

Supplementary Material

Synthesis, Characterisation, and Biological Activity of the Ruthenium Complexes of the N₄-tetradentate (N₄-T_L), 1,6-di(2'-pyridyl)-2,5-dimethyl-2,5-diazahexane (picenMe₂).

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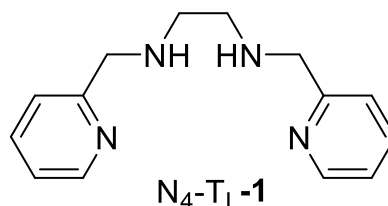
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1. Synthesis

1.1 Synthesis of N_4 -TLs such as N,N' -bis(2-pyridylmethyl)-1,2-diaminoethane (picen, N_4 -TL-1)

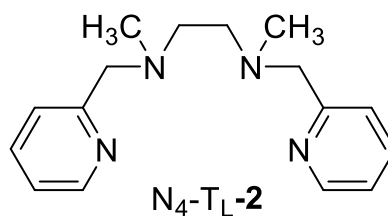
A solution of 2-pyridinecarboxaldehyde (2.145 g, 20 mmol) dissolved in ethyl acetate (20 mL) was added to a solution of 1,2-diaminoethane (0.60 g, 10 mmol) in ethyl acetate (60 mL); this mixture was left stirring for 30 min. The ethyl



acetate was evaporated to produce the diimine N_4 -TL. The diimine N_4 -TL was reduced by the addition of methanol (80 mL) and NaBH_4 (1:5, 2.15 g) and the mixture was left stirring overnight at 25 °C. Methanol was removed under reduced pressure and the remaining residue dissolved in water (50 mL). The mixture was extracted several times with chloroform (5 × 30 mL); the organic phases were combined and dried with Na_2SO_4 . The product was filtered, and chloroform was evaporated under vacuum to obtain a yellow oil of N_4 -TL-1. Yield: 2.28 g (94%). Picen (N_4 -TL-1) $^1\text{H-NMR}$ (400 MHz, D_2O) δ : 8.56 (d, 2H, $J_1 = 4.56$ Hz, H11), 7.94 (t, 2H, $J_1 = 7.74$ Hz, H13), 7.50 (d, 2H, $J_1 = 7.88$ Hz, H14), 7.45 (m, 2H, H12), 3.93 (s, 4H, H16a/b), 2.81 (s, 4H, H1a/b). $^{13}\text{C-NMR}$ (400 MHz, D_2O) δ : 158.03 (C15), 148.55 (C11), 138.30 (C13), 123.28 (C12), 123.05 (C14), 53.34 (C16), 47.15 (C1). ESI-MS (MeOH, m/z): calculated (m/z): 242.33, found (m/z): 243.41. UV-Vis λ_{max} nm ($\epsilon \text{ mol}^{-1} \text{ dm}^{-3} \text{ cm}^{-1}$, CHCl_3): 262 ($7.7 \pm 0.3 \times 10^3$). RP-HPLC Phenomenex C18 (5 μm , 150 × 4.6 mm) 0-40 % B over 15 min, t_R 6.68 min at 254 nm.

1.2 Synthesis of N,N' -bis(2-pyridylmethyl)- N,N' -dimethyl-1,2-diaminoethane (picenMe₂, N_4 -TL-2)

Methylation of picen (N_4 -TL-1) and Me₂picen (N_4 -TL-7) was achieved using the published method of Goldsmith *et al.* A mixture of picen, N_4 -TL-1 (0.277 g, 1.02 mmol), formaldehyde (0.190 g, 6.33 mmol) and formic acid (0.730 g, 16.0 mmol) was stirred and refluxed at 85 °C for 3 days. The

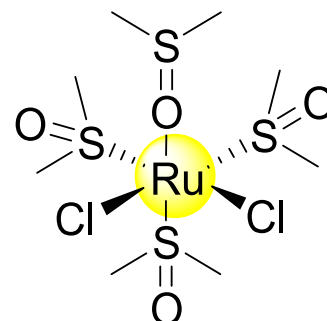


mixture was left to cool to room temperature, and then the pH was increased to pH 12 with 1 M KOH. The methylated product was extracted with chloroform (3 × 20 mL) and dried over Na_2SO_4 . The extract was filtered, and the chloroform was evaporated under reduced pressure to yield product as a viscous brown oil. Yield: 0.26 g (96%). picenMe₂ (N_4 -TL-2) $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ : 8.58 (d, 2H, $J_1 = 4.20$ Hz, H11), 7.71 (t, 2H, $J_1 = 8.00$ Hz, H13), 7.56 (d, 2H, $J_1 = 7.76$ Hz, H14), 7.24 (m, 2H, H12), 4.00 (s, 4H, H16a/b), 3.04 (s, 4H, H1a/b), 2.50 (s, 6H, N-CH₃). $^{13}\text{C-NMR}$ (400 MHz, CDCl_3) δ : 149.34 (C11), 136.96 (C13), 124.23 (C14),

122.86 (C12), 62.35 (C16), 53.58 (C1), 42.12 (N-CH₃). ESI-MS (MeOH, *m/z*): Calculated (*m/z*): 270.38, found (*m/z*): 271.40. UV-Vis λ_{max} nm (ϵ mol⁻¹ dm⁻³ cm⁻¹, CHCl₃): 262 (6.4 ± 0.1 × 10³). RP-HPLC Phenomenex C18 (5 μ m, 150 × 4.6 mm) 0-40 % B over 15 min, *t_R* 7.22 min at 254 nm.

1.3 Synthesis of dichlorotetrakis(dimethylsulfoxide)ruthenium(II) [Ru(DMSO)₄Cl₂]

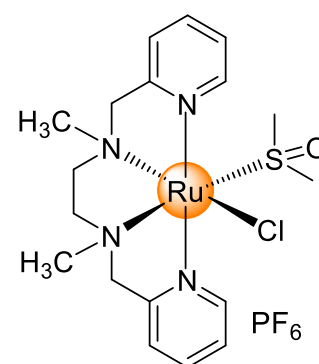
A solution of DMSO (24 mL) was added to RuCl₃.nH₂O (1.0 g, 4.82 mmol), the sealed reaction mixture was flushed with nitrogen for 10 mins. The nitrogen gas was removed, then refluxed at ~189 °C for 5 mins or until the solution turned orange/red. The stoppers were removed, and the mixture continued to be heated while nitrogen was bubbled through the reaction vessel until the solution reduced in



volume by half (12 mL), and a yellow precipitate started to form. The reaction mixture was removed from heat, acetone (40 mL) added and the mixture could cool slowly, whereupon a yellow precipitate formed. The precipitate was collected by vacuum filtration, washed with acetone (2 × 50 mL) and diethyl-ether (2 × 5 mL). Yield: 1.40 g (60%). ¹H-NMR (400 MHz, CDCl₃) δ : 3.53, 3.51, 3.44, and 3.34 (Me of DMSO, S-Ru linked), 2.74 (Me of DMSO, O-Ru linked), 2.65 (Me of free DMSO); ratio S-Ru: O-Ru 4:1. ¹³C-NMR (400 MHz, CDCl₃) δ : 47.7, 46.7, 44.5, 44.3 (Me of DMSO, S-Ru linked), 38.8 (Me of DMSO, O-Ru linked). UV-Vis λ_{max} nm (ϵ mol⁻¹ dm⁻³ cm⁻¹, H₂O): 230 (10.1 ± 0.1 × 10³), 346 (565). RP-HPLC Phenomenex C18 (5 μ m, 150 × 4.6 mm) 0-40 % B over 15 min, *t_R* 6.46 min at 254 nm.

1.4 Synthesis of *cis*- α -[Ru(*p*icenMe₂)(DMSO)Cl](PF₆) (Ru-1)

A solution of [Ru(DMSO)₄Cl₂] (0.34 g, 0.7 mmol), dissolved in water (1.25 mL) and ethanol (7.5 mL), was added dropwise to a warm stirred solution of *p*icenMe₂ (0.108 g, 0.4 mmol) in ethanol (12.5 mL). The yellow mixture was refluxed at 95 °C for 2 h resulting in an orange/red solution. The reaction solution was reduced in volume to ~5 mL by evaporating most of the ethanol, and then a saturated solution of potassium hexafluorophosphate

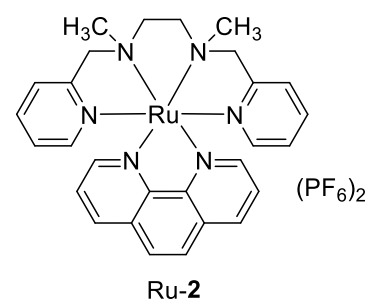


(KFP₆, 1 mL) was added to precipitate the product. The product was left to precipitate 24 – 72 h, before collection by filtration, washed with water (2 × 3 mL), then diethyl ether (2 × 3 mL) and air dried. Yield: 65.8 mg (26%). (Ru-1) ¹H-NMR (400 MHz, DMSO-d₆) δ : 9.14 (d, 1H, *J_I* = 5.65 Hz, H21), 9.10 (d, 1H, *J_I* = 5.23 Hz, H11), 8.06 (t, 1H, *J_I* = 7.72 Hz, H13), 7.96 (t, 1H, *J_I* = 7.68 Hz, H23), 7.74 (d, 1H, *J_I* = 7.68 Hz, H14), 7.70 (d, 1H, *J_I* = 7.72 Hz, H24), 7.59 (m,

1H, H12), 7.59 (m, 1H, H22), 4.96 (d, 1H, $J_1 = 14.88$ Hz, H16a), 4.96 (d, 1H, $J_1 = 15.08$ Hz, H26a), 4.35 (d, 1H, $J_1 = 8.44$ Hz, H16b), 4.35 (d, 1H, $J_1 = 8.44$ Hz, H26b), 3.21 (s, 3H, S-CH₃), 2.63 (m, 1H, H2a/b), 2.55 (s, 3H, N-CH₃), 2.47 (s, 3H, N-CH₃), 2.40 (m, 1H, H1a/b), 2.27 (s, 3H, S-CH₃). ¹³C-NMR (400 MHz, DMSO-d₆) δ : 162.13 (C15), 161.70 (C25), 155.83 (C11), 153.37 (C12), 138.24 (C13), 137.49 (C23), 125.19 (C12), 125.05 (C22), 123.78 (C14), 123.55 (C24), 70.02 (C26), 67.62 (C16), 59.61 (C1), 57.45 (C2), 46.99 (N-CH₃), 45.56 (N-CH₃), 45.45 (S-CH₃), 43.53 (S-CH₃). ESI-MS (MeOH:H₂O, 0.1% Formic acid, [M]⁺ m/z): Calculated (m/z): 485.08, found (m/z): 485.04. UV-Vis λ_{\max} nm (ϵ mol⁻¹ dm⁻³ cm⁻¹, DMSO): 247 ($10.1 \pm 0.09 \times 10^3$), 346 ($8.0 \pm 0.1 \times 10^3$). RP-HPLC Phenomenex C18 (5 μ m, 150 \times 4.6 mm) 10-100 % B over 15 min, t_R 4.44 min at 254 nm.

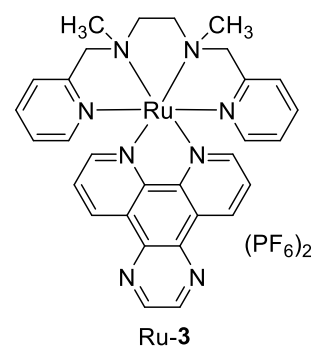
1.5 Synthesis of *cis- α -[Ru(picenMe₂)(phen)](PF₆)₂ (Ru-2)*

Yield: 22.2 mg (67%). (Ru-2) ¹H-NMR (400 MHz, DMSO-d₆) δ : 9.77 (d, 2H, $J_1 = 4.96$ Hz, H7/7'), 8.72 (d, 2H, $J_1 = 7.80$ Hz, H9/9'), 8.25 (s, 2H, H19/19'), 8.07 (m, 2H, H11/21), 7.73 (t, 2H, $J_1 = 7.70$ Hz, H13/23), 7.63 (d, 2H, $J_1 = 7.68$ Hz, H14/24), 7.58 (d, 2H, $J_1 = 5.40$ Hz, H8/8'), 7.06 (t, 2H, $J_1 = 6.58$ Hz, H12/22), 5.14 (d, 2H, $J_1 = 16.84$ Hz, H16/26a), 4.54 (d, 2H, $J_1 = 16.96$ Hz, H16/26b), 2.88 (s, 6H, N-CH₃), 2.74 (m, 4H, H1/2ab). ¹³C-NMR (400 MHz, DMSO-d₆) δ : 161.47 (C15/25), 156.87 (C7/7'), 152.27 (C8/8'), 148.97 (C17/17'), 137.22 (C9/9'), 136.91 (C13/23), 130.49 (C18/18'), 128.37 (C19/19'), 126.74 (C11/21), 125.27 (C12/22), 123.33 (C14/24), 68.49 (C16/26), 60.79 (C1/2), 47.67 (N-CH₃). ESI-MS (MeOH:H₂O, 0.1% Formic acid, [M]⁺ m/z): Calculated (m/z): 697.12, found (m/z): 697.12. UV-Vis λ_{\max} nm (ϵ mol⁻¹ dm⁻³ cm⁻¹, DMSO): 271 ($52.1 \pm 3.0 \times 10^3$), 369 ($15.8 \pm 0.6 \times 10^3$), 442 ($8.2 \pm 0.3 \times 10^3$), 476 ($7.3 \pm 0.3 \times 10^3$). RP-HPLC Phenomenex C18 (5 μ m, 150 \times 4.6 mm) 10-100 % B over 15 min, t_R 8.84 min at 254 nm.



1.6 Synthesis of *cis- α -[Ru(picenMe₂)(dpq)](PF₆)₂ (Ru-3)*

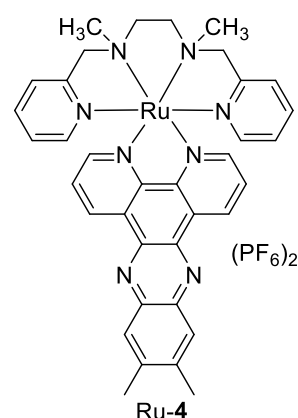
Yield: 17.0 mg (48%). (Ru-3) ¹H-NMR (400 MHz, DMSO-d₆) δ : 9.87 (d, 2H, $J_1 = 4.96$ Hz, H7/7'), 9.53 (d, 2H, $J_1 = 8.24$ Hz, H9/9'), 9.30 (s, 2H, H10/10'), 8.23 (m, 2H, H11/21), 7.75 (t, 2H, $J_1 = 7.76$ Hz, H13/23), 7.67 (t, 4H, $J_1 = 6.83$ Hz, H8/8'/14/24), 7.09 (t, 2H, $J_1 = 6.64$ Hz, H12/22), 5.18 (d, 2H, $J_1 = 16.88$ Hz, H16/26a), 4.56 (d, 2H, $J_1 = 17.04$ Hz, H16/26b), 3.40 (m, 2H, H1/2b), 2.89 (s, 6H, N-CH₃), 2.76 (m, 2H, H1/2a). ¹³C-NMR (400 MHz, DMSO-d₆) δ :



161.38 (C15/25), 157.89 (C7/7'), 152.61 (C8/8'), 150.89 (C17/17'), 147.19 (C10/10'), 139.44 (C19/19'), 137.35 (C13/23), 133.02 (C9/9'), 129.31 (C18/18'), 127.78 (C11/21), 125.32 (C12/22), 123.37 (C14/24), 68.48 (C16/26), 63.25 (C1/2b), 60.84 (C1/2a), 47.65 (N-CH₃). ESI-MS (MeOH:H₂O, 0.1% Formic acid, [M]⁺ *m/z*): Calculated (*m/z*): 603.16, found (*m/z*): 603.16. UV-Vis λ_{max} nm (ε mol⁻¹ dm⁻³ cm⁻¹, DMSO): 297 (25.2 ± 1.2 × 10³), 363 (16.2 ± 0.7 × 10³), 449 (8.1 ± 0.4 × 10³), 476 (7.6 ± 0.4 × 10³). RP-HPLC Phenomenex C18 (5 μm, 150 × 4.6 mm) 10-100 % B over 15 min, *t*_R 5.97 min at 254 nm.

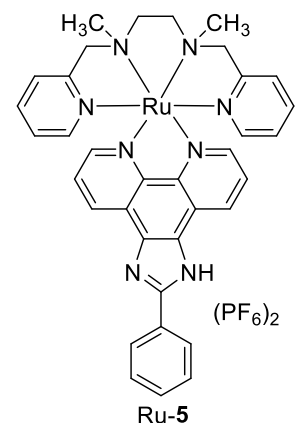
1.7 Synthesis of *cis-α*-[Ru(picenMe₂)(dppzMe₂)](PF₆)₂ (Ru-4)

Yield: 32.3 mg (84%). (Ru-4) ¹H-NMR (400 MHz, DMSO-d₆) δ: 9.83 (d, 2H, *J*₁ = 5.36 Hz, H7/7'), 9.38 (d, 2H, *J*₁ = 8.08 Hz, H9/9'), 8.17 (m, 2H, H11/21), 7.97 (s, 2H, H20/20'), 7.78 (m, 4H, H8/8'/13/23), 7.69 (d, 2H, *J*₁ = 7.64 Hz, H14/24), 7.14 (t, 2H, *J*₁ = 6.52 Hz, H12/22), 5.19 (d, 2H, *J*₁ = 16.84 Hz, H16/26a), 4.58 (d, 2H, *J*₁ = 17.04 Hz, H16/26b), 2.91 (s, 6H, N-CH₃), 2.77 (m, 4H, H1/2ab), 2.57 (s, 6H, Bz-CH₃). ¹³C-NMR (400 MHz, DMSO-d₆) δ: 161.43 (C15/25), 157.53 (C7/7'), 152.76 (C8/8'), 151.74 (C17/17'), 144.19 (C10/10'), 141.59 (C19/19'), 138.91 (C27/27'), 137.39 (C13/23), 132.98 (C9/9'), 129.79 (C18/18'), 128.02 (C11/21), 127.81 (C20/20'), 125.39 (C12/22), 123.42 (C14/24), 68.48 (C16/26), 60.85 (C1/2), 47.64 (N-CH₃), 20.65 (Bz-CH₃). ESI-MS (MeOH:H₂O, 0.1% Formic acid, [M]⁺ *m/z*): Calculated (*m/z*): 681.21, found (*m/z*): 681.20. UV-Vis λ_{max} nm (ε mol⁻¹ dm⁻³ cm⁻¹, DMSO): 276 (99.6 ± 2.4 × 10³), 369 (34.9 ± 1.54 × 10³), 388 (36.0 ± 2.0 × 10³). RP-HPLC Phenomenex C18 (5 μm, 150 × 4.6 mm) 10-100 % B over 15 min, *t*_R 15.86 min at 254 nm.



1.8 Synthesis of *cis-α*-[Ru(picenMe₂)(phenpyrBz)](PF₆)₂ (Ru-5)

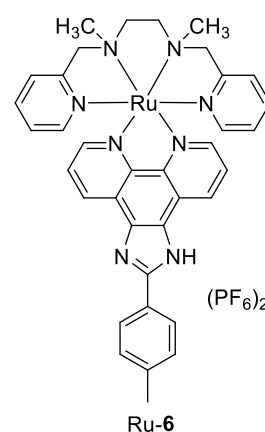
Yield: 24.0 mg (64%). (Ru-5) ¹H-NMR (400 MHz, DMSO-d₆) δ: 14.21 (s, 1H, -NH), 9.70 (d, 2H, *J*₁ = 5.00 Hz, H7/7'), 9.06 (d, 2H, *J*₁ = 8.12 Hz, H11/21), 8.28 (d, 2H, *J*₁ = 7.88 Hz, H9/9'), 8.14 (m, 2H, H30/30'), 7.74 (t, 2H, *J*₁ = 7.60 Hz, H13/23), 7.67–7.56 (m, 7H, H8/8'/14/24/31/31'), 7.09 (t, 2H, *J*₁ = 6.20 Hz, H12/22), 5.18 (d, 2H, *J*₁ = 16.84 Hz, H16/26a), 4.55 (d, 2H, *J*₁ = 17.00 Hz, H16/26b), 2.89 (s, 6H, N-CH₃), 2.76 (m, 4H, H1/2ab). ¹³C-NMR (400 MHz, DMSO-d₆) δ: 161.51 (C15/25), 154.52 (C7/7'), 153.06 (C17/17'), 152.31 (C8/8'/14/24/31/31'/32), 147.29/147.01 (C19/19'), 137.22 (C13/23), 136.94 (C34), 130.84



(C11/21), 129.84 (C18/18'), 129.68 (C8/8'/14/24/31/31'/32), 127.01 (C9/9'/30/30'), 125.31 (C12/22), 123.36 (C8/8'/14/24/31/31'/32), 121.09 (C33), 68.43 (C16/26), 60.85 (C1/2), 47.57 (N-CH₃). ESI-MS (MeOH:H₂O, 0.1% Formic acid, [M]⁺ *m/z*): Calculated (*m/z*): 667.19, found (*m/z*): 667.19. UV-Vis λ_{\max} nm (ϵ mol⁻¹ dm⁻³ cm⁻¹, DMSO): 286 ($58.6 \pm 0.7 \times 10^3$), 301 ($57.5 \pm 0.8 \times 10^3$), 368 ($19.2 \pm 0.2 \times 10^3$), 489 ($8.9 \pm 0.1 \times 10^3$). RP-HPLC Phenomenex C18 5 (5 μ m, 150 \times 4.6 mm) 10-100 % B over 15 min, t_R 6.62 min at 254 nm.

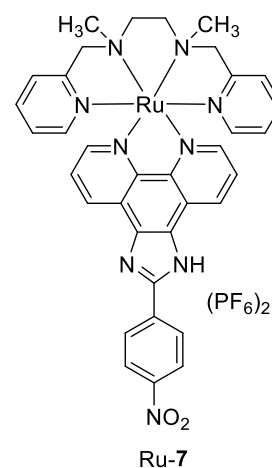
1.9 Synthesis of *cis- α* -[Ru(picenMe₂)(phenpyrBzMe)](PF₆)₂ (Ru-6)

Yield: 26.1 mg (68%). (Ru-6) ¹H-NMR (400 MHz, DMSO-d₆) δ : 14.11 (s, 1H, -NH), 9.69 (d, 2H, $J_I = 5.04$ Hz, H7/7'), 9.03 (m, 4H, H11/21/30/30'), 8.15 (m, 2H, H9/9'), 7.74 (t, 2H, $J_I = 7.52$ Hz, H13/23), 7.65 (d, 2H, $J_I = 7.68$ Hz, H8/8'), 7.44 (m, 4H, H14/24/31/31'), 7.08 (t, 2H, $J_I = 6.44$ Hz, H12/22), 5.17 (d, 2H, $J_I = 16.84$ Hz, H16/26a), 4.54 (d, 2H, $J_I = 17.04$ Hz, H16/26b), 2.89 (s, 6H, N-CH₃), 2.76 (m, 4H, H1/2ab), 2.42 (s, 3H, Bz-CH₃). ¹³C-NMR (400 MHz, DMSO-d₆) δ : 161.51 (C15/25), 154.51 (C7/7'), 153.21 (C17/17'), 152.30 (C14/24/31/31'), 151.52 (C34), 140.70 (C19/19'), 139.99 (C33), 137.21 (C13/23), 130.21 (C8/8'), 130.09 (C11/21/30/30'), 127.11 (C18/18'), 126.93 (C9/9'), 125.30 (C12/22), 124.26 (C32), 123.36 (C14/24/31/31'), 68.43 (C16/26), 60.85 (C1/2), 47.56 (N-CH₃), 21.49 (Bz-CH₃). ESI-MS (MeOH:H₂O, 0.1% Formic acid, [M]⁺ *m/z*): Calculated (*m/z*): 681.21, found (*m/z*): 681.19. UV-Vis λ_{\max} nm (ϵ mol⁻¹ dm⁻³ cm⁻¹, DMSO): 287 ($63.7 \pm 1.6 \times 10^3$), 301 ($60.8 \pm 1.5 \times 10^3$), 371 ($16.9 \pm 0.4 \times 10^3$), 488 ($7.5 \pm 0.2 \times 10^3$). RP-HPLC Phenomenex C18 (5 μ m, 150 \times 4.6 mm) 10-100 % B over 15 min, t_R 7.21 min at 254 nm.



1.10 Synthesis of *cis- α* -[Ru(picenMe₂)(phenpyrBzNO₂)](PF₆)₂ (Ru-7)

Yield: 21.6 mg (55%). (Ru-7) ¹H-NMR (400 MHz, DMSO-d₆) δ : 14.54 (s, 1H, -NH), 9.72 (d, 2H, $J_I = 5.24$ Hz, H7/7'), 9.03 (d, 2H, $J_I = 8.12$ Hz, H11/21), 8.49 (s, 4H, H9/9'/31/31'), 8.15 (m, 2H, H30/30'), 7.74 (t, 2H, $J_I = 4.00$ Hz, H13/23), 7.66 (d, 4H, $J_I = 7.68$ Hz, H8/8'/14/24), 7.09 (t, 2H, $J_I = 6.24$ Hz, H12/22), 5.18 (d, 2H, $J_I = 16.88$ Hz, H16/26a), 4.55 (d, 2H, $J_I = 17.00$ Hz, H16/26b), 2.90 (s, 6H, N-CH₃), 2.77 (m, 4H, H1/2ab). ¹³C-NMR (400 MHz, DMSO-d₆) δ : 161.51 (C15/25), 154.90 (C7/7'), 152.34 (C8/8'/14/24), 150.66 (C17/17'), 148.48 (C18/18'), 147.56 (C19/19'), 137.27 (C13/23), 135.55 (C32/33/34),



130.52 (C11/21), 127.88 (C9/9'31/31'), 126.92 (C30/30'), 125.32 (C12/22), 125.06 (C9/9'/31/31'), 123.38 (C18/18'/14/24), 68.43 (C16/26), 60.85 (C1/2), 47.57 (N-CH₃). ESI-MS (MeOH:H₂O, 0.1% Formic acid, [M]⁺ *m/z*): Calculated (*m/z*): 712.18, found (*m/z*): 712.16. UV-Vis λ_{max} nm (ϵ mol⁻¹ dm⁻³ cm⁻¹, DMSO): 293 ($45.8 \pm 1.3 \times 10^3$), 366 ($48.1 \pm 1.4 \times 10^3$), 488 ($11.23 \pm 0.4 \times 10^3$). RP-HPLC Phenomenex C18 (5 μm , 150 \times 4.6 mm) 10-100 % B over 15 min, t_{R} 7.23 min at 254 nm.

2. Characterisation

2.1 $^1\text{H-NMR}$

400 MHz Bruker Avance NMR using deuterated solvent DMSO, D_2O or CDCl_3 , with temperatures maintained at either 25 or 35 $^\circ\text{C}$, 256 accumulations.

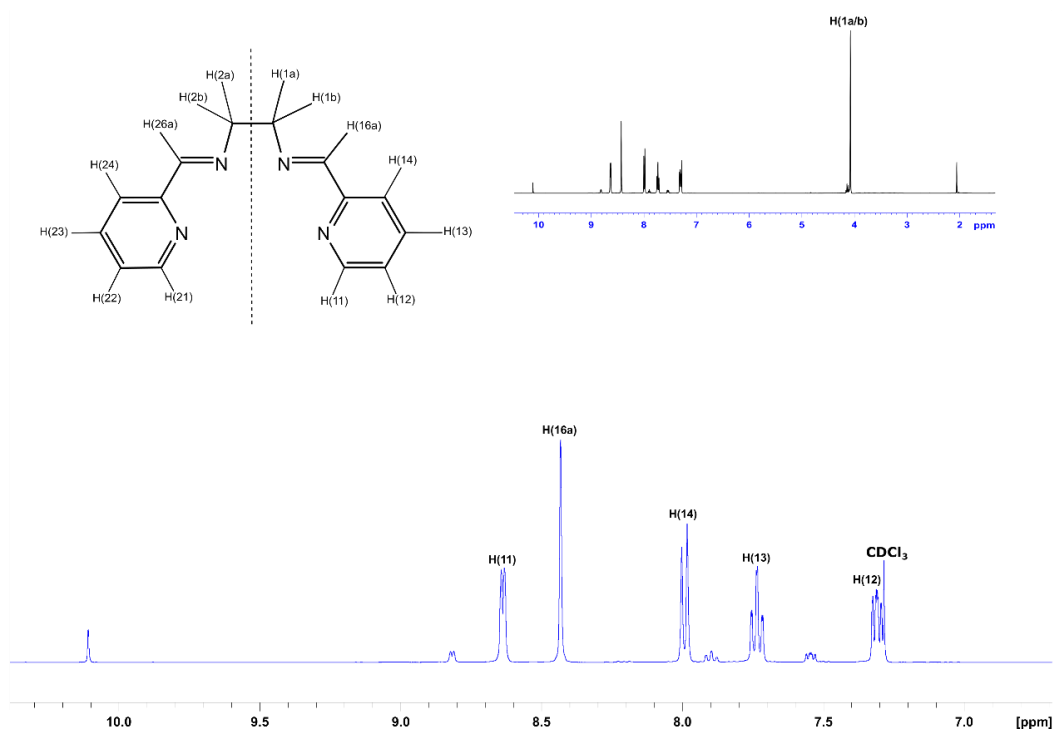


Figure S1: $^1\text{H-NMR}$ spectra of diimine N,N' -bis(pyridylmethyl)-1,2-diaminoethane picen (**1a**).

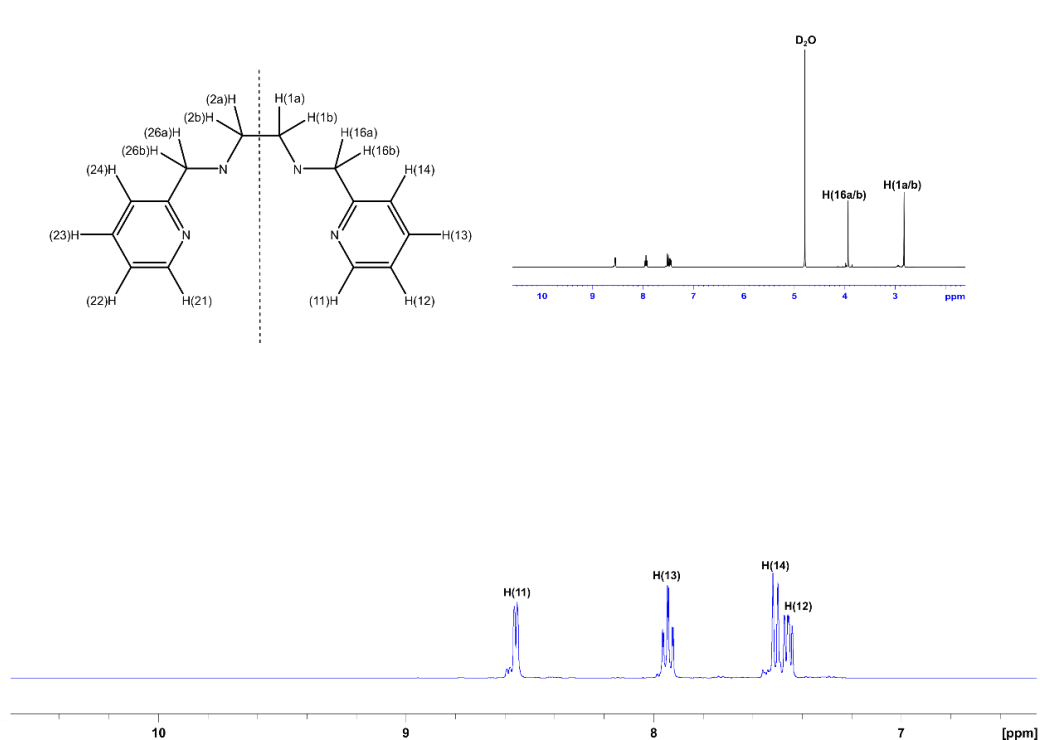


Figure S2: $^1\text{H-NMR}$ spectra of diamine N,N' -bis(pyridylmethyl)-1,2-diaminoethane picen (**1**).

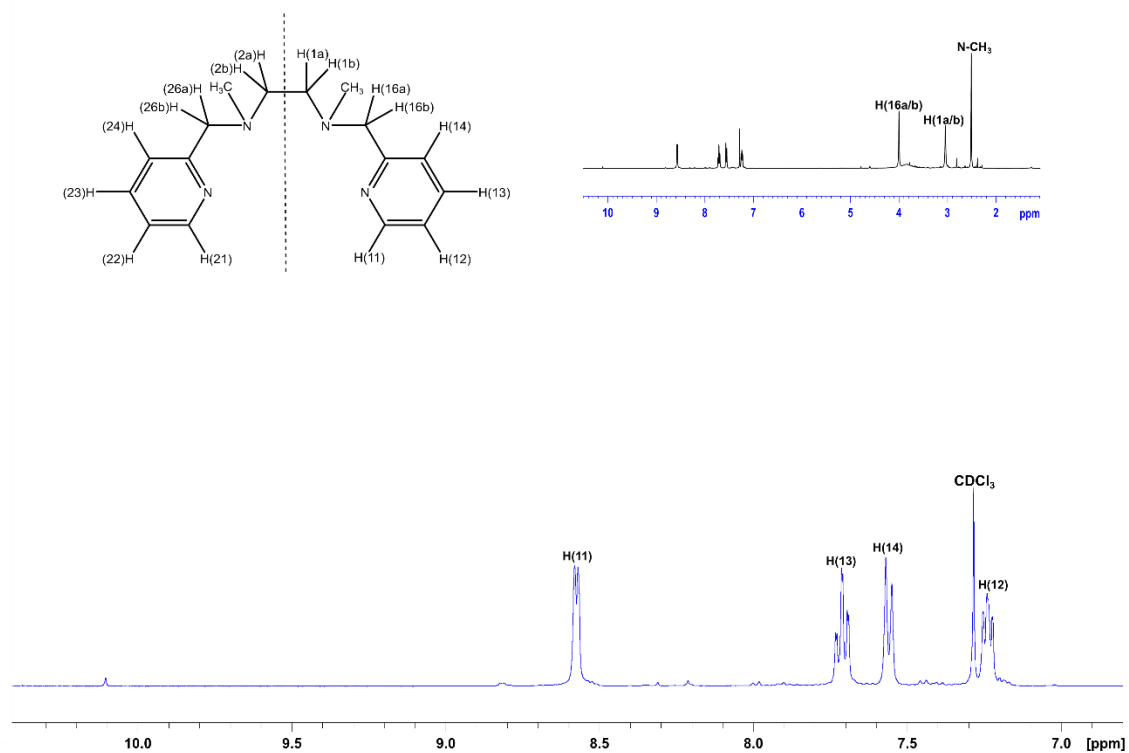


Figure S3: $^1\text{H-NMR}$ spectra of *N,N'*-bis(2-pyridylmethyl)-*N,N'*-dimethyl-1,2-diaminoethane picenMe₂ (**2**).

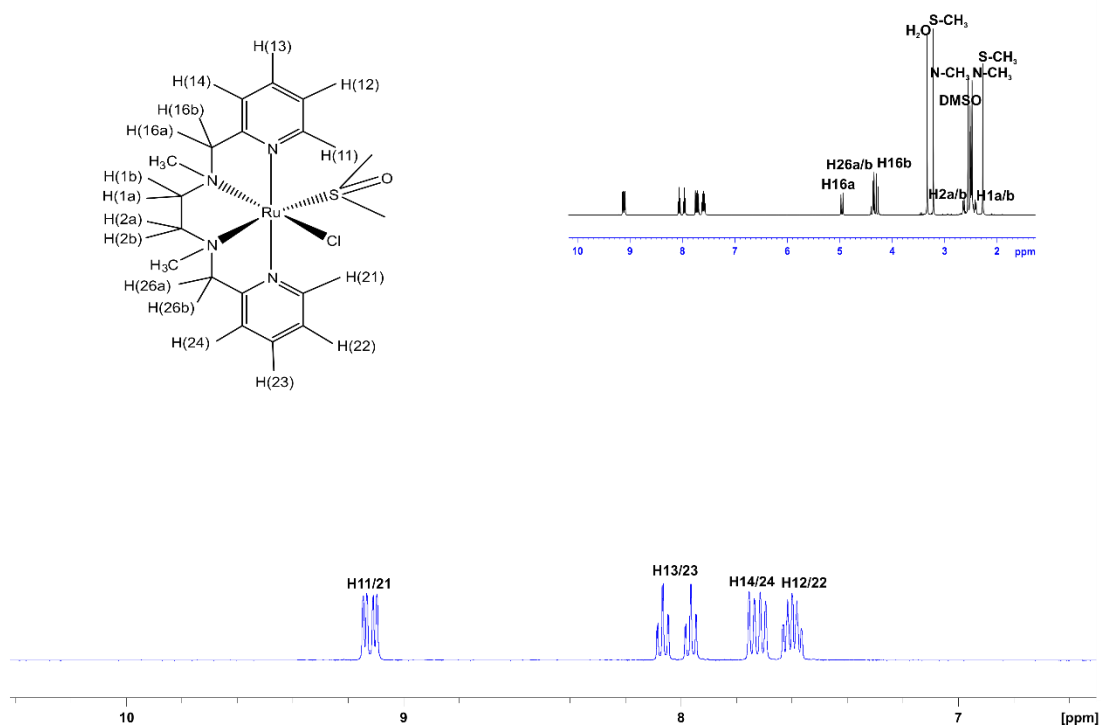


Figure S4: $^1\text{H-NMR}$ spectra of *cis-α*-[Ru(picenMe₂)(DMSO)Cl]PF₆ (**Ru-1**).

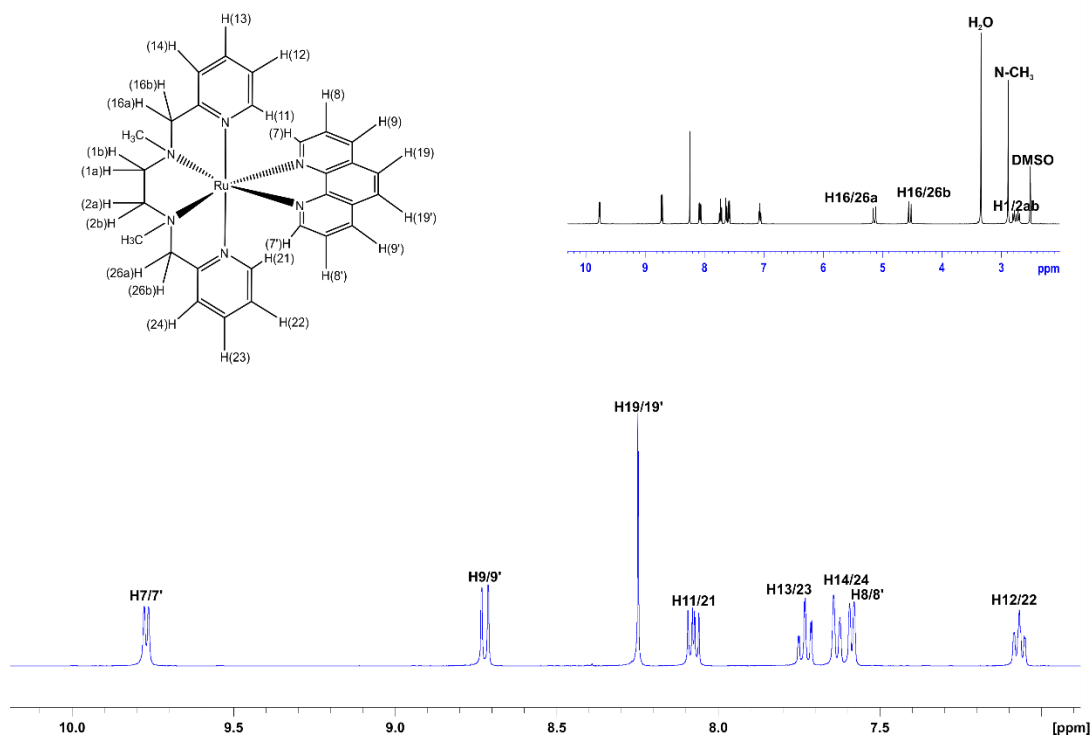


Figure S5: ¹H-NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(phen)](PF₆)₂ (Ru-2).

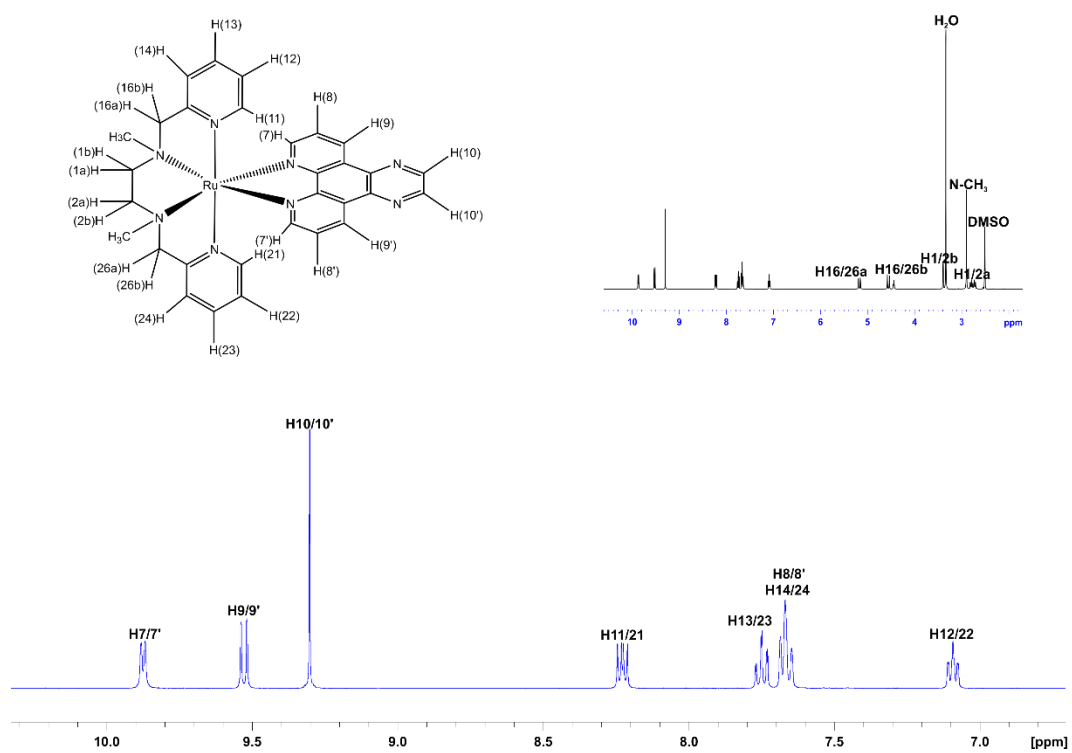


Figure S6: ¹H-NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(DPQ)](PF₆)₂ (Ru-3).

