Supplementary file

Machine Learning-Based QSAR Modeling Assay for the Nitrification Inhibition of 2,4,5-Trichloroaniline-Derived Eco-Friendly Schiff Bases

Tilak Mondal[1]*, Rajesh Kumar[2], Santanu Mukherjee[3,4]*, Nilimesh Mridha[1], Namrata Laskar[1], Avijit Das[1], Pradip Basak[5], Atul Singha[1], Kanchan Sinha[6] and Dinesh Babu Shakyawar[1]

[1]ICAR-National Institute of Natural Fibre Engineering and Technology, Kolkata, India

[2]Indian Agricultural Research Institute, New Delhi, India

[3]School of Agriculture, Shoolini University of Biotechnology and Management Sciences, Solan 173229, India

[4]Department of Environmental and Civil Engineering, Faculty of Engineering, Toyama Prefectural University, 5180 Kurokawa, Imizu, Toyama 939-0398, Japan

[5]Uttar Bangha Krishi Viswavidyalaya, Cooch Behar, West Bengal, India

[6]ICAR-Indian Agricultural Statistics Research Institute, New Delhi, India

***Corresponding Authors:**

Dr. Santanu Mukherjee, School of Agriculture Sciences**,** Shoolini University of Biotechnology and Management Sciences**,** Bajhol, PO Sultanpur, Distt. Solan, Himachal Pradesh 173229, India**;** E-mail: santanu@shooliniuniversity.com

Dr. Tilak Mondal, ICAR-National Institute of Natural Fibre Engineering and Technology, Kolkata, India; E-mail: tilakmondal1987@gmail.com

Supplementary Table 1. Characterized spectral data of synthesized 2,4,5 Trichloro aniline based Schiff base compounds.

Comp No.	IUPAC Name	Physical Property	Spectral analysis (IR, ^{1}H NMR &^{13}C NMR)
C1	*(2,4,5-Trichloro-phenyl)(2,4-dihydroxy-benzylidene)amine*	Yield: 81%; color: dark yellow solid; Melting point: 186ºC; Rf value: 0.7**	IR: 3375 cm^{-1} (O-H, aromatic) 3078 cm^{-1} (C-H, aromatic), 2883 cm^{-1} (C-H, aliphatic), 1509 (C=C, aromatic), 1574 cm^{-1} (C=N), 1239 (C-N), 881 cm^{-1} (C-Cl); ^{1}H NMR: 7.91 (s, 1H, 3-phenyl), 7.32 (s, 1H, 5-phenyl), 8.9 (s, 1H, CH=N), 5.98 (s, 1H, 2-hydroxy), 5.22 (s, 1H, 4- hydroxy), 6.31 (s, 1H, 3-benzylidene), 6.45-6.43 (d, J = 8, 1H, 5- benzylidene), 7.458-7.432 (d, J = 8.4, 1H, 6- benzylidene);^{13}C NMR: 145.3 (1C-phenyl), 128.9 (2C- phenyl), 131.2 (3C- phenyl), 135.7 (4C- phenyl), 131.3 (5C- phenyl), 128.2 (6C- phenyl), 165.4 (CH=N), 112.3 (1C-benzylidene), 163.7(2C- benzylidene), 102.9 (3C-benzylidene), 164.1 (4C-benzylidene), 108.9 (5C-benzylidene), 121.4 (6C-benzylidene)
C2	*(2,4,5-Trichloro-phenyl)(2-methoxy-4-hydroxy-benzylidene)amine*	Yield: 48%; color: white solid; Melting point: 181ºC; Rf value: 0.61**	IR: 3405 cm^{-1} (O-H, aromatic) 3092 cm^{-1} (C-H, aromatic), 2881 cm^{-1} (C-H, aliphatic), 1528 cm^{-1} (C=C, aromatic), 1595 cm^{-1} (C=N), 1242 (C-N), 1265 cm^{-1} (C-O), 865 cm^{-1} (C-Cl); ^{1}H NMR: 7.83 (s, 1H, 3-phenyl), 7.52 (s, 1H, 5-phenyl), 8.42 (s, 1H, CH=N), 3.82 (s, 3H, 2-methoxy), 5.87 (s, 1H, 4- hydroxy), 7.515-7.51 (d, J = 2, 1H, 3-benzylidene), 6.92-6.90 (d, J = 8, 1H, 5- benzylidene), 7.38 (m, 1H, 6-benzylidene);^{13}C NMR: 151.6 (1C-phenyl), 127.9 (2C- phenyl), 127.5 (3C-phenyl), 130.9 (4C- phenyl), 127.4 (5C-phenyl), 125.4 (6C- phenyl), 164.2 (CH=N), 55.9 (3-methoxy), 124.1 (1C-benzylidene), 111.4 (2C- benzylidene), 149.5 (3C- benzylidene), 148.4 (4C-benzylidene), 115.9 (5C- benzylidene), 122.1(6C- benzylidene)

