



Supplementary Information

Synthesis, Characterization and Biological Studies of Ether–Based Ferrocenyl Amides and their Organic Analogues

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a) Synthesis of ether based ferrocenyl amides

i) Synthesis of bis-[4-(4-ferrocenylbenzamide) phenyl] ether (FB1)

4, 4-Diaminodiphenyl ether (0.25 g, 0.9 mmol), dry THF (10 mL), triethylamine (10 mL) and benzoyl chloride (1.8 mmol) were used for the preparation of FB1. Yield 58 %, m.p. 195 °C. Anal. Calc. for C₄₆H₃₆O₃N₂Fe₂(Mr.776): C, 71.13; H, 4.64; N, 3.61. Found: C, 71.15; H, 4.68; N, 3.60%.

ii) Synthesis of bis-[4-(4-ferrocenylbenzamide) phenyl] methane (FB2)

4,4- Diaminodiphenyl methane (0.25 g, 0.9 mmol), dry THF (10 mL), triethylamine (10 mL) and 4-ferrocenyl benzoyl chloride (1.8 mmol) were used for the synthesise of FB2. Yield 55 %, m.p. 180 °C. Anal. Calc. for C₄₇H₃₈O₂N₂Fe₂(Mr.774): C, 72. 87; H, 4.91; N, 3.62. Found: C, 72.84; H, 4.93; N, 3.61%

iii) Synthesis of bis-(1,6-ferrocenylbenzamide) hexane (FB3)

1, 6-Hexanediamine (0.25 g, 0.9 mmol), dry THF (10 mL), triethylamine (10 mL) and 4-ferrocenyl benzoyl chloride (1.8 mmol) were combined to prepare FB3. Yield 60.2 %, m.p. 165 °C. Anal. Calc. for $C_{40}H_{40}O_2N_2Fe_2(Mr.692)$: C, 69.36; H, 5.78; N, 4.05. Found: C, 69.34; H, 5.76; N, 4.04%.

iv) Synthesis of bis-(1, 4-ferrocenylbenzamide) butane (FB4)

1, 4-Butanediamine (0.25 g, 0.9 mmol), dry THF (10 mL), triethylamine (10 mL) and 4-ferrocenyl benzoyl chloride (1.8 mmol) were used to synthesise FB4. Yield 51.5 %, m.p. 173 °C. Anal. Calc. for $C_{38}H_{36}O_2N_2Fe_2(Mr.664)$: C, 68.67; H, 5.42; N, 4.22. Found: C, 68.64; H, 5.46; N, 4.21%.

v) Synthesis of N-(4-naphthaleyl-2-oxy-phenyl)-4-ferrocenyl benzamide (FB5)

4-Naphthaleyl-2-oxy-benzamine (1.8 mmol), dry THF (10 mL), triethylamine (10 mL) and 4-ferrocenyl benzoyl chloride (1.8 mmol) were used for the preparation of FB4. Yield 55.5 %, m.p. 201 °C. Anal. Calc. for C₃₃H₂₅O₂NFe (Mr.523): C, 75.72; H, 4.78; N, 2.68. Found: C, 75.76; H, 4.73; N, 2.67%.

vi) Synthesis of bis-(4-ferrocenylbenzamide) ethane (FB6)

67.93; H, 5.05; N, 4.41%.

Ethylene diamine (0.9 mmol), dry THF (10 mL), triethylamine (10 mL) and 4ferrocenyl benzoyl chloride (1.8 mmol) were amalgamated to get FB6. Yield 60 %, m.p. 183 °C. Anal. Calc. for C₃₆H₃₂O₂N₂Fe₂(Mr.636): C, 67.92; H, 5.03; N, 4.40. Found: C,

vii) Synthesis of N-(4-phenoxyphenyl)-4-ferrocenyl benzamide (FB7)

FB7 was prepared from 4-Phenoxy benzamine (1.8 mmol), dry THF (10 mL), triethylamine (10 mL) and 4ferrocenyl benzoyl chloride (1.8 mmol).

Yield 62 %, m.p. 196 °C. Anal. Calc. for C₂₉H₂₃O₂NFe(Mr.473): C, 73.57; H, 4.86; N, 2.96. Found: C, 73.53; H, 4.83; N, 2.94%.

viii) Synthesis of N-(2-mercaptophenyl)-4-ferrocenyl benzamide (FB8)

For the synthesis of FB8, 4-Aminothiophenol (1.8 mmol), dry THF (10 mL), triethylamine (10 mL) and 4ferrocenyl benzoyl chloride (1.8 mmol) were used.

