Supporting Information

Compound Shape Effects in Minor Groove Binding Affinity and Specificity for Mixed Sequence DNA

Pu Guo[1], Abdelbasset A. Farahat[1,2], Ananya Paul[1], Narinder K. Harika[1], David W. Boykin[1], W. David Wilson[1]*

1. Department of Chemistry and Center for Diagnostics and Therapeutics Georgia State University, 50 Decatur St Se, Atlanta, GA 30303, USA.

2. Department of Pharmaceutical Organic Chemistry, Faculty of Pharmacy, Mansoura University, Mansoura 35516, Egypt

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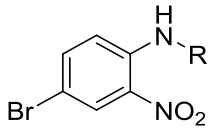
General materials and methods

Synthesis

All commercial reagents were used without further purification. All melting points were determined on a Mel-Temp 3.0 melting point instrument, and are uncorrected. TLC analysis was carried out on silica gel 60 F254 precoated aluminum sheets using UV light for detection. ^{1}HNMR spectra were recorded on a Bruker 400 MHz spectrometer using the indicated solvents. Mass spectra were obtained from the Georgia State University Mass Spectrometry Laboratory, Atlanta, GA. Elemental analysis were performed by Atlantic Microlab Inc., Norcross, GA.

Synthesis of 4-Bromo-*N*-alkyl (aryl)-2-nitroaniline (2a-n).



Amines (40 mmol) were added to 4-bromo-1-fluoro-2-nitrobenzene (4.4 g, 20 mmol) in ethanol (20 ml) and stirred at room temperature for 24 h. The reaction mixture was evaporated under vacuum. In case of aromatic amines, Cs_2CO_3 (6.5 g, 20 mmol) was added to the reaction mixture and heated at 120 ^{o}C in DMA (20 ml) for 24 h, ice water was added and the formed solid was filtered and dried. The products resulting from both aromatic and aliphatic amines were chromatographed on silica gel using hexanes/ethyl acetate as solvent.

4-Bromo-*N*-methyl-2-nitroaniline (2a).[1]

4-Bromo-*N*-ethyl-2-nitroaniline (2b).[2]

Orange solid (3.47 g, 71 %), mp 92-93 ^{o}C (reported mp 86-89 ^{o}C; ^{1}HNMR (DMSO-d_6): δ 8.16 (br s, 1 H), 8.15 (br s, 1 H), 7.64 (dd, *J* = 2, 9.2 Hz, 1 H), 7.03 (d, *J* = 9.2

Hz, 1 H), 3.38 (q, *J* = 6.8 Hz, 2 H), 1.29 (t, *J* = 7.2 Hz, 3 H); ESI-HRMS: m/z calculated for $C_8H_{10}BrN_2O_2$: 244.9920, found: 244.9913 (M^+ + 1).

4-Bromo-*N*-isopropyl-2-nitroaniline (2c).

Orange solid (3.67 g, 72 %), mp 97-98 ^oC ; ^{1}HNMR (DMSO-d_6): δ 8.15 (br s, 1 H), 7.88 (d, *J* = 7.2 Hz, 1 H), 7.64 (d, *J* = 9.2 Hz, 1 H), 7.08 (d, *J* = 9.2 Hz, 1 H), 3.92 (m, 1 H), 1.25 (d, *J* = 6 Hz, 6 H); ESI-HRMS: m/z calculated for $C_9H_{12}BrN_2O_2$: 259.077, found: 259.066 (M^+ + 1).

4-Bromo-*N*-isobutyl-2-nitroaniline (2d).

Orange solid (3.82 g, 70 %), mp 51-52 ^oC ; ^{1}HNMR (DMSO-d_6): δ 8.20 (br s, 1 H), 8.10 (br s, 1 H), 7.57 (d, *J* = 9.2 Hz, 1 H), 6.99 (d, *J* = 9.2 Hz, 1 H), 3.15 (d, *J* = 6 Hz, 2 H), 1.91 (m, 1 H), 0.93 (d, *J* = 6.4 Hz, 6 H); ESI-HRMS: m/z calculated for $C_{10}H_{13}BrN_2O_2$: 295.0058, found: 295.0060 (M^+ + Na).

4-Bromo-*N*-neopentyl-2-nitroaniline (2e).

Orange solid (3.67 g, 64 %), mp 67-68 ^oC ; ^{1}HNMR (DMSO-d_6): δ 8.19 (t, *J* = 5.6 Hz, 1 H), 8.16 (d, *J* = 2 Hz, 1 H), 7.63 (dd, *J* = 2, 9.2 Hz, 1 H), 7.16 (d, *J* = 9.2 Hz, 1 H), 3.20 (d, *J* = 5.6 Hz, 2 H), 0.98 (s, 9 H); ESI-HRMS: m/z calculated for $C_{11}H_{16}BrN_2O_2$: 287.0390, found: 287.0378 (M^+ + 1).

4-Bromo-*N*-butyl-2-nitroaniline (2f).

Orange oil (3.43 g, 63 %); ^{1}HNMR (DMSO-d_6): δ 8.17 (br s, 1 H), 8.14 (br s, 1 H), 7.63 (d, *J* = 9.2 Hz, 1 H), 7.04 (d, *J* = 9.2 Hz, 1 H), 3.35 (m, 2 H), 1.58 (m, 2 H), 1.36 (m, 2 H), 0.91 (t, *J* = 7.2 Hz, 3 H); ESI-HRMS: m/z calculated for $C_{10}H_{14}BrN_2O_2$: 273.0233, found: 273.0221 (M^+ + 1).

4-Bromo-*N*-(3-Methoxypropyl)-2-nitroaniline (2g).

Orange oil (4.1 g, 71 %); ^{1}HNMR (DMSO-d_6): δ 8.36 (t, *J* = 5.2 Hz, 1 H), 8.14 (d, *J* = 2.4 Hz, 1 H), 7.64 (dd, *J* = 2.4, 9.2 Hz, 1 H), 7.02 (d, *J* = 9.2 Hz, 1 H), 3.43 (m, 2 H), 3.37 (m, 2 H), 3.26 (s, 3H), 1.85 (p, *J* = 6 Hz, 2 H); ESI-HRMS: m/z calculated for $C_{10}H_{14}BrN_2O_3$: 289.0182, found: 289.0169 (M^+ + 1).

4-Bromo-*N*-(2-methoxyethyl)-2-nitroaniline (2h).

Orange solid (3.68 g, 67 %), mp 73-74 ^{o}C ; ^{1}HNMR (DMSO-d_6): δ 8.21 (m, 1 H), 8.16 (d, *J* = 2.4 Hz, 1 H), 7.65 (dd, *J* = 2.4, 9.2 Hz, 1 H), 7.09 (d, *J* = 9.2 Hz, 1 H), 3.59 (m, 2 H), 3.52 (m, 2 H), 3.30 (s, 3 H); ESI-HRMS: m/z calculated for $C_9H_{11}BrN_2O_3Na$: 296.9851, found: 296.9862 (M^+ + Na).

4-Bromo-*N*-cyclobutyl-2-nitroaniline (2i).

Orange solid (4.28 g, 79 %), mp 69-70 ^{o}C ; ^{1}HNMR (DMSO-d_6): δ 8.14 (t, *J* = 1.2 Hz, 1 H), 8.02 (d, *J* = 6 Hz, 1 H), 7.64 (dd, *J* = 2, 9.2 Hz, 1 H), 6.89 (d, *J* = 9.2 Hz, 1 H), 4.12 (m, 1 H), 2.42 (m, 2 H), 2.01 (m, 2H), 1.77 (m, 2 H); ESI-HRMS: m/z calculated for $C_{10}H_{12}BrN_2O_2$: 277.0077, found: 277.0064 (M^+ + 1).

4-Bromo-*N*-cyclopentyl-2-nitroaniline (2j).

Orange solid (3.76 g, 66 %), mp 92-93 ^{o}C ; ^{1}HNMR (DMSO-d_6): δ 8.13 (br s, 1 H), 7.96 (d, *J* = 6 Hz, 1 H), 7.64 (d, *J* = 9 Hz, 1 H), 7.07 (d, *J* = 9 Hz, 1 H), 4.03 (m, 1 H), 2.05 (m, 2 H), 1.69 (m, 2 H), 1.55 (m, 4 H); ESI-HRMS: m/z calculated for $C_{11}H_{14}BrN_2O_2$: 285.0233, found: 285.0227 (M^+ + 1).

4-Bromo-*N*-cyclohexyl-2-nitroaniline (2k).[3]

Orange solid (4.02 g, 67 %), mp 115-116 (reported mp 108.5-109.5 ^{o}C); ^{1}HNMR (DMSO-d_6): δ 8.15 (t, *J* = 2 Hz, 1 H), 7.98 (d, *J* = 6 Hz, 1 H), 7.62 (dd, *J* = 2, 9.2 Hz, 1 H), 7.12 (d, *J* = 9.2 Hz, 1 H), 3.63 (m, 1 H), 1.93 (m, 2 H), 1.60 (m, 2H), 1.57 (m, 1 H), 1.35 (m, 4 H), 1.25 (m, 1 H); ESI-HRMS: m/z calculated for $C_{12}H_{16}BrN_2O_2$: 299.0390, found: 299.0376 (M^+ + 1).

4-Bromo-*N*-(cyclopentylmethyl)-2-nitroaniline (2l).

Orange solid (3.52 g, 59 %), mp 98-99 ^{o}C ; ^{1}HNMR (DMSO-d_6): δ 8.19 (t, *J* = 5.2 Hz, 1 H), 8.14 (d, *J* = 2 Hz, 1 H), 7.62 (dd, *J* = 2, 9.2 Hz, 1 H), 7.06 (d, *J* = 9.2 Hz, 1 H), 3.26 (t, *J* = 6.4 Hz, 2 H), 2.21 (m, 1 H), 1.73 (m, 2 H), 1.61 (m, 2 H), 1.53 (m, 2 H), 1.29 (m, 2 H); ESI-HRMS: m/z calculated for $C_{12}H_{16}BrN_2O_2$: 299.0390, found: 299.0396 (M^+ + 1).

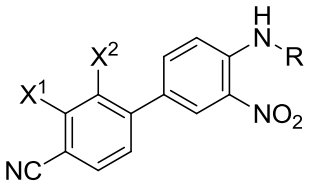
4-Bromo-*N*-phenyl-2-nitroaniline (2m).[4]

Orange solid (2.98 g, 51 %), mp 73-74 °C (reported mp 65-66 °C) ; ^{1}HNMR (DMSO-d_6): δ 9.44 (br s, 1 H), 8.23 (d, *J* = 2.8 Hz, 1 H), 7.63 (dd, *J* = 2.8, 9.2 Hz, 1 H), 7.43 (m, 2 H), 7.32 (d, *J* = 7.6 Hz, 2 H), 7.23 (d, *J* = 7.4 Hz, 1 H), 7.11 (d, *J* = 9.2 Hz, 1 H); ESI-HRMS: m/z calculated for $C_{12}H_{10}BrN_2O_2$: 292.9920, found: 292.9906 (M^+ + 1).

4-Bromo-2-nitro-*N*-(o-tolyl)aniline (2n).

Orange solid (2.51 g, 41 %), mp 74-75 °C ; ^{1}HNMR (DMSO-d_6): δ 9.41 (br s, 1 H), 8.22 (d, *J* = 1.2 Hz, 1 H), 7.57 (d, *J* = 9.2 Hz, 1 H), 7.38 (d, *J* = 6.8 Hz, 1 H), 7.30 (m, 3 H), 6.58 (d, *J* = 9.2 Hz, 1 H), 2.17 (s, 3H).

4'-(alkylamino)-3'-nitro-[1,1'-biphenyl]-4-carbonitrile (3a-q).[5-9]



K_2CO_3 (2.76 g, 20 mmol) in water (5 ml) and 4-cyanophenylboronic acid or its derivatives (11 mmol) methanol (10 ml) were added to a stirred solution of the bromo compound **2** (10 mmol) in dioxane (30 mL) and the mixture was deaerated under nitrogen for 20 min. Tetrakistriphenylphosphine palladium (0.46 g, 0.4 mmol) was added and the reaction mixture was vigorously stirred at 100 °C for 24 h. The solvent was evaporated under reduced pressure, the solid was partitioned between ethyl acetate (200 mL) and 2 M aqueous Na_2CO3 (25 mL) containing 5 mL of concentrated ammonia, to remove palladium residues, then washed with water, passed through celite to remove the catalyst, dried (sodium sulfate) and evaporated. The product was purified using column chromatography on silica gel, and hexanes/ethyl acetate as an eluent.

4'-(Methylamino)-3'-nitro-[1,1'-biphenyl]-4-carbonitrile (3a).[1]

4'-(Ethylamino)-3'-nitro-[1,1'-biphenyl]-4-carbonitrile (3b).

Orange solid (2 g, 78 %), mp 121-122 ^{o}C; ^{1}HNMR (DMSO-d_6): δ 8.40 (br s, 1 H), 8.26 (br s, 1 H), 7.97 (d, *J* = 8.6 Hz, 1 H), 7.87 (br s, 4 H), 7.17 (d, *J* = 8.6 Hz, 1 H), 3.45 (q, *J* = 6.6 Hz, 2 H), 1.25 (t, *J* = 6.6 Hz, 3 H); ESI-HRMS: m/z calculated for $C_{15}H_{14}N_3O_2$: 268.1081, found: 268.1074 (M^+ + 1).

4'-(Isopropylamino)-3'-nitro-[1,1'-biphenyl]-4-carbonitrile (3c).

Orange solid (1.99 g, 71 %), mp 110-111 ^{o}C; ^{1}HNMR ($CDCl_3$): δ 8.49 (d, *J* = 2.4 Hz, 1 H), 8.17 (br s, 1H), 7.73 (m, 3 H), 7.67 (d, *J* = 8.4 Hz, 2 H), 7.01 (d, *J* = 9.2 Hz, 1 H), 3.93 (m, 1 H), 1.39 (d, *J* = 6.4 Hz, 6 H); ESI-HRMS: m/z calculated for $C_{16}H_{16}N_3O_2$: 281.1243, found: 281.1250 (M^+ + 1).

4'-(Isobutylamino)-3'-nitro-[1,1'-biphenyl]-4-carbonitrile (3d).

Orange solid (2.09 g, 71 %), mp 157-158 ^{o}C; ^{1}HNMR (DMSO-d_6): δ 8.41 (br s, 1 H), 8.36 (m, 1 H), 7.95 (d, *J* = 9 Hz, 1 H), 7.87 (m, 4H), 7.20 (d, *J* = 9 Hz, 1 H), 3.26 (t, *J* = 6.2 Hz, 2 H), 1.97 (m, 1 H), 0.97 (d, *J* = 6.4 Hz, 6 H); ESI-HRMS: m/z calculated for $C_{17}H_{18}N_3O_2$: 296.1394, found: 296.1380 (M^+ + 1).

4'-(Neopentylamino)-3'-nitro-[1,1'-biphenyl]-4-carbonitrile (3e).

Orange solid (2.10 g, 68 %), mp 164-165 ^{o}C; ^{1}HNMR (DMSO-d_6): δ 8.42 (br s, 1 H), 8.34 (d, *J* = 5.2 Hz, 1 H), 7.97 (d, *J* = 9 Hz, 1 H), 7.89 (m, 4H), 7.30 (d, *J* = 9 Hz, 1 H), 3.27 (d, *J* = 5.6 Hz, 2 H), 1.01 (s, 9 H); ESI-HRMS: m/z calculated for $C_{18}H_{20}N_3O_2$: 310.1550, found: 310.1539 (M^+ + 1).

4'-(Butylamino)-3'-nitro-[1,1'-biphenyl]-4-carbonitrile (3f).

Orange solid (2.15 g, 73 %), mp 130-131 ^{o}C; ^{1}HNMR (DMSO-d_6): δ 8.42 (br s, 1 H), 8.30 (m, 1 H), 7.98 (d, *J* = 9.2 Hz, 1 H), 7.88 (m, 4H), 7.20 (d, *J* = 9.2 Hz, 1 H),

3.43 (m, 2 H), 1.63 (m, 2 H), 1.40 (m, *J* = 7.2 Hz, 2 H), 0.94 (t, *J* = 7.2 Hz, 3 H); ESI-HRMS: m/z calculated for $C_{17}H_{18}N_3O_2$: 296.1394, found: 296.1379 (M^+ + 1).

4'-((3-Methoxypropyl)amino)-3'-nitro-[1,1'-biphenyl]-4-carbonitrile (3g).

Orange solid (2.14 g, 69 %), mp 75-76 ^oC; ^{1}HNMR (DMSO-d_6): δ 8.46 (t, *J* = 5.4 Hz, 1 H), 8.40 (d, *J* = 2 Hz, 1 H), 7.97 (d, *J* = 9.2 Hz, 1 H), 7.87 (m, 4H), 7.16 (d, *J* = 9.2 Hz, 1 H), 3.47 (m, 4 H), 3.28 (s, 3 H), 1.88 (m, 2 H); ESI-HRMS: m/z calculated for $C_{17}H_{18}N_3O_3$: 312.1343, found: 312.1320 (M^+ + 1).

4'-((2-Methoxyethyl)amino)-3'-nitro-[1,1'-biphenyl]-4-carbonitrile (3h).

Orange solid (1.81 g, 61 %), mp 118-119 ^oC; ^{1}HNMR (DMSO-d_6): δ 8.38 (d, *J* = 1.6 Hz, 1 H), 8.31 (br s, 1 H), 7.95 (d, *J* = 7.6 Hz, 1 H), 7.86 (m, 4 H), 7.20 (m, 1 H), 3.59 (m, 4 H), 3.32 (s, 3 H); ESI-HRMS: m/z calculated for $C_{16}H_{15}N_3O_3Na$: 320.1011, found: 320.1001 (M^+ + Na).

4'-(Cyclobutylamino)-3'-nitro-[1,1'-biphenyl]-4-carbonitrile (3i).

Orange solid (2.31 g, 79 %), mp 159-160 ^oC; ^{1}HNMR (DMSO-d_6): δ 8.39 (br s, 1 H), 8.14 (d, *J* = 5.2 Hz, 1 H), 7.95 (d, *J* = 8.6 Hz, 1 H), 7.87 (m, 4H), 7.03(d, *J* = 8.6 Hz, 1 H), 4.20 (m, 1 H), 2.46 (m, 2 H), 2.04 (m, 2 H), 1.80 (m, 2 H); ESI-HRMS: m/z calculated for $C_{17}H_{16}N_3O_2$: 294.1237, found: 294.1224 (M^+ + 1).

4'-(Cyclopentylamino)-3'-nitro-[1,1'-biphenyl]-4-carbonitrile (3j).

Orange solid (2.19 g, 73 %), mp 166-167 ^oC; ^{1}HNMR (DMSO-d_6): δ 8.40 (br s, 1 H), 8.09 (d, *J* = 6.8 Hz, 1 H), 7.98 (d, *J* = 8.6 Hz, 1 H), 7.88 (m, 4H), 7.22 (d, *J* = 8.6 Hz, 1 H), 4.13 (m, 1 H), 2.09 (m, 2 H), 1.71 (m, 2 H), 1.64 (m, 4 H); ESI-HRMS: m/z calculated for $C_{18}H_{17}N_3O_2$: 307.1315, found: 307.1321 (M^+ + 1).

4'-(Cyclohexylamino)-3'-nitro-[1,1'-biphenyl]-4-carbonitrile (3k).

Orange solid (2.50 g, 78 %), mp 192-193 ^oC; ^{1}HNMR (DMSO-d_6): δ 8.42 (br s, 1 H), 8.11 (d, *J* = 7.8 Hz, 1 H), 7.97 (d, *J* = 9 Hz, 1 H), 7.89 (m, 4H), 7.26 (d, *J* = 9 Hz, 1 H), 3.73 (m, 1 H), 1.98 (m, 2 H), 1.70 (m, 2 H), 1.59 (m, 1 H), 1.41 (m, 4H),

1.25 (m, 1H); ESI-HRMS: m/z calculated for $C_{19}H_{20}N_3O_2$: 322.1550, found: 322.1535 (M^+ + 1).

4'-((Cyclopentylmethyl)amino)-3'-nitro-[1,1'-biphenyl]-4-carbonitrile(3l).

Orange solid (1.89 g, 59 %), mp 181-182 ^oC; ^{1}HNMR ($CDCl_3$): δ 8.49 (d, *J* = 2 Hz, 1 H), 8.27 (br s, 1 H), 7.76-7.67 (m, 5 H), 7.00 (d, *J* = 9.2 Hz, 1 H), 3.31 (m, 2 H), 2.32 (m, 1 H), 1.95 (m, 2 H), 1.68 (m, 2 H), 1.38 (m, 2 H), 0.87 (m, 2 H); ESI-HRMS: m/z calculated for $C_{19}H_{20}N_3O_2$: 322.1550, found: 322.1558 (M^+ + 1).

3'-Nitro-4'-(phenylamino)-[1,1'-biphenyl]-4-carbonitrile (3m).

Orange solid (1.85 g, 59 %), mp 187-188 ^oC; ^{1}HNMR (DMSO-d_6): δ 9.56 (br s, 1 H), 8.47 (d, *J* = 2 Hz, 1 H), 7.94 (dd, *J* = 2, 9.2 Hz, 1 H), 7.90 (m, 4 H), 7.48 (br s, 1 H), 7.45 (d, *J* = 7.6 Hz, 1 H), 7.37 (d, *J* = 7.6 Hz, 2 H), 7.26 (m, 2 H); ESI-HRMS: m/z calculated for $C_{19}H_{14}N_3O_2$: 316.1081, found: 316.1067 (M^+ + 1).

3'-Nitro-4'-(o-tolylamino)-[1,1'-biphenyl]-4-carbonitrile (3n).

Orange solid (1.80 g, 55 %), mp 157-158 ^oC; ^{1}HNMR (DMSO-d_6): δ 9.53 (br s, 1 H), 8.48 (br s, 1 H), 7.88 (m, 5 H), 7.41 (d, *J* = 6.8 Hz, 1 H), 7.32 (m, 3 H), 7.73 (d, *J* = 8.8 Hz, 1 H), 2.21 (s, 3 H); ESI-HRMS: m/z calculated for $C_{20}H_{16}N_3O_2$: 330.1237, found: 330.1221 (M^+ + 1).

3-Chloro-4'-(isopropylamino)-3'-nitro-[1,1'-biphenyl]-4-carbonitrile (3o).

Orange solid (1.73 g, 55 %), mp 146-147 ^oC; ^{1}HNMR (DMSO-d_6): δ 8.45 (d, *J* = 2 Hz, 1 H), 8.07 (br s, 1 H), 8.03 (m, 2 H), 7.98 (d, *J* = 8.4 Hz, 1 H), 7.85 (d, *J* = 8.4 Hz, 1 H), 7.21 (d, *J* = 9.2 Hz, 1 H), 4.04 (m, 1 H), 1.29 (d, *J* = 6 Hz, 6 H), ESI-HRMS: m/z calculated for $C_{16}H_{15}ClN_3O_2$: 316.0847, found: 316.0833 (M^+ + 1).

4'-(Isopropylamino)-3'-nitro-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carbonitrile (3p).

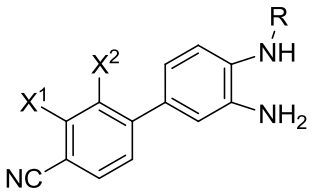
Orange solid (1.77 g, 51 %), mp 141-142 ^oC; ^{1}HNMR (DMSO-d_6): δ 8.53 (d, *J* = 2 Hz, 1 H), 8.23 (br s, 1 H), 8.22 (m, 2 H), 8.08 (dd, *J* = 2, 9.2 Hz, 1 H), 8.04 (d, *J* =

7.6 Hz, 1 H), 7.24 (d, *J* = 9.2 Hz, 1 H), 4.05 (m, 1 H), 1.30 (d, *J* = 6 Hz, 6 H), ESI-HRMS: m/z calculated for $C_{17}H_{15}F_3N_3O_2$: 350.1111, found: 350.1102 (M^+ + 1).

4'-(Isopropylamino)-2-methyl-3'-nitro-[1,1'-biphenyl]-4-carbonitrile (3q).

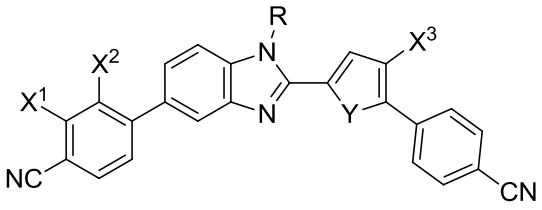
Orange solid (1.79 g, 61 %), mp 135-136 ^oC; ^{1}HNMR (DMSO-d_6): δ 8.03 (d, *J* = 1.6 Hz, 1 H), 7.98 (d, *J* = 7.8 Hz, 1 H), 7.79 (br s, 1 H), 7.71 (d, *J* = 7.8 Hz, 1 H), 7.62 (dd, *J* = 1.6, 8.8 Hz, 1 H), 7.44 (d, *J* = 7.6 Hz, 1 H), 7.19 (d, *J* = 8.8 Hz, 1 H), 4.01 (m, 1 H), 2.31 (s, 3H), 1.30 (d, *J* = 6.8 Hz, 6 H), ESI-HRMS: m/z calculated for $C_{17}H_{18}N_3O_2$: 296.1394, found: 296.1379 (M^+ + 1).

Synthesis of the diamine (4a-q).



$SnCl_2$. $2H_2O$ (4.5 g, 20 mmol) was added to a suspension of the nitro compound **3** (5 mmol) in Ethanol **(**30 ml). The reaction mixture was refluxed for 12 h and concentrated under reduced pressure. The formed residue was neutralized by sodium hydroxide solution in an ice bath. The formed precipitate was filtered, dried under vacuum at room temperature and then dissolved in acetone (50 ml) and filtered. The filtrate was evaporated under reduced pressure and dried under vacuum at room temperature and used directly in the next step.

Synthesis of the bisnitrile compounds (6a-t).[10-14]



Sodium metabisulphite (1.14 g, 6 mmol) was added to a solution of the diamines **3a-r** (3 mmol) and the aldehydes[15] **5a-d** (3 mmol) in DMSO (10 mL) and the mixture was heated at 130 °C for 30 min. The reaction mixture was poured into water, filtered and dried. Purification was by crystallization from acetone.

4-(5-(5-(4-Cyanophenyl)-1-methyl-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzonitrile (6a).[10]

4-(5-(5-(4-Cyanophenyl)-1-ethyl-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzonitrile (6b).

Yellow solid (0.78 g, 61 %), mp > 300 °C; ^{1}HNMR (DMSO-d_6): δ 8.06 (br s, 1 H), 7.97 (m, 9 H), 7.81 (m, 2 H), 7.71 (m, 1 H), 4.60 (br s, 2 H), 1.44 (br s, 3 H); ESI-HRMS: m/z calculated for $C_{27}H_{19}N_4S$: 431.1325, found: 431.1320 (M^+ + 1).

4-(5-(5-(4-Cyanophenyl)-1-isopropyl-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzonitrile (6c).

Yellow solid (0.73 g, 55 %), mp > 300 °C; ^{1}HNMR (DMSO-d_6): δ 8.08 (br s, 1 H), 7.98 (m, 3 H), 7.92 (m, 7 H), 7.64 (m, 2 H), 5.18 (m, 1 H), 1.69 (d, *J* = 6.4 Hz, 6 H); ESI-HRMS: m/z calculated for $C_{28}H_{21}N_4S$: 445.1487, found: 445.1494 (M^+ + 1).

4-(5-(5-(4-Cyanophenyl)-1-isobutyl-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzonitrile (6d).

Yellow solid (0.70 gm, 51 %), mp > 300 °C; ^{1}HNMR (DMSO-d_6): δ 8.06 (br s, 1 H), 7.95 (m, 8 H), 7.84 (m, 3 H), 7.69 (d, *J* = 7.2 Hz, 1 H), 4.43 (d, *J* = 6.8 Hz, 2 H), 2.17 (m, 1 H), 0.89 (d, *J* = 4.8 Hz, 6 H); ESI-HRMS: m/z calculated for $C_{29}H_{23}N_4S$: 459.1638, found: 459.1615 (M^+ + 1).

4-(5-(5-(4-Cyanophenyl)-1-neopentyl-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzonitrile (6e).

Yellow solid (0.86 gm, 61 %), mp > 300 °C; ^{1}HNMR (DMSO-d_6): δ 8.07 (br s, 1 H), 7.96 (m, 4 H), 7.93 (m, 5 H), 7.85 (m, 2 H), 7.68 (d, *J* = 8.4 Hz, 1 H), 4.54 (s, 2

H), 0.83 (s, 9 H); ESI-HRMS: m/z calculated for $C_{30}H_{25}N_4S$: 473.1794, found: 473.1782 ($M^+ + 1$).

4-(1-Butyl-2-(5-(4-cyanophenyl)thiophen-2-yl)-1H-benzo[d]imidazol-5-yl)benzonitrile (6f).

Yellow solid (0.70 gm, 51 %), mp > 300 ^oC; ^{1}HNMR (DMSO-d_6): δ 8.06 (br s, 1 H), 7.97 (m, 4 H), 7.93 (m, 4 H), 7.88 (d, *J* = 4 Hz, 1 H), 7.81 (d, *J* = 4 Hz, 1 H), 7.79 (br s, 1 H), 7.70 (d, *J* = 8 Hz, 1 H), 4.56 (t, *J* = 7.2 Hz, 2 H), 1.79 (m, 2 H), 1.36 (m, 2 H), 0.90 (t, *J* = 7.2 Hz, 3 H); ESI-HRMS: m/z calculated for $C_{30}H_{25}N_4S$: 459.1638, found: 459.1637 ($M^+ + 1$).

4-(5-(5-(4-Cyanophenyl)-1-(3-methoxypropyl)-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzonitrile (6g).

Yellow solid (0.69 gm, 49 %), mp > 300 ^oC; ^{1}HNMR (DMSO-d_6): δ 8.05 (br s, 1 H), 7.92 (m, 9 H), 7.71 (m, 3 H), 4.59 (br s, 2 H), 3.36 (br s, 2 H), 3.22 (s, 3 H), 2.06 (br s, 2 H); ESI-HRMS: m/z calculated for $C_{29}H_{23}N_4OS$: 475.1587, found: 475.1567 ($M^+ + 1$).

4-(5-(5-(4-Cyanophenyl)-1-(2-methoxyethyl)-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzonitrile (6h).

