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Experimental Section

Broth Microdilution Method for MIC Determination. Overnight cultures of bacterial strain were subcultured to 5 x 10^5 CFU/mL in Mueller-Hinton medium (Fluka # 70192). The resulting bacterial suspension was aliquoted (1.0 mL) into culture tubes. Samples were prepared from these culture tubes containing either 256 µg/mL of specified antibiotic or no test compound as a control. Samples were then aliquoted (200 µL) into the first row of wells of a 96-well microtiter plate in which subsequent wells were prefilled with 100 µL of Mueller-Hinton medium based 5 x 10^5 CFU/mL bacterial subculture. Using the multichannel pipettor set at 100 µL, row one wells were mixed 8-10 times. Then, 100 µL were withdrawn and transferred to row two. Row two wells were mixed to serial dilute the rest of the rows of the microtier plate. The microtiter plate sample was then covered with a microtiter plate lid and then placed in a covered plastic container. The chamber was incubated under stationary conditions at 37° C. After 16 hours, the lid was removed and MIC values were recorded.

Procedure to Determine the Inhibitory Effect of Test Compounds on S. Aureus (ATCC# 43300 and ATCC # BAA-44) Biofilm Formation: Inhibition assays were performed by taking an overnight culture of bacterial strain and subculturing it at an OD₆₀₀ of 0.01 into the necessary medium (tryptic soy broth with a 0.5% glucose supplement (TSBG) for MRSA (ATCC # BAA-44) and S. aureus (ATCC # 29213), Luria-Bertani (LB) medium for A. baumannii (ATCC # 19606) and Luria-Bertani medium without NaCl (LBNS) for PA14. Stock solutions of predetermined concentrations of the test compound were then made in the necessary medium. These stock solutions were aliquoted (100 μ L) into the wells of the 96well PVC microtiter plate. Sample plates were then wrapped in GLAD Press n' Seal[®] followed by an incubation under stationary conditions for 24 h at 37 °C (6 h for PA14). After incubation, the medium was discarded from the wells and the plates were washed thoroughly with water. Plates were then stained with 100 µL of 0.1% solution of crystal violet (CV) and then incubated at ambient temperature for 30 min. Plates were washed with water again and the remaining stain was solubilized with 200 µL of 95% ethanol. A sample of 125 μ L of solubilized CV stain from each well was transferred to the corresponding wells of a polystyrene microtiter dish. Biofilm inhibition was quantitated by measuring the OD_{540} of each well in which a negative control lane wherein no biofilm was formed served as a background and was subtracted out.



Biofilm Inhibition (43300)









Biofilm Inhibition (43300)





















Biofilm Inhibition (43300)









Biofilm Inhibition (43300)





































Biofilm Inhibition (BAA-44)



















Procedure to Determine the Dispersal Effect of Test Compounds on S. aureus (ATCC # 43300) Preformed Biofilms: Dispersion assays were performed by taking an overnight culture of bacterial strain and subculturing it at an OD_{600} of 0.01 into the necessary medium (tryptic soy broth with a 0.5% glucose supplement (TSBG) for S. aureus. The resulting bacterial suspension was aliquoted (100 µL) into the wells of a 96-well PVC microtiter plate. Plates were then wrapped in GLAD Press n' Seal[®] followed by an incubation under stationary conditions at 37 °C to establish the biofilms. After 24 h, the medium was discarded from the wells and the plates were washed thoroughly with water. Stock solutions of predetermined concentrations of the test compound were then made in the necessary medium. These stock solutions were aliquoted (100 μ L) into the wells of the 96-well PVC microtiter plate with the established biofilms. Medium alone was added to a subset of the wells to serve as a control. Sample plates were then incubated for 24 h at 37 °C. After incubation, the medium was discarded from the wells and the plates were washed thoroughly with water. Plates were then stained with 100 µL of 0.1% solution of crystal violet (CV) and then incubated at ambient temperature for 30 min. Plates were washed with water again and the remaining stain was solubilized with 200 μ L of 95% ethanol. A sample of 125 μ L of solubilized CV stain from each well was transferred to the corresponding wells of a polystyrene microtiter dish. Biofilm dispersion was quantitated by measuring the OD₅₄₀ of each well in which a negative control lane wherein no biofilm was formed served as a background and was subtracted out.

Growth Curve Analysis

Procedure to Determine the Effect of Test Compounds *S. aureus* (ATCC # 43300 and ATCC # BAA-44) Planktonic Viability via Growth Curve Analysis: Growth curves were

performed by taking an overnight culture of bacterial strain and subculturing it at an OD_{600} of 0.01 into TSBG. The resulting bacterial suspension was then aliquoted (3.0 mL) into culture tubes. The test compound was then added at a predetermined concentration to the medium of the test samples. Controls were employed in which no test compound was added to the bacterial suspension. Samples were then placed in an incubator at 37 °C and shaken at 200 rpm. The OD_{600} of the samples was measured at time intervals starting at 2 hours and ending at 24 hours.











S29






























































Procedure to Determine the Mitigating Effects of Divalent Metal Ions on MRSA (ATCC # 43300) Biofilm Formation Inhibition Induced by Anti-fouling agents Inhibition assays were performed by taking an overnight culture of bacterial strain and subculturing it at an OD₆₀₀ of 0.01 into the tryptic soy broth with a 0.5% glucose supplement. Stock solutions of 8.0 μ M of the appropriate anti-fouling agent were then made in the necessary media. Samples were then doped with 25.0, 50.0, 75.0, 100.0, 150.0 and 200.0 μ M metal ion. Control lanes were doped with 200 μ M metal ion. These stock solutions were aliquoted (100 μ L) into the wells of the 96-well PVC microtiter plate. Sample plates were then wrapped in GLAD Press n' Seal® followed by incubation under stationary conditions for 24 h at 37 °C. After incubation, the media was discarded from the wells and the plates were washed thoroughly with water. Plates were then stained with 110 μ L of 0.1% solution of crystal violet (CV) and then incubated at ambient

temperature for 30 min. Plates were washed with water again and the remaining stain was solubilized with 200 μ L of 95% ethanol. A sample of 125 μ L of solubilized CV stain from each well was transferred to the corresponding wells of a polystyrene microtiter dish. Biofilm inhibition was quantified by measuring the OD₅₄₀ of each well in which a negative control lane wherein no biofilm was formed served as a background and was subtracted out. 200.0 μ M metal ions was found to have no effect on biofilm formation.

























Synthesis Experiemental:

All reagents used for chemical synthesis were purchased from commercially available sources and used without further purification. Chromatography was performed using 60 Å mesh standard grade silica gel from Sorbtech. NMR solvents were obtained from Cambridge Isotope Labs and used as is. All ¹H NMR (300 MHz or 400 MHz) and ¹³C NMR (75 MHz or 100 MHz) spectra were recorded at 25°C on Varian Mercury spectrometers. Chemical shifts (δ) are given in ppm relative to tetramethylsilane or the respective NMR solvent; coupling constants (*J*) are in hertz (Hz). Abbreviations used are s = singlet, bs = broad singlet, d = doublet, dd = doublet of doublets, t = triplet, dt = doublet of triplets, bt = broad triplet, qt = quartet, m = multiplet, bm = broad multiplet, p = pentet, and br = broad. Mass spectra were obtained at the NCSU Department of Chemistry Mass Spectrometry Facility. Funding was obtained from the North Carolina Biotechnology Center and the NCSU Department of Chemistry. Infrared spectra were obtained on a FT/IR-4100 spectrophotometer (v_{max} in cm⁻¹). UV absorbance was recorded on a Genesys 10 scanning UV/visible spectrophotometer (λ_{max} in nm).



N-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide: To a solution of 4-fluoro-3-nitroaniline (10.0 g, 64.05 mmol) in anhydrous CH₂Cl₂ (385 mL), was added DMAP (7.82 g, 10.0 mmol), and 4-pentylbenzoyl chloride (16.9 mL, 83.27 mmol) dropwise. The reaction was stirred under N₂ for 6 hours, after which it was washed with H₂O (3 x 100 mL), saturated aqueous NaHCO₃ (2 x 100 mL), and saturated aqueous NaCl (1 x 100 mL). It was then dried with Na₂SO₄ and purified on silica gel, using EtOAc/Hexanes (90/10) as the eluting solvent. Product was concentrated in vacuo as an cream colored solid (m.p. = 105 - 107 °C, 89%). ¹H NMR (300 MHz, CDCl₃) ö 8.35 (d of d, J₁ = 2.7 Hz, J₂ = 6.3, 1H), 8.04 – 7.99 (m, 2H), 7.80 – 7.77 (m, 2H), 7.32 – 7.24 (m, 2H), 2.68 (t, J = 7.5 Hz, 2H), 1.64 (p, J = 7.5 Hz, 2H), 1.38 – 1.29 (m, 4H), 0.90 (t, 6.9 Hz, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) ö 166.4, 153.5, 150.9, 148.6, 135.0, 134.9, 131.3, 129.3, 127.6, 127.5, 119.2, 119.0, 117.7, 117.6, 36.2, 31.7, 31.1, 22.8, 14.3 ppm; IR vmax (cm⁻¹) 3333, 2854, 1653, 1549, 1341, 1259; HRMS (ESI) calcd for C₁₈H₁₉FN₂O₃ (M+) 331.1452, found 331.1444.

General procedure for the nucleophilic aromatic substation reactions: *N*-(4-fluoro-3nitrophenyl)-4-pentylbenzamide was added to a round bottom flask and dissolved in ethanol (0.5 M). To this mixture the corresponding amine (3-5 equivalents) was added dropwise. The reaction mixture was then heated to reflux and allowed to stir until completion via TLC analysis. The mixture was then cooled to room temperature. Water was added to the reaction mixture, causing the product to precipitate out of solution. This mixture was then cooled to 0°C. The product was then filtered and washed with cold water. The solid was then dried under high vacuum overnight.