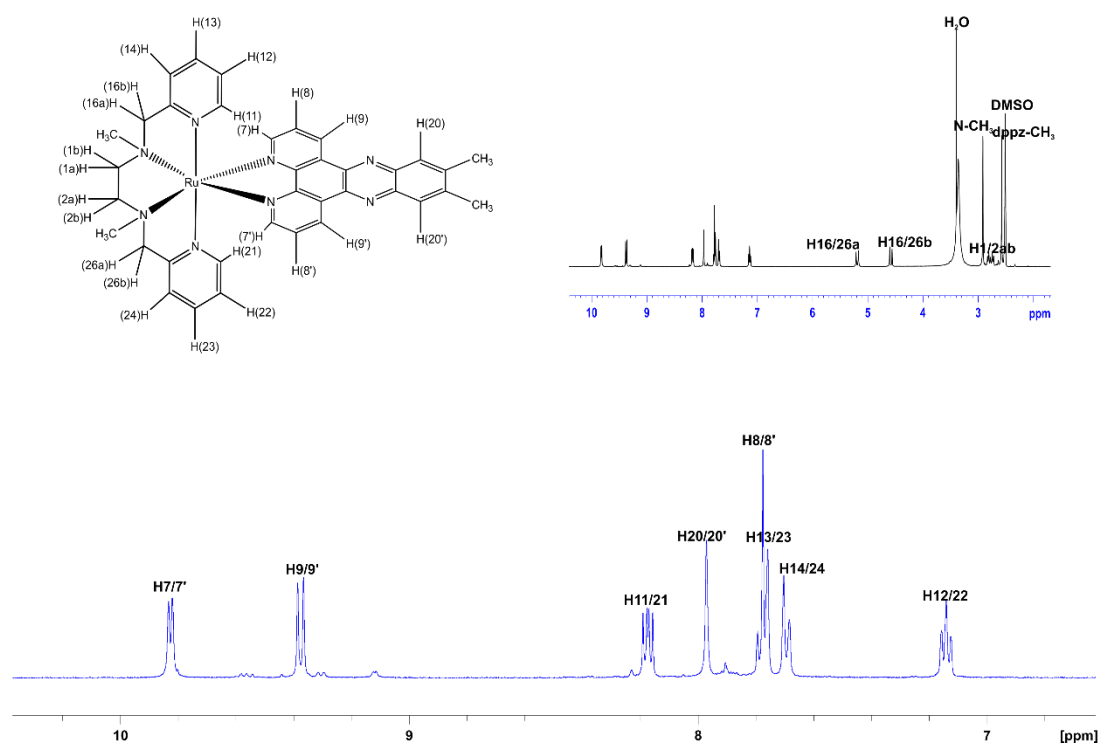


Figure S7: $^1\text{H-NMR}$ spectra of racemic *cis-α*-[Ru(picenMe₂)(DppzMe₂)](PF₆)₂ (Ru-4).

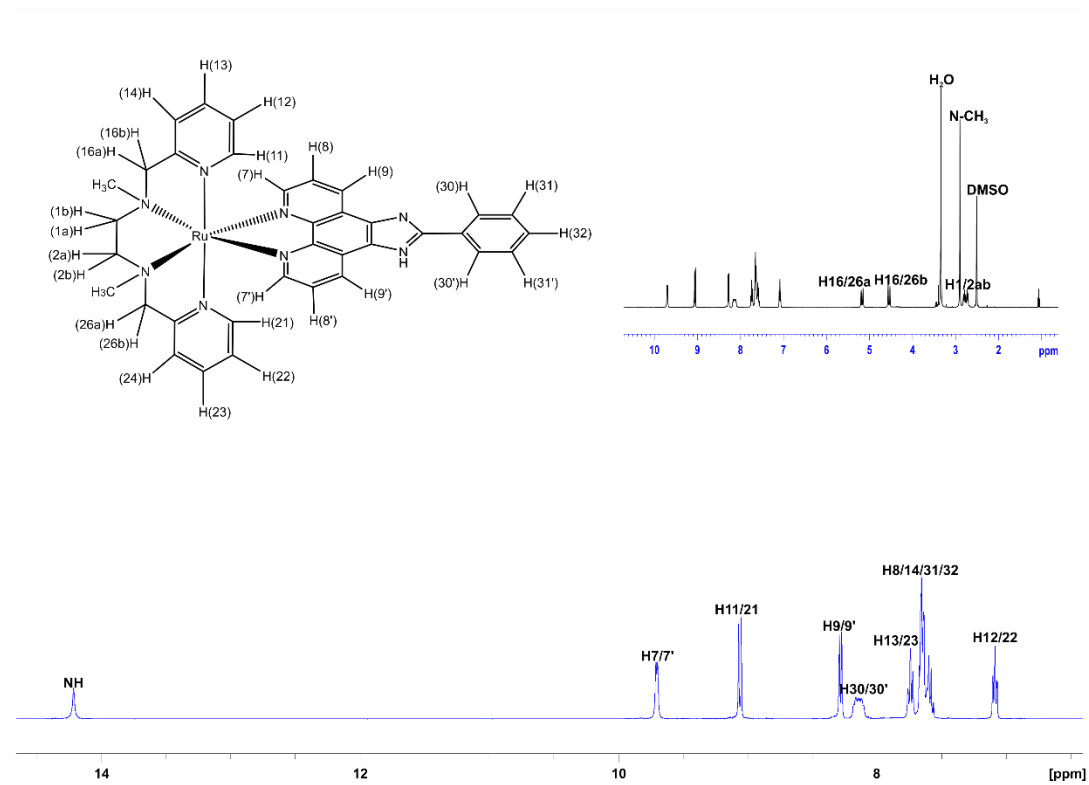


Figure S8: $^1\text{H-NMR}$ spectra of racemic *cis-α*-[Ru(picenMe₂)(phenpyrBz)](PF₆)₂ (Ru-5).

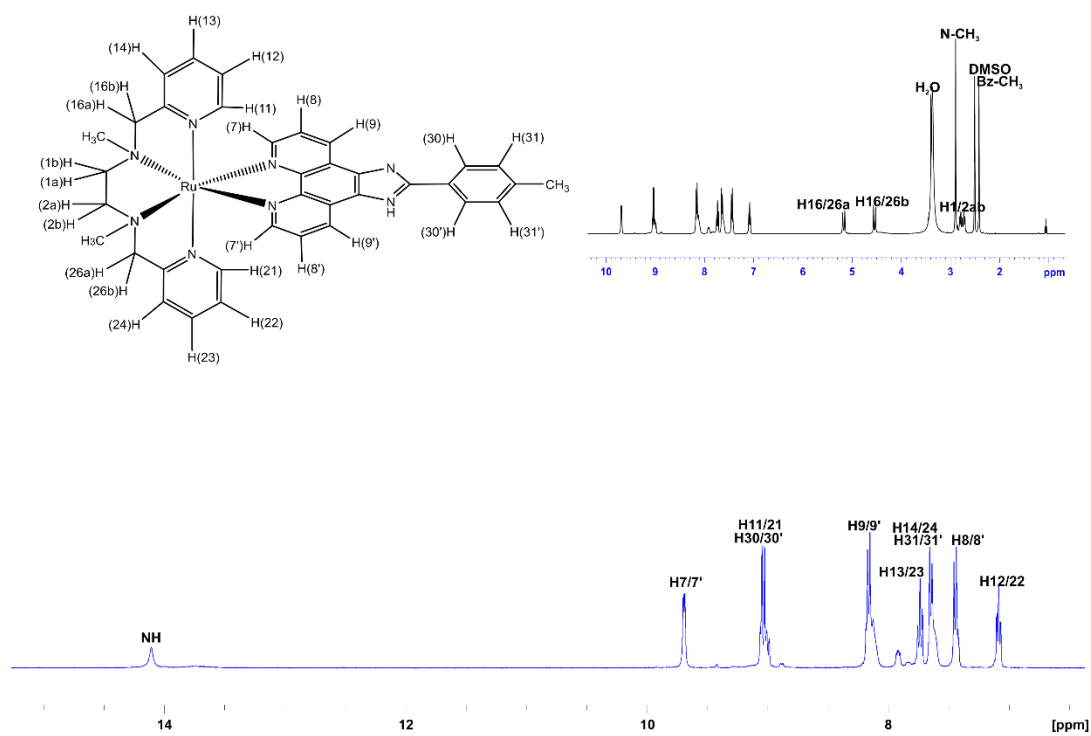


Figure S9: $^1\text{H-NMR}$ spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBzMe)](PF₆)₂ (Ru-6).

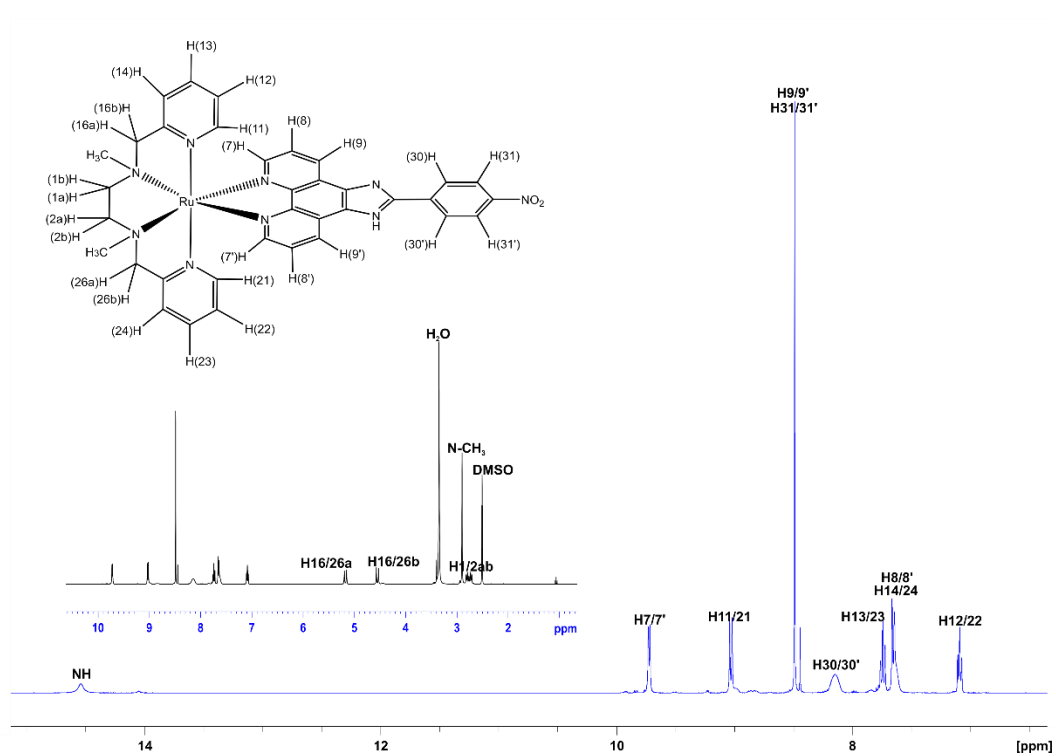


Figure S10: $^1\text{H-NMR}$ spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBzNO₂)](PF₆)₂ (Ru-7).

2.2 ^{13}C -NMR

400 MHz Bruker Avance NMR using deuterated solvent DMSO, D_2O or CDCl_3 , with temperatures maintained at either 25 or 35 $^\circ\text{C}$, 1024 accumulations.

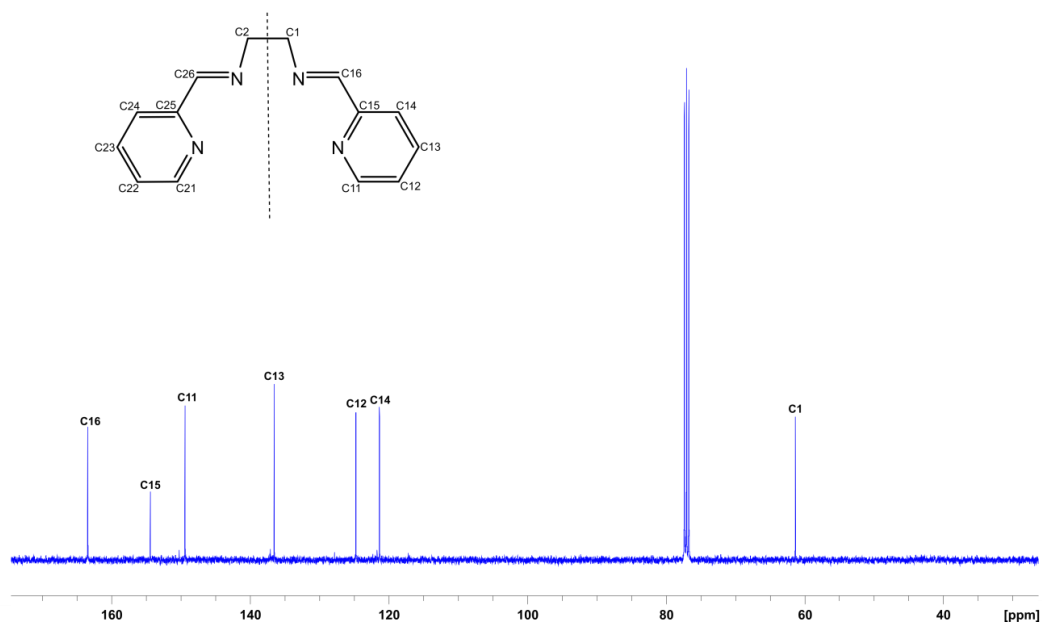


Figure S11: ^{13}C -NMR spectra of diimine N,N' -bis(pyridylmethyl)-1,2-diaminoethane picen (**1a**).

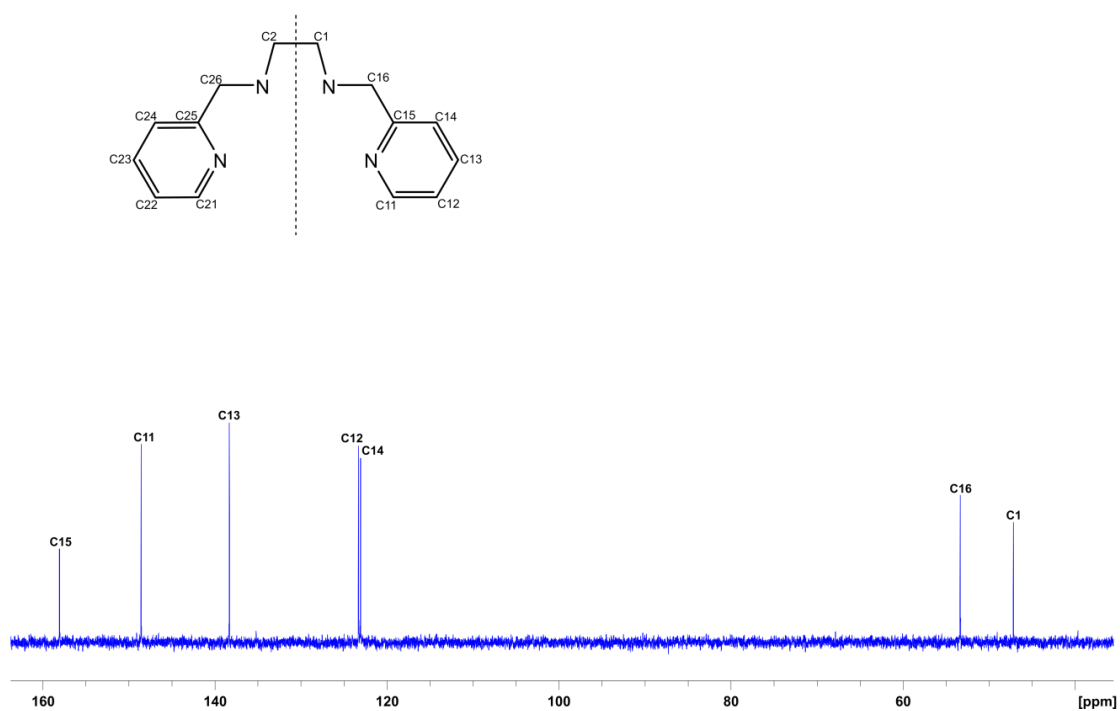


Figure S12: ^{13}C -NMR spectra of diamine N,N' -bis(pyridylmethyl)-1,2-diaminoethane picen (**1**).

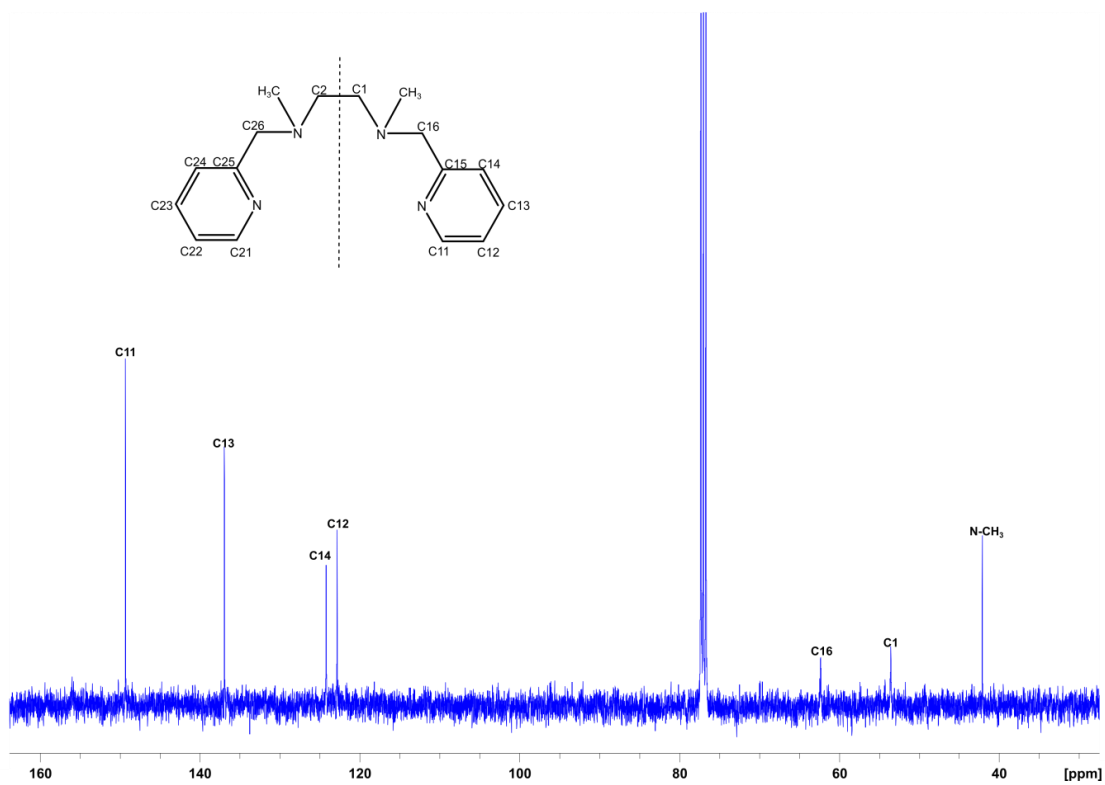


Figure S13: ^{13}C -NMR spectra of *N,N'*-bis(2-pyridylmethyl)-*N,N'*-dimethyl-1,2-diaminoethane picenMe $_2$ (2).

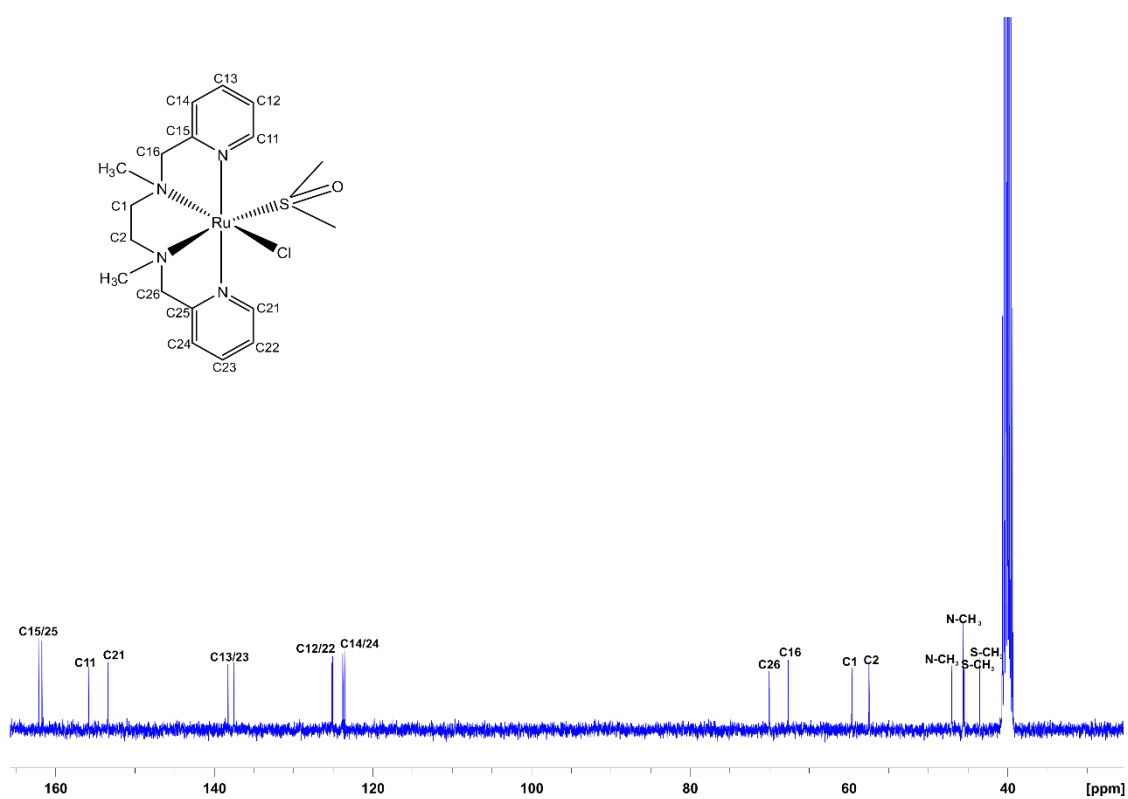


Figure S14: ^{13}C -NMR spectra of *cis*- α -[Ru(picenMe $_2$)(DMSO)Cl]PF $_6$ (Ru-1).

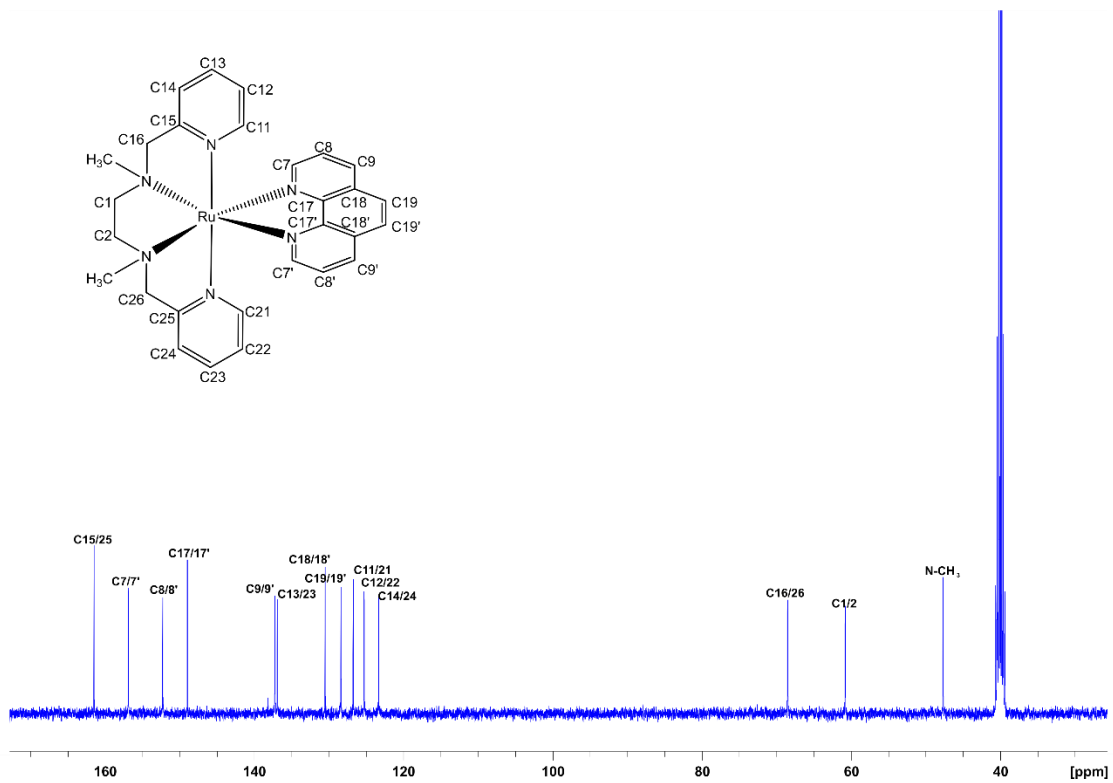


Figure S15: ^{13}C -NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(phen)](PF₆)₂ (Ru-2).

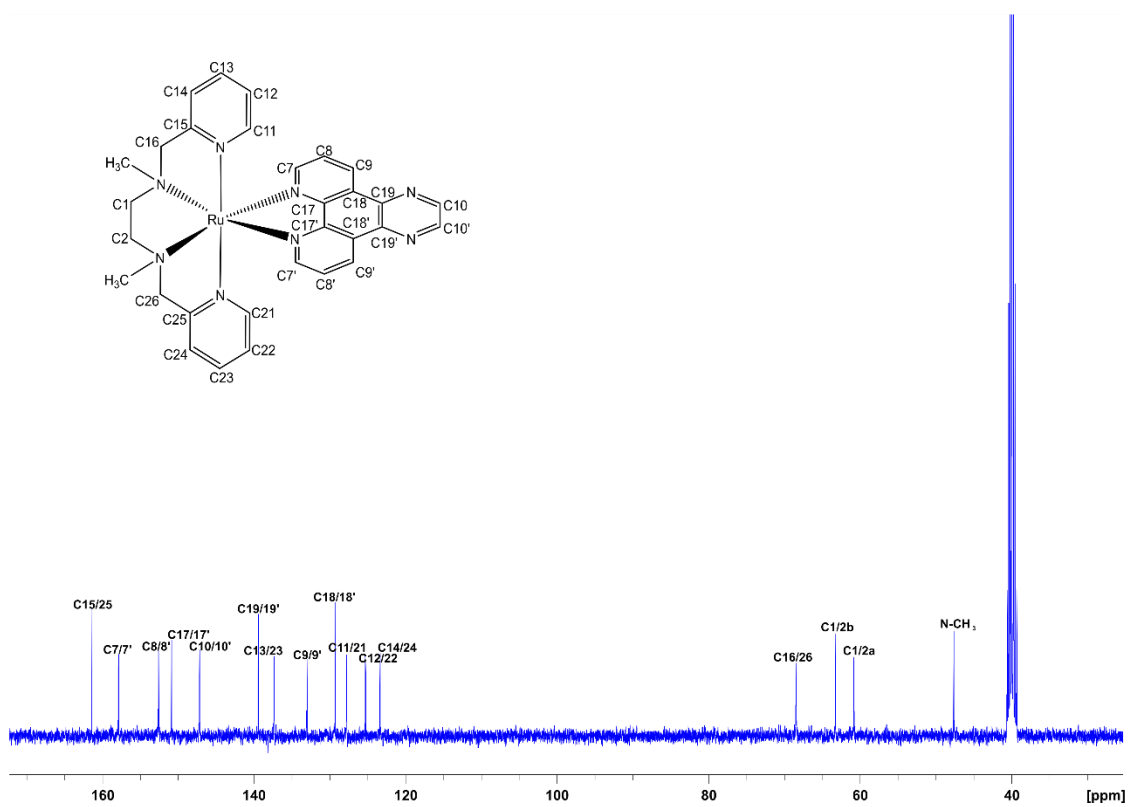


Figure S16: ^{13}C -NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(DPQ)](PF₆)₂ (Ru-3).

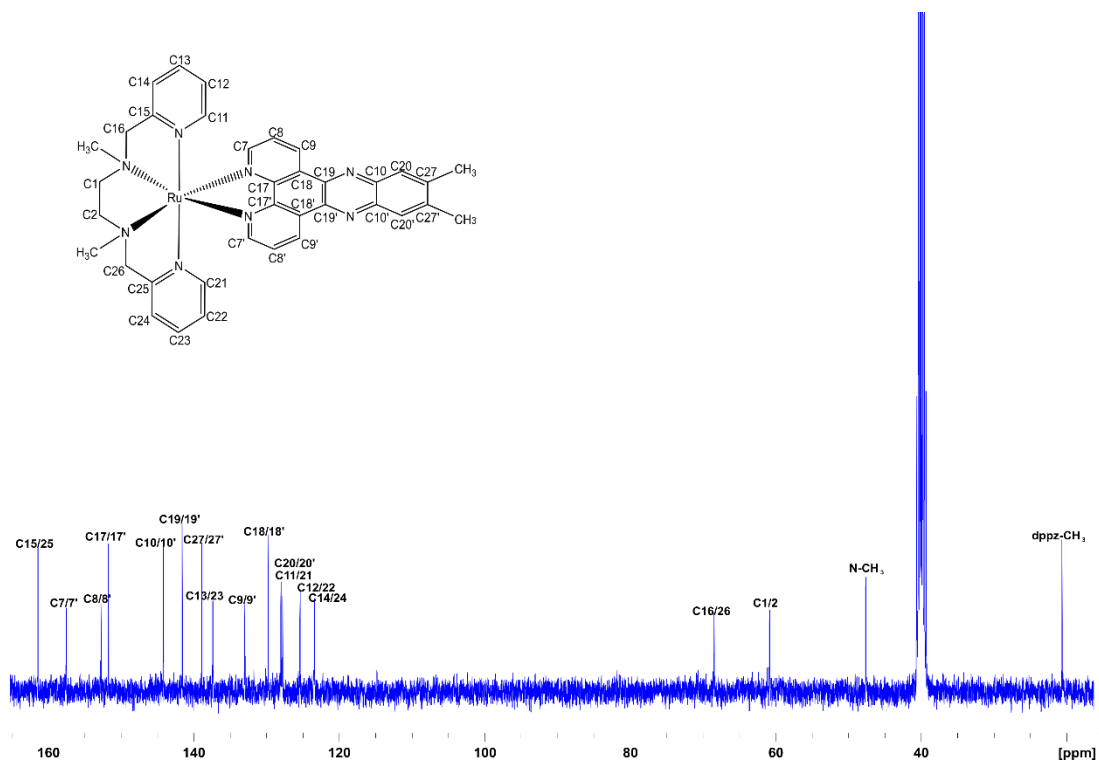


Figure S17: ^{13}C -NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(DppzMe₂)](PF₆)₂ (Ru-4).

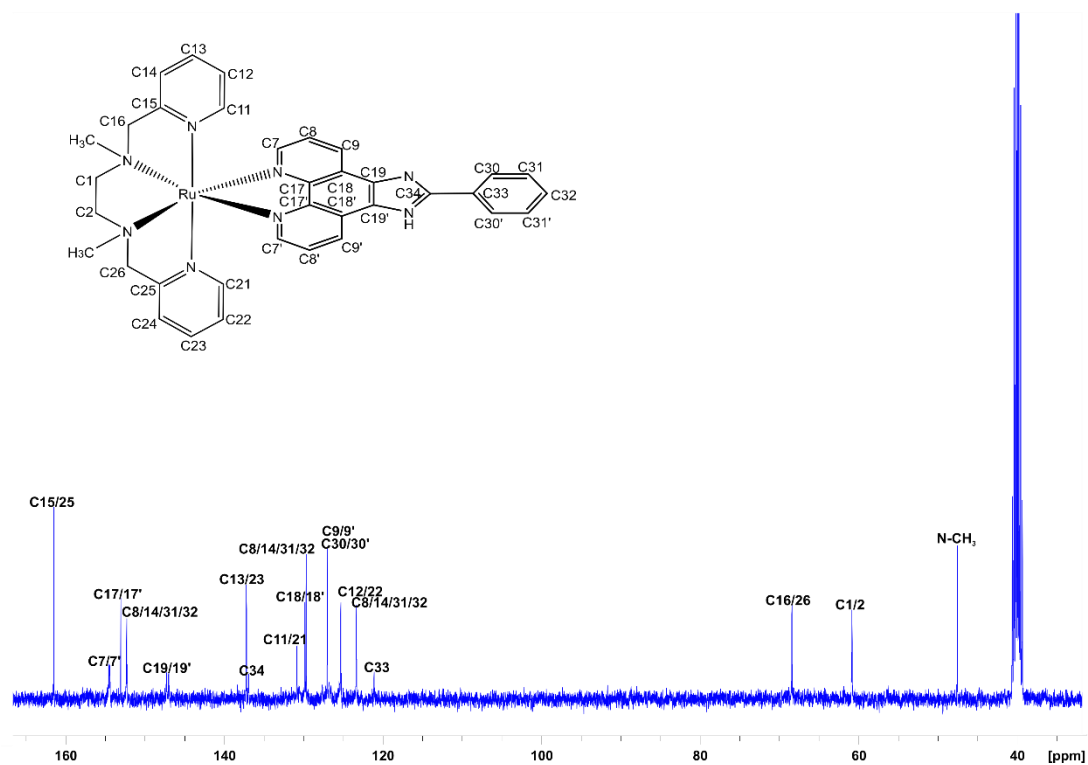


Figure S18: ^{13}C -NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBz)](PF₆)₂ (Ru-5).

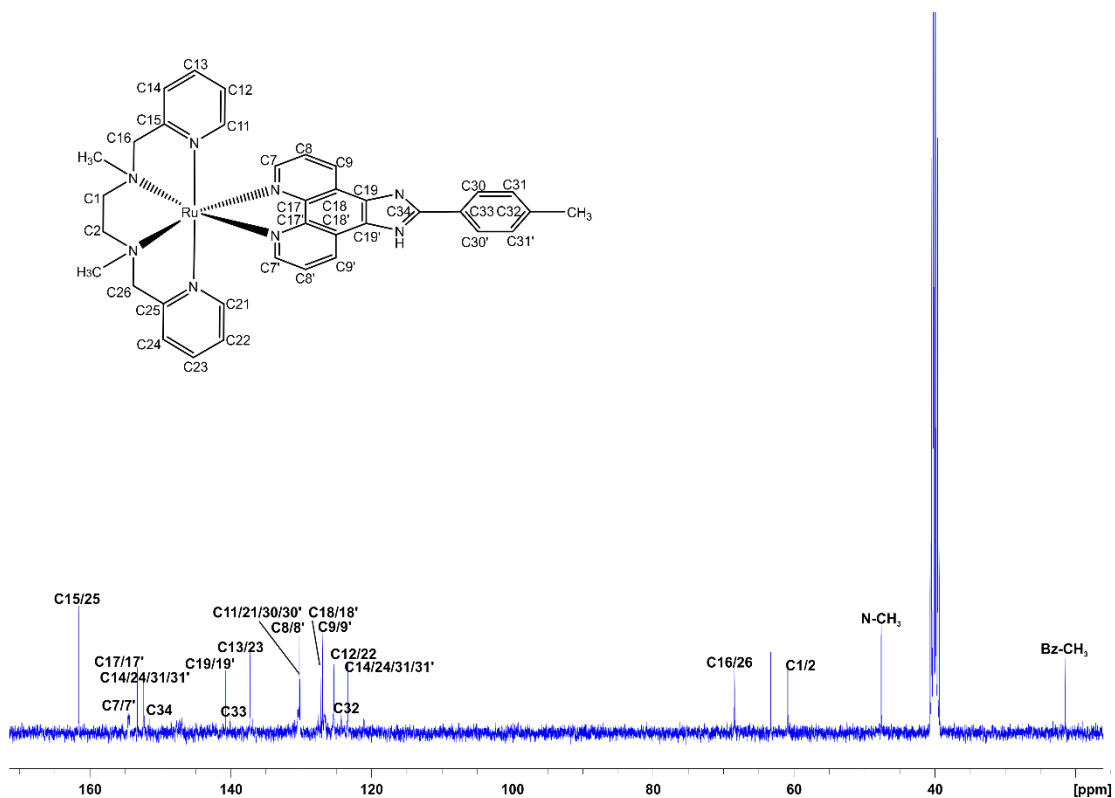


Figure S19: ^{13}C -NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBzMe)](PF₆)₂ (Ru-6).

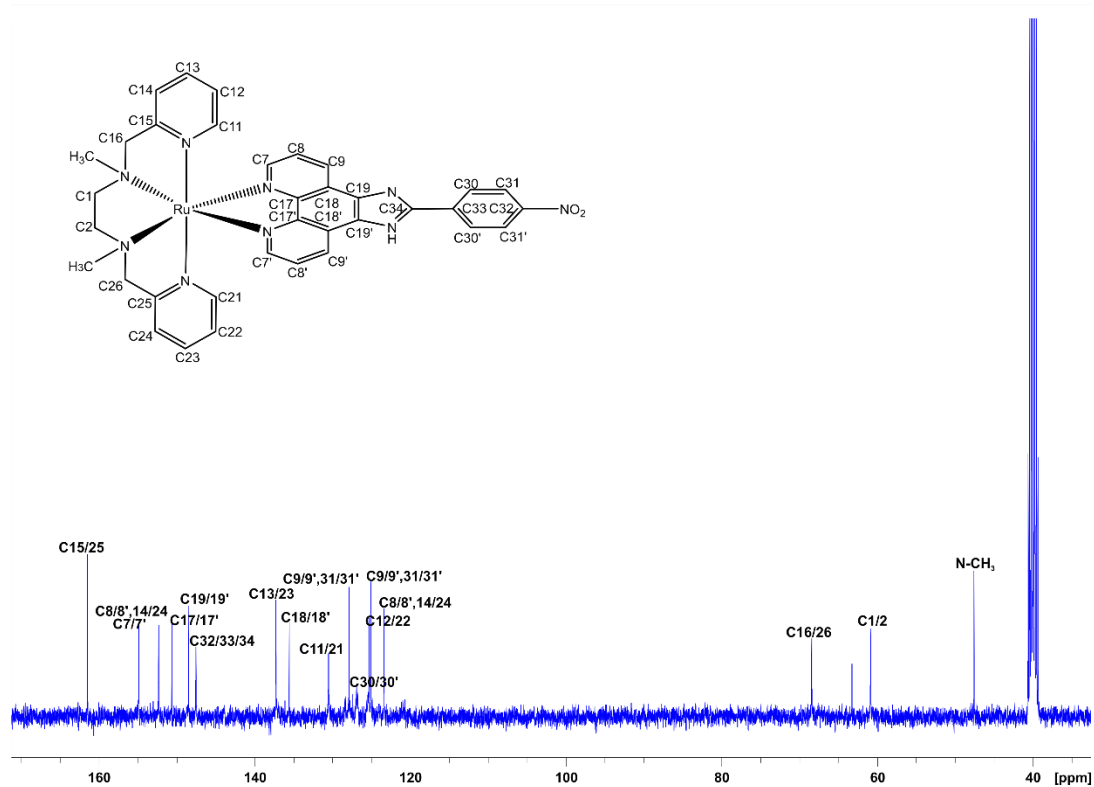


Figure S20: ^{13}C -NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBzNO₂)](PF₆)₂ (Ru-7).

2.3 Dept-NMR

400 MHz Bruker Avance NMR using deuterated solvent DMSO, D₂O or CDCl₃, with temperatures maintained at either 25 or 35 °C, 256 accumulations.

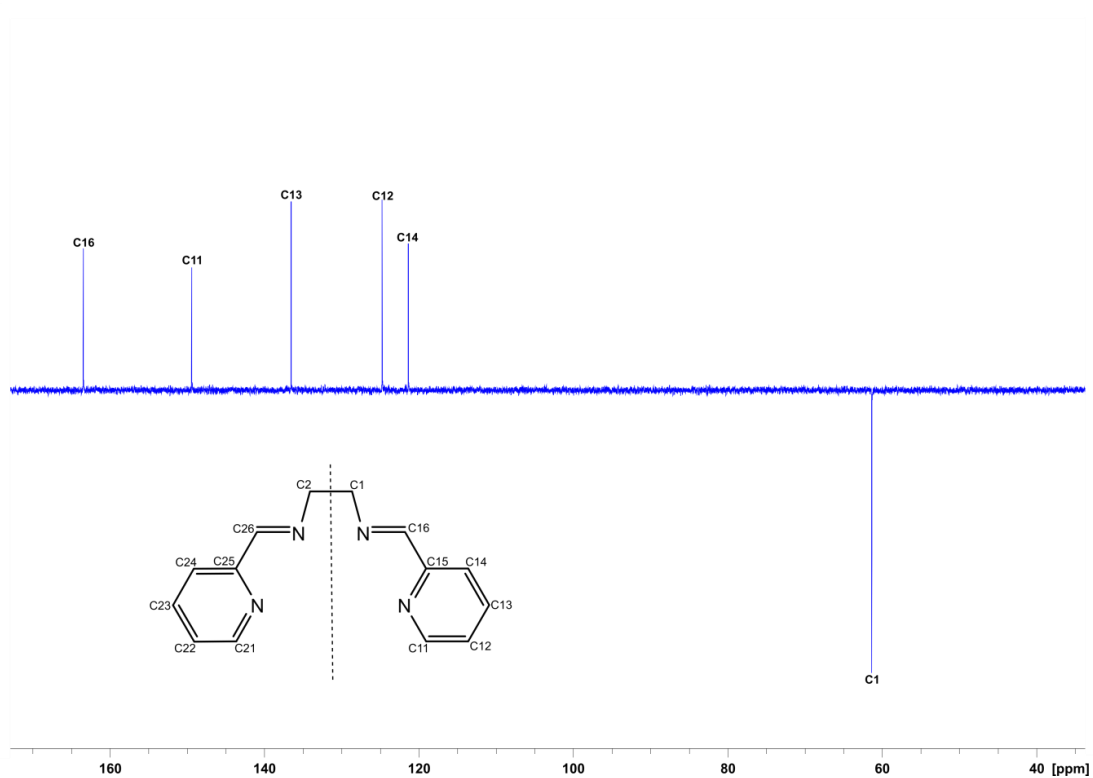


Figure S21: Dept-NMR spectra of diimine *N,N'*-bis(pyridylmethyl)-1,2-diaminoethane picon (**1a**).