Yellow solid (0.92 gm, 67 %), mp > 300 ^oC; ^{1}HNMR (DMSO-d_6): δ 8.06 (br s, 1H), 7.95 (m, 4 H), 7.92 (m, 4 H), 7.88 (m, 2 H), 7.78 (d, *J* = 8.8Hz, 1 H), 7.69 (d, *J* = 8 Hz, 1 H), 4.72 (br s, 2H), 3.81 (br s, 2 H), 3.21 (s, 3 H); ESI-HRMS: m/z calculated for $C_{28}H_{21}N_4OS$: 461.1614, found: 461.1611 ($M^+ + 1$).

4-(5-(5-(4-Cyanophenyl)-1-cyclobutyl-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzonitrile (6i).

Yellow solid (0.83 gm, 61 %), mp > 300 ^oC; ^{1}HNMR (DMSO-d_6): δ 8.10 (br s, 1 H), 8.02 (d, *J* = 8.8 Hz, 2 H), 7.97 (m, 3 H), 7.92 (m, 4 H), 7.88 (d, *J* = 3.7 Hz, 1 H), 7.73 (d, *J* = 3.7 Hz, 1 H), 7.69 (d, *J* = 7.6 Hz, 1 H), 5.44 (m, 1 H), 2.84 (m, 2 H),

2.56 (m, 2 H), 1.91 (m, 2 H); ESI-HRMS: m/z calculated for $C_{29}H_{21}N_4S$: 457.1481, found: 457.1469 (M^+ + 1).

4-(5-(5-(4-Cyanophenyl)-1-cyclopentyl-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzonitrile (6j).

Yellow solid (0.63 gm, 45 %), mp > 300 ^oC; ^{1}HNMR (DMSO-d_6): δ 8.09 (br s, 1 H), 7.93 (m, 8 H), 7.83 (m, 2 H), 7.73 (br s, 1 H), 7.65 (br s, 1 H), 5.31 (m, 1 H), 2.23 (m, 4 H), 2.06 (m, 2 H), 1.78 (m, 2 H); ESI-HRMS: m/z calculated for $C_{30}H_{23}N_4S$: 471.1638, found: 471.1630 (M^+ + 1).

4-(5-(5-(4-Cyanophenyl)-1-cyclohexyl-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzonitrile (6k).

Yellow solid (0.83 gm, 61 %), mp > 300 ^oC; ^{1}HNMR (DMSO-d_6): δ 8.07 (d, *J* = 6 Hz, 1 H), 7.98 (m, 9 H), 7.79 (d, *J* = 8.8 Hz, 1 H), 7.62 (m, 2 H), 4.69 (m, 1 H), 2.35 (m, 2 H), 1.97 (m, 4 H), 1.69 (m, 1 H), 1.46 (m, 3 H); ESI-HRMS: m/z calculated for $C_{29}H_{21}N_4S$: 485.1784, found: 485.1785 (M^+ + 1).

4-(5-(5-(4-Cyanophenyl)-1-(cyclopentylmethyl)-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzonitrile (6l).

Yellow solid (0.58 gm, 40 %), mp > 300 ^oC; ^{1}HNMR (DMSO-d_6): δ 8.06 (br s, 1 H), 7.96 (m, 3 H), 7.93 (m, 4 H), 7.82 (m, 4 H), 7.69 (d, *J* = 7.2 Hz, 1 H), 4.55 (d, *J* = 4.8 Hz, 2 H), 2.38 (m, 1 H), 1.60 (m, 4 H), 1.45 (m, 2 H), 1.29 (m, 2 H); ESI-HRMS: m/z calculated for $C_{31}H_{25}N_4S$: 485.1794, found: 485.1791 (M^+ + 1).

4-(5-(5-(4-Cyanophenyl)-1-phenyl-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzonitrile (6m).

Yellow solid (0.71 gm, 50 %), mp > 300 ^oC; ^{1}HNMR (DMSO-d_6): δ 8.15 (br s, 1 H), 7.93 (m, 4 H), 7.84 (m, 4 H), 7.73 (m, 3 H), 7.65 (m, 4 H), 7.15 (m, 1 H), 6.68 (m, 1 H); ESI-HRMS: m/z calculated for $C_{31}H_{19}N_4S$: 479.1325, found: 479.1314 (M^+ + 1).

4-(5-(5-(4-Cyanophenyl)-1-(o-tolyl)-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzonitrile (6n).

Yellow solid (0.60 gm, 41 %), mp > 300 ^{o}C; ^{1}HNMR (DMSO-d_6): δ 8.17 (br s, 1 H), 7.94 (m, 4 H), 7.89 (d, *J* = 8 Hz, 2 H), 7.83 (d, *J* = 8 Hz, 2 H), 7.62 (m, 4 H), 7.56 (m, 2 H), 7.05 (d, *J* = 8 Hz, 1 H), 6.66 (br s, 1 H), 1.91 (s, 3 H); ESI-HRMS: m/z calculated for $C_{32}H_{21}N_4S$: 493.1481, found: 493.1484 (M^+ + 1).

2-Chloro-4-(2-(5-(4-cyanophenyl)thiophen-2-yl)-1-isopropyl-1H-benzo[d]imidazol-5-yl)benzonitrile (6o).

Yellow solid (0.87 gm, 61 %), mp > 300 ^{o}C; ^{1}HNMR (DMSO-d_6): δ 8.12 (m, 2H), 8.01 (d, *J* = 8 Hz, 1 H), 7.92 (m, 7 H), 7.65 (m, 2 H), 5.18 (m, 1 H), 1.69 (d, *J* = 6 Hz, 6 H); ESI-HRMS: m/z calculated for $C_{28}H_{20}ClN_4S$: 479.1092, found: 479.1086 (M^+ + 1).

4-(2-(5-(4-Cyanophenyl)thiophen-2-yl)-1-isopropyl-1H-benzo[d]imidazol-5-yl)-2-(trifluoromethyl)benzonitrile (6p).

Yellow solid (0.81 gm, 53 %), mp > 300 ^{o}C; ^{1}HNMR (DMSO-d_6): δ 8.26 (m, 4H), 7.99 (m, 3 H), 7.94 (d, *J* = 8 Hz, 2 H), 7.89 (d, *J* = 3.6 Hz, 1 H), 7.75 (d, *J* = 8.4 Hz, 1 H), 7.69 (d, *J* = 3.6 Hz, 1 H), 5.20 (m, 1 H), 1.75 (d, *J* = 6.8 Hz, 3 H), 1.71 (d, *J* = 6.8 Hz, 3 H); ESI-HRMS: m/z calculated for $C_{29}H_{20}F_3N_4S$: 513.1355, found: 513.1349 (M^+ + 1).

4-(2-(5-(4-Cyanophenyl)thiophen-2-yl)-1-isopropyl-1H-benzo[d]imidazol-5-yl)-3-methylbenzonitrile (6q).

Yellow solid (0.85 gm, 62 %), mp > 300 ^{o}C; ^{1}HNMR (DMSO-d_6): δ 7.99 (d, *J* = 8.4 Hz, 2 H), 7.93 (d, *J* = 8.4 Hz, 2 H), 7.90 (d, *J* = 4 Hz, 1 H), 7.84 (br s, 1 H), 7.81 (br s, 1 H), 7.76 (m, 2 H), 7.66 (d, *J* = 4 Hz, 1 H), 7.52 (d, *J* = 8.2 Hz, 1 H), 7.25 (d, *J* = 8.2 Hz, 1 H), 5.18 (m, 1 H), 2.35 (s, 3 H), 1.69 (d, *J* = 6.8 Hz, 6 H); ESI-HRMS: m/z calculated for $C_{29}H_{23}N_4S$: 459.1638, found: 459.1633 (M^+ + 1).

4-(5-(5-(4-Cyanophenyl)-1-isopropyl-1H-benzo[d]imidazol-2-yl)-3-methylthiophen-2-yl)benzonitrile (6r).

Yellow solid (0.53 gm, 39 %), mp > 300 ^{o}C; ^{1}HNMR (DMSO-d_6): δ 8.10 (br s, 1 H), 8.00 (m, 3 H), 7.96 (m, 3 H), 7.79 (m, 3 H), 7.64 (d, *J* = 8.4 Hz, 1 H), 7.58 (br s, 1 H), 5.23(m, 1 H), 2.43 (s, 3 H), 1.74 (d, *J* = 6.8 Hz, 6 H); ESI-HRMS: m/z calculated for $C_{29}H_{23}N_4S$: 459.1638, found: 459.1615 (M^+ + 1).

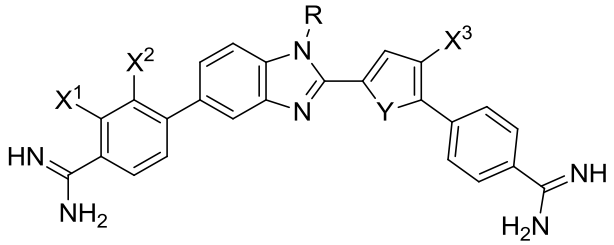
4-(5-(5-(4-Cyanophenyl)-1-methyl-1H-benzo[d]imidazol-2-yl)selenophen-2-yl)benzonitrile (6s).

Yellow solid (0.84 gm, 61 %), mp > 300 ^{o}C; ^{1}HNMR (DMSO-d_6): δ 8.05 (m, 3 H), 7.96 (d, *J* = 8 Hz, 2 H), 7.91 (m, 6 H), 7.76 (d, *J* = 8.4 Hz, 1 H), 7.70 (d, *J* = 8.4 Hz, 1 H), 4.09 (s, 3 H).

4-(5-(5-(4-Cyanophenyl)-1-isopropyl-1H-benzo[d]imidazol-2-yl)selenophen-2-yl)benzonitrile (6t).

Yellow solid (0.75 gm, 51 %), mp > 300 ^{o}C; ^{1}HNMR (DMSO-d_6): δ 8.08 (br s, 1H), 8.04 (br s, 1 H), 7.95 (m, 9 H), 7.85 (br s, 1 H), 7.65 (d, *J* = 8.4 Hz, 1 H), 5.21 (t, *J* = 5.8 Hz, 1 H), 1.70 (d, *J* = 5.8 Hz, 6 H); ESI-HRMS: m/z calculated for $C_{28}H_{21}N_4Se$: 493.0926, found: 493.0915 (M^+ + 1).

Synthesis of the diamidines (7a-t).



The above bis-nitriles (0.6 mmol) were suspended in freshly distilled THF (5 mL), and treated with a 1M $LiN(TMS)_2$[16,17] in THF solution (3.6 mL, 3.6 mmol) and the mixture was stirred for 48 h at room temperature. The reaction mixture was cooled to 0 ^{o}C and HCl saturated ethanol (3 mL) was added. The mixture was stirred for 4

h, and concentrated under reduced pressure, ether was added and the resultant solid was collected by filtration. The diamidine was purified by neutralization with 1M sodium hydroxide solution followed by filtration of the produced solid, washed with water and dried. The free base was stirred with ethanolic HCl for 24 h. The reaction mixture was concentrated under reduced pressure and acetone was added, the solid that formed was filtered and dried under vacuum at 100 ^{o}C for 24 h**.**

4-(5-(5-(4-Carbamimidoylphenyl)-1-methyl-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzimidamide (7a).[15]

4-(5-(5-(4-Carbamimidoylphenyl)-1-ethyl-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzimidamide (7b).

Yellow solid (0.225 gm, 62 %), mp > 300 ^{o}C. ^{1}HNMR (DMSO-d_6): δ 9.58 (s, 2 H), 9.54 (s, 2 H), 9.36 (s, 2 H), 9.34 (s, 2 H), 8.09 (br s, 1 H), 8.03 (d, *J* = 8.4 Hz, 2H), 8.00 (m, 6 H), 7.94 (d, *J* = 4 Hz, 1H), 7.90 (d, *J* = 4 Hz, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.76 (dd, *J* = 1.2, 8.4 Hz, 1H), 4.61 (m, 2 H), 1.46 (t, *J* = 7 Hz, 3H); ESI-HRMS: m/z calculated for $C_{27}H_{26}N_6S$: 233.0964, found: 233.0957 (Double charged amidine base M^+ + 2). Anal. Calcd. For $C_{27}H_{24}N_6S$. 3HCl. 1.75H_2O: C, 53.67; H, 5.09; N, 13.91. Found: C, 53.69; H, 5.18; N, 13.72.

4-(5-(5-(4-Carbamimidoylphenyl)-1-isopropyl-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzimidamide (7c).

Yellow solid (0.260 gm, 72 %), mp > 300 ^{o}C. ^{1}HNMR (DMSO-d_6): δ 9.56 (s, 2 H), 9.51 (s, 2 H), 9.33 (s, 2 H), 9.30 (s, 2 H), 8.13 (s, 1 H), 8.06 (m, 3 H), 8.02 (m, 7 H), 7.79 (d, *J* = 3.2 Hz, 1H), 7.76 (d, *J* = 7.4 Hz, 1H), 5.22 (m, 1H), 1.73 (d, *J* = 6.4 Hz, 6H); ESI-HRMS: m/z calculated for $C_{28}H_{27}N_6S$: 479.2018, found: 479.2012 (Amidine base M^+ + 1). Anal. Calcd. For $C_{28}H_{26}N_6S$. 3HCl. 1.5H_2O: C, 54.79; H, 5.25; N, 13.70. Found: C, 54.91; H, 5.33; N, 13.36.

4-(5-(5-(4-Carbamimidoylphenyl)-1-isobutyl-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzimidamide (7d).

Yellow solid (0.265 gm, 69 %), mp > 300 ^{o}C. ^{1}HNMR (DMSO-d_6): δ 9.51 (s, 2 H), 9.47 (s, 2 H), 9.27 (s, 2 H), 9.24 (s, 2 H), 8.11 (s, 1 H), 8.05 (m, 4 H), 7.95 (m, 6H), 7.91 (d, *J* = 9.2 Hz, 1H), 7.78 (d, *J* = 7.2 Hz, 1H), 4.49 (d, *J* = 6.8 Hz, 2H), 2.20 (m, 1 H), 0.92 (d, *J* = 6 Hz, 6H); ESI-HRMS: m/z calculated for $C_{29}H_{30}N_6S$: 247.1121, found: 247.1113 (Double charged amidine base $M^+ + 2$). Anal. Calcd. For $C_{29}H_{28}N_6S$. 3HCl. 2.10H_2O: C, 54.54; H, 5.56; N, 13.16. Found: C, 54.83; H, 5.69; N, 12.76.

4-(5-(5-(4-Carbamimidoylphenyl)-1-neopentyl-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzimidamide (7e).

Yellow solid (0.050 gm, 13 %), mp > 300 ^{o}C. ^{1}HNMR (DMSO-d_6): δ 9.55 (s, 2 H), 9.51 (s, 2 H), 9.33 (s, 2 H), 9.30 (s, 2 H), 8.12 (s, 1 H), 8.04 (m, 5 H), 7.97 (m, 5 H), 7.93 (d, *J* = 3.6 Hz, 1H), 7.81 (d, *J* = 8 Hz, 1H), 4.61 (s, 2H), 0.86 (s, 9H); ESI-HRMS: m/z calculated for $C_{30}H_{32}N_6S$: 254.1199, found: 254.1192 (Double charged amidine base $M^+ + 2$). Anal. Calcd. For $C_{30}H_{30}N_6S$. 3HCl. 3H_2O: C, 53.87; H, 5.88; N, 12.57. Found: C, 53.50; H, 5.51; N, 12.47.

4-(5-(5-(4-Carbamimidoylphenyl)-1-butyl-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzimidamide (7f).

Yellow solid (0.300 gm, 77 %), mp > 300 ^{o}C. ^{1}HNMR (DMSO-d_6): δ 9.57 (s, 2 H), 9.53 (s, 2 H), 9.35 (s, 2 H), 9.32 (s, 2 H), 8.10 (br s, 1 H), 8.05 (d, *J* = 8.8 Hz, 2H), 8.00 (m, 6 H), 7.98 (d, *J* = 6.8 Hz, 2H), 7.93 (d, *J* = 8.8 Hz, 1H), 7.82 (d, *J* = 8.8 Hz, 1H), 4.64 (t, *J* = 6.6 Hz, 2H), 1.83 (t, *J* = 7.4 Hz, 2H), 1.40 (m, 2H), 0.91 (t, *J* = 7.4 Hz, 3H); ESI-HRMS: m/z calculated for $C_{29}H_{30}N_6S$: 247.1121, found: 247.1112 (Double charged amidine base $M^+ + 2$). Anal. Calcd. For $C_{29}H_{28}N_6S$. 3HCl. 2.25H_2O: C, 54.31; H, 5.58; N, 13.11. Found: C, 53.92; H, 5.48; N, 12.90.

4-(5-(5-(4-Carbamimidoylphenyl)-1-(3-methoxypropyl)-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzimidamide (7g).

Yellow solid (0.060 gm, 10 %), mp > 300 ºC. ^{1}HNMR (DMSO-d_6): δ 9.57 (s, 2 H), 9.53 (s, 2 H), 9.35 (s, 2 H), 9.32 (s, 2 H), 8.10 (br s, 1 H), 8.05 (d, *J* = 8.8 Hz, 2H), 8.00 (m, 6 H), 7.98 (d, *J* = 6.8 Hz, 2H), 7.93 (d, *J* = 8.8 Hz, 1H), 7.82 (d, *J* = 8.8 Hz, 1H), 4.68 (t, *J* = 6.4 Hz, 2H), 3.40 (t, *J* = 5.2 Hz, 2H), 3.22 (s, 3H), 2.11 (m, 2H); ESI-HRMS: m/z calculated for $C_{29}H_{30}N_6OS$: 255.1095, found: 255.1087 (Double charged amidine base M^+ + 2). Anal. Calcd. For $C_{29}H_{28}N_6OS$. 3HCl. 1.25H_2O: C, 54.49; H, 5.28; N, 13.15. Found: C, 54.40; H, 5.30; N, 12.97.

4-(5-(5-(4-Carbamimidoylphenyl)-1-(2-methoxyethyl)-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzimidamide (7h).

Yellow solid (0.260 gm, 68 %), mp > 300 ºC. ^{1}HNMR (DMSO-d_6): δ 9.55 (s, 2 H), 9.50 (s, 2 H), 9.32 (s, 2 H), 9.29 (s, 2 H), 8.11 (br s, 1 H), 8.04 (m, 5H), 7.99 (m, 3H), 7.95 (m, 2H), 7.89 (d, *J* = 8.8 Hz, 1H), 7.80 (d, *J* = 8.8 Hz, 1H), 4.78 (br s, 2H), 3.85 (t, *J* = 4.8 Hz, 2H), 3.22 (s, 3 H); ESI-HRMS: m/z calculated for $C_{28}H_{27}N_6OS$: 495.1967, found: 495.1985 (amidine base M^+ + 1). Anal. Calcd. For $C_{28}H_{26}N_6OS$. 3HCl. 2H_2O: C, 52.65; H, 5.21; N, 13.16. Found: C, 52.63; H, 5.49; N, 13.00.

4-(5-(5-(4-Carbamimidoylphenyl)-1-cyclobutyl-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzimidamide (7i).

Yellow solid (0.162 gm, 40 %), mp > 300 ºC. ^{1}HNMR (DMSO-d_6): δ 9.57 (s, 2 H), 9.54 (s, 2 H), 9.36 (s, 2 H), 9.34 (s, 2 H), 8.15 (br s, 1 H), 8.11 (d, *J* = 8.8 Hz, 1H), 7.05 (d, *J* = 8.4 Hz, 2H), 8.02 (m, 5 H), 7.97 (m, 2H), 7.85 (d, *J* = 3.6 Hz, 1H), 7.81 (d, *J* = 9.2 Hz, 1H), 5.48 (m, 1H), 2.84 (m, 2H), 2.60 (m, 2H), 1.96 (m, 2H); ESI-HRMS: m/z calculated for $C_{29}H_{28}N_6S$: 246.1043, found: 246.1035 (Double charged amidine base M^+ + 2). Anal. Calcd. For $C_{29}H_{26}N_6S$. 3HCl. 2H_2O: C, 54.87; H, 5.24; N, 13.24. Found: C, 54.54; H, 5.12; N, 13.52.

4-(5-(5-(4-Carbamimidoylphenyl)-1-cyclopentyl-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzimidamide (7j).

Yellow solid (0.200 gm, 53 %), mp > 300 ºC. ^{1}HNMR (DMSO-d_6): δ 9.57 (s, 2 H), 9.53 (s, 2 H), 9.34 (s, 2 H), 9.31 (s, 2 H), 8.15 (d, *J* = 1.2 Hz, 1 H), 8.06 (d, *J* = 8.4 Hz, 2 H), 8.02 (m, 5 H), 7.97 (m, 2H), 7.85 (m, 2H), 7.77 (d, *J* = 8.8 Hz, 1 H), 5.34 (m, 1H), 2.26 (m, 4H), 2.06 (m, 2H), 1.81 (m, 2H); ESI-HRMS: m/z calculated for $C_{30}H_{30}N_6S$: 253.1121, found: 253.1116 (Double charged amidine base $M^+ + 2$). Anal. Calcd. For $C_{30}H_{28}N_6S$. 3HCl. 2.75H_2O: C, 54.40; H, 5.55; N, 12.69. Found: C, 54.62; H, 5.42; N, 12.43.

4-(5-(5-(4-Carbamimidoylphenyl)-1-cyclohexyl-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzimidamide (7k).

Yellow solid (0.230 gm, 58 %), mp > 300 ºC. ^{1}HNMR (DMSO-d_6): δ 9.61 (s, 2 H), 9.58 (s, 2 H), 9.39 (s, 2 H), 9.37 (s, 2 H), 8.20 (m, 1 H), 8.14 (br s, 1H), 8.07 (m, 3 H), 8.02 (m, 6 H), 7.86 (m, 1H), 7.81 (d, *J* = 8.4 Hz, 1H), 4.77 (m, 1H), 2.37 (m, 2H), 2.08 (m, 2H), 1.91 (m, 2H), 1.71 (m, 1H), 1.49 (m, 3H); ESI-HRMS: m/z calculated for $C_{31}H_{32}N_6S$: 260.1199, found: 260.1190 (Double charged amidine base $M^+ + 2$). Anal. Calcd. For $C_{31}H_{30}N_6S$. 3HCl. 2.5H_2O: C, 55.42; H, 5.70; N, 12.51. Found: C, 55.17; H, 5.49; N, 12.29.

4-(5-(5-(4-Carbamimidoylphenyl)-1-(cyclopentylmethyl)-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzimidamide (7l).

Yellow solid (0.300 gm, 74 %), mp > 300 ºC. ^{1}HNMR (DMSO-d_6): δ 9.60 (s, 2 H), 9.55 (s, 2 H), 9.36 (s, 2 H), 9.34 (s, 2 H), 8.10 (br s, 2 H), 8.06 (m, 2 H), 8.01 (m, 8 H), 7.83 (d, *J* = 8.4 Hz, 1 H), 4.64 (d, *J* = 6.8 Hz, 2 H), 2.41 (m, 1H), 1.63 (m, 4H), 1.47 (m, 2H), 1.33 (m, 2H); ESI-HRMS: m/z calculated for $C_{31}H_{30}N_6S$: 260.1199, found: 260.1194 (Double charged amidine base $M^+ + 2$). Anal. Calcd. For $C_{31}H_{32}N_6S$. 3HCl. 2.75H_2O: C, 55.05; H, 5.74; N, 12.43. Found: C, 55.09; H, 5.59; N, 12.38.

4-(5-(5-(4-carbamimidoylphenyl)-1-phenyl-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzimidamide (7m).

Yellow solid (0.225 gm, 66 %), mp > 300 ^{o}C. ^{1}HNMR (DMSO-d_6): δ 9.48 (s, 4 H), 9.25 (s, 4 H), 8.21 (d, *J* = 1.2 Hz, 1H), 8.02 (d, *J* = 8.8 Hz, 2H), 7.97 (d, *J* = 8.8 Hz, 2H), 7.91 (br s, 4 H), 7.75 (m, 3H), 7.69 (m, 4H), 7.19 (d, *J* = 8.8 Hz, 1H), 6.73 (d, *J* = 3.6 Hz, 1H); ESI-HRMS: m/z calculated for $C_{31}H_{26}N_6S$: 257.0964, found: 257.0975 (Double charged amidine base M^+ + 2). Anal. Calcd. For $C_{31}H_{24}N_6S$. 3HCl. 0.5H_2O: C, 59.13; H, 4.48; N, 13.35. Found: C, 59.01; H, 4.72; N, 13.16.

4-(5-(5-(4-Carbamimidoylphenyl)-1-(o-tolyl)-1H-benzo[d]imidazol-2-yl)thiophen-2-yl)benzimidamide (7n).

Yellow solid (0.165 gm, 42 %), mp > 300 ^{o}C. ^{1}HNMR (DMSO-d_6): δ 9.52 (s, 4 H), 9.31 (s, 4 H), 8.21 (br s, 1H), 8.01 (m, 4H), 7.93 (d, *J* = 8.2 Hz, 2H), 7.88 (d, *J* = 8.2 Hz, 2H), 7.72 (d, *J* = 8.8 Hz, 1H), 7.65 (m, 3 H), 7.60 (m, 2H), 7.11 (d, *J* = 8.4 Hz, 1H), 7.80 (d, *J* = 3.6 Hz, 1H), 1.95 (s, 3H); ESI-HRMS: m/z calculated for $C_{32}H_{28}N_6S$: 264.1043, found: 264.1038 (Double charged amidine base M^+ + 2). Anal. Calcd. For $C_{32}H_{26}N_6S$. 3HCl. 0.5H_2O: C, 59.70; H, 4.70; N, 13.06. Found: C, 60.02; H, 5.09; N, 13.01.

4-(2-(5-(4-carbamimidoylphenyl)thiophen-2-yl)-1-isopropyl-1H-benzo[d]imidazol-5-yl)-2-chlorobenzimidamide (7o).

Yellow solid (0.110 gm, 28%), mp > 300 ^{o}C. ^{1}HNMR (DMSO-d_6): δ 9.60 (br s, 4 H), 9.33 (br s, 4 H), 8.14 (br s, 1H), 8.07 (m, 4H), 8.00 (m, 2H), 7.98 (d, *J* = 3.2 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.81 (d, *J* = 3.2 Hz, 1H), 7.76 (m, 2H), 5.22 (m, 1H), 1.73 (d, *J* = 6.8 Hz, 6H); ESI-HRMS: m/z calculated for $C_{28}H_{27}ClN_6S$: 257.0848, found: 257.0837 (Double charged amidine base M^+ + 2). Anal. Calcd. For $C_{28}H_{25}ClN_6S$. 3HCl. 2.5H_2O: C, 50.51; H, 5.00; N, 12.63. Found: C, 50.12; H, 4.75; N, 12.46.

4-(2-(5-(4-Carbamimidoylphenyl)thiophen-2-yl)-1-isopropyl-1H-benzo[d]imidazol-5-yl)-2-(trifluoromethyl)benzimidamide (7p).

Yellow solid (0.320 gm, 76 %), mp > 300 ^{o}C. ^{1}HNMR (DMSO-d_6): δ 9.62 (br s, 4 H), 9.59 (s, 2 H), 9.38 (s, 2 H), 8.26 (br s, 2H), 8.19 (s, 1H), 8.05 (m, 3H), 7.98 (m, 3H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.79 (m, 2H), 5.23 (br s, 1H), 1.73 (d, *J* = 4.8 Hz, 6H); ESI-HRMS: m/z calculated for $C_{29}H_{27}F_3N_6S$: 274.0980, found: 274.0971 (Double charged amidine base M^+ + 2). Anal. Calcd. For $C_{29}H_{25}F_3N_6S$. 3HCl. 2.5H_2O: C, 49.77; H, 4.75; N, 12.01. Found: C, 49.72; H, 4.69; N, 11.86.

4-(2-(5-(4-Carbamimidoylphenyl)thiophen-2-yl)-1-isopropyl-1H-benzo[d]imidazol-5-yl)-3-methylbenzimidamide (7q).

Yellow solid (0.16 gm, 42 %), mp > 300 ^{o}C. ^{1}HNMR (DMSO-d_6): δ 9.58 (s, 4 H), 9.40 (s, 4 H), 8.07 (d, *J* = 8.4 Hz, 2H), 8.02 (m, 4H), 7.95 (br s, 1H), 7.91 (m, 2H), 7.86 (d, *J* = 8 Hz, 1H), 7.58 (d, *J* = 8 Hz, 1H), 7.47 (d, *J* = 8.8 Hz, 1H), 5.22 (m, 1H), 2.38 (s, 3H), 1.74 (d, *J* = 6.8 Hz, 6H); ESI-HRMS: m/z calculated for $C_{29}H_{30}N_6S$: 247.1121, found: 247.1114 (Double charged amidine base M^+ + 2). Anal. Calcd. For $C_{29}H_{28}N_6S$. 3HCl. 1.5H_2O: C, 55.48; H, 5.46; N, 13.39. Found: C, 55.45; H, 5.38; N, 13.06.

4-(5-(5-(4-Carbamimidoylphenyl)-1-isopropyl-1H-benzo[d]imidazol-2-yl)-3-methylthiophen-2-yl)benzimidamide (7r).

Yellow solid (0.14 gm, 38 %), mp > 300 ^{o}C. ^{1}HNMR (DMSO-d_6): δ 9.56 (s, 2 H), 9.54 (s, 2 H), 9.36 (s, 2 H), 9.32 (s, 2 H), 8.14 (br s, 1H), 8.07 (d, *J* = 8 Hz, 2H), 8.00 (m, 4H), 7.84 (d, *J* = 8 Hz, 2H), 7.81 (br s, 1H), 7.71 (d, *J* = 8.4 Hz, 1H), 7.64 (br s, 1H), 5.26 (m, 1H), 2.46 (s, 3H), 1.77 (d, *J* = 6.8 Hz, 6H); ESI-HRMS: m/z calculated for $C_{29}H_{30}N_6S$: 247.1121, found: 247.1112 (Double charged amidine base M^+ + 2). Anal. Calcd. For $C_{29}H_{28}N_6S$. 3HCl. 1.5H_2O: C, 55.48; H, 5.46; N, 13.39. Found: C, 55.48; H, 5.52; N, 13.19.

4-(5-(5-(4-Carbamimidoylphenyl)-1-methyl-1H-benzo[d]imidazol-2-yl)selenophen-2-yl)benzimidamide (7s).

Yellow solid (0.150 gm, 39 %), mp > 300 ºC. ^{1}HNMR (DMSO-d_6): δ 9.56 (s, 2 H), 9.52 (s, 2 H), 9.31 (s, 2 H), 9.29 (s, 2 H), 8.24 (d, *J* = 3.6 Hz, 1H), 8.15 (d, *J* = 3.6 Hz, 1H), 8.10 (br s, 1H), 7.99 (m, 9H), 7.85 (d, *J* = 8.8 Hz, 1H), 4.15 (s, 3H); ESI-HRMS: m/z calculated for $C_{26}H_{24}N_6Se$: 250.0608, found: 250.0599 (Double charged amidine base M^+ + 2). Anal. Calcd. For $C_{26}H_{22}N_6Se$. 3HCl. $2H_2O$: C, 48.59; H, 4.55; N, 13.08. Found: C, 48.48; H, 4.39; N, 13.10.

