Supporting Information

A Copper-Catalyzed One-Pot Process to Construct Triazole-Linked Urea Derivatives

Kung-Kai Kuo,^a Siva Senthil Kumar Boominathan,^b Jaya Kishore Vandavasi,^b
Jia-Shing Hsiao,^b Jeh-Jeng Wang^b and Wan-Ping Hu^{c,*}

^a*Department of Surgery, School of Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan.*

^b*Department of Medicinal and Applied Chemistry, Kaohsiung Medical University, Kaohsiung, Taiwan.*

^c*Department of Biotechnology, Kaohsiung Medical University, Kaohsiung, Taiwan.*

Email: wphu@kmu.edu.tw

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General information:

All chemicals were purchased from best grade in commercially available and are used without further purification. All solvents were purchased as HPLC grade and used without any purification or distillation. Analytical thin layer chromatography was performed on aluminum plate coated with silica gel (Merck). Gravity column chromatography was performed using 100-200 mesh silica gel and mixtures of hexane-ethyl acetate were used for elution. Visualization was accomplished using ultraviolet light (254 nm) and chemical staining with acidic potassium permanganate solution and Iodine.

Melting points were determined using "Mel-Temp" melting point apparatus and were uncorrected. Proton nuclear magnetic resonance (^1H NMR) and Carbon nuclear magnetic resonance (^{13}C NMR) spectra's were recorded using a Varian (400 MHz) spectrometer. All spectra were recorded at ambient temperature (298 K). Chemical shifts (δ) are quoted in ppm relative to residual solvent (CHCl_3 : $\delta = 7.26$ ppm for ^1H and $\delta = 77.0$ for ^{13}C ; $(\text{CD}_3)_2\text{SO}$: $\delta = 2.50$ ppm for ^1H). Coupling constants (J) are corrected and quoted to the nearest 0.1 Hz. The following abbreviations are used to indicate the multiplicity of the signals: s = singlet; d = doublet; t = triplet; q = quartet; m = multiplet; bs = broad singlet; dt = doublet of triplet; td = triplet of doublet. High resolution mass spectra (HRMS) were measured on a Micromass Q-TOF spectrometer using EI (electron impact, 70 eV) at the Joint Center for High valued Instruments.

General Experiment Procedure (4a-v):

An oven-dried 50 mL round bottom flask equipped with a magnetic stir bar was charged with Compound **1** (1.0 mmol), **2** (1.0 mmol), **3** (1.0 mmol), $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ (10 mol %), L-ascorbic acid (20 mol %) and DMSO (4.0 mL). The mixture was stirred under open air atmosphere at 60 °C (oil bath temperature) for about 14 hours (checked by TLC). After the starting materials were completely consumed, the reaction mixture was cooled to room temperature, quenched with 15 mL of water, and extracted with ethyl acetate

(3 × 10 mL). The organic layer was washed with saturated salt water and concentrated under reduced pressure. The residue was purified by column chromatography to afford the pure product.

Spectral Characterization Data (4a-v):

1-(2-((1-(2-iodophenyl)-1H-1,2,3-triazol-4-yl)methylcarbamoyl)phenyl)-3-phenylurea (4a):

Light yellow solid; m.p. 155-157 °C; ^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 10.21 (s, 1H), 9.68 (s, 1H), 9.34 (t, J = 5.6 Hz, 1H), 8.38 (s, 1H), 8.23 (dd, J = 7.6, 0.8 Hz, 1H), 8.07 (dd, J = 8.0, 1.2 Hz, 1H), 7.73 (dd, J = 8.0, 2.4 Hz, 1H), 7.59-7.44 (m, 5H), 7.35 (dt, J = 7.6, 2.4 Hz, 2H), 7.27 (t, J = 8.0 Hz, 1H), 7.06 (t, J = 7.8 Hz, 1H), 6.97 (t, J = 7.2 Hz, 1H), 4.68 (d, J = 5.6 Hz, 2H). ^{13}C NMR (100

MHz, $\text{DMSO}-d_6$): δ 168.6, 152.5, 145.1, 139.95, 139.93, 139.8, 131.9, 131.7, 129.5, 128.8, 128.1, 128.0, 124.9, 122.1, 121.2, 121.0, 120.8, 118.7, 95.5, 34.9; HRMS (ESI) $\text{C}_{23}\text{H}_{20}\text{O}_2\text{N}_6\text{I}$ $[\text{M}+\text{H}]^+$ calcd for 539.0687 found 539.0669.

1-(2-((1-(3-methoxyphenyl)-1H-1,2,3-triazol-4-yl)methylcarbamoyl)phenyl)-3-phenylurea (4b):

Yield: (%) Light yellow solid; m.p. 185-187 °C; ^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ = 10.19 (s, 1H), 9.37 (s, 1H), 8.91 (t, J = 5.6 Hz, 1H), 8.38 (s, 1H), 8.31 (d, J = 7.6 Hz, 1H), 7.69-7.65 (m, 1H), 7.52 (d, J = 8.4 Hz, 2H), 7.41-7.32 (m, 4H), 7.23 (t, J = 5.6 Hz, 2H), 7.01-6.92 (m, 3H), 4.72 (d, J = 5.6

Hz, 2H), 3.84 (s, 3H). ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ 168.8, 160.0, 152.6, 145.7, 139.6, 139.4, 137.5, 131.18, 131.1, 128.1, 127.4, 121.6, 120.8, 120.67, 120.62, 118.5, 113.7, 111.7, 105.6, 55.1, 34.9; HRMS (ESI) $\text{C}_{24}\text{H}_{23}\text{O}_3\text{N}_6$ $[\text{M}+\text{H}]^+$ calcd for 443.1826 found 443.1822.

1-(2-((1-(4-bromophenyl)-1H-1,2,3-triazol-4-yl)methylcarbamoyl)phenyl)-3-phenylurea (4c):

Light yellow solid; m.p. 195-197 °C; ^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 10.22 (s, 1H), 9.68 (s, 1H), 9.28 (t, J = 5.6 Hz, 1H), 8.75 (s, 1H), 8.23 (dd, J = 8.4, 0.8 Hz, 1H), 7.88 (d, J = 8.8 Hz, 2H), 7.76-7.26 (m, 3H), 7.50-7.43 (m, 3H), 7.25 (t, J = 7.6 Hz, 1H), 7.05 (t, J = 8.0 Hz, 2H), 6.95 (t, J = 7.2 Hz, 1H),

4.64 (d, $J = 5.2$ Hz, 2H). ^{13}C NMR (100 MHz, DMSO- d_6): δ 168.9, 152.5, 146.4, 139.9, 139.8, 135.9, 132.9, 131.7, 128.8, 128.1, 122.09, 122.03, 121.36, 121.30, 120.9, 120.8, 118.6, 35.0; HRMS (ESI) $\text{C}_{23}\text{H}_{19}\text{O}_2\text{N}_6\text{BrNa}$ $[\text{M}+\text{Na}]^+$ calcd for 513.0645 found 513.0638.

2-(1-methyl-3-phenylureido)-N-((1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl)methyl)benzamide (4d):

Light yellow solid; m.p. 155-157 °C; ^1H NMR (400 MHz, DMSO- d_6): δ 8.84 (t, $J = 6.0$ Hz, 1H), 8.58 (s, 1H), 8.34 (d, $J = 7.6$ Hz, 2H), 8.03 (d, $J = 9.2$ Hz, 2H), 7.81 (s, 1H), 7.59-7.51 (m, 2H), 7.42-7.36 (m, 2H), 7.22 (d, $J = 8.0$ Hz, 2H), 7.05 (t, $J = 7.2$ Hz, 2H), 6.79 (t, $J = 7.2$ Hz, 1H), 4.55

(d, $J = 5.6$ Hz, 1H), 3.19 (s, 3H); ^{13}C NMR (100 MHz, DMSO- d_6): δ 167.6, 155.0, 146.8, 146.6, 141.3, 140.8, 139.8, 135.5, 131.3, 129.0, 128.7, 128.2, 127.3, 125.5, 122.2, 121.3, 120.4, 120.2, 38.3, 34.7; HRMS (ESI) $\text{C}_{24}\text{H}_{22}\text{O}_4\text{N}_7$ $[\text{M}+\text{H}]^+$ calcd for 472.1728 found 471.1717.

