Supporting Information

CsF-Catalyzed transannulation reaction of oxazolones: diastereoselective synthesis of diversified *trans*-*N*-(6-oxo-1,4,5,6-tetrahydropyrimidin-5-yl)benzamides with arylidene azlactones and amidines

Golnaz Parhizkar,[†] Ahmad Reza Khosropour,*[,†] Iraj Mohammadpoor-Baltork,*[,†] Elahehnaz Parhizkar,[‡] Hadi Amiri Rudbari[†]

[†]Department of Chemistry, University of Isfahan, Isfahan 81746-73441, Iran

[‡]Department of Pharmaceutics, School of Pharmacy, Shiraz University of Medical Sciences, Shiraz 71468-64685, Iran

arkhosropour@chem.ui.ac.ir
imbaltork@sci.ui.ac.ir

Contents:

1. General Information

Chemicals were purchased from Fluka and Merck chemical companies. The azlactone[1] and amidine[2] skeletons were accessed following literature protocols. The microwave system used in these experiments includes the following items: Micro-SYNTH labstation, equipped with a glass door, a dual magnetron system with pyramid shaped diffuser, 1000 W delivered power, exhaust system, magnetic stirrer, 'quality pressure' sensor for flammable organic solvents, and a ATCFO fiber optic system for automatic temperature control. The progress of the reactions was monitored by thin layer chromatography (TLC) using 0.25 mm pre-coated silica gel HF_{254} plates. Silica gel (230-400 mesh, silicscycle) was used for column chromatography. Melting points were determined using Stuart Scientific SMP2 apparatus. FT-IR spectra were recorded on a Nicolet-Impact 400D instrument in the range of 400-4000 cm^{-1}. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance 400 MHz Fourier-transform spectrometer. Coupling constants were reported in hertz. Elemental analysis was performed on a LECO, CHNS-932 analyzer. High resolution mass spectrometry (HRMS) spectra were recorded using electrospray ionization with a time-of-flight mass analyzer (ESI-TOF).

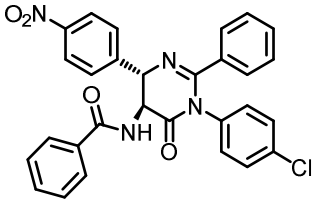
2. Procedures and Analytical Data

General Procedure for the Preparation of Compounds 3{1,1}-3{16,1}

The reaction mixture of azlactones **1**{1}-**1**{16} (0.20 mmol), *N*-(4-chlorophenyl)benzimidamide (**2**{1}, 0.046 g, 0.20 mmol), CsF (0.003 g, 0.10 equivalent), and CH_3CN (1 mL) was subjected to MW irradiation (200 W, 70 °C) for the appropriate time according to Scheme 2. After completion of the reaction as monitored by TLC (eluent: petroleum ether/ethyl acetate, 5:2), the solvent evaporated

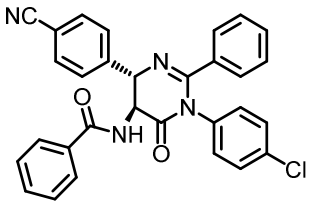
under reduced pressure and the mixture was extracted with ethyl acetate (3×5 mL). The organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. Purification by silica gel column chromatography (20-40% ethyl acetate in petroleum ether) afforded the products **3**{1,1}-**3**{16,1}.

***trans*-*N*-(1-(4-Chlorophenyl)-4-(4-nitrophenyl)-6-oxo-2-phenyl-1,4,5,6-tetrahydropyrimidin-5-yl)benzamide (3{1,1})**



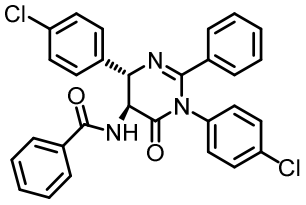
92.3 mg (0.18 mmol, 88%) as a light orange solid. dr > 13:1; m.p. 161-163 °C; IR (KBr): 3325, 3056, 2920, 1671, 1663, 1647, 1520, 1349 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.96 (d, J = 9.2 Hz, 1H), 8.17 (d, J = 8.8 Hz, 2H), 7.77 (d, J = 8.8 Hz, 2H), 7.72 (d, J = 7.2 Hz, 2H), 7.48-7.35 (m, 5H), 7.30-7.23 (m, 7H), 5.34 (d, J = 14 Hz, 1H), 5.17-5.11 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.3, 165.9, 154.4, 147.4, 142.3, 139.7, 139.5, 136.4, 132.1, 131.6, 129.8, 129.7, 128.8, 128.5, 127.8, 127.6, 127.2, 123.4, 123.1, 60.1, 52.5; Anal. calcd for $C_{29}H_{21}ClN_4O_4$ (524.70): C 66.37, H 4.00, N 10.67, found C 66.28, H 4.05, N 10.63; HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{22}ClN_4O_4$ $[M+H]^+$: 525.9624, found 525.9618.

***trans*-*N*-(1-(4-Chlorophenyl)-4-(4-cyanophenyl)-6-oxo-2-phenyl-1,4,5,6-tetrahydropyrimidin-5-yl)benzamide (3{2,1})**



85.8 mg (0.17 mmol, 85%) as a pale yellow solid. dr > 16:1; m.p. 151-153 °C; IR (KBr): 3343, 3059, 2933, 2237, 1674, 1662, 1643 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.91 (d, J = 9.2 Hz, 1H), 7.79 (d, J = 8.8 Hz, 2H), 7.72 (d, J = 7.2 Hz, 2H), 7.69 (d, J = 8.4 Hz, 2H), 7.49-7.36 (m, 5H), 7.29-7.24 (m, 7H), 5.31 (d, J = 14 Hz, 1H), 5.15-5.09 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.4, 166.1, 154.5, 139.8, 138.7, 136.7, 132.2, 131.8, 131.3, 129.6, 129.3, 129.1, 128.5, 128.1, 127.8, 127.6, 127.3, 123.5, 118.6, 111.0, 60.2, 53.1; Anal. calcd for $C_{30}H_{21}ClN_4O_2$ (504.73): C 71.38, H 4.16, N 11.09, found C 71.44, H 4.19, N 11.17; HRMS (ESI-TOF): *m/z* calcd for $C_{30}H_{22}ClN_4O_2$ $[M+H]^+$: 505.9743, found 505.9740.

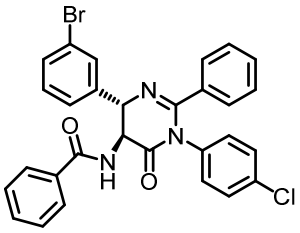
***trans*-*N*-(1,4-Bis(4-chlorophenyl)-6-oxo-2-phenyl-1,4,5,6-tetrahydropyrimidin-5-yl)benzamide (3{3,1})**



87.4 mg (0.17 mmol, 85%) as a pale yellow solid. dr 9:1; m.p. 154-155 °C; IR (KBr): 3348, 3061, 2934, 1672, 1666, 1649 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.82 (d, J = 9.2 Hz, 1H), 7.73 (d, J = 7.2 Hz, 2H), 7.52-7.44 (m, 10H), 7.38-7.34 (m, 3H), 7.29-7.23 (m, 3H), 5.26 (d, J = 14 Hz, 1H), 5.13-5.07 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.9, 166.0, 154.4, 139.7, 136.5, 134.6, 133.7, 131.7, 131.4, 130.3, 129.8, 129.5,

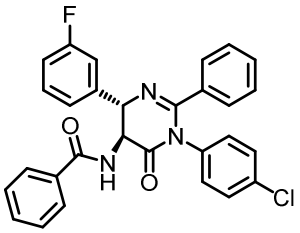
128.9, 128.5, 128.3, 127.8, 127.7, 127.0, 123.5, 60.3, 52.8; Anal. calcd for $C_{29}H_{21}Cl_2N_3O_2$ (514.17): C 67.73, H 4.08, N 8.16, found C 67.61, H 4.15, N 8.11; HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{22}Cl_2N_3O_2$ $[M+H]^+$: 515.4099, found 515.4092.

***trans*-*N*-(4-(3-Bromophenyl)-1-(4-chlorophenyl)-6-oxo-2-phenyl-1,4,5,6-tetrahydropyrimidin-5-yl)benzamide (3{4,1})**



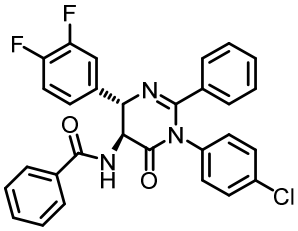
87.1 mg (0.16 mmol, 78%) as a yellow solid. dr 9:1; m.p. 185-188 °C; IR (KBr): 3329, 3053, 2925, 1672, 1660, 1643 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.87 (d, J = 9.2 Hz, 1H), 7.84 (s, 1H), 7.74 (d, J = 7.2 Hz, 2H), 7.49-7.36 (m, 8H), 7.29-7.23 (m, 7H), 5.29 (d, J = 14 Hz, 1H), 5.14-5.08 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.6, 166.2, 154.7, 150.5, 139.4, 136.8, 133.2, 131.6, 131.4, 131.3, 131.1, 130.4, 129.6, 128.8, 128.1, 128.0, 127.9, 127.7, 127.2, 123.2, 121.3, 60.6, 53.4; Anal. calcd for $C_{29}H_{21}BrClN_3O_2$ (558.62): C 62.34, H 3.75, N 7.51, found C 62.23, H 3.84, N 7.46; HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{22}BrClN_3O_2$ $[M+H]^+$: 559.8608, found 559.8611.

***trans*-*N*-(1-(4-Chlorophenyl)-4-(3-fluorophenyl)-6-oxo-2-phenyl-1,4,5,6-tetrahydropyrimidin-5-yl)benzamide (3{5,1})**



79.6 mg (0.16 mmol, 80%) as a yellow solid. dr 10:1; m.p. 140-142 °C; IR (KBr): 3352, 3051, 2919, 1677, 1668, 1645 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.84 (d, J = 9.2 Hz, 1H), 7.74 (d, J = 7.6 Hz, 2H), 7.48-7.33 (m, 8H), 7.31-7.10 (m, 8H), 5.26 (d, J = 14 Hz, 1H), 5.13-5.07 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.8, 166.3, 162.5, 160.4, 154.9, 151.6, 139.8, 136.3, 135.7 (d, J = 9.0 Hz), 131.7, 131.4, 130.1 (d, J = 8.0 Hz), 129.4, 128.6, 128.0, 127.7, 126.9, 124.7 (d, J = 2.0 Hz), 123.9, 115.5 (d, J = 21.0 Hz), 115.3 (d, J = 23.0 Hz), 60.7, 53.7; Anal. calcd for $C_{29}H_{21}ClFN_3O_2$ (497.71): C 69.97, H 4.21, N 8.43, found C 69.85, H 4.28, N 8.35; HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{22}ClFN_3O_2$ $[M+H]^+$: 498.9552, found 498.9545.

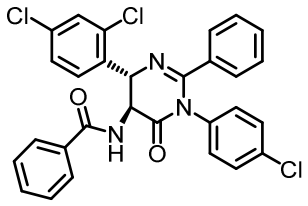
***trans*-*N*-(1-(4-Chlorophenyl)-4-(3,4-difluorophenyl)-6-oxo-2-phenyl-1,4,5,6-tetrahydropyrimidin-5-yl)benzamide (3{6,1})**



83.5 mg (0.16 mmol, 81%) as a yellow solid. dr 8:1; m.p. 156-158 °C; IR (KBr): 3357, 3059, 2928, 1672, 1665, 1644 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.87 (d, J = 9.2 Hz, 1H), 7.75 (d, J = 7.6 Hz, 2H), 7.62 (ddd, J = 12.0, 7.6, 1.6 Hz, 1H), 7.47-7.35 (m, 7H), 7.30-7.23 (m, 7H), 5.31 (d, J = 14 Hz, 1H), 5.16-5.10 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.7, 166.4, 154.9, 150.4 (dd, J = 56.0, 12.0 Hz), 150.3, 147.8 (dd, J = 54.0, 12.0 Hz), 139.9, 136.3, 131.6, 131.4, 131.2, 130.9 (dd, J = 7.0, 4.0 Hz), 129.5, 128.9, 128.4, 127.8, 127.3, 127.0, 125.6 (dd, J = 6.0, 3.0 Hz), 123.8, 117.5 (dd, J = 18.0, 6.0 Hz), 60.8, 53.7; Anal. calcd for $C_{29}H_{20}ClF_2N_3O_2$ (515.70): C 67.53, H 3.87, N 8.14,

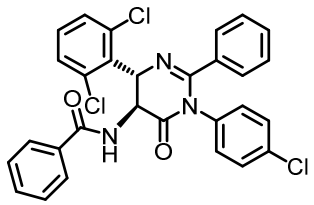
found C 67.40, H 3.82, N 8.09; HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{21}ClF_2N_3O_2$ $[M+H]^+$: 516.9457, found 516.9453.

