Int J Pharm Bio Sci 2014July;5(3): (P) 402 - 421

**Research Article** **Analytical Chemistry**

**International Journal of Pharma and Bio Sciences** **ISSN 0975-6299**

# 3D-QSAR STUDIES FOR SOME SCHIFF BASES AGAINST BACTERIAL PATHOGEN

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## ABSTRACT

3D QSAR viz. 3 descriptor quantitative structure and activity relationship studies for a series of compounds i.e. Schiff base derivatives using their semi-empirical quantum chemical descriptors and their laboratory reported activities against pathogen viz. .*Ralstonia solanaecearum* (ITCC NO –B1- 0002 ) have been carried out and reported in the present paper. Graphs between observed and predicted activities, both in the terms of p(MIC)*cal* and p(MIC) *obs.* are also being reported on the basis of which this may be concluded that some parameters/descriptors have a positive contribution towards the activity. The method has been proved to be useful tool for such type of studies.

**KEY WORDS:** **Semiempirical/3D-qsar/Schiff bases compounds**

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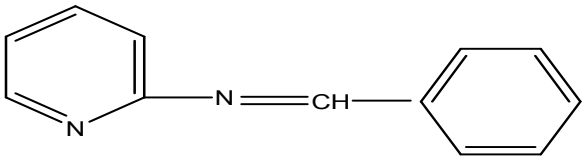
# INTRODUCTION

The battle against the infectious diseases has become a never ending process, as micro-organisms are becoming resistant more quickly than new drugs are being made available. Keeping this view, medicinal chemists are also trying out their best to speed up the drug discovery process for finding the lead molecule by using different techniques which includes QSAR (Quantitative Structure and Activity Relationship) , CADD ( Computer Aided Drug Design), Molecular Modeling, Combinatorial Chemistry and Microwave assisted synthesis. The use of these techniques has reduced the time required for primary screening of the molecule to locate the lead molecule.Previously the studies involve the checking of the antimicrobial activities of naturally occurring and /or synthesized compounds in the laboratory which may include organic compounds and inorganic complexes which were the areas of interest of many workers for so many years.QSAR (Quantitative Structure and Activity Relationship) technique has been developed as a recent and finest technique in the field of drug designing. This technique has its foundation on the statistical analysis particular regression analysis of structural descriptors of compounds under studies with their lab. reported activities. In some of the recent references scientists have even utilized electronic properties or parameters of compounds/ drugs computed on the basis of Quantum Chemical Calculation viz. *ab initio* or semi-empirical studies as descriptors for QSAR studies and correlated these descriptors with activities of the compounds against a certain microorganism, which has been proved as a step ahead in the related field.Schiff bases are the class of compounds in which an aldehyde and an amine condensed form azomethinic linkage to yield a Schiff base. Schiff bases are of interest of many workers for so many years in the field of synthetic organic chemistry as well as in the synthesis and studies of complexes also. A lot of work has been carried out including metal complexes with Schiff bases. Scientists are also trying to locate and study the antimicrobial activities of Schiff bases as well as of their metal complexes against various pathogens.Literature survey carried out in the proposed field (1-32) revealed that on the workers/ scientists have tried many naturally occurring and synthetic compounds to check their activities against various microorganisms. QSAR studies of various series of compounds have also been carried out successfully. Some of the workers have also tried to correlate activities with 2 descriptors and 3 descriptors of the compounds pertaining to 2D- QSAR and 3D-QSAR studies(1-32).Keeping above discussion in mind, in this present paper QSAR precisely 3D-QSAR studies which have been carried out on a new series of compounds i.e. Schiff base derivatives compounds shown in figure) with their activities against. *Ralstonia solanaecearum*ITCC NO –B1- 0002) are reported.

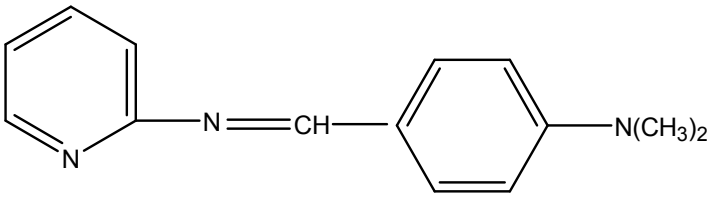
# EXPERIMENTAL

### *Preparation of Schiff bases*

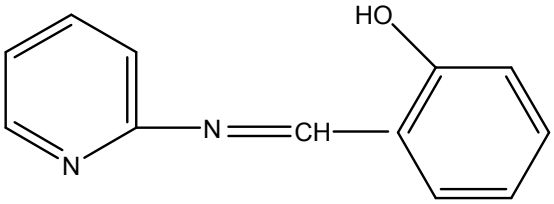
Schiff base compounds under study were synthesized by treating the appropriate amine (~1.0 mmol) with corresponding aldehyde (~1.1mmol) in appropriate solvents such as ethyl alcohol and the reaction mixtures were refluxed for 6 to 12 hours using water condenser. In some cases products were obtained after cooling the reaction mixture as such while in some cases products were obtained after cooling it on ice bath. Schiff bases obtained were then filtered and re-crystallized using appropriate solvents i.e. either alcohol or ether (theyield of the Schiff base compounds ~60- 70 %.)Compounds viz. Schiff bases (SB1-SB15) which are under study are shown in the figure -1. Analytical studies were also carried out for the synthesized compounds. These are given in the tables 1along with their melting points.



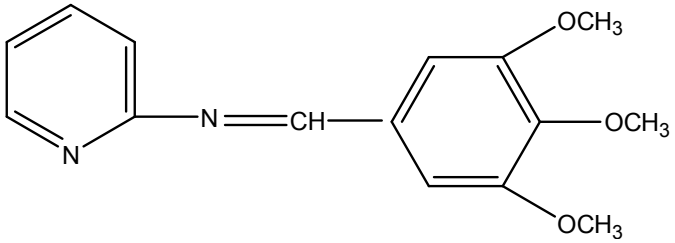

2N – [Benzalidene] Aminopyridine (SB-1)



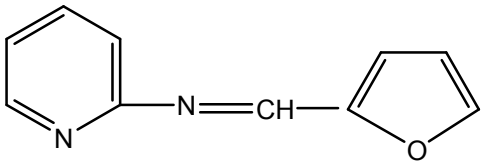

2N – [p-Dimethylaminobenzalidene] aminopyridine (SB-2)



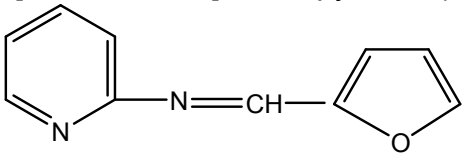

2N – [2-Hydroxybenzalidene] aminopyridine (SB-3)



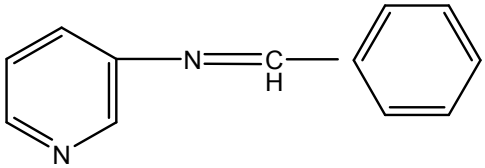

2N – [3,4,5-Trimethoxybenzalidene] aminopyridine (SB-4)