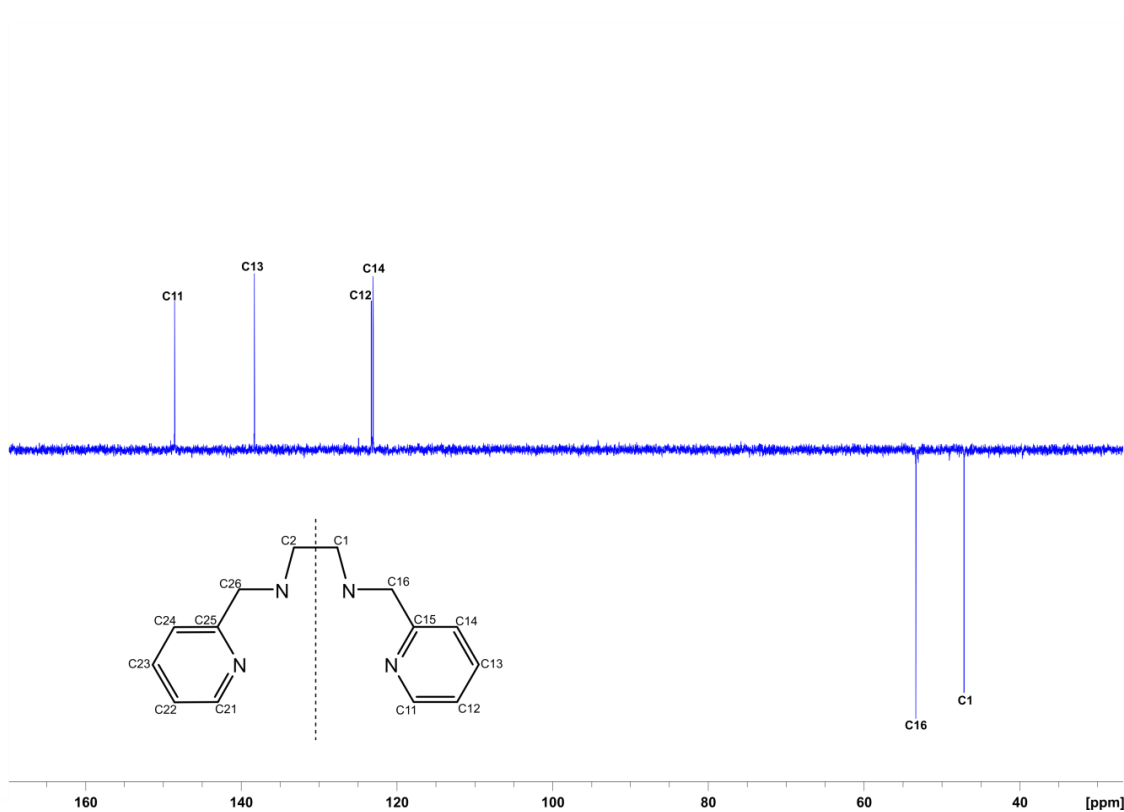


Figure S22: Dept-NMR spectra of diamine *N,N'*-bis(pyridylmethyl)-1,2-diaminoethane picon (**1**).

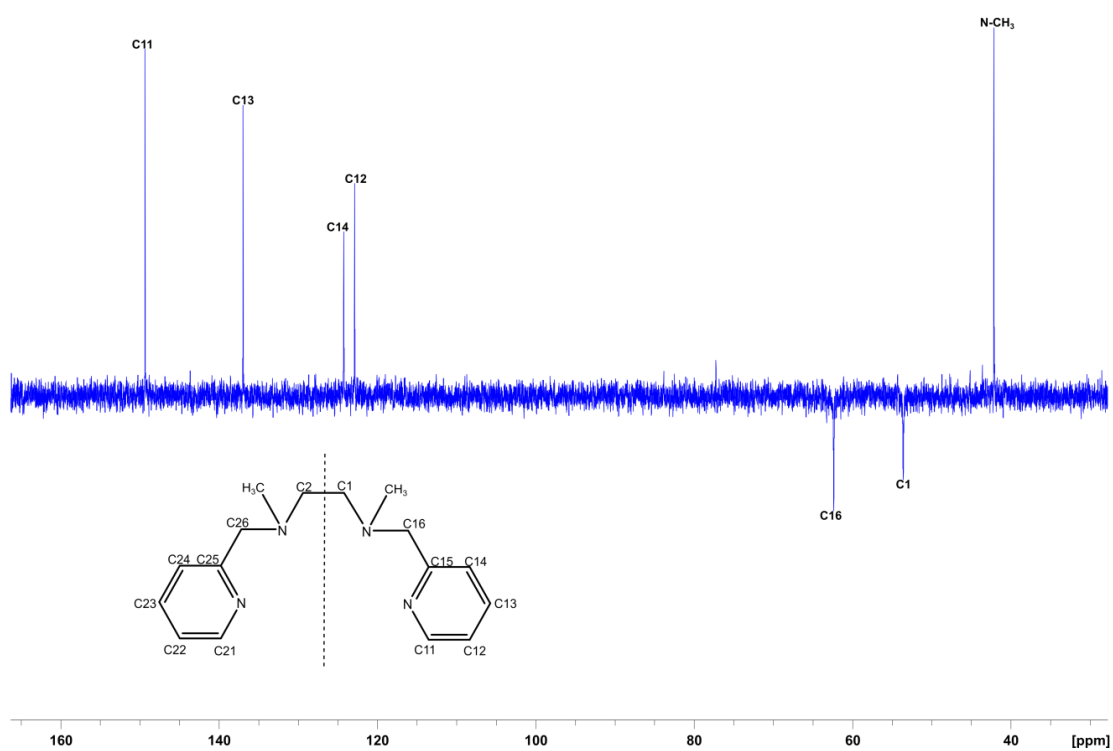


Figure S23: Deft-NMR spectra of *N,N'*-bis(2-pyridylmethyl)-*N,N'*-dimethyl-1,2-diaminoethane picenMe₂ (2).

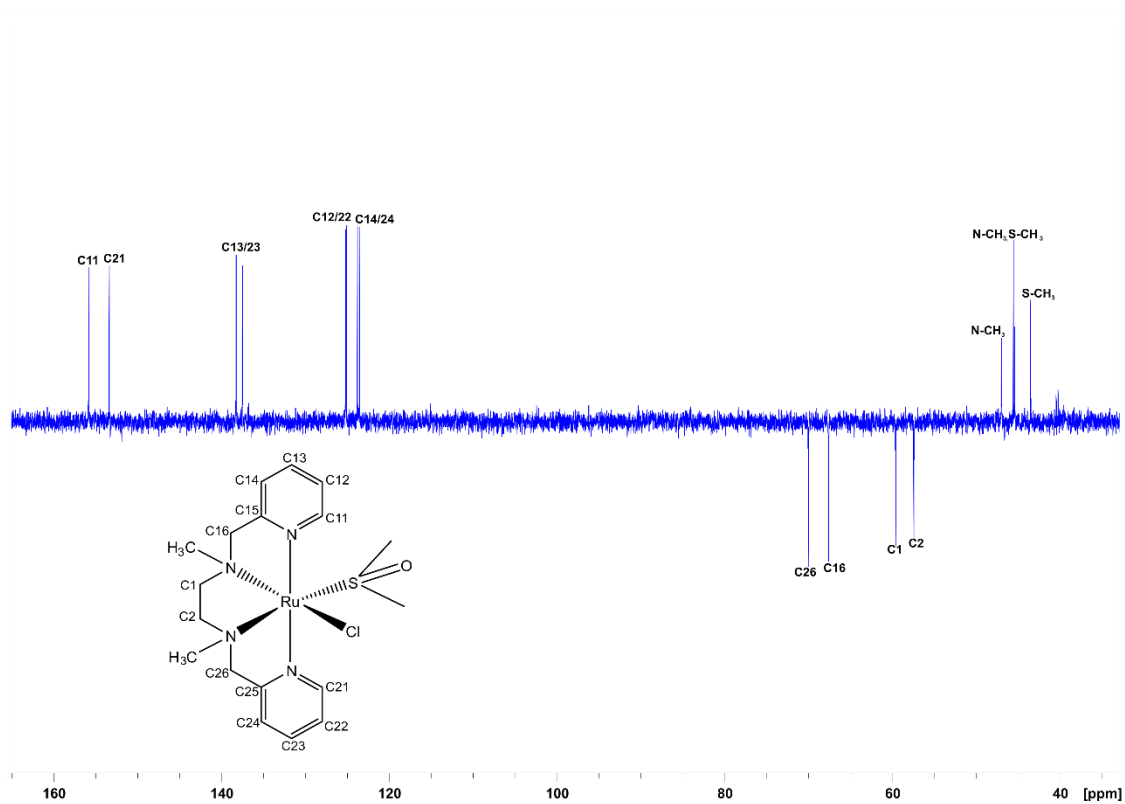


Figure S24: Deft-NMR spectra of *cis-α*-[Ru(picenMe₂)(DMSO)Cl]PF₆ (Ru-1).

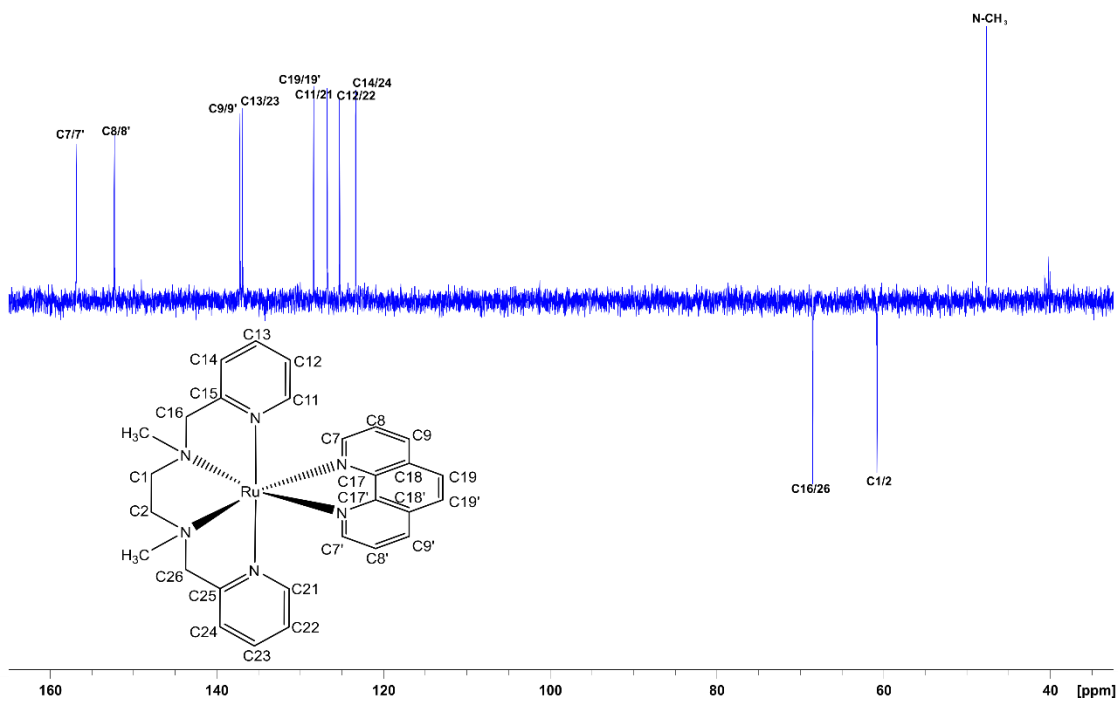


Figure S25: Dept-NMR spectra of racemic *cis-α*-[Ru(picenMe₂)(phen)](PF₆)₂ (Ru-2).

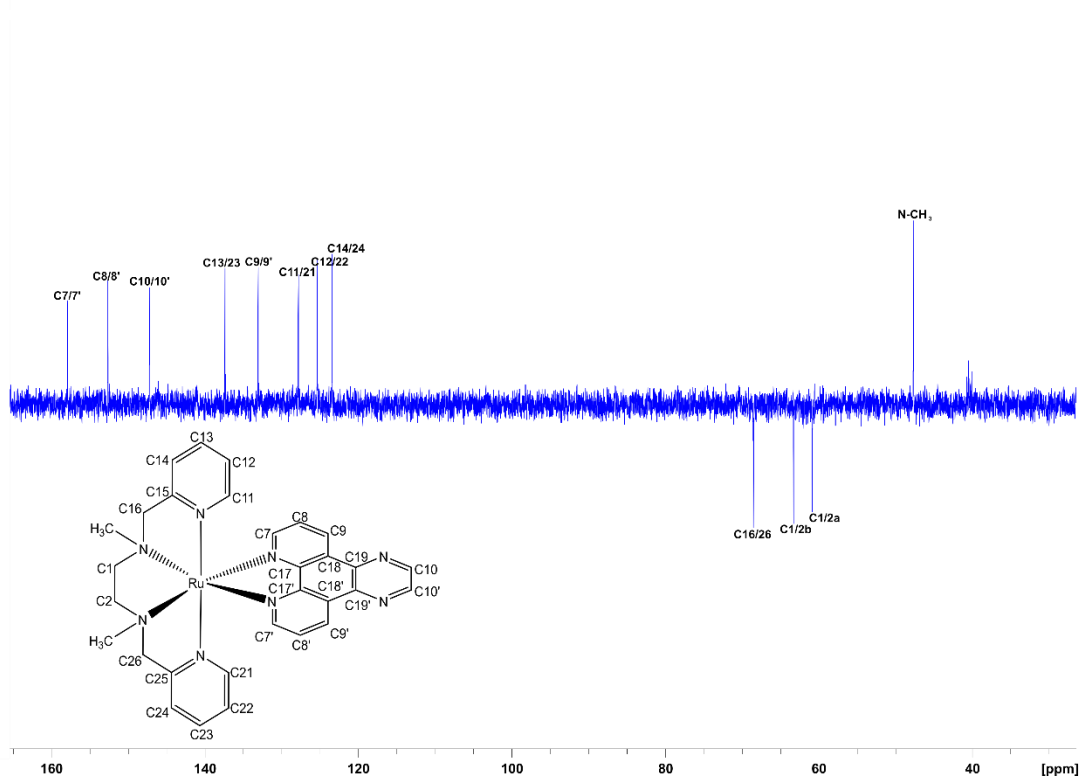


Figure S26: Dept-NMR spectra of racemic *cis-α*-[Ru(picenMe₂)(DPQ)](PF₆)₂ (Ru-3).

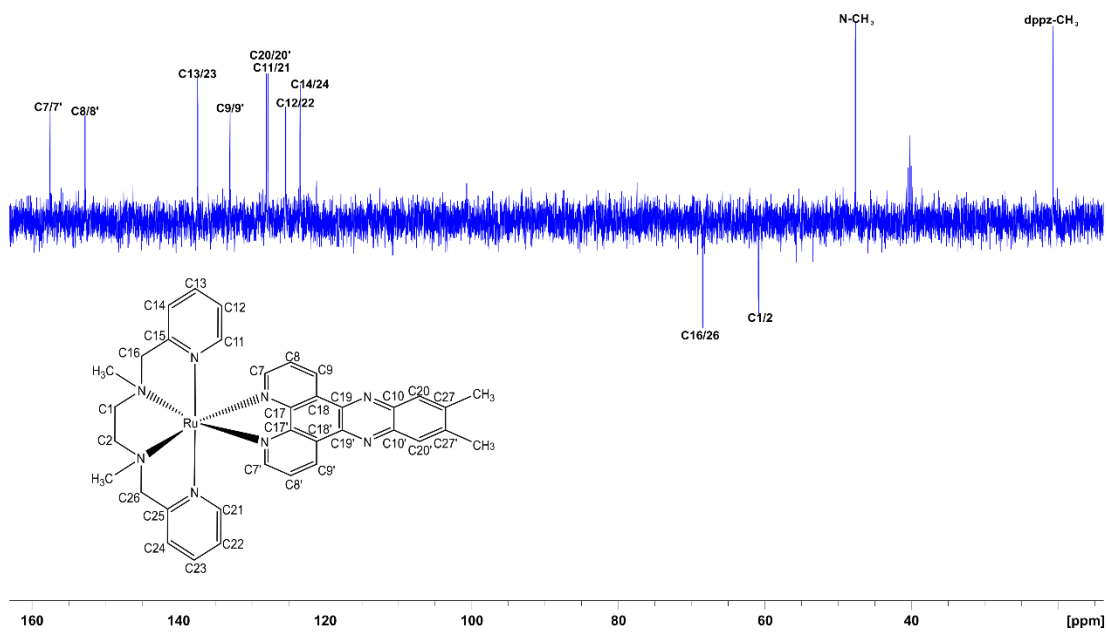


Figure S27: Dept-NMR spectra of racemic *cis-α*-[Ru(picenMe₂)(DppzMe₂)](PF₆)₂ (Ru-4).

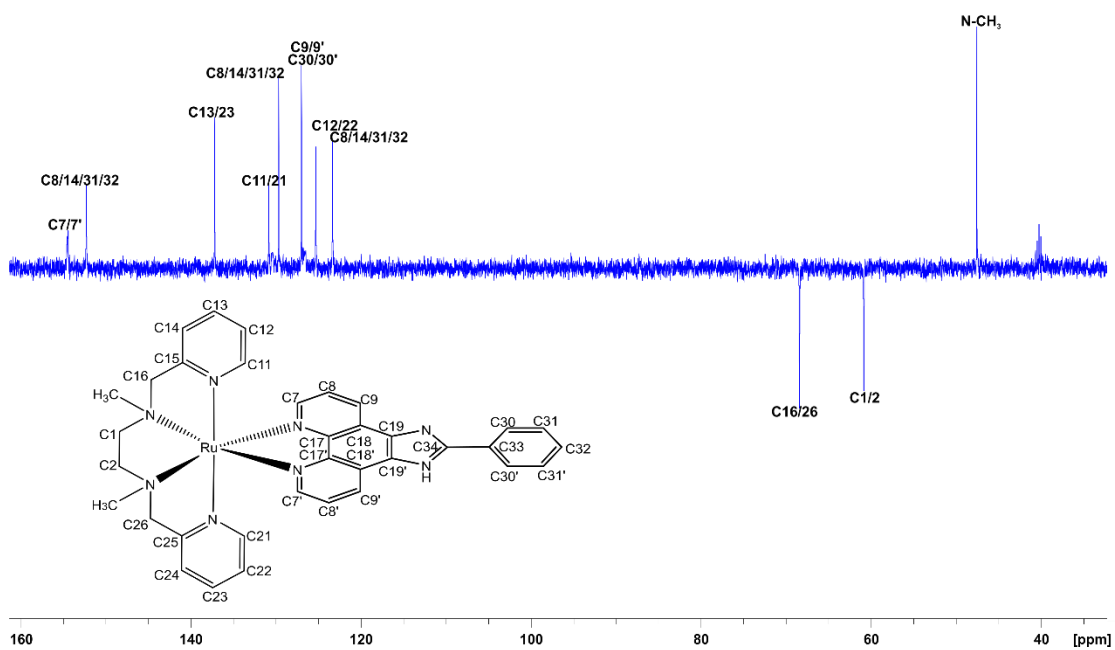


Figure S28: Dept-NMR spectra of racemic *cis-α*-[Ru(picenMe₂)(phenpyrBz)](PF₆)₂ (Ru-5).

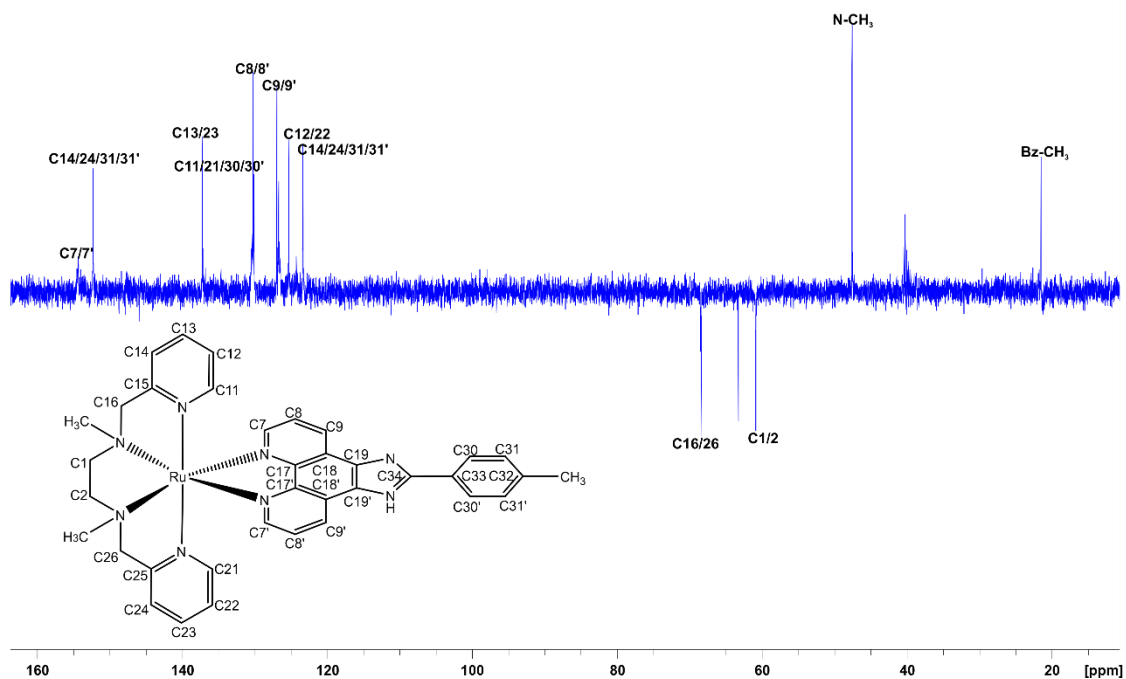


Figure S29: Dept-NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBzMe)](PF₆)₂ (Ru-6).

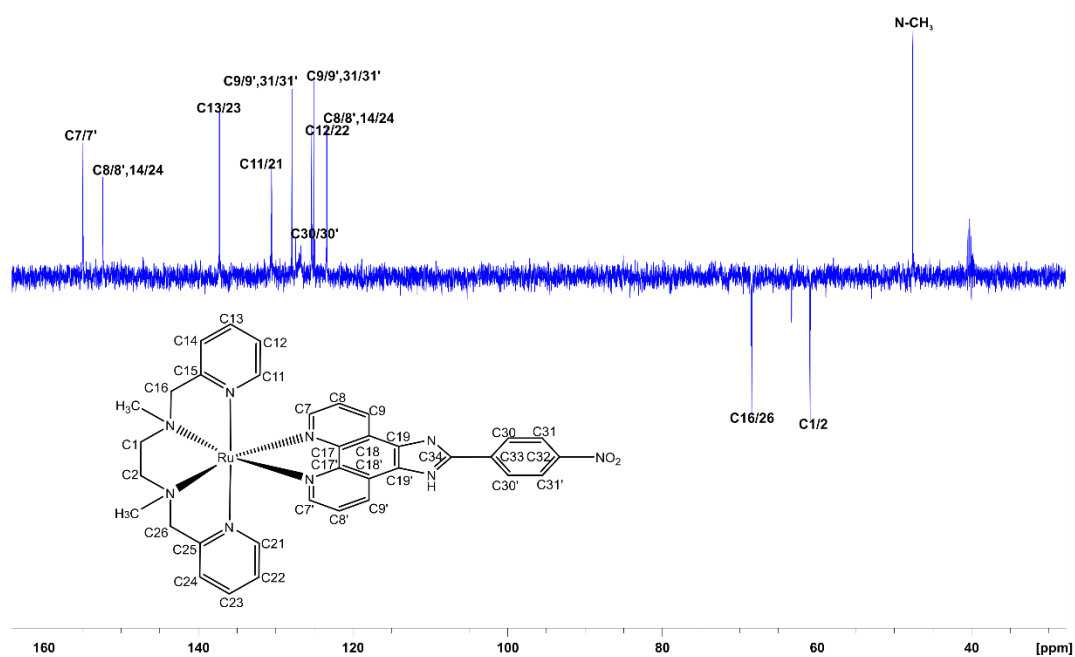


Figure S30: Dept-NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBzNO₂)](PF₆)₂ (Ru-7).

2.4 HMQC-NMR

400 MHz Bruker Avance NMR using deuterated solvent DMSO, D₂O or CDCl₃, with temperatures maintained at either 25 or 35 °C, 4 accumulations.

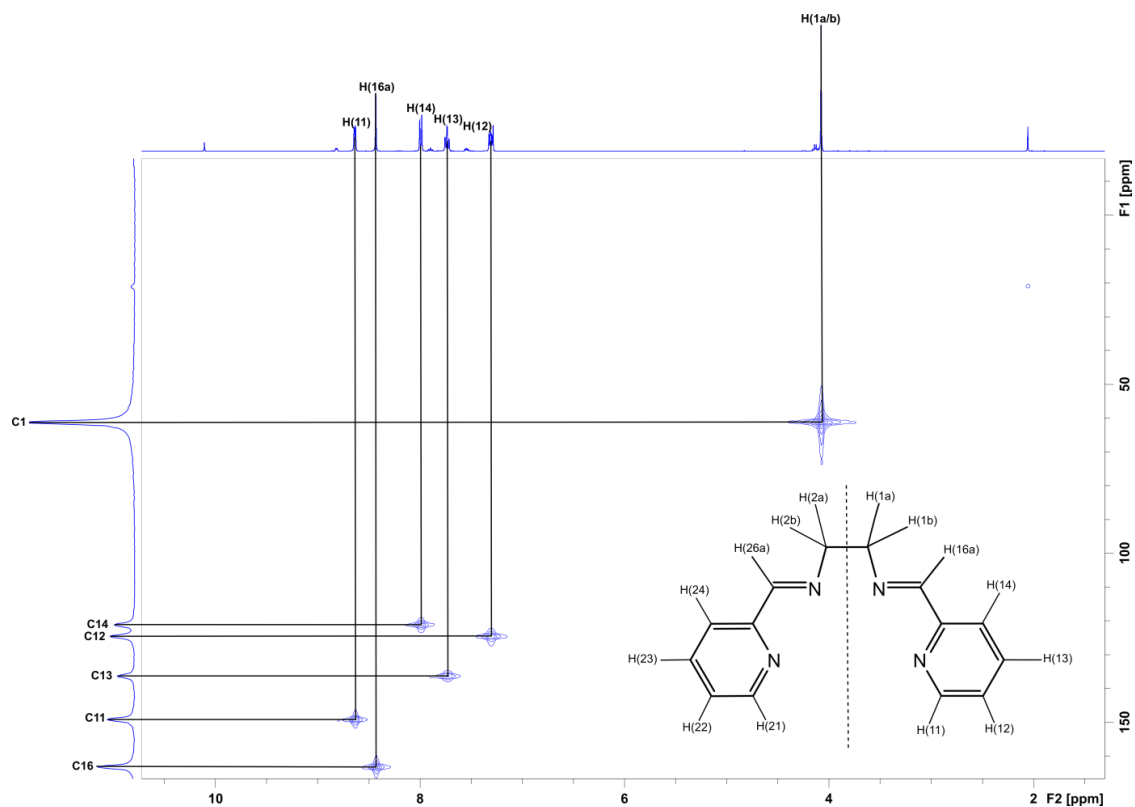


Figure S31: HMQC-NMR spectra of diimine *N,N'*-bis(pyridylmethyl)-1,2-diaminoethane picen (**1a**).

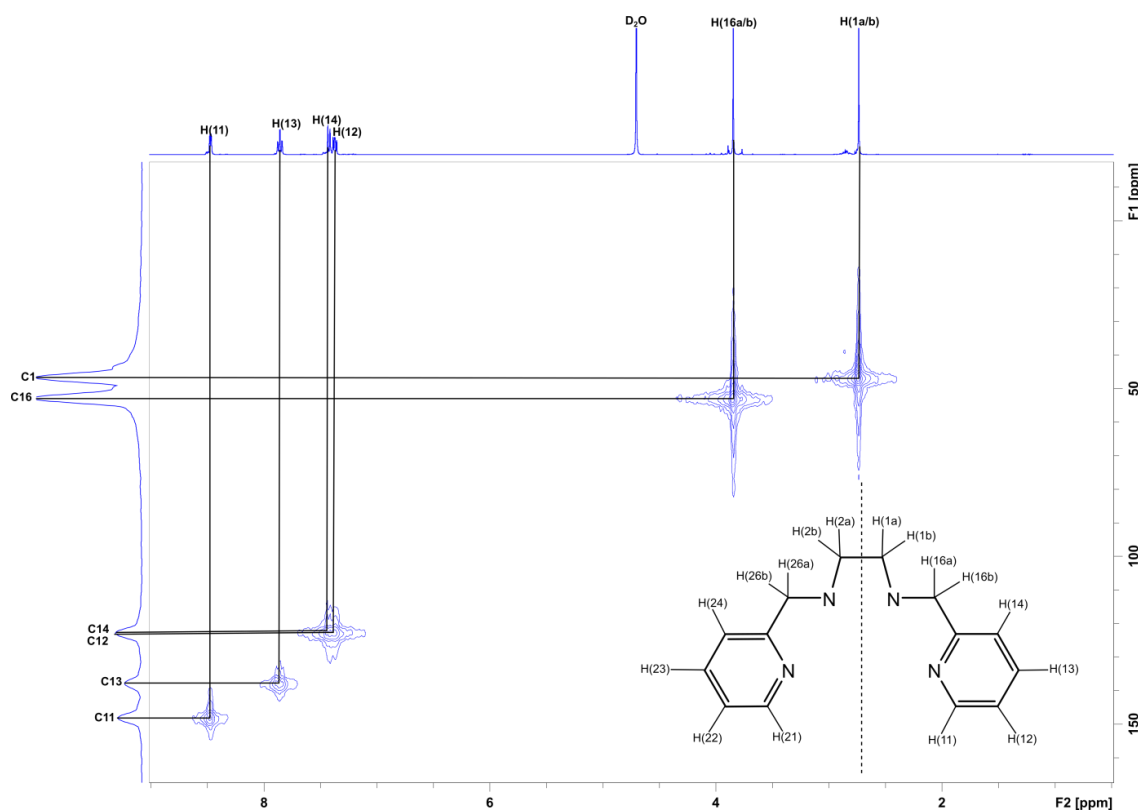


Figure S32: HMQC-NMR spectra of diamine *N,N'*-bis(pyridylmethyl)-1,2-diaminoethane picen (**1**).

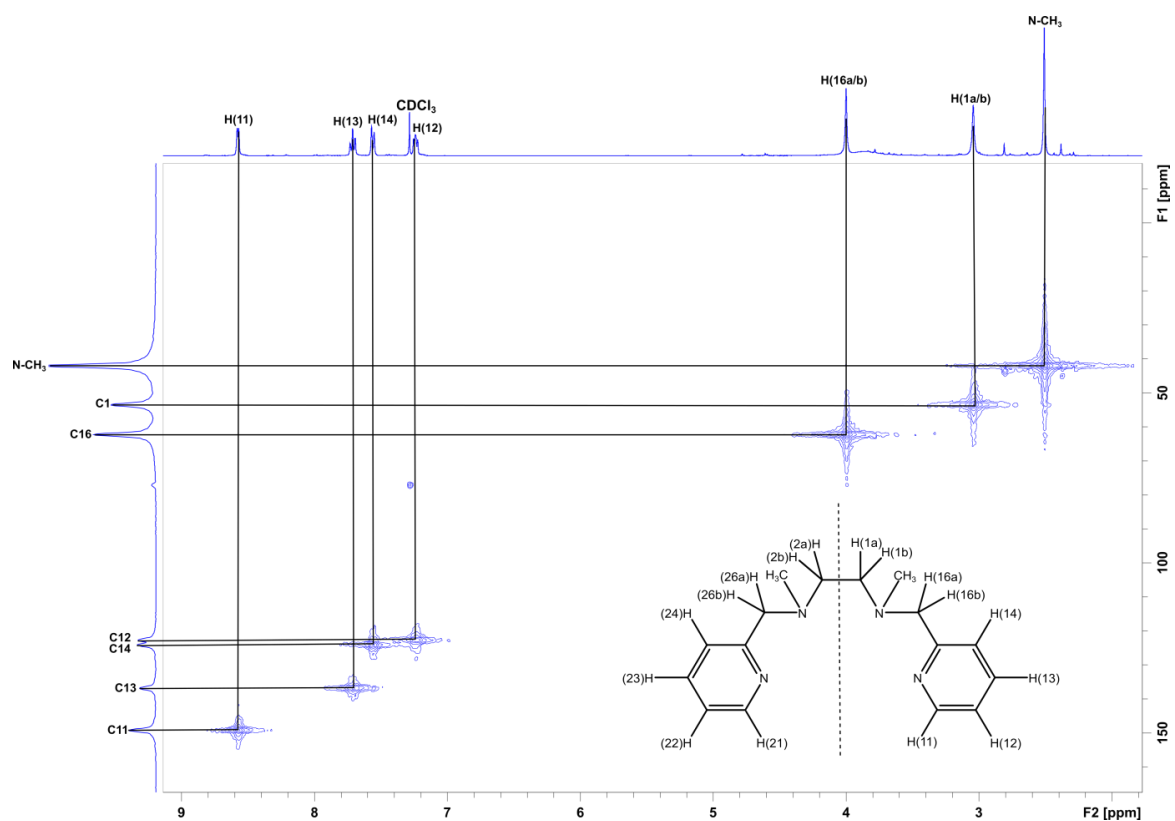


Figure S33: HMQC-NMR spectra of *N,N'*-bis(2-pyridylmethyl)-*N,N'*-dimethyl-1,2-diaminoethane picenMe₂ (2).

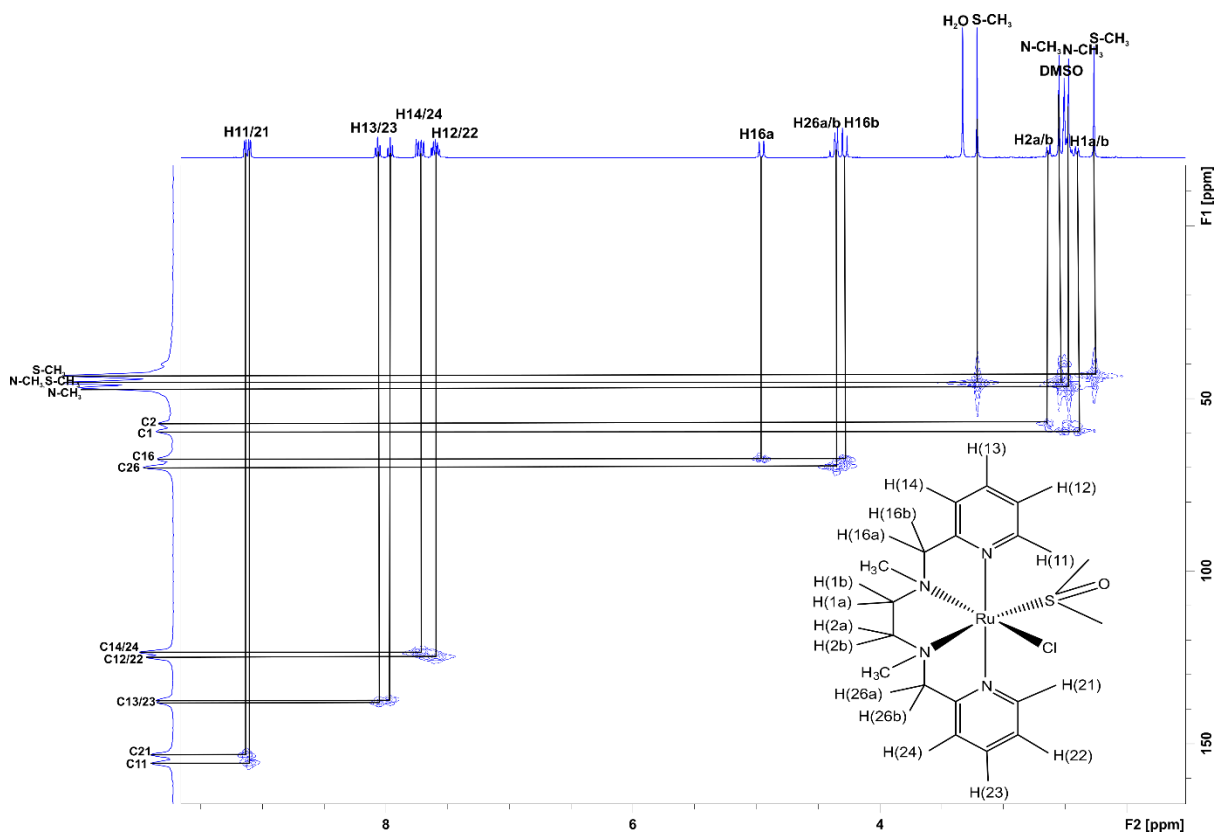


Figure S34: HMQC-NMR spectra of *cis-α*-[Ru(picenMe₂)(DMSO)Cl]PF₆ (Ru-1).

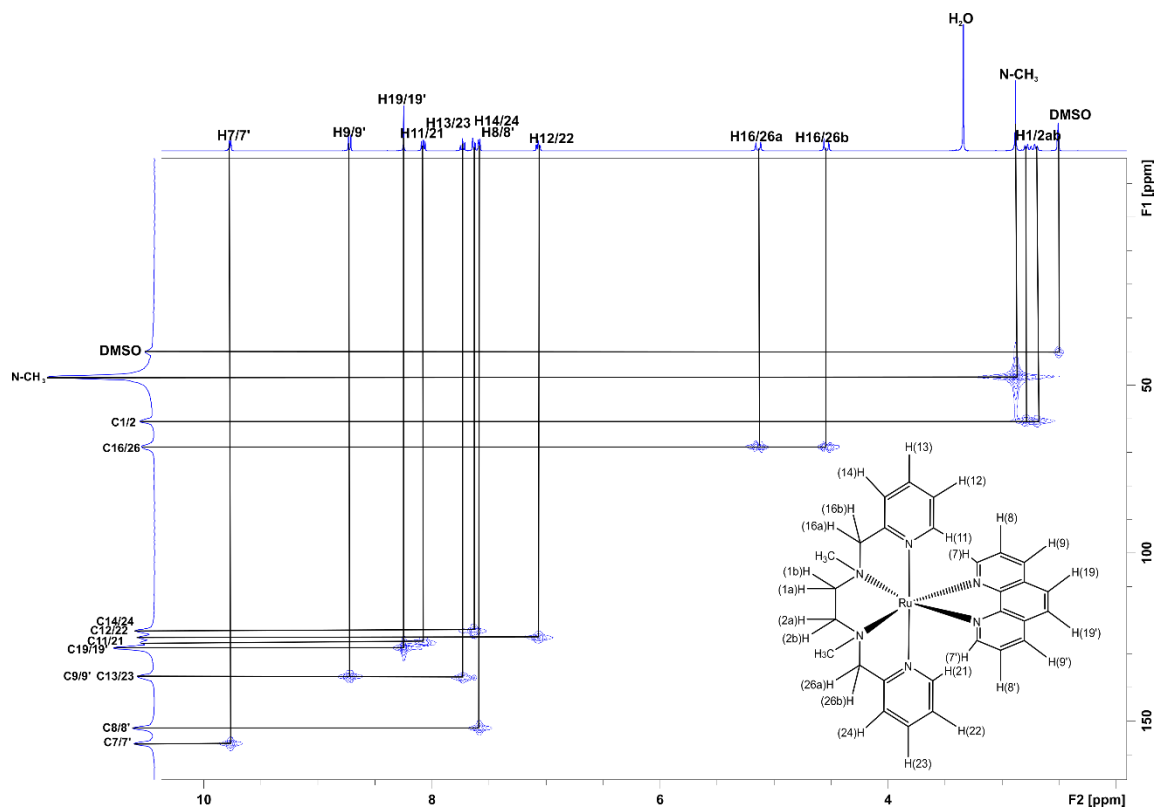


Figure S35: HMQC-NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(phen)](PF₆)₂ (Ru-2).

