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# QSPR Study on Benzene Disulfonamides with log IC50 (CAI) Inhibitory Activities

KEYWORDS: QSAR study on benzene disulfonamides with log Ic50 (CAI) initiatory activities.

**Arunendra kumar pandey**

QSAR & computer chemical laboratories A.P.S. University Rewa (M.P)

**ABSTRACT** *In the present investigation the applicability of various physicochemical parameters are tested for the QSAR study on sulfonamides for the modeling of benzene disulfonamides. The regration analysis shown that even in the multi parameters correlation of physicochemical parameters give significant regration coefficient further more wring combination of physicochemical parameters along with the indicator parameters, a tremendous improvement in the statistics has been observed the results are critically discussed on the basis regration data.*

**Introduction:-**
Quantities structure-property-activity relationship (QSPR./ QSAR) have been established as powerful research tools & are being used in many fields (1-4). These are mathematical models in that property & activities of molecules are predicted from their structure (2), the basis assumption underlying these fields of research in that structure of molecular determines its behaviors (3), these are two kinds of molecular predication used in QSPR as in QSAR studies one of them involves parameters that bears relation to free energy & the other used the topological index or numerical graph invariants, which are produced directly from molecular structure (4).

Several important sulfa drugs have been made by the realized. Presently more than fifty sulfonamides are used in chemical practice.

Be boned this et al (5) have reported correlation of CA inhibitory activities of benzene-sulfonamides with total charge on the- SO2 & NH2 moiety.

Recently, Supuran & Clare (9) have reported quantum chemical QSAR relationship foe a group of anhydrous the activities of these compounds were correlated with Wiener index (6) & the data was subjected to classical regression analysis (7) with care to avoid the collineraty.

IVY Carrol (8) & others prepared & tested the two isomeric sulpha interrupted 8-amino side chain analogues of 4-methly, 5- (Trifluoromethyl) phenenxy) primaquin for anti-malarial activity.

A series of novel azulene-1 carboxylic acid derivatives, azulene, 1 sulphonic acid & related compound were synthesized by Tomigama et al (9), theses compounds were tested for TXAZ recapture antagonistic activity.

J.K. Seydal (10) & others studies the acativity conformation of a set of 36 congener's 4-amino dyphenyl sulfones as inhibitors using both linear free energy & molecular modeling methods. Similarly these are many series of drugs containing sulpher for the treatment of allergy & viral diseases.

Agrawal et al (11-13) have published many papers related to QSAR studies on sulfa drugs where they have proposed mechanism of action of these drugs using topological.

**Materials & Methods:-**
The study was carried on the compounds prepared by Brian W. Clare; Claudin Y. Suparan et al 1998 (table 1). They have used activities of sulfonamides inhibitory activity (Log (CAI)) the seires of benzene disulfonamides.

**Parameters used:-**
We have used chemsketch program of ACD lab for calculation of various physicochemical parameters like molecular weight (MW), molar refraction (MR), molar volume (MV), poacher (PR), Surface Tension (Y), density (D), Polarizarility (α) & index of refraction (N) & adopted stepwise regration analysis for obtaining a model with rest statistics. The calculated parameters for all 72 compounds are reported in table 2.

**Correlation matrix:-**
We have studies the inter correlation of the parameters along with the biological activity & indicator parameters, such a correlation matrix is reported in table 3 parameters showing very good correlation with log CAI, Pr, d, α & IP2 are the parameters with shown good correlation.

**Result & Discussion:-**
Sulfonamides used in the present study are reported in table 1. Table 1 also shown the log (CAI) activity & four indicator parameters IP1, IP2, IP3 & IP4 various physicochemical parameters calculated using ACD lab software are reported in table 2, table 3 shown the correlation with log (CAI) on the basis of correlation matrix, we may infer that N, IP4 & IP5 are the parameters which can be used for modeling the log (CAI) activity the multi parametric is-

Log IC50 (CAI) = 18.5746 (±1.8734) n -0.0329
(±0.0065) r -2.8579 (±0.2819)
d -0.1062 (±0.0077) α -0.1712
(±0.80434) IP1 +0.4349 (±0.0576)
IP4 +0.1548 (±0.0522) IP5 -18.7809
n = 66, SE=0.1325, R=0.9158, F=43.0700, Q=6.9117

Table: - Comparison of estimated biological activity log IC50 (nM) CAI with their observed values using model – 19.

| Compd.No | Observed Log IC50 (nM) CAI | Estimated log IC20 (nM) CAI | |
|---|---|---|---|
| | | Model-19 | Residue |
| 1 | 2.0969 | 2.081 | 0.0159 |
| 2 | 2.0374 | 1.93 | 0.1074 |
| 3 | 2.0569 | 1.913 | 0.1439 |
| 4 | 2.0128 | 2.113 | -0.1002 |
| 5 | 1.9823 | 1.905 | 0.0773 |
| 6 | 1.8388 | 1.93 | -0.0912 |
| 7 | 1.6021 | 1.741 | -0.1389 |
| 8 | 1.5798 | 1.731 | -0.1512 |
| 9 | 1.5441 | 1.359 | 0.1851 |
| 10 | 1.6435 | 1.606 | 0.0375 |
| 11 | 1.415 | 1.477 | -0.62 |
| 12 | 1.4624 | 1.478 | -0.0156 |
| 13 | 1.5185 | 1.478 | 0.0405 |
| 14 | 1.4914 | 1.478 | 0.0134 |