***trans*-*N*-(1-(4-Chlorophenyl)-4-(2,4-dichlorophenyl)-6-oxo-2-phenyl-1,4,5,6-tetrahydropyrimidin-5-yl)benzamide (3{7,1})**



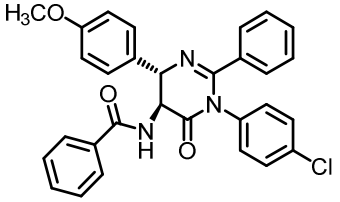
88.8 mg (0.16 mmol, 81%) as a light yellow solid. dr 9:1; m.p. 173-175 °C; IR (KBr): 3351, 3059, 2929, 1673, 1664, 1645 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.92 (d, *J* = 9.2 Hz, 1H), 7.68 (d, *J* = 7.2 Hz, 2H), 7.60 (d, *J* = 7.2 Hz, 1H), 7.55 (d, *J* = 8.4 Hz, 1H), 7.46-7.34 (m, 6H), 7.31-7.24 (m, 7H), 5.32 (d, *J* = 14 Hz, 1H), 5.15-5.09 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.7, 166.0, 154.3, 142.4, 139.8, 136.3, 133.4, 132.6, 132.1, 131.7, 131.3, 129.6, 129.3, 129.0, 128.8, 128.2, 127.9, 127.7, 127.1, 126.9, 123.4, 60.4, 52.9; Anal. calcd for $C_{29}H_{20}Cl_3N_3O_2$ (548.62): C 63.48, H 3.64, N 7.65, found C 63.56, H 3.67, N 7.57; HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{21}Cl_3N_3O_2$ $[M+H]^+$: 549.8550, found 549.8555.

***trans*-*N*-(1-(4-Chlorophenyl)-4-(2,6-dichlorophenyl)-6-oxo-2-phenyl-1,4,5,6-tetrahydropyrimidin-5-yl)benzamide (3{8,1})**



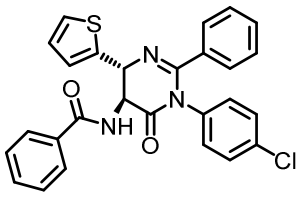
85.5 mg (0.16 mmol, 78%) as a pale yellow solid. dr 12:1; m.p. 175-178 °C; IR (KBr): 3349, 3058, 2929, 1675, 1662, 1644 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.82 (d, *J* = 9.2 Hz, 1H), 7.68 (d, *J* = 7.2 Hz, 2H), 7.46-7.33 (m, 6H), 7.31-7.21 (m, 9H), 5.27 (d, *J* = 14 Hz, 1H), 5.13-5.07 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.6, 166.0, 154.3, 140.5, 139.5, 136.4, 133.4, 132.4, 131.6, 131.3, 130.1, 129.7, 129.1, 128.7, 128.1, 127.9, 127.7, 126.9, 123.5, 60.3, 53.0; Anal. calcd for $C_{29}H_{20}Cl_3N_3O_2$ (548.62): C 63.48, H 3.64, N 7.65, found C 63.41, H 3.71, N 7.55; HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{21}Cl_3N_3O_2$ $[M+H]^+$: 549.8550, found 549.8557.

***trans*-*N*-(1-(4-Chlorophenyl)-4-(4-methoxyphenyl)-6-oxo-2-phenyl-1,4,5,6-tetrahydropyrimidin-5-yl)benzamide (3{9,1})**



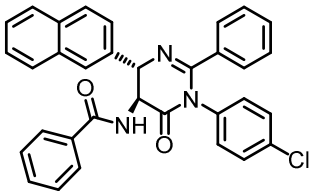
64.2 mg (0.13 mmol, 63%) as a yellow solid. dr 11:1; m.p. 151-152 °C; IR (KBr): 3335, 3065, 2927, 1670, 1663, 1644, 1249, 1036 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.73 (d, *J* = 9.2 Hz, 1H), 7.78 (d, *J* = 6.8 Hz, 2H), 7.54 (d, *J* = 8.8 Hz, 2H), 7.47-7.35 (m, 5H), 7.30-7.22 (m, 7H), 6.90 (d, *J* = 8.8 Hz, 2H), 5.24 (d, *J* = 14 Hz, 1H), 5.11-5.05 (m, 1H), 3.74 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.9, 166.8, 159.4, 154.5, 139.8, 136.7, 131.7, 131.5, 131.3, 129.8, 129.6, 128.9, 128.1, 127.8, 127.3, 127.0, 126.6, 123.4, 113.2, 60.2, 55.0, 52.7; Anal. calcd for $C_{30}H_{24}ClN_3O_3$ (509.72): C 70.68, H 4.70, N 8.23, found C 70.79, H 4.77, N 8.16; HRMS (ESI-TOF): *m/z* calcd for $C_{30}H_{25}ClN_3O_3$ $[M+H]^+$: 510.9908, found 510.9901.

***trans*-*N*-(1-(4-Chlorophenyl)-6-oxo-2-phenyl-4-(thiophen-2-yl)-1,4,5,6-tetrahydropyrimidin-5-yl)benzamide (3{10,1})**



79.6 mg (0.16 mmol, 82%) as a pale yellow solid. dr 9:1; m.p. 131-134 °C; IR (KBr): 3327, 3060, 2928, 1673, 1664, 1642 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.93 (d, J = 9.2 Hz, 1H), 7.84 (d, J = 7.2 Hz, 2H), 7.61 (dd, J = 6.0, 1.2 Hz, 1H), 7.50-7.46 (m, 2H), 7.43-7.36 (m, 4H), 7.29-7.24 (m, 7H), 7.05 (dd, J = 5.2, 3.6 Hz, 1H), 5.31 (d, J = 14 Hz, 1H), 5.15-5.09 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.8, 166.5, 154.2, 149.2, 139.7, 136.4, 132.1, 131.6, 131.5, 129.7, 129.5, 129.2, 128.9, 128.5, 127.8, 127.6, 127.1, 126.9, 123.3, 60.1, 52.7; Anal. calcd for $C_{27}H_{20}ClN_3O_2S$ (485.76): C 66.75, H 4.11, N 8.64, S 6.59, found C 66.80, H 4.17, N 8.57, S 6.68; HRMS (ESI-TOF): *m/z* calcd for $C_{27}H_{21}ClN_3O_2S$ $[M+H]^+$: 486.9925, found 486.9917.

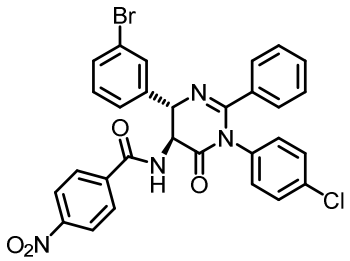
***trans*-*N*-(1-(4-Chlorophenyl)-4-(naphthalen-2-yl)-6-oxo-2-phenyl-1,4,5,6-tetrahydropyrimidin-5-yl)benzamide (3{11,1})**



79.4 mg (0.15 mmol, 75%) as a yellow solid. dr 8:1; m.p. 167-169 °C; IR (KBr): 3333, 3056, 2929, 1671, 1661, 1644 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.85 (d, J = 9.2 Hz, 1H), 8.13 (s, 1H), 7.82-7.77 (m, 3H), 7.72 (d, J = 7.2 Hz, 2H), 7.67 (dd, J = 8.4, 1.2 Hz, 1H), 7.47-7.34 (m, 7H), 7.28-7.23 (m, 7H), 5.28 (d, J = 14 Hz, 1H), 5.13-5.07 (m,

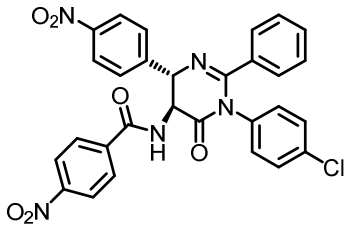
1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.9, 166.2, 154.6, 152.8, 139.8, 136.4, 132.8, 132.5, 131.6, 131.4, 131.1, 129.6, 128.8, 128.3, 128.1, 128.1, 127.8, 127.6, 127.5, 127.4, 127.2, 126.9, 126.5, 126.3, 123.3, 60.0, 52.4; Anal. calcd for $C_{33}H_{24}ClN_3O_2$ (529.76): C 74.81, H 4.53, N 7.92, found C 74.97, H 4.62, N 7.95; HRMS (ESI-TOF): *m/z* calcd for $C_{33}H_{25}ClN_3O_2$ $[M+H]^+$: 531.0235, found 531.0231.

***trans*-*N*-(4-(3-Bromophenyl)-1-(4-chlorophenyl)-6-oxo-2-phenyl-1,4,5,6-tetrahydropyrimidin-5-yl)-4-nitrobenzamide (3{12,1})**



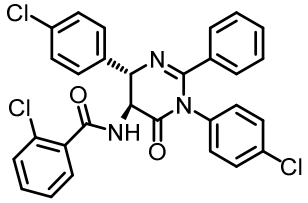
88.1 mg (0.15 mmol, 73%) as an orange solid. dr 9:1; m.p. 195-196 °C; IR (KBr): 3308, 3052, 2921, 1675, 1664, 1645, 1516, 1340 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.94 (d, *J* = 9.2 Hz, 1H), 8.21 (d, *J* = 8.8 Hz, 2H), 8.03 (d, *J* = 8.8 Hz, 2H), 7.85 (s, 1H), 7.49-7.36 (m, 5H), 7.30-7.24 (m, 7H), 5.32 (d, *J* = 14 Hz, 1H), 5.15-5.09 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 169.1, 166.8, 154.7, 149.1, 139.8, 139.6, 136.7, 133.3, 131.7, 131.4, 131.3, 131.1, 130.2, 129.6, 129.0, 128.3, 127.6, 127.1, 123.8, 123.7, 121.1, 60.4, 52.6; Anal. calcd for $C_{29}H_{20}BrClN_4O_4$ (603.60): C 57.70, H 3.31, N 9.27, found C 57.61, H 3.38, N 9.19; HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{21}BrClN_4O_4$ $[M+H]^+$: 604.8584, found 604.8579.

***trans*-*N*-(1-(4-Chlorophenyl)-4-(4-nitrophenyl)-6-oxo-2-phenyl-1,4,5,6-tetrahydropyrimidin-5-yl)-4-nitrobenzamide (3{13,1})**



84.3 mg (0.15 mmol, 74%) as an orange solid. dr 10:1; m.p. 191-193 °C; IR (KBr): 3302, 3048, 2920, 1669, 1660, 1641, 1514, 1342 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 9.03 (d, J = 9.2 Hz, 1H), 8.26 (d, J = 8.8 Hz, 2H), 8.18 (d, J = 8.8 Hz, 2H), 8.04 (d, J = 8.8 Hz, 2H), 7.77 (d, J = 8.8 Hz, 2H), 7.46-7.36 (m, 4H), 7.31-7.26 (m, 5H), 5.36 (d, J = 14 Hz, 1H), 5.18-5.12 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 169.7, 166.8, 154.7, 149.2, 147.3, 142.3, 139.9, 139.8, 136.7, 131.6, 129.7, 129.1, 128.8, 128.7, 127.6, 127.1, 123.8, 123.6, 123.4, 60.6, 53.0; Anal. calcd for $C_{29}H_{20}ClN_5O_6$ (569.68): C 61.13, H 3.51, N 12.28, found C 61.22, H 3.45, N 12.37; HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{21}ClN_5O_6$ $[M+H]^+$: 570.9599, found 570.9588.

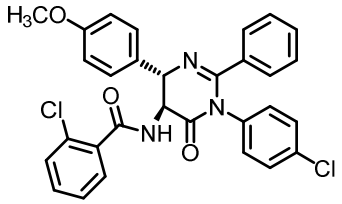
***trans*-*N*-(1,4-Bis(4-chlorophenyl)-6-oxo-2-phenyl-1,4,5,6-tetrahydropyrimidin-5-yl)-2-chlorobenzamide (3{14,1})**



79.0 mg (0.14 mmol, 72%) as a pale yellow solid. dr 9:1; m.p. 174-175 °C; IR (KBr): 3345, 3056, 2929, 1675, 1662, 1644 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.96 (d, J = 9.2 Hz, 1H), 7.57 (d, J = 7.6 Hz, 2H), 7.45-7.36 (m, 6H), 7.35-7.26 (m, 9H), 5.32 (d, J = 14 Hz, 1H), 5.16-5.10 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.7, 166.2, 154.5, 151.5, 139.9, 136.5, 134.1, 133.3, 132.5, 131.4, 131.1, 130.6, 130.1, 129.6,

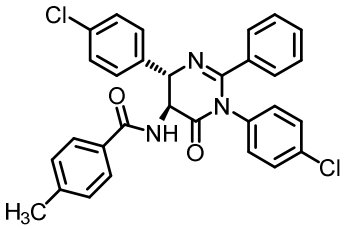
129.4, 129.1, 128.8, 128.0, 127.8, 127.2, 123.8, 60.1, 52.7; Anal. calcd for $C_{29}H_{20}Cl_3N_3O_2$ (548.62): C 63.48, H 3.64, N 7.65, found C 63.43, H 3.69, N 7.57; HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{21}Cl_3N_3O_2$ $[M+H]^+$: 549.8550, found 549.8544.

trans-2-Chloro-_N_-(1-(4-chlorophenyl)-4-(4-methoxyphenyl)-6-oxo-2-phenyl-1,4,5,6-tetrahydropyrimidin-5-yl)benzamide (3{15,1})



66.3 mg (0.12 mmol, 61%) as a yellow solid. dr 15:1; m.p. 176-178 °C; IR (KBr): 3346, 3063, 2927, 1672, 1663, 1642, 1248, 1036 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.83 (d, J = 9.2 Hz, 1H), 7.57 (d, J = 8.0 Hz, 2H), 7.47-7.35 (m, 4H), 7.34-7.25 (m, 9H), 6.91 (d, J = 8.8 Hz, 2H), 5.26 (d, J = 14 Hz, 1H), 5.14-5.08 (m, 1H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.6, 165.8, 159.5, 154.2, 153.6, 139.4, 136.2, 131.4, 131.2, 130.1, 129.9, 129.6, 129.3, 128.8, 128.7, 127.5, 127.1, 126.9, 126.3, 123.3, 113.4, 60.0, 55.0, 52.5; Anal. calcd for $C_{30}H_{23}Cl_2N_3O_3$ (544.17): C 66.21, H 4.22, N 7.71, found C 66.35, H 4.31, N 7.63; HRMS (ESI-TOF): *m/z* calcd for $C_{30}H_{24}Cl_2N_3O_3$ $[M+H]^+$: 545.4358, found 545.4351.

trans-_N_-(1,4-Bis(4-chlorophenyl)-6-oxo-2-phenyl-1,4,5,6-tetrahydropyrimidin-5-yl)-4-methylbenzamide (3{16,1})

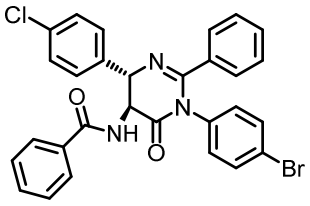


60.2 mg (0.11 mmol, 57%) as a yellow solid. dr 9:1; m.p. 167-169 °C; IR (KBr): 3361, 3061, 2932, 1673, 1664, 1645, 1378 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.76 (d, J = 9.2 Hz, 1H), 7.61 (d, J = 8.0 Hz, 2H), 7.55 (d, J = 8.8 Hz, 2H), 7.46-7.36 (m, 4H), 7.28-7.23 (m, 7H), 7.16 (d, J = 7.6 Hz, 2H), 5.25 (d, J = 14 Hz, 1H), 5.12-5.06 (m, 1H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.3, 165.8, 154.3, 140.1, 139.6, 136.4, 133.2, 132.5, 131.4, 131.3, 130.2, 130.0, 129.7, 129.5, 128.9, 127.9, 127.7, 127.1, 123.5, 60.0, 52.4, 21.8; Anal. calcd for $C_{30}H_{23}Cl_2N_3O_2$ (528.18): C 68.21, H 4.35, N 7.95, found C 68.29, H 4.42, N 7.99; HRMS (ESI-TOF): *m/z* calcd for $C_{30}H_{24}Cl_2N_3O_2$ $[M+H]^+$: 529.4364, found 529.4355.

