Supporting Information

Modified Pyridine Substituted Coumarins – A New Class of Antimicrobial and Antitubercular Agents

Rakesh R. Giri, Hemali B. Lad, Varun G. Bhila, Chirag V. Patel and D. I. Brahmabhatt*

Department of Chemistry, Sardar Patel University, Vallabh Vidyanagar 388120, Gujarat, India

E-mail: drdib317@gmail.com

Spectral and analytical data of compounds 7a-f:

4-Methyl-3-phenyl-6-(4-phenyl-5H-indeno[1,2-b]pyridin-2-yl)coumarin (7a): IR (KBr, $\nu_{\max}$, cm^{-1}): 700 and 746(C-H bending of mono substituted benzene ring), 1439(C=N aromatic stretching), 1612(C=C aromatic stretching), 1709(C=O δ -lactone stretching), 2919(C-H aliphatic stretching), 3052(C-H aromatic stretching); ^1H NMR (400MHz, CDCl_3 , δ): 2.48(3H, s, CH_3), 4.04(2H, s, C_5' protons), 7.28-7.71(15H, m, Ar-H), 8.29(1H, concealed dd, C_9' -H), 8.33(1H, dd, $J = 2.0$ and 8.8 Hz, C_7 -H), 8.52(1H, d, $J = 2.0$ Hz, C_5 -H); ^{13}C NMR (100MHz, CDCl_3 , δ): 16.80(CH_3), 34.45(CH_2), 117.14(CH), 117.93(CH), 120.78(C), 121.40(CH), 123.86(CH), 125.06(CH), 127.32(CH), 127.54(C), 128.23(CH), 128.25(CH), 128.46(CH), 128.77(CH), 128.98(CH), 129.01(CH), 130.11(CH), 130.17(CH), 133.30(C), 134.51(C), 136.09(C), 138.65(C), 140.86(C), 144.20(C), 146.73(C), 147.97(C), 153.12(C), 155.59(C), 161.35 (δ -lactone CO); Anal. Calcd. for $\text{C}_{34}\text{H}_{23}\text{NO}_2$: C, 85.51; H, 4.85; N, 2.93%. Found: C, 85.38; H, 5.01; N, 2.87%.

4-Methyl-3-phenyl-6-(4-(4-methylphenyl)-5H-indeno[1,2-b]pyridin-2-yl)coumarin (7b): IR (KBr, $\nu_{\max}$, cm^{-1}): 833(C-H bending of p-disubstituted benzene ring), 1443(C=N aromatic

stretching), 1606(C=C aromatic stretching), 1704(C=O δ -lactone stretching), 2918(C-H aliphatic stretching), 3050(C-H aromatic stretching); ^1H NMR (400MHz, CDCl_3 , δ): 2.49 and 2.50(6H, 2s, 2 x CH_3), 4.06(2H, s, C_5' protons), 7.37-7.71(14H, m, Ar-H), 8.28(1H, concealed dd, C_9' -H), 8.34(1H, dd, $J = 1.6$ and 8.4 Hz, C_7 -H), 8.55(1H, d, $J = 1.6$ Hz, C_5 -H); ^{13}C NMR (100MHz, CDCl_3 , δ): 16.79(CH_3), 21.35(CH_3), 34.51(CH_2), 117.02(CH), 117.23(CH), 117.80(CH), 117.88(CH), 120.74(C), 121.37(CH), 123.72(CH), 123.93(CH), 124.97(CH), 125.06(CH), 127.28(C), 128.12(CH), 128.20(CH), 128.44(CH), 130.14(CH), 133.20(C), 134.52(C), 135.70(C), 136.19(C), 138.83(C), 140.92(C), 144.20(C), 146.62(C), 148.02(C), 153.07(C), 155.54(C), 160.93(C), 161.31 (δ -lactone CO); Anal. Calcd. for $\text{C}_{35}\text{H}_{25}\text{NO}_2$: C, 85.52; H, 5.13; N, 2.85%. Found: C, 85.43; H, 5.29; N, 2.77%.

