

Supplementary Material

Second Generation Analogs of the Cancer Drug Clinical Candidate Tipifarnib for Anti-Chagas Disease Drug Discovery

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4-(3-Chlorophenyl)-6-((4-chlorophenyl)(hydroxy)(1-methyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one (19). TLC ($\text{CH}_2\text{Cl}_2:\text{MeOH}$ 9:1 v/v): R_f = 0.45; ^1H NMR (300 MHz, CD_3OD , δ): 8.95 (d, J = 1.2 Hz, 1H), 7.78 (m, 2H), 7.51 (ddd, J = 1.5, 1.5, 9.0 Hz, 1H), 7.47 (d, J = 7.2 Hz, 1H), 7.41 (m, 2H), 7.35 (dd, J = 1.5, 1.5 Hz, 1H), 7.26 (m, 4H), 6.85 (d, J = 1.5 Hz, 1H), 6.66 (s, 1H), 3.83 (s, 3H), 3.69 (s, 3H) ESI-MS m/z 490.5 ($M + \text{H}^+$)⁺ MW: 490.4 g/mol. Mono-TFA salt FW: 604.40 g/mol.

4-(phenyl)-6-((4-chlorophenyl)(hydroxy)(1-methyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one. TLC ($\text{CH}_2\text{Cl}_2:\text{MeOH}$ 9:1 v/v): R_f = 0.45; ^1H NMR (300 MHz, CD_3OD , δ): 7.76 (dd, 1H), 7.70 (d, 1H), 7.63 (s, 1H), 7.46 (m, 3H), 7.38 (d, J = 2.1 Hz 1H), 7.31 (m, 4H), 7.20 (m, 2H), 6.94 (d, J = 0.6 Hz 1H), 6.63 (s, 1H), 3.83 (s, 3H), 3.44 (s, 3H) ESI-MS m/z 457.0 ($M + \text{H}^+$)⁺ MW: 455.94 g/mol.

4-(phenyl)-6-((4-chlorophenyl)(methoxy)(1-methyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one (10) 6.5 mg (0.014 mmols) of the previous compound was dissolved in 10 mL of MeOH and 6.5 mg tunic acid was added. The reaction was heated to reflux for 48 hours. One spot by TLC. Solvents were removed under reduced pressure to produce a colorless, oily semi-solid. Product was purified by HPLC using a water-methanol gradient with 0.08% v/v trifluoroacetic acid. 0-5 minutes 20% MeOH, 5-25 minutes 20-65% MeOH, 25-30 minutes 65-100% MeOH. Product elutes at 27.8 minutes. 5.6 mg (0.0096 mmols) produced as a mono-TFA salt. Yield 67%. TLC ($\text{CH}_2\text{Cl}_2:$ MeOH 9:1 v/v): R_f = 0.55; ^1H NMR (300 MHz, CD_3OD , δ): 9.00 (s, 1H), 7.80 (dd, 1H), 7.75 (d, 1H), 7.57 (m, 5H), 7.40 (m, 6H), 6.70 (s, 1H), 3.82 (s, 3H), 3.55 (s, 3H) 3.22 (s, 3H) ESI-MS m/z 470.4 ($M + \text{H}^+$)⁺ MW: 469.96 g/mol. Mono-TFA salt FW: 583.99 g/mol.

4-(4-chlorophenyl)-6-((4-chlorophenyl)(methoxy)(1-methyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one (11). TLC (CH₂Cl₂: MeOH 9:1 v/v): R_f = 0.55; ¹H NMR (300 MHz, CD₃OD, δ): 9.00 (s, 1H), 7.83 (dd, *J* = 9.0, 2.4 Hz, 1H), 7.73 (d, *J* = 9 Hz, 1H), 7.62 (d, *J* = 1.5 Hz, 1H), 7.54 (m, 3H), 7.39 (m, 6H), 6.67 (s, 1H), 3.81 (s, 3H), 3.56 (s, 3H) 3.23 (s, 3H) ESI-MS m/z 504.6 (M + H⁺)⁺ MW: 504.41 g/mol. Mono-TFA salt FW: 618.43 g/mol.

4-(3-chlorophenyl)-6-((4-chlorophenyl)(methoxy)(1-methyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one (3). TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.55; ¹H NMR (300 MHz, CD₃OD, δ): 9.01 (s, 1H), 7.85 (dd, *J* = 9.1 Hz, 2.1 Hz, 1H), 7.74 (d, *J* = 9.0 Hz, 1H), 7.62 (d, *J* = 1.5 Hz, 1H), 7.53 (m, 3H), 7.44 (m, 1H), 7.40 (s, 4H), 7.35 (m, 1H), 6.68 (s, 1H), 3.81 (s, 3H), 3.56 (s, 3H) 3.24 (s, 3H) ESI-MS m/z 504.6 (M + H⁺)⁺ MW: 504.41 g/mol. Mono-TFA salt FW: 618.43 g/mol.

