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Article

Chemoinformatics Analysis of the Colour Fastness Properties of Acid and Direct Dyes in Textile Coloration

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Abstract: The efficiency of chemoinformatics methods based on a fragment approach for the analysis of relationships between the chemical structure of textile dyes and colour fastness of the dyeings have been shown by examining a large set of properties, including the light fastness of acid dyes on wool and polyamide fibres, the sensitivity of acid dyes on wool to oxygen bleaching, the wash fastness of acid dyes on wool, the adsorption of direct dyes on cotton, and the photodegradation of azo dyes in solution. An analysis of the developed regression models depicted the contribution of ten substructural molecular fragments for each indicator of the colour fastness properties of acid and direct azo dyes on textile materials. The similarity of several individual multi-atomic fragments for acid and direct azo dyes was found for wool, polyamide, and cotton fibres, which indicates the coinciding mechanisms of the physicochemical processes that accompany the destruction of dyes while testing the light fastness and sensitivity of the dyeings to oxygen bleaching, as well as their adsorption/desorption with the wash fastness and dyeability of wool and cotton.

Keywords: acid dyes; direct dyes; cotton; wool; polyamide fibres; light fastness; wash fastness; chemoinformatics analysis

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1. Introduction

The study of structure–property relationships was essential for textile chemistry research in previous years. It was based on a detailed study of the physicochemical aspects of dye coloration and the properties of dyes that were adsorbed by the fibres [1–9]. Currently, QSPR/QSAR research (QSPR/QSAR-quantitative structure–property/activity relationships) and chemoinformatics analysis cover almost every fundamental and applied field in chemical studies.

Presently, 27,000 individual products under 13,000 generic names are incorporated in the Colour Index [10]. A lot of information regarding the properties of commercial textile dyes for all the technical groups of dyes is provided on the website, World Dye Variety [11]. Water-soluble dyes contribute to about 50% of the total amount of dyes. The Max Weaver Dye Library [12] at Eastman Kodak Company represents a collection of 98,000 vials of custom-made water-soluble dyes. As a part of this collection, temporary, water-soluble hair dyes were collected and analysed for this research [13,14]. Some results from recent research on the bio-elimination of large groups of commercial acids indicates that direct and reactive dyes [15–17] are suitable for the discussion about dye affinity for cellulose. A chemometric analysis of different classes of dyes was performed through a series of research studies. The different dye classes studied included: acid dyes for silk [18–20], acid dyes for wool and nylon [21], and disperse dyes for synthetic fibres [22–24]. One of the early examples of software for QSPR analysis was the software, SPARC, which was widely used up to now for predicting the ionization constants, pKa, and hydrophobicity, LogP, of organic compounds—such as azo dyes and their related compounds [25].

The problem with QSPR analysis of the dye affinity for textile fibres and the physicochemical properties of dyeings became a key point in the development of new ideas during the eve of 2000. A fundamental contribution to the problem was provided through the research of S. Timofei and co-authors [26]. A review cited above makes reference to 14 papers from their research published since 1994 that were based on the application of the comparative molecular field analysis method. The beginning of their research started directly with vat, disperse, acid, and direct dyes. Later on, the authors continued the modification of the method for acid dyes, which is represented in their recent research [27]. Their results and a database for anionic dyes are used in this research [28–31]. Recent studies [32,33] have continued the development of the chemoinformatics approach based on the experimental data that showed the affinity of anionic dyes for cellulose fibres, which were collected in the abovementioned research [26,27].

A wide variety of empirical properties of water-soluble dyes are covered by chemoinformatics research, for example, the tinctorial properties of acid dyes on cellulose fibres in the domestic washing of mixed cellulose/polyamide/wool materials [34], the photodegradation [35] and catalytic elimination [36] of dyes in wastewater, the behavior of dyes during the advanced oxidation process [37,38], the ecotoxicity of dyes [39–41], etc.

Acid and direct dyes as anionic water-soluble dyes play an important role in fundamental research on colour fading properties [42–45] and adsorption on fibrous materials [2,3,34,46–50]. Reactive dyes are a special class of anionic dyes due to their irreversible chemical fixation on the fibres, therefore their wash fastness properties could not be analysed within a single concept for anionic dyes. Studies on the substantivity of the hydrolysed forms of reactive dyes [51] do not provide information about the chemical structure of these dyes. On the other hand, fundamental research on the colour fading properties of reactive dyes by peroxide [52] and the light fastness of the dyeings [53] does not contain sufficient information for the application of the statistical tools of chemoinformatics.

Recent advances in QSPR methods are analysed in several reviews [54–57]. The particular problems with the chemoinformatics of dyes are reviewed in Refs. [58,59]. Analysis of the chemical structure and property relationships of dyes usually applies multiple linear regression models or neuro-models based on chemoinformatics software, the most typical of which are listed below in Table 1.

Table 1. Examples of modern software for structure–property analysis of organic compounds.

Software	Number of Descriptors
SPARC, by L.A. Carreira et al., ARChem, USA, 1994 [60]	not specified
CODESSA, by A.R. Katritzky, M. Karelson, R. Petrukhin, University of Florida USA, 2001-2005 [61]	about 1500
DRAGON, by Kode Chemoinformatics, R. Todecini et al., Pisa, Italy, 1994 [62]	5270
NASAWIN, by I.I. Baskin et al., Moscow State University, Russia, 1995 [63–66]	unlimited
CORAL, Mario Negri Institute, E. Benfenati, A.A. Toropov, A.P. Toropova, Italy, 2010 [67]	unlimited
OCHEM, I.I. Tetko, et al., International project, 2011 [68]	unlimited

Different kinds of descriptors are represented by the physicochemical parameters, functional groups, topology and geometry of the molecules, fragments of a different kind, etc. Those descriptors are collected, and the databases are arranged through the use of chemoinformatics software—for example, ChemAxon [69].

The fragment approach mentioned above [30,63–66] explores the descriptors based on the chemical structure of the molecule through the defragmentation of the molecule on the substructures of chains, branches, and cycles of atoms. The idea of the fragment approach was used in the research done by Refs. [70–72], which focused on the problems in textile chemistry and the photophysics of fluorescent BODIPY dyes.

Current research aims to develop a database of acid and direct dyes for textile coloration and QSPR analysis using the fragment approach and the software, NASAWIN. This is a universal method of calculating atomic fragments without any reference to the physicochemical properties of the molecule, meeting the clear understanding of the chemists and providing an easy interpretation of the results, which are useful for developing the different chemical and physicochemical properties of dyed fabrics. Each database of dyes is characterised by multiple linear regression models with substructural fragments that describe dye sorption in terms of the fibres, wash fastness, and light fastness of anionic dyes adsorbed on cotton, wool, and polyamide fibres. The results of the analysis provide new insight into dye structure–property relationships and the role of the nature of fibres in textile coloration, which is useful for developing new dyes and dyeings on high-performance textile materials. Several results for the prediction of a series of dyes demonstrate the robustness of the developed models.