1-(2-((1-(3,4,5-trimethoxyphenyl)-1H-1,2,3-triazol-4-yl)methylcarbamoyl)phenyl)-3-phenylurea (4e):

(4e): White solid; m.p. 195-197 °C; ^1H NMR (400 MHz, DMSO- d_6): δ 10.28 (s, 1H), 9.67 (s, 1H), 9.28 (t, $J = 5.6$ Hz, 1H), 8.72 (s, 1H), 8.25 (d, $J = 8.4$ Hz, 1H), 7.74 (d, $J = 8.8$ Hz, 1H), 7.49-7.43 (m, 3H), 7.25 (t, $J = 8.4$ Hz, 2H), 7.18 (s, 2H), 7.05 (t, $J = 8.0$ Hz, 1H), 6.95 (t, $J = 7.6$ Hz, 1H),

4.65 (d, $J = 5.6$ Hz, 2H), 3.84 (s, 6H), 3.69 (s, 3H). ^{13}C NMR (100 MHz, DMSO- d_6): δ 168.5, 153.5, 152.4, 145.8, 140.0, 139.9, 137.2, 132.6, 131.6, 128.6, 128.1, 121.9, 121.4, 121.0, 120.6, 120.5, 118.5, 98.0, 60.2, 56.3, 34.9; HRMS (ESI) $\text{C}_{26}\text{H}_{26}\text{O}_5\text{N}_6\text{Na}$ $[\text{M}+\text{Na}]^+$ calcd for 525.1857 found 525.1853.

1-(2-((1-decyl-1H-1,2,3-triazol-4-yl)methylcarbamoyl)phenyl)-3-phenylurea (4f): White solid; m.p.

140-142 °C; ^1H NMR (400 MHz, DMSO- d_6): δ 10.25 (s, 1H), 9.68 (s, 1H), 9.21 (t, $J = 4.5$ Hz, 1H), 8.24 (d, $J = 8.4$ Hz, 1H), 8.00 (s, 1H), 7.68 (d, $J = 9.2$ Hz, 1H), 7.51 (d, $J = 7.6$ Hz, 2H), 7.43 (t, $J = 8.0$ Hz, 1H), 7.25 (t, $J = 8.0$ Hz, 2H), 7.02 (t, $J = 6.8$ Hz, 1H), 6.95 (t, $J = 7.6$ Hz, 1H), 4.54 (d, $J = 6.4$ Hz, 2H), 4.28

(t, $J = 6.8$ Hz, 2H), 1.79-1.73 (m, 2H), 1.25-1.19 (m, 14H), 0.83 (t, $J = 6.8$ Hz, 3H); ^{13}C NMR (100 MHz, DMSO- d_6): δ 168.5, 152.5, 139.77, 139.72, 131.1, 128.2, 127.5, 121.6, 120.8, 120.6, 120.59, 120.52, 49.6,

34.9, 31.2, 29.7, 29.0, 28.9, 28.8, 28.6, 28.4, 25.9, 22.1, 13.7; HRMS (ESI) $C_{27}H_{37}N_6O_2$ $[M+H]^+$ calcd for 477.2972 found 477.2973.

1-(2-((1-(4-iodophenyl)-1H-1,2,3-triazol-4-yl)methylcarbamoyl)phenyl)-3-(4-bromophenyl)urea

(4g): Light yellow solid; m.p. 198-200 °C; 1H NMR (400 MHz, DMSO- d_6): δ 10.31 (s, 1H), 9.83 (s, 1H),

9.33 (t, $J = 5.6$ Hz, 1H), 8.38 (s, 1H), 8.21 (d, $J = 8.4$ Hz, 1H), 8.06 (d, $J = 7.6$ Hz, 1H), 7.73 (d, $J = 7.6$ Hz, 1H), 7.54 (t, $J = 8.0$ Hz, 1H), 7.49-7.41 (m, 6H), 7.34 (td, $J = 8.0, 1.6$ Hz, 1H), 7.05 (t, $J = 7.6$ Hz, 1H), 4.66 (d, $J = 5.2$ Hz, 2H); ^{13}C NMR (100 MHz, DMSO- d_6): δ 168.6, 152.4, 145.1, 139.95, 139.92, 139.7, 139.4, 131.9, 131.7, 131.56, 131.53, 128.1, 128.0, 124.9, 121.4, 121.0, 120.8, 120.5, 113.5, 95.5, 34.9; HRMS (ESI) $C_{23}H_{18}$

O_2N_6BrI Na $[M+Na]^+$ calcd for 638.9612 found 638.9603.

1-(2-((1-(3-methoxyphenyl)-1H-1,2,3-triazol-4-yl)methylcarbamoyl)phenyl)-3-(4-bromophenyl)urea (4h):

White solid; m.p. 140-142 °C; 1H NMR (400 MHz, DMSO- d_6 and $CDCl_3$): δ 10.27 (s, 1H), 9.81 (s, 1H), 9.24 (t, $J = 5.4$ Hz, 2H), 8.56 (s, 1H), 8.18 (d, $J = 8.4$ Hz, 1H), 7.75-7.69 (m, 3H), 7.45-7.34 (m, 5H), 7.04-7.00 (m, 3H), 4.60 (d, $J = 5.6$ Hz, 2H), 3.76 (s, 3H); ^{13}C NMR (100 MHz, DMSO- d_6 and $CDCl_3$): δ 168.7, 159.1, 152.4, 145.7, 139.5, 139.1, 131.2, 131.0, 130.0, 127.6, 121.3, 120.9, 120.7, 120.6, 120.1, 119.9, 114.4,

113.4, 55.2, 35.0; HRMS (ESI) $C_{24}H_{21}BrN_6O_3$ $[M+H]^+$ calcd for 521.0931 found 521.0934.

1-(2-((1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl)methylcarbamoyl)phenyl)-3-(4-bromophenyl)urea

(4i): Light yellow solid ; m.p. 225-227 °C; 1H NMR (400 MHz, DMSO- d_6): δ 10.31 (s, 1H), 9.83 (s, 1H), 9.33 (t, $J = 5.6$ Hz, 1H), 8.93 (s, 1H), 8.40 (d, $J = 9.2$ Hz, 2H), 8.22 (d, $J = 8.8$ Hz, 3H), 7.75 (d, $J = 7.20$ Hz, 1H), 7.48-7.40 (m, 5H), 7.07 (t, $J = 7.2$ Hz, 1H), 4.65 (d, $J = 5.6$ Hz, 2H); ^{13}C NMR (100 MHz, DMSO- d_6): δ 168.7, 152.4, 146.9, 146.7, 140.9, 139.7,

139.4, 131.8, 131.5, 128.1, 125.6, 121.6, 121.4, 120.9, 120.8, 120.5, 120.4, 113.5, 35.0; HRMS (ESI) $C_{23}H_{18}N_7O_4Br$ $[M+H]^+$ calcd for 536.3401 found 536.3405.