N-(4-(methylamino)-3-nitrophenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide, methyl amine was reacted with *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide to produce N-(4-(methylamino)-3-nitrophenyl)-4-pentylbenzamide as an orange solid (m.p. = 162-164 °C, 89%). ¹H NMR (300 MHz, CDCl₃) ö 8.23 (d, J = 2.1 Hz, 1H), 7.98 (d of d, J₁ = 2.1 Hz, J₂ = 6.9 Hz, 1H), 7.77 (m, 3H), 7.29 (d, J = 6.3 Hz, 2H), 6.88 (d, J = 6.9 Hz, 1H), 3.05 (s, 3H), 2.67 (t, J = 5.7 Hz, 2H), 1.64 (p, J = 5.7 Hz, 2H), 1.37-1.25 (m, 4H), 0.90 (t, J = 5.1 Hz, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) ö 166.3, 147.9, 144.3, 131.9, 131.5, 131.2, 129.2, 127.4, 126.8, 118.5, 114.2,

36.2, 31.8, 31.2, 30.2, 22.8, 14.3 ppm; IR vmax (cm⁻¹) 3394, 2955, 1638, 1528; HRMS (ESI) calcd for C₁₉H₂₃N₃O₃ (M+) 342.1812, found 342.1799.



N-(4-(isopropylamino)-3-nitrophenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide, isopropyl amine was reacted with *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide to produce *N*-(4-(isopropylamino)-3-nitrophenyl)-4-pentylbenzamide as a red solid (m.p. = $135-137^{\circ}$ C, 89%). ¹H NMR (400 MHz, CDCl₃) δ 8.27 (bs, 1H), 8.21 (d, *J* = 2.4 Hz, 1H), 7.95 (d, *J* = 7.2 Hz, 1H), 7.89 (dd, *J*₁ = 2.4Hz, *J*₂ = 9.6 Hz, 1H), 7.79 (d, *J* = 8 Hz, 2H), 7.22 (d, *J* = 8 Hz, 2H), 6.80 (d, *J* = 9.6 Hz, 1H), 3.81 (septet, *J* = 6 Hz, 1H), 2.63 (t, *J* = 7.6 Hz, 2H), 1.61 (p, *J* = 7.6 Hz, 2H), 1.36-1.25 (m, 10H), 0.89 (t, *J* = 6.4 Hz, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 166.3, 147.6, 142.6, 131.7, 131.5, 130.7, 128.8, 127.4, 126.4, 118.7, 114.7, 44.2, 36.0, 31.6, 31.0, 22.9, 22.7, 14.2 ppm; IR v_{max} (cm⁻¹) 3428, 1638, 1523, 1238; HRMS (ESI) calcd for C₂₁H₂₇N₃O₃ (M+) 370.2125, found 370.2128.



N-(4-(butylamino)-3-nitrophenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide, butyl amine was reacted with *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide to produce *N*-(4-(butylamino)-3-nitrophenyl)-4-pentylbenzamide as a red solid (m.p. = 138-140°C, 91%). ¹H NMR (400 MHz, CDCl₃) δ 8.21 (d, *J* = 2.8 H, 1H), 8.02 (t, *J* = 4.8 Hz, 1H), 7.94 (dd, *J_I* = 2.4 Hz, *J₂* = 9.2 Hz, 1H), 7.83 (bs, 1H), 7.78 (d, *J* = 8.4 Hz, 2H), 7.28 (d, *J* = 8.4 Hz, 2H), 6.87 (d, *J* = 9.2 Hz, 1H), 3.32 (q, *J* = 6.4 Hz, 2H), 2.67 (t, *J* = 7.2 Hz, 2H), 1.72 (p, *J* = 7.2 Hz, 2H), 1.66-1.61 (m, 2H), 1.49 (sextet, *J* = 7.6 Hz, 2H), 1.34-1.30 (m, 4H), 0.99 (t, *J* = 7.2 Hz, 3H), 0.90 (t, *J* = 6.8 Hz, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 166.1, 147.8, 143.5, 131.8, 131.3, 130.9, 129.0, 127.3, 126.5, 118.4, 114.6, 43.1, 36.0, 31.6, 31.3, 31.1, 22.7, 20.4, 14.2, 14.0 ppm; IR v_{max} (cm⁻¹) 3426, 1634, 1520, 1239; HRMS (ESI) calcd for C₂₂H₂₉N₃O₃ (M+) 384.2282, found 384.2277.



N-(4-(hexylamino)-3-nitrophenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide, hexyl amine was reacted with *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide to produce *N*-(4-(hexylamino)-3-nitrophenyl)-4-pentylbenzamide as a red solid (m.p. = 132-135°C, 91%). ¹H NMR (400 MHz, CDCl₃) δ 8.21-8.20 (m, 2H), 7.98 (t, *J* = 4.8 Hz, 1H), 7.88 (dd, *J_I* = 2.4 Hz, *J₂* = 9.2 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 2H), 6.78 (d, *J* = 9.2 Hz, 1H), 3.27 (q, *J* = 6.8 Hz, 2H), 2.63 (t, *J* = 7.6 Hz, 2H), 1.71 (p, *J* = 7.2 Hz, 2H), 1.61 (p, *J* = 6.8 Hz, 2H), 1.45-1.29 (m, 10H), 0.92-0.87 (m, 6H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 166.3, 147.6, 143.4, 131.7, 131.5, 130.7, 128.9, 127.3, 126.6, 118.5, 114.4, 43.4, 35.6, 31.7, 31.6, 31.0, 29.1, 26.9, 22.7, 22.7, 14.2 ppm; IR v_{max} (cm⁻¹) 3426, 1634, 1520, 1239; HRMS (ESI) calcd for C₂₄H₃₃N₃O₃ (M+) 412.2595, found 412.2589.



N-(4-(octylamino)-3-nitrophenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide, octyl amine was reacted with *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide to produce *N*-(4-(octylamino)-3-nitrophenyl)-4-pentylbenzamide as a red solid (m.p. = $126-129^{\circ}$ C, 91%). ¹H NMR (400 MHz, CDCl₃) δ 8.21 (d, *J* = 2.4 H, 1H), 8.02 (t, *J* = 4.8 Hz, 1H), 7.94 (dd, *J*₁ = 2.0 Hz, *J*₂ = 8.8 Hz, 1H), 7.87 (bs, 1H), 7.78 (d, *J* = 8.0 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 6.85 (d, *J* = 9.6 Hz, 1H), 3.30 (q, *J* = 7.2 Hz, 2H), 2.66 (t, *J* = 8.4 Hz, 2H), 1.76-1.60 (m, 4H), 1.44-1.29

(m, 14H), 0.91-0.87 (m, 6H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 166.1, 147.7, 143.5, 131.8, 131.3, 130.8, 129.0, 127.3, 126.5, 118.4, 114.6, 43.4, 36.0, 32.0, 31.6, 31.1, 29.5, 29.4, 29.2, 27.3, 22.8, 22.7, 14.3, 14.2 ppm; IR v_{max} (cm⁻¹) 3426, 1634, 1520, 1239; HRMS (ESI) calcd for C₂₆H₃₇N₃O₃ (M+) 440.2908, found 440.2907.



N-(4-(dodecylamino)-3-nitrophenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide, dodecyl amine was reacted with *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide to produce N-(4-(dodecylamino)-3-nitrophenyl)-4-pentylbenzamide as a red solid (m.p. = 125-127 °C, 83%).

¹H NMR (300 MHz, CDCl₃) ö 8.21 (d, J = 3 Hz, 1H), 8.00 (m, 2H), 7.93 (dd, J₁ = 2.1 Hz, J₂ = 9 Hz, 1H), 7.26 (d, J = 7.8 Hz, 2H), 6.83 (d, J = 9.3 Hz, 1H), 3.29 (q, J = 5.4 Hz, 2H), 2.66 (t, J = 7.5 Hz, 2H), 1.72 (p, J = 7.2 Hz, 2H), 1.63 (p, J = 7.2 Hz, 2H), 1.44-1.27 (m, 23H), 0.89 (m, 6H) ppm; ¹³C NMR (100 MHz, CDCl₃) ö 166.3, 147.8, 143.6, 131.9, 131.5, 130.9, 129.1, 127.4, 126.7, 118.5, 114.6, 43.6, 36.2, 32.2, 31.8, 31.2, 30.0, 29.9, 29.9, 29.8, 29.7, 29.6, 29.4, 27.4, 23.0, 22.8, 14.5, 14.3 ppm; IR vmax 3359, 2853, 1650, 1531, 1237 (cm⁻¹); HRMS (ESI) calcd for C₃₀H₄₅N₃O₃ (M+) 496.3534, found 496.3526.



N-(4-(cyclopentylamino)-3-nitrophenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of N-(4-fluoro-3-nitrophenyl)-4cyclopropylamine with N-(4-fluoro-3-nitrophenyl)-4pentylbenzamide, was reacted pentylbenzamide to produce N-(4-(cyclopentylamino)-3-nitrophenyl)-4-pentylbenzamide as an orange solid (m.p. = 123-126 °C, 87%). ¹H NMR (300 MHz, CDCl₃) ö 8.20 (d, J = 2.4 Hz, 1H), 7.94 (s, 1H), 7.90 (d, J = 2.4 Hz, 1H), 7.78 (d, J = 8.4 Hz, 2H), 7.26 (d, J = 8.1 Hz, 2H), 6.89 (d, J = 9.3 Hz, 1H), 3.97 (p, J = 6 Hz, 1H), 2.66 (d, J = 7.5 Hz, 2H), 2.10 (sextet, J = 6.3 Hz, 2H), 1.822-1.606 (m, 8H), 1.345-1.310 (m, 4H), 0.89 (t, J = 6.9 Hz, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) ö 166.5, 147.8, 143.1, 131.9, 131.5, 131.0, 129.1, 127.5, 126.7, 118.7, 115.5, 54.5, 36.2, 33.9, 31.8, 31.2, 24.4, 22.8, 14.4 ppm; IR vmax (cm⁻¹) 3329, 2845, 1675, 1523; HRMS (ESI) calcd for C₂₃H₂₉N₃O₃ (M+) 396.2282, found 396.2268.



