equation is significant for predicting the first oxidation potential of the series of molecules studied. The experimental variance is TSS=0.0987, while the theoretical variance due to the model is ESS=0.0951.

Statistical parameters of the developed model

The statistical parameters of the model are listed in the following table:

Table 8. Statistical parameters of the model

n	R	R^2	R^2_{adj}	s	F
10	0.9815	0.9634	0.9451	0.0245	52.6765

Examination of the data in **Table 8** shows that the correlation coefficient is very high (R = 0.9815). This means that the first oxidation potential is highly correlated with the selected descriptors. The coefficient of determination R^2 = 0.9634 indicates that 96.34% of the experimental variance in the first oxidation potential is explained by the model descriptors. In addition, the standard deviation (s = 0.0245) very close to 0 indicates a good fit and high reliability of the prediction. As for the Fischer coefficient, its value is high (F = 52.6765). This means that the regression equation is significant. While the statistical parameters have yielded satisfactory results, it is imperative to conduct validation tests.

Internal validation of the model

Table 9. Statistical parameters of the LOO internal validation of the model

N	PRESS	Q^2_{LOO}
10	0.0079	0.9200

Table 9 shows that the value of $Q^2_{LOO}$is excellent because Q^2_{LOO}>0.90 (33). This result also shows that Model is resistant to this operation of isolating a molecule and putting it back into the training set. Moreover, 92% of the molecules in the training set have their redox potentials predicted by this model. Consequently, the model has excellent predictive ability with respect to the molecules in the training set. This excellent predictive ability is also confirmed by the very low value of PRESS (0.0079).

Validation externe du modèle

Tableau 10. Paramètres statistiques de la validation externe du modèle

n	R^2_{ext}	Q^2_{ext}
5	0.9802	0.9603

Analysis of the data in Table 10 shows that the model has very high predictive power because Q^2_{ext}=0.9603. This means that 96.03% of the molecules in the test set have their first reduction potentials predicted by the model. In addition, 98.02% of the experimental variance in the first oxidation potential is explained by the descriptors of this model (R^2_{ext}).

Verification of the five (05) Tropsha criteria

Criterion 1: $R^2_{ext} = 0.9802 > 0.70$

Criterion 2: Q^2_{ext}=0.9603>0.60

Criterion 3: $\frac{|R^2_{ext}-R^2_0|}{R^2_{ext}} = 0.01693<0.1$ and k=0.9475 with 0.85<k<1,15

Criterion 4: $\frac{|R^2_{ext}-R'^2_0|}{R^2_{ext}} = 0.01693<0.1$ and k'= 1.0521 with 0.85<k'<1.15

Criterion 5: $|R^2_{ext} - R^2_0|$=0.01666<0.3

All five (05) Tropsha criteria are verified. Consequently, the model performs very well in predicting first oxidation potential. It is therefore acceptable as a prediction model.

Ratio between theoretical redox potential and experimental redox potential: The performance of the model was also studied by analyzing the ratio $\tau = {}^{E_{theo}}/_{E_{exp}}$ of the test series. The obtained values are summarized in **Table 11**.

Tableau 11. Values of the ratio $\tau = {}^{E_{theo}}/_{E_{exp}}$

CODE	E_{exp}	E_{theo}	τ
TTF_11	0.4080	0.4097	1.0043
TTF_12	0.3520	0.3647	1.0361
TTF_13	0.4600	0.4678	1.0170
TTF_14	0.4800	0.4822	1.0045
TTF_15	0.3290	0.3396	1.0322

Analysis of the data in **Table 11** shows that the values of the ratio $\tau = {}^{E_{theo}}/_{E_{exp}}$ are approximately equal to unity. This shows that the model is very effective in predicting the redox potential of the series of studied molecules and can be used to predict other TTF molecules. **Figure 2** illustrates these different observations.