4-Methyl-3-phenyl-6-(4-(4-methoxyphenyl)-5H-indeno[1,2-b]pyridin-2-yl)coumarin (7c): IR (KBr, ν_{max} , cm^{-1}): 826(C-H bending of p-disubstituted benzene ring), 1439(C=N aromatic stretching), 1609(C=C aromatic stretching), 1712(C=O δ -lactone stretching), 2918(C-H aliphatic stretching), 3052(C-H aromatic stretching); ^1H NMR (400MHz, CDCl_3 , δ): 2.49(3H, s, CH_3), 3.93(3H, s, OCH_3), 4.06(2H, s, C_5' protons), 7.10-7.69(14H, m, Ar-H), 8.28(1H, concealed dd, C_9' -H), 8.33(1H, dd, $J = 2.0$ and 8.8 Hz, C_7 -H), 8.55(1H, d, $J = 2.0$ Hz, C_5 -H); ^{13}C NMR (100MHz, CDCl_3 , δ): 16.81(CH_3), 34.63(CH_2), 55.48(OCH_3), 114.40(CH), 117.13(CH), 117.70(CH), 120.77(C), 121.43(CH), 123.88(CH), 125.05(CH), 127.28(CH), 127.53(C), 128.25(CH), 128.47(CH), 128.91(CH), 129.53(CH), 130.11(CH), 130.90(C), 133.04(C), 134.52(C), 136.28(C), 140.96(C), 144.18(C), 146.30(C), 148.00(C), 153.09(C), 155.61(C), 160.11(C), 160.93(C), 161.35 (δ -lactone CO); Anal. Calcd. for $\text{C}_{35}\text{H}_{25}\text{NO}_3$: C, 82.82; H, 4.96; N, 2.76%. Found: C, 82.66; H, 5.10; N, 2.71%.

4-Methyl-3-phenyl-6-(4-(4-fluorophenyl)-5H-indeno[1,2-b]pyridin-2-yl)coumarin (7d): IR (KBr, $\nu_{\max}$, cm^{-1}): 826(C-H bending of p-disubstituted benzene ring), 1439(C=N aromatic stretching), 1609(C=C aromatic stretching), 1704(C=O δ -lactone stretching), 2919(C-H aliphatic stretching), 3047(C-H aromatic stretching); ^1H NMR (400MHz, CDCl_3 , δ): 2.49(3H, s, CH_3), 4.03(2H, s, C_5' protons), 7.26-7.70(14H, m, Ar-H), 8.28(1H, concealed dd, C_9' -H), 8.33(1H, dd, $J = 2.0$ and 8.4 Hz, C_7 -H), 8.56(1H, d, $J = 2.0$ Hz, C_5 -H); ^{13}C NMR (100MHz, CDCl_3 , δ): 16.81(CH_3), 34.44(CH_2), 115.94(CH), 116.15(CH), 117.19(CH), 117.78(CH), 120.82(C), 121.43(CH), 123.87(CH), 125.09(CH), 127.37(CH), 127.59(C), 128.26(CH), 128.47(CH), 129.08(CH), 129.97(CH), 130.08(CH), 130.14(CH), 133.18(C), 134.49(C), 134.68(C), 135.60(C), 136.04(C), 140.76(C), 144.14(C), 145.69(C), 147.99(C), 152.84(C), 153.15(C), 155.77(C), 160.86(C), 161.49(C), 161.81 (δ -lactone CO); Anal. Calcd. for $\text{C}_{34}\text{H}_{22}\text{FNO}_2$: C, 82.41; H, 4.47; N, 2.83%. Found: C, 82.35; H, 4.32; N, 2.89%.

4-Methyl-3-phenyl-6-(4-(4-chlorophenyl)-5H-indeno[1,2-b]pyridin-2-yl)coumarin (7e): IR (KBr, $\nu_{\max}$, cm^{-1}): 824(C-H bending of p-disubstituted benzene ring), 1441(C=N aromatic stretching), 1604(C=C aromatic stretching), 1710(C=O δ -lactone stretching), 2918(C-H aliphatic stretching), 3056(C-H aromatic stretching); ^1H NMR (400MHz, CDCl_3 , δ): 2.48(3H, s, CH_3), 4.01(2H, s, C_5' protons), 7.28-7.66(14H, m, Ar-H), 8.28(1H, concealed dd, C_9' -H), 8.32(1H, dd, $J = 2.0$ and 8.4 Hz, C_7 -H), 8.55(1H, d, $J = 2.0$ Hz, C_5 -H); ^{13}C NMR (100MHz, CDCl_3 , δ): 16.79(CH_3), 34.36(CH_2), 117.45(CH), 117.72(CH), 120.82(C), 121.52(CH), 123.87(CH), 124.96(CH), 125.28(CH), 127.61(C), 128.35(CH), 128.56(CH), 129.06(CH), 129.39(CH), 129.69(CH), 130.19(CH), 130.48(CH), 133.07(C), 134.47(C), 134.94(C), 135.95(C), 137.04(C), 140.76(C), 144.03(C), 145.50(C), 147.91(C), 153.18(C), 155.78(C), 160.86(C), 161.56 (δ -lactone CO); Anal. Calcd. for $\text{C}_{34}\text{H}_{22}\text{ClNO}_2$: C, 79.76; H, 4.33; N, 2.74%. Found: C, 79.68; H, 4.45; N, 2.58%.