C3	*(2,4,5-Trichloro-phenyl)(3,4,5-trimethoxy-benzylidene)amine*	Yield: 72%; color: light yellow solid; Melting point: 117ºC; Rf value: 0.47**	IR: 3067 cm^{-1} (C-H, aromatic), 2884 cm^{-1} (C-H, aliphatic), 1521 cm^{-1} (C=C, aromatic), 1582 cm^{-1} (C=N), 1237 (C-N), 1255 cm^{-1} (C-O), 878 cm^{-1} (C-Cl); ^{1}H NMR: 7.86 (s, 1H, 3-phenyl), 7.56 (s, 1H, 5-phenyl), 8.49 (s, 1H, CH=N), 3.74 (s, 6H, 3,5-dimethoxy), 3.83 (s, 3H, 4-methoxy), 7.27 (s, 2H, 2,6 – benzylidene);^{13}C NMR: 153.6 (1C-phenyl), 127.3 (2C- phenyl), 131.1 (3C-phenyl), 134.1 (4C- phenyl), 126.4 (5C-phenyl), 122.1 (6C- phenyl), 164.4 (CH=N), 56.2 (3,5-dimethoxy), 60.6(4-methoxy), 128.4 (1C- benzylidene), 106.9(2,6 -benzylidene), 149.1 (3,5-benzylidene), 141.7 (4- benzylidene)
C4	*(2,4,5-Trichloro-phenyl)(3,4-dimethoxy-benzylidene)amine*	Yield: 75%; color: light yellow solid; Melting point: 109ºC; Rf value: 0.43**	IR: 3075 cm^{-1} (C-H, aromatic), 2882 cm^{-1} (C-H, aliphatic), 1526 cm^{-1} (C=C, aromatic), 1597 cm^{-1} (C=N), 1239 (C-N), 1248 cm^{-1} (C-O), 872 cm^{-1} (C-Cl); ^{1}H NMR: 7.84 (s, 1H, 3-phenyl), 7.56 (s, 1H, 5-phenyl), 8.48 (s, 1H, CH=N), 3.83 (s, 6H, 3,4-dimethoxy), 7.52(s,1H,2-benzylidene, 7.11-7.09 (d, J = 8, 1H, 5-benzylidene), 7.48-7.46 (d, J = 8, 1H, 6-benzylidene);^{13}C NMR: 153.1 (1-phenyl), 128.1 (2- phenyl), 128.7 (3- phenyl), 131.0 (4- phenyl), 130.9 (5- phenyl), 124.7 (6-phenyl), 164.1 (CH=N), 55.9 (3-methoxy), 56.1 (4-methoxy), 125.3 (1- benzylidene), 111.8 (2 -benzylidene), 149.3 (3-benzylidene), 149.4 (4- benzylidene), 110.3 (5- benzylidene), 122.1 (6-benzylidene)
C5	*(2,4,5-Trichloro-phenyl)(4-methoxy-benzylidene)amine*	Yield: 67%; color: white solid; Melting point: 98ºC; Rf value: 0.52**	IR: 3088 cm^{-1} (C-H, aromatic), 2887 cm^{-1} (C-H, aliphatic), 1532 cm^{-1} (C=C, aromatic), 1558 cm^{-1} (C=N), 1232 (C-N), 1245 cm^{-1} (C-O), 876 cm^{-1} (C-Cl); ^{1}H NMR: 7.72 (s, 1H, 3-phenyl), 7.48 (s, 1H, 5-phenyl), 8.51 (s, 1H, CH=N), 3.57 (s, 1H, 4- methoxy), 7.81-7.83 (d, J = 8 , 2H, 2,6 -benzylidene), 6.93-6.908 (d, J = 8.8, 2H, 3,5- benzylidene);^{13}C NMR: 149.3 (1-

			phenyl), 127.4 (2- phenyl), 128.5 (3-phenyl), 131.6 (4- phenyl), 131.0 (5-phenyl), 122. (6-phenyl), 163.9 (CH=N), 55.9 (4-methoxy), 123.4 (1-benzylidene), 128.1 (2,6-benzylidene), 114.8 (3,5-benzylidene), 163.1 (4- benzylidene)
C6	*(2,4,5-Trichloro-phenyl)(4-nitro - benzylidene)amine*	Yield: 82%; color: dark yellow solid; Melting point: 64ºC; Rf value: 0.72**	IR: 3064 cm^{-1} (C-H, aromatic), 2896 cm^{-1} (C-H, aliphatic), 1542 cm^{-1} (C=C, aromatic), 1524 cm^{-1} (C=N), 1227 (C-N), 1235 cm^{-1} (C-O), 825 cm^{-1} (C-Cl); ^{1}H NMR: 8.73 (s, 1H, 3-phenyl), 7.44 (s, 1H, 5-phenyl), 8.4 (s, 1H, CH=N), 8.19-8.17 & 8.15-8.13 (dd, *J* = 8 & 8, 2H, 2,6-benzylidene), 8.38-8.37 (d, *J* = 4, 2H, 3,5-benzylidene); ^{13}C NMR: 151.06 (1-phenyl), 115.72 (2- phenyl), 130.38 (3-phenyl), 131.25 (4- phenyl), 122.07 (5-phenyl), 116.93 (6- phenyl), 162.7 (CH=N), 140.5 (1-benzylidene), 130.66 (2,6-benzylidene), 124.71 (3,5-benzylidene), 145.54 (4-benzylidene)
C7	*(2,4,5-Trichloro-phenyl)(4-bromo-benzylidene)amine*	Yield: 75%; color: gray solid; Melting point: 69ºC; Rf value: 0.6**	IR: 3062 cm^{-1} (C-H, aromatic), 2927 cm^{-1} (C-H, aliphatic), 1558 cm^{-1} (C=N), 1532 cm^{-1} (C=C, aromatic), 1257 cm^{-1} (C-N), 826 (C-Cl); ^{1}H NMR: 8.09 (s, 1H, 3-phenyl), 7.87 (s, 1H, 5-phenyl), 8.60 (s, 1H, CH=N), 7.50 (t, 2H, 2,6-benzylidene), 7.76-7.74 (d, *J* = 8, 2H, 3,5- benzylidene); ^{13}C NMR: 148.54 (1-phenyl), 127.72 (2-phenyl), 129.06 (3- phenyl), 131.74 (4-phenyl), 137.92 (5- phenyl), 122.64 (6-phenyl), 163.84 (CH=N), 135.32 (1-benzylidene), 131.61 (2- benzylidene), 122.04 (3- benzylidene), 131.61 (4-benzylidene), 128.67 (5- benzylidene), 131.09 (6- benzylidene)
C8	*(2,4,5-Trichloro-phenyl)(3-methyl-benzylidene)amine*	Yield: 73%; color: gray solid; Melting point: 101ºC; Rf value: 0.53**	IR: 3075 cm^{-1} (C-H, aromatic), 2923 cm^{-1} (C-H, aliphatic), 1541 cm^{-1} (C=N), 1562 cm^{-1} (C=C, aromatic), 1263 cm^{-1} (C-N), 842 (C-Cl); ^{1}H NMR: 7.74 (s, 1H, 3-phenyl), 7.13 (s, 1H, 5-phenyl), 8.32 (s, 1H, CH=N), 2.55 (s, 3H, 3-methyl),