N-(4-(4-butylphenylamino)-3-nitrophenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of N-(4-fluoro-3-nitrophenyl)-4pentylbenzamide, 4-pentylaniline with N-(4-fluoro-3-nitrophenyl)-4was reacted pentylbenzamide to produce N-(3-nitro-4-((4-pentylphenyl)amino)phenyl)-4-pentylbenzamide as an orange solid (m.p. = $163-168 \,^{\circ}C$, 37%). ¹H NMR (300 MHz, CDCl₃) ö 9.41 (s, 1H), 8.30 (d, J = 2.4 Hz, 1H), 7.94 (s, 1H), 7.80 (t, J = 8.1 Hz, 3H), 7.29-7.16 (m, 7H), 2.69-2.60 (m, 4H), 1.65 (m, 4H), 1.35 (m, 9H), 0.91-0.87 (m, 6H) ppm; ¹³C NMR (100 MHz, CDCl₃) ö 166.2, 148.0, 141.2, 141.1, 136.4, 131.9, 130.4, 130.0, 129.2, 128.5, 127.4, 124.7, 118.0, 117.1, 36.2, 35.7, 31.8, 31.7, 22.9, 22.8, 14.4, 14.4 ppm; IR vmax (cm⁻¹) 3341, 2955, 2853, 1633, 1539, 1225; HRMS (ESI) calcd for $C_{29}H_{35}N_3O_3$ (M+) 474.2751, found 474.2736.



N-(4-(benzylamino)-3-nitrophenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide, benzylamine was reacted with *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide to produce *N*-(4-(benzylamino)-3-nitrophenyl)-4-pentylbenzamide as a red solid (m.p. = $170-172^{\circ}$ C, 89%). ¹H NMR (400 MHz, CDCl₃) δ 8.40 (t, *J* = 5.2 Hz, 1H), 8.28 (d, *J* = 2.4 Hz, 1H), 7.87 (dd, *J*₁ = 2.4 Hz, *J*₂ = 9.2 Hz, 1H), 7.77 (d, *J* = 8 Hz, 2H), 7.75 (bs, 1H), 7.40-7.26 (m, 7H), 6.85 (d, *J* = 9.2 Hz, 1H), 4.58 (d, J = 6 Hz, 2H), 2.69 (t, J = 7.6 Hz, 2H), 1.64 (p, J = 7.6 Hz, 2H), 1.34-1.30 (m, 4H), 0.90 (t, J = 6.8 Hz, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 166.0, 147.8, 143.0, 137.5, 131.8, 131.5, 131.0, 129.2, 129.1, 128.0, 127.3, 127.2, 127.2, 118.3, 115.0, 47.4, 36.0, 31.6, 31.1, 22.7, 14.2 ppm; IR v_{max} (cm⁻¹) 3426, 1634, 1520, 1239; HRMS (ESI) calcd for C₂₅H₂₇N₃O₃ (M+) 418.2125, found 418.2118.



N-(4-(4-methoxybenzylamino)-3-nitrophenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide, 4-methoxybenzylamine was reacted with *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide to produce N-(4-((4-methoxybenzyl)amino)-3-nitrophenyl)-4-pentylbenzamide as a dark red solid (m.p. = $172-174 \,^{\circ}$ C, 88%). ¹H NMR (300 MHz, CDCl₃) ö 8.29-8.25 (m, 2H), 8.06 (s, 1H), 7.83 (d of d, J₁ = 2.4 Hz, J₂ = 9.3 Hz, 1H), 7.77 (d, J = 8.4 Hz, 2H), 7.27-7.22 (m, 3H), 6.88 (d, J = 9 Hz, 2H), 6.80 (d, J = 9.9 Hz, 1H), 4.45 (d, J = 5.1 Hz, 2H), 3.78 (s, 3H), 2.64 (t, J = 7.2 Hz, 2H), 1.61 (p, J = 7.5 Hz, 2H), 1.32-1.28 (m, 4H), 0.89 (t, J = 6.6 Hz, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) ö 166.3, 159.5, 147.9, 143.0, 131.9 131.5, 131.3, 129.5, 129.1, 128.8, 127.4, 127.2, 118.5, 115.1, 114.7, 55.7, 47.1, 36.1, 31.7, 31.2, 22.8, 14.3 ppm; IR vmax (cm⁻¹) 3397, 2955, 1656, 1528, 1233; HRMS (ESI) calcd for C₂₆H₂₉N₃O₄ (M+) 448.2231, found 448.2215.



N-(3-nitro-4-(phenethylamino)phenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide, 2phenylethanamine was reacted with *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide to produce *N*-(3-nitro-4-(phenethylamino)phenyl)-4-pentylbenzamide as a red solid (m.p. = 154-155°C, 94%). ¹H NMR (400 MHz, CDCl₃) δ 8.21 (d, *J* = 2.4 Hz, 1H), 8.01 (bs, 1H), 7.92 (dd, *J*₁ = 2.8 Hz, *J*₂ = 9.2 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.36-7.33 (m, 2H), 7.28-7.25 (m, 5H), 6.83 (d, *J* = 9.6 Hz, 1H), 3.55 (t, *J* = 6.8 Hz, 2H), 3.01 (t, *J* = 6.8 Hz, 2H), 2.65 (t, *J* = 8.0 Hz, 2H), 1.63 (p, *J* = 8.0 Hz, 2H), 1.34-1.30 (m, 4H), 0.90 (t, *J* = 6.4 Hz, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 166.2, 147.7, 143.0, 138.4, 131.7, 131.3, 131.1, 129.0, 129.0, 128.9, 127.3, 127.0, 126.8, 118.4, 114.4, 44.8, 36.0, 35.5, 31.6, 31.0, 22.7, 14.22 ppm; IR v_{max} (cm⁻¹) 3426, 1636, 1524, 1245; HRMS (ESI) calcd for C₂₆H₂₉N₃O₃ (M+), 4432.2282, found 432.2281.



N-(4-(2-methoxyphenethylamino)-3-nitrophenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide, 2-(2-methoxyphenyl)ethanamine was reacted with *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide to produce *N*-(4-(2-methoxyphenethylamino)-3-nitrophenyl)-4-pentylbenzamide as a red solid (m.p. = 144-146°C, 92%). ¹H NMR (400 MHz, CDCl₃) δ 8.20-8.17 (m, 2H), 7.96-7.94 (m, 2H), 7.79 (d, *J* = 7.6 Hz, 2H), 7.27-7.20 (m, 4H), 6.95-6.89 (m, 3H), 3.90 (s, 3H), 3.53 (q, *J* = 6.4 Hz, 2H), 3.04 (t, *J* = 6.8 Hz, 2H), 2.66 (t, *J* = 7.2 Hz, 2H), 1.64 (p, *J* = 7.6 Hz, 2H), 1.34-1.30 (m, 4H), 0.90 (t, *J* = 7.2 Hz, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 166.1, 157.7, 147.7, 143.4, 131.8, 131.2, 130.9, 130.7, 129.0, 128.4, 127.3, 127.0, 126.5, 120.9, 118.3, 114.6, 110.5, 55.5, 44.1, 36.0, 31.6, 31.0, 30.1, 22.7, 14.2 ppm; IR v_{max} (cm⁻¹) 3426, 1636, 1524, 1450, 1245 1110; HRMS (ESI) calcd for C₂₇H₃₁N₃O₄ (M+), 462.2387, found 462.2383.



N-(4-(3-methoxyphenethylamino)-3-nitrophenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide, 2-(3-methoxyphenyl)ethanamine was reacted with *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide to produce *N*-(4-(3-methoxyphenethylamino)-3-nitrophenyl)-4-pentylbenzamide as a orange solid (m.p. = $105-108^{\circ}$ C, 91%). ¹H NMR (400 MHz, CDCl₃) δ 8.21 (d, *J* = 2.8 Hz, 1H), 8.04 (bs, 1H), 7.94-7.92 (m, 2H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.28-7.24 (m, 3H), 6.87-6.80 (m, 4H), 3.82 (s, 3H), 3.56 (bs, 2H), 2.99 (t, *J* = 7.2 Hz, 2H), 2.66 (t, *J* = 7.2 Hz, 2H), 1.64 (p, *J* = 7.6 Hz, 2H), 1.37-1.30 (m, 4H), 0.90 (t, *J* = 6.8 Hz, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 166.2, 160.1, 147.8, 143.0, 140.0, 131.8, 131.2, 131.1, 130.1, 129.0, 127.3, 126.8, 121.2, 118.4, 114.6, 114.4, 112.5, 55.4, 44.8, 36.0, 35.5, 31.6, 31.1, 22.7, 14.2 ppm; IR v_{max} (cm⁻¹) 3426, 1636, 1524, 1450, 1245 1110; HRMS (ESI) calcd for C₂₇H₃₁N₃O₄ (M+), 462.2387, found 462.2393.



N-(4-(4-methoxyphenethylamino)-3-nitrophenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of N-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide, 2-(4-methoxyphenyl)ethanamine was reacted with N-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide to produce N-(4-(4-methoxyphenethylamino)-3-nitrophenyl)-4-

pentylbenzamide as a orange solid (m.p. = 174-178°C, 88%). ¹H NMR (400 MHz, CDCl₃) δ 8.21 (d, *J* = 2.8 Hz, 1H), 8.05 (t, *J* = 4.8 Hz, 1H), 7.96 (dd, *J*₁ = 2.8 Hz, *J*₂ = 9.6 Hz, 1H), 7.79-7.75 (m, 3H), 7.29 (d, *J* = 8.4 Hz, 2H), 7.19 (d, *J* = 8.4 Hz, 2H), 6.88 (d, *J* = 8.8 Hz, 3H), 3.80 (s, 3H), 3.55 (q, *J* = 7.2 Hz, 2H), 2.97 (t, *J* = 7.2 Hz, 2H), 2.67 (t, *J* = 7.6 Hz, 2H), 1.64 (p, *J* = 8.0 Hz, 2H), 1.34-1.30 (m, 4H), 0.90 (t, *J* = 6.8 Hz, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 166.0, 158.7, 147.8, 143.1, 131.8, 131.1, 130.4, 130.2, 129.9, 129.1, 127.2, 126.7, 118.3, 114.6, 114.5, 55.5, 45.1, 36.0, 34.6, 31.6, 31.1, 22.7, 14.2 ppm; IR v_{max} (cm⁻¹) 3426, 1634, 1520, 1456, 1239 1116; HRMS (ESI) calcd for C₂₇H₃₁N₃O₄ (M+), 462.2387, found 462.2377.