4-Methyl-3-phenyl-6-(4-(3,4-dimethoxyphenyl)-5H-indeno[1,2-b]pyridin-2-yl)coumarin (7f): IR (KBr, $\nu_{\max}$, cm^{-1}): 830(C-H bending of trisubstituted benzene ring), 1440(C=N aromatic stretching), 1608(C=C aromatic stretching), 1709(C=O δ -lactone stretching), 2929(C-H aliphatic stretching), 3052(C-H aromatic stretching); ^1H NMR (400MHz, CDCl_3 , δ): 2.48(3H, s, CH_3), 4.01(6H, s, 2 x OCH_3), 4.05(2H, s, C_5' protons), 7.06-7.69(13H, m, Ar-H), 8.28(1H, concealed dd, C_9' -H), 8.32(1H, dd, $J = 2.0$ and 8.8 Hz, C_7 -H), 8.56(1H, d, $J = 2.0$ Hz, C_5 -H); ^{13}C NMR (100MHz, CDCl_3 , δ): 16.81(CH_3), 34.64(CH_2), 56.08(OCH_3), 56.20(OCH_3), 111.45(CH), 117.10(CH), 117.68(CH), 120.79(C), 120.96(CH), 121.32(CH), 121.44(CH), 123.88(CH), 127.32(CH), 127.54(C), 128.27(CH), 128.47(CH), 128.96(CH), 129.70(CH), 130.10(CH), 130.20(CH), 131.27(C), 133.07(C), 134.49(C), 136.20(C), 140.94(C), 144.11(C), 146.57(C), 147.98(C), 149.31(C), 149.65(C), 153.10(C), 155.63(C), 160.90(C), 161.37 (δ -lactone CO); Anal. Calcd. for $\text{C}_{36}\text{H}_{27}\text{NO}_4$: C, 80.43; H, 5.06; N, 2.61%. Found: C, 80.51; H, 5.14; N, 2.49%.

Spectral and analytical data of compounds 8a-f:

4-Methyl-3-phenyl-6-(1-phenyl-9,10-dihydro-4-aza-phenanthren-3-yl)coumarin (8a): IR (KBr, $\nu_{\max}$, cm^{-1}): 700 and 752(C-H bending of mono substituted benzene ring), 1544(C=N aromatic stretching), 1608(C=C aromatic stretching), 1721(C=O δ -lactone stretching), 2919(C-H aliphatic stretching), 3053(C-H aromatic stretching); ^1H NMR (400MHz, CDCl_3 , δ): 2.47(3H, s, CH_3), 2.89-3.00(4H, m, C_9' and C_{10}' protons), 7.27-7.65(15H, m, Ar-H), 8.37(1H, dd, $J = 1.6$ and 8.4 Hz, C_7 -H), 8.53(1H, d, $J = 1.6$ Hz, C_5 -H), 8.58(1H, concealed dd, C_5' -H); ^{13}C NMR (100MHz, CDCl_3 , δ): 16.81(CH_3), 25.30(CH_2), 28.11(CH_2), 117.12(CH), 119.66(CH), 120.69(C), 123.39(CH), 125.61(CH), 127.14(CH), 127.52(CH), 127.63(C), 128.21(CH), 128.25(CH), 128.40(C), 128.45(CH), 128.58(CH), 128.78(CH), 129.32(CH), 129.90(CH), 130.10(CH),

134.53(C), 134.96(C), 135.91(C), 138.31(C), 139.14(C), 147.95(C), 149.62(C), 152.85(C), 153.00(C), 153.11(C), 160.92 (δ -lactone CO); Anal. Calcd. for $C_{35}H_{25}NO_2$: C, 85.52; H, 5.13; N, 2.85%. Found: C, 85.38; H, 5.18; N, 2.81%.

4-Methyl-3-phenyl-6-(1-(4-methylphenyl)-9,10-dihydro-4-aza-phenanthren-3-yl)coumarin (8b):

IR (KBr, $\nu_{\max}$, cm^{-1}): 828(C-H bending of p-disubstituted benzene ring), 1538(C=N aromatic stretching), 1613(C=C aromatic stretching), 1721(C=O δ -lactone stretching), 2928(C-H aliphatic stretching), 3053(C-H aromatic stretching); ^1H NMR (400MHz, CDCl_3 , δ): 2.46 and 2.48(6H, 2 s, 2 x CH_3), 2.88-3.01(4H, m, C_9' and C_{10}' protons), 7.26-7.64(14H, m, Ar-H), 8.37(1H, dd, $J = 1.6$ and 8.8 Hz, C_7 -H), 8.52(1H, d, $J = 1.6$ Hz, C_5 -H), 8.57(1H, concealed dd, C_5' -H); ^{13}C NMR (100MHz, CDCl_3 , δ): 16.80(CH_3), 21.30(CH_3), 25.33(CH_2), 28.13(CH_2), 117.12(CH), 119.78(CH), 120.69(C), 123.41(CH), 125.63(CH), 127.14(CH), 127.51(C), 127.61(CH), 128.25(CH), 128.45(CH), 128.50(C), 128.70(CH), 129.27(CH), 129.31(CH), 129.93(CH), 130.10(CH), 134.52(C), 134.90(C), 135.84(C), 136.14(C), 138.18(C), 138.32(C), 147.95(C), 149.68(C), 152.78(C), 152.92(C), 153.10(C), 160.91 (δ -lactone CO); Anal. Calcd. for $C_{36}H_{27}NO_2$: C, 85.52; H, 5.38; N, 2.77%. Found: C, 85.43; H, 5.49; N, 2.71%.