1-(2-((1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl)methylcarbamoyl)phenyl)-3-(4-chlorophenyl)urea

(4j): Light yellow solid; m.p. 308-310 °C; ¹H NMR (400 MHz, DMSO-*d*₆): δ 10.26 (s, 1H), 9.81 (s, 1H), 9.32 (t, *J* = 5.6 Hz, 1H), 8.89 (s, 1H), 8.39 (d, *J* = 9.2 Hz, 2H), 8.20-8.17 (m, 3H), 7.43 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.51-7.43 (m, 3H), 7.29-7.26 (m, 2H), 7.06 (t, *J* = 7.2 Hz, 1H), 4.66 (d, *J* = 5.6 Hz, 2H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ 168.7, 152.4, 146.9, 146.7, 140.9, 139.7, 138.9, 131.7, 128.6, 128.1, 125.6, 125.5, 121.6, 121.4,

120.8, 120.5, 120.0, 35.0; HRMS (ESI) C₂₃H₁₉N₇O₄Cl [M+H]⁺ calcd for 492.1182 found 492.1175.

1-(2-((1-(3-methoxyphenyl)-1H-1,2,3-triazol-4-yl)methylcarbamoyl)phenyl)-3-(4-chlorophenyl)urea (4k):

Light yellow solid; m.p. 180-182 °C; ¹H NMR (400 MHz, DMSO-*d*₆ and CDCl₃): δ 10.35 (s, 1H), 9.79 (s, 1H), 9.25 (t, *J* = 5.6 Hz, 1H), 8.66 (s, 1H), 8.25 (d, *J* = 8.0 Hz, 1H), 7.52 (d, *J* = 8.8 Hz, 2H), 7.45-7.38 (m, 4H), 7.23 (d, *J* = 9.2 Hz, 2H), 7.03-6.96 (m, 2H), 4.65 (d, *J* = 5.6 Hz, 2H), 3.81 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆ and CDCl₃): δ 168.6, 160.2, 152.3, 145.9, 139.9, 138.9, 137.7, 131.5, 130.6, 128.3, 128.0, 125.5, 121.1,

121.0, 120.6, 119.9, 114.0, 111.8, 105.6, 55.5, 35.0; HRMS (ESI) C₂₄H₂₁N₆O₃ClNa [M+Na]⁺ calcd for 499.1256 found 499.1249.

1-(2-((1-benzyl-1H-1,2,3-triazol-4-yl)methylcarbamoyl)phenyl)-3-(4-chlorophenyl)urea (4l):

White solid; m.p. 170-172 °C; ¹H NMR (400 MHz, DMSO-*d*₆): δ 10.36 (s, 1H), 9.84 (s, 1H), 9.23 (t, *J* = 5.6 Hz, 1H), 8.23 (d, *J* = 8.0 Hz, 1H), 8.06 (s, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.54 (d, *J* = 8.8 Hz, 2H), 7.44 (t, *J* = 7.2 Hz, 1H), 7.35-7.26 (m, 7H), 7.03 (t, *J* = 7.2 Hz, 1H), 5.55 (s, 2H), 4.55 (d, *J* = 5.6 Hz, 2H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ 168.5, 152.4, 145.2, 139.9, 139.0, 136.1, 131.7, 128.5, 128.6, 128.2, 128.1, 125.6, 123.1, 121.3, 120.7, 120.5, 120.1, 52.9, 35.0; HRMS (ESI)

C₂₄H₂₂N₆O₂Cl [M+H]⁺ calcd for 461.1487 found 461.1475.

1-(2-((1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl)methylcarbamoyl)phenyl)-3-(3-methoxyphenyl)urea

(4m): White solid; m.p. 330-332 °C; ^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 10.14 (s, 1H), 9.64 (s, 1H), 9.28 (t, $J = 5.6$ Hz, 1H), 8.87 (s, 1H), 8.38 (d, $J = 9.2$ Hz, 2H), 8.18-8.15 (m, 3H), 7.69 (dd, $J = 8.8, 1.6$ Hz, 1H), 7.41 (t, $J = 8.0$ Hz, 1H), 7.13-7.08 (m, 2H), 7.03-6.98 (m, 2H), 6.49-6.47 (m, 1H), 4.63 (d, $J = 6.0$ Hz, 2H), 3.66 (s, 3H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ

168.7, 159.6, 152.4, 146.9, 146.6, 141.2, 140.9, 139.8, 131.6, 129.57, 129.52, 128.1, 1255.6, 121.6, 121.2, 120.98, 120.92, 120.5, 110.8, 107.3, 104.3, 54.9, 35.0; HRMS (ESI) $\text{C}_{24}\text{H}_{21}\text{N}_7\text{O}_5$ $[\text{M}]^+$ calcd for 487.4710 found 487.4705. (Compound have some residual solvent from the reaction mixture, thus the NMR contains traces of DMF peaks)

1-(2-((1-(4-bromophenyl)-1H-1,2,3-triazol-4-yl)methylcarbamoyl)phenyl)-3-(3-methoxyphenyl)urea (4n):

Light yellow solid; m.p. 190-192 °C; ^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 10.22 (s, 1H), 9.70 (s, 1H), 9.30 (t, $J = 5.6$ Hz, 1H), 8.75 (s, 1H), 8.23 (d, $J = 8.0$ Hz, 1H), 7.88-7.86 (d, $J = 7.2$ Hz, 2H), 7.76-7.72 (m, 3H), 7.45 (td $J = 8.8, 1.6$ Hz, 1H), 7.21-7.13 (m, 2H), 7.05-7.03 (m, 2H), 6.53 (dd, $J = 7.2, 2.0$ Hz, 1H), 4.64 (d, $J = 6.0$ Hz, 2H), 3.71 (s, 3H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ 168.9, 159.7, 152.5, 146.4,

141.2, 139.8, 135.9, 132.8, 131.7, 129.5, 128.1, 121.9, 121.3, 121.2, 121.0, 120.9, 110.9, 107.4, 104.4, 55.0, 35.0; HRMS (ESI) $\text{C}_{24}\text{H}_{22}\text{O}_3\text{N}_6\text{Br}$ $[\text{M}+1]^+$ calcd for 521.0931 found 521.0934.

1-(2-((1-(3-methoxyphenyl)-1H-1,2,3-triazol-4-yl)methylcarbamoyl)-5-chlorophenyl)-3-phenylurea

(4o): White solid; m.p. 178-180 °C; ^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 10.47 (s, 1H), 9.83 (s, 1H), 9.37 (t, $J = 5.6$ Hz, 1H), 8.75 (s, 1H), 8.41 (d, $J = 2.4$ Hz, 2H), 7.77 (d, $J = 8.4$ Hz, 1H), 7.50-7.46 (m, 5H), 7.26 (t, $J = 8.0$ Hz, 5H), 7.13 (dd, $J = 8.8, 2.4$ Hz, 1H), 7.049-7.034 (m, 1H),

6.97 (m, 1H), 4.64 (d, $J = 5.6$ Hz, 2H), 3.83 (s, 3H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ 167.9, 160.0, 152.1, 141.2, 138.7, 137.5, 136.8, 130.9, 130.2, 128.9, 120.7, 120.4, 120.2, 119.7, 118.2, 113.76, 113.71, 111.7, 105.6, 55.2, 34.9; HRMS (ESI) $\text{C}_{24}\text{H}_{21}\text{N}_6\text{O}_3\text{Cl}$ $[\text{M}+\text{H}]^+$ calcd for 476.9147 found 476.9149.

1-(2-((1-(4-bromophenyl)-1H-1,2,3-triazol-4-yl)methylcarbamoyl)-5-chlorophenyl)-3-(4-

bromophenyl)urea (4p): White solid; m.p. 260-262 °C; ¹H NMR (400 MHz, DMSO-*d*₆): δ 10.52 (s, 1H), 9.99 (s, 1H), 9.40 (t, *J* = 5.6 Hz, 1H), 8.74 (s, 1H), 8.39 (d, *J* = 2.0 Hz, 1H), 7.89-7.86 (m, 2H), 7.79-7.75 (m, 2H), 7.50-7.44 (m, 5H), 7.15 (dd, *J* = 8.4, 2.0 Hz, 1H), 4.65 (d, *J* = 5.6 Hz, 2H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ 167.8, 152.2, 146.2, 141.3,

139.1, 136.4, 135.9, 132.9, 131.66, 131.60, 129.9, 122.0, 121.39, 121.32, 121.0, 120.7, 120.4, 119.7, 118.9, 113.8, 35.0; HRMS (ESI) C₂₃H₁₈ClN₆Br₂ [M+H]⁺ calcd for 602.9541 found 602.9525.