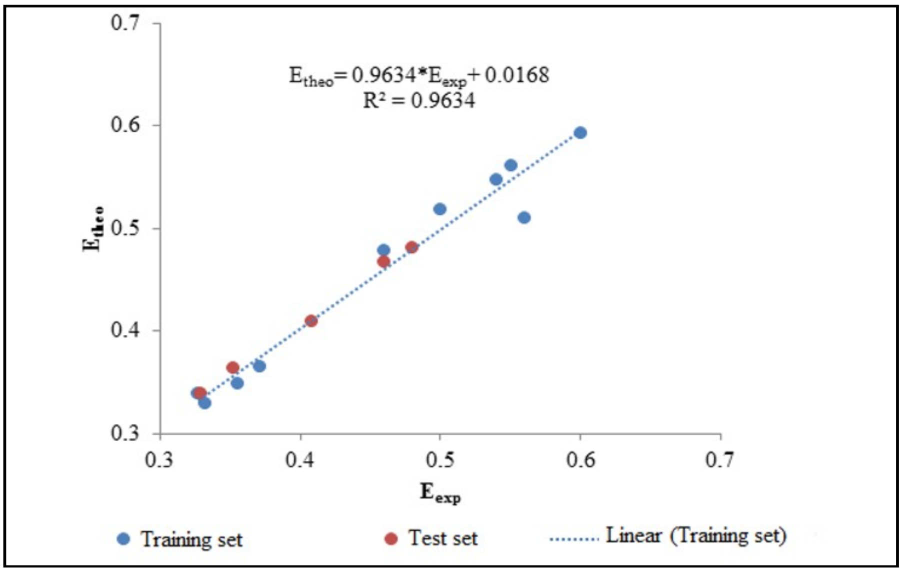


Figure 2. Regression line of the model

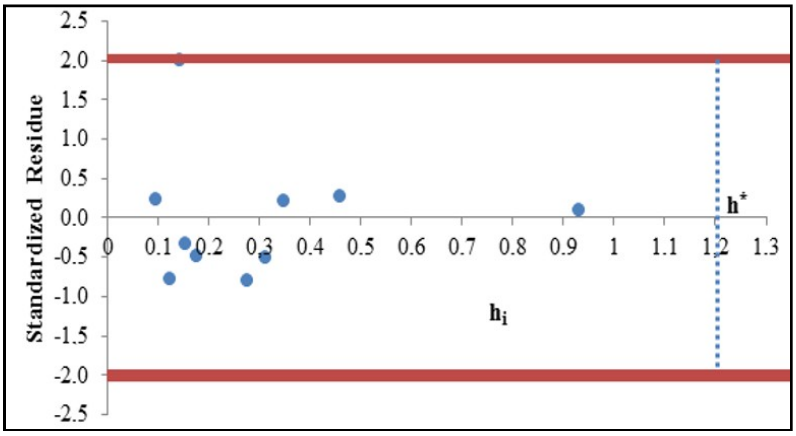


Figure 3. Williams diagram of the model

Applicability Domain of the model: The Applicability Domain (AD) of the model was determined by analyzing the Williams diagram below (**Figure 3**). Analysis of the Williams diagram shows that all observations have standardized residuals between (-2σ; 2σ). In addition, the leverage values obtained are less than the threshold value h^*=1.2. This proves the absence of outliers. The validation results and the domain of applicability show that the model can be used to predict future TTF first oxidation potentials belonging to its domain of applicability.

CONCLUSION

Tetrathiafulvalene (TTF) molecules and existing TTF-TCNQ charge transfer complexes have generally exhibited attractive redox and electrical properties. Improving their properties and searching for new, even better molecules is therefore a challenge for scientific research. Our study in particular consisted of conducting a QSPR study linking the experimental first oxidation potential of a series of TTF molecules to quantum descriptors derived from conceptual DFT. In the model developed, Ethéo is a function of three parameters: the dipole momentμ_D, the smallest Mulliken charge q^- of the molecule, and the infrared IR corresponding to the vibration of the C=C double bond of the TTF nucleus. This model presented very satisfactory statistical parameters (R=0.9815, R^2=0.9634, s=0.0245, F=52.6765). It appears that the dipole moment μ_D is the main descriptor in predicting the redox potential. The model developed can be used as a prediction model for future TTFs within the applicability domain, given that the validation parameters are very satisfactory. Finally, it should be noted that even though a high Q^2_{LOO} value is a necessary condition for a model's robustness and high predictive power with respect to the molecules in the training set, this condition alone is not sufficient, as it can lead to an overestimation of the model's predictive power when applied to truly external compounds.

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