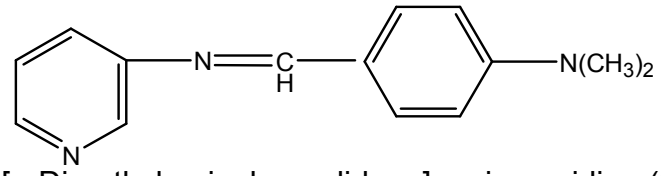

2N – [Furfuralidene] aminopyridine (SB-5)



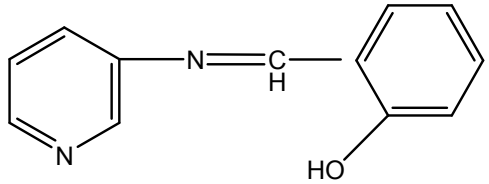

3N – [Furfuralidene] aminopyridine (SB-6)



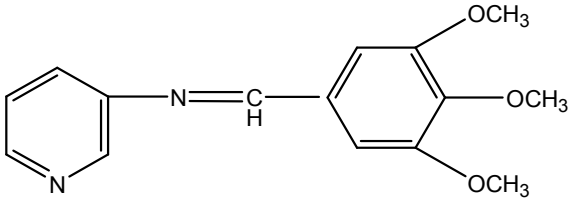

3N – [Benzalidene] aminopyridine (SB-7)



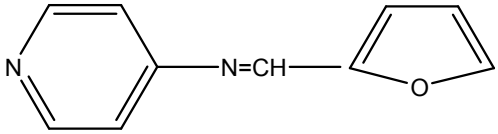

3N – [p-Dimethylaminobenzalidene] aminopyridine (SB-8)



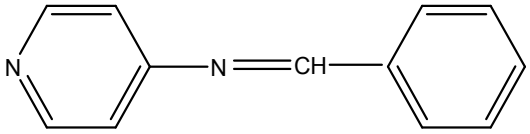

3N – [2-Hydroxybenzalidene] aminopyridine (SB-9)



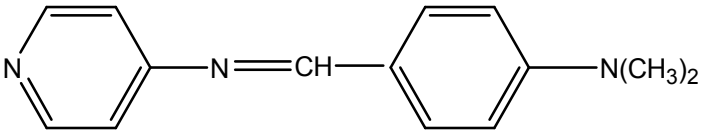

3N – [3,4,5-Trimethoxybenzalidene] aminopyridine (SB-10)



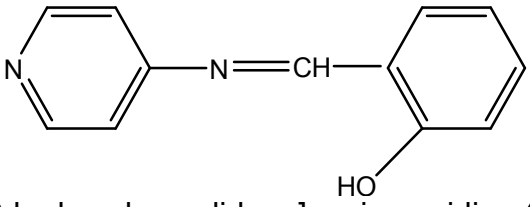

4N – [Furfuralidene] aminopyridine (SB-11)



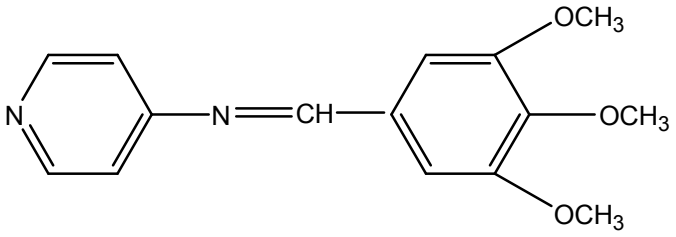

4N – [Benzalidene] aminopyridine (SB-12)




4N – [p-Dimethylaminobenzalidene] aminopyridine (SB-13)




4N – [2-hydroxybenzalidene] aminopyridine (SB-14)




4N – [3,4,5-Trimethoxy benzalidene] aminopyridine (SB-15)

**Figure-1**
***Schiff Base Compounds Under Study***

**Table 1**
***Analytical studies for the Schiff bases under study***

| Compound | M. Pt. ($^0$C) | C Found (Calcd.) | H Found (Calcd.) | N Found (Calcd.) |
|---|---|---|---|---|
| SB-1 | 180-185 | 76.26 (79.3%) | 5.85 (5.4%) | 18.28 (15.3%) |
| SB-2 | 185-190 | 76.76 (74.6%) | 5.67 (6.66%) | 15.34 (18.6%) |
| SB-3 | 190-192 | 70.9 (72.0%) | 6.65 (5.0%) | 13.05 (14.0%) |
| SB-4 | 182-185 | 64.69 (64.6%) | 6.004 (6.1%) | 7.41 (10.7%) |
| SB-5 | 168-172 | 67.46 (69.7%) | 4.76 (4.6%) | 14.86 (16.2%) |
| SB-6 | 172-175 | 67.64 (69.7%) | 4.67 (4.6%) | 14.96 (16.2%) |
| SB-7 | 182-189 | 77.62 (79.3%) | 5.05 (5.4%) | 17.82 (15.3%) |
| SB-8 | 188-192 | 79.67 (74.6%) | 7.67 (6.66%) | 16.89 (18.6%) |
| SB-9 | 175-180 | 70.91 (72.0%) | 6.67 (5.0%) | 13.50 (14.0%) |
| SB-10 | 185-189 | 64.96 (64.6%) | 6.40 (6.1%) | 7.42 (10.7%) |
| SB-11 | 170-174 | 64.56 (69.7%) | 6.00 (4.6%) | 14.20 (16.2%) |
| SB-12 | 183-188 | 76.82 (79.3%) | 5.80 (5.4%) | 18.80 (15.3%) |
| SB-13 | 187-190 | 78.67 (74.6%) | 7.77 (6.66%) | 16.98 (18.6%) |
| SB-14 | 176-181 | 70.9 (72.0%) | 6.66 (5.0%) | 12.4 (14.0%) |
| SB-15 | 183-186 | 66.08 (64.6%) | 6.115 (6.1%) | 7.813 (10.7%) |

These compounds were also established on the basis of modern spectroscopic studies viz. i.r. spectral studies. N.M.R. spectral and Mass spectral studies for some of the representative compounds were also carried out . Analysis of the studies is given below:-

***I.R. spectral studies***

Assignments of peaks are given in the table-2 for Schiff base compounds. I.R spectral analysis show that (C=N) stretching azomethine peaks are predominant in the spectra of every Schiff base compound. This peak appears ca 1635-1590 $cm^{-1}$ in the spectra of compounds under study. Apart from these peaks ring stretching

peaks, N- phenyl stretching peak, ring breathing of benzene, C-N-C bending, C-H out of plane deformation of mono substituted benzene and Out of plane bending of mono substituted benzene are also reported in the table-2.

### *NMR spectral studies*

NMR spectral studies are of less interest for the compounds under study. However, these spectra were also recorded for some representative compounds on NMR spectrometer Bruker DRX-300 with due acknowledgement to C.D.R.I. Lucknow. Some notable peaks in these spectra are listed below:-

**SB1:** 1.062(s);1.220 (s); 2.118-2.065 (d); 2.490 (s); 3.021(s); 3.341(s); 5.833 (s); 6.161(s); 6.458-6.393 (t); 6.584- 6.520 (t); 6.680-6.636(t); 7.227-7.206 (d); 7.302-7.278 (d); 7.376-7.353 (d); 7.464-7.736 (d); 7.534- 7.509 (d); 7.665-7.585 (q); 7.828- 7.687 (q).