1-(2-((1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl)methylcarbamoyl)-5-chlorophenyl)-3-(4-

bromophenyl)urea (4q): White solid; m.p. 340-342 °C; ¹H NMR (400 MHz, DMSO-*d*₆): δ 10.54 (s, 1H), 9.97 (s, 1H), 9.42 (t, *J* = 5.2 Hz, 1H), 8.94 (s, 1H), 8.42-8.40 (m, 3H), 8.23-8.20 (m, 2H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.48-7.38 (m, 4H), 7.15 (d, *J* = 9.2 Hz, 1H), 4.66 (d, *J* = 5.2 Hz, 2H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ 167.8, 152.1, 146.7, 141.3, 140.9, 139.0, 136.3, 131.5, 129.9, 125.6, 121.6, 121.0, 120.67, 120.6,

119.7, 118.9, 113.8; HRMS (ESI) C₂₃H₁₇N₇O₄BrClNa [M+Na]⁺ calcd for 592.0106 found 592.0095.

1-(2-((1-(3,4,5-trimethoxyphenyl)-1H-1,2,3-triazol-4-yl)methylcarbamoyl)-5-chlorophenyl)-3-(4-

bromophenyl)urea (4r): White solid; m.p. 185-187 °C; ¹H NMR (400 MHz, DMSO-*d*₆): δ 10.58 (s, 1H), 9.97 (s, 1H), 9.39 (t, *J* = 5.2 Hz, 1H), 8.73 (s, 1H), 8.41 (d, *J* = 2.0 Hz, 1H), 7.78 (d, *J* = 8.4 Hz, 1H), 7.49-7.42 (m, 4H), 7.18-7.13 (m, 3H), 4.65 (d, *J* = 5.6 Hz, 2H), 3.85 (s, 6H), 3.69 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ 167.7, 153.6, 152.1, 145.7,

141.4, 139.1, 137.3, 136.4, 132.6, 131.5, 129.9, 121.5, 121.9, 120.6, 119.6, 118.6, 113.8, 98.0, 60.3, 56.3, 35.0; HRMS (ESI) C₂₆H₂₃N₆O₅BrCl [M-H]⁺ calcd for 613.0596 found 613.0599.

1-(2-((1-(4-methoxyphenyl)-1H-1,2,3-triazol-4-yl)methylcarbamoyl)-5-chlorophenyl)-3-(4-

bromophenyl)urea (4s): White solid; m.p. 120-122 °C; ¹H NMR (400 MHz, DMSO-*d*₆): δ 10.57 (s, 1H), 9.98 (s, 1H), 9.38 (t, *J* = 5.6 Hz, 1H), 8.75 (s, 1H), 8.43 (d, *J* = 2.0 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.49-7.42 (m, 7H), 7.14 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.05-7.02 (m, 1H), 4.64 (d, *J* = 5.6 Hz, 2H), 3.83 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ 167.9, 160.1, 152.0, 145.7, 141.3, 129.0, 137.6, 136.2, 131.4, 130.8, 129.1,

121.2, 120.7, 120.5, 119.5, 118.6, 114.2, 113.6, 111.9, 105.6, 55.6, 35.0; HRMS (ESI) C₂₄H₂₁N₆O₃BrCl [M+H]⁺ calcd for 555.0542 found 555.0537.

1-(2-((1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl)methylcarbamoyl)-5-chlorophenyl)-3-(3-

methoxyphenyl)urea (4t): Yellow solid; m.p. 340-342 °C; ¹H NMR (400 MHz, DMSO-*d*₆): δ 10.43 (s, 1H), 9.82 (s, 1H), 9.40 (t, *J* = 5.6 Hz, 1H), 8.94 (s, 1H), 8.41-8.39 (m, 3H), 8.22-8.16 (m, 2H), 7.77 (d, *J* = 7.2 Hz, 1H), 7.18-7.04 (m, 4H), 6.55 (dd, *J* = 7.2, 2.0 Hz, 1H), 4.66 (d, *J* = 5.2 Hz, 2H), 3.70 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ 167.9,

162.5, 159.6, 152.2, 146.77, 146.71, 141.4, 140.94, 140.91, 136.3, 129.8, 129.5, 125.6, 121.6, 120.8, 120.5, 119.7, 118.9, 111.0, 107.7, 104.4, 54.9, 35.0; HRMS (ESI) C₂₄H₁₉N₇O₅Cl [M-H]⁺ calcd for 520.1131 found 520.1138. (Compound have some residual solvent from the reaction mixture, thus the NMR contains traces of DMF peaks)

1-(2-((1-(4-bromophenyl)-1H-1,2,3-triazol-4-yl)methylcarbamoyl)phenyl)-1-methyl-3-phenylurea

(4u): yellow solid; m.p. 215-218 °C; ¹H NMR (400 MHz, DMSO-*d*₆): δ 8.79 (t, *J* = 5.6 Hz, 1H), 8.45 (s, 1H), 7.80 (bs, 1H), 7.72 (s, 4H), 7.58-7.51 (m, 2H), 7.43-7.36 (m, 2H), 7.26 (d, *J* = 7.2 Hz, 2H), 7.09 (t, *J* = 8.4 Hz, 2H), 6.84 (t, *J* = 7.6 Hz, 1H), 4.52 (d, *J* = 4.8 Hz, 2H), 3.18 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ 167.5, 155.0, 146.3, 141.2, 139.8, 135.8, 135.5, 132.7, 131.2, 129.0, 128.7, 128.2, 127.3, 122.2, 121.9, 121.2, 120.8, 120.1, 38.3, 34.7; HRMS (ESI) C₂₄H₂₂N₆O₂Br [M]⁺ calcd for 505.0982 found 505.0968.

1-(2-((1-benzyl-1H-1,2,3-triazol-4-yl)methylcarbamoyl)-5-chlorophenyl)-1-methyl-3-phenylurea

(4v): White solid; m.p. 255-258 °C; ^1H NMR (400 MHz, $\text{DMSO}-d_6$): δ 8.74 (t, $J = 5.6$ Hz, 1H), 7.89 (s, 1H), 7.84 (s, 1H), 7.54-7.50 (m, 2H), 7.41-7.30 (m, 6H), 7.23-7.18 (m, 4H), 6.94 (t, $J = 7.2$ Hz, 1H), 5.33 (s, 2H), 4.42 (d, $J = 5.6$ Hz, 2H), 3.15 (s, 3H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$): δ 167.5, 155.0, 145.3, 141.3, 140.0, 136.0, 135.6, 131.2,

128.9, 128.8, 128.6, 128.4, 128.2, 127.9, 127.2, 122.8, 122.2, 119.9, 52.7, 38.2, 34.9; HRMS (ESI) $\text{C}_{25}\text{H}_{23}\text{N}_6\text{O}_2\text{Cl}$ $[\text{M}]^+$ calcd for 474.9402 found 474.9408.

Cytotoxicity studies of synthesized compounds on BCC cell lines:

The synthesized triazole linked urea derivatives 4a-v, were further assessed for *in vitro* cytotoxicity on the BCC cell lines. The respective cells were cultured with agents at a concentration of 5mM for 24 hrs before growth and viability were assessed using the MTT assay. The potency of the compounds indicated by IC50 values (50% inhibitory concentration) was calculated from the plotted absorbance data for the dose response curves. IC50 values (in μM) were expressed as the average of two independent experiments.