			7.51(s,1H, 2-benzylidene), 7.34-7.33 (d, *J* = 4, 1H, 4- benzylidene), 7.42(m, 1H, 5-benzylidene), 7.65 (t, 1H, 6-benzylidene);^{13}C NMR: 148.78 (1-phenyl), 129.87 (2- phenyl), 135.05 (3- phenyl), 138.78 (4- phenyl), 136.26 (5- phenyl), 121.06 (6- phenyl), 163.39 (CH=N), 21.17 (methyl), 131.16 (1-benzylidene), 130.69 (2- benzylidene), 141.77 (3- benzylidene), 133.17 (4- benzylidene), 128.90 (5-benzylidene), 127.85 (6- benzylidene)
C9	*(2,4,5-Trichloro-phenyl)(4-chloro-benzylidene)amine*	Yield: 80%; color: white solid; Melting point: 104ºC; Rf value: 0.58**	IR: 3067 cm^{-1} (C-H, aromatic), 2884 cm^{-1} (C-H, aliphatic), 1542 cm^{-1} (C=N), 1492 cm^{-1} (C=C, aromatic), 1266 cm^{-1} (C-N), 802 (C-Cl); ^{1}H NMR: 7.85 (s, 1H, 3-phenyl), 7.63 (s, 1H, 5-phenyl), 8.62 (s, 1H, CH=N), 7.94-7.93 (d, *J* = 4, 2H, 2,6-benzylidene), 7.60-7.58 ((d, *J* = 8, 2H, 3,5- benzylidene); ^{13}C NMR: 148.62 (1-phenyl), 127.73 (2-phenyl), 130.38 (3-phenyl), 134.56 (4-phenyl), 131.24 (5-phenyl), 122.01 (6-phenyl), 163.68 (CH=N), 129.55 (1-benzylidene), 131.1 (2,6-benzylidene), 128.87 (3,5-benzylidene), 137.5 (4- benzylidene)
C10	*(2,4,5-Trichloro-phenyl)(2-pyridylidene)amine*	Yield: 67%; color: creamy white solid; Melting point: 108ºC; Rf value: 0.39**	IR: 3094 cm^{-1} (C-H, aromatic), 2873 cm^{-1} (C-H, aliphatic), 1556 cm^{-1} (C=N), 1512 cm^{-1} (C=C, aromatic), 1275 cm^{-1} (C-N), 837 (C-Cl); ^{1}H NMR: 7.69 (s, 1H, 3-phenyl), 7.26 (s, 1H, 5-phenyl), 8.64 (s, 1H, CH=N), 7.954-7.951 (d, *J* = 1.2, 1H, 3-pyridylidene), 7.62 (t, 1H, 4-pyridylidene), 7.17 (t, 1H, ,5-pyridylidene), 7.60-7.58 (d, *J* = 8, 1H, 6-pyridylidene);^{13}C NMR: 138.06 (1-phenyl), 130.39 (2-phenyl), 133.5 (3-phenyl), 134.12 (4-phenyl), 129.4 (5-phenyl), 114.79 (6-phenyl), 155.25 (CH=N), 149.10(1-pyridylidene), 148.2 (3-pyridylidene), 118.5 (4-pyridylidene), 123.18 (5-pyridylidene), 124.62 (6-pyridylidene)
C11	*(2,4,5-Trichloro-*	Yield: 77%; color:	IR: 3082 cm^{-1} (C-H, aromatic), 2868 cm^{-1}

