Electronic Supplementary Information

of

Promising Anticancer Mono- and Dinuclear Ruthenium(III) Dithiocarbamato Complexes: Systematic Solution Studies

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Table S1. Selected bond lengths (Å) and angles (°) for $[Ru(DMDT)_3]$.

Ru-S(23)	2.3789(7)	S(23)-Ru-S(13)	73.16(2)
Ru-S(13)	2.3852(7)	S(23)-Ru-S(21)	98.64(3)
Ru-S(21)	2.3852(7)	S(13)-Ru-S(21)	95.30(3)
Ru-S(22)	2.3876(7)	S(23)-Ru-S(22)	166.06(3)
Ru-S(12)	2.3888(8)	S(13)-Ru-S(22)	98.72(3)
Ru-S(11)	2.3976(7)	S(21)-Ru-S(22)	93.31(3)
S(11)-C(11)	1.720(2)	S(23)-Ru-S(12)	96.87(3)
S(21)-C(11)	1.714(2)	S(13)-Ru-S(12)	99.14(3)
S(23)-C(13)	1.714(2)	S(21)-Ru-S(12)	161.31(3)
S(22)-C(12)	1.702(3)	S(22)-Ru-S(12)	72.86(3)
S(13)-C(13)	1.719(2)	S(23)-Ru-S(11)	93.30(3)
S(12)-C(12)	1.711(3)	S(13)-Ru-S(11)	160.80(2)
N(11)-C(11)	1.324(3)	S(21)-Ru-S(11)	72.89(2)
N(11)-C(21)	1.457(3)	S(22)-Ru-S(11)	97.07(3)
N(11)-C(31)	1.462(3)	S(12)-Ru-S(11)	95.91(3)
C(13)-N(13)	1.318(3)	C(11)-S(11)-Ru	87.41(8)
C(23)-N(13)	1.457(3)	C(11)-S(21)-Ru	87.95(8)
N(12)-C(12)	1.346(3)	C(13)-S(23)-Ru	87.79(8)
N(12)-C(22)	1.453(4)	C(12)-S(22)-Ru	87.5(1)
N(12)-C(32)	1.465(4)	C(13)-S(13)-Ru	87.48(8)
N(13)-C(33)	1.460(3)	C(12)-S(12)-Ru	87.2(1)

Table S2. Selected bond lengths (Å) and angles (°) for $[Ru(PDT)_3]\cdot CHCl_3$.

Ru-S(22)	2.373(1)	S(22)-Ru-S(23)	92.98(4)
Ru-S(23)	2.375(1)	S(22)-Ru-S(21)	91.78(4)
Ru-S(21)	2.390(1)	S(23)-Ru-S(21)	94.44(4)
Ru-S(11)	2.392(1)	S(22)-Ru-S(11)	100.68(4)
Ru-S(12)	2.396(1)	S(23)-Ru-S(11)	161.66(4)
Ru-S(13)	2.410(1)	S(21)-Ru-S(11)	73.13(4)
S(21)-C(11)	1.711(4)	S(22)-Ru-S(12)	73.29(4)
S(13)-C(13)	1.722(4)	S(23)-Ru-S(12)	100.14(4)
S(11)-C(11)	1.717(4)	S(21)-Ru-S(12)	159.54(4)
S(12)-C(12)	1.724(4)	S(11)-Ru-S(12)	95.51(4)
S(22)-C(12)	1.708(4)	S(22)-Ru-S(13)	163.18(4)
S(23)-C(13)	1.705(4)	S(23)-Ru-S(13)	73.00(4)
N(12)-C(12)	1.318(5)	S(21)-Ru-S(13)	98.40(4)
N(12)-C(22)	1.453(5)	S(11)-Ru-S(13)	95.09(4)
N(12)-C(52)	1.471(5)	S(12)-Ru-S(13)	99.55(4)
N(11)-C(11)	1.321(5)	C(11)-S(21)-Ru	87.3(1)
N(11)-C(21)	1.471(5)	C(13)-S(13)-Ru	86.4(1)
N(11)-C(51)	1.473(5)	C(11)-S(11)-Ru	87.1(1)
N(13)-C(13)	1.316(5)	C(12)-S(12)-Ru	86.5(1)
N(13)-C(23)	1.457(5)	C(12)-S(22)-Ru	87.6(1)
N(13)-C(53)	1.481(5)	C(13)-S(23)-Ru	87.9(1)
C(23)-C(33)	1.506(6)		
C(52)-C(42)	1.506(6)		
C(32)-C(22)	1.518(6)		
C(32)-C(42)	1.523(6)		
C(53)-C(43)	1.498(7)		
C(51)-C(41)	1.502(6)		
C(41)-C(31)	1.462(7)		
C(21)-C(31)	1.536(6)		
C(33)-C(43)	1.470(7)		

Table S3. Selected bond lengths (Å) and angles (°) for $[Ru(ESDT)_3]$.

