

Supporting Information for

Aryl-substituted aminobenzimidazoles targeting the hepatitis C virus internal ribosome entry site

Kejia Ding, Annie Wang, Mark A. Boerneke, Sergey M. Dibrov and Thomas Hermann*

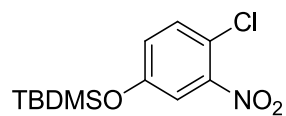
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Experimental Procedures

General Notes: All chemical reagents were obtained from commercial suppliers listed on UCSD Market Place website and used without further purification. Anhydrous solvents were obtained using a two-column purification system (Glasscontour Systems, Irvine, CA). Non-aqueous reactions were carried out under anhydrous conditions using oven-dried glassware under an inert atmosphere. The inert atmosphere was created via balloons filled with Argon (Ar) gas or via a Schlenk line apparatus. Analytical thin-layer chromatography (TLC) was carried out on precoated 60 F254 aluminum backed silica gel plates from EMD Millipore. TLC plates were visualized by UV and/or stained by ninhydrin solution followed by heating. Flash column chromatography was performed using SiliaFlash P60 40-63 μm 60 \AA silica gel from Silicycle. Organic solvents were removed by rotary evaporation below 30 $^{\circ}\text{C}$ at approximately 15 mmHg. NMR spectra were recorded at room temperature (22 $^{\circ}\text{C}$) on a Varian Mercury 400 MHz instrument with chemical shifts reported relative to residual deuterated solvent peaks. Deuterated solvents used include deuteriochloroform (CDCl_3), deuteromethanol (CD_3OD), and deuterodimethyl sulfoxide (DMSO-d_6). Chemical shifts (δ) are in parts per million (ppm); multiplicities are indicated by s (singlet), d (doublet), t (triplet), q (quartet), dd (doublet of doublet), or m (multiplet); coupling constants (J) are reported in Hertz (Hz). Mass spectra were obtained on a Micromass Quattro Ultima Triple Quadrupole using the ESI method at the UCSD Molecular Mass Spectrometry Facility.

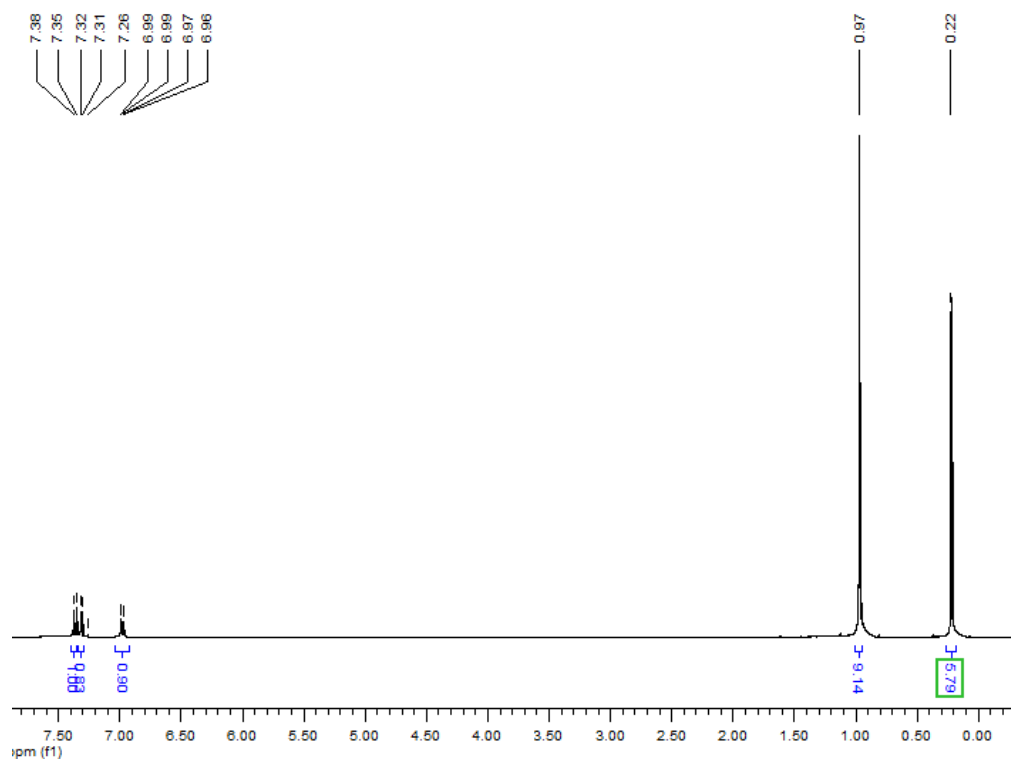
Abbreviations: ACN = acetonitrile; BINAP = 2,2'-bis(diphenylphosphino)-1,1'-binaphthalene; dba = dibenzylideneacetone; DCM = dichloromethane; DIPC = N,N'-diisopropylcarbodiimide; DIPEA = N,N-diisopropylethylamine; DMF = dimethylformamide; DMSO = dimethyl sulfoxide; RT = room temperature; TBDMSCl = tert-butyldimethylsilyl chloride;

***tert*-butyl(4-chloro-3-nitrophenoxy)dimethylsilane (9a)**

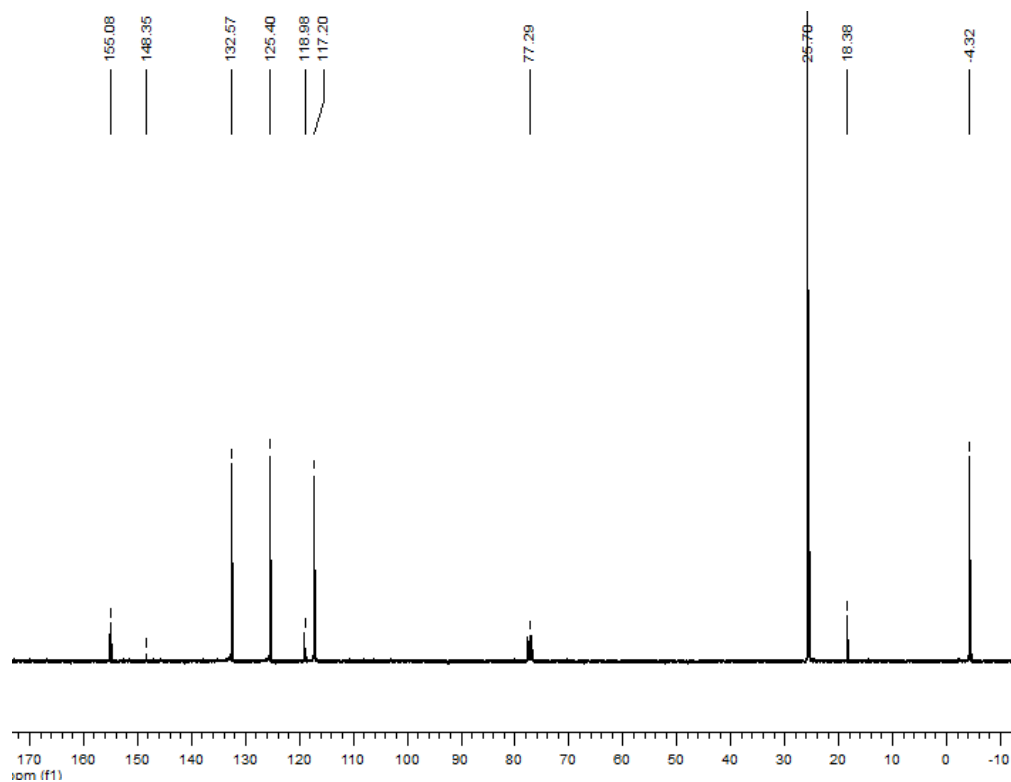


To a 100 ml round-bottom flask was added 4-chloro-3-nitrophenol (200 mg, 1.16 mmol), DCM (30 ml), *tert*-butyldimethylchlorosilane (174 mg, 1.16 mmol), and triethylamine (161 μ l, 1.16 mmol). The reaction was stirred at RT for 2.5 hours, then concentrated and purified via flash column (hexane – DCM : 80 % - 20 %) to yield the product as a clear oil (324 mg, 94 % yield). ^1H NMR (400 MHz, CDCl_3): δ 7.38 (d, $J = 8$ Hz, 1H), 7.32 (d, $J = 2$ Hz, 1H), 6.99 (dd, $J_1 = 8$ Hz, $J_2 = 2$ Hz, 1H), 0.97 (s, 9H), 0.22 (s, 6H). ^{13}C NMR (400 MHz, CDCl_3): δ 155.08, 148.35, 132.56, 125.39, 118.98, 117.20, 25.70, 18.37, -4.32.

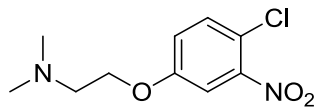
tert-butyl(4-chloro-3-nitrophenoxy)dimethylsilane (**9a**) ^1H NMR (400 MHz, CDCl_3)



tert-butyl(4-chloro-3-nitrophenoxy)dimethylsilane (**9a**) ^{13}C NMR (400 MHz, CDCl_3)

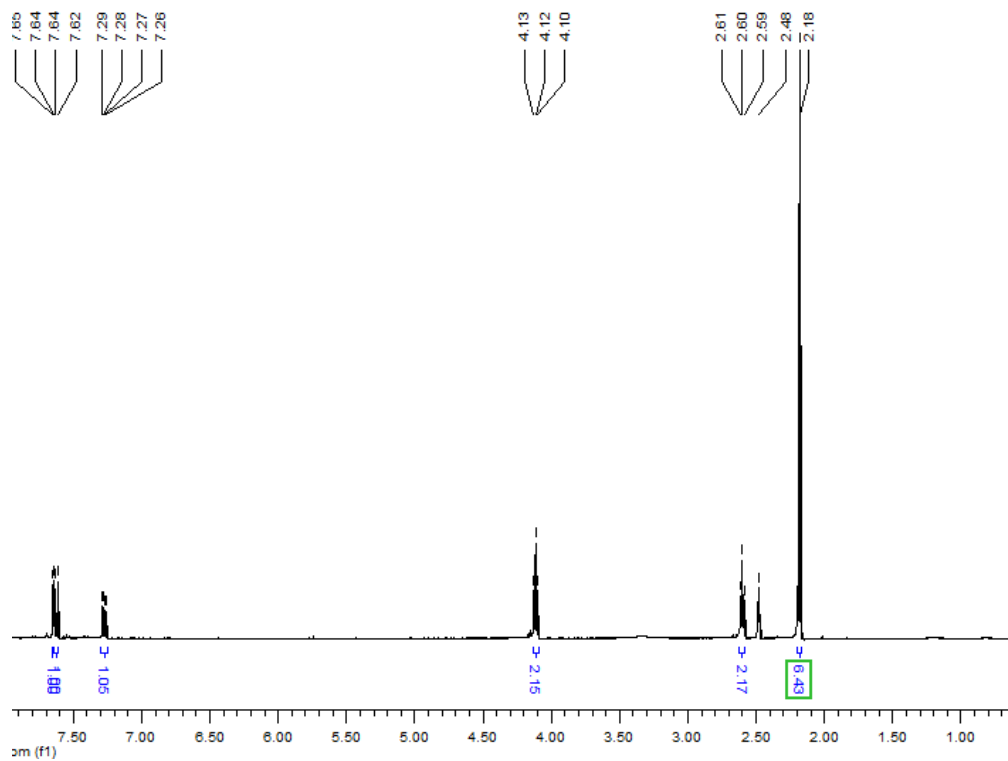


2-(4-chloro-3-nitrophenoxy)-*N,N*-dimethylethanamine (9b)

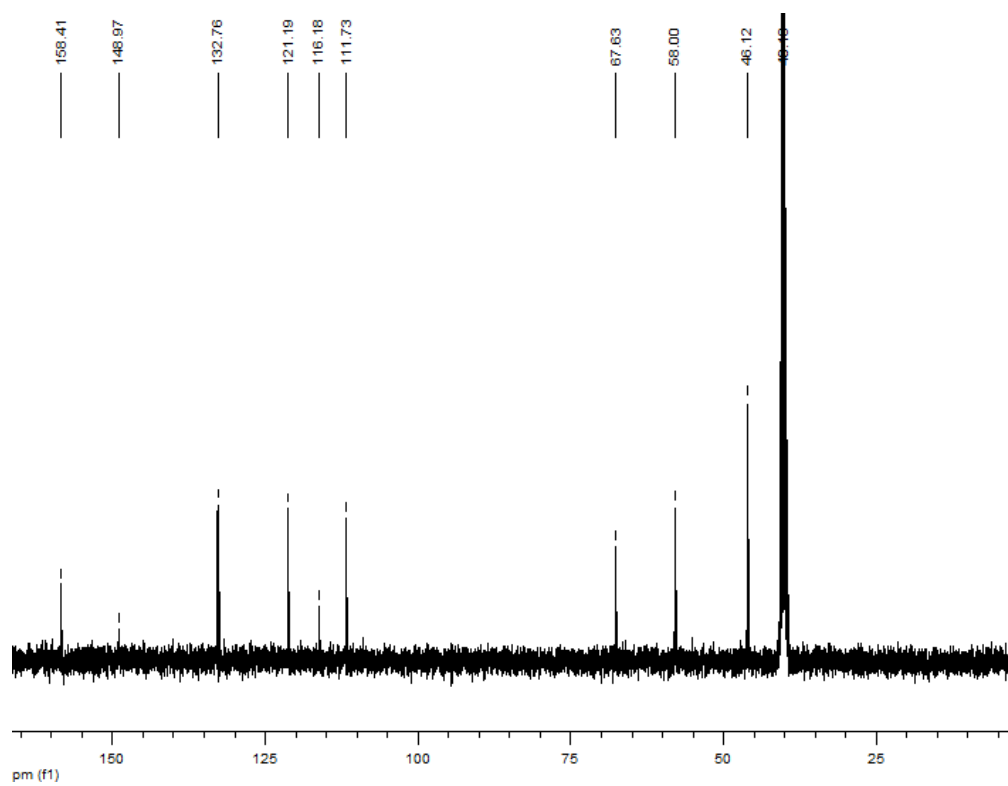


To a 100 ml round-bottom flask was added 2-dimethylaminoethyl chloride hydrochloride (1.0 g, 6.9 mmol, 1.2 eq), ACN (50 ml), 4-chloro-3-nitrophenol (1.0 g, 5.8 mmol) and finally K_2CO_3 (1.7 g, 12.7 mmol). The reaction was stirred under Ar and heated to reflux for 26 hours before cooling to RT and filtration. After removal of solvent, the residue was extracted with EtOAc and water (150 ml ea.). The water layer was extracted with additional 100 ml of EtOAc. The combined organic layers were then washed with water, brine and dried over Na_2SO_4 . After filtration and concentration, the crude was purified with flash column chromatography (DCM – MeOH : 90 % - 10 %) to yield a yellow oil as the product (1.3 g, 94 % yield). 1H NMR (400 MHz, DMSO- d_6): δ 7.65 (d, $J = 3$ Hz), 7.64 (d, $J = 9$ Hz, 1H), 7.29 (dd, $J_1 = 9$ Hz, $J_2 = 3$ Hz, 1H), 4.12 (t, $J = 5$ Hz, 2H), 2.60 (t, $J = 5$ Hz, 2H), 2.18 (s, 6H). ^{13}C NMR (400 MHz, DMSO- d_6): δ 158.41, 148.96, 132.76, 121.19, 116.18, 111.72, 67.62, 58.00, 46.12.

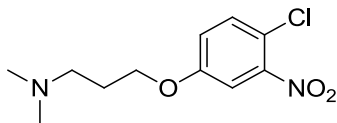
2-(4-chloro-3-nitrophenoxy)-*N,N*-dimethylethanamine (**9b**) ^1H NMR (400 MHz, DMSO- d_6)



2-(4-chloro-3-nitrophenoxy)-*N,N*-dimethylethanamine (**9b**) ^{13}C NMR (400 MHz, DMSO- d_6)

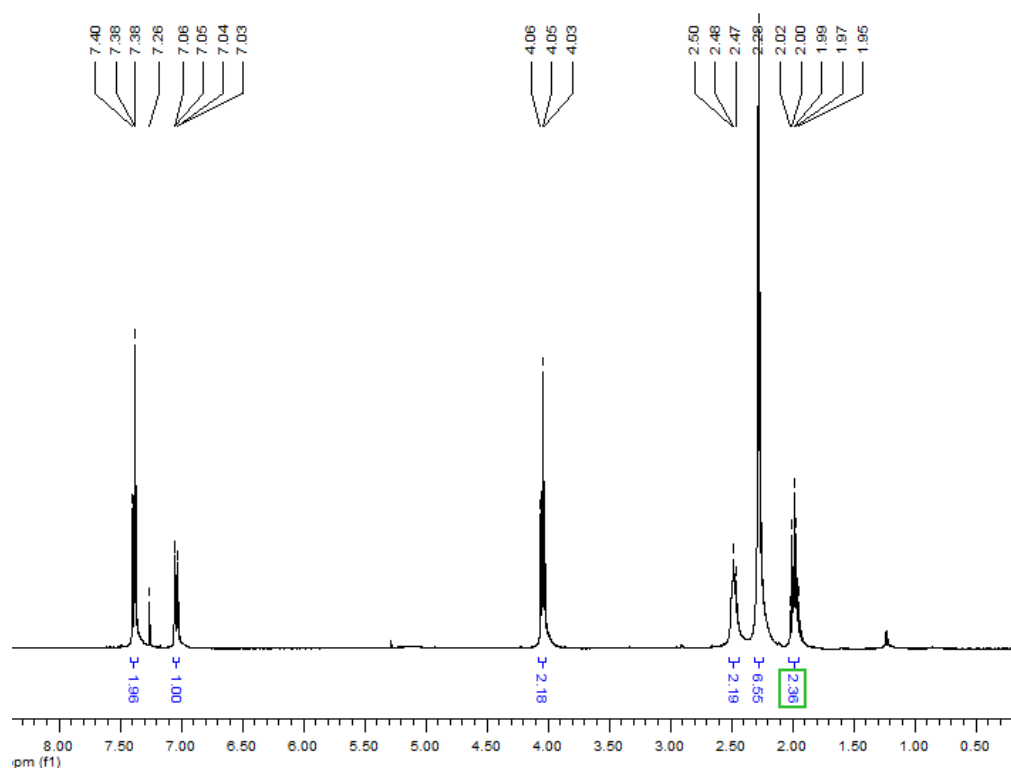


3-(4-chloro-3-nitrophenoxy)-*N,N*-dimethylpropan-1-amine (9c)

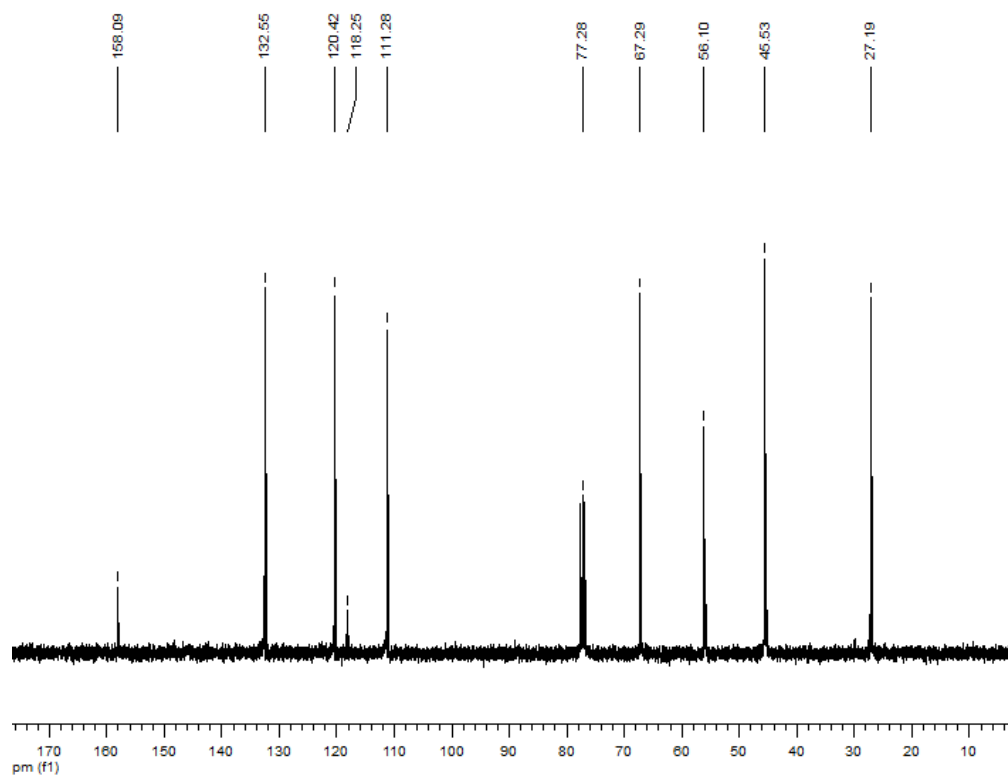


To a 250 ml round-bottom flask was added 4-chloro-3-nitrophenol (2.0 g, 11.5 mmol), DMF (100 ml), *N,N*-dimethylaminopropylchloride hydrochloride (2.2 g, 13.8 mmol, 1.2 eq), and K_2CO_3 (3.1 g, 23.0 mmol). The reaction was stirred and heated to 60 °C for 16 hours before cooling to RT, filtration and concentration. The crude was purified via flash column chromatography (DCM – MeOH : 90 % - 10 %) to yield the product as a yellow oil (2.4 g, 79 % yield). 1H NMR (400 MHz, $CDCl_3$): δ 7.40 – 7.38 (m, 2H), 7.06 (dd, $J_1 = 9$ Hz, $J_2 = 3$ Hz, 1H), 4.06 (t, $J = 6$ Hz, 2H), 2.50 (t, $J = 7$ Hz, 2H), 2.27 (s, 6H), 2.02 (p, $J = 6$ Hz, 2H). ^{13}C NMR (400 MHz, $CDCl_3$): δ 158.08, 132.54, 120.41, 118.24, 111.27, 67.29, 56.10, 45.53, 27.19. MS (ESI) calculated exact mass for $C_{11}H_{15}ClN_2O_3 = 258.08$. Found $[M+H]^+ = 259.00$.

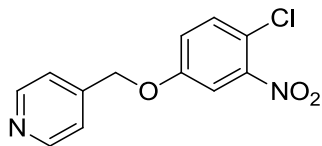
3-(4-chloro-3-nitrophenoxy)-*N,N*-dimethylpropan-1-amine (**9c**) ^1H NMR (400 MHz, CDCl_3)



3-(4-chloro-3-nitrophenoxy)-*N,N*-dimethylpropan-1-amine (**9c**) ^{13}C NMR (400 MHz, CDCl_3)

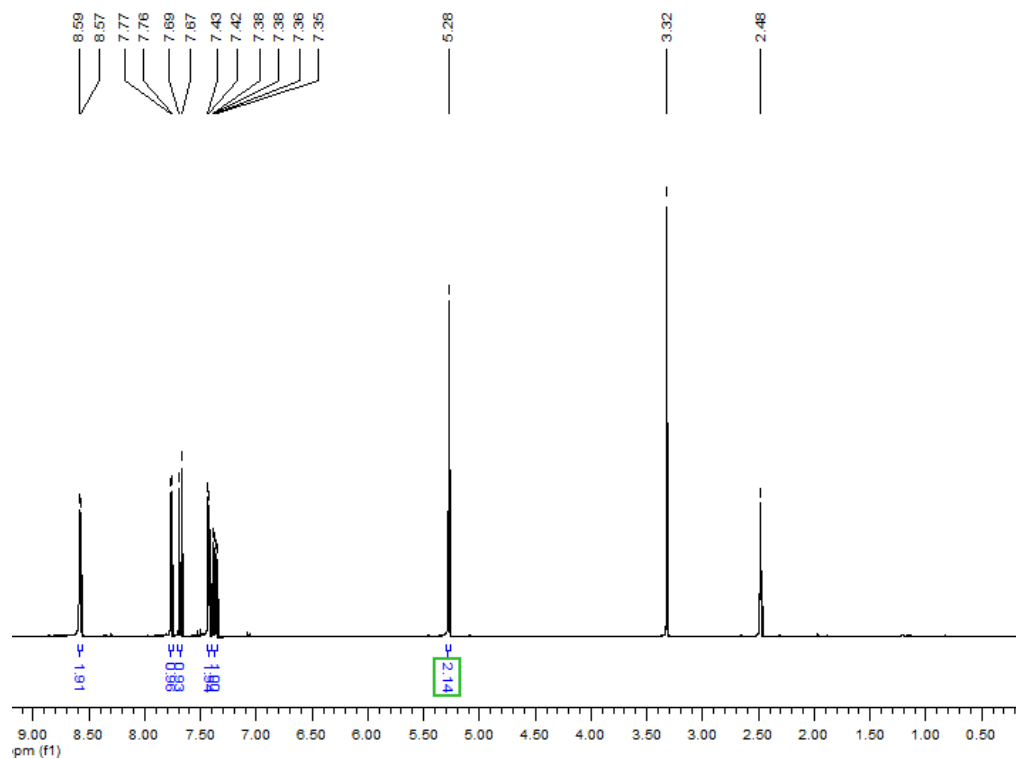


4-((4-chloro-3-nitrophenoxy)methyl)pyridine (9d)

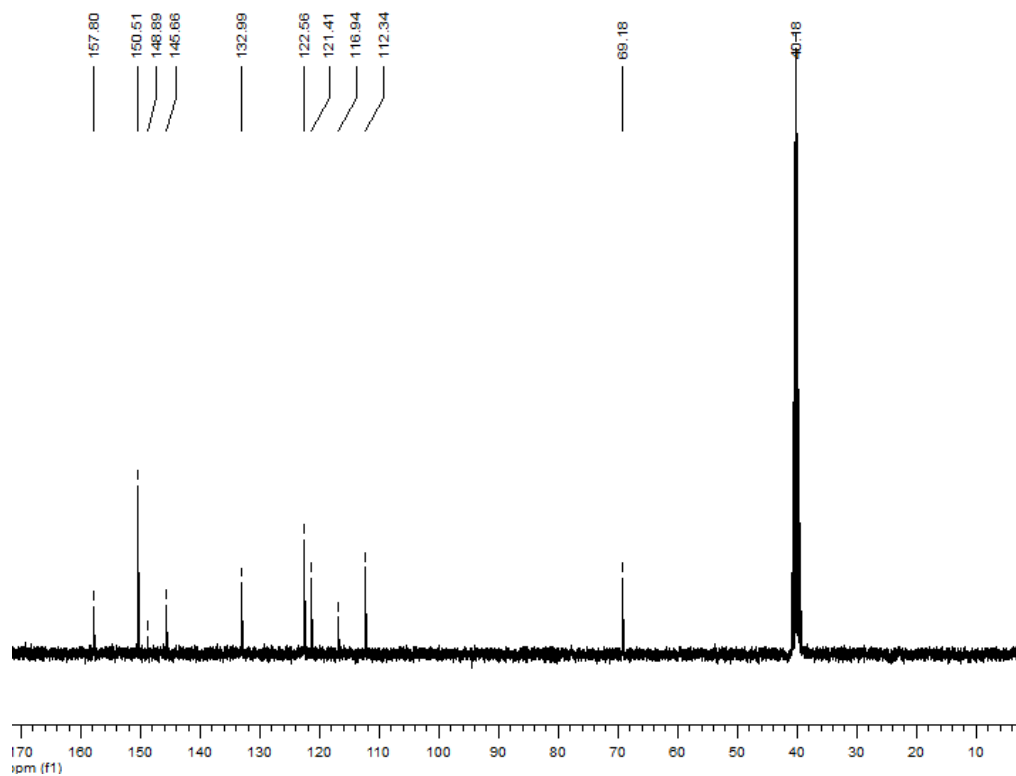


To a 250 ml round-bottom flask was added 4-chloro-3-nitrophenol (1.6 g, 9.2 mmol), DMF (100 ml), 4-picolylchloride hydrochloride (1.5 g, 9.2 mmol) and K_2CO_3 (2.54 g, 18.3 mmol). The reaction was stirred and heated to 60 °C for 28 hours before cooling to RT, filtration and concentration. The crude was purified via flash column (Hexane – EtOAc : 40 % - 60 %) to yield a slightly yellow solid product (1.3 g, 52 % yield). 1H NMR (400 MHz, DMSO- d_6): δ 8.59 (d, $J = 6$ Hz, 2H), 7.77 (d, $J = 3$ Hz, 1H), 7.69 (d, $J = 9$ Hz, 1H), 7.43 (d, $J = 6$ Hz, 2H), 7.38 (dd, $J_1 = 9$ Hz, $J_2 = 3$ Hz, 1H), 5.28 (s, 2H). ^{13}C NMR (400 MHz, DMSO- d_6): δ 157.80, 150.50, 148.89, 145.65, 132.99, 122.55, 121.41, 116.94, 112.23, 67.17. MS (ESI) calculated exact mass for $C_{12}H_9ClN_2O_3 = 264.03$. Found $[M+H]^+ = 264.97$.

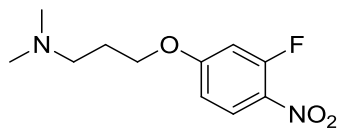
4-((4-chloro-3-nitrophenoxy)methyl)pyridine (**9d**) ^1H NMR (400 MHz, DMSO- d_6)



4-((4-chloro-3-nitrophenoxy)methyl)pyridine (**9d**) ^{13}C NMR (400 MHz, DMSO- d_6)

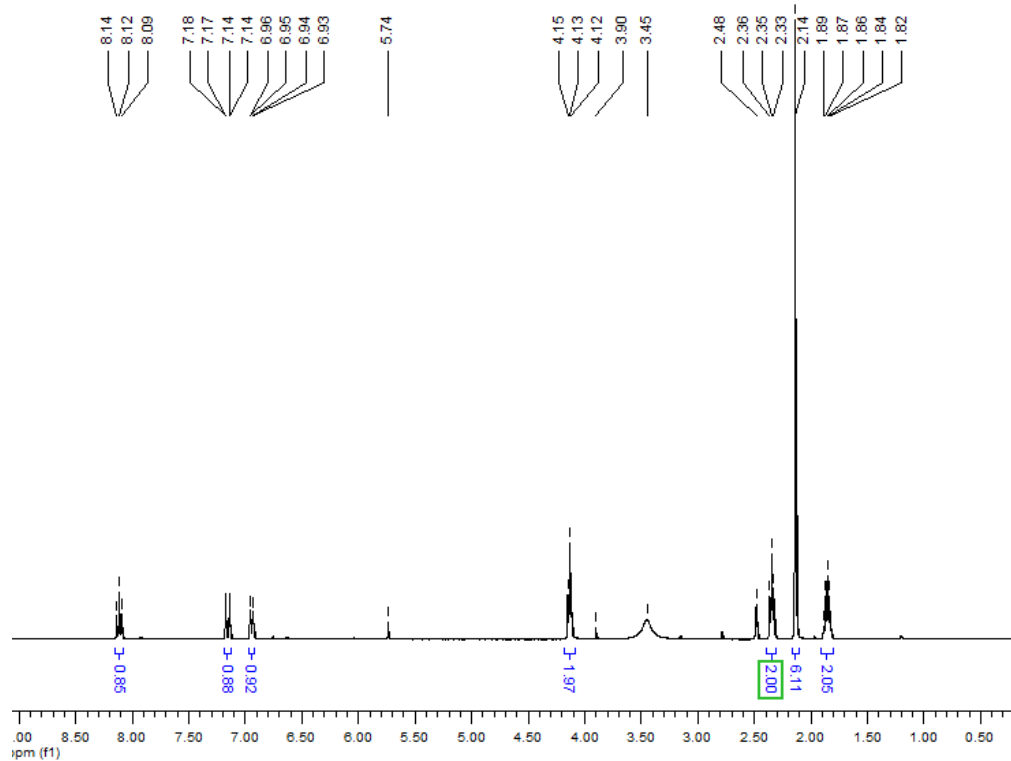


3-(3-fluoro-4-nitrophenoxy)-*N,N*-dimethylpropan-1-amine (9f)

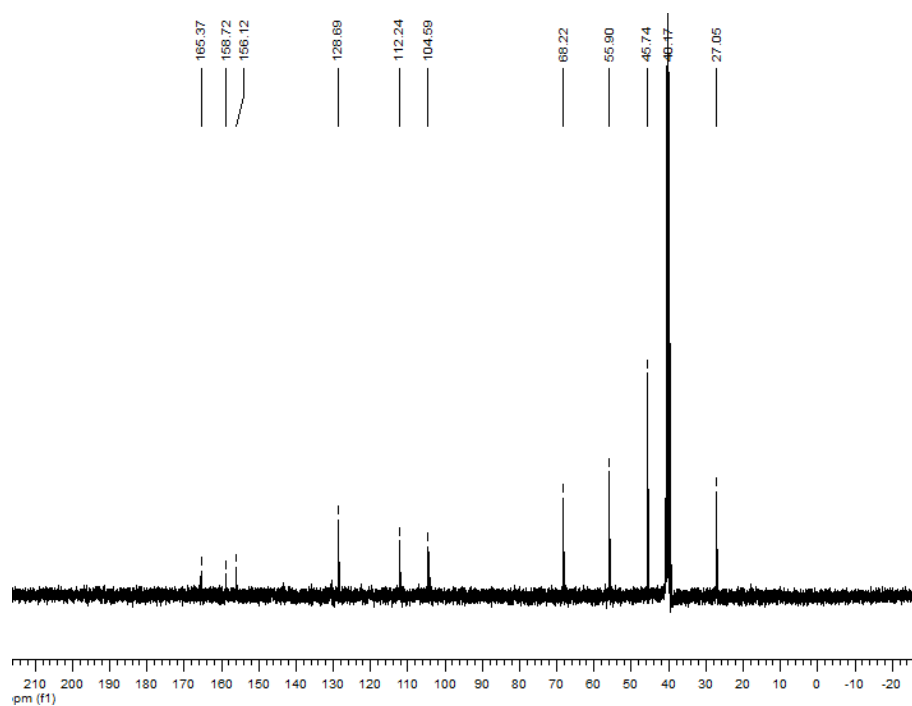


To a 250 ml round-bottom flask was added 3-fluoro-4-nitrophenol (2.0 g, 12.7 mmol), DMF (100 ml), *N,N*-dimethylaminopropylchloride hydrochloride (2.4 g, 15.3 mmol, 1.2 eq), and K_2CO_3 (3.9 g, 28.0 mmol). The reaction was stirred and heated to 60 °C for 18 hours before cooling to RT, filtration and concentration. The crude was purified via flash column (DCM – MeOH : 90 % - 10 %) to yield a yellow oil as the product (2.0 g, 64 % yield). 1H NMR (400 MHz, DMSO- d_6): δ 8.14 (t, $J = 9$ Hz, 1H), 7.18 (dd, $J_1 = 14$ Hz, $J_2 = 3$ Hz, 1H), 6.96 (dd, $J_1 = 9$ Hz, $J_2 = 2$ Hz, 1H), 4.15 (t, $J = 7$ Hz, 2H), 2.36 (t, $J = 7$ Hz, 2H), 2.14 (s, 6H), 1.89 (p, $J = 6$ Hz, 2H). ^{13}C NMR (400 MHz, DMSO- d_6): δ 165.37, 158.72, 156.11, 128.69, 112.23, 104.59, 68.22, 55.90, 45.74, 27.05. MS (ESI) calculated exact mass for $C_{11}H_{16}FN_2O_3 = 242.11$. Found $[M+H]^+ = 243.06$.

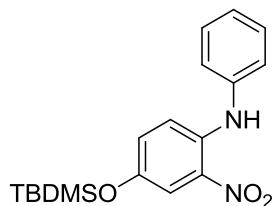
3-(3-fluoro-4-nitrophenoxyl)-*N,N*-dimethylpropan-1-amine (**9f**) ¹H NMR (400 MHz, DMSO-d₆)



3-(3-fluoro-4-nitrophenoxyl)-*N,N*-dimethylpropan-1-amine (**9f**) ¹³C NMR (400 MHz, DMSO-d₆)

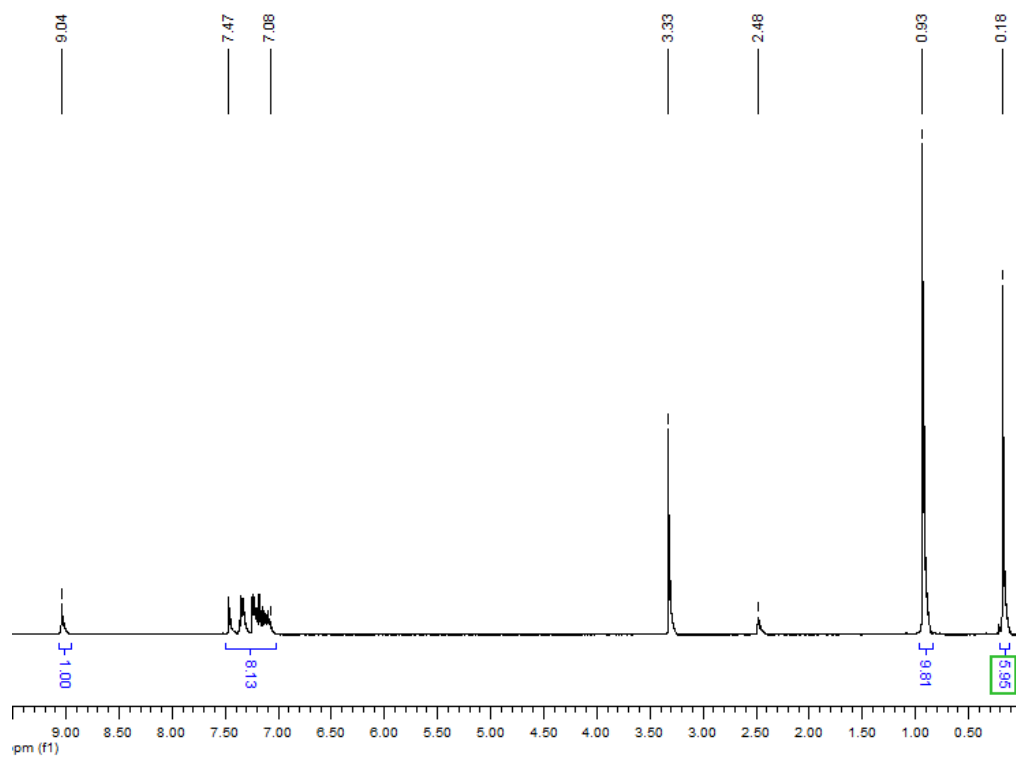


4-((*tert*-butyldimethylsilyl)oxy)-2-nitro-*N*-phenylaniline (**11a**)

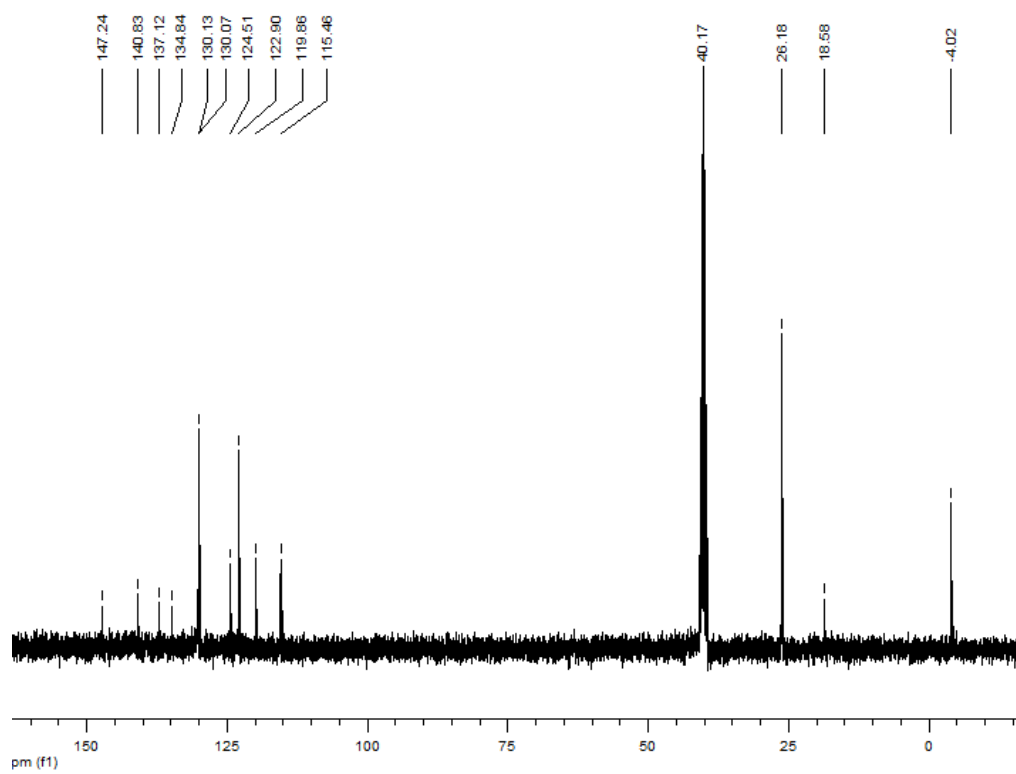


To a 100 ml round bottom flask was added *tert*-butyl(4-chloro-3-nitrophenoxy)dimethylsilane (**9a**) (1.5 g, 5.3 mmol), toluene (40 ml), aniline (730 μ l, 8 mmol), Pd₂(dba)₃ (243 mg, 0.26 mmol, 5 mol %), *rac*-BINAP (248 mg, 0.39 mmol, 7.5 mol %), and Cs₂CO₃ (2.6 g, 8 mmol). The reaction was stirred and heated to reflux under Ar for 26 hr. It was then cooled to RT and extracted with water (2 x 100 ml). The organic layer was washed with brine and dried over Na₂SO₄. After filtration and evaporation of solvent, the crude was purified via flash column chromatography (Hexane – Hexane : 80 % - 20 %) to give deep red oil product (1.38 g, 76 % yield). ¹H NMR (400 MHz, DMSO-d₆): δ 9.03 (s, 1H), 7.47-7.07 (m, 8H), 0.93 (s, 9H), 0.18 (s, 6H). ¹³C NMR (400 MHz, DMSO-d₆): δ 147.23, 140.82, 137.12, 134.84, 130.13, 130.06, 124.50, 122.89, 119.86, 115.46, 26.18, 18.58, -4.01. MS (ESI) calculated exact mass for C₁₈H₂₄N₂O₃Si = 344.16. Found [M+H]⁺ = 345.20.

