Computational Technique 3D-QSPR Applied on FBAS By Using CoMFA Technique

Mahwish
University of Karachi, Pakistan

Syed Ishrat Ali
Government College University Hyderabad, Pakistan.

Nosheen Ahmed
Government Degree Girls College Buffer Zone, Karachi, Pakistan
Email: nosh_aga@hotmail.com

Mushtaque Hussain
Government College University Hyderabad, Pakistan

Received on: 25 -07-2024 Accepted on: 26- 08 -2024

Abstract

CoMFA (Comparative Molecular Field Analysis) is a 3D QSAR technique based on data from known active molecules. To apply CoMFA, all that is needed are the activities and the 3D structures of the molecules.3D-QSPR studies are certainly of great importance in different branches of chemistry. This technique leads to locate the close relationship between bulk properties of compounds and their molecular structure.

Keywords: 3D QSAR, CoMFA, Computational Technique

1. Introduction

CoMFA (Comparative Molecular Field Analysis) is a 3D QSAR technique based on data from known active molecules. CoMFA can be applied, as it often is, when the 3D structure of the receptor is unknown. To apply CoMFA, all that is needed are the activities and the 3D structures of the molecules.3D-QSPR studies are certainly of great importance in different branches of chemistry. This technique leads to locate the close relationship between bulk properties of compounds and their molecular structure.

One of the most important technique used to predict different properties of a molecule initiate from information of its molecular structure is known as three-dimensional quantitative structure property relationship (3D-QSPR) [**1-2**]. 3D-QSPR study has great importance in pharmaceutical chemistry, medicinal chemistry and drug discovery [**3-4**].

This technique is used to find the close relationship between properties of compound and its molecular structure. Once the model is developed then it can be used to predict the properties

of unknown molecule.

2. Experimental work

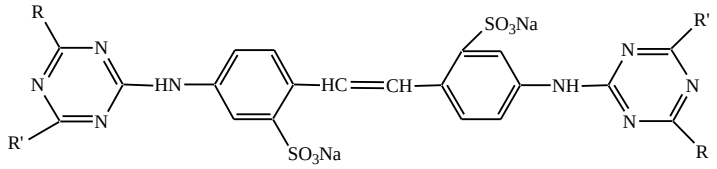
In this research 3D-QSPR technique with the help of CoMFA was applied on the following sets of FBAs.

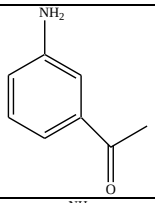
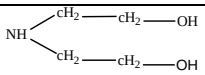
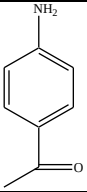
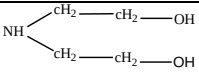
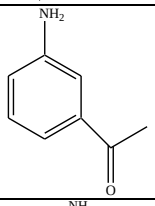
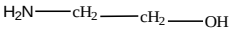
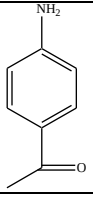
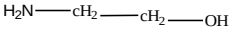
Data set 1: Sixteen compounds (**M_1-M_{16}**) were provided from our synthesized FBAs.

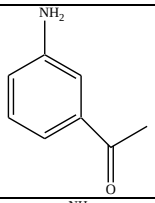
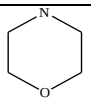
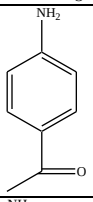
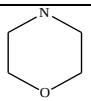
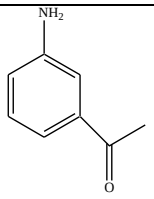
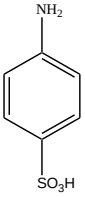
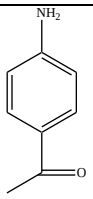
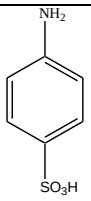
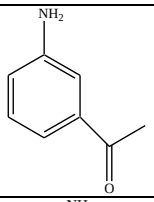
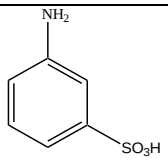
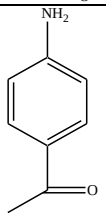
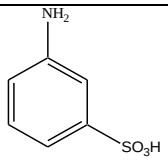
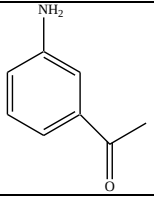
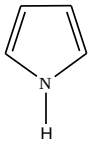
Data set 2: Ten compounds were taken from [**5-6**].

