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SUPPLEMENTARY MATERIAL TO

New ruthenium(II) bipyridyl complex: synthesis, crystal structure and cytotoxicity

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CHARACTERIZATION DATA FOR THE SYNTHESIZED COMPOUND

Yield: 110 mg, (74 %); m.p.: >300 °C; Anal. Calcd. for $C_{27}H_{20}F_6N_5O_4PRu \cdot 0.5H_2O$: C, 44.21; H, 2.89; N, 9.55 %. Found: C, 43.83; H, 2.87; N, 9.59 %; IR (ATR, cm^{-1}): 3089*w*, 1605*m*, 1469*m*, 1450*m*, 1315*w*, 1161*w*, 1030*w*, 840*s*, 767*s*, 727*w*, 556*m*; ^{1}H-NMR (500 MHz, DMSO-d_6, δ / ppm): 8.84–8.81 (2H, *m*, Ar-H), 8.76 (2H, *t*, J = 8.3 Hz, Ar-H), 8.69 (*d*, 1H, J = 5.5 Hz, Ar-H), 8.25 (1H, *bd*, J = 1.5 Hz, Ar-H), 8.19 (2H, *bt*, J = 7.8 Hz, Ar-H), 8.02 (2H, *p*, J = 7.9 Hz, Ar-H), 7.97 (1H, *d*, J = 5.5 Hz, Ar-H), 7.84–7.78 (3H, *m*, Ar-H), 7.72 (1H, *d*, J = 5.5 Hz, Ar-H), 7.62–7.60 (2H, *m*, Ar-H), 7.39 (2H, *p*, J = 6.3 Hz, Ar-H); ESI-MS (*m*/*z*): Calcd. for [M^+–PF_6^-, 100]: 580.06. Found: 580.05.

TABLE S-I. Crystal data and structure refinement for complex **1**

Identification code	Ru24K176
Empirical formula	$C_{27}H_{22}F_6N_5O_5PRu$
Formula weight	742.54
Temperature, K	100.0(1)
Crystal system	monoclinic
Space group	$P2_1/n$
a / Å	12.4042(3)

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TABLE S-I. Continued

b / Å	14.3080(5)
c / Å	15.9245(5)
α / °	90
β / °	98.475(3)
γ / °	90
Volume, Å^3	2795.41(15)
Z	4
ρ_{calc} / g cm^{-3}	1.764
μ / mm^{-1}	5.895
F(000)	1488.0
Crystal size, mm^3	0.24 × 0.124 × 0.075
Radiation	CuK_α (λ = 1.54184 nm)

TABLE S-II. Fractional atomic coordinates and equivalent isotropic displacements

Atom	*x*	*y*	*z*	*U*(eq)
Ru1	4002.2(2)	4572.2(2)	3119.9(2)	20.03(10)
O1	5550(2)	4998(2)	3690.0(16)	23.6(6)
O2	6866(2)	6034(2)	3566.2(17)	29.2(7)
O3	4372(3)	8500(2)	503.2(19)	36.0(8)
O4	5984(2)	8542(2)	1349.8(18)	29.1(7)
N1	3154(3)	5434(2)	3820(2)	21.8(7)
N2	2444(3)	4296(2)	2589.3(19)	19.9(7)
N3	4044(3)	3397(2)	3864(2)	22.1(7)
N4	4800(3)	3654(3)	2432(2)	26.0(7)
N5	4239(3)	5710(2)	2387(2)	21.0(7)
C1	3596(3)	5993(3)	4457(3)	27.6(9)
C2	2999(4)	6647(3)	4815(3)	30.0(1)
C3	1889(4)	6737(3)	4523(3)	29.8(10)
C4	1416(3)	6134(3)	3893(2)	28.3(9)
C5	2059(3)	5496(3)	3550(2)	22.9(8)
C6	1660(3)	4829(3)	2873(2)	24.7(9)
C7	564(3)	4715(3)	2543(3)	27.4(9)
C8	257(4)	4052(3)	1922(3)	30.3(10)
C9	1055(4)	3508(3)	1637(3)	29.1(10)
C10	2134(3)	3643(3)	1986(2)	25.4(9)
C11	3584(3)	3307(3)	4578(2)	26.6(9)
C12	3657(4)	2473(3)	5033(3)	32.4(10)
C13	4178(4)	1714(3)	4744(3)	36.1(11)
C14	4659(4)	1815(3)	4022(3)	33.3(10)
C15	4595(3)	2653(3)	3594(3)	26.5(9)
C16	5087(3)	2821(3)	2822(3)	27.7(9)
C17	5785(4)	2212(4)	2506(3)	37.2(11)
C18	6164(4)	2419(4)	1745(3)	42.5(13)
C19	5817(4)	3225(4)	1332(3)	41.4(12)
C20	5157(4)	3834(3)	1690(3)	31.1(10)
C21	5953(3)	5696(3)	3341(2)	22.8(8)

TABLE S-II. Continued

Atom	x	y	z	U(eq)
C22	5221(3)	6147(3)	2607(2)	22.1(8)
C23	5525(3)	6920(3)	2195(2)	23.7(9)
C24	4798(3)	7301(3)	1527(2)	23.2(8)
C25	3806(3)	6847(3)	1293(3)	26.9(9)
C26	3553(3)	6068(3)	1732(2)	25.9(9)
C27	5026(3)	8171(3)	1068(3)	26.7(9)
P1	7650.8(10)	497.8(9)	4461.6(7)	33.2(3)
F1	8807(3)	480(2)	4202(3)	87.5(14)
F2	8120(4)	844(3)	5379.3(19)	78.7(12)
F3	6465(3)	506(3)	4750(3)	83.7(13)
F4	7111(5)	158(3)	3565(2)	111(2)
F5	7781(3)	–558(2)	4774(2)	57.5(9)
F6	7496(3)	1556(2)	4148.8(19)	49.9(8)