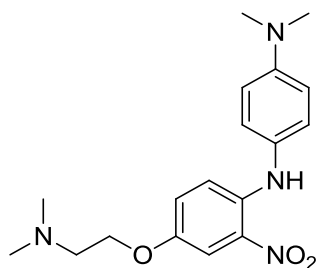
4-((*tert*-butyldimethylsilyl)oxy)-2-nitro-*N*-phenylaniline (**11a**) ^1H NMR (400 MHz, DMSO- d_6)



4-((*tert*-butyldimethylsilyl)oxy)-2-nitro-*N*-phenylaniline (**11a**) ^{13}C NMR (400 MHz, DMSO- d_6)

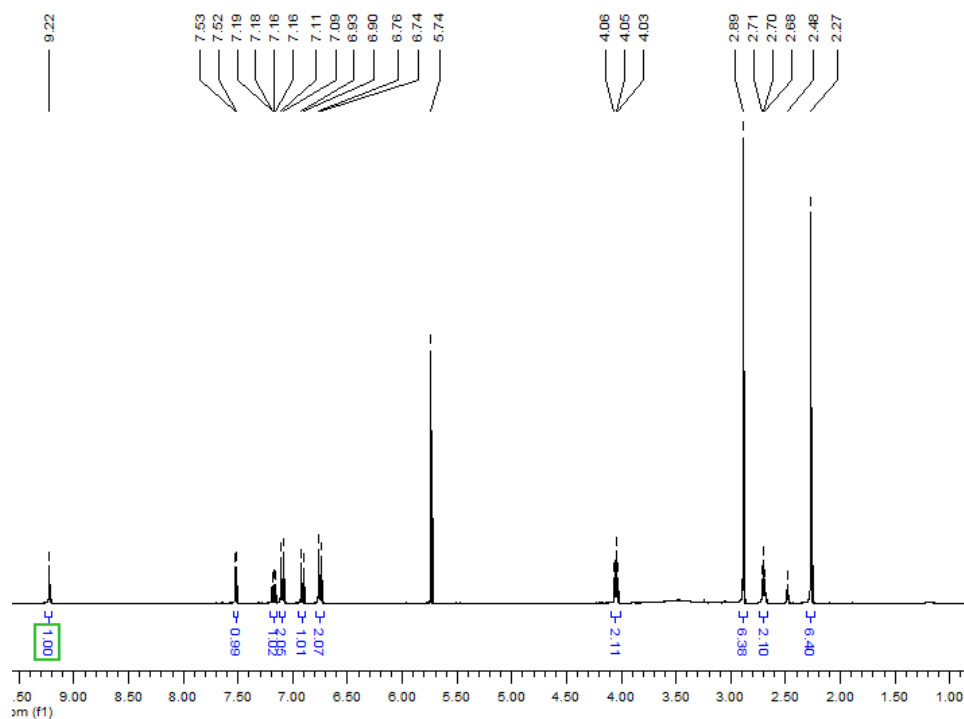


***N*¹-(4-(2-dimethylamino)ethoxy)-2-nitrophenyl)-*N*⁴,*N*⁴-dimethylbenzene-1,4-diamine (11x)**

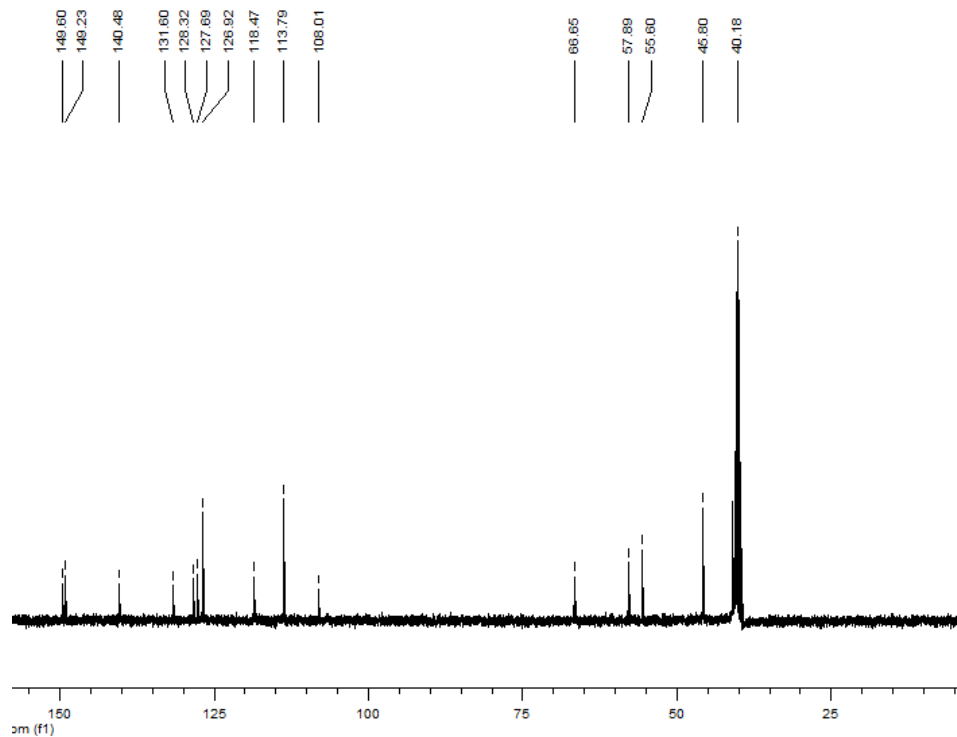


To a 50 ml round-bottom flask was added 2-(4-chloro-3-nitrophenoxy)-*N,N*-dimethylethanamine (**9b**) (290 mg, 1.2 mmol), toluene (20 ml), *N*¹,*N*¹-dimethylbenzene-1,4-diamine (162 mg, 1.2 mmol), Pd₂(dba)₃ (54 mg, 0.06 mmol, 5 mol %), rac-BINAP (55 mg, 0.09 mmol, 7.5 mol %), and Cs₂CO₃ (376 mg, 1.2 mmol). The reaction was stirred and heated to reflux under Ar for 21 hours before cooling to RT. It was filtered and extracted with water (2 x 20 ml). The organic layer was dried over Na₂SO₄. After filtration and removal of solvent, the crude was purified via flash column (DCM – MeOH : 80 % - 20 %) to yield a dark red oil (136 mg, 33 % yield). ¹H NMR (400 MHz, DMSO-d₆): δ 9.22 (s, 1H), 7.53 (d, *J* = 3 Hz, 1H), 7.19 (dd, *J*₁ = 9 Hz, *J*₂ = 3 Hz, 1H), 7.11 (d, *J* = 9 Hz, 2H), 6.93 (d, *J* = 9 Hz, 1H), 6.76 (d, *J* = 9 Hz, 2H), 4.06 (t, *J* = 6 Hz, 2H), 2.88 (s, 6H), 2.71 (t, *J* = 6 Hz, 2H), 2.27 (s, 6H). ¹³C NMR (400 MHz, DMSO-d₆): δ 149.60, 149.22, 140.47, 131.59, 128.31, 127.68, 126.92, 118.46, 113.78, 108.01, 66.64, 57.89, 55.60, 45.79. MS (ESI) calculated exact mass for C₁₉H₂₂N₄O₂ = 344.18. Found [M+H]⁺ = 345.2.

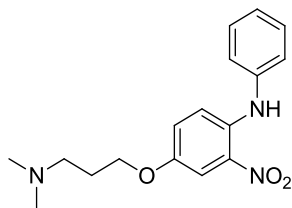
N^1 -(4-(2-dimethylamino)ethoxy)-2-nitrophenyl)- N^4,N^4 -dimethylbenzene-1,4-diamine (**11x**) ^1H
NMR (400 MHz, DMSO-d6)



N^1 -(4-(2-dimethylamino)ethoxy)-2-nitrophenyl)- N^4,N^4 -dimethylbenzene-1,4-diamine (**11x**) ^{13}C
NMR (400 MHz, DMSO-d6)

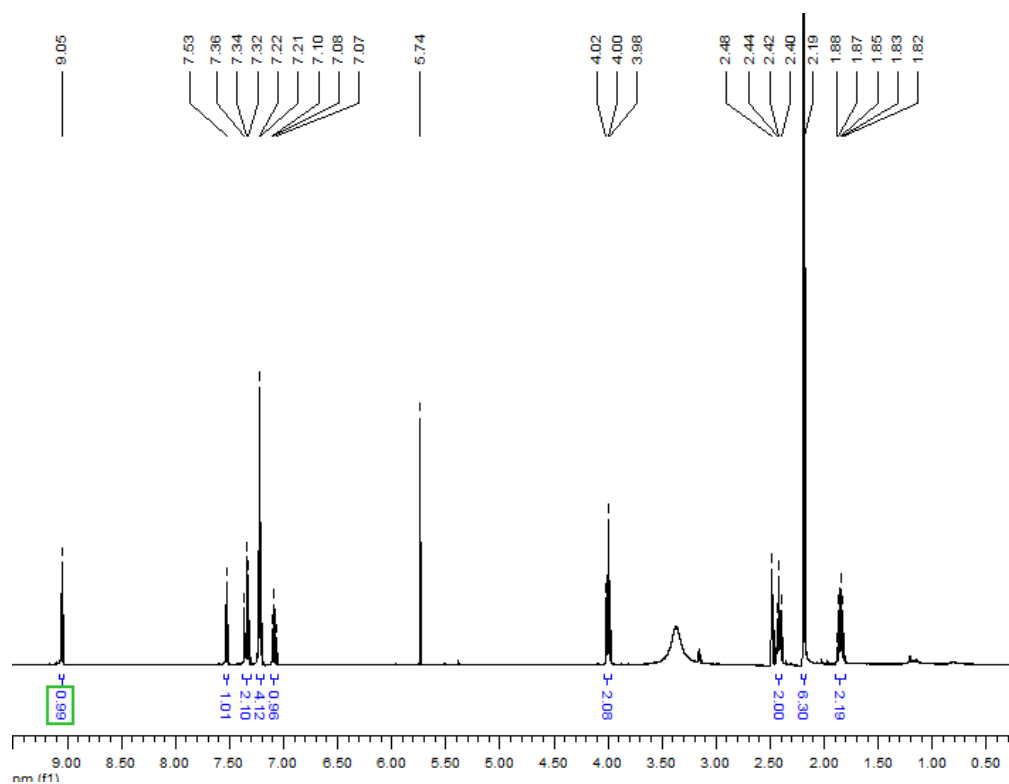


4-(3-(dimethylamino)propoxy)-2-nitro-*N*-phenylaniline (**11c**)

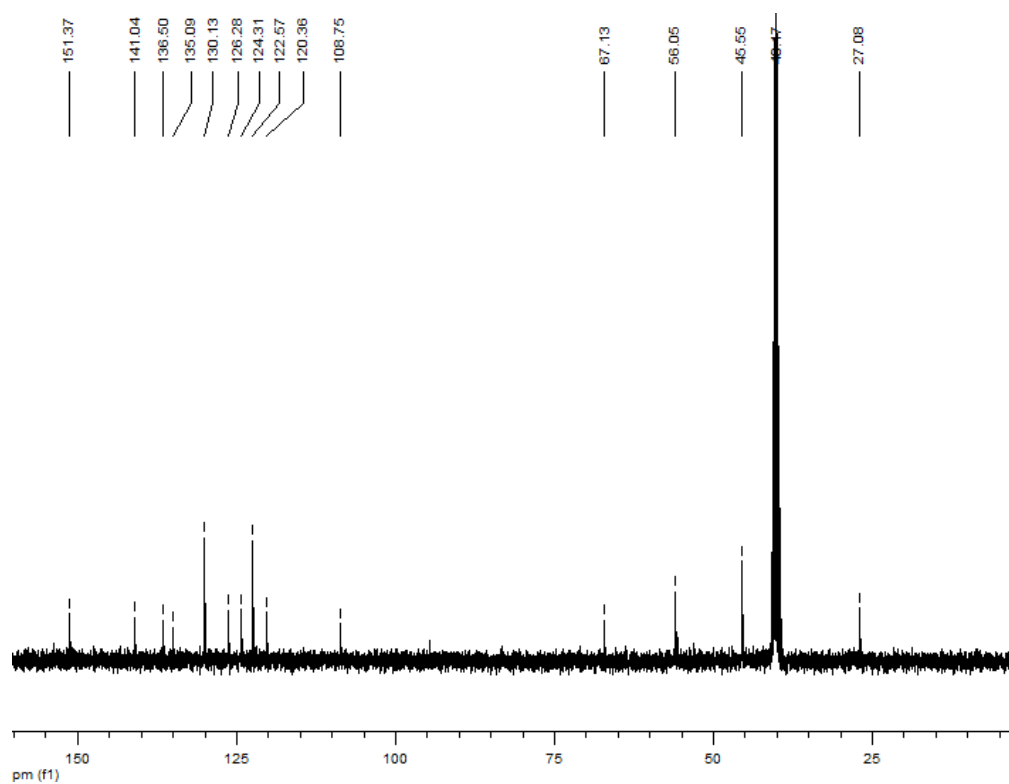


To a 100 ml round bottom flask was added 3-(4-chloro-3-nitrophenoxy)-*N,N*-dimethylpropan-1-amine (**9c**) (1.5 g, 5.7 mmol), toluene (50 ml), aniline (525 μ l, 5.7 mmol), Pd2(dba)₃ (263 mg, 0.29 mmol, 5 mol %), rac-BINAP (269 mg, 0.43 mmol, 7.5 mol %), and Cs₂CO₃ (1.8 g, 5.7 mmol). The reaction was stirred and heated to reflux under Ar for 24 hours before cooling to RT, filtration and extraction twice with water (100 ml ea.). The organic layer was then washed with brine and dried over Na₂SO₄. After filtration and removal of solvent, the crude product was purified via flash column chromatography (DCM – MeOH : 90 % - 10 %) to yield a red oil as the product (1.1 g, 63 % yield). ¹H NMR (400 MHz, DMSO-d₆): δ 9.05 (s, 1H), 7.53 (s, 1H), 7.36 (t, J = 8 Hz, 2H), 7.22 – 7.21 (m, 4H), 7.10 (t, J = 7 Hz, 1H), 4.02 (t, J = 7 Hz, 2H), 2.44 (t, J = 7 Hz, 2H), 2.19 (s, 6H), 1.88 (p, J = 7 Hz, 2H). ¹³C NMR (400 MHz, DMSO-d₆): δ 151.37, 141.03, 136.49, 135.09, 130.12, 126.28, 124.31, 122.56, 120.35, 108.74, 67.13, 56.04, 45.55, 27.08. MS (ESI) calculated exact mass for C₁₇H₂₁N₃O₃ = 315.16. Found [M+H]⁺ = 316.07.

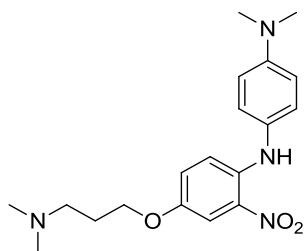
4-(3-(dimethylamino)propoxy)-2-nitro-*N*-phenylaniline (**11c**) ^1H NMR (400 MHz, DMSO- d_6)



4-(3-(dimethylamino)propoxy)-2-nitro-*N*-phenylaniline (**11c**) ^{13}C NMR (400 MHz, DMSO- d_6)

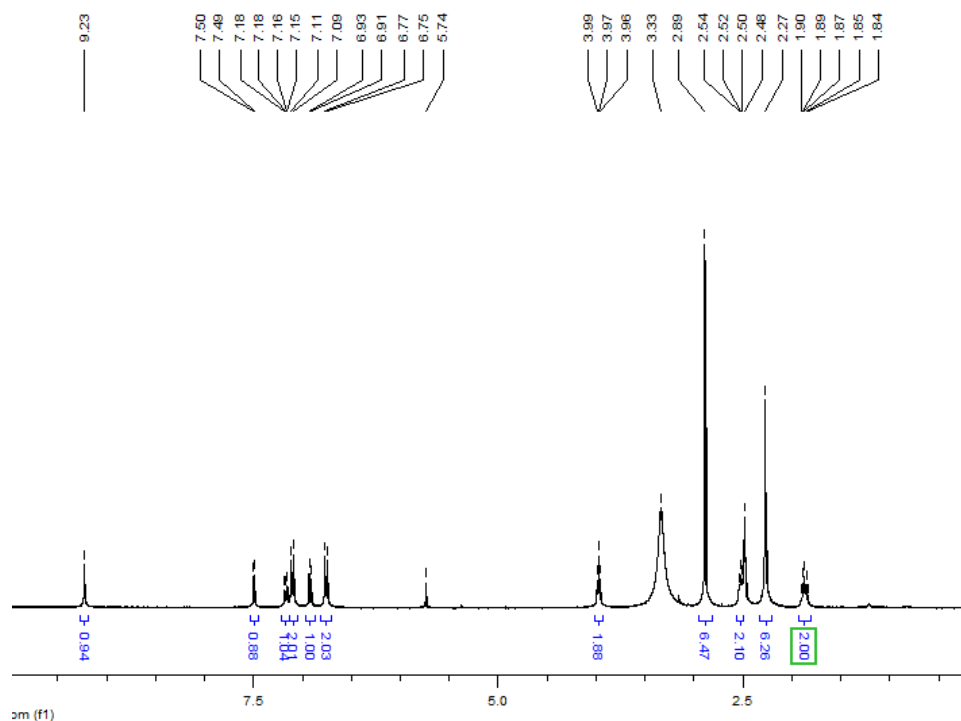


***N*¹-(4-(3-(dimethylamino)propoxy)-2-nitrophenyl)-*N*⁴,*N*⁴-dimethylbenzene-1,4-diamine
(11e)**

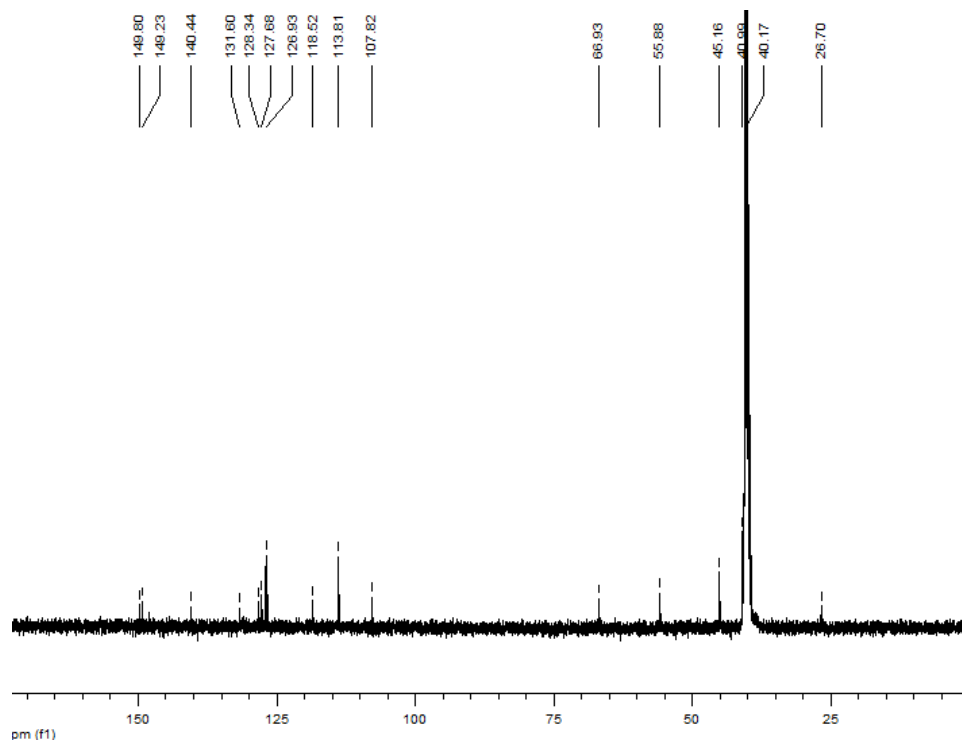


To a 250 ml round-bottom flask was added *N,N*-dimethyl-*p*-nitroaniline (957 mg, 5.7 mmol) and MeOH (100 ml). The flask was flushed with Ar gas before Pd/C (50 mg, 10 wt %) was added. The reaction was then sealed under H₂ atm and stirred at RT for 3.5 hours before filtered and concentrated. The oil residue was dissolved in toluene (100 ml). 3-(4-chloro-3-nitrophenoxy)-*N,N*-dimethylpropan-1-amine (**9c**) (1.5 g, 5.7 mmol) was added, followed by Pd₂(dba)₃ (264 mg, 0.3 mmol, 5 mol %) and rac-BINAP (269 mg, 0.4 mmol, 7.5 mol %) and Cs₂CO₃ (1.8 g, 5.7 mmol). The reaction was stirred and heated to reflux for 24 hours before filtered and extracted with water (2 x 150 ml). The organic layer was then washed with brine and dried over Na₂SO₄. The crude was filtered, concentrated and purified via flash column (DCM – MeOH : 90 % - 10 %) to yield red oil product (637 mg, 31 % yield). ¹H NMR (400 MHz, DMSO-*d*₆): δ 9.23 (s, 1H), 7.50 (d, *J* = 2 Hz, 1H), 7.18 (dd, *J*₁ = 2 Hz, *J*₂ = 8 Hz, 1H), 7.11 (d, *J* = 8 Hz, 2H), 6.93 (d, *J* = 10 Hz, 1H), 6.77 (d, *J* = 8 Hz, 2H), 3.99 (t, *J* = 6 Hz, 2H), 2.89 (s, 6H), 2.54 (t, *J* = 7 Hz, 2H), 2.27 (s, 6H), 1.90 (p, *J* = 7 Hz, 2H). ¹³C NMR (400 MHz, DMSO-*d*₆): δ 149.79, 149.23, 140.43, 131.59, 128.34, 127.68, 126.93, 118.51, 113.80, 107.81, 66.92, 55.88, 45.15, 40.98, 26.70. MS (ESI) calculated exact mass for C₁₉H₂₆N₄O₃ = 358.20. Found [M+H]⁺ = 359.18.

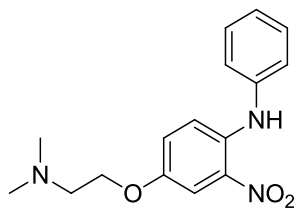
N^1 -(4-(3-(dimethylamino)propoxy)-2-nitrophenyl)- N^4,N^4 -dimethylbenzene-1,4-diamine (**11e**) ^1H
 NMR (400 MHz, DMSO- d_6)



N^1 -(4-(3-(dimethylamino)propoxy)-2-nitrophenyl)- N^4,N^4 -dimethylbenzene-1,4-diamine (**11e**) ^{13}C
 NMR (400 MHz, DMSO- d_6)

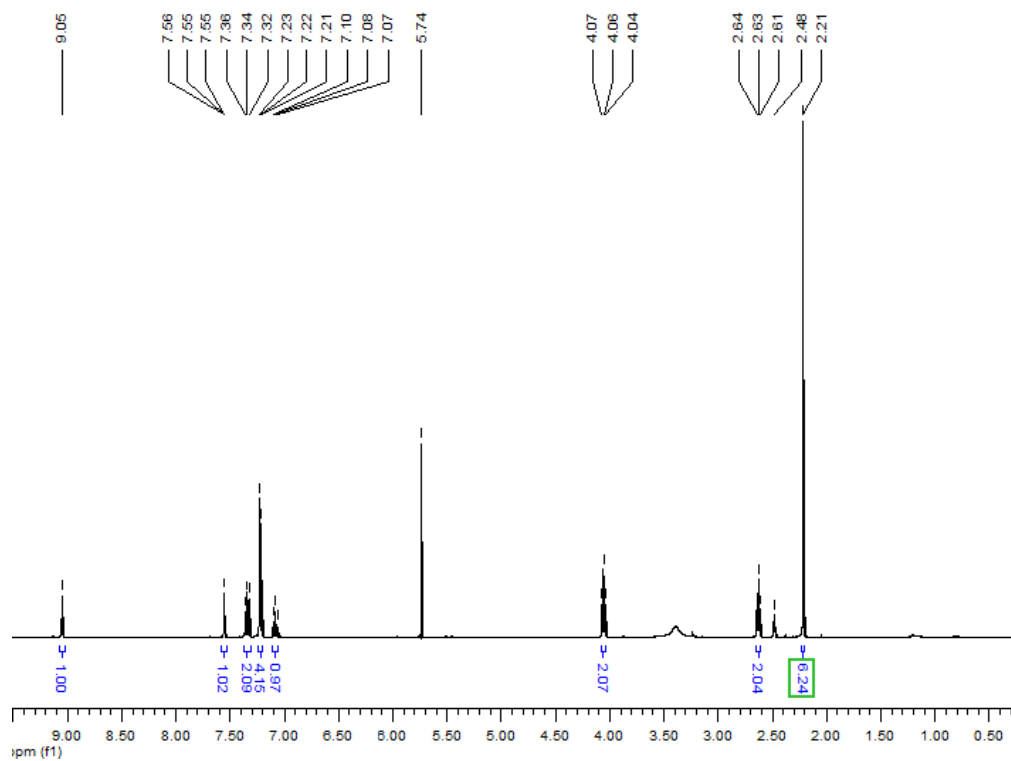


4-(2-(dimethylamino)ethoxy)-2-nitro-*N*-phenylaniline (**11b**)

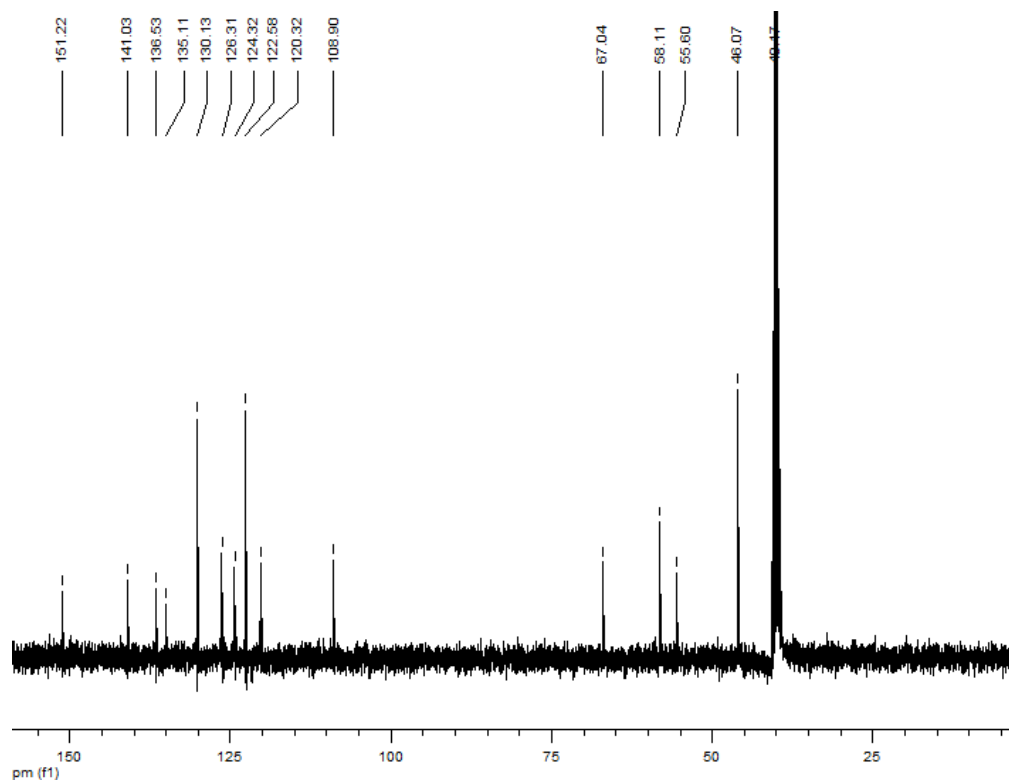


To a 100 ml round bottom flask was added 2-(4-chloro-3-nitrophenoxy)-*N,N*-dimethylethanamine (**9b**) (1.3 g, 5.3 mmol), toluene (50 ml), aniline (520 μ l, 5.7 mmol), Pd₂(dba)₃ (264 mg, 0.29 mmol, 5 mol %), rac-BINAP (269 mg, 0.43 mmol, 7.5 mol %), Cs₂CO₃ (1.8 g, 5.7 mmol). The reaction was stirred and heated to reflux for 28 hr before cooling to RT, followed by filtration and extraction with water twice (100 ml ea). The organic layer was then washed with brine and dried over Na₂SO₄. After filtration and concentration, the crude was purified via flash column (DCM – MeOH : 90 % - 10 %) to yield a red oil product (990 mg, 62 % yield). ¹H NMR (400 MHz, DMSO-d₆): δ 9.05 (s, 1H), 7.55 (t, *J* = 2 Hz, 1H), 7.34 (t, *J* = 8 Hz, 2H), 7.23 – 7.21 (m, 4H), 7.10 (t, *J* = 8 Hz, 1H), 4.07 (t, *J* = 6 Hz, 2H), 2.64 (t, *J* = 6 Hz, 2H), 2.21 (s, 6H). ¹³C NMR (400 MHz, DMSO-d₆): δ 151.21, 141.03, 136.53, 135.10, 130.12, 126.30, 124.31, 122.57, 120.32, 108.90, 67.04, 58.10, 55.10, 55.60, 46.07. MS (ESI) calculated exact mass for C₁₆H₁₉N₃O₃ = 301.14. Found [M+H]⁺ = 302.0.

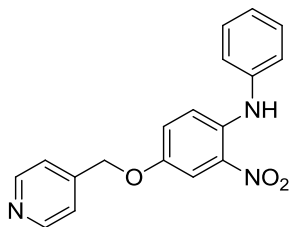
4-(2-(dimethylamino)ethoxy)-2-nitro-*N*-phenylaniline (**11b**) ^1H NMR (400 MHz, DMSO- d_6)



4-(2-(dimethylamino)ethoxy)-2-nitro-*N*-phenylaniline (**11b**) ^{13}C NMR (400 MHz, DMSO- d_6)

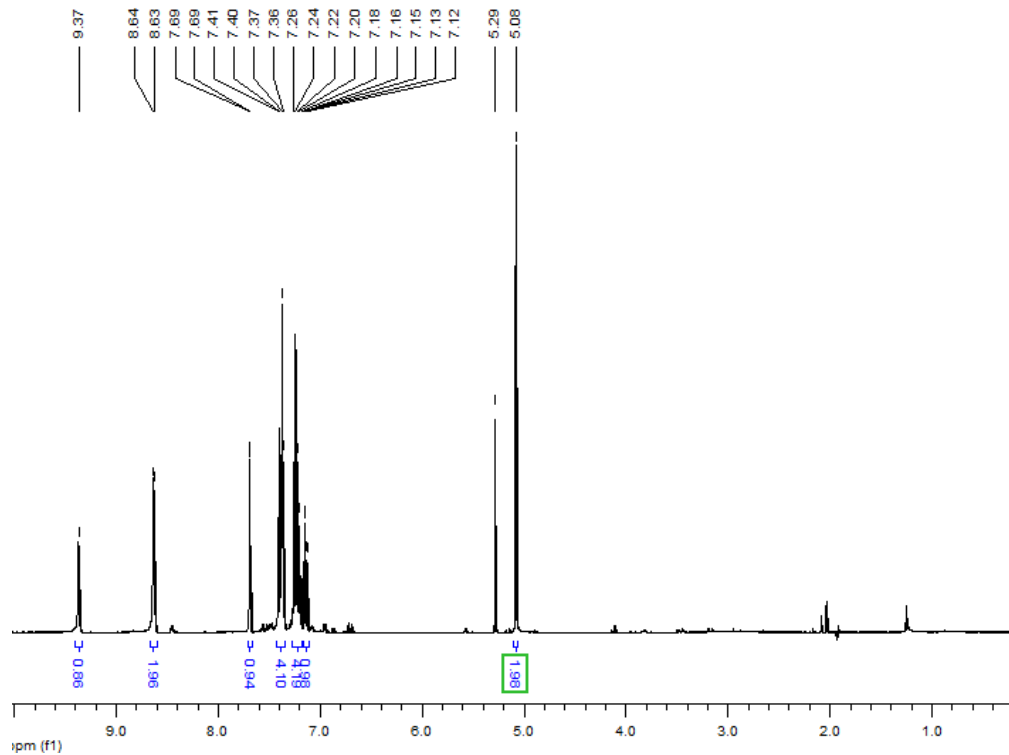


2-nitro-N-phenyl-4-(pyridine-4-ylmethoxy)aniline (11d)

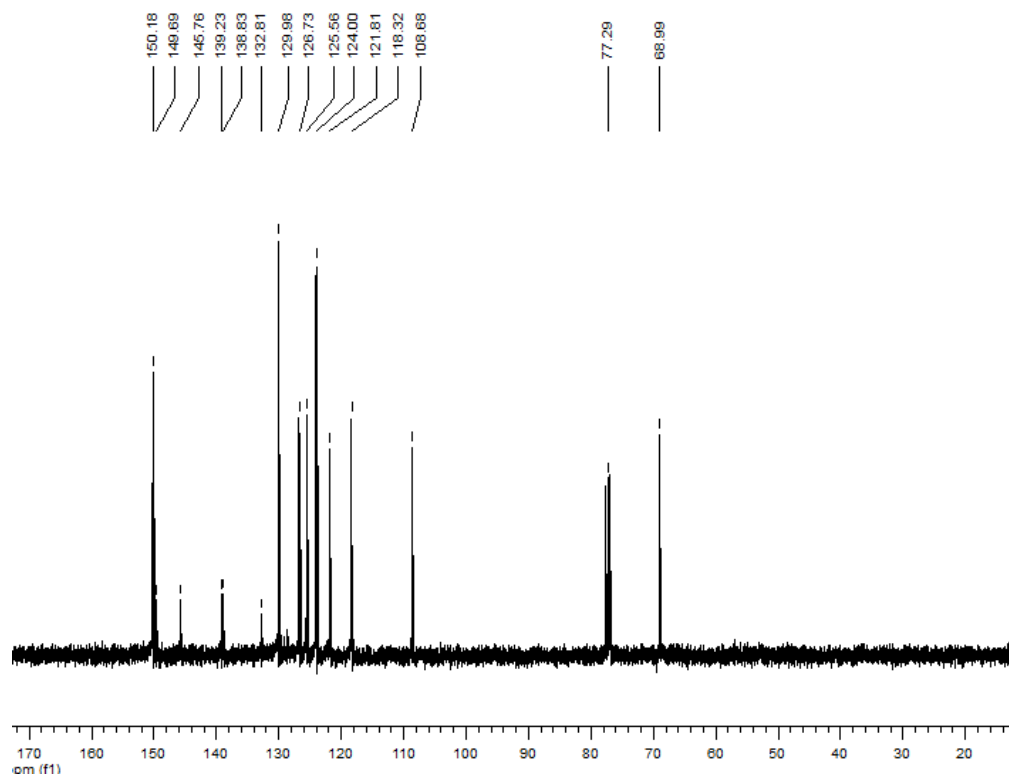


To a 250 ml round-bottom flask was added 4-((4-chloro-3-nitrophenoxy)methyl)pyridine (**9d**) (1.56 g, 5.9 mmol), toluene (100 ml), aniline (646 μ l, 7.0 mmol, 1.2 eq), Pd₂(dba)₃ (265 mg, 0.3 mmol, 5 mol %), rac-BINAP (273 mg, 0.4 mmol, 7.5 mol %) and Cs₂CO₃ (1.9 g, 5.9 mmol). The reaction was stirred and heated to reflux under Ar atm for 19 hours before cooling to RT. After filtration, it was extracted with water (2 x 100 ml), washed with brine and dried over Na₂SO₄. The crude solution was filtered and concentrated before purified via flash column chromatography (DCM – EtOAc : 60 % - 40 %) to yield red solid product (1.73 g, 91 % yield). ¹H NMR (400 MHz, CDCl₃): δ 9.37 (s, 1H), 8.64 (d, *J* = 6 Hz, 2H), 7.69 (d, *J* = 3Hz, 1H), 7.41 – 7.36 (m, 4H), 7.26 – 7.18 (m, 4H), 7.16 (dd, *J*₁ = 9 Hz, *J*₂ = 3 Hz, 1H), 5.08 (s, 2H). ¹³C NMR (400 MHz, CDCl₃): δ 150.17, 149.69, 145.76, 139.22, 138.82, 132.81, 129.97, 126.73, 125.55, 124.00, 121.81, 118.31, 108.68, 68.98. MS (ESI) calculated exact mass for C₁₈H₁₅N₃O₃ = 321.11. Found [M+H]⁺ = 322.08.

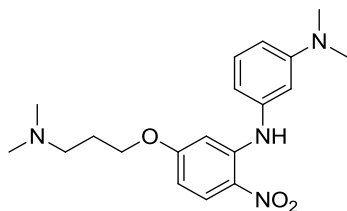
2-nitro-N-phenyl-4-(pyridine-4-ylmethoxy)aniline (**11d**) ^1H NMR (400 MHz, CDCl_3)



2-nitro-N-phenyl-4-(pyridine-4-ylmethoxy)aniline (**11d**) ^{13}C NMR (400 MHz, CDCl_3)

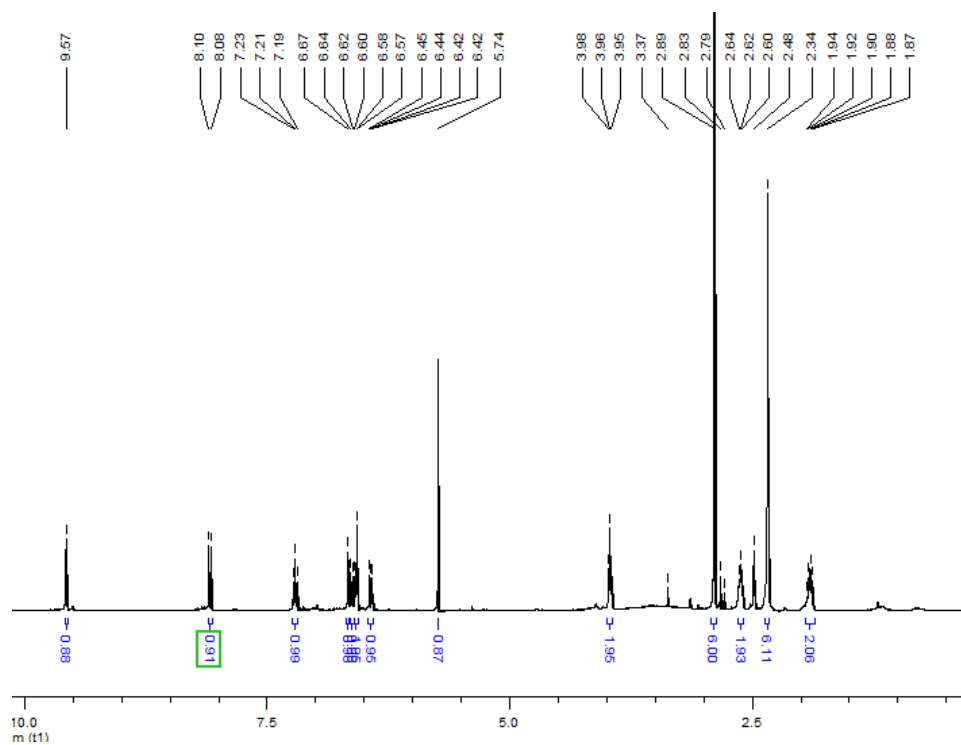


***N*¹-(5-(3-(dimethylamino)propoxy)-2-nitrophenyl)-*N*³,*N*³-dimethylbenzene-1,3-diamine (11g)**

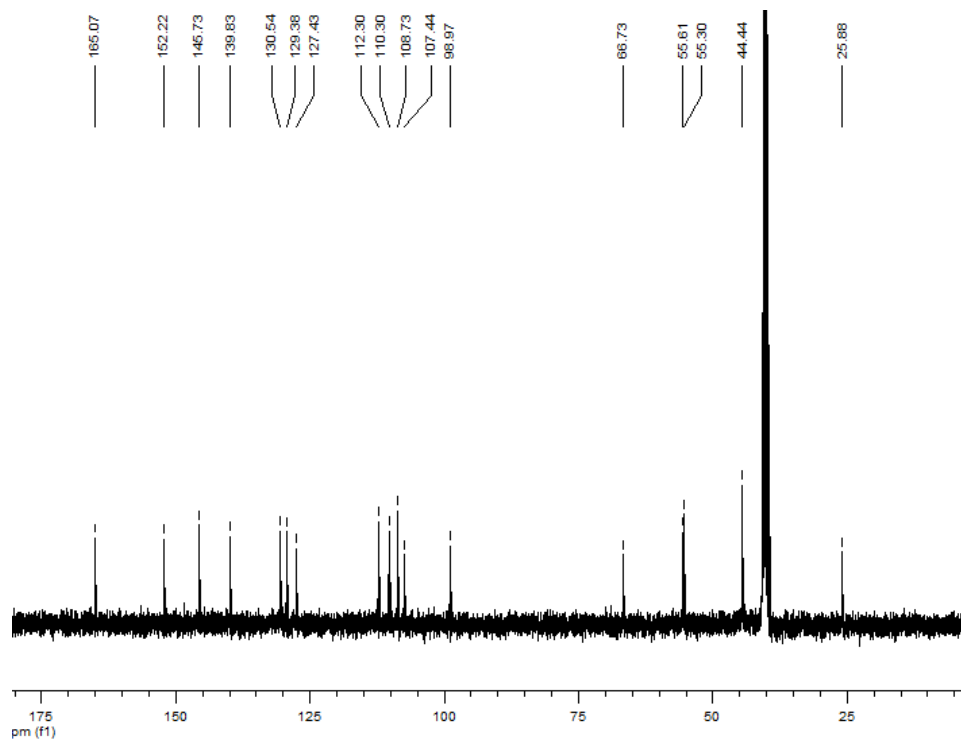


To a 250 ml round bottom flask was added 3-(3-fluoro-4-nitrophenoxy)-*N,N*-dimethylpropan-1-amine (**9f**) (3.83 g, 15.8 mmol), ACN (100 ml), *N*¹,*N*¹-dimethylbenzene-1,3-diamine (2.05 g, 15.0 mmol), and Cs₂CO₃ (5.0 g, 15.8 mmol). The reaction was stirred and heated to reflux under Ar for 41 hr before cooling to RT, followed by filtration and concentration. The dark residue was dissolved in DCM (200 ml) and extracted with water (2 x 100 ml). The organic layer was collected and washed with brine and dried over Na₂SO₄. After filtration and evaporation of solvent, the crude was purified via flash column chromatography (DCM – MeOH : 90 % - 10 %) to yield yellow oil product (2.02 g, 36 % yield). ¹H NMR (400 MHz, DMSO-d₆): δ 9.57 (s, 1H), 8.10 (d, *J* = 10 Hz, 1H), 7.23 (t, *J* = 8 Hz, 1H), 6.67 (s, 1H), 6.64 (d, *J* = 8 Hz, 1H), 6.58 (dd, *J*₁ = 8 Hz, *J*₂ = 2 Hz, 2H), 6.45 (dd, *J*₁ = 10 Hz, *J*₂ = 2Hz, 1H), 5.74 (d, *J* = 1 Hz, 1H), 3.98 (t, *J* = 6 Hz, 2H), 2.89 (s, 6H), 2.64 (t, *J* = 7 Hz, 2H), 2.34 (s, 6H), 1.94 (p, *J* = 7 Hz, 2H). ¹³C NMR (400 MHz, DMSO-d₆): δ 165.06, 152.21, 145.72, 139.82, 130.54, 129.37, 127.43, 112.29, 110.30, 108.73, 107.43, 98.97, 66.73, 55.61, 55.29, 44.44, 25.87. MS (ESI) calculated exact mass for C₁₉H₂₆N₄O₃ = 358.20. Found [M+H]⁺ = 349.18.