2. Materials and Methods

2.1. Database for Colour Fastness of Wool, Polyamide, and Cotton Fibres Dyed with Acid and Direct Dyes

The experimental data for the chemoinformatics analysis of colour fastness properties of textiles are provided in various sources of information.

The data for the light fastness, oxygen bleaching sensitivity, and wash fastness of commercial azo dyes on wool are taken from the World Dye Variety [11]. The information reported by different companies corresponds to the ISO standards. Validation of data presented on the web is performed by comparing the selected entries for the properties of the dyeings with those published in the literature. Data for the oxygen bleaching of azo dye on polyamide and cotton are not available on the web or in the literature. In general, this topic is discussed in systematic research for both cotton [24–29] and nylon fibres [32,33], however, detailed information for various dyes is not reported.

The data for the research on light fastness in acid azo dyes on polyamide fibres (Nylon 6.6) were collected from the following publications: Grecu and Pieroni 1981 [73]; Carpignano et al. 1983, 1985 [74,75]; Barni et al. 1984 [76]; De Giorgi et al. 1994, 1997 [19,21]; Kraska 1984 [77]; Blus 1992, 1993, 2005 [78–81]; Kraska and Blus 1996 [82]. In total, the database includes acid dyes with azobenzene, azonaphthalene, and azopyrazolone structures.

The data representing the adsorption of direct dyes on cotton were collected from Refs. [83,84] for the different initial concentrations of dye in the dyebath: 0.1%, 0.5%, 1.0%, and 2.5% of the weight of the fabric. Such information is suitable for the discussion of the mechanism of adsorption of newly synthesised disazo and trisazo direct dyes, which were studied by one group of researchers. The abovementioned experimental data for the affinity of direct dyes are less reliable due to the various approaches used to evaluate the physicochemical quantity in the collected research papers. The data for the wash fastness of direct dyes that were reported in scientific research have been omitted due to the low statistical reliability of the chemoinformatics results.

As a whole, the database explored in the research serves as an example of the collection of miscellaneous properties that reflect the colour fastness of anionic azo dyes on fibres of various natures.

2.2. Chemoinformatics Tools

The database was prepared using JChem for Office software [69], implementing tools for drawing dye molecules, checking their chemical structure, and generating an sdf-file. Further analysis of the database by NASAWIN [66] makes it possible to decompose the whole database of dyes into sub-molecular descriptors without the calculation of any special physicochemical parameters of the molecules. Originally, the total amount of fragment descriptors for the database of about 130 dye molecules, as an example, counts around 6000 descriptors, which yields a so-called underdetermined system of linear equations. Further calculation procedures, including the partial square regression (PLS) method, and removing the correlated parameters yield an overestimated matrix for the determination of the regression coefficients of the multiple linear regression model. Finally, the single-step procedure of eliminating the regression coefficients based on Student-criteria, Fischer-criteria, and the regression coefficient yields a multiple linear regression model with a limited number of descriptors (usually about ten), thereby characterising the properties of the database with appropriate precision.

Statistical parameters attributed to the model are represented by the following quantities: N–total amount of compounds included in the database; R–regression coefficient, which shows how close the data points are to fitting a curve or line; R—adj-adjusted regression coefficient, which indicates how well the terms fit a curve or line but adjusts for the number of terms in a model; RMSE–root-mean-square error, i.e., square root of mean square error, a measure of the differences between the values predicted by a model and the values observed; MAE–mean absolute error, a measure of the average vertical distance between each point and the Y = X line; s–standard deviation, a measure of how much the data is spread out; F–Fischer number, which characterises how small the dispersion of the predicted data is related to the average dispersion of the data; T-stat–Student number for each regression coefficient of the model.

3. Results and Discussion

3.1. Light Fastness of Commercial Acid Azo Dyes on Wool

The results of the chemoinformatics analysis of the database for the light fastness of commercial acid azonaphthalene dyes are shown below in Figure 1. Table 2 shows the molecular fragments for the exemplified dye congeners along with the values of the regression coefficients for the multiple linear regression model and corresponding Student numbers T-stat. The sign of the regression coefficient characterises the positive or negative impact of the correspondent fragment on the light fastness of dyed fabrics, and the absolute value of the coefficient shows the impact of the descriptor on the light fastness. Student number T-stat characterises the reliability of the coefficient; the standard deviation of the coefficient could be evaluated as the relation coeff/T-stat. The results represented below display the high statistical quality of the regression coefficients.

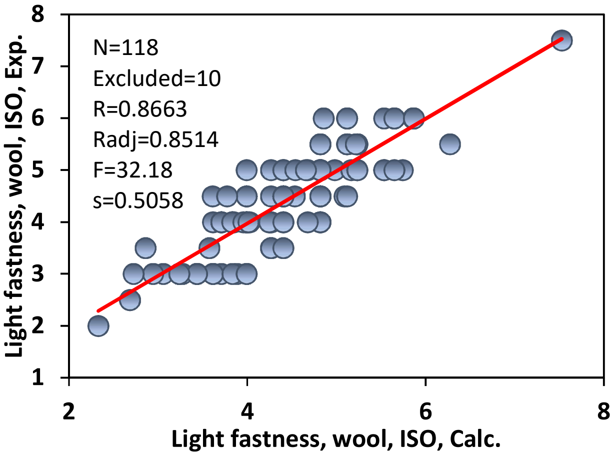
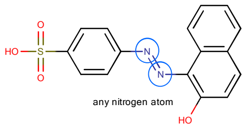
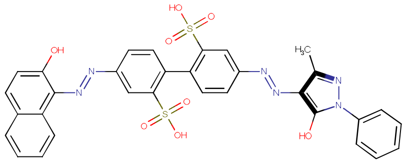
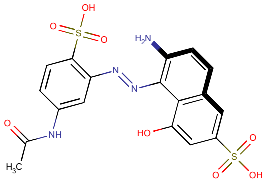
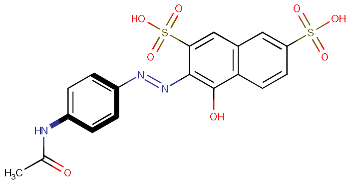
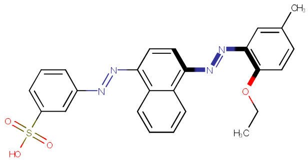
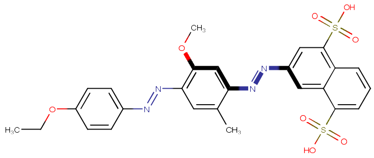
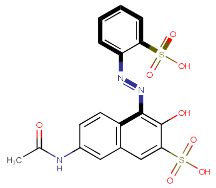
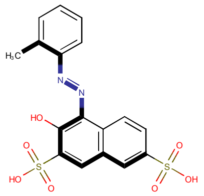
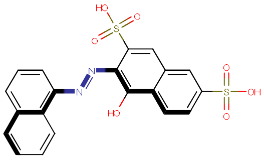
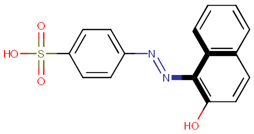


Figure 1. Correlation between calculated and experimental values of light fastness of commercial azo acid dyes on wool.