General Procedure for the Preparation of Compounds 3{3,2}-3{3,7}

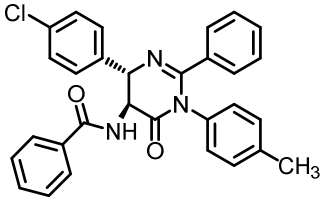
The reaction mixture of (*Z*)-4-(4-chlorobenzylidene)-2-phenyloxazol-5(4*H*)-one (**1**{3}, 0.056 g, 0.20 mmol), amidines **2**{2}-**2**{7} (0.20 mmol), CsF (0.003 g, 0.10 equivalent), and CH_3CN (1 mL) was subjected to MW irradiation (200 W, 70 °C) for the appropriate time according to Scheme 3. After completion of the reaction as monitored by TLC (eluent: petroleum ether/ethyl acetate, 5:2), the solvent evaporated under reduced pressure and the mixture was extracted with ethyl acetate (3×5 mL). The organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. Purification by silica gel column chromatography (20-40% ethyl acetate in petroleum ether) afforded the products **3**{3,2}-**3**{3,7}.

***trans*-*N*-(1-(4-Bromophenyl)-4-(4-chlorophenyl)-6-oxo-2-phenyl-1,4,5,6-tetrahydropyrimidin-5-yl)benzamide (3{3,2})**



93.8 mg (0.17 mmol, 84%) as a yellow solid. dr 9:1; m.p. 179-181 °C; IR (KBr): 3331, 3056, 2925, 1674, 1662, 1643 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.81 (d, J = 9.2 Hz, 1H), 7.71 (d, J = 7.2 Hz, 2H), 7.49-7.43 (m, 10H), 7.39-7.35 (m, 2H), 7.24-7.18 (m, 4H), 5.24 (d, J = 14 Hz, 1H), 5.12-5.06 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.7, 165.9, 154.2, 150.1, 136.7, 134.5, 133.7, 132.9, 131.6, 131.3, 130.3, 129.8, 129.0, 128.6, 128.4, 128.2, 127.7, 123.9, 113.7, 60.2, 52.8; Anal. calcd for $C_{29}H_{21}BrClN_3O_2$ (558.62): C 62.34, H 3.75, N 7.51, found C 62.26, H 3.83, N 7.44; HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{22}BrClN_3O_2$ $[M+H]^+$: 559.8608, found 559.8603.

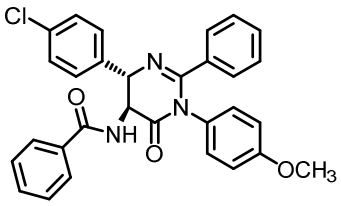
***trans*-*N*-(4-(4-Chlorophenyl)-6-oxo-2-phenyl-1-(*p*-tolyl)-1,4,5,6-tetrahydropyrimidin-5-yl)benzamide (3{3,3})**



81.9 mg (0.17 mmol, 83%) as a yellow solid. dr 10:1; m.p. 158-160 °C; IR (KBr): 3358, 3059, 2930, 1673, 1664, 1644, 1375 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.80 (d, J = 9.2 Hz, 1H), 7.72 (d, J = 7.2 Hz, 2H), 7.52-7.44 (m, 8H), 7.38-7.34 (m, 3H), 7.27-7.18 (m, 5H), 5.26 (d, J = 14 Hz, 1H), 5.13-5.07 (m, 1H), 2.41 (s, 3H); ^{13}C NMR (100 MHz,

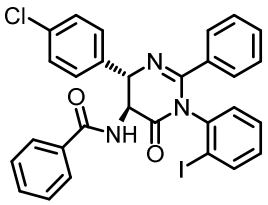
DMSO-d_6): δ 168.6, 166.1, 154.4, 139.6, 138.2, 134.7, 133.6, 131.6, 130.4, 129.7, 129.3, 128.5, 128.4, 128.4, 128.1, 127.8, 127.7, 126.5, 123.4, 60.2, 52.7, 21.8; Anal. calcd for $C_{30}H_{24}ClN_3O_2$ (493.73): C 72.97, H 4.86, N 8.50, found C 73.04, H 4.96, N 8.43; HRMS (ESI-TOF): *m/z* calcd for $C_{30}H_{25}ClN_3O_2$ $[M+H]^+$: 494.9914, found 494.9907.

***trans*-*N*-(4-(4-Chlorophenyl)-1-(4-methoxyphenyl)-6-oxo-2-phenyl-1,4,5,6-tetrahydropyrimidin-5-yl)benzamide (3{3,4})**



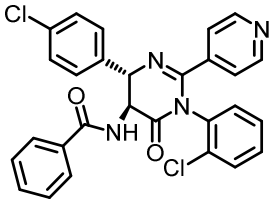
86.6 mg (0.17 mmol, 85%) as a light yellow solid. dr 8:1; m.p. 149-151 °C; IR (KBr): 3337, 3065, 2929, 1673, 1663, 1644, 1249, 1035 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.80 (d, *J* = 9.2 Hz, 1H), 7.73 (d, *J* = 7.2 Hz, 2H), 7.54 (d, *J* = 8.8 Hz, 2H), 7.49-7.36 (m, 5H), 7.29-7.23 (m, 7H), 6.88 (d, *J* = 8.8 Hz, 2H), 5.26 (d, *J* = 14 Hz, 1H), 5.12-5.06 (m, 1H), 3.74 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.8, 166.3, 159.3, 154.4, 139.8, 134.7, 133.6, 131.8, 130.3, 129.7, 129.6, 128.6, 128.5, 128.3, 128.1, 127.7, 126.6, 123.5, 113.2, 60.1, 55.0, 52.6; Anal. calcd for $C_{30}H_{24}ClN_3O_3$ (509.72): C 70.68, H 4.70, N 8.23, found C 70.80, H 4.79, N 8.31; HRMS (ESI-TOF): *m/z* calcd for $C_{30}H_{25}ClN_3O_3$ $[M+H]^+$: 510.9908, found 510.9905.

***trans*-*N*-(4-(4-Chlorophenyl)-1-(2-iodophenyl)-6-oxo-2-phenyl-1,4,5,6-tetrahydropyrimidin-5-yl)benzamide (3{3,5})**



95.6 mg (0.16 mmol, 79%) as a dark yellow solid. dr 10:1; m.p. 199-201 °C; IR (KBr): 3327, 3056, 2926, 1674, 1663, 1641 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.82 (d, J = 9.2 Hz, 1H), 7.82 (d, J = 7.6 Hz, 1H), 7.73 (d, J = 7.2 Hz, 2H), 7.52-7.44 (m, 7H), 7.38-7.34 (m, 3H), 7.29-7.23 (m, 3H), 7.11 (d, J = 6.4 Hz, 1H), 7.03-7.00 (m, 1H), 5.26 (d, J = 14 Hz, 1H), 5.11-5.05 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.5, 165.8, 153.9, 138.7, 134.6, 133.7, 133.6, 131.8, 131.1, 130.4, 130.3, 129.9, 129.8, 129.7, 128.8, 128.5, 128.5, 128.3, 127.7, 123.8, 121.9, 60.1, 52.6; Anal. calcd for $C_{29}H_{21}ClIN_3O_2$ (605.62): C 57.50, H 3.46, N 6.93, found C 57.37, H 3.54, N 6.81; HRMS (ESI-TOF): *m/z* calcd for $C_{29}H_{22}ClIN_3O_2$ $[M+H]^+$: 606.8613, found 606.8605.

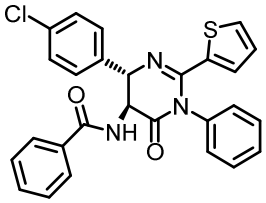
***trans*-*N*-(1-(2-Chlorophenyl)-4-(4-chlorophenyl)-6-oxo-2-(pyridin-4-yl)-1,4,5,6-tetrahydropyrimidin-5-yl)benzamide (3{3,6})**



82.4 mg (0.16 mmol, 80%) as a yellow solid. dr 9:1; m.p. 157-159 °C; IR (KBr): 3348, 3056, 2925, 1675, 1664, 1644 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.81 (d, J = 9.2 Hz, 1H), 8.54 (d, J = 5.2 Hz, 2H), 7.87 (d, J = 4.8 Hz, 2H), 7.73 (d, J = 7.2 Hz, 2H), 7.51-7.44 (m, 5H), 7.38-7.34 (m, 3H), 7.29-7.21 (m, 3H), 5.26 (d, J = 14 Hz, 1H), 5.13-5.07 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.4, 165.7, 152.6, 149.8, 147.0,

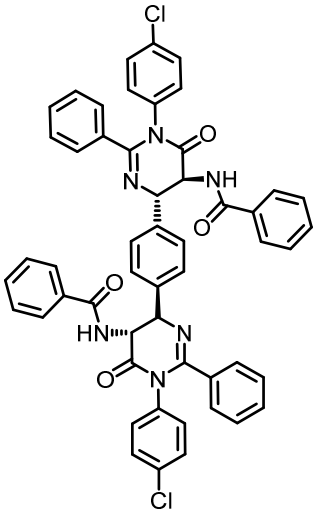
142.6, 134.5, 133.6, 131.7, 130.4, 130.2, 129.7, 128.7, 128.5, 128.3, 127.6, 126.2, 124.1, 123.5, 121.3, 60.4, 52.6; Anal. calcd for $C_{28}H_{20}Cl_2N_4O_2$ (515.16): C 65.27, H 3.88, N 10.87, found C 65.41, H 3.81, N 10.98; HRMS (ESI-TOF): *m/z* calcd for $C_{28}H_{21}Cl_2N_4O_2$ $[M+H]^+$: 516.3980, found 516.3977.

***trans*-*N*-(4-(4-Chlorophenyl)-6-oxo-1-phenyl-2-(thiophen-2-yl)-1,4,5,6-tetrahydropyrimidin-5-yl)benzamide (3{3,7})**



75.7 mg (0.16 mmol, 78%) as a pale yellow solid. dr 12:1; m.p. 136-138 °C; IR (KBr): 3329, 3059, 2928, 1673, 1662, 1642 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.80 (d, *J* = 9.2 Hz, 1H), 7.74 (d, *J* = 7.2 Hz, 2H), 7.63 (dd, *J* = 6.0, 1.2 Hz, 1H), 7.52-7.44 (m, 7H), 7.38-7.34 (m, 3H), 7.29-7.23 (m, 3H), 7.06 (dd, *J* = 5.2, 3.6 Hz, 1H), 5.26 (d, *J* = 14 Hz, 1H), 5.13-5.07 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.1, 165.4, 150.4, 149.4, 141.7, 134.7, 133.8, 131.8, 130.3, 129.8, 129.5, 129.1, 128.5, 128.3, 127.8, 127.6, 127.2, 122.6, 121.9, 59.9, 52.3; Anal. calcd for $C_{27}H_{20}ClN_3O_2S$ (485.76): C 66.75, H 4.11, N 8.64, S 6.59, found C 66.83, H 4.15, N 8.55, S 6.67; HRMS (ESI-TOF): *m/z* calcd for $C_{27}H_{21}ClN_3O_2S$ $[M+H]^+$: 486.9925, found 486.9919.