N-(4-(2-(naphthalen-2-yl)ethylamino)-3-nitrophenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide 2-(2-naphthyl)ethylamine was reacted with *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide to produce N-(4-((2-(naphthalen-2-yl)ethyl)amino)-3-nitrophenyl)-4-pentylbenzamide as an orange solid (m.p. = 199-200 °C, 77%). ¹H NMR (400 MHz, DMSO d₆) ö 10.25 (s, 1H), 8.68 (d, J = 2.1 Hz, 1H), 8.18 (t, J = 5.6 Hz, 1H), 7.99 (d of d, J₁ = 2 Hz, J₂ = 9.2 Hz, 1 H), 7.93-7.87 (m, 6H), 7.56-7.49 (m, 3H), 7.39 (d, J = 9.6 Hz, 2H), 7.27 (d, J = 9.6 Hz, 1H), 3.76 (q, J = 7.6 Hz, 2H), 3.17 (t, J = 7.6 Hz, 2H), 2.68 (t, J = 7.6 Hz, 2H), 1.64 (p, J = 8 Hz, 2H), 1.38-1.29 (m, 4H), 0.90 (t, J = 6.8 Hz, 3H) ppm; ¹³C NMR (75 MHz, DMSO d₆) ö 166.1, 147.4, 143.0, 137.5, 134.1, 132.9, 131.6, 130.8, 129.2, 128.9, 128.8, 128.5, 128.5, 128.4, 128.3,

127.9, 127.1, 126.4, 117.3, 115.8, 44.6, 35.9, 35.6, 31.8, 31.3, 22.9, 14.9 ppm; IR vmax (cm⁻¹) 2917, 2849, 1642, 1524 ; HRMS (ESI) calcd for C₃₀H₃₁N₃O₃ (M+) 504.2258, found 504.2250.



N-(4-(2-(naphthalen-1-yl)ethylamino)-3-nitrophenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide, 2-(naphthalen-1-yl)ethanamine was reacted with *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide to N-(4-((4-(1H-indol-2-yl)butyl)amino)-3-nitrophenyl)-4-pentylbenzamide: as a red solid (m.p. = 156-158 °C, 64%). ¹H NMR (300 MHz, CDCl₃) ö 8.20 (d, J = 2.1 Hz, 1H), 8.06 (d, J = 7.8 Hz, 1H), 7.94-7.87 (m, 2H), 7.87 (t, J = 6.3 Hz, 4H), 7.59-7.41 (m, 4H), 7.29 (s, 2H), 6.84 (d, J = 9.3 Hz, 1H), 3.71 (t, J = 7.2 Hz, 2H), 3.50 (t, J = 7.8 Hz, 2H), 2.66 (t, J = 7.5 Hz, 2H), 1.63 (p, J = 7.5 Hz, 2H), 1.33-1.26 (m, 4H), 0.90 (t, J = 6.6 Hz, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) ö166.2, 148.0, 143.1, 134.5, 134.4, 132.0, 131.9, 131.2, 129.4, 129.2, 128.1, 127.6, 127.4, 126.9, 126.7, 126.1, 126.0, 123.5, 118.5, 114.7, 44.1, 36.2, 32.9, 31.7, 31.2, 22.8, 14.3 ppm; IR vmax (cm⁻¹) 2919, 2843, 1645, 1522; HRMS (ESI) calcd for C₃₀H₃₁N₃O₃ (M+) 482.2438, found 482.2421.



N-(3-nitro-4-(2-(pyridin-2-yl)ethylamino)phenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide, 2-(pyridin-2-yl)ethanamine was reacted with *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide to produce *N*-(3-nitro-4-(2-(pyridin-2-yl)ethylamino)phenyl)-4-pentylbenzamide as a orange solid (m.p. = 126-128°C, 88%). ¹H NMR (400 MHz, CDCl₃) δ 8.58 (d, *J* = 4.8 Hz, 1H), 8.26-8.22 (m, 2H), 8.13 (bs, 1H), 7.88 (dd, *J*₁ = 2.4 Hz, *J*₂ = 9.2 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 2H), 7.64 (dt, *J*₁ = 1.2 Hz, *J*₂ = 7.2 Hz, 1H), 7.25-7.16 (m, 4H), 6.87 (d, *J* = 9.6 Hz, 1H), 3.73 (q, *J* = 6.4 Hz, 2H), 3.17 (t, 7.2 Hz, 2H), 2.64 (t, *J* = 7.2 Hz, 2H), 1.62 (p, *J* = 7.6 Hz, 2H), 1.36-1.28 (m, 4H), 0.89 (t, *J* = 7.2 Hz, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 166.2, 158.5, 149.8, 147.6, 143.0, 136.9, 131.8, 131.3, 131.0, 128.9, 127.3, 126.8, 123.7, 122.1, 118.5, 114.3, 42.9, 37.3, 36.0, 31.6, 31.0, 22.7, 14.2 ppm; IR v_{max} (cm⁻¹) 3430, 1640, 1521, 1241; HRMS (ESI) calcd for C₂₅H₂₈N₄O₃ (M+) 433.234, found 433.2229.



N-(4-(2-(1*H*-indol-3-yl)ethylamino)-3-nitrophenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide, tryptamine was reacted with *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide as a red solid (m.p. = $167-171^{\circ}$ C, 86°). ¹H NMR (400 MHz, CDCl₃) δ 8.20 (d, *J* = 2.4 Hz, 1H), 8.10-8.08 (m, 3H), 7.91 (dd, *J*₁ = 2.4 Hz, *J*₂ = 9.2 Hz, 1H), 7.77 (d, 8.0 Hz, 2H), 7.73 (bs, 1H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.22 (t, *J* = 8.0 Hz, 1H), 7.17-7.13 (m, 2H), 6.88 (d, *J* = 9.2 Hz, 1H), 3.64 (q, *J* = 6.8 Hz, 2H), 3.21 (t, *J* = 6.4 Hz, 2H), 2.67 (t, *J* = 7.6 Hz, 2H), 1.64 (p, *J* = 8.0 Hz, 2H), 1.34-1.30 (m, 4H), 0.90 (t, *J* = 7.2 Hz, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 166.0, 147.8, 143.3, 136.7, 131.8, 131.1, 131.0, 129.1, 127.2, 16.6, 122.7, 122.6, 119.8, 118.7, 118.3, 114.7, 112.5, 111.6, 43.5, 36.0, 31.6, 31.1, 25.2, 22.7, 14.2 ppm; IR v_{max} (cm⁻¹) 3426, 1634, 1520, 1456, 1239; HRMS (ESI) calcd for C₂₈H₃₀N₄O₃ (M+), 493.2210 found 493.2209.



N-(4-(2-(1H-benzo[d]imidazol-2-yl)ethylamino)-3-nitrophenyl)-4-pentylbenzamide:

Following the general procedure for the nucleophilic aromatic substitution of *N*-(4-fluoro-3nitrophenyl)-4-pentylbenzamide 2-(2-aminoethyl)benzimidazole dihydrochloride was reacted
with *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide to produce N-(4-((2-(1H-benzo[d]imidazol-2-yl)ethyl)amino)-3-nitrophenyl)-4-pentylbenzamide as an orange solid (m.p. = 207-209 °C, 82%). ¹H NMR (400 MHz, DMSO d₆) ö 12.33 (s, 1H), 10.21 (s, 1H), 8.65 (d, J = 2.8 Hz, 1H), 8.36 (t, J = 6 Hz, 1H), 7.94 (d of d, J₁ = 2.4 Hz, J₂ = 9.2 Hz, 1H), 7.89 (d, J = 8.4 Hz, 2H), 7.56 (d, J = 6.4 Hz, 1H), 7.44 (d, J = 6.4 Hz, 1H), 7.34 (d, J = 8 Hz, 2H), 7.23 (d, J = 10 Hz, 1Hz), 7.15-7.09 (m, 2H), 3.86 (q, J = 6.8 Hz, 2H), 3.19 (t, J = 6.8 Hz, 2H), 2.64 (t, J = 7.2 Hz, 2H), 1.60 (p, J = 7.6 Hz, 2H), 1.34-1.23 (m, 4H), 0.86 (t, J = 6.8 Hz, 3H) ppm; ¹³C NMR (100 MHz, DMSO d₆) ö 166.1, 153.4, 147.3, 144.2, 142.8, 135.2, 132.9, 131.5, 131.1, 129.2, 128.8, 128.5, 122.6, 121.9, 119.2, 117.4, 115.6, 111.8, 41.7, 35.9, 31.8, 31.3, 29.1, 22.9, 14.9 ppm; IR vmax (cm⁻¹) 3354, 2955, 1645, 1512, 1332 ; HRMS (ESI) calcd for C₂₇H₂₉N₅O₃ (M+) 472.2343, found 472.2333.



N-(3-nitro-4-(3-phenylpropylamino)phenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide, 3-phenylpropan-1-amine was reacted with *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide to produce *N*-(3-nitro-4-(3-phenylpropylamino)phenyl)-4-pentylbenzamide as a red solid (m.p. = $150-152^{\circ}$ C, 91°). ¹H NMR (400 MHz, CDCl₃) δ 8.23 (d, *J* = 2.4 Hz, 1H), 8.05 (t, *J* = 5.6 Hz, 1H), 7.93-7.89 (m, 2H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.33-7.20 (m, 5H), 6.78 (d, *J* = 9.2 Hz, 1H), 3.32 (q, *J* = 6.8 Hz, 2H), 2.78 (t, *J* = 7.2 Hz, 2H), 2.66 (t, *J* = 7.6 Hz, 2H), 2.06 (p, *J*

= 7.2 Hz, 2H), 1.63 (t, J = 7.6 Hz, 2H), 1.37-1.30 (m, 4H), 0.90 (t, J = 6.0 Hz, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 166.1, 147.8, 143.3, 141.0, 131.8, 131.3, 131.0, 129.0, 128.8, 128.6, 127.3, 126.7, 126.4, 118.4, 114.5 ppm; IR v_{max} (cm⁻¹) 3426, 1634, 1520, 1239; HRMS (ESI) calcd for C₂₇H₃₁N₃O₃ (M+) 446.2438, found 446.2450.