**SB3:-** 2.260 (s); 2.490 (s); 2.997 (s); 3.326 (s); 6.179-6.159 (d); 6.205(s0; 6.572-6.460 (d); 6.731- 6.599 (q); 6.925 (s); 6.991-6.971 (d); 7.100-7.073 (d);7.338-7.282 (t);7.463- 7.442 (d); 7.668-7.486( t); 7.919(s); 9.776 (s); 10.250(s); 10.695 (s) ppm respectively.

### *MASS spectral studies*

Mass spectral studies of some representative Schiff base compounds have been carried out. Notable peaks in different compounds are:- base peaks at SB-1 :-228, SB-3 :-154, SB-4:-273, SB-5: -173, with parent ion peaks at SB-1 :-181, SB-3 :-199, SB-4:- 273, SB-5: -173,. These parent peaks confirm the mol. weights of the compounds under study. Mass spectral analyses of the compounds are given in tables 3-6.

**Table-2**

***IR spectral analysis for the Schiff base compounds under study***

| Assignment/ Compound | (C=N) Stretching azomethine | Ring stret-ching | N-Phenyl stret-ching | v(C-N) | Ring breathing of benzene | C-N-C Ben-ding | C-H out of plane deformation of mono substituted benzene | Out of plane bending of mono substituted benzene |
|---|---|---|---|---|---|---|---|---|
| SB-1 | 1600.1s | 1515.8m<br>1457.4s<br>1434.4s | 1396.3w<br>1320.5m | 1151.2m | 1088m<br>988m | 925w<br>857w<br>813w | 767m<br>695m | 534m |
| SB-2 | 1597s | 1530w<br>1488w<br>1438w | 1370m<br>1312w | 1165m | 1065w<br>991w | 937w<br>815m | 725w<br>695w | 511w |
| SB-3 | 1608s | 1552m<br>1496m<br>1428m | 1400w<br>1353w | 1185s | 1145m<br>993m | 913m<br>845m | 754m<br>695sh | 527w |
| SB-4 | 1591s | 1555sh<br>1503m<br>1421m | 1391m<br>1330s | 1186s | 1127s<br>989m | 915w | 771w<br>677w | 523w |
| SB-5 | 1600s | 1569w<br>1482m<br>1439m | 1392w<br>1313m | 1150w | 1125sh<br>988w | 925w | 771m<br>695sh | 553w |
| SB-6 | 1624s | 1583s<br>1525m<br>1482s | 1390sh<br>1293m | 1186w | 1131w<br>990sh | 925w | 797m<br>705m | 550w |
| SB-7 | 1635s | 1583w<br>1482w<br>1420w | 1294w | 1187m | 1132m | 883s | 798m<br>706m | 550w |
| SB-8 | 1599s | 1551m<br>1527w<br>1437w | 1398m<br>1330w | 1169s | 1124w<br>1064w | 942w | 817m<br>708m | 516m |
| SB-9 | 1595s | 1535w<br>1480w<br>1438w | 1375m<br>1312w | 1160m | 1060w<br>991w | 935w<br>815m | 725w<br>695w | 515w |
| SB-10 | 1624s | 1583s<br>1539s<br>1502s | 1372m<br>1329s | 1186s | 1126s<br>1041s | 950w | 842w<br>710m | 515w |

| Assignment/ Compound | (C=N) Stretching azomethine | Ring stret-ching | N-Phenyl stret-ching | v(C-N) | Ring breathing of benzene | C-N-C Ben-ding | C-H out of plane deformation of mono substituted benzene | Out of plane bending of mono substituted benzene |
|---|---|---|---|---|---|---|---|---|
| SB-11 | 1600vs | 1585sh 1513m 1423w | 1372sh 1309m | 1214s | 1129m 1087m | 933m | 868w 816m | 531m |
| SB-12 | 1605s | 1510m 1455s 1434s | 1395w 1325m | 1150m | 1088m 988m | 925w 857w 813w | 760m 690m | 534m |
| SB-13 | 1600s | 1585sh 1512m | 1431w 1331w | 1216w | 1166w 1085sh | 935sh | 820m 725w | 534w |
| SB-14 | 1604s | 1527s 1510sh | 1478w 1435w 1343m | 1269w | 1197m 1085sh | 940sh | 828w 760m | 525w |
| SB-15 | 1590vs | 1505s 1461s 1425m | 1425m 1391s 1330s | 1236m | 1188w 1127s | 990m | 843m 757m | 533m |

## Table-3
## *Mass spectral data for Schiff base (SB-1)*

| m/e | %relative abundance |
|---|---|
| 228 | 100 (Base peak) |
| 227 | 10 |
| 212 | 15 |
| 197 | 15 |
| 189 | 18 |
| 185 | 18 |
| 181 | 18 (Parent peak) |
| 155 | 35 |
| 154 | 75 |
| 144 | 25 |
| 136 | 65 |
| 122 | 45 |
| 110 | 62 |
| 98 | 60 |
| 97 | 15 |
| 95 | 100 |

## Table-4
## *Mass spectral data for Schiff base (SB-3)*

| m/e | %relative abundance |
|---|---|
| 199 | 10 (parent peak) |
| 189 | 05 |
| 164 | 10 |
| 155 | 28 |
| 154 | 100 (base peak) |
| 150 | 40 |
| 138 | 30 |
| 137 | 52 |
| 136 | 70 |
| 107 | 22 |
| 95 | 15 |

**Table -5**
***Mass spectral data for Schiff base (SB-4)***

| m/e | %relative abundance |
|---|---|
| 173 | 10 |
| 197 | 10 |
| 219 | 10 |
| 273 | 100 (base peak) |
| 274 | 20 |
| 295 | 02 |
| 305 | 15 |
| 323 | 05 |
| 415 | 04 |
| 420 | 02 |
| 441 | 02 |

**Table -6**
***Mass spectral data for Schiff base (SB-5)***

| m/e | %relative abundance |
|---|---|
| 173 | 100 (base peak) |
| 174 | 20 |
| 189 | 04 |
| 195 | 10 |
| 205 | 03 |
| 211 | 04 |
| 227 | 04 |
| 278 | 03 |

***Antimicrobial activities of the compounds under study***

**Procurement of pathogens:-**ITCC certified Pathogens viz. *Ralstonia solanacearum* (ITCC NO –B1- 0002) were procured from plant pathology division, I.A.R.I., New Delhi with due acknowledgement. Their sub- cultures have been made and the anti-microbial studies of the compounds under study were carried out against these pathogens at Birla Institute of Professional Studies with due acknowledgements. MIC (minimum inhibitory concentration) have been recorded which is then subjected to further studies to get QSAR equations. Experimental procedures that have been adopted for anti microbial studies are mentioned below:

***Experimental procedure for Anti bacterial studies***

Pure cultures that were obtained from IARI were revived. Fresh inoculation of *Ralstonia solanacearum* was done by taking a loopful from IARI culture tube and streaking was done on sterile nutrient agar petri plate and slant and incubated at $28^0$c for 48 hrs to revive the culture. After 48 hrs on revival of test organism, a loopful this has been taken and dispensed in 50 mL of medium in a conical flask and kept for further 48 hrs for the preparation of inoculum. Culture media were autoclaved at $121^0$c for 15 lbs pressure for 15 minutes. Plates were made by dispensing the media approx 15-20 mL in each plate. Plates were kept inverted in the incubator at $28^0$c overnight for sterility checking. Whatmann 1 filter paper discs of 6 mm diameter were punched out from barge sheet and were autoclaved for 15 minutes. About 100µL of actively growing pathogen inoculated nutrient broth was used to inoculate sterile nutrient agar plates through spread plate method. The whatmann paper discs were dispensed on glass plates and each was loaded with about 5 µL. Volume of pre designated dilutions were used for analysis. The discs were left air dried in the laminar air flow and were then carefully transferred to inoculated positions. The plates were then

inoculated at $28^0$c for 48 minimum hrs. Some of the results of anti bacterial studies are shown in Figure 2.