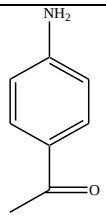
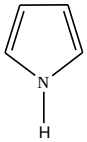
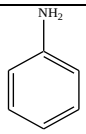
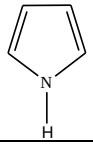
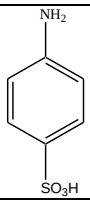
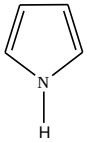
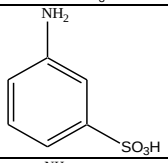
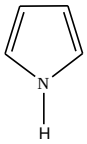
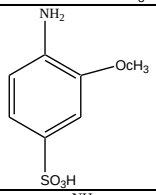
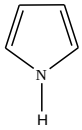
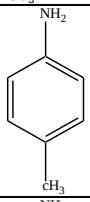
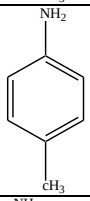
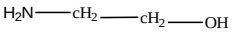
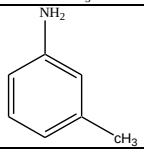
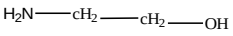
Complete data of 26 compounds is given in **Table 1.1** and **1.2**.

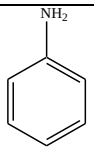
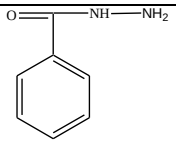
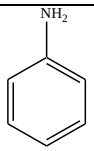
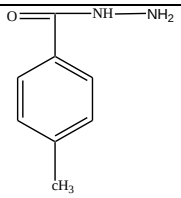
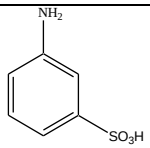
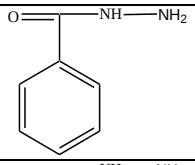
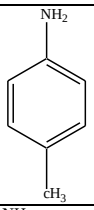
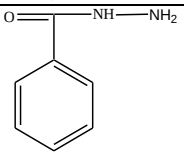
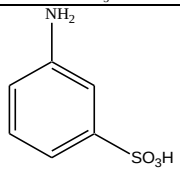
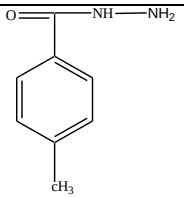
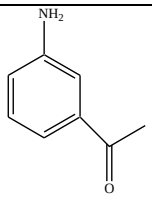
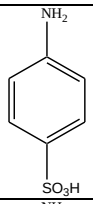
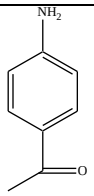
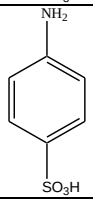
Table 1.1:- Structures of Fluorescent Brighteners and their Absorptivity's ($dm^3mol^{-1}cm^{-1}\times10^4$).



S. No.	Sample Code	R	R'
01	**M_1**		
02	**M_2**		
03	**M_3**		
04	**M_4**		

05	**M_5**		
06	**M_6**		
07	**M_7**		
08	**M_8**		
09	**M_9**		
10	**M_{10}**		
11	**M_{11}**		

12	**M_{12}**		
13	**M_{13}**		
14	**M_{14}**		
15	**M_{15}**		
16	**M_{16}**		
17	**5a**		
18	**5b**		
19	**5c**		

20	**5d**		
21	**5e**		
22	**K5I**		
23	**K5II**		
24	**K5III**		
25	**K5IV**		
26	**K5V**		

S. No.	Sample Code	R	R’	Absorptivity $dm^3mol^{-1}cm^{-1}\times10^4$

01	**M_1**	m-aminoacetophenone	diethanol amine	14.0
02	**M_2**	p-aminoacetophenone	diethanol amine	8.10
03	**M_3**	m-aminoacetophenone	monoethanol amine	2.50
04	**M_4**	p-aminoacetophenone	monoethanol amine	4.10
05	**M_5**	m-aminoacetophenone	morpholine	4.70
06	**M_6**	p-aminoacetophenone	morpholine	8.70
07	**M_7**	m-aminoacetophenone	p-aminosulfonic acid	2.90
08	**M_8**	p-aminoacetophenone	p-aminosulfonic acid	5.10
09	**M_9**	m-aminoacetophenone	m-aminosulfonic acid	8.10
10	**M_{10}**	p-aminoacetophenone	m-aminosulfonic acid	7.70
11	**M_{11}**	m-aminoacetophenone	pyrrole	0.55
12	**M_{12}**	p-aminoacetophenone	pyrrole	0.85
13	**M_{13}**	Aniline	pyrrole	0.84
14	**M_{14}**	p-aminosulfonic acid	pyrrole	0.97
15	**M_{15}**	m-aminosulfonic acid	pyrrole	0.97
16	**M_{16}**	p-methoxyaminosulfonic acid	pyrrole	0.96
17	**5a**	m-aminosulfonic acid	benzoylhydrazine	4.20
18	**5b**	p-toluidine	diethanol amine	4.00
19	**5c**	p-toluidine	morpholine	4.20
20	**5d**	p-toluidine	monoethanol amine	4.10
21	**5e**	m-toluidine	monoethanol amine	4.10
22	**K5I**	Aniline	benzohydrazide	4.10
23	**K5II**	Aniline	p-tolyl-hydrazide	4.00
24	**K5III**	m-aminosulfonic acid	benzohydrazide	4.50
25	**K5IV**	p-toluidine	benzohydrazide	4.30
26	**K5V**	m-aminosulfonic acid	p-tolyl-hydrazide	4.50