Table 2. Coefficients of multiple linear regression model for light fastness of wool dyed with commercial azo acid dyes and fragments of exemplified dye congeners.

Regression Coefficient, Molecular Fragment	**Regression Coefficient, Molecular Fragment**	**Regression Coefficient, Molecular Fragment**
Coeff0 = 3.161944, T-stat = 18.3618	Coeff1 = 0.414375, T-stat = 8.8966 LF-W-1  	Coeff2 = −0.604511, T-stat = −4.3458 LF-W-2 
Coeff3 = −1.037494, T-stat = −6.3766 LF-W-3 	Coeff4 = −0.287592, T-stat = −3.3646 LF-W-4 	Coeff5 = 0.685249, T-stat = 4.1154 LF-W-5 
Coeff6 = 0.668728, T-stat = 7.1565 LF-W-6 	Coeff7 = 0.288798, T-stat = 4.1107 LF-W-7 	Coeff8 = −0.492495, T-stat = −3.5045 LF-W-8 
Coeff9 = −0.376856, T-stat = −3.9398 LF-W-9 	Coeff10 = −0.55531, T-stat = −6.5707 LF-W-10 	

Analysis shows that the chemical fragments of the dye molecules increase the light fastness of acid azo dyes on wool, including the nitrogen atoms for all the compounds (fragment 1); the azo-bond connecting aromatic chain, an aromatic chain with m-methoxy- or o-ethoxy-groups (fragment 5 and 6); and the azo group connecting the aromatic chain and the aromatic chain with a sulphonic group (fragment 7). The fragments that decrease the light fastness are exemplified by the aromatic chain with primary amino- or substituted amino groups (fragments 3 and 4). Another two examples are the branch or chain fragments of the aromatic carbon atoms with nitrogen in an sp3-hybridisation form (nitrogen of double azo-bond or nitrogen of pyrazolone cycle) (fragments 2 and 10).

3.2. Colour Fastness to Oxygen Bleaching of Commercial Acid Azo Dyes on Wool

The chemoinformatics analysis of the database for the oxygen bleaching sensitivity of acid azonaphthalene dyes is represented in Figure 2 and Table 3.

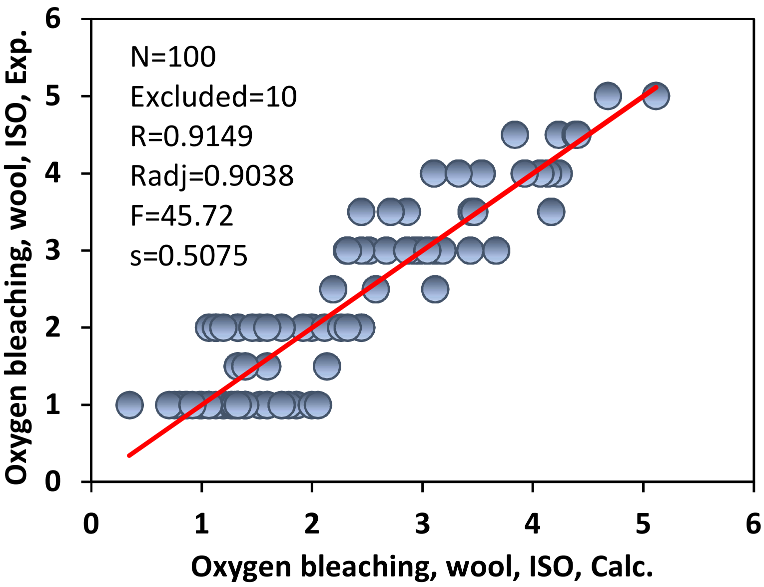


Figure 2. Correlation between calculated and experimental values of oxygen bleaching sensitivity of commercial azo acid dyes on wool fibres.

Oxygen bleaching sensitivity is explained by dye destruction in the domestic washing treatment of textiles, therefore it is quite reasonable that some fragments, which decrease light fastness, increase oxygen beaching sensitivity—for example, the aromatic chain with a primary amino-group or an azo-bond connecting two aromatic chains of carbon atoms from both sides (fragments 3, 4, 7, 9). There is a high negative impact on sensitivity when there is a branch fragment connecting the aliphatic carbon atom and the two aromatic ones (fragment 10). There is a stabilizing effect on OB-sensitivity when there are two azo-bonds in disazo acid dyes with an aliphatic ethyl-group (fragments 5 and 10). Some of the results correlate with common knowledge, for example, polyazo dyes, which were found to be more stable during biodegradation than monoazo dyes in early QSPR analysis [85].

Table 3. Coefficients of multiple linear regression model for oxygen bleaching sensitivity of wool dyed with commercial azo acid dyes and fragments of exemplified dye congeners.