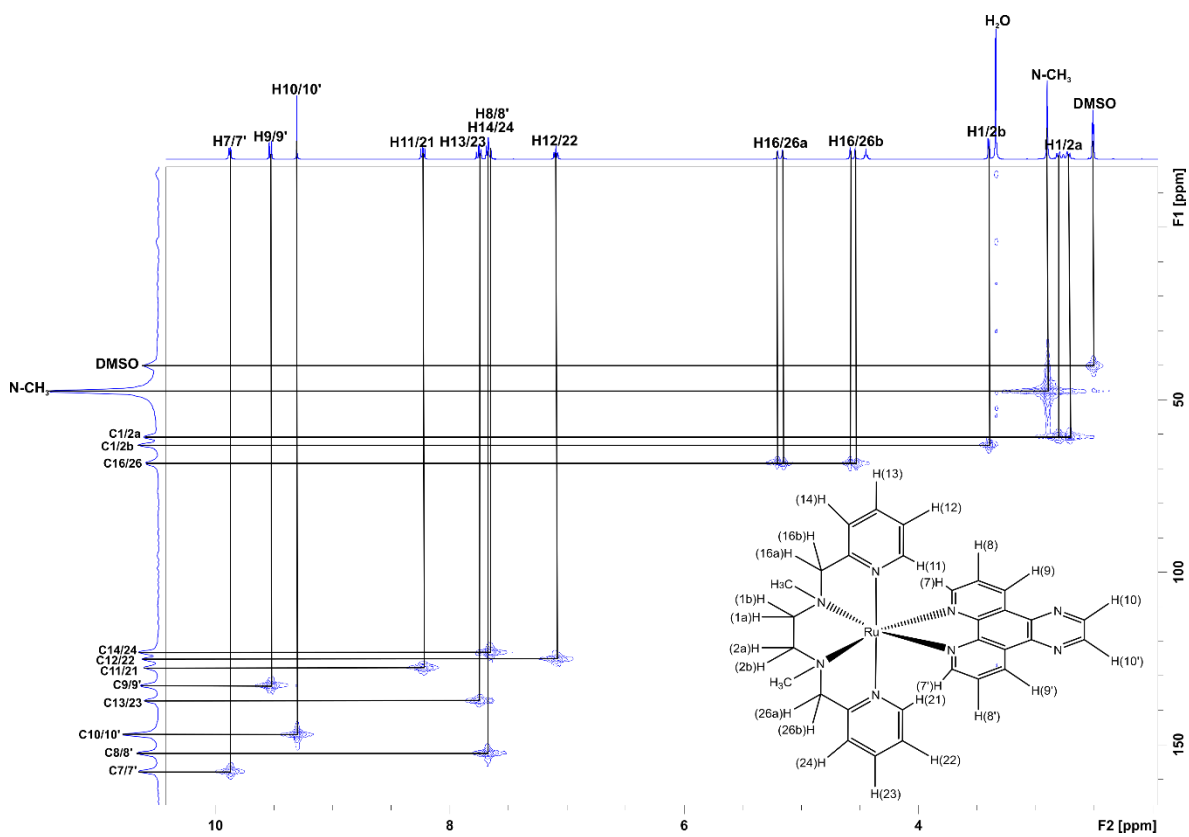


Figure S36: HMQC-NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(DPQ)](PF₆)₂ (Ru-3).

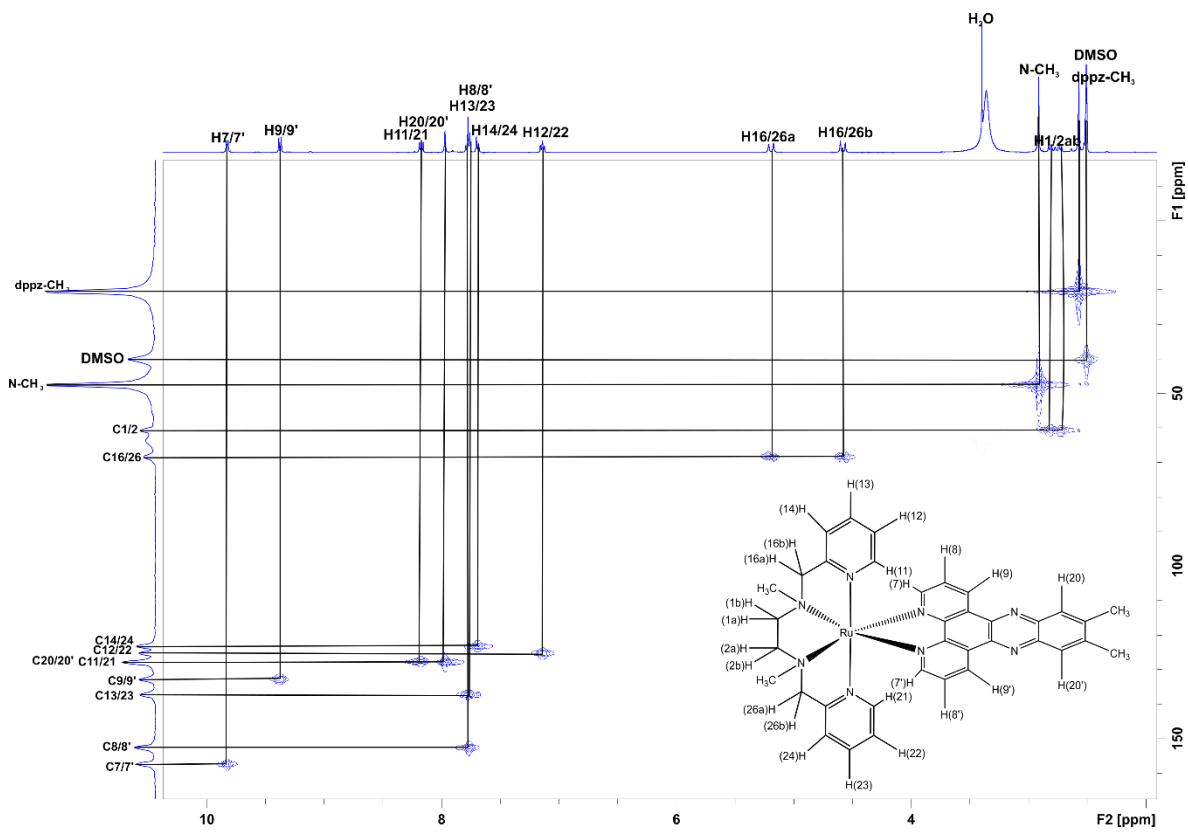


Figure S37: HMQC-NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(DppzMe₂)](PF₆)₂ (Ru-4).

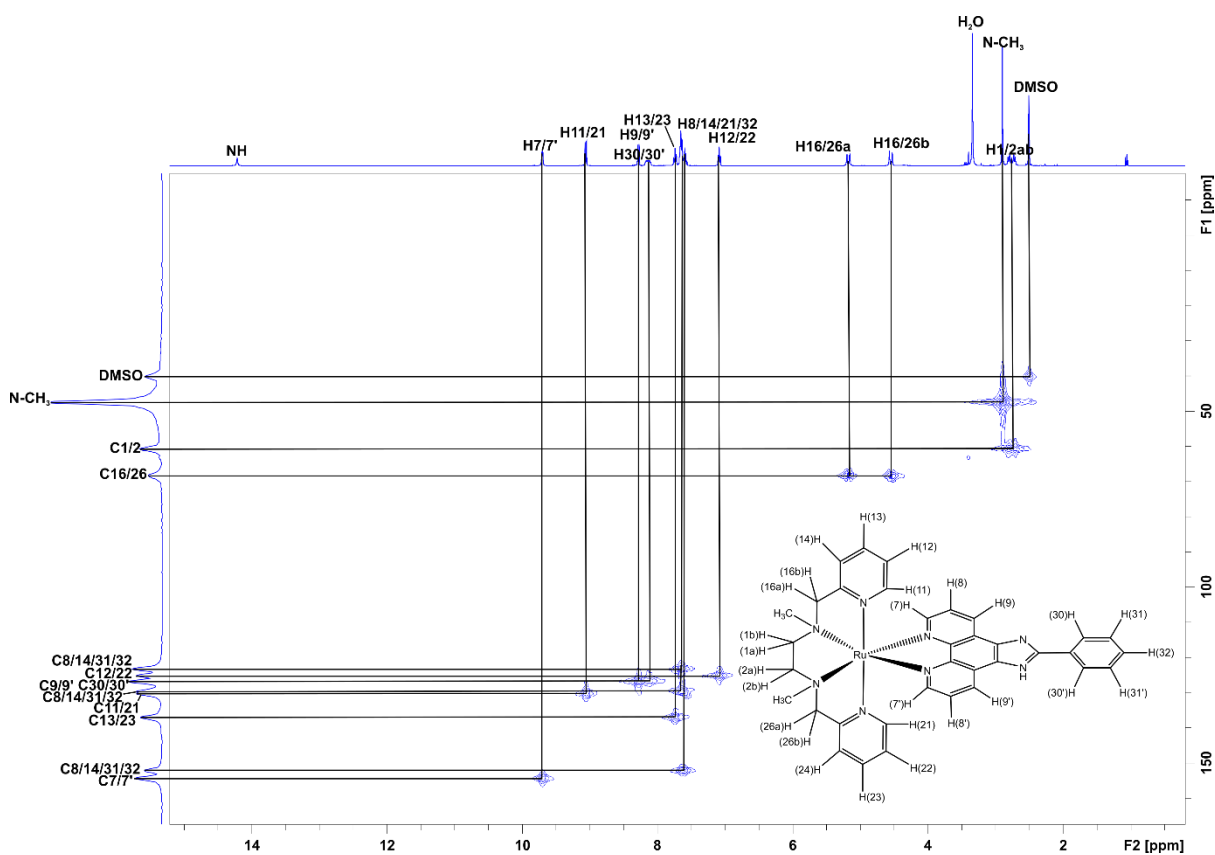


Figure S38: HMQC-NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBz)](PF₆)₂ (Ru-5).

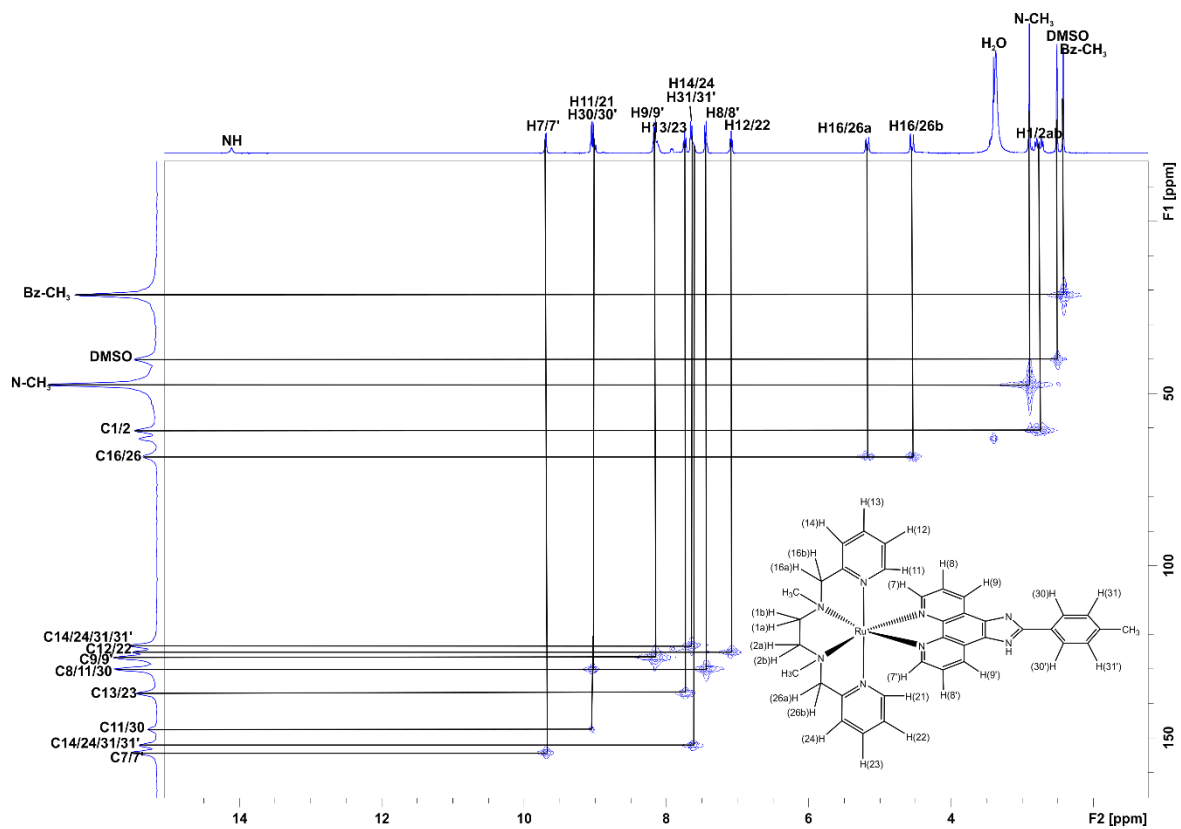


Figure S39: HMQC-NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBzMe)](PF₆)₂ (Ru-6).

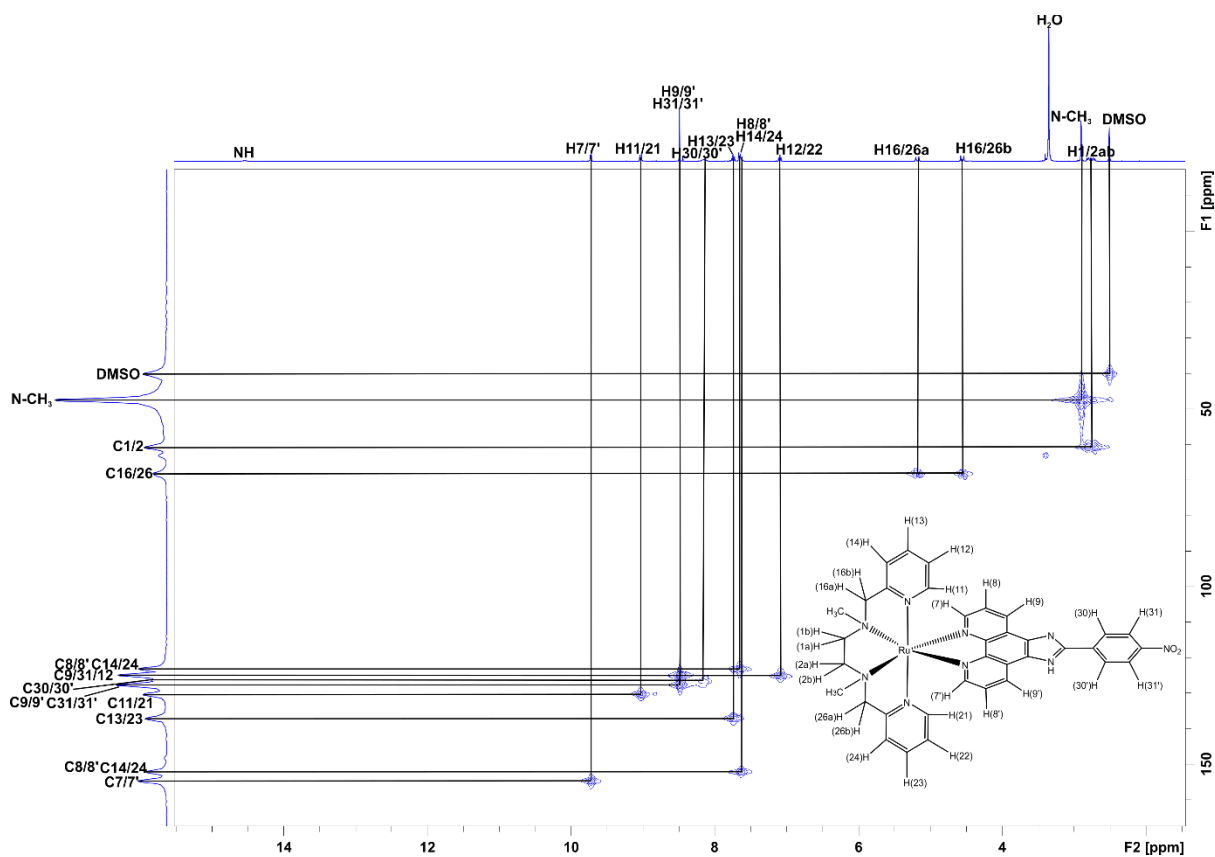


Figure S40: HMQC-NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBzNO₂)](PF₆)₂ (Ru-7).

2.5 COSY-NMR

400 MHz Bruker Avance NMR using deuterated solvent DMSO, D₂O or CDCl₃, with temperatures maintained at either 25 or 35 °C, 2 accumulations.

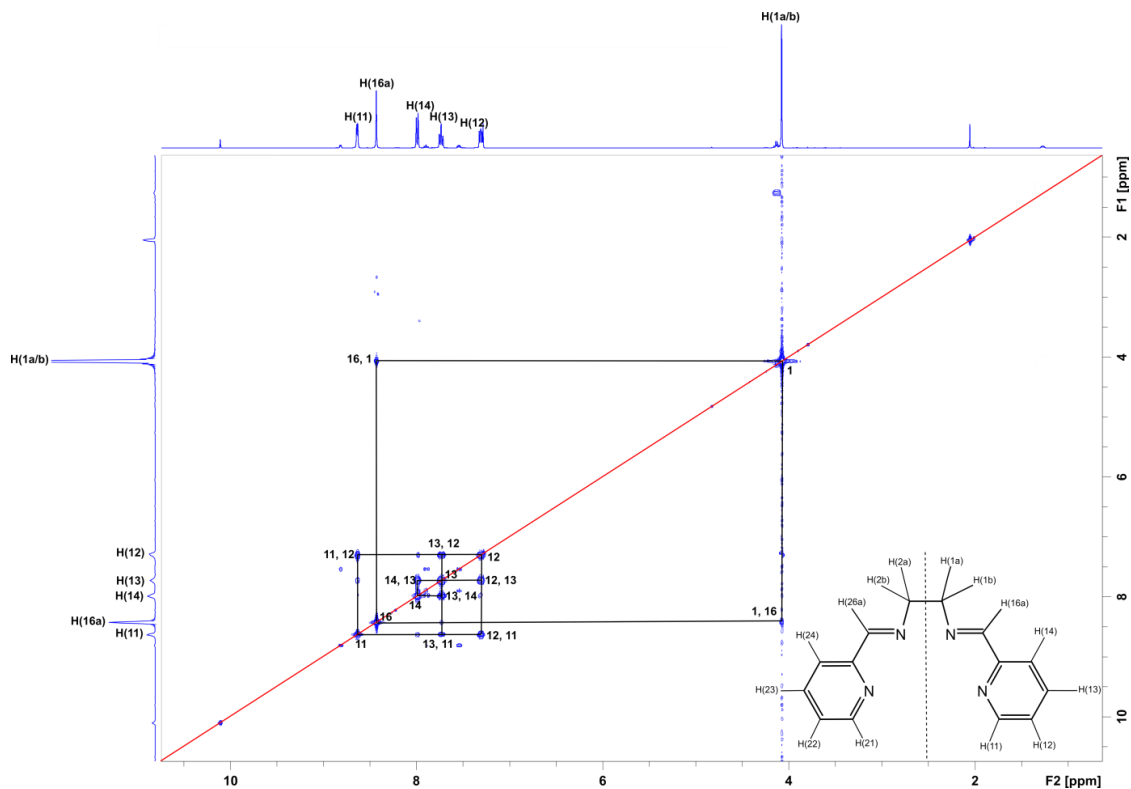


Figure S41: COSY-NMR spectra of diimine *N,N'*-bis(pyridylmethyl)-1,2-diaminoethane picen (**1a**).

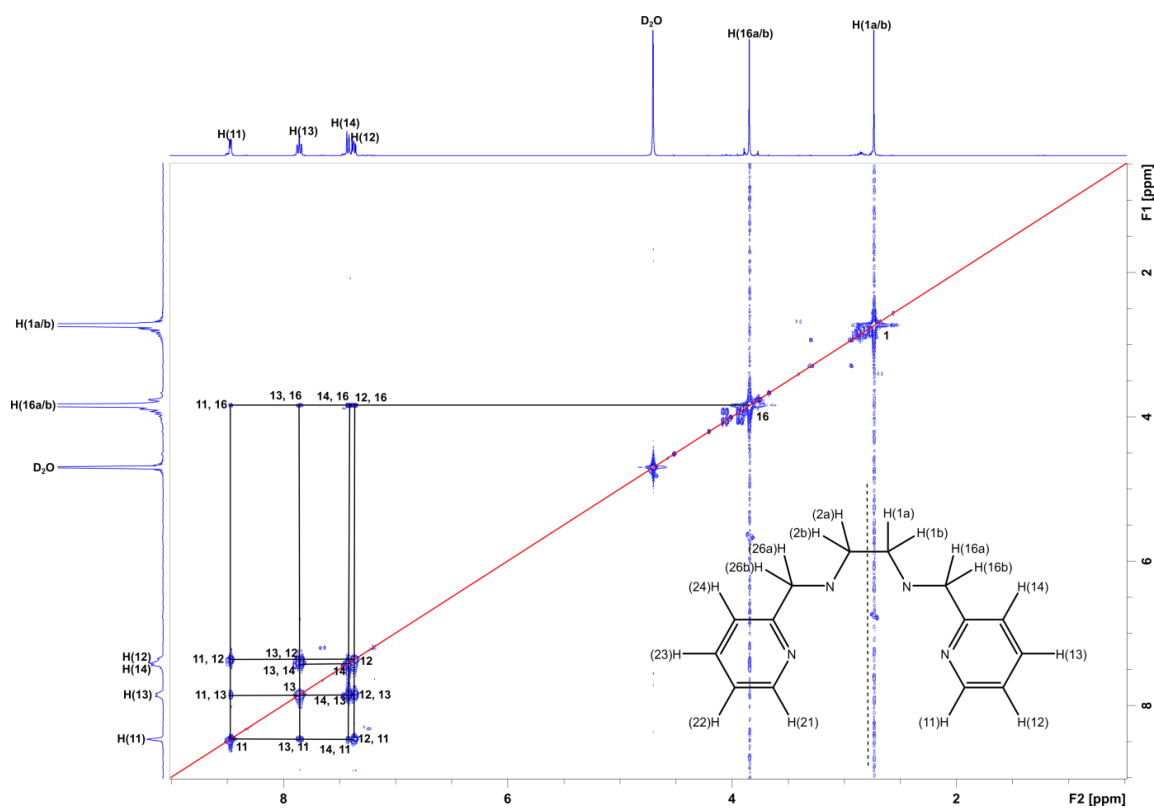


Figure S42: COSY-NMR spectra of diamine *N,N'*-bis(pyridylmethyl)-1,2-diaminoethane picen (**1**).

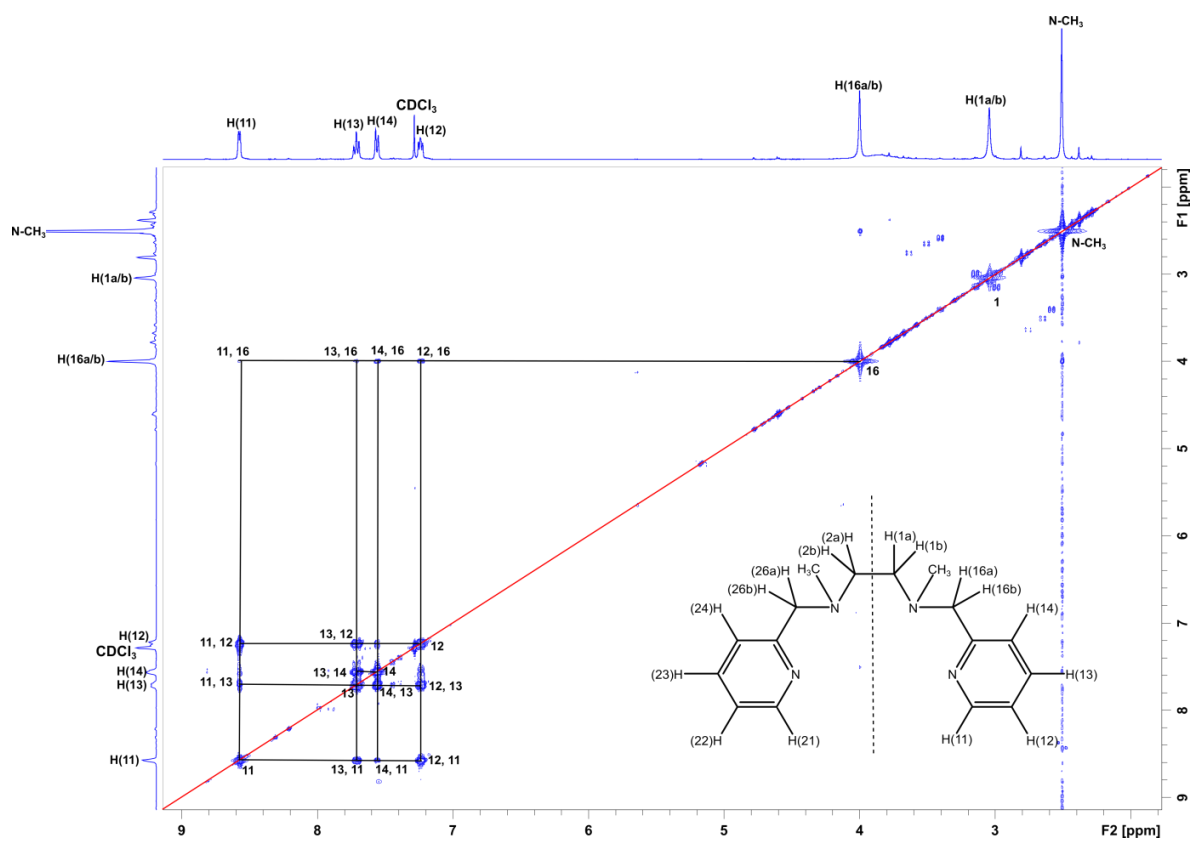


Figure S43: COSY-NMR spectra of *N,N'*-bis(2-pyridylmethyl)-*N,N'*-dimethyl-1,2-diaminoethane picenMe₂ (**2**).

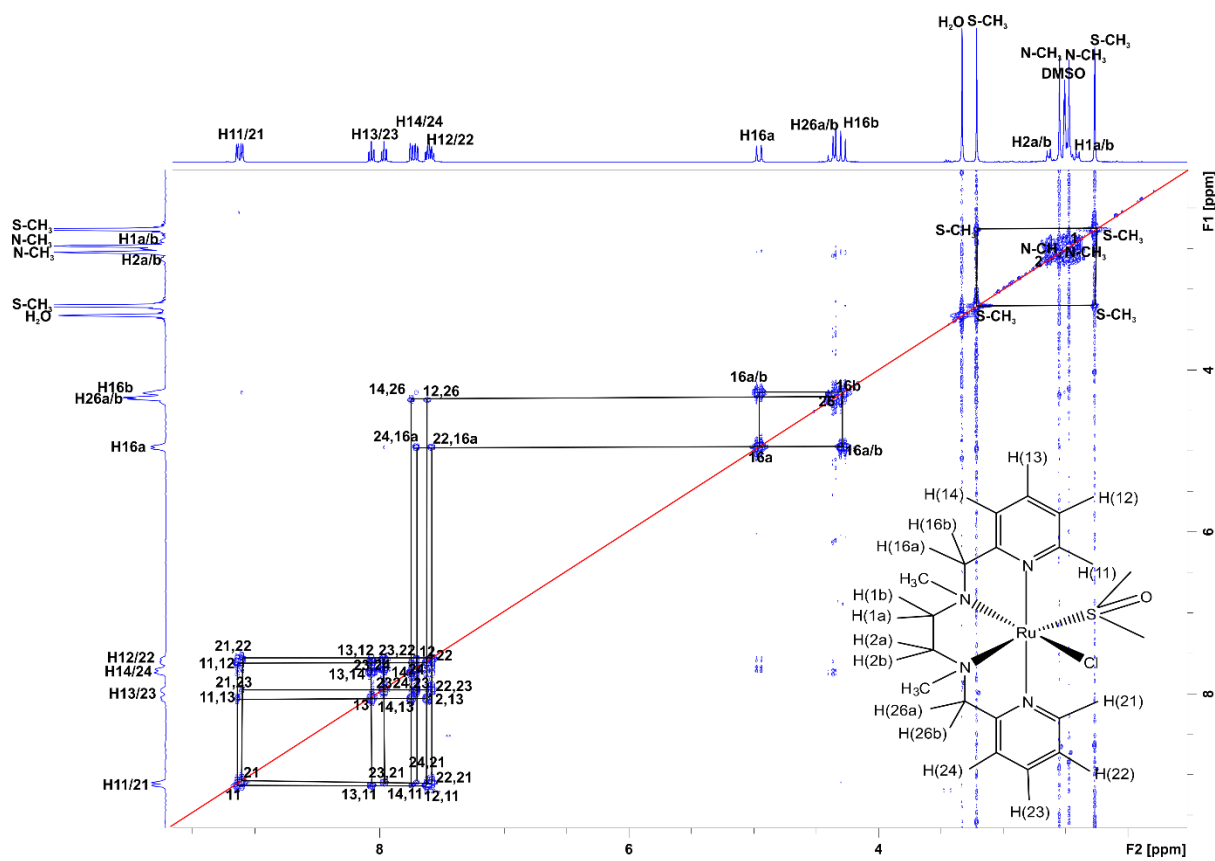


Figure S44: COSY-NMR spectra of *cis-α*-[Ru(picenMe₂)(DMSO)Cl]PF₆ (**Ru-1**).

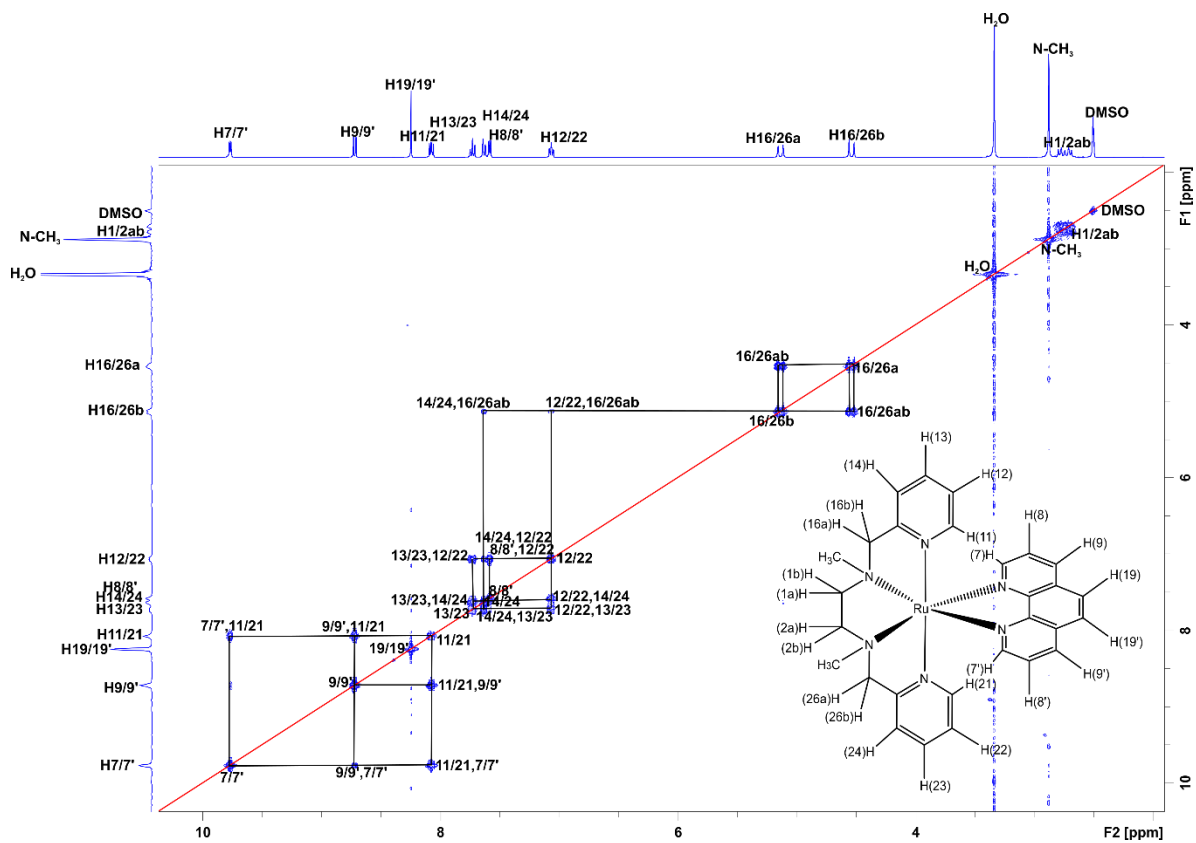


Figure S45: COSY-NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(phen)](PF₆)₂ (Ru-2).

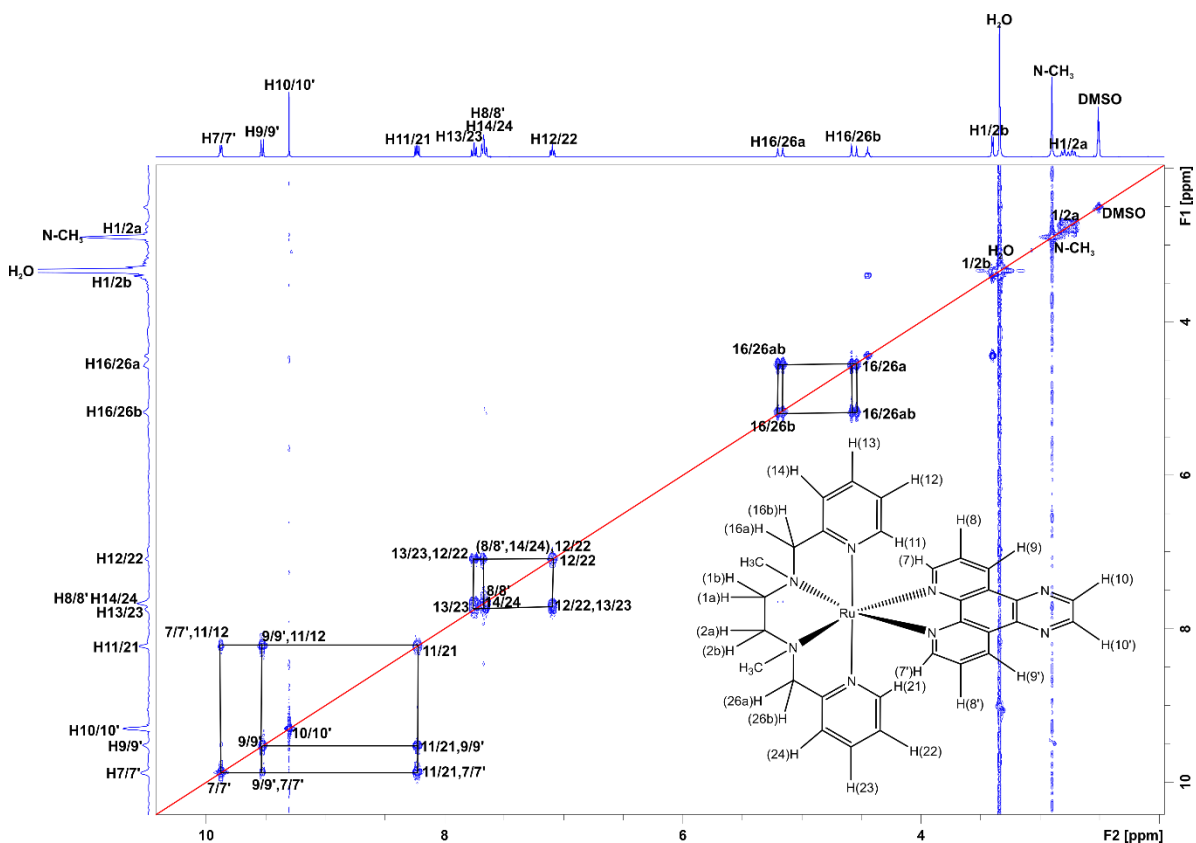


Figure S46: COSY-NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(DPQ)](PF₆)₂ (Ru-3).

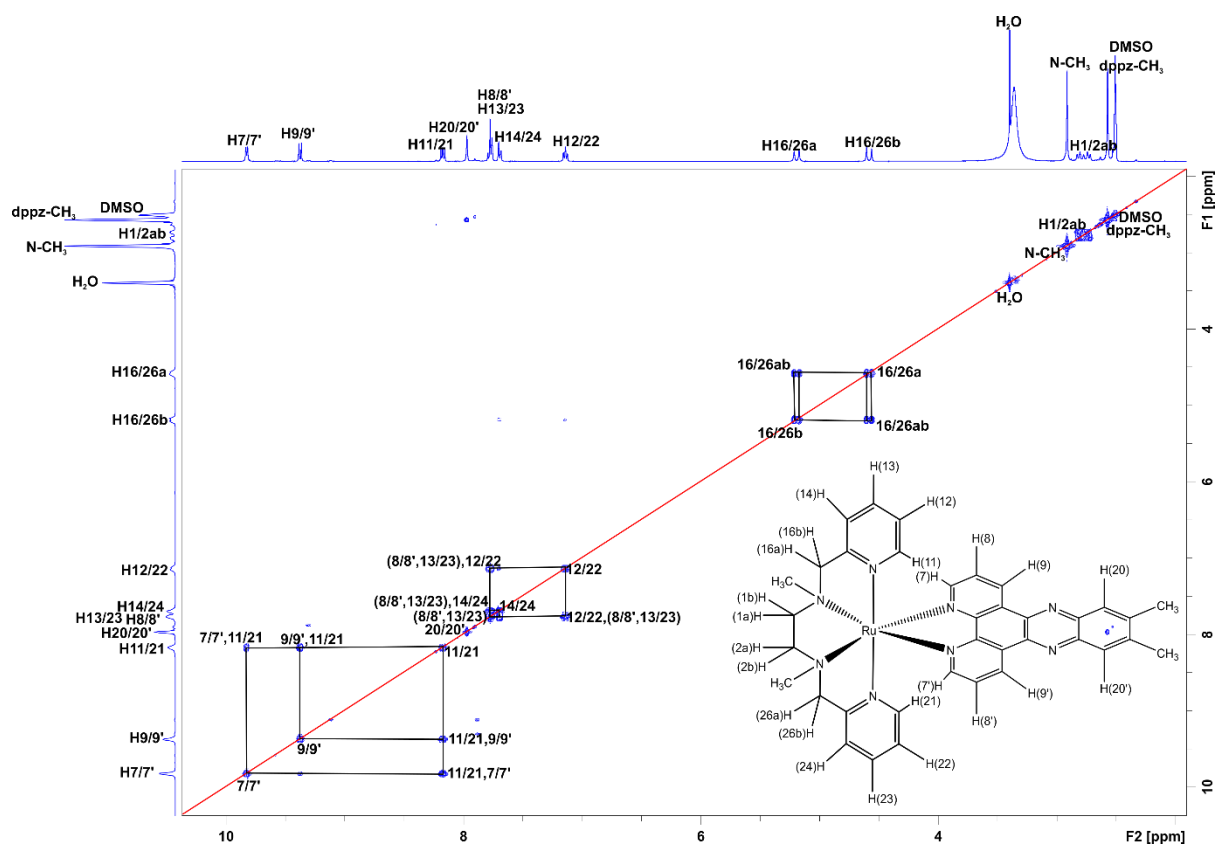


Figure S47: COSY-NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(DppzMe₂)](PF₆)₂ (Ru-4).

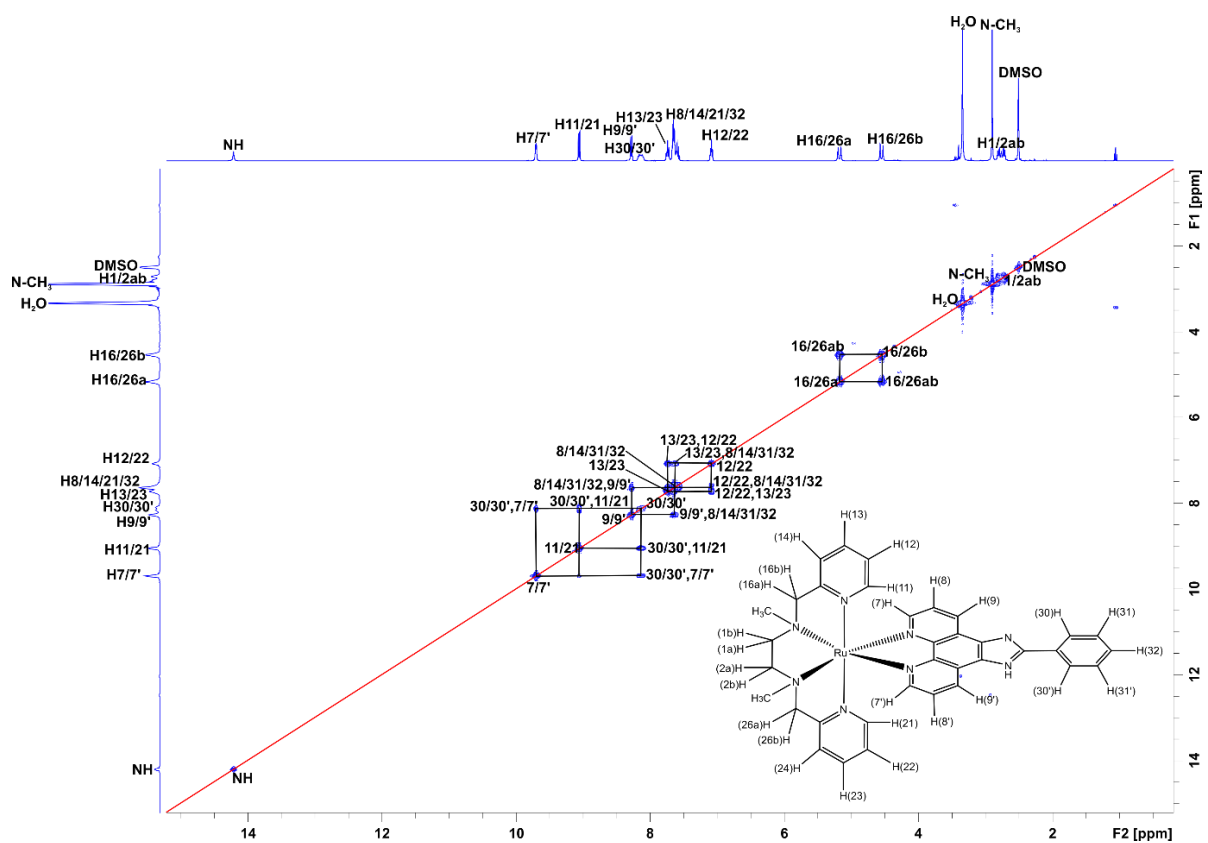


Figure S48: COSY-NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBz)](PF₆)₂ (Ru-5).

