Management Studies, Jan.-Feb. 2016, Vol. 4, No. 1, 33-47
doi: 10.17265/2328-2185/2016.01.004

# Notes on Quantitative Structure-Properties Relationships (QSPR) Part Four: Quantum Multimolecular Polyhedra, Collective Vectors, Quantum Similarity, and Quantum QSPR Fundamental Equation[*]

Ramon Carbó-Dorca
Universitat de Girona, Girona, Catalonia, Spain
Silvia González
Universidad Técnica Particular de Loja, Loja, Ecuador

The nature and origin of a fundamental quantum QSPR (QQSPR) equation are discussed. In principle, as any molecular structure can be associated to quantum mechanical density functions (DF), a molecular set can be reconstructed as a quantum multimolecular polyhedron (QMP), whose vertices are formed by each molecular DF. According to QQSPR theory, complicated kinds of molecular properties, like biological activity or toxicity, of molecular sets can be calculated via the quantum expectation value of an approximate Hermitian operator, which can be evaluated with the geometrical information contained in the attached QMP via quantum similarity matrices. Practical ways of solving the QQSPR problem from the point of view of QMP geometrical structure are provided. Such a development results into a powerful algorithm, which can be implemented within molecular design as an alternative to the current classical QSPR procedures.

*Keywords:* quantum similarity, quantum multimolecular polyhedra (QMP), quantum QSPR (QQSPR), QQSPR fundamental equation, QMP statistical-like collective functions, QMP condensed collective indices, classical QSPR-QSAR

## Introduction

### Quantum Similarity and Quantum Object Sets

Quantum similarity, since the starting paper on this subject (Carbó, Leyda, & Arnau, 1980), intends to deal with molecular sets, described from the point of view of quantum mechanics. In fact, this kind of theoretical setup can be used over any collection of submicroscopic objects. These collections could be described as quantum object sets (QOS), for example the references from many researches (Bultinck & Carbó-Dorca, 2004;

---

[*] **Acknowledgements:** One of the authors (R. C.-D.) wishes to specify that this work has been developed under a Prometeo fellowship and acknowledges the SENESCYT, Government of Ecuador, for granting it.

Ramon Carbó-Dorca, Ph.D., professor, Institut de Química Computacional i Catàlisi, Universitat de Girona, Girona, Catalonia, Spain.

Silvia González, Ph.D., professor, Departamento de Química, Universidad Técnica Particular de Loja, Loja, Ecuador.

Correspondence concerning this article should be addressed to Ramon Carbó-Dorca, Institut de Química Computacional i Catàlisi, Universitat de Girona, Girona, Catalonia, Spain. E-mail: ramoncarbodorca@gmail.com.

Carbó & Besalú, 1995; Carbó-Dorca & Besalú, 1998; 2012a; Carbó-Dorca, 1998a; 1998b; 2001a; 2002), where the development of the quantum similarity theory and practice can be followed.

A set made of submicroscopic elements, when described as a QOS, corresponds to a composite of two sets. It is constructed by the Cartesian product of some set, usually being a well-described molecular set, which is named and acting as the object set, multiplied by a set made of their representation in terms of quantum mechanical density functions (DF), which is named the tag set. Both object and tag sets can be connected in a combined form, so-called, tagged set (Carbó-Dorca, 1998a; 1998b), for which if the tag set is constructed by DF, it becomes a QOS.

This construct becomes always possible within a submicroscopic object structure description. For instance, whenever the object molecular set is represented by $M$ and the tag set of DF by $P$, then, in order to construct the QOS elements, while considering a pair $m_I \in M$ and $\rho_I \in P$, it can be first taken into account that these elements are in a one-to-one correspondence, that is: $\forall I : m_I \leftrightarrow \rho_I$. As a consequence of this close relation, any QOS can be expressed as the Cartesian product: $Q = M \times P$, in such a way that it can be also written:

$$\forall I : q_I = (m_I; \rho_I) \in Q$$

## Molecular Sets and QMP Collective Vectors and Indices

An alternative point of view of a molecular set $M$, other than a QOS construct, can be also taken from the same quantum mechanical description as the QOS was, but taking in consideration the associated tag set of DF only. Then, from such a new viewpoint, the QOS DF tag set can be observed not just as a set of functions, like in the QOS perspective, but as a set of $M$ points belonging to some function space.

Adopting the geometrical perspective as expressed above about the DF tag set of a given QOS, then now the elements of the QOS tag set, can be also considered as forming a so-called quantum polyhedron (QP) (Carbó-Dorca & Besalú, 2012a; Carbó-Dorca, 2014a; 2014b), and thus any QOS can be supposed formed by the object set and a QP instead of a DF tag set. A quantum object represented by a definite DF might be also considered in this geometrical way as a vertex within the QP structure.

Because it can be considered in this manner, any QP becomes in fact the same as the tag set of any QOS, but observed from a geometrical perspective. In any case, a QP can be simply represented as the set of quantum DF acting as their vertices: $P = \{\rho_I | I = 1, 2, \ldots, M\}$. In case of wanting to stress the molecular nature of the elements of the QP, it can be then referred as quantum multimolecular polyhedra (QMP).

## Classical Multimolecular Polyhedra

QMP are also related with the classical manner QSPR or QSAR procedures are based. Molecular sets in the classical case are constructed as some set of $N$-dimensional vectors, which are built up with arbitrarily chosen molecular descriptor parameters (Todeschini & Consonni, 2008). Indeed, even adopting this empirical description, the geometrical structure of a polyhedron, which can be attached to a set of molecules represented as vectors, can be easily retrieved (Carbó-Dorca, Gallegos, & Sánchez, 2009; Carbó-Dorca & Gallegos, 2009a; Carbó-Dorca, 2013a). The vectors associated to each molecule become then the classical multimolecular polyhedron vertices. In the following, the classical description of molecular sets can be considered as a simplified form of the present QMP formalism. A detailed discussion can be found elsewhere (Carbó-Dorca, 2013a) and at the end of the present discussion.

## Quantum Mechanical Expectation Values in QP

The vertices-elements of any QP being originally quantum mechanical DF, it might be also admitted that they individually possess the quantum mechanical meaning of representing the source of knowledge about some observable properties, attached to every quantum object element.