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|---|---|---|---|
| 15 | 2.3829 | | |
| 16 | 2.2253 | 2.032 | 0.1933 |
| 17 | 2.2148 | 2.467 | -0.2522 |
| 18 | 1.7782 | | |
| 19 | 2.2455 | 2.252 | -0.0065 |
| 20 | 2.1761 | 2.102 | 0.0741 |
| 21 | 2.3222 | 2.0484 | 0.2382 |
| 22 | 2.4698 | 2.47 | -0.0002 |
| 23 | 2.4746 | | |
| 24 | 1.9912 | 2.101 | -0.1098 |
| 25 | 1.8129 | 1.913 | -0.1001 |
| 26 | 1.6435 | 1.902 | -0.2585 |
| 27 | 1.6021 | 1.531 | 0.0711 |
| 28 | 1.7708 | 1.777 | -0.0062 |
| 29 | 1.5051 | 1.648 | -0.1429 |
| 30 | 1.5185 | 1.65 | -0.1315 |
| 31 | 1.5441 | 1.65 | -0.1059 |
| 32 | 1.5563 | 1.65 | -0.0937 |
| 33 | 2.4742 | | |
| 34 | 2.2455 | 2.204 | 0.0415 |
| 35 | 2.2672 | 2.204 | 0.0632 |
| 36 | 1.8692 | 1.743 | 0.1262 |
| 37 | 2.017 | 2.06 | -0.043 |
| 38 | 1.9823 | 1.813 | 0.1693 |
| 39 | 1.9546 | 1.876 | 0.0782 |
| 40 | 1.9085 | 1.994 | -0.0855 |
| 41 | 1.9294 | 1.792 | 0.1374 |
| 42 | 1.7782 | 1.812 | -0.0338 |
| 43 | 1.5185 | 1.652 | -0.1335 |
| 44 | 1.4624 | 1.632 | -0.1696 |
| 45 | 1.3802 | 1.282 | 0.0982 |
| 46 | 1.6335 | 1.504 | 0.1295 |
| 47 | 1.3222 | 1.425 | -0.1028 |
| 48 | 1.3802 | 1.531 | -0.1508 |
| 49 | 1.3979 | 1.431 | -0.0331 |
| 50 | 1.301 | 1.431 | -0.13 |
| 51 | 2.3118 | | |
| 52 | 2.0899 | 1.931 | 0.1589 |
| 53 | 2.0374 | 1.931 | 0.1064 |
| 54 | 1.7634 | 1.519 | 0.2444 |
| 55 | 1.9685 | 2.055 | -0.0865 |
| 56 | 1.9085 | 1.756 | 0.1525 |
| 57 | 1.8751 | 1.845 | 0.0301 |
| 58 | 1.8388 | 1.924 | -0.0852 |
| 59 | 1.8451 | 1.717 | 0.1281 |
| 60 | 1.6628 | 1.758 | -0.0952 |
| 61 | 1.4472 | 1.599 | -0.1518 |
| 62 | 1.3802 | 1.582 | -0.2018 |
| 63 | 1.2788 | 1.244 | 0.0348 |
| 64 | 1.5798 | 1.455 | 0.1248 |
| 65 | 1.1761 | 1.373 | -0.1969 |
| 66 | 1.3424 | 1.377 | -0.0346 |
| 67 | 1.3424 | 1.377 | -0.0346 |
| 68 | 1.301 | 1.377 | -0.076 |
| 69 | 2.2718 | | |
| 70 | 2.0043 | 1.851 | 0.1533 |
| 71 | 1.9777 | 1.851 | 0.1267 |
| 72 | 1.699 | 1.487 | 0.212 |

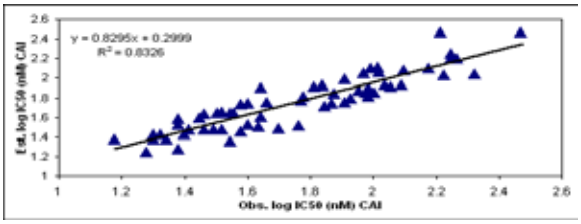


Figure: - Comparison of observed & estimated log IC50 (nM) CAI using model – 19.

**Conclusion:-**

On the basis of above rending we conclude that Log IC50 (CAI) activity can be modeled Wring the Physicochemical parameters n, α, d, α, IP1, IP4 & IP5 has been found to be excellent. Our result better then the earlier reported results.

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