Ph-NCO-I

Pulse Sequence: s2pul

UNITYplus-400 "unity400"

Date: May 9 2013

Solvent: DMSO

Ambient temperature

Total 80 repetitions

Integration value 10 = 1H

Ph-NCO-I

Pulse Sequence: s2pu1

UNITYplus-400 "unity400"

Date: May 9 2013

Solvent: DMSO

Ambient temperature

Total 1600 repetitions

Ph-NCO-OMe

Pulse Sequence: s2pu1

UNITYplus-400 "unity400"

Date: May 17 2013

Solvent: DMSO

Ambient temperature

Total 80 repetitions

Integration value 10 = 1H

Ph-NCO-OMe

Pulse Sequence: s2pu1

UNITYplus-400 "unity400"

Date: May 17 2013

Solvent: DMSO

Ambient temperature

Total 2016 repetitions

X : parts per Million : Proton

Filename = code-4c_Proton-1-3.jdf
 Author = delta
 Experiment = proton.jxp
 Sample_Id = code-4c
 Solvent = DMSO-D6
 Creation_Time = 17-JUN-2016 10:13:25
 Revision_Time = 17-JUN-2016 10:13:01
 Current_Time = 17-JUN-2016 10:13:48
 Comment = single pulse
 Data_Format = 1D COMPLEX
 Dim_Size = 13107
 Dim_Title = Proton
 Dim_Units = [ppm]
 Dimensions = X
 Site = JNM-ECS400

Spectrometer = DELTA2_NMR
 Field_Strength = 9.389766[T] (400[MHz])
 X_Acq_Duration = 2.18365952[s]
 X_Domain = 1H
 X_Freq = 399.78219838[MHz]
 X_Offset = 5[ppm]
 X_Points = 16384
 X_Prescans = 1
 X_Resolution = 0.45794685[Hz]
 X_Sweep = 7.5030012[kHz]
 X_Sweep_Clipped = 6.00240096[kHz]
 Irr_Domain = Proton
 Irr_Freq = 399.78219838[MHz]
 Irr_Offset = 5[ppm]
 Tri_Domain = Proton

Tri_Freq = 399.78219838[MHz]
 Tri_Offset = 5[ppm]
 Clipped = FALSE
 Scans = 16
 Total_Scans = 16
 Relaxation_Delay = 5[s]
 Recvr_Gain = 44
 Temp_Get = 24.9[dC]
 X_90_Width = 12.795[us]
 X_Acq_Time = 2.18365952[s]
 X_Angle = 45[deg]
 X_Atn = 2.4[dB]
 X_Pulse = 6.3975[us]
 Irr_Mode = Off
 Tri_Mode = Off

Ph-NCO-Br

Pulse Sequence: s2pu1

UNITYplus-400 "unity400"

Date: May 13 2013

Solvent: DMSO

Ambient temperature

Total 2208 repetitions

Ph-NCO-NO2-CH3

Pulse Sequence: s2pu1

UNITYplus-400 "unity400"

Date: May 14 2013

Solvent: DMSO

Ambient temperature

Total 64 repetitions

Integration value 10 = 1H

Ph-NCO-NO2-CH3

Pulse Sequence: s2pu1

UNITYplus-400 "unity400"

Date: May 14 2013

Solvent: DMSO

Ambient temperature

Total 20480 repetitions

Ph-NCO-NO2-CH3

Pulse Sequence: DEPT

X : parts per Million : Proton

Filename = code-4e_Proton-1-3.jdf
 Author = delta
 Experiment = proton.jxp
 Sample_Id = code-4e
 Solvent = DMSO-D6
 Creation_Time = 10-JUN-2016 15:53:32
 Revision_Time = 10-JUN-2016 15:55:05
 Current_Time = 10-JUN-2016 15:55:40
 Comment = single pulse
 Data_Format = 1D COMPLEX
 Dim_Size = 13107
 Dim_Title = Proton
 Dim_Units = [ppm]
 Dimensions = X
 Site = JNM-ECS400

Spectrometer = DELTA2_NMR
 Field_Strength = 9.389766[T] (400[MHz])
 X_Acq_Duration = 2.18365952[s]
 X_Domain = 1H
 X_Freq = 399.78219838[MHz]
 X_Offset = 5[ppm]
 X_Points = 16384
 X_Prescans = 1
 X_Resolution = 0.45794685[Hz]
 X_Sweep = 7.5030012[kHz]
 X_Sweep_Clipped = 6.00240096[kHz]
 Irr_Domain = Proton
 Irr_Freq = 399.78219838[MHz]
 Irr_Offset = 5[ppm]
 Tri_Domain = Proton

Tri_Freq = 399.78219838[MHz]
 Tri_Offset = 5[ppm]
 Clipped = FALSE
 Scans = 16
 Total_Scans = 16
 Relaxation_Delay = 5[s]
 Recvr_Gain = 34
 Temp_Get = 23.4[dC]
 X_90_Width = 12.795[us]
 X_Acq_Time = 2.18365952[s]
 X_Angle = 45[deg]
 X_Atn = 2.4[dB]
 X_Pulse = 6.3975[us]
 Irr_Mode = Off
 Tri_Mode = Off

Ph-NCO-3OMe

Pulse Sequence: s2pul

Mercury-400BB "MercuryPlus400"

Date: Oct 25 2012

Solvent: DMSO

Ambient temperature

Total 1600 repetitions

Ph-NCO-3OMe

Pulse Sequence: DEPT

X : parts per Million : Proton

Filename = code-4f_Proton-1-3.jdf
 Author = delta
 Experiment = proton.jxp
 Sample_Id = code-4f
 Solvent = DMSO-D6
 Creation_Time = 10-JUN-2016 16:00:22
 Revision_Time = 10-JUN-2016 16:14:35
 Current_Time = 10-JUN-2016 16:15:06
 Comment = single pulse
 Data_Format = 1D COMPLEX
 Dim_Size = 13107
 Dim_Title = Proton
 Dim_Units = [ppm]
 Dimensions = X
 Site = JNM-ECS400

Spectrometer = DELTA2_NMR
 Field_Strength = 9.389766[T] (400[MHz])
 X_Acq_Duration = 2.18365952[s]
 X_Domain = 1H
 X_Freq = 399.78219838[MHz]
 X_Offset = 5[ppm]
 X_Points = 16384
 X_Prescans = 1
 X_Resolution = 0.45794685[Hz]
 X_Sweep = 7.5030012[kHz]
 X_Sweep_Clipped = 6.00240096[kHz]
 Irr_Domain = Proton
 Irr_Freq = 399.78219838[MHz]
 Irr_Offset = 5[ppm]
 Tri_Domain = Proton

Tri_Freq = 399.78219838[MHz]
 Tri_Offset = 5[ppm]
 Clipped = FALSE
 Scans = 32
 Total_Scans = 32
 Relaxation_Delay = 5[s]
 Recvr_Gain = 30
 Temp_Get = 23.4[dC]
 X_90_Width = 12.795[us]
 X_Acq_Time = 2.18365952[s]
 X_Angle = 45[deg]
 X_Atn = 2.4[dB]
 X_Pulse = 6.3975[us]
 Irr_Mode = Off
 Tri_Mode = Off

PH-NCO-Dec

Pulse Sequence: s2pu1

UNITYplus-400 "unity400"

Date: May 17 2013

Solvent: DMSO

Ambient temperature

Total 4096 repetitions

PH-NCO-Dec

Pulse Sequence: DEPT

X : parts per Million : Proton

Filename = code-4g_Proton-1-3.jdf
 Author = delta
 Experiment = proton.jxp
 Sample Id = code-4g
 Solvent = DMSO-D6
 Creation_Time = 10-JUN-2016 11:28:41
 Revision_Time = 10-JUN-2016 11:30:17
 Current_Time = 10-JUN-2016 11:30:47

Comment = single pulse
 Data Format = 1D COMPLEX
 Dim_Size = 13107
 Dim_Title = Proton
 Dim_Units = [ppm]
 Dimensions = X
 Site = JNM-ECS400