4-Methyl-3-phenyl-6-(1-(4-methoxyphenyl)-9,10-dihydro-4-aza-phenanthren-3-yl)coumarin (8c):

IR (KBr, $\nu_{\max}$, cm^{-1}): 831(C-H bending of p-disubstituted benzene ring), 1541(C=N aromatic stretching), 1609(C=C aromatic stretching), 1719(C=O δ -lactone stretching), 2930(C-H aliphatic stretching), 3056(C-H aromatic stretching); ^1H NMR (400MHz, CDCl_3 , δ): 2.47(3H, s, CH_3), 2.90-3.00(4H, m, C_9' and C_{10}' protons), 3.92 (3H, s, OCH_3), 7.06-7.63(14H, m, Ar-H), 8.36(1H, dd, $J = 1.6$ and 8.4 Hz, C_7 -H), 8.52(1H, d, $J = 1.6$ Hz, C_5 -H), 8.56(1H, concealed dd, C_5' -H); ^{13}C NMR (100MHz, CDCl_3 , δ): 16.77(CH_3), 25.38(CH_2), 28.16(CH_2), 55.52(OCH_3), 114.00(CH), 117.09(CH), 119.82(CH), 120.69(C), 123.31(C), 123.43(CH), 125.51(C), 125.64(CH),

127.15(CH), 127.59(CH), 128.25(CH), 128.45(CH), 129.32(CH), 129.92(CH), 130.07(CH), 130.09(CH), 131.29(C), 134.51(C), 134.93(C), 135.87(C), 138.30(C), 147.96(C), 149.35(C), 152.80(C), 152.93(C), 153.08(C), 159.66(C), 160.93 (δ -lactone CO); Anal. Calcd. for $C_{36}H_{27}NO_3$: C, 82.90; H, 5.22; N, 2.69%. Found: C, 82.81; H, 5.19; N, 2.74%.

4-Methyl-3-phenyl-6-(1-(4-fluorophenyl)-9,10-dihydro-4-aza-phenanthren-3-yl)coumarin (8d):

IR (KBr, $\nu_{\max}$, cm^{-1}): 833(C-H bending of p-disubstituted benzene ring), 1544(C=N aromatic stretching), 1607(C=C aromatic stretching), 1724(C=O δ -lactone stretching), 2922(C-H aliphatic stretching), 3054(C-H aromatic stretching); ^1H NMR (400MHz, CDCl_3 , δ): 2.47(3H, s, CH_3), 2.91-2.96(4H, m, C_9' and C_{10}' protons), 7.21-7.61(14H, m, Ar-H), 8.35(1H, dd, $J = 2.0$ and 8.4 Hz, C_7 -H), 8.53(1H, d, $J = 2.0$ Hz, C_5 -H), 8.57(1H, concealed dd, C_5' -H); ^{13}C NMR (100MHz, CDCl_3 , δ): 16.83(CH_3), 25.28(CH_2), 28.06(CH_2), 115.65(CH), 117.13(CH), 119.63(CH), 120.73(C), 123.31(CH), 123.56(CH), 125.51(CH), 125.78(CH), 127.20(CH), 127.56(C), 128.28(CH), 128.40(C), 128.46(CH), 129.44(CH), 129.75(CH), 129.94(CH), 130.09(CH), 130.57(CH), 134.47(C), 134.78(C), 135.01(C), 135.68(C), 138.22(C), 147.89(C), 148.65(C), 152.94(C), 153.06(C), 153.14(C), 160.87(C), 161.47(C), 163.93 (δ -lactone CO); Anal. Calcd. for $C_{35}H_{24}FNO_2$: C, 82.50; H, 4.75; N, 2.75%. Found: C, 82.37; H, 4.65; N, 2.81%.