	phenyl)(1-napthylidene)amine	brawn solid; Melting point: 136ºC; Rf value: 0.45**	(C-H, aliphatic), 1541 cm^{-1} (C=N), 1522 cm^{-1} (C=C, aromatic), 1278 cm^{-1} (C-N), 826 (C-Cl); ^{1}H NMR: 7.44 (s, 1H, 3-phenyl), 7.11 (s, 1H, 5-phenyl), 8.41 (s, 1H, CH=N), 8.19-8.17 (d, *J* = 8, 1H, 2-napthylidene), 7.93 (m, 1H, 3-napthylidene), 8.07 (m, 1H, 4-napthylidene), 7.66 (m, 2H, 5,8-napthylidene), 7.43 (m, 2H, 6,7-napthylidene);^{13}C NMR: 149.18 (1-phenyl), 127.91 (2- phenyl), 132.45 (3-phenyl), 133.97 (4- phenyl), 133.50 (5-phenyl), 125.24 (6-phenyl), 164.93 (CH=N), 131.04 (1-napthylidene), 128.37 (2- napthylidene), 126.9(3-napthylidene),130.88(4-napthylidene),131.17(4a-napthylidene), 128.71 (5,8- napthylidene),125.9(6,7-napthylidene), 131.27 (8a- napthylidene)
C12	*2,4,5-Trichloro-phenyl)(4-trifluoromethyl-benzylidene)amine*	Yield: 87%; color: light yellow solid; Melting point: 78ºC; Rf value: 0.48**	IR: 3068 cm^{-1} (C-H, aromatic), 2893 cm^{-1} (C-H, aliphatic), 1542 cm^{-1} (C=N), 1512 cm^{-1} (C=C, aromatic), 1267 cm^{-1} (C-N), 881 (C-Cl); ^{1}H NMR: 7.88 (s, 1H, 3-phenyl), 7.662 (s, 1H, 5-phenyl), 8.716 (s, 1H, CH=N), 7.86-7.851 (d, *J* = 3.6, 2H, 2,6-benzylidene), 7.60-7.58 & 8.129-8.109 (d,d, *J* = 8, 2H, 3,5- benzylidene); ^{13}C NMR: 148.28 (1-phenyl), 125.69 (2-phenyl), 127.87 (3- phenyl), 131.13 (4-phenyl), 130.19 (5- phenyl), 122.98 (6-phenyl), 163.68 (CH=N), 120.27 (trifluromethyl), 139.17 (1-benzylidene), 132.31 (2,6-benzylidene), 126.22 (3,5-benzylidene), 129.26 (4-benzylidene)
C13	*(2,4,5-Trichloro-phenyl)(4-methylsulfanyl-benzylidene)amine*	Yield: 61%; color: light yellow solid; Melting point: 142ºC; Rf value: 0.67**	IR: 3096 cm^{-1} (C-H, aromatic), 2897 cm^{-1} (C-H, aliphatic), 1553 cm^{-1} (C=N), 1502 cm^{-1} (C=C, aromatic), 1259 cm^{-1} (C-N), 878 (C-Cl); ^{1}H NMR: 7.55 (s, 1H, 3-phenyl), 7.17 (s, 1H, 5-phenyl), 8.31 (s, 1H, CH=N), 2.55 (s, 3H, methylsulfanyl), 7.87-7.85 & 7.79-7.77 (dd, *J* = 8 & 8, 2H, 2,6-benzylidene), 7.34 (m, 2H, 3,5-benzylidene); ^{13}C NMR: 147.91 (1-

			phenyl), 129.29 (2- phenyl), 130.94 (3-phenyl), 132.94 (4- phenyl), 131.55 (5-phenyl), 116.32 (6- phenyl), 162.4 (CH=N), 120.93 (methylsulfanyl), 127.07 (1-benzylidene), 130.18 (2,6- benzylidene), 125.57 (3,5- benzylidene), 142.46 (4-benzylidene)
C14	*(2,4,5-Trichloro-phenyl)(4-tert-butyl-benzylidene)amine*	Yield: 58%; color: brown semi solid; Melting point: 71ºC; Rf value: 0.41**	IR: 3076 cm^{-1} (C-H, aromatic), 2919 cm^{-1} (C-H, aliphatic), 1606 cm^{-1} (C=N), 1514 cm^{-1} (C=C, aromatic), 1246 cm^{-1} (C-N), 821 (C-Cl); ^{1}H NMR: 7.45 (s, 1H, 3-phenyl), 6.96 (s, 1H, 5-phenyl), 8.56 (s, 1H, CH=N),1.28 (s, 9H, tert-butyl), 7.882-7.859 & 7.83-7.81 (dd, *J* = 9.2 & 8, 2H, 2,6-benzylidene), 7.5 (m, 2H, 3,5-benzylidene); ^{13}C NMR: 155.97 (1-phenyl), 127.5 (2- phenyl), 130.4 (3-phenyl), 134.36 (4- phenyl), 133.21 (5-phenyl), 122.03 (6- phenyl), 164.58 (CH=N), 31.31, 35.5 (tert-butyl), 128.41 (1-benzylidene), 129.89 (2,6- benzylidene), 126.2 (3,5-benzylidene), 149.23 (4-benzylidene)
C15	*(2,4,5-Trichloro-phenyl)(4-ethyl-benzylidene)amine*	Yield: 47%; color: brown semi solid; Melting point: 66ºC; Rf value: 0.52**	IR: 3094 cm^{-1} (C-H, aromatic), 2886 cm^{-1} (C-H, aliphatic), 1558 cm^{-1} (C=N), 1532 cm^{-1} (C=C, aromatic), 1228 cm^{-1} (C-N), 828 (C-Cl); ^{1}H NMR: 7.33 (s, 1H, 3-phenyl), 7.14 (s, 1H, 5-phenyl), 8.42 (s, 1H, CH=N), 1.3 (t, 3H,methyl), 2.7 (q, 2H, methylene), 7.87-7.85 & 7.82-7.80 (dd, *J* = 8 & 8, 2H, 2,6-benzylidene), 7.34 (m, 2H, 3,5- benzylidene); ^{13}C NMR: 149.24 (1-phenyl), 130.97 (2- phenyl), 131.34 (3- phenyl), 145.52 (4- phenyl), 131.62 (5- phenyl), 127.59 (6- phenyl), 163.69 (CH=N), 15.33, 29.18 (ethyl), 121.86 (1-benzylidene), 130.41 (2-benzylidene), 116.99 (3- benzylidene), 162.39 (4- benzylidene), 115.14 (5-benzylidene), 128.46 (6-benzylidene)
C16	*(2,4,5-Trichloro-phenyl)(4-ethoxy-benzylidene)amine*	Yield: 72%; color: gray solid; Melting point: 83ºC; Rf	IR: 3048 cm^{-1} (C-H, aromatic), 2921 cm^{-1} (C-H, aliphatic), 1601 cm^{-1} (C=N), 1527 cm^{-1} (C=C, aromatic), 1242 cm^{-1} (C-N),