By construction, such quantum mechanical characteristic of the QP vertices might be also visualized by means of defining an appropriate Hermitian operator: $\Omega(r)$, which can be used upon every DF to retrieve some attached quantum object property. Also, once defined such an operator, for instance via an approximate computational procedure, one can calculate the corresponding expectation value $\alpha$, attached to every QP DF vertex, by using the integral expression, the following references describe the evolution of theoretical and practical use of this technique with time (Bultinck, Gironés, & Carbó-Dorca, 2005; Carbó, Besalú, Amat, & Fradera, 1996; Carbó & Calabuig, 1990; 1992a; 1992b; Carbó-Dorca & Gallegos, 2009b; Carbó-Dorca & Gironés, 2005; Carbó-Dorca, 2013b):

$$\forall I : \alpha_I = \left\langle \Omega \rho_I \right\rangle = \int_D \Omega(r) \rho_I(r) dr \tag{1}$$

Quantum similarity is theoretically and computationally based on such a quantum mechanical expectation value framework (Carbó & Calabuig, 1992a; Carbó-Dorca & Gallegos, 2009b; Carbó-Dorca, 2013b). This quantum similarity background important fact might be therefore also stated by means of the above integral (1).

Moreover, equation (1), which is a basic element of quantum mechanical theoretical lore, will be also next in this study revealed as the theoretical element, appearing as the building block of quantum QSPR (QQSPR) fundamental equations.

Thus, a basic quantum similarity postulate can be enunciated, indicating that any source of information, which can be extracted from the elements of any QOS, resides on the QP or tag set $P$ (Carbó-Dorca, 1998a; 1998b), containing the quantum mechanical DF, attached into a one-to-one correspondence with the elements of the object set belonging to the QOS.

### Quantum Similarity Integrals

A straightforward example of the above quantum similarity postulate, when considering some QP or QOS tag set, could be attached to the simpler and most used quantum similarity comparison possible, which implies two elements of any QOS and might be defined by the integrals (Carbó & Calabuig, 1990; 1992a; 1992b), involving any pair of DF belonging to the QP: $\rho_I, \rho_J \in P$, say. Then, for all the DF pairs forming a QMP, it might be written the symmetrical integral construction:

$$\forall I, J : Z_{IJ} = \int_D \rho_I(r) \rho_J(r) dr = \int_D \rho_J(r) \rho_I(r) dr = Z_{IJ} \tag{2}$$

As above defined, this kind of double density quantum similarity integrals can be primarily interpreted as comes next.

For instance, in the following way: the expectation values obtained by means of anyone of the two DF used ($\rho_I$ or $\rho_J$) acting as an adequate Hermitian operator on the other DF ($\rho_J$ or $\rho_I$, respectively), which can be considered, at the same time, as attached to some condensed wave function as well, and related in turn to some quantum object of the associated QOS (Carbó & Calabuig, 1992a; 1992b).

### Quantum Similarity Matrix

Moreover, computed over the DF tag elements of the QOS or the vertices of the QP, such set of similarity integrals defines a symmetric matrix: $Z = \{Z_{IJ}\}$, the so-called (quantum) similarity matrix (Bultinck et al., 2005; Carbó & Calabuig, 1990; Carbó-Dorca & Besalú, 1998; Carbó-Dorca & Gironés, 2005; Carbó-Dorca, 2013b) in order to grasp the properties, computation, and aplication of such a matrix.

Similarity matrices can be supposed to act as metric matrices, not necessarily positive definite (Carbó-Dorca, Besalú, & Mercado, 2011; Carbó-Dorca, 2008). This is so because QMP are usually made of essentially different molecular structures. Thus, the DF tag set elements are necessarily and fundamentally different one from the other. Consequently, the DF tag set and accordingly the DF QMP elements become linearly independent set and the matrix of their scalar products, the similarity matrix $Z$, a metric matrix.

Hence, the set of similarity integrals as defined in equation (2), associated to the similarity matrix $Z$, might transform it into a positive definite matrix. This apparently must be so, although in some cases the resultant similarity matrix corresponds to an indefinite but non-singular array (Carbó-Dorca, 2008). This fact is a consequence of the way the similarity matrix elements are obtained numerically, as a superposition of the coordinates associated to two molecular structures (Carbó-Dorca et al., 2011).

The similarity matrix elements (2) can be thus also seen as Euclidian scalar products of two functions. In practice, such scalar products become integrals optimally calculated by superposing the pair of implied molecular structures, via nuclear coordinate translations and rotations (Carbó-Dorca et al., 2011). In any case, the matrix $Z$ can be considered as a metric matrix (Carbó-Dorca et al., 2011; Carbó-Dorca, 2008). Such occurrence will be discussed in detail elsewhere (Carbó-Dorca, 2015a; 2015b), when practical application of the quantum similarity theory on QMP will be exposed.

### Quantum Selfsimilarity

Two additional remarks could be now provided about the similarity matrix $Z$, which can be attached to any QOS or QMP by means of the DF similarity integrals. The first remark corresponds to the diagonal elements of the similarity matrix, which can be named as (quantum) selfsimilarity integrals. They already have implicitly been defined in equation (2). These diagonal elements of the similarity matrix might be also obviously associated to every element of the QOS tag set $P$.

That is, selfsimilarity integrals consist into a subset of the elements of the similarity matrix, which might be defined as the diagonal of such a matrix, according to the formal statement:

$$\mathrm{Diag}(Z) = \{Z_{II} | I = 1, 2, \ldots, M\}$$

Selfsimilarity integrals have been demonstrated to bear an important role when interpreting some aspects of QSPR. One of these aspects corresponds to his direct ability to produce QSPR simple equations, as it is shown in the following references: Amat, Carbó-Dorca, Cooper, Allan, and Ponec (2003); Amat, Carbó-Dorca, and Ponec (1999); Gironés, Carbó-Dorca, and Ponec (2003); Ponec, Amat, and Carbó-Dorca (1999a; 1999b); and Ponec, Girones, and Carbo-Dorca (2002), similar to these associated to Hansch analysis (Hansch & Leo, 1979), but corresponding within quantum similarity theory to a general quantum background based in equation (1) (Carbó-Dorca & Barragán, 2015).

A related aspect of the selfsimilarity integrals can be associated to the connection of the diagonal elements of the similarity matrix with the number of atoms in a given related molecule. The classical and quantum QSPR consequences of this fact, have been broadly discussed in a previous paper (Carbó-Dorca & Gallegos, 2009a), as the culmination of a wide set of studies on the modern structure of QQSPR fundamental equation and its connection with classical QSPR (Carbó-Dorca et al., 2009; Carbó-Dorca & Gallegos, 2009b; Carbó-Dorca, 2013a).

A second supplementary remark can be connected to one of the possible collective indices, which might be generally described in vector sets and in QOS or QP in particular. Previous work, such as works of

Carbó-Dorca and Barragán (2015) and Carbó-Dorca (2013a; 2014b; n.d.), has been done in this direction, essentially related to the definition of a vector set collective distance by means of the construction of a collective variance vector.