4-Methyl-3-phenyl-6-(1-(4-chlorophenyl)-9,10-dihydro-4-aza-phenanthren-3-yl)coumarin (8e):

IR (KBr, $\nu_{\max}$, cm^{-1}): 828(C-H bending of p-disubstituted benzene ring), 1539(C=N aromatic stretching), 1607(C=C aromatic stretching), 1713(C=O δ -lactone stretching), 2944(C-H aliphatic stretching), 3054(C-H aromatic stretching); ^1H NMR (400MHz, CDCl_3 , δ): 2.46(3H, s, CH_3), 2.88-2.97(4H, m, C_9' and C_{10}' protons), 7.27-7.59(14H, m, Ar-H), 8.35(1H, dd, $J = 2.0$ and 8.8 Hz, C_7 -H), 8.52(1H, d, $J = 2.0$ Hz, C_5 -H), 8.56(1H, concealed dd, C_5' -H); ^{13}C NMR (100MHz, CDCl_3 , δ): 16.77(CH_3), 25.26(CH_2), 28.03(CH_2), 117.14(CH), 119.32(CH), 120.73(C),

123.25(CH), 123.56(CH), 125.47(CH), 125.80(CH), 127.21(CH), 127.52(C), 127.57(C), 127.79(C), 128.23(CH), 128.46(CH), 128.84(CH), 129.45(CH), 129.73(CH), 129.98(CH), 134.41(C), 134.47(C), 134.78(C), 135.66(C), 137.46(C), 138.20(C), 147.88(C), 148.40(C), 153.00(C), 153.13(C), 160.86 (δ -lactone CO); Anal. Calcd. for $C_{35}H_{24}ClNO_2$: C, 79.92; H, 4.60; N, 2.66%. Found: C, 79.79; H, 4.55; N, 2.52%.

4-Methyl-3-phenyl-6-(1-(3,4-dimethoxyphenyl)-9,10-dihydro-4-aza-phenanthren-3-yl)coumarin

(8f): IR (KBr, $\nu_{\max}$, cm^{-1}): 832(C-H bending of trisubstituted benzene ring), 1542(C=N aromatic stretching), 1609(C=C aromatic stretching), 1714(C=O δ -lactone stretching), 2919(C-H aliphatic stretching), 3059(C-H aromatic stretching); ^1H NMR (400MHz, CDCl_3 , δ): 2.47(3H, s, CH_3), 2.89-3.02(4H, m, C_9' and C_{10}' protons), 6.96-7.64(13H, m, Ar-H), 8.36(1H, dd, $J = 1.6$ and 8.4 Hz, C_7 -H), 8.54(1H, d, $J = 1.6$ Hz, C_5 -H), 8.56(1H, concealed dd, C_5' -H); ^{13}C NMR (100MHz, CDCl_3 , δ): 16.80(CH_3), 25.44(CH_2), 28.19(CH_2), 56.07(OCH_3), 56.11(OCH_3), 111.20(CH), 112.12(CH), 117.10(CH), 119.68(CH), 120.71(C), 121.28(CH), 123.43(CH), 125.62(CH), 127.14(CH), 127.53(CH), 127.63(C), 128.21(CH), 128.25(CH), 128.40(C), 128.45(CH), 128.58(CH), 128.78(CH), 129.32(CH), 129.90(CH), 130.10(CH), 134.53(C), 134.96(C), 135.91(C), 138.31(C), 139.14(C), 147.95(C), 149.62(C), 152.85(C), 153.00(C), 153.11(C), 160.92 (δ -lactone CO); Anal. Calcd. for $C_{37}H_{29}\text{NO}_4$: C, 80.56; H, 5.30; N, 2.54%. Found: C, 80.48; H, 5.47; N, 2.41%.

Spectral and analytical data of compounds 9a-f:

4-Methyl-3-phenyl-6-(4-phenyl-benzofuro[3,2-b]pyridin-2-yl)coumarin (9a): IR (KBr, $\nu_{\max}$, cm^{-1}): 700 and 752(C-H bending of mono substituted benzene ring), 1464(C=N aromatic stretching), 1609(C=C aromatic stretching), 1715(C=O δ -lactone stretching), 2921(C-H aliphatic stretching), 3055(C-H aromatic stretching); ^1H NMR (400MHz, CDCl_3 , δ): 2.47(3H, s, CH_3), 7.29-7.71(15H,

m, Ar-H), 8.29(1H, dd, $J = 1.6$ and 8.4 Hz, C₇-H), 8.35(1H, concealed dd, C₉'-H), 8.55(1H, d, $J = 1.6$ Hz, C₅-H); ¹³C NMR (100MHz, CDCl₃, δ): 16.82(CH₃), 117.21(CH), 117.96(CH), 120.82(C), 121.45(CH), 123.93(CH), 125.11(CH), 127.37(CH), 127.58(C), 128.24(CH), 128.29(CH), 128.49(CH), 128.86(CH), 129.00(CH), 129.08(CH), 130.14(CH), 130.21(CH), 133.33(C), 134.54(C), 136.11(C), 138.69(C), 140.93(C), 144.25(C), 146.77(C), 147.97(C), 153.17(C), 155.65(C), 161.51 (δ -lactone CO); Anal. Calcd. for C₃₃H₂₁NO₃: C, 82.66; H, 4.41; N, 2.92%. Found: C, 82.49; H, 4.32; N, 2.81%.