4-(4-Fluorophenyl)-6-((4-chlorophenyl)(methoxy)(1-methyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one (12). TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.55; ¹H NMR (300 MHz, CD₃OD, δ): 9.00 (s, 1H), 7.82 (dd, *J* = 8.9, 2.4 Hz, 1H), 7.73 (d, *J* = 9 Hz 1H), 7.61 (d, *J* = 1.2 Hz, 1H), 7.53 (d, *J* = 2.1 Hz, 1H), 7.43 (m, 6H), 7.28 (m, 2H), 6.65 (s, 1H), 3.81 (s, 3H), 3.56 (m, 3H) 3.23 (s, 3H), ESI-MS m/z 488.5 (M + H⁺)⁺ MW: 487.95 g/mol. Mono-TFA salt FW: 601.98 g/mol.

4-(3-fluorophenyl)-6-((4-chlorophenyl)(methoxy)(1-methyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one (6). TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.55; ¹H NMR (300 MHz, CD₃OD, δ): 8.96 (s, 1H), 7.79 (dd, *J* = 9.0, 2.1 Hz, 1H), 7.70 (d, *J* = 8.7 Hz 1H), 7.57 (d, *J* = 1.5 Hz 1H), 7.50 (m, 2H), 7.36 (s, 4H), 7.20 (m, 3H), 6.64 (s, 1H), 3.77 (s, 3H), 3.51 (s, 3H) 3.19 (s, 3H) ESI-MS m/z 488.5 (M + H⁺)⁺ MW: 487.95 g/mol. Mono-TFA salt FW: 601.98 g/mol.

4-(2-fluorophenyl)-6-((4-chlorophenyl)(methoxy)(1-methyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one (9). TLC (CH₂Cl₂:MeOH 9:1 v/v): [R_f = 0.55; ¹H

NMR (300 MHz, CD₃OD, δ): 8.97 (m, 1H), 7.75 (m, 2H), 7.56 (m, 2H), 7.40-7.15 (m, 8H), 6.66 (s, 1H), 3.77 (s, 3H), 3.49 (m, 3H) 3.16 (s, 3H) ESI-MS m/z 488.5 (M + H⁺)⁺ MW: 487.95 g/mol. Mono-TFA salt FW: 601.98 g/mol.

4-(4-Methylphenyl)-6-((4-chlorophenyl)(methoxy)(1-methyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one (13). TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.55; ¹H NMR (300 MHz, CD₃OD, δ): 8.85 (s, 1H), 7.78 (dd, J = 9.0, 1.2 Hz, 1H), 7.68 (d, J = 9.0 Hz, 1H), 7.56 (d, J = 2.1 Hz, 1H), 7.50 (d, J = 1.5 Hz, 1H), 7.35 (s, 4H), 7.30 (d, J = 7.8 Hz, 2H), 7.23 (d, J = 8.1 Hz, 2H), 6.59 (s, 1H), 3.77 (s, 3H), 3.49 (s, 3H), 3.18 (s, 3H) ESI-MS m/z 484.6 (M + H⁺)⁺ MW: 483.99 g/mol. Mono-TFA salt FW: 598.01 g/mol.

4-(3-Methylphenyl)-6-((4-chlorophenyl)(methoxy)(1-methyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one (7). TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.55; ¹H NMR (300 MHz, CD₃OD, δ): 8.96 (s, 1H), 7.77 (dd, J = 9.0, 2.1 Hz, 1H), 7.68 (d, J = 9.0 Hz, 1H), 7.55 (m, 2H), 7.34 (m, 7H), 7.14 (m, 2H), 6.59 (s, 1H), 3.76 (s, 3H), 3.50 (s, 3H) 3.17 (s, 3H) ESI-MS m/z 484.5 (M + H⁺)⁺ MW: 483.99 g/mol. Mono-TFA salt FW: 598.01 g/mol.

4-(2-Methylphenyl)-6-((4-chlorophenyl)(methoxy)(1-methyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one (4). TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.55; ¹H NMR (300 MHz, CD₃OD, δ): 8.94 (m, 1H), 7.74 (m, 2H), 7.50 (m, 1H), 7.34 (m, 7H), 7.13 (m, 1H), 7.07 (m, 1H), 6.56 (s, 1H), 3.79 (s, 3H), 3.48 (m, 3H) 3.13 (m, 3H), 1.95 (m, 3H) ESI-MS m/z 484.5 (M + H⁺)⁺ MW: 483.99 g/mol. Mono-TFA salt FW: 598.01 g/mol.

