

Supporting information

Organoruthenated nitroxoline derivatives impair tumor cell invasion through inhibition of cathepsin B activity

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Table S1: Crystallographic data

Compound	1a	1c	2a·H₂O
Empirical formula	C ₁₉ H ₁₉ N ₂ O ₃ ClRu	C ₁₉ H ₁₉ IN ₂ O ₃ Ru	C ₅₂ H ₆₂ N ₆ O ₁₂ Ru ₂
Formula weight	459.88	551.34	1165.21
Temperature/K	150	150	150
Crystal system	triclinic	triclinic	orthorhombic
Space group	P-1	P-1	Pccn
a/Å	6.0643(4)	7.7724(3)	12.2106(5)
b/Å	11.6144(11)	11.7903(4)	20.2814(11)
c/Å	12.8288(11)	11.9839(5)	20.1035(11)
α/°	98.568(8)	70.324(4)	90
β/°	95.292(6)	85.214(3)	90
γ/°	90.353(7)	88.449(3)	90
Volume/Å ³	889.50(13)	1030.46(7)	4978.6(4)
Z	2	2	4
ρ _{calc} g/cm ³	1.717	1.7768	1.555
μ/mm ⁻¹	1.053	2.278	0.677
F(000)	464.0	532.9	2400.0
Crystal size/mm ³	0.1 × 0.1 × 0.05	0.2 × 0.1 × 0.05	0.3 × 0.2 × 0.1
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.452 to 54.962	5.96 to 54.96	5.602 to 54.956
Index ranges	-7 ≤ h ≤ 7, -15 ≤ k ≤ 15, -16 ≤ l ≤ 16	-10 ≤ h ≤ 10, -15 ≤ k ≤ 16, -16 ≤ l ≤ 16	-15 ≤ h ≤ 14, -24 ≤ k ≤ 26, -26 ≤ l ≤ 21
Reflections collected	8002	18206	25577
Independent reflections	4037 [R _{int} = 0.0786, R _{sigma} = 0.0945]	4721 [R _{int} = 0.0316, R _{sigma} = 0.0375]	5660 [R _{int} = 0.0744, R _{sigma} = 0.0677]
Data/restraints/parameters	4037/0/238	4721/0/238	5660/0/331
Goodness-of-fit on F ²	0.978	1.055	1.010
Final R indexes [I>=2σ (I)]	R ₁ = 0.0457, wR ₂ = 0.0930	R ₁ = 0.0226, wR ₂ = 0.0462	R ₁ = 0.0441, wR ₂ = 0.0943
Final R indexes [all data]	R ₁ = 0.0672, wR ₂ = 0.1003	R ₁ = 0.0296, wR ₂ = 0.0502	R ₁ = 0.0867, wR ₂ = 0.1091
Largest diff. peak/hole / e Å ⁻³	1.32/-1.35	0.84/-0.62	0.56/-0.61