Yield 63.5 %, m.p. 225 °C. Anal. Calc. for C₂₃H₁₉OSNFe(Mr.413): C, 66.83; H, 4.60; N, 3.39. Found: C, 66.83; H, 4.61; N, 3.41%.

ix) Synthesis of N-phenyl-4-ferrocenyl benzamide (FB9)

To synthesise FB9, aniline (1.8 mmol), dry THF (10 mL), triethylamine (10 mL) and 4-ferrocenyl benzoyl chloride (1.8 mmol) were used.

Yield 60 %, m.p.175 °C. Anal. Calc. for C₂₃H₁₉ONFe(Mr.381): C, 72.44; H, 4.99; N, 3.67. Found: C, 72.43; H, 4.97; N, 3.64%.

x) Synthesis of bis-(4-ferrocenylbenzamide) benzene (FB10)

The synthesis of FB10 was carried out by taking Phenylene diamine (0.9 mmol), dry THF (10 mL), triethylamine (10 mL) and 4ferrocenyl benzoyl chloride (1.8 mmol). Yield 53.9 %, m.p. 160 °C. Anal. Calc. for C₄₀H₃₂O₂N₂Fe₂(Mr.684): C, 70.18; H, 4.68; N, 4.09. Found: C, 70.13; H, 4.64; N, 4.09%.

xi) Synthesis of N-4-ferocenylphenyl benzamide (FB11)

The preparation of FB11 involved the use of 4- Ferrocenyl aniline (1.8 mmol), dry THF (10 mL), triethylamine (10 mL) and 4ferrocenyl benzoyl chloride (1.8 mmol). Yield 62%, m.p. 191 °C. Anal. Calc. for C₃₃H₂₇ONFe₂(Mr.565): C, 70.09; H, 4.78; N, 2.48. Found: C, 70.10; H, 4.79; N, 2.49%.

xii) Synthesis of (4-biphenyl-4-oxyphenyl)-4-ferrocenyl benzamide (FB12)

To accomplish the manufacturing of FB12, 4-Biphenyloxy benzamine (1.8 mmol), dry THF (10 mL), triethylamine (10 mL) and 4-ferrocenyl benzoyl chloride (1.8 mmol) were used. Yield 65 %, m.p. 155 °C. Anal. Calc. for C₃₅H₂₇O₂NFe(Mr.549): C, 76.50; H, 4.92; N, 2.55. Found: C, 76.53; H, 4.90; N, 2.59%.

xiii) Synthesis of N-(4-naphthalenyl-1-oxy)phenyl)-4-ferrocenyl benzamide (FB13)

The synthesis of FB13 was completed from N-(4-Naphthalenyl-1-oxy) benzamine (1.8 mmol), dry THF (10 mL), triethylamine (10 mL) and 4-ferrocenyl benzoyl chloride (1.8 mmol). Yield 64.8 %, m.p. 215 °C. Anal. Calc. for C₃₃H₂₅O₂NFe(Mr.523): C, 75.72; H, 4.78; N, 2.68. Found: C, 75.71; H, 4.79; N, 2.63%.

b) Synthesis of organic analogues of ether based ferrocenyl amides

i) Synthesis of bis-((4-benzamide) phenyl) ether (BZ1)

BZ1 was prepared by taking 4, 4-Diaminodiphenyl ether (0.25 g, 0.9 mmol), dry THF (10 mL), triethylamine (10 mL) and benzoyl chloride (1.8 mmol). Yield 50 %, m.p. 192 °C. Anal. Calc. for C₂₆H₂₀O₃N₂(Mr.408): C, 76.47; H, 4.90; N, 6.86. Found: C, 76.45; H, 4.93; N, 6.83%.

ii) Synthesis of bis - ((4-benzamide) phenyl) methane (BZ2)

To synthesise BZ2, 4, 4-Diaminodiphenyl methane (0.25 g, 0.9 mmol), dry THF (10 mL), triethylamine (10 mL) and benzoyl chloride (1.8 mmol) were used.

Yield 52.3 %, m.p. 194 °C. Anal. Calc. for C₂₇H₂₂O₂N₂(Mr.406): C, 79.80; H, 5.41; N, 6.89. Found: C, 79.83; H, 5.39; N, 6.91%.

iii) Synthesis of bis-(1, 6-benzamide) hexane (BZ3)

The synthesis of BZ3 was accomplished by taking 1, 6-Hexanediamine (0.25 g, 0.9 mmol), dry THF (10 mL), triethylamine (10 mL) and benzoyl chloride (1.8 mmol).