In such recent studies, the trace of the similarity matrix, $Tr(Z) = \Sigma_I Z_{II}$ or the sum of the whole set of selfsimilarities attached to the QP, has been also proved to be the leading term in such a definition of collective distance (Carbó-Dorca & Barragán, 2015; Carbó-Dorca, 2013c) and in the setup of quantum QSPR (QQSPR) linear functions. Such characteristic of the selfsimilarity elements and its role will be briefly described next.

## Mathematical Introduction

### Collective QMP Statistical-Like Functions and Condensed Collective Indices

As a consequence of what has been discussed so far, this study pretends to describe several application aspects of the quantum similarity theory, related to the structure and description of QMP and its relation with QQSPR.

In order to analyze the connection of QMP and QQSPR fundamental equations, first the theoretical characteristics of the statistical-like QMP collective functions will be commented (Carbó-Dorca, 2014b), which in their three first relevant orders correspond to variance, skewness, and kurtosis vectors. In any case, higher order extensions of the lower order terms can be also easily described.

In fact, the QMP statistical-like collective functions can be initially written expressed as powers of the centroid shifted original DF set (Carbó-Dorca & Besalú, 2012b; Carbó-Dorca, 2013d; 2013e).

$$P = 1,\ 2,\ 3,\ \ldots :\ \alpha_P = M^{-1}\sum_J (\rho_J - \rho_C)^P \tag{3}$$

where $\alpha_P$ is the corresponding $P$-th order statistical-like function of the QMP and the centroid DF $\rho_C$ might be easily defined by the arithmetic average:

$$\rho_C = M^{-1}\sum_J \rho_J \tag{4}$$

therefore the first power of the series (3) coincides with the arithmetic mean and corresponds to the zero function:

$$\alpha_I = M^{-1}\sum_J (\rho_J - \rho_C) = M^{-1}\sum_J \rho_J - \rho_C = \rho_C - \rho_C = 0\ \rightarrow\ \alpha_1(r)\ \equiv\ \theta(r) \tag{5}$$

The condensed or complete sum structures of the collective QMP statistical-like functions (3) can be easily revealed. They correspond to collective QMP scalar indices, which resume in some kind of statistical-like form, the configuration of the whole QMP DF vertex set.

Integrating the functions described in equation (3), it is obtained:

$$\left\langle \alpha_P \right\rangle = \int_D \alpha_P(r)dr = M^{-1}\sum_I \left\langle (\rho_I - \rho_C)^P \right\rangle = M^{-1}\sum_I \left[ \sum_{K=0}^{P} (-1)^K \binom{P}{K} \left\langle \rho_I^{P-K} (\rho_C)^K \right\rangle \right] \tag{6}$$

The similarity integrals present in the equation (6) above, which appear described with the complete summation symbol as: $\left\langle \rho_I^{P-K} (\rho_C)^K \right\rangle$, correspond to the sums of $P$ DF products integrals. It must be taking also into account that any power $K$ of the centroid function (4), is linked to an expression involving $K$ nested sums of $K$ DF products.

The collective function of order $P$ = 2, which can be taken as the simplest example of what it is said beforehand, will produce, when integrated, the variance condensed collective QMP index (Carbó-Dorca, 2014b), and will appear in a final form, which can be easily deduced like:

$$\begin{aligned}\left\langle \alpha_2 \right\rangle &= \int_D \alpha_2(r)dr = M^{-1}\sum_I \left\langle (\rho_I - \rho_C)^2 \right\rangle = M^{-1}\sum_I \left\langle \rho_I^2 \right\rangle - 2M^{-1}\sum_I \left\langle \rho_I \rho_C \right\rangle + \left\langle \rho_C^2 \right\rangle \\ &= M^{-1}\sum_I \left\langle \rho_I^2 \right\rangle - \left\langle \rho_C^2 \right\rangle \\ &= M^{-1}\sum_I Z_{II} - M^{-2}\sum_I \sum_J Z_{II} \\ &= M^{-1} Tr(Z) - M^{-2}\left\langle Z \right\rangle \end{aligned} \qquad (7)$$

That is a final expression which corresponds to the difference between the average trace of the double density similarity matrix and the average complete sum of its elements.

Expression (7) above possesses the additional interest of being compliant with the axiomatic definition of collective distance (Carbó-Dorca & Barragán, 2015; Carbó-Dorca, 2013c; 2014b; n.d.-b), which in general might be associated to a set of vectors constructing in turn some polyhedron within a vector space. As expressed above, the QMP condensed variance function can be considered as a distance of this collective sort, providing global scalar information about the DF vertex set (Carbó-Dorca & Barragán, 2015; Carbó-Dorca, 2013c, 2014b; n.d.-b). In fact, the condensed collective QMP indices of even order $\alpha_{2K}$ can be considered as a set of generalized collective distances too.

Another interesting feature, which appears to be capital and extensive to any condensed statistical-like QMP function, is the possibility to write the result in the equality sequence (7) above, as a set of molecular contributions $\{A_{2I} | I = 1, 2, \ldots, M\}$:

$$M\left\langle \alpha_2 \right\rangle = \sum_I \left( Z_{II} - M^{-1}\sum_J Z_{IJ} \right) = \sum_I A_{2I}$$

Then, it is easy to define each second order molecular contribution as:

$$I = 1, \ M : A_{2I} = Z_{II} - M^{-1}\sum_J Z_{IJ}$$

Observing equation (6), it is easy to obtain the same individual molecular contributions up to any order to the collective condensed QMP index of order $P$, writing:

$$\forall P : I = 1, \ M : A_{2I} = \sum_{K=0}^{P} (-1)^K \binom{P}{K} \left\langle \rho_I^{P-K} (\rho_C)^K \right\rangle \qquad (8)$$

which constitutes a convenient definition of the set $\{A_{PI} | I = 1, 2, \ldots, M\}$ of $P$-th order molecular contributions, such that:

$$M\left\langle \alpha_2 \right\rangle = \sum_I A_{PI}$$

Such molecular decomposition feature of the condensed collective QMP indices is a determinant characteristic of the condensed indices $\langle \alpha_P \rangle$, which will be revealed fundamental to build up the QQSPR equations.