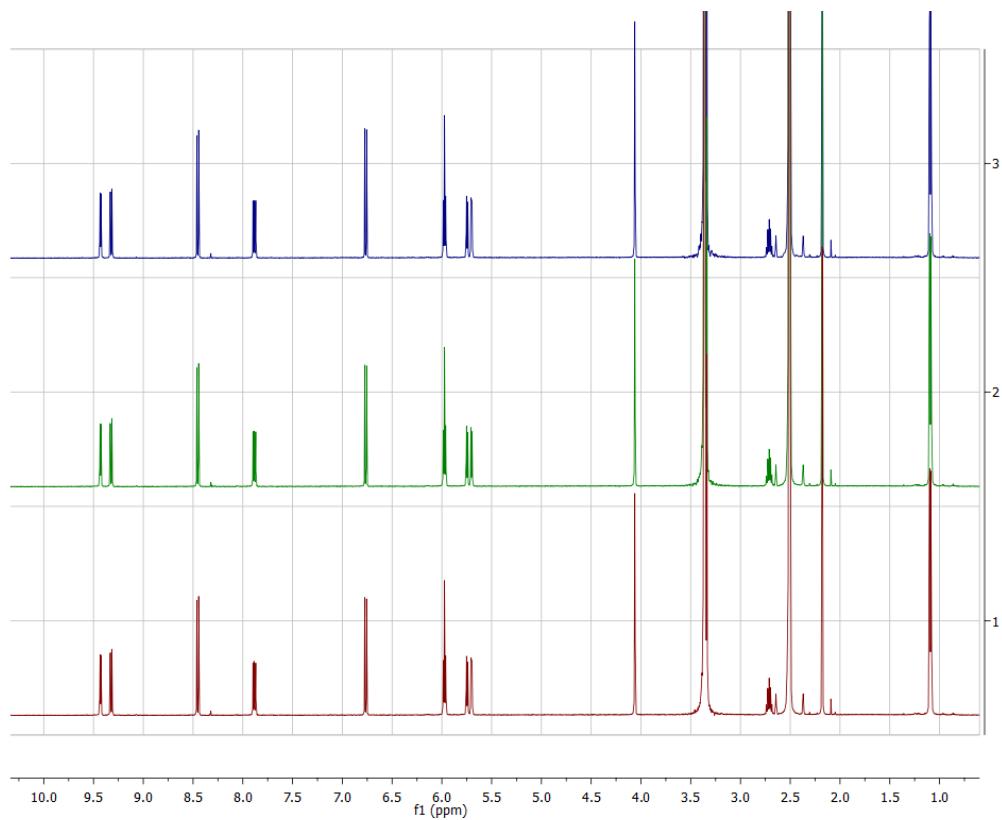


Figure S1: Stability of **1a** in DMSO-d₆ (bottom to top; *t* = 10 min; *t* = 3h; *t* = 72h).

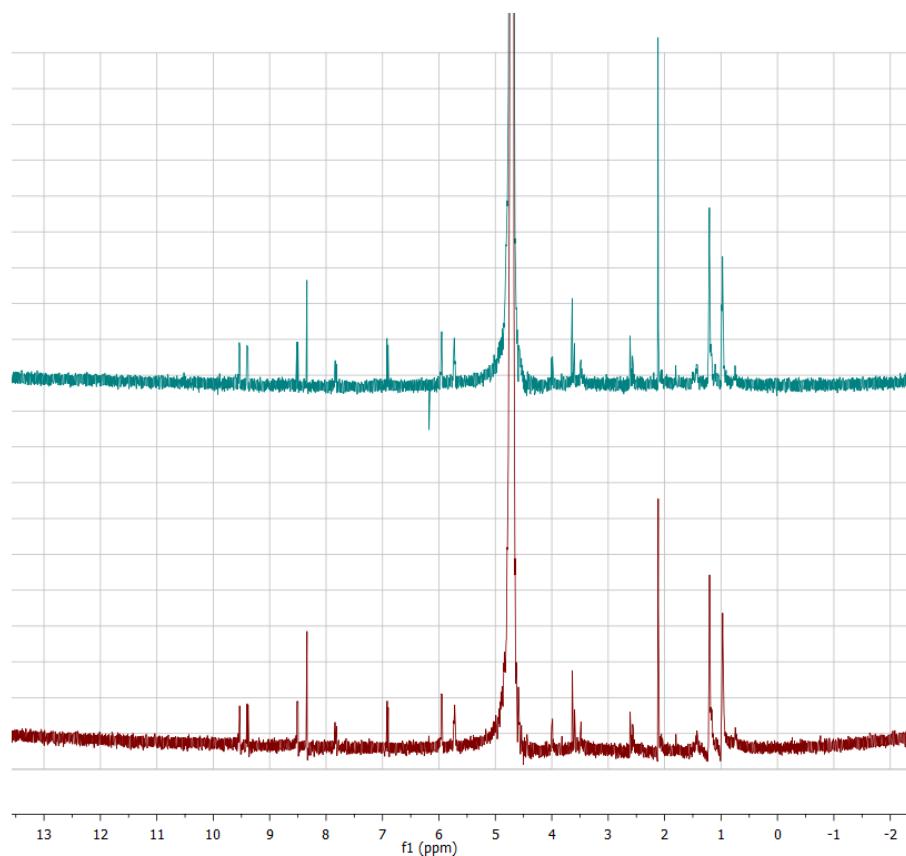


Figure S2: Stability of **1a** in D₂O (bottom to top; *t* = 2h; *t* = 5d).