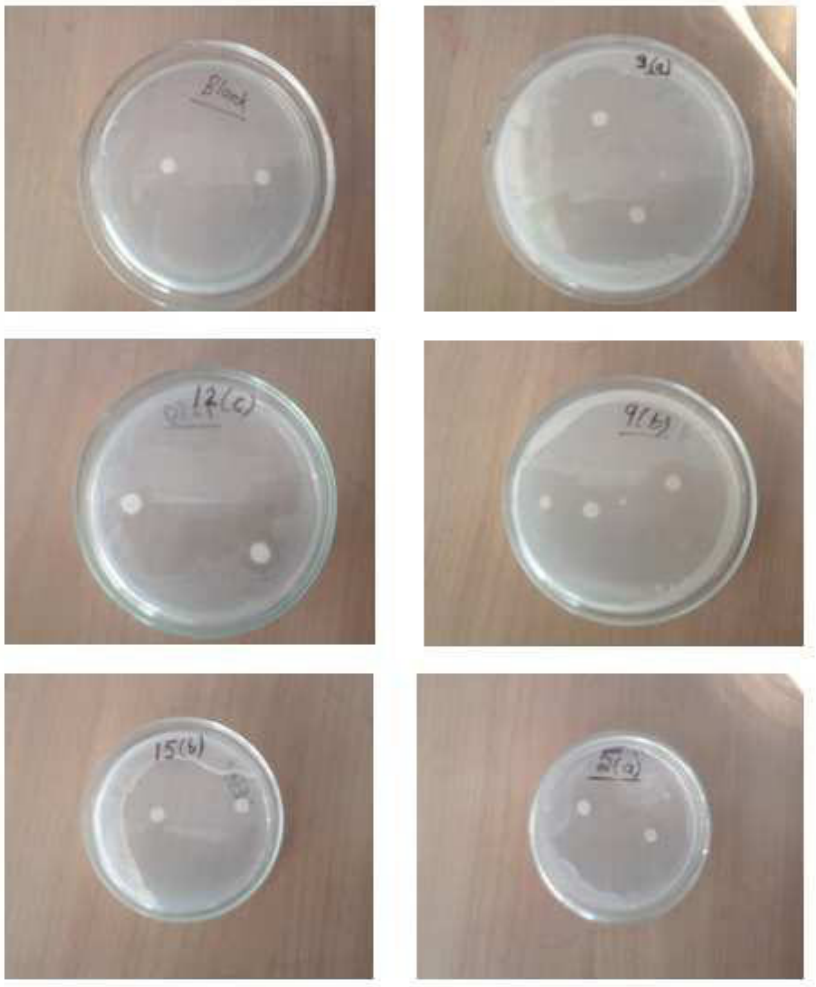



**Figure-2**
***Some notable photographs for anti bacterial studies of compounds under study***

**Table-7**
***Antibacterial analysis of Schiff base compounds under study against Ralstonia solanacearum(ITCC NO –B1- 0002)***

| Compounds under study | Concentrations of compounds/10 ml | | | |
|---|---|---|---|---|
| | 10 mg | 20 mg | 30 mg | 40 mg |
| SB1 | 23 mm | 17 mm | ------- | ----- |
| SB2 | ------- | ---------- | ------- | 05 mm |
| SB3 | -------- | ---------- | ------- | 02 mm |
| SB4 | -------- | ---------- | -------- | 01 mm |
| SB5 | -------- | ---------- | -------- | 03 mm |
| SB6 | 31 mm | ---------- | -------- | -------- |
| SB7 | 27 mm | 29 mm | --------- | --------- |
| SB8 | -------- | --------- | ---------- | 05 mm |
| SB9 | --------- | ---------- | ---------- | 04 mm |
| SB10 | --------- | --------- | ---------- | ------ |
| SB11 | --------- | --------- | ---------- | 02 mm |
| SB12 | -------- | --------- | 10 mm | 12 mm |
| SB13 | -------- | --------- | 27 mm | 28 mm |
| SB14 | -------- | --------- | -------- | ------- |
| SB15 | --------- | ---------- | --------- | 02 mm |

***Computational Details for the computational work***

The AM1 Hamiltonia on Hyperchem 8.0 professional version were used to calculate the QSAR related descriptors such as Hydration energy (Hyd E), log P (log P), Refractivity (REF), Polarizability (POL). mass (mass), Surface area approx (SAA), Surface area Grid (SAG), volume (Vol), Heat of formation (HF) , Zero point energy (ZPE), HOMO energy (HOMO), LUMO energy ( LUMO) and dipole moment ( DM).

All these computations were carried out on Pentium core -2 duo machine having configuration

Intel (R ) core (™) 2 Duo CPU

$T_{5450}$@ 1.66 GHz.

982 MHz, 896 MB RAM

150 GB HDD

with windows – Microsoft windows XP software as an operating system.These descriptors and the activities of the compounds against specified microbes, mentioned in the tables, were taken into consideration in terms of p (MIC) and were subjected to statistical analysis/ regression analysis to get QSAR equations. All these statistical calculations were carried out on the same machine mentioned above using EXCEL software.

## RESULTS AND DISCUSSION

The *in-vitro* anti microbial viz. anti bacterial and anti fungal studies of the Schiff base compounds were carried out as per experimental procedure mentioned in the experimental section at Birla Institute of Medical Research, Gwalior with due acknowledgement. The activities of the compounds were recorded in terms of Minimum Inhibitory Concentration (MIC). Some of the compounds have shown notable activities against the specified pathogen under study while other do not show any activity. The activities are recorded and reported here in the table 7. Figures of some of the plates were also taken showing growth of the pathogens.These labs. reported activities of the Schiff base and pyrazolone compounds under study in terms of p(MIC) have been subjected to QSAR studies with Semi-empirical quantum chemical based certain parameters of the compounds. These parameters/ descriptors are hydration energy (HE), logP(logP), Refractivity(RF), Polarizaility (POL), Mass(Mass), Surface area approx(SAA), Surface area Grid( SAG), Volume (VOL), Heat of formation (HF), Zero point Energy (ZPE), HOMO energy(HOMO), LUMO energy (LUMO) and dipole moment( DM).These parameters are computed on HYPERCHEM 8.0 version software after geometry optimization of the compounds under study as mentioned in the experimental section above. The computed parameters/ descriptors are reported in the tables 8-11. The methods adopted here in this project are AM1, PM3, MNDO and ZINDO respectively. All methods are proved to be good to give optimized geometry and minimized energy for the compounds under study. This fact can also be proved as IR studies which are observed experimentally for the compounds under study match well with the computed IR spectral frequencies using Hyperchem 8.0 professional software especially on the basis of AM1 and PM3 method. The fact of authenticity of AM1 and PM3 may prove to be appropriate in this study, so far as software is concerned.The software Hyperchem 8.0 version was quite fast and provides reasonably good results regarding all parameters viz. physical parameters, spectroscopic parameters and SAR related parameters.