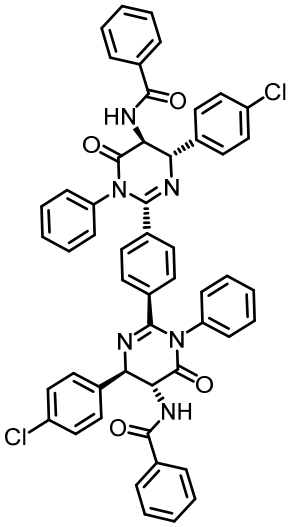
***trans*,*trans*-*N*,*N'*-(1,4-Phenylenebis(1-(4-chlorophenyl)-6-oxo-2-phenyl-1,4,5,6-tetrahydropyrimidine-4,5-diyl))dibenzamide (3{17,1})**



The reaction mixture of (4*Z*,4'*Z*)-4,4'-(1,4-phenylenebis(methanylylidene))bis(2-phenyloxazol-5(4*H*)-one) (**1**{17}, 0.084 g, 0.20 mmol), *N*-(4-chlorophenyl)benzimidamide (**2**{1}, 0.092 g, 0.40 mmol), CsF (0.006 g, 0.20 equivalent), and CH_3CN (2 mL) was subjected to MW irradiation (200 W, 70 °C) for the appropriate time according to Scheme 4. After completion of the reaction as monitored by TLC (eluent: petroleum ether/ethyl acetate, 5:2), the solvent evaporated under reduced pressure and the mixture was extracted with ethyl acetate (3×10 mL). The organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. Purification by silica gel column chromatography (20-40% ethyl acetate in petroleum ether) afforded the product **3**{17,1}. 125.1 mg (0.14 mmol, 71%) as a yellow solid. dr 16:1; m.p. 223-225 °C; IR (KBr): 3345, 3056, 2931, 1672, 1665, 1646 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.77 (d, *J* = 9.2 Hz, 2H), 7.80 (d, *J* = 7.2 Hz, 4H), 7.72 (d, *J* = 7.2 Hz, 4H), 7.59 (s, 4H), 7.55-7.41 (m, 10H), 7.36-7.33 (m, 4H), 7.26-7.23 (m, 6H), 5.24 (d, *J* = 14 Hz, 2H), 5.09-5.03 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 169.4, 166.7, 154.2, 139.6, 136.5, 133.8, 131.7, 131.5, 129.6, 128.9, 128.3, 128.1, 127.9, 127.8, 127.5, 127.1, 123.4, 60.0, 52.4; Anal. calcd for $C_{52}H_{38}Cl_2N_6O_4$ (881.38):

C 70.85, H 4.31, N 9.53, found C 70.73, H 4.40, N 9.40; HRMS (ESI-TOF): *m/z* calcd for $C_{52}H_{39}Cl_2N_6O_4$ $[M+H]^+$: 882.8098, found 882.8089.

***trans*,*trans*-*N*,*N*′-(1,4-Phenylenebis(4-(4-chlorophenyl)-6-oxo-1-phenyl-1,4,5,6-tetrahydropyrimidine-2,5-diyl))dibenzamide (3{3,8})**



The reaction mixture of (*Z*)-4-(4-chlorobenzylidene)-2-phenyloxazol-5(4*H*)-one (**1**{3}, 0.113 g, 0.40 mmol), *N*-phenyl-4-((phenylamino)methyl)benzimidamide (**2**{8}, 0.060 g, 0.20 mmol), CsF (0.006 g, 0.20 equivalent), and CH_3CN (2 mL) was subjected to MW irradiation (200 W, 70 °C) for the appropriate time according to Scheme 4. After completion of the reaction as monitored by TLC (eluent: petroleum ether/ethyl acetate, 5:2), the solvent evaporated under reduced pressure and the mixture was extracted with ethyl acetate (3×10 mL). The organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. Purification by silica gel column chromatography (20-40% ethyl acetate in petroleum ether) afforded the product **3**{3,8}. 119.8 mg (0.14 mmol, 68%) as a yellow solid. dr 19:1; m.p. 213-216 °C; IR (KBr): 3343, 3061, 2927, 1673, 1666,

1645 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.79 (d, J = 9.2 Hz, 2H), 7.76 (d, J = 7.2 Hz, 4H), 7.69 (d, J = 7.2 Hz, 4H), 7.62 (s, 4H), 7.55-7.43 (m, 10H), 7.36-7.33 (m, 4H), 7.26-7.23 (m, 6H), 5.25 (d, J = 14 Hz, 2H), 5.12-5.06 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.7, 165.9, 152.8, 134.4, 133.8, 133.8, 132.7, 131.7, 130.2, 129.6, 128.9, 128.5, 128.3, 128.1, 127.7, 127.5, 123.3, 60.2, 52.6; Anal. calcd for $C_{52}H_{38}Cl_2N_6O_4$ (881.38): C 70.85, H 4.31, N 9.53, found C 70.76, H 4.39, N 9.44; HRMS (ESI-TOF): *m/z* calcd for $C_{52}H_{39}Cl_2N_6O_4$ $[M+H]^+$: 882.8098, found 882.8093.

3. Antimicrobial Assay

The in vitro antibacterial activities of the samples were determined by agar disc diffusion method. American Type Culture Collection (ATCC) strains of *Escherichia coli* (ATCC 25922) as Gram-negative and *Bacillus subtilis* (ATCC 11778) and clinical isolates of *Staphylococcus aureus* as Gram-positive bacteria (standard inoculums concentration was 1-1.5 × 10^8 c.f.u./mL) were grown on nutrient broth medium and incubated at 37 °C for 24 h.

Microorganisms were seeded over sterilized culture medium plates and growth inhibition zones were measured in mm using streptomycin, penicillin, and tetracycline as references antibiotics (positive control). All compounds were dissolved in DMSO in the concentration of 100 μg/mL with DMSO as negative control.

Minimum Inhibitory Concentration (MIC) assay was determined applying broth dilution method. This assay shows the minimum concentration that inhibits the growth of bacteria completely. The compounds (with the concentrations of 200, 100, 50, 25, 12.5 and 6.25 μg/mL) were two fold diluted into nutrient broth medium containing approximately 5 × 10^6 c.f.u./mL of bacteria cells. Samples incubated at 37 °C for 24 h and the lowest concentration (highest dilution) was considered as MIC.

According to measured inhibition zones and MIC assay which are summarized in Table S1, almost all compounds show desirable antibacterial effect.

Table S1. Inhibition Zone (mm ± SD) and Minimum Inhibitory Concentration (μg/mL) of Different *trans*-*N*-(6-Oxo-1,4,5,6-tetrahydropyrimidin-5-yl)benzamides Derivatives Against Selected Bacteria

Microorganism / Sample	Inhibition Zone (mm ± SD)			MIC		
	E. coli	*B. subtilis*	*S. aureus*	*E. coli*	*B. subtilis*	*S. aureus*
3{1,1}	5.8 ± 0.4	11.6 ± 0.2	8.6 ± 0.1	25	25	25
3{2,1}	6.1 ± 0.3	12.3 ± 0.2	8.9 ± 0.4	25	12.5	25
3{3,1}	6.7 ± 0.4	14.3 ± 0.3	10.0 ± 0.2	12.5	6.25	12.5
3{4,1}	6.4 ± 0.2	12.9 ± 0.3	9.2 ± 0.4	12.5	12.5	12.5
3{5,1}	6.5 ± 0.3	12.7 ± 0.1	9.4 ± 0.1	12.5	12.5	12.5
3{6,1}	6.5 ± 0.3	13.4 ± 0.5	9.7 ± 0.3	12.5	6.25	12.5
3{7,1}	6.7 ± 0.4	14.0 ± 0.2	10.3 ± 0.4	12.5	6.25	12.5
3{8,1}	6.8 ± 0.2	15.1 ± 0.4	9.3 ± 0.0	12.5	6.25	12.5
3{9,1}	5.4 ± 0.5	11.5 ± 0.3	7.6 ± 0.3	50	25	50
3{10,1}	5.5 ± 0.3	12.1 ± 0.5	9.2 ± 0.3	25	12.5	25
3{11,1}	5.7 ± 0.4	11.9 ± 0.3	9.1 ± 0.4	25	12.5	25
3{12,1}	6.1 ± 0.2	12.0 ± 0.4	9.8 ± 0.3	25	25	12.5
3{13,1}	5.6 ± 0.1	11.4 ± 0.2	8.4 ± 0.2	50	50	50
3{14,1}	6.7 ± 0.3	14.1 ± 0.3	10.1 ± 0.3	12.5	6.25	12.5
3{15,1}	5.7 ± 0.3	10.9 ± 0.1	6.4 ± 0.2	50	50	50
3{16,1}	6.3 ± 0.2	13.3 ± 0.3	9.6 ± 0.4	25	12.5	12.5
3{17,1}	6.2 ± 0.4	11.2 ± 0.4	8.8 ± 0.3	25	25	50
3{3,2}	6.1 ± 0.2	12.8 ± 0.1	9.5 ± 0.2	25	12.5	12.5
3{3,3}	5.8 ± 0.3	12.9 ± 0.3	9.2 ± 0.1	25	12.5	25
3{3,4}	5.3 ± 0.2	11.7 ± 0.3	7.8 ± 0.4	50	12.5	25
3{3,5}	6.4 ± 0.3	12.9 ± 0.1	9.8 ± 0.2	25	12.5	12.5
3{3,6}	6.3 ± 0.3	13.6 ± 0.2	9.7 ± 0.3	25	12.5	12.5
3{3,7}	5.4 ± 0.2	12.4 ± 0.4	9.5 ± 0.1	50	12.5	12.5
3{3,8}	6.1 ± 0.1	11.4 ± 0.3	9.1 ± 0.3	25	25	25
Streptomycin	9.8 ± 0.3	15.3 ± 0.2	12.4 ± 0.1	6.25	6.25	6.25
Penicillin	7.2 ± 0.2	13.9 ± 0.1	10.8 ± 0.2	25	12.5	25
Tetracycline	11.0 ± 0.3	12.4 ± 0.4	12.1 ± 0.4	12.5	6.25	6.25

The antifungal activity also performed by disk diffusion method on potato dextrose agar medium. Strains of fungi *Candida albicans* (ATCC 10261) and clinical isolates of *Aspergillus flavus* (2-5 × 10^6 spores/mL) were incubated 5 days at 35 °C. Synthesized compounds with the concentration of 100 µg/mL were mixed with agar and allowed to solidify. Fluconazole and nystatin as two antifungal drugs were selected as positive control samples (Table S2).

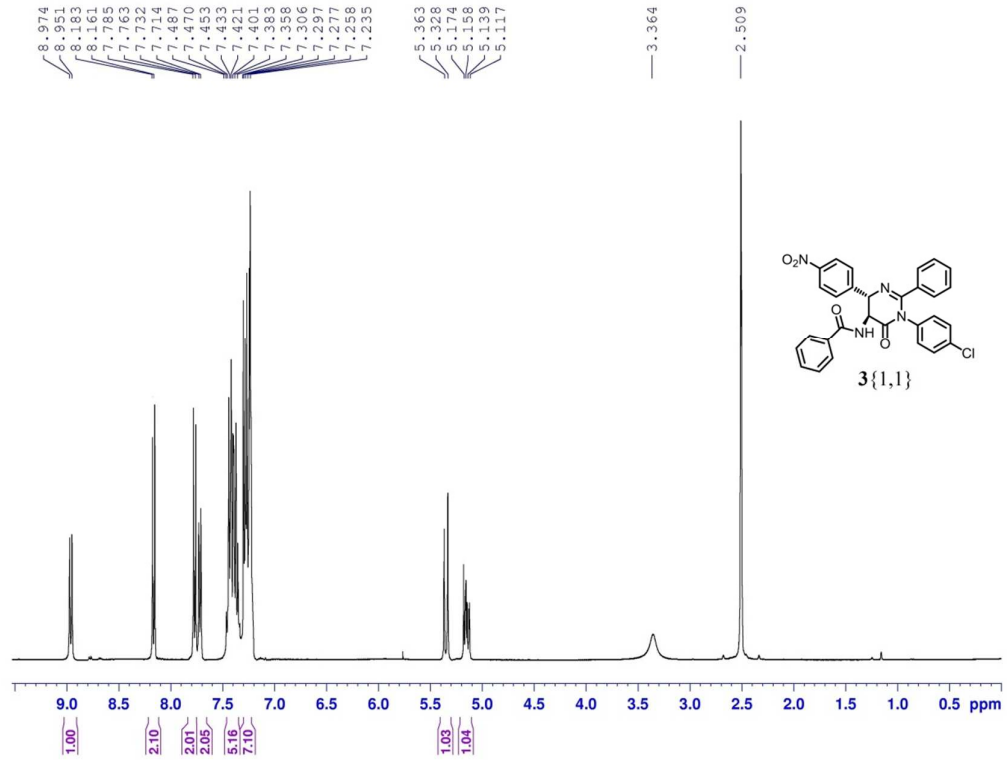
MIC of fungi was performed as the mentioned method for bacteria with differences in fungal concentration and incubation time. The nutrient broth inoculated with 2-5 × 10^4 spores/mL and incubated for 5 days at 35 °C (Table S2).