Yield 52.7 %, m.p. 170 °C. Anal. Calc. for C₂₀H₂₄O₂N₂(Mr.324): C, 74.07; H, 7.40; N, 8.64. Found: C, 74.08; H, 7.39; N, 8.61%.

iv) Synthesis of bis-(1, 4-benzamide) butane (BZ4)

The preparation of BZ4 was carried out from 1, 4-Butanediamine (0.25 g, 0.9 mmol), dry THF (10 mL), triethylamine (10 mL) and benzoyl chloride (1.8 mmol).

Yield = 51.5 %, m.p = 169 °C. Anal. Calc. for C₁₈H₂₀O₂N₂(Mr.296): C, 72.97; H, 6.76; N, 9.50. Found: C, 72.99; H, 6.75; N, 9.51%.

v) Synthesis of N-(4-naphthaleyl-2-oxy-phenyl) benzamide (BZ5)

4-Naphthaleyl-2-oxy-benzamine (1.8 mmol), dry THF (10 mL), triethylamine (10 mL) and benzoyl chloride (1.8 mmol) were used to prepare BZ5.

Yield 55.5 %, m.p. 190 °C. Anal. Calc. for C₂₃H₁₇O₂N(Mr.339): C, 81.41; H, 5.01 ; N, 4.13. Found: C, 81.39; H, 5.02; N, 4.15%.

vi) Synthesis of bis-(1,2-benzamide) ethane (BZ6)

Ethylene diamine (0.9 mmol), dry THF (10 mL), triethylamine (10 mL) and benzoyl chloride (1.8 mmol) were taken for the manufacturing of BZ6.

Yield 60 %, m.p. 171 °C. Anal. Calc. for C16H16O2N2(Mr.268): C, 71.64; H, 5.97; N, 10.44. Found: C, 71.63; H, 5.96; N, 10.41%.

vii) Synthesis of N-(4-phenoxyphenyl) benzamide (BZ7)

BZ7 was prepared by taking 4-Phenoxy benzamine (1.8 mmol), dry THF (10mL), triethylamine (10mL) and benzoyl chloride (1.8mmol).

Yield 62 %, m.p. 188 °C. Anal. Calc. for C19H15O2N(Mr.289): C, 78.89; H, 5.19; N, 4.84. Found: C, 78.88; H, 5.20; N, 4.81%.

viii) Synthesis of N-(2-mercaptophenyl) benzamide (BZ8)

4-Aminothiophenol (1.8 mmol), dry THF (10 mL), triethylamine (10 mL) and benzoyl chloride (1.8 mmol) were used for the preparation of BZ8.

Yield 63.5 %, m.p. 210 °C. Anal. Calc. for C13H11OSN(Mr.229): C, 68.12; H, 4.80; N, 6.11. Found: C, 68.13; H, 4.83; N, 6.10%.

ix) Synthesis of N-phenylbenzamide (BZ9)

BZ9 was prepared from aniline (1.8 mmol), dry THF (10 mL), triethylamine (10 mL) and benzoyl chloride (1.8 mmol).Yield = 60 %, m.p = 162 °C. Anal. Calc. for C₁₃H₁₁ON(Mr.197): C, 79.19; H, 5.58; N, 7.10. Found: C, 79.19; H, 5.53; N, 7.11%.

x) Synthesis of bis-(benzamide) benzene (BZ10)

Phenylene diamine (0.9 mmol), dry THF (10 mL), triethylamine (10 mL) and benzoyl chloride (1.8 mmol) were used for the preparation of BZ10.

Yield 53.9 %, m.p. 152 °C. Anal. Calc. for C₂₀H₁₆O₂N₂(Mr.316): C, 75.94; H, 5.06; N, 8.86. Found: C, 75.93; H, 5.03; N, 8.85%.

xi) Synthesis of N-4-ferocenylphenyl benzamide (BZ11)

BZ11 was synthesise from 4- ferrocenyl aniline (1.8 mmol), dry THF (10 mL), triethylamine (10 mL) and benzoyl chloride (1.8 mmol).

Yield 62 %, m.p. 180 °C. Anal. Calc. for C₂₃H₁₉ONFe(Mr.381): C, 72.44; H, 4.99; N, 3.67. Found: C, 72.44; H, 4.98; N, 3.69%.

xii) Synthesis of (4-biphenyl-4-oxyphenyl)benzamide (BZ12)

To complete the synthesis of BZ12 4-biphenyloxy benzamine (1.8 mmol), dry THF (10 mL), triethylamine (10 mL) and benzoyl chloride (1.8 mmol) were used.

