Angewandte Chemie
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Supporting Information

69451 Weinheim, Germany

"Construction and Screening of a 2-Aminoimidazole Library Accessed by [3+2] Click Chemistry Identifies a Small Molecule Capable of Inhibiting and Dispersing Biofilms Across Bacterial Order, Class and Phylum"

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Supporting Information

1. Experimental Protocols for 2-AIT Conjugate Synthesis

2. Experimental Protocols for Bacterial Biofilm Regulation Studies

3. ^{1}H NMR Spectra for New Compounds

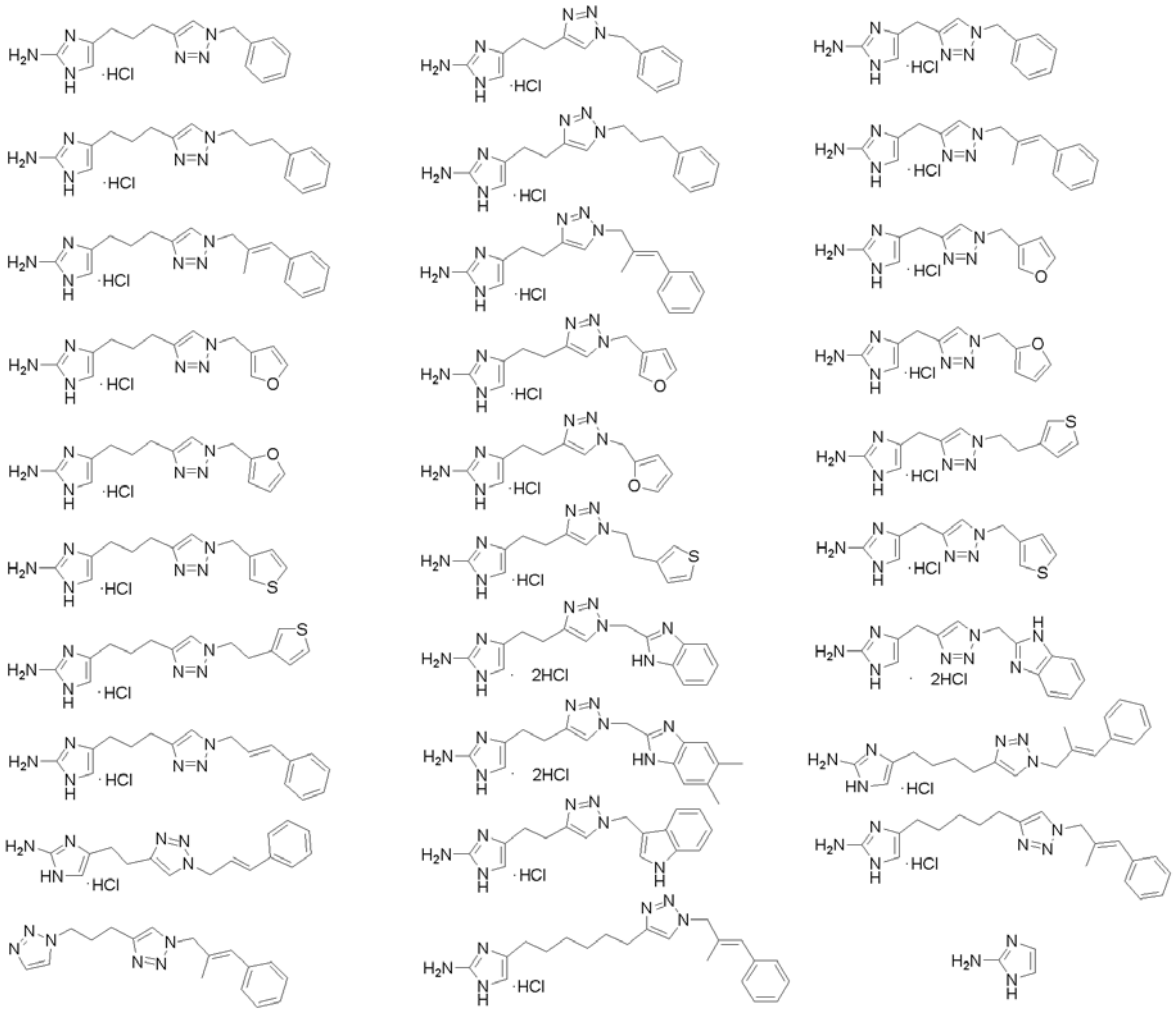
1. Experimental Protocols for 2-AIT Conjugate Synthesis

All reagents used for chemical synthesis were purchased from commercially available sources and used without further purification. Chromatography was performed using 60 Å mesh standard grade silica gel from Sorbtech. NMR solvents were obtained from Cambridge Isotope Labs and used as is. ^{1}H NMR (300 MHz or 400 MHz) and ^{13}C NMR (75 MHz or 100 MHz) spectra were recorded at 25ºC on Varian Mercury spectrometers. Chemical shifts (δ) are given in ppm relative to tetramethylsilane or the respective NMR solvent; coupling constants (*J*) are in hertz (Hz). Abbreviations used are s = singlet, bs = broad singlet, d = doublet, dd = doublet of doublets, t = triplet, dt = doublet of triplets, bt = broad triplet, qt = quartet, m = multiplet, bm = broad multiplet and br = broad. High and low resolution mass spectra were obtained at the North

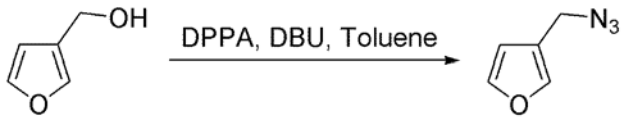
Carolina State Mass Spectrometry Laboratory for Biotechnology. FAB experiments were carried out with a JOEL HX110HF mass spectrometer while ESI experiments were carried out on an Agilent LC-TOF mass spectrometers.

A. baumannii (ATCC # 19606) was purchased from ATCC. *P. aeruginosa* strains PA14 and PAO1 were provided by Dr. Wozniak at Wake Forest School of Medicine while *B. bronchiseptica* strain RB50 was donated by Dr. Deora at the Wake Forest School of Medicine. *S. aureus* (ATCC # 29213) was also obtained from the ATCC.

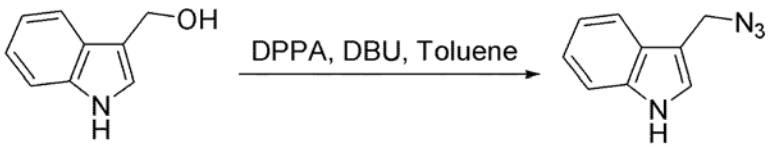
Chemical Library



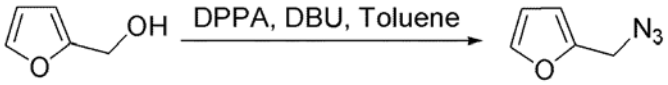
Synthesis



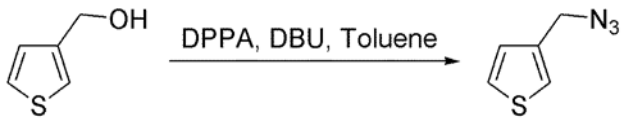
- To a 50 mL round-bottomed flask equipped with a magnetic stir bar was added 3-furan methanol (1.00 g, 10.2 mmol) and a solution of diphenyl phosphoryl azide (3.37 g, 12.2 mmol) in toluene (30 mL). The stirring solution was allowed to cool to 0° C, in which 1, 8 Diazabycyclo [5. 4. 0.] undec-7-ene (1.86 g, 12.2 mmol) was added dropwise. The reaction was allowed to slowly warm to ambient temperature for an additional 16 hours of stirring. After this period, the reaction mixture was washed with water (2 x 20 mL) and then with 5% HCl (20 mL). Volatiles were evaporated under reduced pressure. The resulting residue was then purified by column chromatography (1:9 ethyl acetate:hexane) providing 3-(azidomethyl)furan (1.19 g, 95% yield) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, 1H), δ 7.44 (s, 1H), δ 6.42 (d, 1H), δ 4.20 (s, 2H). ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 144.1, 141.1, 110.4, 92.1, 45.8 ppm; LRMS (EI) calcd for $C_5H_5N_3O$ (M^+) 123, found 123.



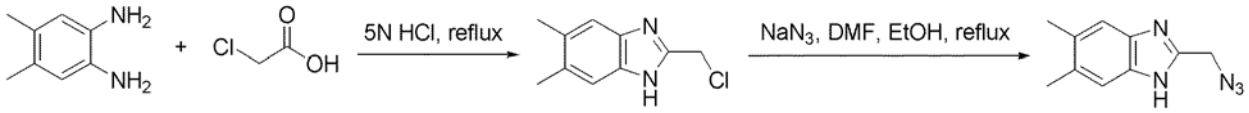
- Following the same procedure used to synthesize 3-(azidomethyl)furan, indole-3-methanol (2.00 g, 13.6 mmol) was converted to 3-(azidomethyl)indole (1.31 g, 56% yield) as a yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.19 (bs, 1H), δ 7.71 (d, 1H), δ 7.39 (m, 2H), δ 7.19 (m, 2H), δ 4.54 (s, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 130.3, 125.9, 125.3, 122.2, 120.3, 120.3, 119.7, 118.7, 111.9 ppm; LRMS (EI) calcd for $C_9H_8N_4$ (M^+) 172, found 172.



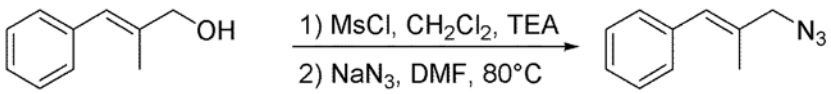
- Following the same procedure used to synthesize 3-(azidomethyl)furan, furfuryl alcohol (2.50 g, 25.5 mmol) was converted to 2-(azidomethyl)furan (2.96 g, 95% yield) as a colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.43 (d, 1H), δ 6.36 (m, 2H), δ 4.29 (s, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.2, 110.7, 109.6, 47.2 ppm; LRMS (EI) calcd for $C_5H_5N_3O$ (M^+) 123, found 123.



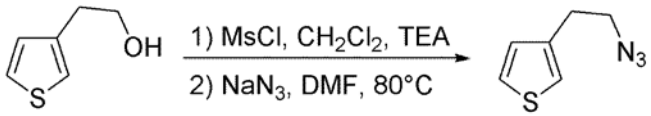
- Following the same procedure used to synthesize 3-(azidomethyl)furan, thiophene-3-methanol (3.14 g, 27.6 mmol) was converted to 3-(azidomethyl)thiophene (3.72 g, 97% yield) as a colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38 (d, 1H), δ 7.23 (s, 1H), δ 7.10 (d, 1H), δ 4.36 (s, 2H) ppm; ^{113}C NMR (75 MHz, $CDCl_3$) δ 136.4, 127.6, 127.1, 124.0, 49.9 ppm; LRMS (EI) calcd for $C_5H_5N_3S$ (M^+) 139, found 139.



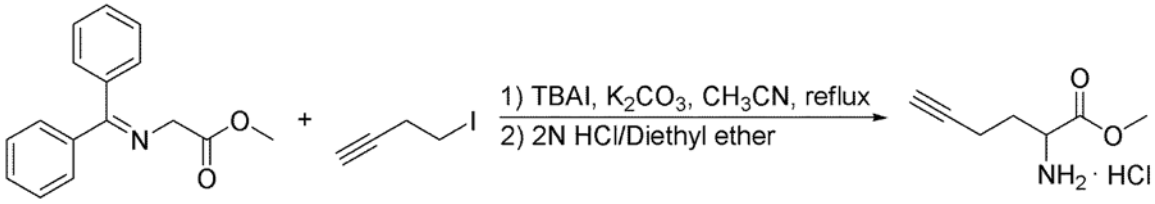
- 2-chloroethyl-5, 6-dimethyl-1H-benzimidazole was synthesized through the treatment of 4, 5-dimethyl-1, 2-phenylenediamine to conditions outlined by Hortelano.[1] The resulting product was transformed to 2-azidomethyl-5, 6-dimethyl-1H-benzimidazole following conditions outlined by Hankovszky resulting in a yellow solid.[2] ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.26 (s, 2H), δ 4.72 (s, 2H), δ 2.37 (s, 6H) ppm; ^{13}C NMR (75 MHz, DMSO) δ 153.7, 134.3, 130.1, 125.1, 124.6, 117.2, 113.6, 48.0, 20.6, 19.6 ppm; HRMS (FAB) calcd for $C_{10}H_{11}N_5$ (M^+) 201.1014, found 201.1010.



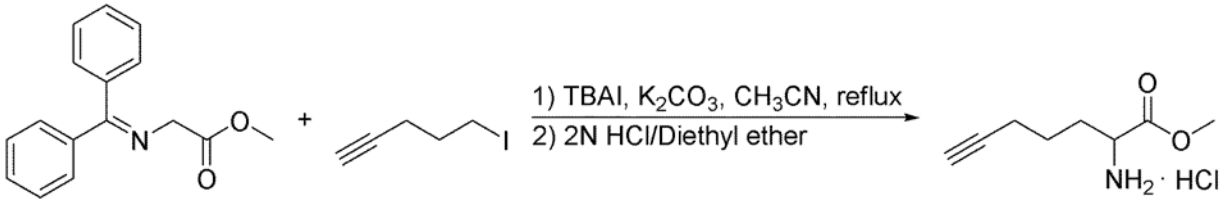
- To a 100 mL round-bottomed flask equipped with a magnetic stir was added trans-2-methyl-3-phenyl-2-propen-1-ol (2.00 g, 13.5 mmol) and 75 mL of methylene chloride. The solution was then cooled to 0° C while stirring. Then, triethylamine (2.75 g, 27.0 mmol) was added followed by a dropwise addition of methanesulfonyl chloride (2.34 g, 20.4 mmol) and a two hour stir period. The reaction mixture was washed with water (2 x 75 mL), dried with sodium sulfate and then concentrated de vacuo. The crude mixture is then dissolved in 75 mL of DMF and then stirred via magnetic stir bar. To this mixture, sodium azide (1.76 g, 27.0 mmol) was added. The reaction mixture was then heated to 80° C and allowed to stir for two hours. At this time, volatiles are concentrated de vacuo and the resulting residue is purified via column chromatography (1:9 ethyl acetate:hexane) providing (3-Azido-2-methyl-propenyl)-benzene (2.08 g, 89% yield) as a colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36 – 7.25 (m, 5H), δ 6.53 (s, 1H), δ 3.87 (s, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 129.4, 129.2, 128.9, 128.6, 128.4, 127.1, 59.9, 52.0, 22.3, 16.5 ppm; LRMS (EI) calcd for $C_{10}H_{11}N_3$ (M^+) 173, found 173.



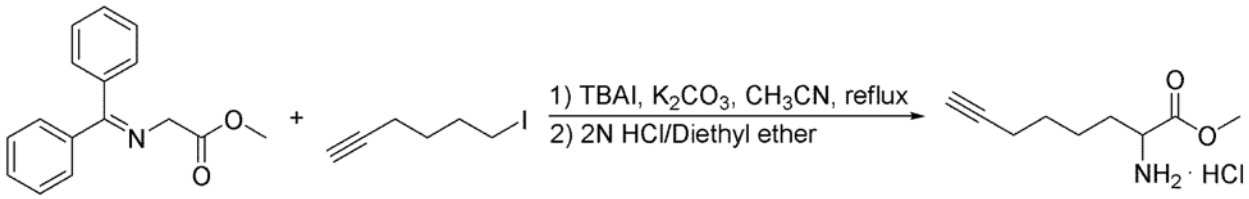
- Following the same procedure used to synthesize (3-Azido-2-methyl-propenyl)-benzene, thiophene-3-ethanol (2.00 g, 15.5 mmol) was converted to 3-(azidomethyl)thiophene (2.06 g, 86% yield) as a colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36 (s, 1H), δ 7.14 (d, 1H), δ 7.04 (d, 1H), δ 3.54 (t, 2H), δ 2.98 (t, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 138.7, 128.4, 126.3, 122.2, 52.0, 30.1 ppm; LRMS (EI) calcd for $C_6H_7N_3S$ (M^+) 153, found 153.



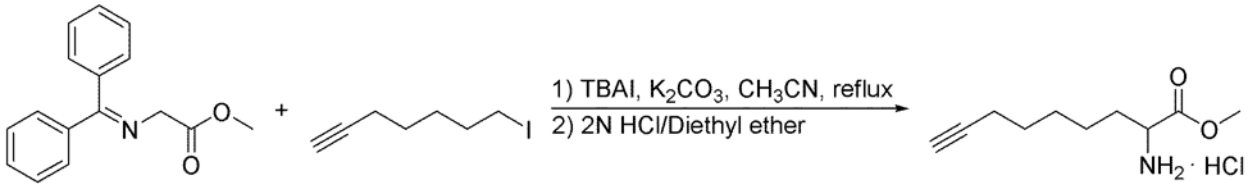
- 2-Amino-hex-5-ynoic acid methyl ester hydrochloride was synthesized using the same methods previously reported for the synthesis of 2-Amino-pent-4-ynoic acid methyl ester hydrochloride.[3] ^{1}H NMR (300 MHz, D_2O) δ 4.16 (t, 1H), δ 3.71 (s, 3H), δ 2.32 (t, 1H), δ 2.29 (m, 2H), δ 2.06 (m, 2H) ppm; ^{13}C NMR (75 MHz, D_2O) δ 170.4, 82.4, 71.4, 53.9, 52.1, 28.7, 14.4 ppm; HRMS (ESI) calcd for $C_7H_{11}NO_2$ (M^+) 142.0859, found 142.862.



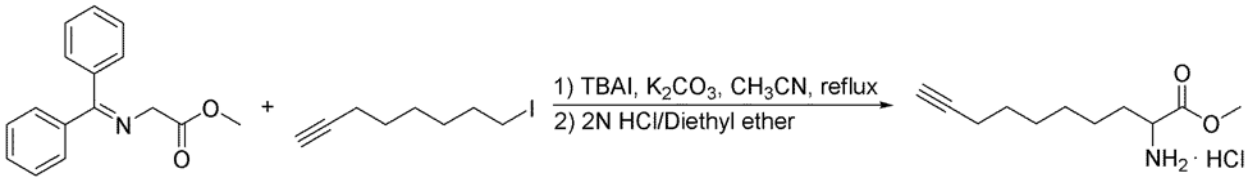
- 2-Amino-hept-6-ynoic acid methyl ester hydrochloride was synthesized using the same methods previously reported for the synthesis of 2-Amino-pent-4-ynoic acid methyl ester hydrochloride.[3] ^{1}H NMR (300 MHz, DMSO) δ 8.75 (s, 2H), δ 3.99 (m, 1H), δ 3.72 (s, 3H), δ 2.82 (t, 1H), δ 2.17 (m, 2H), δ 1.89 (m, 2H), δ 1.51 (m, 2H) ppm; ^{13}C NMR (75 MHz, DMSO) δ 163.7, 83.1, 69.2, 60.9, 30.6, 29.5, 23.9, 17.6 ppm; HRMS (ESI) calcd for $C_8H_{13}NO_2$ (M^+) 156.1019, found 156.1017.



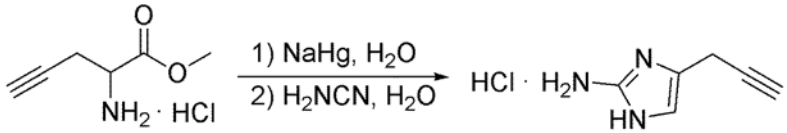
- 2-Amino-oct-7-ynoic acid methyl ester hydrochloride was synthesized using the same methods previously reported for the synthesis of 2-Amino-pent-4-ynoic acid methyl ester hydrochloride.[3] ^{1}H NMR (300 MHz, D_2O) δ 4.16 (t, 1H), δ 3.84 (s, 3H), δ 2.35 (t, 1H), δ 2.24 (m, 2H), δ 1.95 (m, 2H), δ 1.52 (m, 4H) ppm; ^{13}C NMR (75 MHz, D_2O) δ 170.9, 85.6, 69.6, 53.6, 52.9, 29.3, 27.0, 23.4, 17.3 ppm; HRMS (ESI) calcd for $C_9H_{15}NO_2$ (M^+) 170.1176, found 170.1171.



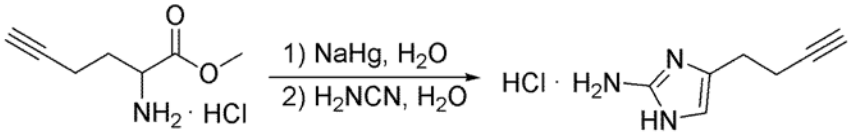
- 2-Amino-non-8-ynoic acid methyl ester hydrochloride was synthesized using the same methods previously reported for the synthesis of 2-Amino-pent-4-ynoic acid methyl ester hydrochloride.[3] ^{1}H NMR (300 MHz, D_2O) δ 4.21 (t, 1H), δ 3.90 (s, 3H), δ 2.41 (t, 1H), δ 2.28 (m, 2H), δ 2.01 (m, 2H), δ 1.51 (m, 6H) ppm; ^{13}C NMR (75 MHz, D_2O) δ 171.1, 86.4, 69.4, 53.7, 53.1, 29.8, 27.5, 27.4, 23.8, 17.6 ppm; HRMS (ESI) calcd for $C_{10}H_{18}NO_2$ (M^+) 184.1332, found 184.1329.



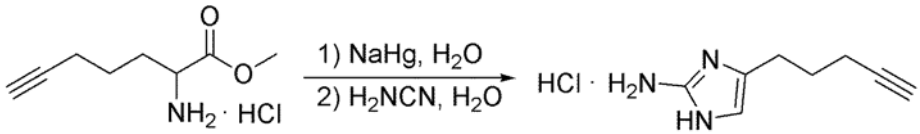
- 2-Amino-dec-9-ynoic acid methyl ester hydrochloride was synthesized using the same methods previously reported for the synthesis of 2-Amino-pent-4-ynoic acid methyl ester hydrochloride.[3] ^{1}H NMR (300 MHz, D_2O) δ 4.16 (t, 1H), δ 3.86 (s, 3H), δ 2.36 (t, 1H), δ 2.21 (m, 2H), δ 1.98 (m, 2H), δ 1.55 – 1.39 (m, 8H) ppm; ^{13}C NMR (75 MHz, D_2O) δ 171.2, 86.7, 69.3, 53.7, 53.1, 29.8, 27.7, 27.7, 27.6, 24.1, 17.6 ppm; HRMS (ESI) calcd for $C_{11}H_{20}NO_2$ (M^+) 198.1488, found 198.1488.



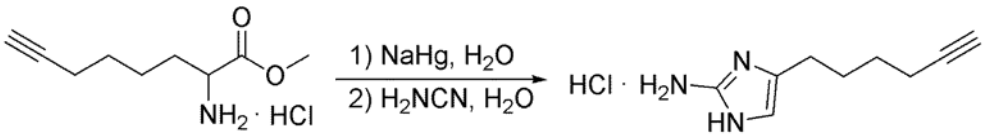
- 2-Amino-pent-4-ynoic acid methyl ester hydrochloride (2.91 g, 17.8 mmol) was treated to an Akabori reduction followed by a cyanamide condensation employing conditions previously reported to produce 4-Prop-2-ynyl-1H-imidazol-2-ylamine hydrochloride (1.65 g, 59% yield) as a yellow oil.[4] ^{1}H NMR (300 MHz, CD_3OD) δ 6.30 (s, 1H), δ 5.02 (d, 2H), δ 2.26 (t, 1H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 150.1, 127.2, 109.6, 83.6, 69.8, 15.9 ppm; HRMS (ESI) calcd for $C_6H_7N_3$ (M^+) 122.0712, found 122.0713.



- 2-Amino-hex-5-ynoic acid methyl ester hydrochloride (2.53 g, 14.2 mmol) was treated to an Akabori reduction followed by a cyanamide condensation employing conditions previously reported to produce 4-But-3-ynyl-1H-imidazol-2-ylamine hydrochloride (1.17 g, 48% yield) as a pale yellow oil.[4] ^{1}H NMR (300 MHz, CD_3OD) δ 6.52 (s, 1H), δ 2.61 (t, 2H), δ 2.42 (m, 2H), δ 2.27 (t, 1H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 147.4, 126.2, 109.4, 81.9, 69.9, 23.8, 17.4 ppm; HRMS (ESI) calcd for $C_7H_{10}N_3$ (M^+) 136.0869, found 136.0865.

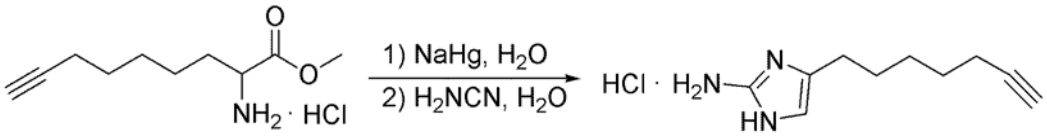


- 2-Amino-hept-6-ynoic acid methyl ester hydrochloride (2.00 g, 10.4 mmol) was treated to an Akabori reduction followed by a cyanamide condensation employing conditions previously reported to produce 4-Pent-4-ynyl-1H-imidazol-2-ylamine hydrochloride (1.75 g, 90% yield) as a pale oil.[4] ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.68 (bs, 2H), δ 6.24 (s, 1H), δ 2.51 (t, 2H), δ 2.17 (t, 1H), δ 1.95 (s, 1H), δ 1.74 (m, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.3, 132.7, 111.6, 84.4, 69.1, 28.0, 26.0, 18.2 ppm; HRMS (ESI) calcd for $C_{10}H_{16}N_3$ (M^+) 150.1026, found 150.1029.

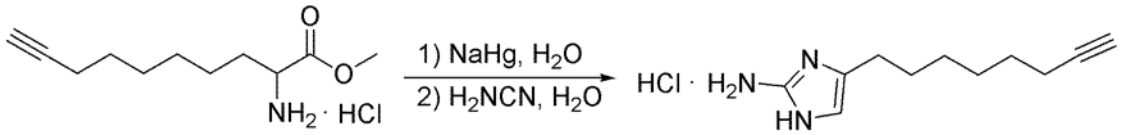


- 2-Amino-oct-7-ynoic acid methyl ester hydrochloride (2.90 g, 14.1 mmol) was treated to an Akabori reduction followed by a cyanamide condensation employing conditions previously reported to produce 4-Hex-5-ynyl-1H-imidazol-2-ylamine hydrochloride (2.45 g, 87% yield) as a pale yellow solid.[4] ^{1}H NMR (300 MHz, CD_3OD) δ 6.43 (s, 1H), δ 2.44 (t, 2H), 2.14 (t, 1H), δ

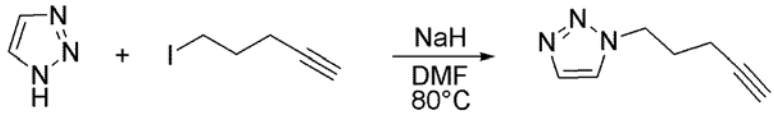
2.12 (m, 2H), δ 1.64 (m, 2H), δ 1.47 (m, 2H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 147.3, 127.6, 108.5, 83.4, 68.7, 27.7, 27.1, 23.8, 17.5 ppm; HRMS (ESI) calcd for $C_9H_{14}N_3$ (M^+) 164.1182, found 164.1182.



- 2-Amino-non-8-ynoic acid methyl ester hydrochloride (2.02g, 9.20mmol) was treated to an Akabori reduction followed by a cyanamide condensation employing conditions previously reported to produce 4-Hept-6-ynyl-1H-imidazol-2-ylamine hydrochloride (1.04 g, 53% yield) as a pale yellow solid.[4] ^{1}H NMR (300 MHz, CD_3OD) δ 6.17 (s, 1H), δ 2.19 (t, 2H), δ 1.90 (t, 1H), δ 1.86 (m, 2H), δ 1.24 – 1.13 (m, 6H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 147.5, 128.3, 108.8, 83.8, 65.5, 28.4, 28.3, 28.2, 24.5, 17.8 ppm; HRMS (ESI) calcd for $C_{10}H_{16}N_3$ (M^+) 178.1338, found 178.1337.



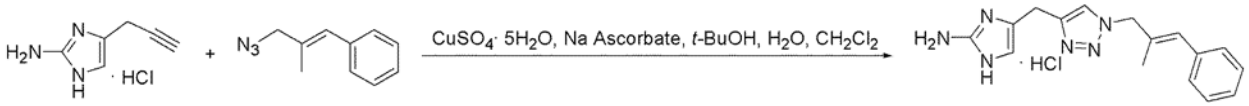
- 2-Amino-dec-9-ynoic acid methyl ester hydrochloride (1.50 g, 6.42 mmol) was treated to an Akabori reduction followed by a cyanamide condensation employing conditions previously reported to produce 4-Oct-7-ynyl-1H-imidazol-2-ylamine hydrochloride (0.774 g, 53% yield) as a pale yellow solid.[4] ^{1}H NMR (400 MHz, CD_3OD) δ 6.09 (s, 1H), δ 2.19 (t, 2H), δ 1.95 (t, 1H), 1.93 (m, 2H), δ 1.39 – 1.11 (m, 8H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 148.5, 131.0, 110.1, 83.9, 68.3, 28.6, 28.5, 28.4, 28.3, 25.7, 17.8 ppm; HRMS (ESI) calcd for $C_{11}H_{18}N_3$ (M^+) 192.1495, found 192.1495.



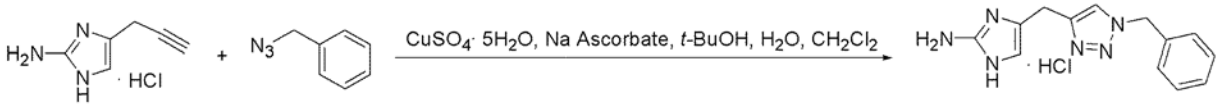
- To a 50 mL round-bottomed flask equipped with a magnetic stir bar was added 1-H-1, 2, 3-triazole (0.192 g, 2.78 mmol) and DMF (10 mL) and then cooled to 0° C while stirring. Then, sodium hydride (60% dispersion in mineral oil) (0.133 g, 3.33 mmol) was added to the reaction mixture and was slowly allowed to warm to ambient temperature. Then, 1-iodo-4-pentyne (0.647 g, 3.33 mmol) was added dropwise. The reaction mixture was then heated to 80° C and allowed to stir for 2.5 hours. Water (20 mL) was then added to the reaction mixture and then extracted with ethyl acetate (2 x 20 mL). The organic phase was dried with sodium sulfate and concentrated de vacuo followed by a purification by column chromatography (ethyl acetate/hexane) to produce 1-Pent-4-ynyl-1H-[1,2,3]triazole (0.349 g, 93% yield) as a colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.67 (s, 1H), δ 7.59 (s, 1H), δ 4.53 (t, 2H), δ 2.20 (t, 2H), δ

2.17 (m, 2H), δ 2.04 (s, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 133.9, 123.9, 82.2, 70.4, 48.7, 28.9. 15.7 ppm; HRMS (ESI) calcd for $C_7H_{10}N_3$ (M^+) 136.0869, found 136.0866.

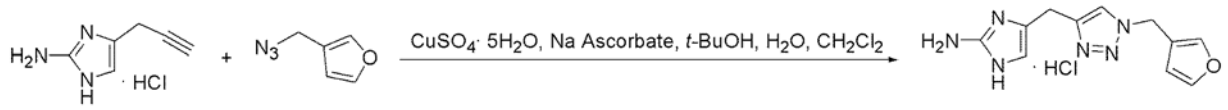
General procedure for click reactions: The terminal alkyne (1.0 equiv.) was dissolved in a 1:1:1 mixture of *tert*-butyl alcohol, water and methylene chloride (ca. 10 mL per 0.300 g of terminal alkyne). To this solution, the appropriate azide (1.2 equiv.) was added while stirring vigorously at room temperature. Copper (II) sulfate pentahydrate (15 mol%) and sodium ascorbate (45 mol%) were then added sequentially to the solution. Reaction mixtures were allowed to stir until completion via TLC analysis (12 – 24 hrs). The solvents were then removed de vacuo in which the resulting residue was dissolved in methanol and purified by flash chromatography (10 – 20% ammonia saturated methanol: methylene chloride). The resulting fractions were evaporated under reduced pressure followed by a 24 hr high vacuum treatment to remove the ammonia. Methanol saturated with HCl is then added to the purified product in which all volatiles were then removed under reduced pressure.



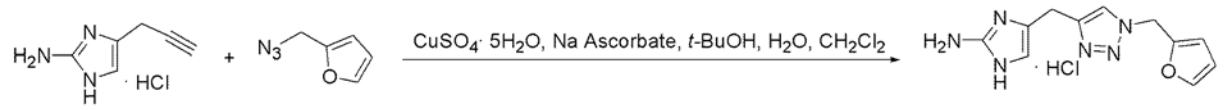
- 4-Prop-2-ynyl-1H-imidazol-2-ylamine hydrochloride (0.127 g, 0.809 mmol) was reacted with (3-Azido-2-methyl-propenyl)-benzene (0.168 g, 0.971 mmol) following the general procedure for click reactions outlined above to produce 4-[1-(2-Methyl-3-phenyl-allyl)-1H-[1,2,3]triazol-4-ylmethyl]-1H-imidazol-2-ylamine hydrochloride (0.244 g, 91% yield) of a pale yellow solid. ^{1}H NMR (300 MHz, D_2O) δ 7.94 (s, 1H), δ 7.40 – 7.35 (m, 5H), δ 6.56 (s, 1H), δ 5.10 (s, 2H), δ 3.99 (s, 2H), δ 1.76 (s, 3H) ppm; ^{13}C NMR (75 MHz, D_2O) δ 145.8, 138.1, 136.9, 136.5, 136.4, 132.8, 128.3, 128.0, 127.6, 125.3, 123.4, 49.3, 23.8, 23.4; HRMS (ESI) calcd for $C_{16}H_{18}N_6$ (M^+) 295.1665, found 295.1665.



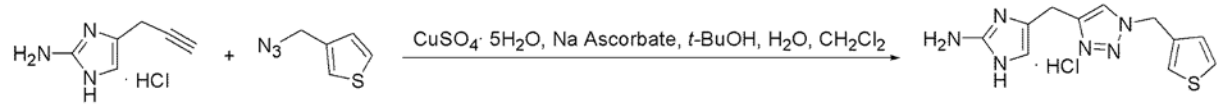
- 4-Prop-2-ynyl-1H-imidazol-2-ylamine hydrochloride (0.095 g, 0.603 mmol) was reacted with benzyl azide (0.096 g, 0.723 mmol) following the general procedure for click reactions outlined above to produce 4-(1-Benzyl-1H-[1,2,3]triazol-4-ylmethyl)-1H-imidazol-2-ylamine hydrochloride (0.151 g, 86% yield) of a pale yellow solid. ^{1}H NMR (300 MHz, D_2O) δ 7.79 **(**s, 1H), δ 7.42 – 7.35 (m, 5H), δ 6.43 (s, 1H), δ 5.58 (s, 2H), δ 3.86 (s, 2H) ppm; ^{13}C NMR (75 MHz, D_2O) δ 145.4, 136.6, 136.4, 128.8, 128.7, 126.9, 126.8, 126.3, 124.1, 121.8, 109.6, 53.3, 24.1 ppm; HRMS (ESI) calcd for $C_{13}H_{16}N_6O$ (M^+) 254.1352, found 254.1352.



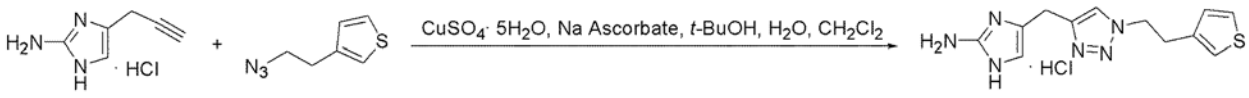
- 4-Prop-2-ynyl-1H-imidazol-2-ylamine hydrochloride (0.101g, 0.639 mmol) was reacted with 3-azidomethyl-furan (0.094 g, 0.767 mmol) following the general procedure for click reactions outlined above to produce 4-(1-Furan-3-ylmethyl-1H-[1,2,3]triazol-4-ylmethyl)-1H-imidazol-2-ylamine hydrochloride (0.077 g, 43% yield) of a pale yellow solid. ^{1}H NMR (300 MHz, CD_3OD) δ 8.12 (s, 1H), δ 7.60 (s, 1H), δ 7.38 (s, 1H), δ 6.53 (s, 1H), δ 6.37 (s, 1H), δ 5.46 (s, 2H), δ 3.95 (s, 2H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 146.1, 145.3, 144.1, 141.0, 123.3, 123.1, 110.3, 110.2, 109.9, 51.3, 19.9 ppm; HRMS (ESI) calcd for $C_{11}H_{12}N_6O$ (M^+) 244.1145, found 244.1145.



- 4-Prop-2-ynyl-1H-imidazol-2-ylamine hydrochloride (0.096 g, 0.061 mmol) was reacted with 2-azidomethyl-furan (0.089 g, 0.729 mmol) following the general procedure for click reactions outlined above to produce 4-(1-Furan-2-ylmethyl-1H-[1,2,3]triazol-4-ylmethyl)-1H-imidazol-2-ylamine hydrochloride (0.078 g, 46% yield) as a pale yellow solid. ^{1}H NMR (300 MHz, CD_3OD) δ 7.93 (s, 1H), δ 7.41 (s, 1H), 6.49 (s, 2H), δ 6.32 (s, 1H), δ 5.56 (s, 2H), δ 3.89 (s, 2H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 146.2, 146.1, 142.4, 141.5, 122.3, 122.2, 108.9, 109.2, 108.8, 51.6, 18.9 ppm; HRMS (ESI) calcd for $C_{11}H_{12}N_6O$ (M^+) 245.1145, found 245.1147.

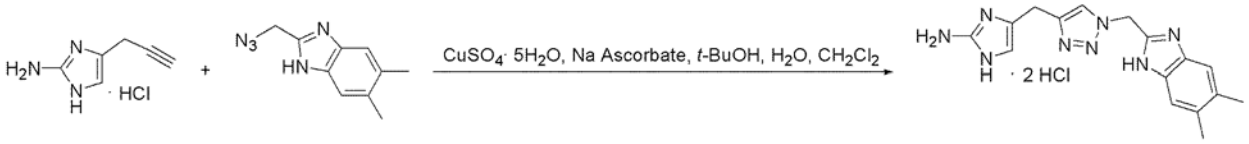


- 4-Prop-2-ynyl-1H-imidazol-2-ylamine hydrochloride (0.096 (0.061 mmol) was reacted with 3-azidomethyl thiophene (0.102 g, 0.732 mmol) following the general procedure for click reactions outlined above to produce 4-(1-Thiophen-3-ylmethyl-1H-[1,2,3]triazol-4-ylmethyl)-1H-imidazol-2-ylamine hydrochloride (0.079 g, 44% yield) of a pale yellow solid. ^{1}H NMR (300 MHz, CD_3OD) δ 8.18 (s, 1H), δ 7.44 (s, 1H), δ 7.30 (d, 1H), δ 6.98 (d, 1H), δ 6.53 (s, 1H), δ 5.57 (s, 2H), δ 3.95 (s, 2H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 145.7, 145.1, 143.7, 139.7, 129.8, 121.8, 111.5, 109.8, 109.2, 52.7, 21.5 ppm; HRMS (ESI) calcd for $C_{11}H_{12}N_6S$ (M^+) 260.0919, found 260.0919.

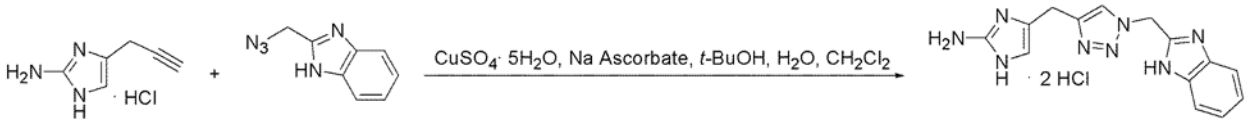


- 4-Prop-2-ynyl-1H-imidazol-2-ylamine hydrochloride (0.101 g, 0.641 mmol was reacted with 3-(2-Azido-ethyl)-thiophene (0.118 g, 0.769 mmol) following the general procedure for click

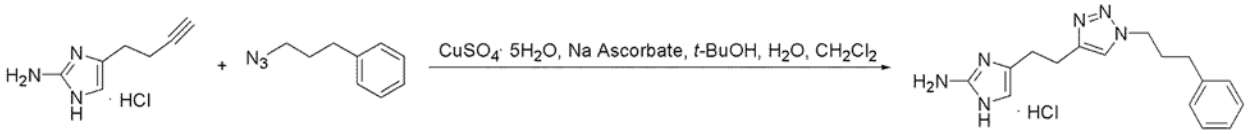
reactions outlined above to produce 4-[1-(2-Thiophen-3-yl-ethyl)-1H-[1,2,3]triazol-4-ylmethyl]-1H-imidazol-2-ylamine hydrochloride (0.119 g, 60% yield) of a pale yellow solid. ^{1}H NMR (300 MHz, CD_3OD) δ 7.42 (s, 1H), δ 7.19 (t, 1H), δ 6.90 (s, 1H), δ 6.78 (d, 1H), δ 6.09 (s, 1H), δ 4.47 (t, 2H), δ 3.67 (s, 2H), δ 3.09 (t, 2H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 151.2, 145.7, 137.7, 130.5, 127.8, 125.8, 122.9, 121.9, 110.3, 50.798, 30.7, 23.3 ppm; HRMS (ESI) calcd for $C_{12}H_{14}N_6S$ (M^+) 274.1001, found 274.1007.



- 4-Prop-2-ynyl-1H-imidazol-2-ylamine hydrochloride (0.047 g, 0.295 mmol) was reacted with 2-azidomethyl-5, 6-dimethyl-1H-benzimidazole (0.071 g, 0.354 mmol) following the general procedure for click reactions outlined above to produce 4-[1-(5,6-Dimethyl-1H-benzoimidazol-2-ylmethyl)-1H-[1,2,3]triazol-4-ylmethyl]-1H-imidazol-2-ylamine dihydrochloride (0.029 g, 25% yield) of a yellow solid. ^{1}H NMR (300 MHz, CD_3OD) δ 8.09 (s, 1H), δ 7.45 (s, 2H), δ 6.52 (s, 1H), δ 6.08 (s, 2H), δ 3.93 (s, 2H), δ 2.35 (s, 6H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 142.2, 136.9, 136.6, 124.5, 124.3, 113.8, 113.4, 110.0, 100.4, 85.8, 80.6, 75.3, 74.1, 45.0, 20.9, 19.28 ppm; HRMS (ESI) calcd for $C_{16}H_{18}N_8$ (M^+) 323.1727, found 323.1734.