4-(5-(5-(4-Carbamimidoylphenyl)-1-isopropyl-1H-benzo[d]imidazol-2-yl)selenophen-2-yl)benzimidamide (7t).

Yellow solid (0.325 gm, 79%), mp > 300 ºC. ^{1}HNMR (DMSO-d_6): δ 9.56 (s, 2 H), 9.53 (s, 2 H), 9.40 (s, 2 H), 9.32 (s, 2 H), 8.11 (m, 3H), 8.09 (m, 9H), 7.79 (d, *J* = 8.4 Hz, 1H), 5.19 (m, 1H), 1.73 (d, *J* = 6.4 Hz, 6H); ESI-HRMS: m/z calculated for $C_{28}H_{28}N_6Se$: 264.0765, found: 264.0756 (Double charged amidine base M^+ + 2). Anal. Calcd. For $C_{28}H_{26}N_6Se$. 3HCl. $2.5H_2O$: C, 49.47; H, 5.04; N, 12.37. Found: C, 49.16; H, 5.13; N, 12.12.

Biophysical Experimental

Materials

In the DNA thermal melting (T_m), circular dichroism (CD) experiments, the hairpin oligomer sequences were used as shown in Figure 1. In SPR experiments, 5′-biotin labeled hairpin DNA oligomers were used. All DNA oligomers were obtained from

Integrated DNA Technologies, Inc. (IDT, Coralville, IA) with reverse-phase HPLC purification and mass spectrometry characterization.

The buffer used in T_m and CD experiments was 50 mM Tris-HCl, 100 mM NaCl, 1 mM EDTA, pH 7.4 (TNE 100). The biosensor-surface plasmon resonance (SPR) experiments were performed in filtered, degassed TNE 100 with 0.05% (v/v) surfactant P20.

UV-vis Thermal Melting (T_m)

DNA thermal melting experiments were performed on a Cary 300 Bio UV-vis spectrophotometer (Varian). The concentration of each hairpin DNA sequence was 3 μM in TNE 100 using 1 cm quartz cuvettes. The solutions of DNA and ligands were tested with the ratio of 2:1 [ligand] / [DNA]. All samples were increased to 95 °C and cooled down to 25 °C slowly before each experiment. The spectrophotometer was set at 260 nm with a 0.5 °C/min increase beginning at 25 °C, which is below the DNA melting temperature and ending above it at 95 °C. The absorbance of the buffer was subtracted, and a graph of normalized absorbance versus temperature was created using KaleidaGraph 4.0 software. The ΔT_m values were calculated using a combination of the derivative function and estimation from the normalized graphs.

Biosensor-Surface Plasmon Resonance (SPR)

SPR measurements were performed with a four-channel Biacore T200 optical biosensor system (GE Healthcare, Inc., Piscataway, NJ). A streptavidin-derivatized (SA) CM5 sensor chip was prepared for use by conditioning with a series of 180 s

injections of 1 M NaCl in 50 mM NaOH (activation buffer) followed by extensive washing with HBS buffer (10 mM HEPES, 150 mM NaCl, 3 mM EDTA, and 0.05% P20, pH 7.4). Biotinylated-DNA samples (AAATTT, AAAGTTTand AAAGCTTT hairpins, Figure1) of 25-30 nM were prepared in HBS buffer and immobilized on the flow cell surface by noncovalent capture. Flow cell 1 was left blank as a reference, while flow cells 2−4 were immobilized separately by manual injection of biotinylated-DNA stock solutions (flow rate of 1 μL/min) until the desired amount of DNA response units (RU) was obtained (250−300 RU). Ligand solutions were prepared with degassed and filtered TNE 100 with 0.05% (v/v) surfactant P20 by serial dilutions from a concentrated stock solution. Typically, a series of different ligand concentrations (2 nM to 500 nM) were injected over the DNA sensor chip at a flow rate of 100 μL/min for 180 s, followed by buffer flow for ligand dissociation (600−1800 s). After each cycle, the sensor chip surface was regenerated with a 10 mM glycine solution (pH 2.5) for 30 s followed by multiple buffer injections to yield a stable baseline for the following cycles. RU_{obs} was plotted as a function of free ligand concentration (C_{free}), and the equilibrium binding constants (K_A) were determined either with a one-site binding model, where $r = (RU_{obs}/RU_{max})$ represents the moles of bound compound/mol of DNA hairpin duplex and K is macroscopic binding constant.

$$\boldsymbol{r = K * C_{free}/1 + K * C_{free}} \qquad \textbf{(1)}$$

RU_{max} can be used as a fitting parameter, and the obtained value compared to the predicted maximal response per bound ligand can also be used to independently evaluate the stoichiometry. Kinetic analyses were performed by globally fitting the binding results for the entire concentration series using a standard 1:1 kinetic model with integrated mass transport-limited binding parameters as described previously.

[18,19] To obtain the optimized kinetic constants (k_a, k_d), we have immobilized different amount of the target DNAs on CM5 chip surfaces in three independent experiments with different sensor chips.

Circular Dichroism (CD)

Circular dichroism experiments were performed on a Jasco J-810 CD and Jasco J-1500 CD spectrometer in 1 cm quartz cuvette at 25 °C. A buffer scan as a baseline was collected first in the same cuvette and subtracted from the scan of following samples. The hairpin DNA sequence AAAGTTT (5 µM), Figure 1, in TNE 100 was added to the cuvette prior to the titration experiments and then the compound was added to the DNA solution and incubated for 10 min to achieve equilibrium binding for the DNA-ligand complex formation. For each titration point, four spectra were averaged from 500 to 230 nm wavelength with scan speed of 50 nm/min, with a response time of 1 s. Baseline-subtracted graphs were created using the KaleidaGraph 4.0 software.

Structural Calculations

Molecular torsional angle map calculations of the compounds were performed in the Spartan'16 software. The "constrain dihedral" command was used with selected compounds to restrain four atoms to define the middle rotation bond and two terminal bonds which formed the dihedral as the calculation targets. The calculation range was set from 0° to 100° or 180° through 11 or 19 steps. Calculations were carried out with the energy profile method at ground state with density functional B3LYP/6-31G* in vacuum. After the calculations, the relative energy (rel. E) (kJ/mol) was displayed in a spreadsheet. The torsional angle map can be created with

the constraint of the torsional angle as the X-axis and rel. E as the Y-axis by using KaleidaGraph 4.0 software.

Ab-Initio Calculations and Molecular Dynamic (MD) Simulation

Optimization and electrostatic potential calculations were performed for the DB2708 molecule using DFT/B3LYP theory with the 6-31+G* basis set in Gaussian 09 (Gaussian, Inc., 2009, Wallingford, CT) with Gauss-view 5.09.[20] Partial charges were derived using the RESP fitting method (Restrained Electrostatic potential).[21,22] AMBER 14 (Assisted Model Building with Energy Refinement) software suite was used to perform molecular dynamic (MD) simulations.[23] Canonical *B*-form *ds*[(5'-CCAAAGTTTGG-3')(5'-CCAAACTTTGG-3')] DNA was built in Nucleic Acid Builder (NAB) tool in AMBER. AMBER preparation and force field parameter files required to run molecular dynamic simulations for DB2708 molecule were produced using ANTECHAMBER.[24] Specific atom types assigned for DB2708 molecule were adapted from the ff99 force field. Most of the force field parameters for DB2708 molecule were derived from the existing set of bonds, angles and dihedrals for the similar atom types in parm99 and GAFF force fields.[25] Some dihedral angle parameters were obtained from previously reported parametrized data.[26, 27] Parameters of DB2708 in frcmod file are listed at the Table S1.

AutoDock Vina program was used to dock the DB2528 in the minor groove of DNA to obtain the initial structure for DB2708-DNA complex.[28] MD simulations were performed in explicit solvation conditions where the DNA-DB2708 complex was placed in a truncated octahedron box filled with TIP3P water using xleap program in AMBER. Sodium ions were used to neutralize the system. A 10 Å cutoff was applied on all van der Waals interactions. The MD simulation was

carried out using the Sander module with SHAKE algorithm applied to constrain all bonds. Initially, the system was relaxed with 500 steps of steepest-descent energy minimization. The temperature of the system was then increased from 0 K to 310 K for over 10 ps under constant-volume conditions. In the final step, the production run on the system was subsequently performed for 500 ns under NPT (constant-pressure) conditions. Coordinate file of DB2708-DNA complex along with water molecules in proximity is also attached.

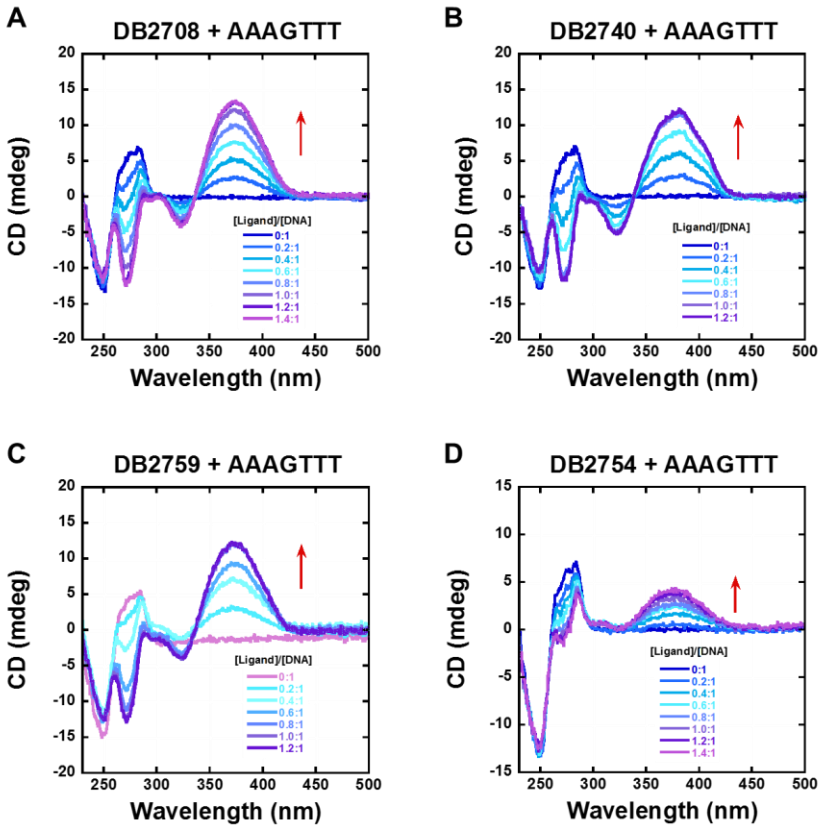


Figure S1. Circular dichroism spectra for the titration of representative compounds, A) DB2708, B) DB2740, C) DB2759 and D) 2754 with a 5 μM AAAGTTT sequence in Tris-HCl buffer (50 mM Tris-HCl, 100 mM NaCl, 1 mM EDTA, pH 7.4) at 25℃. Arrows indicate the changes.

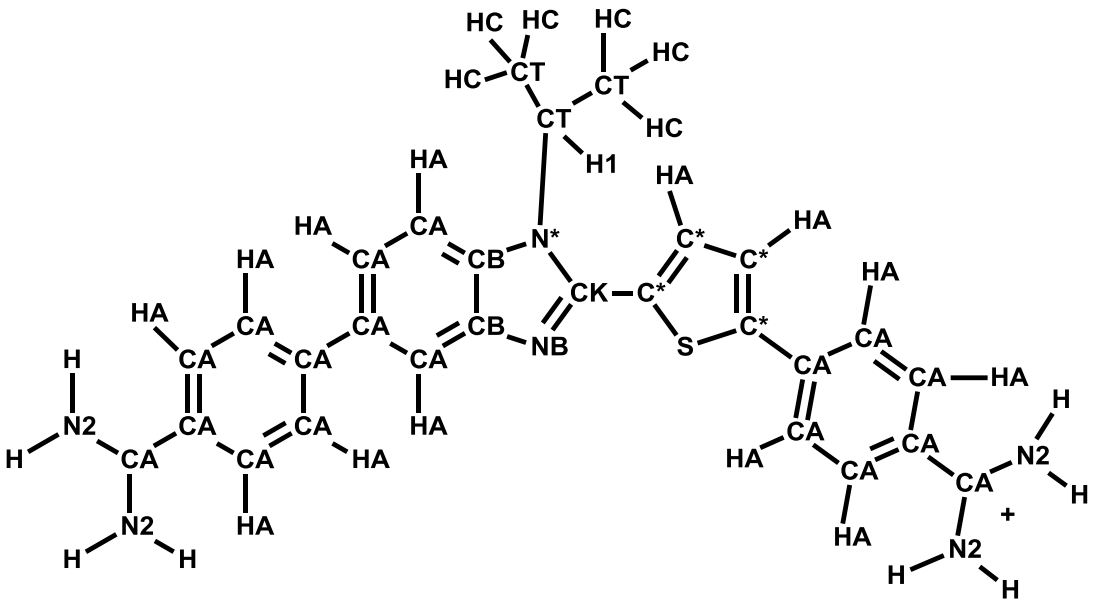
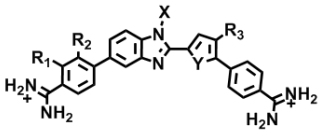
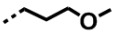


Figure S2. Molecular structure with specific atom types used for the DB2708 molecule.

Table S1. Thermal melting studies (ΔT_m, ℃) of DB2457 and analogues with pure AT and mixed DNA sequences. [a]



Compounds	R_1	R_2	R_3	X	Y	ΔT_m AAATTT (70℃)	ΔT_m AAAGTTT (66℃)	ΔT_m AAAGCTTT (67℃)
DB2457 (7a)	H	H	H	Me	S	6	14	5
DB2737 (7b)	H	H	H	Et	S	7	15	7
DB2708 (7c)	H	H	H	*i*-Pr	S	4	14	5
DB2711 (7d)	H	H	H		S	5	13	5
DB2718 (7e)	H	H	H		S	2	11	4
DB2715 (7f)	H	H	H		S	5	13	5
DB2728 (7g)	H	H	H		S	4	13	5
DB2764 (7h)	H	H	H		S	3	13	5
DB2726 (7i)	H	H	H		S	4	14	4
DB2714 (7j)	H	H	H		S	4	13	5
DB2727 (7k)	H	H	H		S	4	13	3
DB2738 (7l)	H	H	H		S	4	13	5
DB2740(7m)	H	H	H		S	5	17	7
DB2747 (7n)	H	H	H		S	7	16	9
DB2759 (7o)	Cl	H	H	*i*-Pr	S	3	12	3
DB2762 (7p)	CF_3	H	H	*i*-Pr	S	1	8	3
DB2753 (7q)	H	Me	H	*i*-Pr	S	1	3	2
DB2754 (7r)	H	H	Me	*i*-Pr	S	1	4	2
DB2673 (7s)	H	H	H	Me	Se	7	12	5
DB2712 (7t)	H	H	H	*i*-Pr	Se	5	13	6

a. $\Delta T_m = T_m$ (the complex) - T_m (the free DNA). 3 μM DNA sequences were studied in Tris-HCl buffer (50 mM Tris-HCl, 100 mM NaCl, 1 mM EDTA, pH 7.4) with the ratio of 2:1 [ligand]/[DNA]. An average of two independent experiments with a reproducibility of 0.5 ℃.
Full DNA sequences: AAATTT: 5'-CCAAATTTGCCTCTGCAAATTTGG-3';
AAAGTTT: 5'-CCAAAGTTTGCTCTCAAACTTTGG-3';
AAAGCTTT: 5'-CCAAAGCTTTGCTCTCAAAGCTTTGG-3'.

Table S2. Frcmod file of the DB2708 molecule

```
remark goes here
MASS
N2 14.01         0.530              parm99
CA 12.01         0.360              parm99
CB 12.01         0.360              parm99
C* 12.01         0.360              gaff SP2 carbon at non-pure aromatic system
CK 12.01         0.360              parm99
CT 12.01         0.878              parm99
HA 1.008         0.167              parm99
H  1.008         0.161             parm99
HC 1.008         0.135              parm99
H1 1.008         0.135              parm99
N* 14.01         0.530             parm99
NB 14.01         0.530              parm99
S  32.06        2.900             gaff

BOND
CA-CA  469.0    1.400       parm99
CA-CB  469.0    1.404       parm99
CB-CB  520.0    1.370       parm99
CB-N*  436.0    1.374      parm99
CB-NB  414.0    1.391       parm99
CT-N*  337.0    1.475      parm99
CT-CT  310.0    1.526       parm99
CA-HA  367.0    1.080       parm99
CT-H1  340.0    1.090      parm99
CT-HC  340.0    1.090       parm99
CK-N*  440.0    1.371      parm99
CK-NB  529.0    1.304       parm99
CK-C*  418.3    1.4290      SOURCE1   740 0.0069 cc-cc gaff similar to gaussian bond
C*-C*  418.3    1.4290     SOURCE1    740 0.0069  gaff
C*-SS  279.3    1.7370      SOURCE3     52 0.0194  gaff
C*-HA  347.2    1.0850      SOURCE3    7400.0039  gaff
CA-C*  411.7    1.4340      SOURCE1     80 0.0000  gaff
CA-N2  481.0    1.340       parm99
S -C*  279.3    1.7370     SOURCE3      52  0.0194  gaff

ANGLE
CA-CA-CA    63.0      120.00    parm99
CA-CA-CB    63.0      120.00    parm99
CA-CA-HA    50.0      120.00    parm99
CA-CB-CB    63.0      117.30    parm99
CB-CA-HA    50.0      120.00    parm99
CA-CB-NB    70.0      132.40    parm99
CA-CB-N*    70.0      132.40    parm99 CA-CB-NB parm99
CB-CB-N*    70.0      106.20    parm99
CB-CB-NB    70.0      110.40    parm99
CT-CT-CT    40.0      109.50    parm99
CT-CT-H1    50.0      109.50    parm99
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CB-N*-CT    70.0      125.80    parm99
CT-CT-N*    50.0      109.50    parm99
N*-CK-NB    70.0      113.90    parm99
CB-NB-CK    70.0      103.80    parm99
CB-N*-CK    70.0      105.40    parm99
C*-CK-NB    67.53     121.69      CORR       105 cc-cc-nc GAFF
C*-CK-N*    67.53     121.69      CORR       105 cc-cc-nc GAFF
C*-C*-CK    66.24     121.77      CORR  c2-cc-cc GAFF
C*-C*-C*    67.880    110.700 SOURCE3          54   3.4091 gaff
CK-N*-CT    70.0      128.80    parm99
CB-N*-CT    70.0      125.80    parm99
H1-CT-N*    50.0      109.50    parm99
HC-CT-HC    35.0      109.50    parm99
HC-CT-CT    50.0      109.50    parm99
C*-C*-HA    47.14     120.86      CORR       1751 cc-cc-ha GAFF
C*-S -C*    41.930    89.910    SOURCE3          11   2.2164 cc-ss-cc gaff
CA-C*-S     78.690    120.980SOURCE4           28   1.8865 ca-cc-ss gaff
S -C*-C*    80.780    115.020  SOURCE3          2    0.0000 cc-cc-ss gaff
CA-C*-C*    67.660    111.040SOURCE3           9    7.9455 ca-cc-cc gaff
CA-CA-N2    70.0      119.99    parm99, CM-CA-N2, Gaussian-angle
N2-CA-N2    70.0      120.00    parm99
H -N2-H     35.0      120.00    parm99
CA-N2-H     50.0      120.00    parm99
CA-CA-C*    5.99      120.10    SOURCE3          103 0.3451 ca-ca-cc
CK-C*-S     78.460     120.940          SOURCE4          31   1.2422 ce-cc-ss--gaff

DIHE
N2-CA-N2-H     4    9.60        180.0           2.0    parm 99, X -CA-N2-X
H -N2-CA-CA    4    9.60        180.0           2.0    parm 99, X -CA-N2-X
N2-CA-CA-CA    4   -3.118       0.000           -2.0    DB921
N2-CA-CA-CA    4    0.609       90.000           1.0    DB921
CA-CA-CA-CA    4   14.50        180.0           2.0    parm99, X -CA-CA-X
CA-CA-CA-HA    4   14.50        180.0           2.0    parm99, X -CA-CA-X
HA-CA-CA-HA    4   14.50        180.0           2.0    parm99, X -CA-CA-X
CA-CA-CA-CB    4   14.50        180.0           2.0    parm99, X -CA-CA-X
CB-CA-CA-HA    4   14.50        180.0           2.0    parm99, X -CA-CA-X
CA-CA-CB-CB    4   14.00        180.0           2.0    parm99, X -CA-CB-X
HA-CA-CB-N*    4   14.00        180.0           2.0    parm99, X -CA-CB-X
HA-CA-CB-NB    4   14.00        180.0           2.0    parm99, X -CA-CB-X
HA-CA-CB-CB    4   14.00        180.0           2.0    parm99, X -CA-CB-X
CB-CB-N*-CK    4    6.60        180.0           2.0    parm99, X -CB-N*-X
CB-CB-N*-CT    4    6.60        180.0           2.0    parm99,  X -CB-N*-X
H1-CT-N*-CB    1    0.00        000.0           -2.     parm98, TC,PC,PAK FOR OS-CT-N*CK
H1-CT-N*-CB    1    2.50        0.0             1.     parm98, TC,PC,PAK FOR OS-CT-N*CK
CA-CB-N*-CT    4    6.60        180.0           2.0    parm99, X -CB-N*-X
CA-CB-CB-NB    4   21.80        180.0           2.0    parm99, X -CB-CB-X
CA-CB-CB-N*    4   21.80        180.0           2.0    parm99, X -CB-CB-X
CB-N*-CT-CT    1    0.00        000.0           -2.     parm98, TC,PC,PAK FOR OS-CT-N*CK
CB-N*-CT-CT    1    2.50        0.0             1.     parm98, TC,PC,PAK FOR OS-CT-N*CK
N*-CT-CT-HC    9    1.40        0.0             3.     JCC,7,(1986),230, X -CT-CT-X
CA-CA-CB-NB    4   14.00        180.0           2.     intrpol.bsd.on C6H6, X -CA-CB-X
```

CA-CB-NB-CK 2 5.10 180.0 2.0 parm99, X -CB-NB-X
CA-CB-N*-CK 4 6.60 180.0 2. JCC,7,(1986),230, X -CB-N*-X
NB-CK-N*-CB 4 6.80 180.0 2.0 parm99, X -CK-N*-X
N*-CK-NB-CB 2 20.00 180.0 2.0 parm99, X -CK-NB-X
C*-CK-NB-CB 2 20.00 180.0 2.0 parm99, X -CK-NB-X
C*-CK-NB-CB 2 20.00 180.0 2. JCC,7,(1986),230, X -CK-NB-X
NB-CK-C*-S 4 -0.6 180.0 -4.0 DB921 for NB-CK-CA-CA
NB-CK-C*-S 4 3.1 180.0 -2.0 DB921 for NB-CK-CA-CA
NB-CK-C*-S 4 -0.7 360.0 1.0 DB921 for NB-CK-CA-CA
CB-N*-CK-C* 4 6.80 180.0 2.0 parm99, X -CK-N*-X
NB-CK-C*-C* 4 3.1 180.0 -2.0 DB921 for NB-CK-CA-CA
NB-CK-C*-C* 4 -0.6 180.0 -4.0 DB921 for NB-CK-CA-CA
NB-CK-C*-C* 4 -0.7 360.0 1.0 DB921 for NB-CK-CA-CA
N*-CK-C*-C* 4 3.42 180.0 2.0 New parameter for N*-CK-CA-CA
N*-CK-C*-S 4 -0.6 180.0 -4.0 DB921 for NB-CK-CA-CA
N*-CK-C*-S 4 3.1 180.0 -2.0 DB921 for NB-CK-CA-CA
N*-CK-C*-S 4 -0.7 360.0 1.0 DB921 for NB-CK-CA-CA
CT-N*-CK-C* 4 6.80 180.0 2.0 parm99, X -CK-N*-X
CK-C*-C*-C* 4 16.000 180.000 2.0 stat value of parm94 X -cc-cc-X
CK-C*-C*-HA 4 16.000 180.000 2.0 stat value of parm94 X -cc-cc-X
C*-C*-C*-HA 4 16.000 180.000 2.0 stat value of parm94 X -cc-cc-X
C*-S-C*-CA 2 2.200 180.000 2.0 X -c2-ss-X
S-C*-CA-CA 4 3.42 180.0 2.0 New parameter for N*-CK-CA-CA
HA-CA-CA-C* 4 14.50 180.0 2.0 parm99, X -CA-CA-X
CA-CA-CA-C* 4 14.50 180.0 2.0 parm99, X -CA-CA-X
CA-CA-C*-C* 4 3.1 180.0 -2.0 DB921 for NB-CK-CA-CA
CA-CA-C*-C* 4 -0.6 180.0 -4.0 DB921 for NB-CK-CA-CA
CA-CA-C*-C* 4 -0.7 360.0 1.0 DB921 for NB-CK-CA-CA
CA-C*-C*-HA 4 16.000 180.000 2.0 stat value of parm94 X cc-cc-
S -C*-C*-HA 4 16.000 180.000 2.0 statistic value of parm94 X -cc-cc-X
S -C*-C*-C* 4 16.000 180.000 2.0 stat value of parm94 X -cc-cc-X
C*-C*-C*-C* 4 16.000 180.000 2.0 stat value of parm94 X -cc-cc-X
CA-C*-C*-C* 4 16.000 180.000 2.0 stat value of parm94 X -cc-cc-X
HA-C*-C*-HA 4 16.000 180.000 2.0 stat value of parm94 X -cc-cc-X
CK-C*-C*-S 4 16.000 180.000 2.0 stat value of parm94 X -cc-cc-X
C*-S -C*-C* 1 1.100 180.000 2.000 same as X -c2-ss-X, cc-ss-cc-cd
C*-S -C*-CK 1 1.100 180.000 2.000 same as X -c2-ss-X, cc-ss-cc-cc
HC-CT-CT-HC 1 0.15 0.0 3.000 Junmei et al, 199
HC-CT-CT-CT 1 0.16 0.0 3. Junmei et al, 1999
H1-CT-N*-CK 1 0.00 000.0 -2.000 parm98,TC,PC,PAK OS-CT-N*-CK
H1-CT-N*-CK 1 2.50 0.0 1.000 parm98, TC,PC,PAK FOR OS-CT-N*-CK

IMPROPER
CA-CB-CB-NB 1.1 180.0 2.0 Using default value
CA-CA-CA-HA 1.1 180.0 2.0 General improper torsional angle (2 general atom types)
CA-CA-CA-C* 1.1 180.0 2.0 Using default value
CA-CA-CA-C* 1.1 180.0 2.0 Using default value
C*-C*-C*-HA 1.1 180.0 2.0 Using default value
CA-CA-CA-HA 1.1 180.0 2.0 Using default value
CA-CA-CA-CA 1.1 180.0 2.0 Using default value

```
CA-N2-CA-N2      1.1      180.0      2.0      Using default value
CT-CK-N*-CB      1.1      180.0      2.0      Using default value
CA-CB-CB-N*      1.1      180.0      2.0      Using default value
CK-N*-CK-NB      1.1      180.0      2.0      Using default value
C*-C*-C*-S       1.1      180.0      2.0      Using default value
CA-C*-C*-S       1.1      180.0      2.0      Using default value
CA-CA-CA-CA      1.1      180.0      2.0      Using default value
CA-CA-CA-CA      1.1      180.0      2.0      Using default value

NONBON
  H1        1.3870  0.0157          parm99
  H         0.6000  0.0157          parm99
  HA        1.4590  0.0150          parm99
  CT        1.9080  0.1094          parm99
  CA        1.9080  0.0860          parm99 (C*)
  CB        1.9080  0.0860          parm99 (C*)
  CK        1.9080  0.0860          parm99 (C*)
  N*        1.8240  0.1700          parm99 (N)
  NB        1.8240  0.1700          parm99 (N)
  N2        1.8240  0.1700          parm99 (N)
  C*        1.9080  0.0860          parm99
  S         2.0000  0.2500          parm9
  HC        1.4870  0.0157          OPLS
```

References

(1) Farahat, A. A.; Paliakov, E.; Kumar, A.; Barghash, A.-E. M.; Goda, F. E.; Eisa, H. M.; Wenzler, T.; Brun, R.; Liu, Y.; Wilson, W. D.; Boykin, D. W. *Bioorg. Med. Chem.* **2011**, *19* (7), 2156.

(2) McKenzie, B. M.; Miller, A. K.; Wojtecki, R. J.; Johnson, J. C.; Burke, K. A.; Tzeng, K. A.; Mather, P. T.; Rowan, S. J. *Tetrahedron* **2008**, *64* (36), 8488.

(3) Schelz, D.; Rotzler, N. *Dyes and Pigments* **1983**, *4* (4), 305.

(4) Vivian, D. L.; Hartwell, J. L. *J. Org. Chem.* **1953**, *18* (8), 1065.

(5) Farahat, A. A.; Kumar, A.; Say, M.; Barghash, A. E.-D. M.; Goda, F. E.; Eisa, H. M.; Wenzler, T.; Brun, R.; Liu, Y.; Mickelson, L.; Wilson, W. D.; Boykin, D. W. *Bioorg. Med. Chem.* **2010**, *18* (2), 557.

(6) Branowska, D.; Farahat, A. A.; Kumar, A.; Wenzler, T.; Brun, R.; Liu, Y.; Wilson, W. D.; Boykin, D. W. *Bioorg. Med. Chem.* **2010**, *18* (10), 3551.

(7) Reid, C. S.; Farahat, A. A.; Zhu, X.; Pandharkar, T.; Boykin, D. W.; Werbovetz, K. A. *Bioorg. Med. Chem. Lett.* **2012**, *22* (22), 6806.

(8) Farahat, A. A.; Boykin, D. W. *Heterocycles* **2012**, *85* (10), 2437.