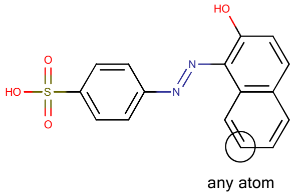
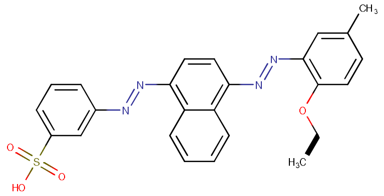
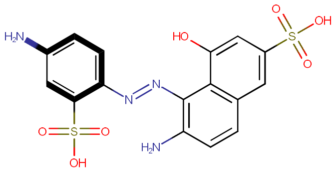
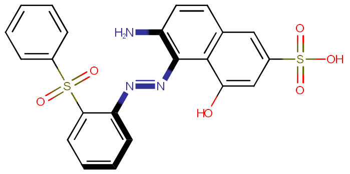
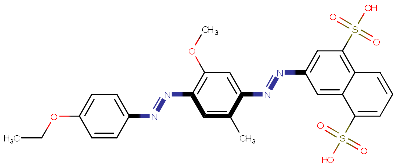
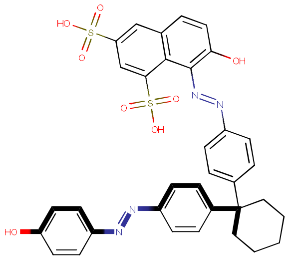
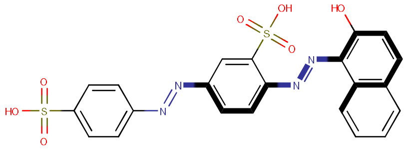
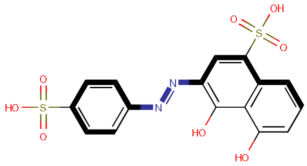
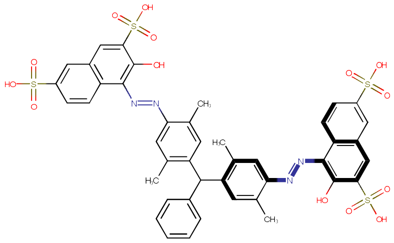
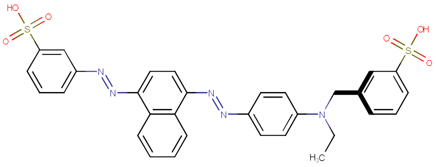
Regression Coefficient, Molecular Fragment	Regression Coefficient, Molecular Fragment	Regression Coefficient, Molecular Fragment
Coeff0 = −0.714316, T-stat = −2.9669	Coeff1 = 0.065831, T-stat = 10.1430 OB-W-1  	Coeff2 = −0.938693, T-stat = −4.1047 OB-W-2 
Coeff3 = 1.477873, T-stat = 4.8356 OB-W-3 	Coeff4 = 2.706476, T-stat = 7.3958 OB-W-4 	Coeff5 = −1.376763, T-stat = −5.2326 OB-W-5 

Table 3. *Cont.*

Regression Coefficient, Molecular Fragment	Regression Coefficient, Molecular Fragment	Regression Coefficient, Molecular Fragment
Coeff6 = 0.101659, T-stat = 4.6905 OB-W-6 	Coeff7 = 1.20228, T-stat = 6.8330 OB-W-7 	Coeff8 = 0.492824, T-stat = 5.1165 OB-W-8 
Coeff9 =−1.134224, T-stat = −5.6996 OB-W-9 	Coeff10 = 2.800875, T-stat = 7.3944 OB-W-10 	

3.3. *Wash Fastness of Commercial Acid Azo Dyes on Wool*

The results of the analysis of the database for the wash fastness of acid azonaphthalene dyes on wool fibres are shown in Figure 3 and Table 4.

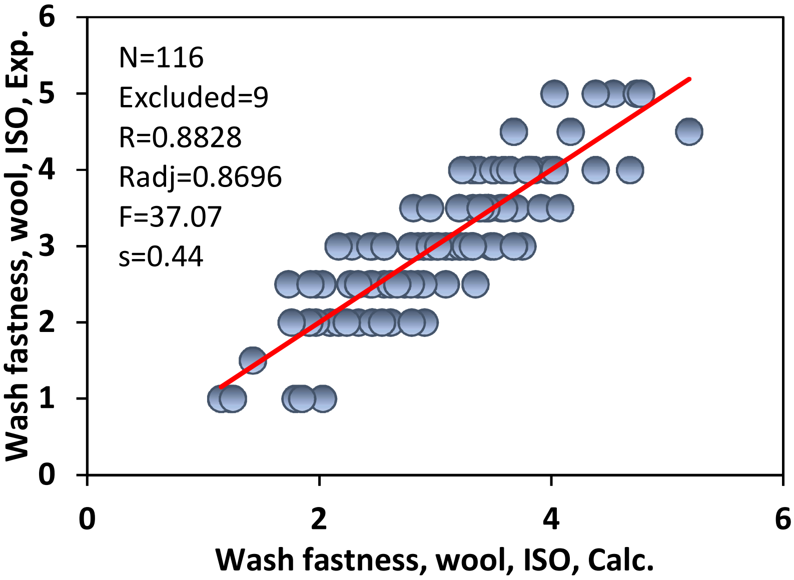
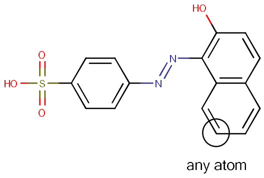
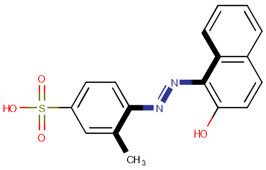
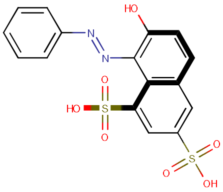
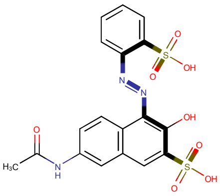
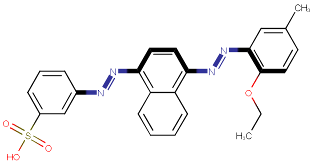
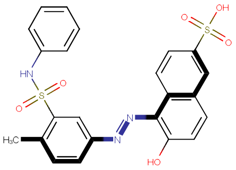
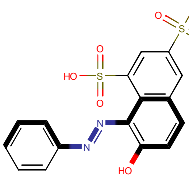
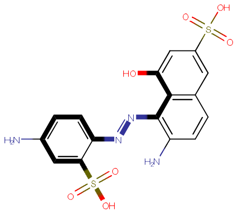
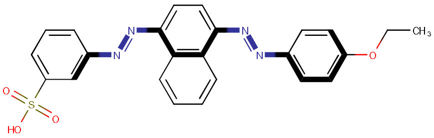
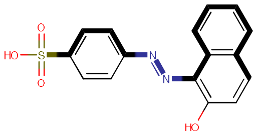


Figure 3. Correlation between calculated and experimental values of wash fastness of commercial azo acid dyes on wool fibres.

Table 4. Coefficients of multiple linear regression model for wash fastness of wool dyed with commercial azo acid dyes and fragments of exemplified dye congeners.

Regression Coefficient, Molecular Fragment	Regression Coefficient, Molecular Fragment	Regression Coefficient, Molecular Fragment
Coeff0 = 0.963902, T-stat = 4.9380	Coeff1 = 0.058948, T-stat = 12.5825 WF-W-1  	Coeff2 = −0.309573, T-stat = −3.9703 WF-W-2 
Coeff3 = −0.335361, T-stat = −3.8736 WF-W-3 	Coeff4 = −0.256796, T-stat = −3.8610 WF-W-4 	Coeff5 = 0.199498, T-stat3 = 3.3687 WF-W-5 
Coeff6 = 0.511187, T-stat = 4.1279 WF-W-6 	Coeff7 = −0.532824, T-stat = −3.5236 WF-W-7 	Coeff8 = −0.938293, T-stat = −3.4897 WF-W-8 
Coeff9 = 0.407356, T-stat = 6.1331 WF-W-9 	Coeff10 = −0.0876, T-stat = −4.8110 WF-W-10 	

Wash fastness is a property that reflects the affinity of the dyes to fibres. A simple correlation analysis demonstrated the properties of disperse dyes on acetate fibres [86,87], which proves this statement directly.