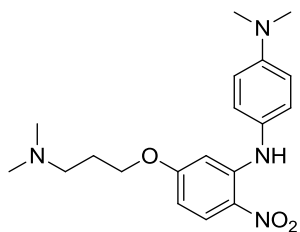
N^1 -(5-(3-(dimethylamino)propoxy)-2-nitrophenyl)- N^3,N^3 -dimethylbenzene-1,3-diamine (**11g**) ^1H
 NMR (400 MHz, DMSO- d_6)



N^1 -(5-(3-(dimethylamino)propoxy)-2-nitrophenyl)- N^3,N^3 -dimethylbenzene-1,3-diamine (**11g**)
 ^{13}C NMR (400 MHz, DMSO- d_6)

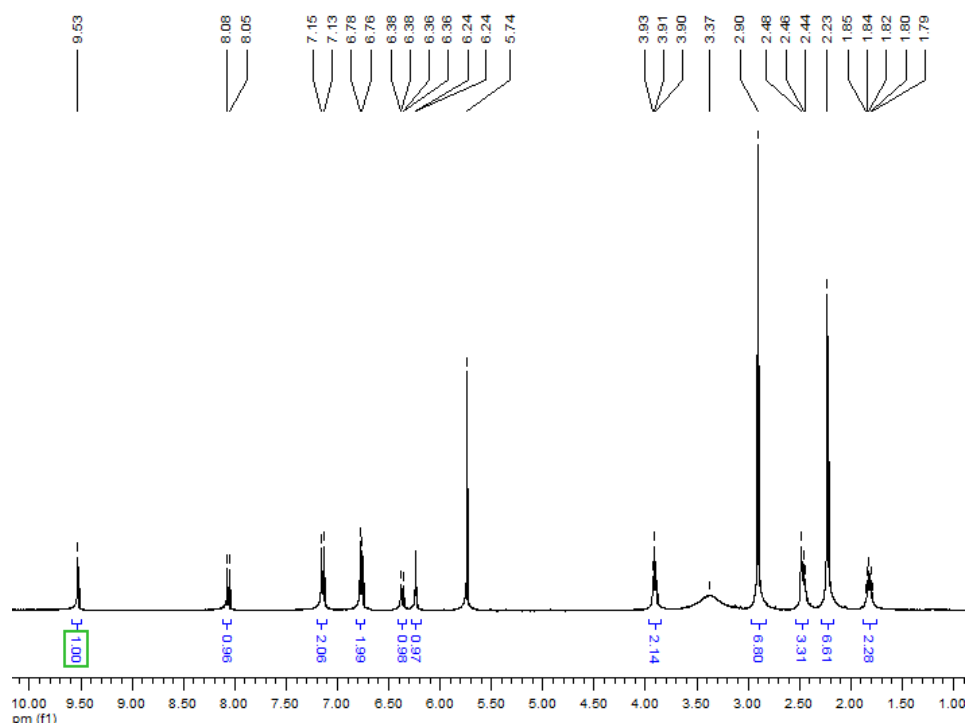


***N*¹-(5-(3-(dimethylamino)propoxy)-2-nitrophenyl)-*N*⁴,*N*⁴-dimethylbenzene-1,4-diamine
(11f)**

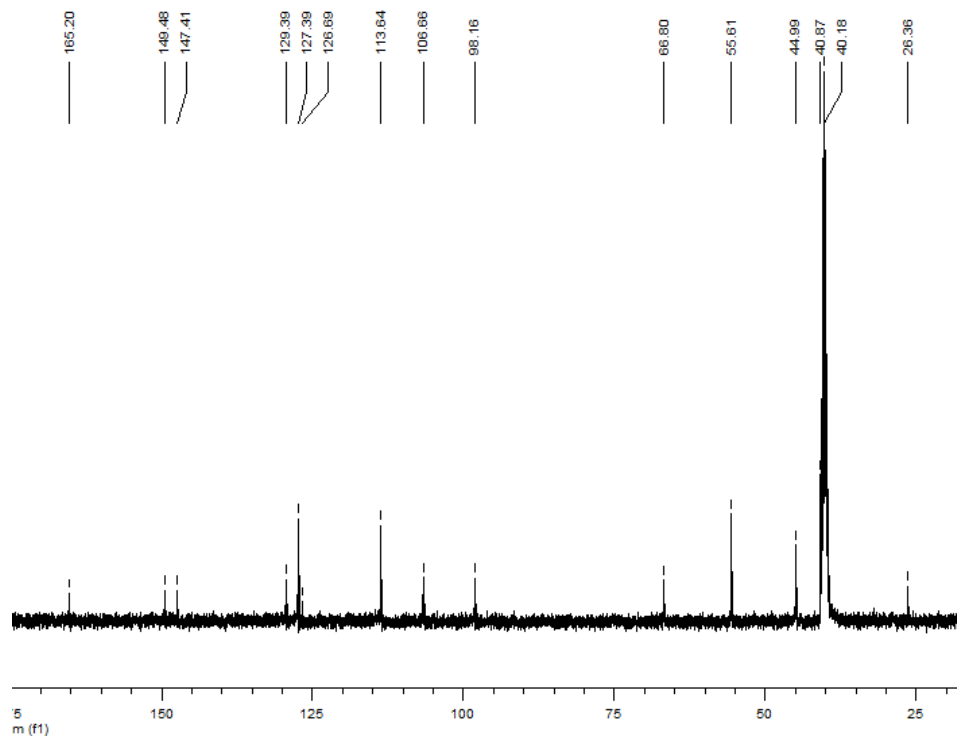


To a 250 ml round bottom flask was added 3-(3-fluoro-4-nitrophenoxy)-*N,N*-dimethylpropan-1-amine (**9f**) (3.6 g, 15.0 mmol), ACN (100 ml), *N*¹,*N*¹-dimethylbenzene-1,4-diamine (2.04 g, 15.0 mmol) and Cs₂CO₃ (4.7 g, 15.0 mmol). The reaction was stirred and heated to reflux under Ar for 21 hr before cooling to RT and concentration. The oil residue was dissolved in chloroform (100 ml) and extracted with water (2 x 100 ml). The organic layer was washed with brine and dried over Na₂SO₄. After filtration and evaporation of solvent *in vacuo*, the crude was purified via flash column chromatography (DCM – MeOH : 90 % - 10 %) to yield red oil product (1.81 g, 34 % yield). ¹H NMR (400 MHz, DMSO-d₆): δ 9.53 (s, 1H), 8.08 (d, J = 10 Hz, 1H), 7.15 (d, J = 9 Hz, 2H), 6.78 (d, J = 9 Hz, 2H), 6.38 (dd, J₁ = 9 Hz, J₂ = 2 Hz, 1H), 6.24 (d, J = 2 Hz, 1H), 3.93 (t, J = 6 Hz, 2H), 2.90 (s, 6H), 2.46 (t, J = 7 Hz, 2H), 2.23 (s, 6H), 1.85 (p, J = 7 Hz, 2H). ¹³C NMR (400 MHz, DMSO-d₆): δ 165.19, 149.48, 147.40, 129.39, 127.38, 126.68, 113.63, 106.66, 98.16, 66.80, 55.61, 44.98, 40.87, 26.35. MS (ESI) calculated exact mass for C₁₉H₂₆N₄O₃ = 358.20. Found [M+H]⁺ = 359.18.

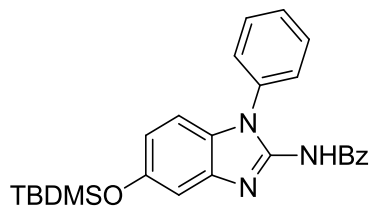
N^1 -(5-(3-(dimethylamino)propoxy)-2-nitrophenyl)- N^4,N^4 -dimethylbenzene-1,4-diamine (**11f**) ^1H
NMR (400 MHz, DMSO- d_6)



N^1 -(5-(3-(dimethylamino)propoxy)-2-nitrophenyl)- N^4,N^4 -dimethylbenzene-1,4-diamine (**11f**) ^{13}C
NMR (400 MHz, DMSO- d_6)

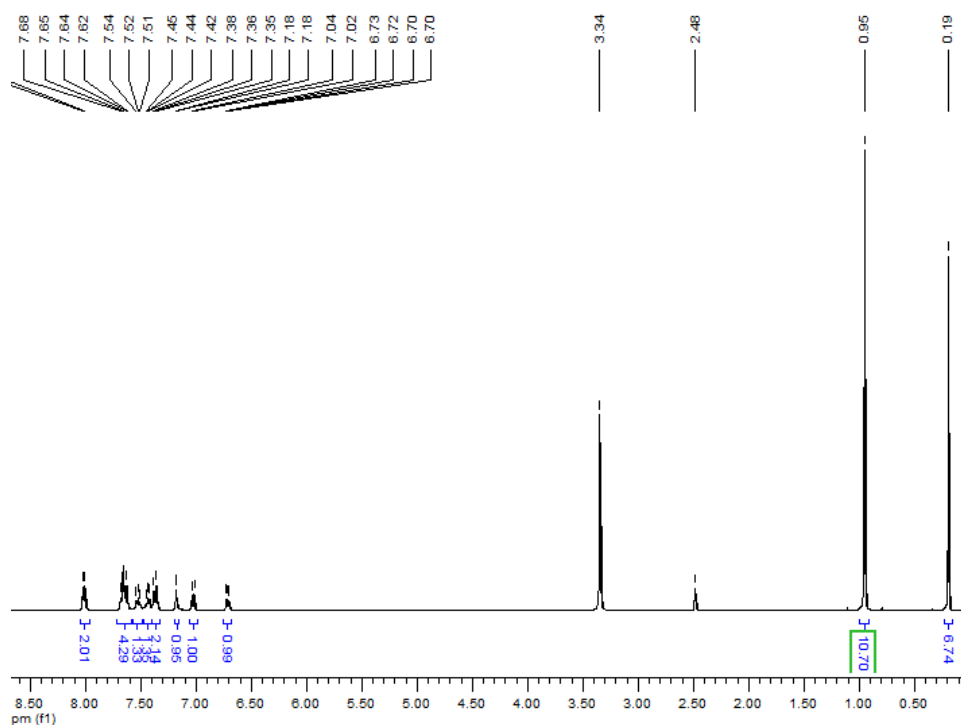


***N*-5-((*tert*-butyldimethylsilyl)oxy)-1-phenyl-1*H*-beno[*d*]imidazol-2-yl)benzamide (4a)**

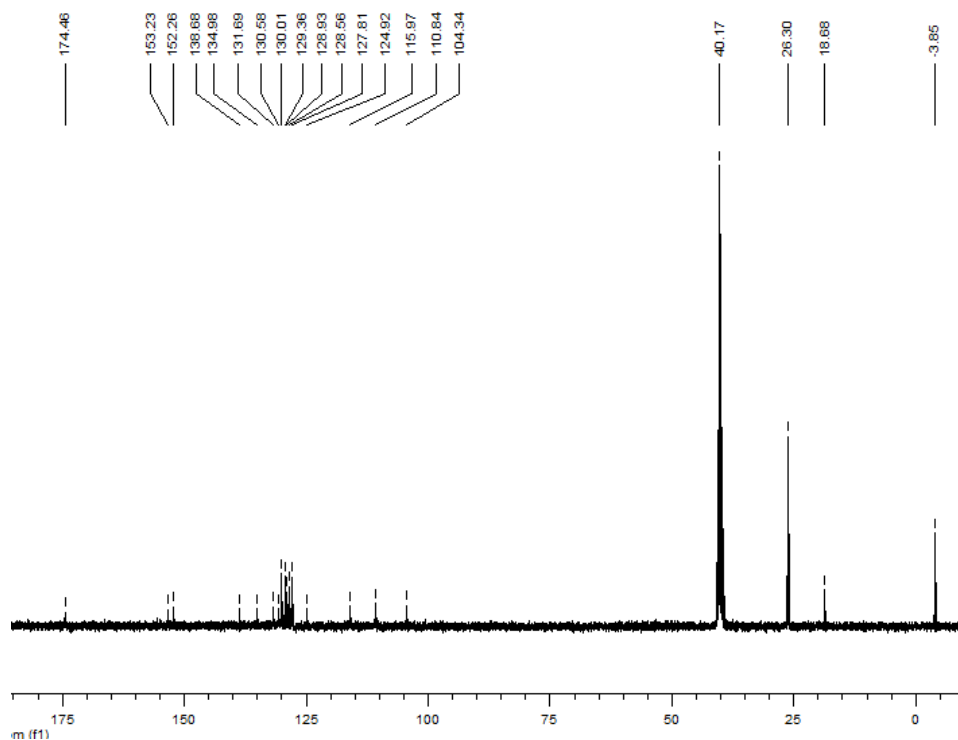


To a 100 ml round-bottom flask was added 4-((*tert*-butyldimethylsilyl)oxy)-2-nitro-*N*-phenylaniline (**11a**) (3.65 g, 10.6 mmol) and methanol (60 ml). The flask was flushed with Ar gas before Pd/C (10 wt%, 100 mg) was added. The reaction was then sealed under H₂ atm and stirred at RT for 25 hours before filtration and concentration. The oil residue was dissolved in DCM (250 ml) and benzoyl isothiocyanate was added (1.5 ml, 10.6 mmol). The reaction was stirred at RT for 24 hours before filtration, concentration and purification via flash column to yield a foam product (3.4 g, 67.4 % yield). It was dissolved in DCM (80 nml) and DIPC (2.22 ml, 14.3 mmol) and DIPEA (2.49 ml, 14.3 mmol) was added. The reaction was stirred at RT for 24 hours before concentration and purification via flash column chromatography (DCM 100 %) to yield white solid product (2.1 g, 66 % yield). ¹H NMR (400 MHz, DMSO-*d*₆): δ 8.02 (d, *J* = 8 Hz, 2H), 7.68 – 7.62 (m, 4H), 7.52 (t, *J* = 7 Hz, 1H), 7.43 (t, *J* = 7 Hz, 1H), 7.38 (t, *J* = 7 Hz, 2H), 7.18 (d, *J* = 2 Hz, 1H), 7.04 (d, *J* = 8 Hz, 1H), 6.73 (dd, *J*₁ = 8 Hz, *J*₂ = 2 Hz, 1H), 0.95 (s, 9H), 0.19 (s, 6H). ¹³C NMR (400 MHz, DMSO-*d*₆): δ 174.45, 153.22, 152.26, 138.68, 134.97, 131.69, 130.57, 130.01, 129.36, 128.92, 128.56, 127.80, 124.92, 115.97, 110.84, 104.33, 26.29, 18.67, -3.85. MS (ESI) calculated exact mass for C₂₆H₂₉N₃O₂Si = 443.20. Found [M+H]⁺ = 444.23.

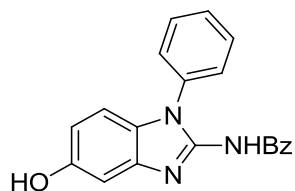
N-(5-((*tert*-butyldimethylsilyl)oxy)-1-phenyl-1*H*-beno[*d*]imidazol-2-yl)benzamide (**4a**) ¹H NMR (400 MHz, DMSO-*d*6)



N-(5-((*tert*-butyldimethylsilyl)oxy)-1-phenyl-1*H*-beno[*d*]imidazol-2-yl)benzamide (**4a**) ¹³C NMR (400 MHz, DMSO-*d*6)

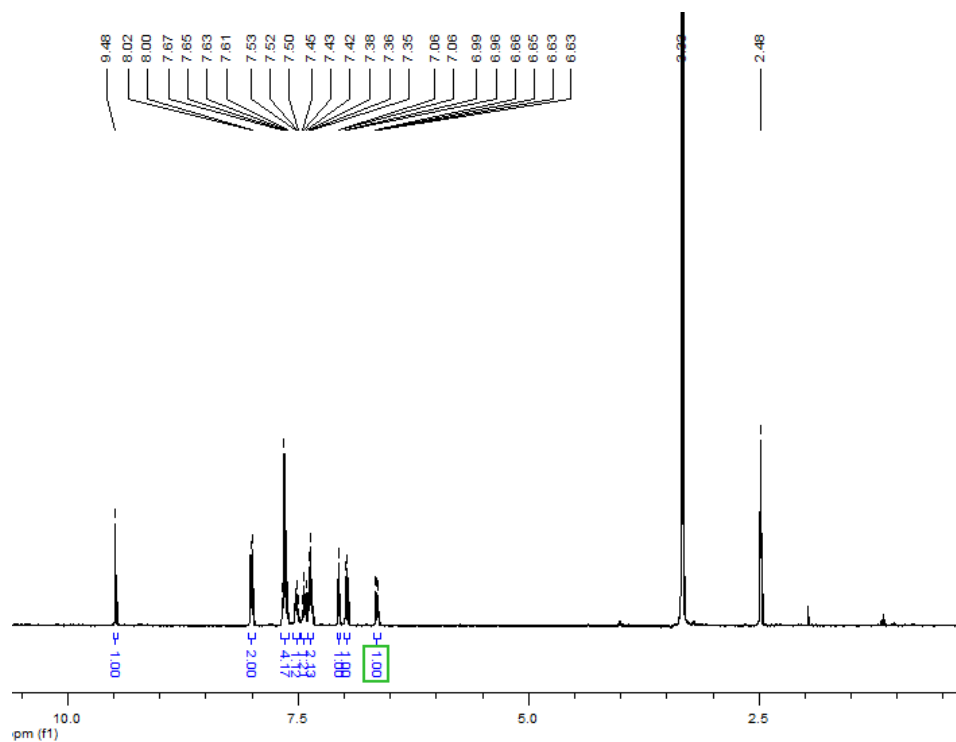


***N*-(5-hydroxy-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)benzamide (4ab)**

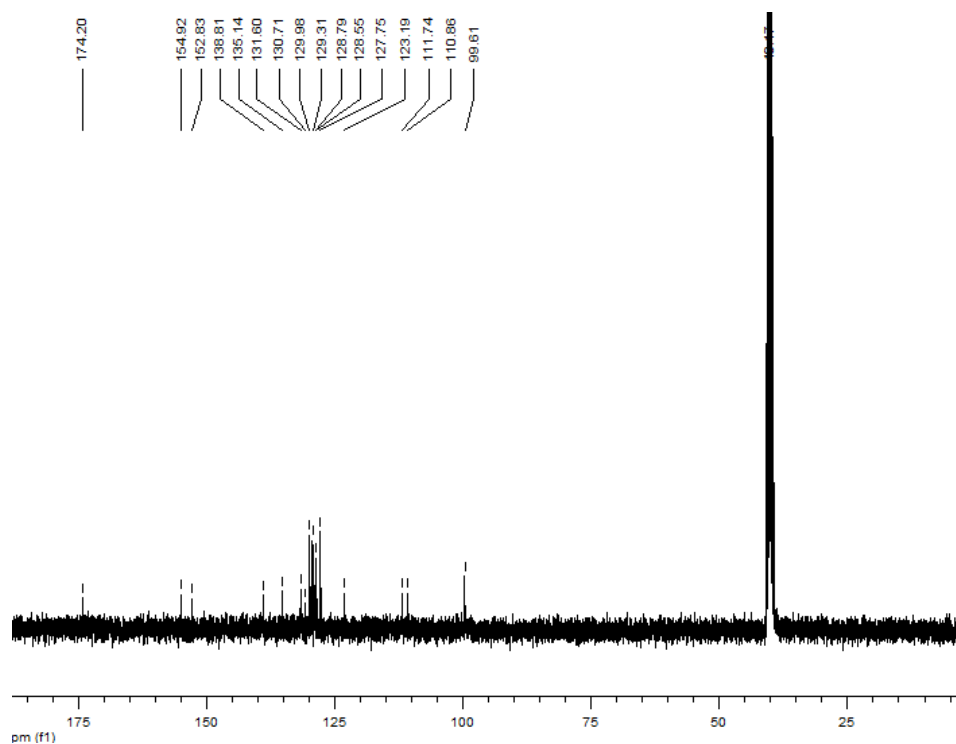


To a 50 ml round-bottom flask was added *N*-(5-((*tert*-butyldimethylsilyl)oxy)-1-phenyl-1*H*-beno[*d*]imidazol-2-yl)benzamide (**4a**) (447 mg, 1.0 mmol) DCM (20 ml) and TBAF (1 ml, 1 M solution in THF, 5 wt% H₂O, 1mmol). The reaction was stirred at RT for 2 hours before concentration and purification via flash column chromatography (DCM – MeOH : 90 % - 10 %) to yield white solid product (257 mg, 78 % yield). ¹H NMR (400 MHz, DMSO-*d*₆): δ 9.48 (s, 1H), 8.02 (d, *J* = 8 Hz, 2H), 7.67 (m, 4H), 7.53 (t, *J* = 7 Hz, 1H), 7.45 (t, *J* = 7 Hz, 1H), 7.38 (t, *J* = 8 Hz, 2H), 7.06 (d, *J* = 2Hz, 1H), 6.99 (d, *J* = 9 Hz, 1H), 6.66 (dd, *J*₁ = 2Hz, *J*₂ = 9Hz, 1H), . ¹³C NMR (400 MHz, DMSO-*d*₆): δ 174.19, 154.91, 152.83, 138.81, 135.14, 131.60, 130.70, 129.97, 129.31, 128.79, 128.55, 127.74, 123.18, 111.73, 110.86, 99.61. MS (ESI) calculated exact mass for C₂₀H₁₅N₃O₂ = 329.12. Found [M+H]⁺ = 330.12.

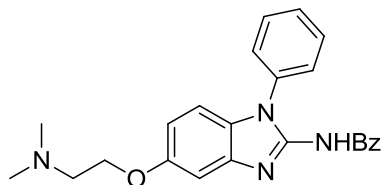
N-(5-hydroxy-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**4ab**) ¹H NMR (400 MHz, DMSO-*d*₆)



N-(5-hydroxy-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**4ab**) ¹³C NMR (400 MHz, DMSO-*d*₆)

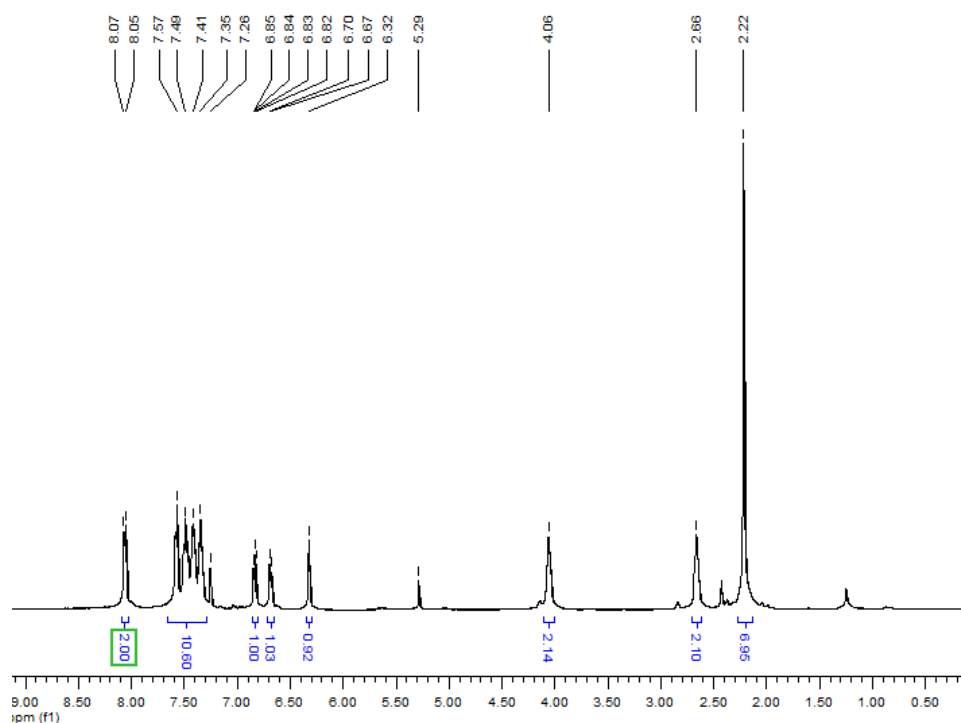


***N*-(5-(2-(dimethylamino)ethoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)benzamide (4bb)**

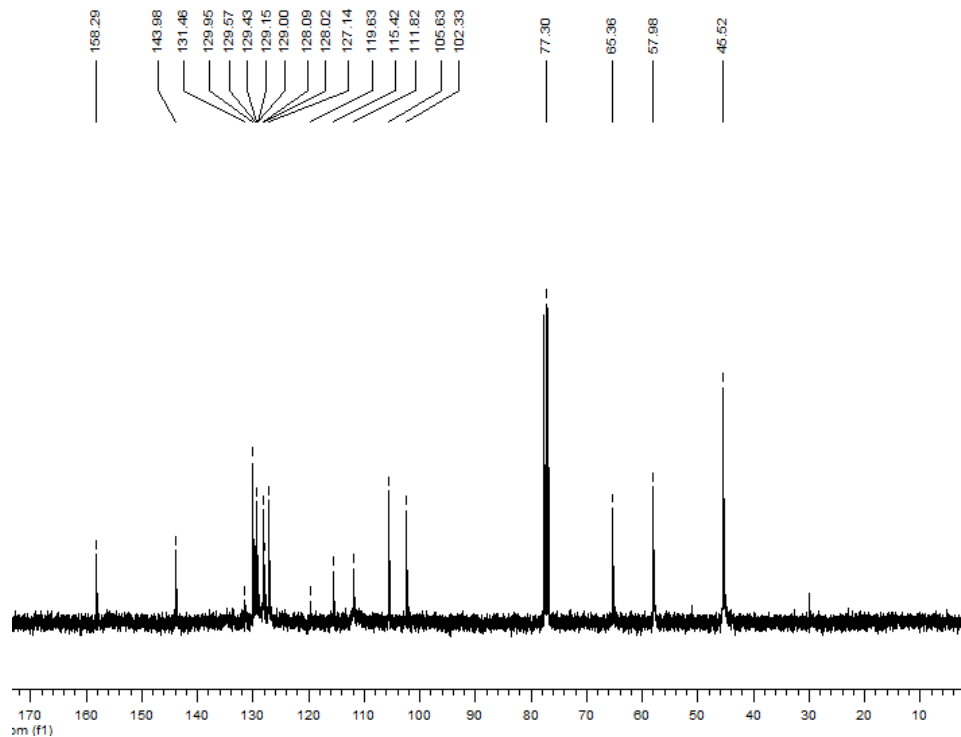


To a 250 ml round-bottom flask was added 4-(2-dimethylamino)ethoxy-2-nitro-*N*-phenylaniline (**11b**) (897 mg, 2.9 mmol) and methanol (100 ml). The flask was flushed with Ar gas before Pd/C (90 mg, 10 wt %) was added. The reaction was then sealed under H₂ atmosphere via balloon. It was stirred at RT for 1.5 hours before filtration and concentration. To the oil residue was added ACN (100 ml) followed by Benzoyl isothiocyanate (432 μ l, 2.9 mmol). The reaction was stirred at RT for 2 hours before DIPC (463 μ l, 2.9 mmol) and K₂CO₃ (411 mg, 2.9 mmol) were added. The reaction was stirred at RT for 20 hours before filtration, concentration and purification via flash column (DCM – MeOH : 90 % - 10 %) to yield off white foam product (572 mg, 48 % yield two steps). ¹H NMR (400 MHz, CDCl₃): δ 8.07 (d, J = 8 Hz, 2H), 7.57 – 7.35 (m, 10 H), 6.85 (dd, J₁ = 8 Hz, J₂ = 4 Hz, 1H), 6.70 (d, J = 9 Hz, 1H), 6.32 (s, 1H), 4.06 (s, 2H), 2.66 (s, 2H), 2.22 (s, 6H). ¹³C NMR (400 MHz, CDCl₃): δ 158.28, 143.98, 131.46, 129.95, 129.56, 129.43, 129.15, 128.99, 128.08, 128.01, 127.14, 119.62, 115.42, 111.81, 105.63, 102.32, 65.36, 57.97, 45.51. MS (ESI) calculated exact mass for C₂₄H₂₄N₄O₂ = 400.19. Found [M+H]⁺ = 401.07.

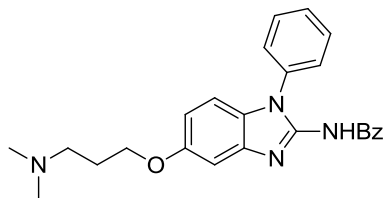
N-(5-(2-(dimethylamino)ethoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**4bb**) ^1H NMR (400 MHz, CDCl_3)



N-(5-(2-(dimethylamino)ethoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**4bb**) ^{13}C NMR (400 MHz, CDCl_3)

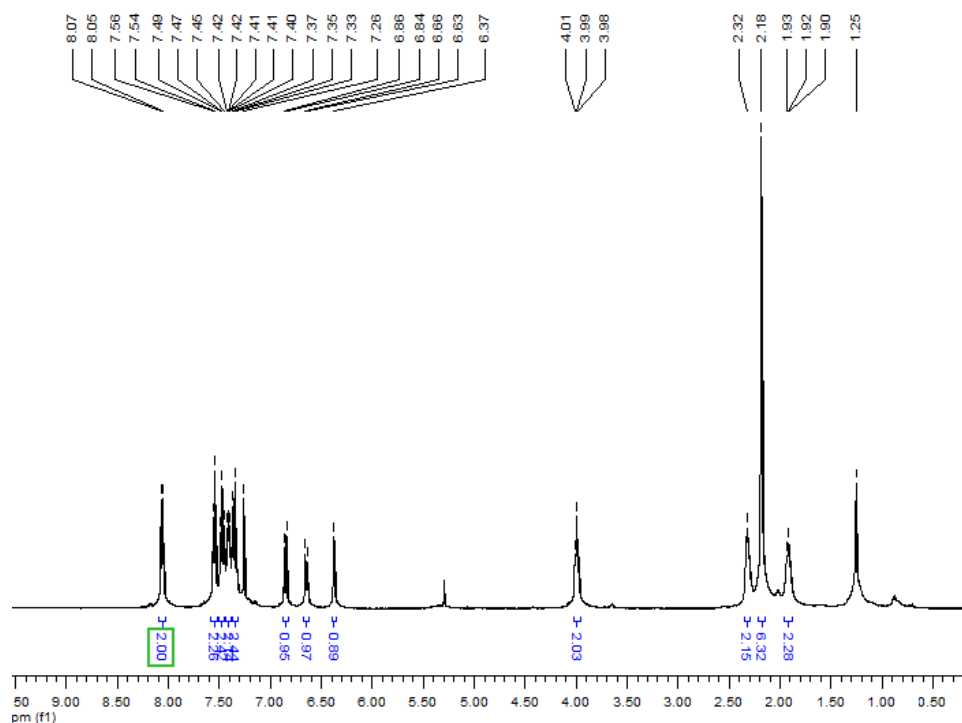


***N*-(5-(3-(dimethylamino)propoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)benzamide (4cb)**

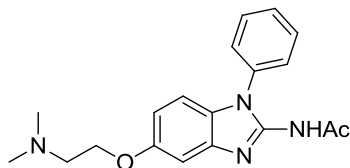


To a 50 ml round-bottom flask was added *N*-(5-hydroxy-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**4ab**) (214 mg, 0.65 mmol), ACN (15 ml), 3-dimethylamino-1-propyl chloride (200 mg, 1.26 mmol, 2 eq), Cs₂CO₃ (616 mg, 1.95 mmol) The reaction was stirred and heated to reflux under Ar atmosphere via balloon for 6 hours before cooling to RT. It was filtered and concentrated before purification via flash column chromatography (DCM – MeOH – 90 % - 10 %) to yield clear oil product (229 mg, 86 %). ¹H NMR (400 MHz, CDCl₃): δ 8.07 (d, J = 8 Hz, 2H), 7.56 (d, J = 8 Hz, 2H), 7.49 (t, J = 7 Hz, 2H), 7.42-7.40 (m, 2H), 7.37 (t, 7 Hz, 2H), 6.86 (d, J = 8 Hz, 1H), 6.66 (d, J = 8 Hz, 1H), 6.37 (s, 1H), 4.01 (t, J = 7 Hz, 2H), 2.32 (s, 2H), 2.18 (s, 6H), 1.93 (m, 2H). MS (ESI) calculated exact mass for C₂₅H₂₆N₄O₂ = 414.21. Found [M+H]⁺ = 415.1.

N-(5-(3-(dimethylamino)propoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**4b**) ^1H
NMR (400 MHz, CDCl_3)

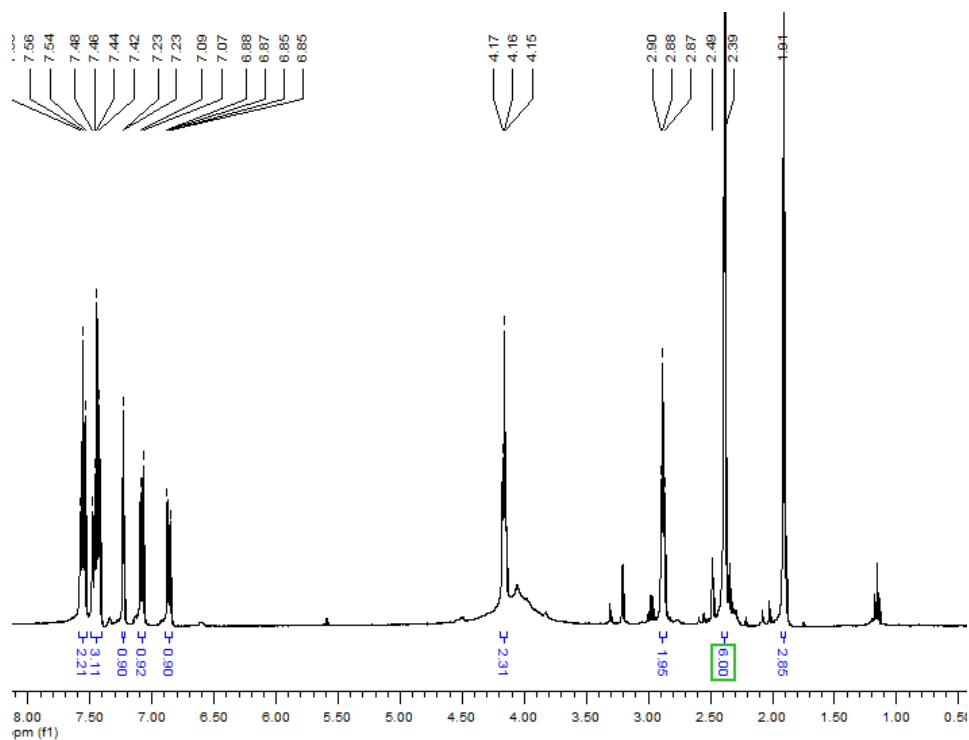


***N*-5-(2-(dimethylamino)ethoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)acetamide (4ba)**

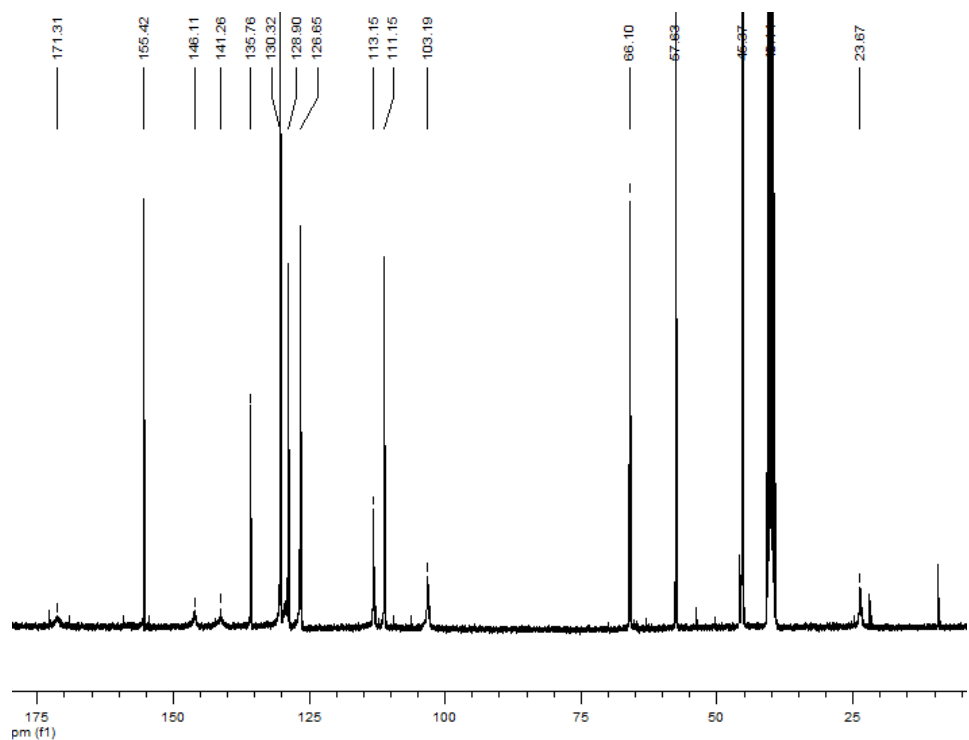


To a 100 ml round-bottom flask was added 4-(2-dimethylamino)ethoxy-2-nitro-*N*-phenylaniline (**11b**) (564 mg, 1.87 mmol) and MeOH (50 ml). The flask was flushed with Ar gas before Pd/C (50 mg, 10 wt %) was added. The reaction was then stirred at RT under H₂ for 26 hr before filtration and concentration, followed by addition of DCM (50 ml). Then, acetyl isothiocyanate (164 μ l, 1.87 mmol) was added. The reaction was stirred at RT for 2 hrs when DIPC (298 μ l, 1.87 mmol) and Et₃N (262 μ l, 1.87 mmol) were added. The reaction was then stirred at RT for 46 hrs before filtration, concentration and extraction with water and DCM (150 ml ea.). The organic layer was washed with water (100 ml), brine and dried with Na₂SO₄. After filtration and removal of solvent *in vacuo*, the crude was purified via flash column chromatography (DCM – MeOH : 80 % - 20 %) to yield clear oil product (144 mg, 23 % yield). ¹H NMR (400 MHz, DMSO-*d*₆): δ 7.58 (t, *J* = 8 Hz, 2H), 7.48-7.42 (m, 3H), 7.23 (d, *J* = 2 Hz, 1H), 7.09 (d, *J* = 9 Hz, 1H), 6.88 (dd, *J*₁ = 9 Hz, *J*₂ = 2 Hz, 1H), 4.17 (t, *J* = 5 Hz, 2H), 2.90 (t, *J* = 5 Hz, 2H), 2.39, (s, 6H), 1.91 (s, 3H). ¹³C NMR (400 MHz, DMSO-*d*₆): δ 171.31, 155.41, 146.10, 141.26, 135.76, 130.31, 128.90, 126.65, 113.14, 111.15, 103.19, 66.09, 57.62, 45.36, 40.13, 23.67. MS (ESI) calculated exact mass for C₁₉H₂₂N₄O₂ = 338.17. Found [M+H]⁺ = 339.15.

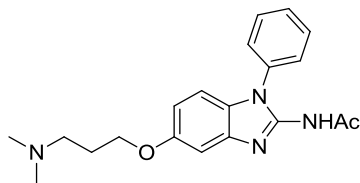
N-(5-(2-(dimethylamino)ethoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)acetamide (**4ba**) ¹H NMR (400 MHz, DMSO-*d*₆)



N-(5-(2-(dimethylamino)ethoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)acetamide (**4ba**) ¹³C NMR (400 MHz, DMSO-*d*₆)

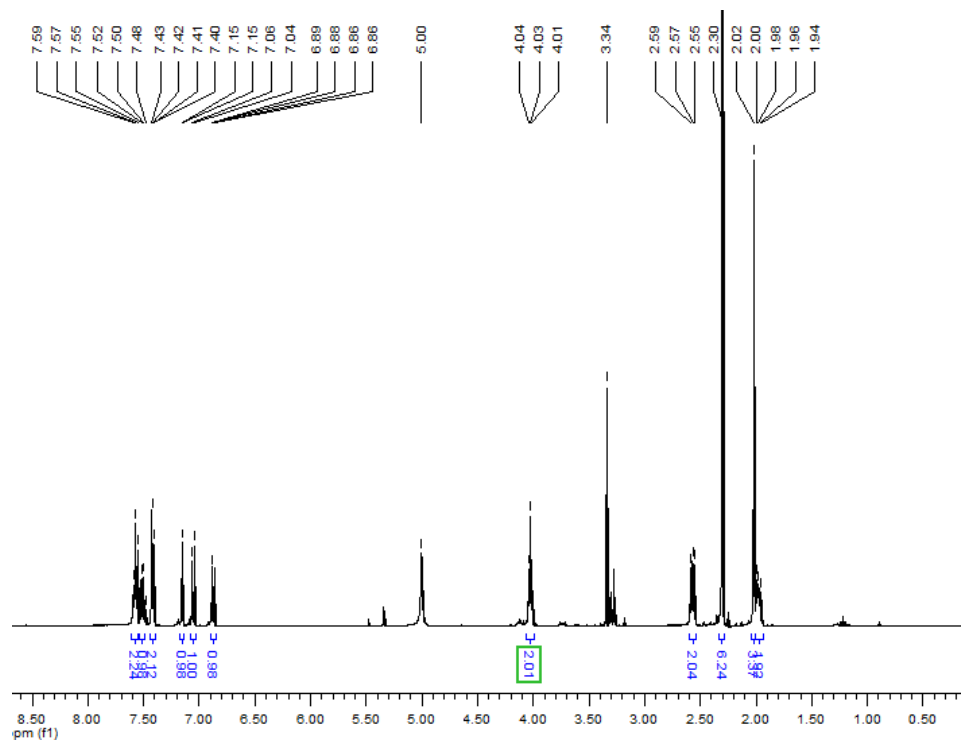


***N*-(5-(3-dimethylamino)propoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)acetamide (4ca)**

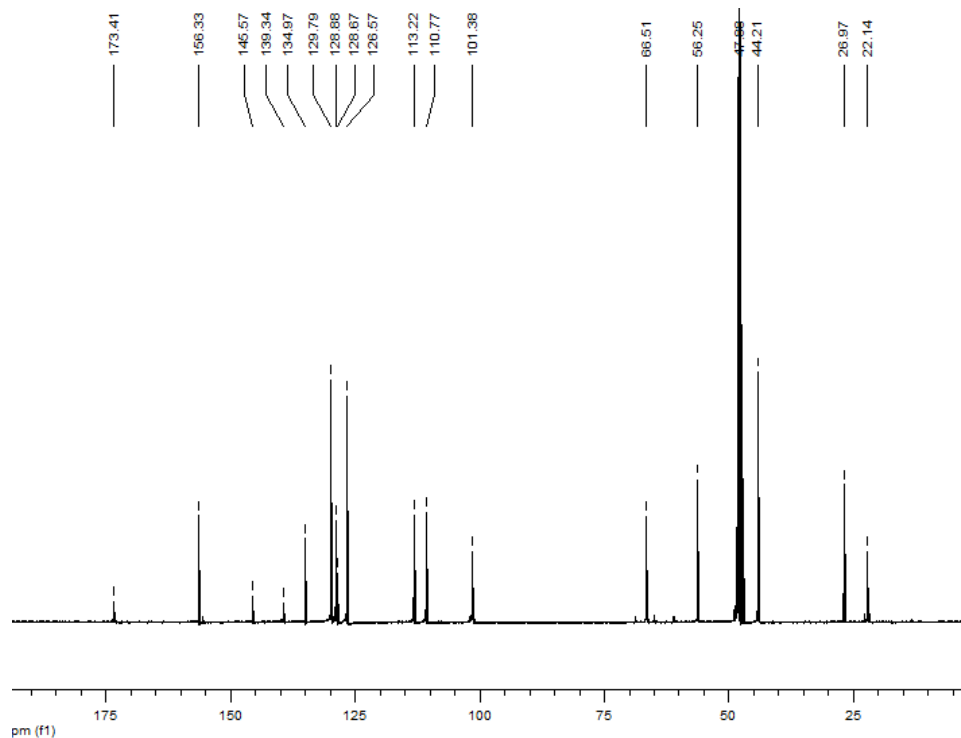


To a 100 ml round-bottom flask was added 4-(3-(dimethylamino)propoxy)-2-nitro-*N*-phenylaniline (**11c**) (682 mg, 2.16 mmol) and MeOH (50 ml). The flask was flushed with Ar gas before Pd/C (50 mg, 10 wt %) was added. The reaction was sealed under H₂ atm and stirred at RT for 7 hr. The metal was filtered and the solvent was removed *in vacuo*. The oil residue was dissolved in ACN and ethyl isothiocyanate (196 μ l, 2.16 mmol) was added dropwise. The reaction was heated to reflux for 19 hr. After cooled to RT, it was concentrated and purified by flash column chromatography (DCM – MeOH : 90 % - 10 %) to yield clear oil product (77 mg, 10 % yield). ¹H NMR (400 MHz, CD₃OD): δ 7.59 (t, *J* = 7 Hz, 2H), 7.52 (d, *J* = 7 Hz, 1H), 7.43 – 7.40 (m, 2H), 7.15 (d, *J* = 2 Hz, 1H), 7.06 (d, *J* = 9 Hz, 1H), 5.89 (dd, *J*₁ = 2 Hz, *J*₂ = 9 Hz, 1H), 4.04 (t, *J* = 6 Hz, 2H), 2.59 (t, *J* = 8 Hz, 2H), 2.30 (s, 6H), 2.02 (s, 3H), 2.00 (p, *J* = 7 Hz, 2H). ¹³C NMR (400 MHz, CD₃OD): δ 173.40, 156.32, 145.56, 139.33, 134.97, 129.78, 128.88, 128.67, 126.56, 113.21, 110.76, 101.38, 66.51, 56.24, 44.21, 26.97, 22.14. MS (ESI) calculated exact mass for C₂₀H₂₄N₄O₂ = 352.19. Found [M+H]⁺ = 353.1.