Spectrometer = DELTA2_NMR
 Field Strength = 9.389766[T] (400[MHz])
 X Acq_Duration = 2.18365952[s]
 X_Domain = 1H
 X_Freq = 399.78219838[MHz]
 X_Offset = 5[ppm]
 X_Points = 16384
 X_Prescans = 1
 X Resolution = 0.45794685[Hz]
 X Sweep = 7.5030012[kHz]
 X Sweep_Clippped = 6.00240096[kHz]
 Irr_Domain = Proton
 Irr_Freq = 399.78219838[MHz]
 Irr_Offset = 5[ppm]
 Tri_Domain = Proton

Tri_Freq = 399.78219838[MHz]
 Tri_Offset = 5[ppm]
 Clipped = FALSE
 Scans = 16
 Total_Scans = 16
 Relaxation_Delay = 5[s]
 Recvr_Gain = 42
 Temp_Get = 23.8[dc]
 X_90_Width = 12.795[us]
 X_Acq_Time = 7.18365952[s]
 X_Angle = 45[deg]
 X_Atn = 2.4[dB]
 X_Pulse = 6.3975[us]
 Irr_Mode = Off
 Tri_Mode = Off

Ph-Br-I

Pulse Sequence: s2pu1

UNITYplus-400 "unity400"

Date: May 13 2013

Solvent: DMSO

Ambient temperature

Total 1072 repetitions

Ph-Br-I

Pulse Sequence: DEPT

X : parts per Million : Proton

Filename = code-4h_Proton-1-3.jdf
 Author = delta
 Experiment = proton.jxp
 Sample_Id = code-4h
 Solvent = DMSO-D6
 Creation Time = 10-JUN-2016 10:04:06
 Revision Time = 10-JUN-2016 10:07:05
 Current Time = 10-JUN-2016 10:08:13
 Comment = single pulse
 Data Format = 1D COMPLEX
 Dim Size = 13107
 Dim Title = Proton
 Dim Units = [ppm]
 Dimensions = X
 Site = JNM-ECS400

Spectrometer = DELTA2_NMR
 Field Strength = 9.389766[T] (400[MHz])
 X Acq_Duration = 2.18365952[s]
 X_Domain = 1H
 X_Freq = 399.78219838[MHz]
 X_Offset = 5[ppm]
 X_Points = 16384
 X_Prescans = 1
 X Resolution = 0.45794685[Hz]
 X Sweep = 7.5030012[kHz]
 X Sweep Clipped = 6.00240096[kHz]
 Irr_Domain = Proton
 Irr_Freq = 399.78219838[MHz]
 Irr_Offset = 5[ppm]
 Tri_Domain = Proton

Tri_Freq = 399.78219838[MHz]
 Tri_Offset = 5[ppm]
 Clipped = FALSE
 Scans = 16
 Total_Scans = 16
 Relaxation_Delay = 5[s]
 Recvr Gain = 38
 Temp_Get = 24[dc]
 X 90_Width = 12.795[us]
 X Acq Time = 2.18365952[s]
 X Angle = 45[deg]
 X_Atn = 2.4[dB]
 X_Pulse = 6.3975[us]
 Irr_Mode = Off
 Tri_Mode = Off

Ph-Br-OMe

Pulse Sequence: s2pu1

UNITYplus-400 "unity400"

Date: May 17 2013

Solvent: DMSO

Ambient temperature

Total 2464 repetitions

X : parts per Million : Proton

Filename = code-4i_Proton-1-3.jdf
 Author = delta
 Experiment = proton.jxp
 Sample Id = code-4i
 Solvent = DMSO-D6
 Creation Time = 10-JUN-2016 11:36:22
 Revision Time = 10-JUN-2016 11:42:06
 Current Time = 10-JUN-2016 11:43:15
 Comment = single pulse
 Data Format = 1D COMPLEX
 Dim Size = 13107
 Dim Title = Proton
 Dim Units = [ppm]
 Dimensions = X
 Site = JNM-ECS400

Spectrometer = DELTA2_NMR
 Field Strength = 9.389766[T] (400[MHz])
 X Acq Duration = 2.18365952[s]
 X Domain = 1H
 X Freq = 399.78219838[MHz]
 X Offset = 5[ppm]
 X Points = 16384
 X Prescans = 1
 X Resolution = 0.45794685[Hz]
 X Sweep = 7.5030012[kHz]
 X Sweep_Clippped = 6.00240096[kHz]
 Irr Domain = Proton
 Irr Freq = 399.78219838[MHz]
 Irr Offset = 5[ppm]
 Tri_Domain = Proton

Tri_Freq = 399.78219838[MHz]
 Tri_Offset = 5[ppm]
 Clipped = FALSE
 Scans = 16
 Total_Scans = 16
 Relaxation_Delay = 5[s]
 Recvr Gain = 38
 Temp Get = 23.8[dC]
 X 90_Width = 12.795[us]
 X Acq Time = 2.18365952[s]
 X Angle = 45[deg]
 X Atn = 2.4[dB]
 X Pulse = 6.3975[us]
 Irr_Mode = Off
 Tri_Mode = Off

Ph-Br-NO2

Pulse Sequence: s2pu1

UNITYplus-400 "unity400"

Date: May 9 2013

Solvent: DMSO

Ambient temperature

Total 3104 repetitions

Ph-C1-NO2

Pulse Sequence: s2pu1

Solvent: DMSO

Ambient temperature

Mercury-400BB "MercuryPlus400"

Pulse 48.1 degrees

Acq. time 4.002 sec

Width 5995.2 Hz

64 repetitions

OBSERVE H1, 400.3997918 MHz

DATA PROCESSING

FT size 65536

Total time 5 min, 7 sec

Ph-C1-NO2

Pulse Sequence: s2pu1

Solvent: DMSO

Ambient temperature

Mercury-400BB "MercuryPlus400"

Pulse 68.7 degrees

Acq. time 1.000 sec

Width 25000.0 Hz

64000 repetitions

OBSERVE C13, 100.6806408 MHz

DECOUPLE H1, 400.4018591 MHz

Power 38 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 21 hr, 51 min, 34 sec

Ph-Cl-OMe

Pulse Sequence: s2pul

Solvent: DMSO

Ambient temperature

Mercury-400BB "MercuryPlus400"

Pulse 48.1 degrees

Acq. time 4.002 sec

Width 5995.2 Hz

64 repetitions

OBSERVE H1, 400.3997920 MHz

DATA PROCESSING

FT size 65536

Total time 5 min, 7 sec

Ph-Cl-OMe

Pulse Sequence: s2pu1

Solvent: DMSO

Ambient temperature

Mercury-400BB "MercuryPlus400"

Pulse 68.7 degrees

Acq. time 1.000 sec

Width 25000.0 Hz

1072 repetitions

OBSERVE C13, 100.6806461 MHz

DECOUPLE H1, 400.4018591 MHz

Power 38 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 21 hr, 51 min, 34 sec

X : parts per Million : Proton

Filename = code-4l_Proton-1-3.jdf
 Author = delta
 Experiment = proton.jxp
 Sample_Id = code-4l
 Solvent = DMSO-D6
 Creation_Time = 10-JUN-2016 16:09:31
 Revision_Time = 10-JUN-2016 16:38:28
 Current_Time = 10-JUN-2016 16:39:01

Comment = single pulse
 Data Format = 1D COMPLEX
 Dim_Size = 13107
 Dim_Title = Proton
 Dim_Units = [ppm]
 Dimensions = X
 Site = JNM-ECS400

Spectrometer = DELTA2_NMR
 Field_Strength = 9.389766[T] (400[MHz])
 X_Acq_Duration = 2.18365952[s]
 X_Domain = 1H
 X_Freq = 399.78219838[MHz]
 X_Offset = 5[ppm]
 X_Points = 16384
 X_Prescans = 1
 X_Resolution = 0.45794685[Hz]
 X_Sweep = 7.5030012[kHz]
 X_Sweep_Clippped = 6.00240096[kHz]
 Irr_Domain = Proton
 Irr_Freq = 399.78219838[MHz]
 Irr_Offset = 5[ppm]
 Tri_Domain = Proton