In our case, wash fastness reflects the intermolecular bonding of acid dyes with wool keratin. Several fragments exhibit positive effects, such as any atom of the molecule (i.e., all atoms of any nature) (fragment 1), the 12- and 15-atom fragment containing two azo-bonds (fragments 5 and 9), as well as the 12- and 13-atomic fragments containing an azo-bond and hydrophobic methyl group (fragment 6). On the other hand, a negative effect is demonstrated when there is a chain of conjugated double bonds containing an azo-bond and hydrophilic hydroxy-group (fragment 7), as well as the four fragments containing sulphonic groups (fragments 3, 4, 8, 10).

3.4. Light Fastness of Acid Dyes on Polyamide (Nylon) Fibres

The database includes acid dyes with azobenzene, azonaphthalene, and azopyrazolone structures. The results of the computational analysis of the database are shown in Figure 4 and Table 5.

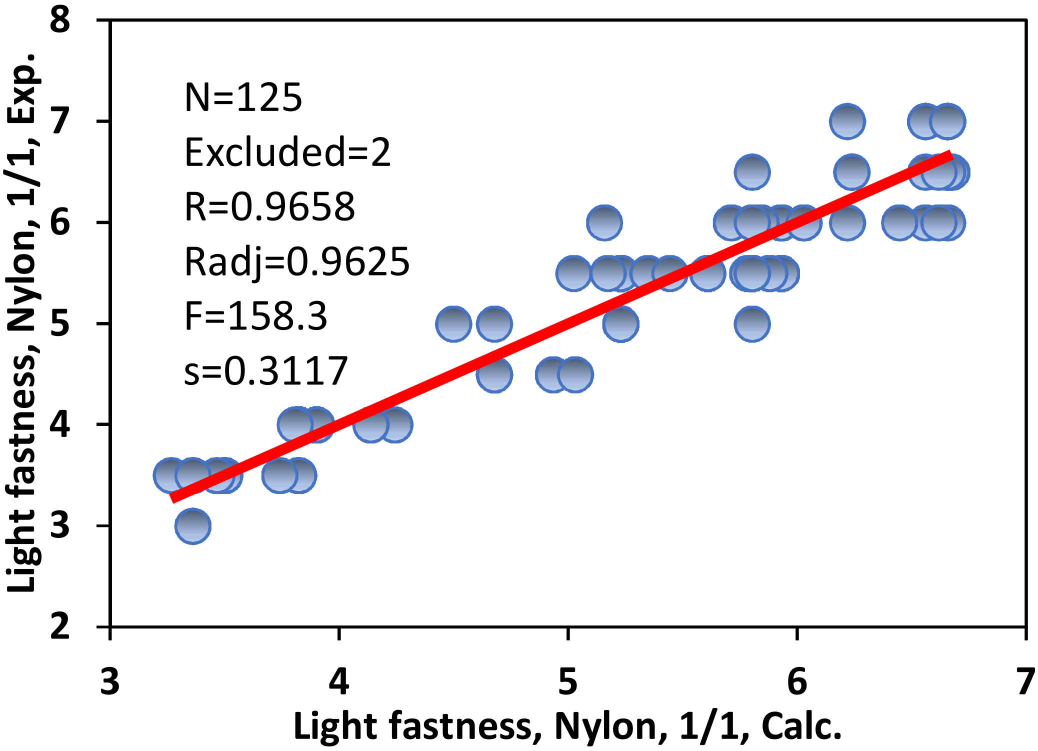
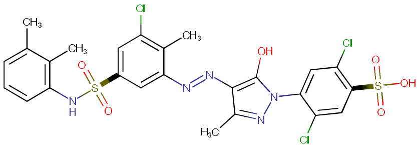
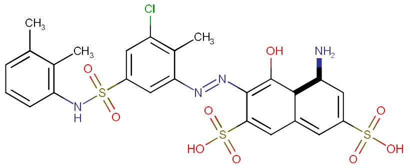
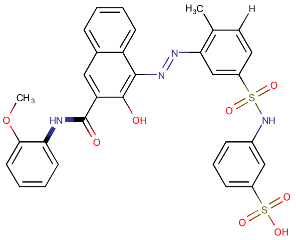
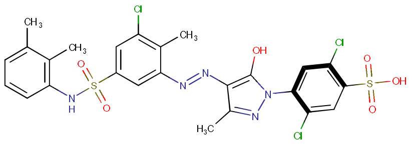
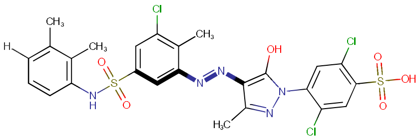
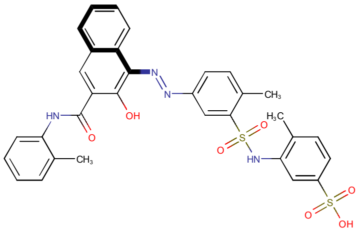
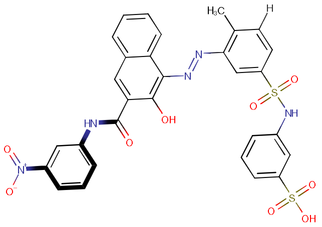
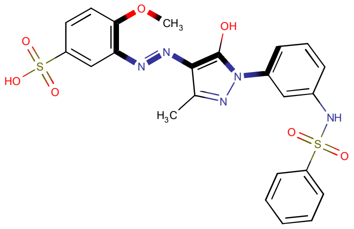
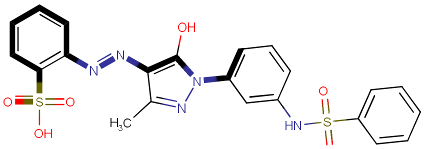
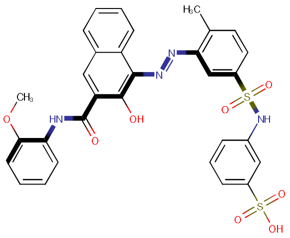


Figure 4. Correlation between calculated and experimental values of light fastness of dyeings on polyamide fibres.