Another characteristic to be noted corresponds to the first term of the sum (8), which can be written in general as:

$$\forall I = 1, \ \mathrm{M} \wedge \mathrm{K} = 0: \ \left\langle \rho_I^{P-K} (\rho_C)^K \right\rangle = \left\langle \rho_I^P \right\rangle = \int_D \rho_I^P(r)dr = Z_{II\ldots I} \qquad (9)$$

which can be seen as the *P*-th order selfsimilarity integral. Therefore, every condensed QMP molecular index has as a first element the corresponding molecular selfsimilarity of the adequate order. While observing the last term of equation (8), it is obtained:

$$\begin{aligned}&\forall I = 1, M \wedge K = P : \left\langle \rho_I^{P-K} (\rho_C)^K \right\rangle = \left\langle (\rho_C)^P \right\rangle \\ &= M^{-P} \sum_{J_1} \sum_{J_2} \ldots \sum_{J_P} \left\langle \rho_{J_1} \rho_{J_2} \ldots \rho_{J_P} \right\rangle = M^{-P} \sum_{J_1} \sum_{J_2} \ldots \sum_{J_P} Z_{J_1 J_2 \ldots J_P} = M^{-P} \left\langle {}^{[P]}Z \right\rangle\end{aligned} \tag{10}$$

which is nothing else than the average of the complete sum of the elements of ${}^{[P]}Z$, the *P*-th order quantum similarity hypermatrix or tensor. Observing equation (7), where $P = 2$, only these two terms, trace and complete sum, are needed for the expression of the condensed variance function, associated to the double DF quantum similarity matrix $Z \equiv {}^{[2]}Z$.

**Isometries and Multiple DF Quantum Similarity Hypermatrix Elements**

Condensing the collective QMP functions of *P*-th order into the set of molecular contributions, as expressed in equation (8), produces integrals involving products of *P* DF. When the order of the collective function is larger than two, as in the variance function connected with equation (7), such high order quantum similarity integrals are difficult to compute (Besalú, Carbó, Cooper, Mestres, & Solà, 1995; Carbó, Calabuig, Besalú, & Martínez, 1992; Carbó-Dorca, 2012; Robert & Carbó-Dorca, 1998) where details of some computations involving high order similarity integrals are provided. This difficulty is not only due to the integral evaluation itself, but also it can be attributed to the fact that the implied three or higher DF products producing quantum similarity integrals, generate higher order dimensional arrays too, like these appearing in equations (8), (9), and (10). Even taking into account the high symmetry of the associated hypermatrices or tensors, in any case depending on the number of molecules, the number of hypermatrix elements can increase accordingly.

Because of this accumulative difficulty, it is worthwhile to try to find out a way to simplify the integral evaluation, substituting it, if possible, by an algebraic algorithm. It has been already discussed in previous work (Carbó-Dorca, 2015; n.d.-a), the possibility to substitute the *P* DF similarity integrals, which in fact can be associated to generalized Euclidian products (Carbó-Dorca, 2001a; 2001b; 2003; Sen & Carbó-Dorca, 2000) for more details in the theory and implementation of such products, by alternative generalized scalar products involving finite dimensional column or row vectors.

The basis of such a simplification can be found into the decomposition of the two DF similarity ($M \times M$) matrix *Z*. Because if there can be found a ($M \times M$) matrix *X*, such that the matrix equality:

$$Z = X^T X \tag{11}$$

holds, and whenever the matrix *X* can be decomposed into its columns as:

$$X = (|x_1\rangle,\ |x_2\rangle,\ \ldots\ |x_M\rangle) \tag{12}$$

then, an isometry can be chosen using the columns of $X : \{|x_1\rangle | I = 1, 2, \ldots M\}$ in order to reconstruct the metric matrix *Z*. From equations (11) and (12), the elements of *Z* might be easily rewritten as:

$$\forall I, J : Z_{IJ} = \left\langle x_I \middle| x_J \right\rangle = \sum_K x_{KI} x_{KJ} = \left\langle \left| x_I \right\rangle * \left| x_J \right\rangle \right\rangle \tag{13}$$

In the expression above, the last element just becomes expressed as the complete sum of the inward product of the two involved column vectors; for more details about these two operations see references from Carbó-Dorca (2001b; 2003; 2015a; 2015b) and Sen and Carbó-Dorca (2000). Then, every element of the similarity matrix *Z* can be associated to simple products of the columns of the matrix *X* entering the decomposition (11). This might be just a trivial result, whenever there could not be possible to reconstruct the *P*-th order quantum similarity integrals in an equivalent manner to the double DF case, as written in equation (13), that is:

$$\begin{aligned}&\forall P \wedge \forall I_K = 1, M \wedge K = 1, P : Z_{I_1} Z_{I_2} \ldots Z_{I_P} = \rho_{J_1} \rho_{J_2} \ldots \rho_{J_P} \\ &\equiv \left\langle \left| x_{I_1} \right\rangle * \left| x_{I_2} \right\rangle * \ldots \left| x_{I_P} \right\rangle \right\rangle = \sum_L \left( x_{LI_1} x_{LI_2} \ldots x_{LI_P} \right)\end{aligned} \tag{14}$$

In this way, the molecular contribution elements discussed earlier, concerning the condensed collective QMP indices can be evaluated.

A simple way to proceed seems to be based on the double DF similarity matrix *Z*, by means of any of the elsewhere described isometric procedures (Carbó-Dorca, 2015a; 2015b) and employ the discussed isometric decomposition (11) to obtain higher order statistical-like vectors and their condensed indices.

The problem consists now into that the matrix *X* of the decomposition (11) is not unique. Thus, there are many ways to fulfill the isometric equality, for an extended discussion and the problems associated to this subject, work of Wilkinson (1988) can be referred to.

After being aware of the many ways to construct isometrically, the statistical-like functions and their condensed scalar forms attached to a QMP, practical computational use of the developed theory indicates that, despite the diverse possibilities at hand, the best is to choose a plausible one and fully develop its use.

Once the QMP indices and their condensed scalar values are well defined, the QQSPR fundamental equation can be set up and its practical development, properties, and use are described.

### QMP Associated to Quantum QSPR Equations, Constructed Employing Some Condensed QMP Collective Indices Sequence

Suppose a well-defined QMP, where the experimental values of a molecular property π are also known for some or all the implied QMP molecular structures, which will be present on it as a DF vertex set forming his geometrical structure.

According to this initial framework, for each molecule with a known property, using the previously described techniques described in this work, condensed QMP collective indices can be computed. The first relevant three in the sequence, say: $\{A_2, A_3, A_4\}$, corresponding respectively to the complete sum of the QMP variance, skewness, and kurtosis collective functions. They can be used in such a way that a linear relationship might be sought associated to the form:

$$\pi \approx \omega_0 I + \omega_2 A_2 + \omega_3 A_3 + \omega_4 A_4 + O(5) \tag{15}$$

### Definition of the QQSPR Operator and Its Action Over DF

Moreover, as written above, such kind of linear relation can be also associated to the expectation value of some unknown operator Ω, which can be written in turn as a linear superposition of Hermitian operators $\{A_P\}$.