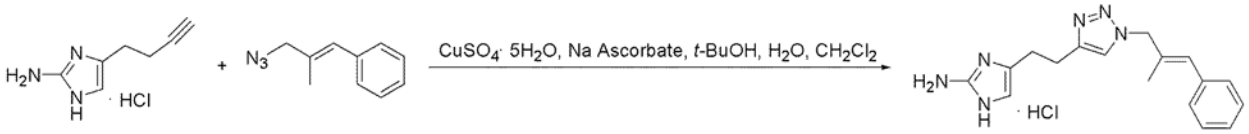


- 4-Prop-2-ynyl-1H-imidazol-2-ylamine hydrochloride (0.091 g, 0.576 mmol) was reacted with 2-azidomethyl-1H-benzimidazole, which was synthesized using previously reported methods,[2](0.120 g,0.691 mmol) following the general procedure for click reactions outlined above to produce 4-[1-(1H-Benzoimidazol-2-ylmethyl)-1H-[1,2,3]triazol-4-ylmethyl]-1H-imidazol-2-ylamine dihydrochloride (0.125 g, 59% yield) of a yellow solid. ^{1}H NMR (300 MHz, CD_3OD) δ 8.01 (s, 1H), δ 7.58 (d, 2H), δ 7.31 (t, 2H), δ 6.44 (s, 1H), δ 5.98 (s, 2H) δ 3.84 (s, 2H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 135.6, 124.7, 123.7, 123.5, 122.8, 112.8, 112.3, 108.4, 83.6, 78.9, 74.0, 73.2, 44.2, 19.3 ppm; HRMS (ESI) calcd for $C_{14}H_{14}N_8$ (M^+) 295.1414, found 295.1420.

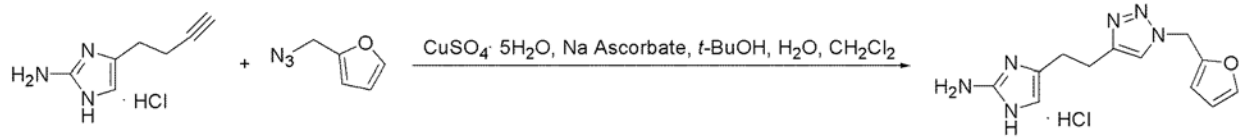


- 4-But-3-ynyl-1H-imidazol-2-ylamine hydrochloride (0.0735 g, 0.428 mmol) was reacted with (3-azido-propyl) benzene, which was synthesized using previously reported methods,[5](0.083 g, 0.514 mmol) following the general procedure for click reactions outlined above to produce 4-{2-

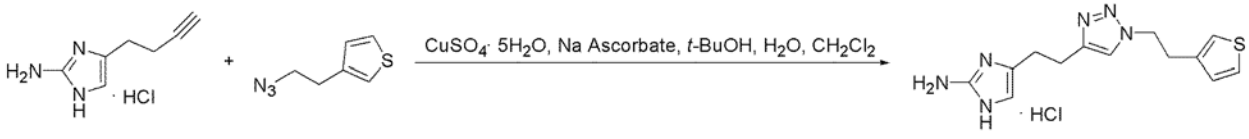
[1-(3-Phenyl-propyl)-1H-[1,2,3]triazol-4-yl]-ethyl}-1H-imidazol-2-ylamine hydrochloride (0.051 g, 36% yield) of a pale yellow oil. ^{1}H NMR (300 MHz, CD_3OD) δ 7.87 (s, 1H), δ 7.32 – 7.22 (m, 5H), δ 6.54 (s, 1H), δ 4.31 (t, 2H), δ 3.05 (t, 2H), δ 2.93 (t, 2H), δ 2.67 (t, 2H), δ 2.23 (m, 2H) ppm; ^{13}C NMR (75 MHz CD_3OD) δ 153.3, 146.6, 140.4, 134.3, 128.8, 128.7, 128.6, 126.6, 121.5, 67.5, 53.9, 32.8, 32.9, 29.5 ppm; HRMS (ESI) calcd for $C_{16}H_{20}N_6$ (M^+) 296.1822, found 296.1828.



- 4-But-3-ynyl-1H-imidazol-2-ylamine hydrochloride (0.062 g, 0.362) was reacted with (3-Azido-2-methyl-propenyl)-benzene (0.075 g, 0.434 mmol) following the general procedure for click reactions outlined above to produce 4-{2-[1-(2-Methyl-3-phenyl-allyl)-1H-[1,2,3]triazol-4-yl]-ethyl}-1H-imidazol-2-ylamine hydrochloride (0.054 g, 43% yield) of a pale yellow oil. ^{1}H NMR (300 MHz, CD_3OD) δ 8.39 (s, 1H), δ 7.12 – 7.07 (m, 5H), δ 6.54 (s, 1H), δ 6.36 (s, 1H), δ 5.09 (s, 2H), δ 3.01 (t, 2H), δ 2.76 (t, 2H), δ 1.60 (s, 3H) ppm; ^{13}C NMR (75 MHz CD_3OD) δ 147.7, 143.1, 136.3, 132.7, 129.9, 128.9, 128.6, 128.5, 128.2, 127.4, 127.1, 124.9, 109.9, 61.2, 23.0, 22.3, 14.7 ppm; HRMS (ESI) calcd for $C_{16}H_{20}N_6$ (M^+) 308.1749, found 308.1742.

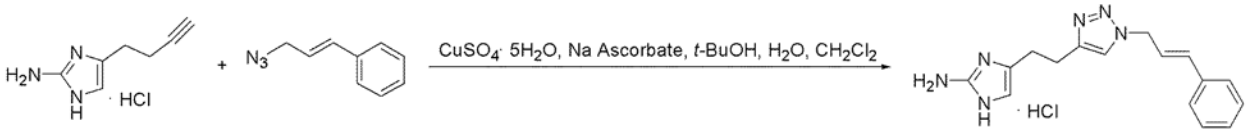


- 4-But-3-ynyl-1H-imidazol-2-ylamine hydrochloride (0.068 g, 0.399 mmol) was reacted with 2-azidomethyl furan (0.059 g, 0.478 mmol) following the general procedure for click reactions outlined above to produce 4-[2-(1-Furan-2-ylmethyl-1H-[1,2,3]triazol-4-yl)-ethyl]-1H-imidazol-2-ylamine hydrochloride (0.085 g, 72% yield) of a pale yellow solid. ^{1}H NMR (300 MHz, CD_3OD) δ 8.06 (s, 1H), δ 7.53 (s, 1H), δ 6.59 (t, 1H), δ 6.49 (s, 1H), δ 6.44 (dd, 1H), δ 3.05 (t, 2H), δ 2.89 (t, 2H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 156.4, 154.9, 147.5, 144.1, 126.0, 125.1, 123.8, 110.7, 109.3, 69.8, 23.8, 17.4 ppm; HRMS (ESI) calcd for $C_{12}H_{14}N_6O$ (M^+) 259.1301, found 259.1305.

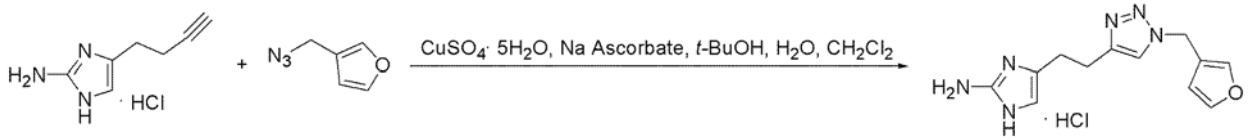


- 4-But-3-ynyl-1H-imidazol-2-ylamine hydrochloride (0.078 g, 0.45 mmol) was reacted with 3-(2-Azido-ethyl)-thiophene (0.083 g, 0.543 mmol) following the general procedure for click reactions outlined above to produce 4-{2-[1-(2-Thiophen-3-yl-ethyl)-1H-[1,2,3]triazol-4-yl]-ethyl}-1H-imidazol-2-ylamine hydrochloride (0.069 g, 47% yield) of a pale yellow oil. ^{1}H NMR

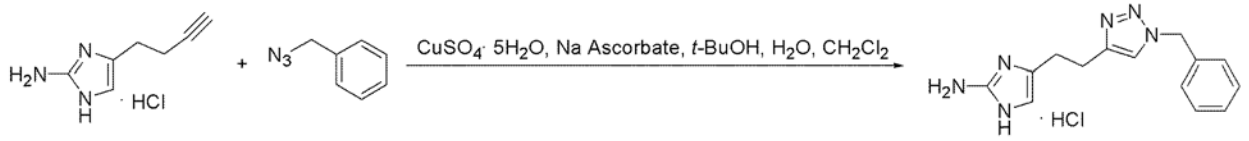
(300 MHz, CD_3OD) δ 7.33 (s, 1H), δ 7.19 (dd, 1H), δ 6.85 (d, 1H), δ 6.72 (d, 1H), δ 6.06 (s, 1H), δ 4.45 (t, 2H), δ 3.08 (t, 2H), δ 2.79 (t, 2H), δ 2.59 (t, 2H), ppm ^{13}C NMR (75 MHz, CD_3OD) δ 149.3, 147.0, 137.7, 132.1, 127.7, 125.8, 122.4, 121.9, 110.6, 50.8, 30.7, 26.6, 24.8 ppm; HRMS (ESI) calcd for $C_{13}H_{17}N_6S$ (M^+) 289.1229, found 289.1231.



- 4-But-3-ynyl-1H-imidazol-2-ylamine hydrochloride (0.066 g, 0.383 mmol) was reacted with (3-azido-propenyl)-benzene, which was synthesized using previously reported methods,[6](0.079 g, 0.460 mmol) following the general procedure for click reactions outlined above to produce 4-{2-[1-(3-Phenyl-allyl)-1H-[1,2,3]triazol-4-yl]-ethyl}-1H-imidazol-2-ylamine hydrochloride (0.049 g, 39% yield) of a pale yellow oil. ^1H NMR (300 MHz, CD_3OD) δ 8.19 (s, 1H), δ 7.44 (d, 2H), δ 7.29 (m, 3H), δ 6.73 (d, 1H), δ 6.53 (s, 1H), δ 6.42 (m, 2H), δ 5.24 (d, 2H), δ 3.07 (t, 2H), δ 2.88 (t, 2H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 148.6, 145.3, 139.4, 139.2, 129.8, 129.7, 129.6, 128.5, 128.4, 127.6, 54.6, 47.3, 45.9, 26.3, 22.6 ppm; HRMS (ESI) calcd for $C_{16}H_{19}N_6$ (M^+) 295.1665, found 295.1670.

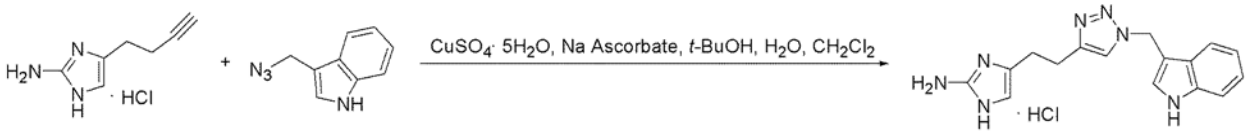


- 4-But-3-ynyl-1H-imidazol-2-ylamine hydrochloride (0.066 g, 0.384 mmol) was reacted with 3-azidomethyl-furan (0.057 g, 0.461 mmol) following the general procedure for click reactions outlined above to produce 4-[2-(1-Furan-3-ylmethyl-1H-[1,2,3]triazol-4-yl)-ethyl]-1H-imidazol-2-ylamine hydrochloride (0.061 g, 54% yield) as a pale yellow solid. ^1H NMR (300 MHz, CD_3OD) δ 7.70 (s, 1H), δ 7.61 (s, 1H), δ 7.46 (s, 1H), δ 6.42 (s, 1H), δ 6.38 (s, 1H), δ 5.41 (s, 2H), δ 2.95 (t, 2H), δ 2.83 (t, 2H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 146.3, 144.2, 141.6, 141.5, 126.5, 122.3, 120.2, 109.9, 109.1, 44.8, 24.2, 23.9 ppm; HRMS (ESI) calcd for $C_{12}H_{14}N_6O$ (M^+) 259.1301, found 259.1306.

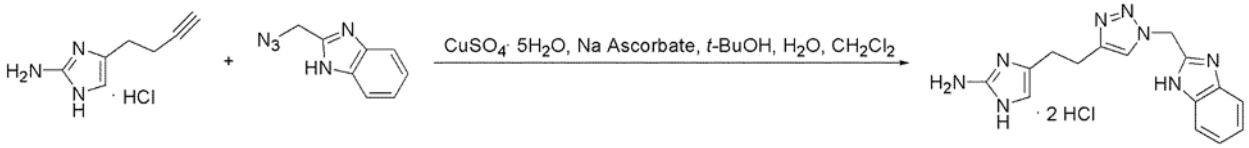


- 4-But-3-ynyl-1H-imidazol-2-ylamine hydrochloride (0.073 g, 0.423 mmol) was reacted with benzyl azide (0.068 g, 0.509 mmol) following the general procedure for click reactions outlined above to produce 4-[2-(1-Benzyl-1H-[1,2,3]triazol-4-yl)-ethyl]-1H-imidazol-2-ylamine hydrochloride (0.059 g, 46% yield) as a pale yellow oil. ^1H NMR (300 MHz, CD_3OD) δ 7.83 (d, 1H), δ 7.37 – 7.24 (m, 5H), δ 6.44 (d, 1H), δ 5.54 (d, 2H), δ 2.96 (m, 2H), δ 2.83 (m, 2H) ppm;

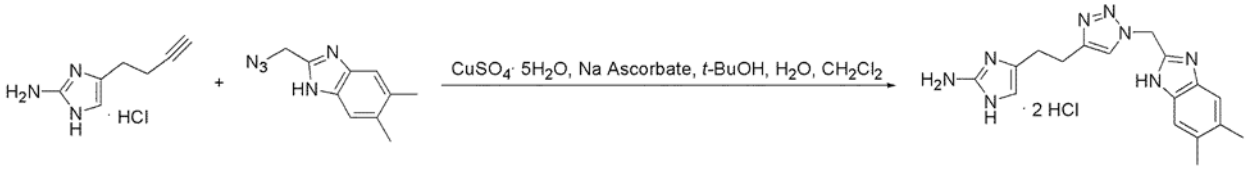
^{13}C NMR (75 MHz, CD_3OD) δ 163.7, 147.3, 146.4, 135.7, 128.8, 128.4, 127.9, 127.8, 126.5, 122.6, 109.1, 53.7, 24.1, 23.9 ppm; HRMS (ESI) calcd for $C_{14}H_{16}N_6$ (M^+) 269.1515, found 269.1513.



- 4-But-3-ynyl-1H-imidazol-2-ylamine hydrochloride (0.073 g, 0.429 mmol) was reacted with 3-azidomethyl-indole (0.089 g, 0.515 mmol) following the general procedure for click reactions outlined above to produce 4-{2-[1-(1H-Indol-3-ylmethyl)-1H-[1,2,3]triazol-4-yl]-ethyl}-1H-imidazol-2-ylamine hydrochloride (0.086 g, 58% yield) as a yellow oil. ^{1}H NMR (300 MHz, CD_3OD) δ 8.11 (s, 1H), δ 7.84 (m, 2H), δ 7.41 (m, 2H), δ 7.06 (d, 1H), δ 5.66 (s, 2H), δ 3.04 (t, 2H), δ 2.85 (t, 2H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 147.5, 144.9, 144.8, 134.7, 131.9, 127.2, 127.1, 127.1, 125.8, 125.3, 124.4, 109.5, 49.9, 23.6, 23.2 ppm; HRMS (ESI) calcd for $C_{17}H_{19}N_7$ (M^+) 321.1701, found 321.1704.

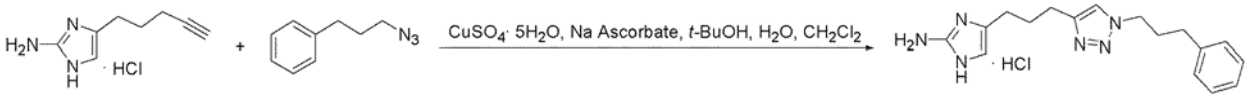


- 4-But-3-ynyl-1H-imidazol-2-ylamine hydrochloride (0.061 g, 0.361 mmol) was reacted with 2-azidomethyl-1-H-benzimidazole (0.075 g, 0.433 mmol) following the general procedure for click reactions outlined above to produce 4-{2-[1-(1H-Benzoimidazol-2-ylmethyl)-1H-[1,2,3]triazol-4-yl]-ethyl}-1H-imidazol-2-ylamine dihydrochloride (0.066 g, 48% yield) of a yellow solid. ^{1}H NMR (300 MHz, CD_3OD) δ 8.05 (s, 1H), δ 7.68 (m. 2H), δ 7.48 (m, 2H), δ 6.38 (s, 1H), δ 6.15 (s, 2H`), δ 2.90 (t, 2H), δ 2.76 (t, 2H) ppm; ^{13}C (75 MHz, CD_3OD) δ 147.4, 146.9, 146.8, 131.3, 127.0, 126.4, 124.1, 114.1, 109.2, 44.7, 24.0, 23.9 ppm; HRMS (ESI) calcd for $C_{15}H_{17}N_8$ (M^+) 309.1570, found 309.1572.

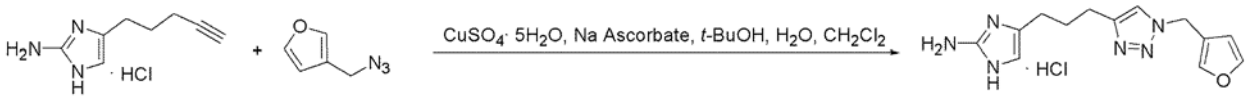


- 4-But-3-ynyl-1H-imidazol-2-ylamine hydrochloride (0.0734 g, 0.432 mmol) was reacted with 2-azidomethyl-5, 6-dimethyl-1H-benzimidazole (0.104 g, 0.518 mmol) following the general procedure for click reactions outlined above to produce 4-{2-[1-(5,6-Dimethyl-1H-benzoimidazol-2-ylmethyl)-1H-[1,2,3]triazol-4-yl]-ethyl}-1H-imidazol-2-ylamine dihydrochloride (0.104 g, 59% yield) of a pale yellow solid. ^{1}H NMR (300 MHz, CD3OD) δ 7.70 (s, 1H), δ 7.19 (s, 2H), δ 6.23 (s, 1H), δ 5.66 (s, 2H), δ 2.85 (t, 2H), δ 2.68 (t, 2H), δ 2.21 (s,

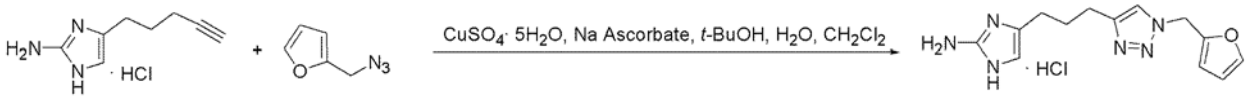
6H) ppm; ^{13}C NMR (75 MHz, CD3OD) δ 148.2, 147.0, 146.9, 132.3, 128.9, 122.8, 120.0, 115.1, 109.7, 100.4, 25.1, 24.4, 19.2 ppm; HRMS (ESI) calcd for $C_{17}H_{20}N_8$ (M^+) 337.1883, found 337.1886.



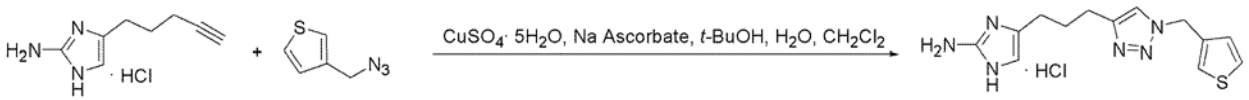
- 4-Pent-4-ynyl-1H-imidazol-2-ylamine hydrochloride (0.050 g, 0.269 mmol) was reacted with (3-azido-propyl) benzene (0.044 g, 0.273 mmol) following the general procedure for click reactions outlined above to produce 4-{3-[1-(3-Phenyl-propyl)-1H-[1,2,3]triazol-4-yl]-propyl}-1H-imidazol-2-ylamine hydrochloride (0.0318 g, 34% yield) as a pale yellow solid. ^{1}H NMR (300 MHz, DMSO) δ 7.91 (s, 1H), δ 7.29 – 7.17 (m, 5H), δ 6.62 (s, 2H), δ 6.57 (s, 1H), δ 4.29 (t, 2H), δ 2.59 (t, 2H), δ 2.53 (t, 2H), δ 2.43 (t, 2H) δ 2.09 (m, 2H), δ 1.83 (m, 2H) ppm; ^{13}C NMR (75 MHz, DMSO) δ 163.6, 156.2, 155.1, 147.4, 146.9, 141.4, 129.1, 127.1, 126.7, 122.6, 109.4, 49.4, 32.6, 32.0, 28.1, 24.9, 24.2 ppm; HRMS (ESI) calcd for $C_{17}H_{22}N_6$ (M^+) 310.1978, found 310.1977.



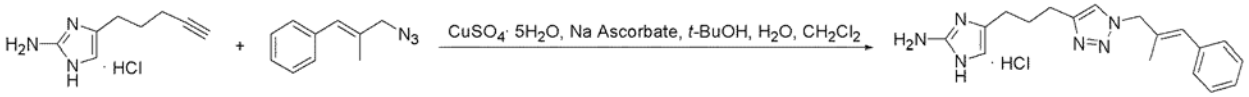
- 4-Pent-4-ynyl-1H-imidazol-2-ylamine hydrochloride (0.063 g, 0.340 mmol) was reacted with 3-azidomethyl-furan (0.050 g, 0.406 mmol) following the general procedure for click reactions outlined above to produce 4-[3-(1-Furan-3-ylmethyl-1H-[1,2,3]triazol-4-yl)-propyl]-1H-imidazol-2-ylamine hydrochloride (0.061g, 58% yield) as a pale yellow solid. ^{1}H NMR (300 MHz, CD_3OD) δ 7.70 (s, 1H), δ 7.56 (s, 1H), δ 7.41 (s, 1H), δ 6.44 (s, 1H), δ 6.35 (s, 1H), δ 5.35 (s, 2H), δ 2.65 (t, 2H), δ 2.45 (t, 2H), δ 1.86 (m, 2H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 147.3, 147.3, 144.2, 141.6, 127.2, 122.1, 120.2, 109.9, 108.8, 44.7, 27.8, 24.2, 23.6 ppms; HRMS (ESI) calcd for $C_{13}H_{16}N_6O$ (M^+) 272.1458, found 272.1462.



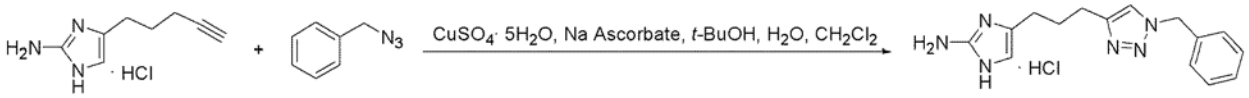
- 4-Pent-4-ynyl-1H-imidazol-2-ylamine hydrochloride (0.093 g, 0.500 mmol) was reacted with 2-azidomethyl-furan (0.074 g, 0.601 mmol) following the general procedure for click reactions outlined above to produce 4-[3-(1-Furan-2-ylmethyl-1H-[1,2,3]triazol-4-yl)-propyl]-1H-imidazol-2-ylamine hydrochloride (0.075, 50% yield) as a pale yellow solid. ^{1}H NMR (300 MHz, DMSO) δ 7.85 (s, 1H), δ 7.65 (s, 1H), δ 6.70 (s, 2H), δ 6.64 (s, 1H), δ 6.52 (t, 1H), δ 6.46 (s, 1H), δ 5.58 (s, 2H), δ 2.61 (t, 2H), δ 2.41 (t, 2H), δ 1.82 (m, 2H) ppm; ^{13}C NMR (75 MHz, DMSO) δ 163.6, 149.4, 147.9, 147.4, 144.3, 128.5, 122.6, 111.5, 110.3, 109.9, 46.3, 28.4, 24.9 ppm; HRMS (ESI) calcd for $C_{13}H_{16}N_6O$ (M^+) 272.1458, found 272.1460.



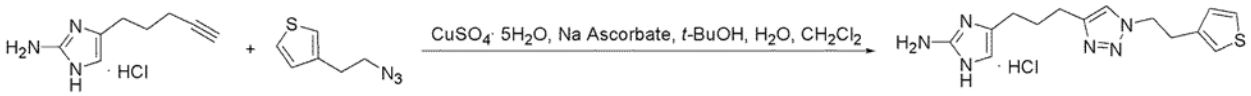
- 4-Pent-4-ynyl-1H-imidazol-2-ylamine hydrochloride (0.090 g, 0.486 mmol) was reacted with 3-Azidomethyl-thiophene (0.081 g, 0.582 mmol) following the general procedure for click reactions outlined above to produce 4-[3-(1-Thiophen-3-ylmethyl-1H-[1,2,3]triazol-4-yl)-propyl]-1H-imidazol-2-ylamine hydrochloride (0.0727 g, 46% yield) as a pale yellow solid. ^{1}H NMR (300 MHz, CD_3OD) δ 7.61 (s, 1H), δ 7.24 (s, 1H), δ 7.23 (d, 1H), δ 6.87 (d, 1H), δ 6.29 (s, 1H), δ 2.54 (t, 2H), 2.33 (t, 2H), δ 1.75 (m, 2H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 147.6, 147.4, 147.3, 136.1, 127.9, 127.0, 126.9, 124.2, 122.2, 109.1, 53.1, 27.9, 24.3; HRMS (ESI) calcd for $C_{13}H_{16}N_6S$ (M^+) 289.1229, found 289.1234.



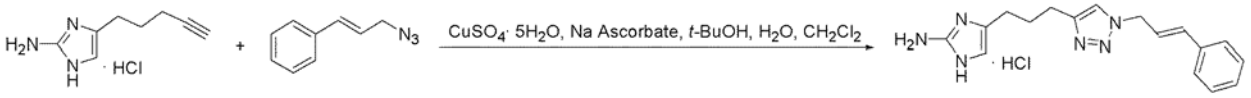
- 4-Pent-4-ynyl-1H-imidazol-2-ylamine hydrochloride (0.096 g, 0.517 mmol) was reacted with (3-Azido-2-methyl-propenyl)-benzene (0.110 g, 0.635 mmol) following the general procedure for click reactions outlined above to produce 5-{3-[1-(2-Methyl-3-phenyl-allyl)-1H-[1,2,3]triazol-4-yl]-propyl}-1H-imidazol-2-ylamine hydrochloride (0.076, 41% yield) as a pale yellow solid. ^{1}H NMR (300 MHz, CD_3OD) δ 7.65 (s, 1H), δ 7.14 – 7.04 (m, 5H), δ 6.35 (s, 1H), δ 6.28 (s, 1H), δ 4.94 (s, 2H), δ 2.57 (t, 2H), δ 2.34 (t, 2H), δ 1.75 (m, 2H), δ 1.57 (s, 3H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 147.5, 136.9, 132.5, 129.7, 128.8, 128.6, 128.4, 128.3, 128.2, 126.9, 122.5, 109.2, 58.1, 61.9, 28.0, 24.3, 24.3, 24.1, 14.6 ppm; HRMS (ESI) calcd for $C_{18}H_{22}N_6$ (M^+) 323.1978, found 323.1984.



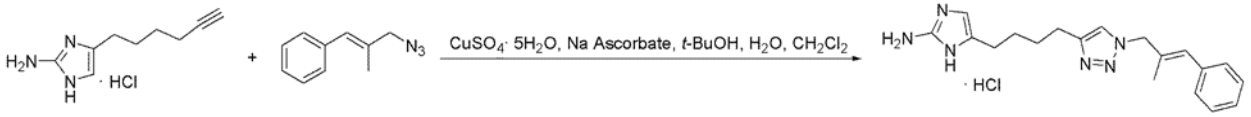
- 4-Pent-4-ynyl-1H-imidazol-2-ylamine hydrochloride (0.081 g, 0.437 mmol) was reacted with benzyl azide (0.071 g, 0.533 mmol) following the general procedure for click reactions outlined above to produce 4-[3-(1-Benzyl-1H-[1,2,3]triazol-4-yl)-propyl]-1H-imidazol-2-ylamine hydrochloride (0.073 g, 53% yield) as a pale yellow solid. ^{1}H NMR (300 MHz, DMSO) δ 7.93 (s, 1H), δ 7.37 – 7.27 (m, 5H), δ 6.63 (s, 2H), δ 6.44 (s, 1H), δ 2.61 (t, 2H), δ 2.40 (t, 2H), δ 1.82 (m, 2H) ppm; ^{13}C NMR (75 MHz, DMSO) δ 163.5, 148.1, 147.4, 135.9, 129.4, 128.7, 128.5, 128.4, 122.8, 122.8, 115.9, 109.9, 53.3, 28.5, 25.0; HRMS (ESI) calcd for $C_{15}H_{18}N_6$ (M^+) 282.1665, found 282.1674.



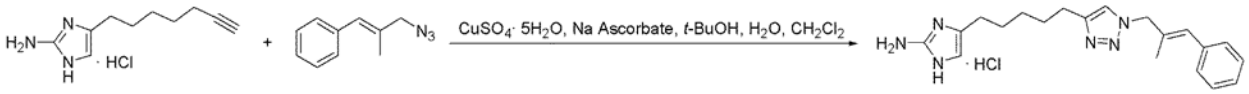
- 4-Pent-4-ynyl-1H-imidazol-2-ylamine hydrochloride (0.090 g, 0.485 mmol) was reacted with 3-(2-Azido-ethyl)-thiophene (0.089 g, 0.581 mmol) following the general procedure for click reactions outlined above to produce 4-{3-[1-(2-Thiophen-3-yl-ethyl)-1H-[1,2,3]triazol-4-yl]-propyl}-1H-imidazol-2-ylamine hydrochloride (0.067 g, 41% yield) as a pale yellow solid. ^{1}H NMR (300 MHz, CD_3OD) δ 7.42 (s, 1H), δ 7.12 (d, 1H), δ 6.83 (s, 1H), δ 6.70 (d, 1H), δ 6.29 (s, 1H), δ 4.41 (t, 2H), δ 3.04 (t, 2H), δ 2.50 (t, 2H), δ 2.29 (t, 2H), δ 1.72 (m, 2H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 146.8, 146.8, 137.7, 127.8, 127.6, 125.7, 122.6, 121.9, 109.0, 50.7, 30.7, 27.9, 23.7 ppm; HRMS (ESI) calcd for $C_{14}H_{18}N_6S$ (M^+) 302.1313, found 302.1317.



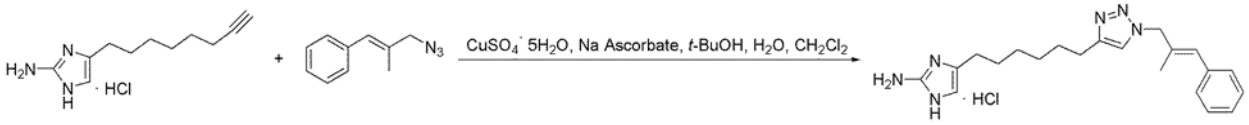
- 4-Pent-4-ynyl-1H-imidazol-2-ylamine hydrochloride (0.115 g, 0.620 mmol) was reacted with (3-azido-propenyl)-benzene (0.119 g, 0.748 mmol) following the general procedure for click reactions outlined above to produce 4-{3-[1-(3-Phenyl-allyl)-1H-[1,2,3]triazol-4-yl]-propyl}-1H-imidazol-2-ylamine hydrochloride (0.082 g, 43% yield) as a pale yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34 – 7.24 (m, 6H), δ 6.67 (d, 1H), δ 6.34 (q, 1H), δ 6.25 (s, 1H), δ 5.08 (d, 2H), δ 2.72 (t, 2H), δ 2.47 (t, 2H), δ 1.91 (m, 2H) ppm; ^{13}C NMR (75 MHz, CD_3OD) 149.1, 137.9, 133.5, 129.5, 128.9, 128.7, 128.3, 128.2, 127.7, 126.8, 54.8, 48.9, 31.3, 29.6, 27.5 ppm ; HRMS (ESI) calcd for $C_{17}H_{21}N_6$ (M^+) 308.1822, found 308.1821.



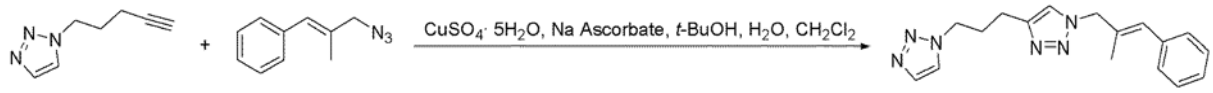
- 4-Hex-5-ynyl-1H-imidazol-2-ylamine hydrochloride (0.089 g, 0.4.47 mmol) was reacted with (3-Azido-2-methyl-propenyl)-benzene (0.085 g, 0.491 mmol) following the general procedure for click reactions outlined above to produce 4-{4-[1-(2-Methyl-3-phenyl-allyl)-1H-[1,2,3]triazol-4-yl]-butyl}-1H-imidazol-2-ylamine (0.132 g, 79% yield) as a pale yellow solid. ^{1}H NMR (300 MHz, CD_3OD) δ 8.36 (s, 1H), 7.03 (m, 5H), 6.49 (s, 1H), 6.25 (s, 1H), 5.05 (s, 2H), δ 2.67 (t, 2H), δ 2.73 (t, 2H), δ 1.56 (s, 3H), δ 1.42 (m, 4H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 147.3, 144.7, 136.4, 132.7, 129.9, 128.9, 128.6, 128.5, 128.3, 127.5, 127.2, 126.9, 108.7, 61.2, 27.4, 27.3, 23.8, 22.8, 14.8 ppm; HRMS (ESI) calcd for $C_{19}H_{24}N_6$ (M^+) 336.2135, found 336.2134.



- 4-Hept-6-ynyl-1H-imidazol-2-ylamine hydrochloride (0.060 g, 0.281 mmol) was reacted with (3-Azido-2-methyl-propenyl)-benzene (0.058 g, 0.336 mmol) following the general procedure for click reactions outlined above to produce 4-{5-[1-(2-Methyl-3-phenyl-allyl)-1H-[1,2,3]triazol-4-yl]-pentyl}-1H-imidazol-2-ylamine hydrochloride (0.064 g, 65% yield) as a pale yellow solid. ^{1}H NMR (300 MHz, CD_3OD) δ 8.23 (s, 1H), δ 6.93 – 6.83 (m, 5H), δ 6.38 (s, 1H), δ 6.08 (s, 1H), δ 4.93 (s, 2H), δ 2.51 (t, 2H), δ 2.09 (t, 2H), δ 1.43 (s, 3H), δ 1.41 (m, 2H), δ 1.25 (m, 2H), δ 1.05 (m, 2H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 147.7, 144.8, 136.3, 132.8, 129.8, 128.9, 128.6, 128.5, 128.2, 127.6, 127.5, 127.0, 108.5, 61.3, 28.0, 27.6, 27.5, 24.0, 22.9, 14.7 ppm; HRMS (ESI) calcd for $C_{20}H_{27}N_6$ (M^+) 351.2291, found 351.2291.



- 4-Oct-7-ynyl-1H-imidazol-2-ylamine hydrochloride (0.098 g, 0.568 mmol) was reacted with (3-Azido-2-methyl-propenyl)-benzene (0.118 g, 0.681 mmol) following the general procedure for click reactions outlined above to produce 4-{6-[1-(2-Methyl-3-phenyl-allyl)-1H-[1,2,3]triazol-4-yl]-hexyl}-1H-imidazol-2-ylamine hydrochloride (0.147 g, 85% yield) as a pale yellow solid. ^{1}H NMR (300 MHz, CD_3OD) δ 8.42 (s, 1H), δ 7.25 – 7.15 (m, 5H), δ 6.65 (s, 1H), δ 6.36 (s, 1H), δ 5.23 (s, 2H), δ 2.78 (t, 2H), δ 2.38 (t, 2H), δ 1.74 (s, 3H), δ 1.64 (m, 2H), δ 1.51 (m, 2H), δ 1.33 (m, 4H) ppm; ^{13}C NMR (75 MHz, CD_3OD) δ 147.5, 136.3, 132.9, 132.8, 129.9, 128.9, 128.6, 128.5, 128.3, 127.7; HRMS (ESI) calcd for $C_{21}H_{29}N_6$ (M^+) 365.2448, found 365.2448.

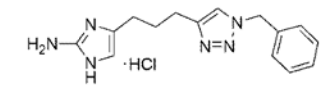


- 1-Pent-4-ynyl-1H-[1,2,3]triazole (0.100 g, 0.739 mmol) was reacted with (3-Azido-2-methyl-propenyl)-benzene (0.154 g, 0.889 mmol) following the general procedure for click reactions outlined above to produce 1-(2-Methyl-3-phenyl-allyl)-4-(3-[1,2,3]triazol-1-yl-propyl)-1H-[1,2,3]triazole (0.227 g, Quantitative) as a white solid. ^{1}H NMR (300 MHz, DMSO) δ 7.91 (s, 1H), δ 7.77 (s, 2H), δ 7.40 – 7.25 (m, 5H), δ 6.47 (s, 1H), δ 5.05 (s, 2H), δ 4.48 (t, 2H), δ 2.62 (t, 2H), δ 2.50 (t, 2H), δ 2.21 (m, 2H), δ 1.74 (s, 3H) ppm; ^{13}C NMR (75 MHz, DMSO) δ 146.4, 137.1, 134.8, 133.6, 132.8, 129.4, 129.3, 129.2, 128.9, 127.6, 123.0, 57.9, 54.0, 32.9, 29.6, 22.7, 16.2 ppm; HRMS (ESI) calcd for $C_{17}H_{21}N_6$ (M^+) 309.1822, found 309.1821.

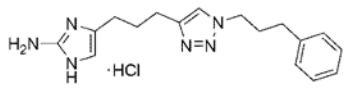
2. Experimental Protocols for Bacterial Biofilm Regulation Studies

General Static Bacterial Biofilm Inhibition Assay Procedure for *A. baumannii, P. aeruginosa, B bronchiseptica* and *S. aureus*: Biofilm inhibition assays were performed by taking an overnight culture of bacterial strain and subculturing it at an OD_{600} of 0.01 into the necessary growth liquid medium (LB for *A. baumannii*, LBNS for *P. aeruginosa*, Stainer-Scholte medium that was supplemented with 10 µL/mL of 100X nutrient complex for *B. bronchiseptica* and TSB w/0.3% glucose for *S. aureus*) for the strain. The compound being tested was then added at a predetermined concentration and then aliquoted (100 µL) into the wells of a 96-well PVC microtiter plate (wells not used for samples are filled with 100 µL of de-ionized water). Plates were then wrapped in GLAD Press n' Seal® and incubated under stationary conditions at 37° C. After 24 hours, the media was discarded from the wells and the plates were washed thoroughly with tap water. Plates were then stained with 100 µL of 0.1% solution of crystal violet (CV) and then incubated at an ambient temperature for 30 minutes. Sample plates were then washed with tap water again and the remaining stain was solubilized with 200 µL of 95% ethanol. Biofilm inhibition was quantitated by measuring the OD_{540} for each well by transferring 125 µL of the solubilized CV stain into a polystyrene microtiter dish for analysis.