Tri_Freq = 399.78219838[MHz]
 Tri_Offset = 5[ppm]
 Clipped = FALSE
 Scans = 32
 Total_Scans = 32
 Relaxation_Delay = 5[s]
 Recvr_Gain = 34
 Temp_Get = 23.4[dC]
 X_90_Width = 12.795[us]
 X_Acq_Time = 2.18365952[s]
 X_Angle = 45[deg]
 X_Atn = 2.4[dB]
 X_Pulse = 6.3975[us]
 Irr_Mode = Off
 Tri_Mode = Off

**JEOL
RESONANCE**

Ph-C1-2H

Pulse Sequence: s2pul

Solvent: DMSO

Ambient temperature

Mercury-400BB "MercuryPlus400"

Pulse 68.7 degrees

Acq. time 1.000 sec

Width 25000.0 Hz

256 repetitions

OBSERVE C13, 100.6806400 MHz

DECOUPLE H1, 400.4018591 MHz

Power 38 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 21 hr, 51 min, 34 sec

Ph-Cl-2H

Pulse Sequence: DEPT

Filename = code-4m_Proton-1-4 jdf
 Author = delta
 Experiment = proton.jxp
 Sample Id = code-4m
 Solvent = DMSO-D6
 Creation Time = 10-JUN-2016 16:18:56
 Revision Time = 10-JUN-2016 16:54:56
 Current Time = 10-JUN-2016 16:56:16

Comment = single pulse
 Data Format = 1D COMPLEX
 Dim Size = 13107
 Dim Title = Proton
 Dim Units = [ppm]
 Dimensions = X
 Site = JNM-ECS400

Spectrometer = DELTA2_NMR
 Field Strength = 9 389766[T] (400[MHz])
 X Acq_Duration = 2 18365952[s]
 X Domain = 1H
 X Freq = 399.78219838[MHz]
 X Offset = 5[ppm]
 X Points = 16384
 X Prescans = 1
 X Resolution = 0 45794685[Hz]
 X Sweep = 7 5030012[kHz]
 X Sweep Clipped = 6.00240096[kHz]
 Irr Domain = Proton
 Irr Freq = 399.78219838[MHz]
 Irr Offset = 5[ppm]
 Tri_Domain = Proton

Tri Freq = 399 78219838[MHz]
 Tri_Offset = 5[ppm]
 Clipped = FALSE
 Scans = 48
 Total_Scans = 48
 Relaxation_Delay = 5[s]
 Recvr Gain = 28
 Temp Get = 23 4[dC]
 X 90_Width = 12 795[us]
 X Acq_Time = 2.18365952[s]
 X Angle = 45[deg]
 X Atn = 2 4[dB]
 X Pulse = 6 3975[us]
 Irr Mode = Off
 Tri_Mode = Off

Ph-OMe-NO2

Pulse Sequence: s2pu1

UNITYplus-400 "unity400"

Date: Jan 30 2013

Solvent: DMSO

Ambient temperature

Total 16000 repetitions

Ph-OMe-Br

Pulse Sequence: s2pu1

UNITYplus-400 "unity400"

Date: May 9 2013

Solvent: DMSO

Ambient temperature

Total 1056 repetitions

Filename = code-4o_Proton-1-3 jdf
 Author = delta
 Experiment = proton.jxp
 Sample Id = code-4o
 Solvent = NONE
 Creation Time = 14-JUN-2016 16:54:30
 Revision Time = 14-JUN-2016 17:12:40
 Current Time = 14-JUN-2016 17:14:36
 Comment = single pulse
 Data Format = 1D COMPLEX
 Dim Size = 13107
 Dim Title = Proton
 Dim Units = [ppm]
 Dimensions = X
 Site = JNM-ECS400

Spectrometer = DELTA2 NMR
 Field Strength = 9 389766[T] (400[MHz])
 X Acq Duration = 2 18365952[s]
 X Domain = 1H
 X Freq = 399 78219838[MHz]
 X Offset = 5[ppm]
 X Points = 16384
 X Prescans = 1
 X Resolution = 0 45794685[Hz]
 X Sweep = 7 5030012[kHz]
 X Sweep Clipped = 6 00240096[kHz]
 Irr Domain = Proton
 Irr Freq = 399.78219838[MHz]
 Irr Offset = 5[ppm]
 Tri Domain = Proton

Tri Freq = 399.78219838[MHz]
 Tri Offset = 5[ppm]
 Clipped = FALSE
 Scans = 128
 Total Scans = 128
 Relaxation Delay = 5[s]
 Recvr Gain = 42
 Temp Get = 23.5[dc]
 X 90 Width = 12 795[us]
 X Acq Time = 2 18365952[s]
 X Angle = 45[deg]
 X Atn = 2 4[dB]
 X Pulse = 6.3975[us]
 Irr Mode = Off
 Tri Mode = Off

Cl-Ph-NCO-OMe

Pulse Sequence: s2pu1

UNITYplus-400 "unity400"

Date: May 16 2013

Solvent: DMSO

Ambient temperature

Total 7472 repetitions

Cl-Ph-Br-Br

Pulse Sequence: s2pu1

UNITYplus-400 "unity400"

Date: Jan 29 2013

Solvent: DMSO

Ambient temperature

File: U0023-4

Total 64 repetitions

Cl-Ph-Br-Br

Pulse Sequence: s2pu1

UNITYplus-400 "unity400"

Date: Jan 29 2013

Solvent: DMSO

Ambient temperature

Total 4304 repetitions

Filename = code-4q_Proton-2-3 jdf
 Author = delta
 Experiment = proton.jxp
 Sample_Id = code-4q
 Solvent = DMSO-D6
 Creation Time = 14-JUN-2016 16:03:55
 Revision Time = 14-JUN-2016 16:10:45
 Current Time = 14-JUN-2016 16:11:28

Comment = single pulse
 Data Format = 1D COMPLEX
 Dim_Size = 13107
 Dim_Title = Proton
 Dim_Units = [ppm]
 Dimensions = X
 Site = JNM-ECS400

Spectrometer = DELTA2_NMR
 Field Strength = 9 389766[T] (400[MHz])
 X Acq_Duration = 2 18365952[s]
 X_Domain = 1H
 X_Freq = 399 78219838[MHz]
 X_Offset = 5[ppm]
 X Points = 16384
 X Prescans = 1
 X Resolution = 0 45794685[Hz]
 X Sweep = 7 5030012[kHz]
 X Sweep Clipped = 6 00240096[kHz]
 Irr_Domain = Proton
 Irr_Freq = 399 78219838[MHz]
 Irr_Offset = 5[ppm]
 Tri_Domain = Proton

Tri_Freq = 399 78219838[MHz]
 Tri_Offset = 5[ppm]
 Clipped = FALSE
 Scans = 8
 Total_Scans = 8
 Relaxation_Delay = 5[s]
 Recvr_Gain = 36
 Temp_Get = 23.6[dC]
 X 90_Width = 12 795[us]
 X Acq_Time = 2 18365952[s]
 X Angle = 45[deg]
 X Atn = 2 4[dB]
 X_Pulse = 6.3975[us]
 Irr_Mode = Off
 Tri_Mode = Off

Cl-Ph-Br-NO2

Pulse Sequence: s2pu1

Solvent: DMSO

Ambient temperature

Mercury-400BB "MercuryPlus400"