Accepting this set up, then it can be written:

$$\Omega \approx \sum_P \omega_P A_P \tag{16}$$

with $A_0 = I$ as the unit operator and owing to the property (5), $A_1 = \theta$ is the zero operator.

Then, when the DF $\rho$ of some quantum object is known, the expectation value associated to both the operator (16) expansion and the DF can be easily written by means of the complete sum:

$$\pi \approx \left\langle \Omega_{\rho} \right\rangle = \sum_{P} \omega_P A_P \tag{17}$$

whenever one can admit that the condensed QMP collective indices $\{A_P\}$ present in equation (15), can be also written by means of the expectation values of the Hermitian operator set $\{A_P\}$:

$$\forall P \ : \ A_P \ = \ A_P \rho \tag{18}$$

So far, this theoretical scheme corresponds to an actual alternative representation of the basic quantum QSPR abstract structure, which has been presented into the literature, since the first applicable descriptions of quantum similarity (Carbó-Dorca et al., 2009; Carbó-Dorca & Gallegos, 2009a; Carbó-Dorca, 2013a; Bultinck et al., 2005; Carbó et al., 1996; Carbó & Calabuig, 1990; 1992a; 1992b; Carbó-Dorca & Gallegos, 2009b; Carbó-Dorca, 2013b).

As usual in these problems, within both fundamental quantum QSPR equations (15) and (17), the set of linear coefficients $\{\omega_P\}$ has to be determined via some mathematical procedure, for example, by means of a least squares technique, it has been proposed in other contexts (Carbó-Dorca et al., 2009; Carbó-Dorca, 2013a).

### A Choice of the QQSPR Operator Series Based on the QMP Structure of Collective Functions

At this moment, the question appears about how one can choose the structure of the expansion leading to some equation like expression (16), thus defining the QQSPR operator. It can be shown that such expression yields the expectation value (17) structure, if a background relation is carefully chosen by means of the QMP collective functions. Such process might be described by the way of constructing the elements of the expectation value set $\{A_P\}$, directly related to the operator set $\{A_P\}$. That is, one can proceed seeking for an answer to the questions about why and how equation (18) is fulfilled.

In order to arrive at some result related with the proposed theoretical description of QMP, one can use the fact that for the series (15), every considered term has to be associated to some molecular DF, according to the expectation value definition, as appearing in equation (18).

In fact equation (15) or what is the same, also equation (17), both have to be attached to some molecular DF, acting as one of the vertices of the background QMP. That is, it must be also allowed to write, for every DF, representing a vertex of the associated polyhedron, connected to a known property value, the set of equalities:

$$\forall I : \pi_I \approx \left\langle \Omega_{\rho_I} \right\rangle = \sum_{P} \omega_P \left\langle A_P \rho_I \right\rangle = \sum_{P} \omega_P A_{PI} \tag{19}$$

To obtain a plausible expression for the molecular contributions, to every expectation value, associated to the QMP $I$-th DF vertex $\{A_{PI}\}$, the structure of the QMP condensed function indices first must be recalled.

The condensed QMP collective function indices are easily obtained by developing the corresponding integral, which can be easily connected to a complete sum (Carbó-Dorca & Besalú, 2012a; Carbó-Dorca, 2014a). The following equality sequence can be retrieved from the definition of the condensed collective QMP functions:

$$\begin{aligned}
\forall P : \left\langle \alpha_P \right\rangle &= M^{-1} \sum_{J} \left\langle (\rho_J - \rho_C)^P \right\rangle \\
&= M^{-1} \sum_{J} \left\langle (\rho_J - \rho_C)^{P-1} (\rho_J - \rho_C) \right\rangle \\
&= M^{-1} \sum_{J} \left\langle \beta_{PJ} \rho_J \right\rangle - M^{-2} \sum_{J} \sum_{I} \left\langle \beta_{PJ} \rho_I \right\rangle = M^{-1} \sum_{I} \left\langle \beta_{PI} \rho_I \right\rangle - M^{-2} \sum_{I} \left\langle \sum_{J} \beta_{PJ} \rho_I \right\rangle \\
&= M^{-1} \sum_{I} (\left\langle \beta_{PI} \rho_I \right\rangle - \left\langle \beta_{PC} \rho_I \right\rangle) = M^{-1} \sum_{I} \left\langle (\beta_{PI} - \beta_{PC}) \rho_I \right\rangle \\
&= M^{-1} \sum_{I} \left\langle \gamma_{PI} \rho_I \right\rangle = M^{-1} \sum_{I} A_{PI}
\end{aligned}$$

where in the above development, the following definitions have been used:

$$\forall P \wedge J = 1, M : \beta_{PJ} = (\rho_J - \rho_C)^{P\text{-}1}$$

also

$$\forall P : \beta_{PC} = M^{-1} \sum_J \beta_{PJ}$$

and

$$\forall P \wedge I = 1, M : \gamma_{PI} = \beta_{PI} - \beta_{PC}$$

Thus, perhaps one might rewrite equation (19) now using the following terms:

$$\forall I = 1, M : \pi_I \approx \langle \Omega_I \rho_I \rangle = \sum_P \omega_P \langle \gamma_{PI} \rho_I \rangle = \sum_P \omega_P A_{PI} \tag{20}$$

and in this way, to every molecular structure within the QMP possessing a well-defined property value, there appears that it can be also constructed a well-defined operator with the form (16):

$$\forall I = 1, M : \Omega_I = \sum_P \omega_P \gamma_{PI} \tag{21}$$

which is able to provide a molecular property estimation as an expectation value using equation (20).

Therefore, every condensed statistical-like collective parameter can be supposed corresponding to an average of the expectation values set:

$$\forall P : \{ A_{PI} | I = 1, 2, \ldots, M\} \rightarrow \langle \alpha_P \rangle, = M^{-1} \sum_I A_{PI}$$

associated to every molecular contribution and to every order of the employed condensed QMP collective indices.

### The Nature of the QQSPR Operator Parameters and the Role of Molecular Operators

Within the definition of each molecular $P$-th order operator as provided in equation (21), it can be observed that there presents a set of common operator parameters $\{\omega_P\}$, which could be obtained via a least squares procedure. Besides the common operator parameters, a set of local molecular operators $\{\gamma_{PI}\}$ does appear as well, which depends both on the order of the approximation of the fundamental QQSPR equation (15) and of every molecular DF vertex constituting the QMP possessing a known property value.