		value: 0.69**	842 (C-Cl); ^{1}H NMR: 7.76 (s, 1H, 3-phenyl), 7.50 (s, 1H, 5-phenyl), 8.46 (s, 1H, CH=N), 1.33 (t, 3H,methyl), 4.1 (q, 2H, methylene), 7.86-7.84 (d, *J* = 8 , 2H, 2,6-benzylidene), 7.029-7.008 (d, *J* = 8.4, 2H,3,5- benzylidene); ^{13}C NMR: 149.24 (1-phenyl), 128.46 (2- phenyl), 131.34 (3-phenyl), 145.52 (4- phenyl), 131.62 (5-phenyl), 127.59 (6- phenyl), 163.69 (CH=N), 14.94 , 63.93 (ethoxy), 121.86 (1-benzylidene), 130.91 (2-benzylidene), 128.56 (3-benzylidene), 162.39 (4-benzylidene), 115.75 (5-benzylidene), 130.41 (6-benzylidene)
C17	*(2,4,5-Trichloro-phenyl)(4-hydroxy-benzylidene)amine*	Yield: 82%; color: white solid; Melting point: 76ºC; Rf value: 0.54**	IR: 3368 cm^{-1} (O-H, aromatic), 3074 cm^{-1} (C-H, aromatic), 2874 cm^{-1} (C-H, aliphatic), 1541 cm^{-1} (C=N), 1524 cm^{-1} (C=C, aromatic), 1256 cm^{-1} (C-N), 864 (C-Cl); ^{1}H NMR: 7.55 (s, 1H, 3-phenyl), 7.18 (s, 1H, 5-phenyl), 8.3 (s, 1H, CH=N), 6.98 (s, 1H, 4- hydroxy), 7.7 (m, 2H,2,6-benzylidene), 6.92-6.90 (d, *J* = 8, 2H, 3,5-benzylidene); ^{13}C NMR: 142.88 (1-phenyl), 128.49 (2- phenyl), 129.69 (3-phenyl), 131.97 (4- phenyl), 131.85 (5-phenyl), 117.61(6- phenyl), 163.43(CH=N), 119.6 (1-benzylidene), 130.73 (2,6-benzylidene), 116.49 (3,5-benzylidene), 163.01 (4-benzylidene)
C18	*(2,4,5-Trichloro-phenyl)(4-methyl-benzylidene)amine*	Yield: 78%; color: white solid; Melting point: 88ºC; Rf value: 0.42**	IR: 3076 cm^{-1} (C-H, aromatic), 2884 cm^{-1} (C-H, aliphatic), 1557 cm^{-1} (C=N), 1537 cm^{-1} (C=C, aromatic), 1234 cm^{-1} (C-N), 854 (C-Cl); ^{1}H NMR: 7.42 (s, 1H, 3-phenyl), 7.11 (s, 1H, 5-phenyl), 8.32 (s, 1H, CH=N), 2.44 (s, 3H,methyl), 7.79-7.77 (d, *J* = 8, 2H, 2,6-benzylidene), 7.34 (m, 2H, 3,5- benzylidene); ^{13}C NMR: 145.62 (1-phenyl), 117.88 (2-phenyl), 130.86 (3- phenyl), 134.17 (4-phenyl), 131.29 (5- phenyl), 116.31 (6-phenyl), 163.04 (CH=N), 21.91 (methyl), 129.37 (1-benzylidene), 129.88 (2,6-benzylidene), 121.20 (3,5-benzylidene), 142.52(4-

			benzylidene)
C19	*(2,4,5-Trichloro-phenyl)(2-napthylidene)amine*	Yield: 84%; color: light yellow solid; Melting point: 166ºC; Rf value: 0.65**	IR: 3087 cm^{-1} (C-H, aromatic), 2896 cm^{-1} (C-H, aliphatic), 1554 cm^{-1} (C=N), 1534 cm^{-1} (C=C, aromatic), 1276 cm^{-1} (C-N), 838 (C-Cl); ^{1}H NMR: 7.48 (s, 1H, 3-phenyl), 6.95 (s, 1H, 5-phenyl), 8.78 (s, 1H, CH=N), 8.4 (m, 1H, 1-napthylidene), 8.05 (m, 1H, 3- napthylidene), 7.9 (m, 1H, 4- napthylidene), 7.72 (m, 2H, 5,8-napthylidene), 7.63 (m, 2H, 6,7-napthylidene);^{13}C NMR: 152.48 (1-phenyl), 126.91 (2- phenyl), 132.45 (3-phenyl), 134.14 (4- phenyl), 133.60 (5-phenyl), 125.28 (6-phenyl), 163.61 (CH=N), 128.27 (1-napthylidene), 128.58 (2- napthylidene), 126.9 (3-napthylidene), 127.88 (4-napthylidene), 135.17 (4a-napthylidene), 128.11 (5,8- napthylidene), 125.9 (6,7-napthylidene), 133.27 (8a-napthylidene)
C20	*(2,4,5-Trichloro-phenyl)(4-iso-propyl-benzylidene)amine*	Yield: 46%; color: white solid; Melting point: 60ºC; Rf value: 0.71**	IR: 3078 cm^{-1} (C-H, aromatic), 2872 cm^{-1} (C-H, aliphatic), 1605 cm^{-1} (C=N), 1522 cm^{-1} (C=C, aromatic), 1256 cm^{-1} (C-N), 841 (C-Cl); ^{1}H NMR: 7.32 (s, 1H, 3-phenyl), 6.85 (s, 1H, 5-phenyl), 8.31 (s, 1H, CH=N), 1.301-1.284 (d, J = 6.8 6H, methyl), 3.01 (m, 1H, CH), 7.40-7.38 (d, J = 8 , 1H, 3-benzylidene), 7.52 (t, 1H, 4-benzylidene), 7.32 (m, 1H,5- benzylidene), 7.83-7.81 (d, J = 8, 1H,6- benzylidene); ^{13}C NMR: 154.79 (1-phenyl), 126.16 (2-phenyl), 131.12 (3- phenyl), 134.66 (4-phenyl), 132.21 (5- phenyl), 124.33 (6-phenyl), 163.48 (CH=N), 23.72, 32.5 (iso-propyl), 128.41 (1-benzylidene), 129.35 (2,6- benzylidene), 126.81 (3,5-benzylidene), 151.23 (4- benzylidene)
C21	*(2,4,5-Trichloro-phenyl)(2-methoxy-4-methoxy-benzylidene)amine*	Yield: 79%; color: light yellow solid; Melting point: 141ºC; Rf value: 0.52**	IR: 3076 cm^{-1} (C-H, aromatic), 2914 cm^{-1} (C-H, aliphatic), 1542 cm^{-1} (C=C, aromatic), 1607 cm^{-1} (C=N), 1238 (C-N), 1248 cm^{-1} (C-O), 878 cm^{-1} (C-Cl); ^{1}H NMR: 7.54 (s, 1H, 3-phenyl), 7.31 (s, 1H, 5-phenyl), 8.47 (s, 1H, CH=N), 3.9 (s, 3H,