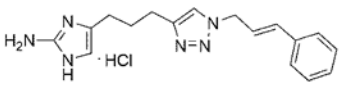
Initial Bacterial Biofilm Inhibition Activity Screening Data



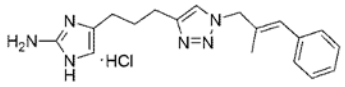
	% Inhibition at 300 µM
A. baumannii	41 ± 3.6%
PAO1	< 10%
RB50	Not Active



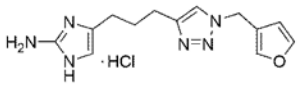
	% Inhibition at 300 µM
A. baumannii	40 ± 4.0%
PAO1	23 ± 2.7%
RB50	< 10 %



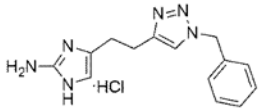
	% Inhibition at 300 µM
A. baumannii	41 ± 1.0%
PAO1	< 10%
RB50	Not Active



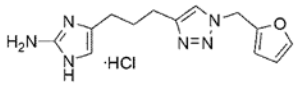
	% Inhibition at 300 µM
A. baumannii	88 ± 3.2%
PAO1	< 10 %
RB50	37 ± 3.1%



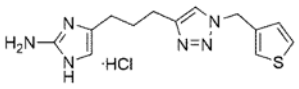
	% Inhibition at 300 µM
A. baumannii	16 ± 2.0%
PAO1	13 ± 3.0%
RB50	Not Active



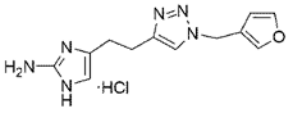
	% Inhibition at 300 µM
A. baumannii	19 ± 1.7%
PAO1	53 ± 3.2%
RB50	16 ± 5.9%



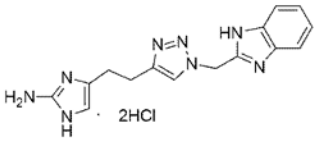
	% Inhibition at 300 µM
A. baumannii	17 ± 1.2 %
PAO1	17 ± 4.6%
RB50	Not Active



	% Inhibition at 300 µM
A. baumannii	30 ± 1.0%
PAO1	37 ± 2.5%
RB50	Not Active

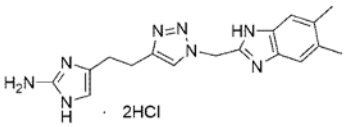


	% Inhibition at 300 µM
A. baumannii	19 ± 1.0%
PAO1	34 ± 3.2%
RB50	< 10%



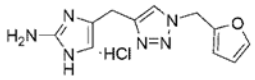
% Inhibition at 300 µM

A. baumannii	25 ± 2.6%
PAO1	< 10 %
RB50	Not Active



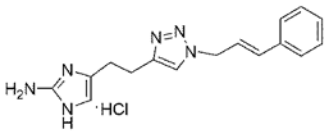
% Inhibition at 300 µM

A. baumannii	55 ± 4.7%
PAO1	< 10%
RB50	< 10%



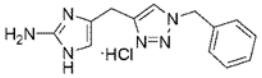
% Inhibition at 300 µM

A. baumannii	18 ± 1.0%
PAO1	21 ± 0.0%
RB50	Not Active



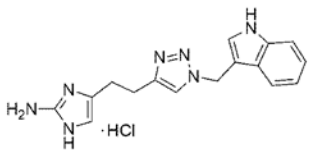
% Inhibition at 300 µM

A. baumannii	36 ± 4.5%
PAO1	32 ± 3.5%
RB50	18 ± 2.9%



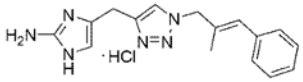
% Inhibition at 300 µM

A. baumannii	17 ± 2.5%
PAO1	Not Active
RB50	< 10 %



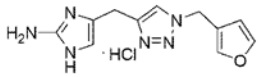
% Inhibition at 300 µM

A. baumannii	20 ± 2.6%
PAO1	59 ± 3.6%
RB50	11 ± 2.5%



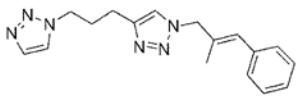
% Inhibition at 300 µM

A. baumannii	34 ± 1.2%
PAO1	31 ± 2.1%
RB50	31 ± 2.1%



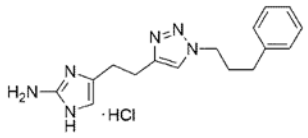
% Inhibition at 300 µM

A. baumannii	< 10%
PAO1	11 ± 2.8%
RB50	Not Active



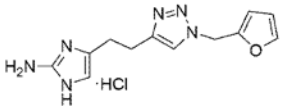
% Inhibition at 300 µM

A. baumannii	12 ± 1.7%
PAO1	Not Active
RB50	Not Active



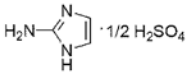
% Inhibition at 300 µM

A. baumannii	46 ± 1.0%
PAO1	38 ± 1.5%
RB50	< 10%



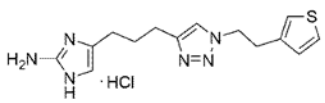
% Inhibition at 300 µM

A. baumannii	14 ± 1.5%
PAO1	34 ± 3.2%
RB50	< 10%



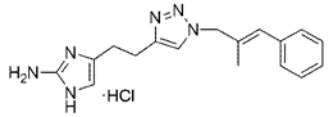
% Inhibition at 300 µM

A. baumannii	Not Active
PAO1	Not Active
RB50	Not Active



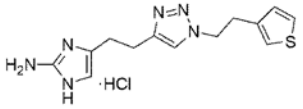
% Inhibition at 300 µM

A. baumannii	33 ± 1.7%
PAO1	17 ± 1.8%
RB50	Not Active



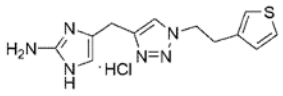
% Inhibition at 300 µM

A. baumannii	46 ± 1.2%
PAO1	Not Active
RB50	Not Active



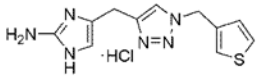
% Inhibition at 300 µM

A. baumannii	23 ± 4.0%
PAO1	44 ± 1.5%
RB50	14 ± 4.7%



% Inhibition at 300 µM

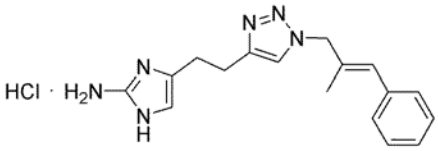
A. baumannii	21 ± 1.7%
PAO1	< 10 %
RB50	< 10 %

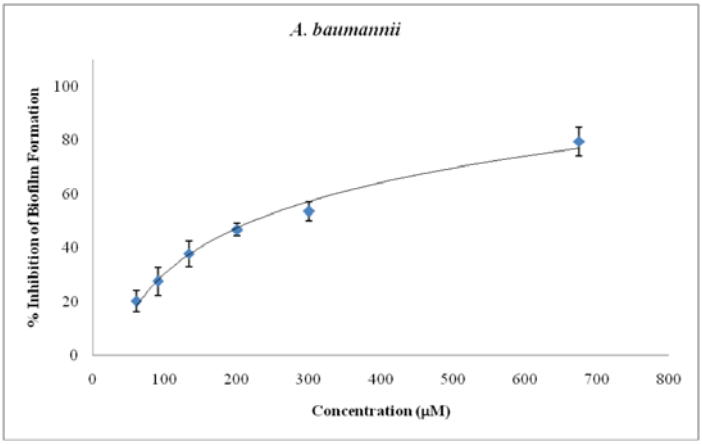


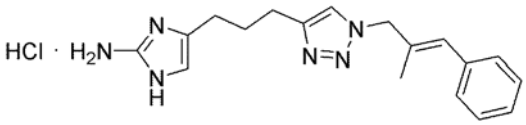
% Inhibition at 300 µM

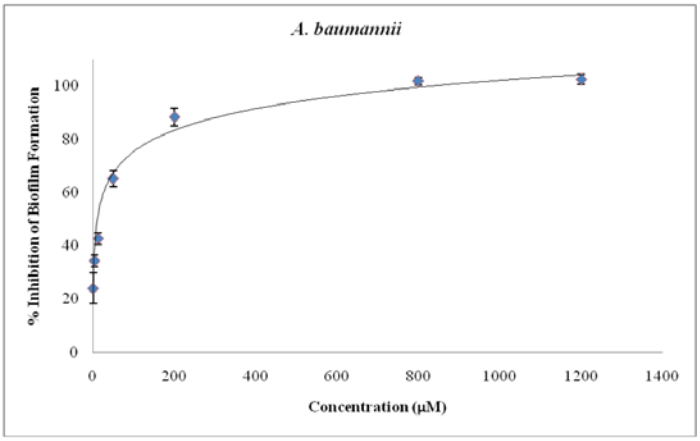
A. baumannii	24 ± 1.0%
PAO1	39 ± 1.0%
RB50	< 10 %

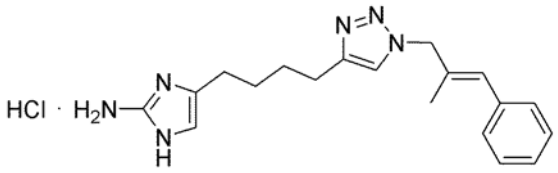
Bacterial Biofilm Inhibition Dose Response Curves

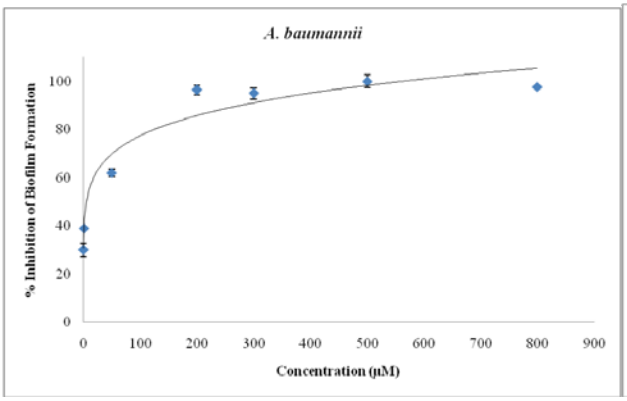


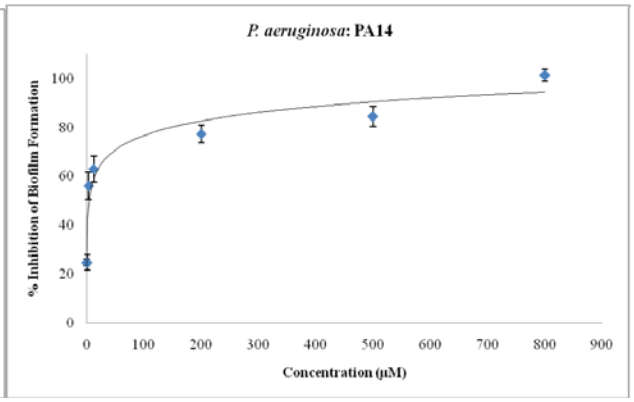


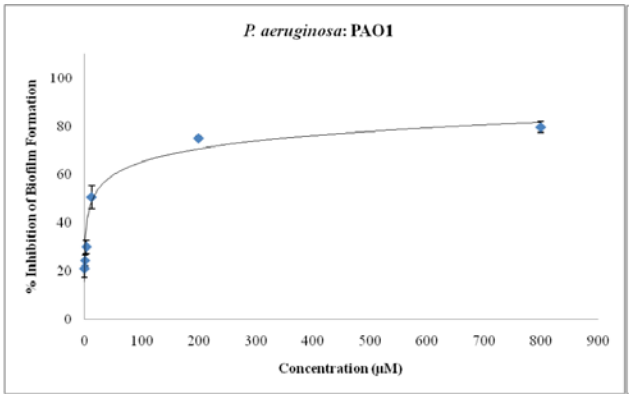


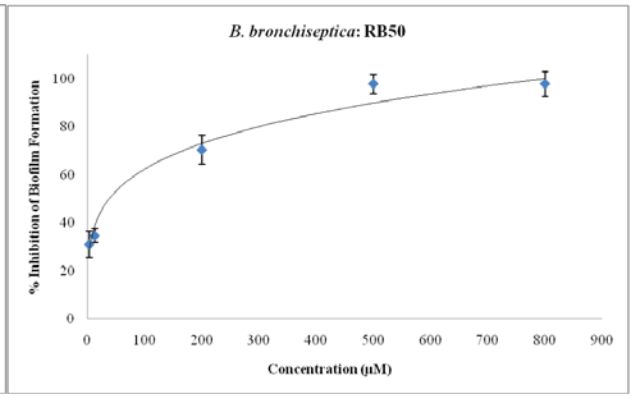


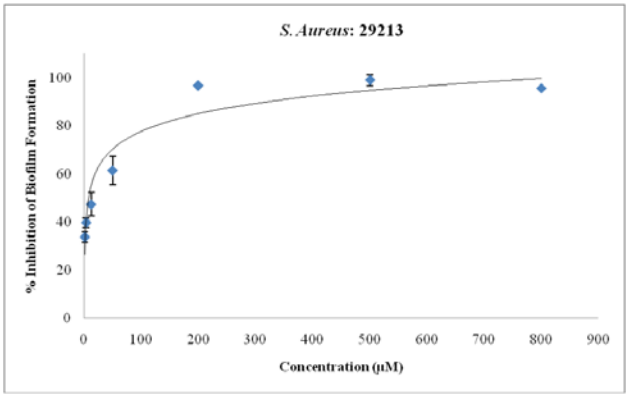

HCl · H2N
N
N
H
N=N
N

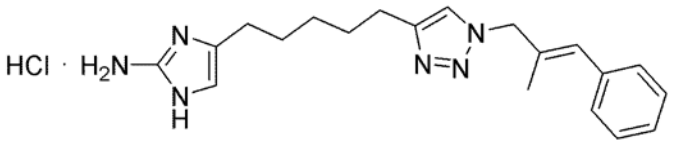

A. baumannii
% Inhibition of Biofilm Formation
Concentration (µM)

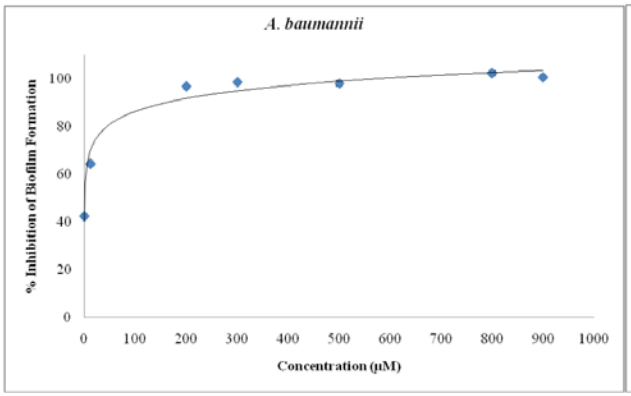

P. aeruginosa: PA14
% Inhibition of Biofilm Formation
Concentration (µM)

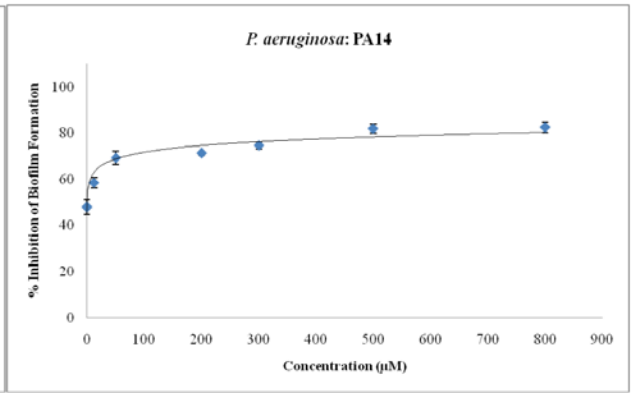

P. aeruginosa: PAO1
% Inhibition of Biofilm Formation
Concentration (µM)

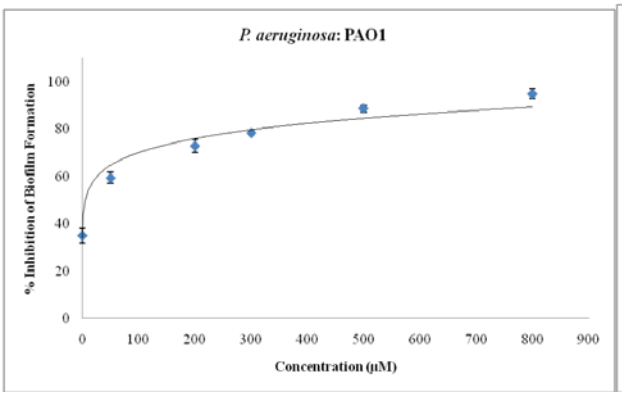

B. bronchiseptica: RB50
% Inhibition of Biofilm Formation
Concentration (µM)

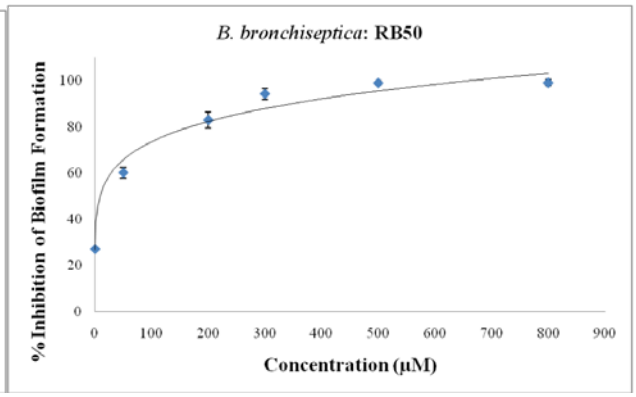

S. Aureus: 29213
% Inhibition of Biofilm Formation
Concentration (µM)

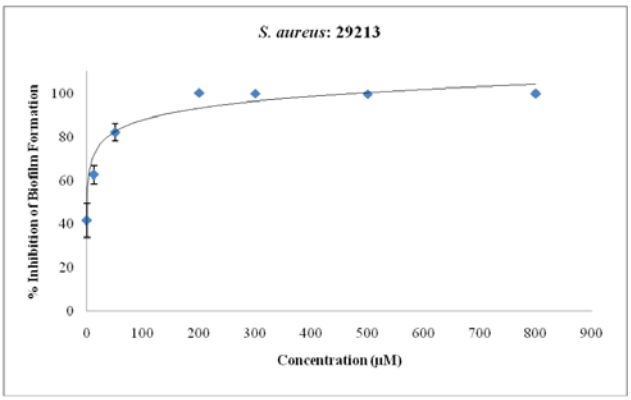

HCl · H2N
N
N
H
N
N=N

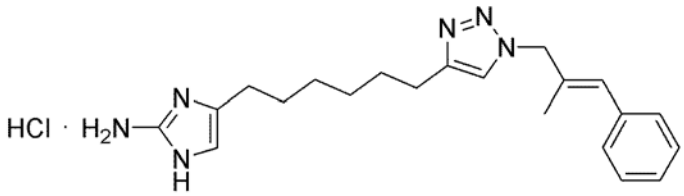

A. baumannii
% Inhibition of Biofilm Formation
Concentration (µM)

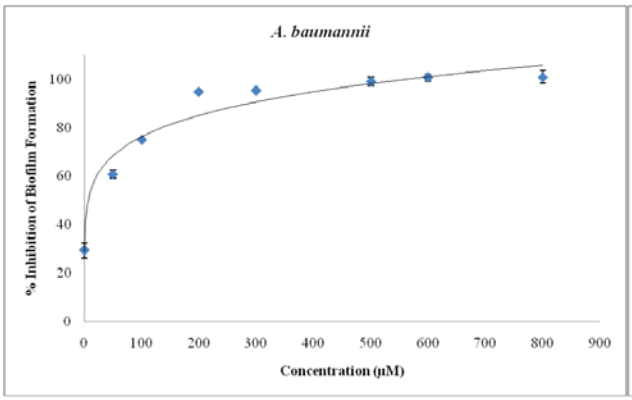

P. aeruginosa: PA14
% Inhibition of Biofilm Formation
Concentration (µM)

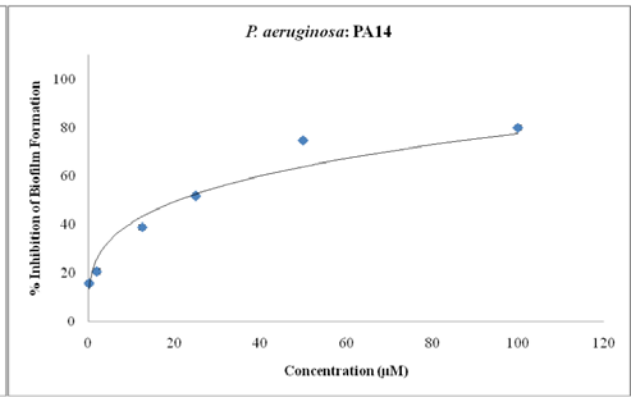

P. aeruginosa: PAO1
% Inhibition of Biofilm Formation
Concentration (µM)

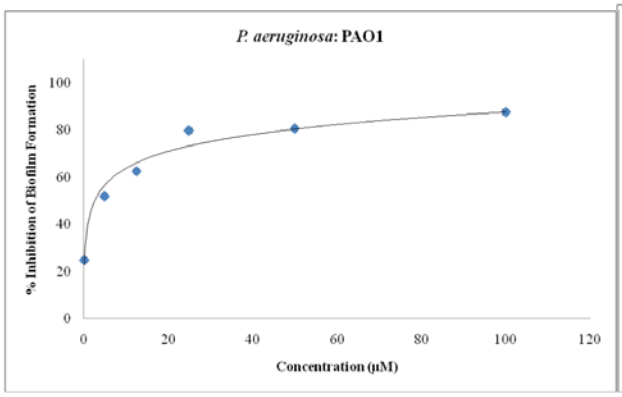

B. bronchiseptica: RB50
% Inhibition of Biofilm Formation
Concentration (µM)

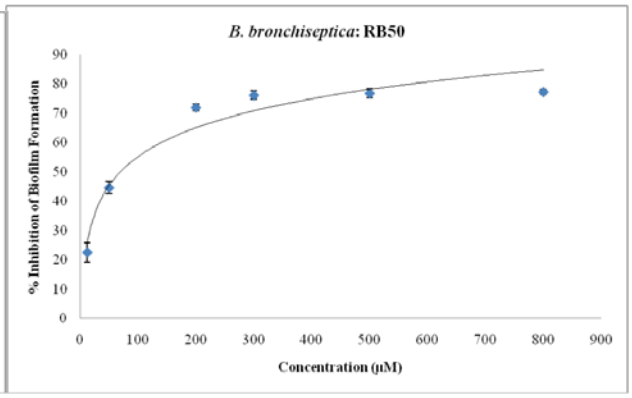

S. aureus: 29213
% Inhibition of Biofilm Formation
Concentration (µM)

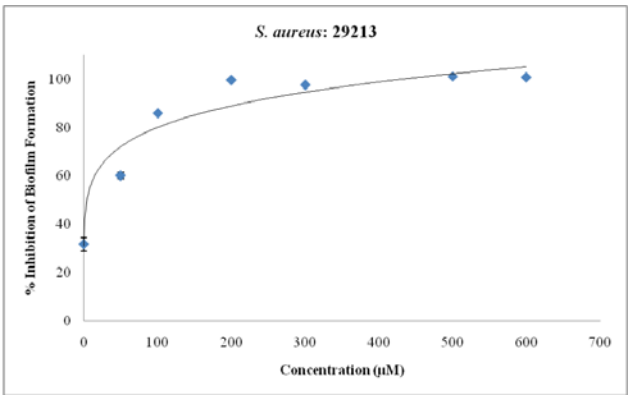

HCl · H2N
N
N
H
N
N


A. baumannii
% Inhibition of Biofilm Formation
Concentration (µM)


P. aeruginosa: PA14
% Inhibition of Biofilm Formation
Concentration (µM)


P. aeruginosa: PAO1
% Inhibition of Biofilm Formation
Concentration (µM)

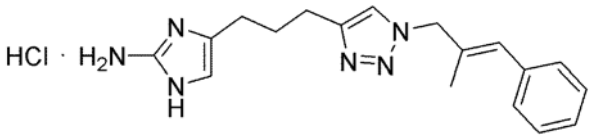

B. bronchiseptica: RB50
% Inhibition of Biofilm Formation
Concentration (µM)

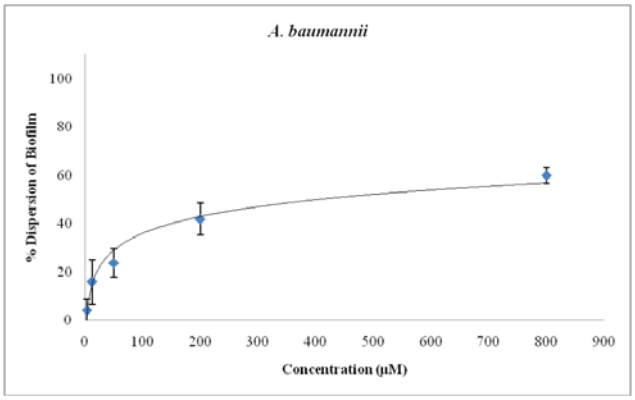

S. aureus: 29213
% Inhibition of Biofilm Formation
Concentration (µM)

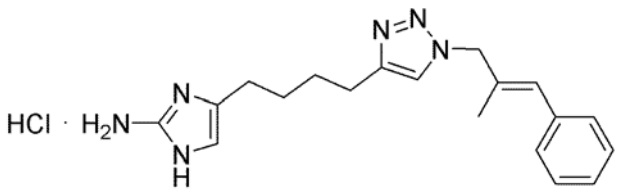
General Static Bacterial Biofilm Dispersion Assay Procedure for *A. baumannii, P. aeruginosa* and *S. aureus*: Dispersion assays were performed by taking an overnight culture of bacterial strain and subculturing it at an OD_{600} of 0.01 into the necessary growth liquid medium. The resulting bacterial suspension was aliquoted (100 µL) into the wells of a 96-well PVC microtiter plate. Plates were then wrapped in GLAD Press n' Seal® followed by an incubation under stationary conditions at an ambient temperature. After 24 hours, the media was discarded from the wells and the plates were washed thoroughly with tap water. Predetermined concentrations of the test compound were then made in the same medium used to initially grow the biofilms and then aliquoted (100 µL) into the wells of the 96-well PVC microtiter plate with the established biofilms. Plates were then wrapped in GLAD Press n' Seal® and incubated under stationary conditions at 37° C. After 24 hours, the media was discarded from the wells and the plates were washed thoroughly with tap water. Plates were then stained with 100 µL of 0.1% solution of crystal violet (CV) and then incubated at room temperature for 30 minutes. Plates were then washed with tap water again and the remaining stain was solubilized with 200 µL of 95% ethanol. Biofilm dispersion was quantitated by measuring the OD_{540} for each well by transferring 125 µL of the solubilized CV stain into a polystyrene microtiter dish for analysis.

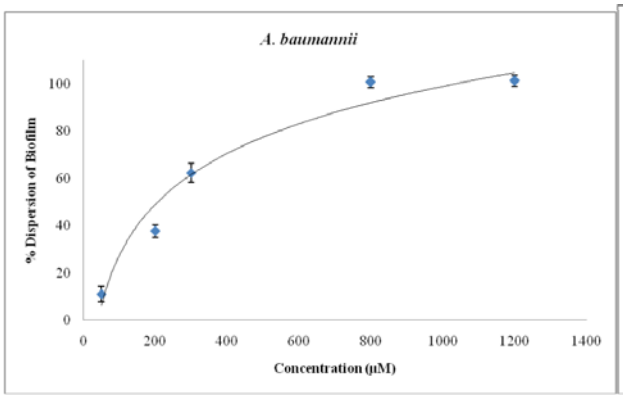
General Static Bacterial Biofilm Dispersion Assay Procedure for *B. bronchiseptica*: This procedure is identical to the general dispersion procedure described above except that initial biofilm formation in the absence of the test compound was carried out at 37° C.

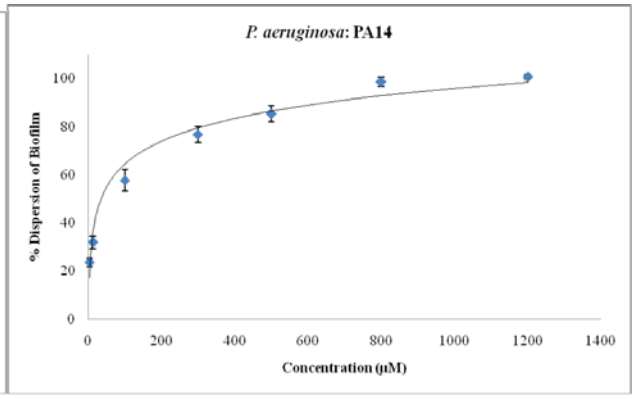
Bacterial Biofilm Dispersion Dose Response Curves

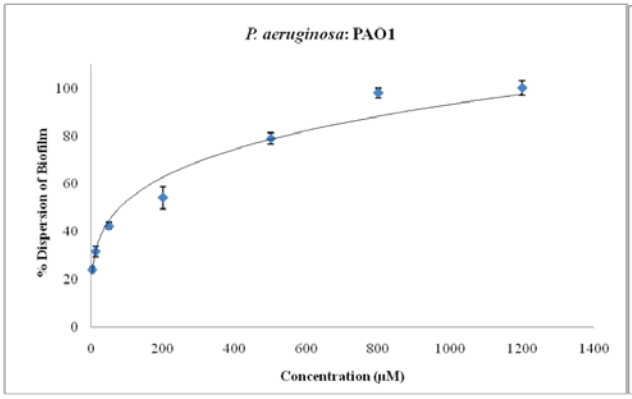


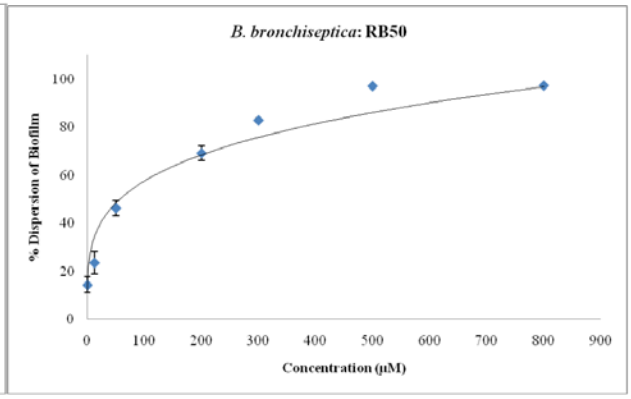


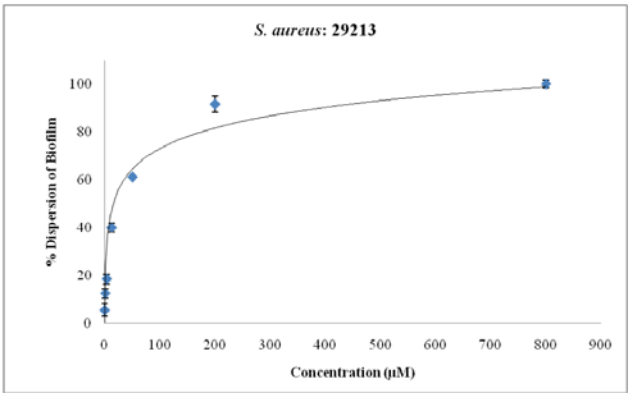

HCl · H2N
N
N
H
N=N
N

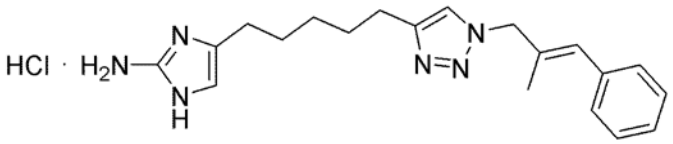

A. baumannii
% Dispersion of Biofilm
Concentration (µM)
0
20
40
60
80
100
0
200
400
600
800
1000
1200
1400

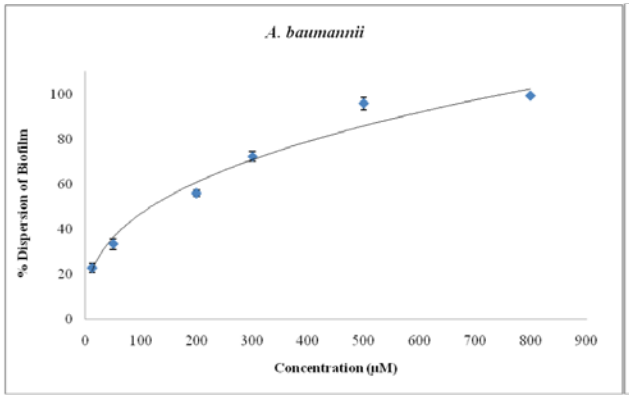

P. aeruginosa: PA14
% Dispersion of Biofilm
Concentration (µM)
0
20
40
60
80
100
0
200
400
600
800
1000
1200
1400

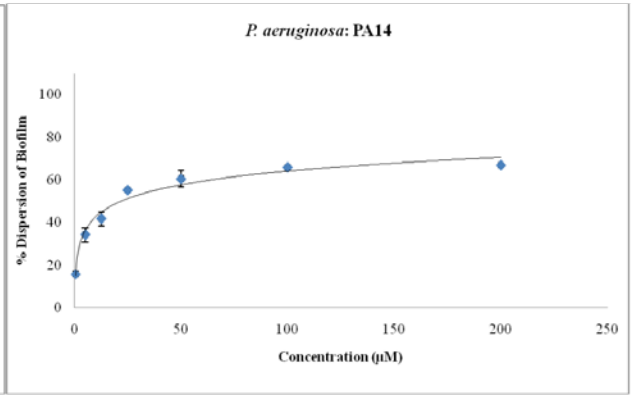

P. aeruginosa: PAO1
% Dispersion of Biofilm
Concentration (µM)
0
20
40
60
80
100
0
200
400
600
800
1000
1200
1400

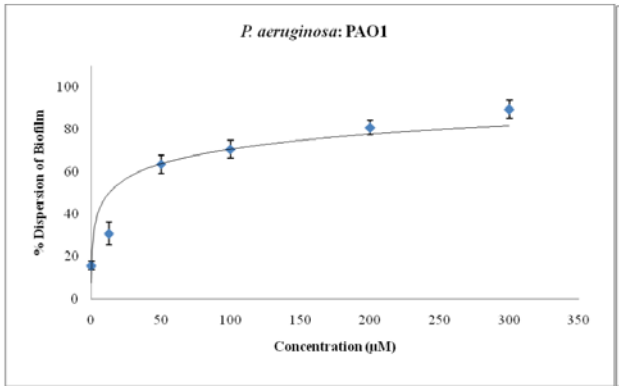

B. bronchiseptica: RB50
% Dispersion of Biofilm
Concentration (µM)
0
20
40
60
80
100
0
100
200
300
400
500
600
700
800
900

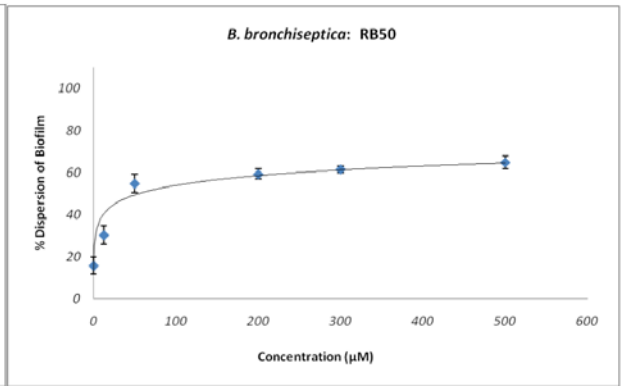

S. aureus: 29213
% Dispersion of Biofilm
Concentration (µM)
0
20
40
60
80
100
0
100
200
300
400
500
600
700
800
900

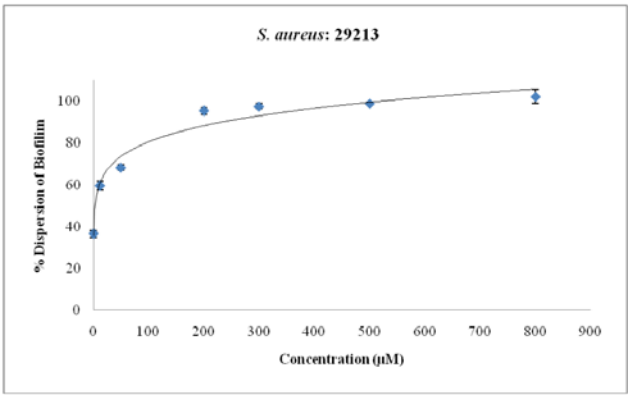

HCl · H2N
N
N
H
N
N=N

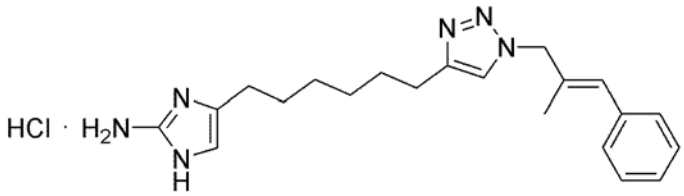

A. baumannii
% Dispersion of Biofilm
Concentration (µM)

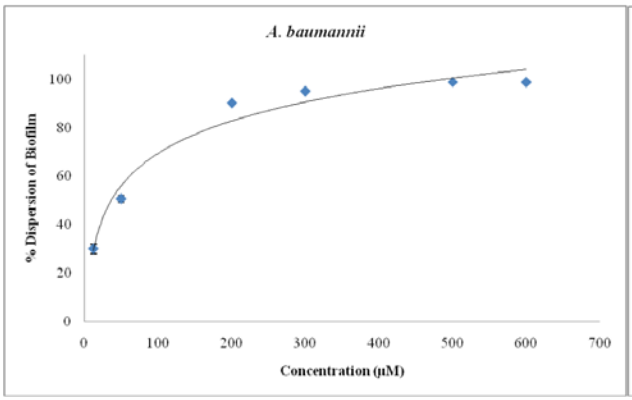

P. aeruginosa: PA14
% Dispersion of Biofilm
Concentration (µM)

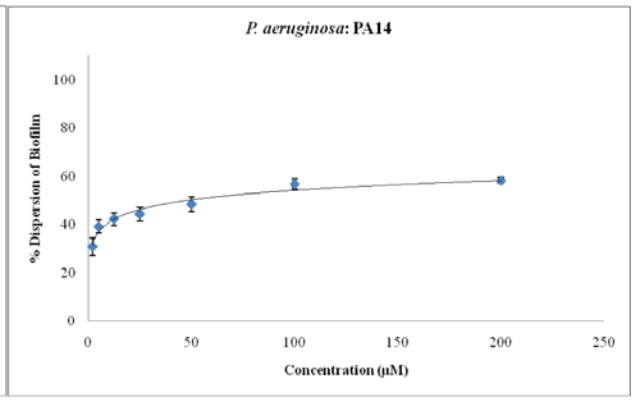

P. aeruginosa: PAO1
% Dispersion of Biofilm
Concentration (µM)

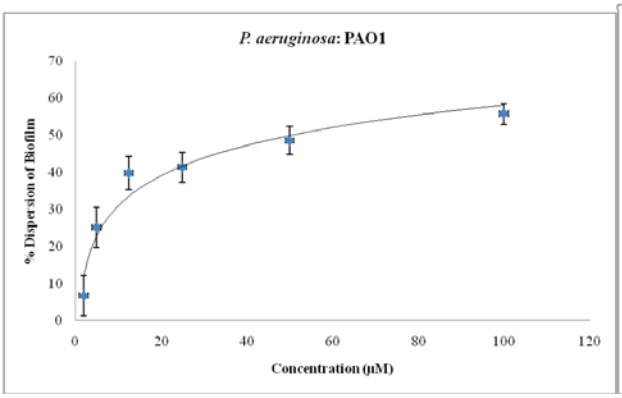

B. bronchiseptica: RB50
% Dispersion of Biofilm
Concentration (µM)

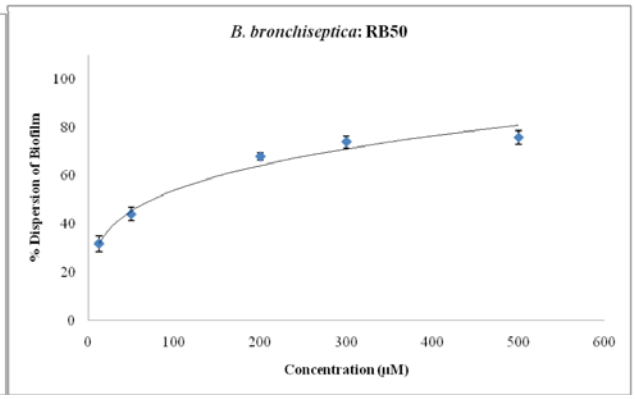

S. aureus: 29213
% Dispersion of Biofilim
Concentration (µM)

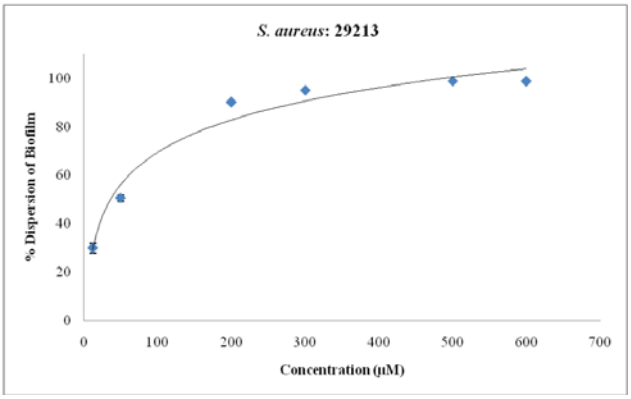

HCl · H2N
N
N
H
N
N
N


A. baumannii
% Dispersion of Biofilm
Concentration (µM)
0
20
40
60
80
100
0
100
200
300
400
500
600
700


P. aeruginosa: PA14
% Dispersion of Biofilm
Concentration (µM)
0
20
40
60
80
100
0
50
100
150
200
250

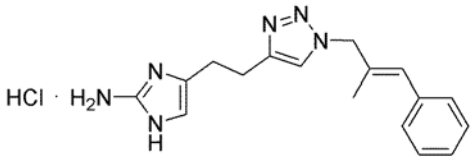

P. aeruginosa: PAO1
% Dispersion of Biofilm
Concentration (µM)
0
10
20
30
40
50
60
70
0
20
40
60
80
100
120

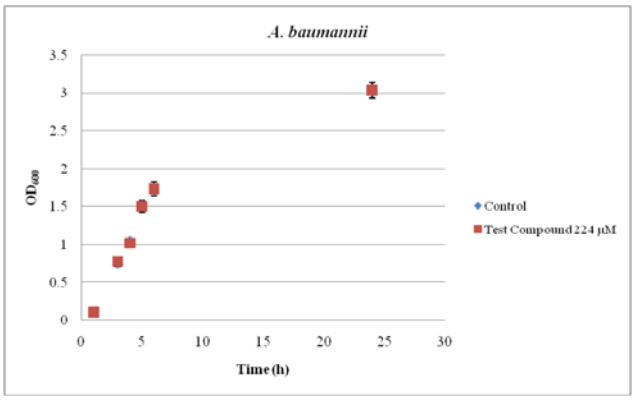

B. bronchiseptica: RB50
% Dispersion of Biofilm
Concentration (µM)
0
20
40
60
80
100
0
100
200
300
400
500
600

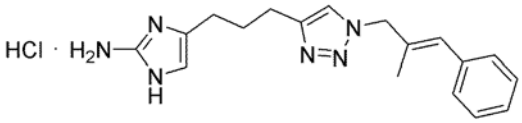

S. aureus: 29213
% Dispersion of Biofilm
Concentration (µM)
0
20
40
60
80
100
0
100
200
300
400
500
600
700

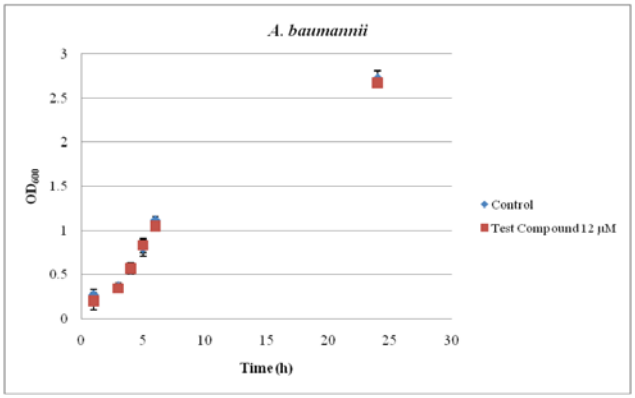
General Procedure for Growth Curves: The bacterial strains were grown in the absence and in the presence of the test compound at the IC_{50} value starting at an OD_{600} of 0.01 in culture tubes in an incubator shaker at 37° C at 200 rpm. The OD_{600} was recorded at 1, 3, 4, 5, 6 and 24 hours.