N-(3-nitro-4-(4-phenylbutylamino)phenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide, 4-phenylbutan-1-amine was reacted with *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide to produce N-(3-nitro-4-((4-phenylbutyl)amino)phenyl)-4-pentylbenzamide as an orange solid (m.p. = 145-148 °C, 86%). ¹H NMR (300 MHz, CDCl₃) ö 8.21 (d, J = 2.4 Hz, 1H), 7.96 (s, 1H), 7.91 (d of d, J₁ = 2.7 Hz, J₂ = 9.3 Hz, 1H), 7.79 (d, J = 8.4 Hz, 2H), 7.32-7.14 (m, 7H), 6.81 (d, J = 9.6 Hz, 1H), 3.30 (t, J = 6.3 Hz, 2H), 2.71-2.63 (m, 4H), 1.77 (m, 4H), 1.63 (p, J = 7.8 Hz, 2H), 1.36-1.28 (m, 4H), 0.90 (t, J = 6.6 Hz, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃) ö 166.3, 147.9, 143.5, 142.1, 131.9, 131.5, 131.0, 129.1, 128.8, 128.7, 127.4, 126.8, 126.3, 118.6, 114.6, 43.4, 36.2, 35.8, 31.8, 31.2, 28.5, 29.0, 28.9, 22.8, 14.4 ppm; IR vmax (cm⁻¹) 2925, 1642, 1527, 1402; HRMS (ESI) calcd for C₂₈H₃₃N₃O₃ (M+) 460.2595, found 460.2580.



N-(4-(4-(1*H*-indol-3-yl)butylamino)-3-nitrophenyl)-4-pentylbenzamide: Following the general procedure for the nucleophilic aromatic substitution of *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide, 4-(1H-indol-2-yl)butan-1-amine was reacted with *N*-(4-fluoro-3-nitrophenyl)-4-pentylbenzamide to N-(4-((4-(1H-indol-2-yl)butyl)amino)-3-nitrophenyl)-4-pentylbenzamide: as an orange solid (m.p. = 179-180 °C, 49%). ¹H NMR (400 MHz, DMSO d₆) ö 10.80 (s, 1H), 10.24 (s, 1H), 8.68 (d, J = 2.4 Hz, 1H), 8.16 (t, J = 5.4 Hz, 1H), 7.95 (d, J = 2.7 Hz, 1H), 7.92 (d, J = 7.8 Hz, 2H), 7.55 (d, J = 7.8 Hz, 1H), 7.39-7.35 (m, 3H), 7.17-7.07 (m, 2H), 6.99 (t, J = 7.5 Hz, 1H), 3.45 (q, J = 6 Hz, 2H), 2.79 (t, J = 6.3 Hz, 2H), 2.68 (t, J = 7.5 Hz, 2H), 1.78 (m, 4H), 1.64 (p, J = 7.8 Hz, 2H), 1.39-1.29 (m, 4H), 0.90 (t, J = 6.3 Hz, 3H) ppm; ¹³C NMR (75 MHz, DMSO d₆) ö 166.1, 147.4, 137.3, 133.8, 133.0, 131.7, 130.7, 129.3, 128.6, 128.2, 123.2, 121.8, 119.3, 119.1, 117.4, 115.7, 115.3, 112.3, 43.2, 35.9, 31.8, 31.4, 29.3, 28.3, 25.3, 26.9, 14.9 ppm; IR vmax (cm⁻¹) 3315, 2975, 1678, 1343; HRMS (ESI) calcd for C₃₀H₃₄N₄O₃ (M+) 499.2704, found 499.2692.

General procedure for the formation of the *N***-1 substituted 2-aminobenzimidazoles:** The appropriate nitro-compound was dissolved in ethanol (0.4 M), and 0.1 equivalents of Pd/C were added to the mixture. The reaction mixture was then heated to reflux. Ammonium formate was

then dissolved in ethanol and added dropwise to the reaction mixture which was allowed to stir until completion, via TLC analysis. The mixture was then cooled to room temperature, and quickly filtered through a pad of celite which was washed with a 1:1 mixture of ethanol and chloroform. The crude product was then placed under an inert atmosphere. Solid cyanogen bromide (10 eq) was then added to the crude product and allowed to stir overnight. The reaction mixture was then concentrated and purified using column chromatography methanol (NH₃ sat) and dichloromethane. The product was then allowed to dry under vacuum overnight. Methanol supplemented with HCl was added to the product forming the HCl salt, which was then dried under high vacuum overnight.



N-(2-amino-1H-benzo[d]imidazol-5-yl)-4-pentylbenzamide hydrochloride: N-(2-amino-1H-benzo[d]imidazol-5-yl)-4-pentylbenzamide hydrochloride was synthesized following the procedure of Huigens *et al.*, *Bioorg Med Chem*, *18*, 663.



N-(2-amino-1-methyl-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide hydrochloride: : N-(4-(methylamino)-3-nitrophenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the *N*-1 substituted 2-aminobenzimidazoles, producing N-(2-amino-1-methyl-1Hbenzo[d]imidazol-5-yl)-4-pentylbenzamide hydrochloride as a white solid (m.p. = decays > 252 °C, 71%). ¹H NMR (300 MHz, CD₃OD) ö 8.01 (d, J = 1.2 Hz, 1H), 7.86 (d, J = 6.3 Hz, 2H), 7.52 (d of d, J₁ = 1.2 Hz, J₂ = 6.6 Hz, 1H), 7.41 (d, J = 6.6 Hz, 1H), 7.32 (d, J = 6.3 Hz, 2H), 3.66 (s, 3H), 2.68 (t, J = 5.7 Hz, 2H), 1.65 (p, J = 5.4 Hz, 2H), 1.40-1.29 (m, 4H), 0.91 (t, J = 4.8 Hz, 3H) ppm; ¹³C NMR (100 MHz, CD₃OD) ö 167.7, 151.1, 147.6, 135.7, 132.2, 129.1, 128.5, 127.9, 127.6, 116.9, 109.8, 104.5, 35.6, 31.4, 31.0, 28.3, 22.4, 13.2 ppm; IR vmax (cm⁻¹) 3237, 2965, 2938, 1673, 1509; HRMS (ESI) calcd for C₂₀H₂₄N₄O (M+) 337.2023, found 337.2020.



N-(2-amino-1-isopropyl-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide hydrochloride: *N*-(4-(isopropylamino)-3-nitrophenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the *N*-1 substituted 2-aminobenzimidazoles, producing *N*-(2-amino-1-isopropyl-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide hydrochloride as a yellow solid (m.p. 155-164°C, 78%). ¹H NMR (400 MHz, CD₃OD) δ 8.06 (d, *J* = 2.0 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 2H), 7.63 (d, *J* = 8.8 Hz, 1H), 7.51 (dd, *J*₁ = 2.0 Hz, *J*₂ = 8.4 Hz, 1H), 7.33 (d, *J* = 8.0 Hz, 2H), 4.75 (septet, *J* = 6.4 Hz, 1H), 2.67 (t, *J* = 7.6 Hz, 2H), 1.67-1.62 (m, 8H), 1.39-1.32 (m, 4H), 0.91 (t, *J* = 6.8 Hz, 3H) ppm; ¹³C NMR (100 MHz, CD₃OD) δ 169.1, 151.1, 149.0, 136.9, 133.5, 131.0, 129.8, 128.9, 126.7, 117.9, 113.6, 106.0, 36.9, 32.7, 32.3, 23.7, 20.4, 14.5 ppm; IR v_{max}

(cm⁻¹) 3237, 2965, 2938, 1673, 1509; HRMS (ESI) calcd for $C_{22}H_{29}N_4O$ (M+) 365.2336, found 365.2339.



N-(2-amino-1-butyl-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide hydrochloride: *N*-(4-(butylamino)-3-nitrophenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the *N*-1 substituted 2-aminobenzimidazoles, producing *N*-(2-amino-1-butyl-1*H*benzo[*d*]imidazol-5-yl)-4-pentylbenzamide hydrochloride as a yellow solid (m.p. 122-126°C, 81%). ¹H NMR (400 MHz, CD₃OD) δ 8.02 (d, *J* = 2.0 Hz, 1H), 7.86 (d, *J* = 8.4 Hz, 2H), 7.54 (dd, *J*₁ = 2.0 Hz, *J*₂ = 8.8 Hz, 1H), 7.42 (d, *J* = 8.8 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 2H), 4.12 (t, *J* = 7.2 Hz, 2H), 2.66 (t, *J* = 7.2 Hz, 2H), 1.77 (p, *J* = 7.2 Hz, 2H), 1.64 (p, *J* = 7.2 Hz, 2H), 1.48-1.30 (m, 6H), 0.98 (t, *J* = 7.6 Hz, 3H), 0.90 (t, *J* = 6.4 Hz, 3H) ppm; ¹³C NMR (100 MHz, CD₃OD) δ 168.9, 115.7, 148.8, 137.0, 133.4, 130.4, 129.8, 128.9, 128.5, 118.3, 111.5, 105.9, 44.0, 36.9, 32.7, 32.2, 31.3, 23.7, 21.0, 14.5, 14.2 ppm; IR vmax (cm⁻¹) 3237, 2965, 2938, 1673, 1509; HRMS (ESI) calcd for C₂₃H₃₁N₄O (M+) 379.2492, found 379.2500.



N-(2-amino-1-hexyl-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide hydrochloride: *N*-(4-(hexylamino)-3-nitrophenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the *N*-1 substituted 2-aminobenzimidazoles, producing *N*-(2-amino-1-hexyl-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide hydrochloride as a yellow solid (m.p. 122-126°C, 81%). ¹H NMR (400 MHz, CD₃OD) δ 8.00 (d, *J* = 1.2 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 2H), 7.54 (dd, *J*₁ = 2.0 Hz, *J*₂ = 8.8 Hz, 1H), 7.39 (d, *J* = 8.8 Hz, 1H), 7.28 (d, *J* = 8.0 Hz, 1H), 4.10 (t, *J* = 6.8 Hz, 2H), 2.64 (t, *J* = 7.6 Hz, 2H), 1.77 (p, *J* = 6.8 Hz, 2H), 1.62 (p, *J* = 7.6 Hz, 2H), 1.37-1.28 (m, 10H), 0.90-0.86 (m, 6H) ppm; ¹³C NMR (100 MHz, CD₃OD) δ 168.8, 151.6, 148.8, 137.0, 133.3, 130.3, 129.8, 128.9, 128.4, 118.2, 111.4, 105.9, 44.1, 36.9, 32.7, 32.2, 29.2, 27.4, 23.7, 23.7, 14.5, 14.5 ppm; IR vmax (cm⁻¹) 3237, 2965, 2938, 1673, 1509; HRMS (ESI) calcd for C₂₅H₃₄N₄O (M+) 407.2805, found 407.2803.