				2-methoxy), 3.88 (s, 3H, 4- methoxy), 6.85 (s,1H, 3-benzylidene), 6.544-6.538 (d, *J* = 2, 1H, 5- benzylidene), 7.82-7.80 (d, *J* = 8, 1H, 6- benzylidene);^{13}C NMR: 142.55 (1C-phenyl), 120.78 (2C- phenyl), 122.81 (3C- phenyl), 131.27 (4C- phenyl), 130.12 (5C- phenyl), 119.04 (6C- phenyl), 188.38 (CH=N), 55.98 (methoxy), 116.31 (1C-benzylidene), 163.62 (2C- benzylidene), 97.93 (3C- benzylidene), 166.19 (4C-benzylidene), 105.96 (5C- benzylidene), 117.85 (6C- benzylidene)

**Ethyl acetate: Hexane - 50:50 developing solvent system was used

Supplementary Table 2. Physicochemical and Topological parameters along with log P used in the study

Compd no.	MW (g/mol)	MR (cm³/mol)	VV (Å³)	Pol (Å³)	Polar 2D SA (Å²)	HbA (count)	Log P	BI	Sz	WI	Wp	RI	PI
								(Unit less)					
C1	316.56	79.76	233.69	29.52	52.82	3	5.05	1.6	1158	758	28	8.97	56
C2	330.59	84.25	251.3	31.46	41.82	3	5.2	1.82	1303	866	30	9.51	58
C3	374.64	95.18	295.18	36.72	40.05	4	5.19	1.87	1886	1266	37	10.99	66
C4	344.62	88.73	268.9	33.74	30.82	3	5.34	1.7	1536	1020	32	10.05	60
C5	314.59	82.27	242.95	30.84	21.95	2	5.5	1.53	1214	794	27	9.1	54
C6	329.56	83.13	239.83	30.26	58.18	5	5.6	1.71	1398	921	29	9.47	58
C7	363.46	83.42	234.88	31.05	12.36	2	6.43	1.66	1010	658	25	8.56	52
C8	298.59	80.84	233.69	29.8	12.36	1	6.17	1.66	1010	658	25	8.56	52
C9	319.01	80.61	230.64	30.08	12.36	1	6.26	1.63	1032	669	25	8.56	52
C10	273.54	71.21	200.61	25.61	24.39	2	4.6	1.62	732	450	22	7.66	46
C11	322.61	88.58	248.45	31.97	12.36	1	6.25	1.46	1419	800	32	9.65	62
C12	352.56	81.78	248.5	30.28	12.36	1	6.54	1.64	1584	1050	31	9.77	64
C13	330.66	88.56	252.55	33.08	12.36	1	6.29	1.53	1214	794	27	9.1	54
C14	340.67	94.47	285.13	35.92	12.36	1	7.2	1.64	1584	1050	31	9.77	64
C15	312.62	85.44	250.68	32	12.36	1	6.62	1.53	1214	794	27	9.1	54
C16	328.62	87.01	259.8	33.1	21.59	2	5.86	1.68	1415	938	28	9.6	56
C17	300.56	77.76	225.17	28.69	32.59	2	5.36	1.63	1032	669	25	8.56	52
C18	298.59	80.84	233.47	29.96	12.36	1	6.17	1.63	1032	669	25	8.56	52
C19	322.61	88.43	248.35	32.31	12.36	1	6.21	1.39	1499	840	31	9.63	62
C20	326.64	89.99	267.94	34.03	12.36	1	6.9	1.71	1398	921	29	9.47	58
C21	344.62	88.73	268.92	33.58	30.82	3	5.34	1.73	1500	1002	32	10.05	60

Supplementary Table 3. Effect of 2,4,5-trichloro aniline based Schiff bases on Ammonium-N (NH_4-N) retention (mg/kg),