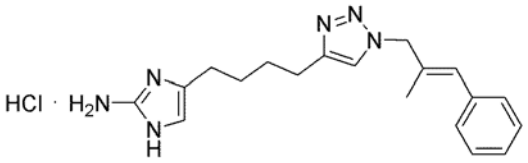
Growth Curves

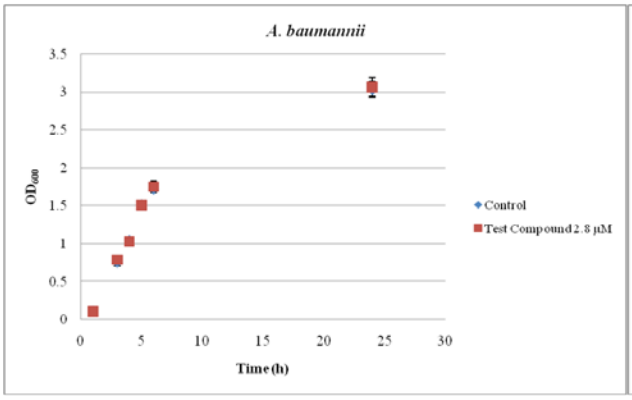


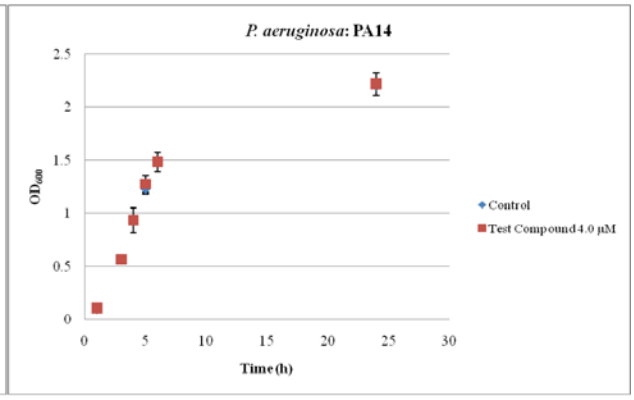


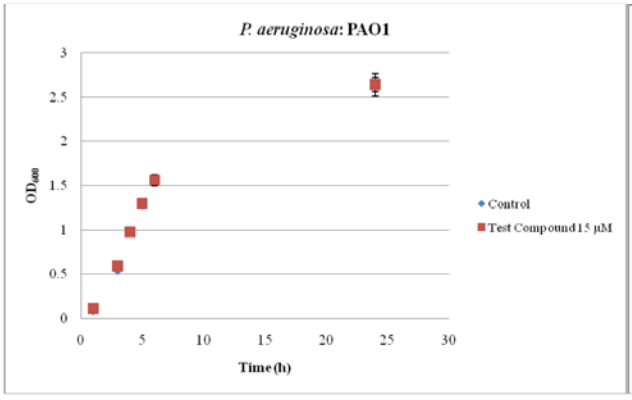


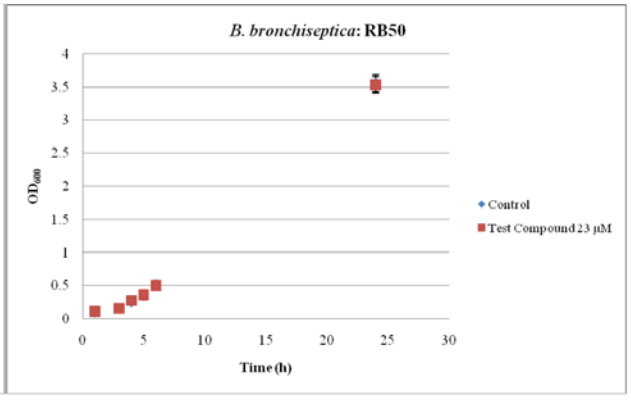


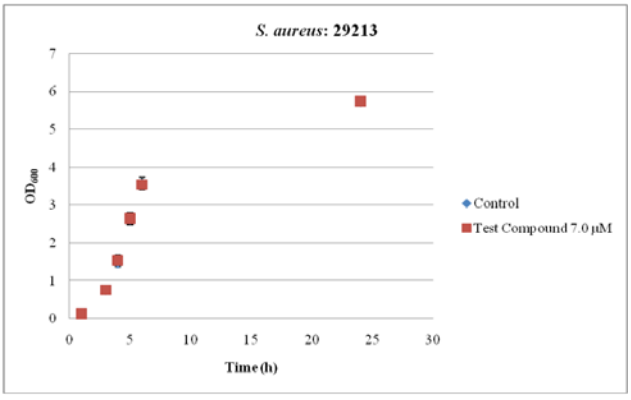

HCl · H2N
N
N
H
N
N

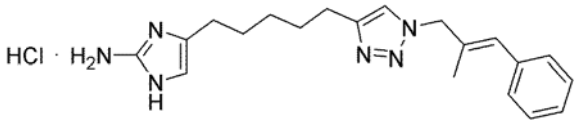

A. baumannii
OD600
Time (h)
Control
Test Compound 2.8 µM

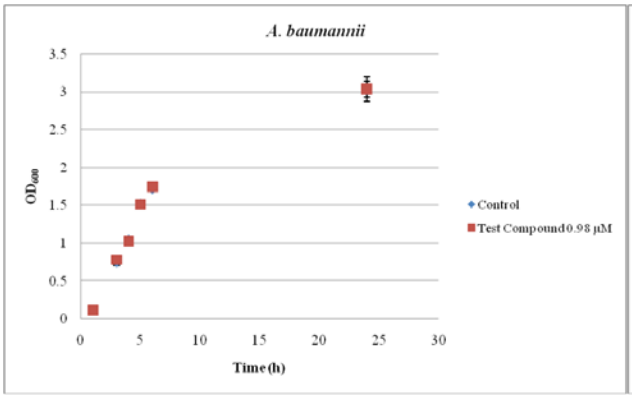

P. aeruginosa: PA14
OD600
Time (h)
Control
Test Compound 4.0 µM

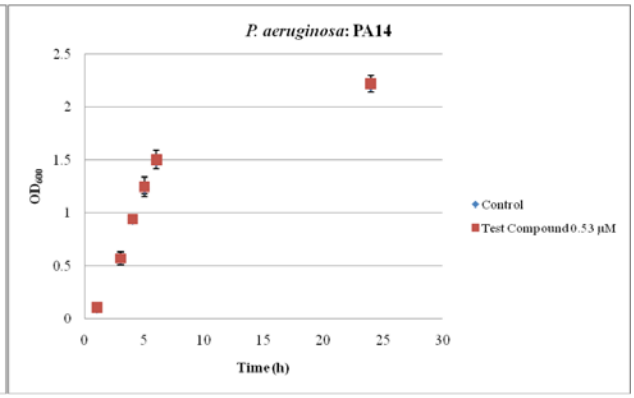

P. aeruginosa: PAO1
OD600
Time (h)
Control
Test Compound 15 µM

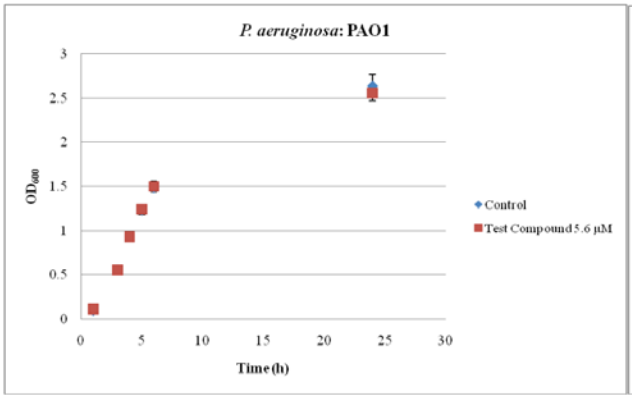

B. bronchiseptica: RB50
OD600
Time (h)
Control
Test Compound 23 µM

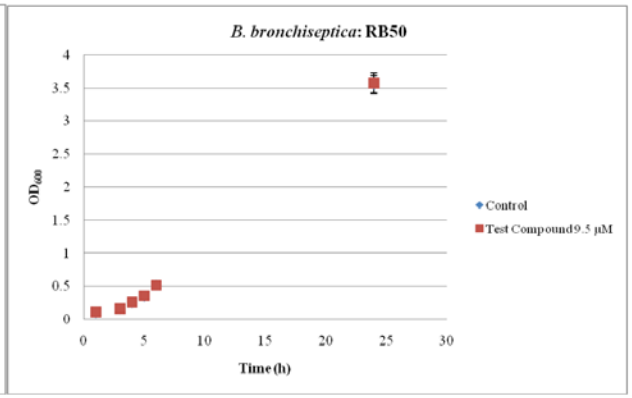

S. aureus: 29213
OD600
Time (h)
Control
Test Compound 7.0 µM

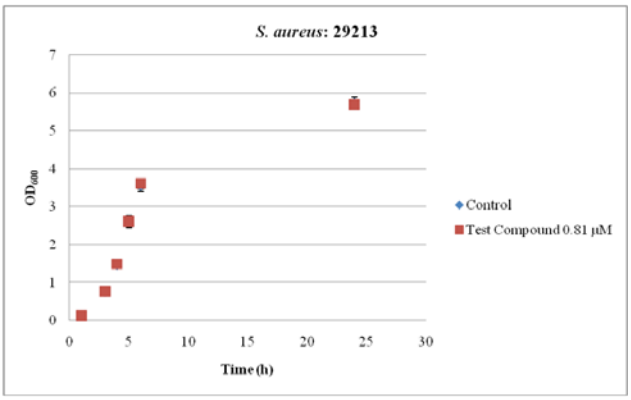

HCl · H2N
N
N
H
N
N=N

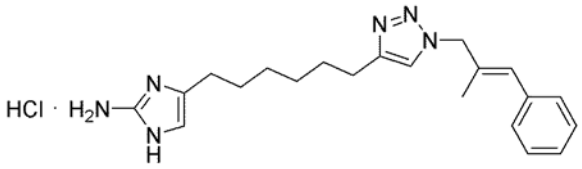

A. baumannii
OD600
Time (h)
Control
Test Compound 0.98 µM

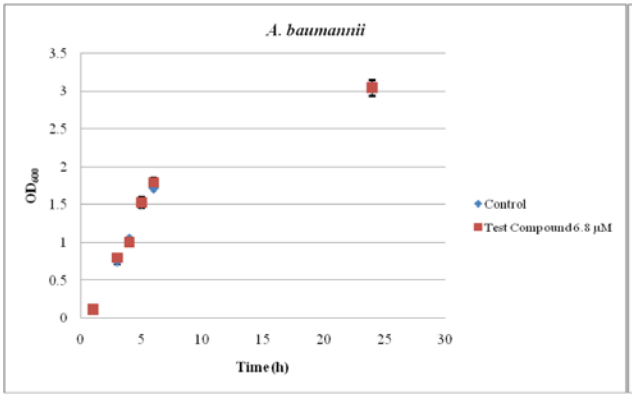

P. aeruginosa: PA14
OD600
Time (h)
Control
Test Compound 0.53 µM

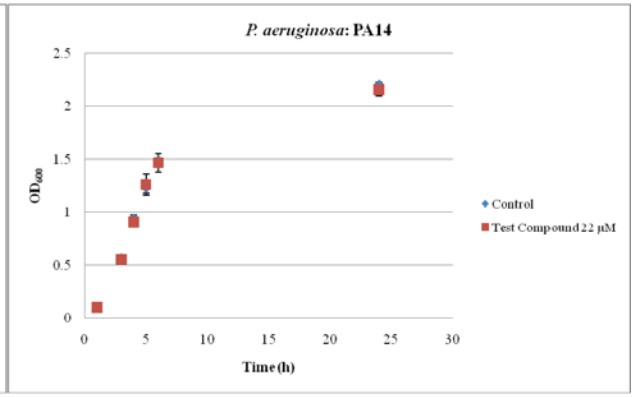

P. aeruginosa: PAO1
OD600
Time (h)
Control
Test Compound 5.6 µM

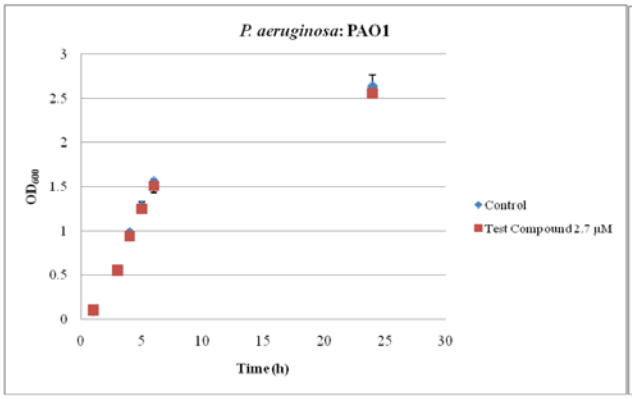

B. bronchiseptica: RB50
OD600
Time (h)
Control
Test Compound 9.5 µM

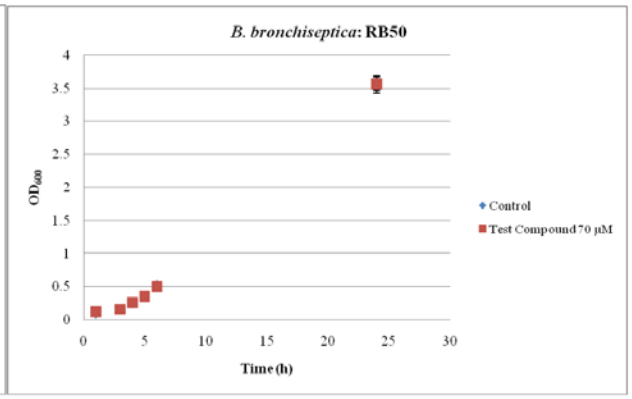

S. aureus: 29213
OD600
Time (h)
Control
Test Compound 0.81 µM

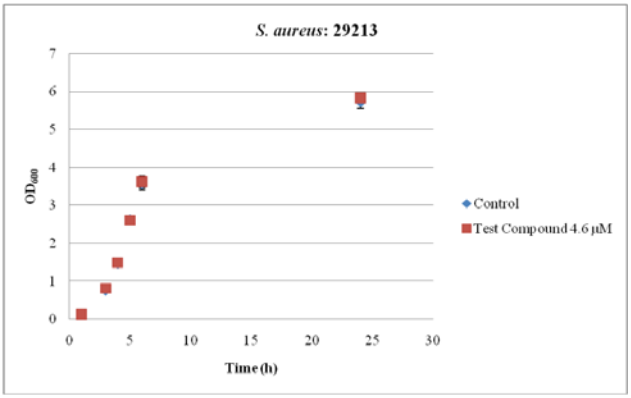

HCl · H2N
N
N
H
N
N


A. baumannii
OD600
Time (h)
Control
Test Compound 6.8 µM


P. aeruginosa: PA14
OD600
Time (h)
Control
Test Compound 22 µM

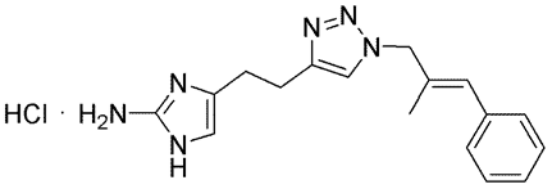

P. aeruginosa: PAO1
OD600
Time (h)
Control
Test Compound 2.7 µM

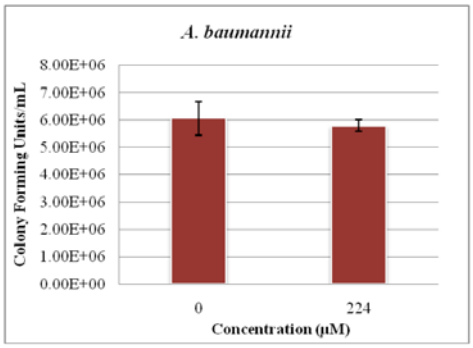

B. bronchiseptica: RB50
OD600
Time (h)
Control
Test Compound 70 µM

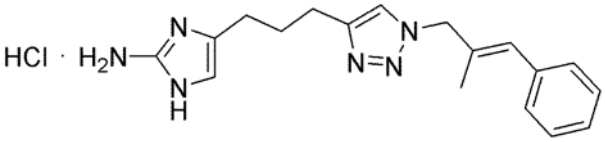

S. aureus: 29213
OD600
Time (h)
Control
Test Compound 4.6 µM

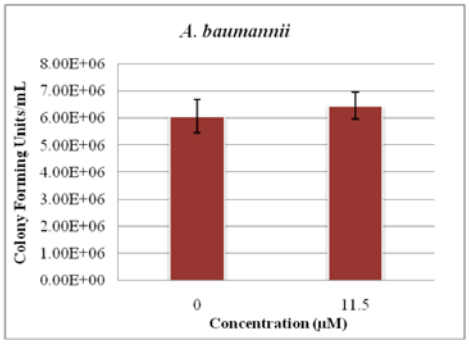
General Colony Count Procedure for *A. baumannii, P. aeruginosa, B. bronchiseptica* and *S. aureus*: Colony counts were performed by incubating either bacterial strain in the presence and absence of the test compound at 37° C in culture tubes until the sample with the absence of the test compound reached an OD_{600} of 0.4 from a starting OD_{600} of 0.01. This typically took three to four hours. Once the OD_{600} of approximately 0.4 was observed, 100 µL were taken from each culture tube from which serial dilutions were made. Then, 10 µL were removed from each serial dilution and plated out on a square gridded petri-dish followed by 16 hours of incubation at 37° C period (48 hours for *B. bronchiseptica*) to grow countable colonies. Viable bacteria were quantified through employment of the track-dilution method.[7]

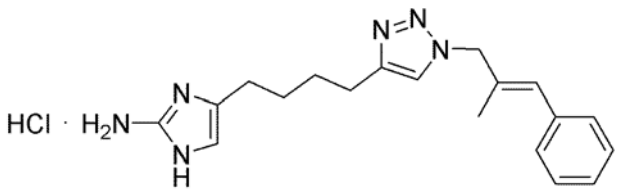
Colony Counts

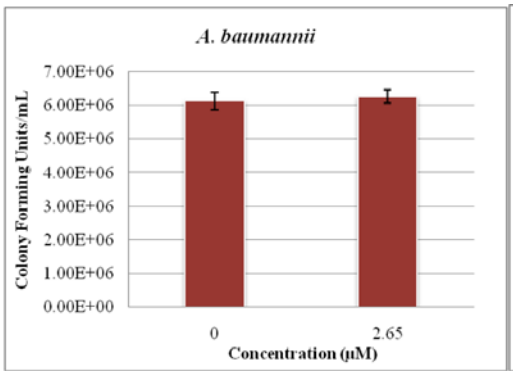


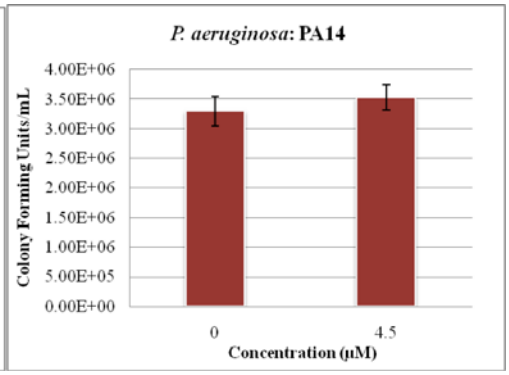


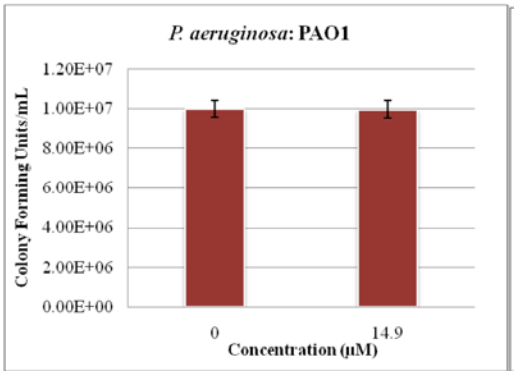


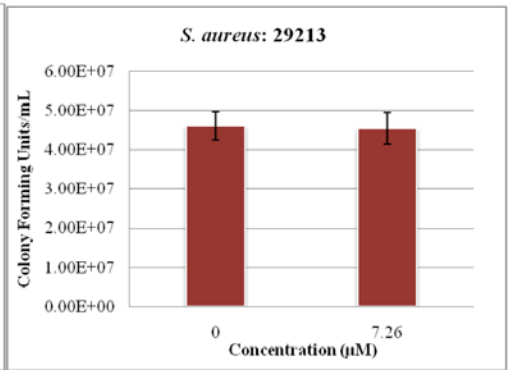


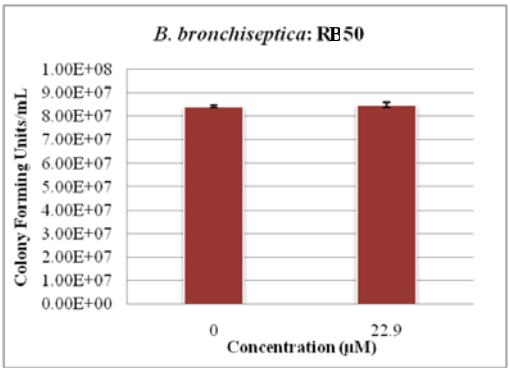

HCl · H2N
N
N
H
N=N
N

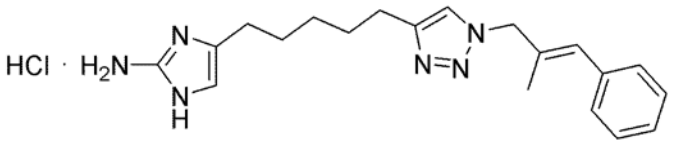

A. baumannii
Colony Forming Units/mL
7.00E+06
6.00E+06
5.00E+06
4.00E+06
3.00E+06
2.00E+06
1.00E+06
0.00E+00
0
2.65
Concentration (µM)

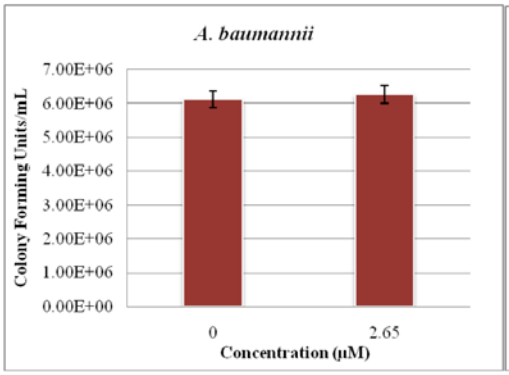

P. aeruginosa: PA14
Colony Forming Units/mL
4.00E+06
3.50E+06
3.00E+06
2.50E+06
2.00E+06
1.50E+06
1.00E+06
5.00E+05
0.00E+00
0
4.5
Concentration (µM)

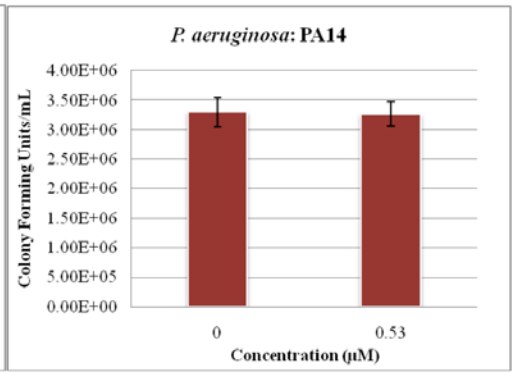

P. aeruginosa: PAO1
Colony Forming Units/mL
1.20E+07
1.00E+07
8.00E+06
6.00E+06
4.00E+06
2.00E+06
0.00E+00
0
14.9
Concentration (µM)

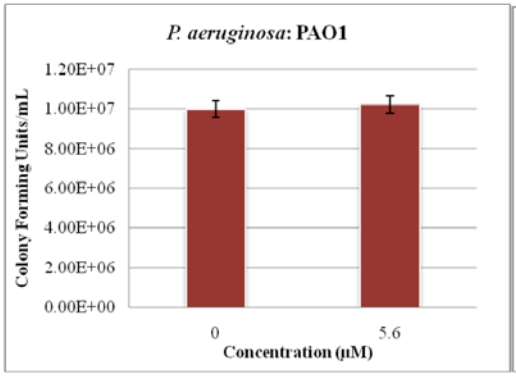

S. aureus: 29213
Colony Forming Units/mL
6.00E+07
5.00E+07
4.00E+07
3.00E+07
2.00E+07
1.00E+07
0.00E+00
0
7.26
Concentration (µM)

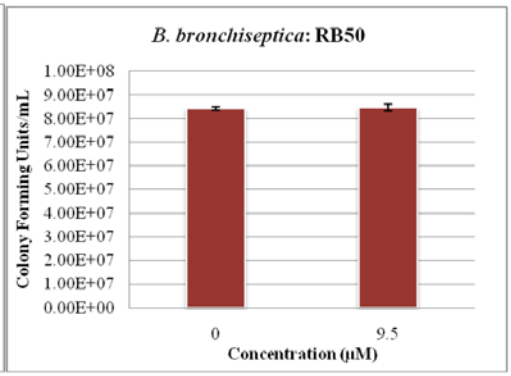

B. bronchiseptica: RB50
Colony Forming Units/mL
1.00E+08
9.00E+07
8.00E+07
7.00E+07
6.00E+07
5.00E+07
4.00E+07
3.00E+07
2.00E+07
1.00E+07
0.00E+00
0
22.9
Concentration (µM)

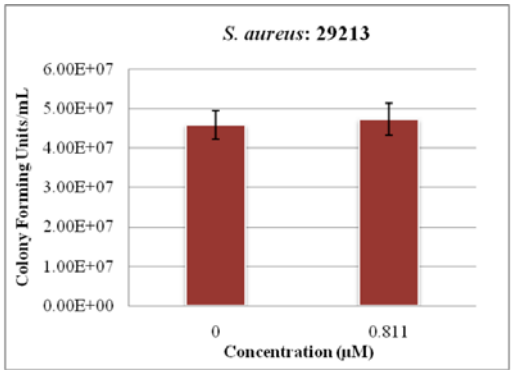

HCl · H2N
N
N
H
N
N=N

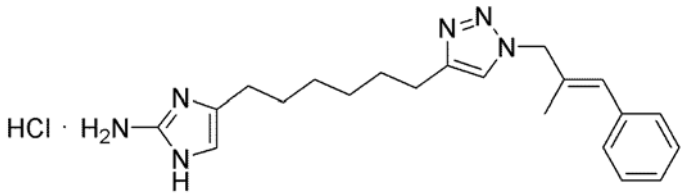

A. baumannii
Colony Forming Units/mL
7.00E+06
6.00E+06
5.00E+06
4.00E+06
3.00E+06
2.00E+06
1.00E+06
0.00E+00
0
2.65
Concentration (µM)

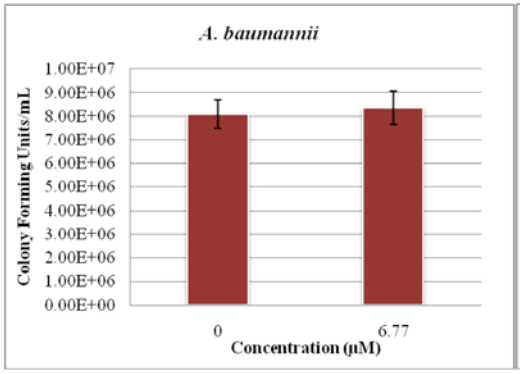

P. aeruginosa: PA14
Colony Forming Units/mL
4.00E+06
3.50E+06
3.00E+06
2.50E+06
2.00E+06
1.50E+06
1.00E+06
5.00E+05
0.00E+00
0
0.53
Concentration (µM)

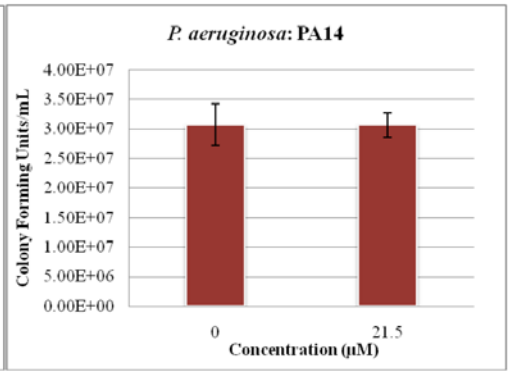

P. aeruginosa: PAO1
Colony Forming Units/mL
1.20E+07
1.00E+07
8.00E+06
6.00E+06
4.00E+06
2.00E+06
0.00E+00
0
5.6
Concentration (µM)

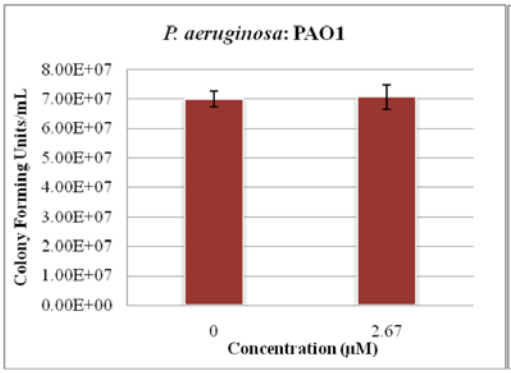

B. bronchiseptica: RB50
Colony Forming Units/mL
1.00E+08
9.00E+07
8.00E+07
7.00E+07
6.00E+07
5.00E+07
4.00E+07
3.00E+07
2.00E+07
1.00E+07
0.00E+00
0
9.5
Concentration (µM)

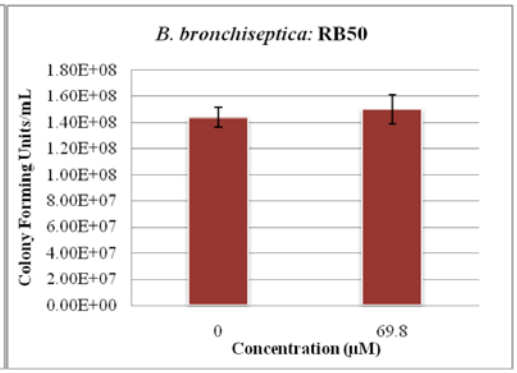

S. aureus: 29213
Colony Forming Units/mL
6.00E+07
5.00E+07
4.00E+07
3.00E+07
2.00E+07
1.00E+07
0.00E+00
0
0.811
Concentration (µM)

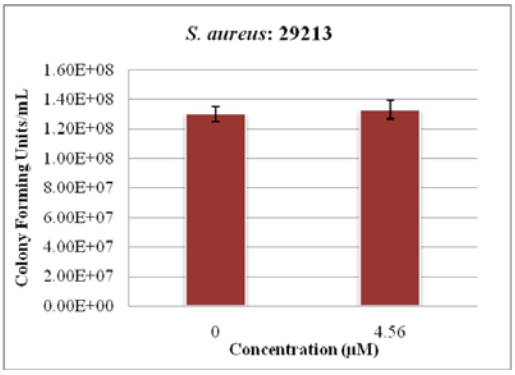

HCl · H2N
N
N
H
N
N


A. baumannii
Colony Forming Units/mL
1.00E+07
9.00E+06
8.00E+06
7.00E+06
6.00E+06
5.00E+06
4.00E+06
3.00E+06
2.00E+06
1.00E+06
0.00E+00
0
6.77
Concentration (µM)


P. aeruginosa: PA14
Colony Forming Units/mL
4.00E+07
3.50E+07
3.00E+07
2.50E+07
2.00E+07
1.50E+07
1.00E+07
5.00E+06
0.00E+00
0
21.5
Concentration (µM)


P. aeruginosa: PAO1
Colony Forming Units/mL
8.00E+07
7.00E+07
6.00E+07
5.00E+07
4.00E+07
3.00E+07
2.00E+07
1.00E+07
0.00E+00
0
2.67
Concentration (µM)


B. bronchiseptica: RB50
Colony Forming Units/mL
1.80E+08
1.60E+08
1.40E+08
1.20E+08
1.00E+08
8.00E+07
6.00E+07
4.00E+07
2.00E+07
0.00E+00
0
69.8
Concentration (µM)


S. aureus: 29213
Colony Forming Units/mL
1.60E+08
1.40E+08
1.20E+08
1.00E+08
8.00E+07
6.00E+07
4.00E+07
2.00E+07
0.00E+00
0
4.56
Concentration (µM)

References:

1. Raban, J.; Chang, H.; Craine, L.; Hortelano, E. J. N-(Arylthio)benzimidazoles. Torsional Barriers and 1, 3-Rearrangement. J. Org. Chem. **1985**, 50 (13), 2205 – 2210.

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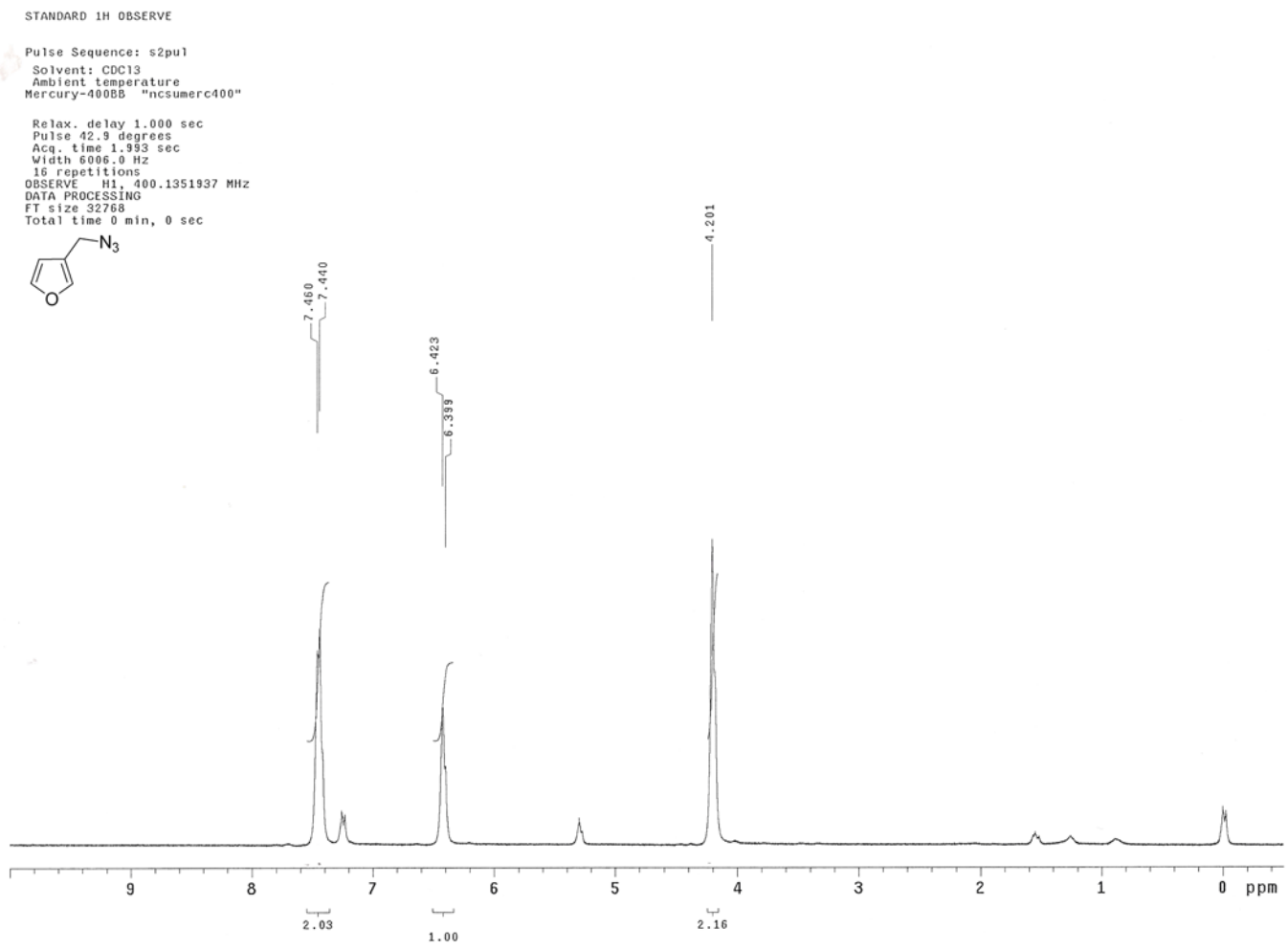
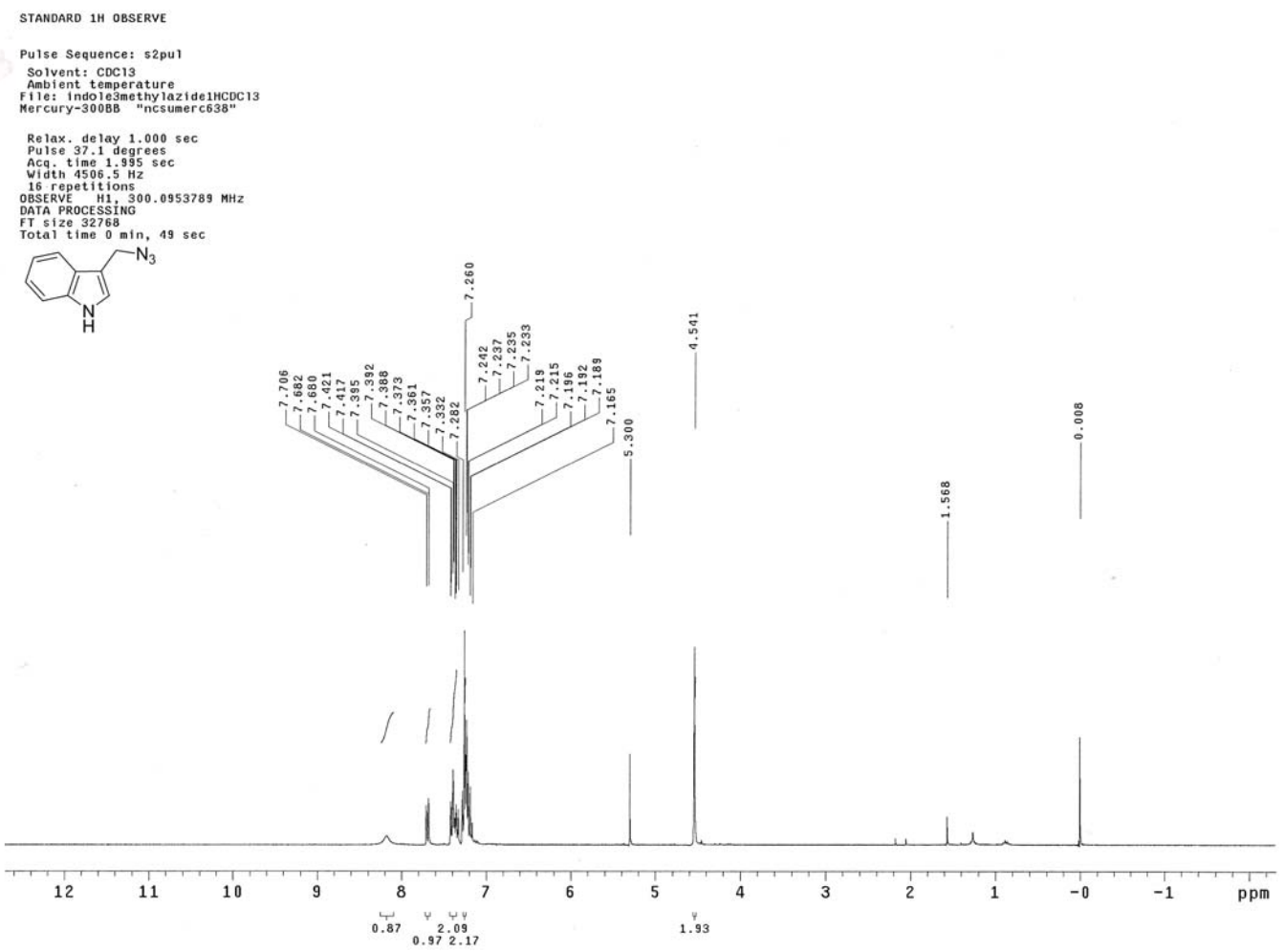
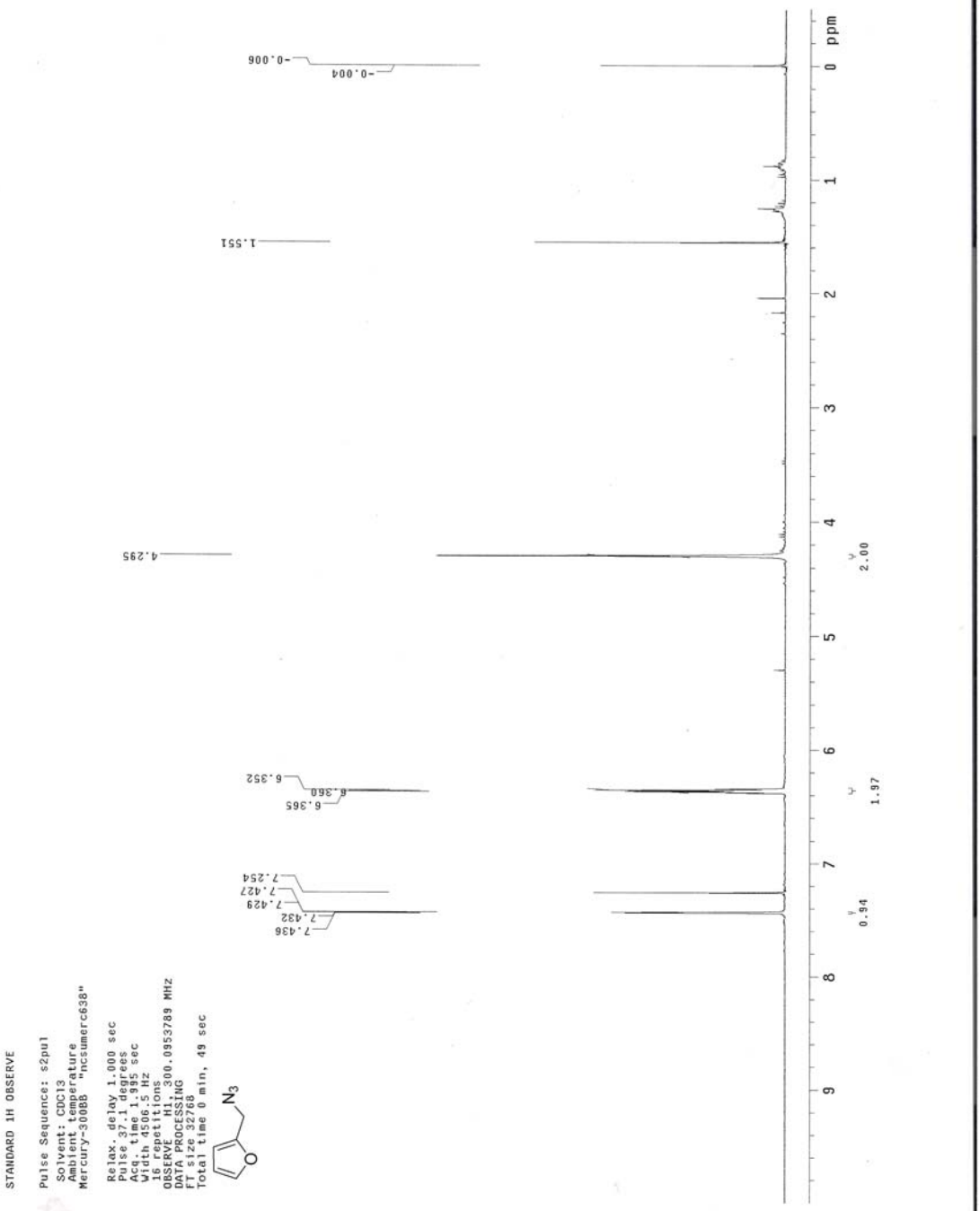
6. Rad, M. N. S.; Behrouz, S.; Khalafi-Nezhad, A. A simple one-pot procedure for the direct conversion of alcohols into azides using TsIm. Tetrahedron Letters **2007**, 48, 3445 – 3449.