## Table-8

***Semi- Empirical AM1 based Computed properties of the Compounds (SB1-SB15) under study and their antibacterial results: p(MIC) on Ralstonia solanacearum (ITCC NO –B1- 0002 )***

| Compd | SAA | SAG | HE | Log P | RF | POL | Mass |
|---|---|---|---|---|---|---|---|
| SB-1 | 328.43 | 403.81 | -5.27 | 1.7 | 63.44 | 22.15 | 182 |
| SB-2 | 431.84 | 474.32 | -4.13 | 0.75 | 77.06 | 27.17 | 225.29 |
| SB-3 | 331.54 | 407.3 | -10.03 | 0.67 | 65.05 | 22.79 | 198.22 |
| SB-4 | 316.5 | 431.39 | -5.44 | -1.28 | 82.56 | 29.57 | 272.3 |
| SB-5 | 307.6 | 373.6 | -8.83 | -0.13 | 53.02 | 19.31 | 172.19 |
| SB-6 | 220.04 | 393.91 | 13.97 | -0.31 | 58.09 | 21.34 | 188.23 |
| SB-7 | 321.31 | 387.75 | -5.91 | 0.13 | 64.08 | 22.15 | 182.22 |
| SB-8 | 419.03 | 458.97 | -4.74 | -0.82 | 77.69 | 27.17 | 225.29 |
| SB-9 | 511.03 | 396.31 | 25.91 | -0.89 | 65.68 | 22.79 | 198.22 |
| SB-10 | 410.85 | 489.58 | -7.99 | -2.85 | 83.2 | 29.57 | 272.3 |
| SB-11 | 300.68 | 362.1 | -9.65 | -1.82 | 53.58 | 19.31 | 172.19 |
| SB-12 | 320.5 | 387.2 | -6.12 | 0.01 | 64 | 22.15 | 182.22 |
| SB-13 | 418.19 | 459.23 | -4.95 | -0.94 | -7.62 | 27.17 | 225.29 |
| SB-14 | 191.46 | 382.67 | -2.87 | -1.02 | 65.61 | 22.79 | 198.22 |
| SB-15 | 386.88 | 482.8 | -8.37 | -2.97 | 83.12 | 29.57 | 272.3 |

| VOL | HF | ZPE | HOMO | LUMO | DM | MIC | P(MIC) obs. |
|---|---|---|---|---|---|---|---|
| 625.06 | 90.6906 | 122.856 | -0.6919 | 0.28678 | 0.846 | 10 | -1 |
| 756.97 | 93.4313 | 168.516 | -0.4682 | 0.46352 | 2.391 | 40 | -1.602 |
| 637.89 | 41.6617 | 125.925 | -0.6392 | 0.31279 | 1.173 | 40 | -1.602 |
| 708.65 | 93.8518 | 183.267 | -0.0233 | 0.78834 | 10.492 | 40 | -1.602 |
| 565.99 | 64.5137 | 296.708 | -0.5966 | 0.31456 | 0.518 | 40 | -1.602 |
| 624.46 | 83.3848 | 129.024 | -1.0503 | 0.41409 | 1.739 | 10 | -1 |
| 603.63 | 93.2951 | 122.589 | -0.8216 | 0.224 | 1.532 | 10 | -1 |
| 737.98 | 101.265 | 168.037 | -0.5746 | 0.41979 | 3.794 | 40 | -1.602 |
| 636.32 | 72.8485 | 123.336 | -0.9824 | 0.01622 | 0.04 | 40 | -1.602 |
| 850.52 | 24.9715 | 185.623 | -0.0456 | 0.04697 | 3.247 | 40 | -1.602 |
| 549.61 | 70.8844 | 103.81 | -0.7422 | 0.21055 | 3.084 | 40 | -1.602 |
| 604.65 | 93.9724 | 122.609 | -0.8569 | 0.15012 | 3.463 | 30 | -1.477 |
| 736.8 | 101.813 | 168.075 | -0.6006 | 0.36356 | 6.029 | 30 | -1.477 |
| 606.8 | 115.656 | 123.955 | -0.1917 | 0.22419 | 3.773 | 40 | -1.602 |
| 813.78 | 25.1947 | 185.703 | -0.5742 | 0.07244 | 2.504 | 40 | -1.602 |

## Table-9

***Semi- Empirical PM3 based Computed properties of the Compounds (SB1-SB15) under study and their antibacterial results p(MIC) on Ralstonia solanacearum (ITCC NO –B1- 0002 )***

| Compd | MIC | P(MIC)Obs. | SAA | SAG | HE | Log P | RF |
|---|---|---|---|---|---|---|---|
| SB-1 | 10 | -1 | 327.9 | 398.57 | -5.21 | 1.7 | 63.44 |
| SB-2 | 40 | -1.602 | 429.81 | 471.29 | -4.09 | 0.75 | 77.06 |
| SB-3 | 40 | -1.602 | 330.69 | 405.7 | -10.08 | 0.67 | 65.05 |
| SB-4 | 40 | -1.602 | 421.13 | 487.55 | -6.75 | -1.28 | 82.56 |
| SB-5 | 40 | -1.602 | 308.07 | 373.46 | -8.7 | -0.13 | 53.02 |
| SB-6 | 10 | -1 | 240.24 | 396.48 | 15.86 | -0.31 | 58.09 |
| SB-7 | 10 | -1 | 321.22 | 386.16 | -5.91 | 0.13 | 64.08 |
| SB-8 | 40 | -1.602 | 407.33 | 448.7 | -4.5 | -0.82 | 77.69 |
| SB-9 | 40 | -1.602 | 806.97 | 394.77 | 31.12 | -0.89 | 65.58 |
| SB-10 | 40 | -1.602 | 346.15 | 448.96 | -6.48 | -2.85 | 83.2 |
| SB-11 | 40 | -1.602 | 300.33 | 358.64 | -9.57 | -1.82 | 53.58 |
| SB-12 | 30 | -1.477 | 320.33 | 386.98 | -6.11 | 0.01 | 64 |
| SB-13 | 30 | -1.477 | 300.14 | 463.82 | -3.11 | -0.94 | 77.62 |
| SB-14 | 40 | -1.602 | -637.25 | 399.25 | 21.37 | -1.02 | 65.61 |
| SB-15 | 40 | -1.602 | 438.28 | 494.15 | -8.31 | -2.97 | 83.12 |