Table S2. Inhibition Zone (mm ± SD) and Minimum Inhibitory Concentration (µg/mL) of Different *trans*-*N*-(6-Oxo-1,4,5,6-tetrahydropyrimidin-5-yl)benzamides Derivatives Against Selected Fungi

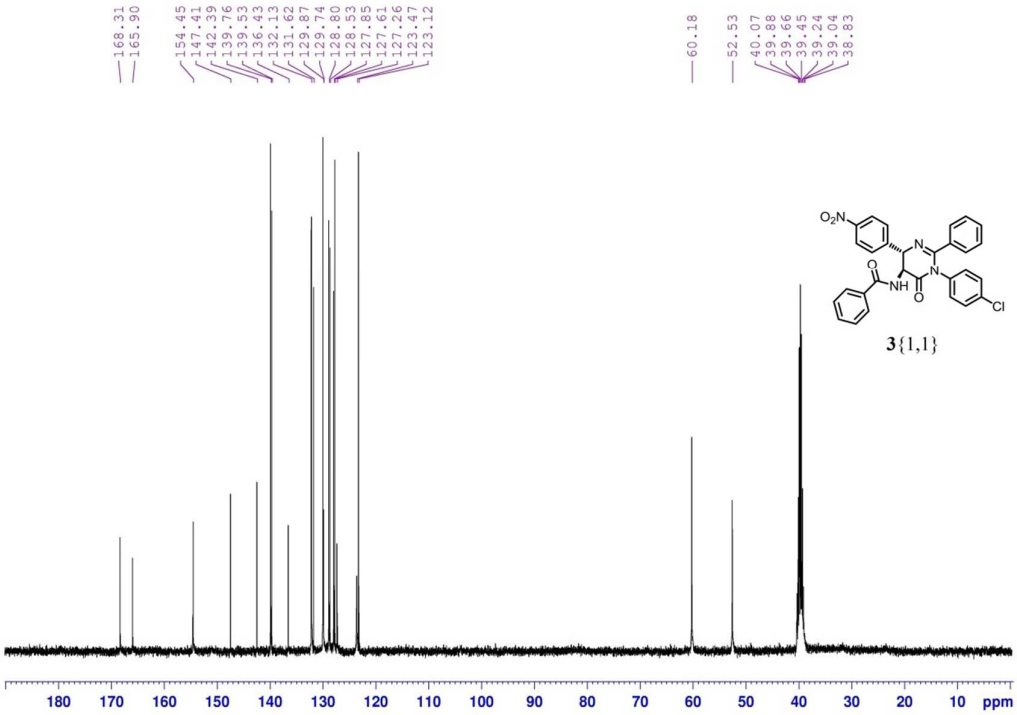
	Inhibition Zone (mm ± SD)		MIC	
Microorganism / Sample	*C. albicans*	*A. flavus*	*C. albicans*	*A. flavus*
3{1,1}	4.9 ± 0.2	5.3 ± 0.3	25	25
3{2,1}	5.2 ± 0.3	5.6 ± 0.2	25	12.5
3{3,1}	6.0 ± 0.4	5.8 ± 0.1	12.5	6.25
3{4,1}	4.7 ± 0.3	5.1 ± 0.1	12.5	12.5
3{5,1}	5.3 ± 0.3	5.7 ± 0.0	12.5	12.5
3{6,1}	5.9 ± 0.1	5.9 ± 0.2	25	12.5
3{7,1}	5.7 ± 0.4	5.5 ± 0.1	12.5	12.5
3{8,1}	6.8 ± 0.2	6.8 ± 0.3	12.5	25
3{9,1}	4.5 ± 0.1	3.4 ± 0.3	100	50
3{10,1}	3.3 ± 0.2	4.1 ± 0.2	25	25
3{11,1}	4.1 ± 0.2	4.3 ± 0.4	25	25
3{12,1}	4.9 ± 0.3	5.3 ± 0.1	25	25
3{13,1}	5.4 ± 0.0	5.6 ± 0.3	50	100
3{14,1}	6.2 ± 0.3	5.9 ± 0.2	12.5	12.5
3{15,1}	4.6 ± 0.1	5.0 ± 0.4	50	50
3{16,1}	6.0 ± 0.4	5.4 ± 0.3	25	12.5
3{17,1}	5.1 ± 0.4	4.3 ± 0.2	25	25
3{3,2}	5.0 ± 0.2	4.9 ± 0.3	50	12.5
3{3,3}	5.4 ± 0.3	5.1 ± 0.1	25	12.5
3{3,4}	4.7 ± 0.3	3.8 ± 0.2	100	12.5
3{3,5}	5.3 ± 0.3	5.1 ± 0.2	50	25
3{3,6}	5.9 ± 0.1	5.7 ± 0.4	50	25
3{3,7}	3.6 ± 0.2	4.2 ± 0.3	50	12.5
3{3,8}	5.6 ± 0.2	4.5 ± 0.3	25	25
Fluconazole	7.2 ± 0.3	8.0 ± 0.2	6.25	12.5
Nystatin	7.9 ± 0.4	7.9 ± 0.3	6.25	6.25