Sl No.	R	7th days			14th days			21st days			28th days		
		1%	5%	10%	1%	5%	10%	1%	5%	10%	1%	5%	10%
1	2,4-$(OH)_2C_6H_3$	130.0	155.8	183.7	109.6	138.7	159.9	88.9	110.6	139.4	64.1	88.1	114.7
2	2-OCH_3-4-OH C_6H_3	121.4	147.7	173.1	105.0	118.6	144.2	81.7	97.1	124.5	52.8	83.5	101.1
3	3,4,5-$(OCH_3)_3C_6H_2$	138.3	170.4	180.3	111.6	136.5	162.2	90.0	121.5	144.9	66.6	104.5	114.4
4	3,4-$(OCH_3)_2$ C_6H_3	106.3	123.1	169.2	87.6	107.2	143.6	69.2	88.2	116.4	47.3	72.8	89.9
5	4-$OCH_3C_6H_4$	126.4	159.5	184.7	107.8	138.5	160.5	83.4	118.6	138.5	66.5	92.7	114.1
6	4-$NO_2C_6H_4$	111.0	142.4	184.9	83.5	116.6	159.6	62.1	94.7	127.5	47.1	69.6	104.4
7	4-BrC_6H_4	117.9	152.9	178.4	86.6	127.6	150.7	62.1	98.8	123.8	42.0	69.6	88.2
8	3-$CH_3C_6H_4$	101.4	142.8	173.3	83.5	116.6	150.8	66.2	89.1	132.8	53.3	69.8	109.1
9	4-ClC_6H_4	92.8	120.4	164.9	71.0	97.4	147.2	51.1	79.7	113.8	33.1	54.8	85.0
10	2-pyridyl	84.1	115.5	146.2	69.0	90.7	115.0	54.6	71.8	102.6	43.0	62.3	82.5
11	1-Napthyl	97.0	124.3	157.0	84.0	104.3	147.6	65.7	87.4	118.2	55.0	71.1	99.3
12	4-$CF_3C_6H_4$	118.0	150.3	173.8	102.8	123.1	157.4	87.1	104.4	140.0	68.8	87.2	116.6
13	4-$SCH_3C_6H_4$	109.0	142.5	177.8	78.3	118.5	155.7	62.1	90.6	134.5	54.3	74.8	111.1
14	4- $C(CH_3)_3$ C_6H_4	122.4	158.9	172.3	98.1	142.4	156.5	84.4	115.1	139.2	64.6	90.8	113.6
15	4-C_2H_5	138.0	162.5	176.4	117.1	144.6	160.5	93.6	119.1	136.5	73.8	98.8	120.2
16	4-$OC_2H_5C_6H_4$	91.4	118.9	148.3	70.3	99.5	120.5	61.1	84.3	108.9	48.8	76.7	89.3
17	4-OHC_6H_4	112.4	150.0	182.5	96.8	120.0	158.1	81.5	102.0	137.6	63.6	85.6	116.5

18	4-$CH_3C_6H_4$	123.1	158.4	178.2	108.8	141.2	167.0	87.0	112.9	148.8	71.4	94.8	119.6
19	2-Naphthyl	113.7	151.3	174.0	91.6	120.6	154.9	78.7	102.8	140.1	64.3	84.2	117.5
20	4-$(CH_3)_2CH$ C_6H_4	133.9	153.7	169.0	113.5	132.3	153.5	93.1	118.2	132.1	73.8	90.0	112.5
21	2,4-$(OCH_3)_2C_6H_3$	145.1	163.2	172.8	115.5	143.8	152.2	97.8	117.3	139.3	79.1	93.9	115.0
	Nitrapyrin (Positive Control)	160.5	179.8	182.6	144.8	165.1	174.3	129.7	142.4	159.2	110.2	125.5	141.1
	DCD (Positive Control)	130.6	148.3	168.2	110.1	138.5	155.8	93.8	119.8	142.8	70.6	104.4	120.5
	Urea (Negative Control)	91.3			63.3			25.3			8.3		
	CD (5%)	4.8			3.9			7.1			3.3		

Supplementary Table 4. Effect of 2,4,5-trichloro aniline based Schiff bases on Nitrate –N (NO_3^--N) reduction(mg/kg)

Sl No.	R	7th days			14th days			21st days			28th days		
		1%	5%	10%	1%	5%	10%	1%	5%	10%	1%	5%	10%
1	2,4-$(OH)_2C_6H_3$	42.2	19.2	5.8	62.2	44.7	11.4	81.3	57.0	20.8	112.7	85.0	33.2
2	2-OCH_3-4-OH C_6H_3	47.1	19.7	10.5	70.9	45.9	18.0	92.5	67.4	33.0	124.1	93.9	53.0
3	3,4,5-$(OCH_3)_3C_6H_2$	38.2	17.6	8.5	58.5	28.6	16.0	78.9	60.8	26.7	97.0	77.0	37.0
4	3,4-$(OCH_3)_2$ C_6H_3	51.8	33.3	17.0	76.3	53.0	29.0	94.2	74.2	44.9	123.5	98.8	63.2
5	4-$OCH_3C_6H_4$	42.2	17.0	6.1	62.1	36.4	16.6	82.4	60.7	28.7	110.8	81.5	50.0
6	4-$NO_2C_6H_4$	30.5	15.6	6.1	55.7	35.4	12.9	84.1	51.8	24.6	108.8	73.5	47.9
7	4-BrC_6H_4	35.2	17.1	13.0	71.3	52.7	29.8	97.1	71.1	45.7	112.3	90.9	61.8
8	3-$CH_3C_6H_4$	46.6	26.2	6.9	59.5	38.8	16	85.8	64.3	35.4	113.7	93.0	64.9