| POL | Mass | VOL | HF | ZPE | HOMO | LUMO | DM |
|---|---|---|---|---|---|---|---|
| 22.15 | 182.22 | 617.65 | 74.5392 | 118.0805 | -0.0237 | 0.26053 | 0.856 |
| 27.17 | 225.29 | 751.72 | 75.0653 | 161.0597 | -0.6047 | 0.12665 | 1.636 |
| 22.79 | 198.22 | 635.43 | 31.13328 | 121.3319 | -0.7363 | 0.07505 | 0.576 |
| 2.57 | 272.3 | 808.85 | 23.0389 | 177.9144 | -0.1781 | 0.2533 | 3.178 |
| 19.31 | 172.19 | 565.62 | 45.417 | 298.6673 | -0.6761 | 0.01641 | 0.0695 |
| 21.34 | 188.23 | 626.51 | 67.5881 | 123.476 | -1.1512 | 0.26996 | 1.601 |
| 22.15 | 152.22 | 601.46 | 84.0827 | 117.0909 | -0.908 | 0.000038 | 1.271 |
| 27.17 | 225.29 | 733.56 | 73.9653 | 163.41169 | -0.4841 | 0.05898 | 2.219 |
| 22.79 | 198.22 | 637.16 | 69.1811 | 118.1698 | -0.0854 | 0.18165 | 0.219 |
| 29.57 | 272.3 | 761.35 | 20.0201 | 180.9994 | -0.2461 | 0.06722 | 3.985 |
| 19.31 | 172.19 | 547.72 | 53.6628 | 99.6895 | -0.8176 | 0.05231 | 3.093 |
| 22.15 | 182.22 | 601.83 | 84.5714 | 17.8388 | -0.9709 | 0.005465 | 3.068 |
| 27.17 | 237.3 | 764.27 | 19.88857 | 166.303 | -0.2295 | 0.19077 | 4.018 |
| 22.79 | 198.22 | 639.93 | 82.8752 | 118.0187 | -0.1425 | 0.1323 | 2.432 |
| 29.57 | 272.3 | 818.5 | 17.18738 | 177.1228 | -0.0148 | 0.10017 | 3.332 |

## Table-10

***Semi- Empirical MNDO based Computed properties of the Compounds (SB1-SB15) under study and their antibacterial results p(MIC) on Ralstonia solanecearum (ITCC NO –B1- 0002 )***

| Compd | MIC | P(MIC)Obs. | SAA | SAG | HE | Log P | RF |
|---|---|---|---|---|---|---|---|
| SB-1 | 10 | -1 | 330.44 | 398.47 | -5.25 | 1.7 | 63.44 |
| SB-2 | 40 | -1.602 | 431.87 | 474.32 | -4.13 | 0.75 | 77.06 |
| SB-3 | 40 | -1.602 | 334.34 | 409.26 | -10.21 | 0.67 | 65.05 |
| SB-4 | 40 | -1.602 | 390.26 | 501.86 | -7.57 | -1.28 | 82.56 |
| SB-5 | 40 | -1.602 | 308.07 | 372.46 | -8.7 | -0.13 | 53.02 |
| SB-6 | 10 | -1 | 363.32 | 421.19 | 28.06 | -0.31 | 58.09 |
| SB-7 | 10 | -1 | 325.42 | 390.74 | -6 | 0.13 | 64.05 |
| SB-8 | 40 | -1.602 | 424.74 | 461.48 | -4.85 | -0.82 | 77.69 |
| SB-9 | 40 | -1.602 | 335.53 | 410.08 | 11.66 | -0.84 | 65.69 |
| SB-10 | 40 | -1.602 | 441.86 | 516.88 | -8.45 | -2.85 | 83.2 |
| SB-11 | 40 | -1.602 | 516.88 | 364.47 | -9.63 | -1.82 | 53.58 |
| SB-12 | 30 | -1.477 | 324.51 | 390.82 | -6.13 | 0.01 | 64 |
| SB-13 | 30 | -1.477 | 424.08 | 462.98 | -5.04 | -0.94 | 77.62 |
| SB-14 | 40 | -1.602 | 85.62 | 385.41 | -2.18 | -1.02 | 65.61 |
| SB-15 | 40 | -1.602 | 373.02 | 493.92 | -8.61 | -2.97 | 83.12 |

| POL | Mass | VOL | HF | ZPE | HOMO | LUMO | DM |
|---|---|---|---|---|---|---|---|
| 22.15 | 182.22 | 620.52 | 72.6814 | 125.5213 | -0.7304 | 0.1807 | 0.115 |
| 27.17 | 225.29 | 756.97 | 83.6483 | 173.1405 | -0.552 | 0.3057 | 1.985 |
| 22.79 | 198.22 | 639.44 | 26.4478 | 128.8318 | -0.6656 | 0.164 | 1.313 |
| 29.57 | 272.3 | 831.31 | 86.8148 | 187.9244 | -0.2584 | 0.7191 | 9.788 |
| 19.31 | 172.19 | 565.62 | 37.5895 | 294.6581 | -0.5852 | 0.2013 | 0.256 |
| 21.34 | 188.23 | 653.43 | 77.1433 | 132.8215 | -1.0426 | 0.2484 | 1.872 |
| 22.15 | 182.22 | 607.45 | 90.8727 | 125.2745 | -0.8436 | 0.0489 | 1.666 |
| 27.17 | 225.29 | 744.34 | 1-1.5124 | 172.8898 | -0.6482 | 0.2094 | 3.487 |
| 22.79 | 198.22 | 653.5 | 76.8839 | 126.1077 | -0.111 | 0.0129 | 0.94 |
| 29.57 | 271.3 | 851.71 | 39.9456 | 190.328 | -0.1264 | 0.0924 | 2.72 |
| 19.31 | 172.19 | 552.73 | 54.2342 | 106.3981 | -0.7498 | 0.1216 | 3.434 |
| 22.15 | 182.22 | 608.03 | 99.2275 | 125.2744 | -0.0444 | 0.07092 | 3.738 |
| 27.17 | 225.29 | 745.39 | 101.729 | 172.9119 | -0.7083 | 0.12267 | 5.8 |
| 22.79 | 198.22 | 611.87 | 118.4008 | 127.213 | -0.3373 | 0.06016 | 3.922 |
| 29.57 | 272.3 | 829.41 | 67.5956 | 189.1327 | -0.911 | 0.7773 | 9.452 |

**Table-11**

***Semi- Empirical ZINDO based Computed properties of the Compounds (SB1-SB15) under study and their antibacterial results p(MIC) on Ralstonia solanacearum (ITCC NO –B1- 0002 )***

| Compd | MIC | P(MIC)Obs. | SAA | SAG | HE | Log P | RF |
|---|---|---|---|---|---|---|---|
| SB-1 | 10 | -1 | 326.31 | 398.74 | -5.13 | 1.7 | 63.44 |
| SB-2 | 40 | -1.602 | 424.59 | 468.15 | -3.98 | 0.75 | 77.06 |
| SB-3 | 40 | -1.602 | 328.99 | 410.75 | -9.8 | 0.67 | 65.05 |
| SB-4 | 40 | -1.602 | 302.76 | 441.39 | -7.29 | -1.29 | 82.56 |
| SB-5 | 40 | -1.602 | 304.93 | 369.03 | -8.63 | -0.013 | 53.02 |
| SB-6 | 10 | -1 | -181.81 | 374.77 | -8.95 | -0.31 | 58.09 |
| SB-7 | 10 | -1 | 319.51 | 385.78 | -5.81 | 0.13 | 64.08 |
| SB-8 | 40 | -1.602 | 417.14 | 454.99 | -4.72 | -0.82 | 77.69 |
| SB-9 | 40 | -1.602 | 208.81 | 396.28 | -7.19 | -0.89 | 65.68 |
| SB-10 | 40 | -1.602 | 369.07 | 456.56 | -7.15 | -2.85 | 83.2 |
| SB-11 | 40 | -1.602 | 296.07 | 355.04 | -9.52 | -1.82 | 53.08 |
| SB-12 | 30 | -1.477 | 318.2 | 381.79 | -6.09 | 0.01 | 64 |
| SB-13 | 30 | -1.477 | 415.76 | 455.86 | -4.93 | -0.94 | 77.62 |
| SB-14 | 40 | -1.602 | -515.87 | 371.28 | 557.06 | -1.02 | 65.61 |
| SB-15 | 40 | -1.602 | 320.41 | 440.74 | -7.49 | -2.49 | 83.12 |