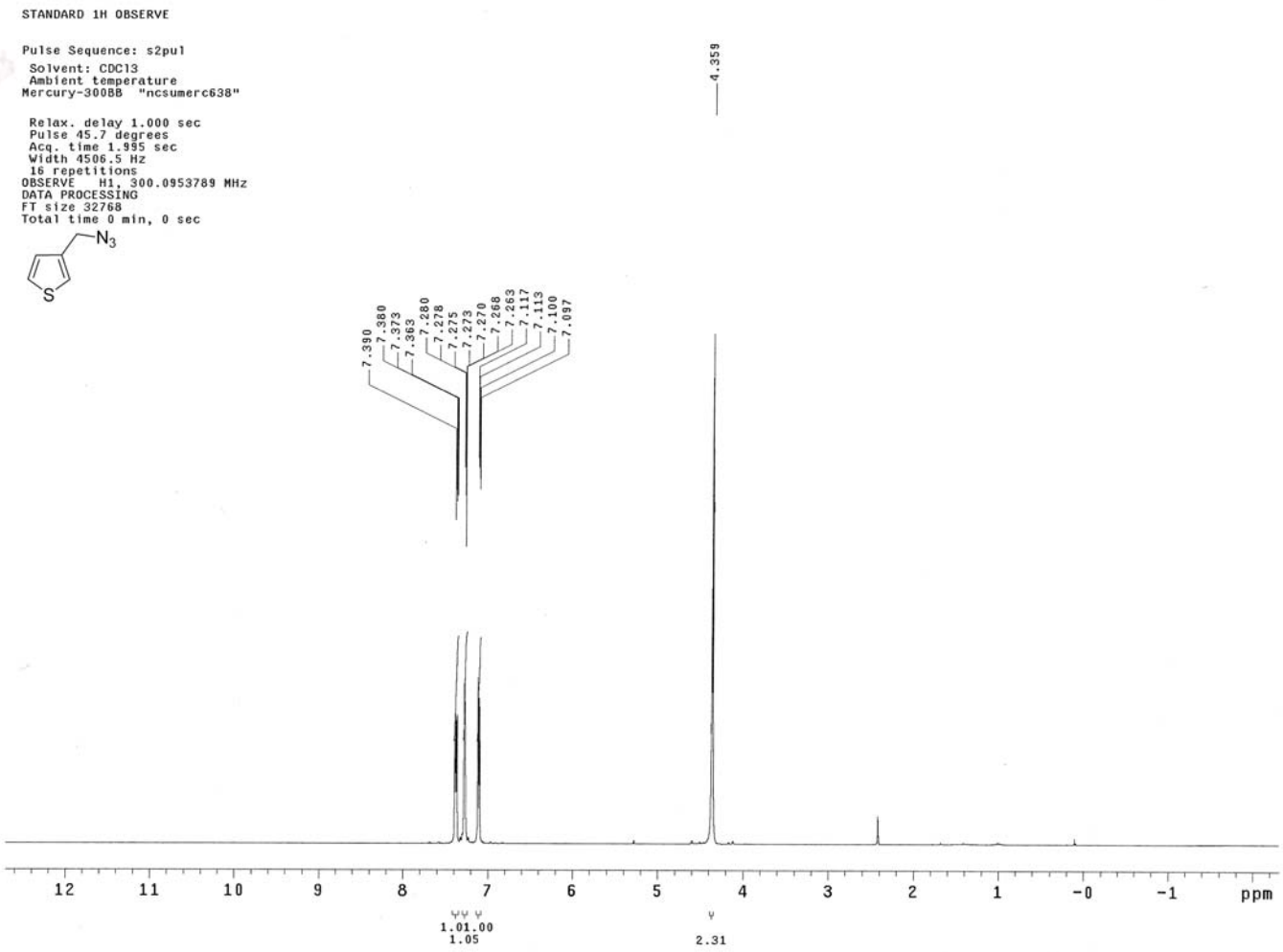
7. Jett, B. D.; Hatter, K. L.; Huycke, M. M.; Gilmore, M. S. Simplified agar plate method for quantifying viable bacteria. Bio Techniques. **1997**, 23, 648-650.

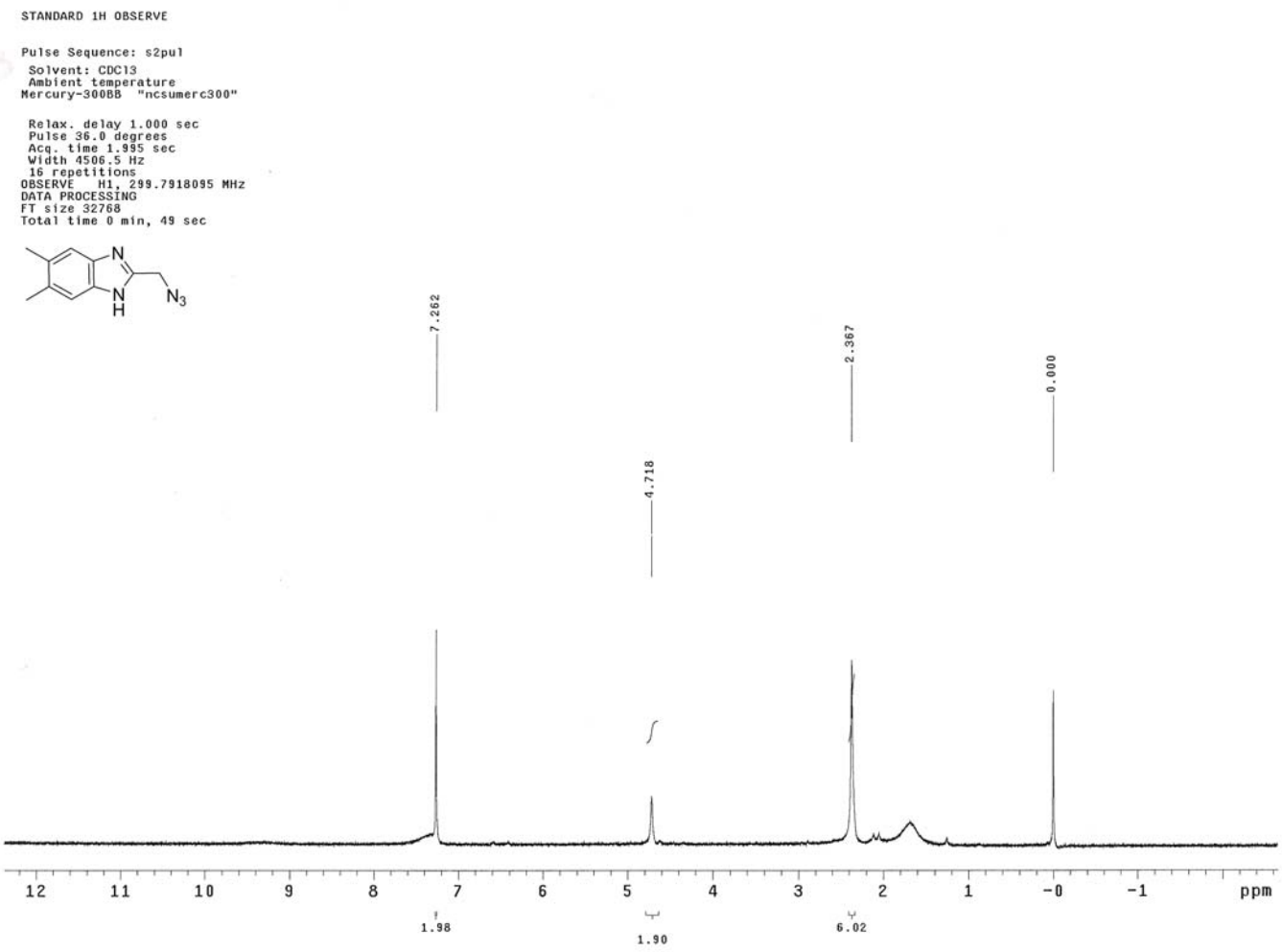
3. ^{1}H NMR Spectra for New Compounds

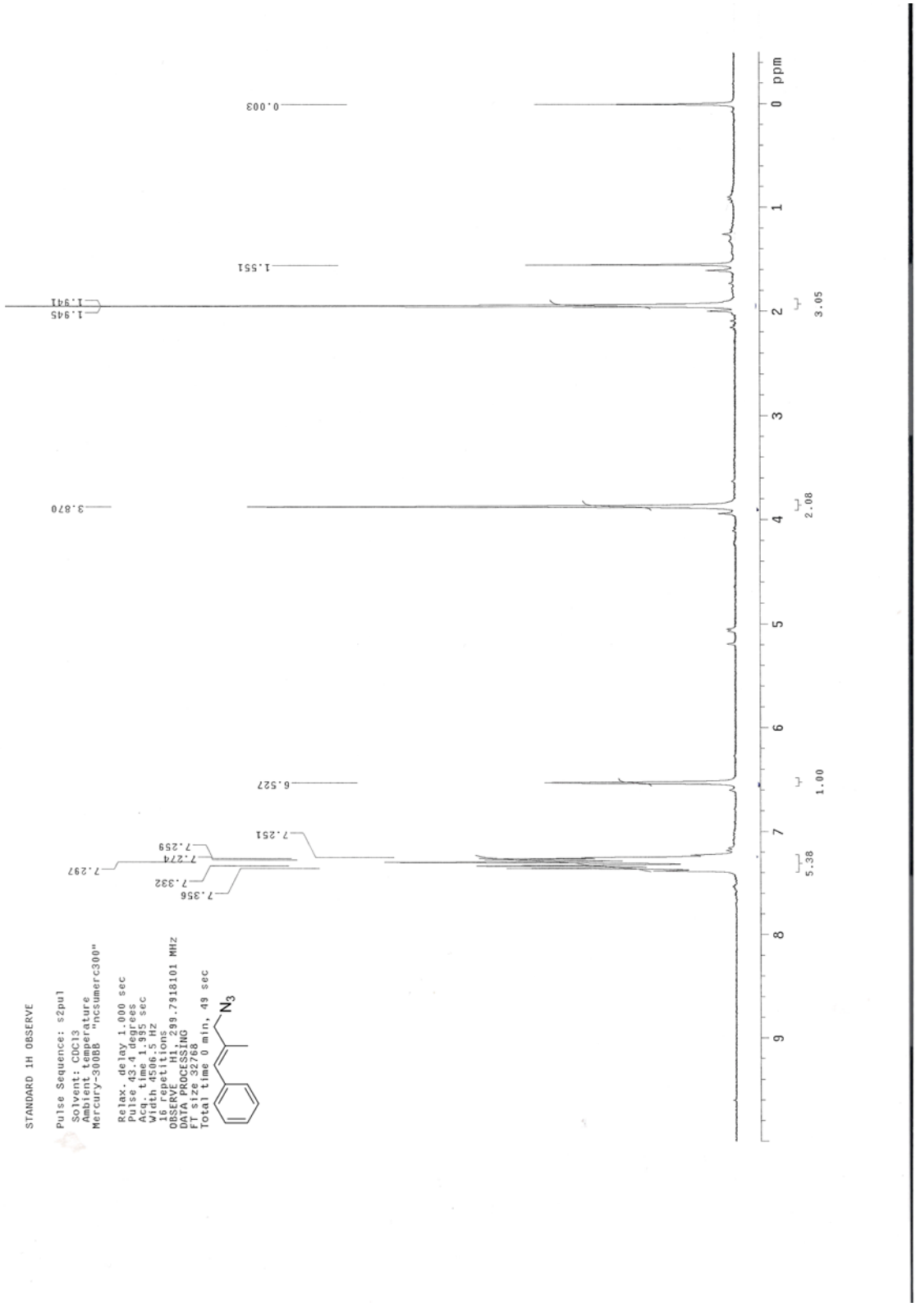

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 42.9 degrees
Acq. time 1.993 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1351937 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 0 sec
N3
O
7.460
7.440
6.423
6.399
4.201
9
8
7
6
5
4
3
2
1
0 ppm
2.03
1.00
2.16

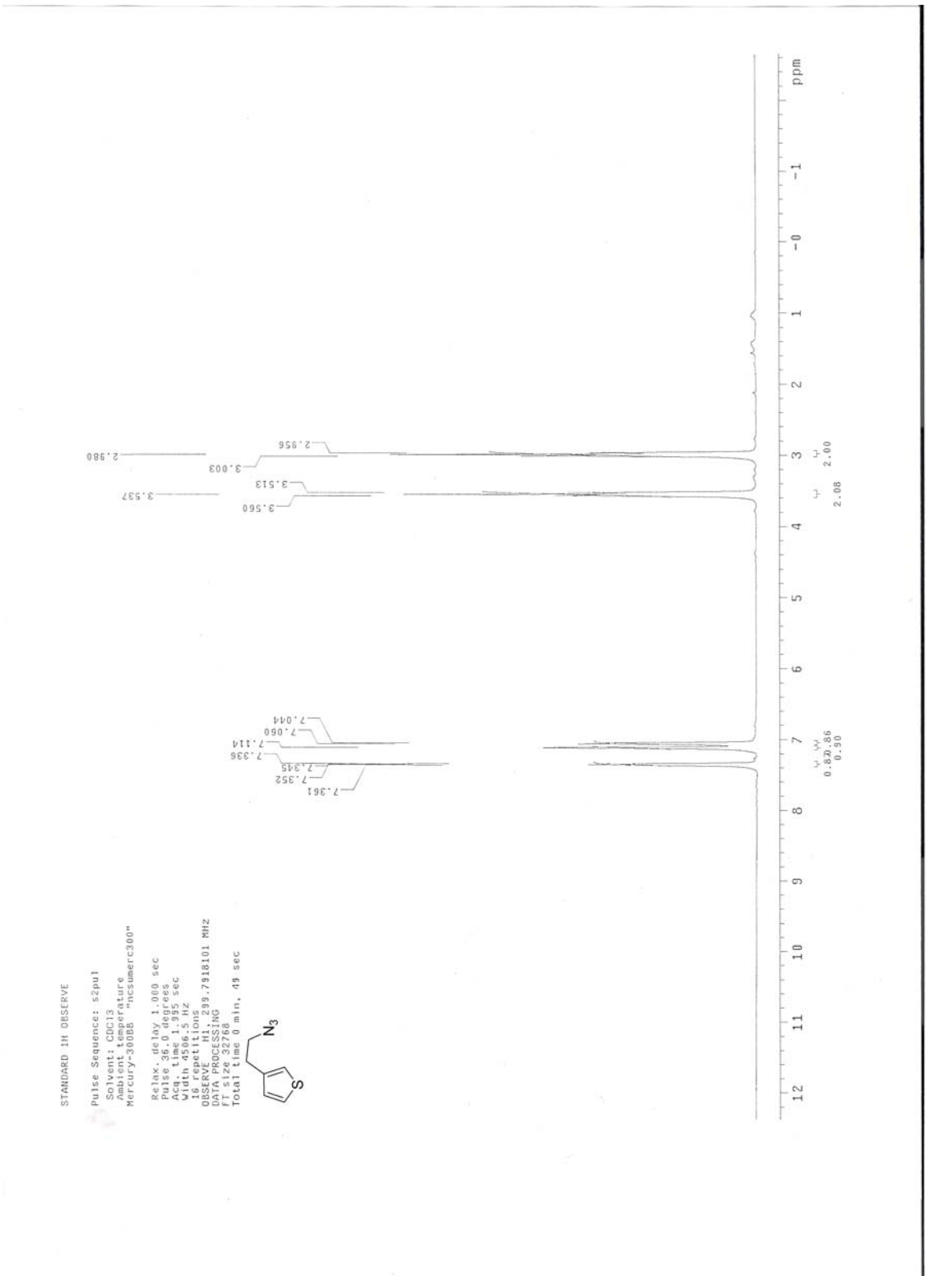

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: indole3methylazide1HCDCl3
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0953789 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
N3
N
H
7.706
7.682
7.680
7.421
7.417
7.395
7.392
7.388
7.373
7.361
7.357
7.332
7.282
7.260
7.242
7.237
7.235
7.233
7.219
7.215
7.196
7.192
7.189
7.165
5.300
4.541
1.568
0.008
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm
0.87
0.97
2.09
2.17
1.93


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0953789 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
N3
O
-0.006
-0.004
1.551
4.295
6.352
6.360
6.365
7.254
7.427
7.429
7.432
7.436
0.94
1.97
2.00
ppm


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 45.7 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0953789 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 0 sec
N3
S
4.359
7.390
7.380
7.373
7.363
7.280
7.278
7.275
7.273
7.270
7.268
7.263
7.117
7.113
7.100
7.097
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm
1.01.00
1.05
2.31

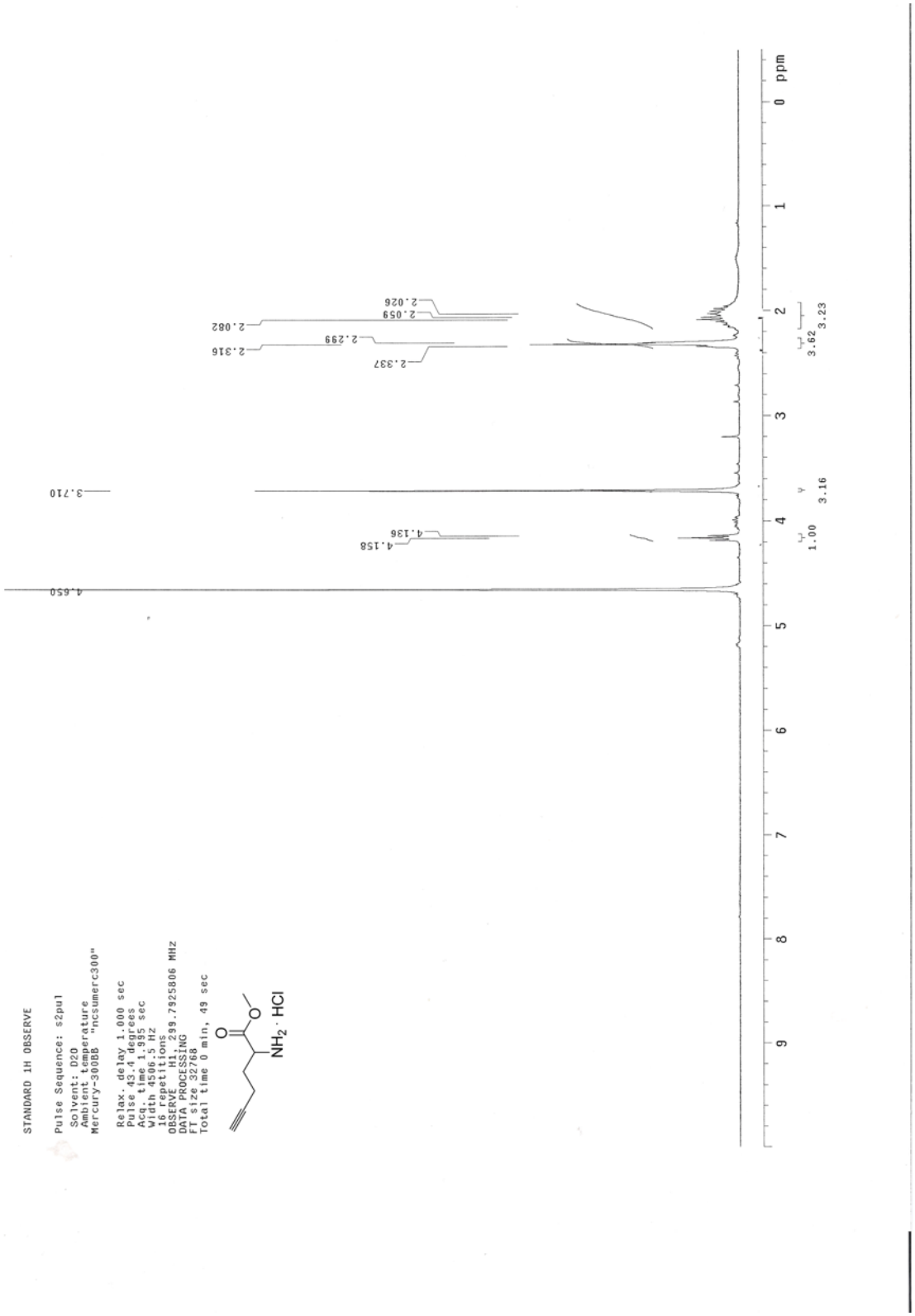

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 299.7918095 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
N
N
H
N3
7.262
4.718
2.367
0.000
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm
1.98
1.90
6.02

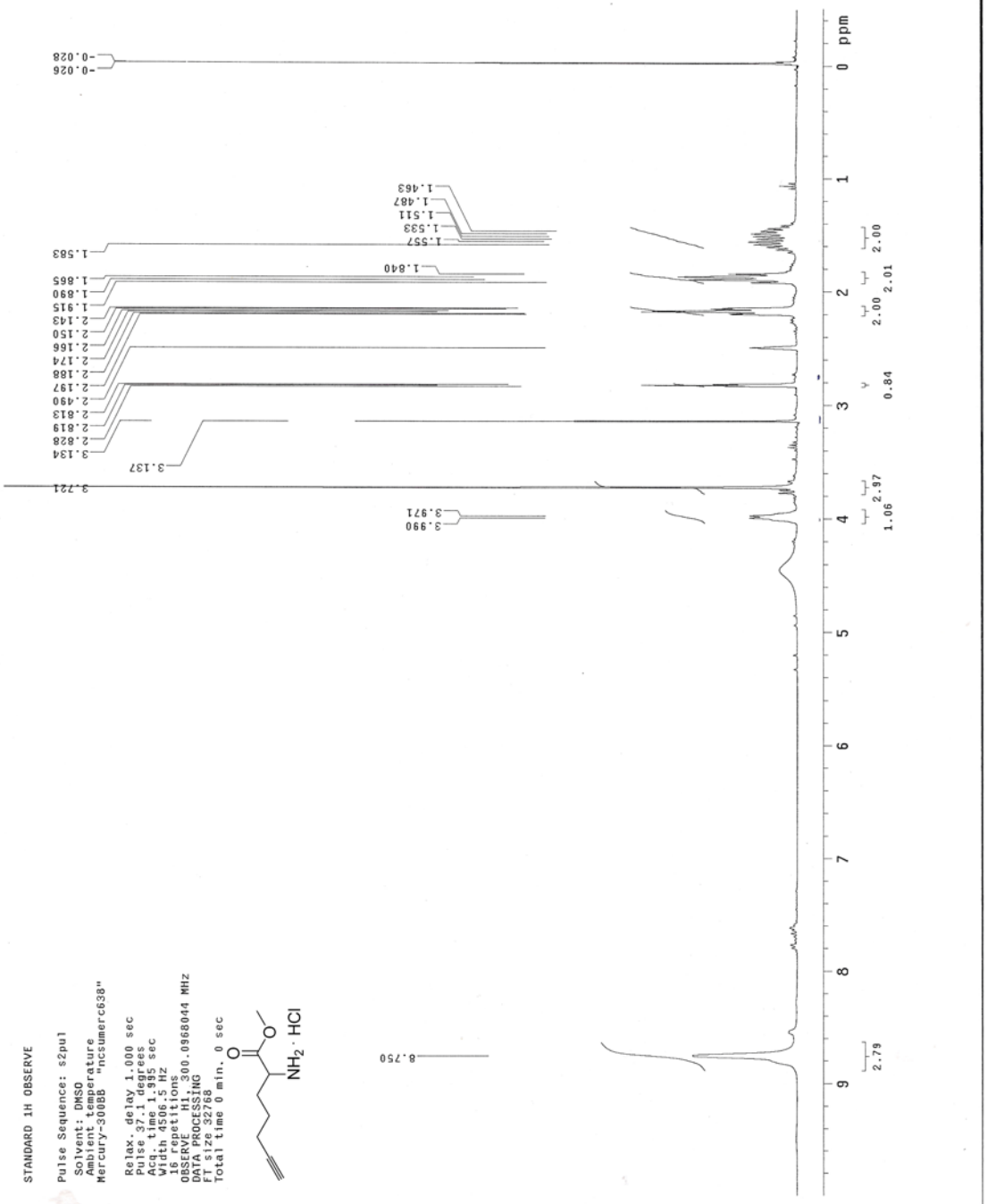

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 43.4 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 299.7918101 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
N3
7.356
7.332
7.297
7.274
7.259
7.251
6.527
3.870
1.945
1.941
1.551
0.003
5.38
1.00
2.08
3.05
ppm


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 2.185 sec
Width 4506.5 HZ
16 repetitions
OBSERVE H1, 299.7918101 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
2.980
3.003
2.956
3.537
3.513
3.560
7.361
7.352
7.315
7.336
7.114
7.060
7.044
2.00
2.08
0.86
0.90
ppm

4.

5.

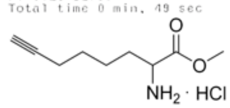

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: D2O
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 43.4 degrees
Acq. time 1.995 sec
Width 4515.5 Hz
16 repetitions
OBSERVE H1, 299.7925806 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
NH2 · HCl
4.650
4.156
4.136
3.710
2.337
2.299
2.316
2.082
2.059
2.026
1.00
3.16
3.62
3.23
ppm

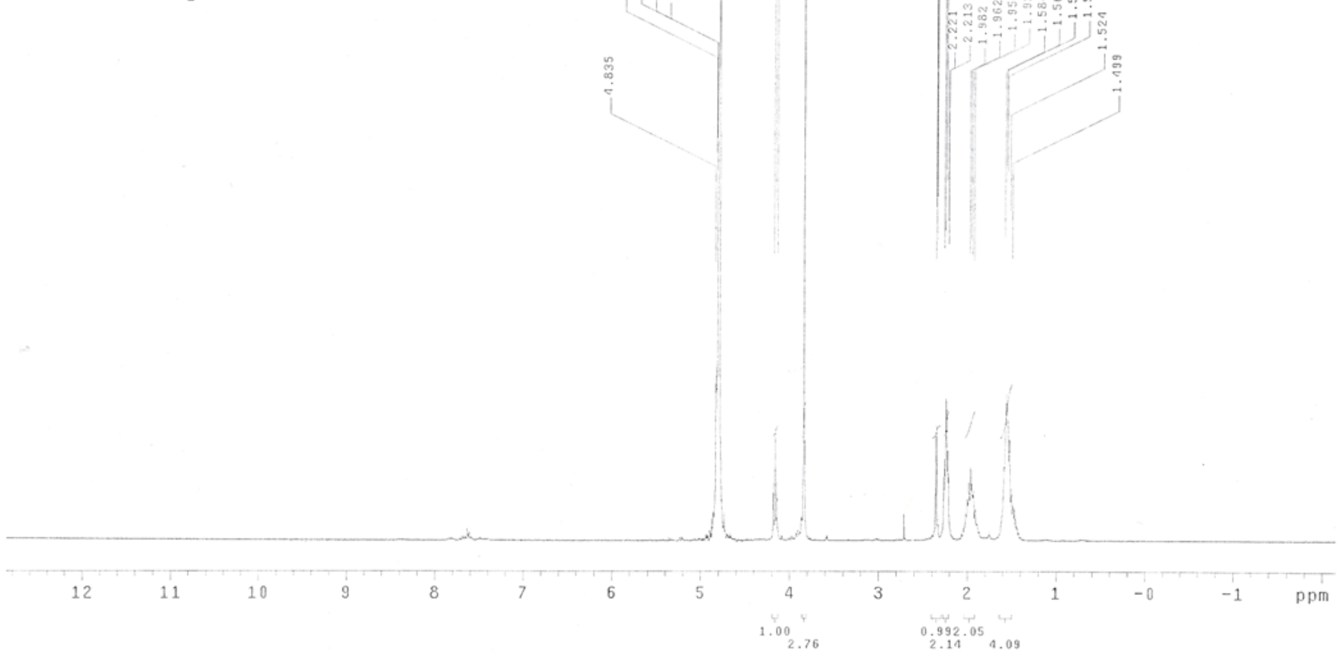

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: DMSO
Ambient temperature
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4516.5 Hz
16 repetitions
OBSERVE H1, 300.0968044 MHz
DATA PROCESSING
FT size 32768
Total time 0 min. 0 sec
NH2 · HCl
-0.026
-0.028
1.463
1.487
1.511
1.533
1.557
1.583
1.840
1.865
1.890
1.915
2.143
2.150
2.166
2.174
2.188
2.197
2.490
2.613
2.619
2.828
3.134
3.137
3.221
3.971
3.990
8.750
ppm
2.79
1.06
2.97
0.84
2.00
2.01
2.00

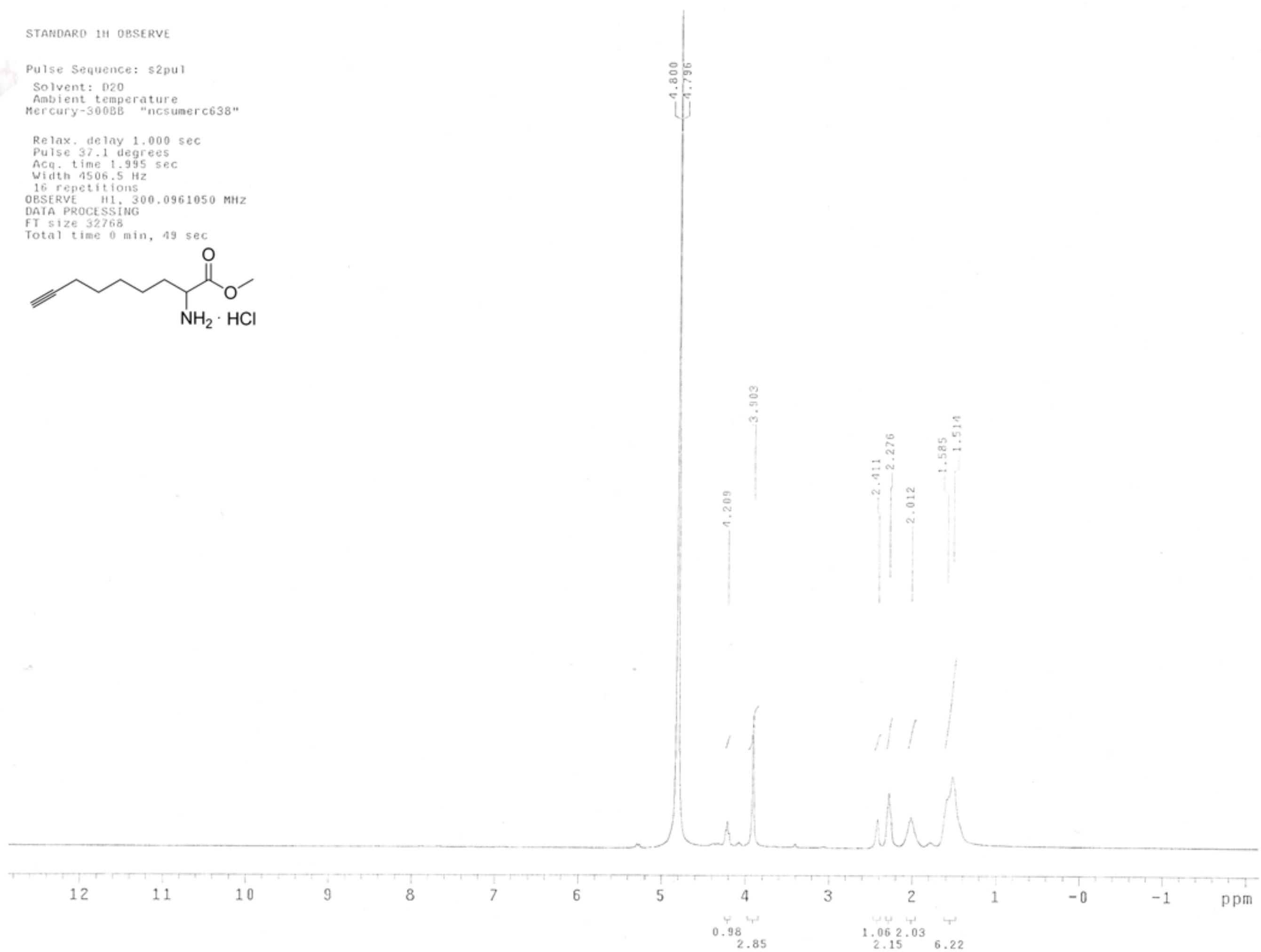
STANDARD 1H OBSERVE

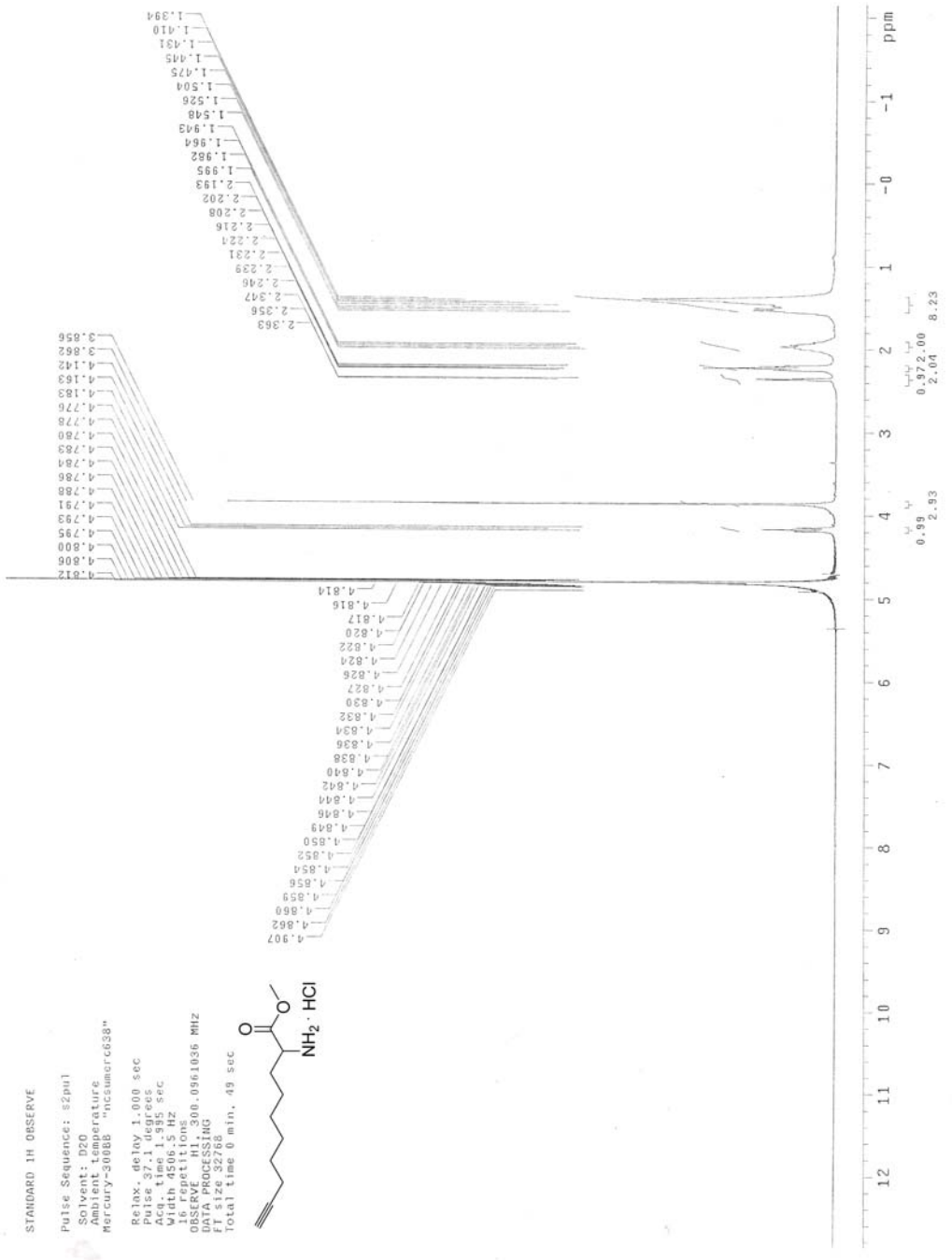
Pulse Sequence: s2pul
Solvent: D2O
Ambient temperature
File: Hexynglycinemethylester-1H-D2O
Mercury-300BB "ncsumerc638"

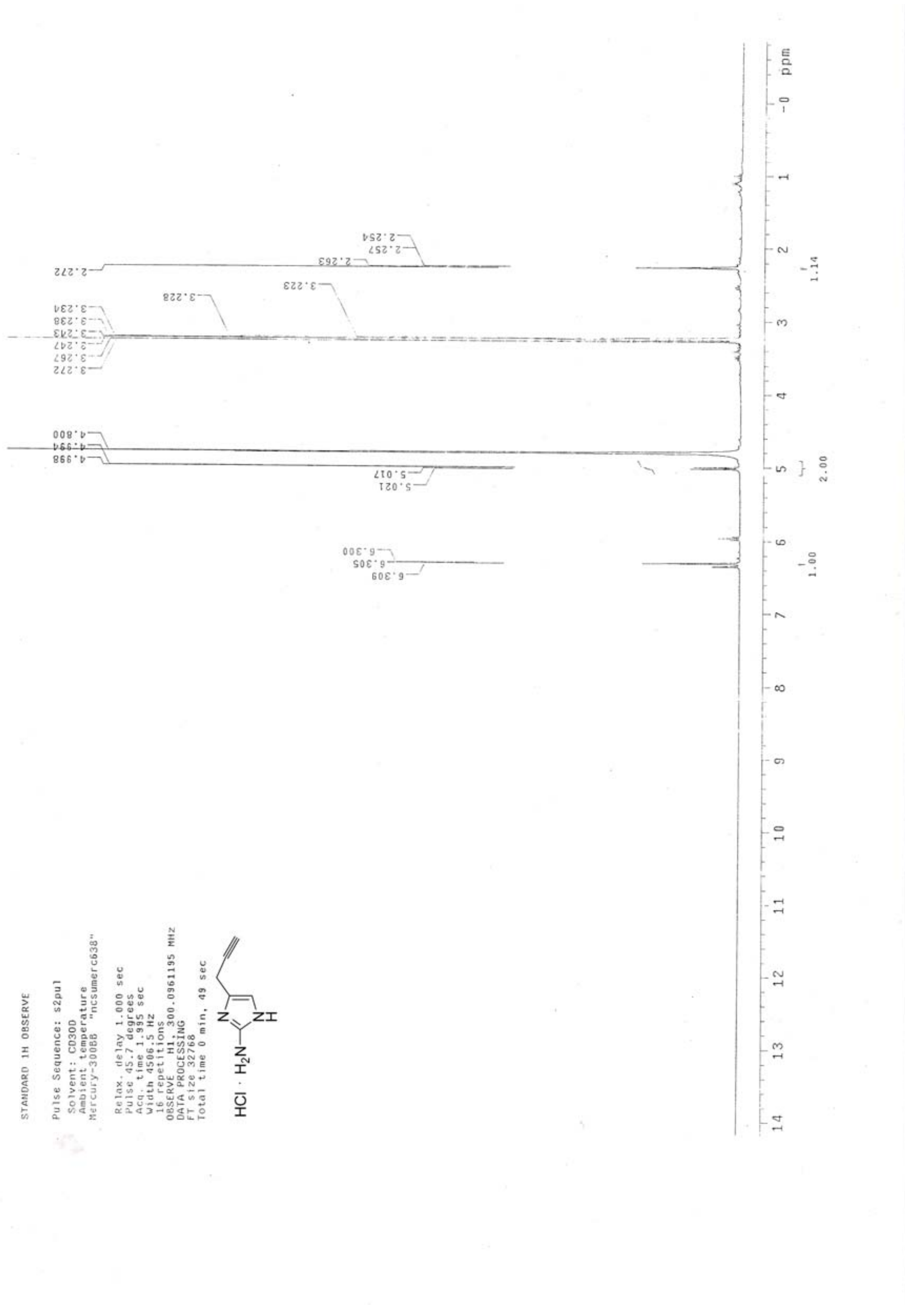
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0961028 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec

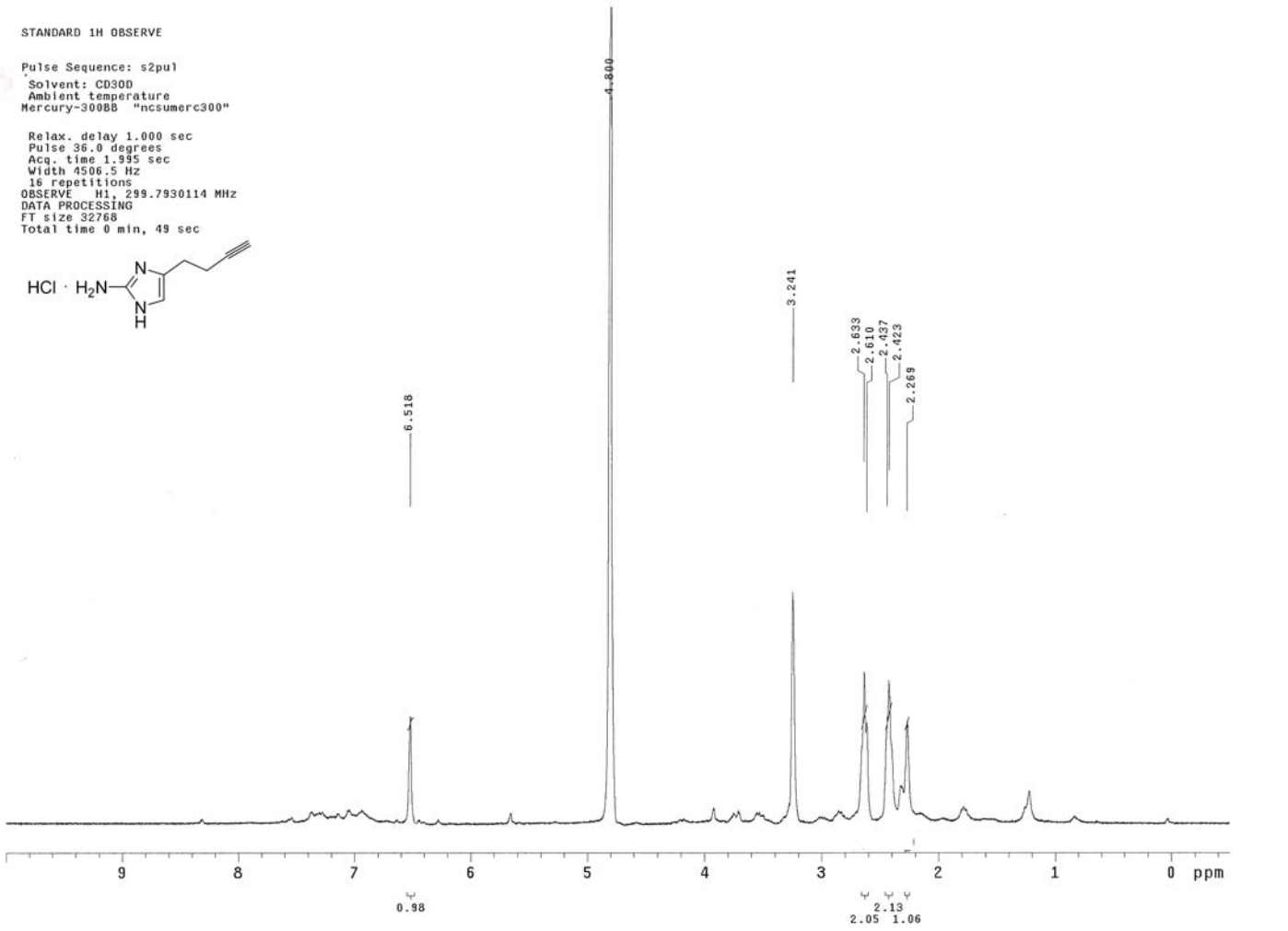





STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: D2O
Ambient temperature
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0961050 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
O
O
NH2 · HCl
4.800
4.796
4.209
3.903
2.411
2.276
2.012
1.585
1.514
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm
0.98
2.85
1.06
2.15
2.03
6.22