The light fastness of polyamide fibres dyed with acid dyes demonstrates the similarity of several descriptors that are responsible for the light fastness of wool. For example, fragments containing primary amino- (fragment 2) or nitrogen atoms with azo-bonds (fragment 6) decrease the light fastness of dyed polyamide fibres. The same role is demonstrated by the substituted amino group in a chain with a nitro-group (fragment 7) and a tri-substituted amino-group in a fragment with an azo group and o-methoxy-group (fragment 8). On the other hand, fragments containing aromatic carbons (fragment 4) as well as azo-bonds with aromatic carbons without other substituents (fragment 5) demonstrate a positive impact.

This positive role is demonstrated by a short C(ar)-S(vi) fragment (fragment 1); a long fragment including a tri-substituted nitrogen atom, azo-bond, and o-sulphonic group (fragment 9); as well as a longer fragment including, in addition, a substituted acetamide group and aromatic carbon atoms (fragment 10).

Table 5. Coefficients of multiple linear regression model for the light fastness of dyeing on polyamide fibres and fragments of exemplified dye congeners with a 1:1 concentration of dye.

Regression Coefficient, Molecular Fragment	**Regression Coefficient, Molecular Fragment**	**Regression Coefficient, Molecular Fragment**
Coeff0 = 4.930911, T-stat = 30.6418	Coeff1 = 0.43608, T-stat = 7.3894 LF-PA-1 	Coeff2 = −2.4247, T-stat =−17.7498 LF-PA-2 
Coeff3 = 0.85488, T-stat = 10.6573 LF-PA-3 	Coeff4 = −0.31445, T-stat = −7.2016 LF-PA-4 	Coeff5 = 0.758169, T-stat = 8.1588 LF-PA-5 
Coeff6 = −1.66501, T-stat = −19.3869 LF-PA-6 	Coeff7 = −0.77779, T-stat = −9.5075 LF-PA-7 	Coeff8 = −0.42405, T-stat = −5.5203 LF-PA-8 
Coeff9 = 0.416039, T-stat = 7.6620 LF-PA-9 	Coeff10 = 0.552282, T-stat = 4.6392 LF-PA-10 	

3.5. Adsorption Properties of Direct Dyes on Cotton Fibres

A dataset of direct dyes on cotton was selected from Refs. [83,84] for four different initial concentrations of dye in a dyebath from 0.1–2.5% of the weight of the fabric. The results for the joint model reflecting the different concentrations in solution are shown in Figure 5. The coefficients of the multiple linear regression model are provided in Table 6 along with the coefficients of the T-statistics.

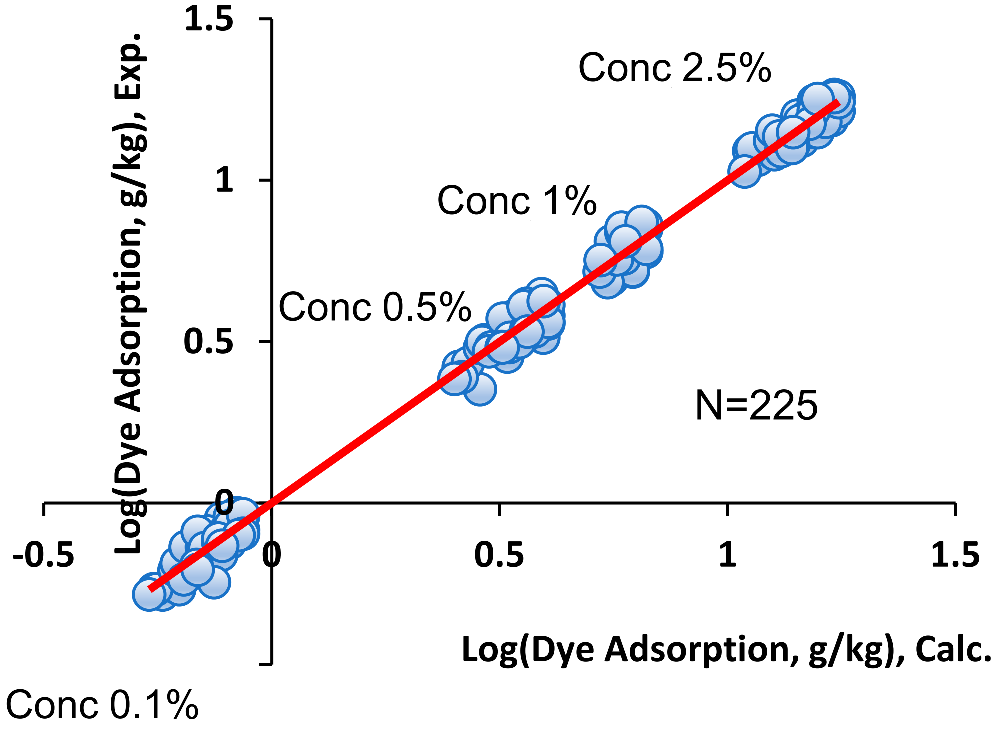
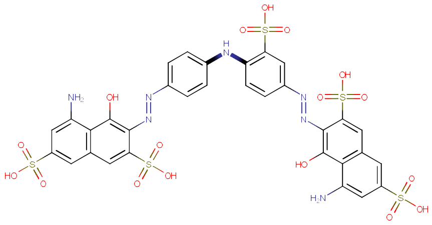
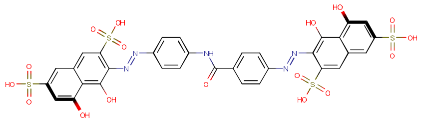
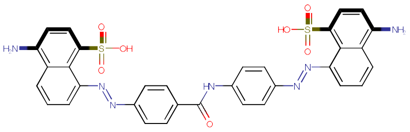
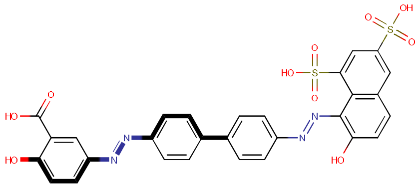
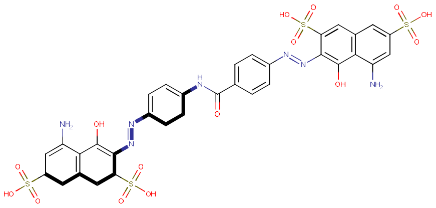
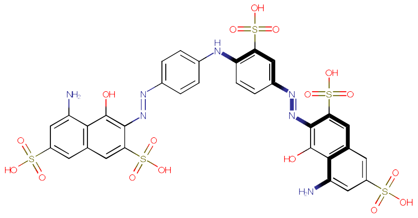
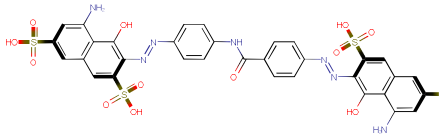


Figure 5. Correlation between calculated and experimental values of dye adsorption on cotton.