### Causal Structure and Other Characteristics of the Fundamental Quantum QSPR Equation

However, as it has been commented many times beforehand in several previous publications (Carbó-Dorca & Gallegos, 2009a; Carbó-Dorca, 2013a; 2013b), the possibility to obtain a QQSPR equation, that is a relation between structure and properties, employing a quantum mechanical bound theoretical result, like the one which is shown in equation (17), makes the obtained relationships somehow causal. This constitutes a clear different contextual aspect in contrast with the usual classical QSPR-QSAR equations structure, which appears to be heavily statistically bound and therefore acausal, a fact which is well known in classical procedures.

It is not necessary to stress the general interest, which has to possess causality in specific scientific areas, and here is not a place where to discuss it. Causality aspects in science have been discussed in deep and its importance revealed, since the publication of the Bunge treatise (2011) many years ago.

Some other not minor aspects, which have been also commented in many instances (Carbó-Dorca & Gallegos, 2009a; Carbó-Dorca, 2013a), about the fundamental quantum QSPR equation, are also of interest in comparison with other current QSAR procedures and will be briefly described.

It must be noted in a first place that QQSPR fundamental equations are defined within the so-called molecular space, in front of the classical problem counterpart, which is circumscribed within the space of descriptors (Todeschini & Consonni, 2008).

QQSPR fundamental equations and their solution to estimate molecular properties can be easily related to a classical procedure (Carbó-Dorca et al., 2009; Carbó-Dorca, 2013a). This simply can be done substituting DF by molecular descriptor vectors, but working in molecular space instead of descriptor space. Classical QSPR procedures appear to be in this sense a simplified particular case of QQSPR theory and procedures.

An extra obvious characteristic, which can be associated to fundamental QQSPR equations, is constituted by the possible universal application to any QMP or even more generally to any QOS.

In addition, one must be aware of the classical QSPR arbitrary choice of molecular descriptor parameters entering the usual computational processes (Todeschini & Consonni, 2008). These parameters are used in turn for the construction of descriptor matrices, just to be manipulated afterwards with least squares techniques and variable reduction procedures closely bound to statistical practice. It is resumed that classical QSPR techniques depend on initial choices of a large number of parameters. Perhaps there can be also, as a result, a lot of possible ways to search for one response, even if this one is found within correct statistical manipulations.

Contrarily, QQSAR parameters and molecular descriptors in the present case study are not arbitrarily chosen by the operator or user. All the information in the QQSAR procedure described here becomes attached to unique quantum similarity matrices and the statistical-like descriptor vectors, connected to the structure of some QMP DF vertices. Quantum descriptors are not arbitrarily chosen but objectively chosen, as they correspond to the only choice of quantum procedures can hold, attached in turn to quantum DF evaluation.

Finally, it can be said that the results of QMP relations between molecular or QO structure, represented by the DF vertices, and submicroscopic object properties are devoid of the typical dimensionality paradox, described around a decade ago which haunts current classical QSPR procedures and statistically bound equations (Carbó-Dorca et al., 2009).

Resuming what has been commented so far, fundamental quantum QSPR equations of type (17) might be used to study structure-properties relationships, within submicroscopic object sets and their QMP geometric representations.

The linear functions obtained by simple mathematical means described here can be considered as the result of causal, universal, and objective procedures, devoid of the dimensionality paradox.

## Practical Implementation of the QQSAR Fundamental Equation

When connecting any QMP vertices with some property and obtaining a QQSPR equation, adapted to the attached molecular DF set, it must be taken into account that in general, while all QMP vertices have to be associated to a DF, not all of them have to be connected with a given property value. Such kind of situation has been already discussed in relation with the QQSPR problem (Carbó-Dorca et al., 2009; Carbó-Dorca, 2013a) and incorporated into the theoretical description and mathematical development finally leading to the QQSPR fundamental equation (20).

In this sense, generally speaking, the whole QMP $P$ can be described by means of the union of two disjoint sets: $K$ and $U$, so that:

$$P = K \cup U \wedge K \cap U = \varnothing$$

In such a way, $K$ might be attached to a set of known values of some property $\{\pi_I^K | I = 1, 2, \dots, M_K\}$ and $U$ to some unknown values of the same property$\{\pi_J^U | J = 1, 2, \dots, M_U\}$, with also $M = M_K + M_U$.

The problem can be clearly seen now consisting into obtaining a QQSPR fundamental equation (20), using the set $K$. Using afterwards, the resultant QQSPR operator parameters to estimate the unknown property values of the molecules of the set $U$ are used.

The following computational steps in form of an algorithm can resume the whole procedure described so far.

**QQSPR Algorithm: QQSPR Operator and Unknown Properties Evaluation**

Knowing a molecular set $M = \{m_I | I = 1, 2, \dots, M\}$ attached in a one-to-one correspondence with a QMP: $P = \{\rho_I | I = 1, 2, \dots, M\}$:

(1) The quantum similarity matrix $Z$ associated to the QMP $P$ can be computed;

(2) The isometric matrix $X$ can be evaluated from $Z = X^T X$;

(3) For every molecule in $M$, the condensed QMP elements of the collective index sequence are computed: $\{A_{PI} | \forall P \wedge I = 1, 2, \dots, M\}$, for example, using the equation (8) and evaluating the necessary quantum similarity integrals using the isometric matrix columns as shown in equation (14);

(4) For every molecule in the subset $K$, the QQSPR equations are set in order to compute the QQSPR operator coefficients $\{\omega_P | \forall P\}$ by means of the known property set $\{\pi_I | I = 1, 2, \dots, M_K\}$:

$$\forall m_I \in K : \pi_I = \sum_P \omega_P A_{PI}$$

$$\Rightarrow \langle \pi | = \{\pi_I | I = 1, 2, \dots, M_K\} \wedge \langle \omega | = \{\omega_P | \forall P\}$$
$$\wedge A_K = \{A_{PI} | \forall P \wedge I = 1, 2, \dots, M\}$$

$$\rightarrow \langle \pi | = \langle \omega | A_K \rightarrow \langle \pi | A_K^T = \omega | A_K A_K^T \rightarrow \langle \omega | = \langle \pi | A_K^T (A_K A_K^T)^{-1}$$

(5) Evaluate the unknown properties using the condensed QMP collective index sequence, attached to the molecular set $U$ and the calculated coefficients $\langle \omega = \{\omega_P | P = 2, 3, \dots\}$ in the previous step:

$$\sum_P \omega_P \gamma_{PI}$$

$$\forall m_J \in U : \pi_J \approx \sum_P \omega_P A_{PJ}$$

$$\Rightarrow \langle^{[U]} \pi | \approx \langle \omega | A_U \leftarrow A_U = \{A_{PJ} | \forall P \wedge J = 1, 2, \dots, M_U\}$$

In this manner, QQSPR procedures based on the previous QQSPR algorithm might include in the problem description and its solution, not only a molecular set $K$ bearing a set of known property values, but also it allows and somehow needs the presence, generally speaking, of any set $U$ of molecules whose property values have to be estimated.