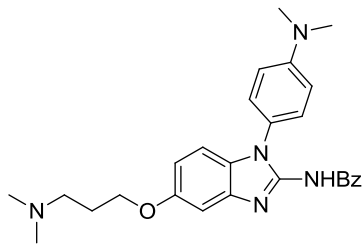
N-(5-(3-dimethylamino)propoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)acetamide (**4ca**) ^1H NMR (400 MHz, CD_3OD)



N-(5-(3-dimethylamino)propoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)acetamide (**4ca**) ^{13}C NMR (400 MHz, CD_3OD)

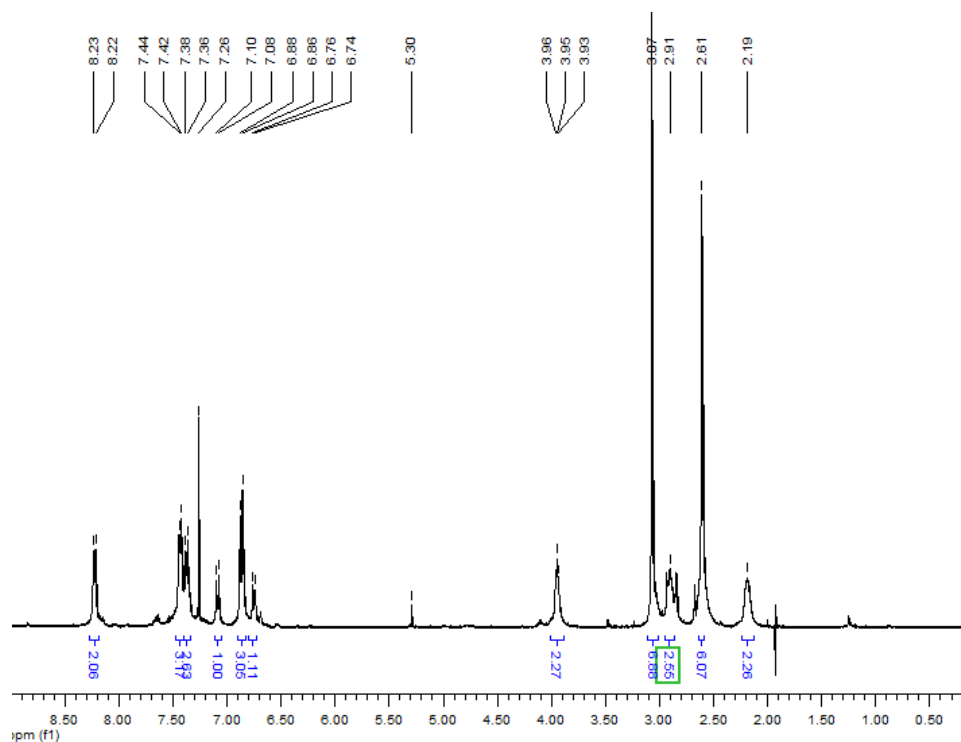


***N*-(1-(4-(dimethylamino)phenyl)-5-(3-(dimethylamino)propoxy)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (4eb)**

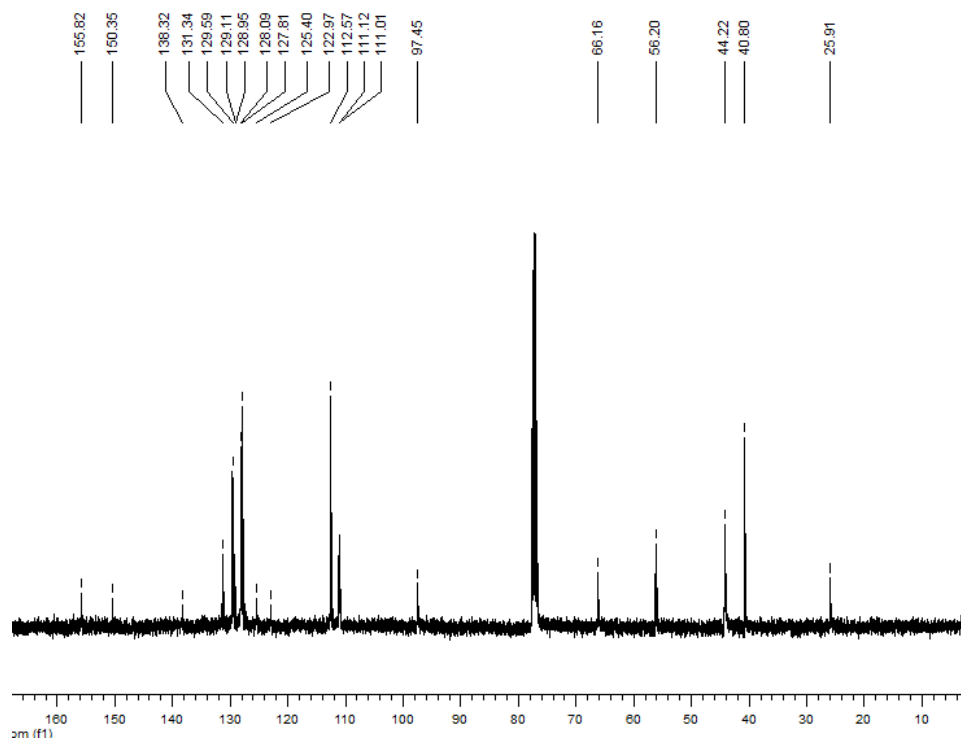


To a 100 ml round-bottom flask was added *N*¹-(4-(3-(dimethylamino)propoxy)-2-nitrophenyl)-*N*⁴,*N*⁴-dimethylbenzene-1,4-diamine (**11e**) (157 mg, 0.4 mmol) and methanol (30 ml). The flask was flushed with Ar gas before Pd/C (10 mg, 10 wt %) was added. The reaction was then sealed under H₂ atm and stirred at RT for 2 hours before filtration and concentration *in vacuo*. The oil residue was dissolved in 50 DCM and benzoyl isothiocyanate was added (65 μl, 0.4 mmol). The reaction was stirred at RT for 1 hour before DIPC (68 μl, 0.4 mmol) and DIPEA (76 μl, 0.4 mmol) were added. The reaction was stirred at RT for 25 hours before pouring into water (50 ml) and extracted. The organic layer was washed with water (50 ml), brine and dried over Na₂SO₄. After filtration and removal of solvent, the crude was purified via flash column chromatography (DCM- MeOH : 80 % - 20 %) to yield slight yellow solid (38 mg, 20 % yield over two steps). ¹H NMR (400 MHz, CDCl₃): δ 8.23 (d, *J* = 7 Hz, 2H), 7.44 – 7.36 (m, 5H), 7.10 (d, *J* = 9 Hz, 1H), 6.88 (m, 3H), 6.76 (d, *J* = 7 Hz, 1H), 3.95 (t, *J* = 5 Hz, 2H), 3.07 (s, 6H), 2.91 (m, 2H), 2.61 (s, 6H), 2.19 (m, 2H). ¹³C NMR (400 MHz, CDCl₃): δ 155.82, 150.34, 138.31, 131.33, 129.10, 128.94, 128.08, 127.81, 125.40, 122.97, 112.56, 111.11, 111.00, 97.44, 66.16, 56.20, 44.21, 40.80, 25.90. MS (ESI) calculated exact mass for C₂₇H₃₁N₅O₂ = 457.25. Found [M+H]⁺ = 458.20 .

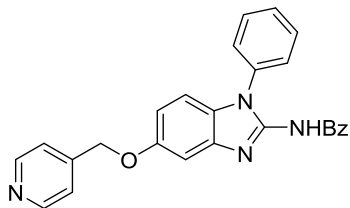
N-(1-(4-(dimethylamino)phenyl)-5-(3-(dimethylamino)propoxy)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**4eb**) ¹H NMR (400 MHz, CDCl₃)



N-(1-(4-(dimethylamino)phenyl)-5-(3-(dimethylamino)propoxy)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**4eb**) ¹³C NMR (400 MHz, CDCl₃)

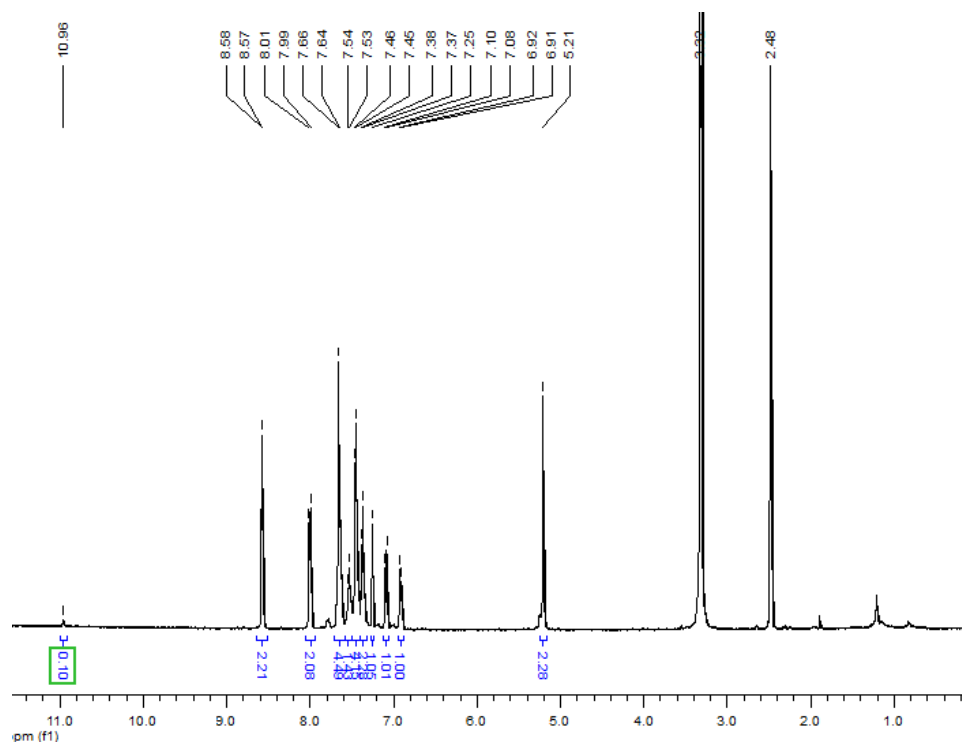


***N*-(1-phenyl-5-(pyridin-4-ylmethoxy)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (4da)**

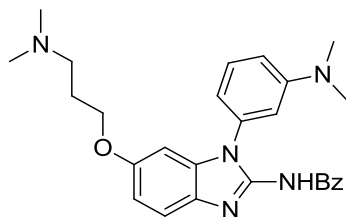


To a 50 ml round-bottom flask was added *N*-(5-hydroxy-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**4ab**) (71 mg, 0.21 mmol), ACN (20 ml), 4-(chloromethyl)pyridine (161 mg, 1.26 mmol, 2 eq), and Cs₂CO₃ (76 mg, 0.24 mmol). The reaction was stirred at RT under Ar atmosphere via balloon for 27 hours before filtration and concentration. It was purified via flash column chromatography (EtOAc – DCM : 40 % - 60 %) to yield white solid product (54 mg, 60 % yield). ¹H NMR (400 MHz, DMSO-*d*₆): δ 8.58 (d, *J* = 4 Hz, 2H), 8.01 (d, *J* = 8 Hz, 2H), 7.66 (m, 4H), 7.54 (m, 1H), 7.46 (m, 4H), 7.38 (m, 2H), 7.25 (s, 1H), 7.10 (d, *J* = 9 Hz, 1H), 6.92 (d, *J* = 6 Hz, 1H), 5.21 (s, 2H). MS (ESI) calculated exact mass for C₂₆H₂₀N₄O₂ = 420.16. Found [M+H]⁺ = 421.1.

N-(1-phenyl-5-(pyridin-4-ylmethoxy)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**4da**) ¹H NMR (400 MHz, DMSO-*d*₆)

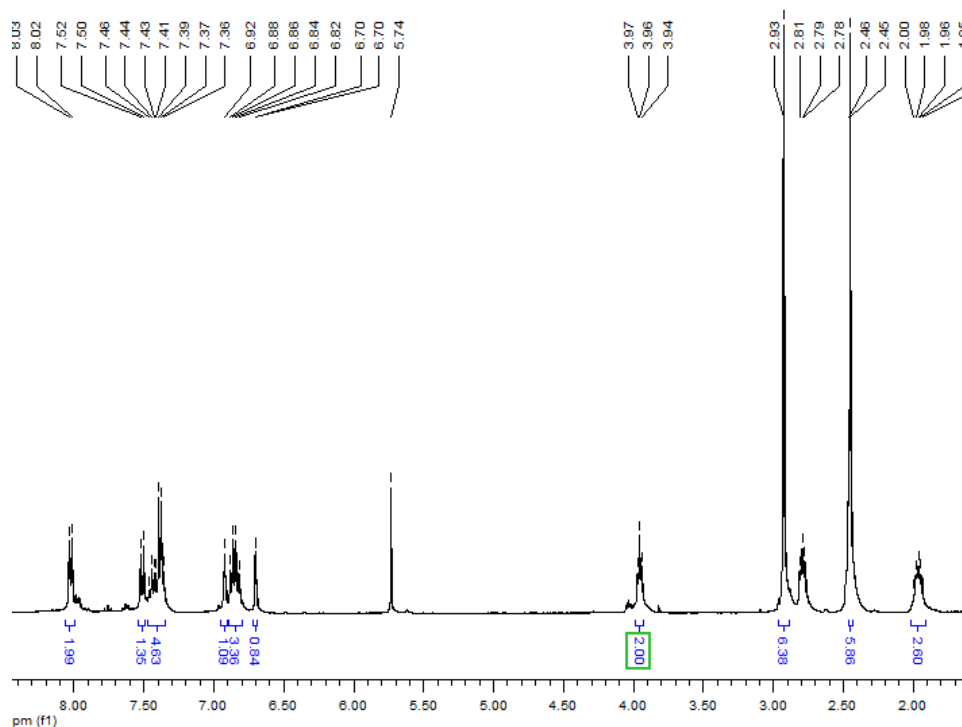


***N*-(1-(3-(dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (4gb)**

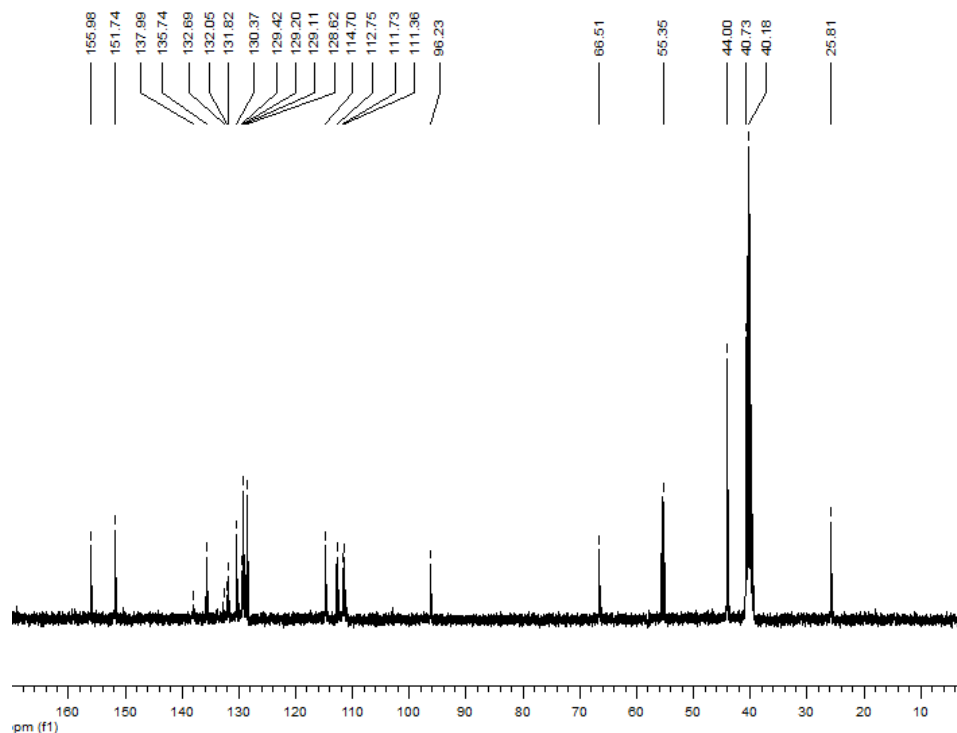


To a 250 ml round-bottom flask was added *N*¹-(5-(3-(dimethylamino)propoxy)-2-nitrophenyl)-*N*³,*N*³-dimethylbenzene-1,3-diamine (**11g**) (1.2 g, 3.2 mmol), methanol (100 ml). The flask was flushed with Ar gas before Pd/C (100 mg, 10 wt %) was added. The reaction was sealed under H₂ and stirred at RT for 22 hours before filtration and concentration. The dark oil residue was dissolved in ACN (100 ml). Benzoylisothiocyanate (386 μl, 3.2 mmol) was added. The reaction was stirred at RT for 3 hours when DIPC (522 μl, 3.2 mmol) and DIPEA (566 μl, 3.2 mmol) were added. The reaction was stirred at RT for 21 hours before filtration, concentration and purification via flash column (DCM – MeOH : 90 % - 10 %) to yield yellow brown foam product (557 mg, 38 % yield). ¹H NMR (400 MHz, DMSO-*d*₆): δ 8.03 (d, *J* = 7 Hz, 2H), 7.52 (d, *J* = 8 Hz, 1H), 7.46 – 7.36 (m, 4H), 6.92 (s, 1H), 6.88 – 6.82 (m, 3H), 6.70 (d, *J* = 2 Hz, 1H), 3.97 (t, *J* = 6 Hz, 2H), 2.93 (s, 6H), 2.81 (t, *J* = 7 Hz, 2H), 2.45 (s, 6H), 2.00 (m, 2H). ¹³C NMR (400 MHz, DMSO-*d*₆): δ 155.97, 151.73, 137.98, 135.74, 132.68, 132.05, 131.82, 130.36, 129.41, 129.20, 129.11, 128.62, 114.70, 112.75, 111.72, 111.36, 96.23, 66.51, 55.34, 44.00, 40.73, 25.81. MS (ESI) calculated exact mass for C₂₇H₃₁N₅O₂ = 457.57. Found [M+H]⁺ = 458.30.

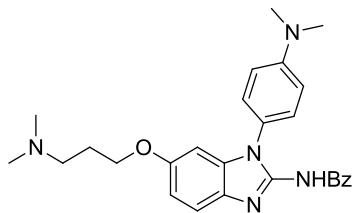
N-(1-(3-(dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**4gb**) ¹H NMR (400 MHz, DMSO-*d*₆)



N-(1-(3-(dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**4gb**) ¹³C NMR (400 MHz, DMSO-*d*₆)

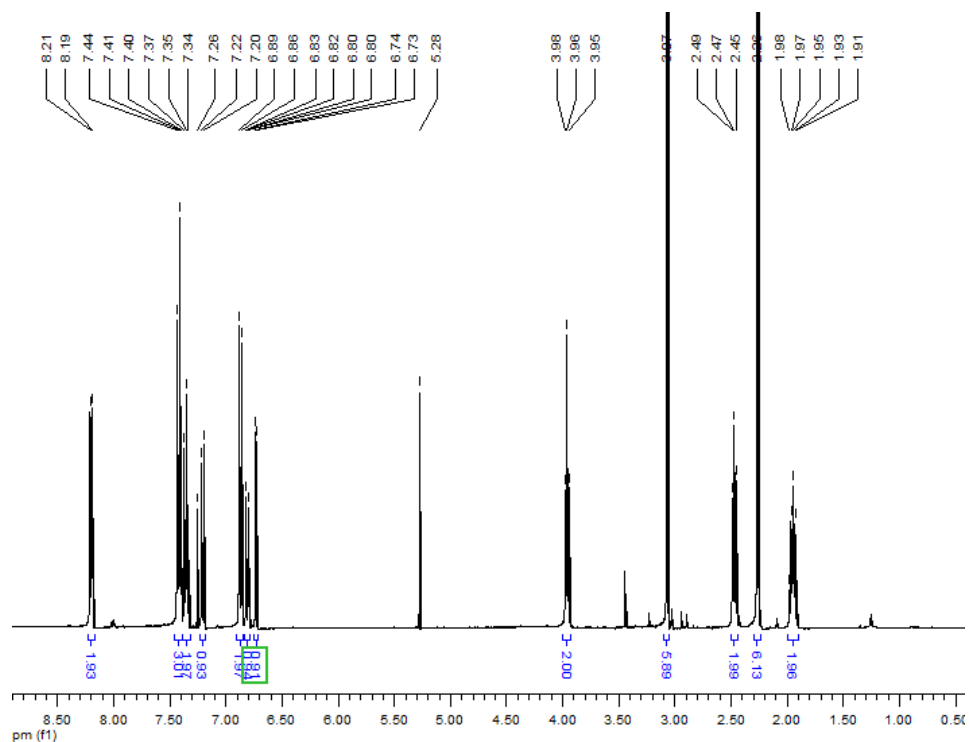


***N*-(1-(4-(dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (4fb)**

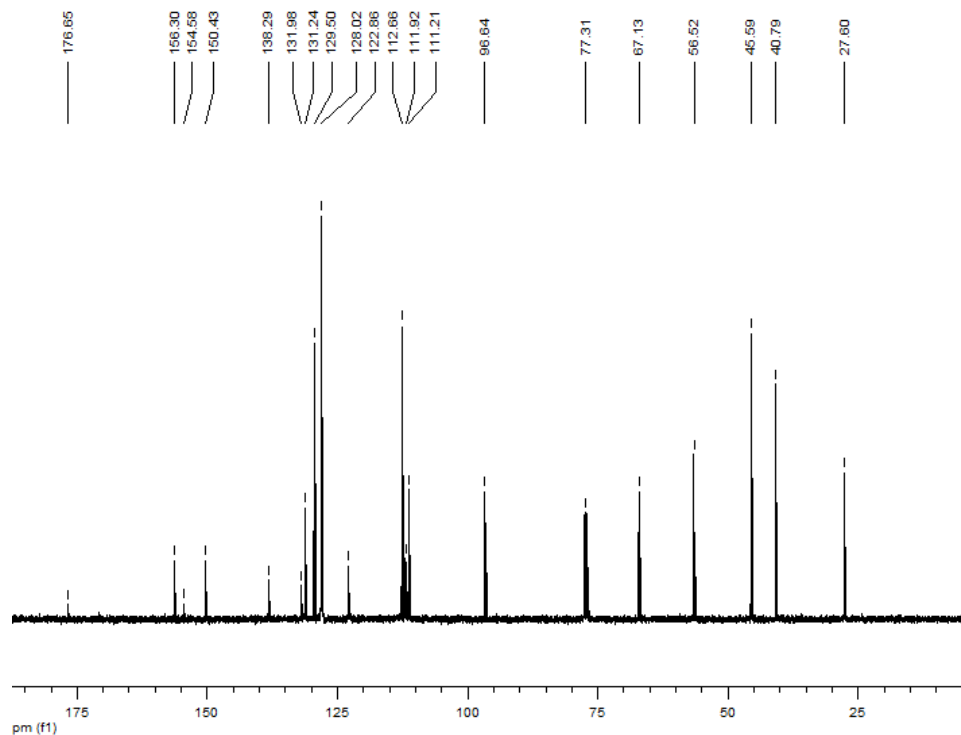


To a 250 ml round bottom flask was added *N*¹-(5-(3-(dimethylamino)propoxy)-2-nitrophenyl)-*N*⁴,*N*⁴-dimethylbenzene-1,4-diamine (**11f**) (1.2 g, 3.35 mmol), MeOH (100 ml). The flask was flushed with Ar gas before Pd/C (120 mg, 10 wt %) was added. The reaction was then sealed under H₂ and stirred at RT for 4.5 hr, when the reaction was filtered and concentrated. The oil residue was dissolved in 100 ml of DCM and benzoyl isothiocyanate (509 μ l, 3.35 mmol) was added. The reaction was stirred at RT under Ar for 1 hr before DIPC (600 μ l, 3.85 mmol) and DIPEA (567 μ l, 3.35 mmol) was added. The reaction was stirred at RT under Ar for 21 hr before extracted with water (2 x 100 ml) and dried over Na₂SO₄. After filtration and evaporation of solvent, the crude was purified via flash column chromatography (DCM – MeOH : 90% - 10 %) to yield white solid product (393 mg, 26 % yield over two steps). ¹H NMR (400 MHz, CDCl₃): δ 8.21 (d, *J* = 7 Hz, 2H), 7.44 – 7.40 (m, 3H), 7.37 (t, *J* = 7 Hz, 2H), 7.22 (d, *J* = 9 Hz, 1H), 6.89 (d, *J* = 9 Hz, 2H), 6.83 (dd, *J*₁ = 9 Hz, *J*₂ = 2 Hz, 1H), 6.74 (d, *J* = 2 Hz, 1H), 3.98 (t, *J* = 6 Hz, 2H), 3.07 (s, 6H), 2.49 (t, *J* = 7 Hz, 2H), 2.26 (s, 6H), 1.98 (p, *J* = 7 Hz, 2H). ¹³C NMR (400 MHz, CDCl₃): δ 176.65, 156.29, 154.58, 150.43, 138.28, 131.97, 131.24, 129.49, 128.01, 122.85, 112.65, 111.91, 111.20, 96.64, 67.12, 56.52, 45.59, 40.78, 27.60. MS (ESI) calculated exact mass for C₂₇H₃₁N₅O₂ = 457.25. Found [M+H]⁺ = 458.24.

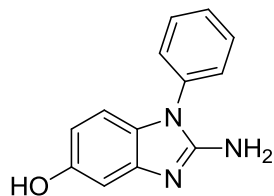
N-(1-(4-(dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**4fb**) ¹H NMR (400 MHz, CDCl₃)



N-(1-(4-(dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**4fb**) ¹³C NMR (400 MHz, CDCl₃)

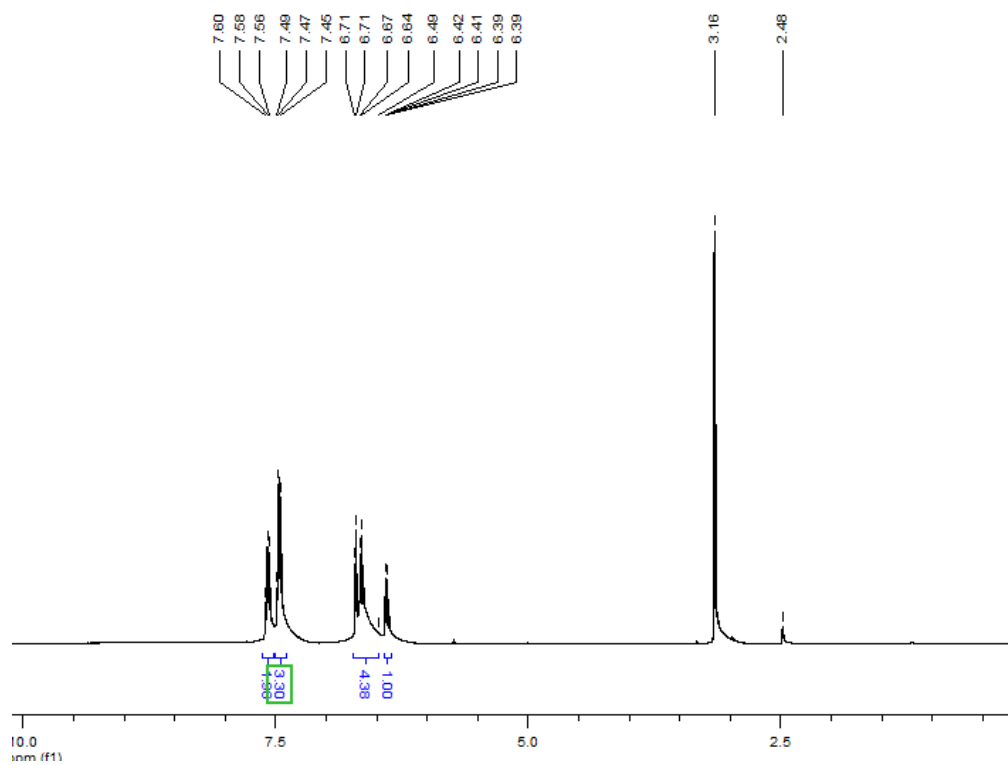


2-amino-1-phenyl-1*H*-benzo[*d*]imidazol-5-ol (3a)

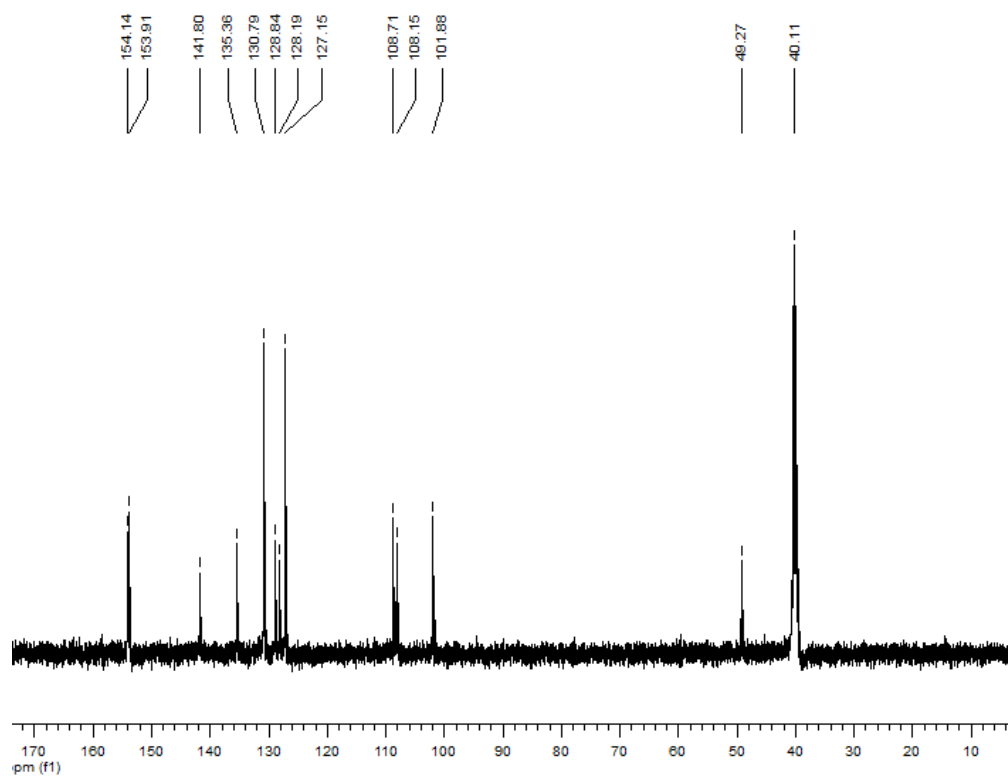


To a 50 ml round-bottom flask was added *N*-(5-hydroxy-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**4ab**) (300 mg, 0.68 mmol), 2N HCl (aq, 10 ml), dioxane (10ml). The reaction was stirred and heated to reflux for 22 hours before cooled to RT and poured into water (100 ml) and extracted with chloroform (150 ml x 2). The organic layers were collected and combined and dried with brine and Na₂SO₄. The crude was filtered, concentrated and purified with flash column (DCM – MeOH : 80 % - 20 %) to yield clear oil product (120 mg, 78 % yield). ¹H NMR (400 MHz, DMSO-*d*₆): δ 7.58 (t, *J* = 7 Hz, 2H), 7.47 (m, 3 H), 6.71 – 6.64 (m, 4 H), 6.42 (dd, *J*₁ = 9 Hz, *J*₂ = 2Hz, 1H). ¹³C NMR (400 MHz, DMSO-*d*₆): δ 154.13, 153.90, 141.79, 135.35, 130.78, 128.84, 128.19, 127.15, 108.70, 108.14, 101.88. MS (ESI) calculated exact mass for C₁₃H₁₁N₃O = 225.09. Found [M+H]⁺ = 226.10.

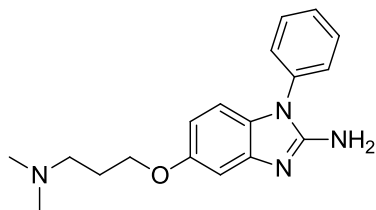
2-amino-1-phenyl-1*H*-benzo[*d*]imidazol-5-ol (**3a**) ¹H NMR (400 MHz, DMSO-*d*₆)



2-amino-1-phenyl-1*H*-benzo[*d*]imidazol-5-ol (**3a**) ¹³C NMR (400 MHz, DMSO-*d*₆)

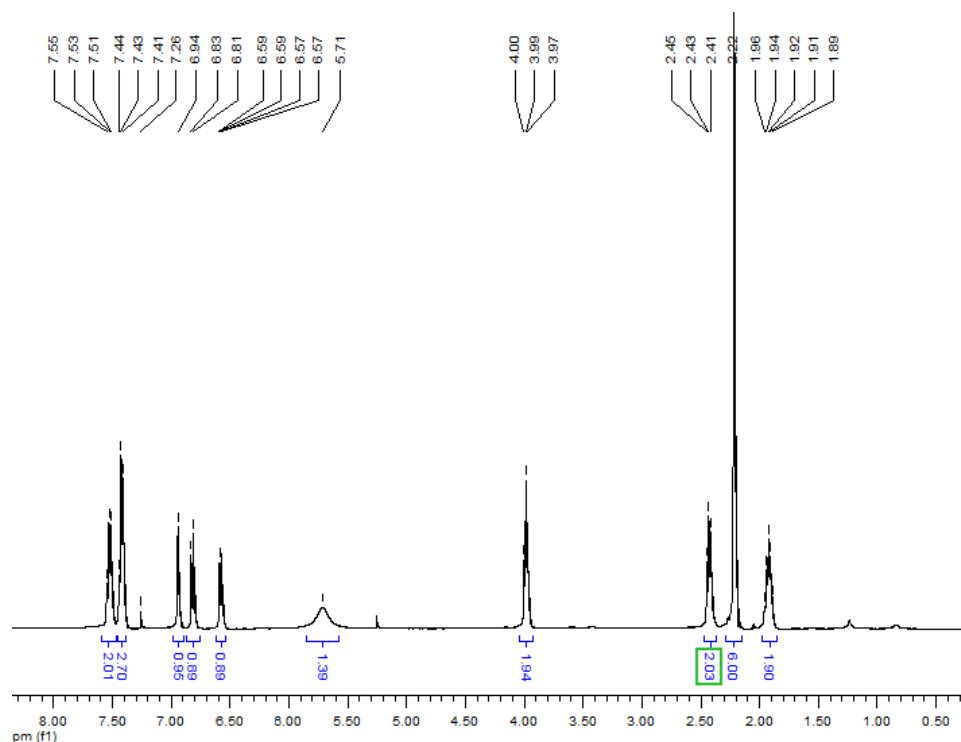


5-(3-(dimethylamino)propoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-amine (3c)

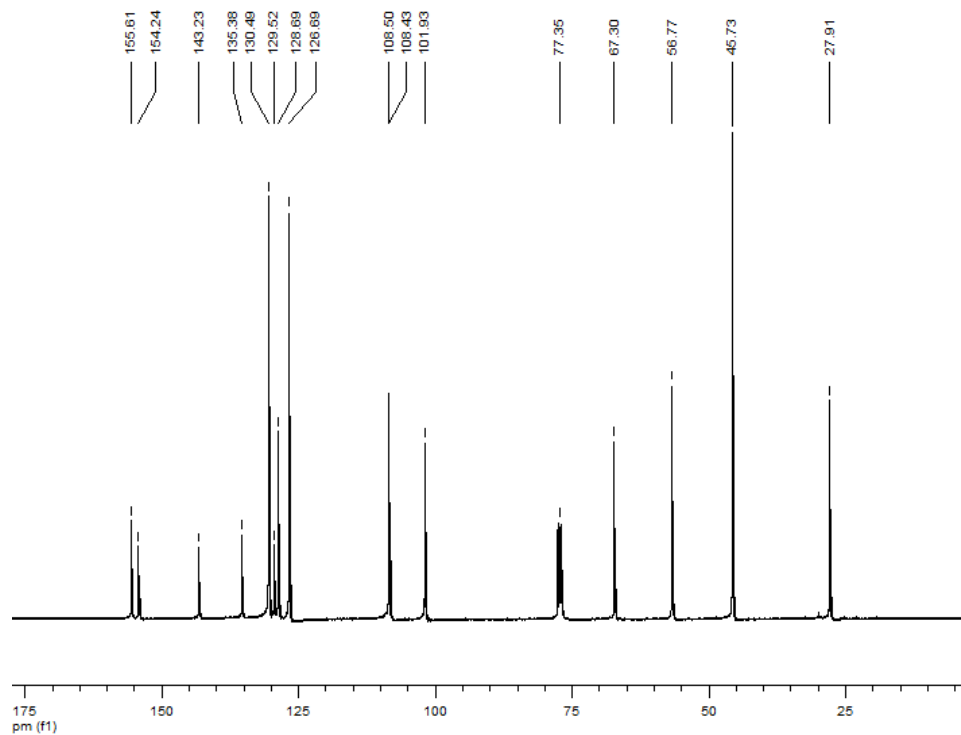


To a 100 ml round-bottom flask was added *N*-(5-(3-(dimethylamino)propoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**4cb**) (264 mg, 0.6 mmol) and 1N HCl aq (40 ml). The reaction was stirred and heated to reflux for 26 hours before cooled to RT and extracted with saturated NaHCO₃ (100 ml). The organic layer was washed with brine and dried over Na₂SO₄. After filtration and evaporation, the crude was purified using flash column chromatography (DCM – MeOH : 80 % - 20 %) to yield slight yellow oil product (190 mg, 94 % yield). ¹H NMR (400 MHz, CDCl₃): δ 7.55 (t, *J* = 8 Hz, 2H), 7.44-7.41 (m, 3H), 6.94 (s, 1H), 6.83 (d, *J* = 8 Hz, 1H), 6.59 (dd, *J*₁ = 8 Hz, *J*₂ = 2 Hz, 1H), 5.71 (broad, 1H), 4.00 (t, *J* = 7 Hz, 2H), 2.45 (t, *J* = 7 Hz, 2H), 2.22 (s, 6H), 1.95 (p, *J* = 7 Hz, 2H). ¹³C NMR (400 MHz, CDCl₃): δ 155.61, 154.24, 143.23, 135.37, 130.48, 129.51, 128.68, 126.69, 108.50, 108.42, 101.92, 67.29, 56.76, 45.73, 27.91. MS (ESI) calculated exact mass for C₁₈H₂₂N₄O = 310.18. Found [M+H]⁺ = 311.1.

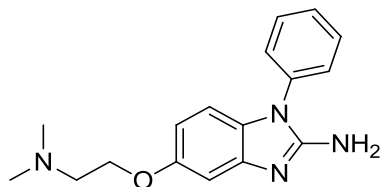
5-(3-(dimethylamino)propoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-amine (**3c**) ^1H NMR (400 MHz, CDCl_3)



5-(3-(dimethylamino)propoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-amine (**3c**) ^{13}C NMR (400 MHz, CDCl_3)

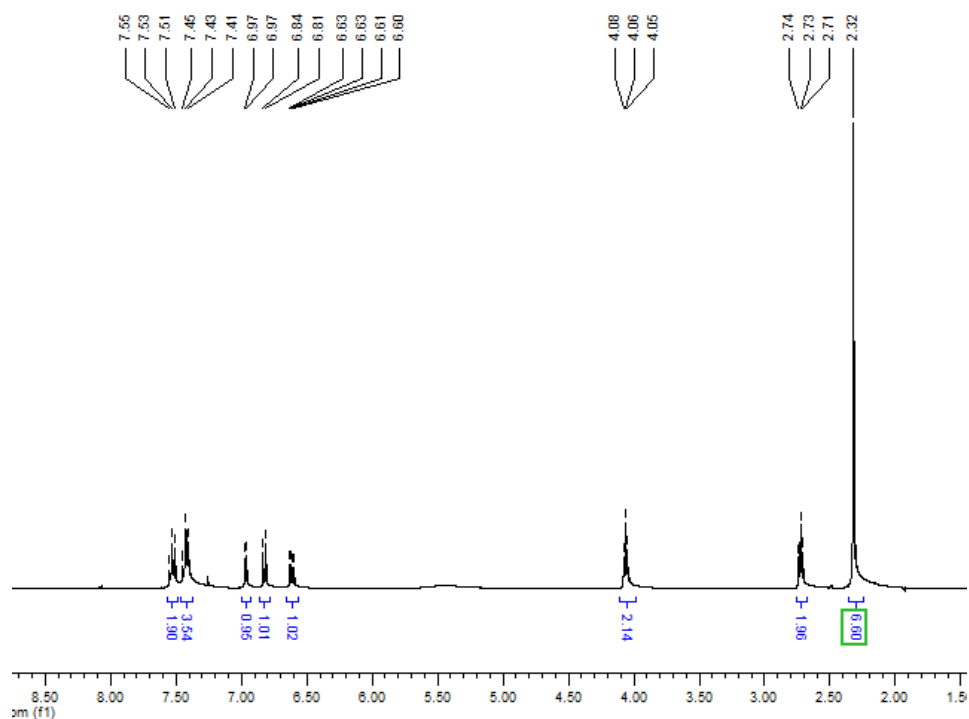


5-(2-(dimethylamino)ethoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-amine (3b)

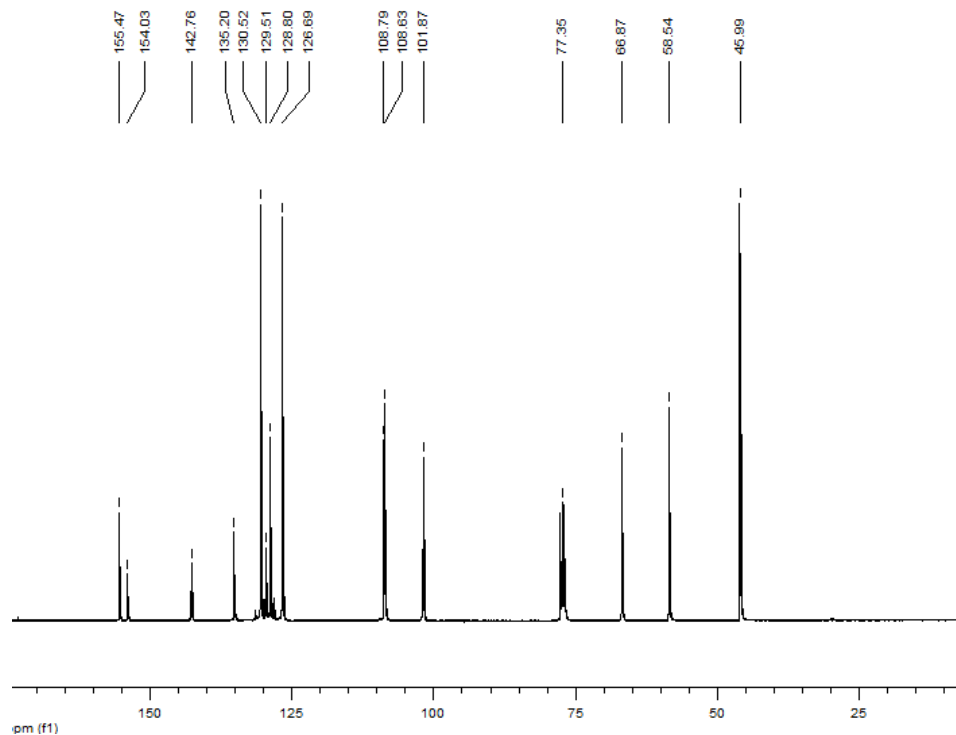


Into a 50 ml round bottom flask was added *N*-(5-(2-(dimethylamino)ethoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**4bb**) (320 mg, 0.8 mmol) and 1N HCl aq (20 ml). The reaction was stirred and heated to reflux for 24 hr before cooling to RT and extraction with saturated NaHCO₃ and DCM (100 ml ea.). The aqueous layer was extracted with more DCM (100 ml). The combined organic layer was washed with brine and dried over Na₂SO₄. After filtration and evaporation of solvent, the crude was purified via flash column chromatography (DCM – MeOH : 80 % - 20 %) to yield white solid (193 mg, 65 % yield). ¹H NMR (400 MHz, CDCl₃): δ 7.55 (t, *J* = 7 Hz, 2H), 7.45 – 7.41 (m, 3H), 6.97 (d, *J* = 2 Hz, 1H), 6.84 (d, *J* = 8 Hz, 1H), 6.63 (dd, *J*₁ = 8 Hz, *J*₂ = 2 Hz, 1H), 4.08 (t, *J* = 6 Hz, 2H), 2.74 (t, *J* = 6 Hz, 2H), 2.32 (s, 6H). ¹³C NMR (400 MHz, CDCl₃): δ 155.47, 154.03, 142.75, 135.19, 130.52, 129.51, 128.80, 126.68, 108.78, 108.63, 101.86, 66.86, 58.53, 45.99. MS (ESI) calculated exact mass for C₁₇H₂₀N₄O = 296.16. Found [M+H]⁺ = 297.15.