It is quite natural that fragments including sulphonic groups exhibit a negative impact that demonstrates a repulsion from the negatively-charged carboxylic end-groups of cellulose fibres, which appeared in the fibres due to the application of different kinds of oxidizing agents during the pre-treatment processes. However, a negative impact from non-ionic polar groups, such as –OH, –NH$_2$, or –NH- groups, disproves the traditional point of view about their significant role in hydrogen bonding with macromolecules of cellulose. Those bonds with polar groups of dyes could be easily destroyed by polar solvents like water.

It was found that only one 13-atom fragment that included a conjugated system of nitrogen with a carbonyl group, azo-bond, and sequence of aromatic bonds was characterised by a positive regression coefficient, Coeff8, which is responsible for the increasing amount of dye adsorption. The other six fragments exhibit a negative effect on direct dye adsorption in cellulose fibres. High coefficient values for T-statistics characterise the high level of reliability of each regression coefficient. As for the total robustness of the regression model, the regression coefficient and Fischer number are extremely high: R = 0.9979, F = 5095. Finally, a standard deviation of the Log (adsorption, g/kg) of direct dyes by cotton is rather low: s = 0.03, which is expressed in the units of Log (g/kg).

Table 6. Coefficients of multiple linear regression model for adsorption of direct dyes on cotton and fragments of exemplified dye congeners.

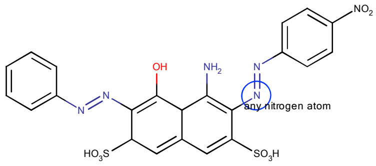
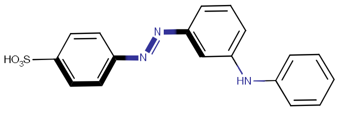
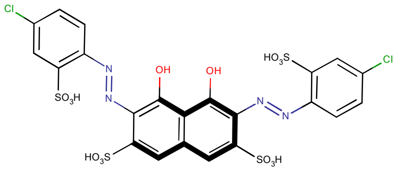
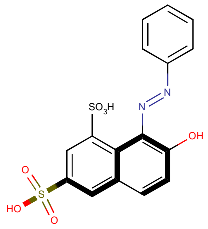
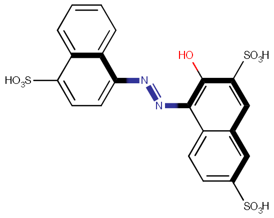
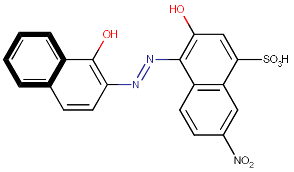
Regression Coefficient, Molecular Fragment	Regression Coefficient, Molecular Fragment	Regression Coefficient, Molecular Fragment
N = 225, R = 0.9979, R_adj = 0.9978, F = 5095, s = 0.0338, RMSE_t = 0.00330, MAE_t = 0.0259 Coeff0 = 0.824114, T-stat = 70.9156 Coeff1(C=1%) = 0.421999, T-stat = 53.6620 Coeff2 (C=0.5%) = −0.21474, T-stat = −27.3063 Coeff3 (C=0.1%) = −0.88427, T-stat = −112.4455		
Coeff4 = −0.13195, T-stat = −11.8450 A-C-4 	Coeff5 = −0.01797, T-stat = −5.4787 A-C-5 	Coeff6 = −0.00622, T-stat = −6.4462 A-C-6 
Coeff7 = −0.01134, T-stat = −3.4668 A-C-7 	Coeff8 = 0.002434, T-stat = 5.8381 A-C-8 	Coeff9 = −0.06541, T-stat = −4.0627 A-C-9 
Coeff10 = −0.01152, T-stat = −6.5432 A-C-10 		

3.6. Photodegradation of Azo Dyes in Solution

Studies of dye photolysis in solution are useful for understanding the fundamental basis for dye destruction as well as the applied aspects of photochemistry of dye removal from wastewater. A small dataset of 22 azo dyes [35], including acid, direct, and disperse dyes, which are characterised by the first-order kinetics constant of photodestruction at different pH levels of the solution, is used as a short example. The results of the chemoinformatics analysis of the process are shown in Table 7 for pH 6.

It is noteworthy that one regression coefficient, Coeff6, has a large positive impact on the rate of photolysis, which indicates the significant role of the unsubstituted benzene ring of the naphthol residue in photofading; other regression coefficients exhibit a negative impact. The highest level of the photostabilisation effect is demonstrated by fragment 4, which is characterised by a long aromatic chain and a sulphonic group. Another fragment that decreases the rate of photodestruction, fragment 5, includes two conjugated aromatic chains connected by an azo-bond.

Table 7. Coefficients of multiple linear regression model for photodegradation of azo dyes in solution at pH 6.

Regression Coefficient, Molecular Fragment	Regression Coefficient, Molecular Fragment	Regression Coefficient, Molecular Fragment
N = 22, R = 0.9814, R_adj = 0.9726, F = 65.43, s = 0.111, RMSE_t = 0.0917, MAE_t = 0.0774 Coeff0 = −2.2095; T-stat = −30.6200		
Coeff1 = −0.0509; T-stat = −3.4380 	Coeff2 = −0.0672; T-stat = −5.7746 	Coeff3 = −0.1204; T-stat = −4.6107 
Coeff4 = −0.2012; T-stat = −5.9598 	Coeff5 = −0.1825; T-stat = −3.3489 	Coeff6 = 0.5413; T-stat = 137513 

3.7. Comparative Analysis of Fragment Descriptors of Regression Models for Different Kinds of Fibres and Colour Fastness Tests

A combination of the models proposed above for various fibres and colour fastness tests is of interest for the comparative analysis of the physicochemical mechanism of dye destruction and their interaction with the fibres. Tables 8–11 demonstrate several molecular fragments of similar chemical nature that indicate the coinciding physicochemical routes of dye destruction and adsorption regardless of the nature of the fibre.

Table 8. Comparison of fragments responsible for the destruction of dyes in light fastness and sensitivity of dyeings to oxygen bleaching tests.