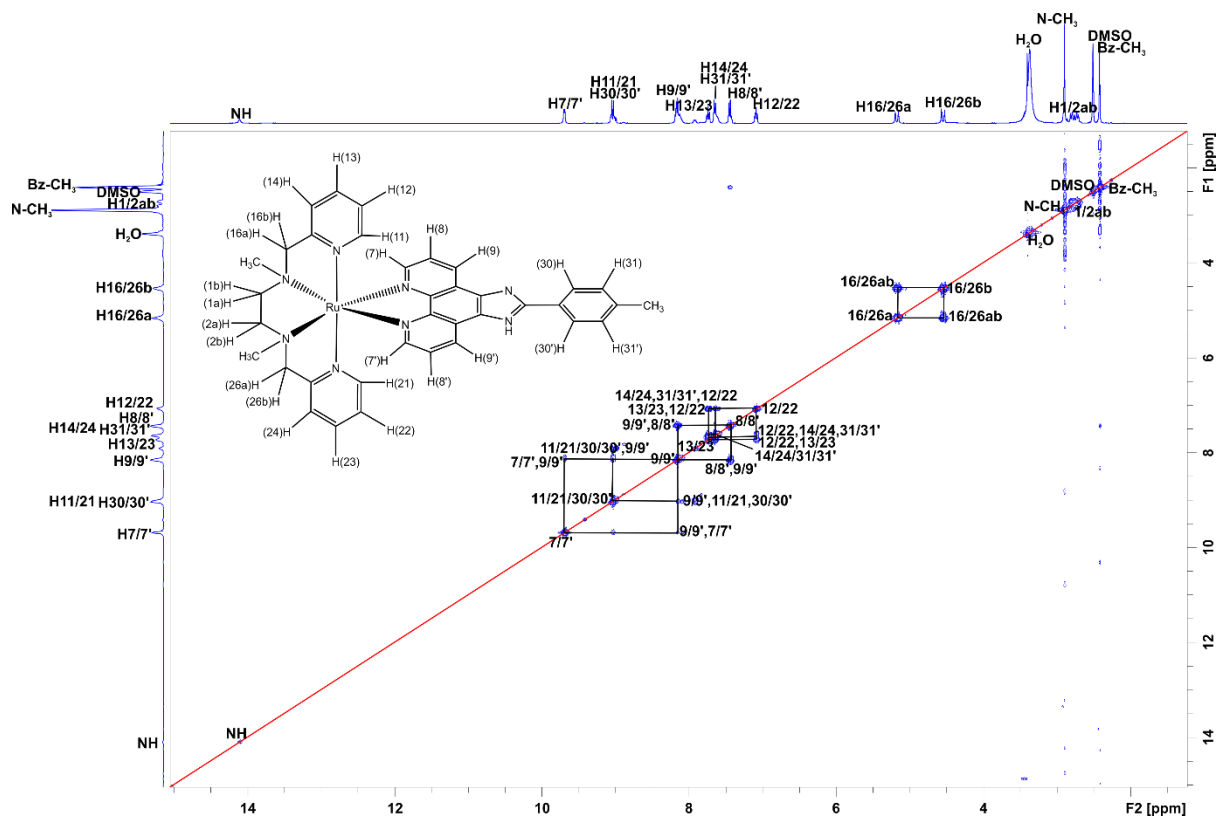


Figure S49: COSY-NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBzMe)](PF₆)₂ (Ru-6).

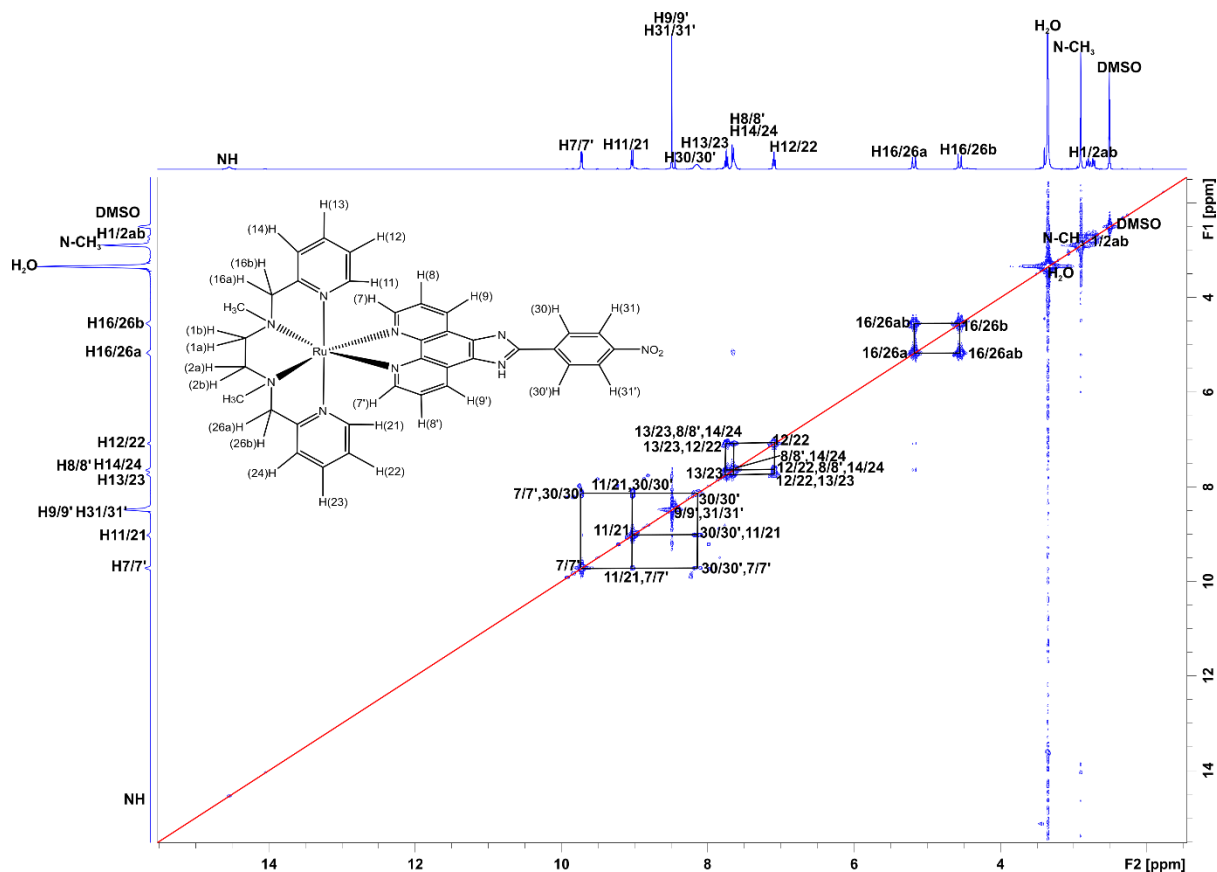


Figure S50: COSY-NMR spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBzNO₂)](PF₆)₂ (Ru-7).

2.6 UV-Vis

1 cm quartz cell, corrected for solvent baseline with either chloroform, acetonitrile or DMSO

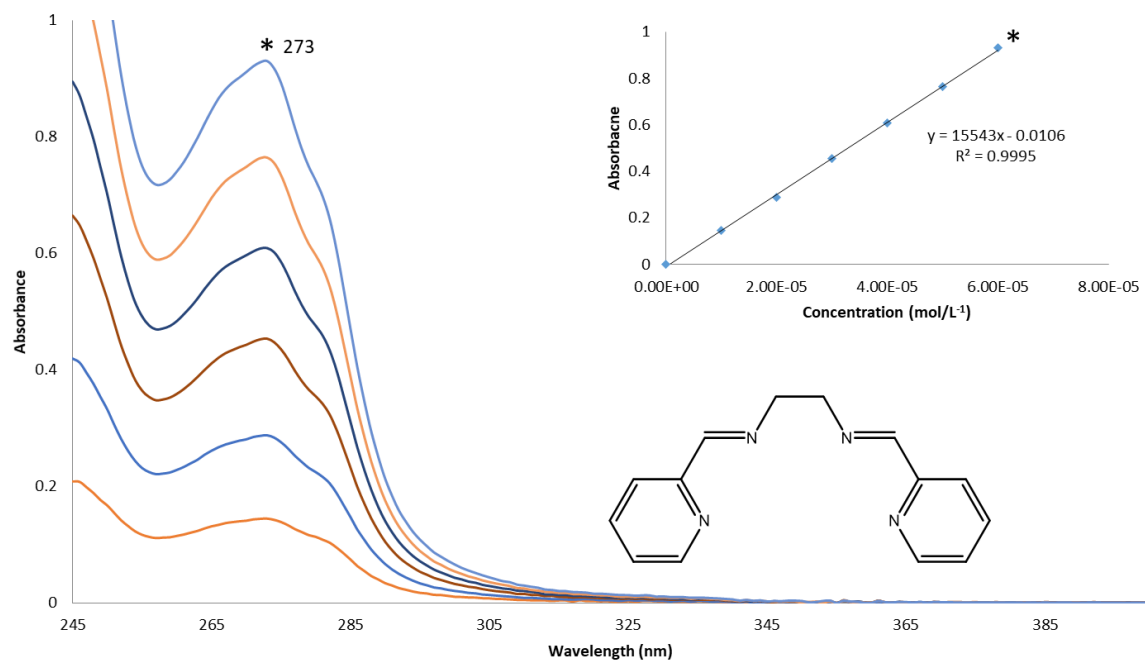


Figure S51: UV-Vis spectra of diimine *N,N'*-bis(pyridylmethyl)-1,2-diaminoethane picen (**1a**).

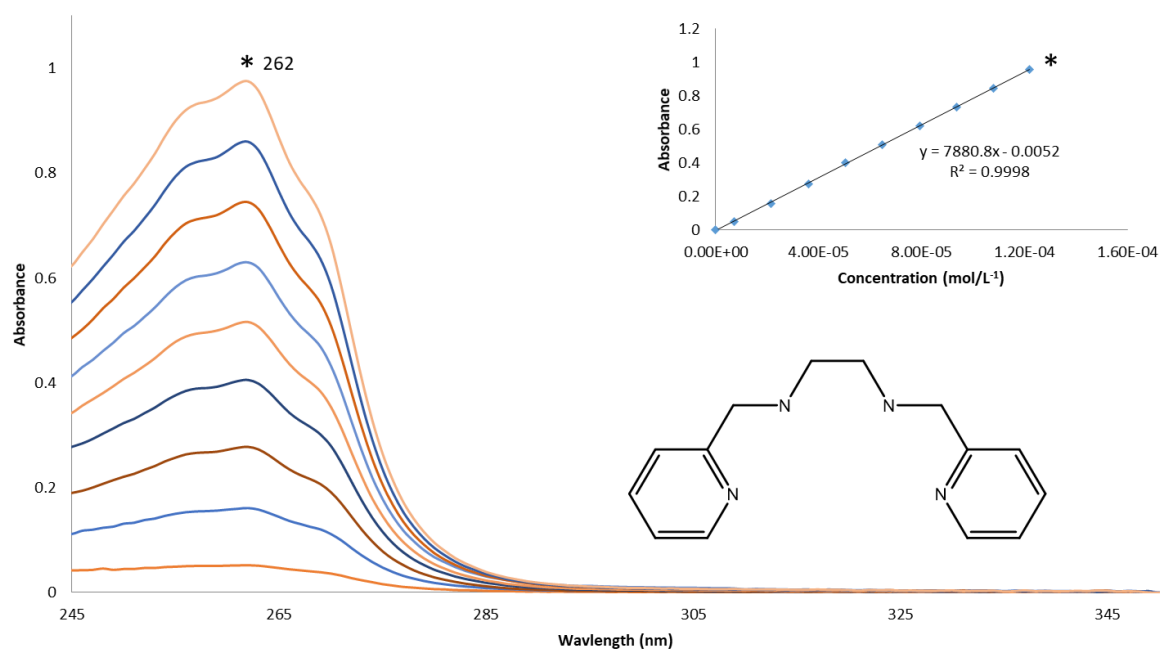


Figure S52: UV-Vis spectra of diamine *N,N'*-bis(pyridylmethyl)-1,2-diaminoethane picen (**1**).

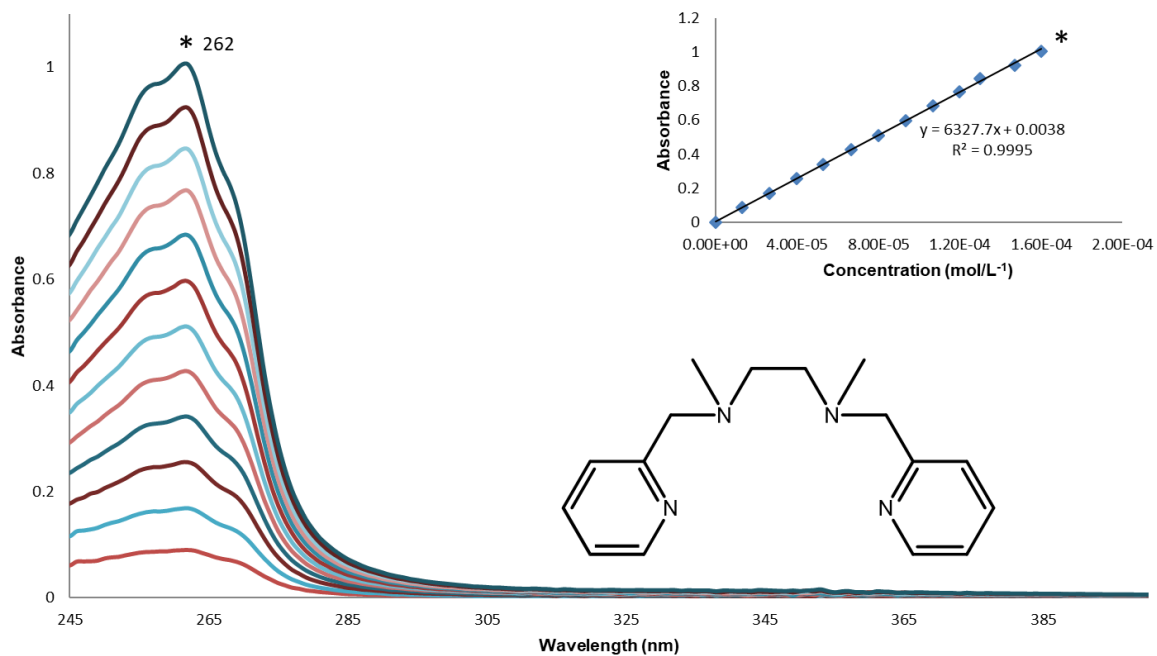


Figure S53: UV-Vis spectra of *N,N'*-bis(2-pyridylmethyl)-*N,N'*-dimethyl-1,2-diaminoethane picenMe₂ (2).

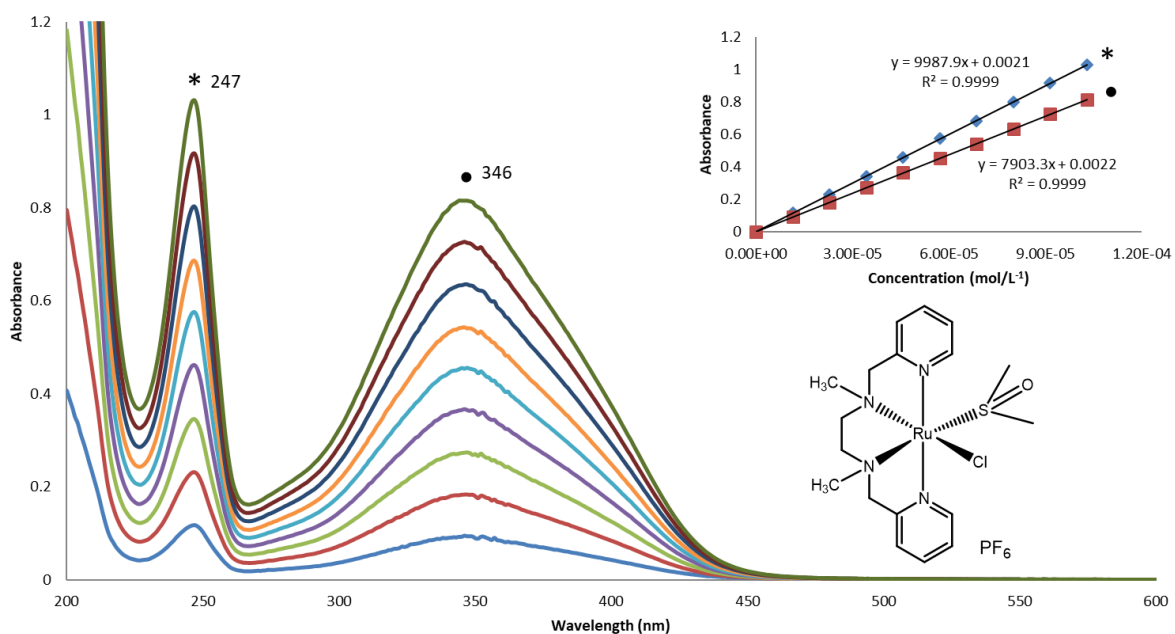


Figure S54: UV-Vis spectra of *cis-α*-[Ru(picenMe₂)(DMSO)Cl]PF₆ (Ru-1).

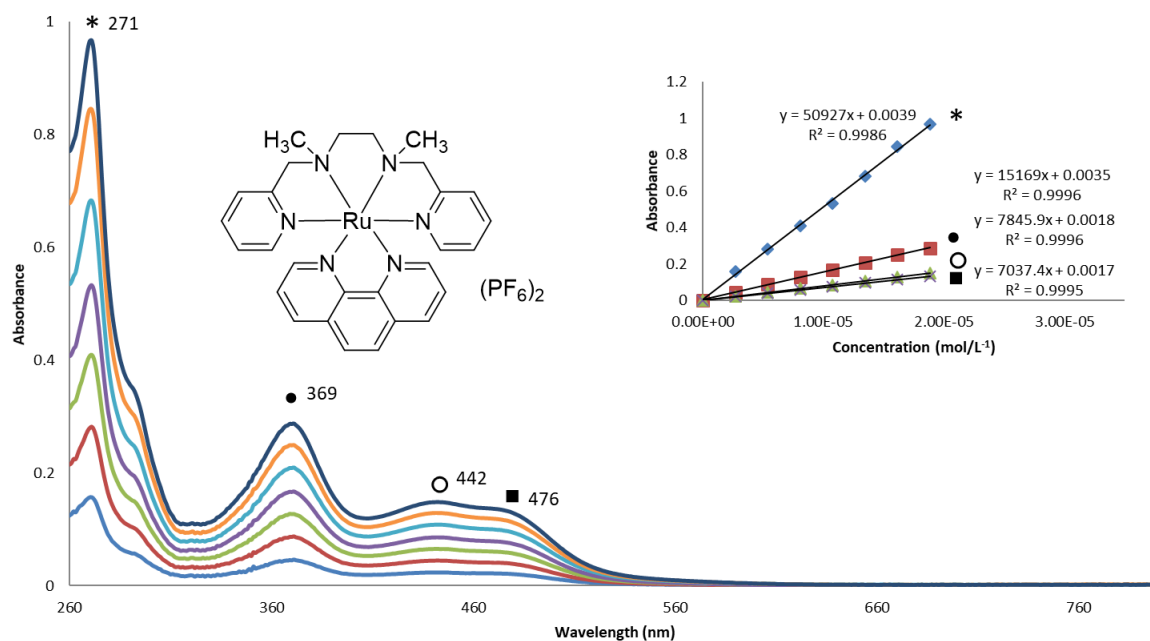


Figure S55: UV-Vis spectra of racemic *cis*- α -[Ru(picenMe₂)(phen)](PF₆)₂ (Ru-2).

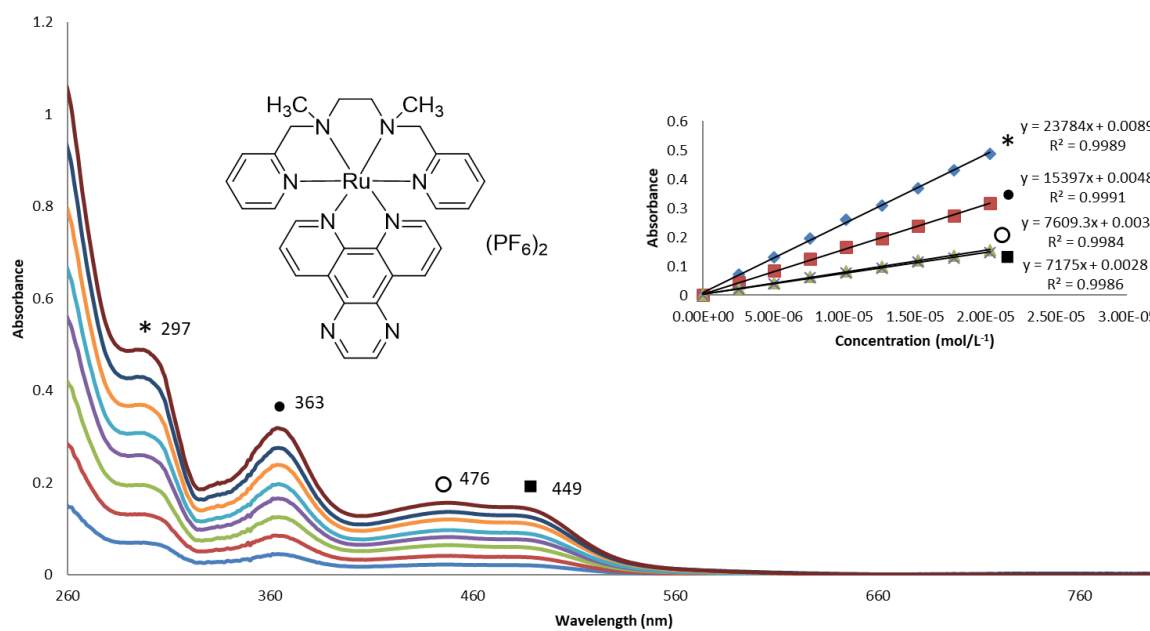


Figure S56: UV-Vis spectra of racemic *cis*- α -[Ru(picenMe₂)(DPQ)](PF₆)₂ (Ru-3).

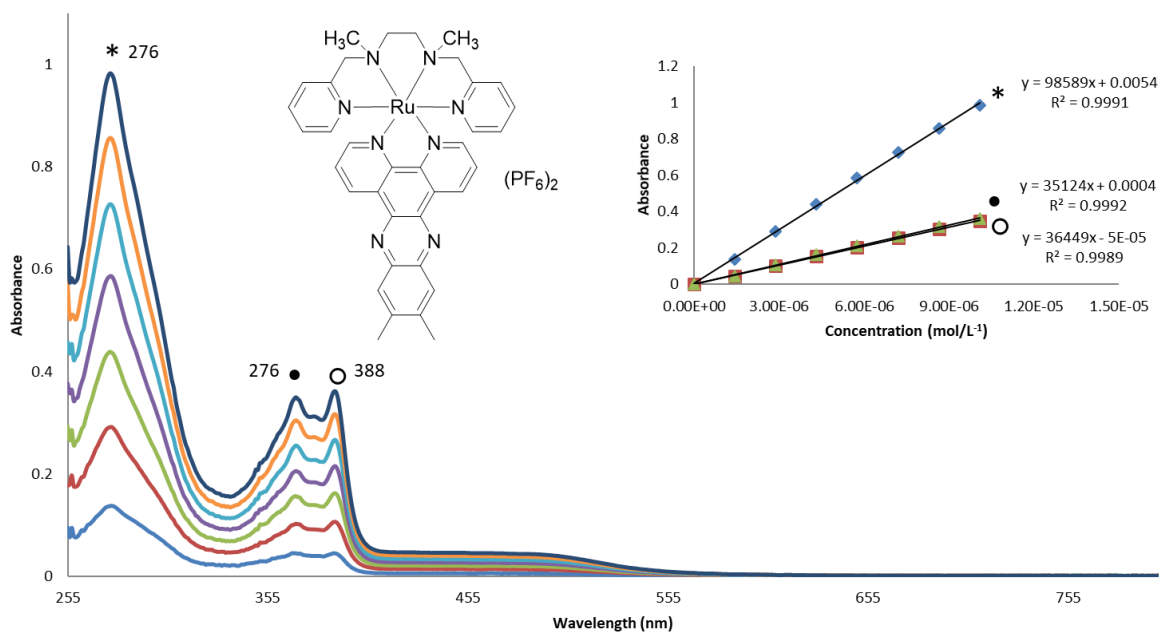


Figure S57: UV-Vis spectra of racemic *cis-α*-[Ru(picenMe₂)(DppzMe₂)](PF₆)₂ (Ru-4).

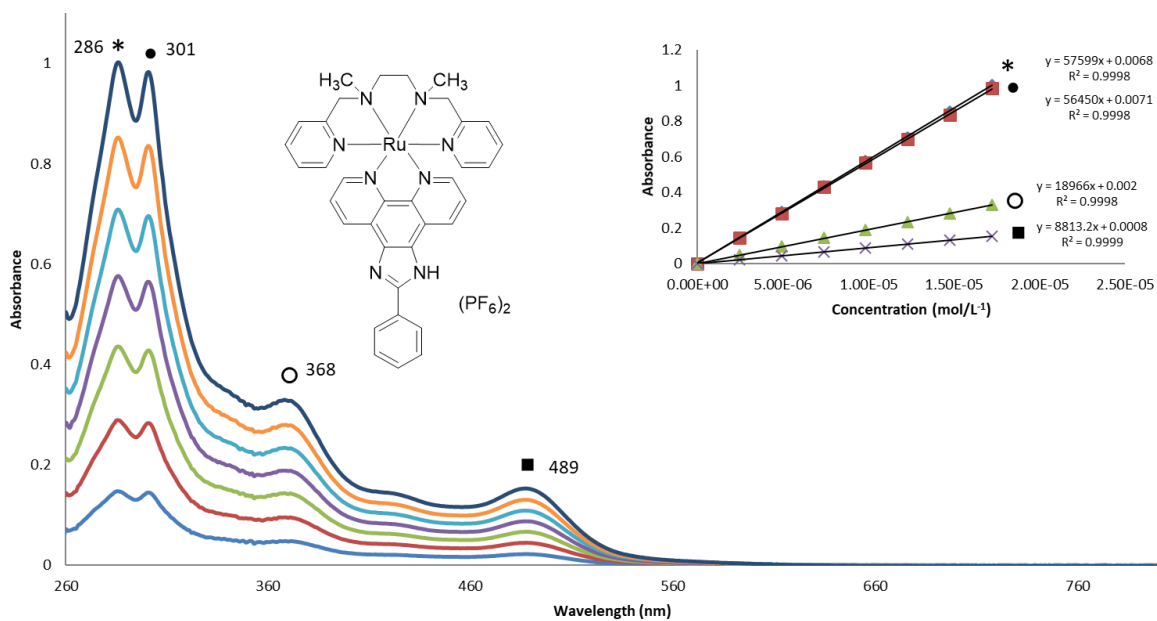


Figure S58: UV-Vis spectra of racemic *cis-α*-[Ru(picenMe₂)(phenpyrBz)](PF₆)₂ (Ru-5).

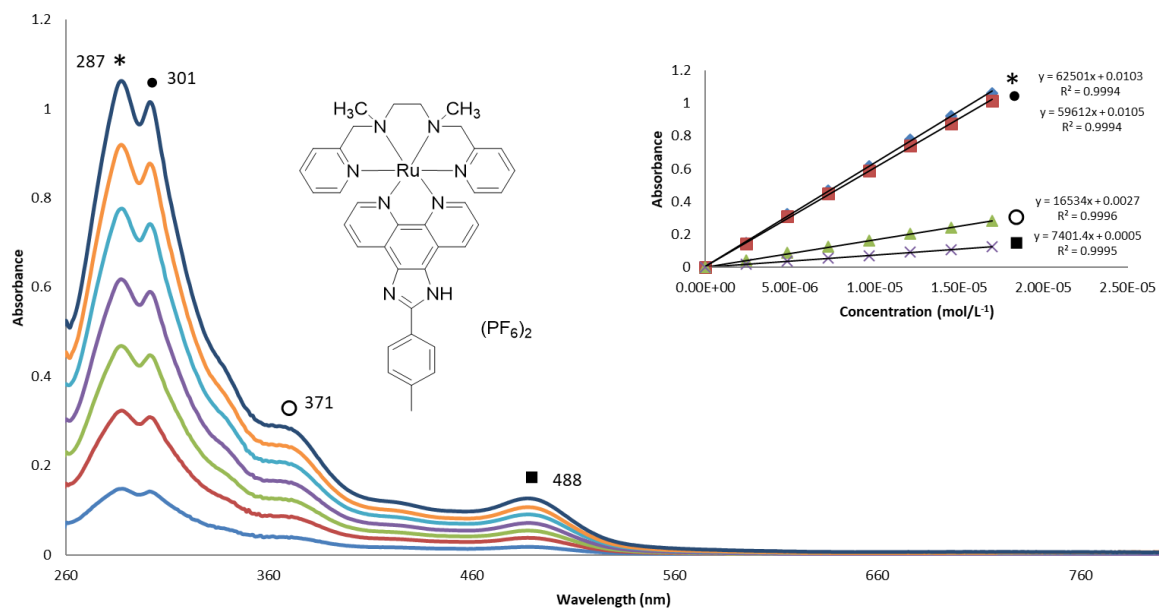


Figure S59: UV-Vis spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBzMe)](PF₆)₂ (Ru-6).

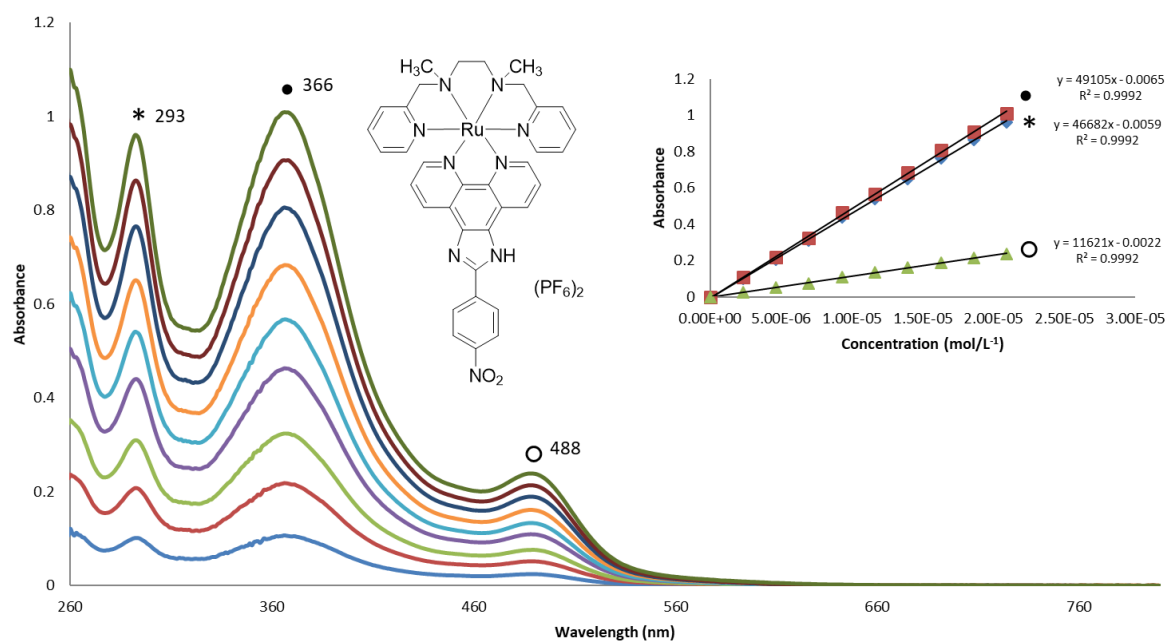


Figure S60: UV-Vis spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBzNO₂)](PF₆)₂ (Ru-7).

2.7 HPLC

Method : C:\CHEM32\1\DATA\20180919-AB_DS 2018-09-19 13-10-23\DLA_10_100_OVER15_5UL.M
(Sequence Method)

Last changed : 9/19/2018 1:10:24 PM by SYSTEM

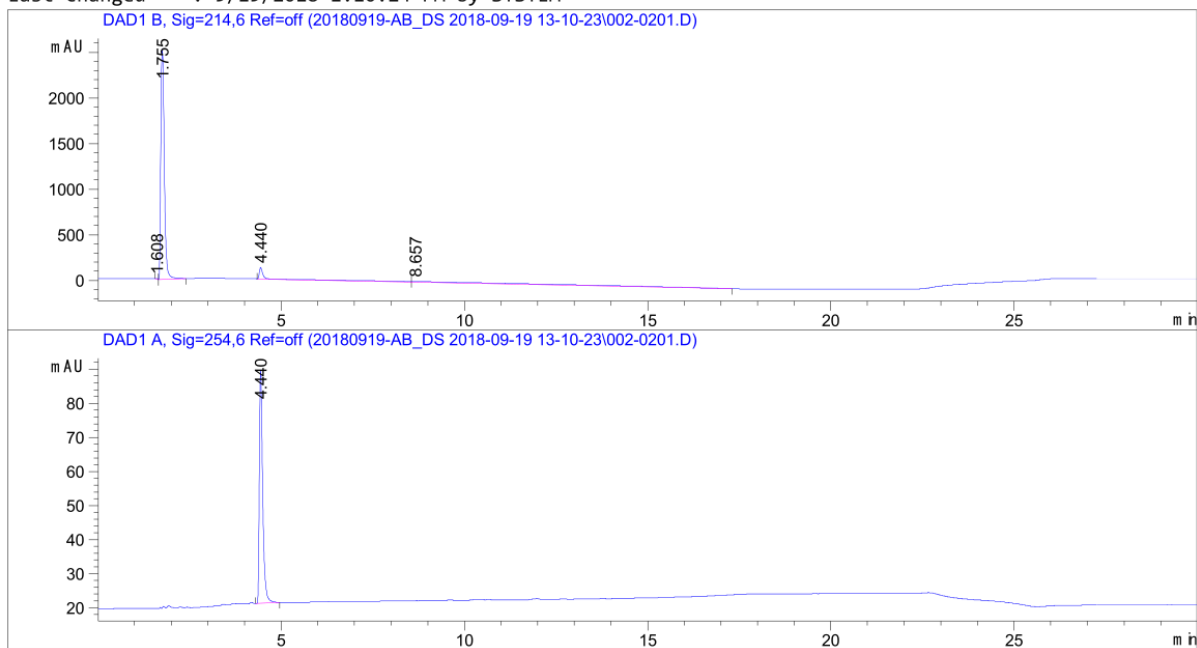


Figure S61: HPLC spectra of *cis*- α -[Ru(picenMe₂)(DMSO)Cl]PF₆ (Ru-1).

Analysis Method : C:\CHEM32\1\DATA\20180308_FLOW LOADING 2018-03-08 15-55-24\10 TO 100 OVER
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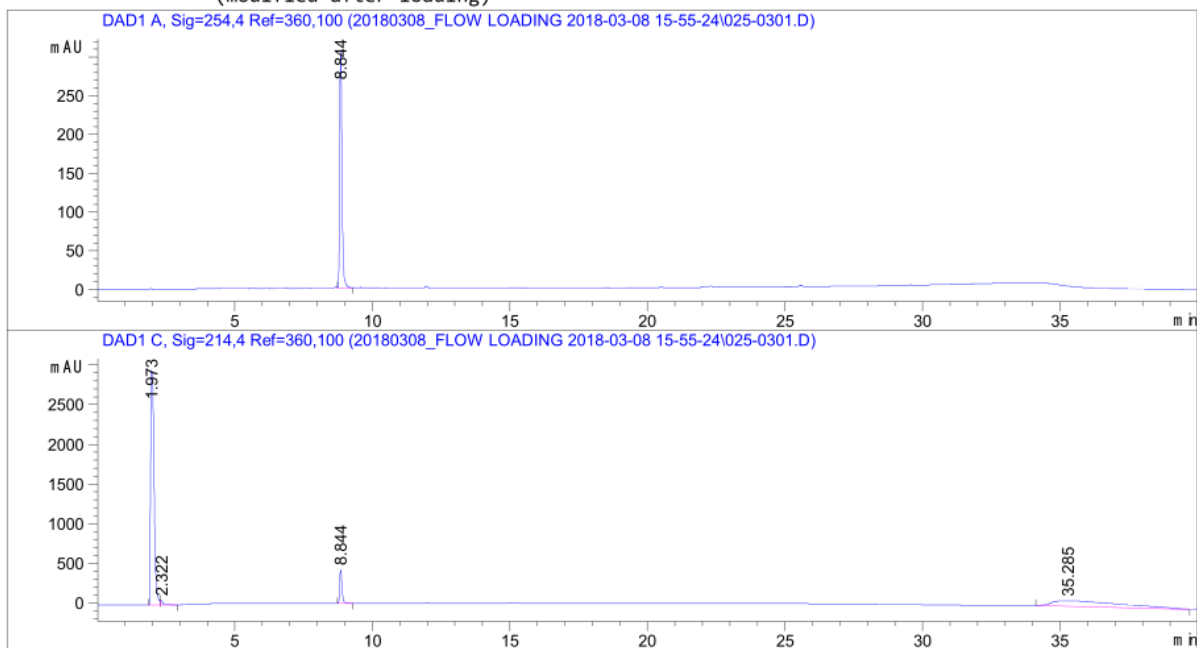


Figure S62: HPLC spectra of racemic *cis*- α -[Ru(picenMe₂)(phen)](PF₆)₂ (Ru-2).

Method : C:\CHEM32\1\DATA\20180216_AB_RUTHENIUM 2018-02-16 09-26-29\10 TO 100 OVER
15 MINS 5UL.M (Sequence Method)
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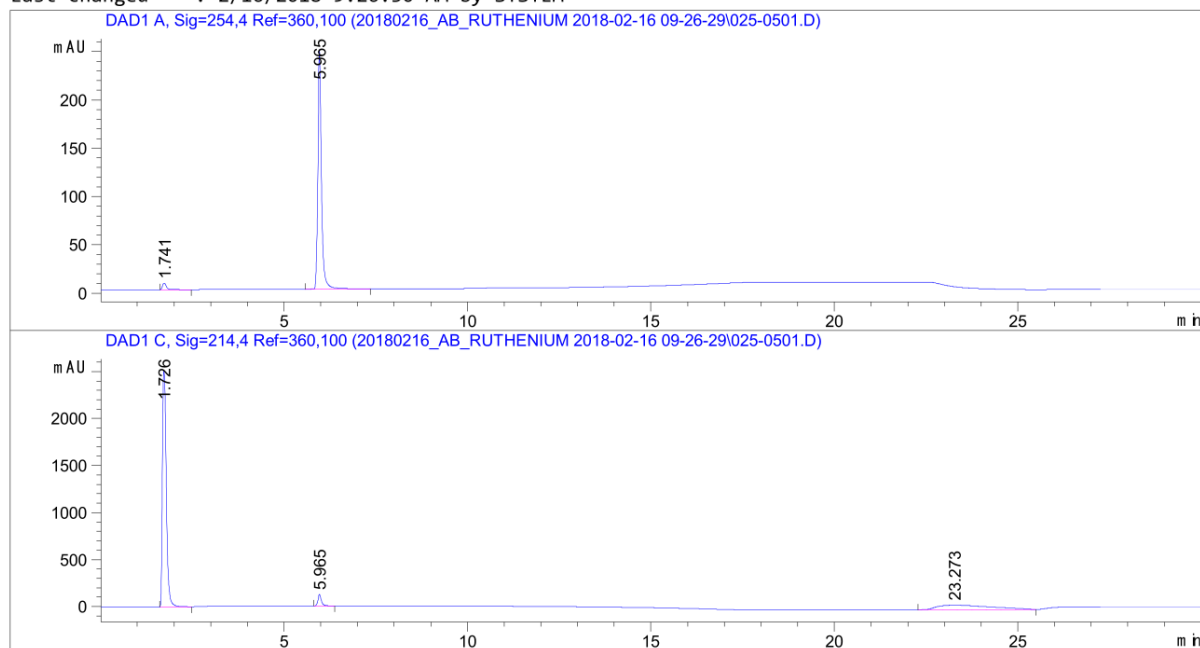


Figure S63: HPLC spectra of racemic *cis*- α -[Ru(picenMe₂)(DPQ)](PF₆)₂ (Ru-3).