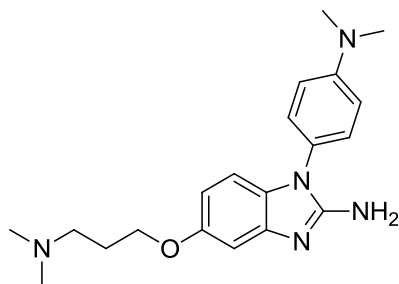
5-(2-(dimethylamino)ethoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-amine (**3b**) ¹H NMR (400 MHz, CDCl₃)



5-(2-(dimethylamino)ethoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-amine (**3b**) ¹³C NMR (400 MHz, CDCl₃)

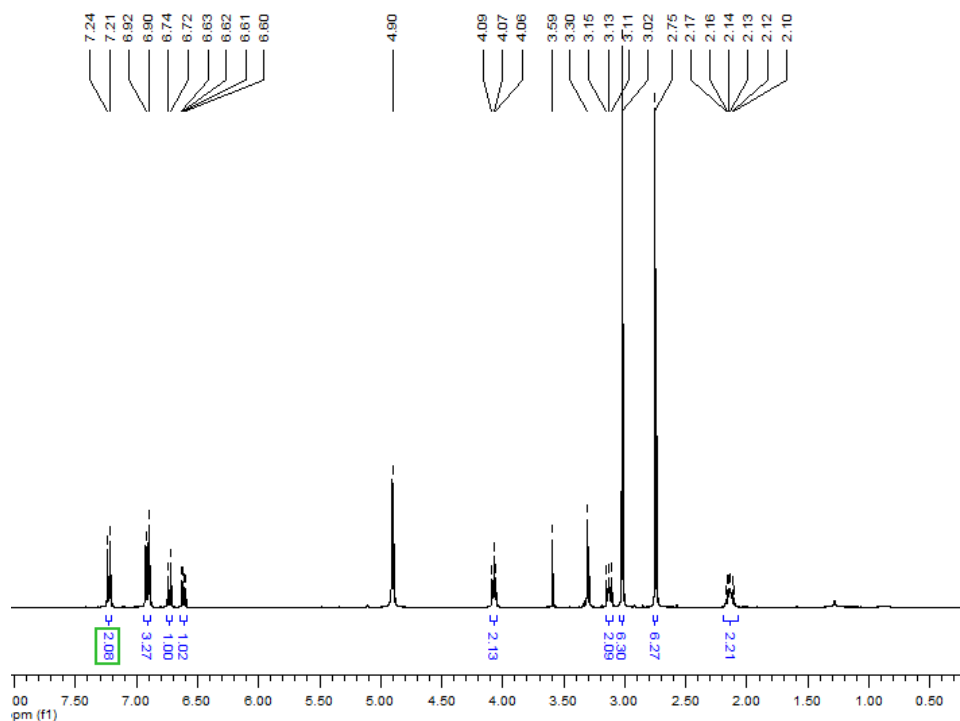


**1-(4-(dimethylamino)phenyl)-5-(3-(dimethylamino)propoxy)-1H-benzo[d]imidazol-2-amine
(3e)**

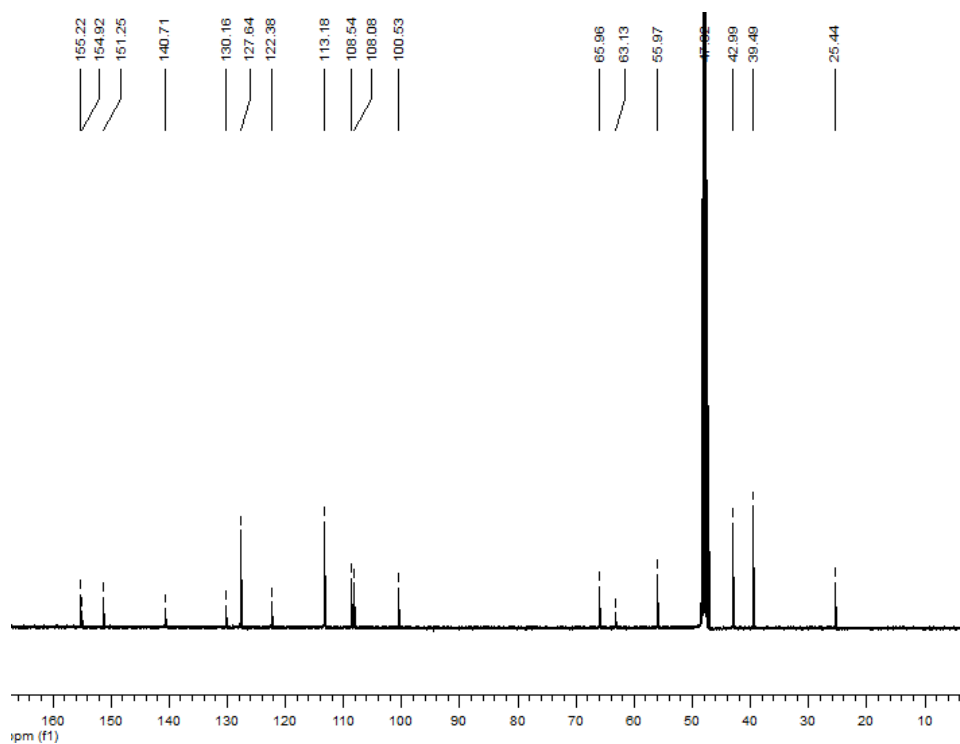


To a 100 ml round-bottom flask was added *N*-(1-(4-(dimethylamino)phenyl)-5-(3-(dimethylamino)propoxy)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**4eb**) (320 mg, 0.7 mmol) and 1N HCl aq (25 ml). The reaction was stirred and heated to reflux for 19 hours, then, at RT 1 M NaOH aq was added until white precipitate formed. It was then extracted with chloroform-ethanol (2 x 100 ml, 2 : 1). The combined organic layers were dried over Na₂SO₄. After filtration and evaporation of solvent, the crude was purified with flash column chromatography (DCM – MeOH : 80 % - 20 %) to yield white solid product (174 mg, 73 % yield). ¹H NMR (400 MHz, CD₃OD): δ 7.23 (d, *J* = 9 Hz, 2H), 6.92 – 6.90 (m, 3H), 6.74 (d, *J* = 8 Hz, 1H), 6.63 (dd, *J*₁ = 8 Hz, *J*₂ = 2 Hz, 1H), 4.09 (t, *J* = 6 Hz, 2H), 3.15 (t, *J* = 8 Hz, 2H), 3.02 (s, 6H), 2.75 (s, 6H), 2.17 – 2.10 (m, 2H). ¹³C NMR (400 MHz, CD₃OD): δ 155.22, 154.91, 151.24, 140.70, 130.15, 127.63, 122.37, 113.18, 108.54, 108.08, 100.52, 65.96, 64.12, 55.97, 42.99, 39.49, 15.44. MS (ESI) calculated exact mass for C₁₉H₂₅N₅O = 353.22. Found [M+H]⁺ = 354.3.

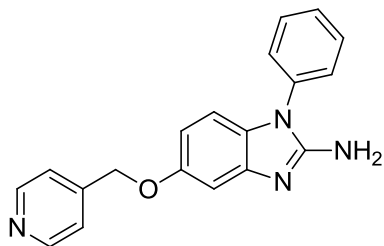
1-(4-(dimethylamino)phenyl)-5-(3-(dimethylamino)propoxy)-1H-benzo[d]imidazol-2-amine (**3e**)
¹H NMR (400 MHz, CD₃OD)



1-(4-(dimethylamino)phenyl)-5-(3-(dimethylamino)propoxy)-1H-benzo[d]imidazol-2-amine (**3e**)
¹³C NMR (400 MHz, CD₃OD)

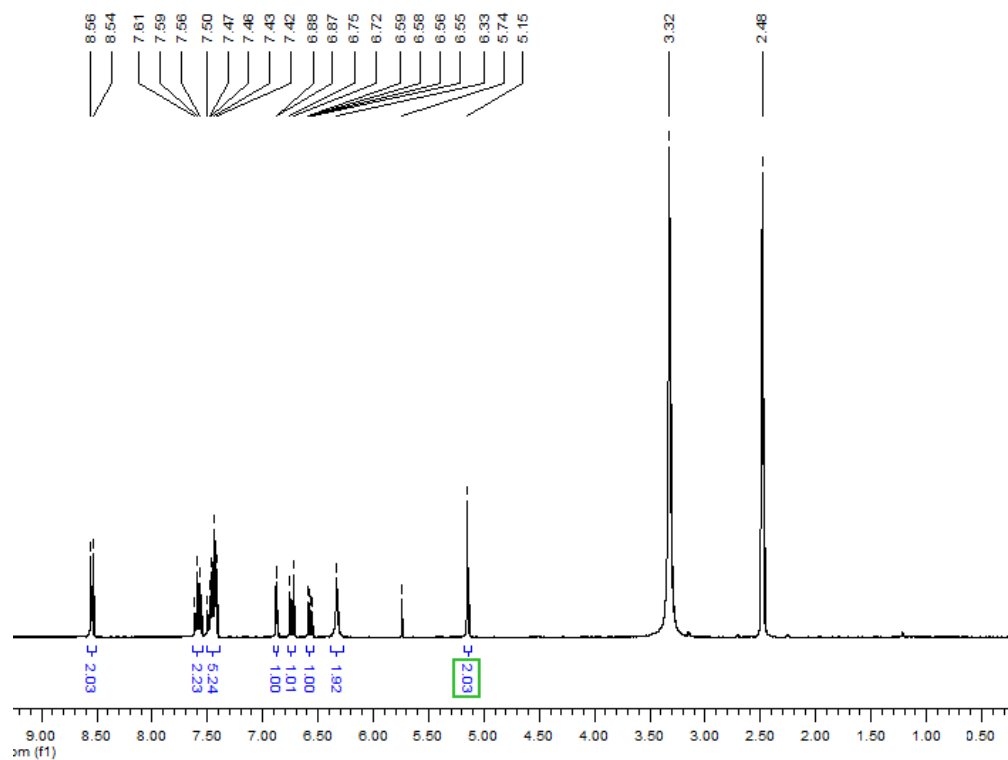


1-phenyl-5-(pyridine-4-ylmethoxy)-1H-benzo[d]imidazol-2-amine (3d)

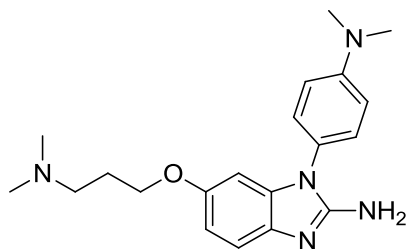


To a 50 ml round-bottom flask was added *N*-(1-phenyl-5-(pyridin-4-ylmethoxy)-1H-benzo[*d*]imidazol-2-yl)benzamide (**4da**) and 1N HCl (20 ml). The reaction was stirred and heated to reflux for 18 hours, then cooled to RT and 1M NaOH added until cloudiness appears. It was then extracted with EtOAc (2 x 20 ml). The organic layers were combined and washed with brine and Na₂SO₄. After filtration and evaporation of solvent *in vacuo*, the crude was purified via flash column chromatography (DCM – MeOH : 90 % - 10 %) to yield white solid product (15 mg, 68 % yield). ¹H NMR (400 MHz, DMSO-*d*₆): δ 8.56 (d, *J* = 6 Hz, 2H), 7.61 (t, *J* = 7 Hz, 2H), 7.50 – 7.42 (m, 5H), 6.88 (d, *J* = 2 Hz, 1H), 6.75 (d, *J* = 9 Hz, 1H), 6.59 (dd, *J*₁ = 9 Hz, *J*₂ = 2Hz, 1H), 6.33 (s, broad, 2H), 5.15 (s, 2H). MS (ESI) calculated exact mass for C₁₉H₁₆N₄O = 316.13. Found [M+H]⁺ = 317.09.

1-phenyl-5-(pyridine-4-ylmethoxy)-1*H*-benzo[*d*]imidazol-2-amine (**3d**) ¹H NMR (400 MHz, DMSO-*d*₆)

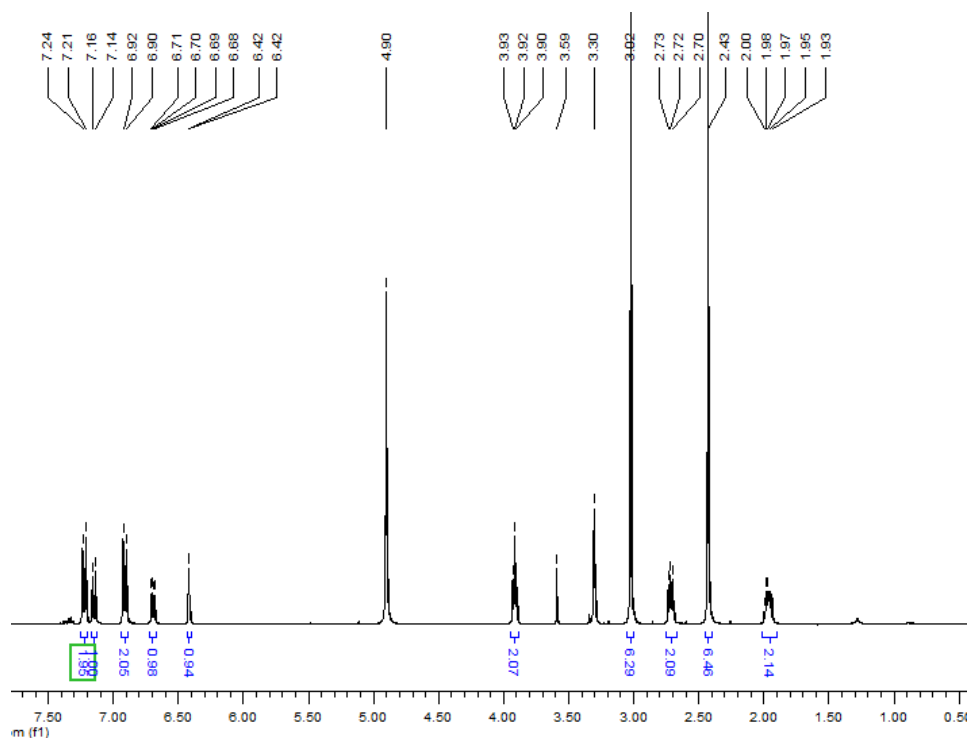


**1-(4-(dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1H-benzo[d]imidazol-2-amine
(3f)**

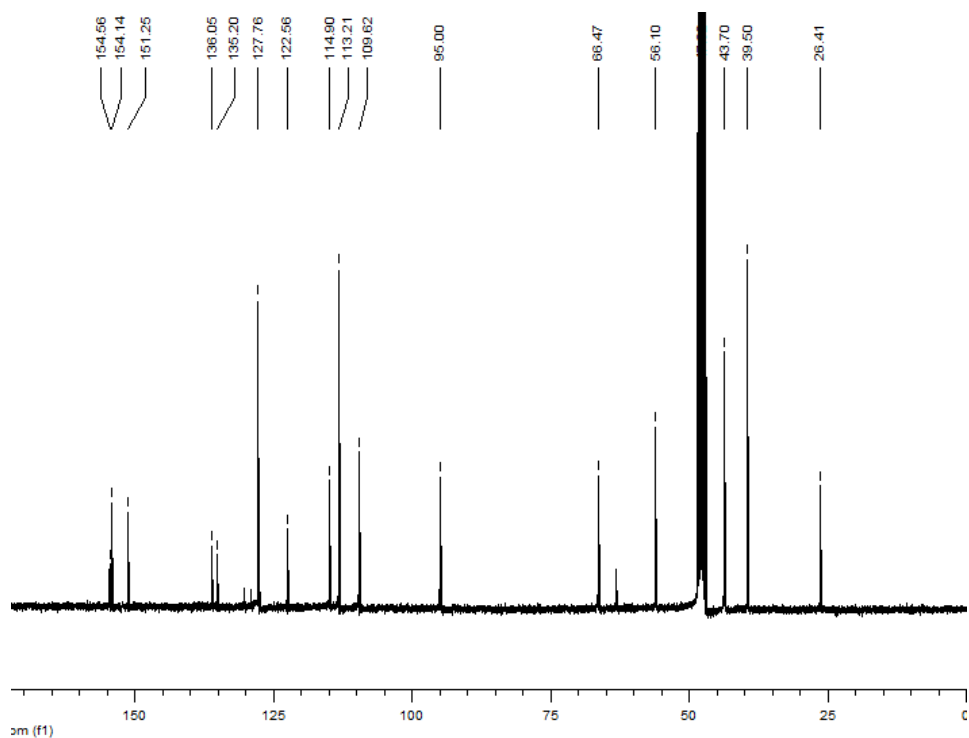


To a 100 ml round-bottom flask was added N-(1-(4-(dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1H-benzo[d]imidazol-2-yl)benzamide (**4fb**) (375 mg, 0.82 mmol) and 1N HCl aq (25 ml). The reaction was stirred and heated to reflux for 19 hr, then cooled to RT. After addition of saturated NaHCO₃ aq and 1M NaOH aq until white precipitate formed, the mixture was extracted with CHCl₃-EtOH (2 : 1, 3 x 150 ml). The combined organic layer was dried over Na₂SO₄. After filtration and concentration, the crude was purified using flash column chromatography (DCM – MeOH : 80 % - 20 %) to yield white solid (240 mg, 83 % yield). ¹H NMR (400 MHz, CD₃OD): δ 7.24 (d, *J* = 9 Hz, 2H), 7.16 (d, *J* = 8 Hz, 1H), 6.92 (d, *J* = 9 Hz, 2H), 6.71 (dd, *J*₁ = 9 Hz, *J*₂ = 2 Hz, 1H), 6.42 (d, *J* = 2 Hz, 1H), 3.93 (t, *J* = 6 Hz, 2H), 3.02 (s, 6H), 2.73 (t, *J* = 7 Hz, 2H), 2.43 (s, 6H), 2.00 (p, *J* = 6 Hz, 2H). ¹³C NMR (400 MHz, DMSO-d₆): δ 154.56, 154.13, 151.24, 136.04, 135.20, 127.76, 122.56, 114.89, 113.21, 109.62, 95.00, 66.46, 56.10, 47.81, 43.70, 39.49, 26.41. MS (ESI) calculated exact mass for C₂₀H₂₇N₅O = 353.22. Found [M+H]⁺ = 354.25.

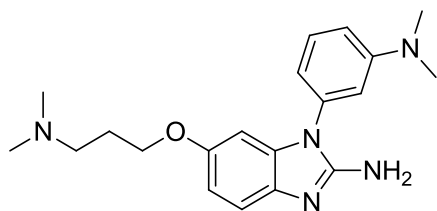
1-(4-(dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1*H*-benzo[*d*]imidazol-2-amine (**3f**)
¹H NMR (400 MHz, CD₃OD)



1-(4-(dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1*H*-benzo[*d*]imidazol-2-amine (**3f**)
¹³C NMR (400 MHz, CD₃OD)

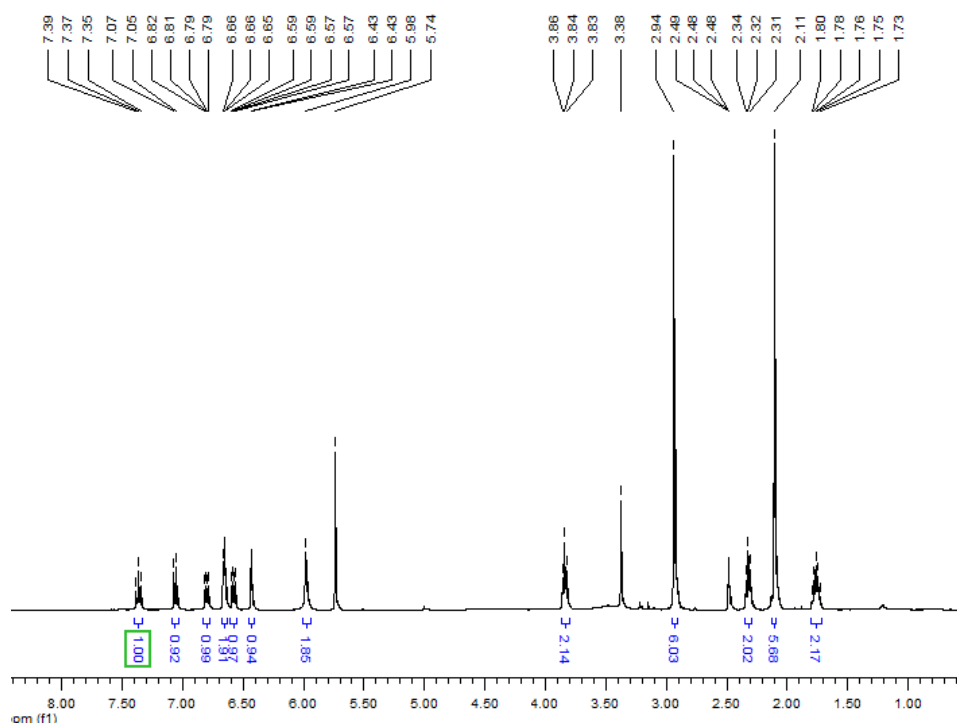


**1-(3-dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1*H*-benzo[*d*]imidazol-2-amine
(3g)**

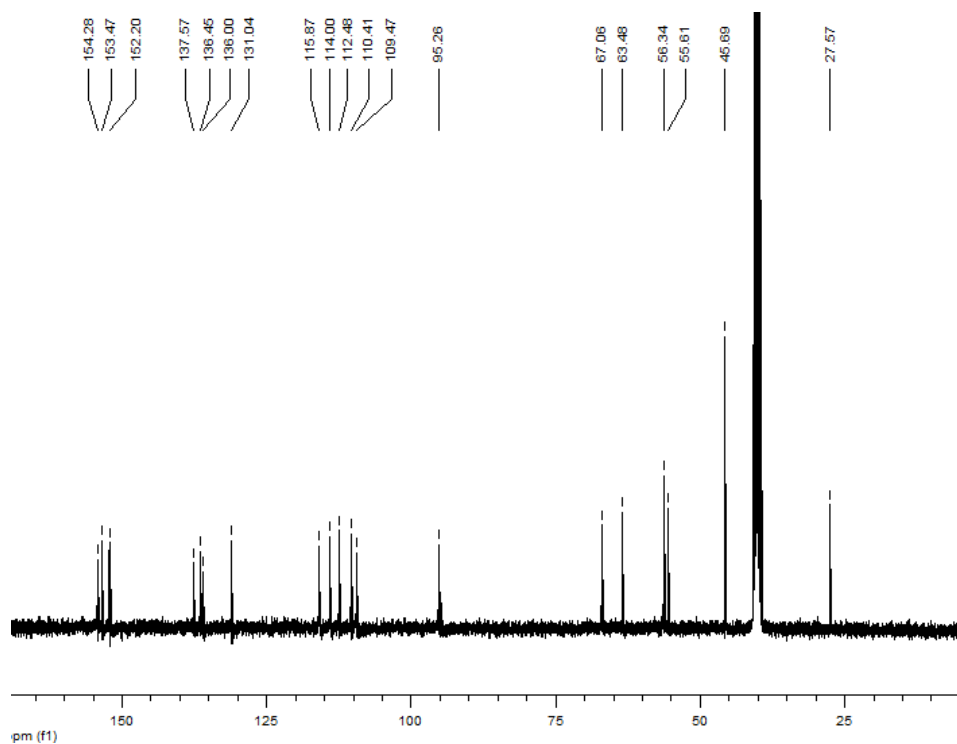


To a 100 ml round bottom flask was added *N*-(1-(3-(dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**4gb**) (432 mg, 0.94 mmol) and 1N HCl aq (50 ml). The reaction was stirred and heated to reflux for 21 hr, then cooled to RT and extracted with saturated NaHCO₃ aq (100 ml) and CHCl₃-EtOH (2 : 1, 100 ml). The aqueous layer was extracted once more with CHCl₃-EtOH (2 : 1, 100 ml). The combined organic layer was dried over Na₂SO₄. After filtration and concentration, the crude was purified via flash column chromatography (DCM – MeOH : 80 % - 20 %) to yield yellow oil product (90.7 mg, 27 % yield). ¹H NMR (400 MHz, DMSO-*d*₆): δ 7.39 (t, *J* = 9 Hz, 1H), 7.07 (d, *J* = 9 Hz, 1H), 6.82 (dd, *J*₁ = 9 Hz, *J*₂ = 2 Hz, 1H), 6.66 (t, *J* = 2 Hz, 2H), 6.59 (dd, *J*₁ = 9 Hz, *J*₂ = 2 Hz, 1H), 6.43 (d, *J* = 2 Hz, 1H), 5.98 (s, 2H), 3.86 (t, *J* = 6 Hz, 2H), 2.94 (s, 6H), 2.34 (t, *J* = 7 Hz, 2H), 2.11 (s, 6H), 1.80 (p, *J* = 7 Hz, 2H). ¹³C NMR (400 MHz, DMSO-*d*₆): δ 154.27, 153.46, 152.19, 137.57, 135.44, 135.99, 131.01, 115.86, 114.00, 112.48, 110.41, 109.46, 95.26, 67.05, 63.47, 56.34, 55.60, 45.69, 27.56.. MS (ESI) calculated exact mass for C₂₀H₂₇N₅O = 353.22. Found [M+H]⁺ = 353.46.

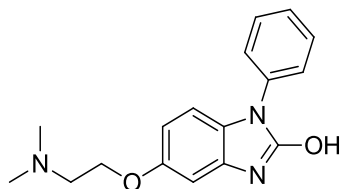
1-(3-dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1*H*-benzo[*d*]imidazol-2-amine (**3g**)
¹H NMR (400 MHz, DMSO-*d*₆)



1-(3-dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1*H*-benzo[*d*]imidazol-2-amine (**3g**)
¹³C NMR (400 MHz, DMSO-*d*₆)

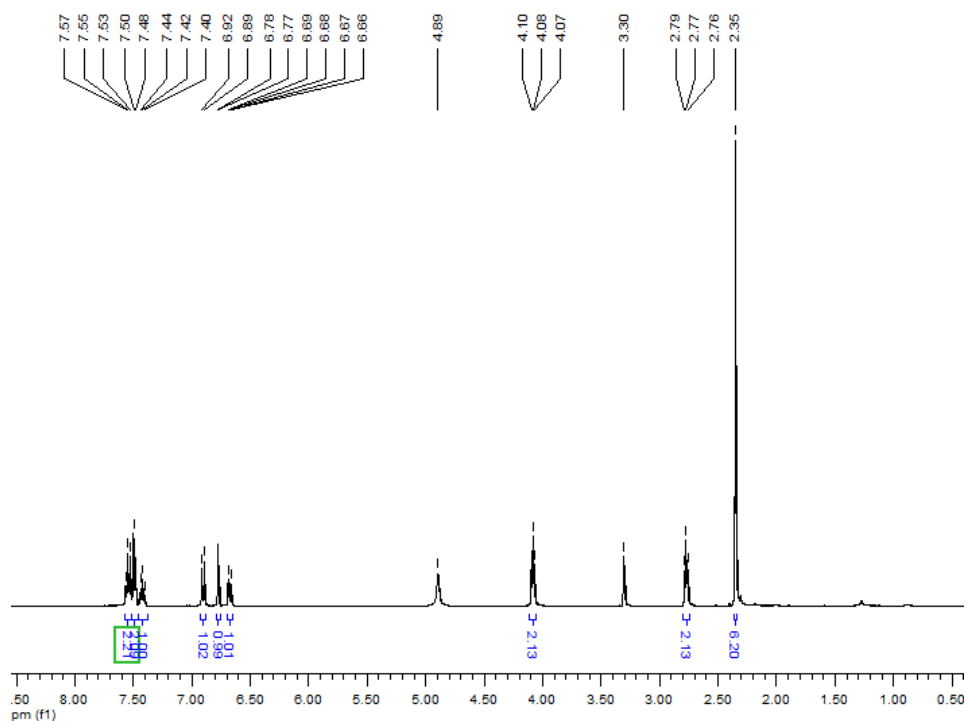


5-(2-(dimethylamino)ethoxy)-1-phenyl-1H-benzo[d]imidazol-2-ol (5b)

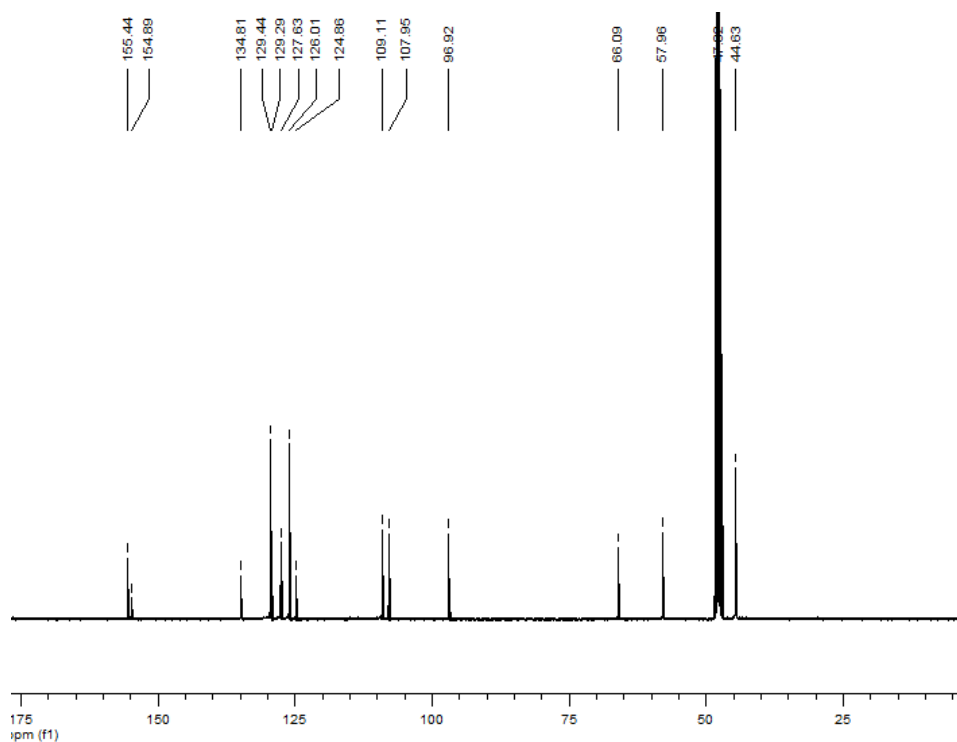


To a 25 ml round bottom flask was added 4-(2-(dimethylamino)ethoxy)-2-nitro-*N*-phenylaniline (**11b**) (56 mg, 0.2 mmol), MeOH (15 ml). The flask was flushed with Ar gas before Pd/C (5 mg, 10 wt %) was added. The reaction was then sealed under Ar and stirred at RT for 26 hr before filtration and concentration. The oil residue obtained was dissolved in DCM (20 ml). While stirred, phosgene (20 % in toluene, 102 μ l, 0.2mmol) was added followed by pyridine (31 μ l, 0.4 mmol). The reaction was stirred at RT for 3 hr, then poured into 20 ml of water and extracted. The DCM layer was collected and the water layer was extracted with 20 ml of DCM. The combined organic layer was washed with brine and dried over Na₂SO₄. After filtration and evaporation of solvent, the crude was purified via flash column chromatography (DCM – MeOH : 60 % - 40 %) to yield oil product (32 mg, 50 % yield). ¹H NMR (400 MHz, CD₃OD): δ 7.57 (t, J = 7 Hz, 2H), 7.50 (d, J = 7 Hz, 2H), 7.44 (t, J = 7 Hz, 1H), 6.92 (d, J = 8 Hz, 1H), 6.78 (d, J = 2 Hz, 1H), 6.69 (dd, J_1 = 8 Hz, J_2 = 2 Hz, 1H), 4.10 (t, J = 5 Hz, 2H), 2.79 (t, J = 5 Hz, 2H), 2.35 (s, 6H). ¹³C NMR (400 MHz, CD₃OD): δ 155.44, 154.89, 134.81, 129.43, 129.28, 127.62, 126.00, 124.86, 109.11, 107.94, 96.92, 66.08, 57.96, 44.62. MS (ESI) calculated exact mass for C₁₇H₁₉N₃O₂ = 297.15. Found [M+H]⁺ = 298.04.

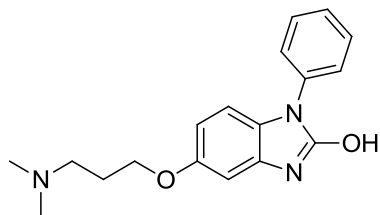
5-(2-(dimethylamino)ethoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-ol (**5b**) ¹H NMR (400 MHz, CD₃OD)



5-(2-(dimethylamino)ethoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-ol (**5b**) ¹³C NMR (400 MHz, CD₃OD)

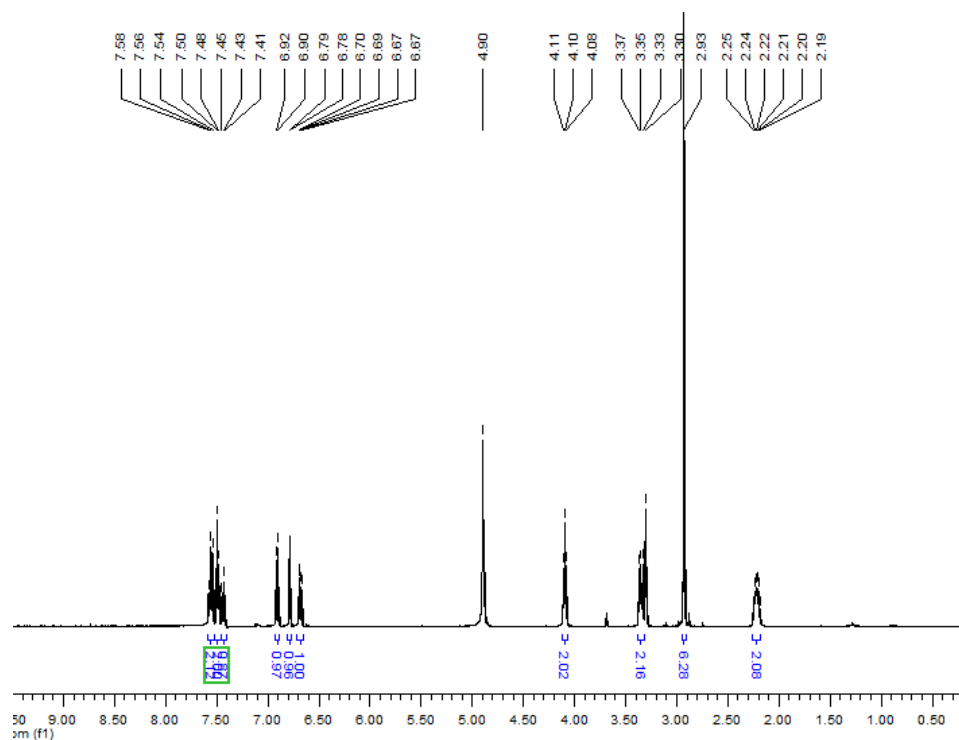


5-(3-(dimethylamino)propoxy)-1-phenyl-1H-benzo[d]imidazol-2-ol (**5c**)

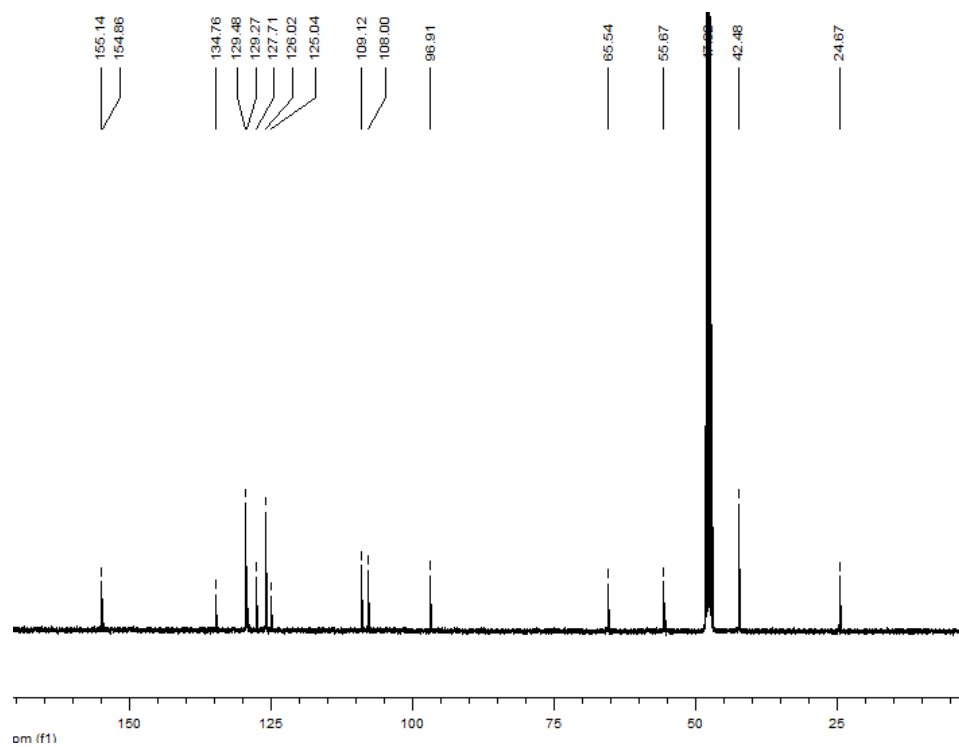


To a 100 ml round-bottom flask was added 4-(3-dimethylamino)propoxy)-2-nitro-*N*-phenylaniline (**11c**) (123 mg, 0.4 mmol) and Methanol (30 ml). The flask was flushed with Ar gas before Pd/C (10 mg, 10 wt %) was added. The reaction was then sealed under H₂ atm and stirred at RT for 1.5 hours before filtration and concentration. The oil residue was dissolved in DCM. Pyridine (63 μ l, 0.8 mmol) and phosgene (214 μ l, 0.4 mmol, 20 wt % solution in toluene) were added. The reaction was stirred at RT for 24 hours before concentrated and purified via flash column (DCM – MeOH : 80 % - 20 %) to yield clear oil product (79 mg, 64 % yield two steps). ¹H NMR (400 MHz, CD₃OD): δ 7.58 (t, J = 8 Hz, 2H), 7.50 (d, J = 9 Hz, 2H), 7.45 (t, J = 7 Hz, 1H), 6.92 (d, J = 6 Hz, 1H), 6.79 (d, J = 2 Hz, 1H), 6.70 (dd, J₁ = 9 Hz, J₂ = 2 Hz, 1H), 4.11 (t, J = 6 Hz, 2H), 3.37 (t, J = 8 Hz, 2H), 2.93 (s, 6H), 2.25 (p, J = 6 Hz, 2H). ¹³C NMR (400 MHz, CD₃OD): δ 155.14, 154.85, 134.76, 129.47, 129.26, 127.70, 126.02, 125.04, 109.11, 107.99, 96.90, 65.53, 55.67, 47.82, 24.67. MS (ESI) calculated exact mass for C₁₈H₂₁N₃O₂ = 311.16. Found [M+H]⁺ = 312.03.

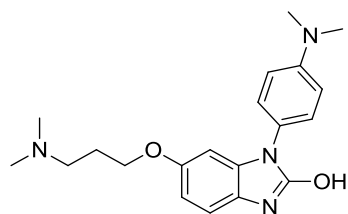
5-(3-(dimethylamino)propoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-ol (**5c**) ¹H NMR (400 MHz, CD₃OD)



5-(3-(dimethylamino)propoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-ol (**5c**) ¹³C NMR (400 MHz, CD₃OD)

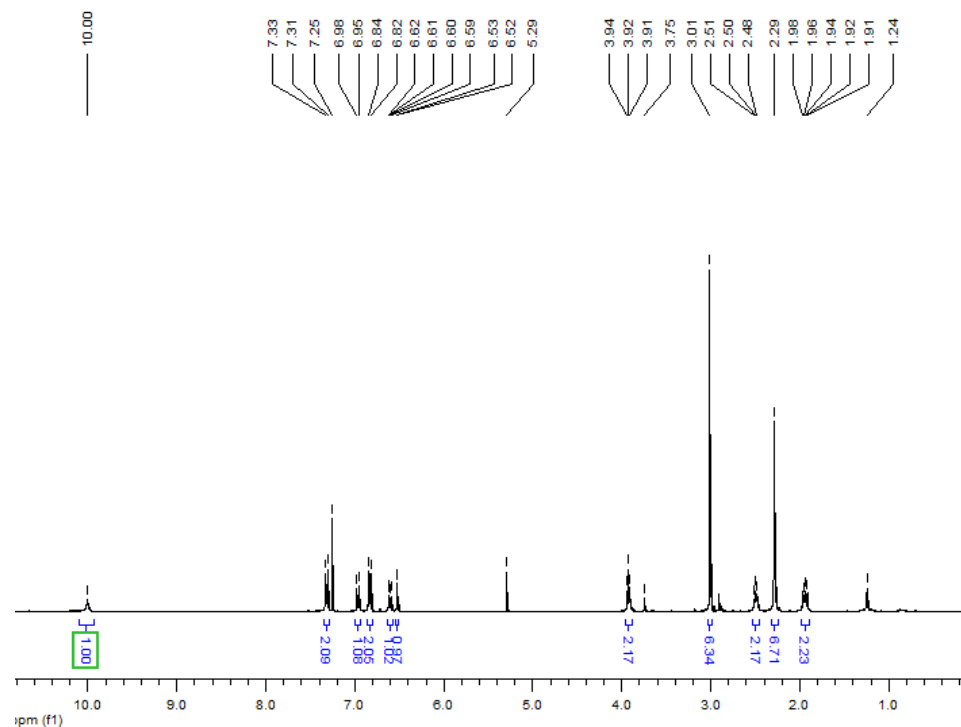


1-(4-(dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1H-benzo[d]imidazol-2-ol (5f)

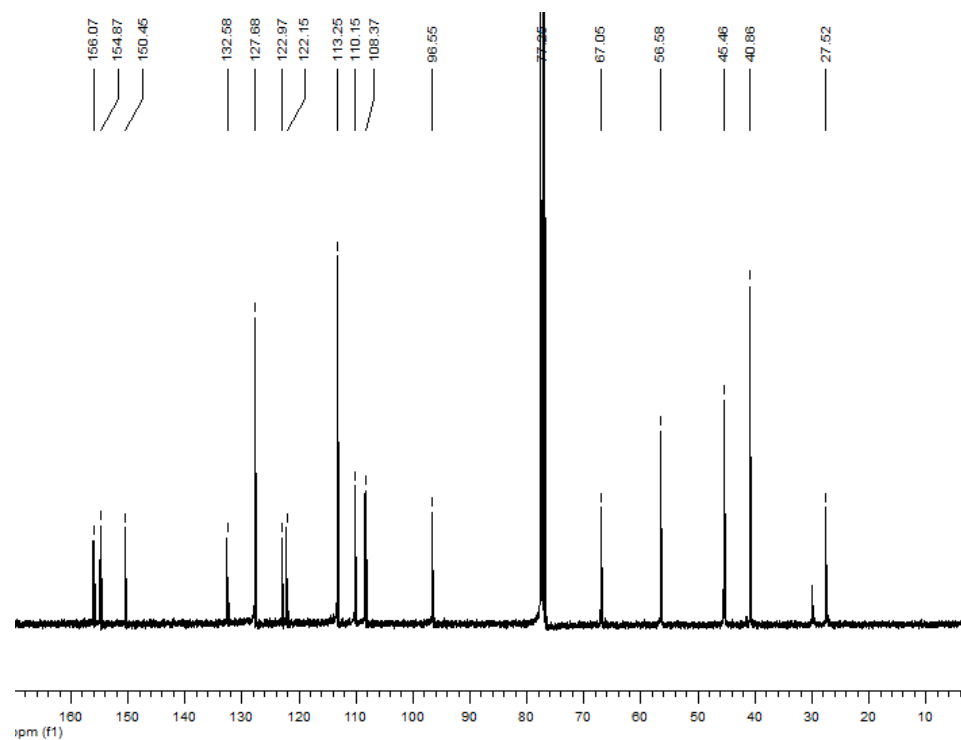


To a 50 ml rb flask was added *N*¹-(5-(3-(dimethylamino)propoxy)-2-nitrophenyl)-*N*⁴,*N*⁴-dimethylbenzene-1,4-diamine (**11f**) (63 mg, 0.17 mmol) and 20 ml of MeOH. The flask was flushed with Ar gas before Pd/C (6 mg, 10 wt %) was added. The reaction was then sealed under H₂ atm and stirred at RT for 1 hour before filtration and concentration. The oil residue was dissolved in DCM (20 ml). Phosgene (96.4 μl, 20 % in toluene, 0.17 mmol) was added followed by pyridine (28 μl, 0.25 mmol). The reaction was stirred at RT for 5 minutes, then poured into water and extracted. The organic layer was collected and washed with brine and Na₂SO₄. After filtration and removal of solvent, the crude was purified via flash column chromatography (DCM – MeOH : 80 % - 20 %) to yield clear oil (26 mg, 43 % yield). ¹H NMR (400 MHz, CDCl₃): δ 10.00 (s, 1H), 7.33 (d, J = 9 Hz, 2H), 6.98 (d, J = 9 Hz, 1H), 6.84 (d, J = 9 Hz, 2H), 6.62 (dd, J₁ = 9 Hz, J₂ = 2 Hz, 1H), 6.53 (d, J = 2 Hz, 1H), 3.94 (t, J = 6 Hz, 2H), 3.01 (s, 6H), 2.51 (t, J = 7 Hz, 2H), 2.29 (s, 6H), 1.98 (m, 2H). ¹³C NMR (400 MHz, CDCl₃): δ 156.06, 154.87, 150.45, 132.57, 127.68, 122.96, 122.14, 113.25, 110.15, 108.37, 96.54, 67.05, 56.58, 45.45, 40.85, 27.52. MS (ESI) calculated exact mass for C₂₇H₃₁N₅O₂ = 354.21. Found [M+H]⁺ = 355.12.