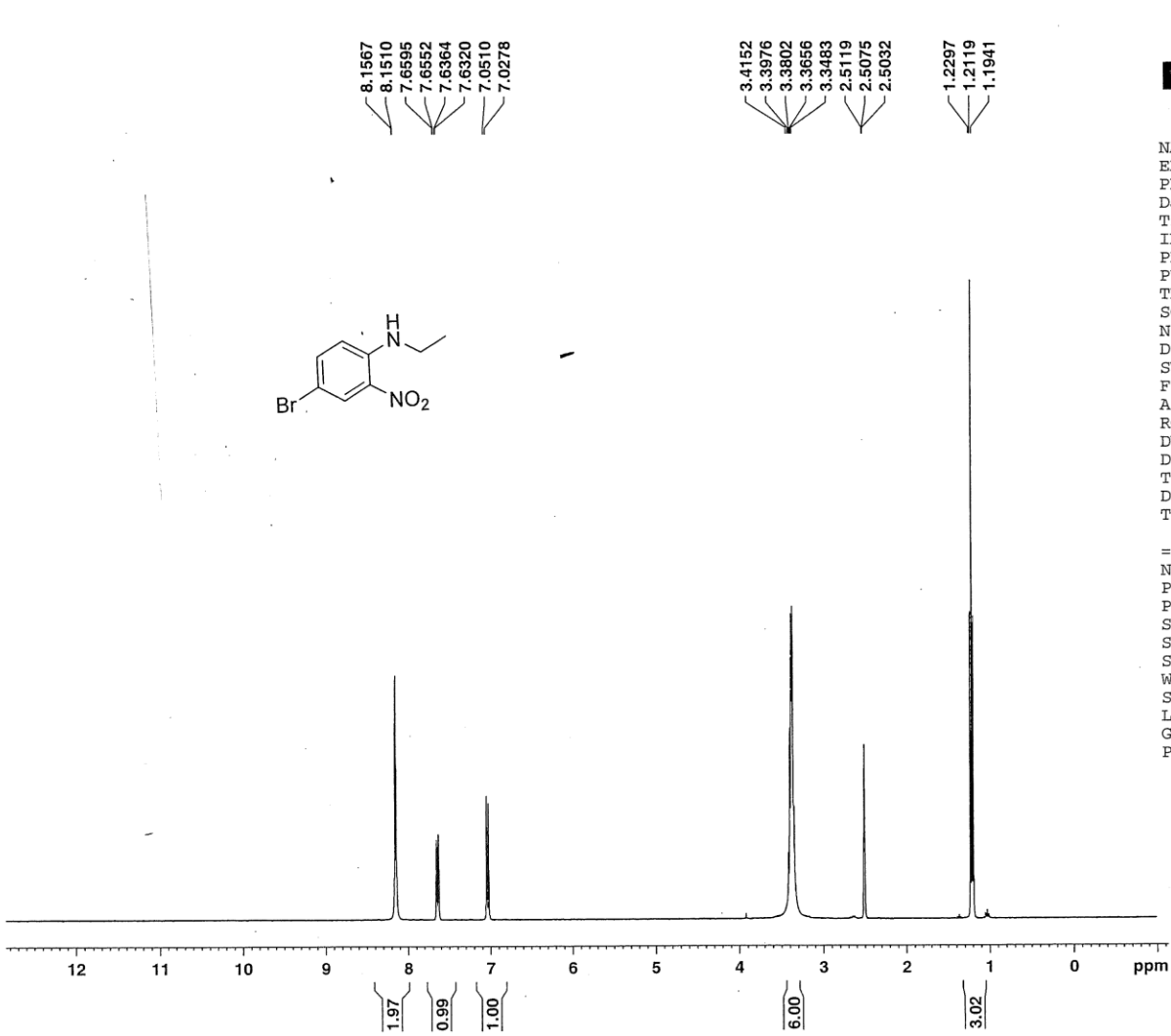
(9) Farahat, A. A.; Boykin, D. W. *J. Heterocyclic Chem.* **2013**, *50* (3), 585.

(10) Farahat, A. A.; Kumar, A.; Barghash, A. E.-D. M.; Goda, F. E.; Eisa, H. M.; Boykin, D. W. *J. Heterocyclic Chem.* **2010**, *47* (1), 167.

(11) Laughlin, S.; Wang, S.; Kumar, A.; Farahat, A. A.; Boykin, D. W.; Wilson, W. D. *Chem. Eur. J.* **2015**, *21* (14), 5528.

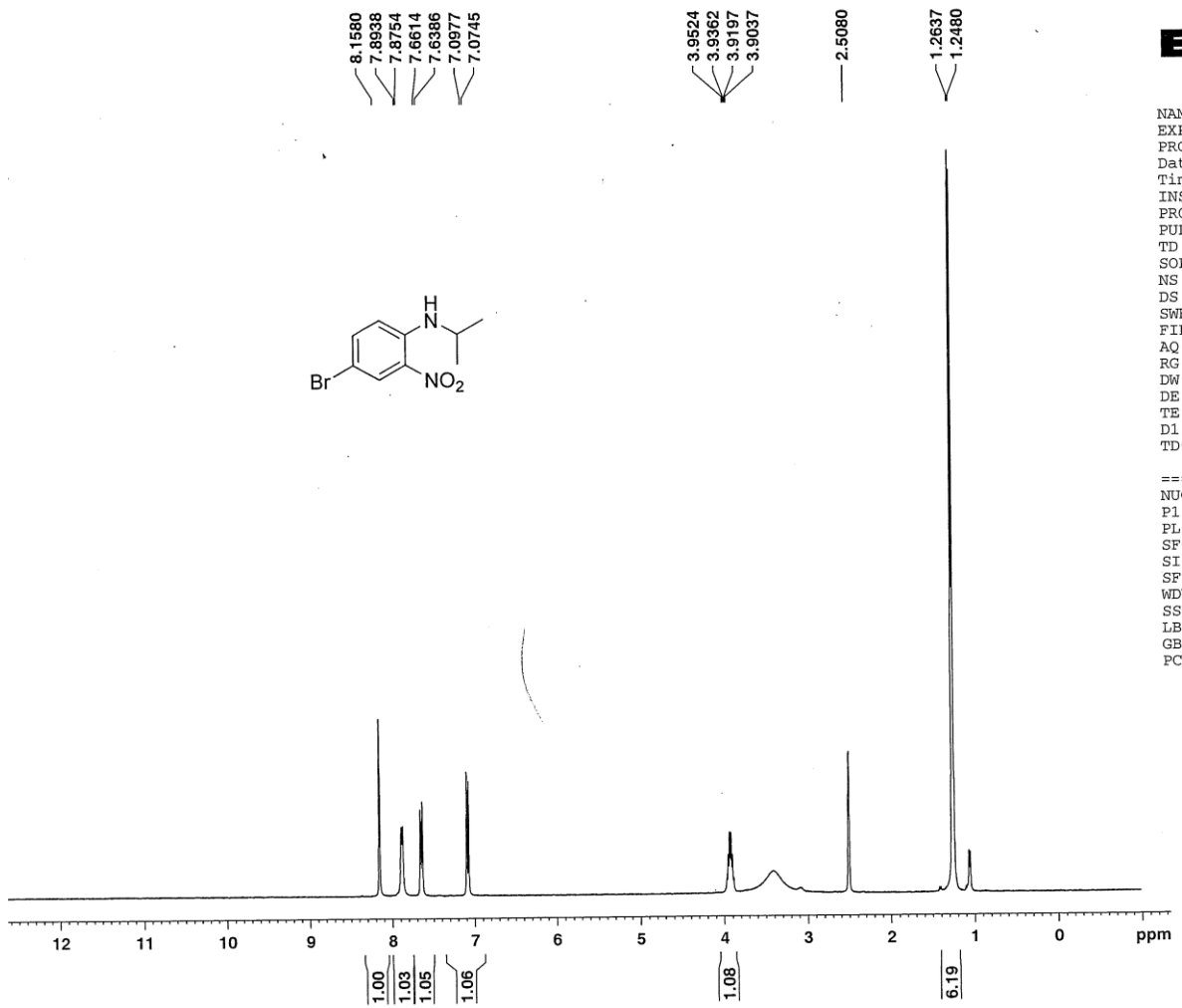
(12) Farahat, A. A.; Bennett-Vaughn, C.; Mineva, E. M.; Kumar, A.; Wenzler, T.; Brun, R.; Liu, Y.; Wilson, W. D.; Boykin, D. W. *Bioorg. Med. Chem. Lett.* **2016**, *26* (24), 5907.

(13) Paul, A.; Kumar, A.; Nanjunda, R.; Farahat, A. A.; Boykin, D. W.; Wilson, W. D. *Org. Biomol. Chem.* **2017**, *15* (4), 827.
(14) Farahat, A. A.; Ismail, M. A.; Kumar, A.; Wenzler, T.; Brun, R.; Paul, A.; Wilson, W. D.; Boykin, D. W. *Eur. J. Med. Chem.* **2018**, *143*, 1590.
(15) Guo, P.; Paul, A.; Kumar, A.; Farahat, A. A.; Kumar, D.; Wang, S.; Boykin, D. W.; Wilson, W. D. *Chem. Eur. J.* **2016**, *22* (43), 15404.
(16) Farahat, A. A.; Kumar, A.; Say, M.; Wenzler, T.; Brun, R.; Paul, A.; Wilson, W. D.; Boykin, D. W. *Eur. J. Med. Chem.* **2017**, *128*, 70.
(17) Munde, M.; Kumar, A.; Peixoto, P.; Depauw, S.; Ismail, M. A.; Farahat, A. A.; Paul, A.; Say, M. V.; David-Cordonnier, M.-H.; Boykin, D. W.; Wilson, W. D. *Biochemistry* **2014**, *53* (7), 1218.
(18) Liu, Y.; Kumar, A.; Depauw, S.; Nhili, R.; David-Cordonnier, M.-H.; Lee, M. P.; Ismail, M. A.; Farahat, A. A.; Say, M.; Chackal-Catoen, S.; Batista-Parra, A.; Neidle, S.; Boykin, D. W.; Wilson, W. D. *J. Am. Chem. Soc.* **2011**, *133* (26), 10171.
(19) Munde, M.; Kumar, A.; Nhili, R.; Depauw, S.; David-Cordonnier, M.-H.; Ismail, M. A.; Stephens, C. E.; Farahat, A. A.; Batista-Parra, A.; Boykin, D. W.; Wilson, W. D. *J. Mol. Biol.* **2010**, *402* (5), 847.
(20) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; GE Scuseria… - Inc.; Wallingford; CT; 2010. *Gaussian 09, revision b. 01, Gaussian*.
(21) Bayly, C. I.; Cieplak, P.; Cornell, W.; Kollman, P. A. *J. Phys. Chem.* **1993**, *97* (40), 10269.
(22) Singh, U. C.; Kollman, P. A. *J. Comput. Chem.* **1984**, *5* (2), 129.
(23) Case, D. A.; Babin, V.; Berryman, J.; Betz, R. M.; Cai, Q.; Cerutti, D. S.; Cheatham, T. E., III; Darden, T. A.; Duke, R. E.; Gohlke, H.; Goetz, A. W.; Gusarov, S.; Homeyer, N.; Janowski, P.; Kaus, J.; Kolossváry, I.; Kovalenko, A.; Lee, T. S.; LeGrand, S.; Luchko, T.; Luo, R.; Madej, B.; Merz, K. M.; Paesani, F.; Roe, D. R.; Roitberg, A.; Sagui, C.; Salomon-Ferrer, R.; Seabra, G.; Simmerling, C. L.; Smith, W.; Swails, J.; Walker, R. C.; Wang, J.; Wolf, R. M.; Wu, X.; Kollman, P. A. AMBER 14, **2014**.
(24) Wang, J.; Wang, W.; Kollman, P. A.; Case, D. A. *J. Mol. Graph. Model.* **2006**, *25* (2), 247.
(25) Harika, N. K.; Germann, M. W.; Wilson, W. D. *Chem. Eur. J.* **2017**, *23 (69)*, 17612.
(26) Athri, P.; Wilson, W. D. *J. Am. Chem. Soc.* **2009**, *131* (22), 7618.
(27) Špačková, N.; Cheatham, T. E.; Ryjáček, F.; Lankaš, F.; van Meervelt, L.; Hobza, P.; Šponer, J. *J. Am. Chem. Soc.* **2003**, *125* (7), 1759.
(28) Trott, O.; Olson, A. J. *J. Comput. Chem.* **2009**, *65*, 455.



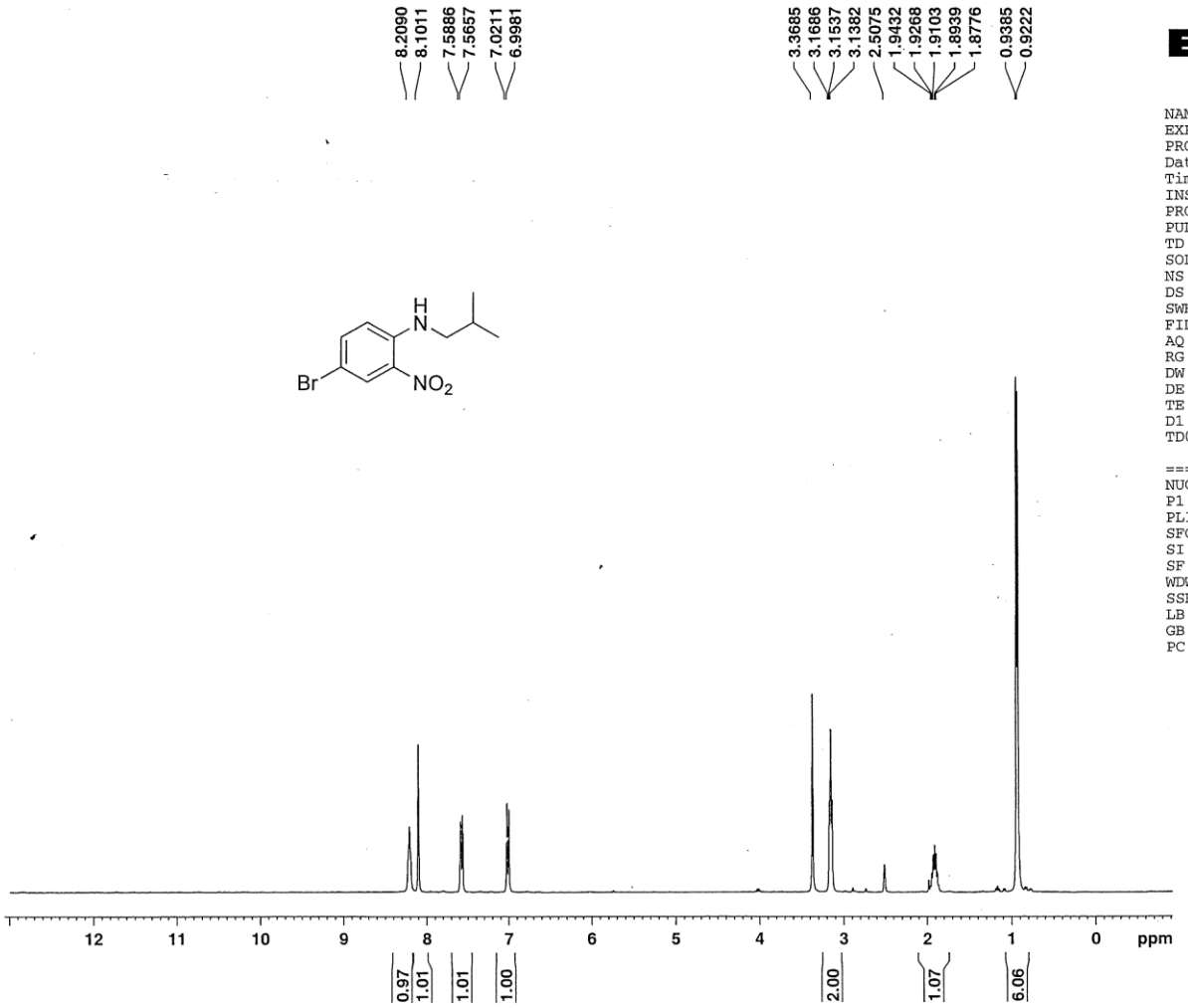
BRUKER

NAME	Br-Ph-NH-ethyl-NO2
EXPNO	1
PROCNO	1
Date_	20170927
Time	14.29
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	4
DS	2
SWH	5592.841 Hz
FIDRES	0.085340 Hz
AQ	5.8589683 sec
RG	228.1
DW	89.400 usec
DE	6.00 usec
TE	295.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	6.40 usec
PL1	0.00 dB
SFO1	400.1324008 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



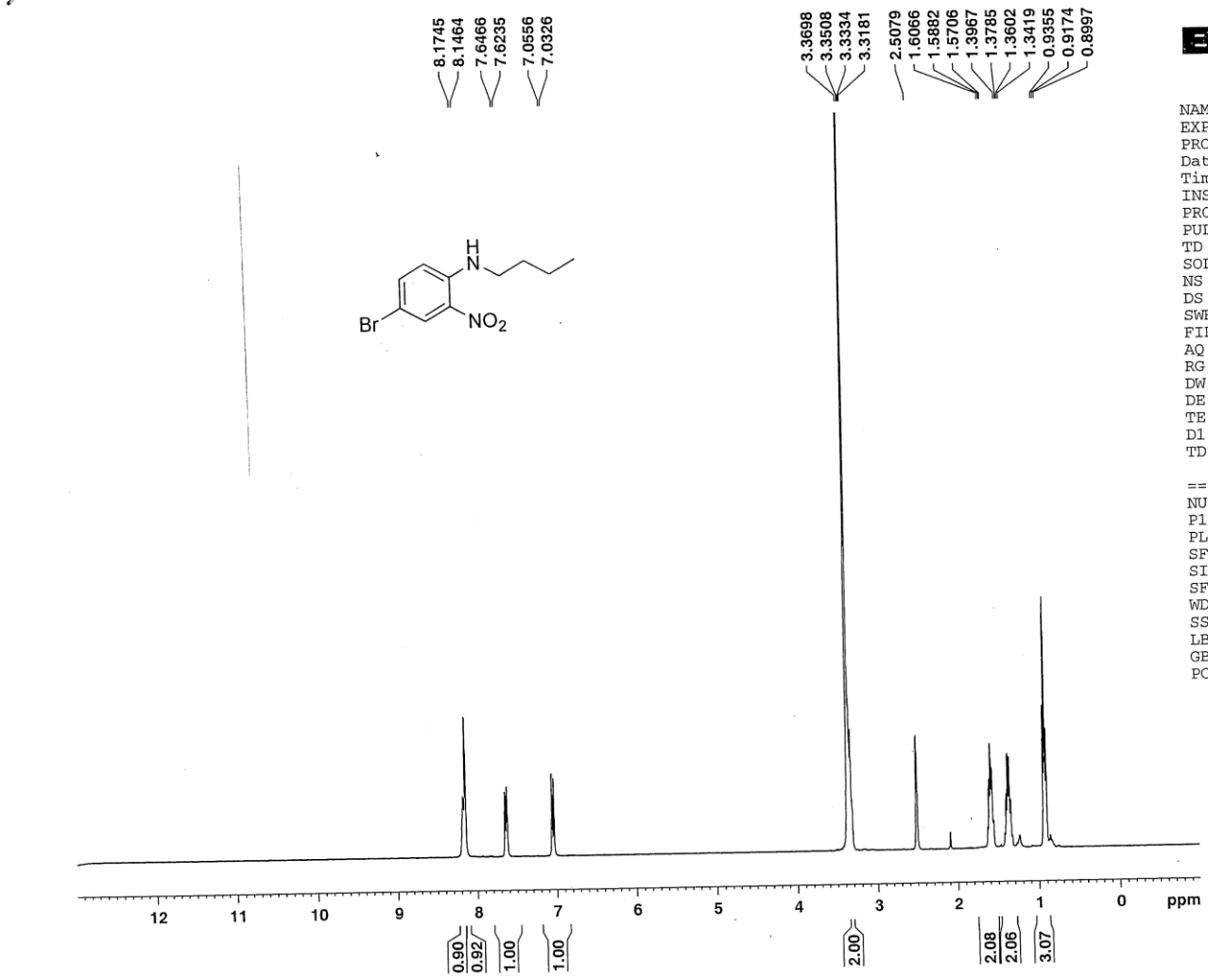
BRUKER

NAME	Br-PH-NH-isopropyl-NO2
EXPNO	1
PROCNO	1
Date_	20170726
Time	12.21
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	4
DS	2
SWH	5592.841 Hz
FIDRES	0.085340 Hz
AQ	5.8589683 sec
RG	181
DW	89.400 usec
DE	6.00 usec
TE	296.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	6.40 usec
PL1	0.00 dB
SFO1	400.1324008 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

NAME	Bromo-Ph-NHisobutyl-NO2
EXPNO	1
PROCNO	1
Date_	20170809
Time	13.19
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	4
DS	2
SWH	5592.841 Hz
FIDRES	0.085340 Hz
AQ	5.8589683 sec
RG	71.8
DW	89.400 usec
DE	6.00 usec
TE	295.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	6.40 usec
PL1	0.00 dB
SFO1	400.1324008 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

NAME	Brph-NH-n-butyl--NO2
EXPNO	1
PROCNO	1
Date_	20170828
Time	11.45
INSTRUM	spect
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PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	4
DS	2
SWH	5592.841 Hz
FIDRES	0.085340 Hz
AQ	5.8589683 sec
RG	161.3
DW	89.400 usec
DE	6.00 usec
TE	296.0 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	6.40 usec
PL1	0.00 dB
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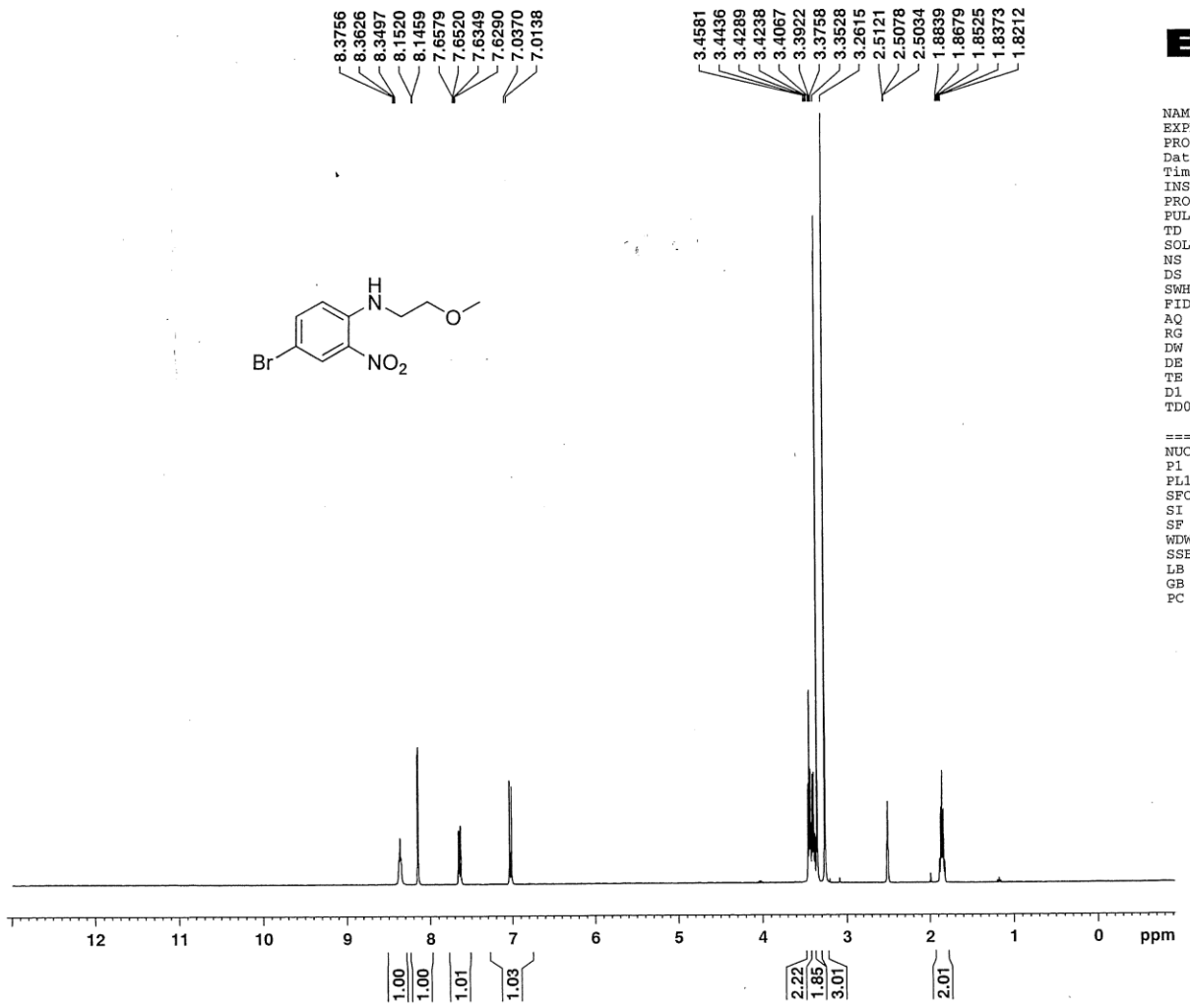
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

NAME	Br-Ph-NH-propylmethoxy-NO2
EXPNO	1
PROCNO	1
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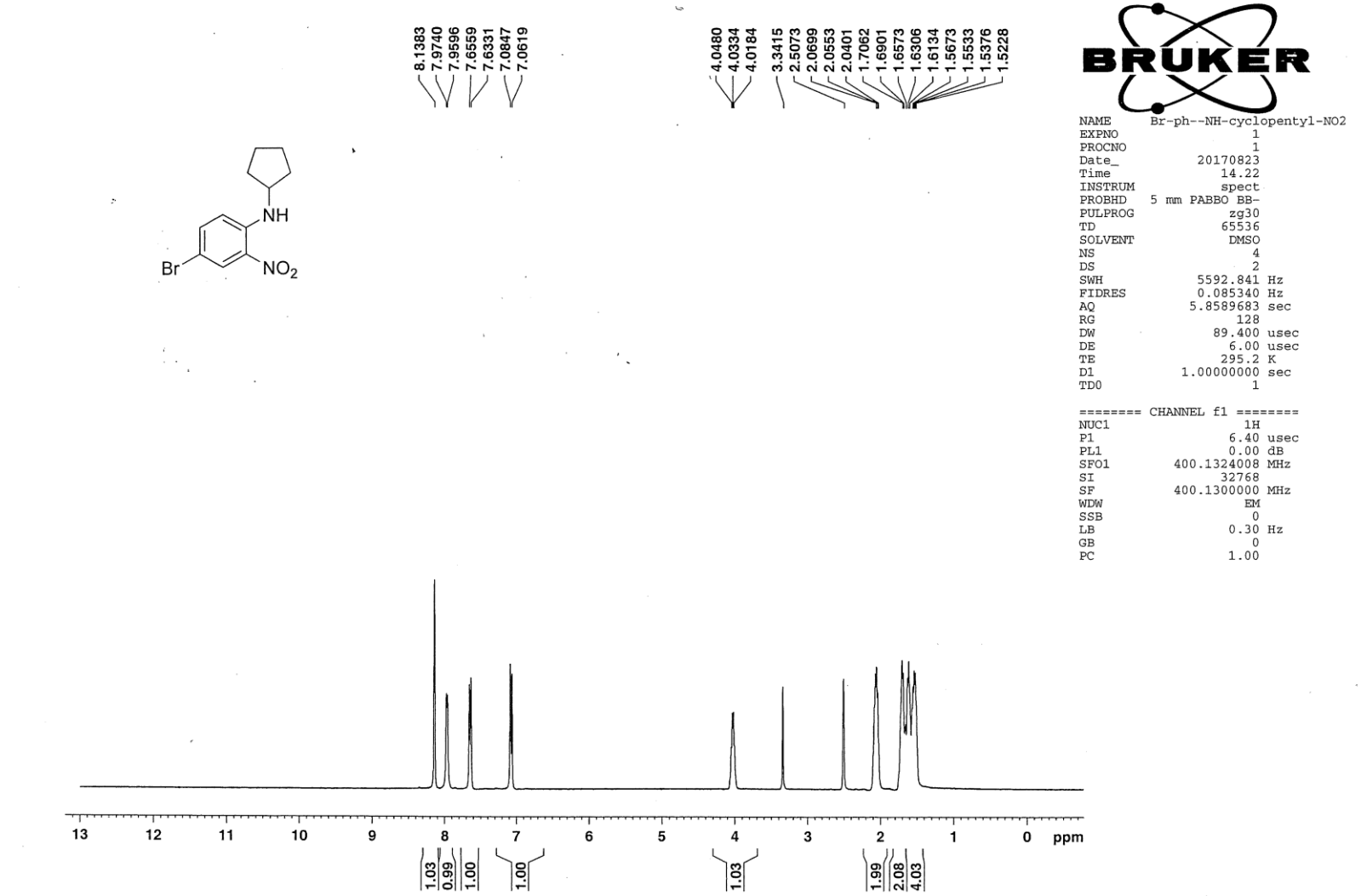
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	4
DS	2
SWH	5592.841 Hz
FIDRES	0.085340 Hz
AQ	5.8589683 sec
RG	181
DW	89.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	6.40 usec
PL1	0.00 dB
SFO1	400.1324008 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