Yield 65 %, m.p. 140 °C. Anal. Calc. for C₂₅H₁₉O₂N(Mr.365): C, 82.19; H, 5.20; N, 3.83. Found: C, 82.20; H, 5.19; N, 3.81%.

xiii) Synthesis of N-(4-naphthalenyl-1-oxy)phenyl)benzamide (BZ13)

The synthesise BZ13 N-(4-naphthalenyl-1-oxy) benzamine (1.8 mmol), dry THF (10 mL), triethylamine (10 mL) and benzoyl chloride (1.8 mmol) were used.

Yield 64.8 %, m.p. 205 °C. Anal. Calc. for C₂₃H₁₇O₂N(Mr.339): C, 81.41; H, 5.01 ; N, 4.13. Found: C, 81.42; H, 5.02; N, 4.12%.

Ferrocenyl Amides	N–H Stretch	CH Aromatic Stretch	Carbonyl Stretch	Double Bond Stretch	Fe–Cp Stretch
FB1	3321	2977	1646	1597, 1524	505
FB2	3282	3095	1644	1534, 1509	507
FB3	3300	2969	1630	1550, 1435	501
FB4	3370	2971	1632	1553, 1442	508
FB5	3392	3046	1630	1500,1460	512
FB6	3304	2956	1633	1582, 1465	500
FB7	3330	3060	1650	1510, 1490	512
FB8	3304	2962	1633	1538, 1505	507
FB9	3350	3031	1633	1510, 1441	510
FB10	3341	3047	1651	1598, 1525	502
FB12	3304	3033	1635	1503, 1482	508
FB13	3390	3045	1628	1503, 1456	506

Table S1. FTIR (cm⁻¹) spectral data of ferrocenyl amides (FB1-FB13)

Table S2. FTIR (cm⁻¹) spectral data of organic analogues (BZ1-BZ13)

Organic Analogues	N–H Stretch	CH(Aromatic Stretch)	Carbonyl Stretch	Double Bond Stretch
BZ1	3327	3050	1649	1519,1505
BZ2	3328	3050	1649	1601,1576
BZ3	3320	3070	1630	1540,1510
BZ5	3337	3043	1647	1600,1598
BZ6	3392	3088	1630	1553,1491
BZ7	3328	3053	1647	1506,1489
BZ8	3371	3060	1670	1590,1545
BZ9	3391	3032	1652	1598,1487
BZ10	3340	3051	1651	1570,1513
BZ11	3300	3053	1651	1596,1537
BZ12	3334	3029	1642	1590,1589
BZ13	3335	3047	1648	1598,1594

Organic analogues	Amide Protons (ppm)	Aromatic Protons (ppm)
BZ-1	10.2	7–7.9 (Ar H)
BZ-2	10.2	7.1–7.9 (Ar H)
BZ-5	10.3	7.1–7.9 (Ar H)
BZ-7	10.33	7–7.9 (Ar H)
BZ-8	10.36	7.2–8 (Ar H)
BZ-10	10.27	7–8 (Ar H)
	10.5	7.2–8.3 (Ar H, Cp H)
FD1		4.0 (s, 5H)
L D I		4.2 (t, 2H)
		4.6 (t, 2H)

Table S3. ¹H NMR spectral data of ferrocenyl amide and organic analogues.

Table S4. ¹³C NMR spectral data of ferrocenyl amides and organic analogues.

Organic Analogues	Carbonyl Carbon (ppm)	Aromatic Carbon (ppm)
BZ-1	165.8	119–135
BZ-7	166	118-135
BZ-8	166.1	127-136
BZ-10	167	120-139
BZ-11	165.7	121-135
FB1	164	116–141 & (Cp–C) 65-86



Figure S1. DPPH free radical scavenging activity.



Figure S2. Hydrogen peroxide scavenging activity.





Figure S3. Alpha glucosidase enzyme inhibition activity of ferrocenyl amides.

Figure S4. Alpha glucosidase enzyme inhibition activity of organic analogues.



Figure S5. Alpha amylase enzyme inhibition activity of ferrocenyl amides.



Figure S6. Alpha amylase enzyme inhibition activities of organic analogues.



Figure S7. Acetylcholinesterase enzyme inhibition activities.



Figure S8. Butyrylcholinesterase enzyme inhibition activities.



Figure S9. Antibacterial activity of gram-negative bacteria.



Figure S10. Antibacterial activity of gram-positive bacteria (Enterobacter aerogenes is also known as Klebsiella aerogenes).