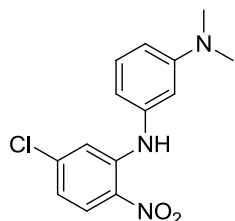
1-(4-(dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1*H*-benzo[*d*]imidazol-2-ol (**5f**) ¹H
NMR (400 MHz, CDCl₃)



1-(4-(dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1*H*-benzo[*d*]imidazol-2-ol (**5f**) ¹³C
NMR (400 MHz, CDCl₃)

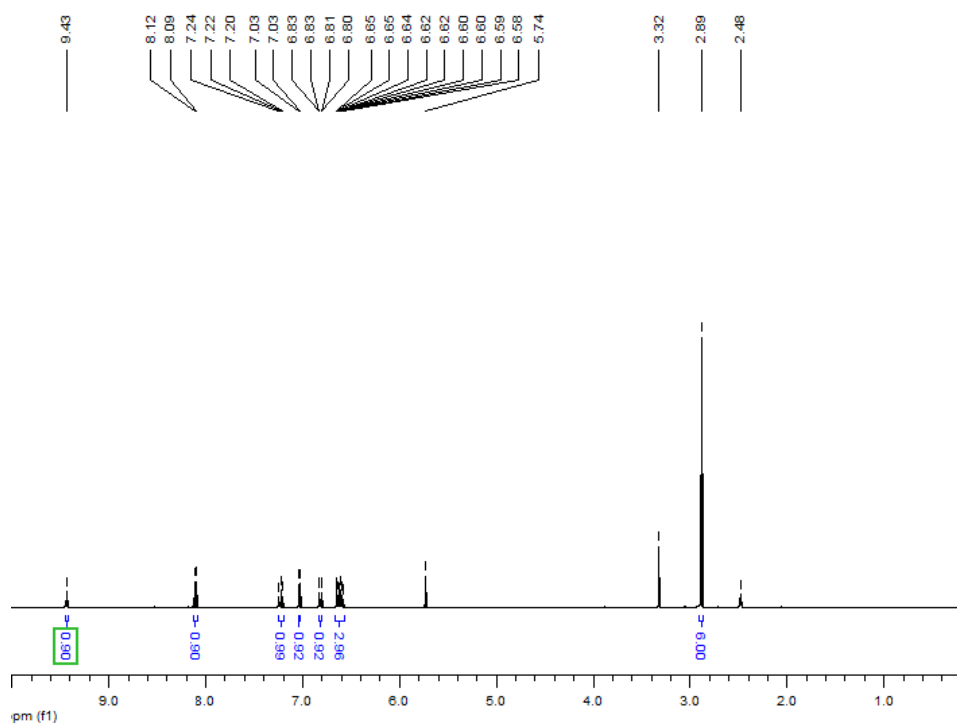


***N*¹-(5-chloro-2-nitrophenyl)-*N*³,*N*³-dimethylbenzene-1,3-diamine (15)**

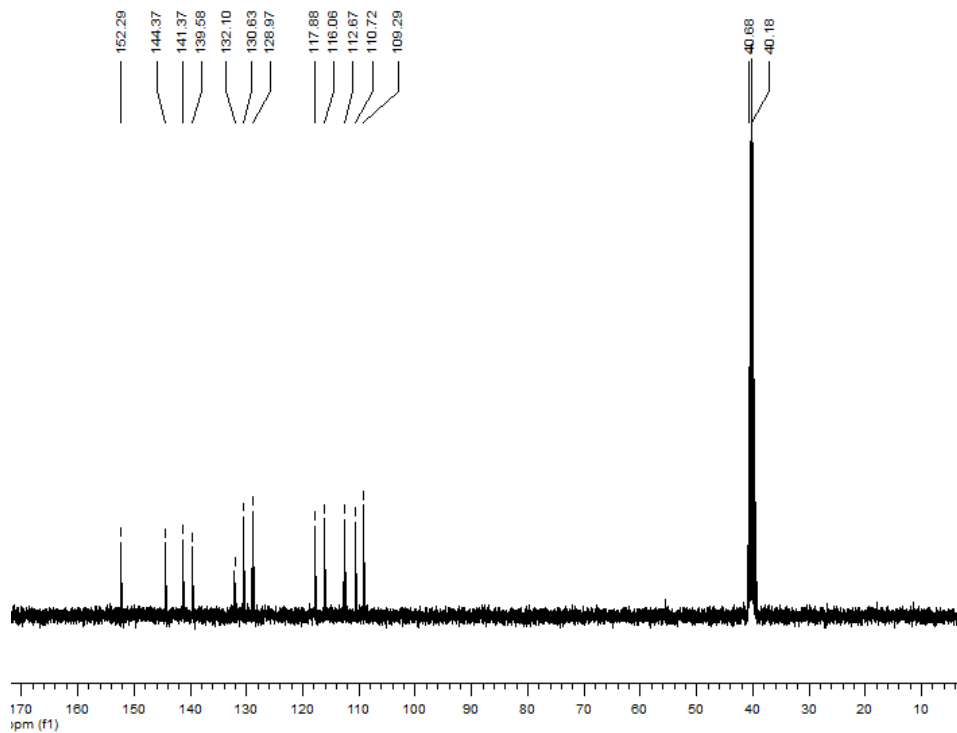


To a 250 ml round-bottom flask was added *N,N*-dimethyl-3-nitroaniline (**14**) (1.2 g, 7.2 mmol), methanol (100 ml). The flask was flushed with Ar gas before Pd/C (120 mg, 10 wt %) was added. The reaction was stirred at RT for 20 hours, then filtered and concentrated to obtain oil product. Toluene (100 ml) was added followed by 2,4-dichloronitrobenzene (**13**) (1.4 g, 7.2 mmol), Pd₂(dba)₃ (330 mg, 0.36 mmol, 5 mol %), *rac*-BINAP (337 mg, 0.54 mmol, 7.5 mol %), and Cs₂CO₃ (2.3 g, 7.2 mmol). The reaction was stirred and heated to reflux under Ar for 21 hours, then cooled to RT, filtered and extracted with water (twice, 150 ml ea.) The organic layer was collected and washed with brine and dried over Na₂SO₄. After filtration and concentration, the crude was purified via flash column (Hexane : EtOAc – 80 % - 20 %) to yield red oil product (900 mg, 43 % two steps). ¹H NMR (400 MHz, DMSO-d₆) δ: 9.43 (s, 1H), 8.12 (d, *J* = 9 Hz, 1H), 7.24 (t, *J* = 8 Hz, 1H), 7.03 (d, *J* = 2 Hz, 1H), 6.83 (dd, *J*₁ = 9 Hz, *J*₂ = 2 Hz, 1H), 6.65-6.58 (m, 3H), 2.89 (s, 6H). ¹³C NMR (400 MHz, DMSO-d₆) δ: 152.28, 144.36, 141.37, 139.58, 132.09, 130.62, 128.97, 117.88, 116.06, 112.66, 110.72, 109.28, 40.67. MS (ESI) calculated exact mass for C₁₄H₁₄ClN₃O₂ = 291.08. Found [M+H]⁺ = 292.0.

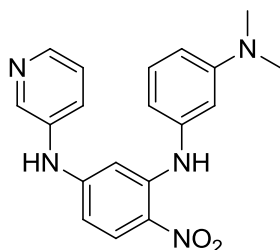
N^1 -(5-chloro-2-nitrophenyl)- N^3,N^3 -dimethylbenzene-1,3-diamine (**15**) ^1H NMR (400 MHz, DMSO- d_6)



N^1 -(5-chloro-2-nitrophenyl)- N^3,N^3 -dimethylbenzene-1,3-diamine (**15**) ^{13}C NMR (400 MHz, DMSO- d_6)

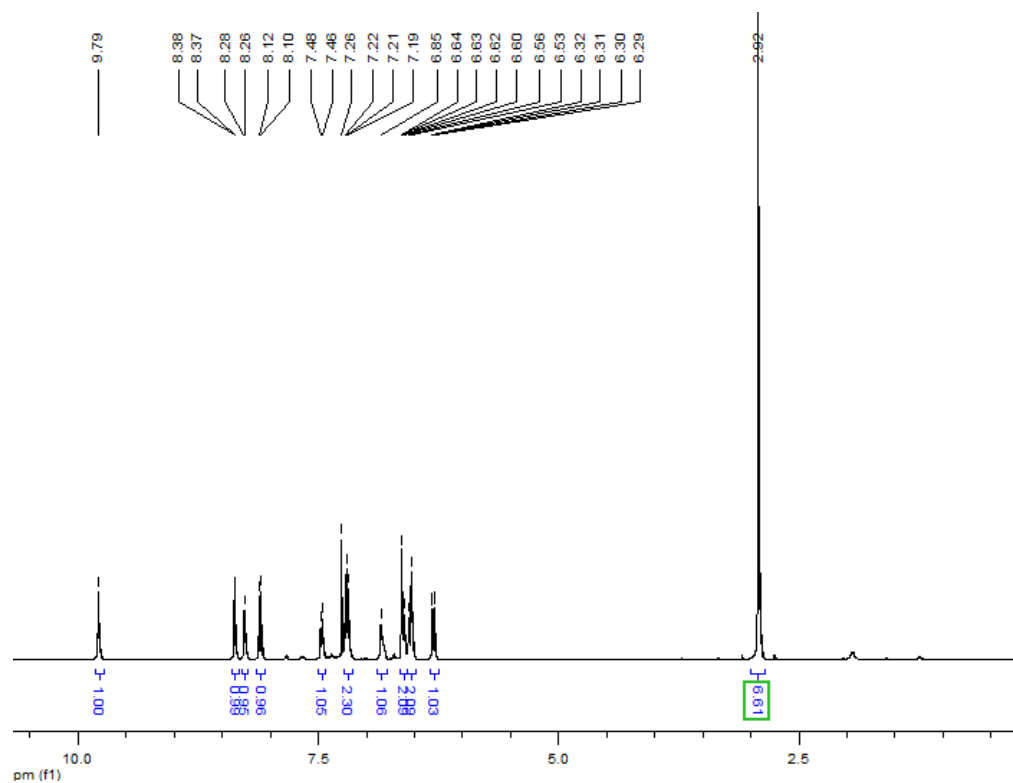


***N*¹,*N*¹-dimethyl-*N*³-(2-nitro-5-(pyridin-3-ylamino)phenyl)benzene-1,3-diamine (17h)**

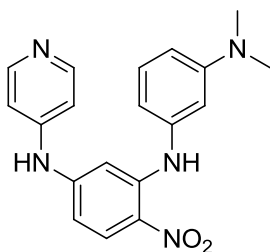


To a 250 ml round-bottom flask was added *N*¹-(5-chloro-2-nitrophenyl)-*N*³,*N*³-dimethylbenzene-1,3-diamine (**15**) (1.47 g, 5.04 mmol), dioxane (100 ml), 3-aminopyridine (569 mg, 6.05 mmol, 1.2 eq), Pd₂(dba)₃ (229 mg, 0.25 mmol, 5 mol %), *rac*-BINAP (235 mg, 0.38 mmol, 7.5 mol %), and Cs₂CO₃ (1.59 g, 5.04 mmol). The reaction was stirred and heated to reflux under Ar for 21 hours, then cooled to RT, filtered and concentrated. The oil residue was extracted with chloroform and water (150 ml ea). The organic layer was collected and extracted with water (150ml), washed with brine and dried over Na₂SO₄. After filtration and concentration, the oil crude was purified via flash column chromatography (DCM – MeOH : 90 % – 10 %) to yield red oil product (757 mg, 43 % yield). ¹H NMR (400 MHz, CDCl₃) δ: 9.79 (s, 1H), 8.38 (d, *J* = 2 Hz, 1H), 8.28 (d, *J* = 6 Hz, 1H), 8.12 (d, *J* = 9 Hz, 1H), 7.48 (d, *J* = 8 Hz, 1H), 7.22 (t, *J* = 5 Hz, 2H), 6.85 (s, 1H), 6.64 – 6.53 (m, 4H), 6.32 (dd, *J*₁ = 9 Hz, *J*₂ = 2 Hz, 1H), 2.92 (s, 6H). MS (ESI) calculated exact mass for C₁₉H₁₉N₅O₂ = 349.15. Found [M+H]⁺ = 350.3.

N^1,N^1 -dimethyl- N^3 -(2-nitro-5-(pyridin-3-ylamino)phenyl)benzene-1,3-diamine (**17h**) ^1H NMR
(400 MHz, CDCl_3)

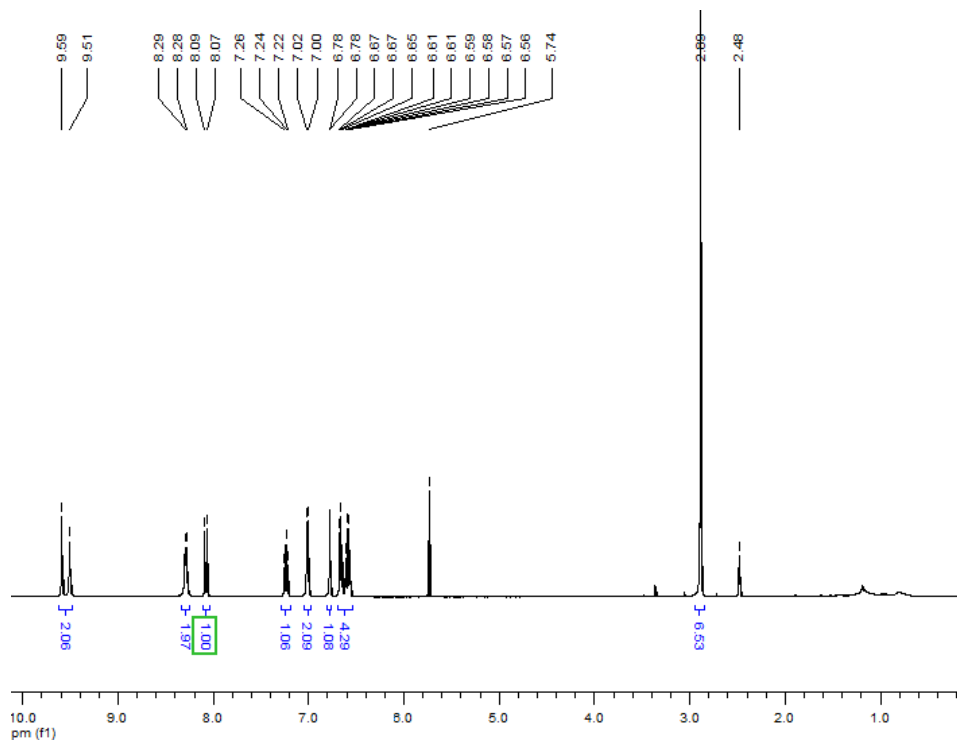


***N*¹,*N*¹-dimethyl-*N*³-(2-nitro-5-(pyridin-4-ylamino)phenyl)benzene-1,3-diamine (17i)**

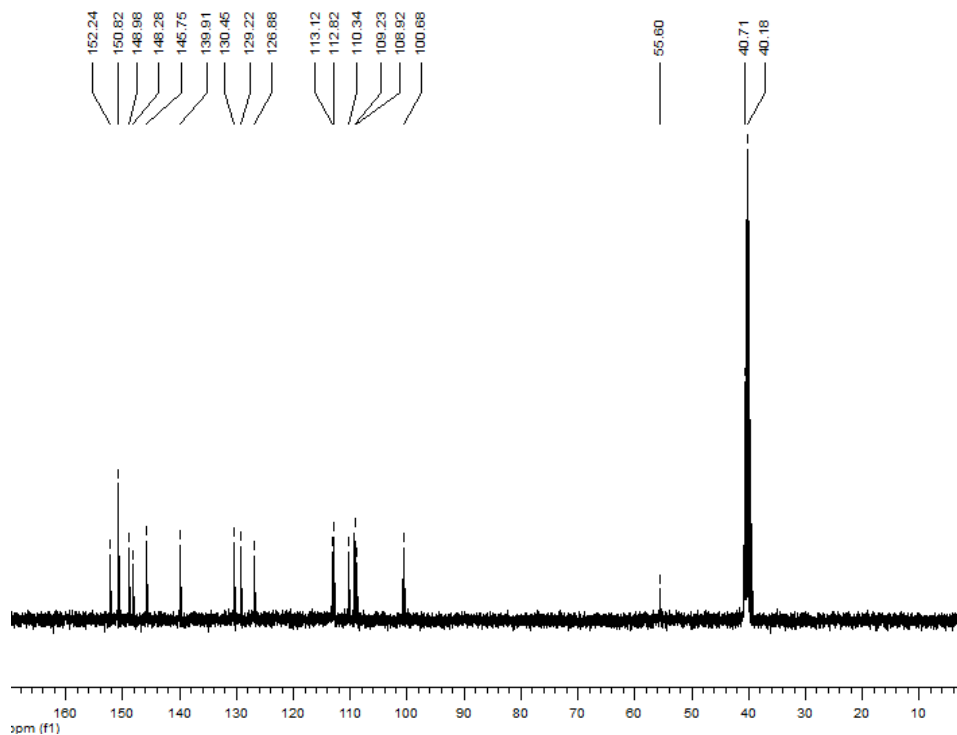


To a 250 ml round-bottom flask was added *N*¹-(5-chloro-2-nitrophenyl)-*N*³,*N*³-dimethylbenzene-1,3-diamine (944 mg, 3.24 mmol), dioxane (100 ml), 4-aminopyridine (335 mg, 3.56 mmol, 1.1 eq), Pd₂(dba)₃ (148 mg, 0.16 mmol, 5 mol %), *rac*-BINAP (151 mg, 0.24 mmol, 7.5 mol %), and Cs₂CO₃ (1.02 g, 3.24 mmol). The reaction was stirred and heated to reflux under Ar for 44 hours, then cooled to RT, filtered and concentrated. The oil residue was extracted with chloroform and water (150 ml ea). The organic layer was collected and extracted with water (150ml), washed with brine and dried over Na₂SO₄. After filtration and concentration, the oil crude was purified via flash column chromatography (DCM – MeOH : 95 % – 5 %) to yield red oil product (390 mg, 34 % yield). ¹H NMR (400 MHz, DMSO-d₆) δ: 9.59 (s, 1H), 9.51 (s, 1H), 8.29 (d, *J* = 4 Hz, 2H), 8.09 (d, *J* = 9 Hz, 1H), 7.26 (t, *J* = 8 Hz, 1H), 7.02 (d, *J* = 6 Hz, 2H), 6.78 (d, *J* = 2Hz, 1H), 6.67 – 6.56 (m, 4H), 2.89 (s, 6H). ¹³C NMR (400 MHz, DMSO-d₆) δ: 152.24, 150.82, 148.98, 148.28, 145.75, 139.90, 130.45, 129.21, 126.87, 113.11, 112.82, 110.34, 109.23, 108.91, 100.68, 40.70. MS (ESI) calculated exact mass for C₁₉H₁₉N₅O₂ = 349.15. Found [M+H]⁺ = 350.3.

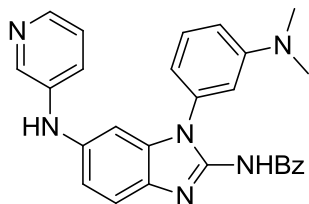
N^1,N^1 -dimethyl- N^3 -(2-nitro-5-(pyridin-4-ylamino)phenyl)benzene-1,3-diamine (**17i**) ^1H NMR (400 MHz, DMSO- d_6)



N^1,N^1 -dimethyl- N^3 -(2-nitro-5-(pyridin-4-ylamino)phenyl)benzene-1,3-diamine (**17i**) ^{13}C NMR (400 MHz, DMSO- d_6)

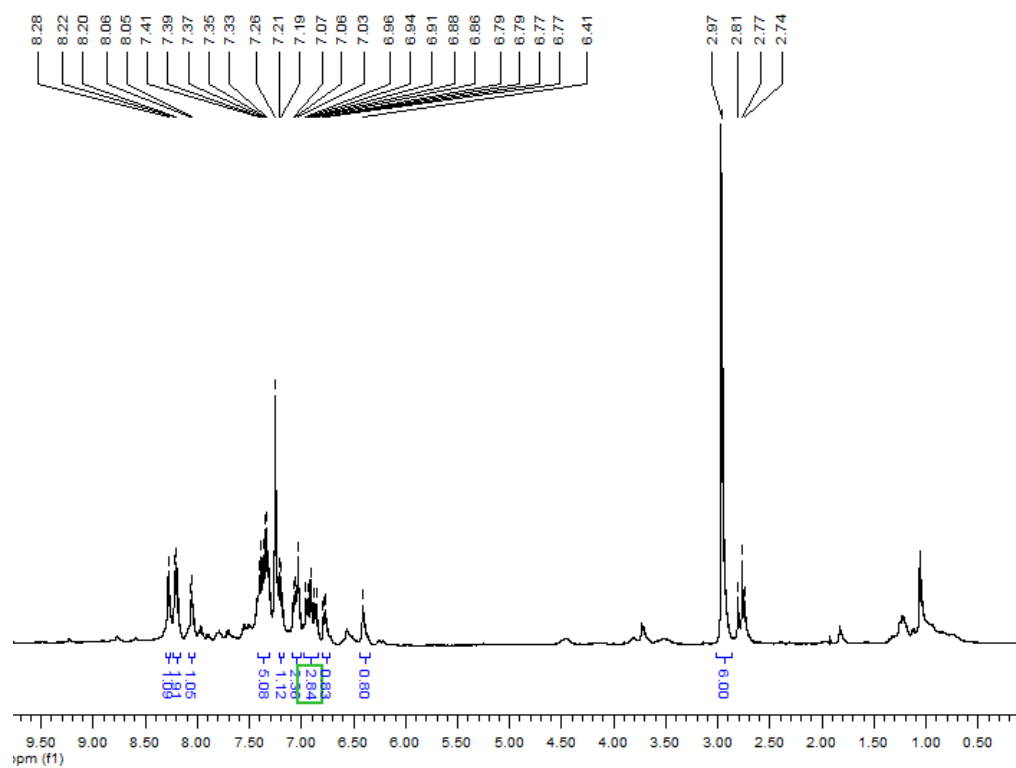


***N*-(1-(3-isopropylphenyl)-6-(pyridin-3-ylamino)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (18h)**

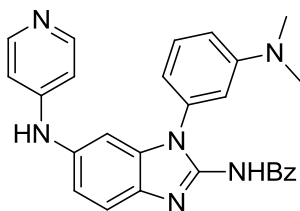


To a 250 ml round bottom flask was added *N*¹,*N*¹-dimethyl-*N*³-(2-nitro-5-(pyridin-3-ylamino)phenyl)benzene-1,3-diamine (**17h**) (757 mg, 2.17 mmol) and methanol (100 ml). The flask was flushed with Ar gas before Pd/C (75 mg, 10 wt%) was added. The reaction was stirred at RT under H₂ atm for 23 hours before filtration and concentration. The oil residue was dissolved in ACN (200 ml) and benzoyl isothiocyanate (322 μl, 2.17 mmol) was added via syringe. The reaction was stirred at RT for 9 hours when DIPC (338 μl, 2.17 mmol) and K₂CO₃ (300 mg, 2.17 mmol) were added. The reaction was stirred at RT for 24 hours before filtration, concentration and purification via flash column (DCM – MeOH : 90 % - 10 %) to yield yellow oil product (312 mg, 32 % yield). ¹H NMR (400 MHz, CDCl₃) δ: 8.28 (s, 1H), 8.22 (d, *J* = 7 Hz, 2H), 8.06 (d, *J* = 4 Hz, 1H), 7.41 – 7.33 (m, 5H), 7.21 (d, *J* = 8 Hz, 1H), 7.07 (m, 2H), 6.96 (m, 3H), 6.79 (dd, *J*₁ = 8 Hz, *J*₂ = 2 Hz, 1H), 6.41 (s, 1H), 2.97 (s, 6H). MS (ESI) calculated exact mass for C₂₈H₂₅N₅O = 448.20. Found [M+H]⁺ = 449.3.

N-(1-(3-isopropylphenyl)-6-(pyridin-3-ylamino)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**18h**) ¹H
NMR (400 MHz, CDCl₃)

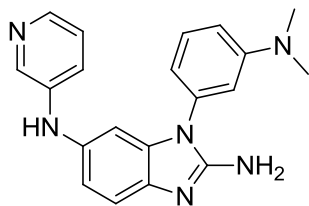


***N*-1-(3-(dimethylamino)phenyl)-6-(pyridin-4-ylamino)-1*H*-benzo[d]imidazol-2-yl)benzamide (18i)**



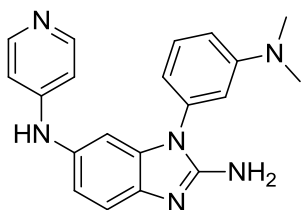
To a 250 ml round bottom flask was added *N*¹,*N*¹-dimethyl-*N*³-(2-nitro-5-(pyridin-4-ylamino)phenyl)benzene-1,3-diamine (**17i**) (390 mg, 1.12 mmol) and methanol (100 ml). The flask was flushed with Ar gas before Pd/C (40 mg, 10 wt%) was added. The reaction was stirred at RT under H₂ atm for 22 hours before filtration and concentration. The oil residue was dissolved in ACN (200 ml) and benzoyl isothiocyanate (166 μl, 1.12 mmol) was added via syringe. The reaction was stirred at RT for 20 hours when DIPC (174 μl, 1.12 mmol) and K₂CO₃ (155 mg, 1.12 mmol) were added. The reaction was stirred at RT for 24 hours before filtration, concentration and purification via flash column (DCM – MeOH : 90 % - 10 %) to yield yellow viscous oil product (108 mg, 22 % yield). ¹H NMR (400 MHz, CD₃OD) δ: 8.07 (d, J = 5 Hz, 2H), 8.01 (d, J = 7 Hz, 2H), 7.62 (d, J = 8 Hz, 1H), 7.48 (t, J = 7 Hz, 1H), 7.37 (m, 3H), 7.21 (d, J = 8 Hz, 1H), 7.12 (s, 1H), 6.95 (d, J = 5 Hz, 2H), 6.89 (s, 1H), 6.86 (m, 2H), 2.94 (s, 6H). MS (ESI) calculated exact mass for C₂₈H₂₅N₅O = 448.20. Found [M+H]⁺ = 449.3.

1-(3-(dimethylamino)phenyl)-*N*⁶-(pyridin-3-yl)-1*H*-benzo[*d*]imidazole-2,6-diamine (3h)



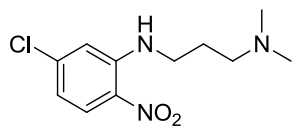
To a 100 ml round bottom flask was added *N*-(1-(3-(dimethylamino)phenyl)-6-(pyridin-3-ylamino)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**18h**) (312 mg, 0.69 mmol) and 1N HCl aq (50 ml). The reaction was heated to reflux while stirred for 24 hours, then cooled to RT and extracted with saturated NaHCO₃ aq and chloroform-EtOH 2:1 (100 ml and 3 x 100 ml). The organic layers were collected and combined and dried over Na₂SO₄. After filtration and concentration the crude was purified via flash column chromatography (DCM – MeOH : 80 % - 20 %) to yield slight brown/yellow oil (92 mg, 39 % yield). ¹H NMR (400 MHz, CD₃OD) δ: 8.12 (d, *J* = 2 Hz, 1H), 7.82 (dd, *J*₁ = 5 Hz, *J*₂ = 1 Hz, 1H), 7.42 (t, *J* = 8 Hz, 1H), 7.33 (m, 1H), 7.25 (d, *J* = 8 Hz, 1H), 7.15 (dd, *J*₁ = 8 Hz, *J*₂ = 5 Hz, 1H), 6.94 (dd, *J*₁ = 8 Hz, *J*₂ = 2 Hz, 1H), 6.88 (dd, *J*₁ = 8 Hz, *J*₂ = 2 Hz, 1H), 6.77 (d, *J* = 2 Hz, 1H), 6.75 (t, *J* = 2Hz, 1H), 6.72 (d, *J* = 8 Hz, 1H), 2.97 (s, 6H). ¹³C NMR (400 MHz, CD₃OD) δ: 154.33, 152.35, 143.56, 138.05, 137.38, 136.38, 135.57, 135.39, 135.04, 130.55, 124.21, 121.11, 115.85, 115.20, 113.66, 112.69, 110.00, 101.69, 39.40. MS (ESI) calculated exact mass for C₂₀H₂₀N₆ = 344.17. Found [M+H]⁺ = 345.2.

1-(3-(dimethylamino)phenyl)-*N*⁶-(pyridin-4-yl)-1*H*-benzo[*d*]imidazole-2,6-diamine (3i)



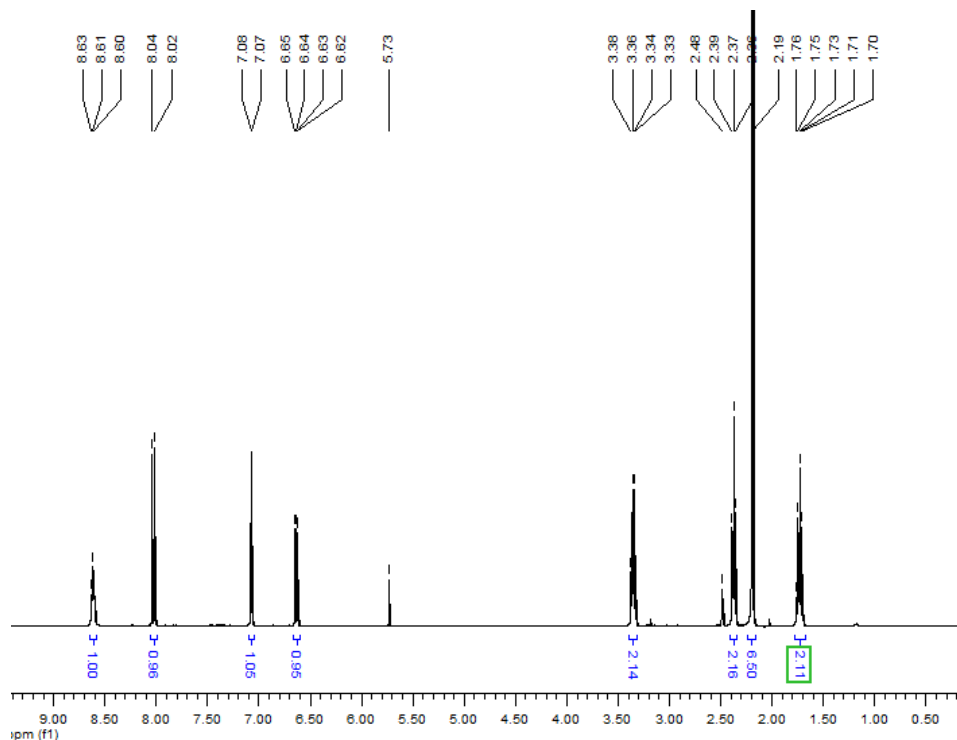
To a 100 ml round bottom flask was added *N*-(1-(3-(dimethylamino)phenyl)-6-(pyridin-4-ylamino)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**18i**) (108 mg, 0.24 mmol) and 1N HCl aq (50 ml). The reaction was heated to reflux while stirred for 28 hours before cooling to RT and extraction with saturated NaHCO₃ aq and chloroform-EtOH 2:1 (100 ml and 3 x 100 ml). The organic layers were collected and combined and dried over Na₂SO₄. After filtration and concentration the crude was purified via flash column chromatography (DCM – MeOH : 80 % - 20 %) to yield slight yellow oil (22 mg, 27 % yield). ¹H NMR (400 MHz, CD₃OD) δ: 7.99 (d, J = 5Hz, 2H), 7.43 (t, J = 8 Hz, 1H), 7.30 (d, J = 8 Hz, 1H), 6.98 (d, J = 8 Hz, 1H), 6.89 (d, J = 8 Hz, 1H), 6.80 (s, 1H), 6.78 – 6.71 (m, 4H), 2.98 (s, 6H). ¹³C NMR (400 MHz, CD₃OD) δ: 154.99, 154.33, 152.37, 147.33, 139.35, 135.60, 135.34, 132.09, 130.59, 117.76, 115.24, 113.63, 112.75, 109.96, 108.31, 104.03, 39.39. MS (ESI) calculated exact mass for C₂₀H₂₀N₆ = 344.17. Found [M+H]⁺ = 345.2.

***N*^l-(5-chloro-2-nitrophenyl)-*N*³,*N*³-dimethylpropane-1,3-diamine (20h)**

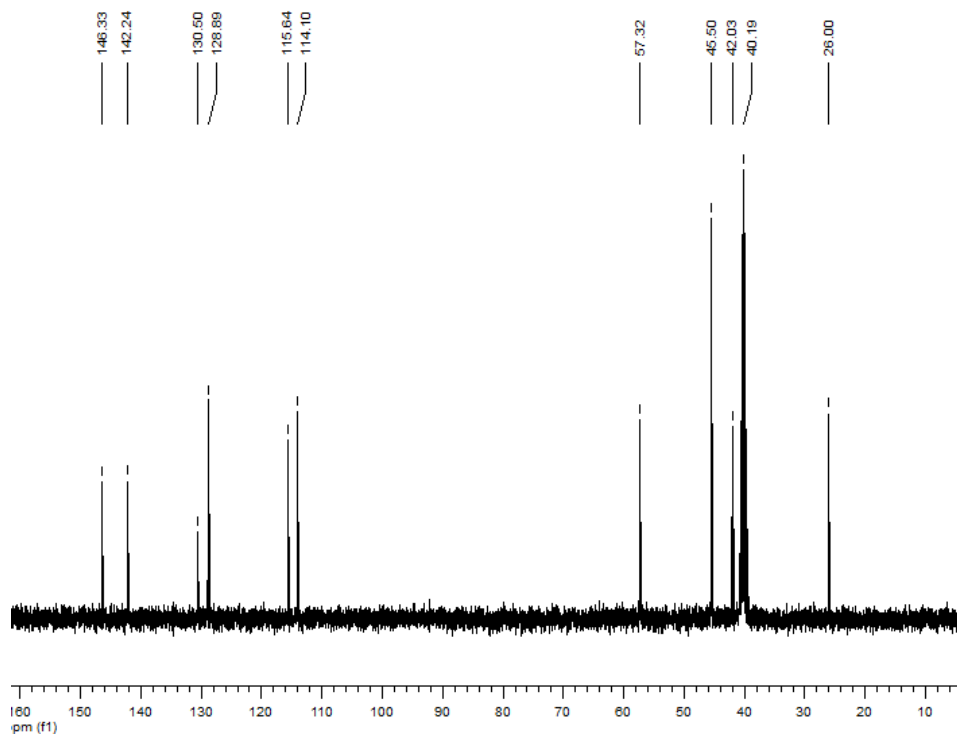


Into a 250 ml round-bottom flask was added 2,4-dichloronitrobenzene (4.0 g, 20.8 mmol), ACN (100 ml) and *N*^l,*N*^l-dimethyl-1,3-propanediamine (**19**) (2.6 ml, 21.0 mmol), and K₂CO₃ (2.9 g, 21.0 mmol). The reaction was stirred and heated to reflux for 24 hours before cooling to RT. It was filtered, concentrated and extracted with DCM (150 ml) and water (150 ml x 2). The organic layer was washed with brine and dried over Na₂SO₄. After filtration and evaporation of solvent *in vacuo*, the oil crude was purified via flash column (DCM – MeOH : 90 % - 10 %) to yield orange color oil product (5.2 g, 97 % yield). ¹H NMR (400 MHz, DMSO-d₆) δ: 8.61 (t, *J* = 5 Hz, 1H), 8.04 (d, *J* = 9 Hz, 1H), 7.08 (d, *J* = 2 Hz, 1H), 6.65 (dd, *J*₁ = 9 Hz, *J*₂ = 2 Hz, 1H), 3.38 (q, *J* = 5 Hz, 2H), 2.39 (t, *J* = 6 Hz, 2H), 2.19 (s, 6H), 1.76 (p, *J* = 6 Hz, 2H). ¹³C NMR (400 MHz, DMSO-d₆) δ: 146.33, 142.24, 130.49, 128.88, 115.64, 114.09, 57.32, 45.50, 42.03, 26.00. MS (ESI) calculated exact mass for C₁₁H₁₆ClN₃O₂ = 257.09. Found [M+H]⁺ = 258.0.

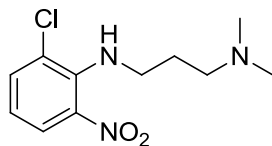
N^1 -(5-chloro-2-nitrophenyl)- N^3,N^3 -dimethylpropane-1,3-diamine (**20h**) ^1H NMR (400 MHz, DMSO- d_6)



N^1 -(5-chloro-2-nitrophenyl)- N^3,N^3 -dimethylpropane-1,3-diamine (**20h**) ^{13}C NMR (400 MHz, DMSO- d_6)

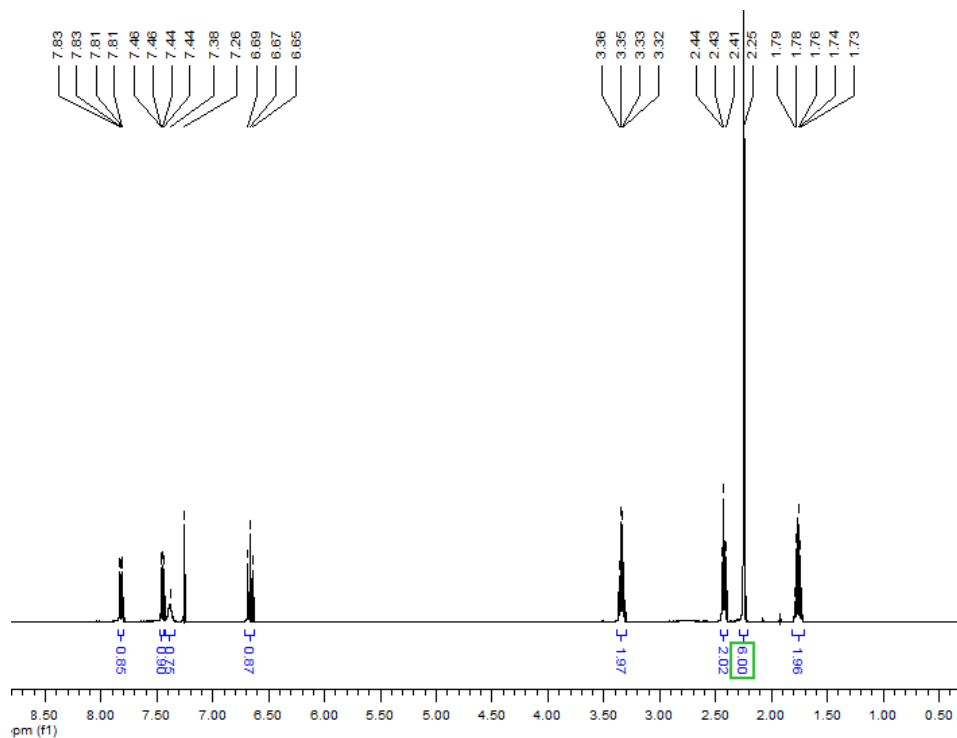


***N*¹-(2-chloro-6-nitrophenyl)-*N*³,*N*³-dimethylpropane-1,3-diamine (20j)**

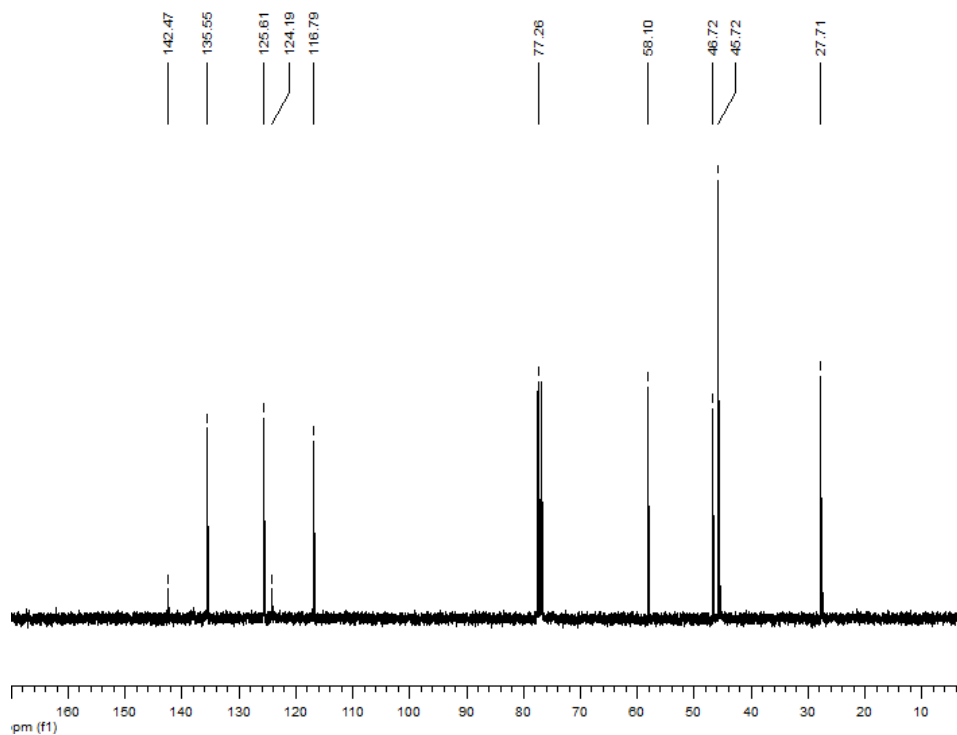


To a 250 ml round bottom flask was added 1,2-dichloro-3-nitrobenzene (7.0 g, 36.5 mmol), ACN (120 ml), *N,N*-dimethyl-1,3-propanediamine (**19**) (4.5 ml, 37.0 mmol), and K₂CO₃ (5.1 g, 37.0 mmol). The reaction was stirred and heated to reflux under Ar atmosphere for 16 hours before cooling to RT. It was filtered and concentrated before purification via flash column chromatography (DCM – MeOH : 95 % - 5 %) to yield yellow oil product (7.98 g, 96 % yield). ¹H NMR (400 MHz, CDCl₃) δ: 7.83 (dd, *J*₁ = 9 Hz, *J*₂ = 2 Hz, 1H), 7.46 (dd, *J*₁ = 8 Hz, *J*₂ = 2 Hz, 1H), 7.38 (s, broad, 1H), 6.69 (t, *J* = 8 Hz, 1H), 3.36 (q, *J* = 5 Hz, 2H), 2.44 (t, *J* = 6 Hz, 2H), 2.26 (s, 6H), 1.79 (p, *J* = 6 Hz, 2H). ¹³C NMR (400 MHz, CDCl₃) δ: 142.46, 135.54, 125.60, 124.19, 116.79, 58.09, 46.71, 45.72, 27.71. MS (ESI) calculated exact mass for C₁₁H₁₆ClN₃O₂ = 257.09. Found [M+H]⁺ = 258.1.