4. ^{1}H and ^{13}C NMR Spectra of the Products

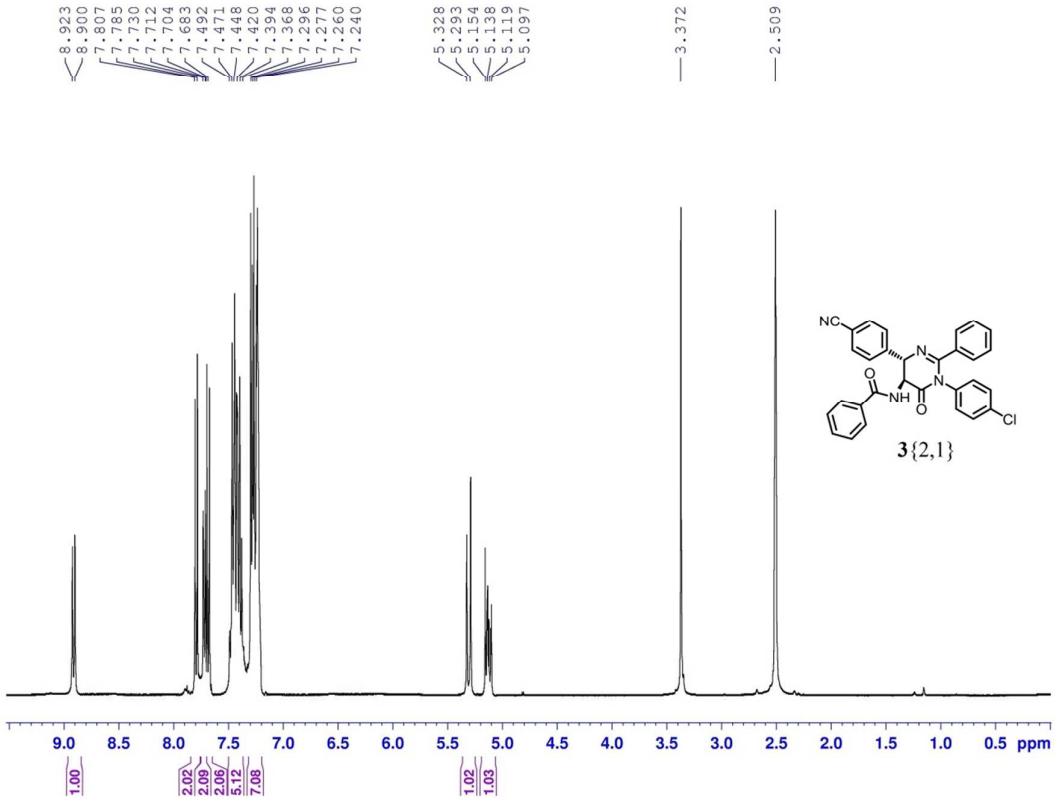
^{1}H NMR of **3**{1,1}



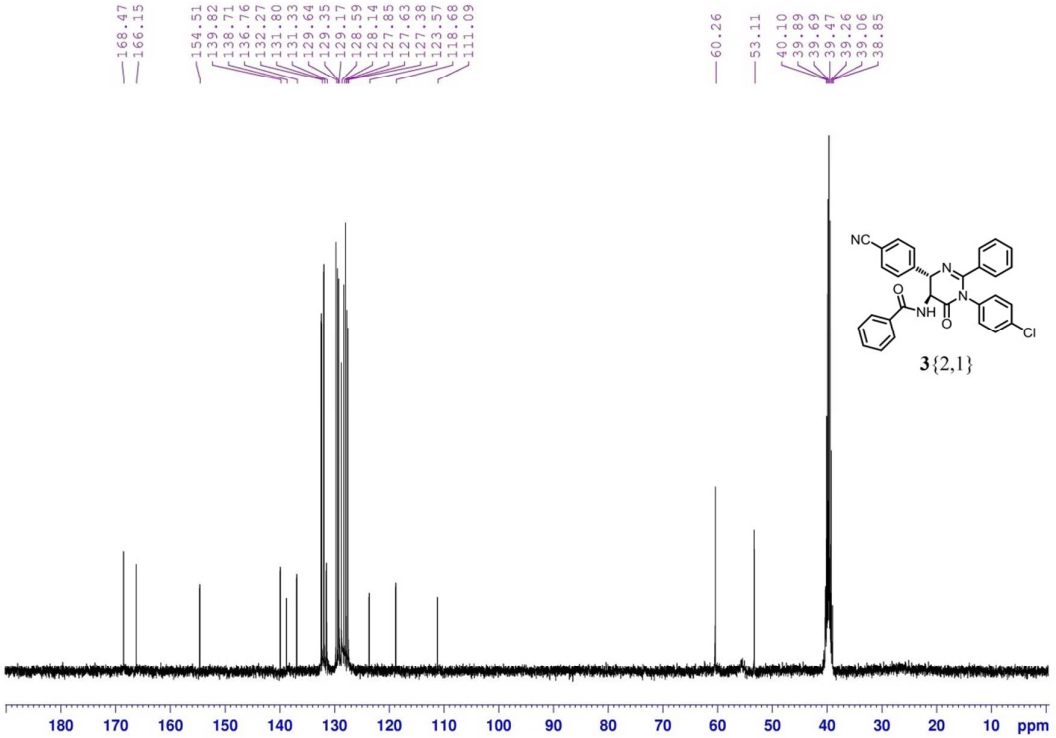
^{13}C NMR of **3**{1,1}



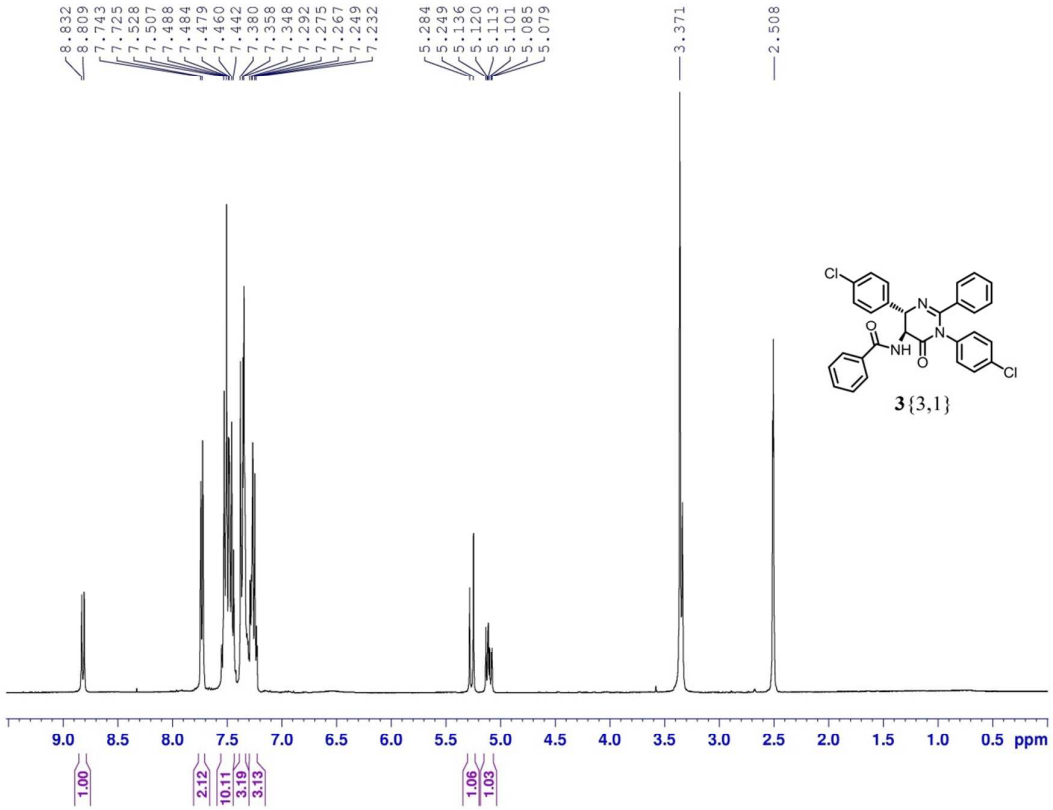
^{1}H NMR of **3**{2,1}



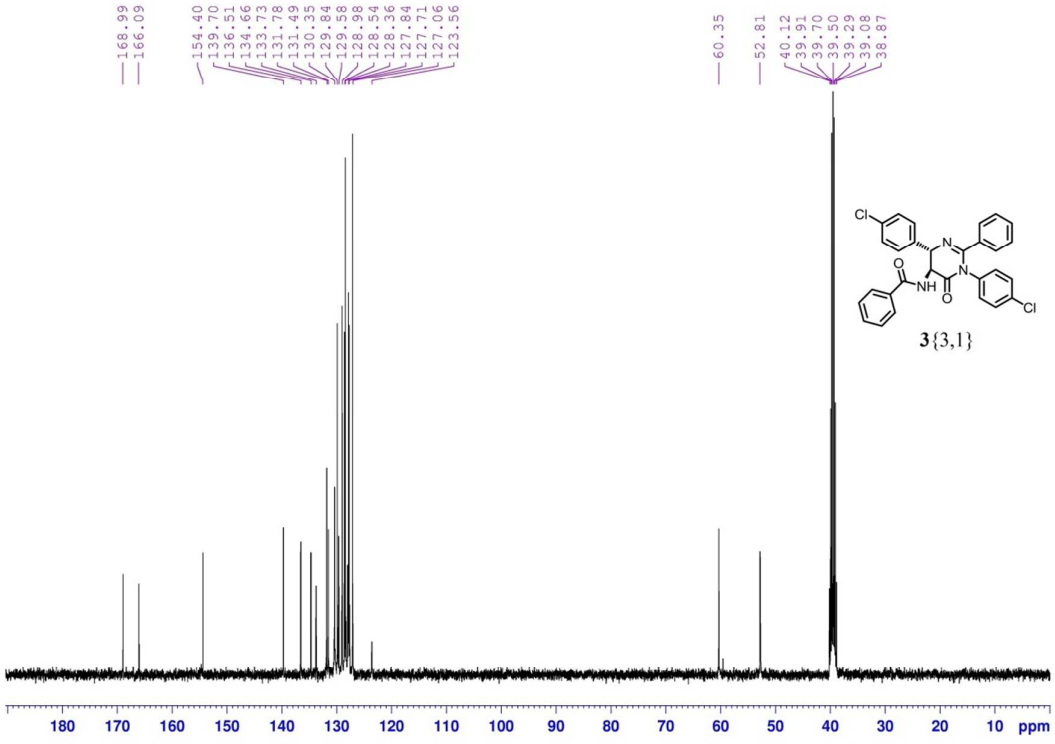
^{13}C NMR of **3**{2,1}



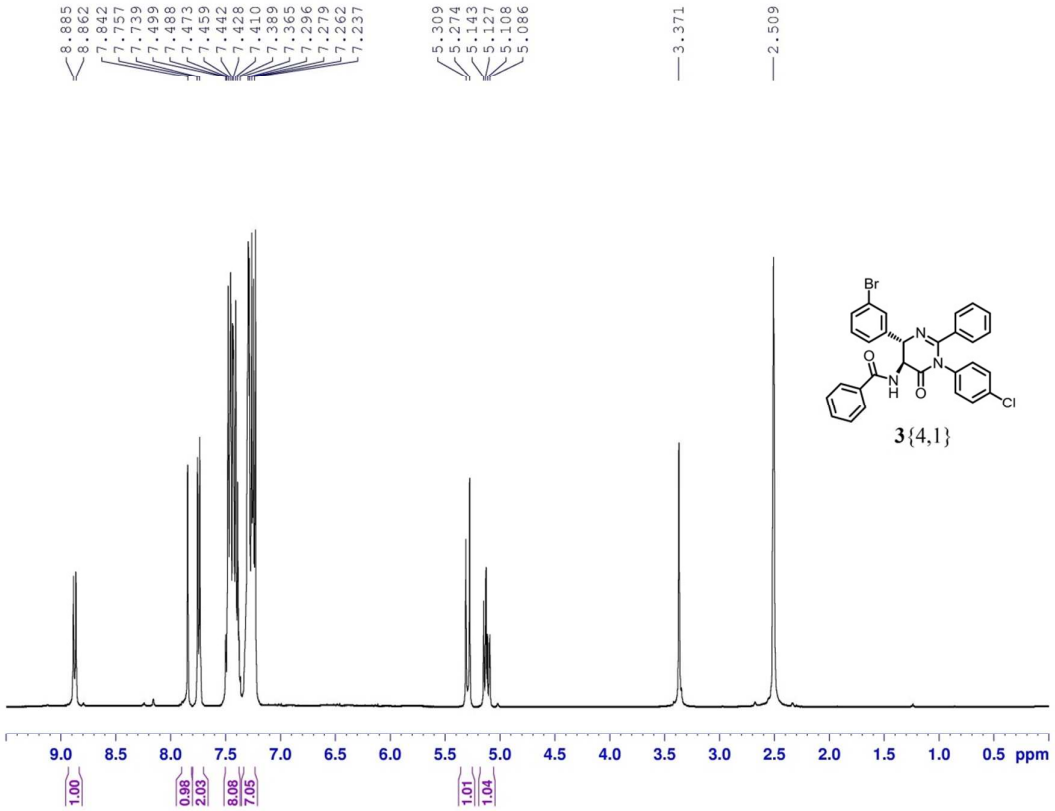
^{1}H NMR of **3**{3,1}



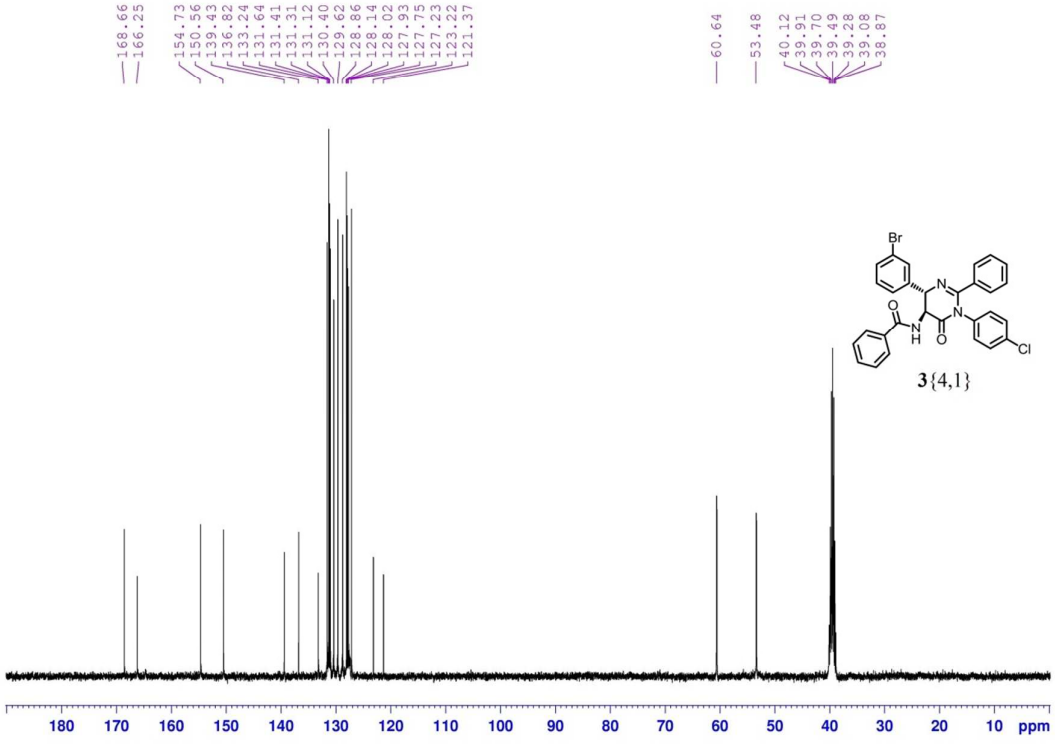
^{13}C NMR of **3**{3,1}



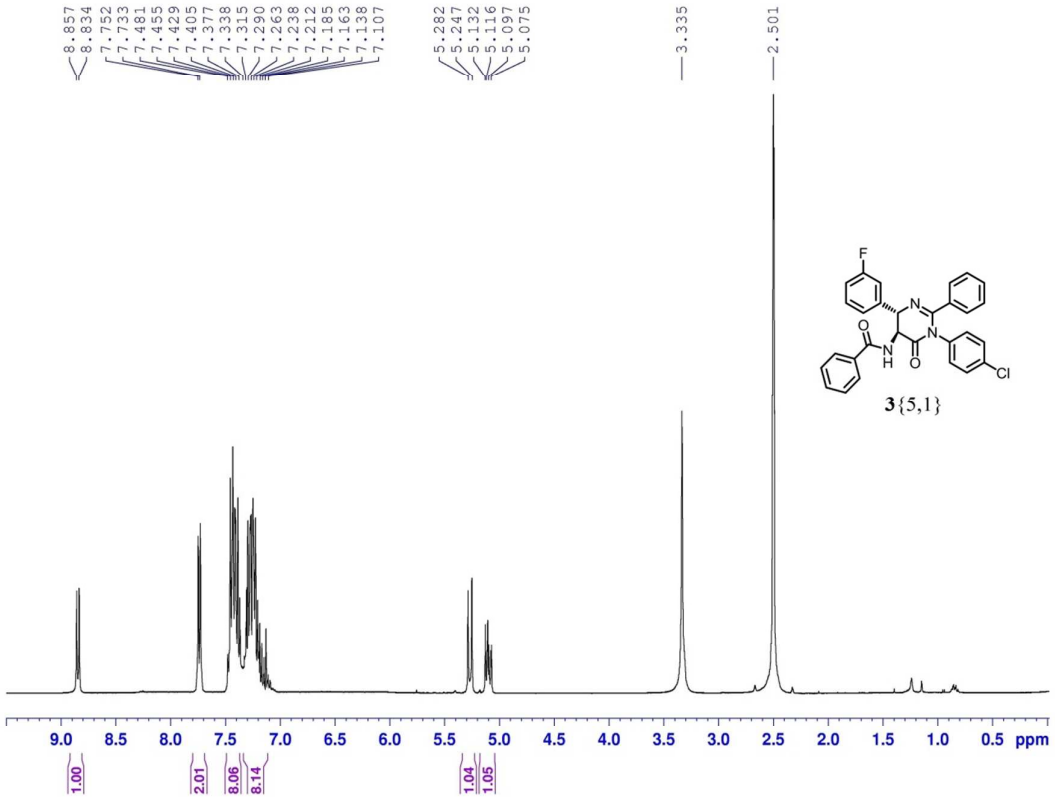
^{1}H NMR of **3**{4,1}



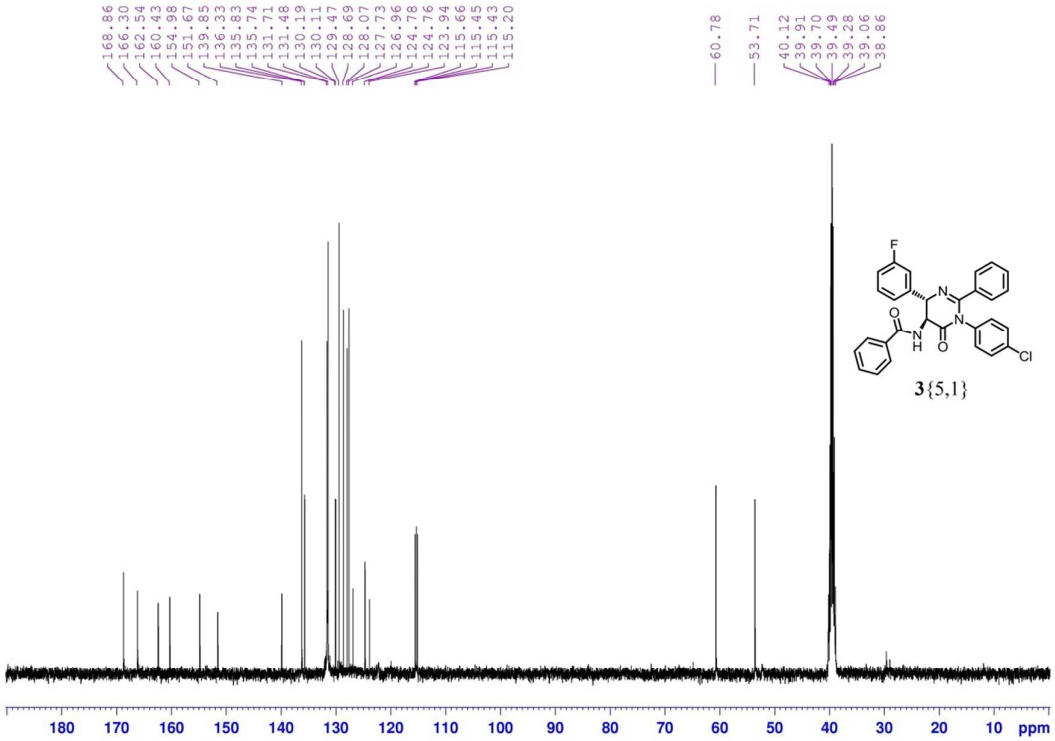
^{13}C NMR of **3**{4,1}



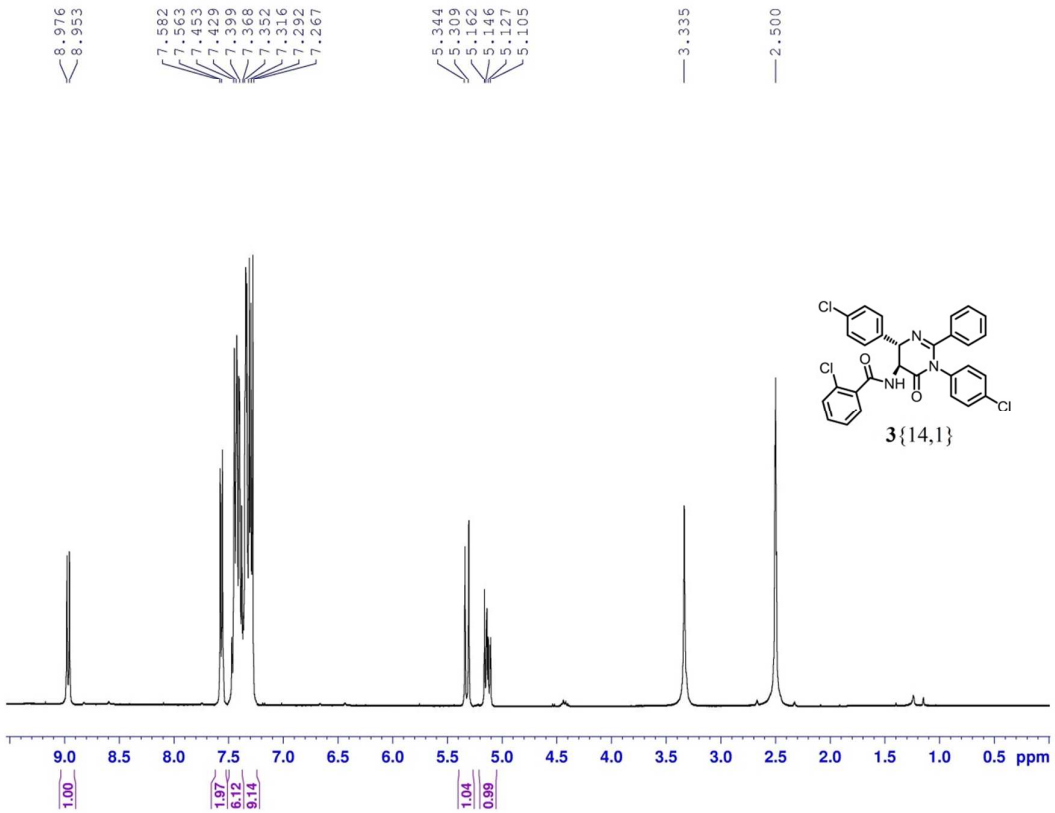
^{1}H NMR of **3**{5,1}



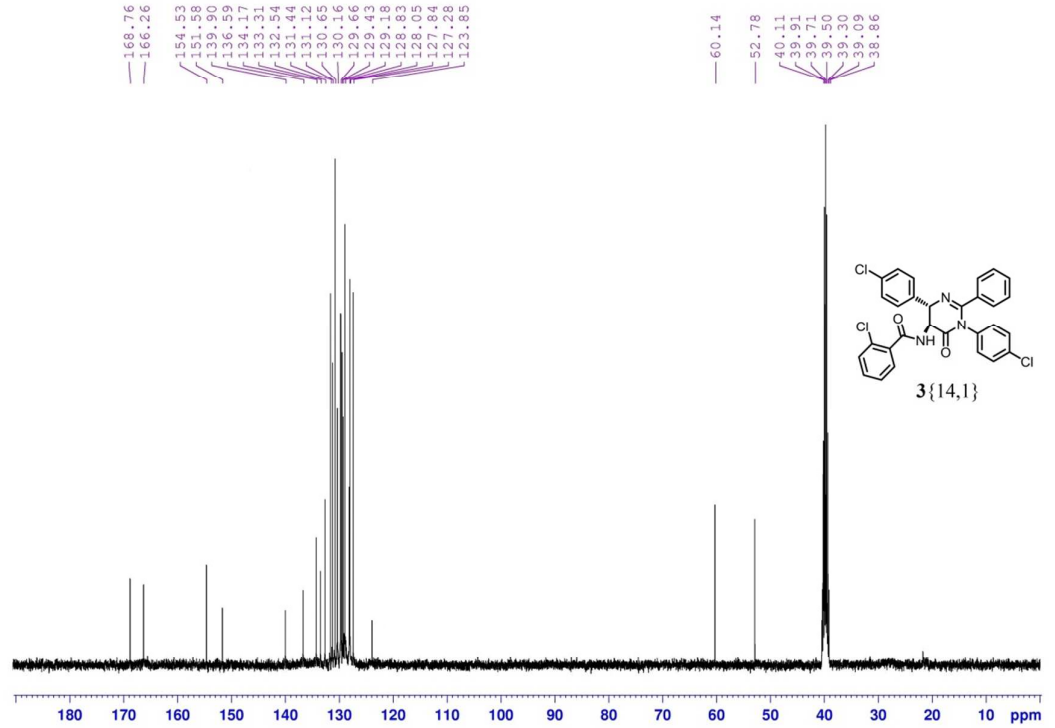
^{13}C NMR of **3**{5,1}



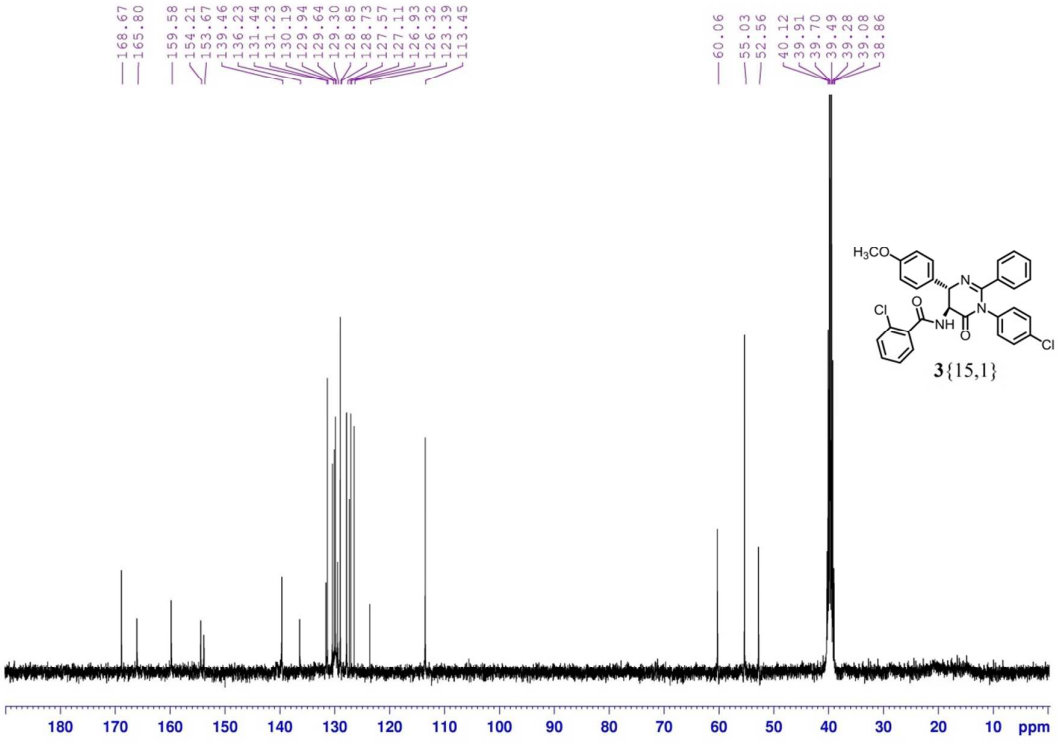
^{1}H NMR of **3**{14,1}



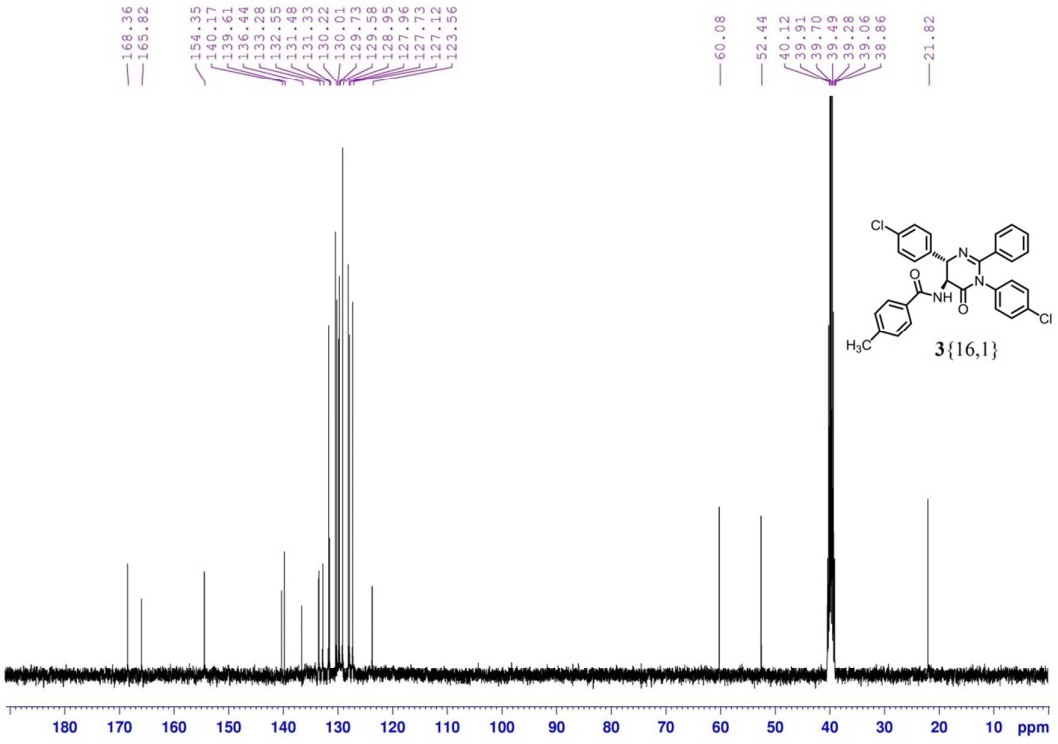
^{13}C NMR of **3**{14,1}



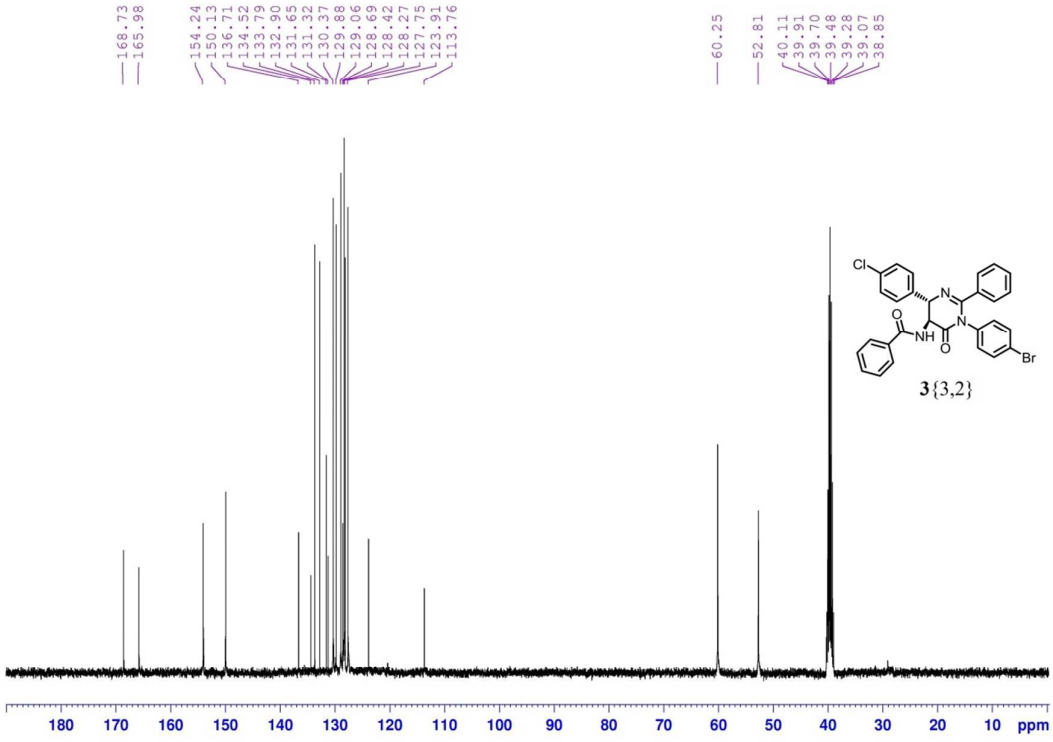
^{13}C NMR of **3**{15,1}



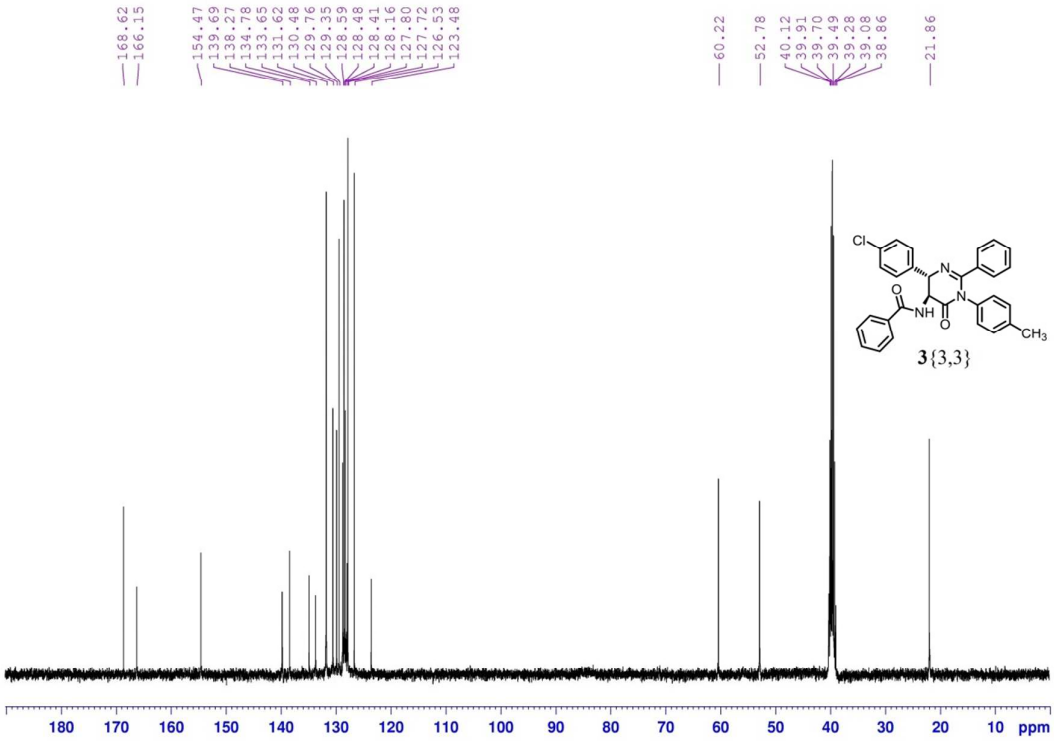
^{13}C NMR of **3**{16,1}