Table 1.2:- Statistical results for FBAs extracted by CoMFA analysis

S.No.	Cross-validated correlation coefficient (q2)

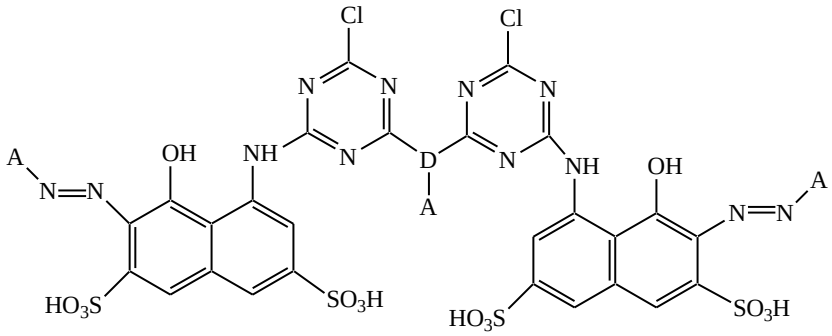
Set 1	-0.288
Set 2	0.32
Set 3	-0.149
Set 4	-0.233
Set 5	-0.474
Set 6	-0.141
Set 7	-0.380
Set 8	-0.379
Set 9	-0.275
Set 10	-0.288
Set 11	-0.487
Set 12	-0.175

3. Results and Discussion

The aim of this research was to create a predictive CoMFA model which correlates with the absorptivity of FBAs with the modification in structure of molecule.

A negative correlation has been observed contrary to earlier studies of our group [**7**]. They confirm the theoretical model existing [**7**]. The explanation relies to describe the fact that reactive dyes form a covalent linkage with the cellulose fiber to provide considerable fastness properties of reactive dyes while FBAs do not appear to form such a covalent linkage with the fiber they actively adsorb on cellulose surface and poor fastness properties are reported as compare with reactive dyes. Reactive dyes as evident are described in **Table 1.3** and **Table 1.4.**

Table 1.3:- Red reactive dye structures and their absorptivity's



(**111-136**)

S.No.	Dye Code	Group A	Bridging Moiety "DA"	Absorbtivity $dm^3mol^{-1}cm^{-1}\times10^4$
111	**JP-01**	anthranilic acid	1,4-phenylenediamine	3.47
112	**JP-02**	anthranilic acid	1,2-phenylenediamine	5.37

113	**JP-03**	anthranilic acid	1,3-phenylenediamine	5.30
114	**JP-04**	anthranilic acid	diaminostilbene-2,2'-disulfonic acid	4.29
115	**JP-05**	anthranilic acid	4,4'diaminebenzoanilide	3.74
116	**JP-06**	anthranilic acid	Ethylene-1,2-diamine	4.94
117	**JP-07**	4-β-sulphatoethyl-sulfonylaniline	1,4-phenylenediamine	5.43
118	**JP-08**	4-β-sulphatoethyl-sulfonylaniline	1,2-phenylenediamine	6.21
119	**JP-09**	4-β-sulphatoethyl-sulfonylaniline	1,3-phenylenediamine	5.81
120	**JP-10**	4-β-sulphatoethyl-sulfonylaniline	diaminostilbene-2,2'-disulfonic acid	5.49
121	**JP-11**	4-β-sulphatoethyl-sulfonylaniline	4,4'diaminebenzoanilide	4.95
122	**JP-12**	4-β-sulphatoethyl-sulfonylaniline	Ethylene-1,2-diamine	6.32
123	**JP-13**	anthranilic acid	1,4-phenylenediamine	4.67
124	**IS-14**	Aniline	diaminostilbene-2,2'-disulfonic acid	2.95
125	**IS-15**	benzene-m-aminosulfonic acid	diaminostilbene-2,2'-disulfonic acid	1.85
126	**IS-16**	benzene-m-aminosulfonic acid	1,4-phenylenediamine	0.71
127	**IS-17**	benzene-p-aminosulfonic acid	1,4-phenylenediamine	1.95
128	**IS-18**	Aniline	1,4-phenylenediamine	0.37
129	**IS-19**	p-toluidine	1,4-phenylenediamine	0.25