Numerical calculations have been performed up to the second order (Carbó-Dorca & Barragán, 2015). Calculations up to third and fourth order are under way (Carbó-Dorca, n.d.-b).

The broad QQSPR characteristic of including into the QMP molecular set elements with unknown properties, as far as the authors know, has not been so clearly described within classical QSPR-QSAR literature. Therefore, it might be considered as an extra powerful distinctive feature, which quantum QSPR, based on QMP geometrical collective mathematical considerations, can easily possess.

### Use of the QQSPR Algorithm in Classical QSPR Procedures

To end this study, some words can be of interest about the possible application of the QQSPR algorithm into a classical description of a molecular polyhedron. Any molecular polyhedron described with a classical discrete vector set instead of DF vertices, as any QMP is composed, can be handled in the same manner as in the quantum environment mathematical structure developed here.

The vector set made of molecular descriptors, which constructs now a classical molecular polyhedron (CMP), can be used to build an attached Gram matrix, which can act as an ersatz of the quantum similarity one, employed throughout this study. Therefore, substituting the matrix $Z$ in the QQSPR algorithm for some Gram matrix $G$, made by the Euclidian products of the discrete classical molecular vector set, allows using the algorithm as it is. Just the steps (a) and (b) of the QQSPR algorithm have to bear the substitution: $Z \Rightarrow G$.

## Conclusions

By means of straightforward geometrical and computational techniques based on quantum similarity theoretical structure, it has found the way to obtain collective information about molecular sets, by considering them as forming quantum molecular polyhedra, whose vertices are quantum mechanical density functions. Such global molecular set geometrical and condensed evidence, taking the form of a sequence of scalar indices, leads to the description of a QQSPR fundamental equation, possessing potential far reaching practical applications, which can be implemented within a set of useful coherent logical properties.

## References

Amat, L., Carbó-Dorca, R., & Ponec, R. (1999). Simple linear QSAR models based on quantum similarity measures. *Journal of Medicinal Chemistry, 42*(25), 5169-5180.

Amat, L., Carbó-Dorca, R., Cooper, D. L., Allan, N. L., & Ponec, R. (2003). Structure—Property relationships and momentum space quantities: Hammett σ—Constants. *Molecular Physics, 101*(21), 3159-3162.

Besalú, E., Carbó, R., Cooper, D. L., Mestres, J., & Solà, M. (1995). Foundations and recent developments of quantum molecular similarity. *Molecular Similarity I (Topics in Current Chemistry), 173*, 31-62.

Bultinck, P., & Carbó-Dorca, R. (2004). A mathematical discussion on density and shape functions, vector semispaces and related questions. *Journal of Mathematical Chemistry, 36*(2), 191-200.

Bultinck, P., Gironés, X., & Carbó-Dorca, R. (2005). Molecular quantum similarity: Theory and applications. In K. B. Lipkowitz, R. Larter, and T. Cundari (Eds.), *Reviews in computational chemistry* (pp. 127-207). Hoboken, USA: John Wiley & Sons, Inc.

Bunge, M. (2011). *Causality and modern science*. New Jersey: Transaction Publishers.

Carbó, R., & Besalú, E. (1995). Theoretical foundation of quantum similarity. In R. Carbó (Ed.), *Molecular similarity and reactivity: From quantum chemical to phenomenological approaches* (pp. 3-30). Amsterdam: Kluwer Academic Publishers.

Carbó, R., & Calabuig, B. (1990). Molecular similarity and quantum chemistry. In M. A. Johnson and G. M. Maggiora (Eds.), *Molecular similarity*. New York: John Wiley & Sons.

Carbó, R., & Calabuig, B. (1992a). Molecular quantum similarity measures and N-dimensional representation of quantum objects. I. Theoretical foundations. *International Journal of Quantum Chemistry, 42*(6), 1681-1693.

Carbó, R., & Calabuig, B. (1992b). Quantum similarity measures, molecular cloud description, and structure-properties relationships. *Journal of Chemical Information and Modeling, 32*(6), 600-606.

Carbó, R., Besalú, E., Amat, L., & Fradera, X. (1996). Quantum molecular similarity measures: Concepts, definitions and applications. In R. Carbó and P. G. Mezey (Eds.), *Advances in molecular similarity* (pp. 1-42). Greenwich (Conn): JAI Press Inc.

Carbó, R., Calabuig, B., Besalú, E., & Martínez, A. (1992). Triple density molecular quantum similarity measures: A general connection between theoretical calculations and experimental results. *Molecular Engineering, 2*(1), 43-64.

Carbó, R., Leyda, L., & Arnau, M. (1980). How similar is a molecule to another? An electron density measure of similarity between two molecular structures. *International Journal of Quantum Chemistry, 17*(6), 1185-1189.

Carbó-Dorca, R. (1998a). Tagged sets, convex sets and quantum similarity measures. *Journal of Mathematical Chemistry, 23*(3-4), 353-364.

Carbó-Dorca, R. (1998b). Fuzzy sets and boolean tagget sets, vector semiespaces and convex sets, QSM and ASA density functions, diagonal vector spaces and quantum chemistry. In R. Carbó and P. G. Mezey (Eds.), *Advances in molecular similarity* (pp. 43-72). Greenwich (Conn): JAI Press Inc.

Carbó-Dorca, R. (2001a). Inward matrix products: Extensions and applications to quantum mechanical foundations of QSAR. *Journal of Molecular Structure: Theochem, 537*(1-3), 41-54.

Carbó-Dorca, R. (2001b). Inward matrix product algebra and calculus as tools to construct space-time frames of arbitrary dimensions. *Journal of Mathematical Chemistry, 30*(2), 227-245.

Carbó-Dorca, R. (2002). Shell partition and metric semispaces: Minkowski norms, root scalar products, distances and cosines of arbitrary order. *Journal of Mathematical Chemistry, 32*(2), 201-223.