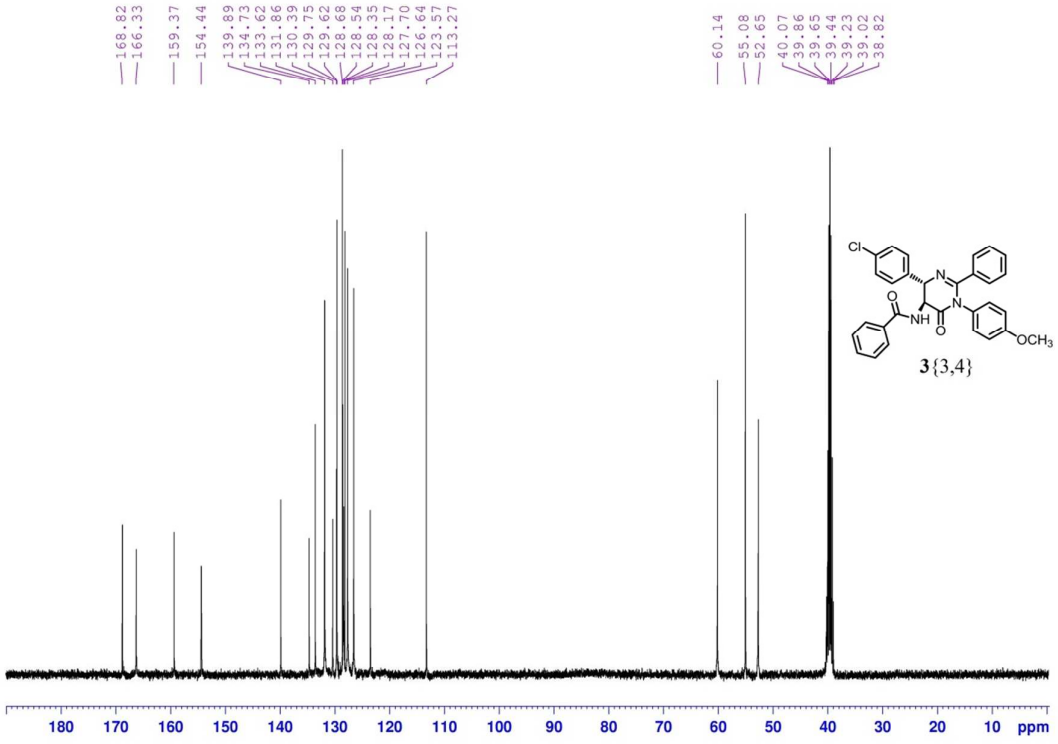
^{13}C NMR of **3**{3,2}



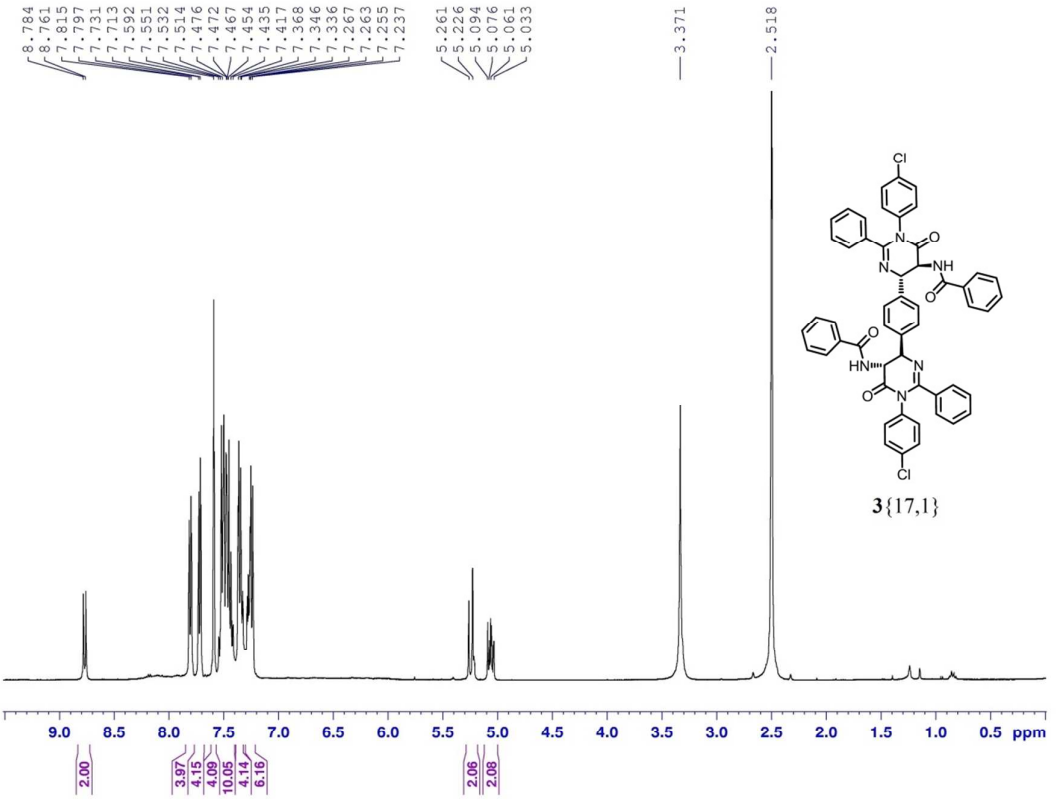
^{13}C NMR of **3**{3,3}



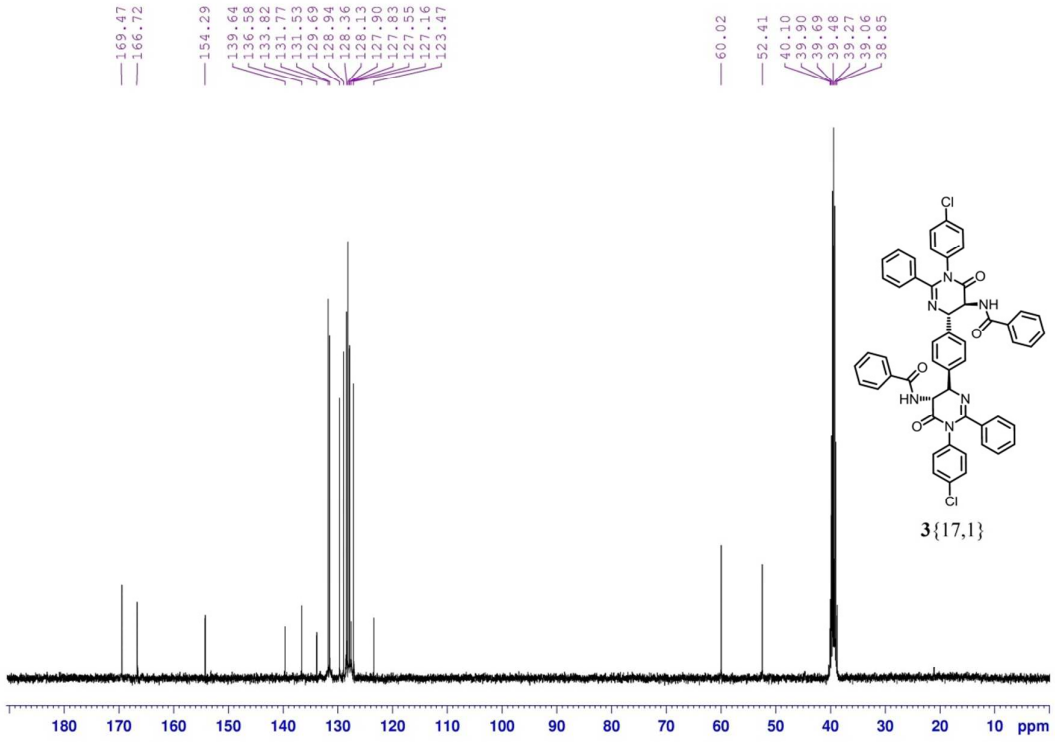
^{13}C NMR of **3**{3,4}



^{1}H NMR of **3**{17,1}

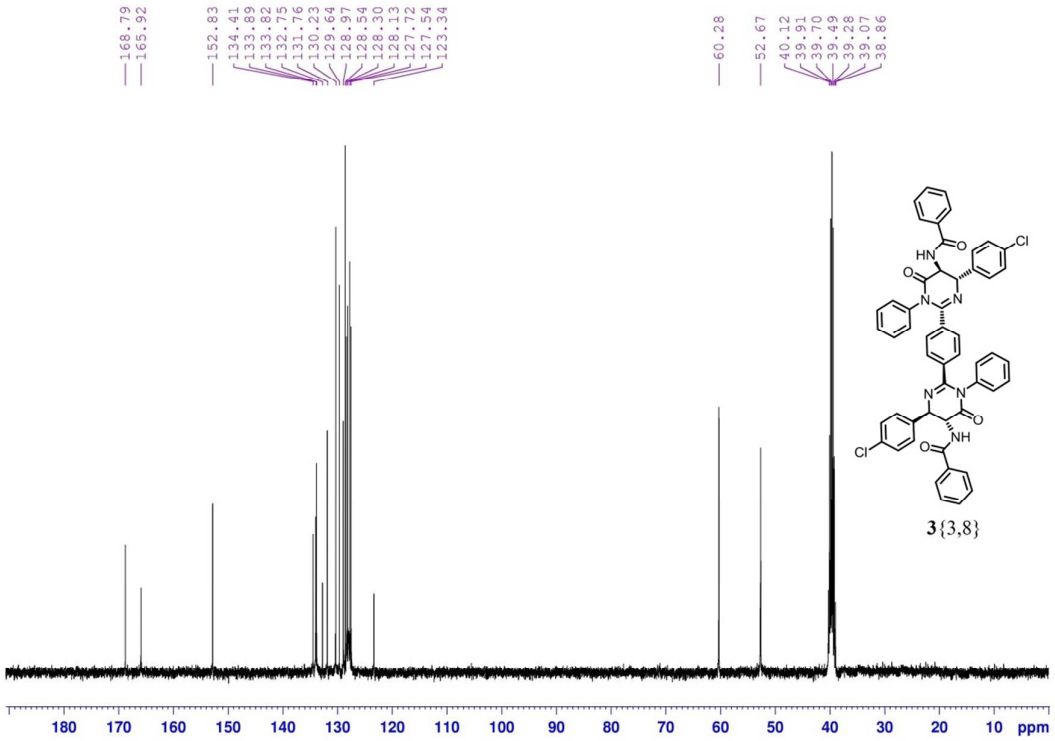


^{13}C NMR of **3**{17,1}



3{17,1}

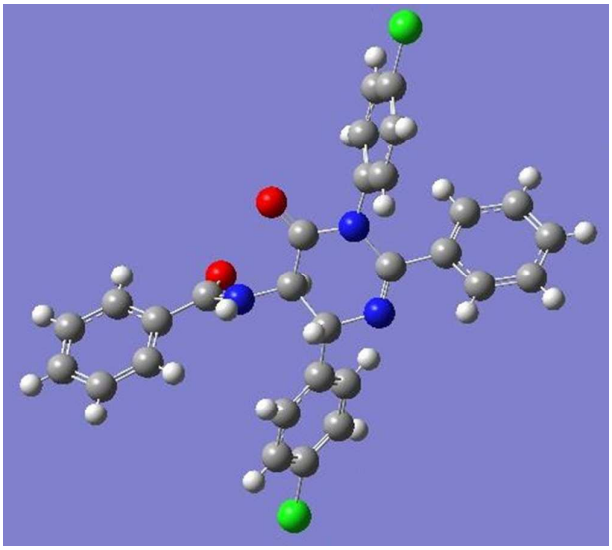
^{13}C NMR of **3**{3,8}



3{3,8}

5. Crystallographic Data for Compound 3{3,1}

X-ray crystal structure of compound **3**{3,1} (after purification and crystallization of the major product)



Crystal data and structure refinement for compound **3**{3,1}

Empirical formula	$C_{29}H_{21}Cl_2N_3O_2$	
Formula weight	514.10	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pna2(1)	
Unit cell dimensions	a = 29.879(6) Å	α = 90°
	b = 10.897(2) Å	β = 90°
	c = 9.1788(18) Å	γ = 90°
Volume	2988.5(10) $Å^3$	
Z	4	
Calculated density	1.317 Mg/m^3	
Absorption coefficient	0.324 mm^{-1}	
F(000)	1232	
Theta range for data collection	2.77 to 25.00°	

Limiting indices	-35<=h<=35, -12<=k<=11, -10<=l<=10