NAME	Br-ph--NH-cyclopentyl-NO2
EXPNO	1
PROCNO	1
Date_	20170823
Time	14.22
INSTRUM	spect
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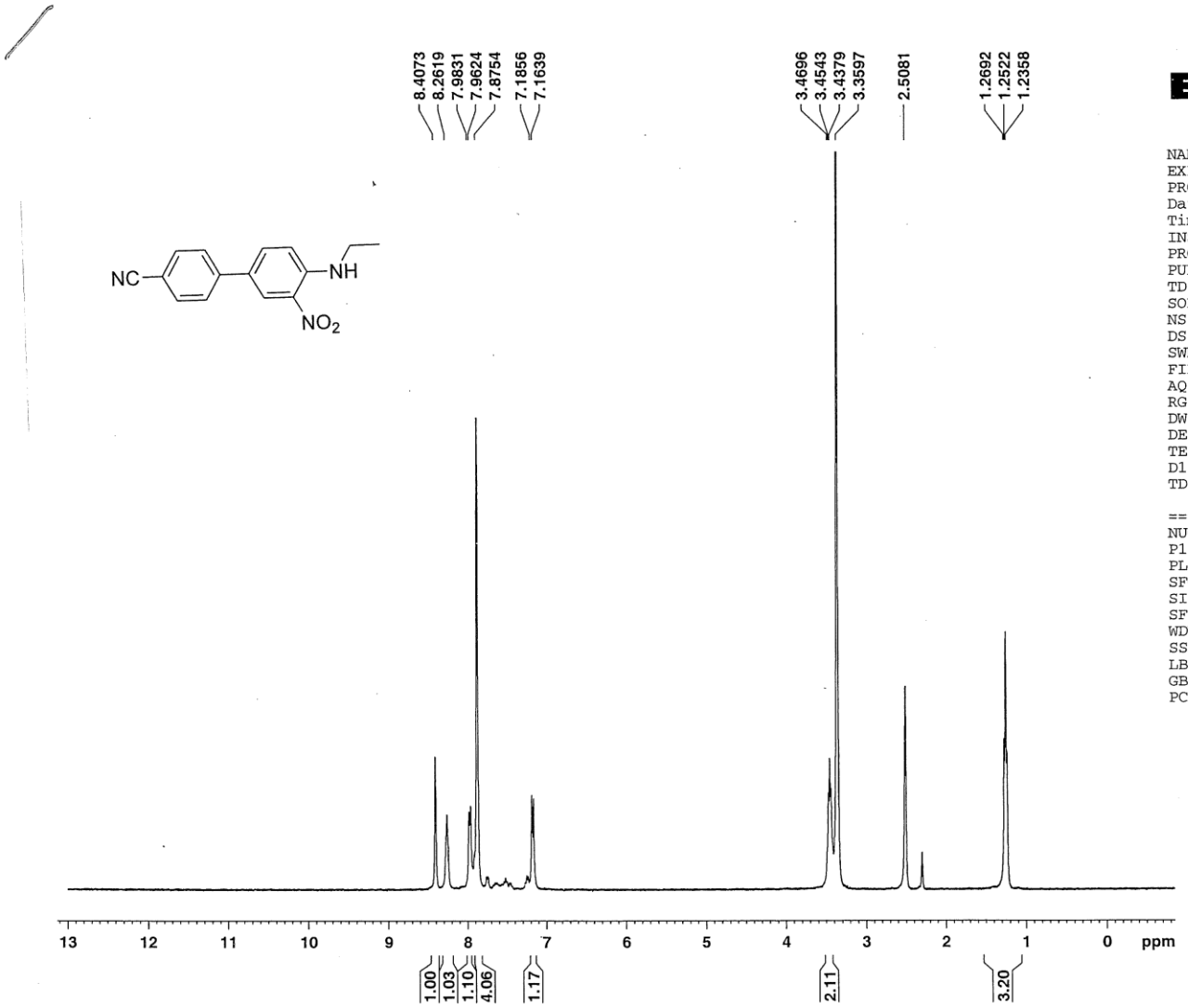
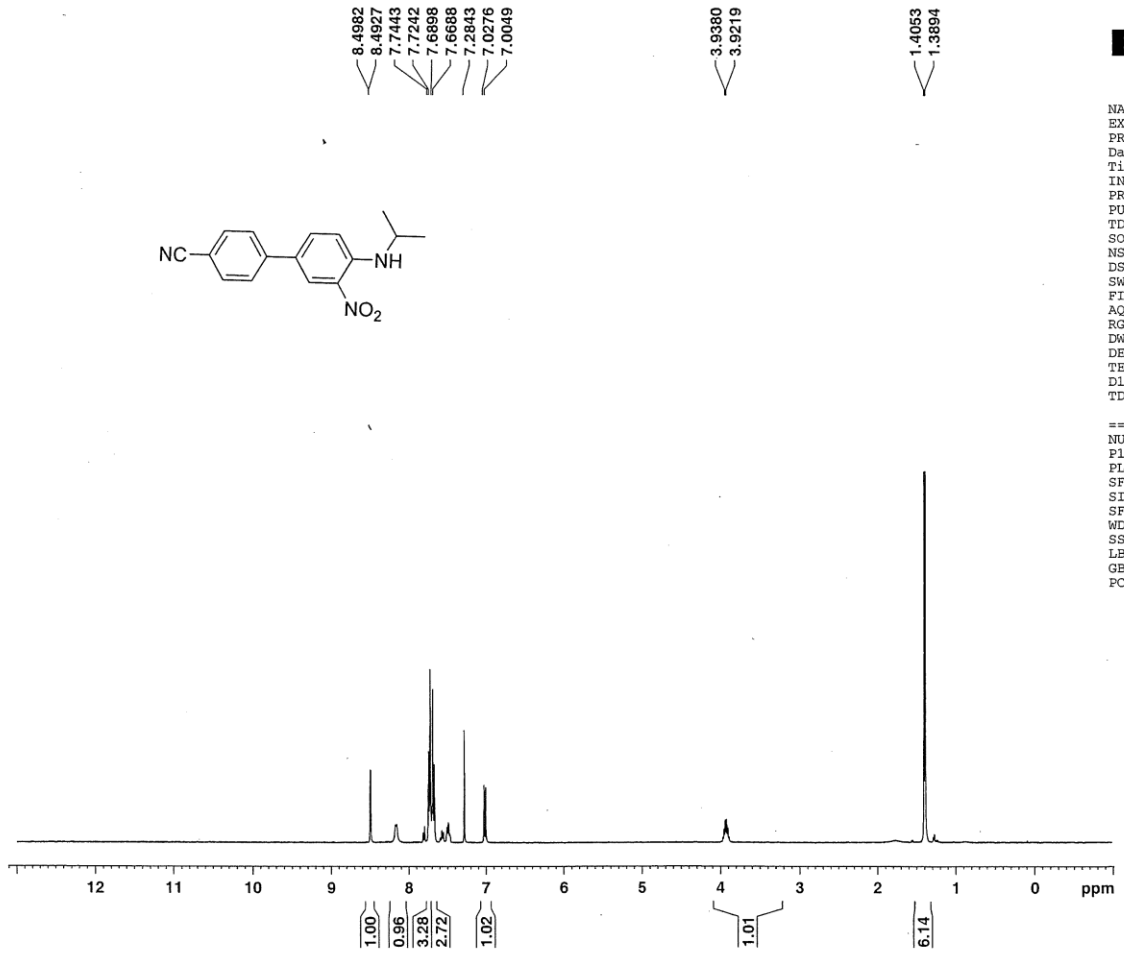
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	4
DS	2
SWH	5592.841 Hz
FIDRES	0.085340 Hz
AQ	5.8589683 sec
RG	128
DW	89.400 usec
DE	6.00 usec
TE	295.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	6.40 usec
PL1	0.00 dB
SFO1	400.1324008 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



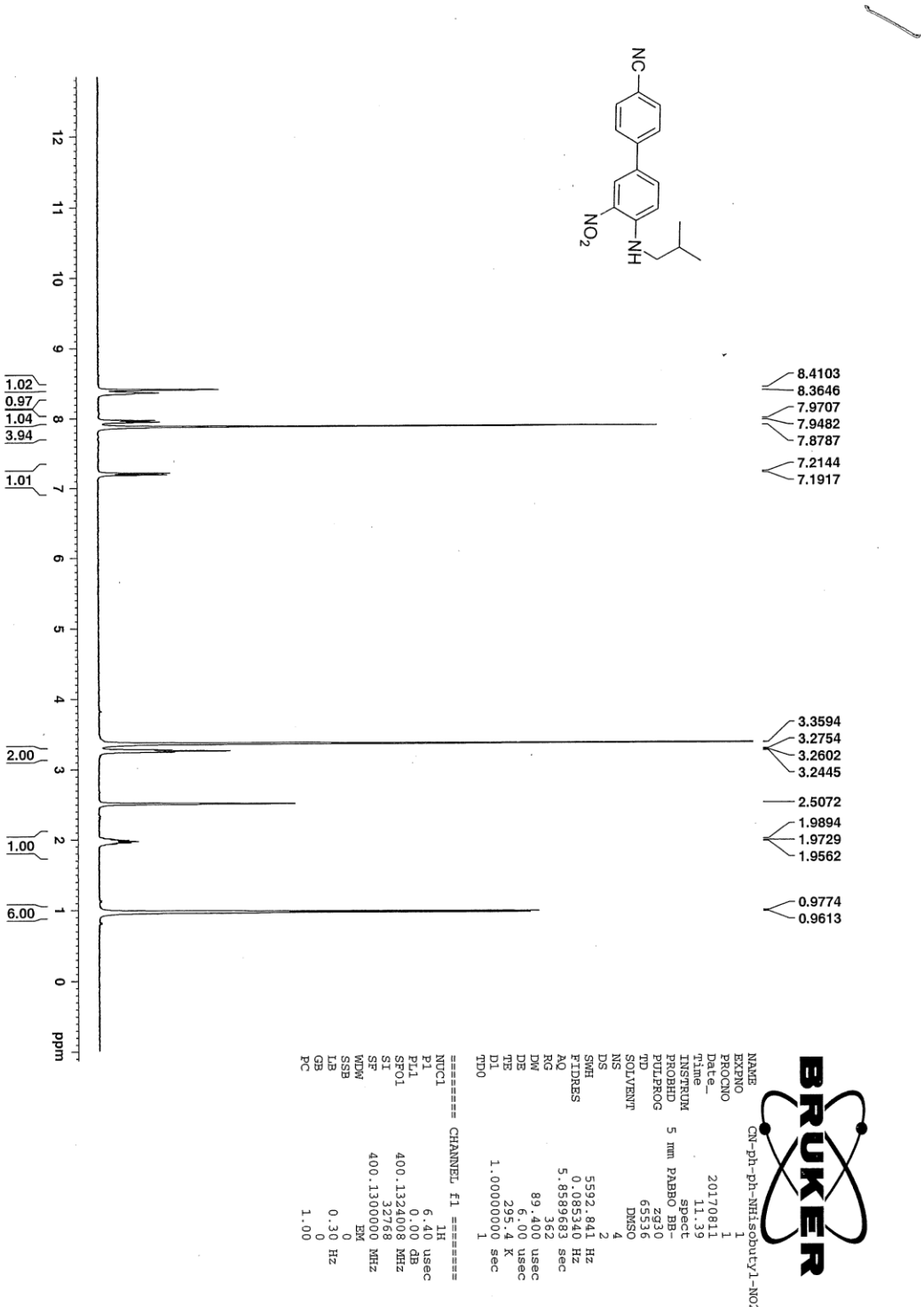
BRUKER

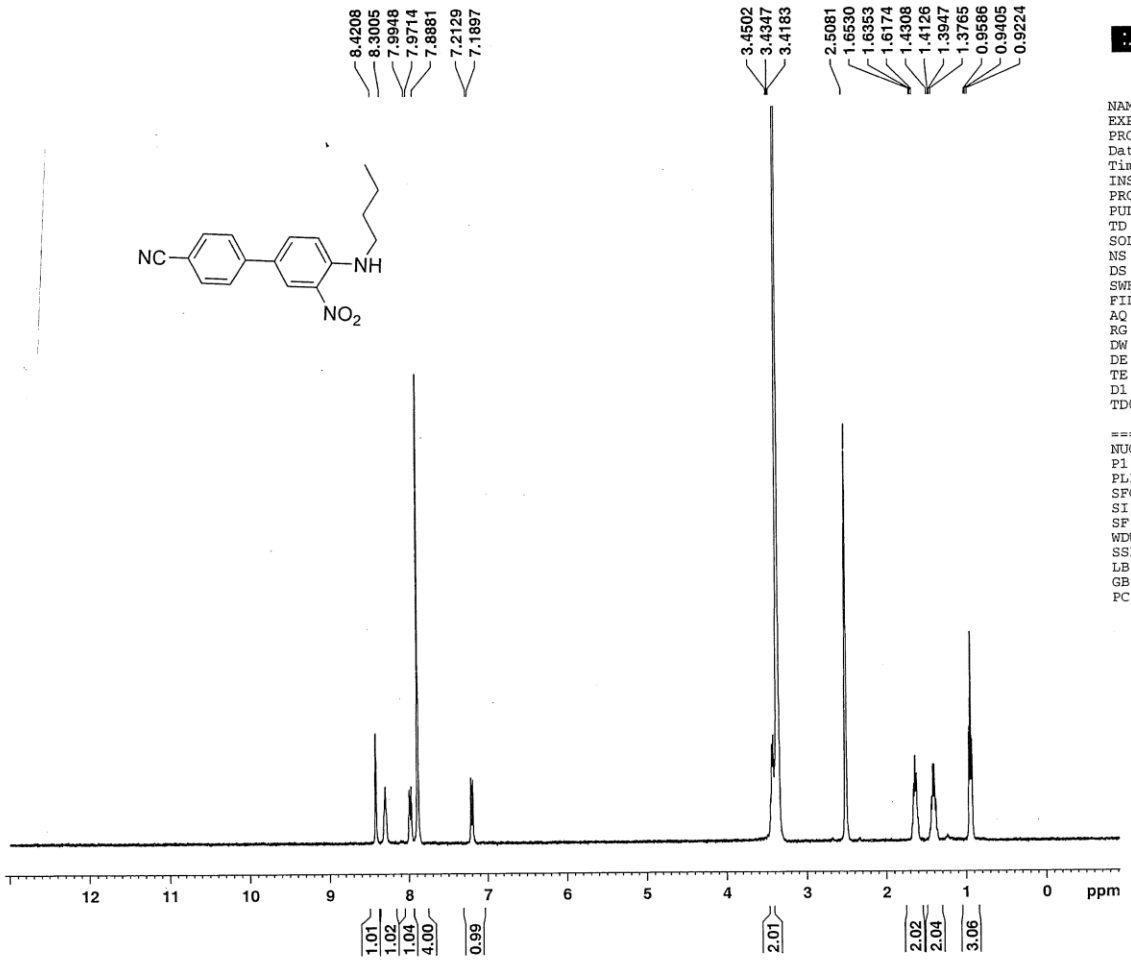
NAME	CN-Ph-Ph-NH-ethyl-NO2
EXPNO	1
PROCNO	1
Date_	20170928
Time	13.36
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	4
DS	2
SWH	5592.841 Hz
FIDRES	0.085340 Hz
AQ	5.8589683 sec
RG	228.1
DW	89.400 usec
DE	6.00 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	6.40 usec
PL1	0.00 dB
SFO1	400.1324008 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

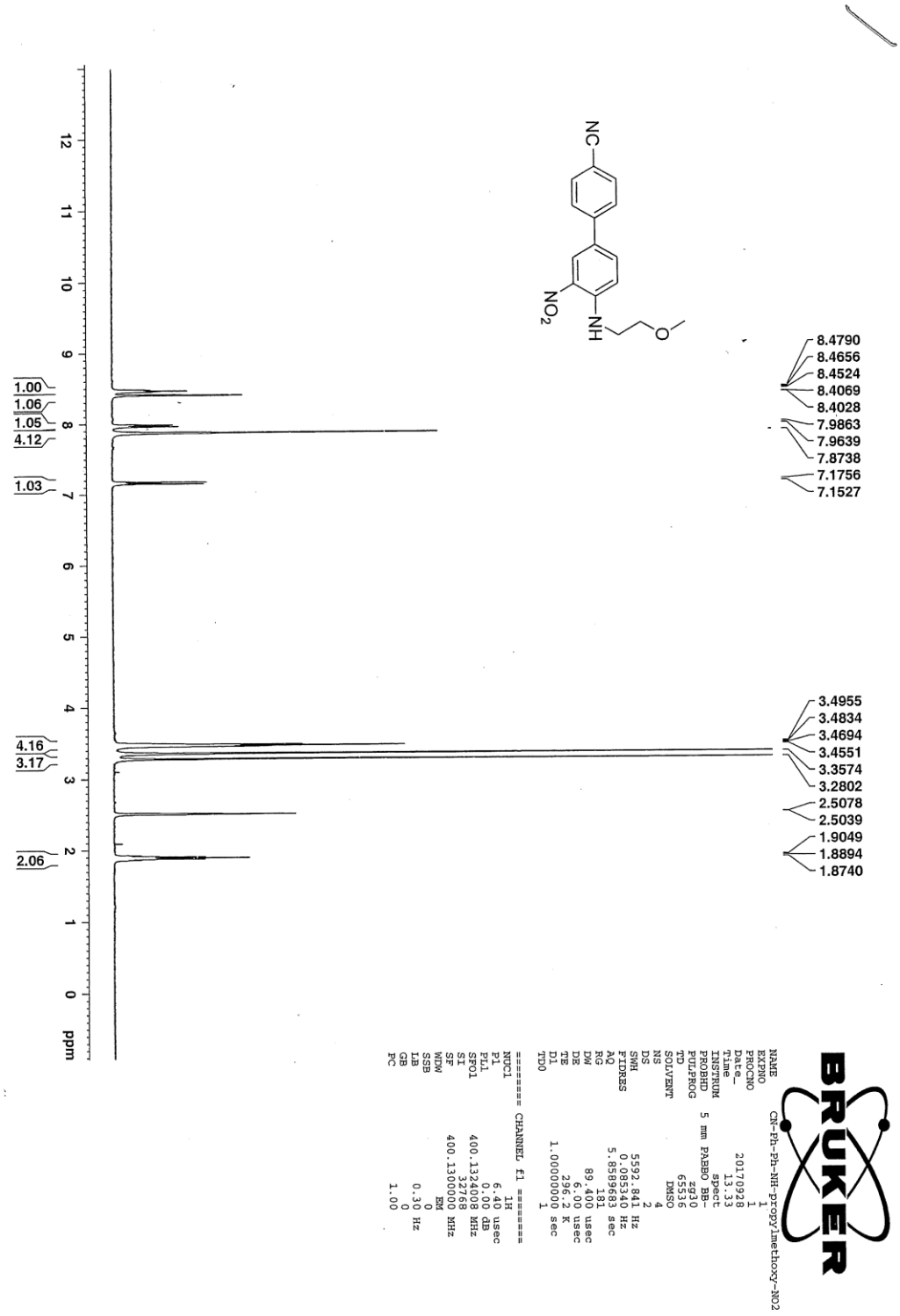
NAME	Cn-ph-ph-NH-isopropyl-NO2
EXPNO	1
PROCNO	1
Date_	20180307
Time	10.40
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	4
DS	2
SWH	5592.841 Hz
FIDRES	0.085340 Hz
AQ	5.8589683 sec
RG	362
DW	89.400 usec
DE	6.00 usec
TE	296.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	6.40 usec
PL1	0.00 dB
SFO1	400.1324008 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

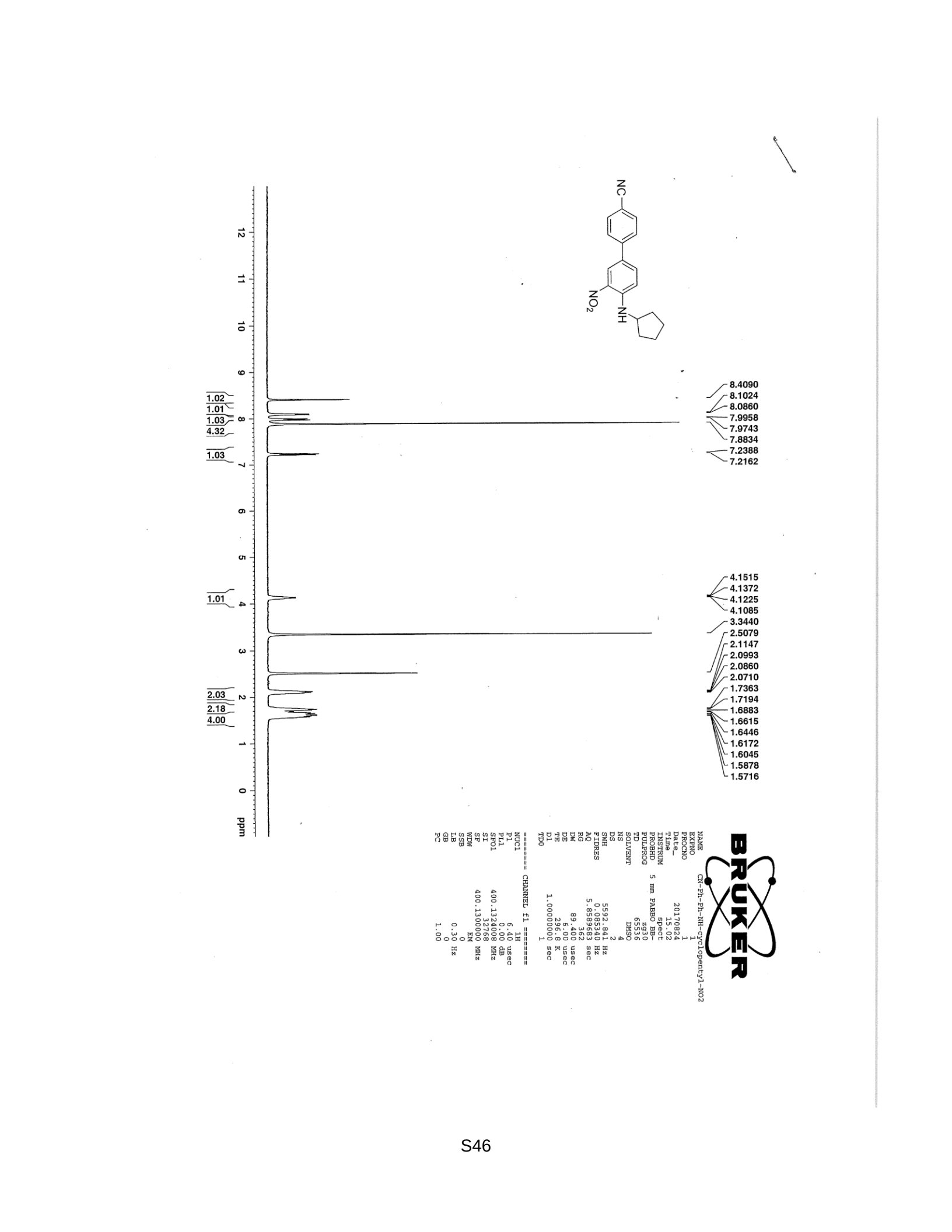

NC
NO2
NH
8.4103
8.3646
7.9707
7.9482
7.8787
7.2144
7.1917
3.3594
3.2754
3.2602
3.2445
2.5072
1.9894
1.9729
1.9562
0.9774
0.9613
1.02
0.97
1.04
3.94
1.01
2.00
1.00
6.00
ppm
NAME CN-ph-ph-NHisobutyl-NO2
EXPNO 1
PROCNO 1
Date_ 20170811
Time_ 11.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 4
DS 2
SWH 5592.841 Hz
FIDRES 0.085340 Hz
AQ 5.8589683 sec
RG 362
DW 89.400 usec
DE 6.00 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 6.40 usec
PL1 0.00 dB
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

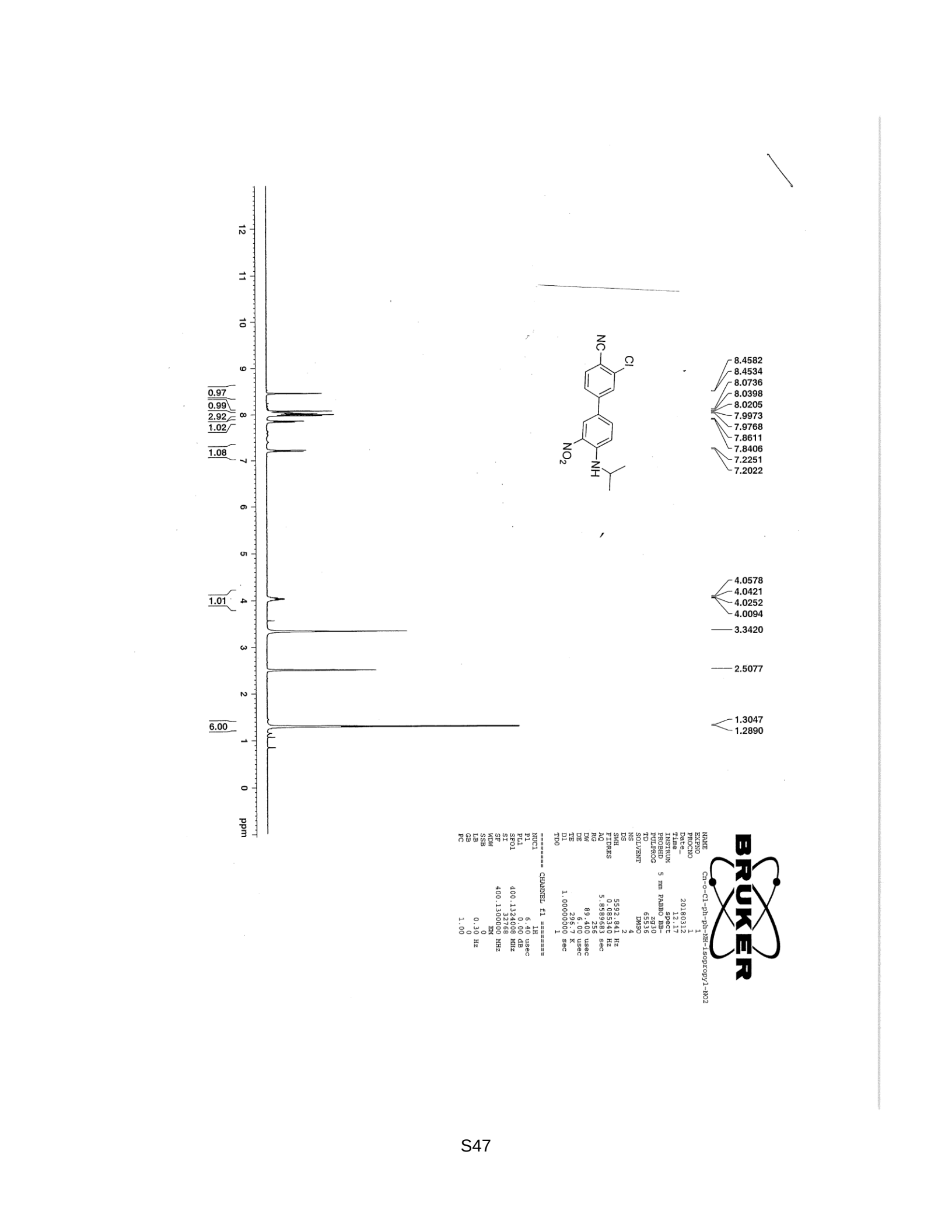


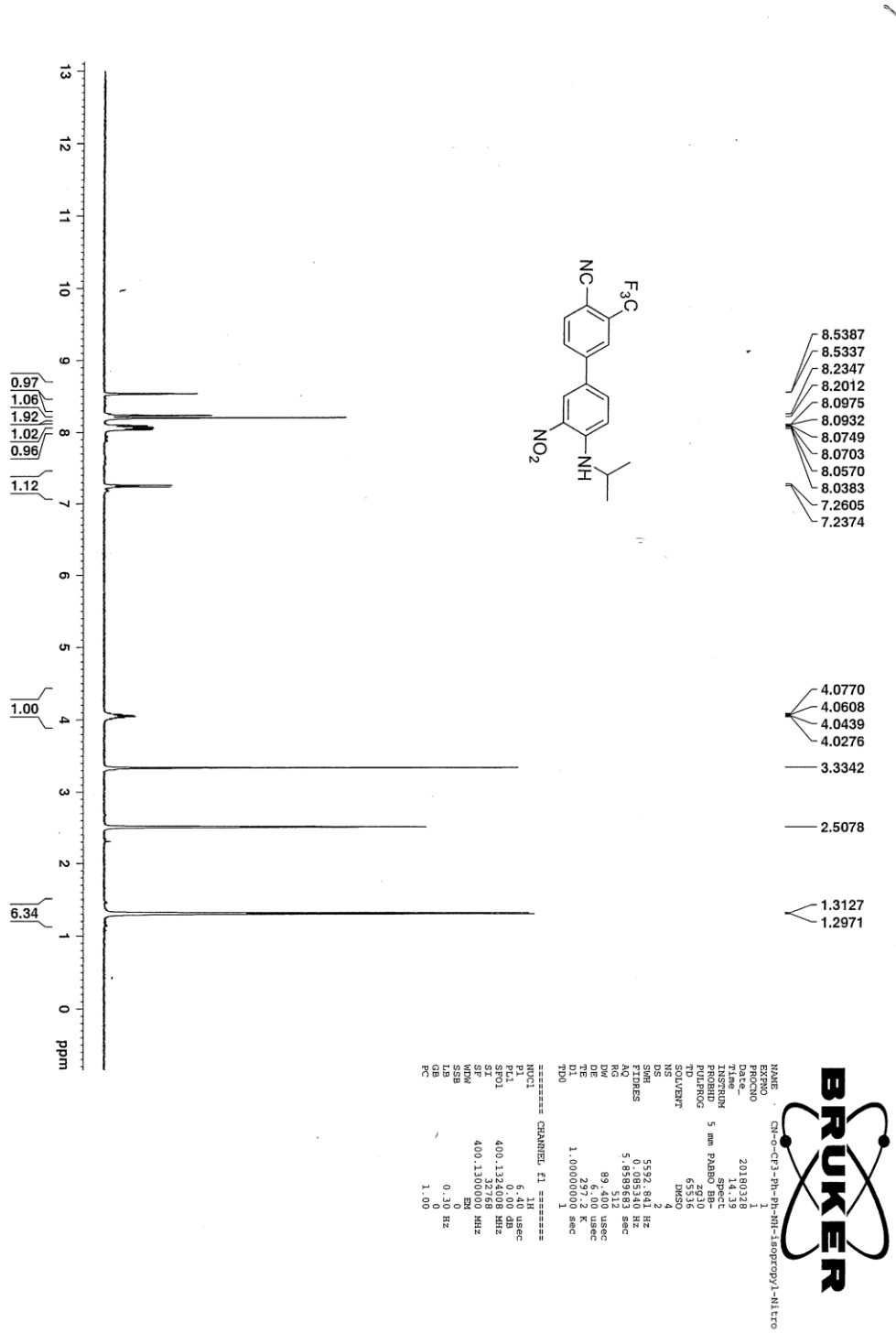
BRUKER

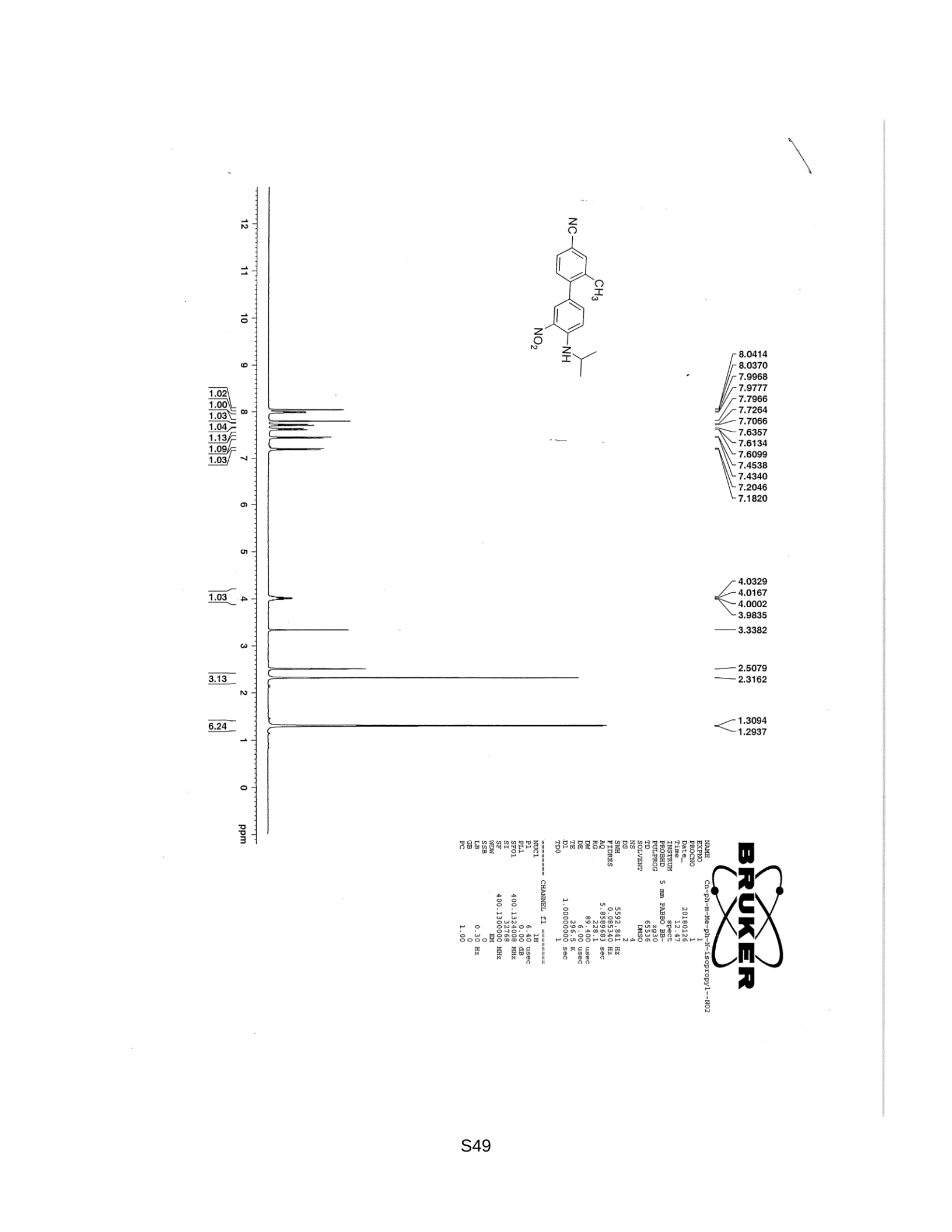
NAME	CN-Ph- Ph-NH-n-butyl-NO2
EXPNO	1
PROCNO	1
Date_	20170829
Time	14.24
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	4
DS	2
SWH	5592.841 Hz
FIDRES	0.085340 Hz
AQ	5.8589683 sec
RG	362
DW	89.400 usec
DE	6.00 usec
TE	296.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	6.40 usec
PL1	0.00 dB
SFO1	400.1324008 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