4-Methyl-3-phenyl-6-(4-(4-methylphenyl)-benzofuro[3,2-b]pyridin-2-yl)coumarin (9b): IR (KBr, $\nu_{\max}$, cm⁻¹): 818(C-H bending of p-disubstituted benzene ring), 1463(C=N aromatic stretching), 1609(C=C aromatic stretching), 1712(C=O δ -lactone stretching), 2917(C-H aliphatic stretching), 3053(C-H aromatic stretching); ¹H NMR (400MHz, CDCl₃, δ): 2.50-2.51(6H, 2 s, 2 x CH₃), 7.37-8.01(14H, m, Ar-H), 8.30(1H, dd, $J = 2.0$ and 8.4 Hz, C₇-H), 8.38(1H, concealed dd, C₉'-H), 8.52(1H, d, $J = 2.0$ Hz, C₅-H); ¹³C NMR (100MHz, CDCl₃, δ): 16.81(CH₃), 21.45(CH₃), 112.19(CH), 112.42(CH), 116.98(CH), 117.16(CH), 120.80(C), 121.51(CH), 121.57(CH), 121.63(CH), 123.43(C), 123.87(CH), 123.96(CH), 127.55(C), 128.58(CH), 128.75(CH), 129.80(CH), 130.11(CH), 130.93(C), 132.83(C), 134.49(C), 136.03(C), 139.82(C), 145.01(C), 146.59(C), 147.95(C), 152.64(C), 152.93(C), 157.89(C), 160.86 (δ -lactone CO); Anal. Calcd. for C₃₄H₂₃NO₃: C, 82.74; H, 4.70; N, 2.84%. Found: C, 82.45; H, 4.62; N, 2.73%.

4-Methyl-3-phenyl-6-(4-(4-methoxyphenyl)-benzofuro[3,2-b]pyridin-2-yl)coumarin (9c): IR (KBr, $\nu_{\max}$, cm⁻¹): 827(C-H bending of p-disubstituted benzene ring), 1466(C=N aromatic stretching), 1609(C=C aromatic stretching), 1711(C=O δ -lactone stretching), 2918(C-H aliphatic stretching), 3053(C-H aromatic stretching); ¹H NMR (400MHz, CDCl₃, δ): 2.50(3H, s, CH₃), 3.95(3H, s, OCH₃), 7.15-8.10(14H, m, Ar-H), 8.29(1H, dd, $J = 2.0$ and 8.4 Hz, C₇-H), 8.37(1H,

concealed dd, C₉'-H), 8.51(1H, d, J = 2.0 Hz, C₅-H); ¹³C NMR (100MHz, CDCl₃, δ): 16.84(CH₃), 55.51(OCH₃), 112.31(CH), 114.58(CH), 116.84(CH), 117.20(CH), 120.88(C), 121.61(CH), 123.49(C), 123.64(CH), 124.03(CH), 126.13(C), 127.62(C), 128.28(CH), 128.47(CH), 129.35(CH), 130.10(CH), 130.16(CH), 130.28(CH), 132.77(C), 134.52(C), 136.25(C), 144.72(C), 146.56(C), 147.95(C), 152.86(C), 153.00(C), 157.94(C), 160.81(C), 160.92 (δ-lactone CO); Anal. Calcd. for C₃₄H₂₃NO₄: C, 80.14; H, 4.55; N, 2.75%. Found: C, 80.21; H, 4.49; N, 2.69%.

4-Methyl-3-phenyl-6-(4-(4-fluorophenyl)-benzofuro[3,2-b]pyridin-2-yl)coumarin (9d): IR (KBr, ν_{max}, cm⁻¹): 826(C-H bending of p-disubstituted benzene ring), 1465(C=N aromatic stretching), 1607(C=C aromatic stretching), 1713(C=O δ-lactone stretching), 2919(C-H aliphatic stretching), 3053(C-H aromatic stretching); ¹H NMR (400MHz, CDCl₃, δ): 2.48(3H, s, CH₃), 7.25-7.71(14H, m, Ar-H), 8.29(1H, dd, J = 2.0 and 8.8 Hz, C₇-H), 8.33(1H, concealed dd, C₉'-H), 8.56(1H, d, J = 2.0 Hz, C₅-H); ¹³C NMR (100MHz, CDCl₃, δ): 16.84(CH₃), 116.21(CH), 117.23(CH), 117.80(CH), 120.77(C), 121.45(CH), 123.84(CH), 125.14(CH), 127.40(CH), 127.52(C), 128.16(CH), 128.36(CH), 128.99(CH), 130.01(CH), 130.07(CH), 130.13(CH), 133.23(CH), 134.52(C), 134.78(C), 135.55(C), 135.94(C), 140.81(C), 144.21(C), 145.79(C), 148.02(C), 152.82(C), 153.25(C), 155.96(C), 160.91(C), 161.52(C), 161.78 (δ-lactone CO); Anal. Calcd. for C₃₃H₂₀FNO₃: C, 79.67; H, 4.05; N, 2.82%. Found: C, 79.78; H, 4.14; N, 2.76%.