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: D2O
Ambient temperature
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.935 sec
Width 4516.5 Hz
32 repetitions
OBSERVE H1, 300.0961036 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
NH2 · HCl
ppm

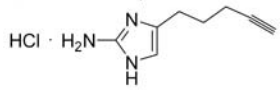

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 45.7 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0961195 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
HCl · H2N
N
NH
2.272
2.254
2.257
2.263
3.234
3.238
3.243
3.247
3.267
3.272
3.228
3.223
4.800
4.994
4.998
5.017
5.021
6.300
6.305
6.309
1.14
2.00
1.00
ppm

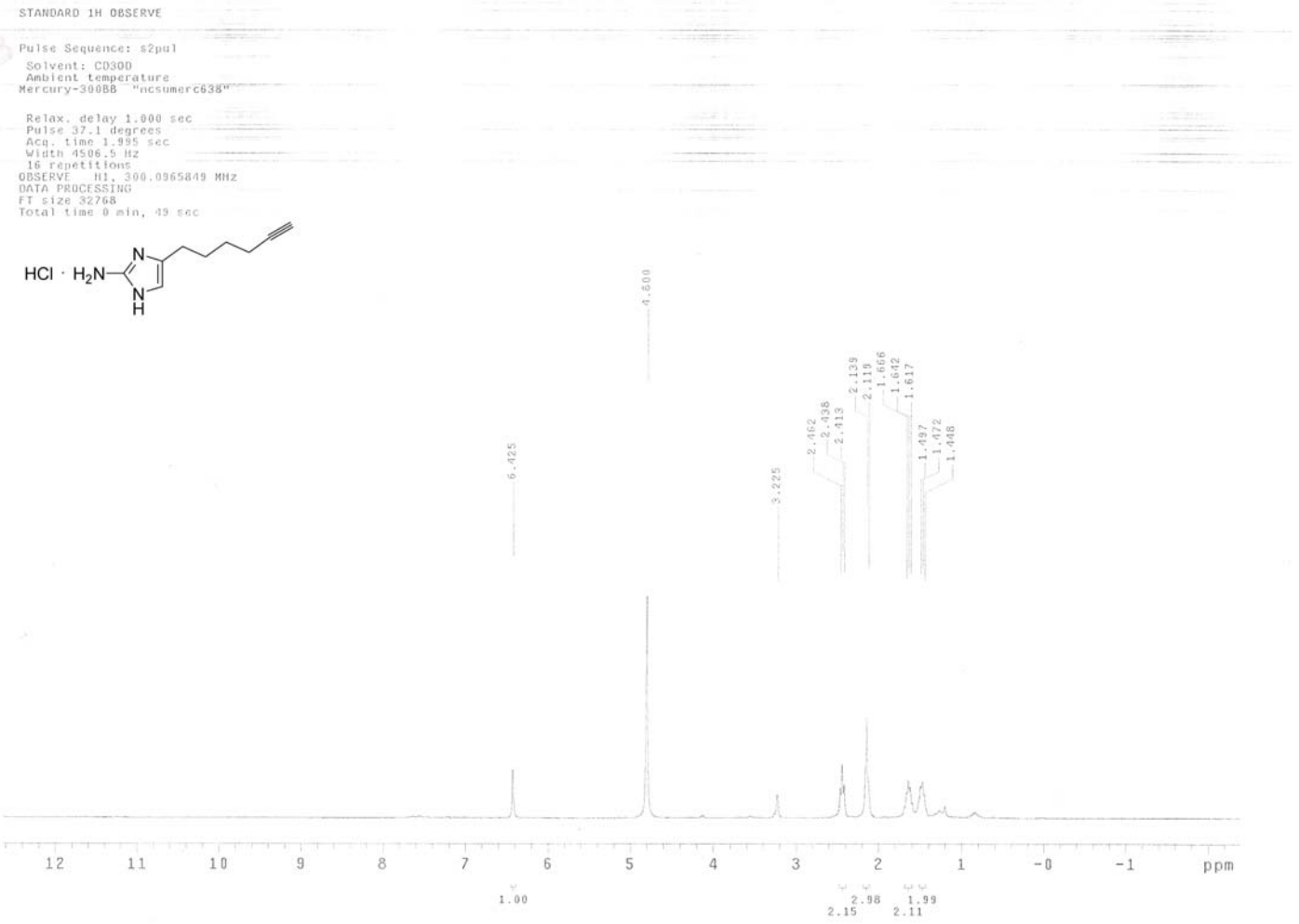

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 299.7930114 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
HCl · H2N
N
N
H
6.518
4.800
3.241
2.633
2.610
2.437
2.423
2.269
9
8
7
6
5
4
3
2
1
0 ppm
0.98
2.13
2.05
1.06

STANDARD 1H OBSERVE

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-300BB "ncsumerc300"

Relax. delay 1.000 sec
Pulse 43.4 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 299.7918101 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec

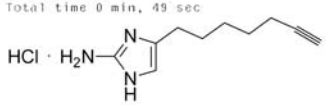


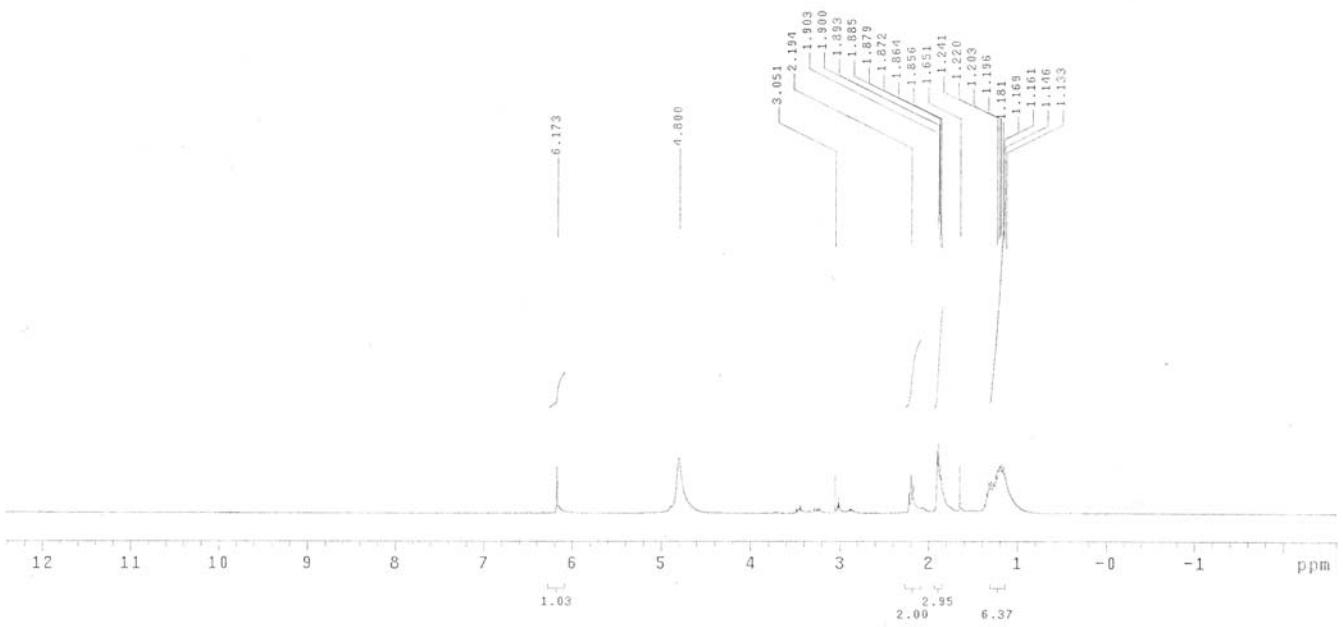

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0965849 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
HCl · H2N
N
N
H
4.600
6.425
3.225
2.462
2.436
2.413
2.139
2.119
1.666
1.642
1.617
1.497
1.472
1.448
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm
1.00
2.15
2.98
2.11
1.99

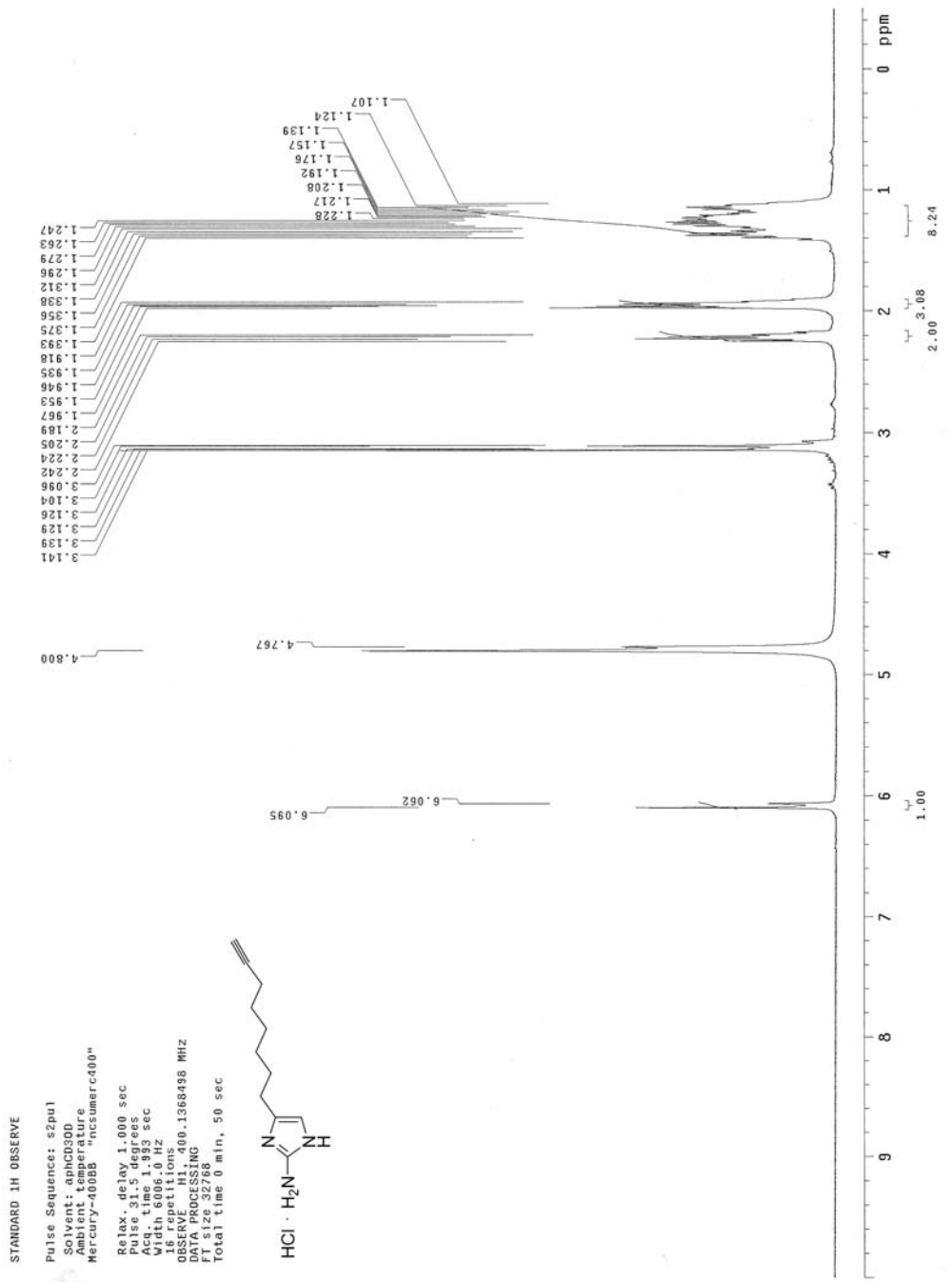
STANDARD 1H OBSERVE

Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc638"

Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0966493 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec



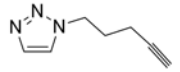


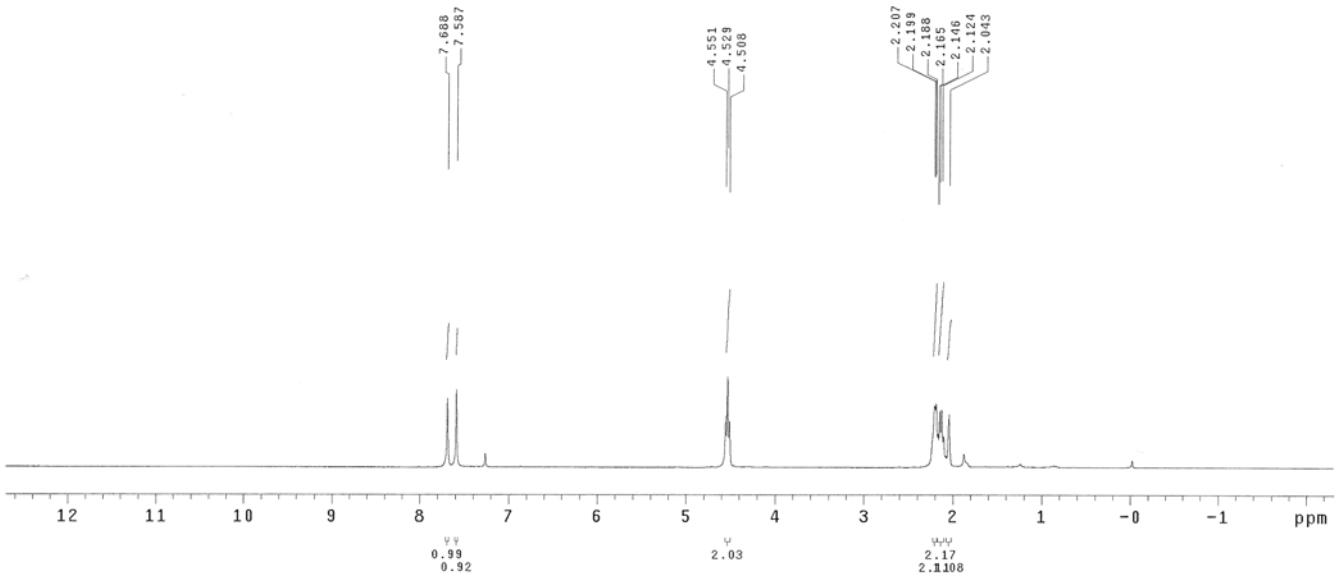

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: apHCD3OD
Ambient temperature
Mercury-400BB "ncsumerc400"
Relax. delay 1.000 sec
Pulse 31.5 degrees
Acq. time 1.993 sec
Width 6006.0 Hz
16 repetitions
OBSERVE H1, 400.1368498 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 50 sec
HCl · H2N
N
N
H
4.800
4.767
6.095
6.062
3.141
3.139
3.129
3.126
3.104
3.096
2.242
2.224
2.205
2.189
1.967
1.953
1.946
1.935
1.918
1.393
1.375
1.356
1.338
1.312
1.296
1.279
1.263
1.247
1.228
1.217
1.208
1.192
1.176
1.157
1.139
1.124
1.107
ppm
2.00
3.08
8.24
1.00

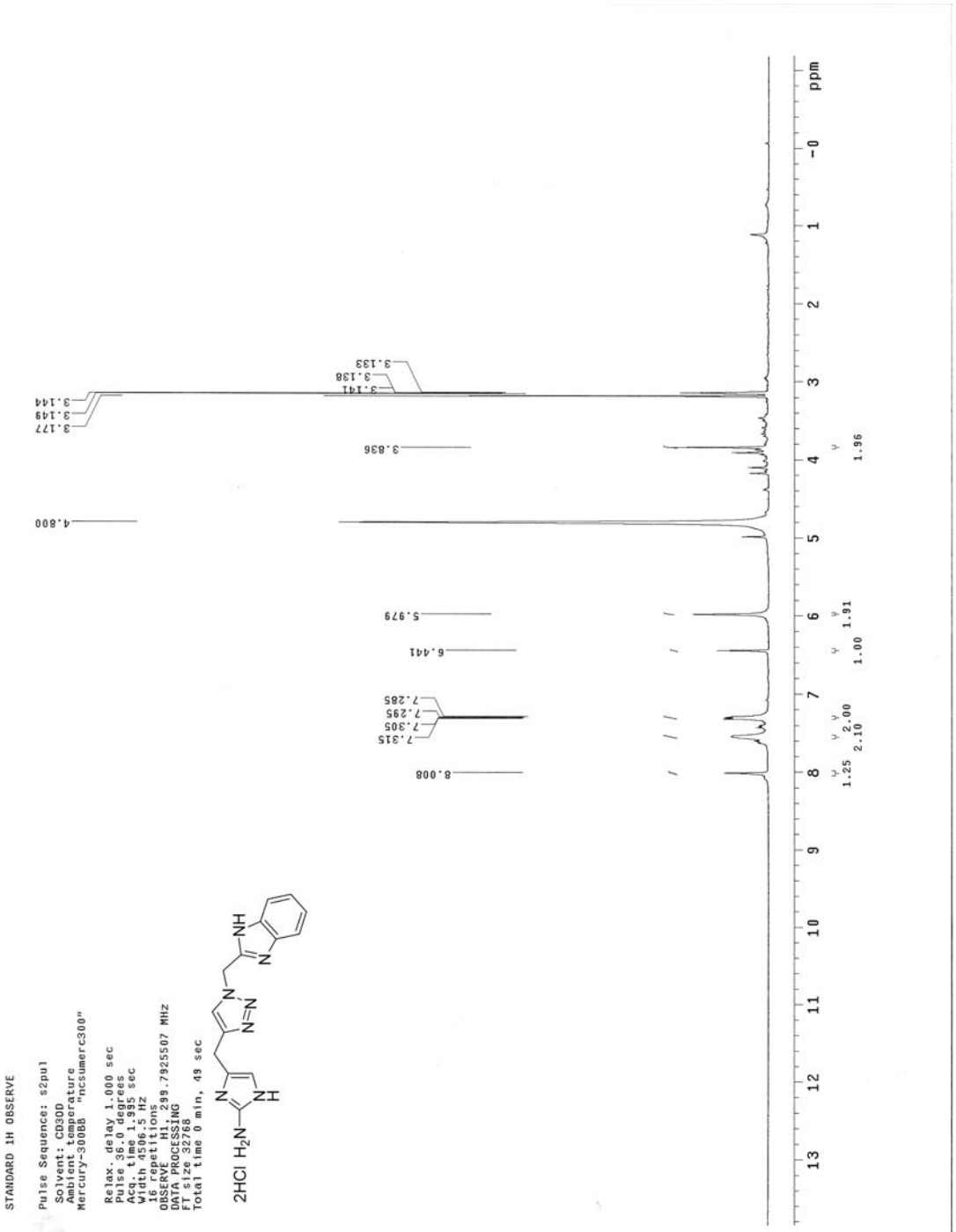
STANDARD 1H OBSERVE

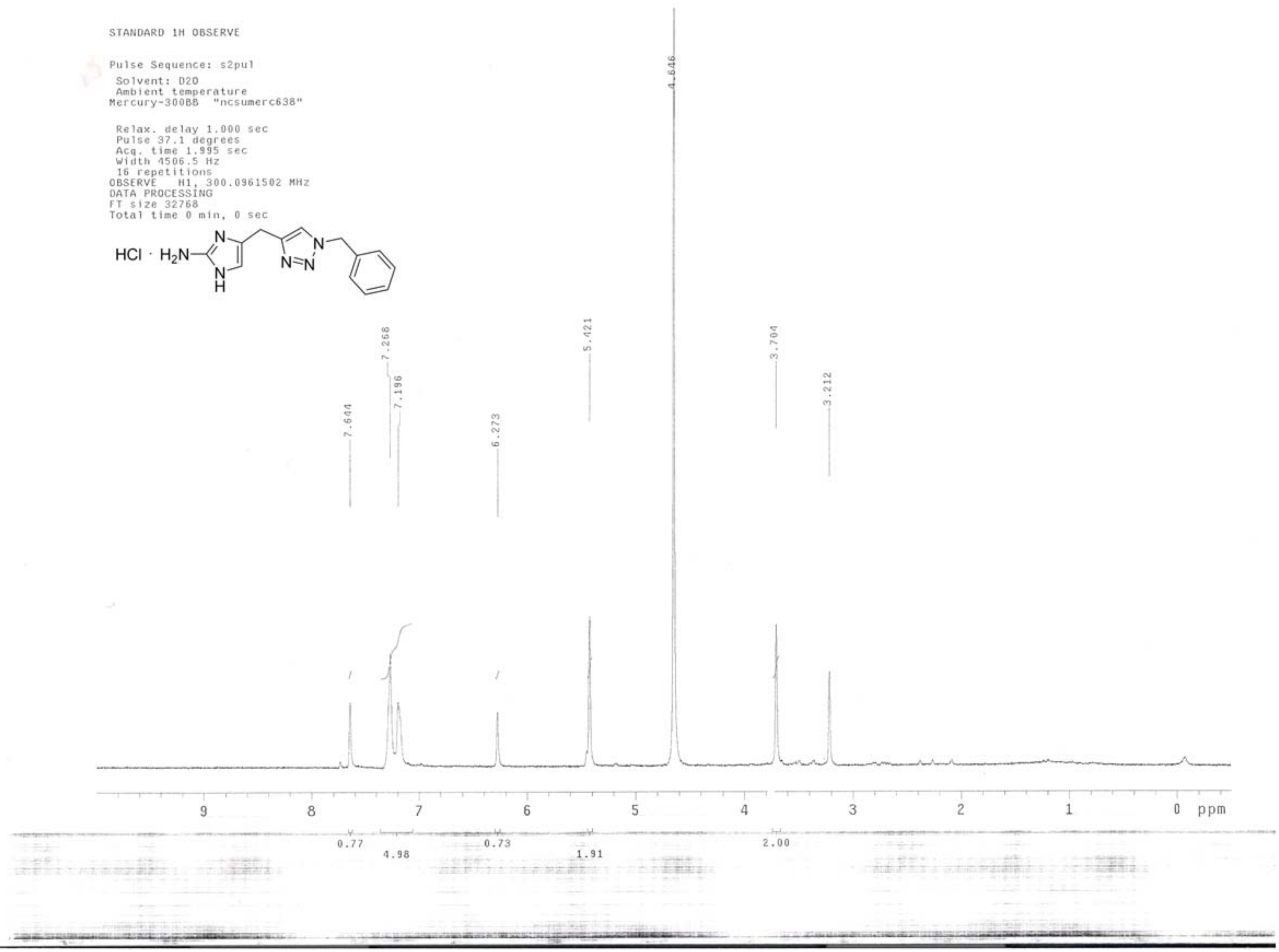
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-300BB "ncsumerc638"

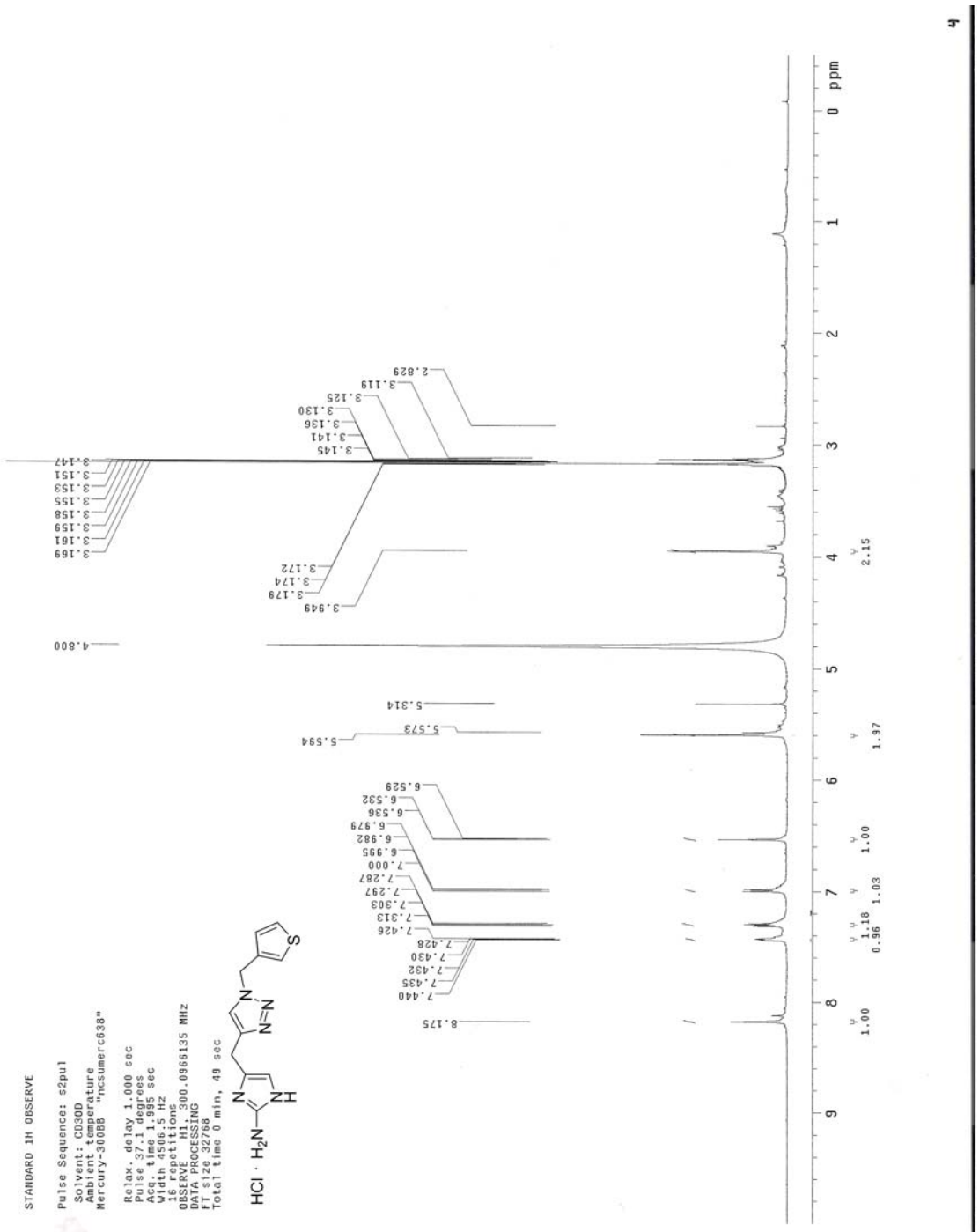
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0953789 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec



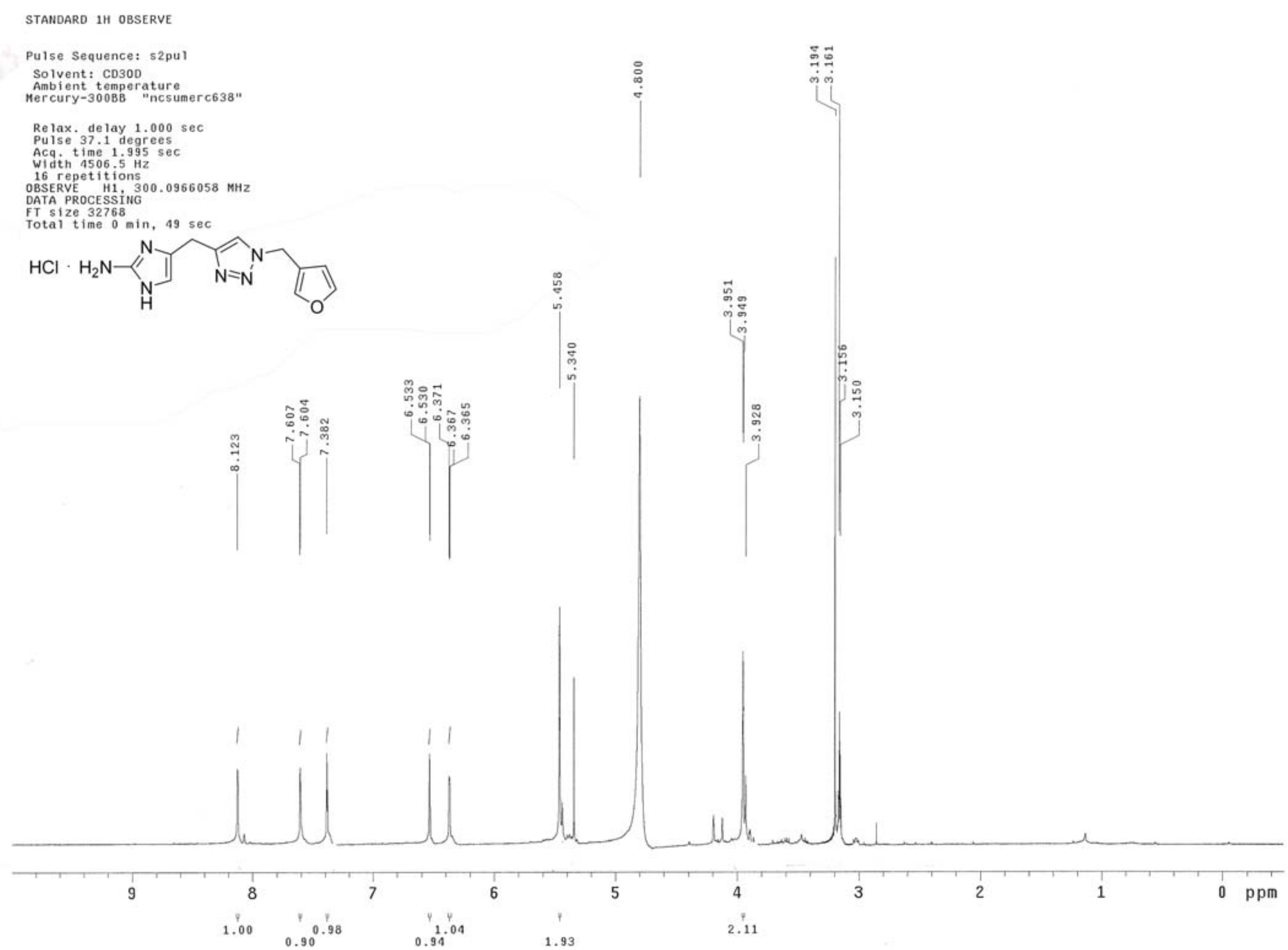



STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 4.855 sec
Width 4506.5 HZ
16 repetitions
OBSERVE H1, 299.7925507 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
2HCl H2N
3.177
3.149
3.144
3.141
3.138
3.133
4.800
3.836
5.979
6.441
7.315
7.305
7.295
7.285
8.008
1.25
2.00
2.10
1.00
1.91
1.96
ppm

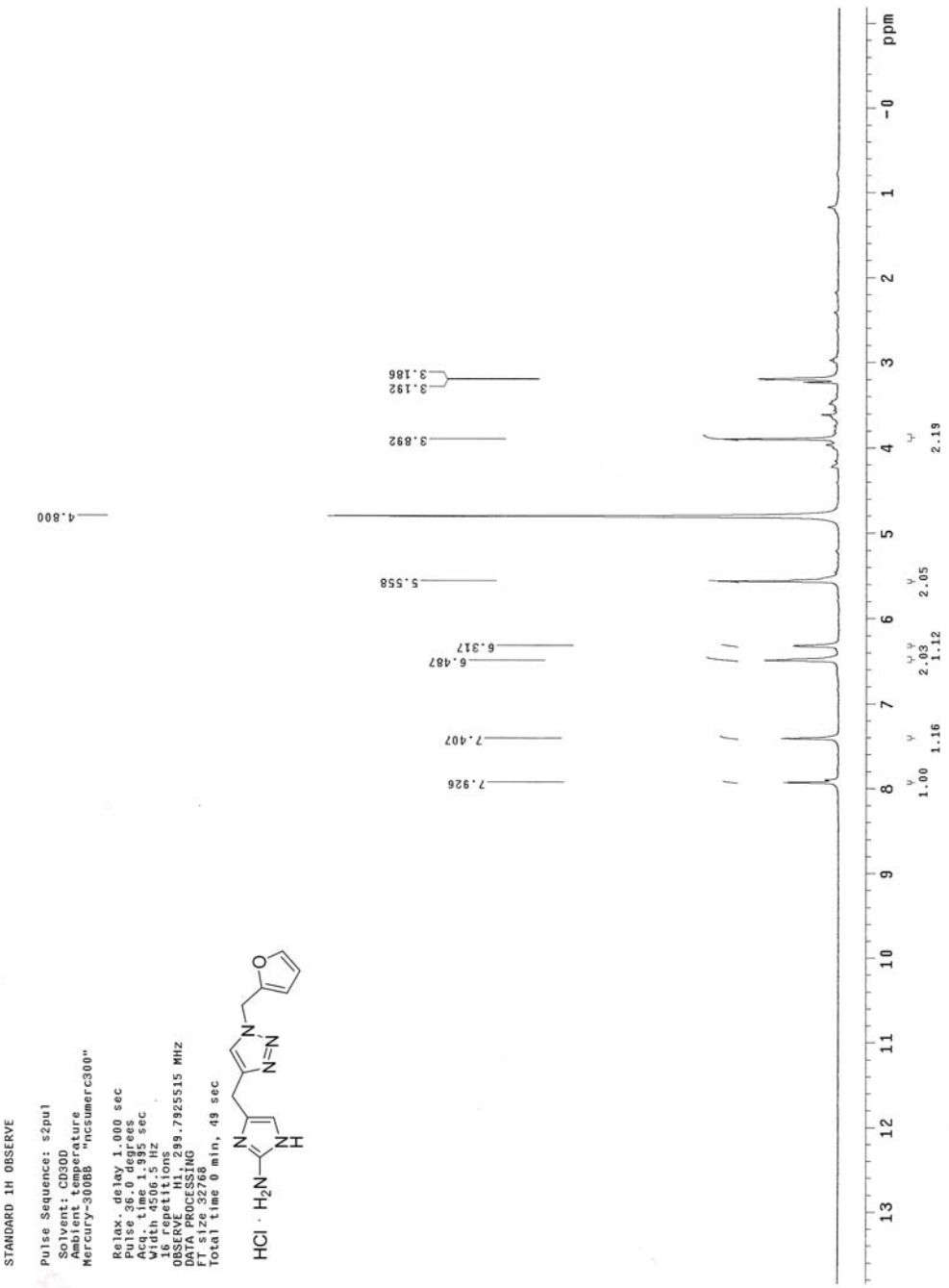

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: D2O
Ambient temperature
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0961502 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 0 sec
HCl · H2N
N
NH
N
N=N
7.644
7.268
7.196
6.273
5.421
4.646
3.704
3.212
9
8
7
6
5
4
3
2
1
0 ppm
0.77
4.98
0.73
1.91
2.00

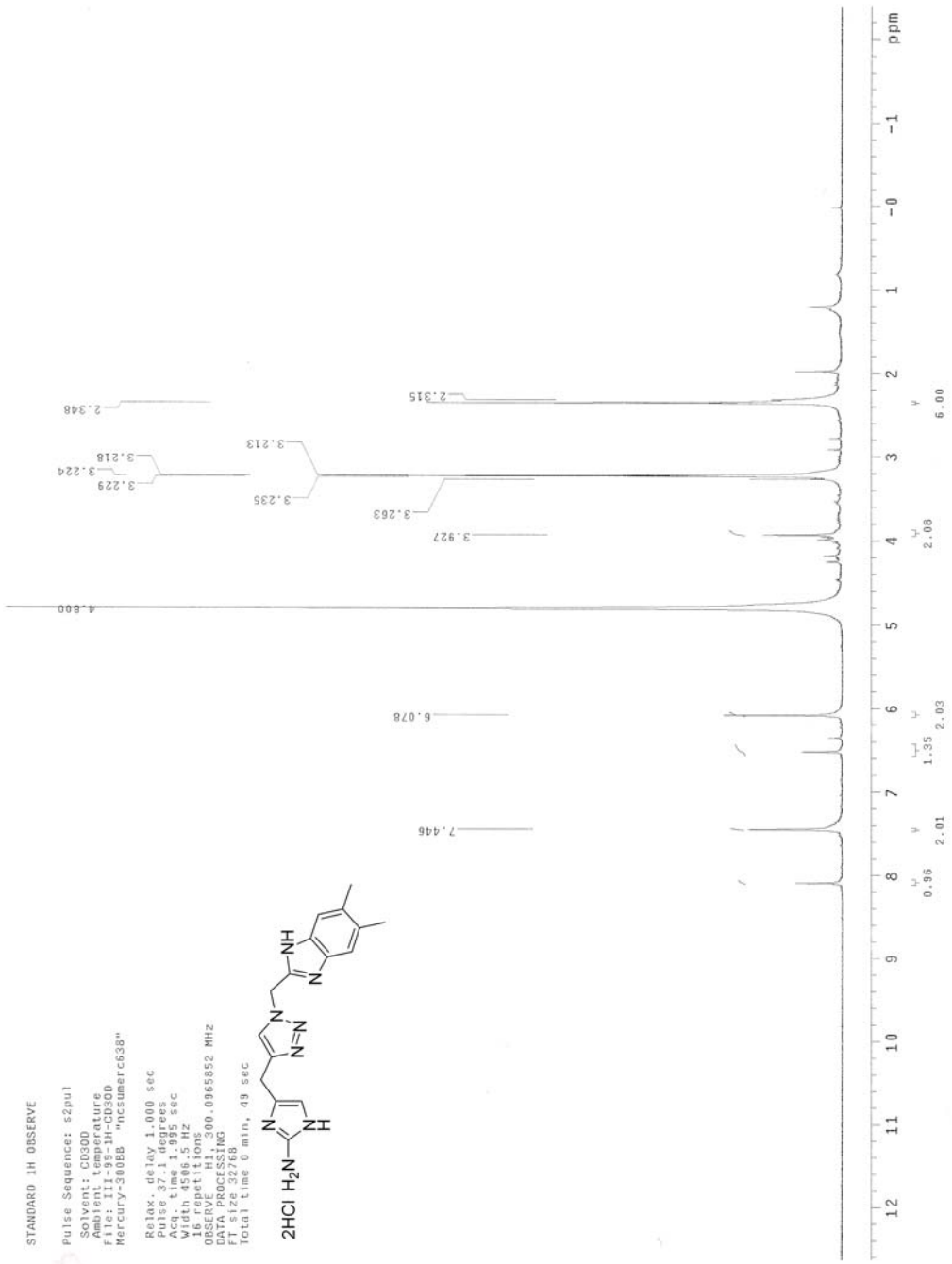

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0966135 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
HCl · H2N
S
N
N
N
H
3.169
3.161
3.159
3.158
3.155
3.153
3.151
3.147
4.800
3.949
3.179
3.174
3.172
3.145
3.141
3.136
3.130
3.125
3.119
2.829
5.314
5.573
5.594
6.529
6.532
6.536
6.979
6.982
6.995
7.000
7.287
7.297
7.303
7.313
7.426
7.428
7.430
7.432
7.435
7.440
8.175
ppm
2.15
1.97
1.00
1.03
0.96
1.18
1.00

4

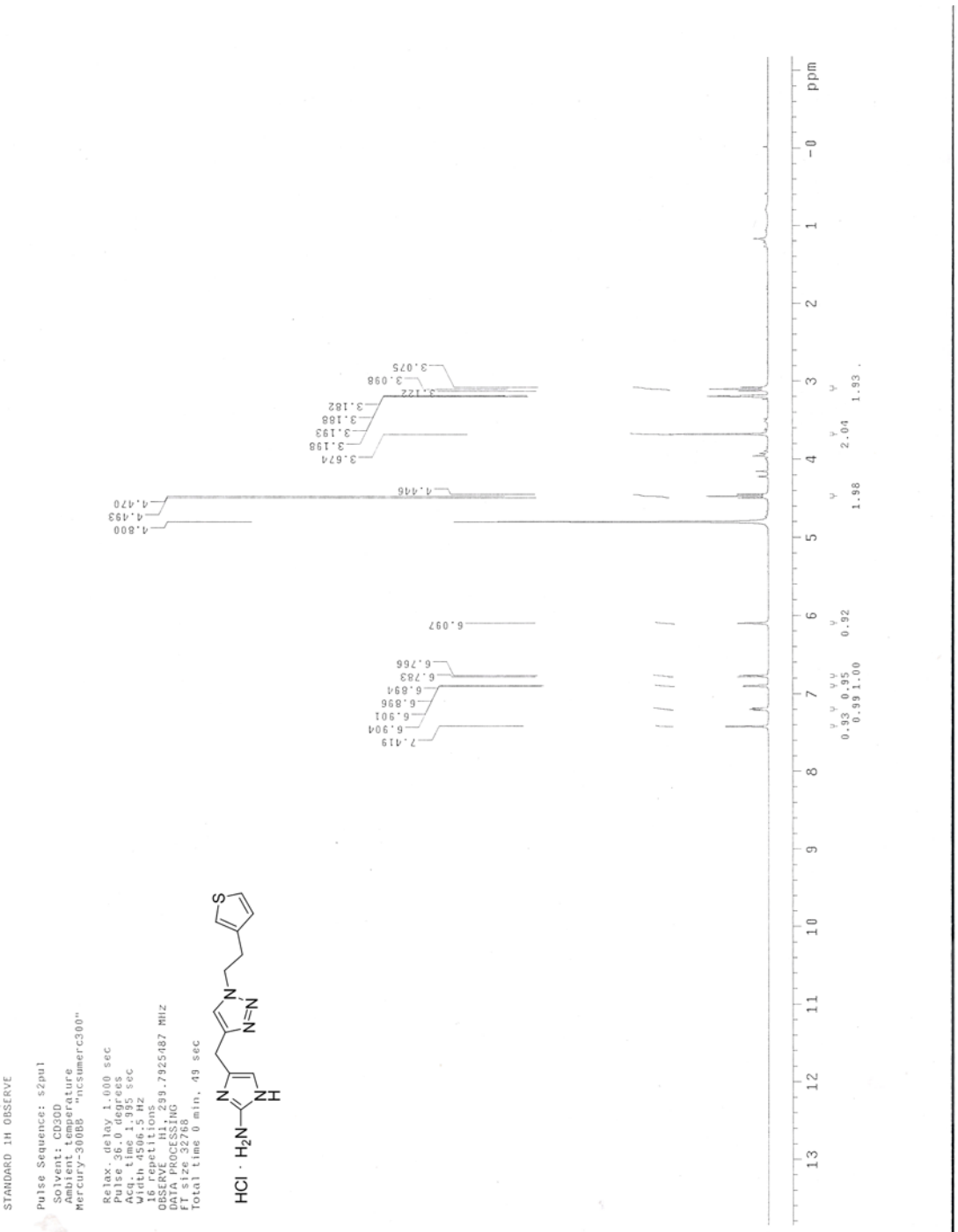

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0966058 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
HCl · H2N
8.123
7.607
7.604
7.382
6.533
6.530
6.371
6.367
6.365
5.458
5.340
4.800
3.951
3.949
3.928
3.194
3.161
3.156
3.150
9
8
7
6
5
4
3
2
1
0 ppm
1.00
0.90
0.98
0.94
1.04
1.93
2.11

6.

