

Supplementary Data

Characterization of small molecule ligands.

Compound 2G: $R_f = 0.15$ (10% CH₃OH in dichloromethane); ¹H NMR (400 MHz CDCl₃) (mixture of rotamers) δ 0.94 (t, 3H, $J = 6.5$ Hz), 1.18-1.38 (m, 2H), 1.46-2.36 (m, 8H), 2.38-2.58 (m, 2H), 2.95 (m, 2H), 3.50-3.68 (m, 5H), 3.71 (s, 6H), 3.79 (s, 3H), 3.80 (s, 3H), 3.81 (s, 3H), 4.36-4.48 (m, 2H), 5.40 (m, 1H), 5.50-5.60 (m, 1H), 6.41 (s, 2H), 6.58-7.20 (m, 7H), 7.56 (br, 1H); ES⁺ HRMS calcd for C₄₅H₅₅N₇O₁₁ (M + H⁺) 870.4038, found 870.3992.

Compound 4G: $R_f = 0.15$ (10% CH₃OH in dichloromethane); ¹H NMR (400 MHz CDCl₃) (mixture of rotamers) δ 0.90 (t, 3H, $J = 7.0$ Hz), 1.28-1.46 (m, 2H), 1.52-1.75 (m, 10H), 2.00-2.31 (m, 2H), 2.40-2.60 (m, 2H), 2.86 (m, 2H), 3.26-3.64 (m, 5H), 3.68 (s, 6H), 3.79 (s, 3H), 3.82 (s, 3H), 3.83 (s, 3H), 4.51-4.80 (m, 2H), 5.43 (m, 1H), 5.59-5.62 (m, 1H), 6.39 (s, 2H), 6.58-7.20 (m, 7H), 7.38 (br, 1H); ES⁺ HRMS calcd for C₄₇H₅₉N₇O₁₁ (M + H⁺) 898.4351, found 898.4318.

Compound 8G: $R_f = 0.13$ (10% CH₃OH in dichloromethane); ¹H NMR (400 MHz CDCl₃) (mixture of rotamers) δ 0.90 (t, 3H, $J = 7.5$ Hz), 1.22-1.46 (m, 2H), 1.52-1.76 (m, 4H), 1.88-2.36 (m, 4H), 2.40-2.62 (m, 2H), 2.81 (m, 2H), 3.50-3.66 (m, 13H), 3.68 (s, 6H), 3.80 (s, 3H), 3.83 (s, 3H), 3.85 (s, 3H), 4.48-4.66 (m, 2H), 5.45 (m, 1H), 5.56-5.65 (m, 1H), 6.41 (s, 2H), 6.60-7.20 (m, 7H), 7.46 (s, 1H); ES⁺ HRMS calcd for C₄₉H₆₃N₇O₁₃ (M + H⁺) 958.4562, found 958.4563.

Compound 2A: $R_f = 0.15$ (10% CH₃OH in dichloromethane); ¹H NMR (400 MHz CDCl₃) (mixture of rotamers) δ 0.91 (t, 3H, $J = 6.8$ Hz), 1.24-1.50 (m, 2H), 1.60-1.80 (m, 4H), 1.86-2.14 (m, 4H), 2.32-2.60 (m, 2H), 2.88 (m, 2H), 3.60-3.70 (m, 5H), 3.71 (s, 6H), 3.79 (s, 3H), 3.83 (s, 3H), 3.84 (s, 3H), 4.38-4.46 (m, 2H), 5.55 (m, 1H), 5.60-5.65 (m, 1H), 6.43 (s, 2H), 6.58-7.10 (m, 7H) 7.80 (s, 1H), 8.28 (s, 1H).; ES⁺ MS calcd for C₄₅H₅₅N₇O₁₀ (M + H⁺) 854.40, found 854.50.