4-(2,6-Dimethylphenyl)-6-((4-chlorophenyl)(methoxy)(1-methyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one (14). TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.55; ¹H NMR (300 MHz, CD₃OD, δ): 8.97 (s, 1H), 7.81 (d, J = 9.0 Hz, 2.1 Hz, 1H), 7.73 (d, J = 9.0 Hz, 1H), 7.50 (d, J = 1.5 Hz, 1H), 7.31 (m, 5H), 7.17 (m, 2H), 6.97 (d, J = 2.1 Hz, 1H), 6.55 (s, 1H), 3.82 (s, 3H), 3.50 (s, 3H) 3.14 (s, 3H), 1.94 (m, 6H) ESI-MS m/z 498.5 (M + H⁺)⁺ MW: 498.02 g/mol. Mono-TFA salt FW: 612.04 g/mol.

4-(3,5-Dimethylphenyl)-6-((4-chlorophenyl)(methoxy)(1-methyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one (17). TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.55; ¹H NMR (300 MHz, CD₃OD, δ): 9.01 (s, 1H), 7.83 (dd, *J* = 9 Hz, 2.1 Hz, 1H), 7.73 (d, *J* = 9 Hz, 1H), 7.60 (m, 2H), 7.39 (m, 4H), 7.17 (s, 1H), 6.99 (m, 2H), 6.62 (s, 1H), 3.81 (s, 3H), 3.56 (s, 3H) 3.23 (s, 3H), 2.39 (s, 6H) [ESI-MS m/z 518.6 (M + H⁺)⁺] MW: 498.02 g/mol. Mono-TFA salt FW: 612.04 g/mol.

4-(3-Trifluoromethylphenyl)-6-((4-chlorophenyl)(methoxy)(1-methyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one (8). TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.55; ¹H NMR (300 MHz, CD₃OD, δ): 8.97 (s, 1H), 7.78 (m, 6H), 7.61 (s, 1H), 7.49 (d, *J* = 2.1 Hz, 1H), 7.39 (s, 4H), 6.73 (s, 1H), 3.83 (s, 3H), 3.54 (s, 3H) 3.22 (s, 3H) ESI-MS m/z 538.5 (M + H⁺)⁺ MW: 537.96 g/mol. Mono-TFA salt FW: 651.98 g/mol.

4-(2-Trifluoromethylphenyl)-6-((4-chlorophenyl)(methoxy)(1-methyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one (5). This compound was prepared as for analogous compounds but with the following modification. Coupling of 2-trifluoromethylbenzylbromide to the Weinreb amide via was done at 0 °C in ether as solvent. TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.55; ¹H NMR (300 MHz, CD₃OD, δ): 8.97 (m, 1H), 7.80 (m, 5H), 7.48 (m, 1H), 7.34 (m, 5H), 7.35 (m, 5H), 6.96 (m, 1H), 6.65 (s, 1H), 3.83 (s, 3H), 3.50 (m, 3H) 3.14 (m, 3H) ESI-MS m/z 538.4 (M + H⁺)⁺ MW: 537.96 g/mol. Mono-TFA salt FW: 651.98 g/mol.

4-(3-chlorophenyl)-6-((β-naphthyl)(methoxy)(1-methyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one (18). TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.55; ¹H NMR (300 MHz, CD₃OD, δ): 8.62 (s, 1H), 7.82 (m, 4H), 7.71 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.55 (m, 3H), 7.47 (d, *J* = 9.0 Hz, 1H), 7.40 (m, 2H), 7.33 (m, 3H), 7.18 (d, *J* = 7.5 Hz, 1H), 6.72 (s, 1H), 3.77 (s, 3H), 3.52 (s, 3H) 3.24 (s, 3H) ESI-MS m/z 520.5 (M + H⁺)⁺ MW: 520.02 g/mol. Mono-TFA salt FW: 634.04 g/mol.

4-(2,6-Dichlorophenyl)-6-((4-chlorophenyl)(methoxy)(1-methyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one (15). TLC (CH₂Cl₂: MeOH 9:1 v/v): R_f = 0.55; ¹H NMR (300 MHz, CD₃OD, δ): 8.99 (s, 1H), 7.82 (dd, *J* = 9.0, 1.8 Hz, 1H), 7.76 (d, *J* = 9.0 Hz, 1H), 7.55 (m, 4H), 7.35 (m, 4H), 6.95 (d, *J* = 2.1 Hz, 1H), 6.66 (s, 1H), 3.83 (s, 3H), 3.53 (s, 3H) 3.18 (s, 3H), ESI-MS m/z 538.6 (M + H⁺)⁺ MW: 538.85 g/mol. Mono-TFA salt FW: 652.88 g/mol.