Pulse 68.7 degrees

Acq time 1 000 sec

Width 25000 0 Hz

656 repetitions

OBSERVE C13 100 6806461 MHz

DECOUPLE H1, 400 4018591 MHz

Power 38 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1 0 Hz

FT size 65536

Total time 21 hr 51 min 34 sec

Filename = code-4r_Proton-1-3 jdf
 Author = delta
 Experiment = proton.jxp
 Sample_Id = code-4r
 Solvent = DMSO-D6
 Creation_Time = 14-JUN-2016 17:38:28
 Revision_Time = 14-JUN-2016 17:41:51
 Current_Time = 14-JUN-2016 17:42:13

Comment = single pulse
 Data Format = 1D COMPLEX
 Dim Size = 13107
 Dim Title = Proton
 Dim Units = [ppm]
 Dimensions = X
 Site = JNM-ECS400

Spectrometer = DELTA2_NMR
 Field Strength = 9.389766[T] (400[MHz])
 X_Acq_Duration = 2.18365952[s]
 X_Domain = 1H
 X_Freq = 399.78219838[MHz]
 X_Offset = 5[ppm]
 X_Points = 16384
 X_Prescans = 1
 X_Resolution = 0.45794685[Hz]
 X_Sweep = 7.5030012[kHz]
 X_Sweep_Clipped = 6.00240096[kHz]
 Irr_Domain = Proton
 Irr_Freq = 399.78219838[MHz]
 Irr_Offset = 5[ppm]
 Tri_Domain = Proton

Tri_Freq = 399.78219838[MHz]
 Tri_Offset = 5[ppm]
 Clipped = FALSE
 Scans = 16
 Total_Scans = 16

Relaxation_Delay = 5[s]
 Recvr_Gain = 38
 Temp_Get = 23.4[dC]
 X_90_Width = 12.795[us]
 X_Acq_Time = 2.18365952[s]
 X_Angle = 45[deg]
 X_Atn = 2.4[dB]
 X_Pulse = 6.3975[us]
 Irr_Mode = Off
 Tri_Mode = Off

Cl-Ph-Br-TMS

Pulse Sequence: s2pu1

Solvent: DMSO

Ambient temperature

Mercury-400BB "MercuryPlus400"

Relax delay 0 500 sec
Pulse 68 7 degrees
Acq time 1 000 sec
Width 25000 0 Hz
16000 repetitions
OBSERVE C13 100 6806415 MHz
DECOUPLE H1 400 4018591 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1 0 Hz
FT size 65536
Total time 7 hr 41 min 13 sec

C1-Ph-Br-OMe

Pulse Sequence: s2pu1

UNITYplus-400 "unity400"

Date: Jan 29 2013

Solvent: DMSO

Ambient temperature

Total 2496 repetitions

X : parts per Million : Proton

Filename = code-4t_Proton-1-3.jdf
 Author = delta
 Experiment = proton.jxp
 Sample Id = code-4t
 Solvent = DMSO-D6
 Creation Time = 14-JUN-2016 15:56:18
 Revision Time = 14-JUN-2016 16:02:55
 Current Time = 14-JUN-2016 16:04:05

Comment = single pulse
 Data Format = 1D COMPLEX
 Dim Size = 13107
 Dim Title = Proton
 Dim Units = [ppm]
 Dimensions = X
 Site = JNM-ECS400

Spectrometer = DELTA2_NMR
 Field Strength = 9.389766[T] (400[MHz])
 X Acq_Duration = 2.18365952[s]
 X Domain = 1H
 X Freq = 399.78219838 [MHz]
 X Offset = 5 [ppm]
 X Points = 16384
 X Prescans = 1
 X Resolution = 0.45794685 [Hz]
 X Sweep = 7.5030012 [kHz]
 X Sweep_Clippped = 6.00240096 [kHz]
 Irr Domain = Proton
 Irr Freq = 399.78219838 [MHz]
 Irr Offset = 5 [ppm]
 Tri_Domain = Proton

Tri_Freq = 399.78219838 [MHz]
 Tri_Offset = 5 [ppm]
 Clipped = FALSE
 Scans = 16
 Total_Scans = 16
 Relaxation_Delay = 5 [s]
 Recvr Gain = 38
 Temp_Get = 23.6 [dC]
 X_90_Width = 12.795 [us]
 X_Acq Time = 2.18365952 [s]
 X_Angle = 45 [deg]
 X_Atn = 2.4 [dB]
 X_Pulse = 6.3975 [us]
 Irr Mode = Off
 Tri_Mode = Off

C1-Ph-OMe-NO2

Pulse Sequence: s2pul1

Solvent: DMSO

Ambient temperature

Mercury-400BB "MercuryPlus400"

Pulse 68.7 degrees

Acq. time 1.000 sec

Width 25000.0 Hz

1600 repetitions

OBSERVE C13, 100.6806392 MHz

DECOUPLE H1, 400.4018591 MHz

Power 38 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 32 min, 47 sec

X : parts per Million : Proton

Filename = code-4u_Proton-1-3.jdf
 Author = delta
 Experiment = proton.jxp
 Sample_Id = code-4u
 Solvent = DMSO-D6
 Creation Time = 17-JUN-2016 10:27:12
 Revision Time = 17-JUN-2016 10:53:42
 Current Time = 17-JUN-2016 10:53:56

Comment = single pulse
 Data Format = 1D COMPLEX
 Dim Size = 13107
 Dim Title = Proton
 Dim Units = [ppm]
 Dimensions = X
 Site = JNM-ECS400

Spectrometer = DELTA2_NMR
 Field Strength = 9.389766[T] (400[MHz])
 X_Acq_Duration = 2.18365952[s]
 X_Domain = 1H
 X_Freq = 399.78219838[MHz]
 X_Offset = 5[ppm]
 X Points = 16384
 X_Prescans = 1
 X Resolution = 0.45794685[Hz]
 X Sweep = 7.5030012[kHz]
 X Sweep_Clippped = 6.00240096[kHz]
 Irr_Domain = Proton
 Irr_Freq = 399.78219838[MHz]
 Irr_Offset = 5[ppm]
 Tri_Domain = Proton

Tri_Freq = 399.78219838[MHz]
 Tri_Offset = 5[ppm]
 Clipped = FALSE
 Scans = 64
 Total_Scans = 64
 Relaxation_Delay = 5[s]
 Recvr Gain = 34
 Temp_Get = 24.8[dC]
 X_90_Width = 12.795[us]
 X_Acq_Time = 2.18365952[s]
 X_Angle = 45[deg]
 X_Atn = 2.4[dB]
 X_Pulse = 6.3975[us]
 Irr_Mode = Off
 Tri_Mode = Off

**JEOL
RESONANCE**

Ph-NCO-Br-CH3

Pulse Sequence: s2pu1

Solvent: DMSO

Ambient temperature

Mercury-400BB "MercuryPlus400"

Relax. delay 0.500 sec

Pulse 68.7 degrees

Acq. time 1.000 sec

Width 25000.0 Hz

464 repetitions

OBSERVE C13, 100.6806415 MHz

DECOUPLE H1, 400.4018591 MHz

Power 38 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 7 hr, 41 min, 13 sec

C1-Ph-NC0-2H-CH3

Pulse Sequence: s2pu1

Solvent: DMSO

Ambient temperature

Mercury-400BB "MercuryPlus400"

Pulse 48.1 degrees

Acq. time 4.002 sec

Width 5995.2 Hz

80 repetitions

OBSERVE H1, 400.3997882 MHz

DATA PROCESSING

Line broadening 0.1 Hz

FT size 65536

Total time 6 min, 23 sec

C1-Ph-NCO-2H-CH3

Pulse Sequence: s2pu1

Solvent: DMSO

Ambient temperature

Mercury-400BB "MercuryPlus400"

Relax. delay 0.500 sec

Pulse 68.7 degrees

Acq. time 1.000 sec

Width 25000.0 Hz

16000 repetitions

OBSERVE C13, 100.6806408 MHz

DECOUPLE H1, 400.4018591 MHz

Power 38 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 7 hr, 41 min, 13 sec