N-(2-amino-1-octyl-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide hydrochloride: *N*-(4-(octylamino)-3-nitrophenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the *N*-1 substituted 2-aminobenzimidazoles, producing *N*-(2-amino-1-octyl-1*H*benzo[*d*]imidazol-5-yl)-4-pentylbenzamide hydrochloride as a yellow solid (m.p. 122-126°C, 71%). ¹H NMR (400 MHz, CD₃OD) δ 8.03 (d, *J* = 2.0 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 2H), 7.53 (dd, *J*₁ = 2.0 Hz, *J*₂ = 8.8 Hz, 1H), 7.43 (d, *J* = 8.8 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 1H), 4.12 (t, *J* = 6.8 Hz, 2H), 2.68 (t, *J* = 7.6 Hz, 2H), 1.80 (p, *J* = 6.8 Hz, 2H), 1.65 (p, *J* = 7.6 Hz, 2H), 1.37-1.28 (m, 14H), 0.92-0.86 (m, 6H) ppm; ¹³C NMR (100 MHz, CD₃OD) δ 169.0, 151.7, 148.9, 137.1, 133.5, 130.4, 129.8, 128.9, 128.5, 118.3, 111.5, 106.0, 44.1, 36.9, 33.0, 32.7, 32.3, 30.5, 30.4, 29.2, 27.7, 23.8, 23.7, 14.6, 14.5 ppm IR vmax (cm⁻¹) 3237, 2965, 2938, 1673, 1509; HRMS (ESI) calcd for C₂₇H₃₈N₄O (M+) 435.3118, found 435.3113.



N-(2-amino-1-dodecyl-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide hydrochloride: N-(4-(dodecylamino)-3-nitrophenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the *N*-1 substituted 2-aminobenzimidazoles, producing N-(2-amino-1-dodecyl-1H-benzo[d]imidazol-5-yl)-4-pentylbenzamide hydrochloride a purple solid (m.p. = decays >78 °C, 45%). ¹H NMR (300 MHz, CD₃OD) ö 8.05 (d, J = 1.5 Hz, 1H), 7.87 (d, J = 8.4 Hz, 2H), 7.53 (d of d, J₁ = 1.8 Hz, J₂ = 8.7 Hz, 1H), 7.44 (d, J = 8.7 Hz, 1H) 7.34 (d, J = 8.4 Hz, 2H), 4.14 (t, J = 7.5 Hz, 2H), 2.69 (t, J = 7.5 Hz, 2H), 1.81 (p, J = 7.2 Hz, 2H), 1.66 (p, J = 7.8 Hz, 2H), 1.37-1.20 (m, 24H), 0.93-0.86 (m, 6H) ppm; ¹³C NMR (100 MHz, CD₃OD) ö 167.7, 150.5, 147.6. 135.8, 132.2, 129.2, 128.5, 127.6, 127.2, 116.9, 110.2, 104.6, 94.6, 42.8, 35.6, 31.9, 31.4, 31.0, 29.6, 29.4, 29.4, 29.3, 29.2, 27.9, 26.4, 22.5, 22.4, 13..3, 13.2; IR vmax (cm⁻¹) 3249, 2956, 2933, 2854, 1668, 1501; HRMS (ESI) calcd for C₃₁H₄₆N₄O (M+) 491.3744, found 491.3734.



N-(2-amino-1-cyclopentyl-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide hydrochloride: N-(4-(cvclopentylamino)-3-nitrophenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the N-1 substituted 2-aminobenzimidazoles, producing N-(2amino-1-cyclopentyl-1H-benzo[d]imidazol-5-yl)-4-pentylbenzamide hydrochloride as a white solid (m.p. = decays > 136 °C, 31%). ¹H NMR (300 MHz, CD₃OD) \ddot{o} 8.11 (s, 1H), 7.90 (d, J = 8.1 Hz, 2H), 7.52 (s, 2H), 7.38 (d, J = 8.1 Hz, 2H), 2.73 (d, J = 7.5 Hz, 2H), 2.22-2.10 (m, 6H), 1.88 (m, 2H), 1.70 (p, J = 7.5 Hz, 2H), 1.40-1.37 (m, 4H), 0.95 (t, J = 6.9 Hz, 3H) ppm; ^{13}C NMR (75 MHz, CD₃OD) ö 169.8, 152.6, 149.7, 137.7, 134.2, 131.9, 130.6, 129.6, 127.0, 118.5, 114.0, 106.9, 58.2, 37.6, 33.4, 33.0, 30.6, 26.6, 24.4, 15.2 ppm; IR vmax (cm⁻¹) 3250, 2955, 2963, 1671, 1502; HRMS (ESI) calcd for C₂₄H₃₀N₄O (M+) 391.2492, found 391.2481



N-(2-amino-1-(4-pentylphenyl)-1H-benzo[d]imidazol-5-yl)-4-pentylbenzamide: N-(3-nitro-4-((4-pentylphenyl)amino)phenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the N-1 substituted 2-aminobenzimidazoles, producing N-(2-amino-1-(4pentylphenyl)-1H-benzo[d]imidazol-5-yl)-4-pentylbenzamide pentylbenzamide hydrochloride as a light blue solid (m.p. = decays > 130 °C, 44%). ¹H NMR (300 MHz, CD₃OD) \ddot{o} 8.16 (d, J = 1.8

Hz, 1H), 7.90 (d, 8.4 Hz, 2H), 7.55 (q, J = 8.4 Hz, 4H), 7.48 (d of d, $J_1 = 1.8$ Hz, $J_2 = 8..47$ Hz, 1H), 7.37 (d, J = 8.4 Hz, 2H), 7.02 (d, J = 9 Hz, 1H), 2.81 (t, J = 7.5 Hz, 2H), 2.73 (t, J = 7.5 Hz, 2H), 1.78-1.65 (m, 4H), 1.47-1.31 (m, 8H), 1.00-0.92 (m, 6H) ppm; ¹³C NMR (75 MHz, CD₃OD) ö 169.8, 149.7, 148.3, 138.1, 134.2, 132.8, 131.4, 130.7, 130.6, 129.6, 129.2, 119.1, 112.2, 106.8, 37.6, 37.5, 33.5, 33.4, 33.1, 24.5, 24.4, 15.2 ppm; IR vmax (cm⁻¹) 3258, 2959, 1668, 1501; HRMS (ESI) calcd for C₃₀H₃₆N₄O (M+) 469.2962, found 469.2943.



N-(2-amino-1-benzyl-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide hydrochloride: N-(4-(benzylamino)-3-nitrophenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the *N*-1 substituted 2-aminobenzimidazoles, producing N-(2-amino-1-benzyl-1Hbenzo[d]imidazol-5-yl)-4-pentylbenzamide hydrochloride as a faint pink solid (m.p. = decays > 140 °C, 19%). ¹H NMR (400 MHz, CD₃OD) ö 8.11 (d, J = 2 Hz, 1H), 7.89 (d, J = 8 Hz, 1H), 7.48-7.31 (m, 9H), 5.44 (s, 2H), 2.72 (t, J = 7.6 Hz, 2H), 1.69 (p, J = 7.6 Hz, 2H), 1.39-1.32 (m, 4H) 0.94 (t, J = 6.4 Hz, 3H) ppm; ¹³C NMR (100 MHz, CD₃OD) ö 169.8, 153.0, 138.0, 136.2, 134.2, 131.3, 131.1, 130.6, 130.3, 129.6, 129.2, 128.8, 119.0, 112.6, 106.8, 47.9, 37.6, 33.4, 33.0, 24.4, 15.2 ppm; IR vmax (cm⁻¹) 3255, 2951, 2934, 1660, 1496; HRMS (ESI) calcd for C₂₆H₂₈N₄O (M+) 413.2336, found 413.2332.



N-(2-amino-1-(4-methoxybenzyl)-1H-benzo[d]imidazol-5-yl)-4-pentylbenzamide

hydrochloride: N-(4-((4-methoxybenzyl)amino)-3-nitrophenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the *N*-1 substituted 2-aminobenzimidazoles, producing N-(2-amino-1-(4-methoxybenzyl)-1H-benzo[d]imidazol-5-yl)-4-pentylbenzamide hydrochloride as a white solid (m.p. = decays > 238 °C, 32%). ¹H NMR (400 MHz, CD₃OD) ö 8.10 (d, J = 2 Hz, 1H), 7.89 (d, J = 8.4 Hz, 2H), 7.46 (d of d, J₁ = 2 Hz, J₂ = 8.8 Hz, 1H), 7.38-7.28 (m, 5H), 6.96 (2, J = 8.8 Hz, 2H), 5.35 (s, 2H), 3.80 (s, 3H), 2.72 (t, J = 7.6 Hz, 2H), 1.69 (p, J = 8 Hz, 2H), 1.45-1.32 (m, 4H), 0.96 (t, J = 6.8 Hz, 3H) ppm; ¹³C NMR (100 MHz, CD₃OD) ö 167.8, 160.1, 150.8, 147.6, 135.9, 132.1, 129.3, 128.5, 128.4, 127.5, 127.1 126.0, 116.9, 114.3, 110.7, 104.7, 54.6, 45.5, 35.6, 31.4, 31.0, 22.4, 13.2 ppm; IR vmax (cm⁻¹) 3251, 2961, 2940, 1669, 1508, 1221; HRMS (ESI) calcd for C₂₇H₃₀N₄O₂ (M+) 443.2442, found 443.2422



N-(2-amino-1-phenethyl-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide hydrochloride: *N*-(3-nitro-4-(phenethylamino)phenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the *N*-1 substituted 2-aminobenzimidazoles, producing *N*-(2-amino-1-phenethyl-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide hydrochloride as a yellow solid (m.p. 103-106°C, 89%). ¹H NMR (400 MHz, CD₃OD) δ 7.99 (d, *J* = 2.0 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.42 (dd, *J*₁ = 2.0 Hz, *J*₂ = 8.8 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.24-7.16 (m, 5H), 7.13-7.11 (m, 2H), 4.37 (t, *J* = 6.8 Hz, 2H), 3.10 (t, *J* = 6.4 Hz, 2H), 2.68 (t, *J* = 7.2 Hz, 2H), 1.65 (p, *J* = 7.6 Hz, 2H), 1.38-1.31 (m, 4H), 0.90 (t, *J* = 7.2 Hz, 3H) ppm; ¹³C NMR (100 MHz, CD₃OD) δ 169.0, 151.8, 148.9, 138.5, 136.9, 133.4, 130.2, 129.9, 129.8, 128.9, 128.3, 128.3, 118.0, 111.6, 105.7, 45.5, 36.9, 34.8, 32.7, 32.3, 23.7, 14.5 ppm; IR vmax (cm⁻¹) 3250, 2948, 2940, 1674, 1502; HRMS (ESI) calcd for C₂₇H₃₀N₄O (M+) 427.2492, found 427.2489.



