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Short Communication

Estimation of chemical shift of sulfonamide using Balaban Indices

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Abstract

The paper describes the estimation of chemical shifts in NMR using Balaban, Balaban type Indices. The statistically significant models are governed by a variety of statistical parameter.

Keywords: QSAR Method, Balaban Indices, NMR Chemical Shift.

Introduction

Molecular descriptors are some numerical values which able to take out tiny pieces of chemical information from the different molecular representations. Molecular descriptors are now in performance a key responsibility in scientific study.

Once the arrangement of lead compound is known, the remedial chemist moves on to study its SAR. The plan is to determine which parts of the molecule are significant to biological activity and which are not. X-ray crystallography and NMR can be used to cram and recognize vital binding interactions between drug and active site.

SAR is synthesizing compounds, where one exacting functional set of the molecule is detached or distorted. In this way it is possible to find out which groups are necessary and which are not for biological effect. A original use of NMR chemical shift of the $-SO_2NH_2$ proton as a molecular descriptors is described by Khadikar *et al*[1]. for model the inhibition constant for benzene sulfonamides against the zinc enzyme carbonic anhydrase (pk_i).

Materials and methods

The series of 21 sulfonamides used by us are shown in Table-1. The log K_i and NMR chemical shift values of these compounds are taken from literature[2-8]. In Table-2 the values of their carbonic anhydrase inhibition, NMR chemical shift and indicator parameters are reported. The various graph theoretical descriptors used by us are as follows:

Balaban, Balaban type Indices: J, $J_{hez,}$ J_{hetm}, J_{hete}, J_{hetv}, J_{hetp}

All these descriptors are designed by DRAGON[9] software. The structure optimization was done using ACD labs software[10].

Result and discussion

Modeling chemical shift (δ) using Balaban, Balaban type Indices: Balaban Index (J) is very judicious index and it can be subjective easily yielding special types of Balaban Indices. We have use J_{hetz} (Balaban type Index from z weighted distance matrix), J_{hetm} (Balaban type Index from mass weighted distance matrix), J_{hetv} (Balaban type index from Van der Waal's weighted distance matrix), J_{hete} (Balaban type Index from electro negativity subjective distance matrix) and J_{hetp} (Balaban type Index from polarisability weighted distance matrix). Khadikar et al.[1] have used this Index fruitfully in emergent some QSPR/QSAR models.

A regression analysis using Balaban, Balaban type Indices is done to model (δ). Models showing high-quality statically information. Table-3 shows that the value of the models goes on rising with addition of indices. Third model is not statistically considerable as some of the coefficients are less than the respective standard deviations. The hexaparametric model is found to be the most suitable model among all the six models.

$\delta = 9.2592\ (\pm 1.0537) + 283.6294\ (\pm 189.6604)\ J_{hetz} - 6.5704\ (\pm 3.0186)\ J + 20.7873\ (\pm 10.1862)\ J_{hetp} - 20.7354\ (\pm 12.1207)\ J_{hetv} + 8.4237\ (\pm 3.8158)\ J_{hete} - 286.921\ (\pm 189.6146)\ J_{hetm.}$

Validation: Several validation techniques have been proposed in order to estimate the model prediction capabilities. To be an excellent model it is necessary that its statistics and analytical power both should be excellent. The predictive power of the model can be obtained by calculating Pogliani's quality factor Q, also called quality factor.

This quality factor Q is defined as the ratio of correlation coefficient to the standard error of estimation. Another parameter used for validation purposes is PRESS i.e. Predictive Error, Sum of Squares.

Conclusion

We bring to a close that Balaban Index J in grouping with W, $1\chi v$, $3\chi v$ and $2\chi v$ indices can be successfully used to model chemical shift δ.

Table-1: Structural details of carbonic anhydrase inhibitor used in present investgation.