Carbó-Dorca, R. (2003). Applications of inward matrix products and matrix wave functions to Hückel MO theory, Slater extended wave functions, spin extended functions, and Hartree method. *International Journal of Quantum Chemistry, 91*(5), 607-617.

Carbó-Dorca, R. (2008). A quantum similarity matrix (QSM) Aufbau procedure. *Journal of Mathematical Chemistry, 44*(1), 228-234.

Carbó-Dorca, R. (2012). Triple density quantum similarity measures and the tensorial representation of quantum object sets. In T. Chakraborty (Ed.), *Quantum chemistry: Theory and practice*. London: Taylor & Francis Group.

Carbó-Dorca, R. (2013a). Notes on quantitative structure-property relationships (QSPR), part 3: Density functions origin shift as a source of quantum QSPR algorithms in molecular spaces. *Journal of Computational Chemistry, 34*(9), 766-779.

Carbó-Dorca, R. (2013b). Quantum similarity. In S. K. Ghosh and P. K. Chattaraj (Eds.), *Concepts and methods in modern theoretical chemistry: Electronic structure and reactivity* (pp. 349-365). London: CRC Press Taylor & Francis.

Carbó-Dorca, R. (2013c). Collective euclidian distances and quantum similarity. *Journal of Mathematical Chemistry, 51*(1), 338-353.

Carbó-Dorca, R. (2013d). Mathematical aspects of the LCAO MO first order density function (5): Centroid shifting of MO shape functions basis set, properties and applications. *Journal of Mathematical Chemistry, 51*(1), 289-296.

Carbó-Dorca, R. (2013e). Variational principle, Hohenberg-Kohn theorem, and density function origin shifts. *Journal of Mathematical Chemistry, 51*(5), 1397-1409.

Carbó-Dorca, R. (2014a). Multimolecular polyhedra and QSPR. *Journal of Mathematical Chemistry, 52*(7), 1848-1856.

Carbó-Dorca, R. (2014b). Quantum polyhedra, definitions, statistics and the construction of a collective quantum similarity index. *Journal of Mathematical Chemistry, 53*(1), 171-182.

Carbó-Dorca, R. (2015a). An isometric representation problem related with quantum multimolecular polyhedra and similarity. *Journal of Mathematical Chemistry, 53*(8), 1876-1884.

Carbó-Dorca, R. (2015b). An isometric representation problem in quantum multimolecular polyhedra and similarity: (2) Synisometry. *Journal of Mathematical Chemistry, 53*(1), 1876-1884.

Carbó-Dorca, R. (n.d.). Collective vectors, condensed indices and quantum similarity. *Frontiers in Computational Chemistry* (IQCC Technical Report TC-2015-2, in preparation).

Carbó-Dorca, R., & Barragán, D. (2015). Communications on quantum similarity (4): Collective distances computed by means of similarity matrices, as generators of intrinsic ordering among quantum multimolecular polyhedra. *WIREs, 5*(5), 380-404.

Carbó-Dorca, R., & Besalú, E. (1998). A general survey of molecular quantum similarity. *Journal of Molecular Structure: Theochem, 451*(1-2), 11-23.

Carbó-Dorca, R., & Besalú, E. (2012a). Shells, point cloud huts, generalized scalar products, cosines and similarity tensor representations in vector semispaces. *Journal of Mathematical Chemistry, 50*(1), 210-219.

Carbó-Dorca, R., & Besalú, E. (2012b). Centroid origin shift of quantum object sets and molecular point clouds description and element comparisons. *Journal of Mathematical Chemistry, 50*(5), 1161-1178.

Carbó-Dorca, R., & Gallegos, S. A. (2009a). Quantum similarity and quantum QSPR (QQSPR). *Encyclopedia of Complexity and Systems Science, 8,* 7422-7480.

Carbó-Dorca, R., & Gallegos, S. A. (2009b). Notes on quantitative structure-properties relationships (QSPR) part 2: The role of the number of atoms as a molecular descriptor. *Journal of Computational Chemistry, 30*(13), 2099-2104.

Carbó-Dorca, R., & Gironés, X. (2005). Foundation of quantum similarity measures and their relationship to QSPR: Density function structure, approximations, and application examples. *International Journal of Quantum Chemistry, 101*(1), 8-20.

Carbó-Dorca, R., Besalú, E., & Mercado, L. D. (2011). Communications on quantum similarity, part 3: A geometric-quantum similarity molecular superposition algorithm. *Journal of Computational Chemistry, 32*(4), 582-599.

Carbó-Dorca, R., Gallegos, S. A., & Sánchez, A. J. (2009). Notes on quantitative structure-properties relationships (QSPR) part 1: A discussion on a QSPR dimensionality paradox (QSPR DP) and its quantum resolution. *Journal of Computational Chemistry, 30*(7), 1146-1159.

Gironés, X., Carbó-Dorca, R., & Ponec, R. (2003). Molecular basis of LFER. Modeling of the electronic substituent effect using fragment quantum self-similarity measures. *Journal of Chemical Information and Computer Sciences, 43*(6), 2033-2038.

Hansch, C., & Leo, A. (1979). *Substituent constants for correlation analysis in chemistry and biology*. New York: Wiley.

Ponec, R., Amat, L., & Carbó-Dorca, R. (1999a). Molecular basis of quantitative structure-properties relationships (QSPR): A quantum similarity approach. *Journal of Computer-Aided Molecular Design, 13*(3), 259-270.

Ponec, R., Amat, L., & Carbó-Dorca, R. (1999b). Quantum similarity approach to LFER: Substituent and solvent effects on the acidities of carboxylic acids. *Journal of Physical Organic Chemistry, 12*(6), 447-454.

Ponec, R., Girones, X., & Carbo-Dorca, R. (2002). Molecular basis of linear free energy relationships. The nature of inductive effect in aliphatic series. *Journal of Chemical Information and Modeling, 42*(3), 564-570.

Robert, D., & Carbo-Dorca, R. (1998). Analyzing the triple density molecular quantum similarity measures with the INDSCAL model. *Journal of Chemical Information and Modeling, 38*(4), 620-623.

Sen, K. D., & Carbó-Dorca, R. (2000). Inward matrix products, generalised density functions and Rayleigh-Schrödinger perturbation theory. *Journal of Molecular Structure: Theochem, 501-502,* 173-176.

Todeschini, R., & Consonni, V. (2008). *Handbook of molecular descriptors*. Weinheim: Wiley Online Library.

Wilkinson, J. H. (1988). *The algebraic eigenvalue problem*. Oxford: Oxford University Press.