Analysis Method : C:\CHEM32\1\DATA\20180308_FLOW LOADING 2018-03-08 15-55-24\10 TO 100 OVER
30 MINS 10UL_150 X 4.6 MM.M (Sequence Method)
Last changed : 3/9/2018 10:57:54 AM by SYSTEM
(modified after loading)

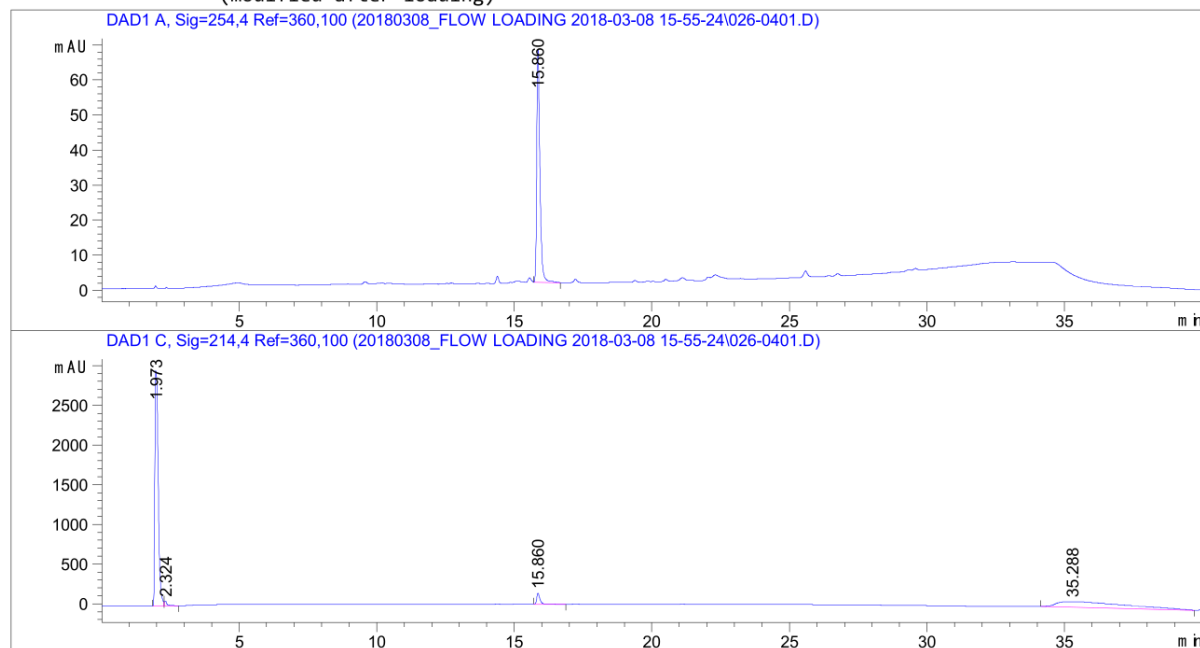


Figure S64: HPLC spectra of racemic *cis*- α -[Ru(picenMe₂)(DppzMe₂)](PF₆)₂ (Ru-4).

Method : C:\CHEM32\1\DATA\05132018-FINALPUREHALIDES 2018-05-14 15-48-42\10 TO 100
OVER 15 MINS 5UL.M (Sequence Method)
Last changed : 5/14/2018 3:48:43 PM by SYSTEM

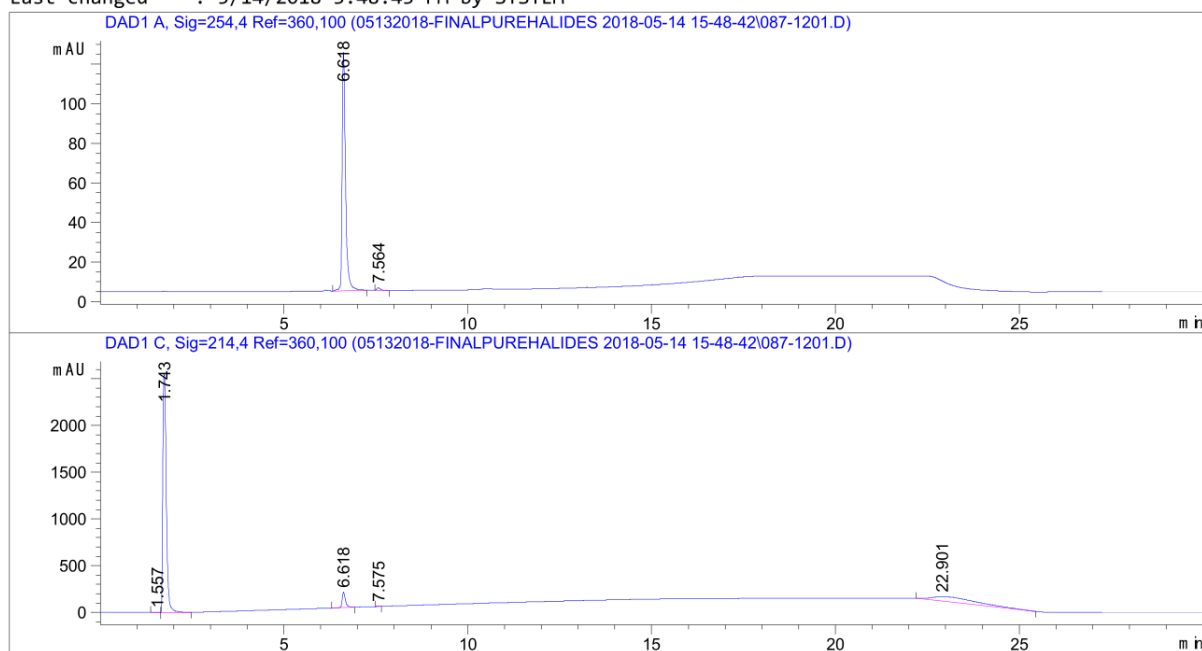


Figure S65: HPLC spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBz)](PF₆)₂ (Ru-5).

Method : C:\CHEM32\1\DATA\05132018-FINALPUREHALIDES 2018-05-14 15-48-42\10 TO 100
OVER 15 MINS 5UL.M (Sequence Method)
Last changed : 5/14/2018 3:48:43 PM by SYSTEM

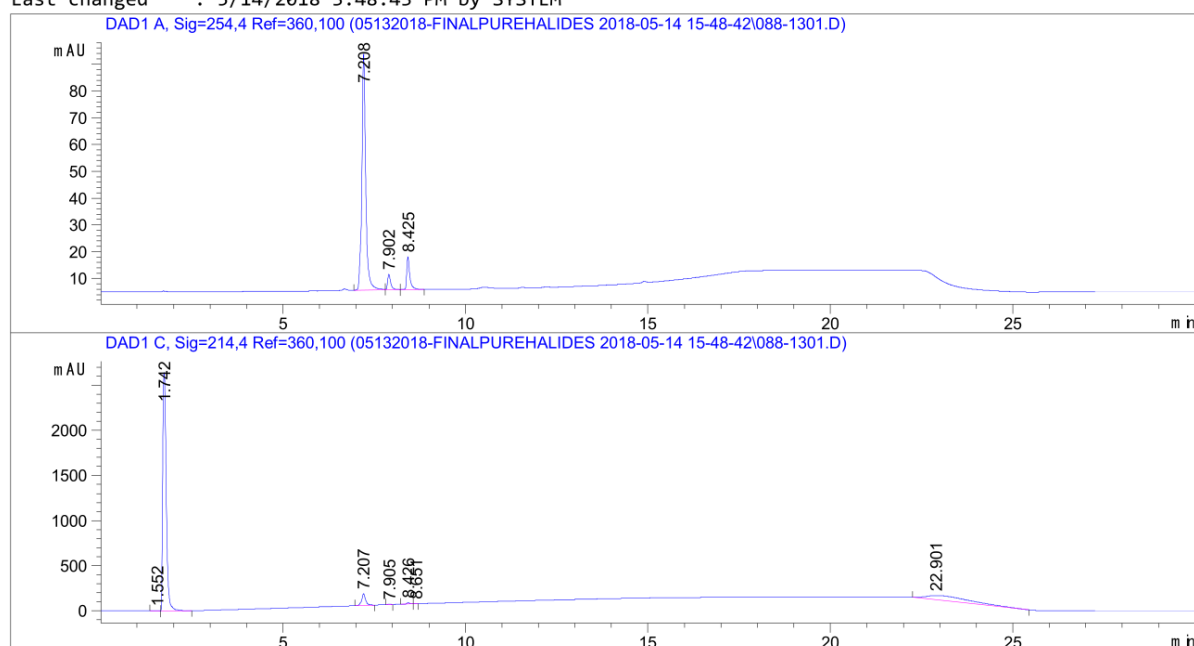


Figure S66: HPLC spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBzMe)](PF₆)₂ (Ru-6).

Method : C:\CHEM32\1\DATA\05132018-FINALPUREHALIDES 2018-05-14 15-48-42\10 TO 100
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Last changed : 5/14/2018 3:48:43 PM by SYSTEM

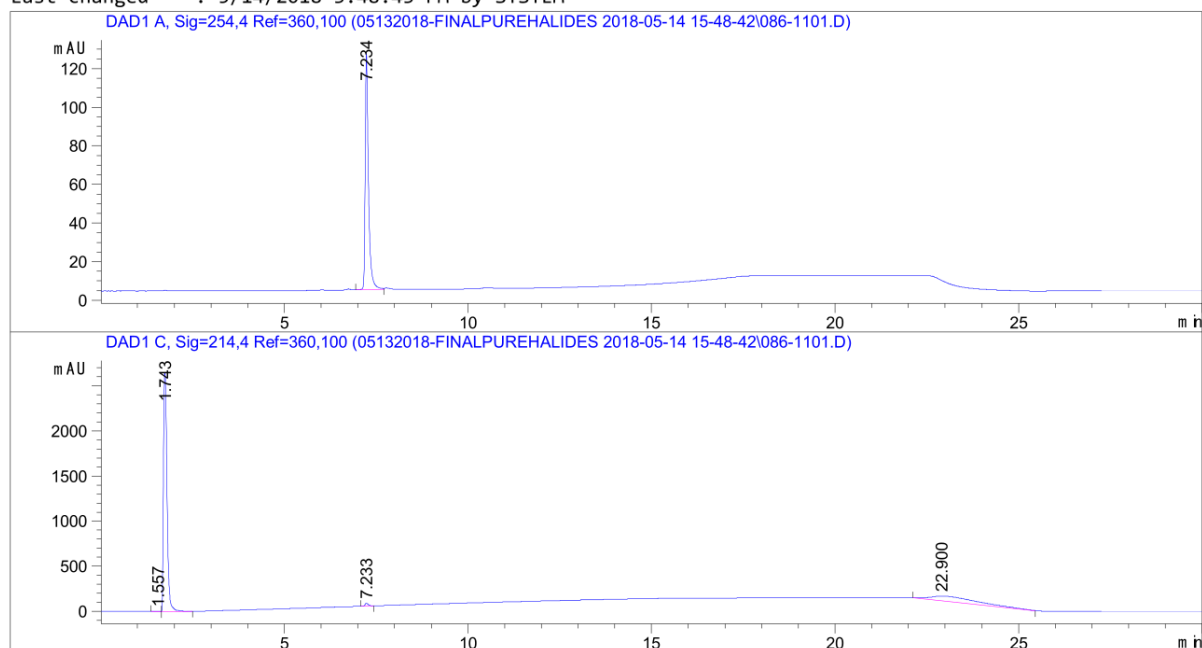


Figure S67: HPLC spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBzNO₂)](PF₆)₂ (Ru-7).

2.9 ESI-MS

Samples were prepared in trace amounts in a solution of methanol or DMSO and diluted into water/methanol mixture, cone voltage set to 30 V for each sample.



Figure S68: ESI-MS spectra of diamine *N,N'*-bis(pyridylmethyl)-1,2-diaminoethane picen (**1**).

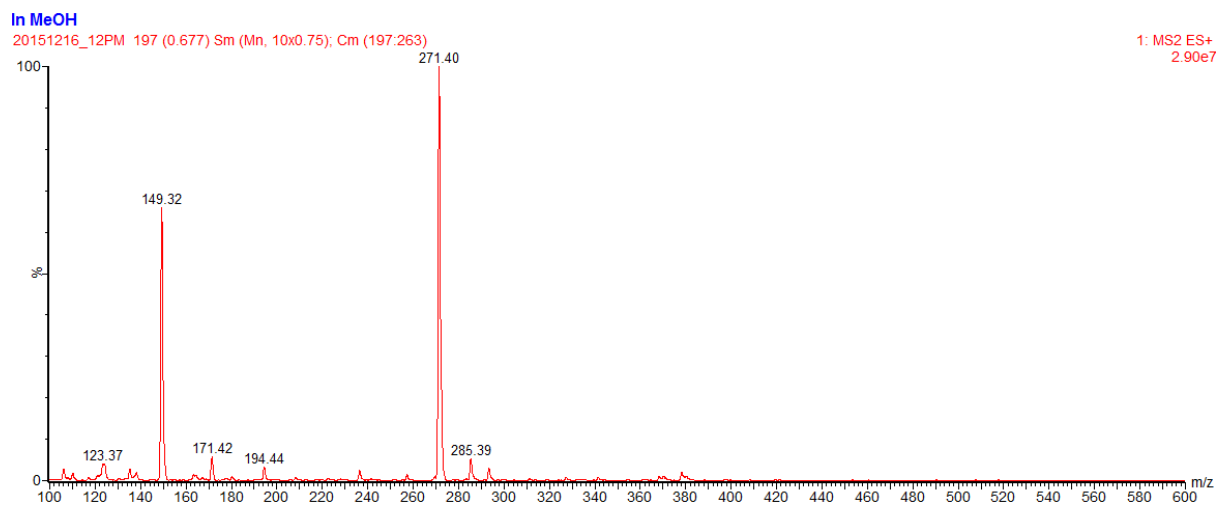


Figure S69: ESI-MS spectra of *N,N'*-bis(2-pyridylmethyl)-*N,N'*-dimethyl-1,2-diaminoethane picenMe₂ (**2**).

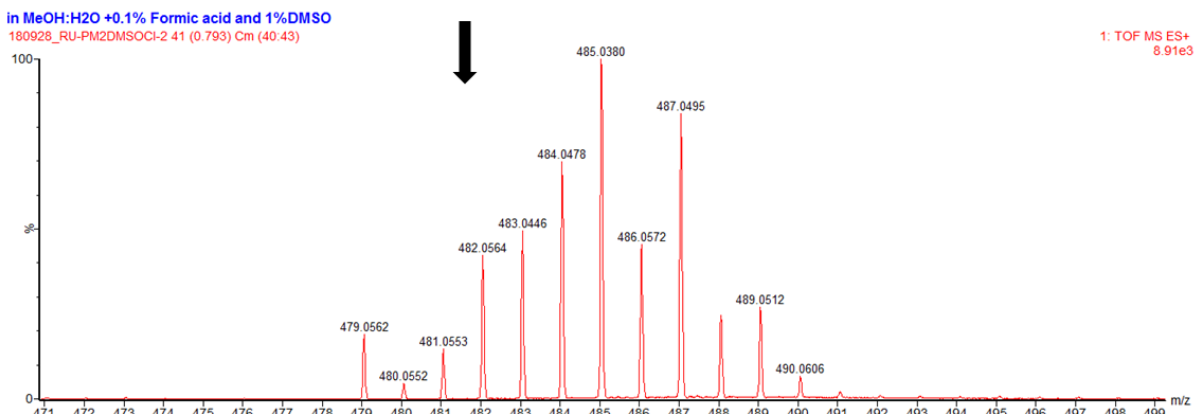
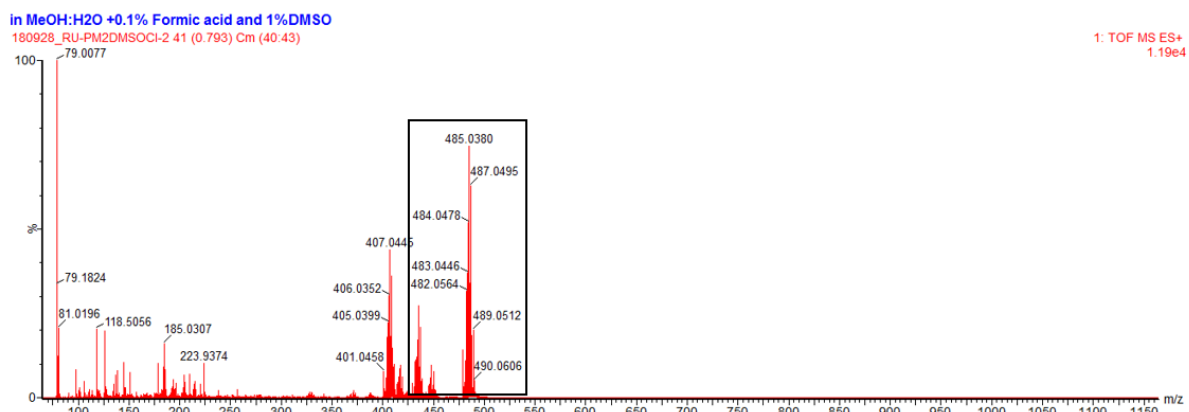


Figure S70: ESI-MS spectra of *cis*- α -[Ru(picenMe₂)(DMSO)Cl]PF₆ (Ru-1).

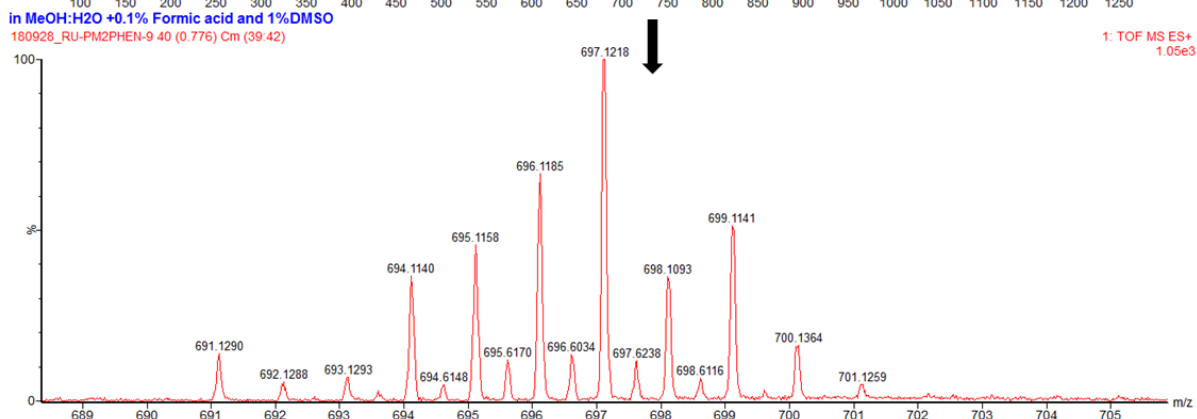
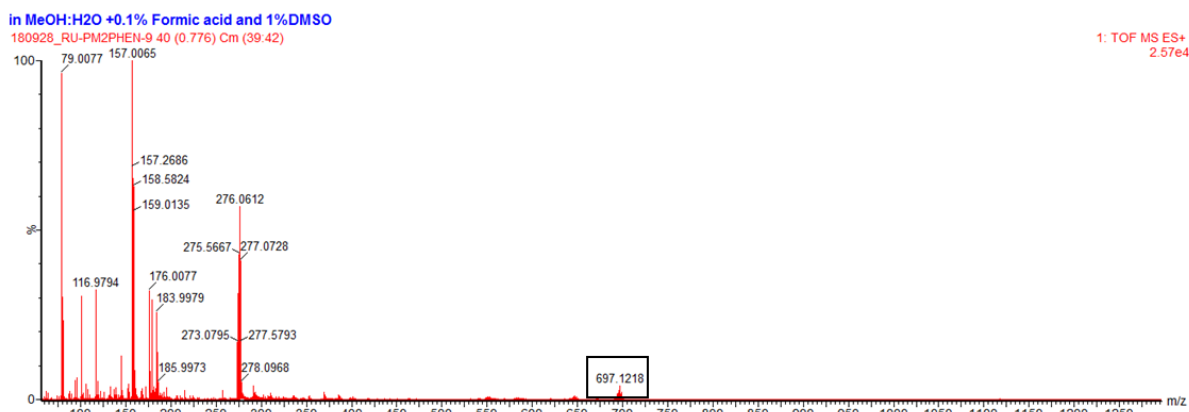
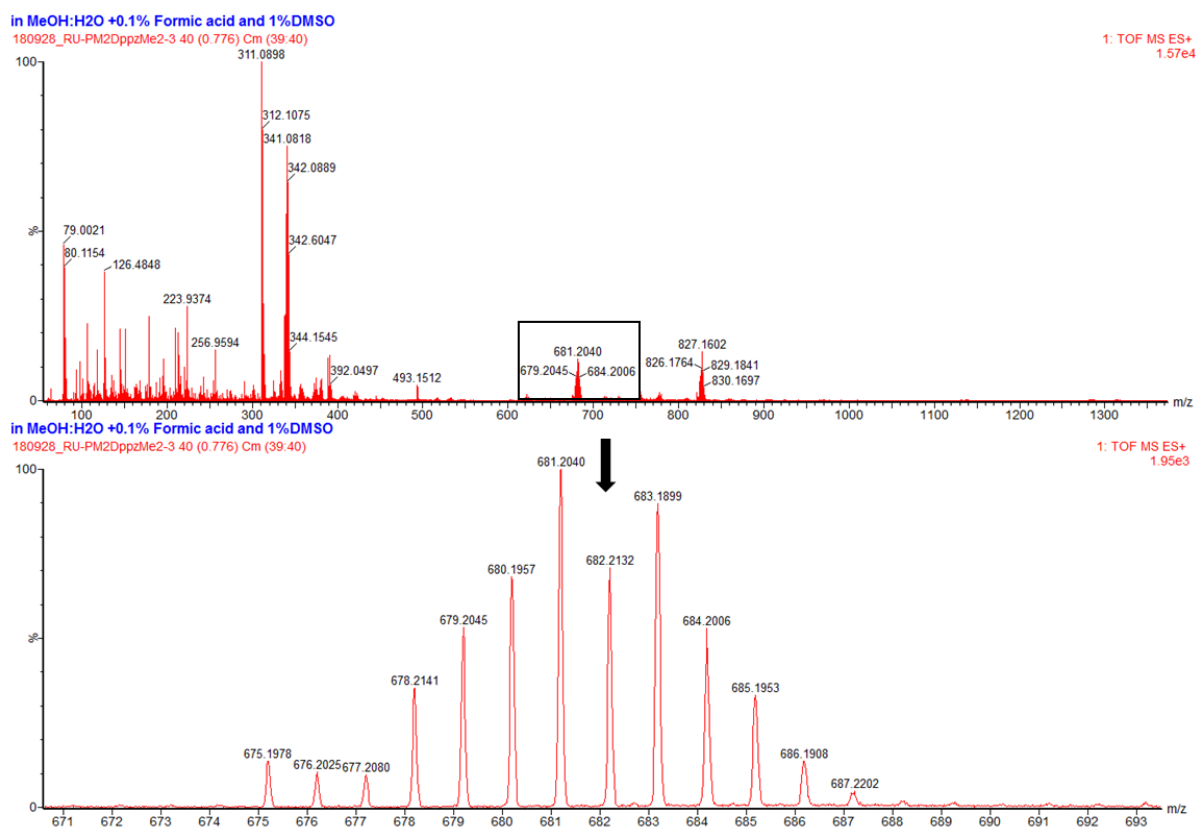
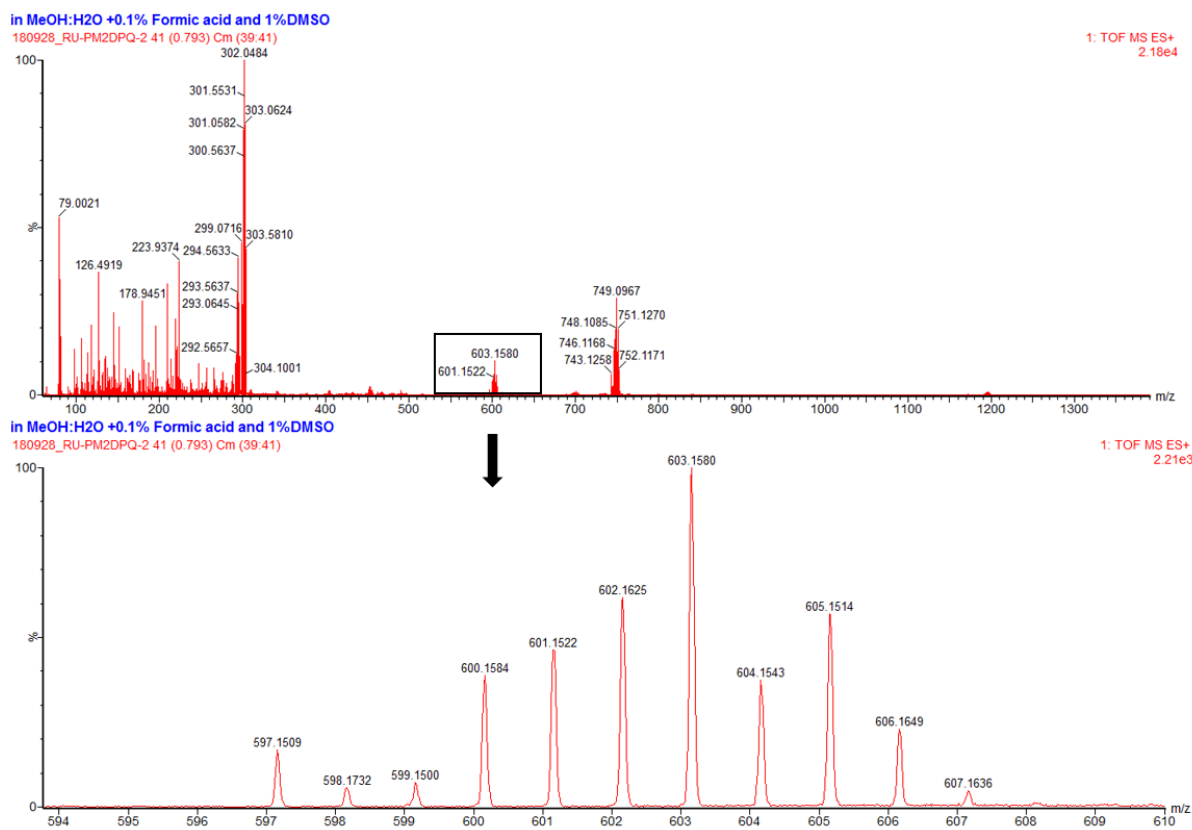


Figure S72: ESI-MS spectra of racemic *cis*- α -[Ru(picenMe₂)(phen)](PF₆)₂ (Ru-2).



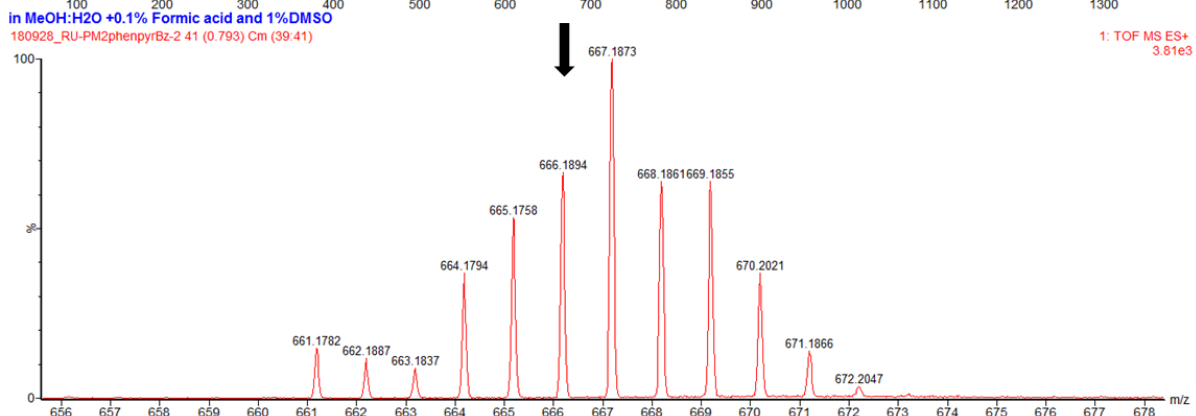
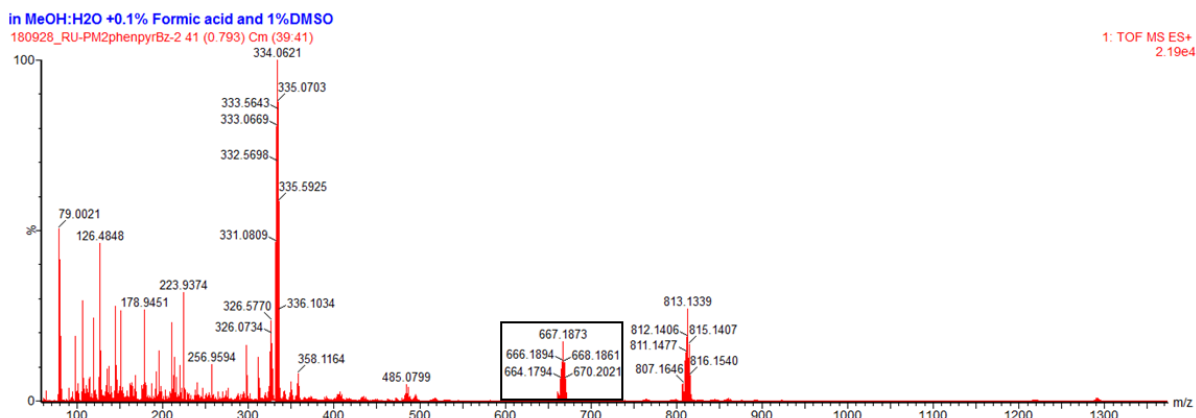


Figure S75: ESI-MS spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBz)](PF₆)₂ (Ru-5).

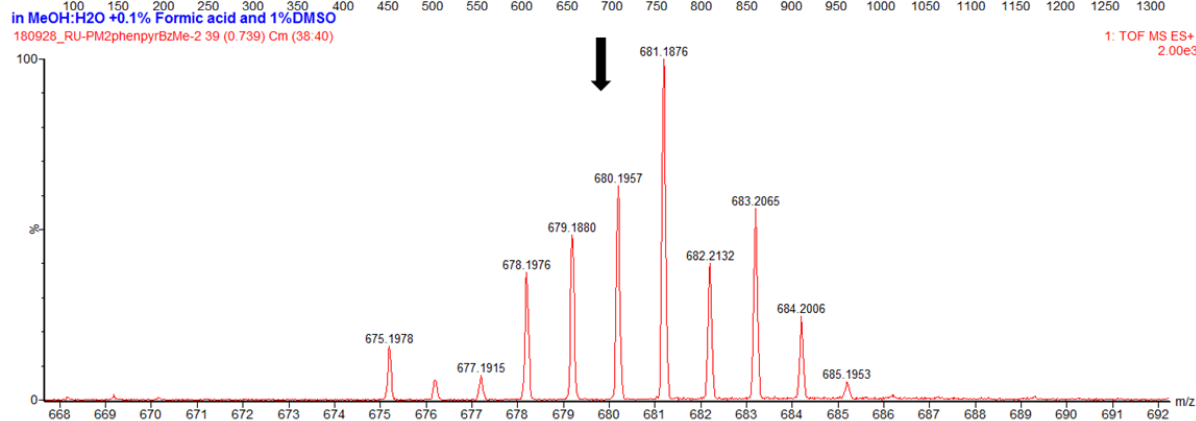
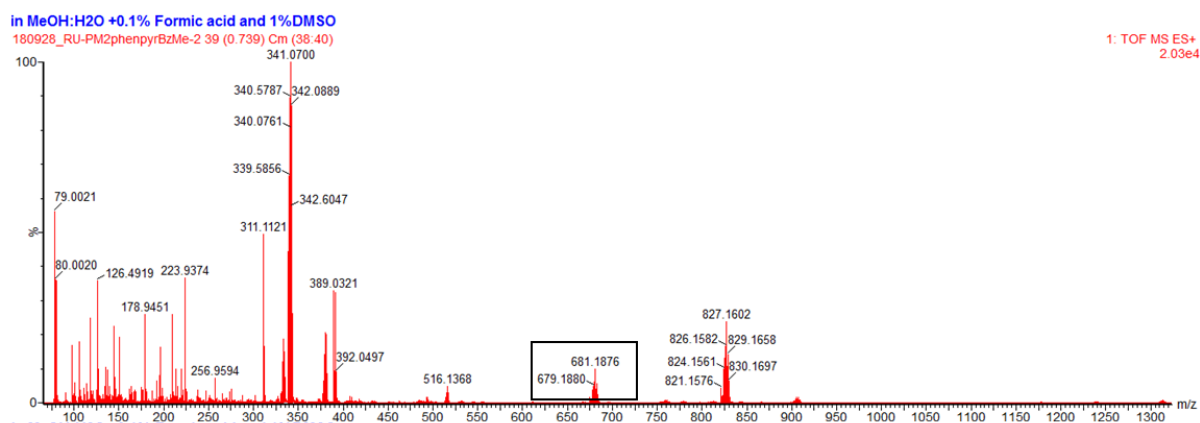


Figure S76: ESI-MS spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBzMe)](PF₆)₂ (Ru-6).

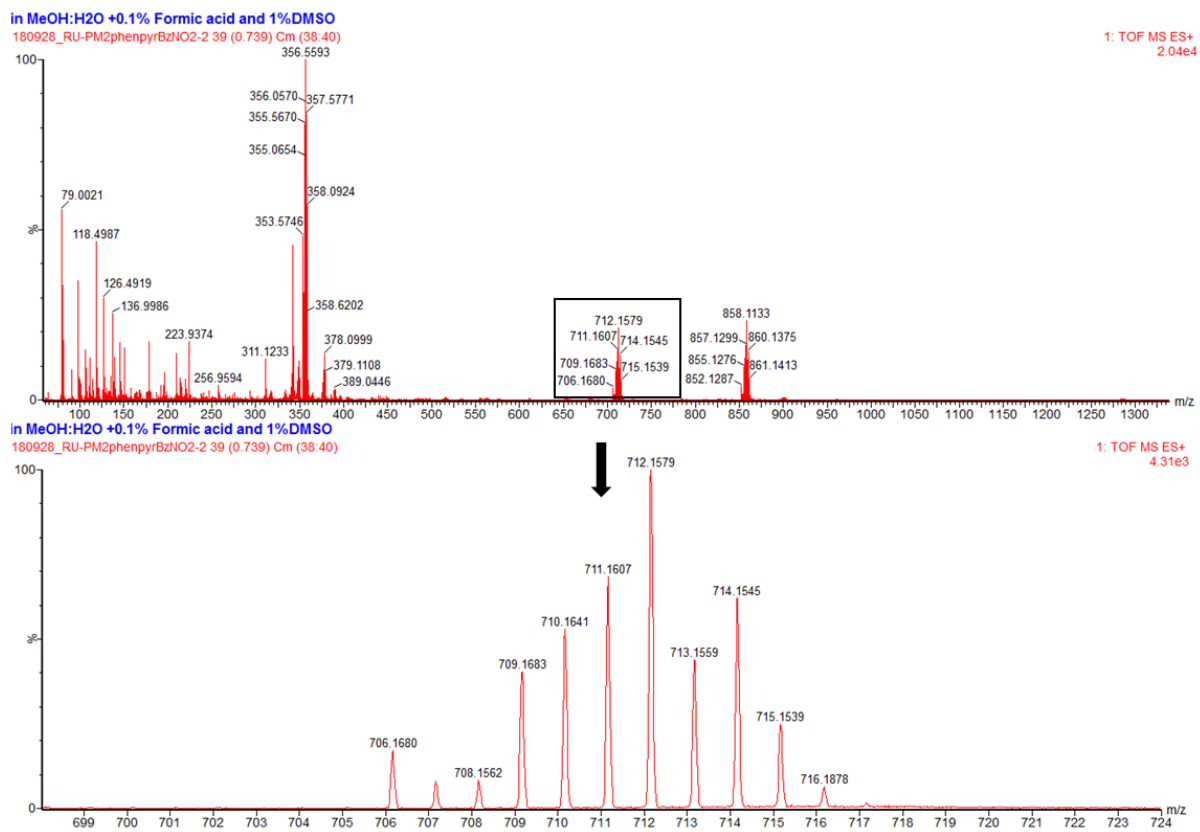


Figure S77: ESI-MS spectra of racemic *cis*- α -[Ru(picenMe₂)(phenpyrBzNO₂)](PF₆)₂ (Ru-7).

2.10 Crystallography

Crystals obtained via slow evaporation from either acetone/water mixture or diffusion of diethyl ether. The single crystal X-ray diffraction measurements for Ru-2-5 were carried out on the MX1 beamline at the Australian Synchrotron at 100 °C, a part of Australian Nuclear Science and Technology Organisation (ANSTO). Diffraction data were collected using a Si<111> monochromated synchrotron X-ray radiation ($\lambda = 0.71080$) at 100(2) K and were corrected for Lorentz and polarization effects using the XDS software.

Ru-2

racemic *cis*- α -[Ru(picenMe₂)(phen)](PF₆)₂

Deposition Number: 1959523

Data Block Name: data_p21byn-_a

Unit Cell Parameters: a 18.585(4), b 17.674(4), c 20.028(4)

Space Group: P21/n

Table S1. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for Ru-2. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{II} tensor.

Atom	x	y	z	U(eq)
Ru1	947.1 (2)	7298.6 (2)	6452.7 (2)	10.86 (7)
N1	1527.1 (14)	6641.3 (15)	7268.1 (13)	14.8 (5)
N2	1920.4 (15)	7981.0 (14)	6847.7 (13)	15.4 (5)
N3	1547.2 (14)	6983.3 (15)	5701.8 (13)	15.8 (6)
N4	469.9 (14)	7998.3 (15)	5634.5 (13)	15.0 (5)
N5	259.3 (15)	7676.5 (14)	7066.3 (13)	15.0 (5)
N6	53.3 (14)	6543.1 (14)	6174.0 (13)	13.6 (5)
C1	1409.8 (18)	5899.0 (18)	7366.9 (17)	18.3 (7)
C2	1820 (2)	5503 (2)	7928.6 (18)	23.6 (8)
C3	2379 (2)	5871 (2)	8402.7 (18)	28.3 (8)
C4	2509 (2)	6627 (2)	8303.3 (17)	26.8 (8)
C5	2069.7 (18)	6999.6 (19)	7735.9 (16)	18.4 (7)
C6	2172.9 (19)	7824.4 (19)	7602.4 (16)	20.5 (7)
C7	1850.9 (19)	8813.3 (17)	6733.7 (17)	19.5 (7)
C8	2511.8 (18)	7685.4 (19)	6526.6 (17)	19.4 (7)
C9	2171.2 (18)	7543.9 (19)	5774.2 (17)	18.7 (7)
C10	1870.5 (19)	6205.6 (18)	5751.3 (17)	20.1 (7)
C11	1036.7 (18)	7100.9 (19)	5007.6 (16)	19.3 (7)
C12	575.3 (18)	7799.9 (18)	5011.9 (16)	18.0 (7)
C13	266 (2)	8217 (2)	4421.0 (17)	24.8 (8)
C14	-154 (2)	8847 (2)	4468.9 (19)	29.1 (8)
C15	-253 (2)	9056.5 (19)	5102.2 (19)	24.9 (8)
C16	67.9 (18)	8627.4 (18)	5671.9 (17)	19.3 (7)
C17	-49.2 (19)	5967.9 (18)	5728.5 (17)	20.2 (7)
C18	-663.0 (19)	5483.8 (18)	5612.6 (18)	21.7 (7)

C19	-1205.8 (19)	5591.9 (18)	5954.0 (18)	22.2 (7)
C20	-1125.3 (18)	6197.4 (18)	6420.7 (16)	17.2 (7)
C21	-487.7 (17)	6654.0 (17)	6518.8 (15)	13.7 (6)
C22	-383.8 (18)	7269.1 (17)	6985.7 (15)	13.8 (6)
C23	-1674.3 (19)	6378 (2)	6785.6 (18)	24.3 (8)
C24	-1586.1 (19)	6981 (2)	7211.3 (18)	24.5 (8)
C25	-936.0 (19)	7450.0 (19)	7325.6 (16)	18.4 (7)
C26	-826 (2)	8080 (2)	7762.6 (17)	24.5 (8)
C27	-187 (2)	8492.3 (19)	7837.5 (17)	24.6 (8)
C28	341 (2)	8272.8 (18)	7489.5 (17)	20.2 (7)
Ru2	5893.0 (2)	7643.9 (2)	5763.3 (2)	13.88 (8)
N7	5438.4 (15)	8212.3 (15)	4847.3 (14)	17.8 (6)
N8	4726.8 (15)	7649.6 (15)	5737.5 (14)	17.6 (6)
N9	5906.4 (16)	8561.6 (16)	6475.0 (14)	21.2 (6)
N10	6261.4 (15)	7098.5 (16)	6702.5 (14)	18.9 (6)
N11	6976.3 (15)	7717.1 (15)	5639.2 (14)	19.4 (6)
N12	5934.2 (15)	6686.7 (15)	5165.6 (13)	16.7 (6)
C29	5819 (2)	8637.0 (19)	4488.6 (17)	21.2 (7)
C30	5478 (2)	8963 (2)	3862.7 (18)	26.8 (8)
C31	4725 (2)	8854.4 (19)	3589.9 (17)	24.5 (8)
C32	4326 (2)	8436.1 (19)	3960.4 (17)	20.9 (7)
C33	4697.9 (18)	8120.1 (18)	4581.2 (16)	17.0 (7)
C34	4310.1 (19)	7636.3 (19)	4998.7 (17)	19.5 (7)
C35	4445.4 (19)	7036 (2)	6113.3 (18)	23.1 (7)
C36	4575.7 (19)	8396.3 (19)	6029.4 (17)	22.1 (7)
C37	5175 (2)	8558 (2)	6660.2 (18)	24.6 (8)
C38	6046 (2)	9333.3 (19)	6235 (2)	29.9 (8)
C39	6482 (2)	8377 (2)	7118.3 (17)	25.1 (8)
C40	6464.5 (19)	7550 (2)	7264.1 (18)	21.7 (7)
C41	6651 (2)	7259 (2)	7929.7 (19)	29.5 (8)
C42	6659 (2)	6483 (2)	8019.7 (19)	34.9 (9)
C43	6479 (2)	6017 (2)	7449.1 (19)	31.3 (9)
C44	6274.1 (19)	6340 (2)	6798.2 (18)	24.5 (8)
C45	7506.0 (19)	8231 (2)	5880.4 (18)	25.4 (8)
C46	8187 (2)	8245 (2)	5696.8 (19)	29.4 (8)
C47	8334 (2)	7720 (2)	5254 (2)	30.7 (9)
C48	7802.9 (19)	7159 (2)	4993.3 (17)	24.4 (8)
C49	7130.2 (18)	7179.2 (19)	5199.9 (16)	18.6 (7)
C50	6578.2 (18)	6623.4 (19)	4952.3 (16)	18.1 (7)
C51	7912 (2)	6574 (2)	4538.7 (18)	30.8 (9)
C52	7399 (2)	6032 (2)	4321.5 (18)	31.6 (9)
C53	6714.8 (19)	6031 (2)	4532.5 (16)	22.1 (7)
C54	6176 (2)	5465 (2)	4340.1 (17)	26.4 (8)
C55	5534 (2)	5529.5 (19)	4547.5 (17)	25.0 (8)
C56	5430.0 (19)	6139.7 (19)	4954.5 (17)	21.6 (7)

P1	4377.4 (5)	8751.0 (5)	8310.8 (4)	16.92 (18)
F1	4705.6 (11)	9502.3 (11)	8051.6 (10)	26.6 (4)
F2	5132.6 (11)	8316.1 (11)	8325.0 (11)	28.5 (5)
F3	4039.8 (12)	8503.3 (13)	7526.2 (10)	32.5 (5)
F4	4044.3 (12)	8002.6 (11)	8569.9 (11)	31.5 (5)
F5	3618.2 (12)	9191.9 (12)	8300.8 (11)	30.6 (5)
F6	4702.5 (13)	9006.5 (13)	9096.4 (10)	34.4 (5)
P2	4234.7 (5)	5533.2 (5)	7457.7 (4)	21.5 (2)
F7	4698.1 (13)	6265.7 (12)	7761.4 (11)	33.7 (5)
F8	4809.7 (14)	5009.4 (13)	7999.2 (11)	38.9 (6)
F9	4736.4 (12)	5432.4 (12)	6917.4 (10)	30.1 (5)
F10	3772.9 (12)	4783.4 (11)	7145.4 (10)	30.4 (5)
F11	3660.8 (12)	6032.6 (12)	6906.2 (12)	35.6 (5)
F12	3746.5 (14)	5609.2 (14)	8000.7 (12)	40.8 (6)
P3	2998.8 (5)	5879.7 (5)	3976.0 (4)	20.37 (19)
F13	3248.6 (15)	6037.7 (14)	4787.5 (11)	43.2 (6)
F14	3074.4 (12)	6766.4 (12)	3832.1 (12)	33.2 (5)
F15	3849.3 (12)	5763.6 (14)	3971.8 (13)	40.5 (6)
F16	2755.7 (15)	5734.4 (14)	3167.5 (11)	44.9 (6)
F17	2928.2 (12)	4994.4 (12)	4116.5 (11)	30.5 (5)
F18	2150.7 (12)	6009.5 (13)	3986.7 (14)	41.7 (6)
P4	2320.6 (5)	4520.4 (5)	10100.0 (4)	21.03 (19)
F19	2554.4 (15)	4792.0 (13)	10886.4 (11)	44.9 (6)
F20	3163.2 (13)	4447.7 (15)	10089.4 (14)	50.5 (7)
F21	2305.6 (14)	5380.8 (12)	9868.7 (11)	36.7 (5)
F22	2079.8 (12)	4255.1 (12)	9313 (1)	30.1 (5)
F23	1456.2 (13)	4592.5 (14)	10101.3 (12)	41.4 (6)
F24	2309.3 (17)	3656.9 (13)	10334.8 (13)	51.0 (7)

Table S2. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for Ru-2. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^2U_{11}+2hka*b*U_{12}+\dots]$.