| POL | Mass | VOL | HF | ZPE | HOMO | LUMO | DM |
|---|---|---|---|---|---|---|---|
| 22.15 | 183.22 | 614.22 | -5357.263 | 166.065 | -7.266 | 5.3892 | 0.767 |
| 27.17 | 225.29 | 744.51 | -6733.5149 | 229.561 | -5.7525 | 5.6997 | 1.445 |
| 22.29 | 198.22 | 636.3 | -5499.3121 | 169.919 | -7.177 | 5.8793 | 2.46 |
| 29.57 | 272.3 | 735.94 | -7446.8667 | 255.6673 | -4.8535 | 5.0977 | 3.882 |
| 19.31 | 172.19 | 561.53 | -4598.1684 | 328.6815 | -6.9848 | 5.6676 | 1.415 |
| 21.34 | 188.23 | 584.88 | -5392.7584 | 180.5573 | -5.7055 | 4.316 | 1.846 |
| 22.15 | 182.22 | 599.51 | -5342.8922 | 166.099 | -6.8912 | 5.4596 | 1.358 |
| 27.17 | 225.29 | 729.78 | -6719.1172 | 229.5434 | -5.7808 | 5.7748 | 3.079 |
| 22.79 | 198.22 | 620.61 | -5502.9938 | 170.1358 | -6.8308 | 5.0378 | 7.069 |
| 29.57 | 272.3 | 770.33 | -7388.4733 | 252.558 | -6.6451 | 5.8622 | 2.089 |
| 19.31 | 172.19 | 542.8 | -4583.9114 | 140.7262 | -7.2156 | 5.4445 | 3.347 |
| 22.15 | 182.22 | 599.36 | -5344.7538 | 166.1238 | -7.2369 | 5.1767 | 3.849 |
| 27.17 | 225.29 | 728.99 | -6721.2763 | 229.5709 | -5.9184 | 5.4844 | 5.915 |
| 22.79 | 198.22 | 590.34 | -5460.0367 | 169.2597 | -3.8549 | 6.7071 | 4.554 |
| 29.17 | 272.3 | 741.15 | -7519.3218 | 253.8556 | -4.1665 | 6.5701 | 7.667 |

This final equation was used to get the predicted activities for all the series of compounds and against all microorganisms under study. The final 3D QSAR equations are reported as under:-

**AM1/Schiff base compounds (SB1-SB15)/Antibacterial** *Ralstonia solanacearum* (ITCC NO –B1-0002 ) **/3D-equation**

p(MIC) = 0.077622896(LogP)+0.000856497(Mass)-0.331649544(HOMO)-1.791057168
N = 15, SD = 0.22465569, r = 0.591026026, F test = 1.96839243

**PM3/Schiff base compounds (SB1-SB15)/Antibacterial** *Ralstonia solanacearum* (ITCC NO –B1-0002 ) **/3D-equation**

p(MIC) = 0.056443566(LogP)-0.001595606(Mass)+0.0005943254(HF)-1.125807305
N = 15, SD = 0.231861138, r = 0.541469338, F test = 1.520953363

**MNDO/Schiff base compounds (SB1-SB15)/Antibacterial** *Ralstonia solanacearum* (ITCC NO – B1- 0002) **/3D-equation**

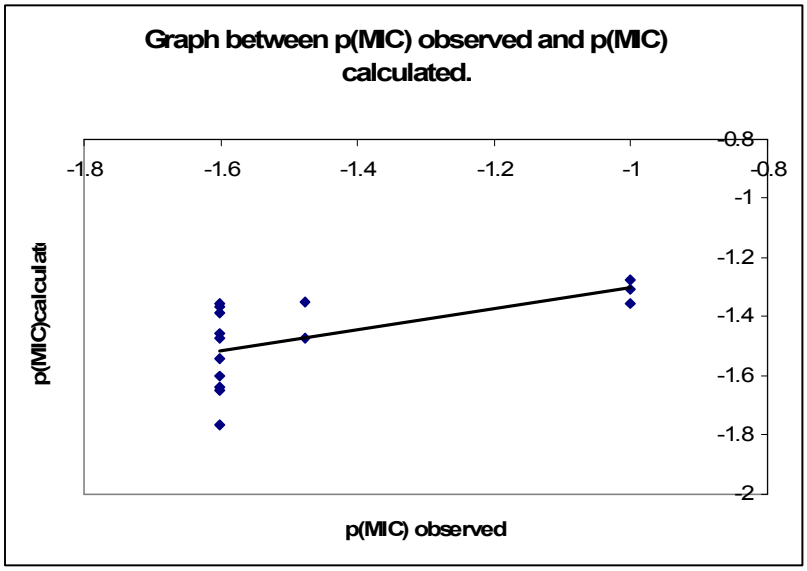
p(MIC) = 0.007929358(HE)+0.0752524(LogP)-0.304572259(HOMO)-1.560126502
N = 15, SD = 0.189418682, r = 0.726822244, F test = 4.10615069

**ZINDO/Schiff base compounds (SB1-SB15)/Antibacterial** *Ralstonia solanacearum* (ITCC NO – B1- 0002**) /3D-equation**
p(MIC) = 0.052848(LogP)-0.15035(LUMO)-0.02495(DM)-0.51054
N = 15, SD = 0.212191386, r = 0.638768901, F test = 2.527296013

Graphs were also drawn between observed activities and predicted activities, both in the terms of p(MIC) form 3 D-QSAR equations for this series of compounds. These trend line graphs are shown in figure 3-6.

**Figure -3**

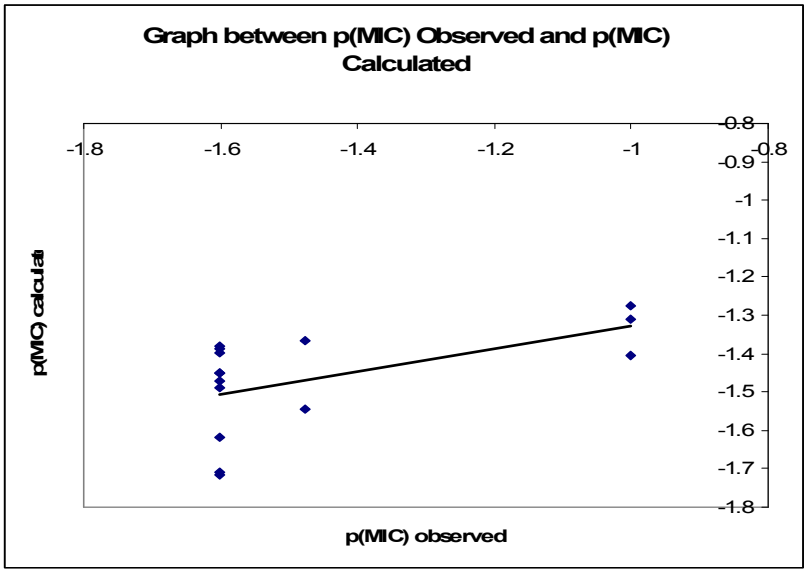
***Trend line Graph between p(MIC) observed and AM1 computed p(MIC) calculated for the Schiff base compounds (SB1-SB15)under study for their antibacterial activities on Ralstonia solanacearum (ITCC NO –B1- 0002)***




| p(MIC) observed | p(MIC) cal. |
|---|---|
| -1 | -1.274 |
| -1.602 | -1.385 |
| -1.602 | -1.357 |
| -1.602 | -1.649 |
| -1.602 | -1.456 |
| -1 | -1.306 |
| -1 | -1.352 |
| -1.602 | -1.471 |
| -1.602 | -1.365 |
| -1.602 | -1.764 |
| -1.602 | -1.539 |
| -1.477 | -1.35 |
| -1.477 | -1.472 |
| -1.602 | -1.637 |
| -1.602 | -1.598 |