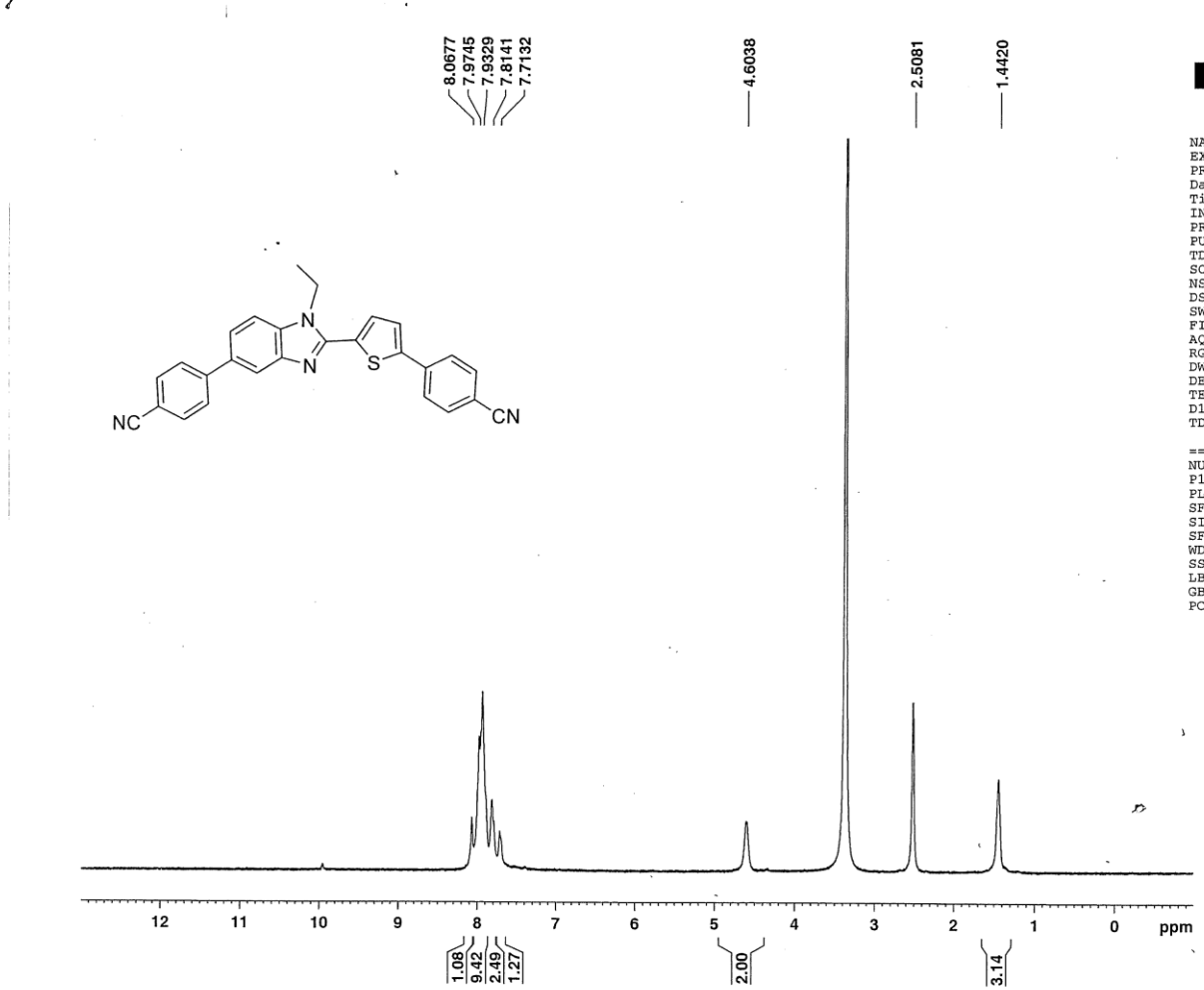

NC
NO2
NH
O
8.4790
8.4656
8.4524
8.4069
8.4028
7.9863
7.9639
7.8738
7.1756
7.1527
3.4955
3.4834
3.4694
3.4551
3.3574
3.2802
2.5078
2.5039
1.9049
1.8894
1.8740
1.00
1.06
1.05
4.12
1.03
4.16
3.17
2.06
ppm
NAME CN-Ph-Ph-NH-propylmethoxy-NO2
EXPNO 1
PROCNO 1
Date_ 20170928
Time 13.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 4
DS 2
SWH 5592.841 Hz
FIDRES 0.085360 Hz
AQ 5.8589569 sec
RG 181
DW 89.400 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 6.40 usec
PL1 0.00 dB
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


NC
NO2
NH
8.4090
8.1024
8.0860
7.9958
7.9743
7.8834
7.2388
7.2162
4.1515
4.1372
4.1225
4.1085
3.3440
2.5079
2.1147
2.0993
2.0860
2.0710
1.7363
1.7194
1.6883
1.6615
1.6446
1.6172
1.6045
1.5878
1.5716
1.02
1.01
1.03
4.32
1.03
1.01
2.03
2.18
4.00
ppm
NAME CN-Ph-Ph-NH-cyclopentyl-NO2
EXPNO 1
PROCNO 1
Date_ 20170824
Time 15.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 4
DS 2
SWH 5592.841 Hz
FIDRES 0.085340 Hz
AQ 5.8589603 sec
RG 362
DW 89.400 usec
DE 6.00 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 6.40 usec
PL1 0.00 dB
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


NC
Cl
NO2
NH
8.4582
8.4534
8.0736
8.0398
8.0205
7.9973
7.9768
7.8611
7.8406
7.2251
7.2022
4.0578
4.0421
4.0252
4.0094
3.3420
2.5077
1.3047
1.2890
0.97
0.99
2.92
1.02
1.08
1.01
6.00
ppm
BRUKER
Cn-o-Cl-ph-ph-NH-isopropyl-NO2
NAME 1
EXPNO 1
PROCNO 1
Date_ 20180312
Time 12.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG 65536
TD DMSO
SOLVENT 4
NS 2
DS 5592.841 Hz
SWH 0.085340 Hz
FIDRES 5.8589683 sec
AQ 256
RG 89.400 usec
DW 6.000 usec
DE 296.0 K
TE 1.00000000 sec
D1 1
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 6.40 usec
PL1 0.00 dB
SFO1 400.1324008 MHz
SI 131072
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

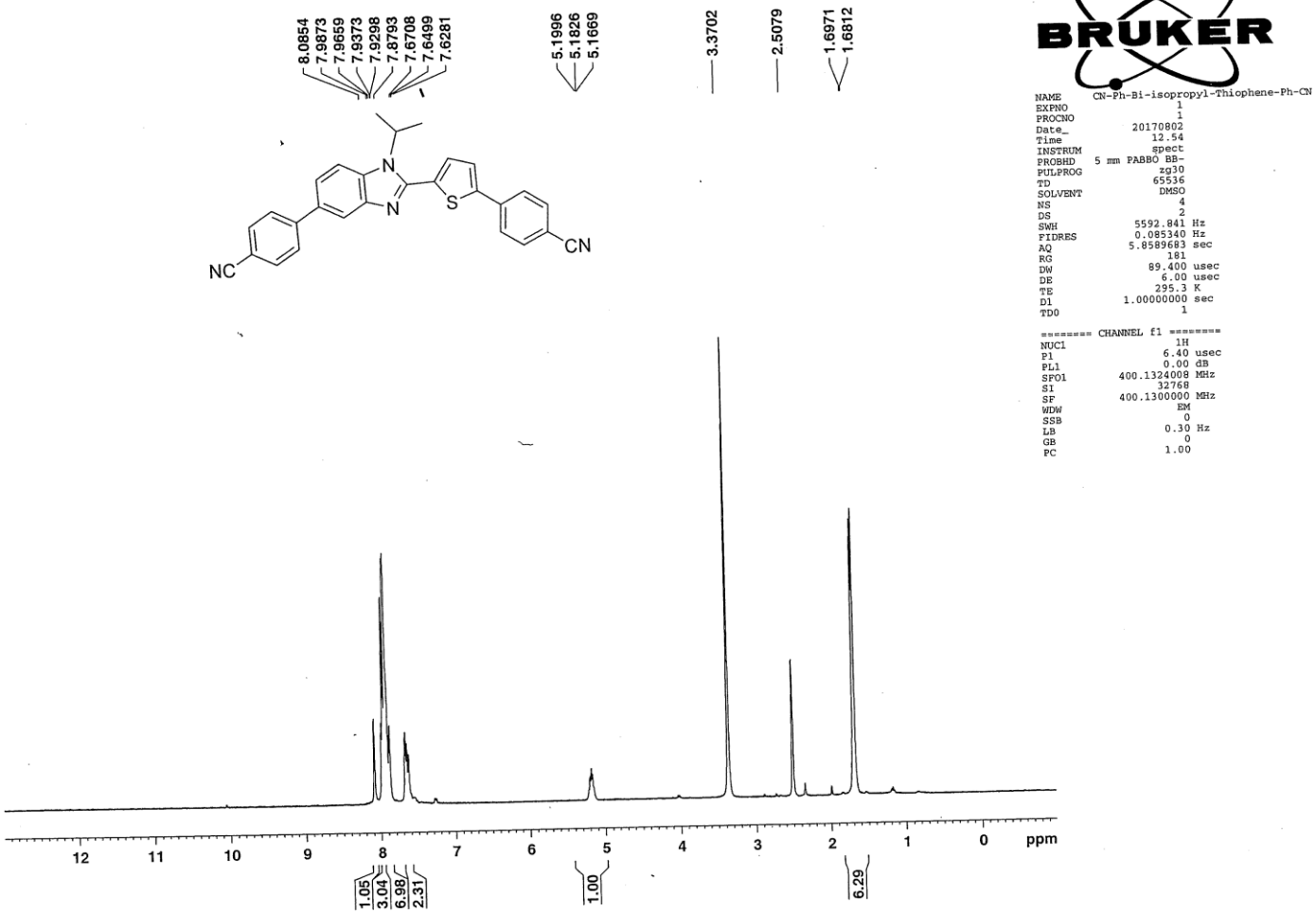

8.5387
8.5337
8.2347
8.2012
8.0975
8.0932
8.0749
8.0703
8.0570
8.0383
7.2605
7.2374
4.0770
4.0608
4.0439
4.0276
3.3342
2.5078
1.3127
1.2971
0.97
1.06
1.92
1.02
0.96
1.12
1.00
6.34
ppm
NC
F3C
NO2
NH
NAME CN-o-CF3-Ph-Ph-NH-isopropyl-Nitro
EXPNO 1
PROCNO 1
Date_ 20180328
Time 14.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 4
DS 2
SWH 5592.841 Hz
FIDRES 0.085281 Hz
AQ 5.8595240 sec
RG 512
DW 89.400 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 6.40 usec
PL1 0.00 dB
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


NC
CH3
NO2
NH
8.0414
8.0370
7.9968
7.9777
7.7966
7.7264
7.7066
7.6357
7.6134
7.6099
7.4538
7.4340
7.2046
7.1820
4.0329
4.0167
4.0002
3.9835
3.3382
2.5079
2.3162
1.3094
1.2937
1.02
1.00
1.03
1.04
1.13
1.09
1.03
1.03
3.13
6.24
ppm
NAME Cn-ph-m-Me-ph-N-isopropyl--NO2
EXPNO 1
PROCNO 1
Date_ 20180126
Time 12.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 4
DS 2
SWH 5592.841 Hz
FIDRES 0.085340 Hz
AQ 5.8589683 sec
RG 8228.01
DW 89.400 usec
DE 6.00 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 6.40 usec
PL1 0.00 dB
SFO1 400.1324008 MHz
SI 131072
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

NAME	cn-Ph-Bi-N-Ethyl-Thi-Ph-Cn
EXPNO	1
PROCNO	1
Date_	20171004
Time	13.21
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	4
DS	2
SWH	5592.841 Hz
FIDRES	0.085340 Hz
AQ	5.8589683 sec
RG	228.1
DW	89.400 usec
DE	6.00 usec
TE	297.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	6.40 usec
PL1	0.00 dB
SFO1	400.1324008 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

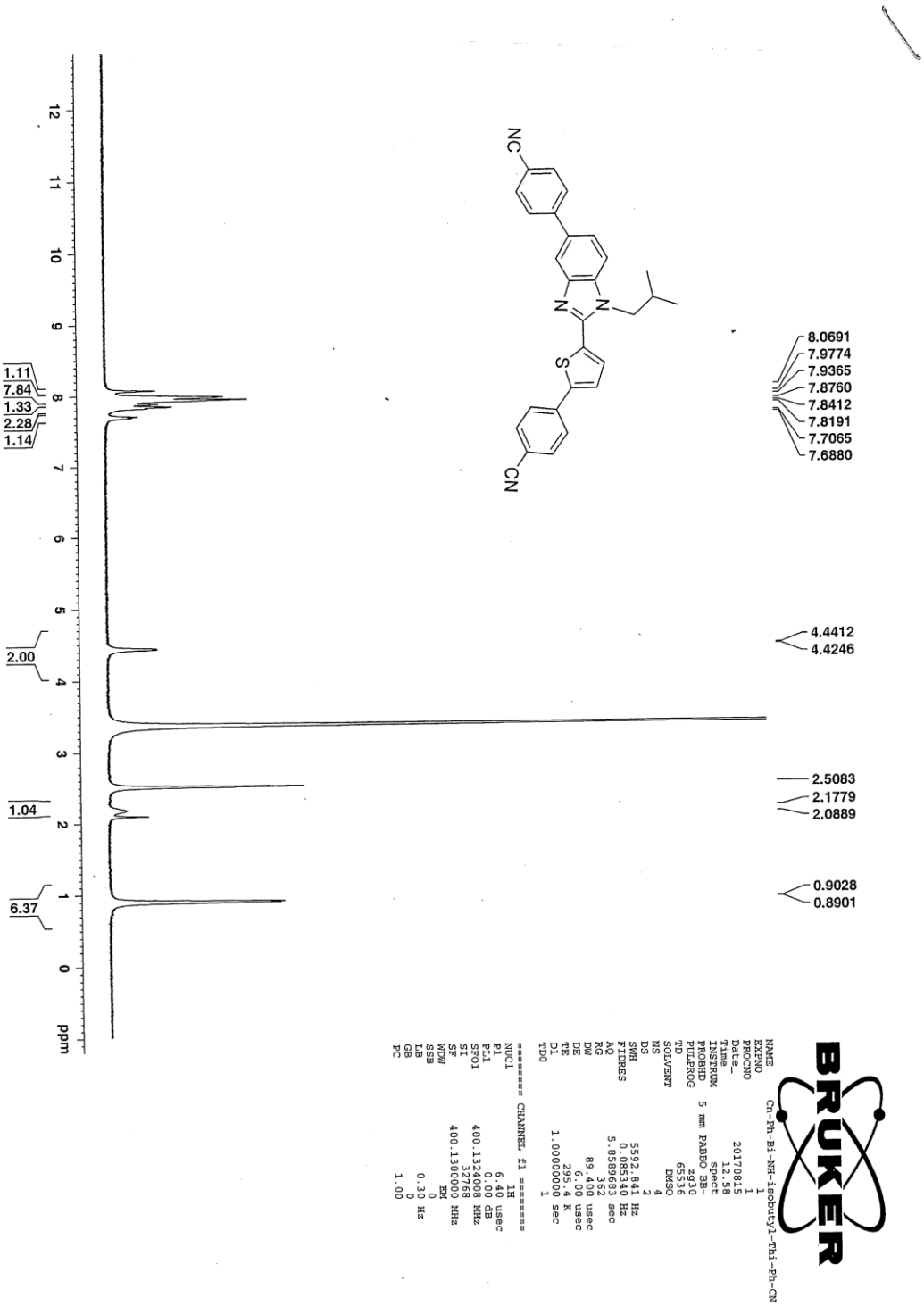


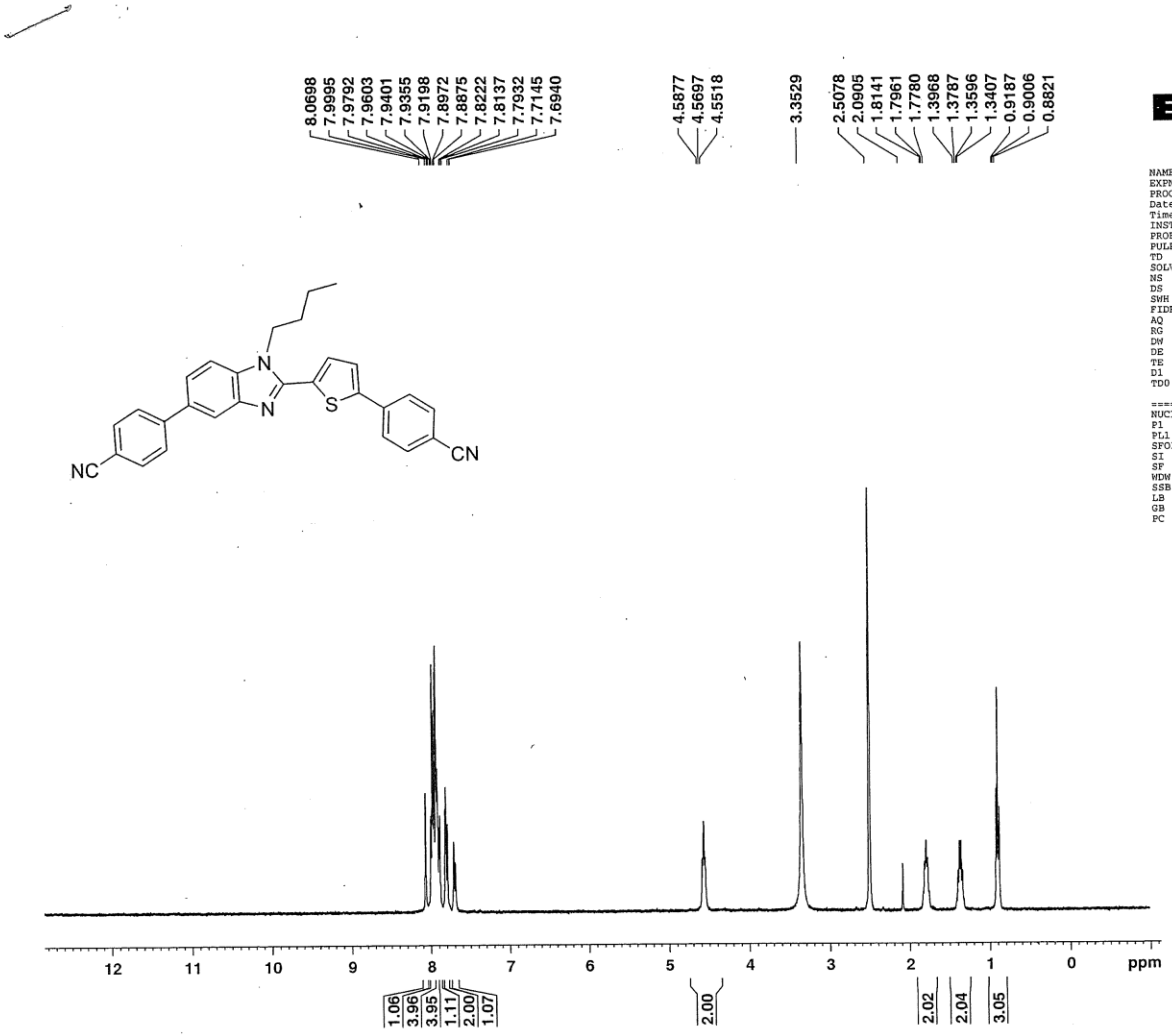
BRUKER

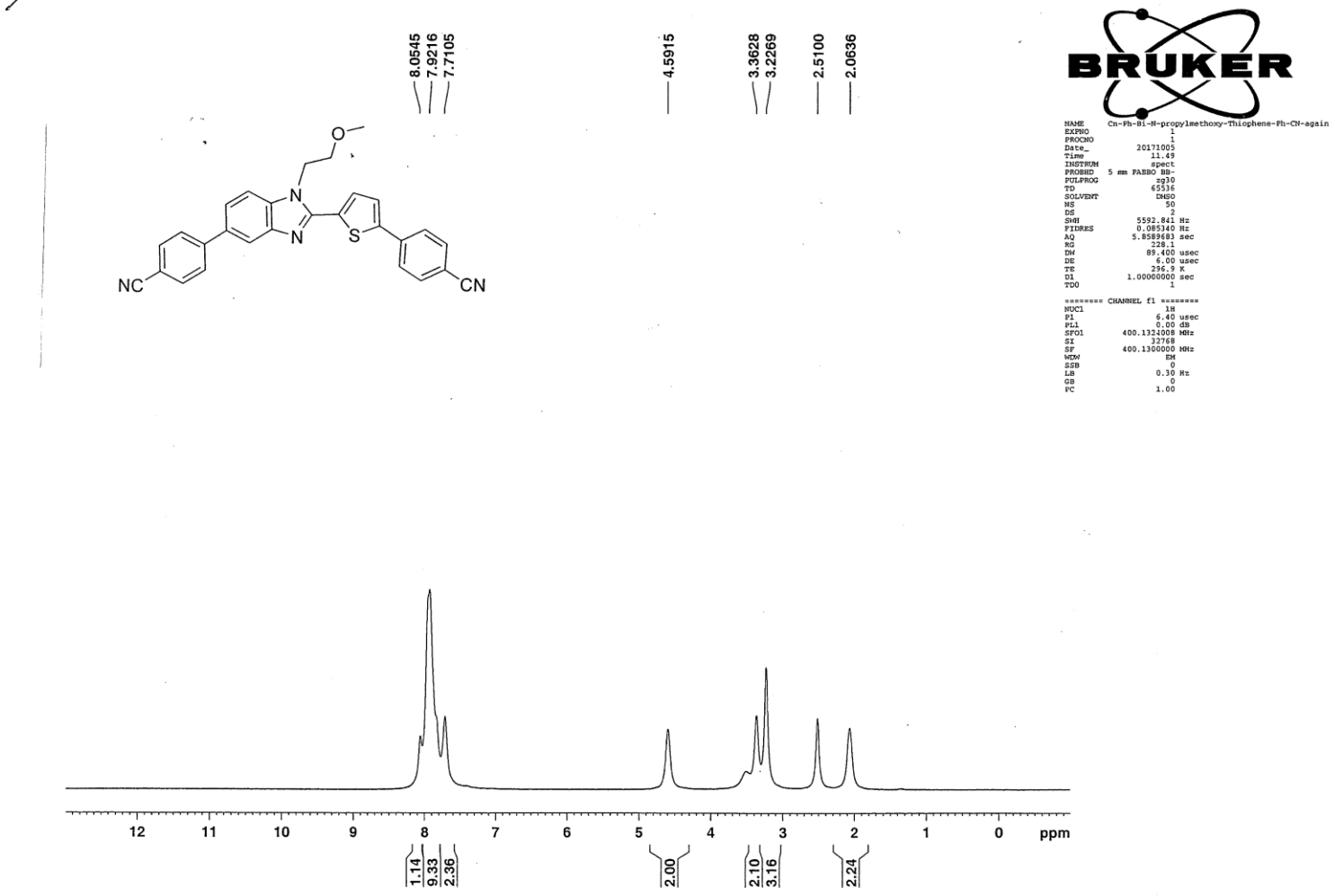
NAME	CN-Ph-Bi-isopropyl-Thiophene-Ph-CN
EXPNO	1
PROCNO	1
Date_	20170802
Time	12.54
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	4
DS	2
SWH	5592.841 Hz
FIDRES	0.085340 Hz
AQ	5.8589683 sec
RG	181
DW	89.400 usec
DE	6.00 usec
TE	295.3 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	6.40 usec
PL1	0.00 dB
SFO1	400.1324008 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

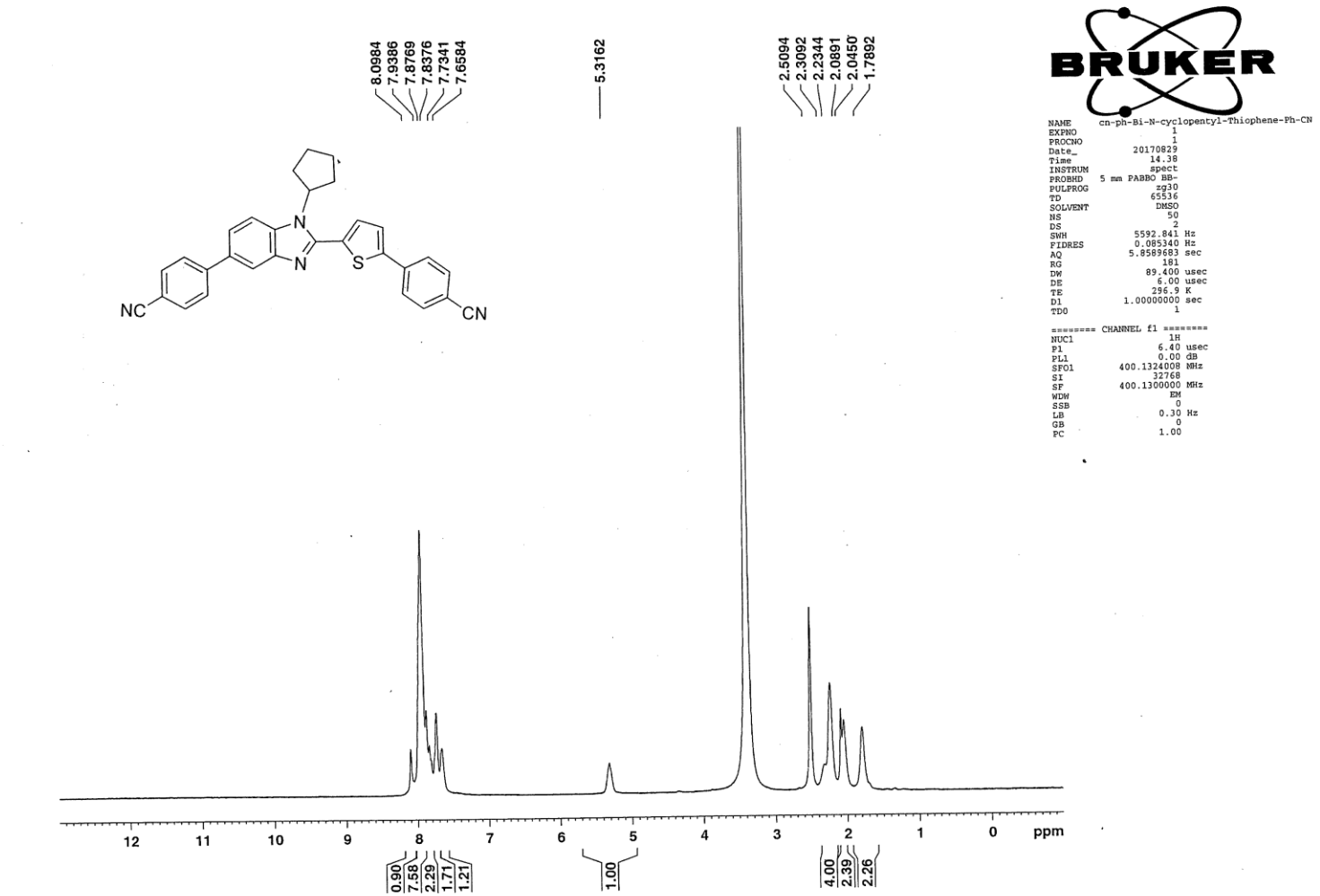

NC
N
N
S
CN
8.0691
7.9774
7.9365
7.8760
7.8412
7.8191
7.7065
7.6880
4.4412
4.4246
2.5083
2.1779
2.0889
0.9028
0.8901
1.11
7.84
1.33
2.28
1.14
2.00
1.04
6.37
ppm
NAME Cn-Ph-Ei-NH-isobutyl-Thi-Ph-CN
EXPNO 1
PROCNO 1
Date_ 20170815
Time 12.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 2
DS 2
SWH 5592.841 Hz
FIDRES 0.085340 Hz
AQ 5.8589683 sec
RG 362
DW 89.400 usec
DE 6.00 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 6.40 usec
PL1 0.00 dB
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