The Primary or Substituted Amino Group	Azo-Bond and the Primary or Substituted Amino Group	Aromatic Chain and Nitrogen of Azo Group
Coeff3 = −1.037494, T-stat = −6.3766 LF-W-3, Table 2		Coeff10 = −0.55531, T-stat = −6.5707 LF-W-10, Table 2
Coeff3 = 1.477873, T-stat = 4.8356 OB-W-3, Table 3	Coeff4 = 2.706476, T-stat = 7.3958 OB-W-4, Table 3	
Coeff2 = −2.4247, T-stat = −17.7498 LF-PA-2, Table 5	Coeff8 = −0.42405, T-stat = −5.5203 LF-PA-8, Table 5	Coeff6 = −1.66501, T-stat = −19.3869 LF-PA-6, Table 5

Table 9. Comparison of fragments responsible for stabilization of dyes in light fastness and sensitivity of dyeings to oxygen bleaching tests.

Azo Group in a Chain of Conjugated Double Bonds	Azo Group in a Chain of Conjugated Double Bonds and Sulphonic Group	Azo-Bond in a Chain of Conjugated Double Bonds and Carbamide Group
	Coeff7 = 0.288798, T-stat = 4.1107 LF-W-7, Table 2	
Coeff9 = −1.134224, T-stat = −5.6996 OB-W-9, Table 3		
Coeff5 = 0.758169, T-stat = 8.1588 LF-PA-5, Table 5	Coeff9 = 0.416039, T-stat = 7.6620 LF-PA-9, Table 5	Coeff10 = 0.552282, T-stat = 4.6392 LF-PA-10, Table 5

Table 10. Comparison of fragments responsible for positive impact on wash fastness and sorption of dyes on wool and cotton.

Two Azo-Bonds in a Chain of Conjugated Double Bonds	Azo-Bond in a Chain of Conjugated Double Bonds and Terminal Hydrophobic Terminal Group
Coeff5 = 0.199498, T-stat = 3.3687 WF-W-5, Table 4	Coeff6 = 0.511187, T-stat = 4.1279 WF-W-6, Table 4
Coeff8 = 0.002434, T-stat = 5.8381 A-C-8, Table 6	

Table 11. Comparison of fragments responsible for negative impact on wash fastness and adsorption of dyes on wool and cotton.

Sulphonic Group	Azo-Bond and Hydrophilic Terminal Group
Coeff3 = −0.335361, T-stat = −3.8736 WF-W-3, Table 4	Coeff7 = −0.532824, T-stat = −3.5236 WF-W-7, Table 4
Coeff10 = −0.01152, T-stat = −6.5432 A-C-10, Table 6	Coeff9 = −0.06541, T-stat = −4.0627 A-C-9, Table 6

A negative (destructive) effect on dye chromophore was observed in the tests for the light fastness of dyeings on wool and polyamide, as well as the sensitivity of the dyeings on wool for oxygen bleaching, which are controlled by the fragments shown in Table 8, including primary or substituted amino groups, an azo-bond as a part of a chain of conjugated double bonds with primary or substituted amino groups, a chain of aromatic carbon atoms, and the nitrogen atom of an azo-bond.

A positive (stabilizing) effect on the dye chromophore was observed in the tests for the light fastness of dyes on wool and polyamide fibres as well as the sensitivity of the dyes on wool to oxygen bleaching, which is explained by the fragments shown in Table 9, including an azo group as a part of a chain of conjugated double bonds, an azo group as a part of a chain of conjugated double bonds and a sulphonic group, and an azo-bond as a part of a chain of conjugated double bonds and a carbamide group.

A comparison of the molecular fragments controlling the light fastness of dyed textiles demonstrates the similarity of several fragments during the photolysis of azo dyes in solution. For instance, in the case of polyamide fibres, molecular fragment 4’s (LF-PA-4, Table 5) decrease of the light fastness of azo acid dye is comparable to fragment 6’s (Table 7) increase of the rate of dye photodestruction in water. On the other hand, the high stabilising effect of the sulphonic group on light fastness is demonstrated by molecular fragment 1 (LF-PA-1, Table 5), which corresponds with fragment 4’s (Table 7) decrease in the rate of dye photodestruction. Similarly, the positive role of the sulphonic group for dyed wool fibres is displayed by fragment 7 (LF-W-7, Table 2)

The fragment shown in Table 10 has a positive effect on the wash fastness of the dyeings on wool and the adsorption on cotton fibres, including two azo groups as a part of a chain of conjugated double bonds and a chain of conjugated double bonds containing an azo group and hydrophobic substituent.

Both chain fragments play the role of a bulky hydrophobic fragment.

In contrast to the above, the fragments presented in Table 11 decrease the wash fastness of acid dyes on wool and the adsorption of direct dyes on cotton. These fragments include an aromatic chain with a terminal sulfonic group or an azo group as a part of a chain of conjugated double bonds with hydrophilic substituents such as –NH_2 or –OH.

4. Conclusions

The application of chemoinformatics tools for the analysis of large databases of dyes demonstrated the efficiency of the method for analyzing the dye chemical structure–

property relationships in several case studies that explored: the light fastness of acid dyes on wool and acid dyes on polyamide, the sensitivity of acid dyes on wool to oxygen bleaching, the wash fastness of acid dyes on wool, the adsorption of direct dyes on cotton, and the photodestruction of azo dyes in solution. The fragment approach of QSPR depicts several substructural descriptors that reflect the mechanism of destruction and the dye–fibre interaction.

The similarity of the fragments for acid and direct azo dyes on fibres of different natures is shown; furthermore, this indicates the coinciding mechanisms of the physicochemical destruction of dyes in light fastness tests and the adsorption/desorption in wash fastness and dyeability tests. It is found that the light fastness of dyeings on wool and polyamide, as well as the sensitivity of dyes on wool fiber to oxygen bleaching, is decreased in the presence of molecular fragments, such as fragments that contain primary or substituted amino groups, an azo-bond and primary or substituted amino group, and a chain of conjugated double bonds with a nitrogen atom on the azo group. The positive (stabilising) effect on dye chromophore is demonstrated by the fragments with an azo group as a part of a chain of conjugated double bonds and the sulfonic group as a substituent or an azo group as a part of conjugated double bonds with a carbamide group. The fragment represented by two azo groups as a part of a chain of conjugated double bonds has a positive effect on the wash fastness on wool and the sorption on cotton fibres. On the contrary, a negative effect is demonstrated by the fragments with a chain of conjugated double bonds with a terminal sulfonic group or azo groups as a part of a chain of conjugated double bonds with hydrophilic substituents such as –NH_2 or –OH.

Author Contributions: Conceptualization, F.Y.T.; methodology, F.Y.T.; software, F.Y.T.; validation, J.R. and V.G.P.; formal analysis, J.R. and V.G.P.; investigation, J.R. and V.G.P.; data curation, J.R. and V.G.P.; writing—original draft preparation, J.R. and V.G.P.; writing—review and editing, J.R., V.G.P. and F.Y.T. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest: The authors declare no conflict of interests.

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