**Figure -4**

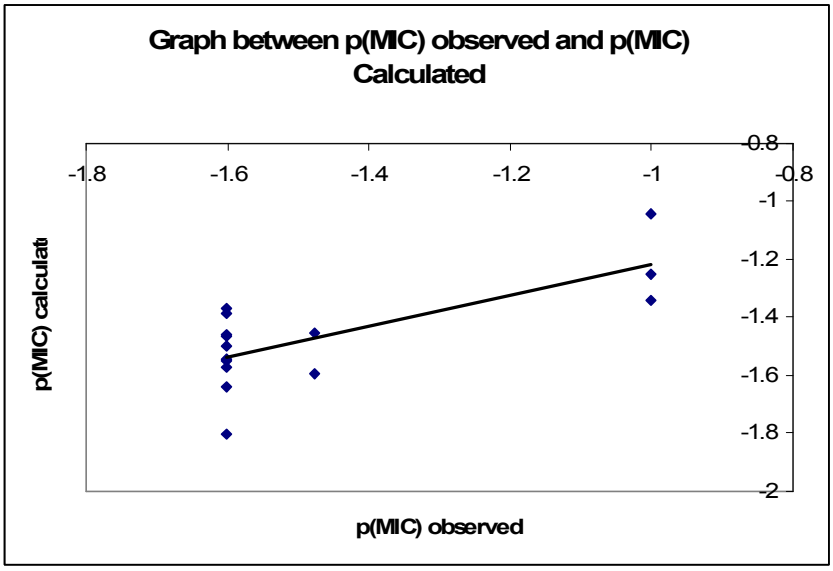
***Trend line Graph between p(MIC) observed and PM3 computed p(MIC) calculated for the Schiff base compounds (SB1-SB15)under study for their antibacterial activities on Ralstonia solanacearum (ITCC NO –B1- 0002 )***




| p(MIC) observed | p(MIC) cal. |
|---|---|
| -1 | -1.276 |
| -1.602 | -1.398 |
| -1.602 | -1.386 |
| -1.602 | -1.619 |
| -1.602 | -1.381 |
| -1 | -1.403 |
| -1 | -1.311 |
| -1.602 | -1.488 |
| -1.602 | -1.451 |
| -1.602 | -1.709 |
| -1.602 | -1.471 |
| -1.477 | -1.366 |
| -1.477 | -1.546 |
| -1.602 | -1.45 |
| -1.602 | -1.718 |

**Figure-5**

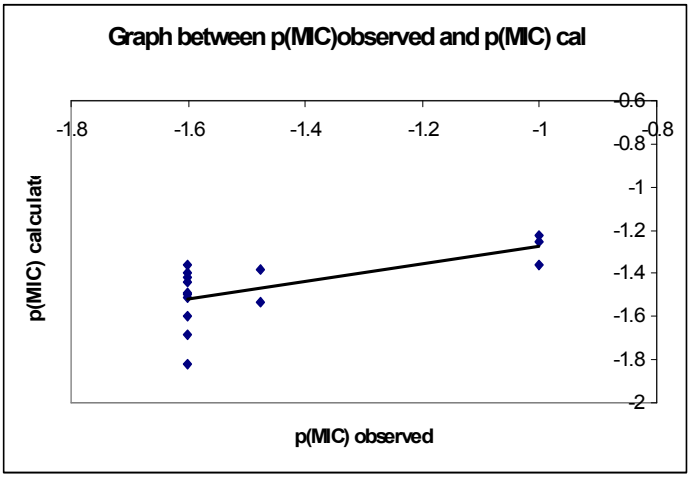
***Trend line Graph between p(MIC) observed and MNDO computed p(MIC) calculated for the Schiff base compounds (SB1-SB15)under study for their antibacterial activities on Ralstonia solanacearum (ITCC NO –B1- 0002 )***




| p(MIC) observed | p(MIC) cal. |
|---|---|
| -1 | -1.251 |
| -1.602 | -1.368 |
| -1.602 | -1.388 |
| -1.602 | -1.638 |
| -1.602 | -1.461 |
| -1 | -1.043 |
| -1 | -1.341 |
| -1.602 | -1.463 |
| -1.602 | -1.497 |
| -1.602 | -1.803 |
| -1.602 | -1.545 |
| -1.477 | -1.594 |
| -1.477 | -1.455 |
| -1.602 | -1.551 |

**Figure -6**

***Trend line Graph between p(MIC) observed and ZINDO computed p(MIC) calculated for the Schiff base compounds (SB1-SB15)under study for their antibacterial activities on Ralstonia solanacearum (ITCC NO –B1- 0002 )***




| p(MIC) observed | p(MIC) cal. |
|---|---|
| -1 | -1.25 |
| -1.602 | -1.364 |
| -1.602 | -1.42 |
| -1.602 | -1.442 |
| -1.602 | -1.399 |
| -1 | -1.222 |
| -1 | -1.358 |
| -1.602 | -1.499 |
| -1.602 | -1.491 |
| -1.602 | -1.595 |
| -1.602 | -1.509 |
| -1.477 | -1.384 |
| -1.477 | -1.532 |
| -1.602 | -1.686 |
| -1.602 | -1.821 |
| -1.602 | -1.574 |

## CONCLUSION

This method has once again proved to be useful for this type of studies. The parameters/ descriptors which contribute positively to p (MIC) in final 3D QSAR equations are listed below:-

**AM1/ Schiff bases (SB1-SB15)/** *Ralstonia solanacearum* (ITCC NO –B1- 0002)**:** Log P , Mass and HOMO

**PM3/ Schiff bases (SB1-SB15)/** *Ralstonia solanacearum* (ITCC NO –B1- 0002)**:** Log P , Mass and HF

**MNDO/ Schiff bases (SB1-SB15)/** *Ralstonia solanacearum* (ITCC NO –B1- 0002)**:** Log P , HE and HOMO
**ZINDO/ Schiff bases (SB1-SB15)/** *Ralstonia solanacearum* (ITCC NO –B1- 0002)**:** Log P , DM and LUMO

In conclusion this may be said that these parameters / descriptors have more impact on (MIC) over all other descriptors computed and reported.

## ACKNOWLEDGEMENT

Author sincerely acknowledges M.P.Council of Science and Technology, Bhopal for financial assistance in the form of Research Project sanctioned to him. {Endt. No. 6051/CST/R&D/2011 Dated 31-03-2011}

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