8.0698
7.9995
7.9792
7.9603
7.9401
7.9355
7.9198
7.8972
7.8875
7.8822
7.8137
7.7932
7.7145
7.6940
4.5877
4.5697
4.5518
3.3529
2.5078
2.0905
1.8141
1.7961
1.7780
1.3968
1.3787
1.3596
1.3407
0.9187
0.9006
0.8821
BRUKER
NAME CN-ph-Bi-N-butyl-thiophene ph CN again
EXPNO 1
PROCNO 1
Date_ 20170905
Time 12.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 4
DS 2
SWH 5592.841 Hz
FIDRES 0.085340 Hz
AQ 5.8589683 sec
RG 322.5
DW 89.400 usec
DE 6.00 usec
TE 297.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 6.40 usec
PL1 0.00 dB
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
N
N
S
NC
CN
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.06
3.96
3.95
1.11
2.00
1.07
2.00
2.02
2.04
3.05



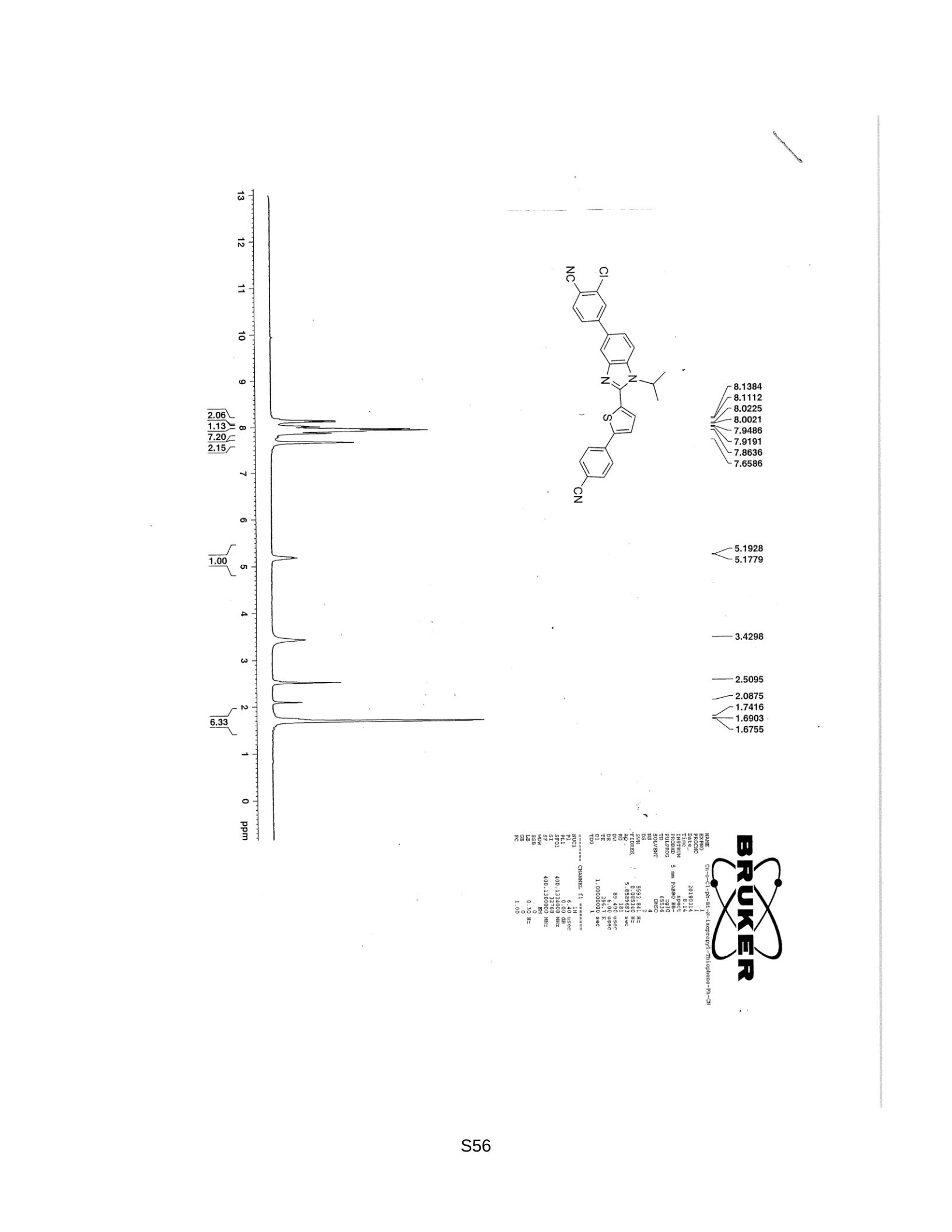
BRUKER

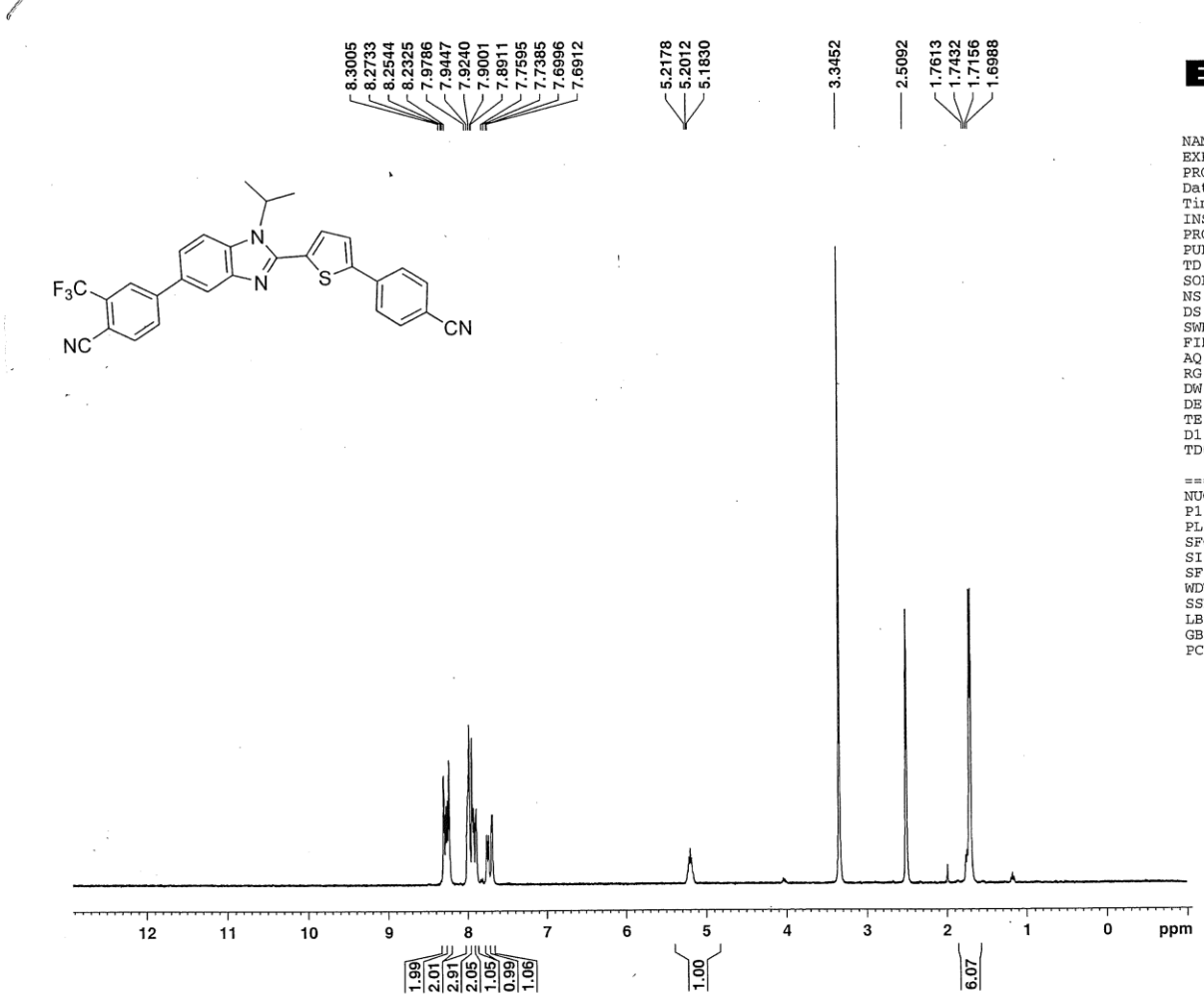
```
NAME          Cn-Ph-Bi-N-propylmethoxy-Thiophene-Ph-CN-again
EXPNO                  1
PROCNO                 1
Date_           20171005
Time              11.48
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD                65536
SOLVENT            DMSO
NS                   50
DS                    2
SWH            5592.841 Hz
FIDRES         0.085340 Hz
AQ             5.8589683 sec
RG                228.1
DW               89.400 usec
DE                6.00 usec
TE               296.9 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                 6.40 usec
PL1                0.00 dB
SFO1         400.1324008 MHz
SI                32768
SF           400.1300000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



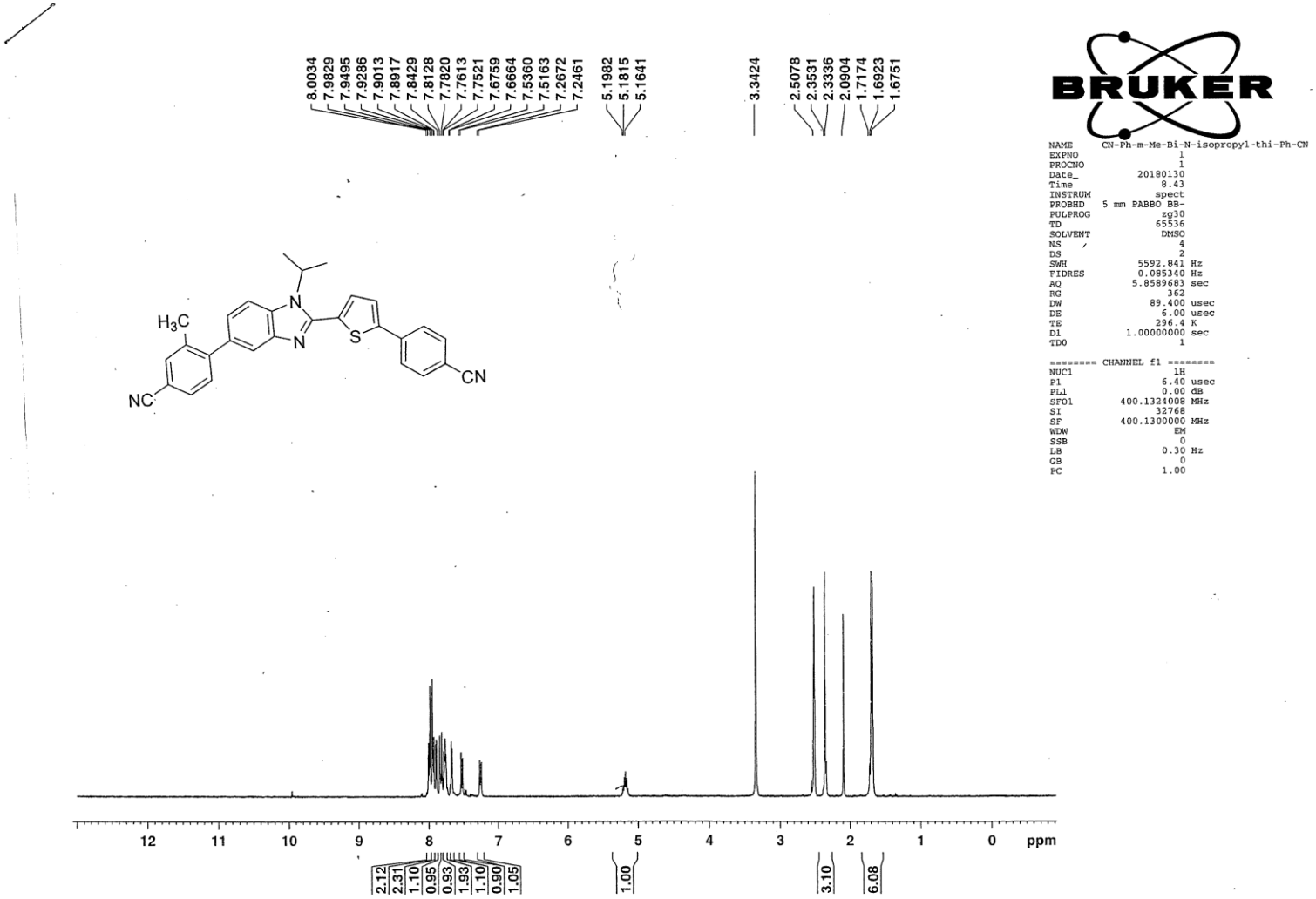
BRUKER

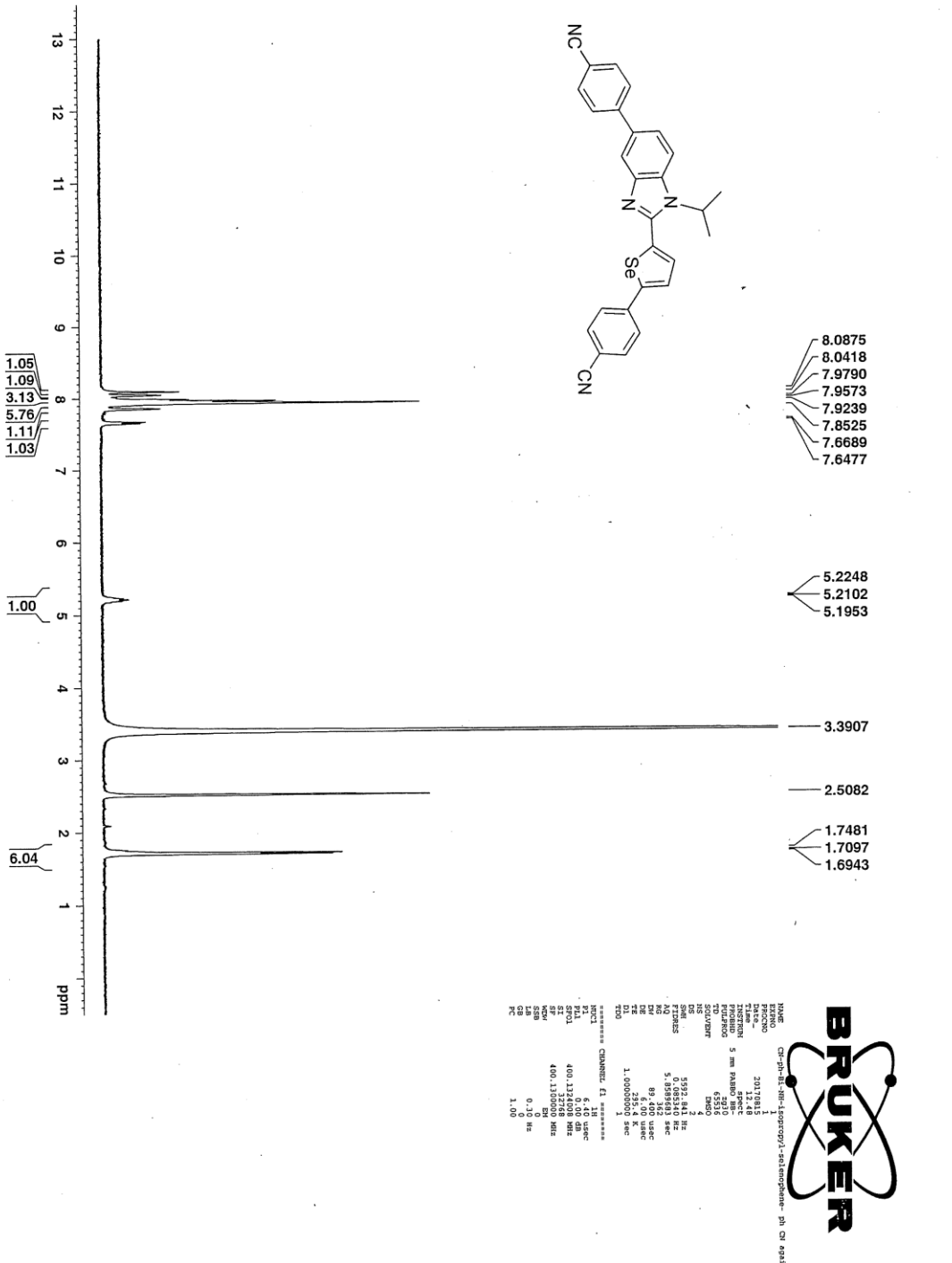
NAME	cn-ph-Bi-N-cyclopentyl-Thiophene-Ph-CN
EXPNO	1
PROCNO	1
Date_	20170829
Time	14.38
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	50
DS	2
SWH	5592.841 Hz
FIDRES	0.085340 Hz
AQ	5.8589683 sec
RG	181
DW	89.400 usec
DE	6.00 usec
TE	296.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	6.40 usec
PL1	0.00 dB
SFO1	400.1324008 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

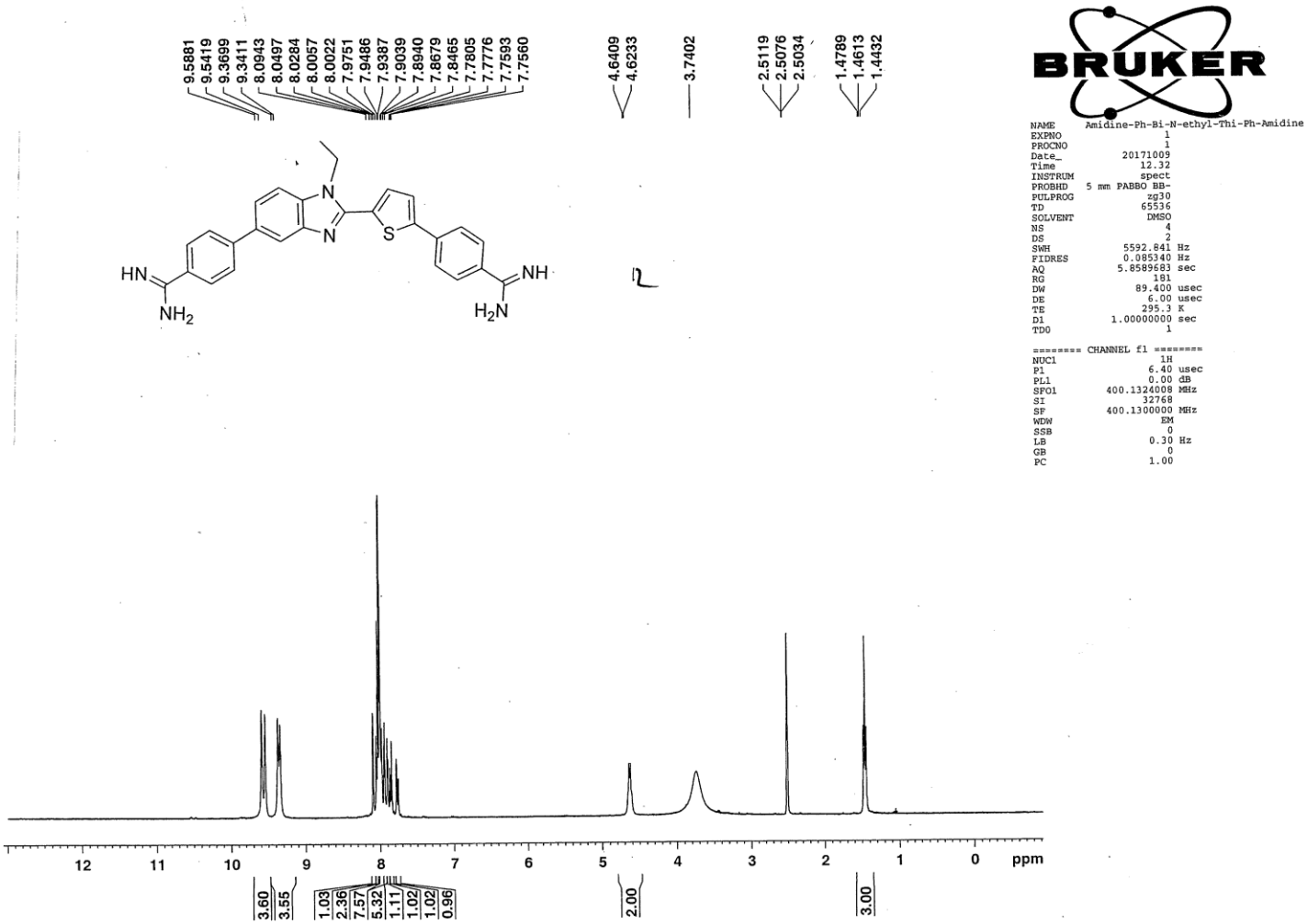

8.1384
8.1112
8.0225
8.0021
7.9486
7.9191
7.8636
7.6586
5.1928
5.1779
3.4298
2.5095
2.0875
1.7416
1.6903
1.6755
2.06
1.13
7.20
2.15
1.00
6.33
ppm
NC
Cl
N
N
S
CN
BRUKER




```
NAME        CF3-biscyano very clean
EXPNO                             1
PROCNO                            1
Date_                      20180417
Time                          13.29
INSTRUM                       spect
PROBHD     5 mm PABBO BB-
PULPROG                       zg30
TD                           65536
SOLVENT                       DMSO
NS                                4
DS                                2
SWH                     5592.841 Hz
FIDRES                  0.085340 Hz
AQ                      5.8589683 sec
RG                              256
DW                         89.400 usec
DE                          6.00 usec
TE                          297.0 K
D1                     1.00000000 sec
TD0                               1