9	4-ClC_6H_4	55.0	32.4	14.8	81.8	57.5	28.5	110.6	82.9	53.3	137.0	107.0	84.2
10	2-pyridyl	64.0	40.7	18.8	87.1	63.4	31.6	102.9	86.3	57.5	126.2	106.1	80.2
11	1-Napthyl	52.3	34.7	16.5	80.3	56.8	34.8	104.3	85.0	55.2	123.6	104.8	78.6
12	4-$CF_3C_6H_4$	40.5	19.1	4.4	67.6	37.0	17.6	93.9	68.7	37.3	117.3	91.5	62.2
13	4-$SCH_3C_6H_4$	54.4	34.5	14.8	79.6	54.4	29.9	103.5	79.0	51.2	126.6	100.3	77.3
14	4- $C(CH_3)_3$ C_6H_4	37.8	17.1	11.5	57.3	38.1	19.5	78.6	49.7	32.0	109.3	81.2	42.1
15	4-C_2H_5	30.3	14.8	5.7	51.0	29.9	15.7	84.0	60.8	28.2	110.0	83.2	46.7
16	4-$OC_2H_5C_6H_4$	80.0	55.6	23.9	101.4	79.4	43.3	126.9	102.7	67.2	137.3	116.1	91.1
17	4-OHC_6H_4	34.7	20.3	8.0	58.9	37.1	17.3	80.6	57.5	38.1	99.9	73.3	56.2
18	4-$CH_3C_6H_4$	32.6	18.4	6.3	53.3	34.4	13.5	81.6	56.0	27.3	103.2	74.3	48.2
19	2-Naphthyl	39.6	20.7	8.1	65.7	40.6	19.8	92.9	61.4	42.0	109.6	86.9	70.9
20	4-$(CH_3)_2CH$ C_6H_4	24.8	11.3	11.2	46.8	23.0	18.6	65.4	45.5	27.4	92.8	66.0	41.7
21	2,4-$(OCH_3)_2C_6H_3$	22.8	9.5	10.4	40.5	24.2	21.4	64.2	45.6	35.4	92.6	66.8	50.2
	Nitrapyrin (Positive Control)	21.6	7.6	2.3	35.3	21.6	10.4	54.1	35.8	18.0	68.0	51.5	29.3
	DCD (Positive Control)	40.8	22.4	7.1	63.6	40.0	40.0	82.9	57.4	57.4	109.4	72.3	72.3
	Urea (Negative Control)	86.4			113.6			139.5			165.1		
	CD (5%)	2.7			5.3			2.9			3.1		

Supplementary Table 5. Pait t-test within the treatment concentration

Treatment Pair	t-test value	D.F.	H0: 1per>5per	P-value
1per-5per	-30.59	21	Reject H0 (1per>5per)	<0.001
1per-10per	-30.61	21	Reject H0 (1per>10per)	<0.001
5per-10per	-21.77	21	Reject H0 (5per>10per)	<0.001

Supplementary Table 6. Summary of Stepwise regression model based on three treatment concentration

Parameter	Estimate	S.E.	t-value	p-value
At 2.5% treatment dose				
Intercept	-29.87	29.96	-1.00	0.34
VV	1.82	0.73	2.49	0.03*
Pol	-10.89	4.52	-2.41	0.03*
Sz	-0.04	0.02	-1.71	0.11
At 5% treatment dose				
Intercept	48.37	76.50	0.63	0.55
MW	0.22	0.17	1.34	0.22
VV	4.43	1.46	3.03	0.02*
Pol	-30.32	10.32	-2.94	0.02*
Polar.2D.SA	0.60	0.25	2.45	0.04*
Log.P	23.03	10.38	2.22	0.06
BI	-57.39	33.49	-1.71	0.13
WI	-0.09	0.05	-1.71	0.13
Wp	8.29	4.52	1.84	0.11
PI	-7.71	3.51	-2.20	0.06
At 10% treatment dose				
Intercept	-401.70	180.30	-2.23	0.07
MR	-56.96	10.61	-5.37	0.00**
VV	13.07	2.23	5.87	0.00**
Pol	33.86	11.15	3.04	0.02*
HbA	56.15	9.71	5.78	0.00**

Log.P	94.31	16.90	5.58	0.00**
Sz	0.89	0.18	5.03	0.00**
WI	-2.13	0.39	-5.48	0.00**
Wp	-11.94	6.40	-1.87	0.11
RI	88.94	30.65	2.90	0.03*
PI	7.73	2.90	2.67	0.04*

Supplementary Table 7. Hyperparameters of the random forest models based on three treatment concentration

At 2.5% treatment dose	Type of random forest	Regression
	Number of trees (ntree)	500
	No. of variables tried at each split (mtry)	4
	Mean of squared residuals	88.62
At 5% treatment dose	Type of random forest	Regression
	Number of trees (ntree)	500
	No. of variables tried at each split (mtry)	4
	Mean of squared residuals	80.92
At 10% treatment dose	Type of random forest	Regression
	Number of trees (ntree)	500
	No. of variables tried at each split (mtry)	4
	Mean of squared residuals	107.84

Supplementary Table 8. Hyperparameters of the SVR models based on three treatment concentration

Treatment concentration	Type	Kernel	Cost (C)	Gamma	Epsilon (ε)	No. of Support Vectors
At 2.5%	eps-regression	radial	1	0.25	0.1	15

At 5%	eps-regression	radial	1	0.25	0.1	16
At 10%	eps-regression	radial	1	0.25	0.1	16

Supplementary Table 9. Predictive abilities of different models in terms of RMSE for nitrification inhabitation activity

Model	Nitrification inhabitation activity at 1% of treatment dose		Nitrification inhabitation activity at 5% of treatment dose		Nitrification inhabitation activity at 10% of treatment dose	
	RMSE		RMSE		RMSE	
	Training	Testing	Training	Testing	Training	Testing
Stepwise Regression	5.62	11.67	4.16	18.66	2.83	69.16
Random Forest	4.34	5.22	4.04	8.83	4.88	7.47
SVR	6.08	4.7	6.13	8.21	6.01	7.94
ANN	0.02	1.13	0.07	2.23	0.07	2.56