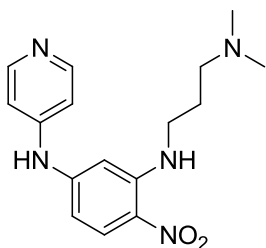
N^1 -(2-chloro-6-nitrophenyl)- N^3,N^3 -dimethylpropane-1,3-diamine (**20j**) ^1H NMR (400 MHz, CDCl_3)



N^1 -(2-chloro-6-nitrophenyl)- N^3,N^3 -dimethylpropane-1,3-diamine (**20j**) ^{13}C NMR (400 MHz, CDCl_3)

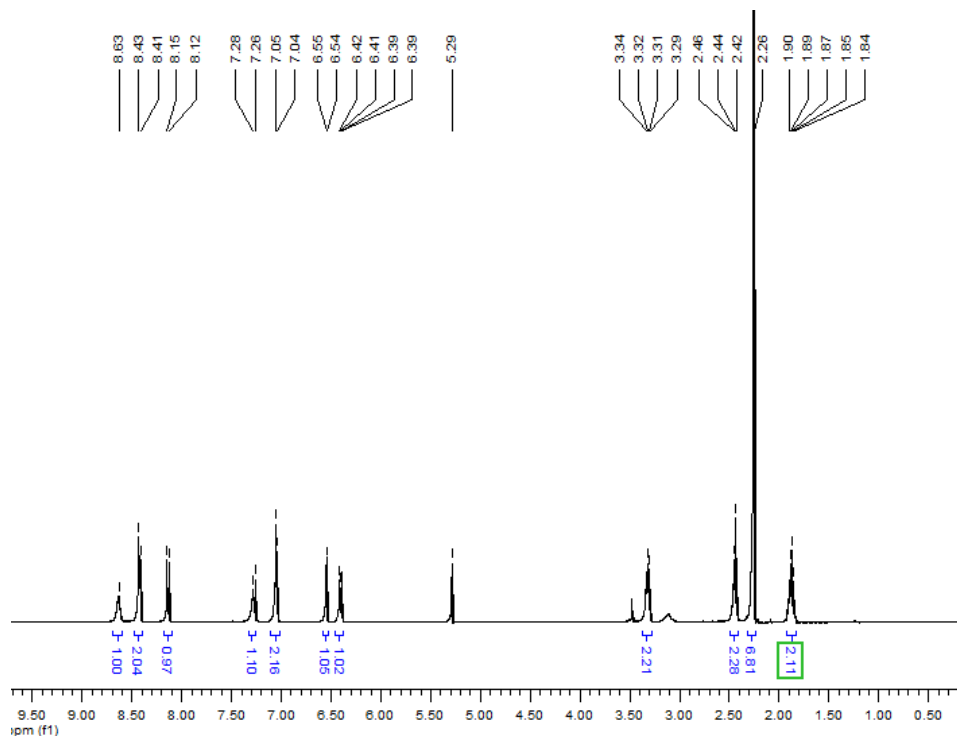


***N*³-(3-(dimethylamino)propyl)-4-nitro-*N*¹-(pyridin-4-yl)benzene-1,3-diamine (22i)**

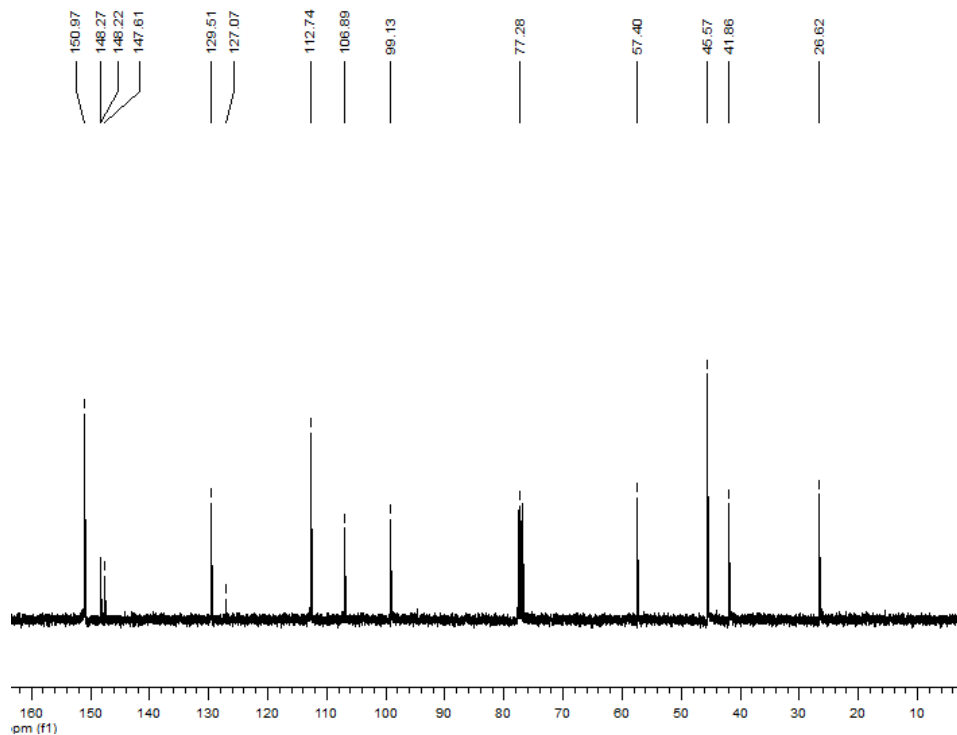


Into a 100 ml round-bottom flask was added *N*¹-(5-chloro-2-nitrophenyl)-*N*³,*N*³-dimethylpropane-1,3-diamine (**20h**) (934 mg, 3.6 mmol), 2-aminopyridine (245 mg, 3.95 mmol), dioxane (50 ml), Pd₂(dba)₃ (166 mg, 0.18 mmol, 5 mol %), rac-BINAP (170 mg, 0.27 mmol, 7.5 mol %), Cs₂CO₃ (1.1 g, 3.6 mmol). The reaction was stirred and heated to reflux under Ar for 20 hours before cooling to RT. It was filtered, concentrated and purified via flash column (DCM – MeOH : 90 % -10 %) to yield yellow oil product (908 mg, 80 % yield). ¹H NMR (400 MHz, CDCl₃) δ: 8.63 (s, 1H), 8.43 (d, *J* = 6Hz, 2H), 8.15 (d, *J* = 9 Hz, 1H), 7.28 (s, 1H), 7.05 (d, *J* = 6 Hz, 2H), 6.55 (d, *J* = 2 Hz, 1H), 6.42 (dd, *J*₁ = 9 hz, *J*₂ = 2Hz, 1H), 3.34 (p, *J* = 5 Hz, 2H), 2.46 (t, *J* = 7 Hz, 2H), 2.25 (s, 6H), 1.90 (p, *J* = 7 Hz, 2H). ¹³C NMR (400 MHz, CDCl₃) δ: 150.96, 148.27, 148.21, 147.61, 129.50, 127.06, 112.73, 106.89, 99.12, 57.40, 45.57, 41.86, 26.62. MS (ESI) calculated exact mass for C₁₆H₂₁N₅O₂ = 315.17. Found [M+H]⁺ = 316.2.

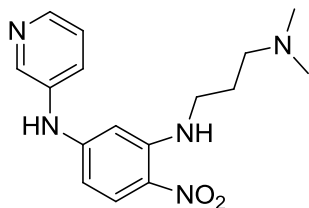
N^3 -(3-(dimethylamino)propyl)-4-nitro- N^1 -(pyridin-4-yl)benzene-1,3-diamine (**22i**) ^1H NMR (400 MHz, CDCl_3)



N^3 -(3-(dimethylamino)propyl)-4-nitro- N^1 -(pyridin-4-yl)benzene-1,3-diamine (**22i**) ^{13}C NMR (400 MHz, CDCl_3)

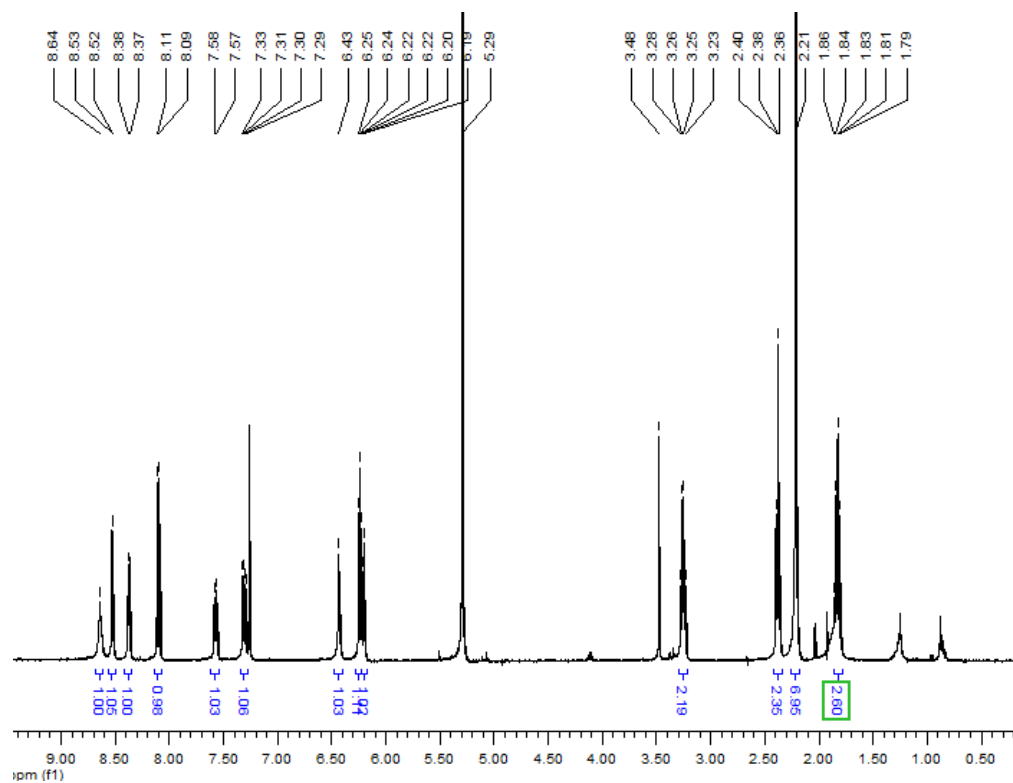


***N*³-(3-(dimethylamino)propyl)-4-nitro-*N*¹-(pyridin-3-yl)benzene-1,3-diamine (22h)**

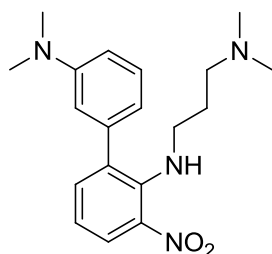


To a 100 ml round-bottom flask was added *N*¹-(5-chloro-2-nitrophenyl)-*N*³,*N*³-dimethylpropane-1,3-diamine (**20h**) (489 mg, 2.16 mmol), toluene (40 ml), 3-aminopyridine (223 mg, 2.37 mmol), Pd₂(dba)₃ (99 mg, 0.11 mmol, 5 mol %), rac-BINAP (101 mg, 0.16 mmol, 7.5 mol%), and Cs₂CO₃ (748 mg, 2.37 mmol, 1.1 eq). The reaction was stirred and heated to reflux under Ar atmosphere for 19 hours before cooling to RT, filtration and concentration. The crude was purified via flash column chromatography (DCM – MeOH (80 % - 20 %)) to yield yellow oil product (269 mg, 40 % yield). ¹H NMR (400 MHz, CDCl₃) δ: 8.64 (s, 1H), 8.53 (d, *J* = 2 Hz, 1H), 8.38 (d, *J* = 5 Hz, 1H), 8.11 (d, *J* = 9 Hz, 1H), 7.58 (d, *J* = 7 Hz, 1H), 7.33 (dd, *J*₁ = 8 Hz, *J*₂ = 5 Hz, 1H), 6.43 (s, 1H), 6.25 (d, *J* = 2 Hz, 1H), 6.22 (dd, *J*₁ = 9 Hz, *J*₂ = 2 Hz, 1H), 3.28 (q, *J* = 5 Hz, 2H), 2.40 (t, *J* = 7 Hz, 2H), 2.21 (s, 6H), 1.86 – 1.79 (m, 2H). MS (ESI) calculated exact mass for C₁₆H₂₁N₅O₂ = 315.17. Found [M+H]⁺ = 316.2.

N^3 -(3-(dimethylamino)propyl)-4-nitro- N^1 -(pyridin-3-yl)benzene-1,3-diamine (**22h**) ^1H NMR (400 MHz, CDCl_3)

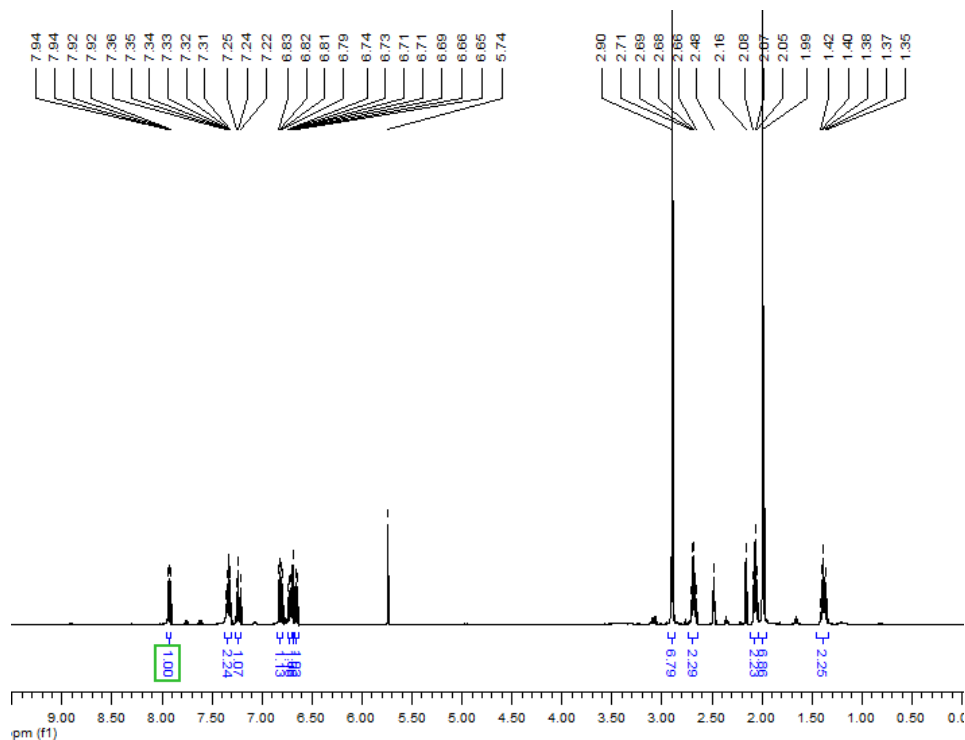


***N*²-(3-(dimethylamino)propyl)-*N*³,*N*³'-dimethyl-3-nitro-[1,1'-biphenyl]-2,3'-diamine (23)**

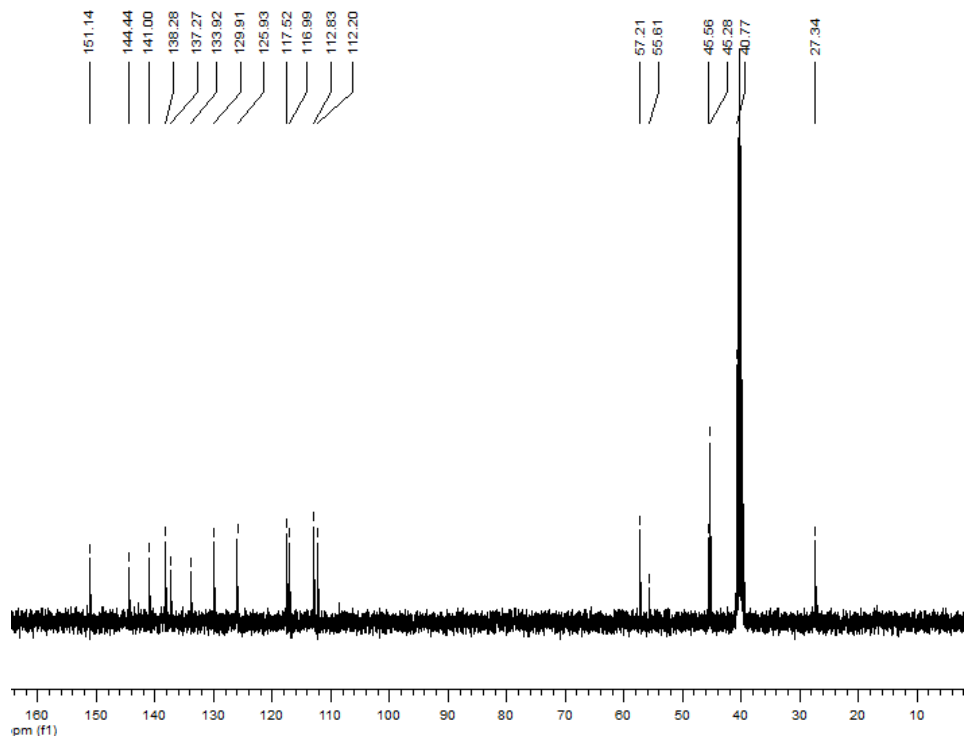


To a 100 ml round bottom flask was added *N*¹-(2-chloro-6-nitrophenyl)-*N*³,*N*³'-dimethylpropane-1,3-diamine (**20j**) (1.0 g, 3.9 mmol), dioxane (40 ml), 3-(*N,N*-dimethylamino)phenylboronic acid (768 mg, 4.6 mmol, 1.2 eq), Pd₂(dba)₃ (178 mg, 0.19 mmol, 5 mol %), rac-BINAP (181 mg, 0.29 mmol, 5 mol %), and Cs₂CO₃ (1.47 g, 4.6 mmol). The reaction was stirred and heated to reflux under Ar atmosphere for 53 hours before cooling to RT, filtration and concentration. The resulting oil residue was purified via flash column chromatography (DCM – MeOH : 90 % - 10 %) to yield red color oil product (803 mg, 60 % yield). ¹H NMR (400 MHz, DMSO) δ: 7.94 (dd, *J*₁ = 8 Hz, *J*₂ = 2 Hz, 1H), 7.36 – 7.31 (m, 2H), 7.25 (t, *J* = 8 Hz, 1H), 6.83 (dd, *J*₁ = 7 Hz, *J*₂ = 8 Hz, 1H), 6.74 (dd, *J*₁ = 9 Hz, *J*₂ = 2 Hz, 1H), 6.69 (s, 1H), 6.66 (d, *J* = 7 Hz, 1H), 2.90 (s, 6H), 2.71 (q, *J* = 6 Hz, 2H), 2.08 (t, *J* = 7 Hz, 2H), 1.99 (s, 6H), 1.42 (p, *J* = 6 Hz, 2H). ¹³C NMR (400 MHz, DMSO) δ: 151.14, 144.44, 141.00, 138.27, 133.91, 129.90, 125.92, 117.52, 116.99, 112.83, 112.19, 57.20, 45.56, 45.28, 40.76, 27.33. MS (ESI) calculated exact mass for C₁₉H₂₆N₄O₂ = 342.21. Found [M+H]⁺ = 343.2.

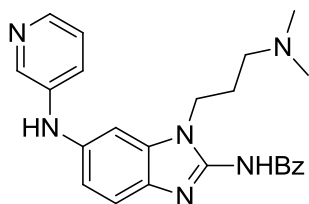
N^2 -(3-(dimethylamino)propyl)- N^3,N^3 -dimethyl-3-nitro-[1,1'-biphenyl]-2,3'-diamine (23) ^1H
 NMR (400 MHz, DMSO)



N^2 -(3-(dimethylamino)propyl)- N^3,N^3 -dimethyl-3-nitro-[1,1'-biphenyl]-2,3'-diamine (23) ^{13}C
 NMR (400 MHz, DMSO)

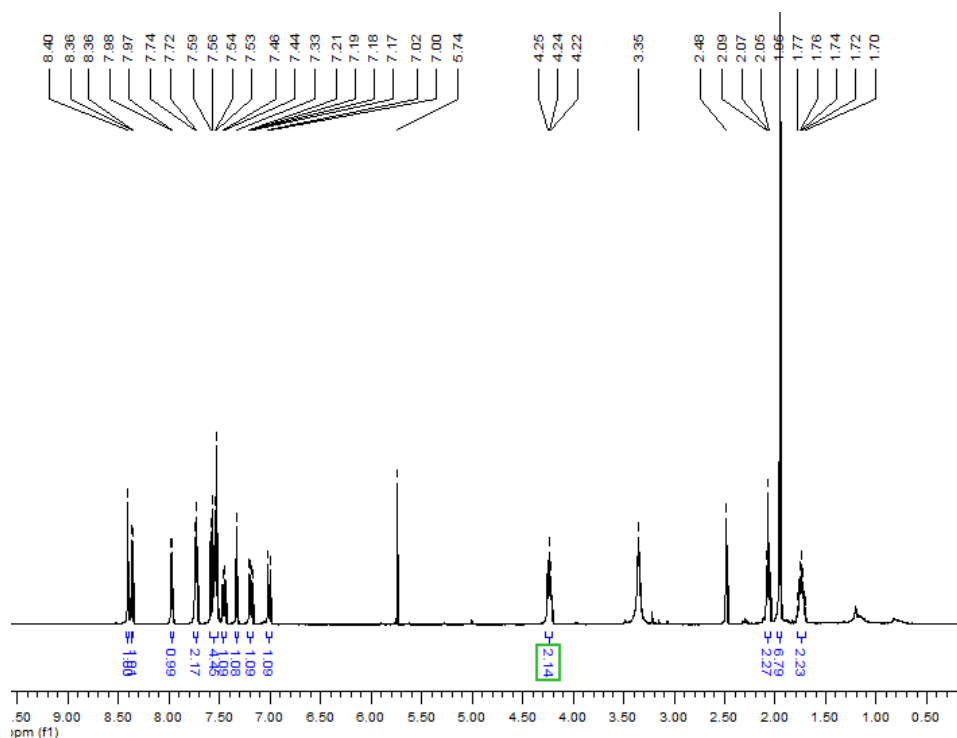


***N*-1-(3-(dimethylamino)propyl)-6-(pyridin-3-ylamino)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (24h)**

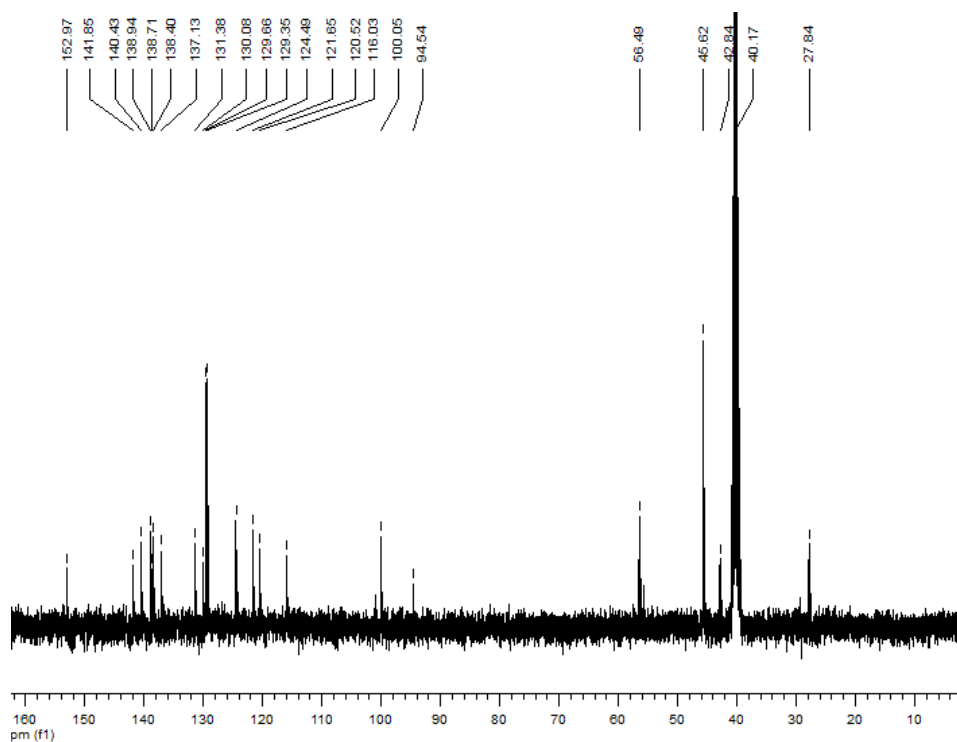


Into a 250 ml round-bottom flask was added *N*³-(3-(dimethylamino)propyl)-4-nitro-*N*¹-(pyridine-3-yl)benzene-1,3-diamine (**22h**) (474 mg, 1.5 mmol) and methanol (100 ml). The flask was flushed with Ar gas before Pd/C (40 mg, 10 wt %) was added. The flask was then sealed under H₂ atmosphere via balloon. The reaction was stirred at RT for 1.5 hours before filtration and concentration. The oil residue was dissolved in ACN (100 ml) and benzoylisothiocyanate (222 μl, 1.5 mmol) was added. The reaction was stirred at RT for 18 hours when DIPC (233 μl, 1.5 mmol) and K₂CO₃ (207 mg, 1.5 mmol) was added. The reaction was stirred at RT for 24 hours before filtered and concentrated. It was purified via flash column chromatography (DCM – MeOH : 90 % - 10 % to 70 % - 30 %) to yield white solid (403 mg, 65 % yield). ¹H NMR (400 MHz, DMSO-d₆) δ: 8.40 (s, 1H), 8.36 (d, *J* = 3 Hz, 1H), 7.98 (d, *J* = 5 Hz, 1H), 7.74 (d, *J* = 8 Hz, 2H), 7.59 – 7.53 (m, 4H), 7.46 (d, *J* = 8 Hz, 1H), 7.33 (s, 1H), 7.21 (dd, *J*₁ = 8 Hz, *J*₂ = 5 Hz, 1H), 7.02 (d, *J* = 8 Hz, 1H), 4.25 (t, *J* = 7 Hz, 2H), 2.09 (t, *J* = 6 Hz, 2H), 1.95 (s, 6H), 1.77 (p, *J* = 7 Hz, 2H). ¹³C NMR (400 MHz, DMSO-d₆) δ: 152.96, 141.84, 140.42, 138.93, 138.70, 138.40, 137.12, 131.37, 130.07, 129.66, 129.34, 124.48, 121.65, 120.52, 116.03, 100.05, 94.54, 56.48, 45.62, 42.83, 27.83. MS (ESI) calculated exact mass for C₂₄H₂₆N₆O = 414.22. Found [M+H]⁺ = 415.3.

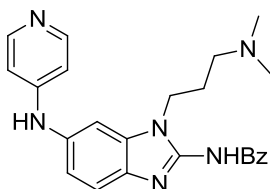
N-(1-(3-(dimethylamino)propyl)-6-(pyridin-3-ylamino)-1*H*-benzo[*d*]imidazol-2-yl)benzamide
(**24h**) ^1H NMR (400 MHz, DMSO- d_6)



N-(1-(3-(dimethylamino)propyl)-6-(pyridin-3-ylamino)-1*H*-benzo[*d*]imidazol-2-yl)benzamide
(**24h**) ^{13}C NMR (400 MHz, DMSO- d_6)

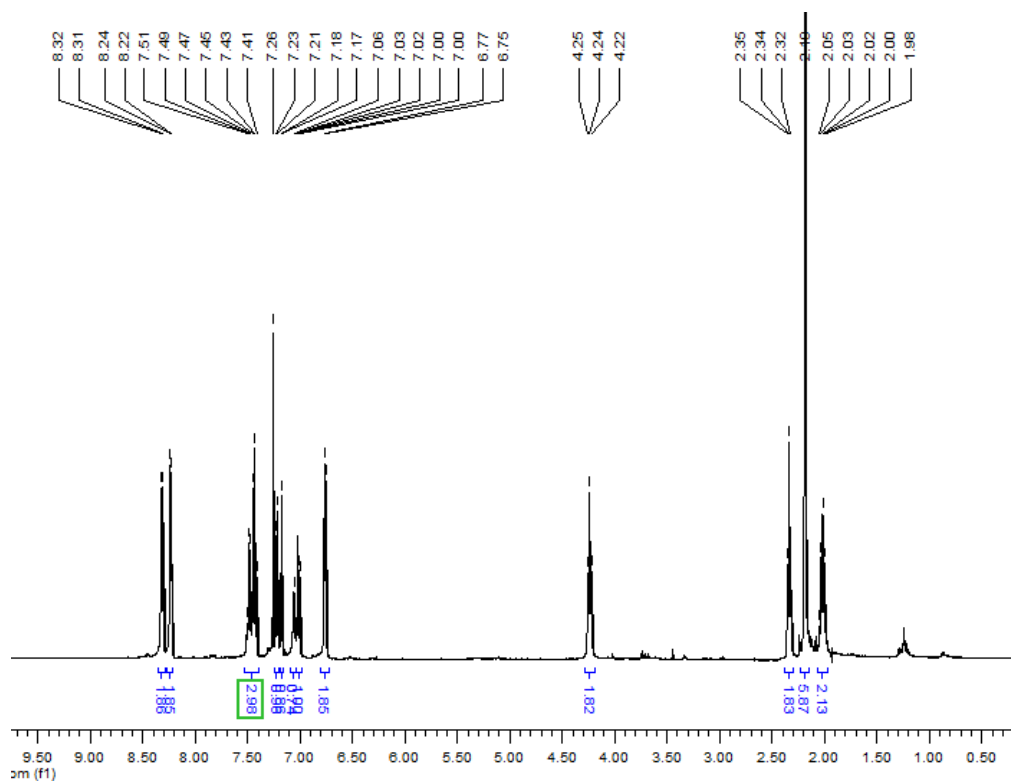


***N*-(1-(3-(dimethylamino)propyl)-6-(pyridin-4-ylamino)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**24i**)**

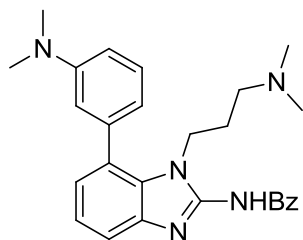


To a 250 ml round-bottom flask was added *N*³-(3-(dimethylamino)propyl)-4-nitro-*N*¹-(pyridin-4-yl)benzene-1,3-diamine (**22i**) (907 mg, 2.87 mmol) and methanol (100 ml). The flask was flushed with Ar gas before Pd/C was added. The reaction was then stirred under H₂ atmosphere for 19 hours before filtration and concentration. The oil residue was dissolved in ACN (250 ml) and benzoyl isothiocyanate (425 μl, 2.87 mmol) was added. The reaction was stirred at RT for 24 hours when DIPC (446 μl, 2.87 mmol) and K₂CO₃ (396 mg, 2.87 mmol) was added. The reaction was stirred at RT for 25 hours before filtered and concentrated. The crude was purified via flash column chromatography (DCM – MeOH : 90 % - 10 %) to yield dark yellow viscous sticky oil product (398mg, 33% yield). ¹H NMR (400 MHz, DMSO) δ: 8.32 (d, *J* = 7 Hz, 2H), 8.24 (d, *J* = 6 Hz, 2H), 7.51 – 7.41 (m, 3H), 7.23 (d, *J* = 9 Hz, 1H), 7.18 (d, *J* = 2Hz, 1H), 7.05 (s, 1H), 7.03 (dd, *J*₁ = 8 Hz, *J*₂ = 2 Hz, 1H), 6.77 (d, *J* = 6 Hz, 2H), 4.25 (t, *J* = 7 Hz, 2H), 2.35 (t, *J* = 7 Hz, 2H), 2.18 (s, 6H), 1.05 – 1.98 (m, 2H). MS (ESI) calculated exact mass for C₂₄H₂₆N₆O = 414.22. Found [M+H]⁺ = 415.2.

N-(1-(3-(dimethylamino)propyl)-6-(pyridin-4-ylamino)-1*H*-benzo[*d*]imidazol-2-yl)benzamide
(24i) ¹H NMR (400 MHz, DMSO)

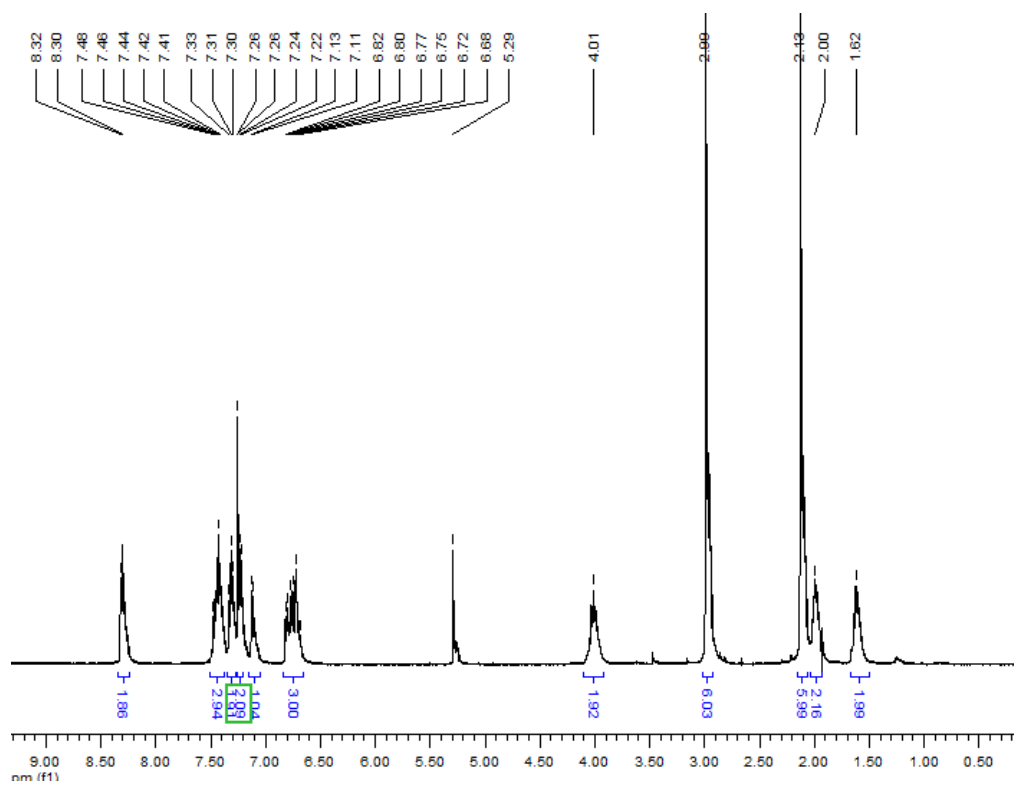


***N*-(7-(3-(dimethylamino)phenyl)-1-(3-(dimethylamino)propyl)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (24j)**

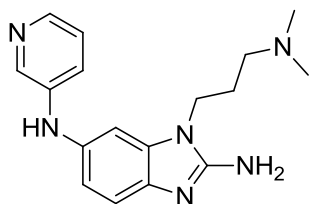


To a 250 ml rb flask was added *N*²-(3-(dimethylamino)propyl)-*N*³,*N*^{3'}-dimethyl-3-nitro-[1,1'-biphenyl]-2,3'-diamine (**23**) (558 mg, 1.63 mmol) and methanol (100 ml). The flask was flushed with Ar gas before Pd/C (60 mg) was added. The reaction was stirred at RT under H₂ atmosphere for 22 hours before filtration and concentration. The oil residue was dissolved in ACN (100ml) and Benzoyl isothiocyanate (240 μl, 1.63 mmol) was added. The reaction was stirred at RT for 27 hours when DIPC (254 μl, 1.63 mmol) and K₂CO₃ (225 mg, 1.63 mmol) were added. The reaction was stirred at RT for 44 hours before filtration, concentration and purification via flash column chromatography (DCM – MeOH : 90 % - 10 %) to yield slight yellow-gray color oil product (280 mg, 39 % yield). ¹H NMR (400 MHz, CDCl₃) δ: 8.32 (d, *J* = 7 Hz, 2H), 7.48 – 7.41 (m, 3H), 7.31 (t, *J* = 8 Hz, 2H), 7.25-7.21 (m, 2H), 7.12 (d, *J* = 7 Hz, 1H), 6.82 – 6.68 (m, 3H), 4.01 (m, 2H), 2.99 (s, 6H), 2.12 (s, 6H), 2.00 (m, 2H), 1.62 (m, 2H). MS (ESI) calculated exact mass for C₂₇H₃₁N₅ = 441.25. Found [M+H]⁺ = 442.3.

N-(7-(3-(dimethylamino)phenyl)-1-(3-(dimethylamino)propyl)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (**24j**) ¹H NMR (400 MHz, CDCl₃)

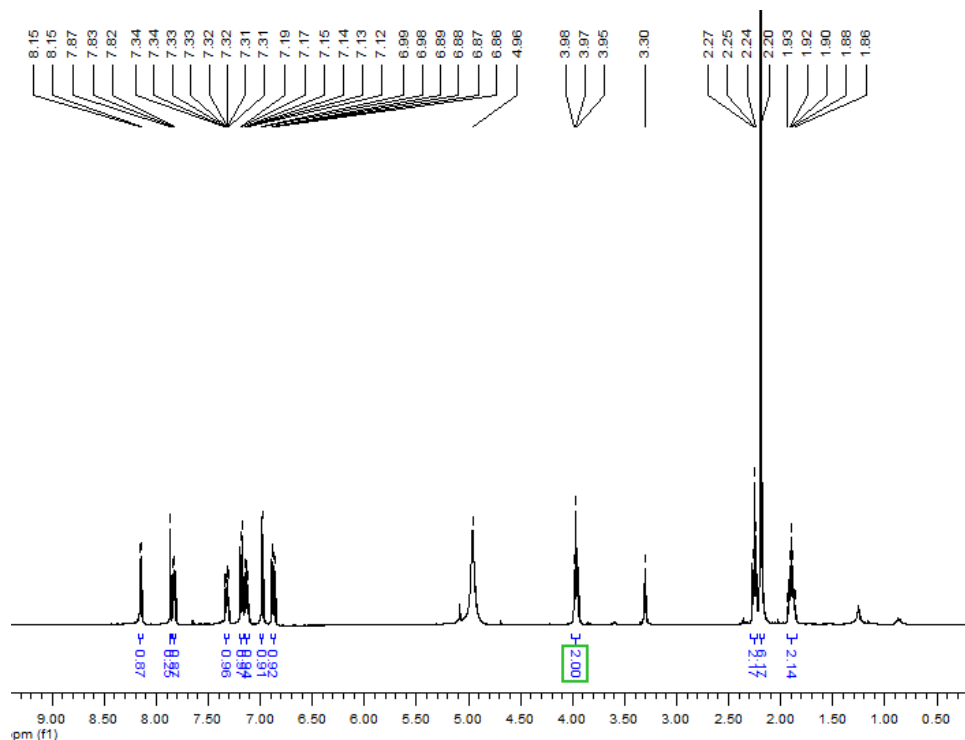


1-(3-(dimethylamino)propyl)-*N*⁶-(pyridin-3-yl)-1*H*-benzo[*d*]imidazole-2,6-diamine (6h)

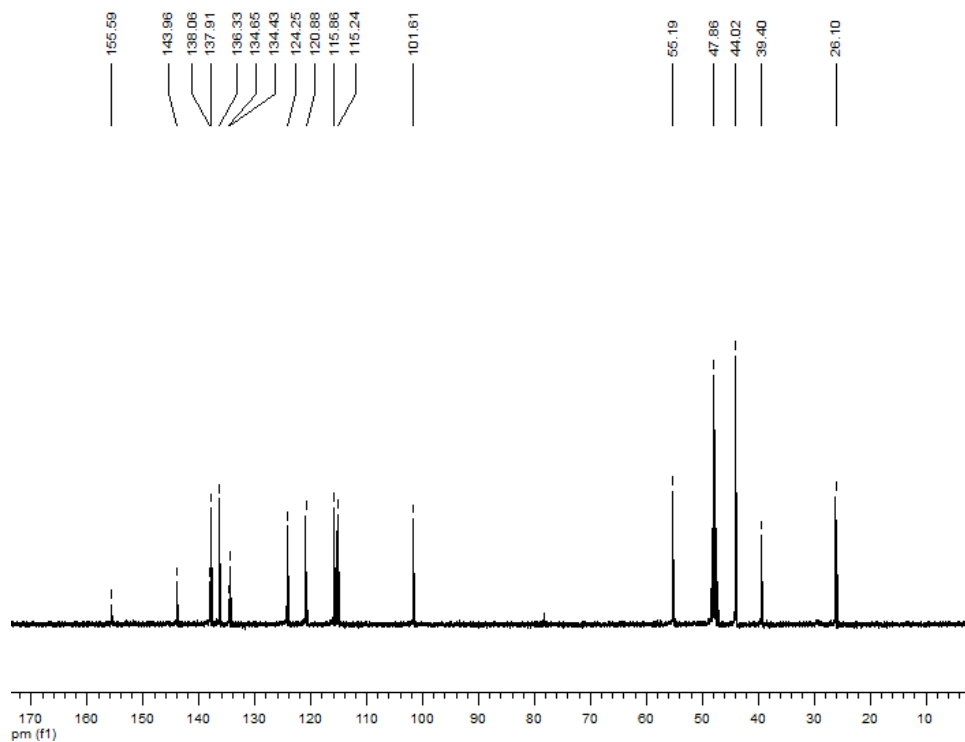


To a 100 ml round bottom flask was added *N*³-(3-(dimethylamino)propyl)-4-nitro-*N*¹-(pyridin-3-yl)benzene-1,3-diamine (**24h**) (403 mg, 1.30 mmol) and 1M HCl aq. (50 ml). The reaction was stirred and heated to reflux for 19 hours before cooling to RT and extracted with saturated NaHCO₃ aq and CHCl₃-EtOH : 2 – 1 (100ml and 2 x 200 ml). The combined organic layer was dried over Na₂SO₄. It was filtered and concentrated before purified via flash column chromatography (DCM – MeOH : 80 % - 20 %) to yield dark yellow oil product (228 mg, 56 % yield). ¹H NMR (400 MHz, CD₃OD) δ: 8.15 (d, *J* = 3 Hz, 1H), 7.83 (d, *J* = 5 Hz, 1H), 7.34 – 7.31 (m, 1H), 7.19 (d, *J* = 8 Hz, 1H), 7.15 (dd, *J*₁ = 8 Hz, *J*₂ = 5 Hz, 1H), 6.99 (d, *J* = 2 Hz, 1H), 6.89 (dd, *J*₁ = 8 Hz, *J*₂ = 2 Hz, 1H), 3.98 (t, *J* = 6 Hz, 2H), 2.27 (t, *J* = 7 Hz, 2H), 2.19 (s, 6H), 1.93 – 1.86 (m, 2H). ¹³C NMR (400 MHz, CD₃OD) δ: 155.59, 143.95, 138.06, 137.91, 136.33, 134.65, 134.42, 124.25, 120.87, 115.86, 115.23, 101.61, 55.19, 44.01, 39.40, 26.10. MS (ESI) calculated exact mass for C₁₇H₂₂N₆ = 310.19. Found [M+H]⁺ = 311.3.