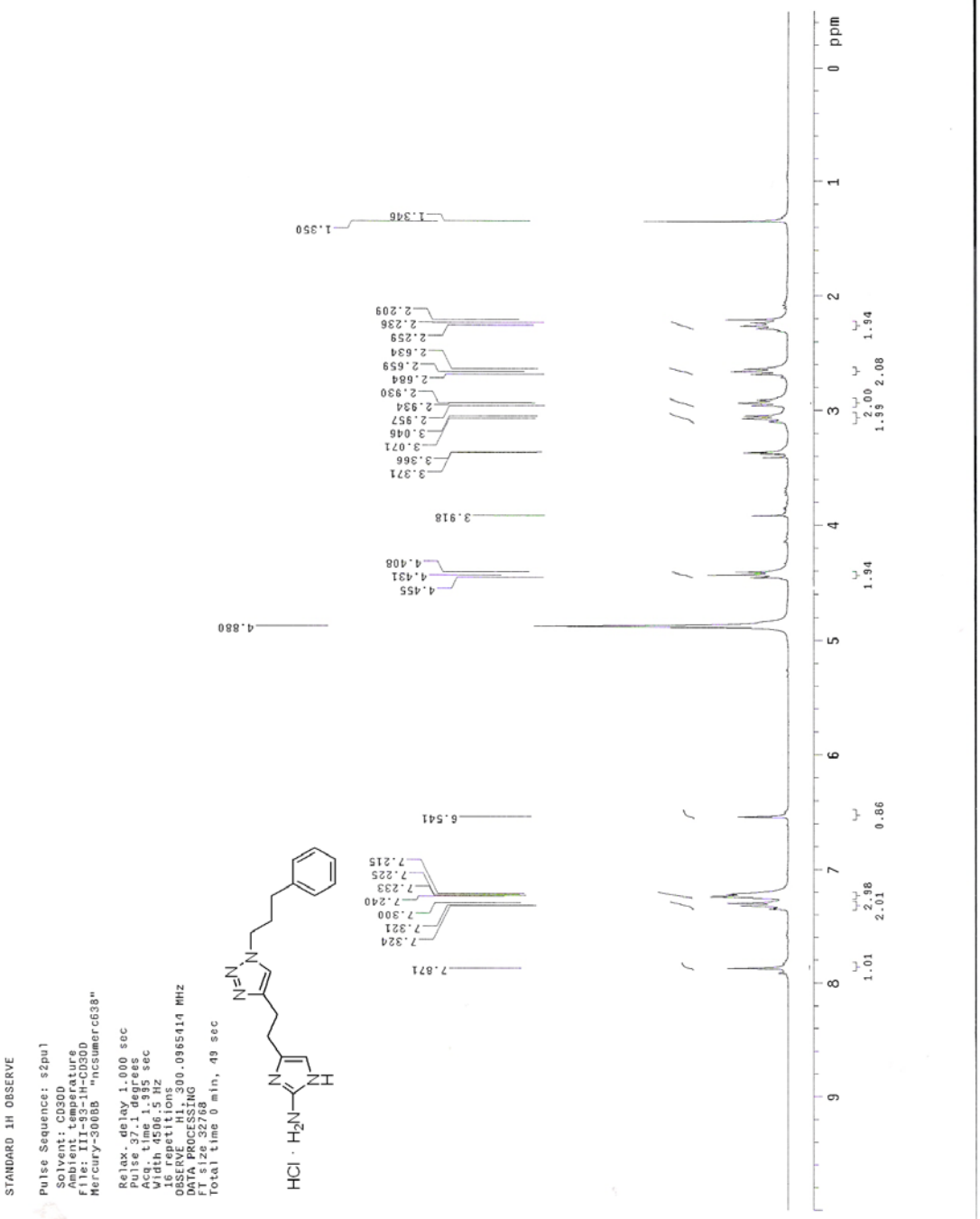

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 299.7925515 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
HCl · H2N
4.800
3.892
3.192
3.186
5.558
6.487
6.317
7.407
7.926
1.00
1.16
2.03
1.12
2.05
2.19
ppm

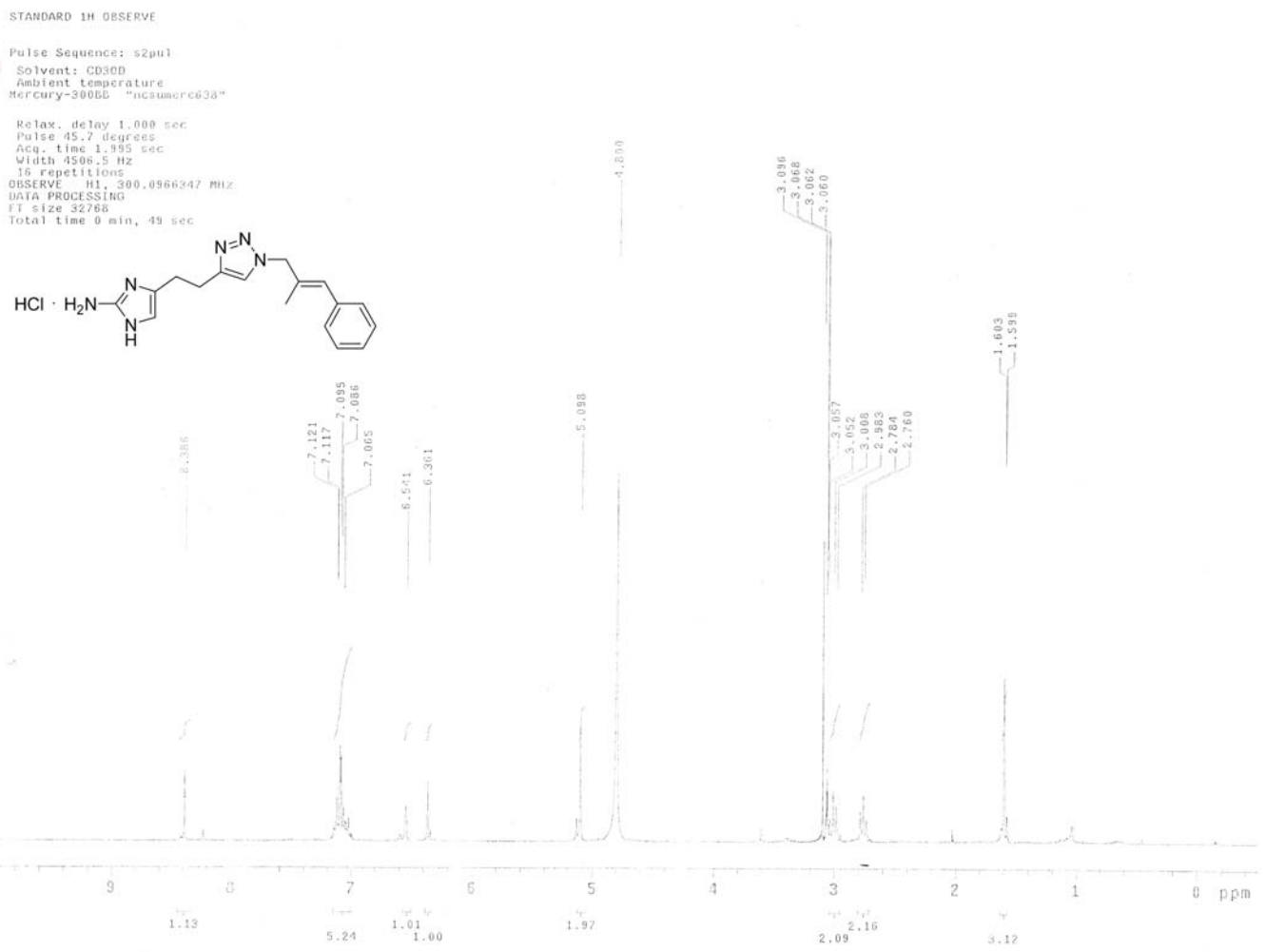

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
File: III-93-1H-CD3OD
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4516.5 Hz
16 repetitions
OBSERVE H1, 300.0965852 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
2HCl H2N
4.800
7.446
6.078
3.927
3.263
3.235
3.213
3.229
3.224
3.218
2.348
2.315
ppm
6.00
2.08
1.35
2.03
2.01
0.96

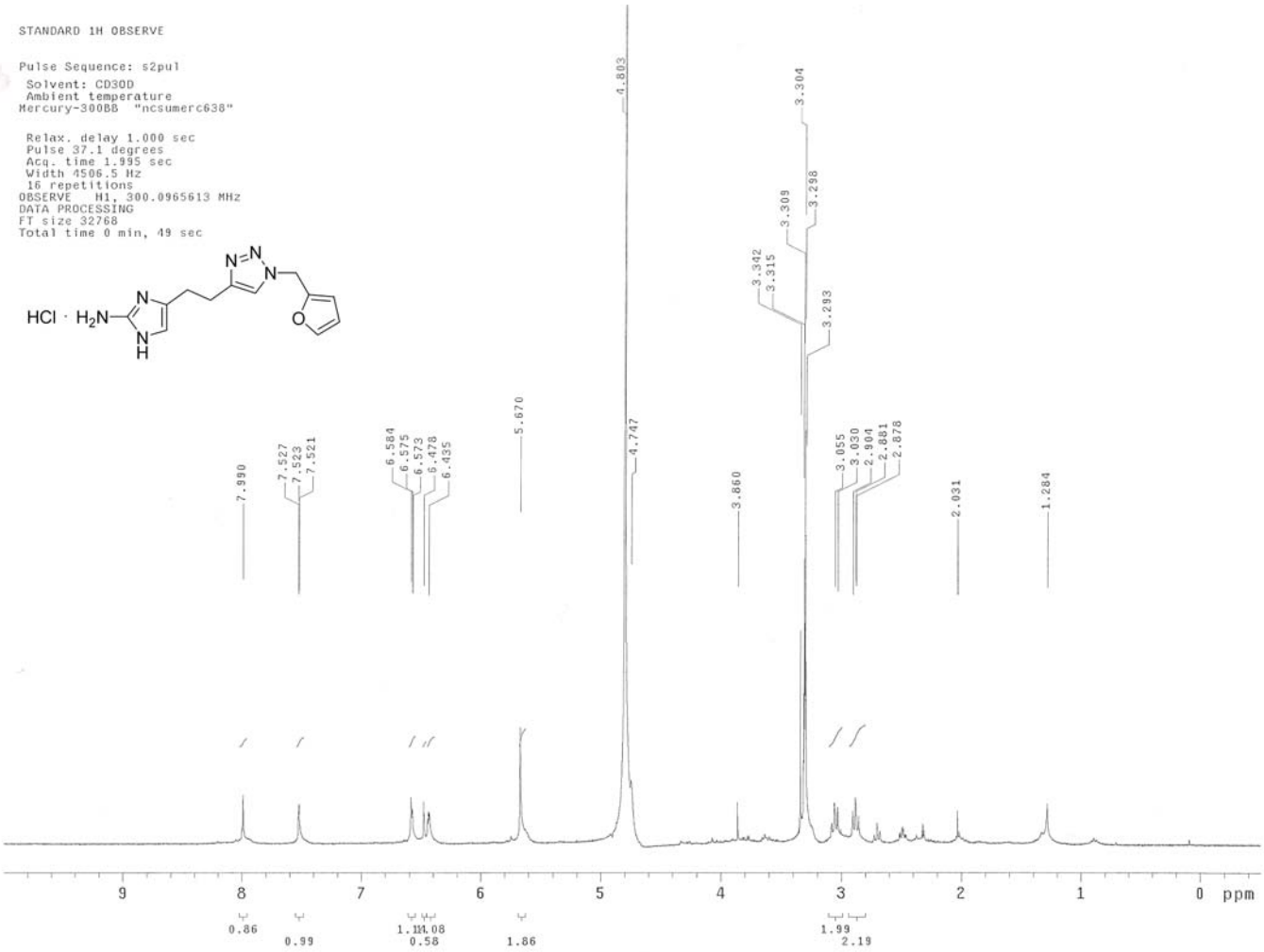
7.


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 299.7925487 MHz
DATA PROCESSING
FT size 32768
Total time 0 min. 49 sec
HCl · H2N
4.800
4.493
4.470
4.446
3.674
3.198
3.193
3.188
3.182
3.122
3.098
3.075
7.419
6.904
6.901
6.896
6.894
6.783
6.766
6.097
0.93
0.95
0.99
1.00
0.92
1.98
2.04
1.93
ppm

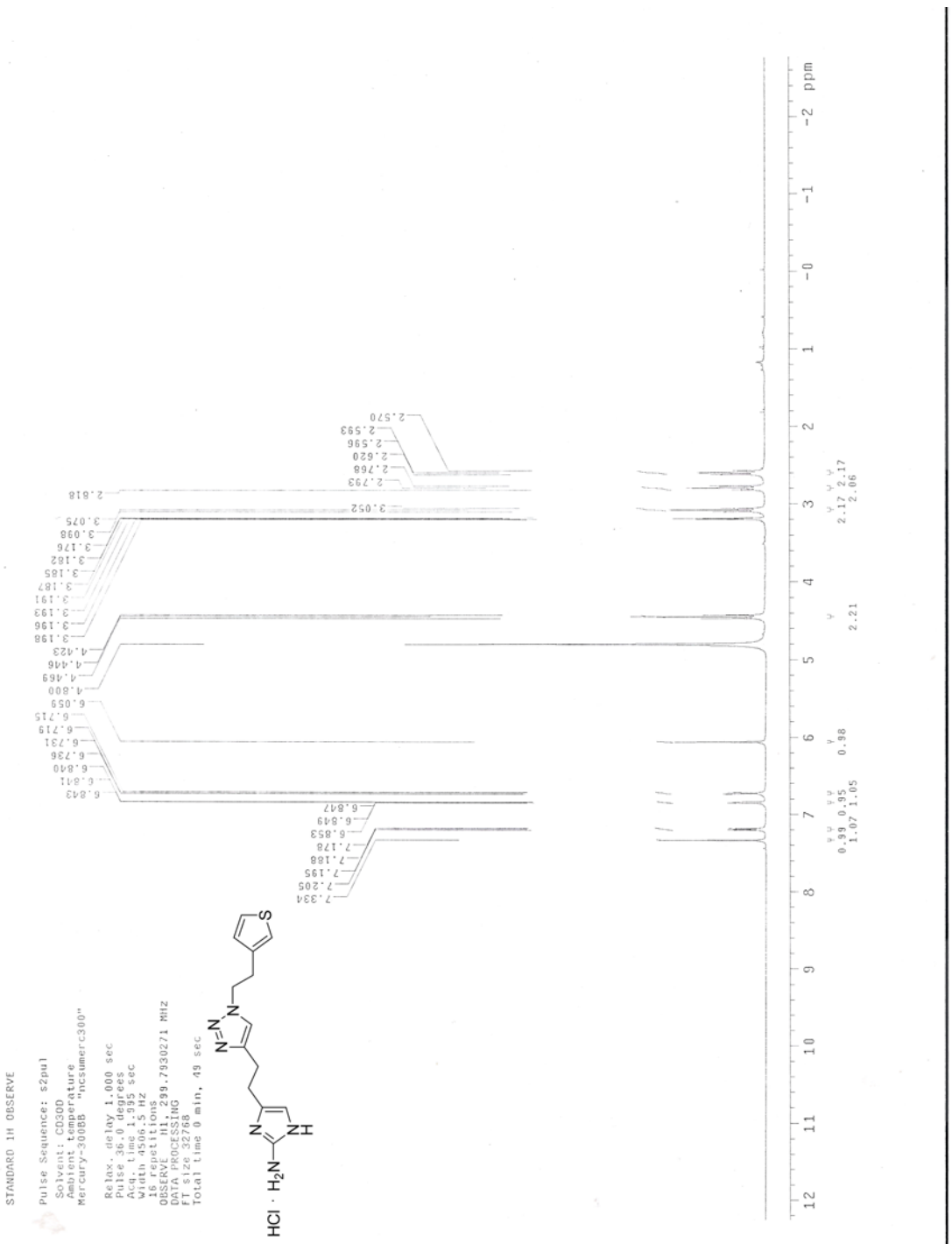
8.


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
File: II-eg-1H-CD3OD
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 37.0 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0965414 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
HCl · H2N
1.350
1.346
2.209
2.236
2.259
2.634
2.659
2.684
2.930
2.934
2.957
3.046
3.071
3.366
3.371
3.918
4.408
4.431
4.455
4.880
6.541
7.215
7.225
7.233
7.240
7.300
7.321
7.324
7.871
1.01
2.98
2.01
0.86
1.94
2.00
1.99
2.08
1.94
ppm

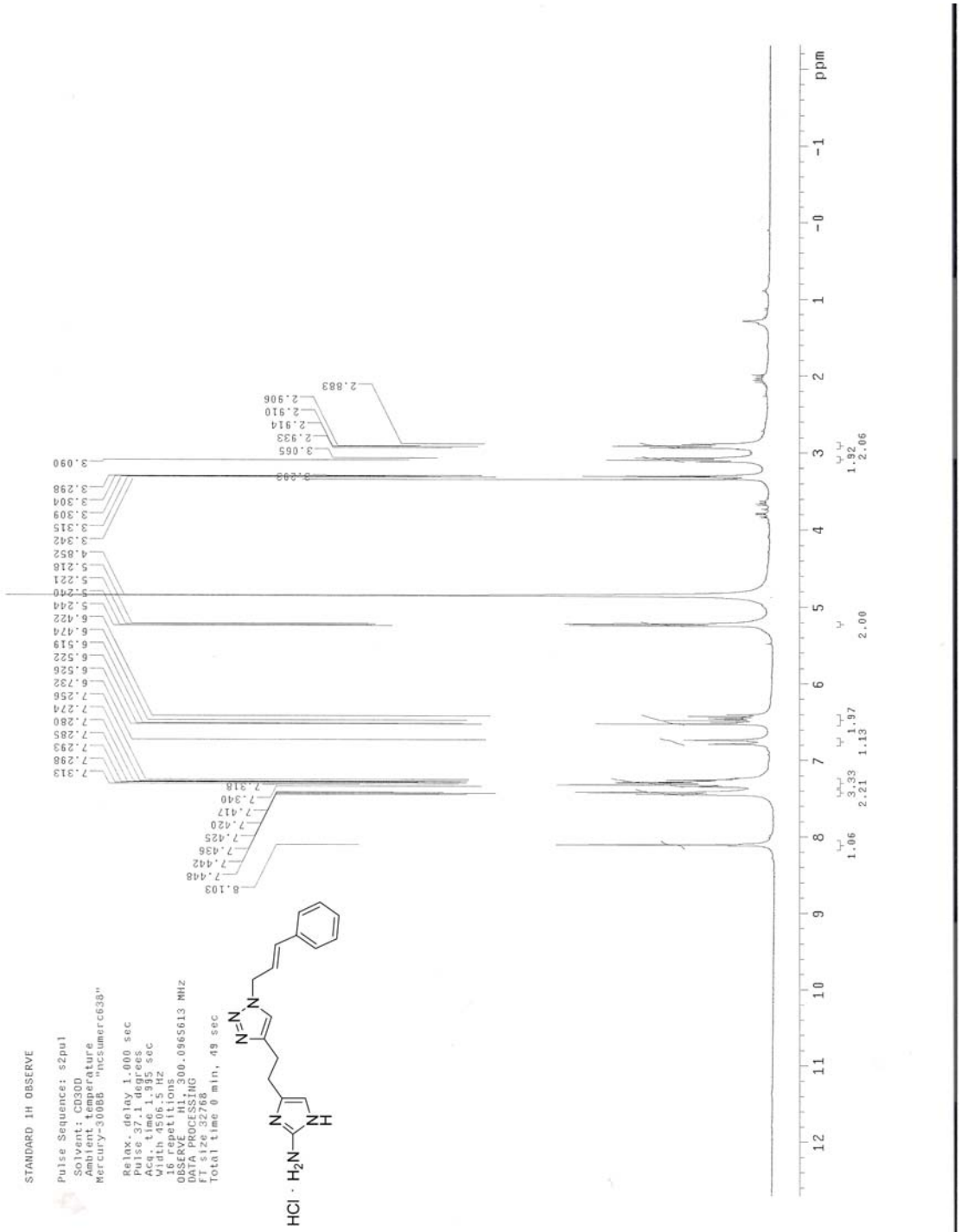

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ucsumerc638"
Relax. delay 1.000 sec
Pulse 45.7 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0966347 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
HCl · H2N
8.366
7.121
7.117
7.095
7.086
7.065
6.541
6.361
5.098
4.809
3.096
3.068
3.062
3.060
3.057
3.052
3.008
2.983
2.784
2.760
1.603
1.598
9
8
7
6
5
4
3
2
1
0 ppm
1.13
5.24
1.01
1.00
1.97
2.09
2.16
3.12

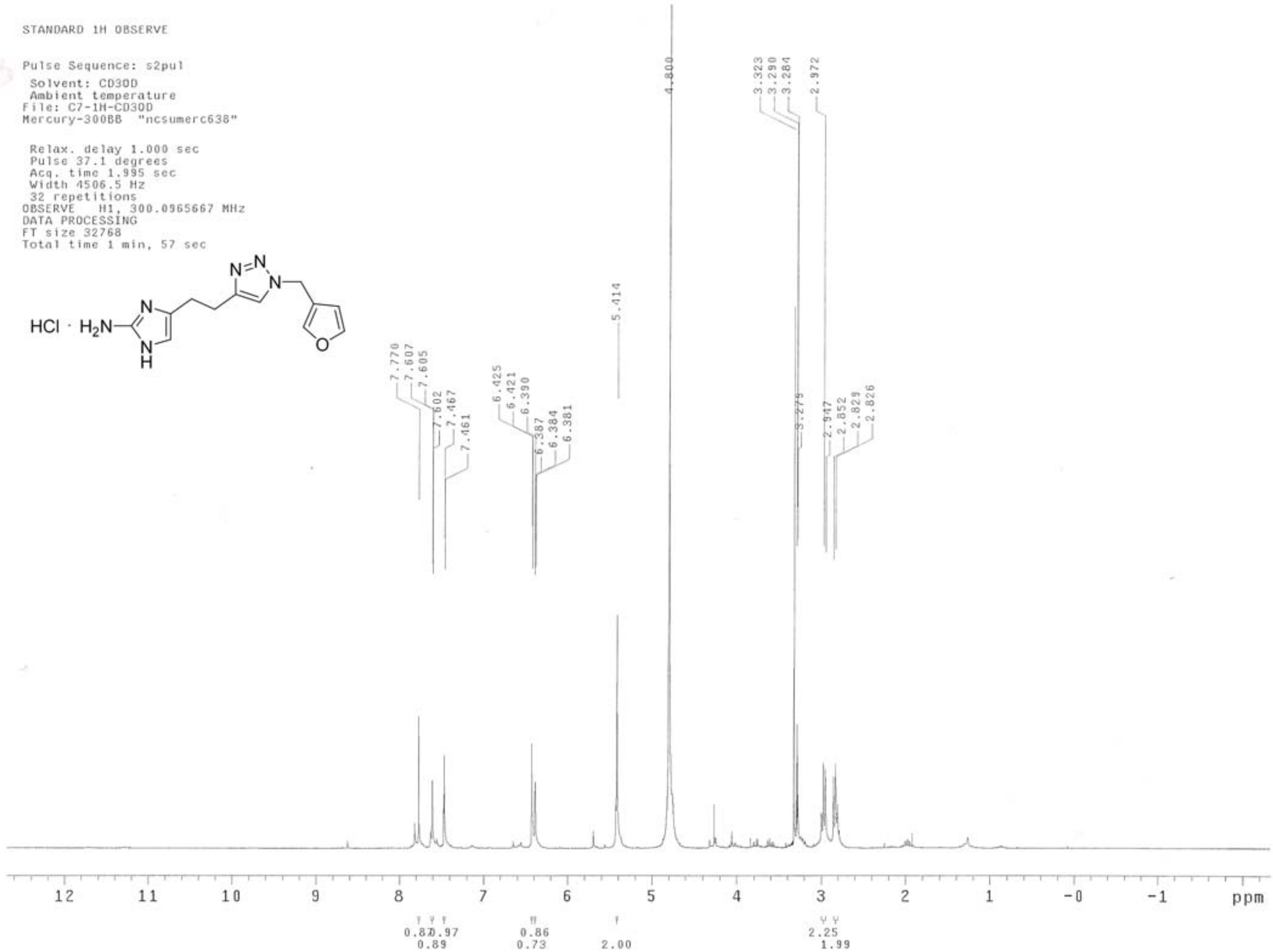

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0965613 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
HCl · H2N
7.990
7.527
7.523
7.521
6.584
6.575
6.573
6.478
6.435
5.670
4.883
4.747
3.860
3.342
3.315
3.309
3.304
3.298
3.293
3.055
3.030
2.904
2.881
2.878
2.031
1.284
9
8
7
6
5
4
3
2
1
0 ppm
0.86
0.99
1.11
1.08
0.58
1.86
1.99
2.19

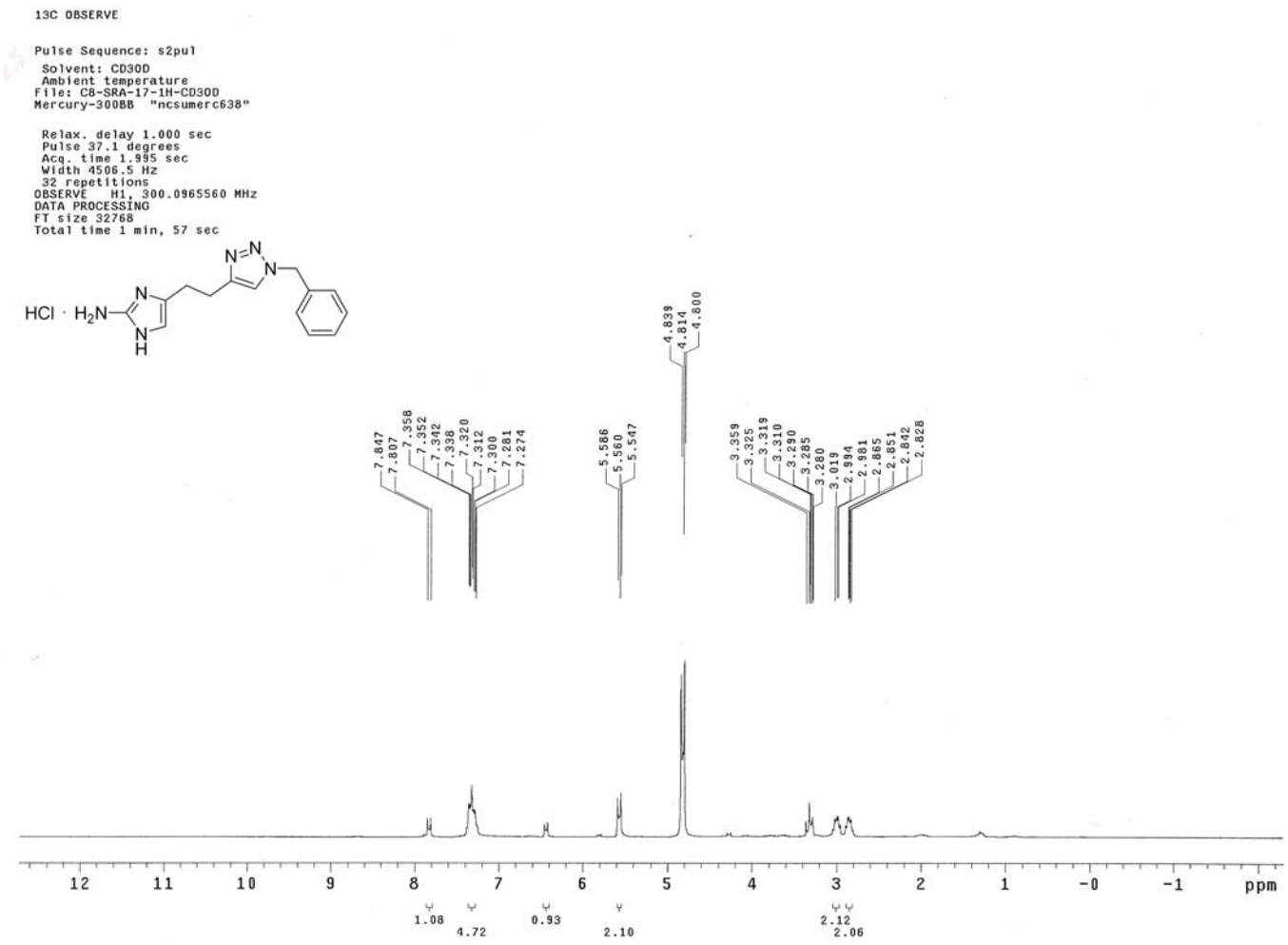
9.


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 4.095 sec
Width 4506.5 HZ
16 repetitions
OBSERVE H1, 299.7930271 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
HCl · H2N
ppm

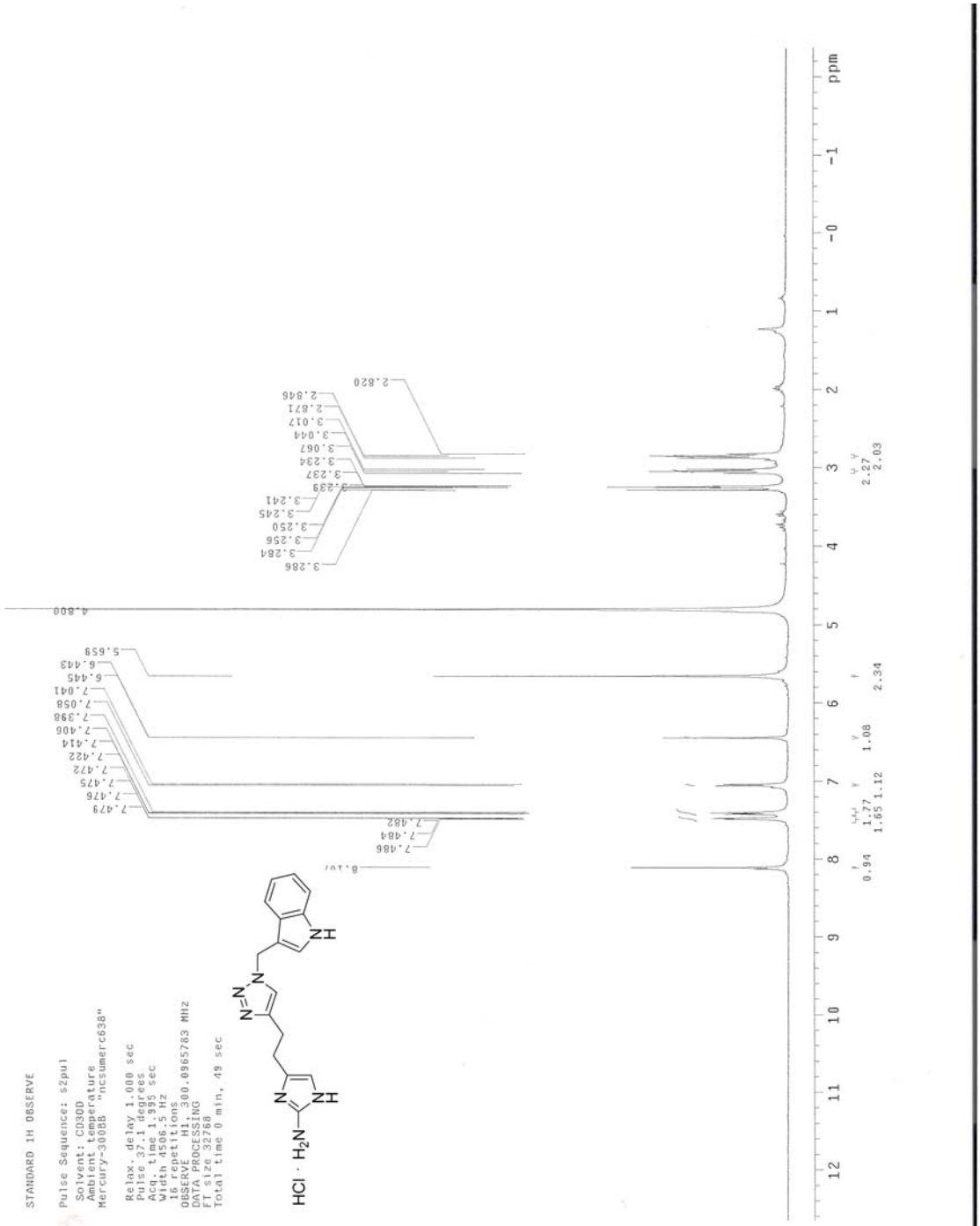
10.


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0965613 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
HCl · H2N
ppm


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
File: C7-1H-CD3OD
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
32 repetitions
OBSERVE H1, 300.0965667 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 57 sec
HCl · H2N
N
H
N
N=N
N
O
7.770
7.607
7.605
7.602
7.467
7.461
6.425
6.421
6.390
6.387
6.384
6.381
5.414
4.800
3.323
3.290
3.284
3.279
2.972
2.947
2.852
2.829
2.826
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm
0.87
0.97
0.89
0.86
0.73
2.00
2.25
1.99


13C OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
File: C8-SRA-17-1H-CD3OD
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
32 repetitions
OBSERVE H1, 300.0965560 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 57 sec
HCl · H2N
7.847
7.807
7.358
7.352
7.342
7.338
7.320
7.312
7.300
7.281
7.274
5.586
5.560
5.547
4.839
4.814
4.800
3.359
3.325
3.319
3.310
3.290
3.285
3.280
3.019
2.994
2.981
2.865
2.851
2.842
2.828
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm
1.08
4.72
0.93
2.10
2.12
2.06

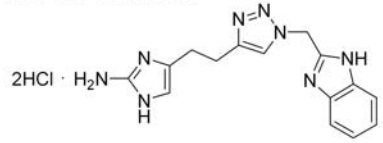
11.

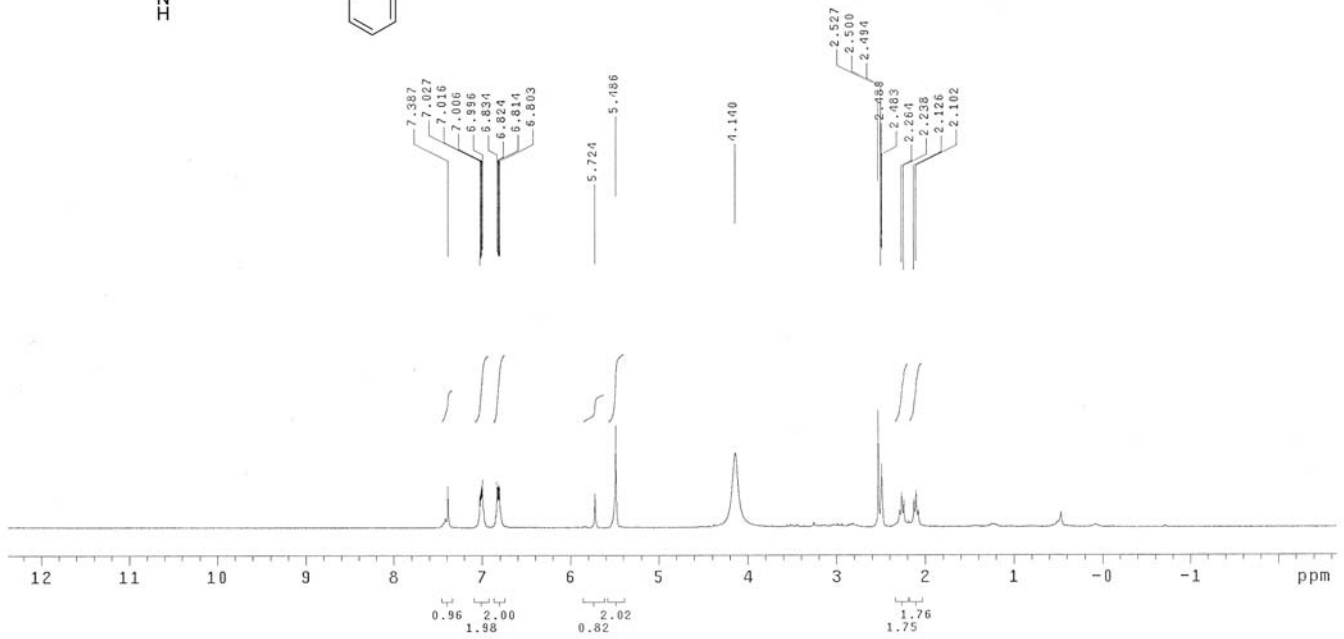

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0965783 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
HCl · H2N
ppm

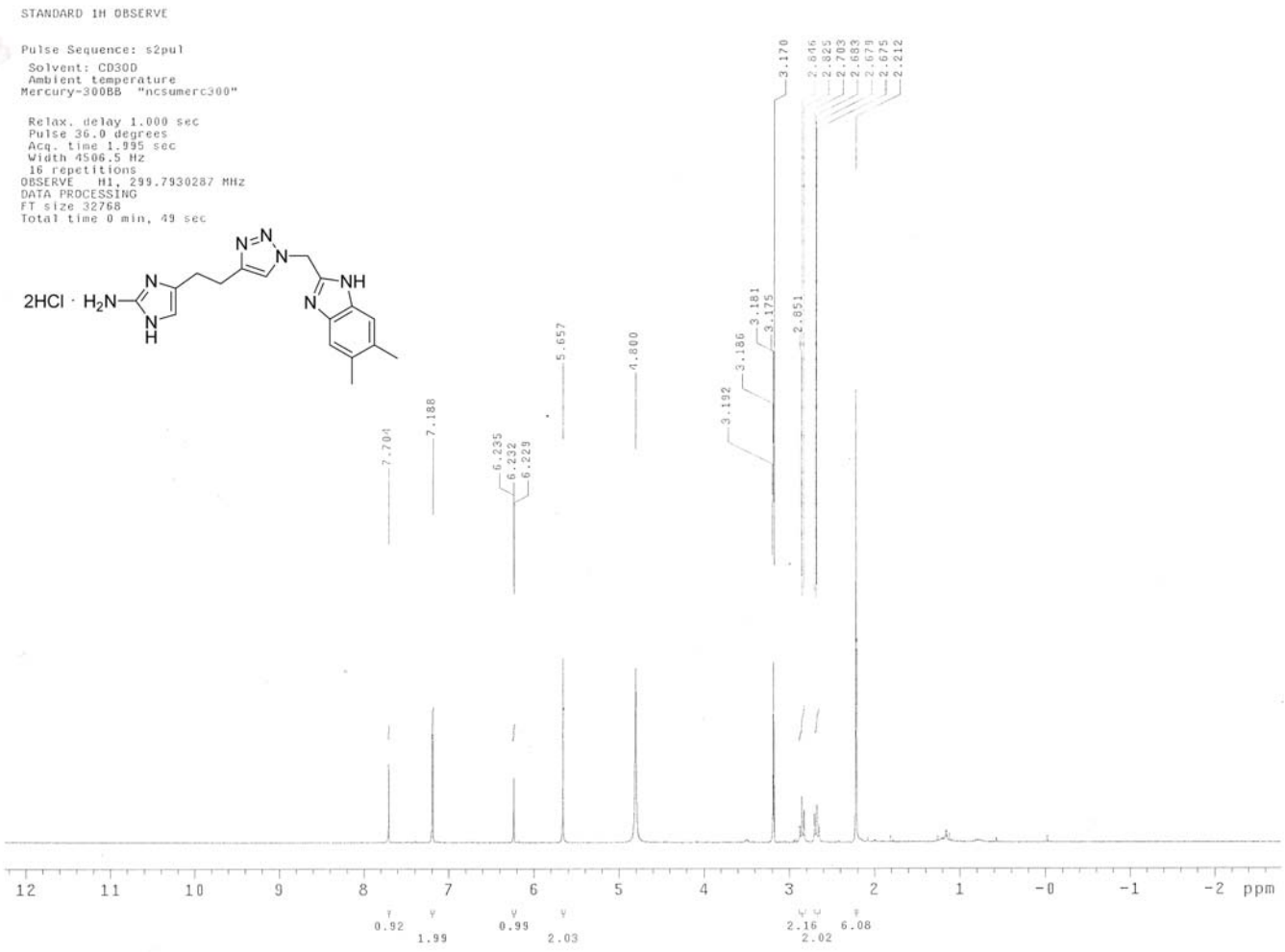
STANDARD 1H OBSERVE

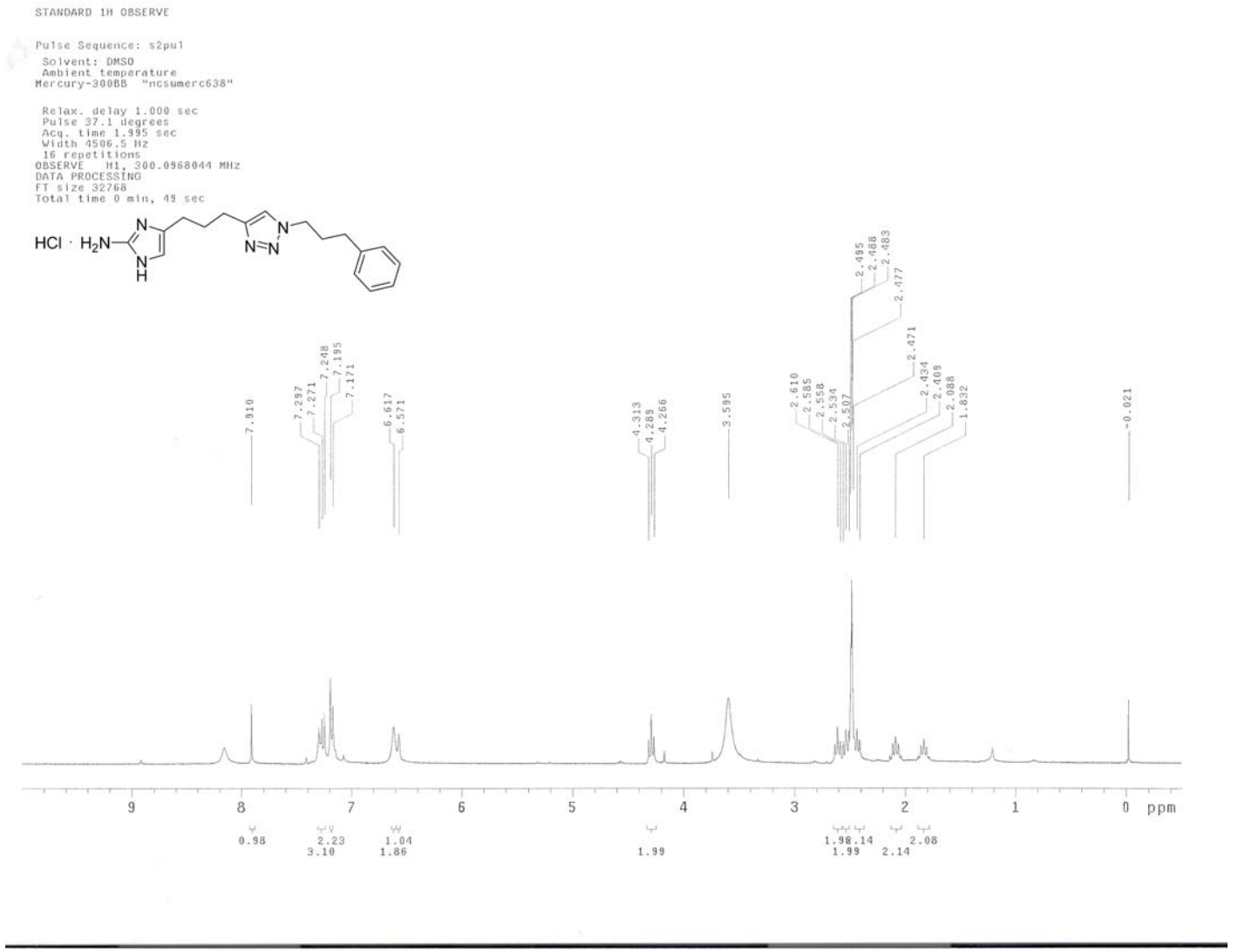
Pulse Sequence: s2pul
Solvent: DMSO
Ambient temperature
File: C11-1H-CD3OD
Mercury-300BB "ncsumerc300"