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
Ru1	10.49(14)	12.74(13)	10.85(13)	-2.77(9)	5.49(10)	-3.05(9)
N1	13.8(14)	19.8(14)	13.1(13)	-3.2(10)	7.8(11)	-0.5(10)
N2	16.3(15)	16.4(13)	14.5(13)	-3(1)	5.8(11)	-1.8(10)
N3	12.9(14)	18.7(14)	17.6(13)	-2.9(11)	7.0(11)	-2.2(11)
N4	11.7(14)	18.0(13)	16.3(13)	-2.7(11)	5.4(11)	-5.7(10)
N5	16.5(15)	15.2(13)	14.8(13)	-0.4(10)	6.9(11)	-1.5(10)
N6	10.1(14)	17.0(13)	14.3(12)	-1.5(10)	4.1(10)	-0.4(10)
C1	17.7(18)	18.6(16)	22.2(16)	0.1(13)	11.7(14)	1.8(13)
C2	24(2)	23.7(18)	27.6(18)	6.6(14)	15.4(16)	6.6(14)
C3	28(2)	38(2)	20.2(17)	9.4(15)	8.2(15)	10.3(16)
C4	25(2)	39(2)	15.7(16)	0.0(15)	4.1(14)	1.9(16)
C5	18.0(18)	23.9(17)	15.3(15)	-2.7(13)	7.7(13)	-0.7(13)
C6	19.4(19)	24.5(17)	15.5(16)	-4.2(13)	0.3(14)	-6.6(13)
C7	19.7(19)	15.8(16)	24.2(17)	-3.4(13)	7.7(14)	-8.0(13)
C8	11.0(18)	24.5(17)	24.0(17)	-4.9(13)	6.9(14)	-5.4(13)
C9	13.8(18)	24.7(17)	20.0(17)	-1.6(13)	8.8(14)	-4.6(13)
C10	19.4(18)	20.9(17)	21.8(17)	-5.7(13)	8.7(14)	0.3(13)
C11	19.4(19)	26.5(17)	12.8(15)	-5.2(13)	5.2(13)	-1.1(14)
C12	17.0(18)	22.6(17)	15.9(16)	-2.5(13)	6.6(13)	-6.5(13)
C13	27(2)	30.2(19)	17.1(16)	2.7(14)	6.2(14)	-6.0(15)
C14	29(2)	34(2)	22.2(18)	10.5(15)	2.2(15)	-1.6(16)
C15	24(2)	19.2(17)	31.6(19)	5.9(14)	7.0(16)	-1.1(14)
C16	14.5(18)	21.4(17)	22.4(17)	1.4(13)	5.0(14)	-4.3(13)
C17	18.0(18)	22.0(17)	21.9(17)	-9.5(13)	7.5(14)	-2.4(13)
C18	17.4(19)	18.8(16)	26.8(18)	-7.0(14)	1.7(15)	-5.0(13)
C19	17.5(19)	19.4(17)	27.0(18)	2.6(14)	0.7(15)	-7.4(13)
C20	14.0(18)	20.5(16)	17.4(16)	6.7(12)	4.8(13)	-1.1(13)
C21	13.3(17)	16.1(15)	11.7(14)	3.5(12)	2.9(12)	0.4(12)
C22	14.3(17)	15.6(15)	12.0(14)	4.5(12)	4.1(13)	2.8(12)
C23	10.4(18)	37(2)	26.0(18)	4.0(15)	5.3(14)	-6.2(14)
C24	15.2(19)	38(2)	24.7(18)	3.1(15)	13.1(15)	1.3(14)
C25	16.5(18)	24.7(17)	15.9(16)	4.1(13)	7.3(14)	3.4(13)
C26	25(2)	34(2)	18.5(17)	-0.1(14)	13.7(15)	7.5(15)
C27	34(2)	22.8(17)	20.3(17)	-6.4(14)	12.3(15)	1.7(15)
C28	26(2)	17.3(16)	20.0(16)	-6.1(13)	10.0(14)	-3.8(13)
Ru2	11.21(15)	17.61(14)	14.41(13)	1.9(1)	6.18(10)	-2.36(9)
N7	20.7(16)	17.3(13)	19.1(14)	0.4(11)	11.8(12)	-0.7(11)
N8	12.8(15)	23.6(14)	17.9(14)	4.8(11)	6.5(11)	-1.2(11)
N9	23.4(17)	22.4(15)	19.1(14)	0.0(11)	7.8(12)	-2.1(11)
N10	12.3(15)	26.5(15)	18.4(14)	3.1(11)	4.8(11)	-1.9(11)
N11	15.8(16)	24.4(15)	18.5(14)	6.9(11)	5.2(12)	-0.1(11)
N12	14.9(15)	20.0(14)	15.0(13)	4.7(11)	3.2(11)	0.5(11)

C29	20.6 (19)	23.8 (17)	22.4 (17)	3.4 (14)	11.4 (14)	-3.6 (14)
C30	35 (2)	25.0 (18)	25.1 (18)	6.0 (14)	15.2 (17)	-3.0 (15)
C31	34 (2)	25.6 (18)	13.7 (16)	4.6 (13)	6.6 (15)	4.6 (15)
C32	20.3 (19)	23.3 (17)	18.1 (16)	-0.5 (13)	2.8 (14)	0.9 (13)
C33	16.3 (18)	19.0 (16)	17.1 (15)	-2.4 (13)	6.9 (13)	-0.2 (12)
C34	12.8 (18)	26.3 (18)	19.5 (16)	4.4 (13)	4.3 (14)	-1.8 (13)
C35	16.1 (19)	31.2 (19)	24.8 (18)	11.0 (15)	10.2 (15)	-1.7 (14)
C36	20.3 (19)	26.6 (18)	22.4 (17)	6.2 (14)	11.2 (14)	5.0 (14)
C37	26 (2)	28.4 (19)	23.3 (18)	-0.1 (14)	13.5 (15)	1.9 (15)
C38	41 (2)	19.0 (17)	31 (2)	-1.5 (15)	12.4 (18)	-7.4 (16)
C39	22 (2)	31.2 (19)	20.1 (17)	-4.2 (14)	2.4 (14)	-6.5 (15)
C40	10.6 (18)	32.6 (19)	23.2 (17)	0.9 (14)	6.4 (14)	-0.8 (13)
C41	18 (2)	51 (2)	18.7 (18)	4.3 (16)	2.5 (15)	1.2 (16)
C42	27 (2)	52 (3)	21.8 (19)	15.9 (18)	-0.6 (16)	6.1 (18)
C43	23 (2)	38 (2)	32 (2)	17.9 (17)	4.4 (16)	4.1 (16)
C44	19 (2)	29.9 (19)	25.4 (18)	5.4 (15)	6.9 (15)	2.1 (14)
C45	17.6 (19)	33 (2)	24.8 (18)	5.6 (15)	4.2 (15)	-7.7 (14)
C46	15 (2)	41 (2)	32 (2)	10.7 (17)	3.1 (15)	-8.0 (15)
C47	10.6 (19)	50 (2)	32 (2)	19.3 (18)	5.4 (16)	1.5 (16)
C48	13.3 (19)	42 (2)	18.4 (17)	15.7 (15)	4.4 (14)	7.4 (15)
C49	14.0 (18)	26.4 (17)	15.1 (16)	9.5 (13)	3.4 (13)	3.8 (13)
C50	15.0 (18)	27.3 (17)	12.1 (15)	9.1 (13)	3.5 (13)	5.5 (13)
C51	24 (2)	50 (2)	22.4 (18)	11.6 (17)	13.8 (16)	14.3 (18)
C52	34 (2)	46 (2)	17.6 (17)	3.7 (16)	10.8 (16)	18.3 (18)
C53	20 (2)	33.3 (19)	11.4 (15)	3.6 (14)	1.1 (13)	7.7 (14)
C54	36 (2)	28.9 (19)	12.8 (16)	0.6 (14)	2.3 (15)	10.1 (16)
C55	31 (2)	22.7 (18)	18.1 (17)	-0.1 (14)	0.2 (15)	0.4 (15)
C56	20.4 (19)	24.0 (17)	19.8 (17)	2.0 (13)	4.2 (14)	-0.4 (14)
P1	17.3 (5)	20.6 (4)	14.0 (4)	0.8 (3)	6.0 (3)	0.8 (3)
F1	27.5 (12)	23 (1)	31.0 (11)	6.6 (8)	10.4 (9)	-1.3 (8)
F2	21.5 (11)	30.2 (11)	36.5 (12)	5.7 (9)	12.2 (9)	6.9 (8)
F3	26.3 (12)	51.4 (14)	19.5 (10)	-9.9 (9)	5.3 (9)	-11.9 (10)
F4	33.5 (13)	22.9 (11)	44.8 (13)	7.2 (9)	22.2 (11)	-1.1 (9)
F5	25.3 (12)	36.1 (12)	36.0 (12)	12.5 (9)	18 (1)	13.2 (9)
F6	43.1 (14)	42.3 (13)	15 (1)	-3.0 (9)	2.1 (9)	-0.5 (10)
P2	29.4 (5)	19.1 (4)	17.6 (4)	-0.9 (3)	8.8 (4)	-5.3 (4)
F7	40.2 (14)	28.4 (11)	33.1 (12)	-9.7 (9)	10.3 (10)	-12.4 (10)
F8	49.2 (15)	36.4 (13)	25.3 (11)	6.5 (9)	-1.1 (10)	2.4 (11)
F9	34.7 (13)	33.0 (12)	25.9 (11)	-4.9 (9)	13.6 (9)	-6.2 (9)
F10	44.1 (14)	23.8 (11)	23.7 (10)	1.0 (8)	9.3 (9)	-13.4 (9)
F11	30.7 (13)	28.8 (11)	44.2 (13)	11.7 (10)	3.5 (10)	1.0 (9)
F12	46.7 (15)	48.7 (14)	35.9 (13)	-11.9 (11)	27.1 (11)	-13.4 (11)
P3	14.0 (5)	28.5 (5)	18.8 (4)	5.8 (3)	4.3 (3)	-3.9 (3)
F13	62.7 (18)	42.6 (14)	21.4 (11)	0.3 (10)	5.1 (11)	-14.8 (12)
F14	29.1 (13)	29.7 (12)	43.1 (13)	13.4 (10)	13.3 (10)	-2.7 (9)

F15	18.7(12)	48.2(14)	58.4(15)	22.0(12)	16.9(11)	4.4(10)
F16	56.0(17)	53.1(15)	18.3(11)	1.8(10)	-4.5(10)	9.7(12)
F17	25.6(12)	27.9(11)	34.5(12)	5.7(9)	1.1(9)	-7.8(9)
F18	20.1(13)	40.6(13)	70.8(17)	7.1(12)	23.3(12)	-2.6(10)
P4	28.6(5)	18.0(4)	16.1(4)	-1.2(3)	4.8(4)	5.4(3)
F19	68.0(18)	39.7(13)	19.4(11)	-6.6(10)	-3.4(11)	22.2(12)
F20	22.0(14)	58.8(17)	66.8(17)	-25.4(14)	3.7(12)	8.9(11)
F21	54.3(16)	20.2(11)	36.1(12)	4.1(9)	12.5(11)	7(1)
F22	29.4(12)	41.7(12)	20.1(10)	-11.7(9)	8.0(9)	0.2(9)
F23	35.4(14)	51.9(15)	43.5(14)	-16.0(11)	22.1(11)	-2.6(11)
F24	94(2)	21.5(12)	42.3(14)	4.3(10)	25.5(14)	9.1(12)

Table S3. Bond Lengths for Ru-2.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ru1	N1	2.073 (3)	N9	C38	1.490 (4)
Ru1	N2	2.153 (3)	N9	C39	1.490 (4)
Ru1	N3	2.158 (3)	N10	C40	1.354 (5)
Ru1	N4	2.067 (3)	N10	C44	1.353 (4)
Ru1	N5	2.092 (3)	N11	C45	1.337 (4)
Ru1	N6	2.095 (3)	N11	C49	1.373 (4)
N1	C1	1.353 (4)	N12	C50	1.372 (4)
N1	C5	1.350 (4)	N12	C56	1.339 (4)
N2	C6	1.492 (4)	C29	C30	1.382 (5)
N2	C7	1.489 (4)	C30	C31	1.381 (5)
N2	C8	1.499 (4)	C31	C32	1.387 (5)
N3	C9	1.504 (4)	C32	C33	1.380 (5)
N3	C10	1.493 (4)	C33	C34	1.501 (4)
N3	C11	1.489 (4)	C36	C37	1.488 (5)
N4	C12	1.356 (4)	C39	C40	1.493 (5)
N4	C16	1.352 (4)	C40	C41	1.389 (5)
N5	C22	1.370 (4)	C41	C42	1.382 (6)
N5	C28	1.337 (4)	C42	C43	1.380 (6)
N6	C17	1.334 (4)	C43	C44	1.386 (5)
N6	C21	1.369 (4)	C45	C46	1.403 (5)
C1	C2	1.381 (5)	C46	C47	1.358 (6)
C2	C3	1.382 (5)	C47	C48	1.403 (5)
C3	C4	1.381 (5)	C48	C49	1.412 (5)
C4	C5	1.388 (5)	C48	C51	1.426 (5)
C5	C6	1.503 (5)	C49	C50	1.417 (5)
C8	C9	1.502 (5)	C50	C53	1.405 (5)
C11	C12	1.505 (5)	C51	C52	1.343 (6)
C12	C13	1.390 (5)	C52	C53	1.437 (5)
C13	C14	1.377 (5)	C53	C54	1.399 (5)
C14	C15	1.377 (5)	C54	C55	1.363 (5)
C15	C16	1.375 (5)	C55	C56	1.394 (5)
C17	C18	1.398 (5)	P1	F1	1.601 (2)
C18	C19	1.366 (5)	P1	F2	1.594 (2)
C19	C20	1.404 (5)	P1	F3	1.600 (2)
C20	C21	1.406 (4)	P1	F4	1.601 (2)
C20	C23	1.432 (5)	P1	F5	1.607 (2)
C21	C22	1.415 (4)	P1	F6	1.603 (2)
C22	C25	1.403 (4)	P2	F7	1.589 (2)
C23	C24	1.349 (5)	P2	F8	1.611 (2)
C24	C25	1.436 (5)	P2	F9	1.606 (2)
C25	C26	1.400 (5)	P2	F10	1.617 (2)
C26	C27	1.368 (5)	P2	F11	1.596 (2)
C27	C28	1.394 (5)	P2	F12	1.587 (2)

Ru2	N7	2.077 (3)	P3	F13	1.599 (2)
Ru2	N8	2.155 (3)	P3	F14	1.606 (2)
Ru2	N9	2.155 (3)	P3	F15	1.596 (2)
Ru2	N10	2.071 (3)	P3	F16	1.589 (2)
Ru2	N11	2.093 (3)	P3	F17	1.601 (2)
Ru2	N12	2.085 (3)	P3	F18	1.598 (2)
N7	C29	1.355 (4)	P4	F19	1.599 (2)
N7	C33	1.355 (4)	P4	F20	1.577 (3)
N8	C34	1.489 (4)	P4	F21	1.588 (2)
N8	C35	1.487 (4)	P4	F22	1.597 (2)
N8	C36	1.498 (4)	P4	F23	1.612 (2)
N9	C37	1.496 (4)	P4	F24	1.599 (2)

Table S4. Bond Angles for Ru-2

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Ru1	N2	78.53 (10)	C40	N10	Ru2	116.1 (2)
N1	Ru1	N3	98.45 (10)	C44	N10	Ru2	125.4 (2)
N1	Ru1	N5	89.42 (10)	C44	N10	C40	118.4 (3)
N1	Ru1	N6	94.24 (10)	C45	N11	Ru2	129.9 (2)
N2	Ru1	N3	82.38 (10)	C45	N11	C49	116.7 (3)
N4	Ru1	N1	174.28 (10)	C49	N11	Ru2	113.2 (2)
N4	Ru1	N2	96.33 (10)	C50	N12	Ru2	113.9 (2)
N4	Ru1	N3	78.23 (10)	C56	N12	Ru2	130.1 (2)
N4	Ru1	N5	94.05 (10)	C56	N12	C50	116.0 (3)
N4	Ru1	N6	90.91 (10)	N7	C29	C30	122.0 (3)
N5	Ru1	N2	100.72 (10)	C31	C30	C29	119.4 (3)
N5	Ru1	N3	172.00 (10)	C30	C31	C32	119.1 (3)
N5	Ru1	N6	78.45 (10)	C33	C32	C31	118.9 (3)
N6	Ru1	N2	172.75 (10)	N7	C33	C32	122.4 (3)
N6	Ru1	N3	99.40 (10)	N7	C33	C34	115.6 (3)
C1	N1	Ru1	126.0 (2)	C32	C33	C34	122.0 (3)
C5	N1	Ru1	115.8 (2)	N8	C34	C33	110.0 (3)
C5	N1	C1	118.2 (3)	C37	C36	N8	109.1 (3)
C6	N2	Ru1	106.89 (19)	C36	C37	N9	108.9 (3)
C6	N2	C8	107.0 (3)	N9	C39	C40	109.7 (3)
C7	N2	Ru1	117.7 (2)	N10	C40	C39	115.5 (3)
C7	N2	C6	109.4 (2)	N10	C40	C41	122.0 (3)
C7	N2	C8	108.9 (2)	C41	C40	C39	122.6 (3)
C8	N2	Ru1	106.61 (18)	C42	C41	C40	119.0 (4)
C9	N3	Ru1	106.45 (18)	C43	C42	C41	119.4 (3)
C10	N3	Ru1	117.45 (19)	C42	C43	C44	119.1 (4)
C10	N3	C9	108.2 (2)	N10	C44	C43	122.1 (4)
C11	N3	Ru1	107.17 (18)	N11	C45	C46	123.2 (4)
C11	N3	C9	107.1 (2)	C47	C46	C45	120.1 (3)
C11	N3	C10	110.0 (2)	C46	C47	C48	119.1 (3)
C12	N4	Ru1	116.2 (2)	C47	C48	C49	117.7 (3)
C16	N4	Ru1	125.5 (2)	C47	C48	C51	123.4 (3)
C16	N4	C12	118.2 (3)	C49	C48	C51	118.8 (3)
C22	N5	Ru1	114.0 (2)	N11	C49	C48	123.1 (3)
C28	N5	Ru1	129.4 (2)	N11	C49	C50	117.1 (3)
C28	N5	C22	116.5 (3)	C48	C49	C50	119.8 (3)
C17	N6	Ru1	129.4 (2)	N12	C50	C49	116.5 (3)
C17	N6	C21	116.5 (3)	N12	C50	C53	123.3 (3)
C21	N6	Ru1	114.1 (2)	C53	C50	C49	120.2 (3)
N1	C1	C2	122.3 (3)	C52	C51	C48	121.4 (3)
C1	C2	C3	119.2 (3)	C51	C52	C53	120.9 (3)
C4	C3	C2	119.0 (3)	C50	C53	C52	118.7 (3)
C3	C4	C5	119.2 (3)	C54	C53	C50	118.2 (3)

N1	C5	C4	122.0 (3)	C54	C53	C52	123.0 (3)
N1	C5	C6	116.0 (3)	C55	C54	C53	118.5 (3)
C4	C5	C6	122.0 (3)	C54	C55	C56	120.2 (3)
N2	C6	C5	109.8 (3)	N12	C56	C55	123.7 (3)
N2	C8	C9	108.6 (3)	F1	P1	F4	179.64 (12)
C8	C9	N3	109.1 (3)	F1	P1	F5	89.91 (11)
N3	C11	C12	109.9 (3)	F1	P1	F6	90.24 (12)
N4	C12	C11	115.5 (3)	F2	P1	F1	90.02 (11)
N4	C12	C13	121.5 (3)	F2	P1	F3	90.72 (12)
C13	C12	C11	123.0 (3)	F2	P1	F4	90.34 (11)
C14	C13	C12	119.3 (3)	F2	P1	F5	179.65 (14)
C13	C14	C15	119.4 (3)	F2	P1	F6	90.26 (12)
C16	C15	C14	119.1 (3)	F3	P1	F1	89.77 (12)
N4	C16	C15	122.6 (3)	F3	P1	F4	90.22 (12)
N6	C17	C18	123.5 (3)	F3	P1	F5	89.63 (12)
C19	C18	C17	120.3 (3)	F3	P1	F6	179.03 (14)
C18	C19	C20	118.1 (3)	F4	P1	F5	89.72 (11)
C19	C20	C21	118.4 (3)	F4	P1	F6	89.76 (12)
C19	C20	C23	122.6 (3)	F6	P1	F5	89.40 (12)
C21	C20	C23	119.0 (3)	F7	P2	F8	90.34 (13)
N6	C21	C20	123.2 (3)	F7	P2	F9	89.87 (12)
N6	C21	C22	116.6 (3)	F7	P2	F10	179.20 (14)
C20	C21	C22	120.3 (3)	F7	P2	F11	91.07 (13)
N5	C22	C21	116.9 (3)	F8	P2	F10	89.30 (12)
N5	C22	C25	123.1 (3)	F9	P2	F8	89.46 (13)
C25	C22	C21	120.0 (3)	F9	P2	F10	89.42 (11)
C24	C23	C20	120.6 (3)	F11	P2	F8	178.38 (13)
C23	C24	C25	121.4 (3)	F11	P2	F9	89.72 (13)
C22	C25	C24	118.7 (3)	F11	P2	F10	89.29 (12)
C26	C25	C22	118.3 (3)	F12	P2	F7	90.97 (12)
C26	C25	C24	123.0 (3)	F12	P2	F8	89.08 (14)
C27	C26	C25	118.6 (3)	F12	P2	F9	178.33 (14)
C26	C27	C28	119.8 (3)	F12	P2	F10	89.73 (12)
N5	C28	C27	123.7 (3)	F12	P2	F11	91.71 (14)
N7	Ru2	N8	78.01 (10)	F13	P3	F14	89.76 (13)
N7	Ru2	N9	98.91 (10)	F13	P3	F17	90.44 (12)
N7	Ru2	N11	93.20 (11)	F15	P3	F13	89.54 (15)
N7	Ru2	N12	87.17 (10)	F15	P3	F14	89.61 (12)
N8	Ru2	N9	81.80 (11)	F15	P3	F17	90.01 (12)
N10	Ru2	N7	174.97 (10)	F15	P3	F18	179.02 (15)
N10	Ru2	N8	97.22 (10)	F16	P3	F13	179.15 (15)
N10	Ru2	N9	78.65 (11)	F16	P3	F14	89.43 (13)
N10	Ru2	N11	91.58 (11)	F16	P3	F15	90.18 (15)
N10	Ru2	N12	95.31 (11)	F16	P3	F17	90.36 (13)
N11	Ru2	N8	171.19 (10)	F16	P3	F18	90.40 (15)

N11	Ru2	N9	100.36 (11)	F17	P3	F14	179.57 (13)
N12	Ru2	N8	99.86 (11)	F18	P3	F13	89.87 (15)
N12	Ru2	N9	173.91 (10)	F18	P3	F14	89.61 (12)
N12	Ru2	N11	78.89 (11)	F18	P3	F17	90.77 (12)
C29	N7	Ru2	125.8 (2)	F19	P4	F23	89.99 (14)
C29	N7	C33	118.2 (3)	F20	P4	F19	90.68 (15)
C33	N7	Ru2	116.0 (2)	F20	P4	F21	91.10 (15)
C34	N8	Ru2	107.07 (19)	F20	P4	F22	89.80 (13)
C34	N8	C36	107.5 (2)	F20	P4	F23	179.33 (14)
C35	N8	Ru2	117.6 (2)	F20	P4	F24	90.71 (16)
C35	N8	C34	109.3 (3)	F21	P4	F19	88.88 (13)
C35	N8	C36	108.7 (3)	F21	P4	F22	90.76 (12)
C36	N8	Ru2	106.28 (19)	F21	P4	F23	88.86 (13)
C37	N9	Ru2	107.5 (2)	F21	P4	F24	178.20 (15)
C38	N9	Ru2	116.7 (2)	F22	P4	F19	179.40 (14)
C38	N9	C37	109.0 (3)	F22	P4	F23	89.53 (12)
C39	N9	Ru2	107.1 (2)	F22	P4	F24	89.37 (13)
C39	N9	C37	106.5 (3)	F24	P4	F19	90.98 (13)
C39	N9	C38	109.5 (3)	F24	P4	F23	89.34 (15)

Table S5 Hydrogen Atom Coordinates ($\text{\AA}\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2\times 10^3$) for Ru-2.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
H1	1040	5646	7045	22
H2	1721	4995	7987	28
H3	2663	5614	8783	34
H4	2887	6884	8613	32
H6A	1888	8129	7848	25
H6B	2693	7959	7769	25
H7A	1767	8919	6250	29
H7B	2300	9057	6981	29
H7C	1440	9000	6896	29
H8A	2717	7219	6751	23
H8B	2911	8052	6581	23
H9A	2544	7346	5558	22
H9B	1983	8014	5547	22
H10A	2269	6167	6161	30
H10B	2057	6108	5354	30
H10C	1493	5842	5771	30
H11A	714	6665	4884	23
H11B	1323	7155	4667	23
H13	343	8071	3998	30
H14	-368	9128	4077	35
H15	-533	9482	5144	30
H16	6	8776	6099	23
H17	306	5885	5482	24
H18	-702	5086	5301	26
H19	-1617	5274	5879	27
H23	-2095	6076	6729	29
H24	-1954	7095	7435	29
H26	-1179	8216	7997	29
H27	-106	8918	8120	30
H28	774	8557	7555	24
H29	6326	8711	4669	25
H30	5751	9254	3627	32
H31	4490	9059	3163	29
H32	3816	8370	3793	25
H34A	3809	7823	4953	23
H34B	4277	7121	4828	23
H35A	4572	6554	5954	35
H35B	3915	7077	6030	35
H35C	4668	7083	6599	35
H36A	4560	8793	5691	26
H36B	4098	8382	6143	26
H37A	5177	8174	7007	30

H37B	5090	9046	6849	30
H38A	6492	9328	6075	45
H38B	6102	9685	6610	45
H38C	5634	9484	5865	45
H39A	6388	8663	7501	30
H39B	6969	8517	7065	30
H41	6769	7581	8309	35
H42	6784	6277	8461	42
H43	6496	5494	7501	38
H44	6141	6025	6415	29
H45	7419	8596	6185	30
H46	8537	8614	5879	35
H47	8781	7731	5125	37
H51	8347	6567	4389	37
H52	7489	5653	4031	38
H54	6255	5055	4077	32
H55	5164	5165	4417	30
H56	4986	6168	5087	26

Ru-3

racemic *cis-α*-[Ru(picenMe₂)(dpq)](PF₆)₂

Deposition Number: 1959524

Data Block Name: data_p4_a_sq

Unit Cell Parameters: a 17.450(3), b 17.450(3), c 12.557(3)

Space Group: P41

Table S6. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for Ru-3. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{II} tensor.

Atom	x	y	z	U(eq)
Ru1	8142.8 (4)	3454.2 (4)	8012.6 (5)	31.5 (2)
N1	8298 (4)	3651 (4)	9619 (6)	30.7 (15)
N2	9356 (4)	3701 (4)	8077 (6)	32.7 (15)
N3	8562 (4)	2291 (4)	7948 (7)	37.6 (16)
N4	8063 (5)	3219 (5)	6397 (6)	39.8 (19)
N5	7715 (4)	4564 (4)	7881 (6)	34.8 (16)
N6	6959 (4)	3255 (4)	8119 (6)	34.7 (16)
C1	7814 (6)	3476 (5)	10408 (8)	35.7 (18)
C2	7941 (6)	3676 (6)	11455 (8)	44 (2)
C3	8621 (5)	4056 (5)	11728 (7)	38 (2)
C4	9137 (5)	4235 (5)	10926 (7)	36 (2)
C5	8958 (5)	4032 (5)	9879 (7)	33.7 (19)
C6	9480 (5)	4243 (5)	8977 (7)	34.4 (19)
C7	9726 (5)	4019 (5)	7107 (7)	37 (2)
C8	9754 (6)	2966 (6)	8350 (7)	38 (2)
C9	9399 (6)	2336 (5)	7707 (7)	40 (2)
C10	8434 (6)	1810 (6)	8935 (8)	44 (2)
C11	8179 (6)	1908 (6)	7019 (7)	42 (2)
C12	8119 (5)	2468 (6)	6102 (7)	39 (2)
C13	8061 (6)	2231 (6)	5076 (8)	46 (2)
C14	7961 (6)	2799 (6)	4287 (7)	43 (2)
C15	7922 (6)	3545 (6)	4546 (8)	41 (2)
C16	7977 (5)	3748 (6)	5625 (8)	41 (2)
C17	8094 (6)	5229 (5)	7726 (7)	39 (2)
C18	7738 (5)	5935 (5)	7684 (7)	37 (2)
C19	6973 (6)	5987 (5)	7809 (6)	36 (2)
C20	6552 (5)	5320 (5)	7950 (7)	33.5 (17)
C21	6940 (5)	4626 (5)	7984 (7)	32.9 (17)
C22	5704 (5)	5329 (4)	8040 (7)	36.3 (18)
C23	5339 (4)	6005 (4)	7993 (6)	28.1 (16)

C24	4579 (5)	5984 (6)	8014 (8)	49 (2)
C25	4182 (5)	5301 (5)	8072 (7)	45 (2)
C26	4542 (4)	4621 (5)	8105 (6)	30.9 (17)
C27	5316 (4)	4637 (5)	8098 (7)	36.2 (19)
C28	5727 (5)	3915 (6)	8122 (7)	40 (2)
C29	6522 (5)	3915 (5)	8091 (7)	32.7 (17)
C30	5361 (5)	3190 (5)	8223 (6)	37 (2)
C31	5772 (6)	2557 (6)	8282 (7)	44 (2)
C32	6580 (6)	2605 (6)	8228 (7)	42 (2)
P1	9773.0 (14)	6582.1 (14)	8923.4 (18)	36.2 (5)
F1	10476 (3)	6997 (3)	8343 (5)	47.8 (14)
F2	9688 (3)	6016 (3)	7920 (5)	43.5 (12)
F3	10337 (3)	5989 (3)	9477 (5)	50.4 (14)
F4	9053 (3)	6172 (4)	9491 (4)	52.2 (15)
F5	9854 (4)	7150 (4)	9922 (4)	54.9 (16)
F6	9200 (3)	7175 (4)	8362 (5)	50.4 (14)
P2	6126.2 (17)	2007.4 (15)	11587 (2)	48.0 (6)
F7	6848 (5)	1815 (5)	10873 (8)	100 (3)
F8	5624 (6)	1507 (5)	10792 (7)	92 (3)
F9	6276 (6)	1263 (4)	12289 (7)	85 (2)
F10	5408 (4)	2213 (5)	12275 (7)	80 (2)
F11	6634 (4)	2498 (4)	12376 (7)	73 (2)
F12	6012 (5)	2757 (4)	10889 (6)	77 (2)
O1	9639 (8)	2319 (7)	11139 (9)	38 (3)
O2	11054 (9)	2067 (9)	10313 (13)	61 (4)

Table S7. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for Ru-3. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
Ru1	39.4 (4)	35.3 (4)	19.7 (3)	1.5 (3)	-3.9 (3)	-5.9 (3)
N1	36 (4)	33 (4)	22 (4)	2 (3)	-1 (3)	7 (3)
N2	38 (4)	38 (4)	22 (3)	-1 (3)	-1 (3)	-5 (3)
N3	48 (4)	35 (4)	29 (4)	-5 (4)	-2 (4)	-1 (3)
N4	47 (5)	43 (4)	30 (4)	2 (4)	-8 (3)	-17 (4)
N5	47 (4)	40 (4)	17 (3)	1 (3)	-5 (3)	-9 (3)
N6	37 (4)	45 (4)	22 (4)	1 (3)	-2 (3)	-10 (3)
C1	47 (5)	36 (5)	24 (4)	4 (4)	-4 (4)	-7 (4)
C2	53 (6)	46 (5)	34 (6)	2 (4)	-3 (4)	12 (5)
C3	47 (5)	44 (5)	22 (4)	-4 (4)	-5 (4)	-7 (4)
C4	41 (5)	43 (5)	24 (4)	1 (4)	-8 (4)	-1 (4)
C5	43 (5)	35 (5)	24 (4)	-3 (3)	-1 (4)	-8 (4)
C6	38 (5)	40 (5)	26 (4)	0 (4)	-8 (4)	-4 (4)
C7	41 (5)	37 (5)	33 (5)	8 (4)	4 (4)	-6 (4)
C8	43 (5)	48 (5)	22 (4)	-3 (4)	-2 (3)	3 (4)
C9	56 (6)	33 (5)	31 (5)	-3 (4)	-3 (4)	4 (4)
C10	56 (6)	48 (6)	30 (5)	3 (4)	-1 (4)	-4 (5)
C11	59 (6)	43 (5)	25 (4)	-7 (4)	1 (4)	-11 (4)
C12	37 (5)	48 (5)	31 (5)	0 (4)	-3 (4)	-8 (4)
C13	53 (6)	51 (6)	33 (5)	-2 (4)	4 (4)	-14 (5)
C14	43 (5)	64 (7)	22 (4)	11 (4)	3 (4)	-6 (5)
C15	42 (5)	59 (6)	22 (5)	1 (4)	1 (4)	-17 (5)
C16	43 (5)	50 (5)	31 (5)	8 (5)	2 (4)	-8 (4)
C17	45 (5)	45 (5)	26 (5)	6 (4)	-6 (3)	-13 (4)
C18	39 (5)	38 (5)	33 (5)	0 (4)	-5 (4)	-4 (4)
C19	51 (5)	39 (5)	19 (4)	3 (3)	-3 (4)	-2 (4)
C20	44 (5)	42 (4)	14 (3)	-2 (4)	-1 (4)	-3 (4)
C21	41 (4)	43 (4)	15 (3)	-2 (4)	-3 (4)	-2 (3)
C22	49 (5)	49 (5)	10 (3)	1 (4)	0 (4)	-2 (4)
C23	33 (4)	37 (4)	14 (3)	0 (3)	3 (3)	5 (3)
C24	71 (7)	60 (6)	18 (4)	-3 (5)	6 (5)	1 (5)
C25	47 (5)	70 (6)	16 (4)	-2 (5)	-5 (4)	5 (4)
C26	37 (4)	49 (5)	7 (3)	-4 (3)	-1 (3)	-3 (4)
C27	44 (5)	54 (5)	11 (4)	-4 (4)	0 (4)	1 (4)
C28	49 (5)	53 (5)	18 (4)	-7 (4)	2 (4)	-9 (4)
C29	45 (5)	38 (4)	15 (3)	-2 (3)	2 (4)	-5 (3)
C30	38 (5)	50 (5)	24 (5)	1 (4)	-2 (3)	-8 (4)
C31	64 (6)	46 (5)	23 (4)	-6 (4)	1 (4)	-23 (5)
C32	53 (6)	41 (5)	33 (5)	2 (4)	3 (4)	-4 (4)
P1	39.6 (12)	43.2 (13)	25.9 (11)	-4.3 (9)	0.4 (9)	0.2 (10)
F1	46 (3)	52 (3)	45 (3)	-2 (3)	1 (2)	-11 (3)
F2	44 (3)	52 (3)	34 (3)	-10 (3)	3 (2)	-9 (2)

F3	43 (3)	55 (3)	53 (3)	3 (3)	-7 (3)	3 (3)
F4	46 (3)	80 (4)	30 (3)	0 (3)	11 (2)	-10 (3)
F5	78 (4)	56 (4)	30 (3)	-15 (3)	1 (3)	-3 (3)
F6	49 (3)	60 (4)	42 (3)	-4 (3)	1 (2)	16 (3)
P2	54.1 (16)	40.6 (14)	49.3 (15)	-5.0 (11)	10.3 (12)	-0.9 (11)
F7	109 (7)	63 (5)	128 (8)	4 (5)	72 (6)	12 (4)
F8	127 (7)	80 (5)	70 (5)	-22 (4)	-14 (5)	-26 (5)
F9	119 (7)	54 (4)	81 (5)	1 (4)	2 (5)	-1 (4)
F10	60 (4)	81 (5)	100 (6)	-29 (5)	30 (4)	-8 (4)
F11	57 (4)	61 (4)	102 (6)	-6 (4)	-18 (4)	-12 (3)
F12	118 (7)	52 (4)	60 (4)	8 (3)	4 (4)	17 (4)
O1	64 (8)	30 (6)	18 (6)	-10 (5)	-13 (5)	-2 (6)
O2	62 (9)	62 (9)	59 (10)	22 (8)	-17 (8)	1 (7)

Table S8. Bond Lengths for Ru-3.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ru1	N1	2.064 (7)	C15	C16	1.405 (14)
Ru1	N2	2.161 (7)	C17	C18	1.380 (14)
Ru1	N3	2.158 (7)	C18	C19	1.348 (13)
Ru1	N4	2.075 (8)	C19	C20	1.387 (12)
Ru1	N5	2.082 (8)	C20	C21	1.389 (12)
Ru1	N6	2.099 (7)	C20	C22	1.485 (12)
N1	C1	1.338 (13)	C21	C29	1.447 (11)
N1	C5	1.369 (12)	C22	C23	1.342 (10)
N2	C6	1.489 (11)	C22	C27	1.386 (10)
N2	C7	1.486 (11)	C23	C24	1.327 (11)
N2	C8	1.498 (12)	C24	C25	1.381 (11)
N3	C9	1.493 (13)	C25	C26	1.343 (10)
N3	C10	1.514 (13)	C26	C27	1.351 (10)
N3	C11	1.502 (12)	C27	C28	1.450 (13)
N4	C12	1.364 (13)	C28	C29	1.387 (13)
N4	C16	1.347 (13)	C28	C30	1.423 (13)
N5	C17	1.350 (11)	C30	C31	1.318 (15)
N5	C21	1.361 (11)	C31	C32	1.414 (15)
N6	C29	1.382 (12)	P1	F1	1.600 (6)
N6	C32	1.320 (12)	P1	F2	1.608 (6)
C1	C2	1.378 (14)	P1	F3	1.588 (6)
C2	C3	1.402 (14)	P1	F4	1.613 (6)
C3	C4	1.386 (13)	P1	F5	1.605 (6)
C4	C5	1.397 (12)	P1	F6	1.602 (6)
C5	C6	1.500 (12)	P2	F7	1.582 (8)
C8	C9	1.498 (12)	P2	F8	1.588 (8)
C11	C12	1.515 (13)	P2	F9	1.591 (8)
C12	C13	1.357 (13)	P2	F10	1.565 (7)
C13	C14	1.413 (14)	P2	F11	1.582 (8)
C14	C15	1.343 (15)	P2	F12	1.587 (7)