4-(3-Chlorophenyl)-6-((4-chlorophenyl)(methylamino)(1-ethyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one (25). TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.45; ¹H NMR (300 MHz, CD₃OD, δ): 9.05 (s, 1H), 7.83 (dd, *J* = 8.7, 1.8 Hz, 1H), 7.77 (d, *J* = 9.0 Hz, 1H), 7.45 (m, 10H), 6.70 (s, 1H), 4.10 (q, 2H), 3.84 (s, 3H), 2.20 (s, 3H), 1.15 (t, 3H) ESI-MS m/z 517.5 (M + H⁺)⁺ MW: 517.45 g/mol. Bis-TFA salt FW: 745.50 g/mol.

4-(3-Chlorophenyl)-6-((4-chlorophenyl)(amino)(1-ethyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one (24). TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.45; ¹H NMR (300 MHz, CD₃OD, δ): 8.98 (s, 1H), 7.85 (m, 2H), 7.46 (m, 4H), 7.32 (m, 1H), 7.22 (m, 4H), 7.02 (s, 1H), 6.85 (d, *J* = 1.5 Hz, 1H), 6.68 (s, 1H), 3.97 (m, 2H), 3.84 (s, 3H), 1.27 (t, 3H) ESI-MS m/z 503.3 (M + H⁺)⁺ MW: 503.42 g/mol. Bis-TFA salt FW: 731.47.

4-(3-Chlorophenyl)-6-((4-chlorophenyl)(methoxy)(1-ethyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one (26). TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.45; ¹H NMR (300 MHz, CD₃OD, δ): 9.15 (s, 1H), 7.85 (dd, *J* = 9.0, 2.1 Hz, 1H), 7.75 (d, *J* = 9.0 Hz, 1H), 7.54 (m, 3H), 7.47 (m, 1H), 7.37 (m, 6H), 6.68 (s, 1H), 4.00 (m, 2H), 3.81 (s, 3H), 3.24 (s, 3H), 1.26 (t, 3H) ESI-MS m/z 518.6 (M + H⁺)⁺ MW: 518.43 g/mol. Mono-TFA salt FW: 632.46 g/mol.

4-(3-Chlorophenyl)-6-((4-chlorophenyl)(hydroxy)(1-ethyl-1H-imidazol-5-yl)methyl)-1-methylquinolin-2(1H)-one (27). TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.45; ¹H NMR (300 MHz, CD₃OD, δ): 9.09 (s, 1H), 7.84 (dd, *J* = 9.0, 2.1 Hz, 1H), 7.78 (d, *J* = 9.0 Hz, 1H) 7.47 (m, 4H), 7.36 (m, 1H), 7.27 (m, 4H), 6.83 (d, *J* = 1.5 Hz, 1H), 6.68 (s, 1H), 4.13 (m,

2H), 3.85 (s, 3H), 1.35 (t, 3H) ESI-MS m/z 504.6 ($M + H^+$)⁺ MW: 504.41 g/mol. Mono-TFA salt FW: 618.43 g/mol.

4-(3-Chloro-phenyl)-6-[methoxy-(3-methyl-3*H*-imidazol-4-yl)-*p*-tolyl-methyl]-1-methyl-1*H*-quinolin-2-one (28). TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.55; ¹H NMR (300 MHz, CD₃OD, δ): 8.98 (s, 1H), 7.85 (dd, J = 9.1 Hz, 2.1 Hz, 1H), 7.73 (d, J = 9.0 Hz, 1H), 7.57-7.52 (m, 3H), 7.50 (d, J = 3.2 Hz 3H), 7.44-7.43 (m, 1H), 7.36-7.33 (m, 1H), 7.28-7.18 (m, 5H), 6.66 (s, 1H), 3.80 (s, 3H), 3.55 (s, 3H) 3.22 (s, 3H), 2.33 (s, 3H) ESI-MS m/z 484.5 ($M + H^+$)⁺ MW: 483.99 g/mol. Mono-TFA salt FW: 598.01 g/mol.