Reflections collected / unique	9566 / 4944 [R(int) = 0.0490]
Completeness to theta = 25.00	98.3 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4944 / 1 / 371
Goodness-of-fit on F^2	0.931
Final R indices [I>2sigma(I)]	R1 = 0.0348, wR2 = 0.0580
R indices (all data)	R1 = 0.0945, wR2 = 0.0686
Largest diff. peak and hole	0.131 and -0.147 e.$Å^{-3}$

6. References

(1) (a) Paul, S.; Nanda, P.; Gupta, R.; Loupy, A. Calcium acetate catalyzed synthesis of 4-arylidene-2-phenyl-5(4*H*)-oxazolones under solvent-free conditions. *Tetrahedron Lett.* **2004**, *45*, 425-427. (b) Roiban, G.-D.; Soler, T.; Grosu, I.; Cativiela, C.; Urriolabeitia, E. P. Unsaturated 4,4'-bis-[5(4*H*)-oxazolones]: Synthesis and evaluation of their *ortho*-palladation through C–H bond activation. *Inorg. Chim. Acta* **2011**, *368*, 247-251.

(2) Patil, U. D.; Mahulikar, P. P. A convenient, $TiCl_4$/$SnCl_4$-mediated synthesis of *N*-phenyl or *N*-aryl benzamidines and *N*-phenylpicolinamidines. *ISRN Organic Chemistry* **2012**, *2012*, 1-6.