130	**IS-20**	p-toluidine	diaminostilbene-2,2'-disulfonic acid	1.92
131	**IS-21**	p-toluidine	1,3-phenylenediamine	0.47
132	**IS-22**	p-toluidine	1,4-phenylenediamine	2.44
133	**IS-23**	p-toluidine	1,3-phenylenediamine	1.74
134	**IS-24**	m-toluidine	1,4-phenylenediamine	0.47
135	**IS-25**	m-toluidine	1,3-phenylenediamine	1.40
136	**IS-26**	m-toluidine	diaminostilbene-2,2'-disulfonic acid	2.32

Table 1.4:- Actual and predicted absorptivity of red reactive dyes of training and test sets

S.No.	Compounds	Experimental absorptivity	Predicted absorptivity by CoMFA
Training set			
112	**JP-02**	5.37	5.38
113	**JP-03**	5.30	5.46
114	**JP-04**	4.29	4.18
115	**JP-05**	3.74	3.67
116	**JP-06**	4.94	4.91
117	**JP-07**	5.43	5.66
118	**JP-08**	6.21	6.24
119	**JP-09**	5.81	5.85
120	**JP-10**	5.49	5.37
122	**JP-12**	6.32	6.51
123	**JP-13**	4.67	4.35
124	**IS-14**	2.95	2.52
125	**IS-15**	1.85	1.95
126	**IS-16**	0.71	0.67
127	**IS-17**	1.95	2.02
128	**IS-18**	0.37	0.43
129	**IS-19**	0.25	0.31
130	**IS-20**	1.92	1.35
132	**IS-22**	0.47	0.75
133	**IS-23**	2.44	2.41
134	**IS-24**	0.47	1.08
135	**IS-25**	1.40	1.39

Test set			
111	**JP-1**	3.47	5.40
121	**JP-11**	4.95	4.37
131	**IS-21**	0.47	2.18

4. Conclusion

The aim of this research was to create a predictive CoMFA model which correlates with the absorptivity of FBAs. A negative correlation has been observed. The explanation relies to describe the fact that FBAs do not appear to form such a covalent linkage with the fiber they actively adsorb on fiber surface and do not exhibit high value of absorptivity.

In future we will try to correlate predictive CoMFA model with other properties of FBAs like color co-ordinates L*, a*, b* and spectroscopic data.

Reference

1. Cao D., Liang Y., Xu Q., Yun, Y., LI H.(2011). Toward better QSAR/QSPR modeling: simultaneous outlier detection and variable selection using distribution of model features. *J. Comput-Aided Mol. Des*,vol 25,pp.1-14
2. Puri S., Chickos J. S., Welsh W. J.(2002).Three-dimensional quantitative structure property relationship (3D-QSPR) models for prediction of thermodynamic properties of polychlorinated biphenyls (PCBs): Enthalpy of sublimation. *J.Chem. Inf. Comput. Sci*. Vol.42, pp.109-116.
3. Katritzky A. R., Fara D. C., Petrukhin R. O., Tatham D. B., Maran U., Lomaka A., Karelson M.(2002). The present utility and future potential for medicinal chemistry of QSAR/QSPR with whole molecule descriptors. *Curr. Top. Med.Chem.* Vol.2,pp.1333-1356.
4. Katritzky A. R., Maran U., Lobanov V. S., Karelson M.(2000).Structurally diverse quantitative structure-property relationship correlations of technologically relevant physical properties. *J. Chem. Inf. Comput. Sci*.Vol.40,pp.1-18.
5. Hussain M, Khan K.M., Ali S. A., Parveen R., Shim W. S.(2009). Symmetrically substituted 4,4'-bis-(1,3,5-triazinylamino)stilbene-2,2'-disulfonate derivaties as fluorescent brighteners.*The Open Textile Journal*, Vol.2,pp.53-58.
6. Hussain M, Khan K.M., Ali S. A., Parveen R., Shim W. S.(2009).Synthesis and properties of symmetrically substituted 4,4'-bis-(1,3,5-triazinyl)-diamino stilbene -2,2'-disulfonic acid derivatives as UV absorbing and fluorescent whitening agents. *Fibers and Polymers*. Vol.10,pp. 407-412.
7. Mahmood U., Rashid S., Ali S.I.,Parveen R.,Qasmi Z, Ambreen N., Khan K. M.,Perveen S. W.(2011). Voelter, 3D-QSPR method of computational technique applied on red reactive dyes by using CoMFA strategy, *International Journal of Molecular Sciences*, Vol.12, pp.8862-8877.