4-Methyl-3-phenyl-6-(4-(4-chlorophenyl)-benzofuro[3,2-b]pyridin-2-yl)coumarin (9e): IR (KBr, ν_{max}, cm⁻¹): 830(C-H bending of p-disubstituted benzene ring), 1466(C=N aromatic stretching), 1610(C=C aromatic stretching), 1712(C=O δ-lactone stretching), 2922(C-H aliphatic stretching), 3056(C-H aromatic stretching); ¹H NMR (400MHz, CDCl₃, δ): 2.46(3H, s, CH₃), 6.98-8.42(14H, m, Ar-H), 8.43(1H, concealed dd, C₇-H), 8.56(1H, concealed dd, C₉'-H), 8.72(1H, concealed d,

C₅-H); ¹³C NMR (100MHz, CDCl₃, δ): 16.89(CH₃), 116.95(CH), 117.12(CH), 120.91(C), 121.63(CH), 121.84(CH), 123.32(C), 124.03(CH), 127.74(C), 128.33(CH), 128.54(CH), 129.43(CH), 130.06(CH), 130.23(CH), 131.70(CH), 132.23(C), 132.80(CH), 133.39(CH), 134.44(C), 135.91(C), 142.32(C), 145.27(C), 146.32(C), 147.92(C), 150.83(C), 153.14(C), 154.96(C), 158.03(C), 160.93 (δ-lactone CO); Anal. Calcd. for C₃₃H₂₀ClNO₃: C, 77.12; H, 3.92; N, 2.73%. Found: C, 77.01; H, 3.84; N, 2.59%.

4-Methyl-3-phenyl-6-(4-(3,4-dimethoxyphenyl)-benzofuro[3,2-b]pyridin-2-yl)coumarin (9f): IR (KBr, ν_{max}, cm⁻¹): 823(C-H bending of trisubstituted benzene ring), 1465(C=N aromatic stretching), 1605(C=C aromatic stretching), 1717(C=O δ-lactone stretching), 2920(C-H aliphatic stretching), 3057(C-H aromatic stretching); ¹H NMR (400MHz, CDCl₃, δ): 2.47(3H, s, CH₃), 4.00 and 4.03(6H, s, 2 x OCH₃), 7.07-7.70(13H, m, Ar-H), 8.32(1H, dd, *J* = 2.0 and 8.8 Hz, C₇-H), 8.36(1H, concealed dd, C_{9'}-H), 8.57(1H, d, *J* = 2.0 Hz, C₅-H); ¹³C NMR (100MHz, CDCl₃, δ): 16.85(CH₃), 56.10(OCH₃), 56.17(OCH₃), 115.36(CH), 117.14(CH), 117.63(CH), 120.75(C), 121.07(CH), 121.36(CH), 121.47(CH), 123.90(CH), 127.31(CH), 127.55(C), 128.30(CH), 128.49(CH), 129.02(CH), 129.77(CH), 130.16(CH), 130.20(CH), 131.31(C), 132.99(C), 134.52(C), 136.17(C), 141.04(C), 144.15(C), 146.63(C), 148.01(C), 149.34(C), 149.69(C), 153.18(C), 155.76(C), 160.89 (δ-lactone CO); Anal. Calcd. for C₃₅H₂₅NO₅: C, 77.91; H, 4.67; N, 2.60%. Found: C, 78.02; H, 4.54; N, 2.52%.

Biological bioassay

Methodology for in vitro antimicrobial screening (broth microdilution method):

In vitro antimicrobial activity of all the compounds and standard drugs were assessed against Gram-positive bacteria viz. *Staphylococcus aureus* (MTCC 96) and *Bacillus subtilis* (MTCC