Table S9. Bond Angles for Ru-3.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Ru1	N2	78.6 (3)	C19	C18	C17	120.0 (9)
N1	Ru1	N3	98.6 (3)	C18	C19	C20	118.9 (9)
N1	Ru1	N4	175.9 (3)	C19	C20	C21	118.5 (8)
N1	Ru1	N5	88.2 (3)	C19	C20	C22	121.9 (8)
N1	Ru1	N6	95.4 (3)	C21	C20	C22	119.6 (7)
N3	Ru1	N2	81.8 (3)	N5	C21	C20	123.4 (8)
N4	Ru1	N2	98.1 (3)	N5	C21	C29	116.2 (8)
N4	Ru1	N3	78.5 (3)	C20	C21	C29	120.3 (8)
N4	Ru1	N5	94.7 (3)	C23	C22	C20	118.6 (7)
N4	Ru1	N6	87.9 (3)	C23	C22	C27	122.4 (8)
N5	Ru1	N2	99.8 (3)	C27	C22	C20	118.8 (7)
N5	Ru1	N3	173.2 (3)	C24	C23	C22	116.7 (8)
N5	Ru1	N6	78.8 (3)	C23	C24	C25	121.8 (9)
N6	Ru1	N2	173.9 (3)	C26	C25	C24	121.9 (9)
N6	Ru1	N3	100.4 (3)	C25	C26	C27	116.7 (8)
C1	N1	Ru1	127.0 (7)	C22	C27	C28	121.1 (8)
C1	N1	C5	117.7 (8)	C26	C27	C22	120.4 (8)
C5	N1	Ru1	115.2 (6)	C26	C27	C28	118.5 (8)
C6	N2	Ru1	107.3 (5)	C29	C28	C27	119.6 (8)
C6	N2	C8	107.6 (7)	C29	C28	C30	116.8 (9)
C7	N2	Ru1	118.0 (6)	C30	C28	C27	123.5 (8)
C7	N2	C6	108.7 (7)	N6	C29	C21	116.0 (7)
C7	N2	C8	107.9 (7)	N6	C29	C28	123.5 (8)
C8	N2	Ru1	107.0 (5)	C28	C29	C21	120.5 (8)
C9	N3	Ru1	106.9 (5)	C31	C30	C28	120.4 (9)
C9	N3	C10	109.8 (7)	C30	C31	C32	119.4 (9)
C9	N3	C11	107.5 (7)	N6	C32	C31	123.7 (10)
C10	N3	Ru1	116.2 (6)	F1	P1	F2	89.5 (3)
C11	N3	Ru1	107.3 (6)	F1	P1	F4	178.8 (4)
C11	N3	C10	108.8 (7)	F1	P1	F5	90.5 (3)
C12	N4	Ru1	116.7 (6)	F1	P1	F6	89.2 (3)
C16	N4	Ru1	125.1 (7)	F2	P1	F4	90.1 (3)
C16	N4	C12	118.1 (9)	F3	P1	F1	91.1 (3)
C17	N5	Ru1	129.4 (7)	F3	P1	F2	90.0 (3)
C17	N5	C21	115.6 (8)	F3	P1	F4	90.0 (3)
C21	N5	Ru1	115.0 (6)	F3	P1	F5	90.3 (4)
C29	N6	Ru1	113.8 (5)	F3	P1	F6	179.6 (4)
C32	N6	Ru1	130.0 (7)	F5	P1	F2	179.7 (4)
C32	N6	C29	116.2 (8)	F5	P1	F4	89.8 (3)
N1	C1	C2	123.1 (9)	F6	P1	F2	89.6 (3)
C1	C2	C3	119.3 (10)	F6	P1	F4	89.7 (4)
C4	C3	C2	118.6 (8)	F6	P1	F5	90.0 (3)
C3	C4	C5	118.8 (8)	F7	P2	F8	88.1 (6)

N1	C5	C4	122.4 (8)	F7	P2	F9	90.6 (5)
N1	C5	C6	116.7 (7)	F7	P2	F12	87.8 (5)
C4	C5	C6	120.9 (8)	F8	P2	F9	89.5 (5)
N2	C6	C5	109.2 (7)	F10	P2	F7	178.7 (6)
C9	C8	N2	108.2 (7)	F10	P2	F8	91.8 (5)
N3	C9	C8	109.5 (7)	F10	P2	F9	90.7 (5)
N3	C11	C12	109.4 (8)	F10	P2	F11	88.8 (5)
N4	C12	C11	114.8 (8)	F10	P2	F12	90.9 (5)
C13	C12	N4	123.0 (9)	F11	P2	F7	91.3 (5)
C13	C12	C11	122.0 (9)	F11	P2	F8	179.3 (5)
C12	C13	C14	117.5 (10)	F11	P2	F9	90.1 (5)
C15	C14	C13	121.1 (9)	F11	P2	F12	88.2 (4)
C14	C15	C16	118.4 (10)	F12	P2	F8	92.1 (5)
N4	C16	C15	121.9 (10)	F12	P2	F9	177.7 (5)
N5	C17	C18	123.6 (9)				

Table S10 Hydrogen Atom Coordinates ($\text{\AA}\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2\times 10^3$) for Ru-3.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
H1	7370	3205	10242	43
H2	7580	3560	11974	53
H3	8723	4186	12432	45
H4	9594	4486	11082	43
H6A	9374	4762	8746	41
H6B	10009	4218	9210	41
H7A	9694	3652	6540	56
H7B	10254	4130	7256	56
H7C	9468	4482	6900	56
H8A	10296	3005	8189	45
H8B	9698	2858	9104	45
H9A	9473	2436	6954	48
H9B	9642	1852	7878	48
H10A	8741	2006	9508	66
H10B	8579	1289	8791	66
H10C	7903	1828	9131	66
H11A	7671	1736	7224	51
H11B	8474	1463	6802	51
H13	8087	1714	4899	55
H14	7920	2654	3576	51
H15	7861	3917	4023	49
H16	7952	4263	5813	50
H17	8623	5211	7642	46
H18	8027	6375	7570	44
H19	6731	6462	7801	43
H23	5606	6466	7949	34
H24	4307	6442	7988	59
H25	3649	5312	8088	53
H26	4272	4162	8132	37
H30	4829	3162	8248	45
H31	5532	2084	8359	53
H32	6860	2153	8270	51

Ru-4racemic *cis-α*-[Ru(picenMe₂)(dppzMe₂)](PF₆)₂

Deposition Number: 1959525

Data Block Name: data_fdd2_a

Unit Cell Parameters: a 23.752(5), b 15.729(3), c 19.930(4)

Space Group: Fdd2

Table S11. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for Ru-4. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{II} tensor.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
Ru1	2500	2500	2884.0 (3)	15.08 (15)
N1	2231.1 (16)	3751 (2)	2849 (2)	19.6 (7)
N2	1902 (2)	2454 (3)	2064 (3)	21.2 (12)
N3	3044 (2)	2691 (3)	3694 (2)	17.6 (10)
N4	3092.6 (17)	2557 (3)	6108 (2)	19.5 (8)
C1	2483 (2)	4418 (3)	3156 (3)	23 (1)
C2	2264 (2)	5221 (3)	3132 (3)	29.2 (12)
C3	1762 (2)	5370 (3)	2800 (3)	31.0 (11)
C4	1500 (2)	4693 (3)	2491 (3)	29.1 (11)
C5	1743 (2)	3895 (3)	2520 (2)	22.6 (10)
C6	1476 (2)	3127 (3)	2198 (3)	23.4 (11)
C7	1615 (2)	1638 (3)	1938 (2)	24.8 (10)
C8	2222 (3)	2714 (4)	1449 (3)	26.3 (13)
C9	3594 (2)	2893 (3)	3693 (3)	19.5 (10)
C10	3910.5 (19)	3003 (3)	4270 (2)	20.1 (9)
C11	3666 (2)	2888 (3)	4889 (2)	19.4 (9)
C12	3093 (2)	2673 (3)	4911 (2)	17.0 (9)
C13	2803 (2)	2591 (3)	4309 (3)	17.1 (12)
C14	2800.3 (19)	2556 (3)	5547 (2)	17.7 (9)
C15	2803 (2)	2510 (3)	6690 (2)	18.8 (10)
C16	3082 (3)	2476 (3)	7310 (3)	21.6 (16)
C17	2805.6 (17)	2477 (4)	7902 (5)	22.1 (8)
C18	3123 (3)	2449 (4)	8558 (3)	24.0 (16)
P1	2643.9 (6)	5197.1 (9)	5180.0 (7)	27.3 (3)
F1	3113.7 (13)	5885 (2)	5366 (2)	43.1 (8)
F2	2936 (2)	4533 (3)	5658 (3)	69.0 (14)
F3	3018.7 (16)	4857 (3)	4581 (2)	64.1 (14)
F4	2171.0 (14)	4510 (2)	4999 (2)	41.8 (10)
F5	2350.9 (16)	5848 (3)	4678 (2)	59.1 (11)
F6	2250.0 (18)	5539 (3)	5760 (2)	60.0 (13)

Table S12. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for Ru-4. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
Ru1	18.9(2)	12.0(2)	14.3(2)	0	0	-0.6(3)
N1	22.8(18)	18.8(19)	17.1(17)	0.3(17)	-0.3(17)	-0.2(15)
N2	25(3)	19(2)	21(2)	-2.8(17)	-1(2)	-3.2(18)
N3	23(2)	12.0(19)	18(2)	1.3(18)	2.4(19)	5.4(19)
N4	19.3(19)	21(2)	18.1(19)	0.9(16)	-0.3(16)	-0.3(16)
C1	25(2)	18(2)	26(2)	-0.4(18)	-6(2)	-1.7(19)
C2	36(3)	16(2)	36(3)	-5(2)	-3(2)	0(2)
C3	38(3)	20(2)	35(3)	0(2)	-5(3)	4.6(19)
C4	31(3)	25(3)	32(3)	0(2)	-7(2)	2(2)
C5	25(2)	23(2)	20(2)	0.6(19)	-2.5(19)	-0.3(19)
C6	27(3)	21(3)	23(3)	1(2)	-6(2)	-1(2)
C7	31(3)	24(2)	20(2)	-4.7(19)	-2(2)	-8(2)
C8	34(3)	29(3)	16(3)	3(3)	-4(2)	-12(3)
C9	21(2)	16(2)	22(2)	0.6(19)	3(2)	2.1(19)
C10	18(2)	19(2)	23(2)	-0.6(19)	3.7(19)	-1.0(18)
C11	21(2)	19(2)	18(2)	-1.3(18)	-4.3(18)	1.2(18)
C12	20(2)	11(2)	21(2)	-1.9(17)	-1.8(19)	3.1(17)
C13	16(3)	15(2)	20(3)	2(2)	2(2)	0.4(19)
C14	18(2)	16(2)	19(2)	0.9(16)	-2.0(19)	1.1(16)
C15	21(2)	19(2)	17(2)	-0.2(18)	1.7(18)	1.4(19)
C16	17(3)	26(3)	21(3)	-1(2)	-3(2)	-1.4(19)
C17	23(2)	22(2)	22(2)	-0.2(17)	-2(4)	-2(3)
C18	28(4)	26(3)	18(3)	-1(2)	-6(2)	-2(2)
P1	23.4(7)	25.4(7)	33.2(8)	-6.2(5)	1.5(6)	-0.3(5)
F1	30.3(16)	40.3(17)	59(2)	-20.8(19)	7.2(17)	-9.0(13)
F2	71(3)	47(2)	89(3)	11(2)	-43(3)	0(2)
F3	30(2)	96(3)	66(3)	-48(3)	3(2)	-1(2)
F4	27.0(18)	31.1(19)	67(3)	-11.0(18)	-5.7(18)	-0.8(14)
F5	40(2)	61(3)	77(3)	29(2)	-3(2)	-6.1(19)
F6	52(3)	71(3)	57(3)	-38(2)	29(2)	-25(2)

Table S13. Bond Lengths for Ru-4. ^{1/2-X,1/2-Y,+Z}

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ru1	N1 ¹	2.070 (4)	C8	C8 ¹	1.483 (13)
Ru1	N1	2.070 (4)	C9	C10	1.384 (7)
Ru1	N2	2.166 (5)	C10	C11	1.376 (7)
Ru1	N2 ¹	2.166 (5)	C11	C12	1.402 (7)
Ru1	N3 ¹	2.089 (5)	C12	C13	1.388 (8)
Ru1	N3	2.089 (5)	C12	C14	1.457 (6)
N1	C1	1.354 (6)	C13	C13 ¹	1.466 (12)
N1	C5	1.351 (6)	C14	C14 ¹	1.437 (9)
N2	C6	1.489 (7)	C15	C15 ¹	1.439 (10)
N2	C7	1.475 (6)	C15	C16	1.403 (8)
N2	C8	1.499 (8)	C16	C17	1.350 (12)
N3	C9	1.345 (7)	C17	C17 ¹	1.454 (8)
N3	C13	1.363 (8)	C17	C18	1.510 (11)
N4	C14	1.317 (6)	P1	F1	1.597 (3)
N4	C15	1.350 (6)	P1	F2	1.575 (4)
C1	C2	1.367 (7)	P1	F3	1.583 (4)
C2	C3	1.384 (8)	P1	F4	1.600 (4)
C3	C4	1.378 (7)	P1	F5	1.591 (4)
C4	C5	1.384 (7)	P1	F6	1.582 (4)
C5	C6	1.507 (7)			

Table S14. Bond Angles for Ru-4. ^{1/2}-X,^{1/2}-Y,+Z

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1 ¹	Ru1	N1	176.1 (2)	C8 ¹	C8	N2	109.1 (4)
N1 ¹	Ru1	N2	98.31 (16)	N3	C9	C10	123.8 (5)
N1	Ru1	N2	78.70 (15)	C11	C10	C9	119.9 (4)
N1 ¹	Ru1	N2 ¹	78.70 (15)	C10	C11	C12	118.0 (4)
N1	Ru1	N2 ¹	98.31 (16)	C11	C12	C14	121.3 (4)
N1 ¹	Ru1	N3 ¹	94.59 (17)	C13	C12	C11	118.5 (4)
N1 ¹	Ru1	N3	88.43 (17)	C13	C12	C14	120.2 (4)
N1	Ru1	N3 ¹	88.42 (17)	N3	C13	C12	123.9 (5)
N1	Ru1	N3	94.59 (17)	N3	C13	C13 ¹	115.8 (3)
N2 ¹	Ru1	N2	82.1 (3)	C12	C13	C13 ¹	120.3 (3)
N3 ¹	Ru1	N2	99.94 (14)	N4	C14	C12	119.2 (4)
N3	Ru1	N2	173.24 (18)	N4	C14	C14 ¹	121.6 (3)
N3 ¹	Ru1	N2 ¹	173.24 (18)	C14 ¹	C14	C12	119.2 (2)
N3	Ru1	N2 ¹	99.94 (14)	N4	C15	C15 ¹	120.7 (3)
N3 ¹	Ru1	N3	78.8 (3)	N4	C15	C16	121.2 (5)
C1	N1	Ru1	125.8 (3)	C16	C15	C15 ¹	118.1 (4)
C5	N1	Ru1	116.1 (3)	C17	C16	C15	122.7 (6)
C5	N1	C1	118.0 (4)	C16	C17	C17 ¹	119.1 (4)
C6	N2	Ru1	106.6 (3)	C16	C17	C18	121.0 (4)
C6	N2	C8	107.3 (4)	C17 ¹	C17	C18	120.0 (4)
C7	N2	Ru1	117.5 (3)	F1	P1	F4	179.6 (2)
C7	N2	C6	109.6 (5)	F2	P1	F1	90.1 (2)
C7	N2	C8	109.4 (4)	F2	P1	F3	89.1 (3)
C8	N2	Ru1	106.0 (4)	F2	P1	F4	89.8 (2)
C9	N3	Ru1	129.4 (4)	F2	P1	F5	178.2 (3)
C9	N3	C13	115.9 (5)	F2	P1	F6	92.5 (3)
C13	N3	Ru1	114.8 (4)	F3	P1	F1	90.6 (2)
C14	N4	C15	117.4 (4)	F3	P1	F4	89.8 (2)
N1	C1	C2	122.2 (5)	F3	P1	F5	89.4 (3)
C1	C2	C3	120.1 (5)	F5	P1	F1	90.9 (2)
C4	C3	C2	118.2 (5)	F5	P1	F4	89.2 (2)
C3	C4	C5	119.6 (5)	F6	P1	F1	90.8 (2)
N1	C5	C4	122.0 (4)	F6	P1	F3	177.9 (3)
N1	C5	C6	115.7 (4)	F6	P1	F4	88.8 (2)
C4	C5	C6	122.3 (4)	F6	P1	F5	89.0 (3)
N2	C6	C5	111.1 (4)				

Table S15. Hydrogen Atom Coordinates ($\text{\AA}\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2\times 10^3$) for Ru-4.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
H1	2815	4326	3392	28
H2	2452	5667	3340	35
H3	1606	5912	2785	37
H4	1161	4773	2264	35
H6A	1186	2903	2492	28
H6B	1299	3293	1780	28
H7A	1885	1223	1793	37
H7B	1335	1714	1595	37
H7C	1437	1446	2343	37
H8A	2013	2556	1051	32
H8B	2273	3326	1446	32
H9	3772	2962	3281	23
H10	4288	3155	4239	24
H11	3874	2950	5281	23
H16	3473	2452	7313	26
H18A	3024	2935	8824	36
H18B	3520	2455	8471	36
H18C	3026	1939	8796	36

Ru-5racemic *cis- α* -[Ru(picenMe₂)(phenpyrBz)](PF₆)₂

Deposition Number: 1959526

Data Block Name: data_cc_a

Unit Cell Parameters: a 19.664(4), b 15.844(3), c 14.416(3)

Space Group: cc

Table S16. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for Ru-5. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{II} tensor.

Atom	x	y	z	U(eq)
Ru1	1805.5 (2)	6250.6 (2)	5043.6 (2)	20.54 (11)
N1	1419 (2)	5023 (2)	4460 (3)	23.3 (7)
N2	427 (3)	6389 (3)	3879 (4)	24.0 (9)
N3	1575 (3)	6284 (2)	6342 (4)	21.8 (10)
N4	2121 (2)	7487 (2)	5614 (3)	24.9 (7)
N5	2097 (3)	6399 (3)	3890 (4)	24.5 (9)
N6	3116 (3)	5991 (3)	6129 (3)	24.0 (8)
N7	4680 (3)	6360 (2)	4030 (4)	23.6 (8)
N8	5536 (3)	6088 (2)	5932 (3)	26.9 (8)
C1	1920 (3)	4333 (3)	4926 (4)	27.8 (10)
C2	1612 (3)	3531 (3)	4483 (4)	30.6 (10)
C3	776 (3)	3422 (3)	3542 (4)	32.6 (11)
C4	258 (3)	4136 (3)	3043 (4)	28.7 (9)
C5	602 (3)	4917 (3)	3513 (4)	25.4 (9)
C6	83 (3)	5722 (3)	2980 (4)	24.3 (9)
C7	83 (3)	7226 (3)	3298 (4)	28.5 (9)
C8	125 (4)	6211 (3)	4585 (5)	25.2 (13)
C9	704 (3)	6617 (3)	5755 (4)	27.1 (10)
C10	1658 (3)	5478 (3)	6928 (4)	27.4 (9)
C11	2186 (3)	6916 (3)	7232 (4)	27.5 (10)
C12	2280 (3)	7650 (3)	6657 (4)	27.1 (9)
C13	2539 (3)	8438 (3)	7159 (4)	31.2 (10)
C14	2617 (3)	9094 (3)	6590 (4)	33.8 (11)
C15	2454 (4)	8924 (3)	5531 (5)	34.5 (10)
C16	2204 (3)	8121 (3)	5067 (4)	28.1 (9)
C17	1583 (3)	6610 (3)	2761 (4)	24.7 (9)
C18	1864 (3)	6759 (3)	2094 (4)	26.2 (9)
C19	2716 (3)	6667 (3)	2577 (4)	24.8 (9)
C20	3277 (3)	6430 (3)	3749 (4)	24.5 (9)
C21	2955 (3)	6315 (3)	4386 (4)	23.6 (11)

C22	3501 (4)	6097 (3)	5598 (4)	24.4 (11)
C23	4382 (3)	6007 (3)	6199 (4)	23.8 (9)
C24	4890 (3)	5781 (3)	7385 (4)	25.5 (9)
C25	4498 (3)	5657 (3)	7903 (4)	28.7 (9)
C26	3616 (3)	5759 (3)	7250 (4)	26.5 (10)
C27	4169 (3)	6313 (2)	4380 (4)	24.6 (10)
C28	4711 (3)	6131 (3)	5561 (4)	25.9 (10)
C29	5498 (4)	6220 (2)	4991 (4)	25.4 (11)
C30	6216 (3)	6206 (3)	4952 (5)	22.9 (10)
C31	6114 (3)	6062 (3)	3915 (4)	28.1 (10)
C32	6792 (3)	6035 (4)	3877 (4)	33.8 (11)
C33	7612 (4)	6161 (3)	4902 (5)	33.7 (13)
C34	7728 (4)	6310 (3)	5937 (5)	29.5 (11)
C35	7050 (4)	6329 (3)	5984 (4)	26.6 (10)
P1	4049.9 (9)	8901.8 (8)	4558.6 (11)	31.7 (3)
F1	3062 (2)	8725 (2)	3865 (3)	55.1 (10)
F2	4013 (2)	9630 (2)	5294 (3)	49.6 (8)
F3	3857 (2)	9583.1 (18)	3605 (2)	39.2 (7)
F4	4268 (3)	8216 (2)	5526 (3)	49.4 (9)
F5	4099 (2)	8183 (2)	3826 (3)	46.4 (8)
F6	5054 (2)	9079 (2)	5263 (3)	47.8 (8)
P2	9137.3 (8)	8481.9 (9)	5512.6 (11)	32.4 (3)
F7	9267 (2)	8130 (2)	4582 (3)	49.4 (9)
F8	8567 (2)	9229 (2)	4642 (3)	46.1 (8)
F9	8304 (2)	7926 (2)	4930 (3)	49.0 (8)
F10	9954 (2)	9062 (3)	6087 (3)	65.6 (11)
F11	9001 (2)	8824 (2)	6444 (3)	45.3 (8)
F12	9711 (3)	7743 (2)	6384 (3)	61.3 (11)

Table S17. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for Ru-5. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
Ru1	23.68 (18)	16.25 (16)	22.29 (16)	0.04 (12)	14.19 (13)	0.15 (13)
N1	26.8 (19)	21.8 (18)	25.5 (17)	0.1 (14)	18.0 (15)	-0.8 (14)
N2	27 (2)	19.9 (17)	24.8 (19)	2.5 (15)	15.2 (16)	2.6 (16)
N3	27 (2)	21 (2)	23 (2)	1.6 (13)	18.0 (19)	1.3 (13)
N4	25.1 (18)	23.3 (19)	25.3 (17)	0.0 (14)	14.7 (14)	0.5 (14)
N5	27 (2)	17.8 (16)	25 (2)	0.2 (16)	14.4 (19)	1.8 (17)
N6	31 (2)	17.6 (18)	25.8 (19)	-2.0 (16)	18.6 (17)	-4.0 (17)
N7	22 (2)	26.1 (18)	24.6 (18)	1.3 (14)	14.7 (16)	0.2 (14)
N8	26 (2)	25.3 (18)	25.4 (19)	1.8 (15)	13.3 (17)	1.0 (15)
C1	39 (3)	23 (2)	27 (2)	2.0 (17)	22.4 (19)	3.0 (18)
C2	44 (3)	21 (2)	35 (2)	0 (2)	28 (2)	1 (2)
C3	49 (3)	21 (2)	35 (2)	-3.6 (18)	30 (2)	-5 (2)
C4	33 (2)	25 (2)	30 (2)	-2.8 (18)	19.9 (19)	-5.7 (19)
C5	28 (2)	26 (2)	27 (2)	1.6 (17)	19.4 (18)	3.5 (18)
C6	26 (2)	21 (2)	22 (2)	-3.2 (17)	13.1 (18)	-0.7 (18)
C7	31 (2)	21 (2)	31 (2)	3.9 (16)	17.3 (19)	5.1 (16)
C8	27 (3)	24 (3)	27 (3)	1.9 (16)	18 (2)	1.7 (17)
C9	30 (2)	24 (3)	29 (2)	-0.9 (18)	18.6 (19)	1.1 (18)
C10	34 (2)	22 (2)	31 (2)	6.2 (16)	22.0 (19)	1.8 (17)
C11	34 (3)	22 (2)	30 (2)	-2.8 (18)	21 (2)	-0.2 (18)
C12	27 (2)	26 (2)	28 (2)	0.9 (17)	15.8 (18)	1.3 (17)
C13	34 (3)	25 (2)	30 (2)	-6.9 (18)	17 (2)	-1.9 (18)
C14	36 (3)	20 (2)	42 (3)	-7.0 (19)	22 (2)	-4.7 (18)
C15	36 (3)	24 (2)	45 (3)	-1 (2)	25 (2)	-1 (2)
C16	33 (2)	25 (2)	25 (2)	-0.5 (17)	17.1 (18)	-1.3 (18)
C17	25 (2)	21 (2)	26 (2)	-1.1 (16)	14.6 (18)	0.7 (16)
C18	26 (2)	25 (2)	24 (2)	1.5 (16)	13.2 (17)	-0.9 (17)
C19	30 (2)	23 (2)	26 (2)	-0.5 (16)	19.2 (19)	-1.2 (16)
C20	26 (2)	18.1 (18)	27 (2)	-1.1 (17)	15.2 (19)	-1.1 (17)
C21	30 (3)	15 (2)	26 (2)	-1.9 (15)	17 (2)	-0.9 (15)
C22	31 (3)	16.4 (19)	23 (2)	2.3 (18)	15 (2)	1.0 (19)
C23	26 (2)	16.7 (19)	29 (2)	-1.6 (16)	16.6 (19)	-1.2 (17)
C24	24 (2)	18.9 (19)	29 (2)	-1.3 (16)	13.9 (18)	-1.2 (16)
C25	33 (2)	22 (2)	28 (2)	-0.4 (17)	16.9 (19)	-1.1 (18)
C26	32 (3)	19 (2)	25 (2)	0.2 (17)	16 (2)	1.3 (18)
C27	29 (3)	20 (2)	28 (2)	0.1 (15)	19 (2)	-0.2 (16)
C28	22 (2)	24 (2)	29 (2)	-0.3 (17)	15 (2)	0.6 (16)
C29	31 (3)	20 (2)	24 (2)	-0.5 (15)	16 (2)	-0.6 (16)
C30	20 (3)	23 (2)	29 (3)	0.7 (15)	17 (2)	-0.6 (14)
C31	31 (3)	29 (2)	27 (2)	-1.9 (19)	20 (2)	-4 (2)
C32	35 (3)	35 (3)	34 (3)	-1 (2)	22 (2)	-4 (2)
C33	37 (3)	34 (3)	38 (3)	4 (2)	27 (3)	-1 (2)

C34	29 (3)	30 (3)	33 (3)	2.9 (17)	20 (2)	3.6 (17)
C35	31 (3)	27 (2)	25 (2)	2.1 (16)	18 (2)	3.6 (17)
P1	34.0 (7)	29.1 (6)	25.7 (6)	-0.1 (5)	14.6 (6)	-6.0 (5)
F1	43 (2)	80 (3)	38.4 (19)	-4.6 (16)	22.6 (17)	-22.4 (16)
F2	65 (2)	37.3 (17)	35.9 (15)	-0.7 (13)	25.3 (15)	9.0 (15)
F3	44.1 (17)	32.9 (15)	33.3 (14)	9.7 (12)	19.5 (13)	-1.4 (12)
F4	74 (3)	30.8 (16)	38.0 (16)	0.6 (14)	31.4 (18)	-7.6 (16)
F5	69 (2)	32.1 (16)	41.9 (17)	-6.5 (13)	35.0 (17)	-8.1 (15)
F6	33.7 (16)	44.2 (19)	46.2 (18)	8.6 (15)	14.0 (14)	-1.0 (14)
P2	32.7 (7)	32.0 (7)	28.5 (6)	0.1 (5)	16.3 (5)	7.0 (6)
F7	52 (2)	64 (2)	35.5 (17)	6.0 (15)	27.8 (16)	25.5 (17)
F8	51.5 (19)	31.2 (16)	40.0 (17)	0.9 (13)	19.3 (15)	7.8 (14)
F9	58 (2)	46.8 (18)	38.4 (16)	-5.6 (14)	27.3 (15)	-15.4 (16)
F10	40 (2)	96 (3)	44 (2)	-6 (2)	16.1 (17)	-19 (2)
F11	40.3 (19)	56 (2)	34.6 (16)	-7.8 (13)	20.1 (15)	10.4 (13)
F12	76 (3)	65 (2)	38.4 (16)	21.0 (16)	32.4 (17)	46 (2)

Table S18. Bond Lengths for Ru-5.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ru1	N1	2.073 (4)	C14	C15	1.385 (8)
Ru1	N2	2.173 (4)	C15	C16	1.383 (7)
Ru1	N3	2.177 (5)	C17	C18	1.388 (6)
Ru1	N4	2.070 (4)	C18	C19	1.380 (7)
Ru1	N5	2.073 (5)	C19	C20	1.402 (6)
Ru1	N6	2.095 (4)	C20	C21	1.408 (7)
N1	C1	1.348 (6)	C20	C27	1.419 (7)
N1	C5	1.352 (6)	C21	C22	1.435 (7)
N2	C6	1.482 (6)	C22	C23	1.400 (8)
N2	C7	1.494 (6)	C23	C24	1.410 (6)
N2	C8	1.482 (7)	C23	C28	1.421 (7)
N3	C9	1.476 (7)	C24	C25	1.371 (7)
N3	C10	1.485 (5)	C25	C26	1.397 (7)
N3	C11	1.494 (6)	C27	C28	1.388 (7)
N4	C12	1.362 (6)	C29	C30	1.447 (8)
N4	C16	1.347 (6)	C30	C31	1.401 (7)
N5	C17	1.341 (6)	C30	C35	1.413 (8)
N5	C21	1.386 (8)	C31	C32	1.368 (8)
N6	C22	1.375 (7)	C32	C33	1.396 (9)
N6	C26	1.340 (6)	C33	C34	1.387 (8)
N7	C27	1.372 (7)	C34	C35	1.376 (9)
N7	C29	1.366 (7)	P1	F1	1.584 (4)
N8	C28	1.371 (7)	P1	F2	1.598 (3)
N8	C29	1.328 (7)	P1	F3	1.603 (3)
C1	C2	1.387 (6)	P1	F4	1.608 (3)
C2	C3	1.371 (7)	P1	F5	1.596 (3)
C3	C4	1.396 (7)	P1	F6	1.608 (4)
C4	C5	1.377 (6)	P2	F7	1.609 (3)
C5	C6	1.520 (6)	P2	F8	1.593 (3)
C8	C9	1.495 (7)	P2	F9	1.583 (3)
C11	C12	1.503 (6)	P2	F10	1.582 (4)
C12	C13	1.378 (6)	P2	F11	1.614 (3)
C13	C14	1.387 (7)	P2	F12	1.585 (3)

Table S19. Bond Angles for Ru-5.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Ru1	N2	78.49 (15)	C19	C20	C21	119.0 (4)
N1	Ru1	N3	99.00 (13)	C19	C20	C27	125.3 (4)
N1	Ru1	N6	95.91 (15)	C21	C20	C27	115.7 (4)
N2	Ru1	N3	81.50 (18)	N5	C21	C20	122.6 (5)
N4	Ru1	N1	176.40 (16)	N5	C21	C22	115.8 (5)
N4	Ru1	N2	98.41 (15)	C20	C21	C22	121.7 (5)
N4	Ru1	N3	78.63 (14)	N6	C22	C21	116.6 (5)
N4	Ru1	N5	92.89 (16)	N6	C22	C23	122.4 (4)
N4	Ru1	N6	87.19 (15)	C23	C22	C21	121.0 (5)
N5	Ru1	N1	89.52 (15)	C22	C23	C24	118.8 (4)
N5	Ru1	N2	100.84 (17)	C22	C23	C28	117.5 (4)
N5	Ru1	N3	171.47 (15)	C24	C23	C28	123.7 (4)
N5	Ru1	N6	79.11 (17)	C25	C24	C23	118.5 (4)
N6	Ru1	N2	174.39 (18)	C24	C25	C26	119.6 (4)
N6	Ru1	N3	99.37 (17)	N6	C26	C25	123.6 (4)
C1	N1	Ru1	125.5 (3)	N7	C27	C20	130.8 (4)
C1	N1	C5	117.9 (4)	N7	C27	C28	105.8 (4)
C5	N1	Ru1	116.6 (3)	C28	C27	C20	123.4 (5)
C6	N2	Ru1	107.6 (3)	N8	C28	C23	129.4 (4)
C6	N2	C7	109.3 (3)	N8	C28	C27	109.9 (4)
C6	N2	C8	107.7 (4)	C27	C28	C23	120.7 (4)
C7	N2	Ru1	117.0 (3)	N7	C29	C30	122.8 (5)
C8	N2	Ru1	106.2 (3)	N8	C29	N7	111.7 (5)
C8	N2	C7	108.7 (4)	N8	C29	C30	125.6 (5)
C9	N3	Ru1	106.7 (3)	C31	C30	C29	122.0 (5)
C9	N3	C10	109.0 (4)	C31	C30	C35	118.3 (5)
C9	N3	C11	107.9 (3)	C35	C30	C29	119.7 (5)
C10	N3	Ru1	117.3 (3)	C32	C31	C30	122.1 (5)
C10	N3	C11	109.4 (4)	C31	C32	C33	119.0 (5)
C11	N3	Ru1	106.2 (3)	C34	C33	C32	119.9 (6)
C12	N4	Ru1	115.6 (3)	C35	C34	C33	121.5 (6)
C16	N4	Ru1	125.8 (3)	C34	C35	C30	119.2 (5)
C16	N4	C12	118.5 (4)	F1	P1	F2	91.0 (2)
C17	N5	Ru1	129.2 (4)	F1	P1	F3	90.69 (19)
C17	N5	C21	116.1 (5)	F1	P1	F4	90.7 (2)
C21	N5	Ru1	114.5 (4)	F1	P1	F5	89.8 (2)
C22	N6	Ru1	113.8 (3)	F1	P1	F6	179.9 (2)
C26	N6	Ru1	129.2 (3)	F2	P1	F3	90.07 (18)
C26	N6	C22	117.0 (4)	F2	P1	F4	90.39 (18)
C29	N7	C27	107.0 (4)	F2	P1	F6	89.1 (2)
C29	N8	C28	105.6 (4)	F3	P1	F4	178.5 (2)
N1	C1	C2	121.9 (5)	F3	P1	F6	89.39 (18)
C3	C2	C1	120.0 (5)	F5	P1	F2	179.1 (2)

C2	C3	C4	118.3 (4)	F5	P1	F3	89.46 (18)
C5	C4	C3	119.1 (5)	F5	P1	F4	90.06 (18)
N1	C5	C4	122.7 (4)	F5	P1	F6	90.1 (2)
N1	C5	C6	115.6 (4)	F6	P1	F4	89.2 (2)
C4	C5	C6	121.7 (4)	F7	P2	F11	179.3 (2)
N2	C6	C5	110.1 (4)	F8	P2	F7	89.51 (19)
N2	C8	C9	110.2 (4)	F8	P2	F11	90.83 (18)
N3	C9	C8	108.9 (4)	F9	P2	F7	89.9 (2)
N3	C11	C12	110.3 (4)	F9	P2	F8	89.11 (19)
N4	C12	C11	116.1 (4)	F9	P2	F11	89.4 (2)
N4	C12	C13	121.1 (4)	F9	P2	F12	91.3 (2)
C13	C12	C11	122.7 (4)	F10	P2	F7	91.0 (2)
C12	C13	C14	120.4 (4)	F10	P2	F8	89.4 (2)
C15	C14	C13	118.2 (4)	F10	P2	F9	178.3 (2)
C16	C15	C14	119.4 (5)	F10	P2	F11	89.7 (2)
N4	C16	C15	122.4 (4)	F10	P2	F12	90.1 (2)
N5	C17	C18	124.1 (4)	F12	P2	F7	90.54 (18)
C19	C18	C17	120.1 (4)	F12	P2	F8	179.6 (3)
C18	C19	C20	118.0 (4)	F12	P2	F11	89.12 (18)

Table S20. Hydrogen Atom Coordinates ($\text{\AA}\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2\times 10^3$) for Ru-5.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
H7	4517	6459	3336	28
H8	5986	5994	6628	32
H1	2488	4397	5563	33
H2	1972	3066	4824	37
H3	559	2887	3244	39
H4	-311	4084	2403	34
H6A	104	5911	2358	29
H6B	-508	5611	2652	29
H7A	218	7643	3869	43
H7B	-524	7189	2728	43
H7C	335	7384	2924	43
H8A	112	5606	4676	30
H8B	-449	6427	4189	30
H9A	702	7224	5669	32
H9B	507	6495	6216	32
H10A	1213	5098	6374	41
H10B	1612	5585	7543	41
H10C	2203	5228	7245	41
H11A	2737	6652	7782	33
H11B	1979	7116	7658	33
H13	2663	8531	7883	37
H14	2774	9632	6912	41
H15	2512	9347	5135	41
H16	2090	8014	4351	34
H17	1003	6659	2402	30
H18	1478	6921	1320	31
H19	2912	6760	2137	30
H24	5477	5718	7807	31
H25	4818	5506	8683	34
H26	3362	5660	7614	32
H31	5567	5983	3230	34
H32	6708	5934	3179	41
H33	8080	6145	4892	40
H34	8276	6398	6614	35
H35	7139	6422	6688	32

3. Cytotoxicity

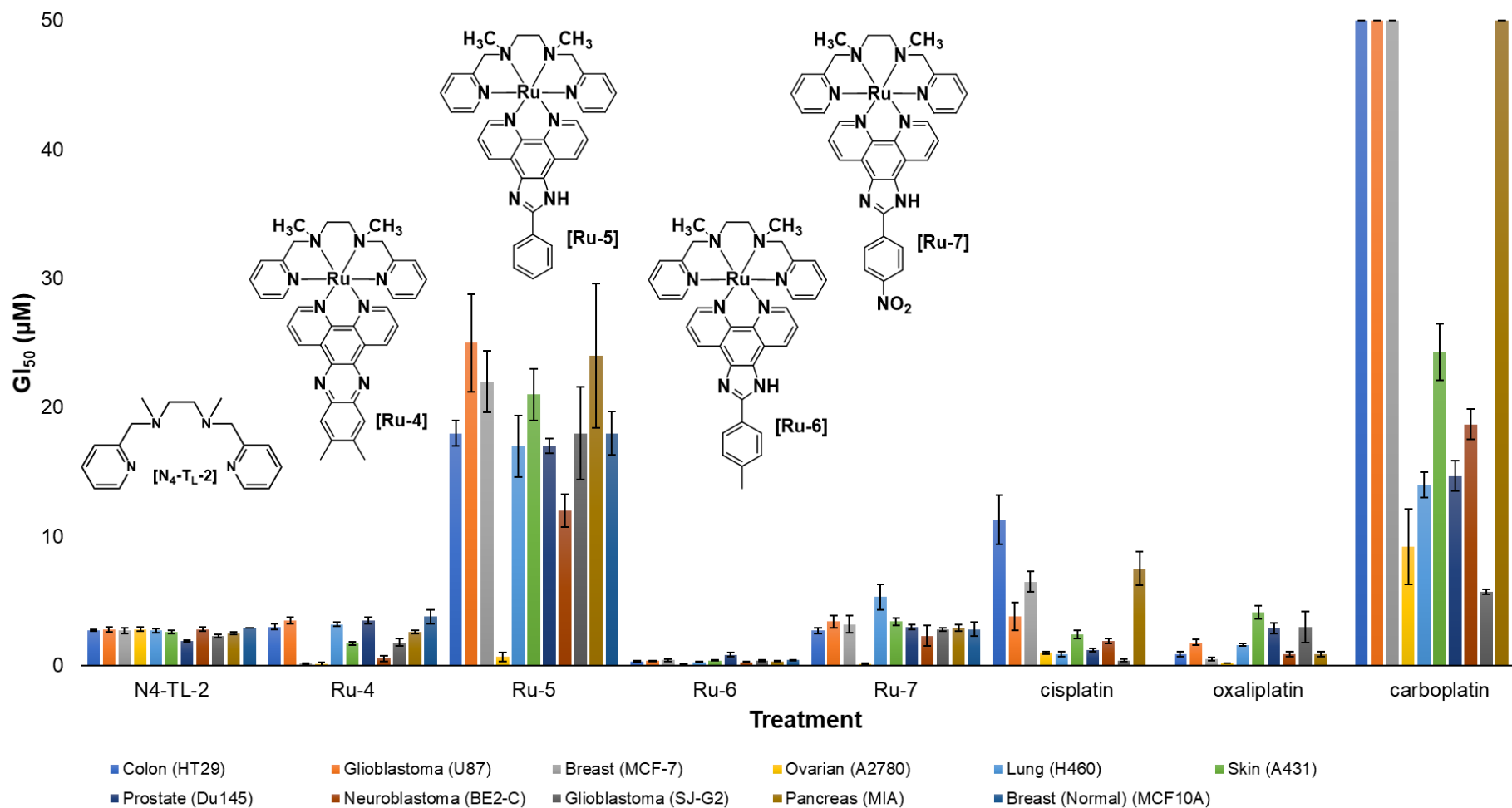


Figure S78: GI₅₀ values of N₄-TL-2, Ru-4, Ru-5, Ru-6 and Ru-7 in multiple cell lines: colon (HT29), glioblastoma (U87 and SJ-G2), ovarian (A2780), lung (H460), skin (A431), prostate (Du145), neuroblastoma (BE2-C), pancreas (MIA), breast (MCF-7), and breast normal (MCF10A).