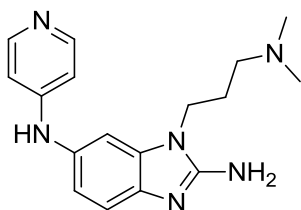
1-(3-(dimethylamino)propyl)-*N*⁶-(pyridin-3-yl)-1*H*-benzo[*d*]imidazole-2,6-diamine (**6h**) ¹H
NMR (400 MHz, CD₃OD)



1-(3-(dimethylamino)propyl)-*N*⁶-(pyridin-3-yl)-1*H*-benzo[*d*]imidazole-2,6-diamine (**6h**) ¹³C
NMR (400 MHz, CD₃OD)

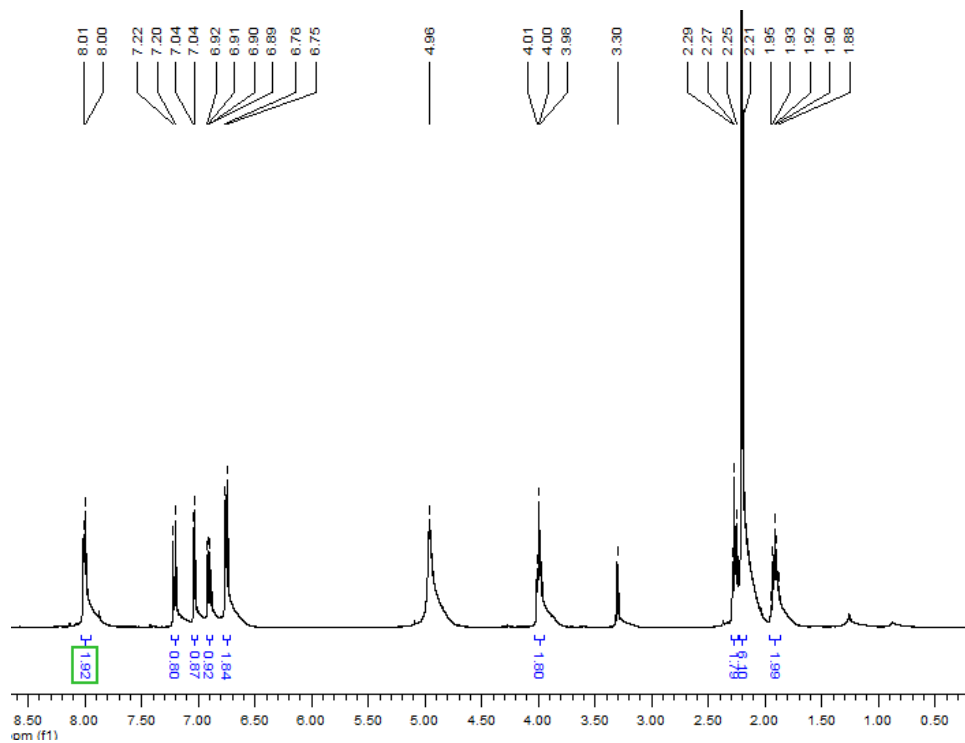


1-(3-(dimethylamino)propyl)-*N*⁶-(pyridin-4-yl)-1*H*-benzo[*d*]imidazole-2,6-diamine (6i)

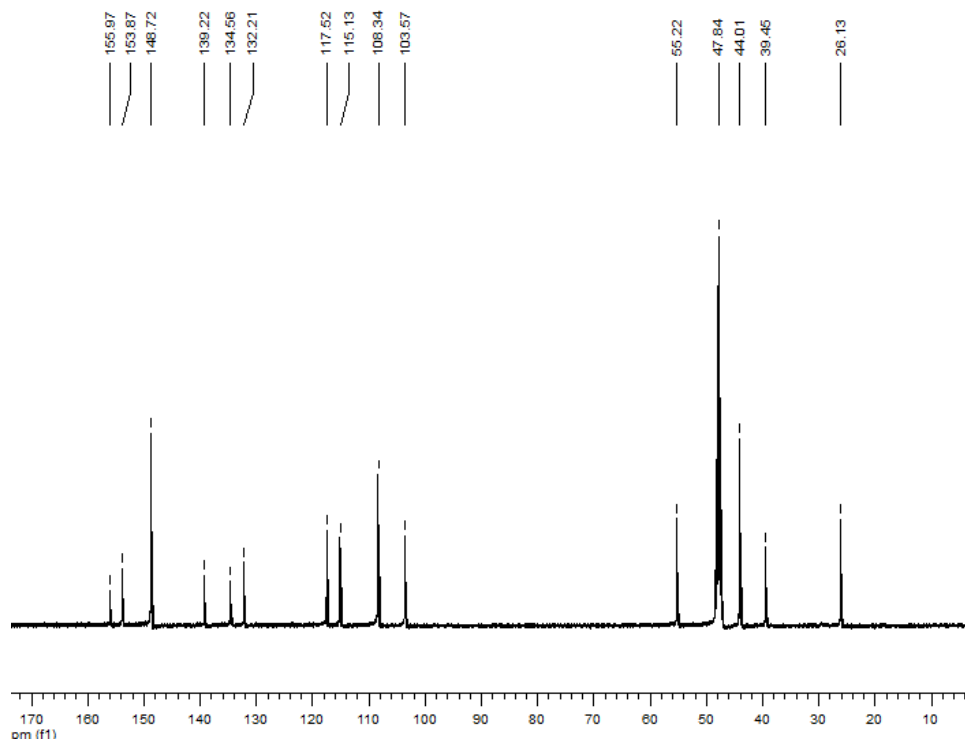


To a 100 ml round bottom flask was added *N*³-(3-(dimethylamino)propyl)-4-nitro-*N*¹-(pyridin-4-yl)benzene-1,3-diamine (**24i**) (652 mg, 1.57 mmol) and 1N HCl aq (50 ml). The reaction was stirred and heated to reflux for 21 hours before cooling to RT and extracted with saturated NaHCO₃ aq and CHCl₃-EtOH : 2 – 1 (100ml and 2 x 200 ml). The combined organic layers was dried over Na₂SO₄. It was filtered and concentrated before purification via flash column chromatography (DCM – MeOH : 80 % - 20 %) to yield off white solid product (208 mg, 43 % yield). ¹H NMR (400 MHz, CD₃OD) δ: 8.01 (d, *J* = 6 Hz, 2H), 7.22 (d, *J* = 8 Hz, 1H), 7.04 (d, *J* = 2 Hz, 1H), 6.92 (dd, *J*₁ = 8 Hz, *J*₂ = 2 Hz, 1H), 6.76 (d, *J* = 6 Hz, 2H), 4.01 (t, *J* = 7 Hz, 2H), 2.29 (t, *J* = 7 Hz, 2H), 2.20 (s, 6H), 1.95 – 1.88 (m, 2H). ¹³C NMR (400 MHz, CD₃OD) δ: 155.96, 153.86, 148.72, 139.21, 134.56, 132.20, 117.51, 115.12, 108.33, 103.57, 55.22, 44.01, 39.44, 26.13. MS (ESI) calculated exact mass for C₁₇H₂₂N₆ = 310.19. Found [M+H]⁺ = 311.3.

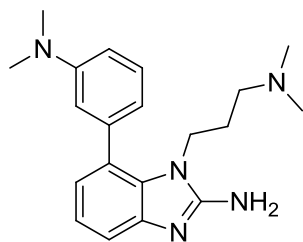
1-(3-(dimethylamino)propyl)-*N*⁶-(pyridin-4-yl)-1*H*-benzo[*d*]imidazole-2,6-diamine (**6i**) ¹H NMR (400 MHz, CD₃OD)



1-(3-(dimethylamino)propyl)-*N*⁶-(pyridin-4-yl)-1*H*-benzo[*d*]imidazole-2,6-diamine (**6i**) ¹³C NMR (400 MHz, CD₃OD)



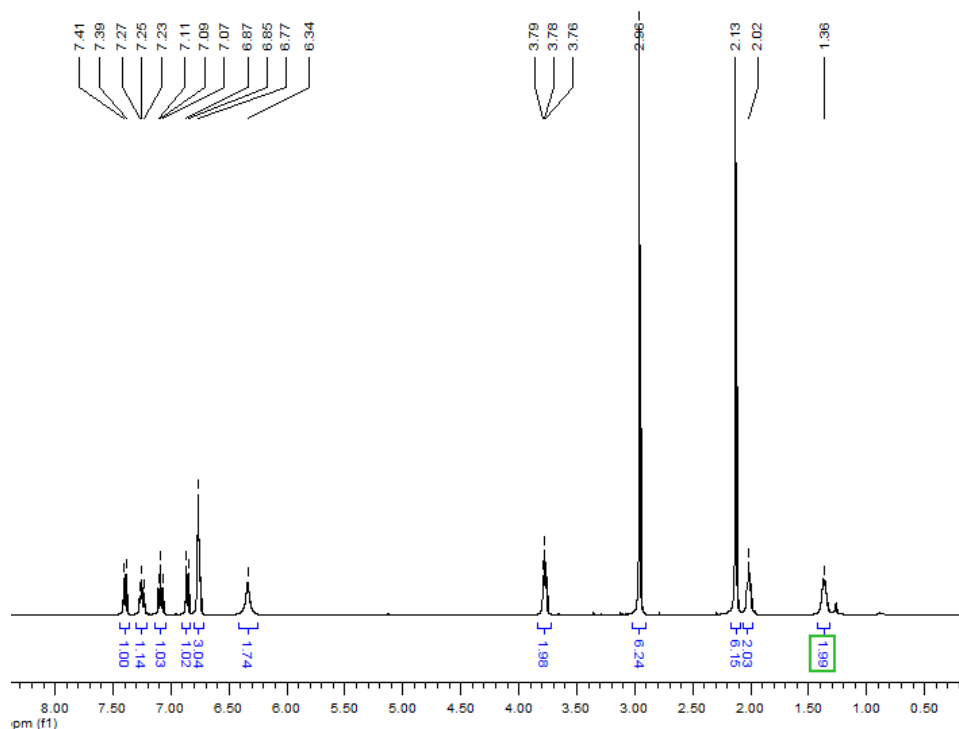
**7-(3-(dimethylamino)phenyl)-1-(3-(dimethylamino)propyl)-1H-benzo[d]imidazol-2-amine
(6j)**



Into a 100 ml round bottom flask was added N-(7-(3-(dimethylamino)phenyl)-1-(3-(dimethylamino)propyl)-1H-benzo[d]imidazol-2-yl)benzamide (**24j**) (210 mg, 0.5 mmol) and 1N HCl aq (40 ml). The reaction was stirred and heated to reflux for 17 hours before cooling to RT and poured into 200 ml of saturated NaHCO₃. It was extracted with chloroform (100 ml) five times. The combined organic layers were dried over Na₂SO₄. After filtration and evaporation of solvent *in vacuo*, the crude was purified via flash column (DCM – MeOH : 70 % - 30 %) to yield slight yellow oil product (73 mg, 46 % yield). ¹H NMR (400 MHz, CDCl₃) δ: 7.40 (d, *J* = 7 Hz, 1H), 7.27 (t, *J* = 7 Hz, 1H), 7.11 (t, *J* = 7 Hz, 1H), 6.87 (d, *J* = 8 Hz, 1H), 6.76 (s, 6H), 6.34 (s, broad, 2H), 3.79 (t, *J* = 6 Hz, 2H), 2.96 (s, 6H), 2.13 (s, 6H), 2.02 (s, 2H), 1.36 (s, 2H). ¹³C NMR (400 MHz, CDCl₃) δ: 156.84, 149.97, 143.37, 140.32, 131.17, 128.54, 126.01, 122.13, 120.61, 118.72, 115.26, 114.64, 111.71, 54.00, 44.59, 40.85, 40.13, 27.04. MS (ESI) calculated exact mass for C₂₀H₂₇N₅ = 337.23. Found [M+H]⁺ = 338.3.

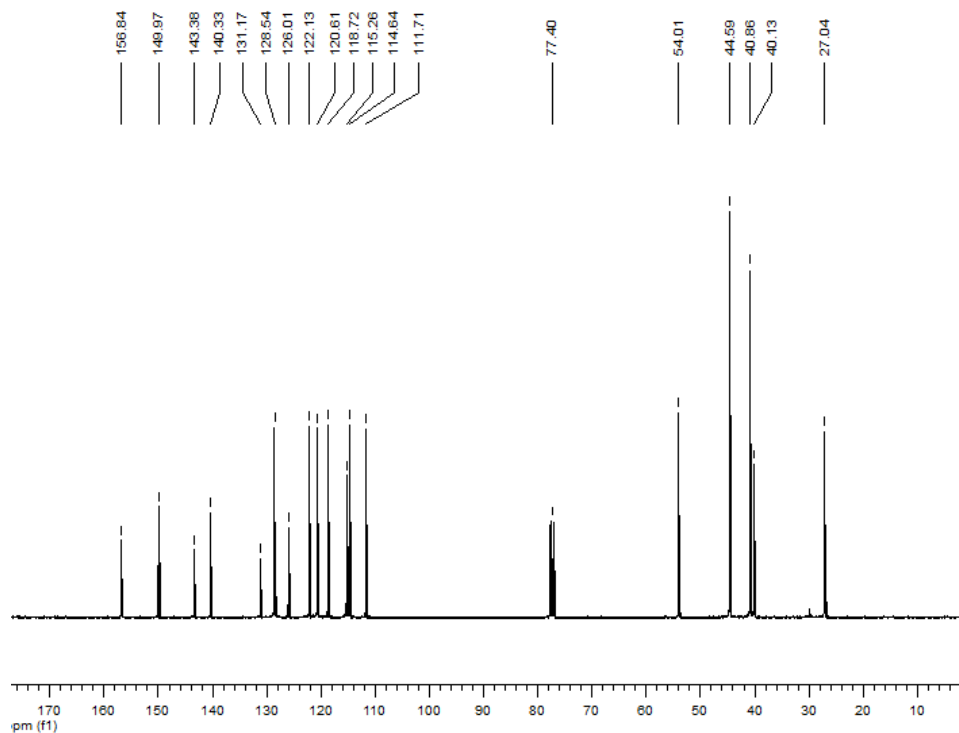
7-(3-(dimethylamino)phenyl)-1-(3-(dimethylamino)propyl)-1*H*-benzo[*d*]imidazol-2-amine **(6j)**

¹H NMR (400 MHz, CDCl₃)



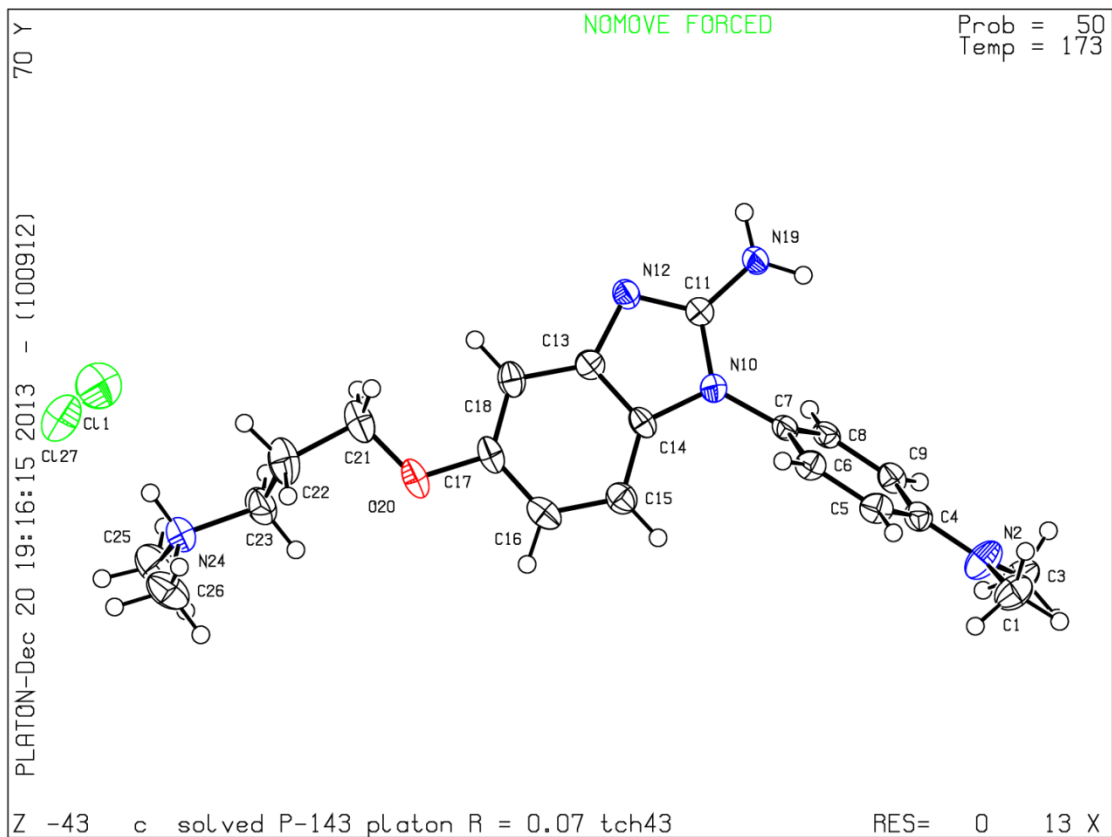
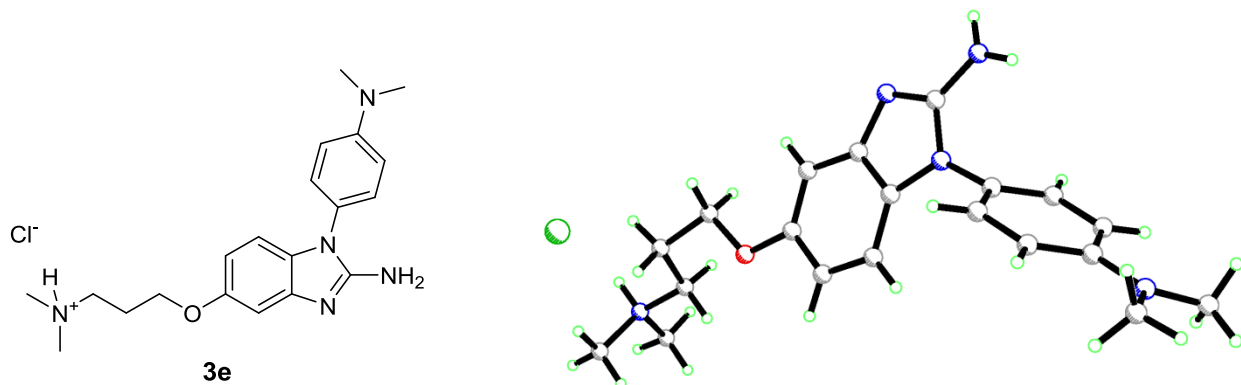
7-(3-(dimethylamino)phenyl)-1-(3-(dimethylamino)propyl)-1*H*-benzo[*d*]imidazol-2-amine **(6j)**

¹³C NMR (400 MHz, CDCl₃)



Crystal structure of compound **3e**:

1-(4-(dimethylamino)phenyl)-5-(3-(dimethylamino)propoxy)-1H-benzo[d]imidazol-2-amine, hydrochloride



Supplementary Table 1. Crystal data and structure refinement for compound **3e**.^a

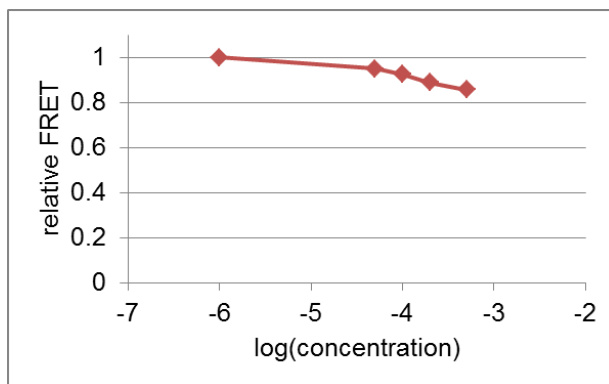
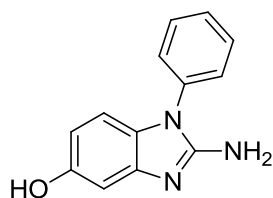
CCDC deposit number	978337
Empirical formula	C ₂₀ H ₂₈ Cl N ₅ O
Formula weight	389.92
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 9.4134(9) Å α = 103.600(5)°. b = 9.6736(9) Å β = 91.925(5)°. c = 15.249(2) Å γ = 115.963(3)°.
Volume	1198.5(2) Å ³
Z	2
Density (calculated)	1.080 Mg/m ³
Absorption coefficient	0.176 mm ⁻¹
F(000)	416
Crystal size	0.40 x 0.30 x 0.30 mm ³
Theta range for data collection	2.54 to 24.19°
Index ranges	-10 ≤ h ≤ 10, -11 ≤ k ≤ 11, -17 ≤ l ≤ 16
Reflections collected	12741
Independent reflections	3757 [R(int) = 0.0401]
Completeness to theta = 24.19°	97.6 %
Absorption correction	semi-empirical from equivalents
Max. and min. transmission	0.9490 and 0.9329
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3757 / 0 / 252
Goodness-of-fit on F ²	1.080
Final R indices [I > 2σ(I)]	R1 = 0.0713, wR2 = 0.1999
R indices (all data)	R1 = 0.1039, wR2 = 0.2152
Largest diff. peak and hole	0.675 and -0.475 e. Å ⁻³

^aAll nonhydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-97). Hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-97. Hydrogen atom H(24) was located in electron difference map and was allowed to refine freely. Solvent molecules could not be modeled satisfactorily. Therefore, SQUEEZE from the PLATON program suite was used to remove the contribution of the disordered molecules, indicating 58 electrons in the solvent accessible voids of 233 Å³. This is equivalent to one chloroform molecule.

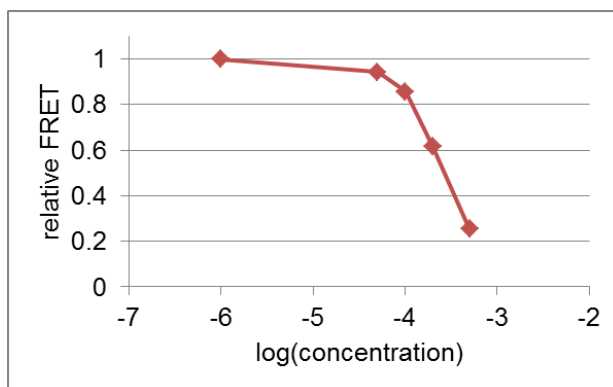
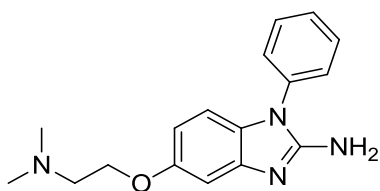
FRET Assay

Compounds were tested for binding to the IRES Ila RNA by triplicate titration in the Ila FRET assay as previously described (Zhou, S.; Rynearson, K. D.; Ding, K.; Brunn, N. D.; Hermann, T. *Bioorg. Med. Chem.* **2013**, *21*, 6139). Titration curves are shown below.

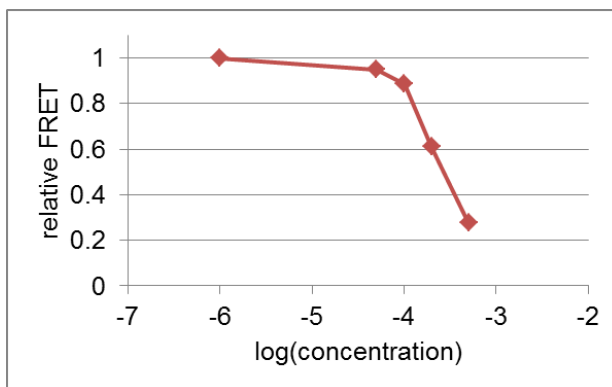
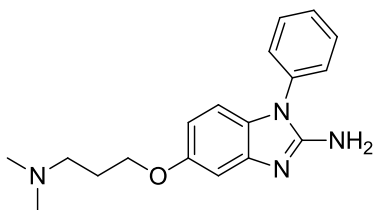
2-amino-1-phenyl-1H-benzo[d]imidazol-5-ol (3a)



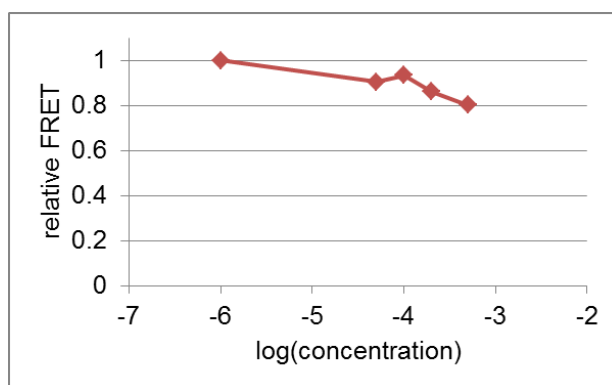
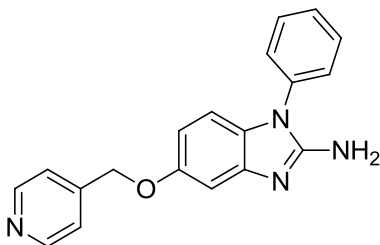
5-(2-(dimethylamino)ethoxy)-1-phenyl-1H-benzo[d]imidazol-2-amine (3b)



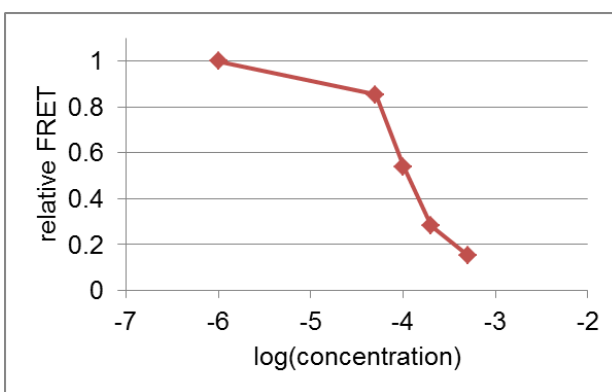
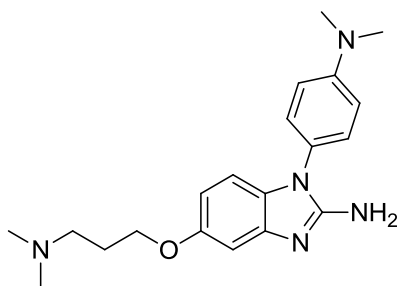
5-(3-(dimethylamino)propoxy)-1-phenyl-1H-benzo[d]imidazol-2-amine (3c)



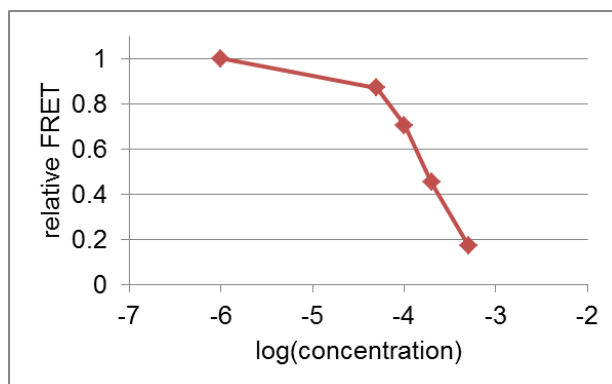
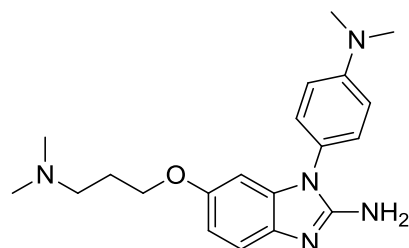
1-phenyl-5-(pyridine-4-ylmethoxy)-1H-benzo[d]imidazol-2-amine (3d)



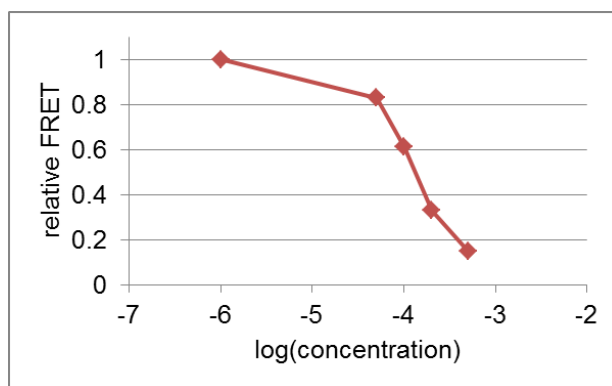
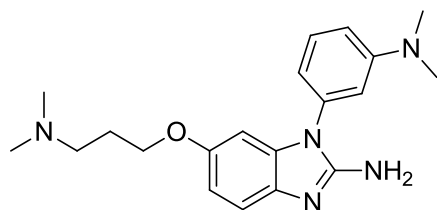
1-(4-(dimethylamino)phenyl)-5-(3-(dimethylamino)propoxy)-1H-benzo[d]imidazol-2-amine (3e)



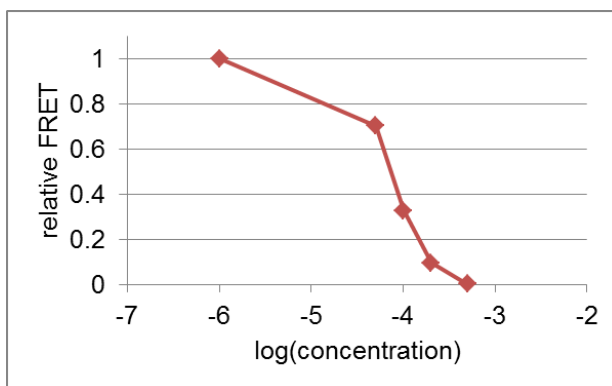
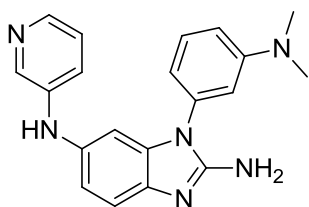
1-(4-(dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1H-benzo[d]imidazol-2-amine (3f)



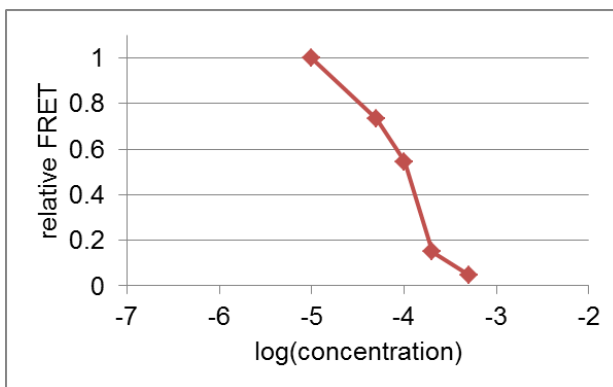
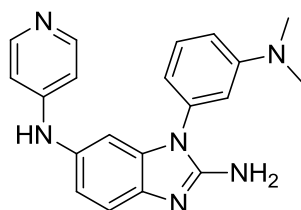
1-(3-(dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1H-benzo[d]imidazol-2-amine (3g)



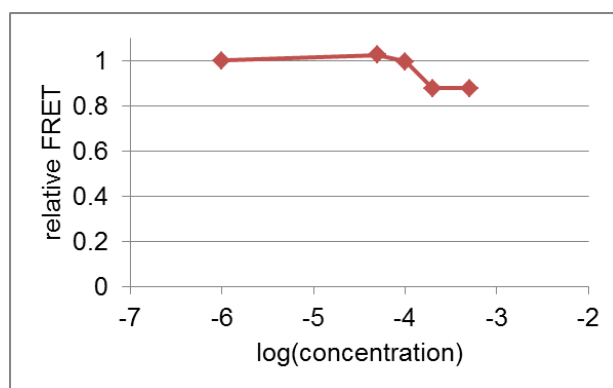
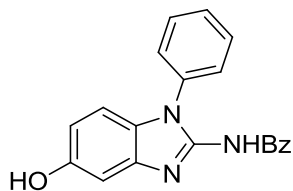
1-(3-(dimethylamino)phenyl)-N⁶-(pyridin-3-yl)-1H-benzo[d]imidazole-2,6-diamine (3h)



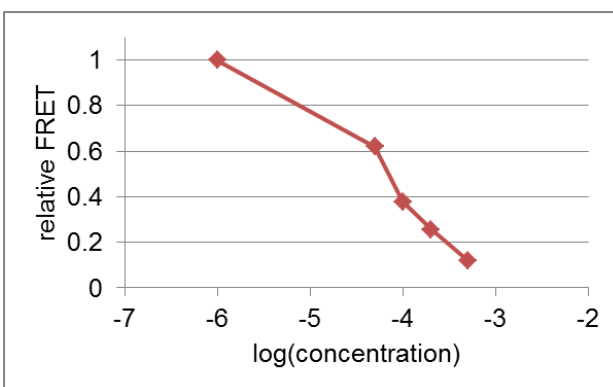
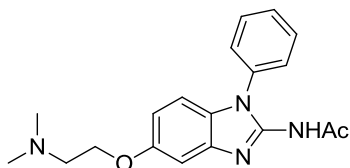
1-(3-(dimethylamino)phenyl)-*N*⁶-(pyridin-4-yl)-1*H*-benzo[*d*]imidazole-2,6-diamine (3i)



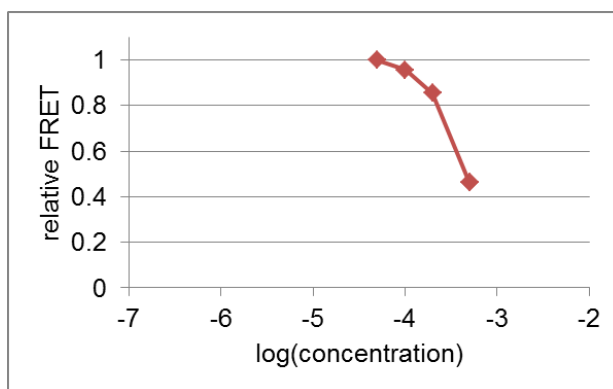
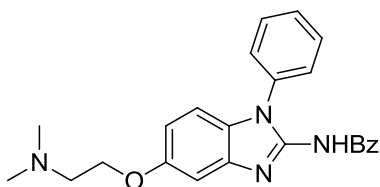
***N*-(5-hydroxy-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)benzamide (4ab)**



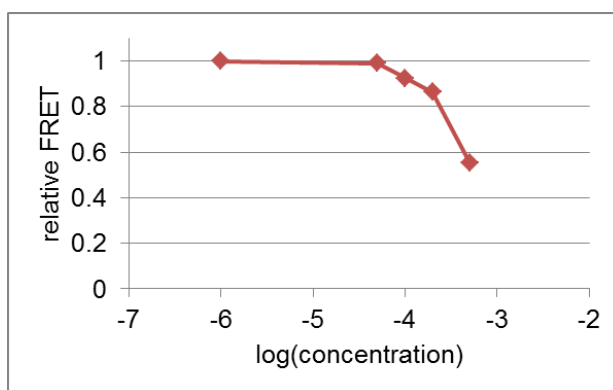
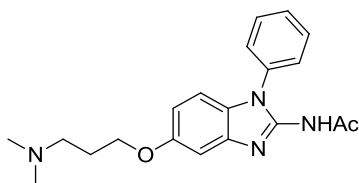
***N*-(5-(2-(dimethylamino)ethoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)acetamide (4ba)**



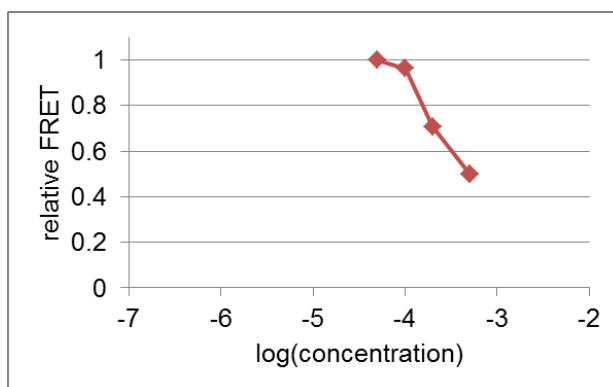
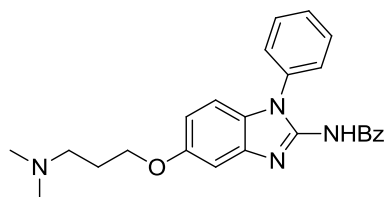
***N*-(5-(2-(dimethylamino)ethoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)benzamide (4bb)**



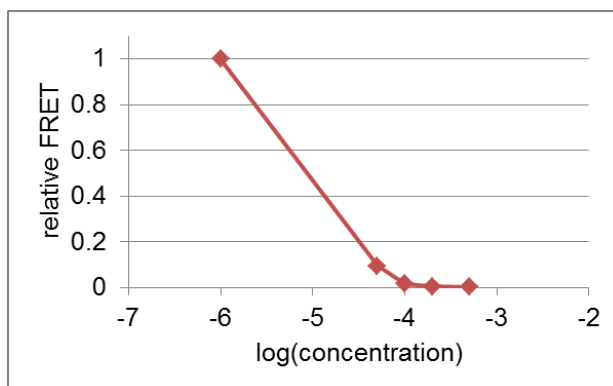
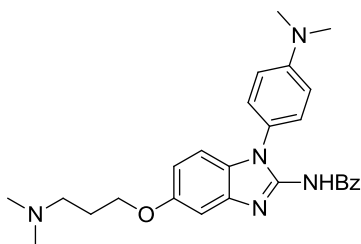
***N*-(5-(3-(dimethylamino)propoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)acetamide (4ca)**



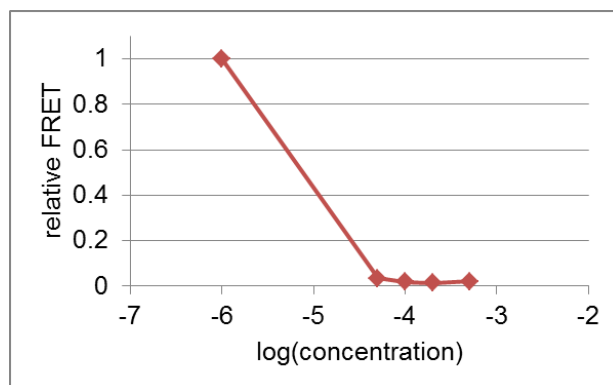
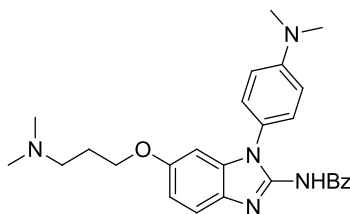
***N*-(5-(3-(dimethylamino)propoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)benzamide (4cb)**



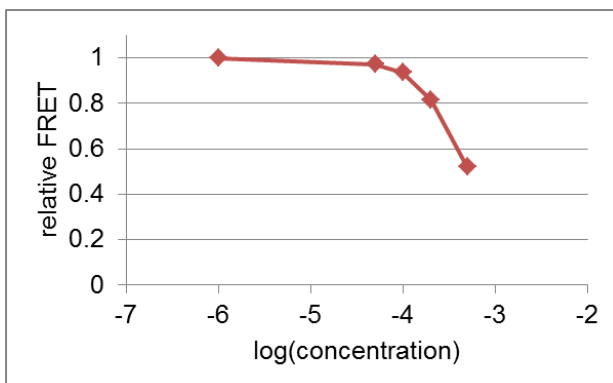
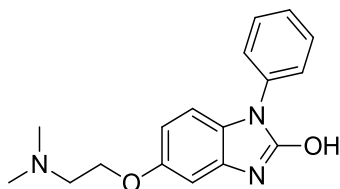
***N*-(1-(4-(dimethylamino)phenyl)-5-(3-(dimethylamino)propoxy)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (4eb)**



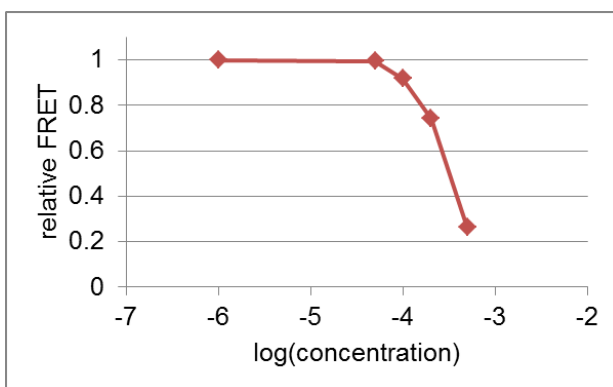
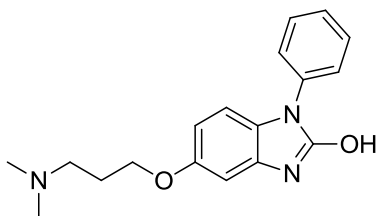
***N*-(1-(4-(dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1*H*-benzo[*d*]imidazol-2-yl)benzamide (4fb)**



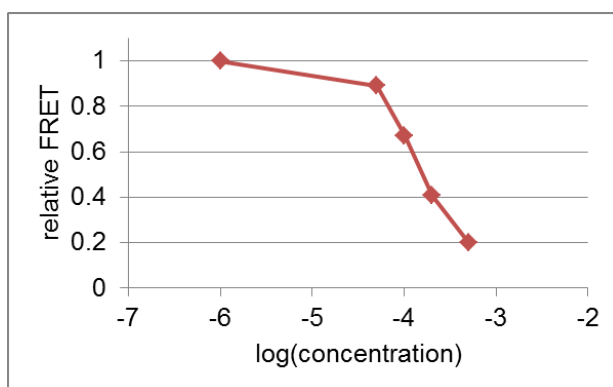
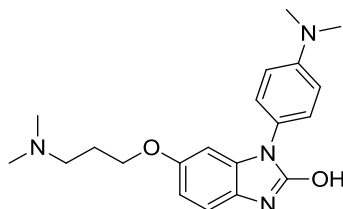
5-(2-(dimethylamino)ethoxy)-1-phenyl-1*H*-benzo[*d*]imidazol-2-ol (5b)



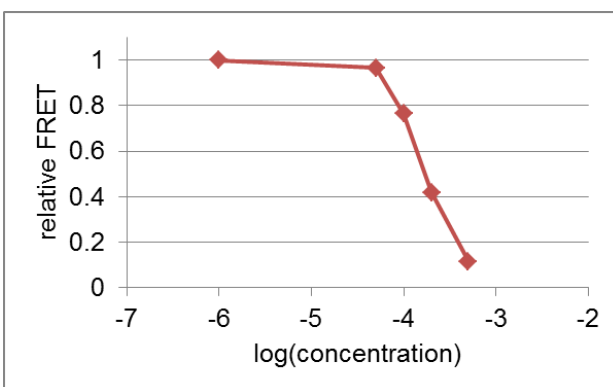
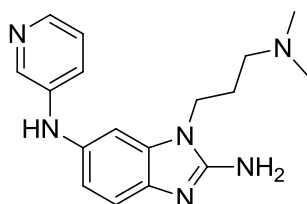
5-(3-(dimethylamino)propoxy)-1-phenyl-1H-benzo[d]imidazol-2-ol (5c)



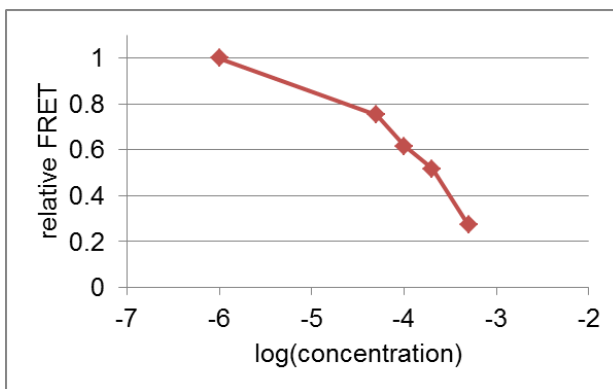
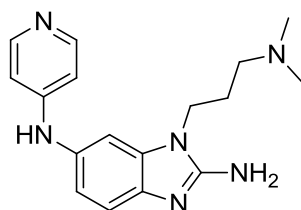
1-(4-(dimethylamino)phenyl)-6-(3-(dimethylamino)propoxy)-1H-benzo[d]imidazol-2-ol (5f)



1-(3-(dimethylamino)propyl)-N⁶-(pyridin-3-yl)-1H-benzo[d]imidazole-2,6-diamine (6h)



1-(3-(dimethylamino)propyl)-*N*⁶-(pyridin-4-yl)-1*H*-benzo[*d*]imidazole-2,6-diamine (6i)



7-(3-(dimethylamino)phenyl)-1-(3-(dimethylamino)propyl)-1*H*-benzo[*d*]imidazol-2-amine (6j)