441); Gram-negative bacteria viz. *Salmonella typhi* (MTCC 98 and *Escherichia coli* (MTCC 443) and two fungi viz. *Aspergillus niger* (MTCC 282) and *Candida albicans* (MTCC 227) by the broth microdilution MIC (Minimum Inhibitory Concentration) method according to NCCLS (national committee for clinical laboratory standards). The strains employed for the activity were procured from (MTCC–Micro Type Culture Collection) Institute of Microbial Technology, Chandigarh. Mueller Hinton Broth was used as nutrient medium to grow and dilute the compound suspension for the test bacteria and Sabouraud dextrose broth used for fungal nutrition. Ampicillin, Norfloxacin, Chloramphenicol and Ciprofloxacin were used as standard antibacterial drugs whereas Griseofulvin and Nystatin were used as standard antifungal drugs. Bacterial strains were primarily inoculated into Mueller–Hinton agar and, after overnight growth, a number of colonies were directly suspended in saline solution until the turbidity matched the turbidity of the McFarland standard (approximately 10^8 CFU/mL) i.e. inoculum size for test strain was adjusted to 10^8 CFU/mL (colony forming unit) per milliliter well by comparing the turbidity (turbidimetric method). Similarly, fungi were inoculated on Sabouraud dextrose broth; the procedures of inoculum standardization were also similar. DMSO was used as diluent to get desired concentration of synthesized compounds and standard drugs to test upon standard microbial strains i.e. the compounds were dissolved in DMSO and the solutions were diluted with a culture medium. Each compound and standard drugs were diluted obtaining 2000 µg/mL concentration, as a stock solution. By further progressive dilutions with the test medium, the required concentrations were obtained for primary and secondary screening. In primary screening 1000, 500, and 250 µg/mL concentrations of the synthesized compounds were taken. The active compounds found in this primary screening were further diluted to obtain 200, 100, 62.5, 50, 25, 12.5 and 6.25 µg/mL concentrations for secondary screening to test in a second set

of dilution against all microorganisms. Briefly, the control tube containing no antibiotic is immediately sub cultured [before inoculation] by spreading a loopful evenly over a quarter of plate of medium suitable for the growth of the test organism. The tubes are then put for incubation at 37 °C for 24 h for bacteria and 48 h for fungi. Growth or a lack of growth in the tubes containing the antimicrobial agent was determined by comparison with the growth control, indicated by turbidity. The lowest concentration that completely inhibited visible growth of the organism was recorded as the minimum inhibitory concentration (MIC, µg/mL) i.e. the amount of growth from the control tube before incubation (which represents the original inoculum) is compared. A set of tubes containing only seeded broth and the solvent controls were maintained under identical conditions so as to make sure that the solvent had no influence on strain growth. The results were summarized in **Table 2** as the minimum inhibitory concentration (MIC, µg/mL).

In vitro evaluation of antituberculosis activity:

The determination of antituberculosis activity of the synthesized compounds against *Mycobacterium tuberculosis* H37Rv were performed by Lowenstein-Jensen method [29] with slight modification where 250 µg/mL dilution of each test compound were added liquid Lowenstein-Jensen Medium and then media were sterilized by inspissations method. A culture of *Mycobacterium tuberculosis* H37Rv growing on Lowenstein-Jensen medium was harvested in 0.85% saline in bijoux bottles. All test compound make solution of 250 µg/mL concentration of compounds was prepared in DMSO. These tubes were then incubated at 37 °C for 24 h followed by streaking of *M. tuberculosis* H37Rv (5×10^4 bacilli per tube). These tubes were then incubated at 37 °C. Growth of bacilli was seen after 12 days, 22 days and finally 28 days of incubation. Tubes having the compounds were compared with control tubes where medium alone

was incubated with *M. tuberculosis* H37Rv. The concentration at which no development of colonies occurred or < 20 colonies was taken as MIC concentration of test compound. The screening results are summarized as % inhibition (**Table 3**) relative to standard drugs isoniazid and rifampicin.

IR spectrum of compound 7a

^1H -NMR spectrum of compound 7a

^{13}C -APT spectrum of compound 7a

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Sample Information

Analyzed by : P.P.VIKARIYA
Analyzed : 7/3/2012 1:28:42 PM
Sample Name : R-103
Sample ID : R-103
Data File : D:\OUT OF DEPinsh\R-103.QID
D:\Project-1\DI1.qgm
Tuning File : C:\GCMSolution\System\Tune1\060612.qgt

Line# 1 R Time: 6.942 (Scan# 798)
MassPulse: 142
RawMode: Averaged 1.292-9.892 (120-1152) BasePeak: 44(68276)
BG Mode: None Group 1 - Event 1

Mass spectrum of compound 7a

IR spectrum of compound 8a

^1H -NMR spectrum of compound 8a

^{13}C -APT spectrum of compound 8a

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Sample Information

Analyzed by : P.P.VIKARIYA
Analyzed : 7/3/2012 12:30:23 PM
Sample Name : R-100
Sample ID : R-100
Data File : D:\OUT OF DE\Peaksh\R-100.qgd
D:\Project-1\DI1.qgm
Tuning File : C:\GCMSolution\System1\060612.qgt

Mass spectrum of compound 8a

IR spectrum of compound 9a

^1H -NMR spectrum of compound 9a

^{13}C -APT spectrum of compound 9a

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Sample Information

Analyzed by : P.P.VIKARIYA
Analyzed : 7/3/2012 2:48:22 PM
Sample Name : R-127
Sample ID : R-127
Data File : D:\OUT OF DE\Peaksh\R-127.QGD
D:\Project-1\DI-1.qgm
Tuning File : C:\GCMSolution\System1\060612.qgt

Mass spectrum of compound 9a