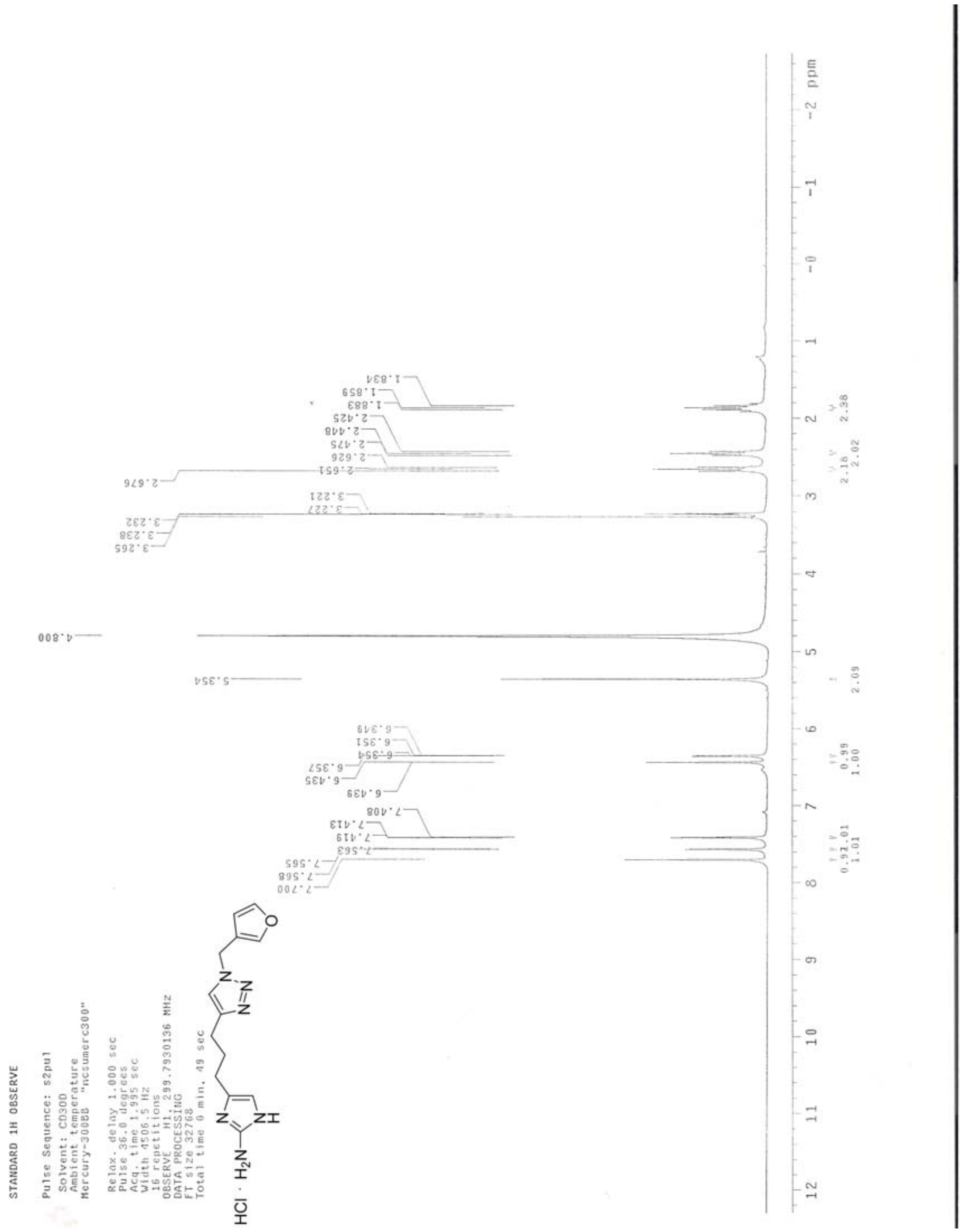
Relax. delay 1.000 sec
Pulse 35.0 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 299.7932341 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec






STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 299.7930287 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
2HCl · H2N
7.704
7.188
6.235
6.232
6.229
5.657
4.800
3.192
3.186
3.181
3.175
3.170
2.851
2.846
2.825
2.703
2.683
2.679
2.675
2.212
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
-2
ppm
0.92
1.99
0.99
2.03
2.16
2.02
6.08

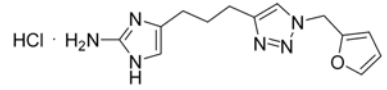

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: DMSO
Ambient temperature
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0968044 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
HCl · H2N
N
N
H
N=N
7.910
7.297
7.271
7.248
7.195
7.171
6.617
6.571
4.313
4.289
4.266
3.595
2.610
2.585
2.558
2.534
2.507
2.495
2.488
2.483
2.477
2.471
2.434
2.409
2.088
1.832
-0.021
9
8
7
6
5
4
3
2
1
0 ppm
0.98
2.23
3.10
1.04
1.86
1.99
1.98
1.99
14
2.14
2.08

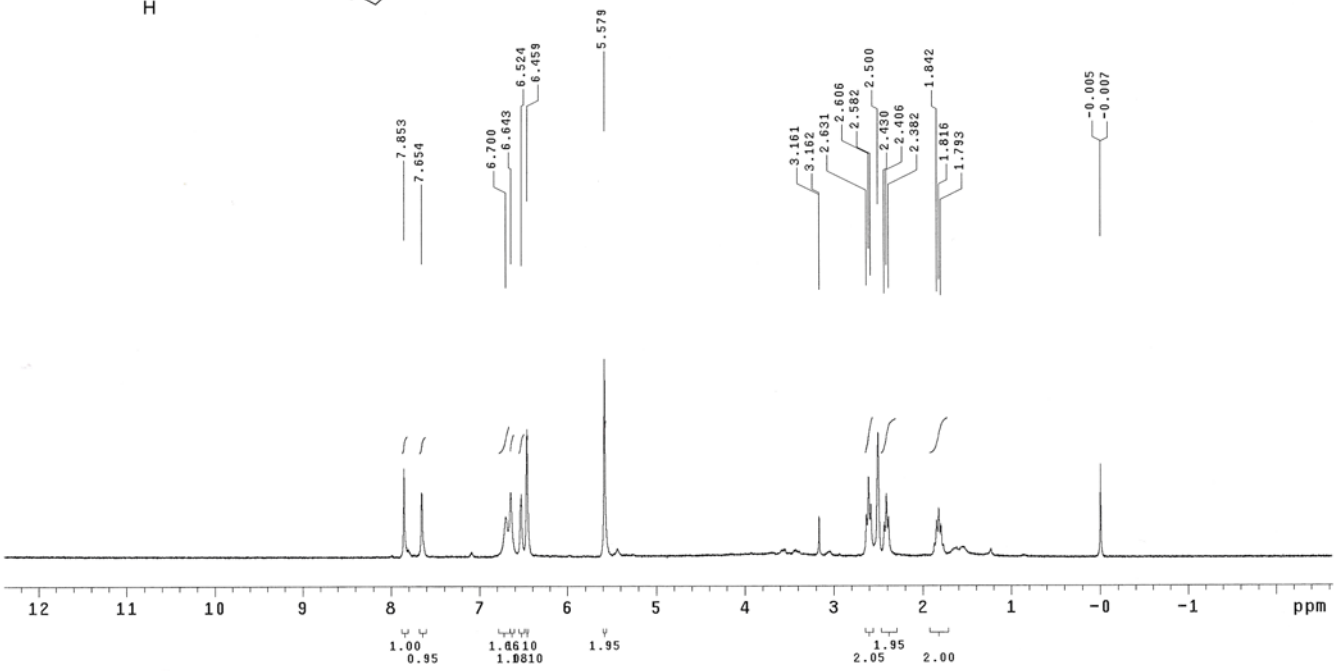

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 299.7930136 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
ppm

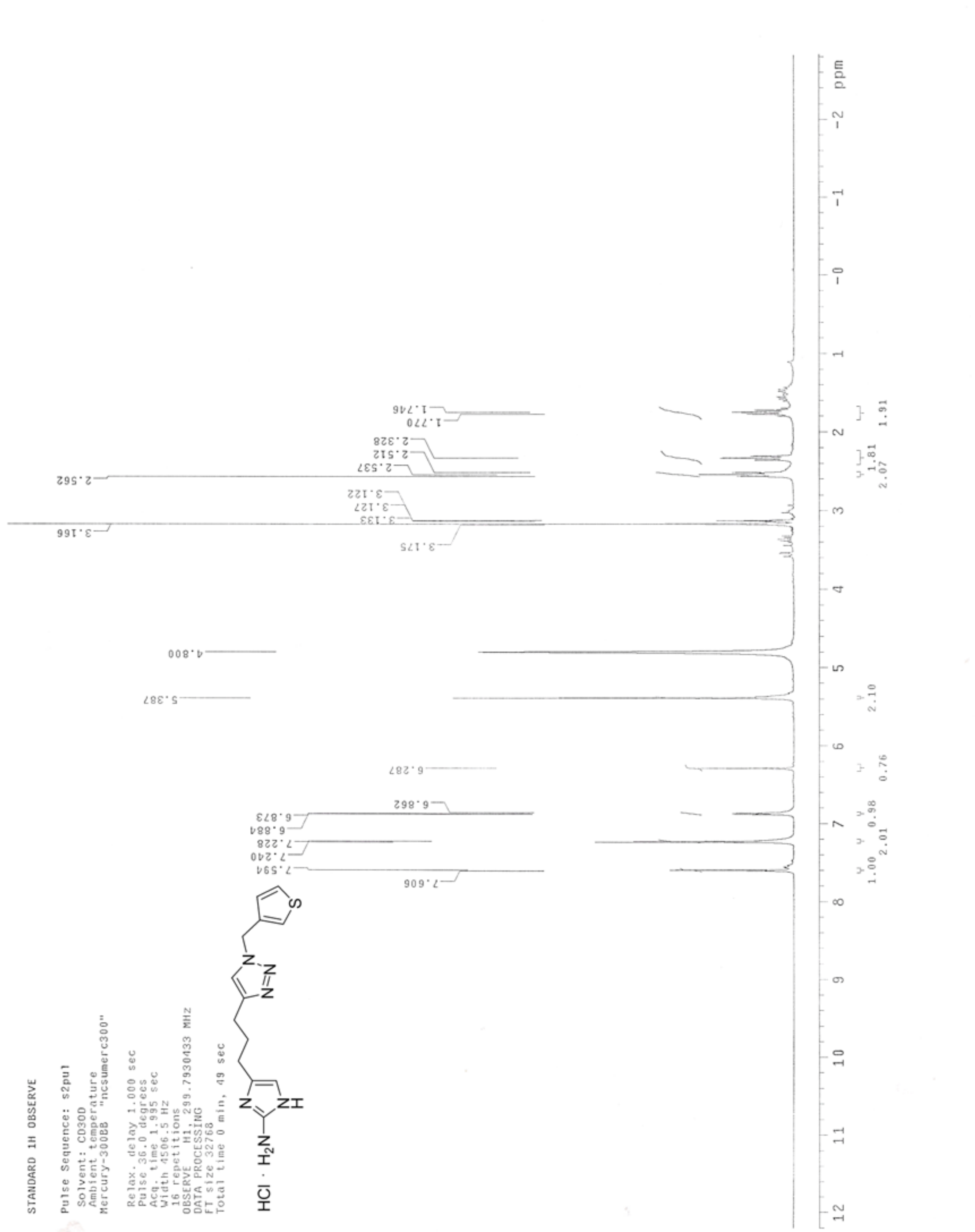
STANDARD 1H OBSERVE

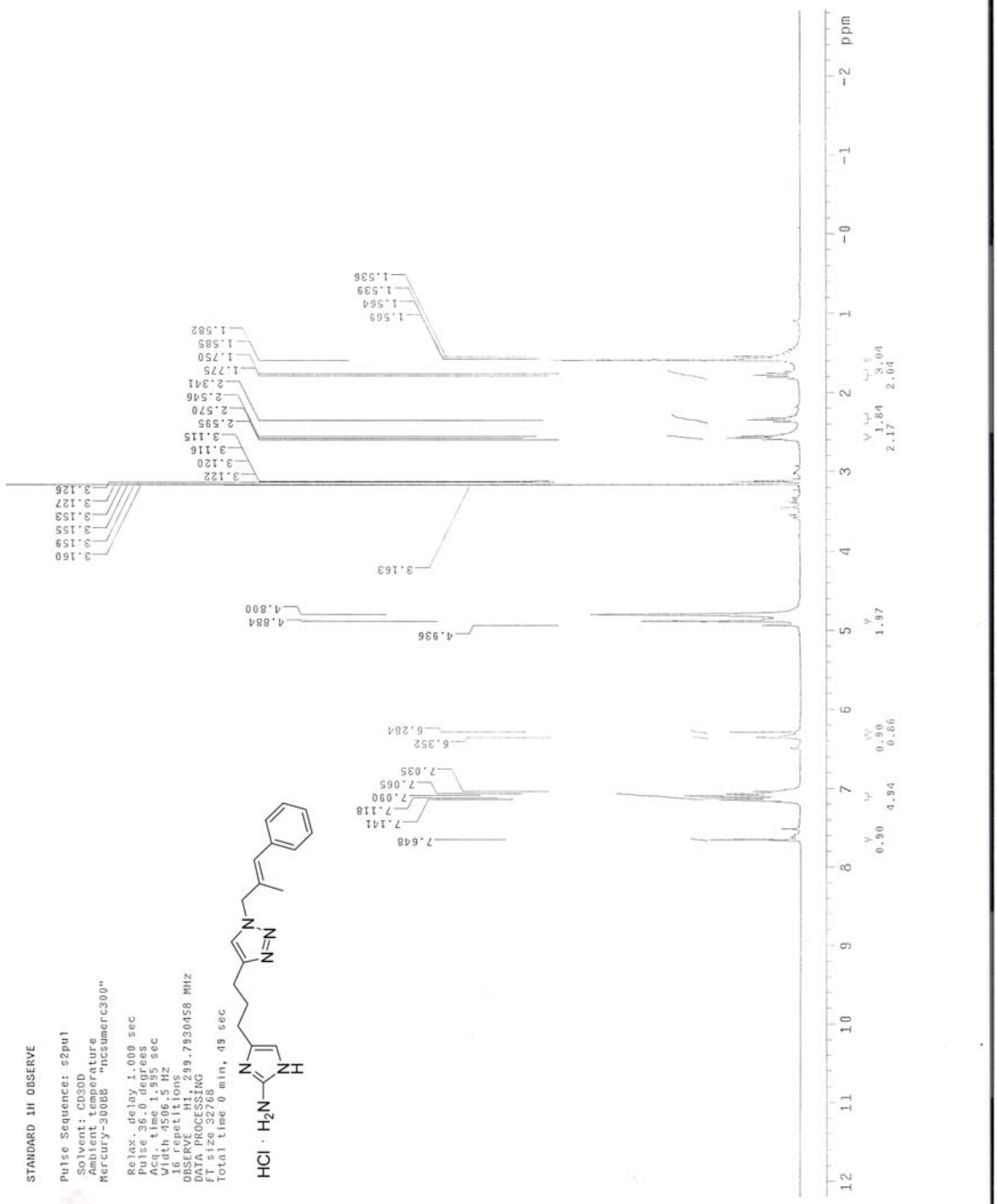
Pulse Sequence: s2pul
Solvent: DMSO
Ambient temperature
File: III-84-1H-DMSO
Mercury-300BB "ncsumerc300"

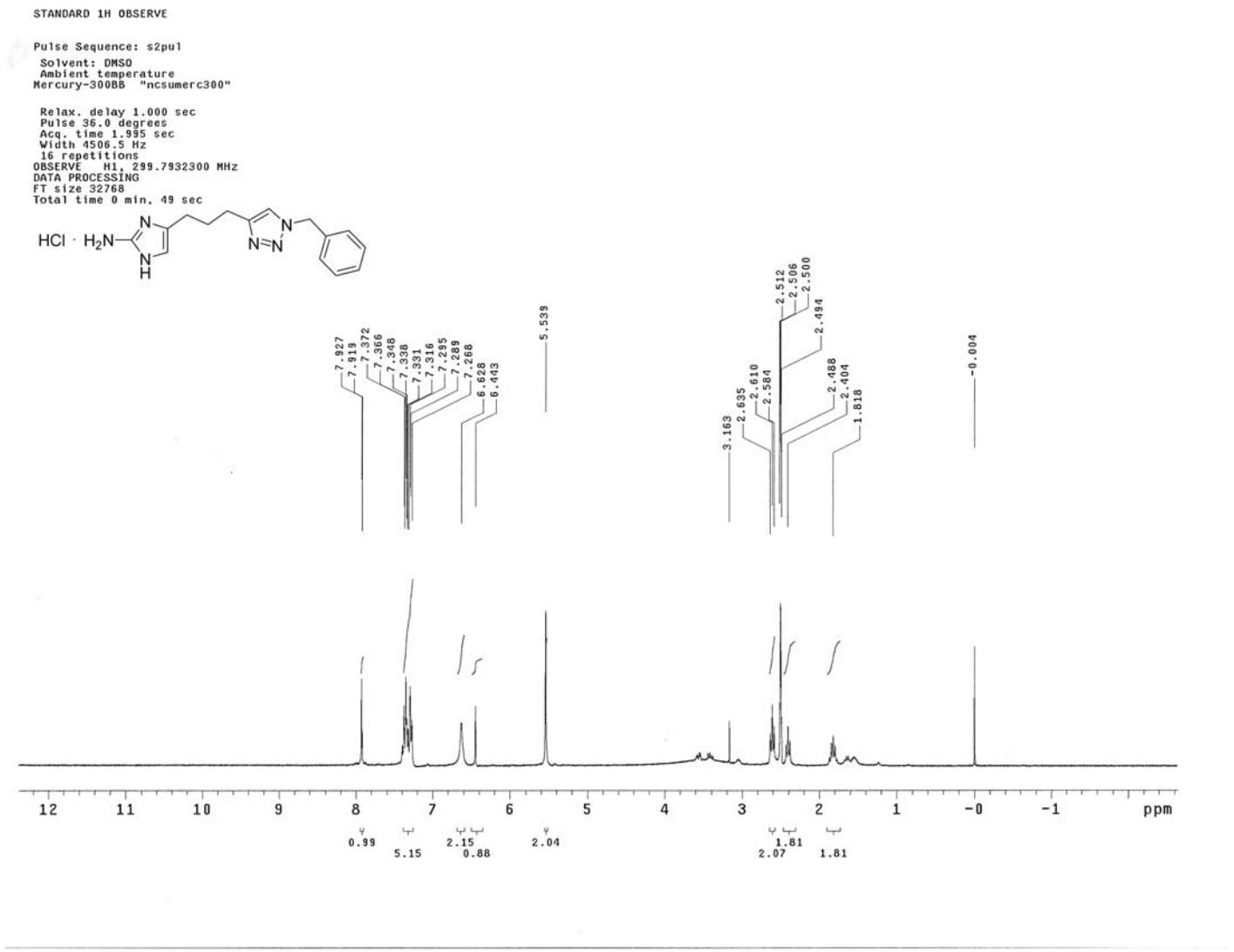
Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 299.7932286 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec






STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 299.7930433 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
HCl · H2N
ppm

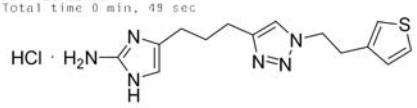

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 299.7930458 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
HCl · H2N
ppm

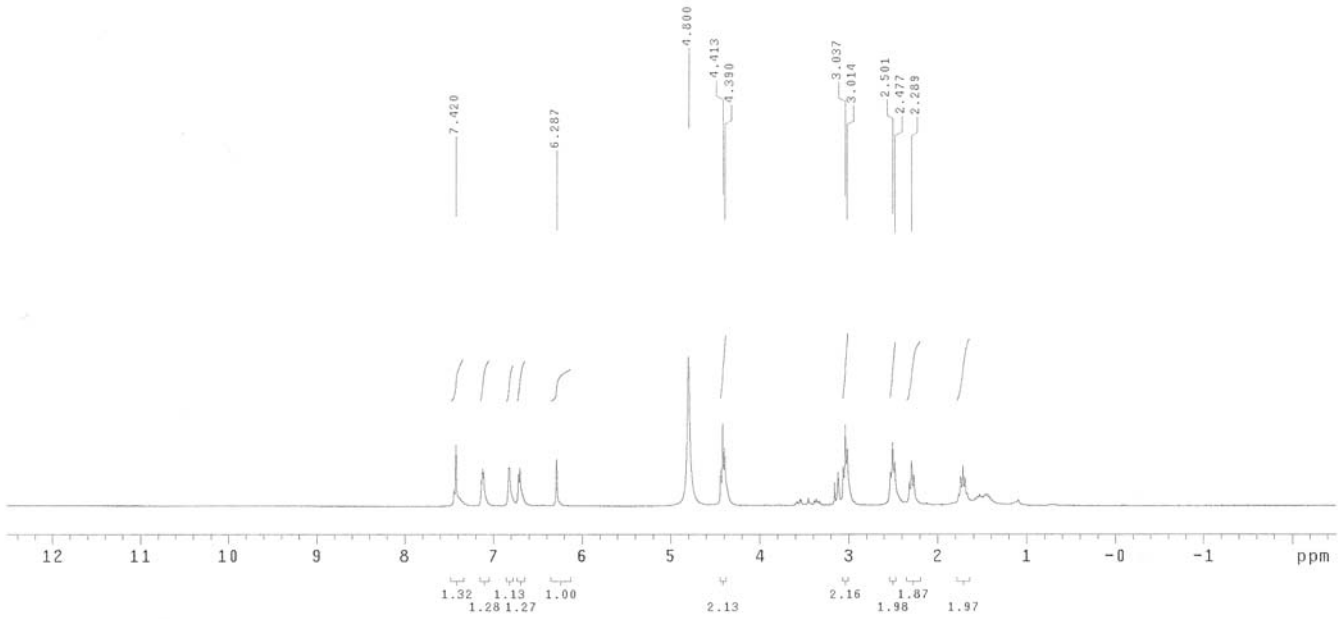

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: DMSO
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 299.7932300 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
HCl · H2N
7.927
7.919
7.372
7.366
7.348
7.338
7.331
7.316
7.295
7.289
7.268
6.628
6.443
5.539
3.163
2.635
2.610
2.584
2.512
2.506
2.500
2.494
2.488
2.404
1.818
-0.004
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm
0.99
5.15
2.15
0.88
2.04
2.07
1.81
1.81

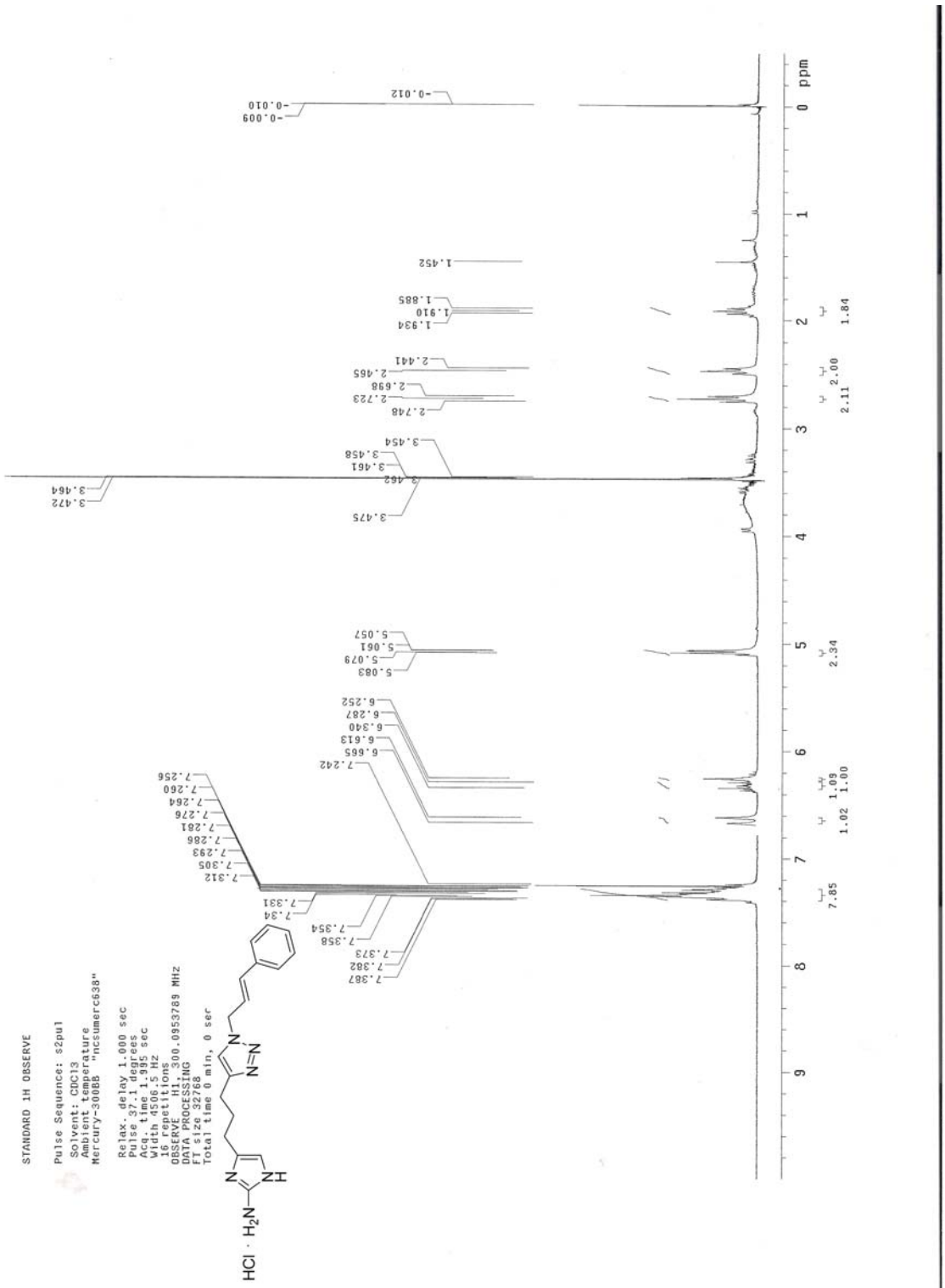
STANDARD 1H OBSERVE

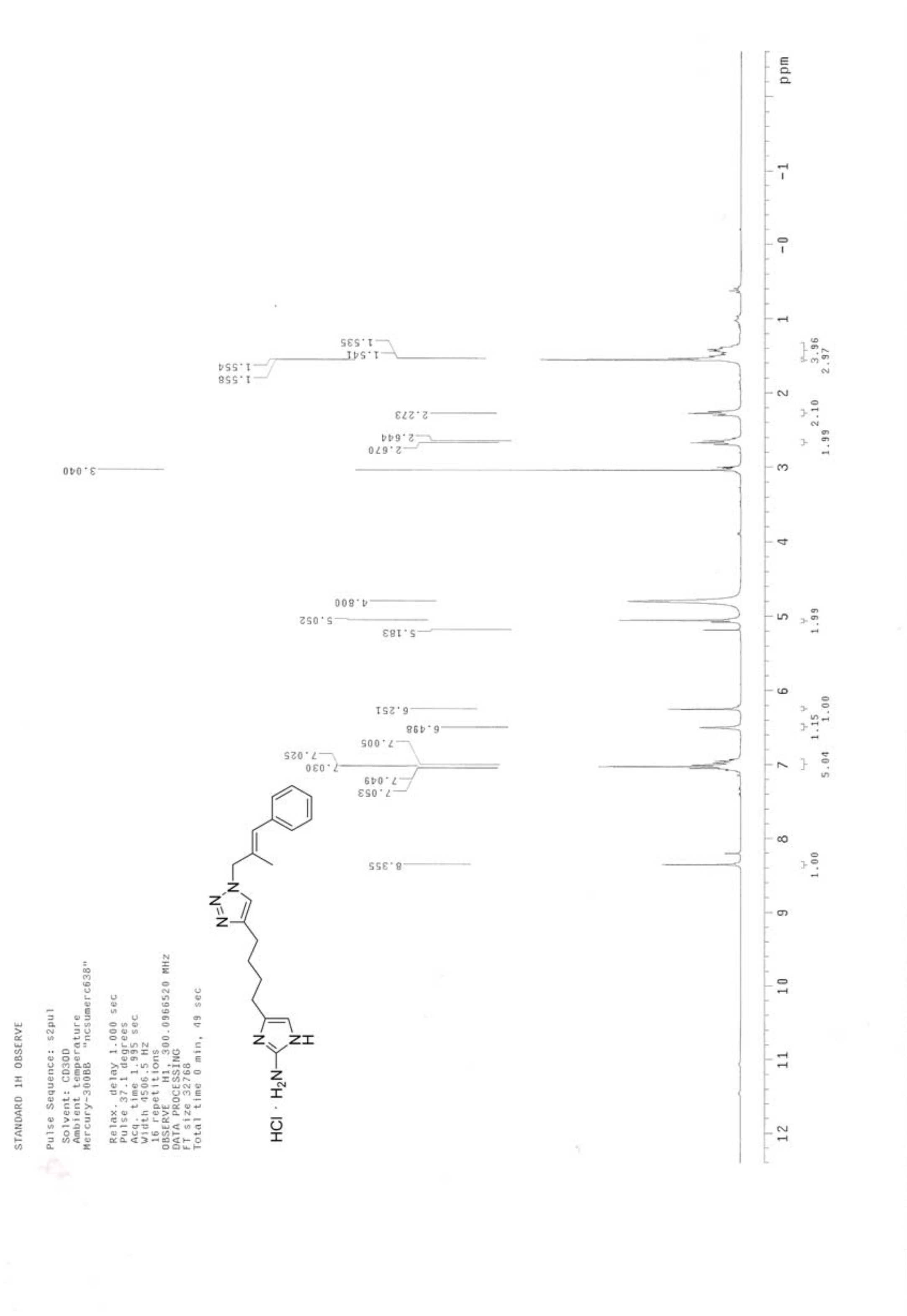
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc638"

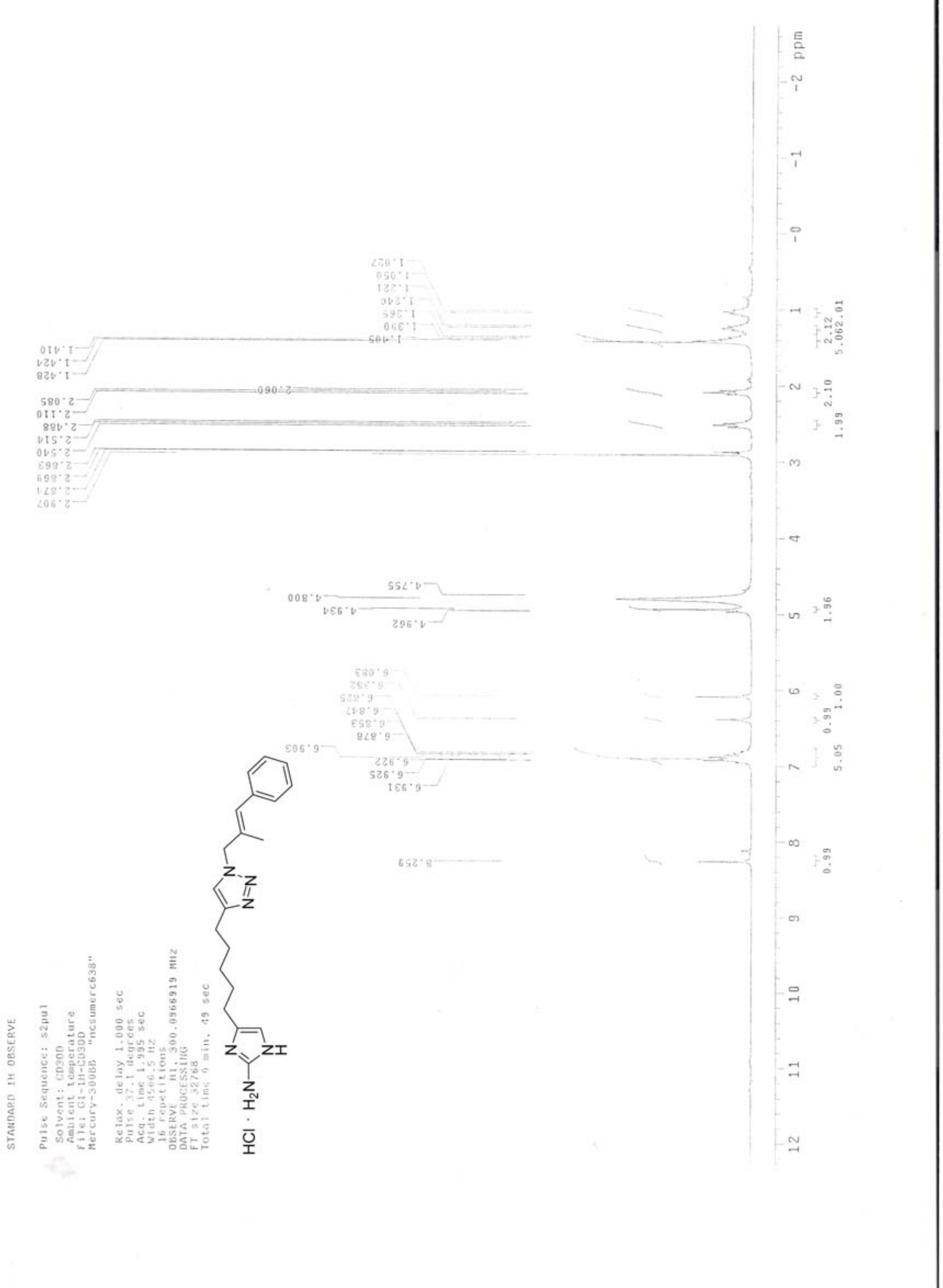
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0966171 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec

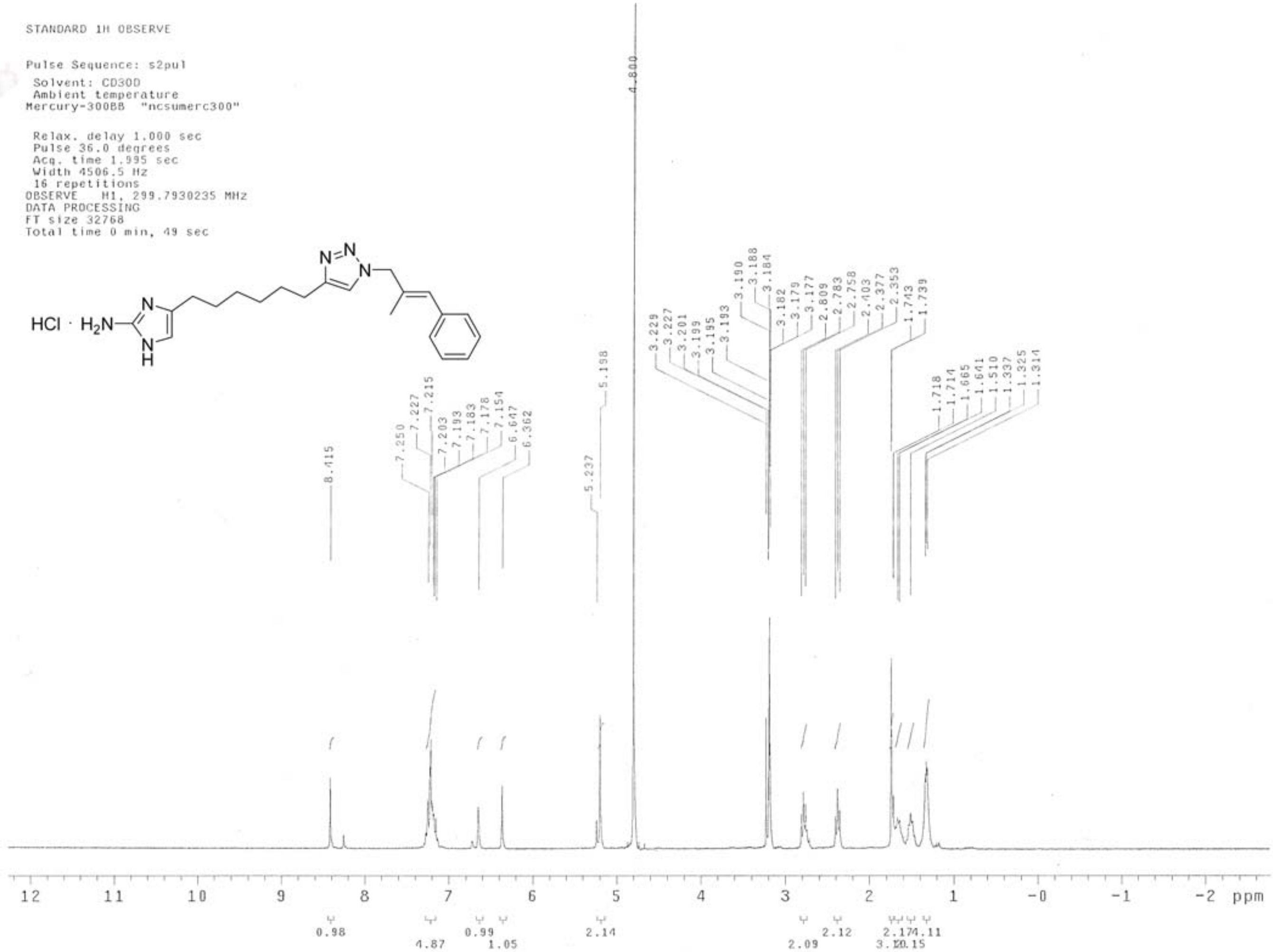





STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0953789 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 0 ser
HCl · H2N
ppm


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0966520 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
HCl · H2N
N
NH
N=N
N
8.355
7.053
7.049
7.030
7.025
7.005
6.498
6.251
5.183
5.052
4.800
3.040
2.670
2.644
2.273
1.558
1.554
1.541
1.535
1.00
5.04
1.15
1.00
1.99
1.99
2.10
2.97
3.96
ppm


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
File: G1-1H-CD3OD
Mercury-300BB "ncsumerc638"
Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 300.0966919 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
HCl · H2N
N
NH
N
N=N
8.259
6.931
6.925
6.922
6.903
6.878
6.853
6.847
6.825
6.392
6.083
4.962
4.934
4.800
4.755
2.907
2.871
2.869
2.863
2.540
2.514
2.488
2.110
2.085
2.060
1.428
1.424
1.410
1.405
1.390
1.365
1.246
1.221
1.050
1.027
0.99
5.05
0.99
1.00
1.96
1.99
2.10
2.12
5.06
2.01
ppm


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-300BB "ncsumerc300"
Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
16 repetitions
OBSERVE H1, 299.7930235 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 49 sec
HCl · H2N
N
H
N=N
N
8.415
7.250 7.227 7.215 7.203 7.193 7.183 7.178 7.154 6.647 6.362
5.237 5.198
4.800
3.229 3.227 3.201 3.199 3.195 3.193 3.190 3.188 3.184 3.182 3.179 3.177 2.809 2.783 2.758 2.403 2.377 2.353 1.743 1.739
1.718 1.714 1.665 1.641 1.510 1.337 1.325 1.314
12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 -2 ppm
0.98 4.87 0.99 1.05 2.14 2.09 2.12 2.17 3.10 4.11 0.15

STANDARD 1H OBSERVE

Pulse Sequence: s2pul
Solvent: DMSO
Ambient temperature
File: A7ditriazole-1H-DMSO
Mercury-300BB "ncsumerc638"

Relax. delay 1.000 sec
Pulse 37.1 degrees
Acq. time 1.995 sec
Width 4506.5 Hz
32 repetitions
OBSERVE H1, 300.0967992 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 57 sec