======== CHANNEL f1 ========
NUC1                           1H
P1                         6.40 usec
PL1                         0.00 dB
SFO1                400.1324008 MHz
SI                         32768
SF                  400.1300000 MHz
WDW                           EM
SSB                            0
LB                          0.30 Hz
GB                             0
PC                          1.00
```

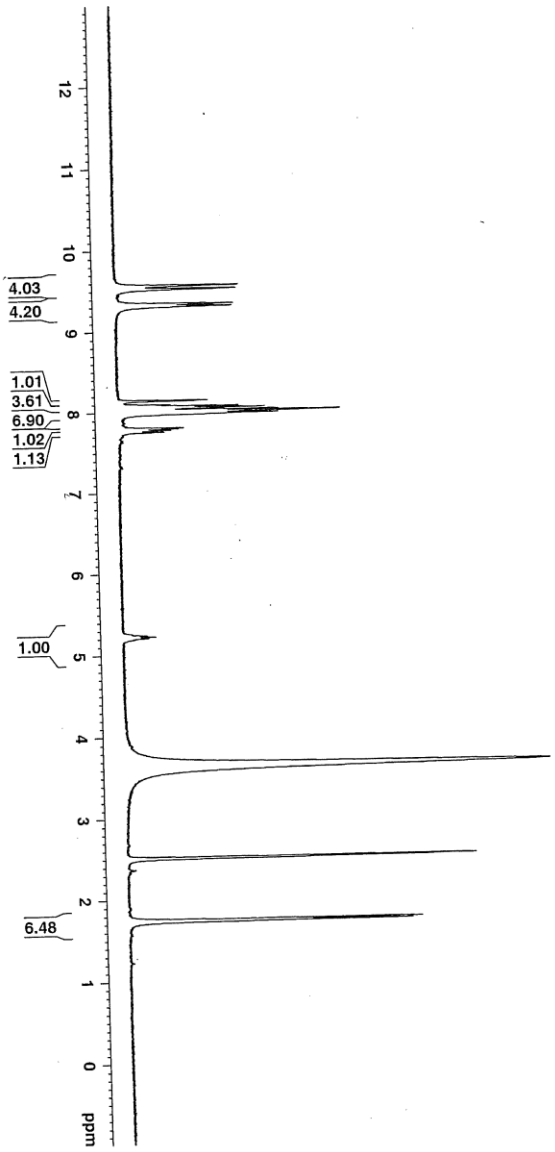

8.0034
7.9829
7.9495
7.9286
7.9013
7.8917
7.8429
7.8128
7.7820
7.7613
7.7521
7.6759
7.6664
7.5360
7.5163
7.2672
7.2461
5.1982
5.1815
5.1641
3.3424
2.5078
2.3531
2.3336
2.0904
1.7174
1.6923
1.6751
BRUKER
NAME CN-Ph-m-Me-Bi-N-isopropyl-thi-Ph-CN
EXPNO 1
PROCNO 1
Date_ 20180130
Time 8.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 4
DS 2
SWH 5592.841 Hz
FIDRES 0.085340 Hz
AQ 5.8589683 sec
RG 362
DW 89.400 usec
DE 6.00 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 6.40 usec
PL1 0.00 dB
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
H3C
N
N
S
CN
NC
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.12
2.31
1.10
0.95
0.93
1.93
1.10
0.90
1.05
1.00
3.10
6.08

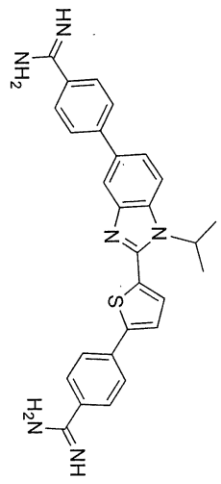

NC
N
N
Se
CN
8.0875
8.0418
7.9790
7.9573
7.9239
7.8525
7.6689
7.6477
5.2248
5.2102
5.1953
3.3907
2.5082
1.7481
1.7097
1.6943
1.05
1.09
3.13
5.76
1.11
1.03
1.00
6.04
ppm
BRUKER



BRUKER

NAME	Amidine-Ph-Bi-N-ethyl-Thi-Ph-Amidine
EXPNO	1
PROCNO	1
Date_	20171009
Time	12.32
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	4
DS	2
SWH	5592.841 Hz
FIDRES	0.085340 Hz
AQ	5.8589683 sec
RG	181
DW	89.400 usec
DE	6.00 usec
TE	295.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	6.40 usec
PL1	0.00 dB
SFO1	400.1324008 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00





9.5613
9.5196
9.3348
9.3056
8.1392
8.0868
8.0681
8.0478
8.0205
8.0025
7.9776
7.7992
7.7913
7.7722
7.7510

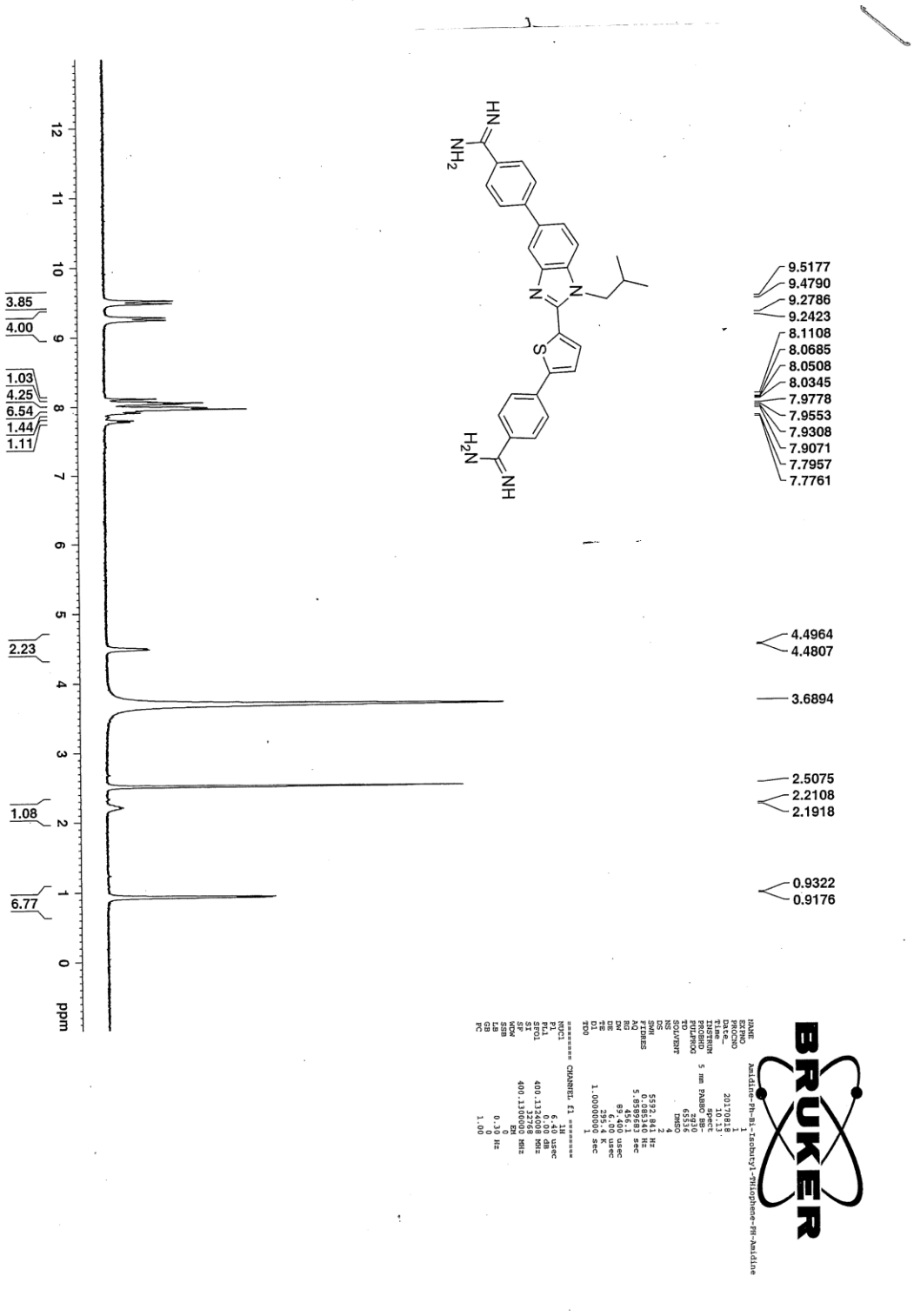
5.2377
5.2212
5.2035

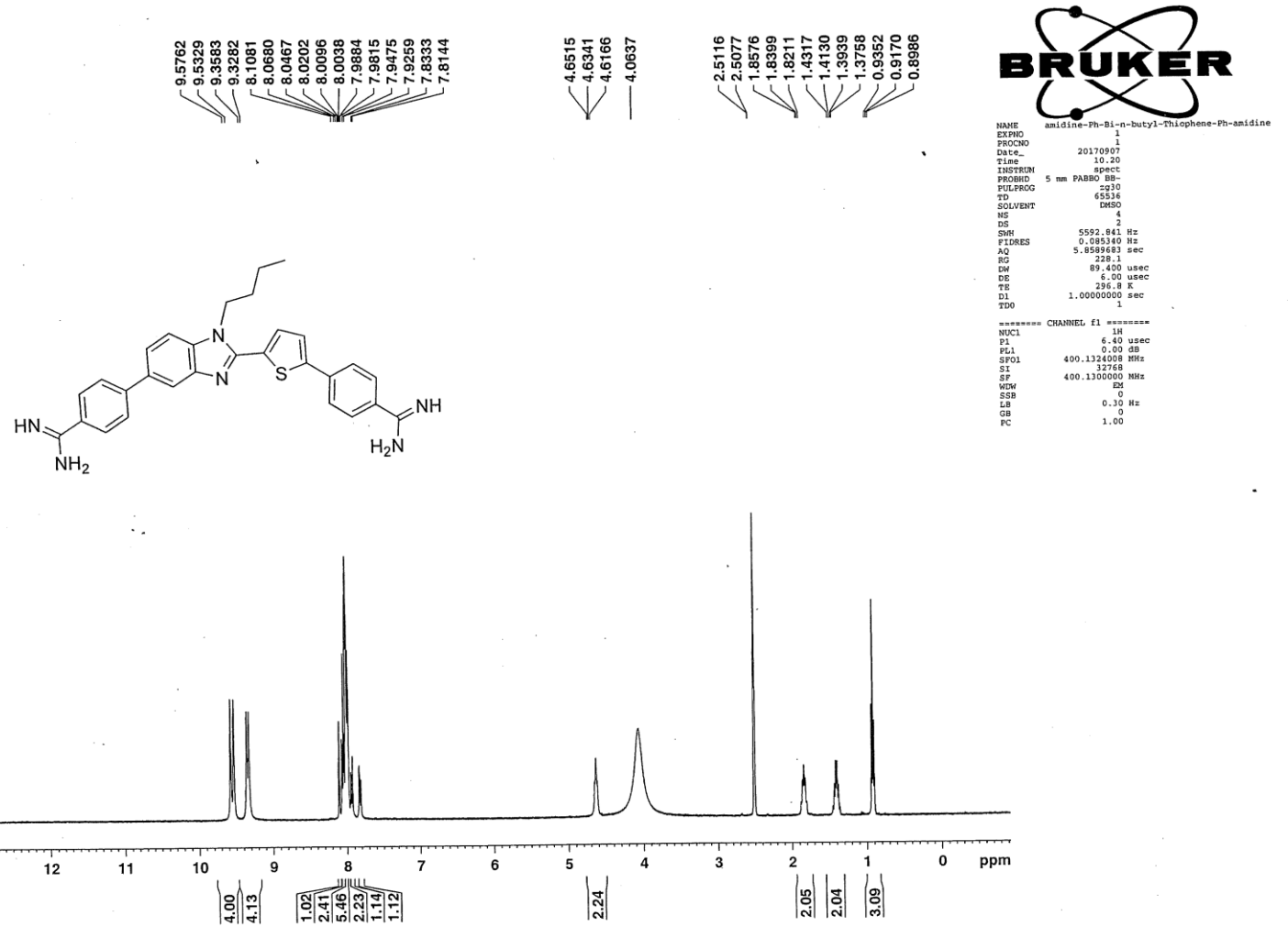
3.6442

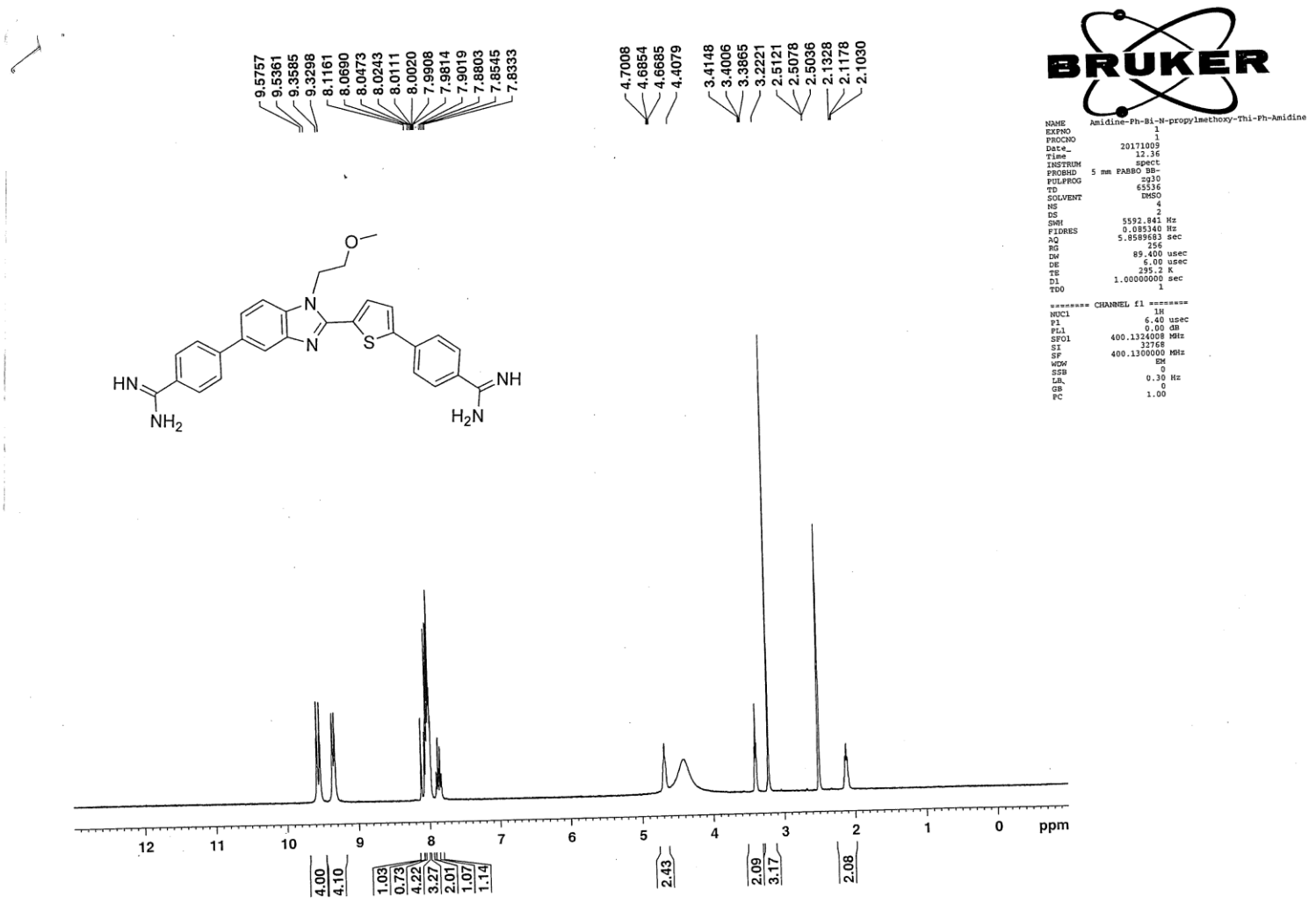
2.5078

1.7428
1.7265

NAME EXPNO PROCNO Date_ Time Solvent INSTRUM PROBHD PULPROG TD SOLVENT NS DS SWH FIDRES AQ RG DW DE TE D1 TD0 ======== CHANNEL f1 ======== NUC1 P1 PLW1 SFO1 SI SF WDW SSB LB GB PC
amidine-Ph-Bz-wf-isopropyl-Thiophene-Ph-amidine
1
1
20170807
9.39
<DMSO>
5 mm PABBO BB-
zg30
65536
DMSO
2
4
5592.841 Hz
0.085340 Hz
5.8932325 sec
89.00 usec
0.00 usec
296.3 K
1.00000000 sec
1
6.40 usec
400.1324009 MHz
32768
400.1300000 MHz
CDCl3
0.30 Hz
0.30
1.00


3.85
4.00
1.03
4.25
6.54
1.44
1.11
2.23
1.08
6.77
ppm
9.5177
9.4790
9.2786
9.2423
8.1108
8.0685
8.0508
8.0345
7.9778
7.9553
7.9308
7.9071
7.7957
7.7761
4.4964
4.4807
3.6894
2.5075
2.2108
2.1918
0.9322
0.9176
HN
NH2
N
N
S
H2N
NH
BRUKER


9.5762
9.5329
9.3583
9.3282
8.1081
8.0680
8.0467
8.0202
8.0096
8.0038
7.9884
7.9815
7.9475
7.9259
7.8333
7.8144
4.6515
4.6341
4.6166
4.0637
2.5116
2.5077
1.8576
1.8399
1.8211
1.4317
1.4130
1.3939
1.3758
0.9352
0.9170
0.8986
BRUKER
NAME amidine-Ph-Bi-n-butyl-Thiophene-Ph-amidine
EXPNO 1
PROCNO 1
Date_ 20170907
Time 10.20
INSTRUN spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 4
DS 2
SWH 5592.841 Hz
FIDRES 0.085340 Hz
AQ 5.8589683 sec
RG 228.1
DW 89.400 usec
DE 6.00 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 6.40 usec
PL1 0.00 dB
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HN
NH2
N
N
S
NH
H2N
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.00
4.13
1.02
2.41
5.46
2.23
1.14
1.12
2.24
2.05
2.04
3.09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9.5361
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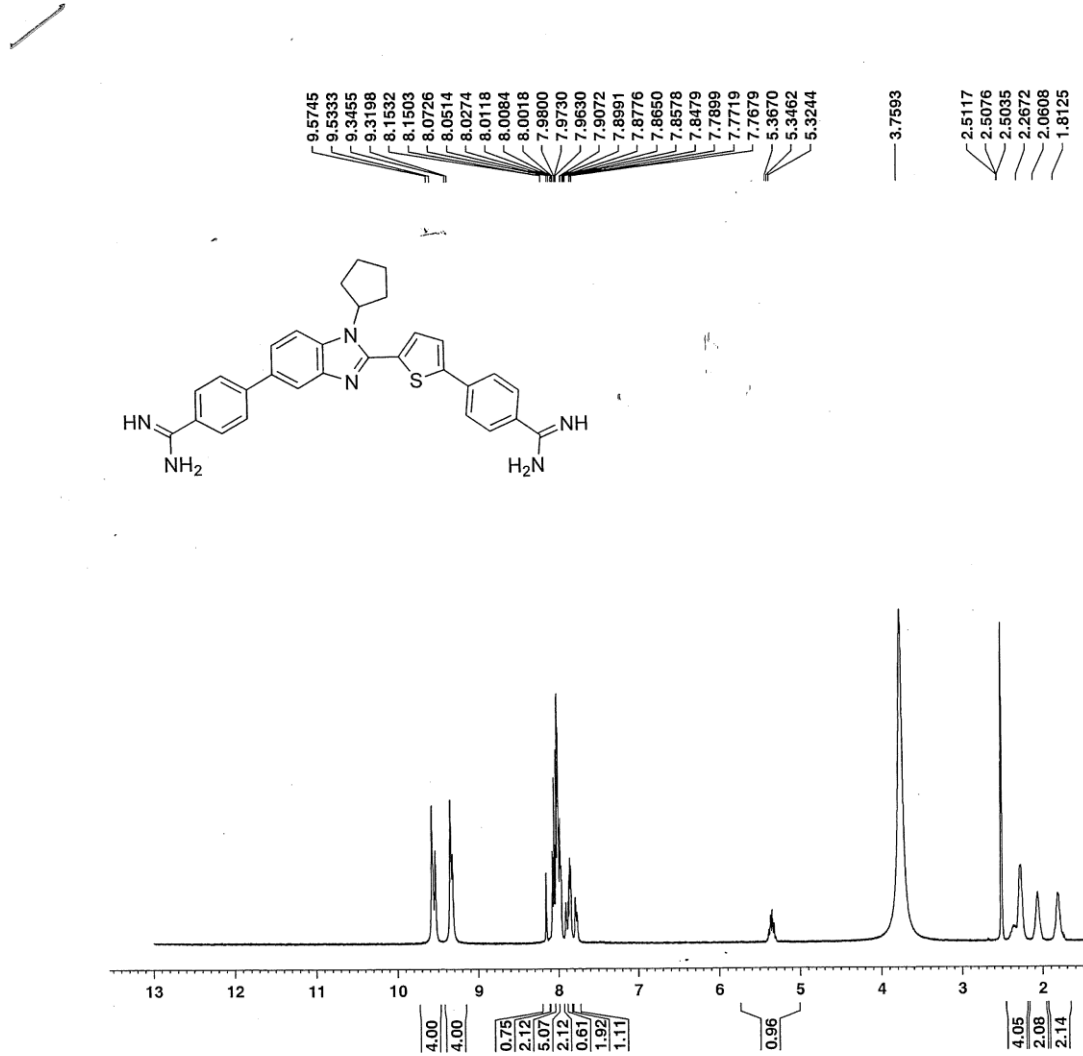
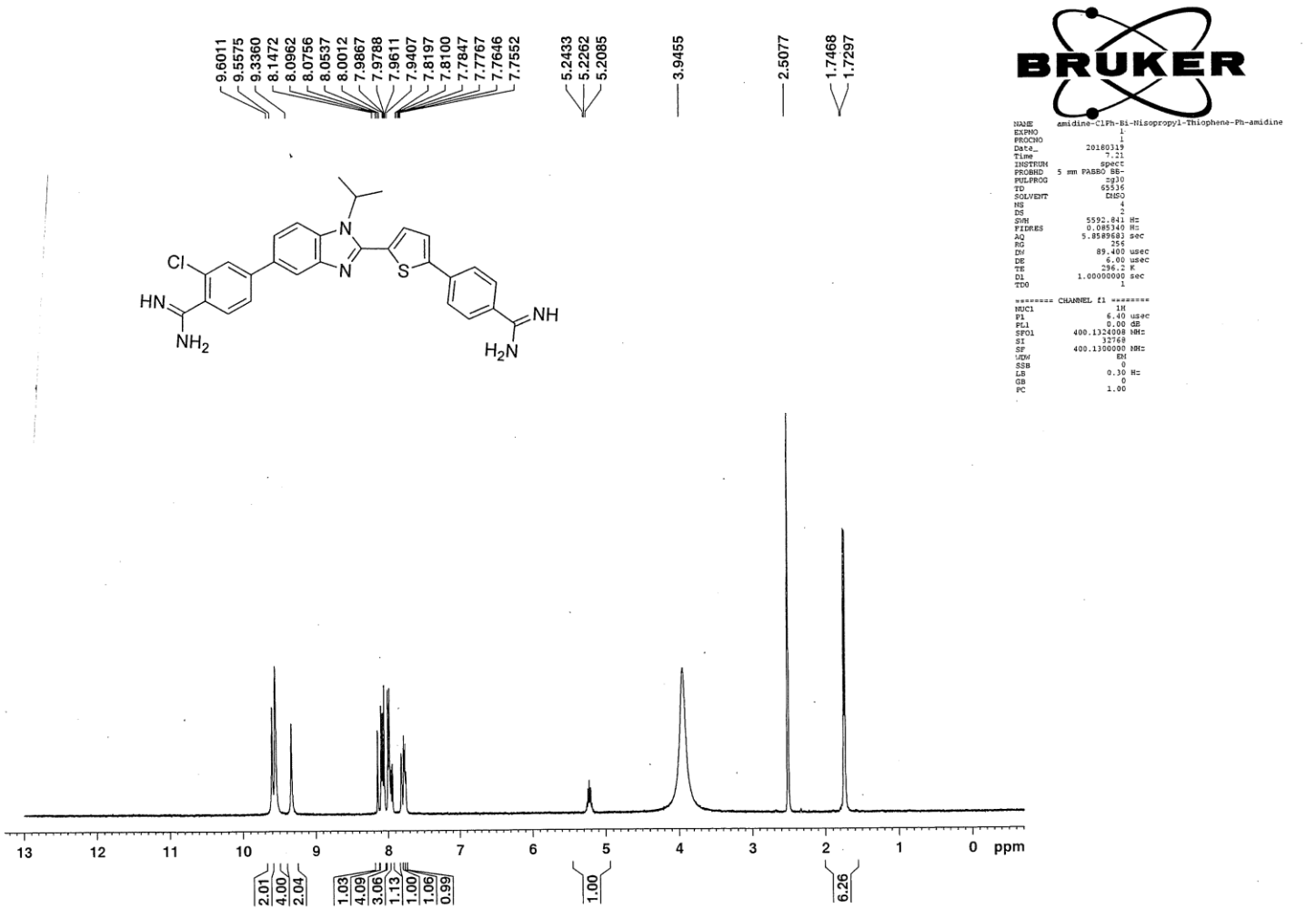
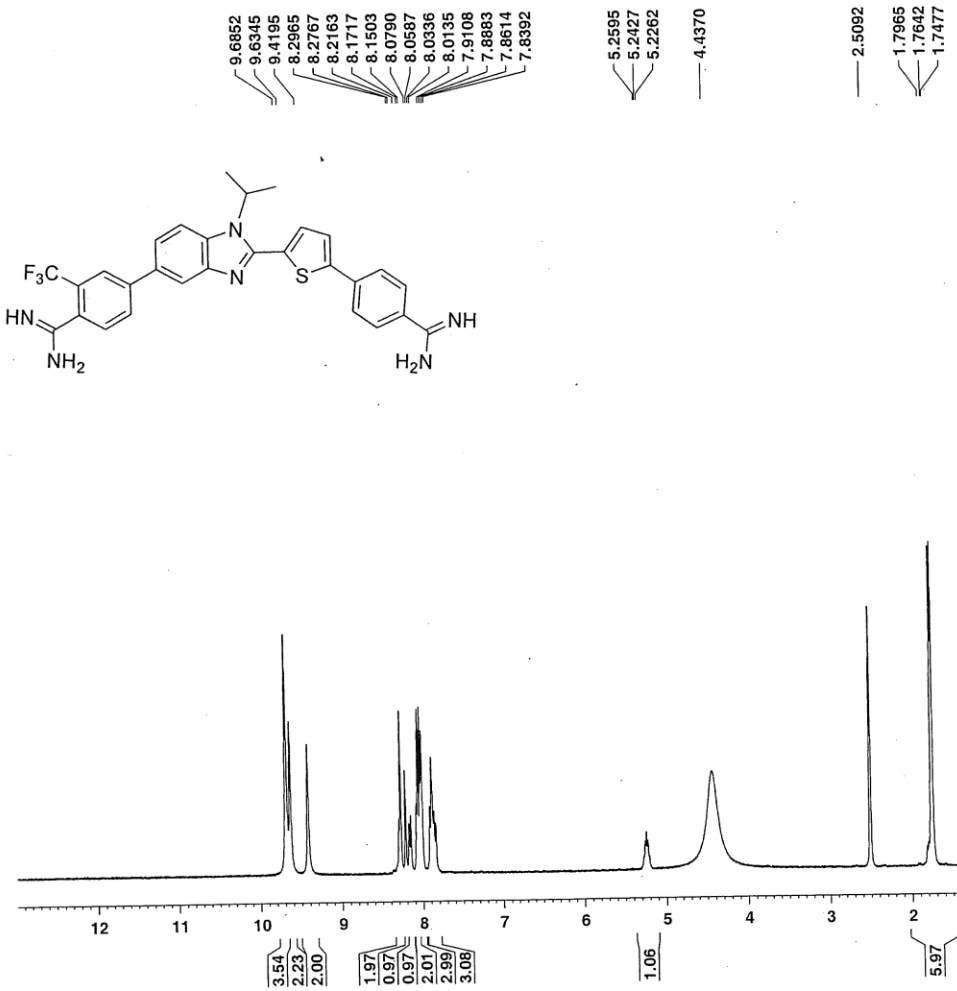
9.3298
8.1161
8.0690
8.0473
8.0243
8.0111
8.0020
7.9908
7.9814
7.9019
7.8803
7.8545
7.8333
4.7008
4.6854
4.6685
4.4079
3.4148
3.4006
3.3865
3.2221
2.5121
2.5078
2.5036
2.1328
2.1178
2.1030
BRUKER
NAME Amidine-Ph-Bi-N-propylmethoxy-Thi-Ph-Amidine
EXPNO 1
PROCNO 1
Date_ 20171009
Time 12.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 4
DS 2
SWH 5592.841 Hz
FIDRES 0.085340 Hz
AQ 5.8589683 sec
RG 256
DW 89.400 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 6.40 usec
PL1 0.00 dB
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HN
NH2
N
N
O
S
NH
H2N
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.00
4.10
1.03
0.73
4.22
3.27
2.01
1.07
1.14
2.43
2.09
3.17
2.08

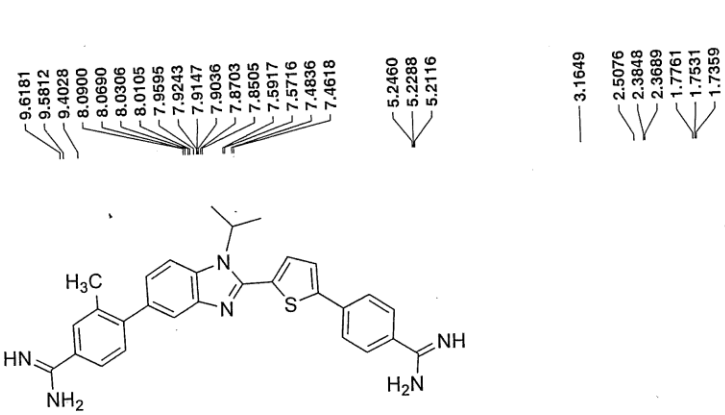

9.5745
9.5333
9.3455
9.3198
8.1532
8.1503
8.0726
8.0514
8.0274
8.0118
8.0084
8.0018
7.9800
7.9730
7.9630
7.9072
7.8991
7.8776
7.8650
7.8578
7.8479
7.7899
7.7719
7.7679
5.3670
5.3462
5.3244
3.7593
2.5117
2.5076
2.5035
2.2672
2.0608
1.8125
BRUKER
NAME amidine-Ph-Bi-N-cyclopentyl-Thiophene-Ph-amidine
EXPNO 1
PROCNO 1
Date_ 20170831
Time 16.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 4
DS 2
SWH 5592.841 Hz
FIDRES 0.085340 Hz
AQ 5.8589683 sec
RG 181
DW 89.400 usec
DE 6.00 usec
TE 295.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 6.40 usec
PL1 0.00 dB
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HN
NH2
N
N
S
NH
H2N
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
4.00
4.00
0.75
2.12
5.07
2.12
0.61
1.92
1.11
0.96
4.05
2.08
2.14


9.6011
9.5575
9.3360
8.1472
8.0962
8.0756
8.0537
8.0012
7.9867
7.9788
7.9611
7.9407
7.8197
7.8100
7.7847
7.7767
7.7646
7.7552
5.2433
5.2262
5.2085
3.9455
2.5077
1.7468
1.7297
Cl
HN
NH2
N
N
S
NH
H2N
BRUKER
NAME amidine-ClPh-Bi-Nisopropyl-Thiophene-Ph-amidine
EXPNO 1
PROCNO 1
Date_ 20180319
Time 7.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 4
DS 2
SWH 5592.841 Hz
FIDRES 0.085340 Hz
AQ 5.8589683 sec
RG 256
DW 89.400 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 6.40 usec
PL1 0.00 dB
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
4.00
2.04
1.03
4.09
3.06
1.13
1.00
1.06
0.99
1.00
6.26



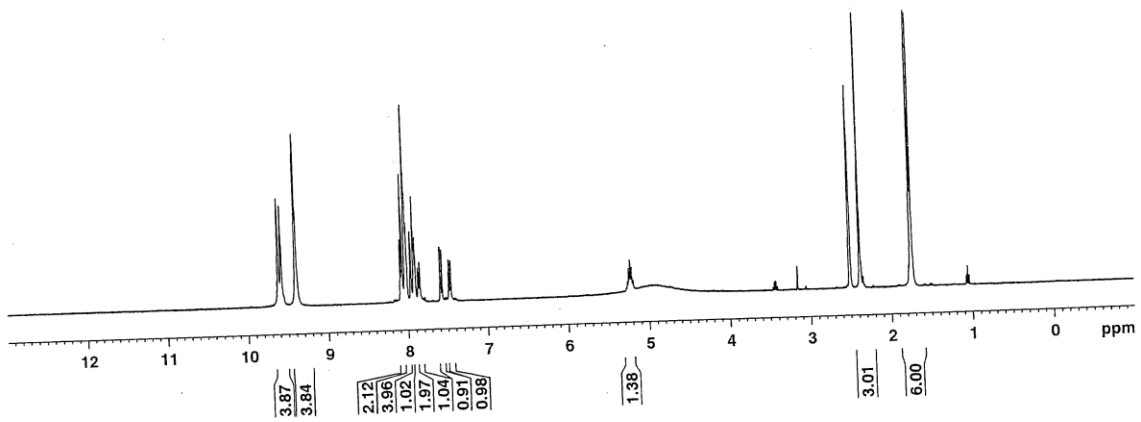
BRUKER

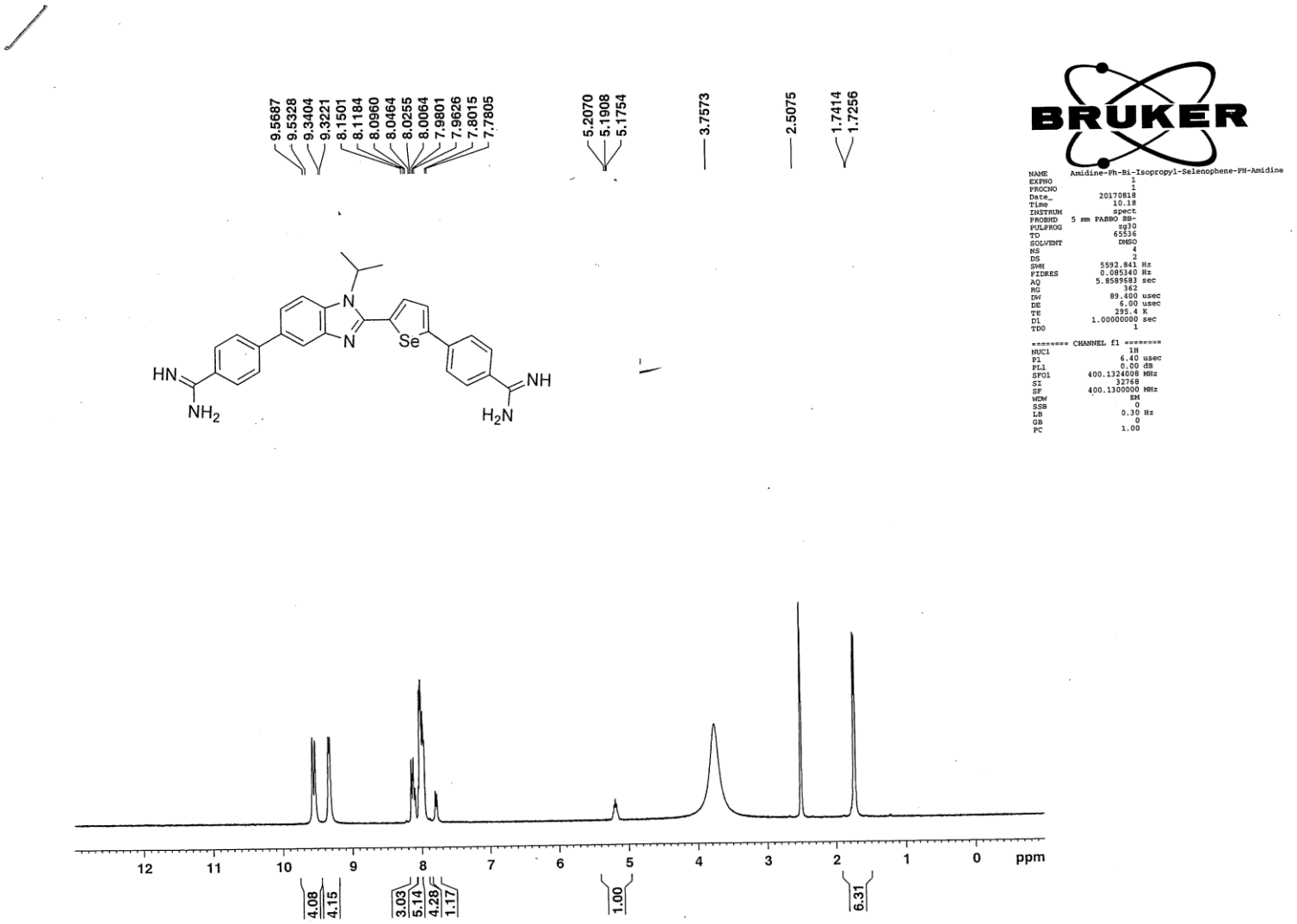
NAME	CF3 diamidine again
EXPNO	1
PROCNO	1
Date_	20180419
Time	11.24
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	4
DS	2
SWH	5592.841 Hz
FIDRES	0.085340 Hz
AQ	5.8589683 sec
RG	228.1
DW	89.400 usec
DE	6.00 usec
TE	297.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	6.40 usec
PL1	0.00 dB
SFO1	400.1324008 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



NAME amidine-Ph-m-Me-Bi-N-isopropyl-thi-Ph-amidine
EXPNO 1
PROCNO 1
Date_ 20180201
Time 9.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 4
DS 2
SWH 5592.841 Hz
FIDRES 0.085340 Hz
AQ 5.8589683 sec
RG 228.1
DW 89.400 usec
DE 6.00 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 6.40 usec
PL1 0.00 dB
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00




9.5687
9.5328
9.3404
9.3221
8.1501
8.1184
8.0960
8.0464
8.0255
8.0064
7.9801
7.9626
7.8015
7.7805
5.2070
5.1908
5.1754
3.7573
2.5075
1.7414
1.7256
BRUKER
NAME Amidine-Ph-Bi-Isopropyl-Selenophene-PH-Amidine
EXPNO 1
PROCNO 1
Date_ 20170818
Time 10.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 4
DS 2
SWH 5592.841 Hz
FIDRES 0.085340 Hz
AQ 5.8589683 sec
RG 362
DW 89.400 usec
DE 6.00 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 6.40 usec
PL1 0.00 dB
SFO1 400.1324008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HN
NH2
N
N
Se
NH
H2N
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.08
4.15
3.03
5.14
4.28
1.17
1.00
6.31