TABLE S-III. Bond lengths for complex **1**

Atom	Atom	Length, Å	Atom	Atom	Length, Å
Ru1	O1	2.090(3)	C6	C7	1.393(5)
Ru1	N1	2.053(3)	C7	C8	1.382(6)
Ru1	N2	2.031(3)	C8	C9	1.387(6)
Ru1	N3	2.054(3)	C9	C10	1.384(6)
Ru1	N4	2.056(4)	C11	C12	1.393(6)
Ru1	N5	2.049(3)	C12	C13	1.377(7)
O1	C21	1.279(5)	C13	C14	1.379(7)
O2	C21	1.235(5)	C14	C15	1.375(6)
O3	C27	1.213(5)	C15	C16	1.470(6)
O4	C27	1.319(5)	C16	C17	1.376(6)
N1	C1	1.344(5)	C17	C18	1.393(7)
N1	C5	1.366(5)	C18	C19	1.365(7)
N2	C6	1.365(5)	C19	C20	1.375(6)
N2	C10	1.354(5)	C21	C22	1.515(5)
N3	C11	1.351(5)	C22	C23	1.366(6)
N3	C15	1.368(5)	C23	C24	1.399(5)
N4	C16	1.366(5)	C24	C25	1.393(6)
N4	C20	1.346(5)	C24	C27	1.492(6)
N5	C22	1.368(5)	C25	C26	1.378(6)
N5	C26	1.346(5)	P1	F1	1.551(4)
C1	C2	1.369(6)	P1	F2	1.571(3)
C2	C3	1.392(6)	P1	F3	1.605(4)
C3	C4	1.386(6)	P1	F4	1.562(4)
C4	C5	1.377(6)	P1	F5	1.592(3)
C5	C6	1.470(5)	P1	F6	1.596(3)

TABLE S-IV. Bond angles for complex **1**

Atom	Atom	Atom	Angle, °	Atom	Atom	Atom	Angle, °
N1	Ru1	O1	95.76(12)	N3	C11	C12	121.1(4)
N1	Ru1	N3	98.62(13)	C13	C12	C11	119.9(4)
N1	Ru1	N4	177.05(13)	C12	C13	C14	118.6(4)
N2	Ru1	O1	173.99(12)	C15	C14	C13	120.2(5)
N2	Ru1	N1	79.07(13)	N3	C15	C14	121.2(4)
N2	Ru1	N3	91.27(13)	N3	C15	C16	115.0(4)
N2	Ru1	N4	99.03(13)	C14	C15	C16	123.8(4)
N2	Ru1	N5	97.22(13)	N4	C16	C15	114.3(4)
N3	Ru1	O1	92.55(11)	N4	C16	C17	121.4(4)
N3	Ru1	N4	79.10(14)	C17	C16	C15	124.3(4)
N4	Ru1	O1	86.25(12)	C16	C17	C18	119.7(5)
N5	Ru1	O1	79.38(12)	C19	C18	C17	118.4(5)
N5	Ru1	N1	87.69(13)	C18	C19	C20	120.0(5)
N5	Ru1	N3	170.27(13)	N4	C20	C19	122.4(5)
N5	Ru1	N4	94.81(14)	O1	C21	C22	116.1(3)
C21	O1	Ru1	115.6(2)	O2	C21	O1	125.4(4)
C1	N1	Ru1	125.7(3)	O2	C21	C22	118.5(4)
C1	N1	C5	118.3(4)	N5	C22	C21	114.3(3)
C5	N1	Ru1	115.7(3)	C23	C22	N5	123.1(4)
C6	N2	Ru1	115.7(3)	C23	C22	C21	122.6(4)
C10	N2	Ru1	125.7(3)	C22	C23	C24	119.2(4)
C10	N2	C6	118.6(3)	C23	C24	C27	123.4(4)
C11	N3	Ru1	125.8(3)	C25	C24	C23	117.8(4)
C11	N3	C15	118.9(4)	C25	C24	C27	118.7(4)
C15	N3	Ru1	115.3(3)	C26	C25	C24	120.0(4)
C16	N4	Ru1	115.4(3)	N5	C26	C25	122.4(4)
C20	N4	Ru1	126.3(3)	O3	C27	O4	124.5(4)
C20	N4	C16	118.0(4)	O3	C27	C24	122.2(4)
C22	N5	Ru1	114.5(3)	O4	C27	C24	113.3(3)
C26	N5	Ru1	128.0(3)	F1	P1	F2	91.3(3)
C26	N5	C22	117.5(3)	F1	P1	F3	178.8(2)
N1	C1	C2	122.4(4)	F1	P1	F4	92.3(3)
C1	C2	C3	119.5(4)	F1	P1	F5	90.72(18)
C4	C3	C2	118.5(4)	F1	P1	F6	90.30(19)
C5	C4	C3	119.4(4)	F2	P1	F3	87.7(2)
N1	C5	C4	121.7(4)	F2	P1	F5	90.1(2)
N1	C5	C6	113.6(4)	F2	P1	F6	90.1(2)
C4	C5	C6	124.7(4)	F4	P1	F2	176.4(3)
N2	C6	C5	115.2(4)	F4	P1	F3	88.7(3)
N2	C6	C7	120.9(4)	F4	P1	F5	90.0(2)
C7	C6	C5	123.9(4)	F4	P1	F6	89.68(19)
C8	C7	C6	120.0(4)	F5	P1	F3	88.45(18)
C7	C8	C9	119.0(4)	F5	P1	F6	178.94(19)
C10	C9	C8	118.9(4)	F6	P1	F3	90.53(18)
N2	C10	C9	122.5(4)				