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N-(2-amino-1-(2-methoxyphenethyl)-1H-benzo[d]imidazol-5-yl)-4-pentylbenzamide

hydrochloride: *N*-(4-(2-methoxyphenethylamino)-3-nitrophenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the *N*-1 substituted 2-aminobenzimidazoles, producing *N*-(2-amino-1-(2-methoxyphenethyl)-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide hydrochloride as a pink solid (m.p. 111-114°C, 72%). ¹H NMR (400 MHz, CD₃OD) δ 7.99 (d, *J* = 2.0 Hz, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.37-7.29 (m, 3H), 7.17-7.09 (m, 2H), 6.97 (d, *J* = 8.8 Hz, 1H), 6.83-6.75 (m, 2H), 4.34 (t, *J* = 6.4 Hz, 2H), 3.63 (s, 3H), 3.11 (t, *J* = 6.8 Hz, 2H), 2.69 (t, *J* = 7.2 Hz, 2H), 1.66 (p, *J* = 7.6 Hz, 2H), 1.37-1.29 (m, 4H), 0.91 (t, *J* = 6.4 Hz, 3H) ppm; ¹³C NMR (100 MHz, CD₃OD) δ 168.8, 159.1, 151.8, 148.8, 136.6, 133.4, 131.9, 130.0, 129.9, 129.8, 128.8, 128.7, 126.5, 121.9, 117.8, 111.4, 111.3, 105.4, 55.8, 44.3, 36.9, 32.7, 32.2, 29.7, 23.7, 14.5 ppm; IR vmax (cm⁻¹) 3250, 2948, 2940, 1674, 1502, 1247, 1040; HRMS (ESI) calcd for C₂₈H₃₂N₄O₂ (M+) 457.2598, found 457.2600.



N-(2-amino-1-(3-methoxyphenethyl)-1H-benzo[d]imidazol-5-yl)-4-pentylbenzamide hydrochloride: N-(4-(3-methoxyphenethylamino)-3-nitrophenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the N-1 substituted 2-

aminobenzimidazoles, producing *N*-(2-amino-1-(3-methoxyphenethyl)-1*H*-benzo[*d*]imidazol-5yl)-4-pentylbenzamide hydrochloride as a pink solid (m.p. 113-116°C, 72%). ¹H NMR (400 MHz, CD₃OD) δ 8.01 (d, *J* = 1.6 Hz, 1H), 7.86 (d, *J* = 8.4 Hz, 2H), 7.41 (dd, *J*₁ = 1.6 Hz, *J*₂ = 8.8 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.22 (d, *J* = 8.8 Hz, 1H), 7.13 (t, *J* = 8.0 Hz, 1H), 6.75 (dd, *J*₁ = 1.6 Hz, *J*₂ = 8.4 Hz, 1H), 6.70 (d, *J* = 7.2 Hz, 1H), 6.66 (d, *J* = 2.0 Hz, 1H), 4.39 (t, *J* = 6.8 Hz, 2H), 3.68 (s, 3H), 3.09 (t, *J* = 6.4 Hz, 2H), 2.69 (t, *J* = 7.6 Hz, 2H), 1.66 (p, *J* = 7.6 Hz, 2H), 1.36-1.32 (m, 4H), 0.91 (t, *J* = 7.2 Hz, 3H) ppm; ¹³C NMR (100 MHz, CD₃OD) δ 169.0, 161.6, 151.9, 148.9, 139.9, 137.0, 133.5, 131.0, 130.3, 129.9, 128.9, 128.4, 122.5, 148.0, 115.7, 113.9, 111.7, 105.8, 55.8, 45.4, 36.9, 34.8, 32.7, 32.3, 23.7, 14.5 ppm; IR vmax (cm⁻¹) 3250, 2948, 2940, 1674, 1502, 1247, 1040; HRMS (ESI) calcd for C₂₈H₃₂N₄O₂ (M+) 457.2598, found 457.2591.



N-(2-amino-1-(4-methoxyphenethyl)-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide

hydrochloride: *N*-(4-(4-methoxyphenethylamino)-3-nitrophenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the *N*-1 substituted 2-aminobenzimidazoles, producing *N*-(2-amino-1-(4-methoxyphenethyl)-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide hydrochloride as a pink solid (m.p. 164° C (decomposition), 72%). ¹H

NMR (400 MHz, CD₃OD) δ 7.99 (d, J = 2.0 Hz, 1H), 7.86 (d, J = 8.4 Hz, 2H), 7.43 (dd, $J_1 = 1.6$ Hz, $J_2 = 8.4$ Hz, 1H), 7.32 (d, J = 8.0 Hz, 2H), 7.20 (d, J = 8.8 Hz, 1H), 7.01 (d, J = 8.4 Hz, 2H), 6.76 (d, J = 8.8 Hz, 2H), 4.33 (t, J = 6.4 Hz, 2H), 3.71 (s, 3H), 3.03 (t, J = 6.4 Hz, 2H), 2.68 (t, J = 7.2 Hz, 2H), 1.65 (p, J = 8.0 Hz, 2H), 1.35-1.27 (m, 4H), 0.91 (t, J = 7.2 Hz, 3H) ppm; ¹³C NMR (100 MHz, CD₃OD) δ 169.0, 160.5, 151.8, 14.9, 136.9, 133.4, 131.3, 130.3, 130.2, 129.8, 128.9, 128.3, 118.0, 115.2, 111.7, 105.8, 55.8, 45.7, 36.9, 34.0, 32.7, 32.3, 23.7, 14.5 ppm IR vmax (cm⁻¹) 3250, 2948, 2940, 1674, 1502, 1247, 1040; HRMS (ESI) calcd for C₂₈H₃₂N₄O₂ (M+) 457.2598, found 457.2567.



N-(2-amino-1-(2-(naphthalen-2-yl)ethyl)-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide hydrochloride: N-(4-((2-(naphthalen-2-yl)ethyl)amino)-3-nitrophenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the *N*-1 substituted 2aminobenzimidazoles, producing N-(2-amino-1-(2-(naphthalen-2-yl)ethyl)-1Hbenzo[d]imidazol-6-yl)-4-pentylbenzamide hydrochloride as a light brown solid (m.p. = decays > 165 °C, 28%), ¹H NMR (400 MHz, CD₃OD) ö 8.04 (d, J = 1.6 Hz, 1H), 7.88 (d, J = 8.8 Hz, 2H), 7.83-7.79 (m, 2H), 7.74-7.72 (m, 1H), 7.57 (s, 1H), 7.48-7.42 (m, 2H), 7.40-7.30 (m, 5H), 4.52 (t, J = 6.8 Hz, 2H), 3.32 (t, J = 6.8 Hz, 2H), 2.73 (t, J = 8 Hz, 2H), 1.69 (p, J = 8 Hz, 2H), 1.43-1.31 (m, 4H), 0.94 (t, J = 6.8 Hz, 3H) ppm; ¹³C NMR (100 MHz, CD₃OD) ö 169.8, 152.6, 149.7, 137.7, 136.7, 135.8, 134.8, 134.2, 131.1, 130.6, 130.4, 129.6, 129.6, 129.5, 129.4, 129.1, 129.0, 128.1, 127.7, 118.8, 112.4, 106.5, 46.0, 37.6, 35.7, 33.4, 33.0, 24.4, 15.2 ppm; IR vmax (cm⁻¹) 3310, 2867, 2843, 1671, 1532; HRMS (ESI) calcd for $C_{31}H_{32}N_4O$ (M+) 477.2649, found 477.2635.



N-(2-amino-1-(2-(naphthalen-1-yl)ethyl)-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide hydrochloride: N-(4-((4-(1H-indol-2-yl)butyl)amino)-3-nitrophenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the *N*-1 substituted 2aminobenzimidazoles, producing N-(4-((4-(1H-indol-2-yl)butyl)amino)-3-nitrophenyl)-4pentylbenzamide hydrochloride as a white solid (m.p. = decays > 160 °C, 70%), ¹H NMR (400 MHz, CD₃OD) ö 7.98 (d, J = 7.2 Hz, 1H), 7.92 (d, J = 2.4 Hz, 1H), 7.85 (d of d, J₁ = 2 Hz, J₂ = 8.4 Hz, 3H), 7.73 (d, J = 8 Hz, 1H), 7.52-7.47 (m, 2H), 7.35 (d of d, J₁ = 2.4 Hz, J₂ = 8.4 Hz, 2H), 7.27 (t, J = 7.6 Hz, 1H), 7.22-7.16 (m, 2H), 6.67 (d, J = 8.8 Hz, 1H), 4.56 (t, J = 6 Hz, 2H), 3.63 (t, J = 6.8 Hz, 2H), 2.71 (t, J = 7.6 Hz, 2H), 1.68 (p, J = 7.2 Hz, 2H), 1.38-1.36 (m, 5H), 0.94 (t, J = 6.8 Hz, 3H) ppm; ¹³C NMR (100 MHz, CD₃OD) ö 168.8, 151.6, 148.7, 136.6, 135.4, 134.6, 133.3, 133.2, 130.0, 129.9, 129.7, 129.0, 128.7, 128.5, 128.3, 127.4, 126.8, 126.5, 123.8, 117.5, 111.0, 105.4, 44.9, 36.7, 32.5 32.1, 31.4, 23.5, 14.4 ppm; IR vmax (cm⁻¹) 3313, 2874, 2853, 1668, 1541; HRMS (ESI) calcd for C₃₁H₃₂N₄O (M+) 477.2649, found 477.2644.