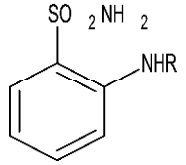
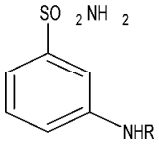
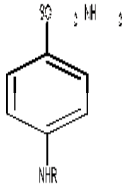
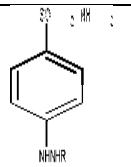
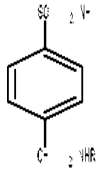
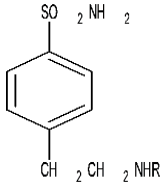
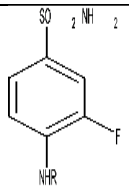
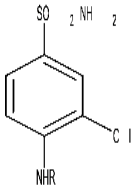
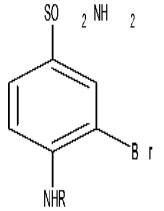
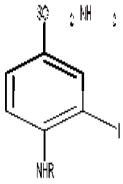
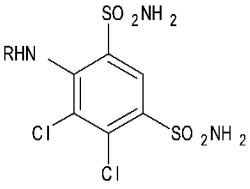
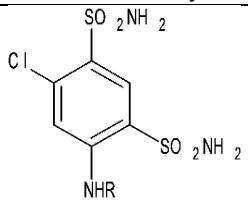
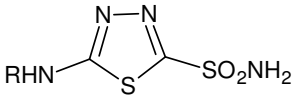
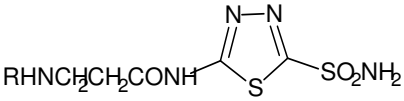
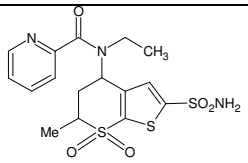
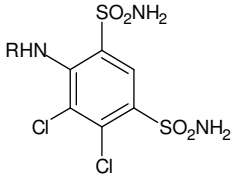
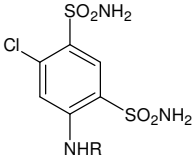
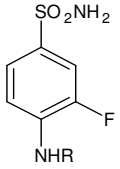
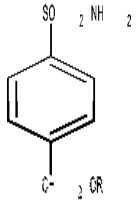
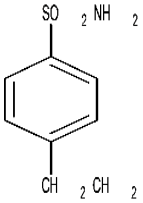
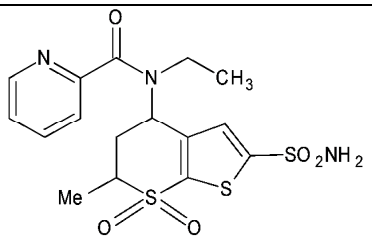
 1. R= Picolinoyl	 2. R= Picolinoyl	 3. R= Picolinoyl
 4. R= Picolinoyl	 5. R= Picolinoyl	 6. R= Picolinoyl
 7. R= Picolinoyl	 8. R= Picolinoyl	 9. R= Picolinoyl
 10. R= Picolinoyl	 11. R= Picolinoyl	 12. R= Picolinoyl
 13. R= Picolinoyl	 14. R= Picolinoyl	 15. R= Picolinoyl
 16. R= Picolinoyl	 17. R= Picolinoyl	 18. R= Picolinoyl
 19. R= Picolinoyl	 20. R= Picolinoyl	 21. R= Picolinoyl

Table-2: log Ki, chemical shift and indicator parameter (I_1, I_2, I_3) used in the present study.

Compoud No.	LogKi	$\Delta(SO_2NH_2)$	I_1	I_2	I_3
1	4.33	7.50	0	0	0
2	4.29	7.60	0	0	0
3	4.17	7.56	0	0	0
4	4.35	7.59	0	0	0
5	3.04	7.67	0	0	0
6	3.04	7.67	0	0	0
7	2.72	6.60	0	0	1
8	2.78	6.70	0	0	1
9	2.79	6.65	0	0	1
10	2.78	6.60	0	0	1
11	2.71	7.68	0	0	0
12	2.78	7.75	0	0	0
13	1.60	6.94	1	0	0
14	1.49	6.96	1	0	0
15	1.30	6.88	1	0	0
16	1.00	8.10	0	1	0
17	1.04	8.10	0	1	0
18	1.00	8.15	0	1	0
19	3.32	7.49	0	0	0
20	3.31	6.95	0	0	0
21	3.20	8.25	0	1	0

I_1: When five members hetero - cyclic ring alone is present (i.e. five-member hetero-cyclic sulfonamide), I_2: When five – member ring is fused with benzene- nucleus. I_3: When di - substitution on benzene rings.

Table-3: Model using Balaban indices.

Parameter used	Se	R^2	R^2 A	F
J	4.3810	0.6964	0.6862	68.8152
J, J_{hetp}	4.4556	0.6964	0.6755	33.2657
J, J_{hetp}, J_{hetv}, J_{hete}	4.6106	0.6861	0.6525	20.4055
J, J_{hetv}, J_{hete}, J_{hetm},	4.4128	0.7277	0.6817	17.5981
J_{hetp}, J_{hetv}, J_{hete}, J_{hetm}, J_{hetz}	4.4959	0.7228	0.6696	13.5655
J, J_{hetp}, J_{hetv}, J_{hete}, J_{hetm}, J_{hetz}	4.5315	0.7293	0.6643	11.2264

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