4-(3-Chloro-phenyl)-6-[methoxy-(3-methyl-3*H*-imidazol-4-yl)-(4-trifluoromethyl-phenyl)-methyl]-1-methyl-1*H*-quinolin-2-one (29). TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.50; ¹H NMR (300 MHz, CD₃OD, δ): 9.01 (s, 1H), 7.88 (dd, J = 9.0 Hz, 2.4 Hz, 1H), 7.78- 7.61 (m, 6H), 7.56-7.51 (m, 3H), 7.44-7.43 (m, 1H), 7.38-7.32 (m, 1H), 6.65 (s, 1H), 3.79 (s, 3H), 3.54 (s, 3H) 3.26 (s, 3H) ESI-MS m/z 538.5 ($M + H^+$)⁺ MW: 537.96 g/mol. Mono-TFA salt FW: 651.98 g/mol.

4-(3-Chloro-phenyl)-6-[(4-ethyl-phenyl)-methoxy-(3-methyl-3*H*-imidazol-4-yl)-methyl]-1-methyl-1*H*-quinolin-2-one (30). TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.55; ¹H NMR (300 MHz, CD₃OD, δ): 9.00 (s, 1H), 7.84 (dd, J = 9.1 Hz, 3.0 Hz, 1H), 7.74 (d, J = 9.0 Hz, 1H), 7.60-7.52 (m, 3H), 7.45-7.43 (m, 1H), 7.37-7.33 (m, 1H), 7.32-7.22 (m, 4H), 6.67 (s, 1H), 3.80 (s, 3H), 3.55 (s, 3H) 3.22 (s, 3H), 2.88 (q, J = 3.3 Hz, 1.8 Hz, 2H), 1.21 (t, J = 7.2 Hz, 3H) ESI-MS m/z 498.5 ($M + H^+$)⁺ MW: 498.02 g/mol. Mono-TFA salt FW: 612.04 g/mol.

4-(3-Chloro-phenyl)-6-[(4-isopropyl-phenyl)-methoxy-(3-methyl-3*H*-imidazol-4-yl)-methyl]-1-methyl-1*H*-quinolin-2-one (31). TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.55; ¹H NMR (300 MHz, CD₃OD, δ): 8.98 (s, 1H), 7.84 (dd, J = 9.3 Hz, 2.4 Hz, 1H), 7.73 (d, J = 9.0 Hz, 1H), 7.58-7.51 (m, 4H), 7.46-7.44 (m, 1H), 7.34-7.24 (m, 5H), 6.68 (s, 1H),

3.83(s, 3H), 3.55 (s, 3H) 3.23 (s, 3H), 2.58-2.55 (m, 1H), 1.20 (d, J = 6.9 Hz, 6H) ESI-MS m/z 512.6 ($M + H$)⁺ MW: 511.20 g/mol. Mono-TFA salt FW: 626.07 g/mol.

4-Biphenyl-3-yl-6-[(4-chloro-phenyl)-methoxy-(3-methyl-3*H*-imidazol-4-yl)-methyl]-1-methyl-1*H*-quinolin-2-one (32). TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.55; ¹H NMR (300 MHz, CD₃OD, δ): 8.95 (s, 1H), 7.85-7.70 (m, 3H), 7.69-7.53 (m, 6H), 7.52-7.48 (m, 2H), 7.45-7.32 (m, 4H), 7.25 (d, J = 9.0 Hz, 2H), 6.66 (s, 1H), 4.06 (s, 2H), 3.83 (s, 3H), 3.51 (s, 3H) 3.21 (s, 3H) ESI-MS m/z 546.6 ($M + H$)⁺ MW: 546.06 g/mol. Mono-TFA salt FW: 660.08 g/mol.

4-(3-Benzyl-phenyl)-6-[(4-chloro-phenyl)-methoxy-(3-methyl-3*H*-imidazol-4-yl)-methyl]-1-methyl-1*H*-quinolin-2-one (33). TLC (CH₂Cl₂:MeOH 9:1 v/v): R_f = 0.55; ¹H NMR (300 MHz, CD₃OD, δ): 9.02 (s, 1H), 7.73 (dd, J = 6.6 Hz, 3.0 Hz, 1H), 7.66 (d, J = 12.0 Hz, 1H), 7.58 (dd, J = 4.5 Hz, 3.0 Hz, 2H), 7.50-7.38 (m, 2H), 7.37-7.20 (m, 11H), 6.61 (s, 1H), 4.06 (s, 2H), 3.78 (s, 3H), 3.51 (s, 3H) 3.24 (s, 3H) ESI-MS m/z 560.6 ($M + H$)⁺ MW: 560.08 g/mol. Mono-TFA salt FW: 674.11 g/mol.

11/04/06 MeOD m/z = 518, Methyl ether of JK-4

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