N-(2-amino-1-(2-(pyridin-2-yl)ethyl)-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide

hvdrochloride: N-(3-nitro-4-(2-(pyridin-2-yl)ethylamino)phenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the N-1 substituted 2aminobenzimidazoles, producing N-(2-amino-1-(2-(pyridin-2-yl)ethyl)-1H-benzo[d]imidazol-5yl)-4-pentylbenzamide hydrochloride red solid (m.p. 181-184°C. 9 as а %). ¹H NMR (300 MHz, CD₃OD) δ 8.93 (m, 1H), 8.80 (m, 1H), 8.64 (d, J = 8.1 Hz, 1H), 8.08-8.04 (m, 2H), 7.86 64 (d, J = 8.4 Hz, 2H), 7.49 (dd, $J_1 = 2.1$ Hz, $J_2 = 9.0$ Hz, 1H), 7.40-7.34 (m, 2H), 4.56 (t, J = 7.2 Hz, 2H), 3.43 (t, J = 7.5 Hz, 2H), 2.71 (t, J = 7.5 Hz, 2H), 1.67 (p, J = 6.9 Hz, 2H), 1.37-1.29 (m, 4H), 0.92 (t, J = 6.9 Hz, 3H)) ppm; ¹³C NMR (100 MHz, CD₃OD) δ 168.8, 159.1, 151.8, 148.8, 136.6, 133.4, 131.9, 129.9, 129.8, 128.8, 128.7, 126.5, 121.9, 117.8, 111.4, 111.3, 105.4, 44.4, 36.9, 32.7, 32.3, 5*.6, 23.7, 14.5 ppm; IR vmax (cm⁻¹) 3321,2984, 1683, 1543, 1246; HRMS (ESI) calcd for C₂₆H₂₉N₅O (M+) 428.2445, found 428.2452



N-(1-(2-(1*H*-indol-3-yl)ethyl)-2-amino-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide

hydrochloride: *N*-(4-(2-(1*H*-indol-3-yl)ethylamino)-3-nitrophenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the *N*-1 substituted 2-aminobenzimidazoles, producing *N*-(1-(2-(1*H*-indol-3-yl)ethyl)-2-amino-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide hydrochloride as a white solid (m.p. 175°C (decomposition), 65%). ¹H NMR (400 MHz, CD₃OD) δ 7.90 (d, *J* = 1.6 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 2H), 7.33-7.26 (m, 4H), 7.22 (d, *J* = 8.0 Hz, 1H), 7.03 (t, *J* = 7.6 Hz, 1H), 6.94-6.89 (m, 3H), 4.30 (t, *J* = 6.0 Hz, 2H), 3.19 (t, *J* = 6.0 Hz, 2H), 2.64 (t, *J* = 7.6 Hz, 2H), 1.61 (p, *J* = 7.2 Hz, 2H), 1.39-1.26 (m, 4H), 0.89 (t, *J* = 6.8 Hz, 3H) ppm; ¹³C NMR (100 MHz, CD₃OD) δ 168.8, 151.6, 148.8, 138.1, 136.7, 133.4, 130.1, 129.8, 128.8, 128.6, 128.5, 124.5, 122.6, 120.1, 118.5, 117.4, 112.6, 111.3, 111.1, 105.6, 45.3, 36.8, 32.7, 32.2, 24.6, 23.7, 14.5 ppm; IR vmax (cm⁻¹) 3210, 2983, 2852, 1665, 1543, 1265; HRMS (ESI) calcd for C₂₉H₃₁N₅O (M+) 466.2601, found 466.2599.



N-(1-(2-(1H-benzo[d]imidazol-2-yl)ethyl)-2-amino-1H-benzo[d]imidazol-5-yl)-4-

pentylbenzamide hydrochloride: N-(4-((2-(1H-benzo[d]imidazol-2-yl)ethyl)amino)-3nitrophenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the *N*-1 substituted 2-aminobenzimidazoles, producing N N-(1-(2-(1H-benzo[d]imidazol-2-yl)ethyl)-2-amino-1H-benzo[d]imidazol-5-yl)-4-pentylbenzamide hydrochloride as a white solid (m.p. = decays > 225 °C, 38%). ¹H NMR (400 MHz, CD₃OD) ö 8.07 (d, J = 2 Hz, 1H), 7.84 (d, J = 8 Hz, 2H), 7.76-7.74 (m, 2H), 7.59-7.57 (m, 2H), 7.34-7.30 (m, 3H), 7.21 (d, J = 8.8 Hz, 1H), 4.77 (t, J = 7.2 Hz, 2H), 3.73 (t, J = 6.4 Hz, 2H), 2.69 (t, J = 7.6 Hz, 2H), 1.66 (p, J = 7.2 Hz, 2H), 1.36-1.29 (m, 4H), 0.91 (t, J = 7.2 Hz, 3H) ppm; ¹³C NMR (100 MHz, CD₃OD) ö 169.8, 152.5, 151.9, 149.7, 138.1, 134.1, 133.6, 131.3, 130.6, 129.5, 128.6, 128.5, 118.9, 115.8, 111.3, 106.9, 42.5, 37.6, 33.4, 33.0, 27.7, 24.4, 15.2 ppm; IR vmax (cm⁻¹) 3321,2984, 1683, 1543, 1246; HRMS (ESI) calcd for C₂₈H₃₀N₆O (M+) 467.2554, found 467.2545.



N-(2-amino-1-(3-phenylpropyl)-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide

hydrochloride: *N*-(3-nitro-4-(3-phenylpropylamino)phenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the *N*-1 substituted 2-aminobenzimidazoles, producing *N*-(2-amino-1-(3-phenylpropyl)-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide hydrochloride as a yellow solid (m.p. 154°C (decomposition), 69%). ¹H NMR (400 MHz, CD₃OD) δ 8.00 (d, *J* = 1.6 Hz, 1H), 7.86 (d, *J* = 8.4 Hz, 2H), 7.50 (dd, *J*₁ = 1.6 Hz, *J*₂ = 8.8 Hz, 1H), 7.34-7.29 (m, 3H), 7.26-7.23 (m, 2H), 7.19-7.14 (m, 3H), 4.17 (t, *J* = 6.8 Hz, 2H), 2.74 (t, *J* = 7.6 Hz, 2H), 2.68 (t, *J* = 7.2 Hz, 2H), 2.14 (p, *J* = 7.6 Hz, 2H), 1.65 (p, *J* = 8.0 Hz, 2H),1.39-1.31 (m, 4H), 0.91 (t, *J* = 7.2 Hz, 3H) ppm; ¹³C NMR (100 MHz, CD₃OD) δ 169.4, 152.9, 149.2, 142.3, 137.4, 133.8, 130.8, 130.2, 130.4, 129.8, 129.2, 128.8, 127.8, 118.6, 111.7, 106.3, 44.1, 37.2, 34.1, 33.1, 32.6, 30.9, 24.0, 14.9 ppm; IR vmax (cm⁻¹) 3250, 2948, 2940, 1674, 1502; HRMS (ESI) calcd for C₂₈H₃₂N₄O (M+) 441.2649, found 441.2646.



N-(2-amino-1-(4-phenylbutyl)-1H-benzo[d]imidazol-5-yl)-4-pentylbenzamide

hydrochloride: N-(4-(methylamino)-3-nitrophenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the *N*-1 substituted 2-aminobenzimidazoles, producing N-(2-amino-1-(4-phenylbutyl)-1H-benzo[d]imidazol-5-yl)-4-pentylbenzamide hydrochloride as a faint pink solid (m.p. = decays > 187 C, 50%). ¹H NMR (400 MHz, CD₃OD) ö 8.05 (d, J = 1.6 Hz, 1H), 7.90 (d, J = 8.4 Hz, 2H), 7.54 (d of d, J₁ = 2 Hz, J₂ = 8.8 Hz, 1H), 7.41-7.34 (m, 3H), 7.28-7.24 (m, 2H), 7.19-7.15 (m, 3H), 4.16 (t, J = 6.8 Hz, 2H), 2.70 (q, J = 8.4 Hz, 4H), 1.89-1.64 (m, 6H), 1.42-1.32 (m, 4H), 0.93 (t, J = 7.2 Hz, 3H) ppm; ¹³C NMR (100 MHz, CD₃OD) ö 167.7, 150.4, 147.6, 141.8, 135.7, 132.1, 129.1, 128.5, 128.2, 127.6, 127.2, 125.8, 116.9, 110.2, 104.7, 42.6, 35.6, 35.1, 31.4, 31.0, 28.2, 27.3, 22.4, 13.2 ppm; IR vmax (cm⁻¹) 3250, 2948, 2940, 1674, 1502; HRMS (ESI) calcd for C₂₆H₂₈N₄O (M+) 455.2805, found 455.2790.



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N-(1-(4-(1*H*-indol-3-yl)butyl)-2-amino-1*H*-benzo[*d*]imidazol-5-yl)-4-pentylbenzamide

hydrochloride: N-(4-((4-(1H-indol-2-yl)butyl)amino)-3-nitrophenyl)-4-pentylbenzamide was subjected to the general procedure for the formation of the *N*-1 substituted 2-aminobenzimidazoles, producing N-(1-(4-(1H-indol-3-yl)butyl)-2-amino-1H-benzo[d]imidazol-5-yl)-4-pentylbenzamide hydrochloride as a brown solid (m.p. = decays > 120 °C, 35%), ¹H NMR (300 MHz, CD₃OD) ö 8.03 (d, J = 1.5 Hz, 1H), 7.90 (d, J = 8.7 Hz, 2H), 7.51-7.45 (m, 2H), 7.39-7.30 (m, 4H), 7.10 (d of t, J₁ = 1.2 Hz, J₂ = 7.2 Hz, 1H), 7.02-6.96 (m, 2H), 4.14 (t, J = 6.3 Hz, 2H), 2.85 (t, J = 6.6 Hz, 2H), 2.73 (t, J = 7.5 Hz, 2H), 1.89-1.87 (m, 4H), 1.70 (p, J = 7.8 Hz, 2H), 1.40-1.31 (m, 5H), 0.95 (t, J = 6.9 Hz, 3H) ppm; ¹³C NMR (100 MHz, CD₃OD) ö 169.9, 152.4, 149.7, 139.1, 137.7, 134.2, 131.1, 130.6, 129.6, 129.5, 129.2, 123.9, 123.1, 120.3, 120.1, 119.0, 116.4, 113.1, 112.2, 106.7, 44.7, 37.6, 33.4, 33.0, 29.3, 29.0, 26.5, 24.4, 15.2 ppm; IR vmax (cm⁻¹) 3210, 2983, 2852, 1665, 1543, 1265; HRMS (ESI) calcd for C₃₁H₃₂N₄O (M+) 494.2914, found 494.2905.























































































































S155



S156



5157



























5170



S1/1















5178



5179












5185