Ru-S(1)	2.365(2)	S(1)-Ru-S(1)#1	100.5(1)
Ru-S(2)	2.369(2)	S(1)-Ru-S(2)	72.78(9)
Ru-S(3)	2.371(3)	S(1)-Ru-S(2)#1	95.16(9)
S(1)-C(11)	1.677(9)	S(2)-Ru-S(2)#1	161.4(1)
S(2)-C(11)	1.726(8)	S(1)-Ru-S(3)	95.2(1)
N(11)-C(11)	1.33(1)	S(1)#1-Ru-S(3)	160.15(9)
N(11)-C(31)	1.39(1)	S(2)-Ru-S(3)	101.11(9)
N(11)-C(21)	1.41(2)	S(1)-Ru-S(3)#1	160.15(9)
C(31)-C(41)	1.54(2)	S(2)-Ru-S(3)#1	93.85(9)
O(11)-C(41)	1.20(2)	S(3)-Ru-S(3)#1	72.6(2)
C(41)-O(21)	1.31(2)	C(11)-S(1)-Ru	88.6(3)
O(21)-C(61)	1.49(2)		
O(21)-C(51)	1.54(2)		
C(51)-C(71)	1.53(2)		
C(61)-C(81)	1.51(2)		
S(3)-C(12)	1.685(6)		
C(12)-N(12)	1.38(2)		
N(12)-C(22)	1.49(2)		
N(12)-C(32)	1.56(3)		
C(32)-C(42)	1.60(2)		
O(12)-C(42)	1.26(2)		
O(22)-C(42)	1.36(3)		
O(22)-C(52)	1.48(2)		
C(52)-C(62)	1.50(2)		

Symmetry code #1 = x,-y,-z+1/2.

Table S4. UV-visible spectral data for BSA in the presence of dimethyl sulfoxide (dmso), $[Ru(ESDT)_3]$ and α-$[Ru_2(ESDT)_5]Cl$ complexes in phosphate buffered saline solution.

	λ_{max} in nm				
BSA : complex (% v/v of dmso)	without dmso	5:1 0.02 %	1:1 0.10 %	1:2 0.19 %	1:5 0.48 %
BSA + dmso	208	219	224.4	227.2	230
BSA + $[Ru(ESDT)_3]$	–	220	227.2	227.6	230
BSA + α-$[Ru_2(ESDT)_5]Cl$	–	219.2	225.2	227.6	230

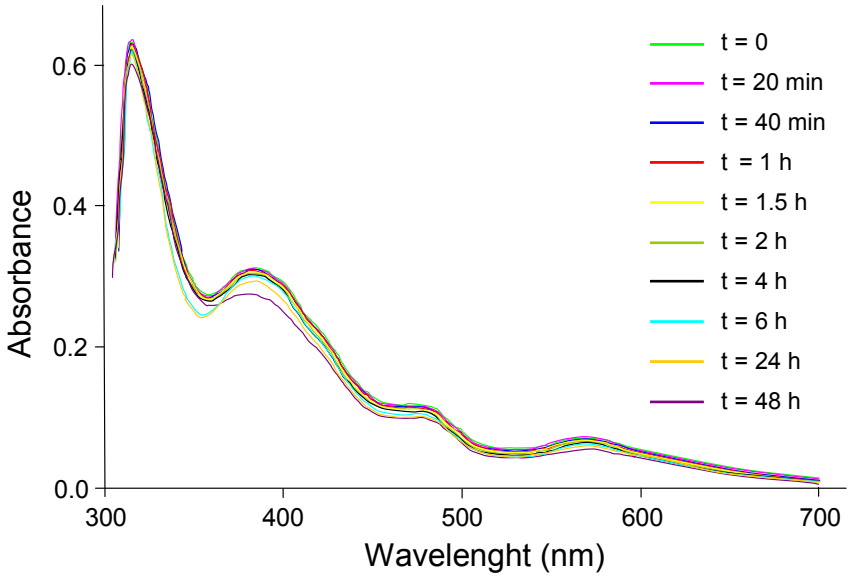

Figure S1. UV-visible spectra of $[Ru(ESDT)_3]$ in DMEM growth medium / 0.5 % (v/v) dimethyl sulfoxide at room temperature followed for 48 h, $c_{complex} = 2.3 \cdot 10^{-5}$ mol·dm^{-3}.

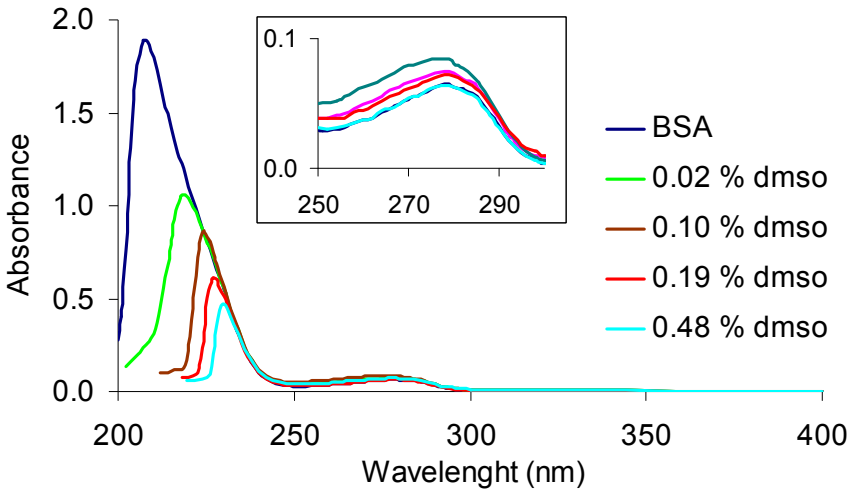

Figure S2. UV-visible spectra of BSA in phosphate buffered saline with dimethyl sulfoxide (dmso) at room temperature, $c_{BSA} = 1.4 \cdot 10^{-6}$ mol·dm^{-3}.

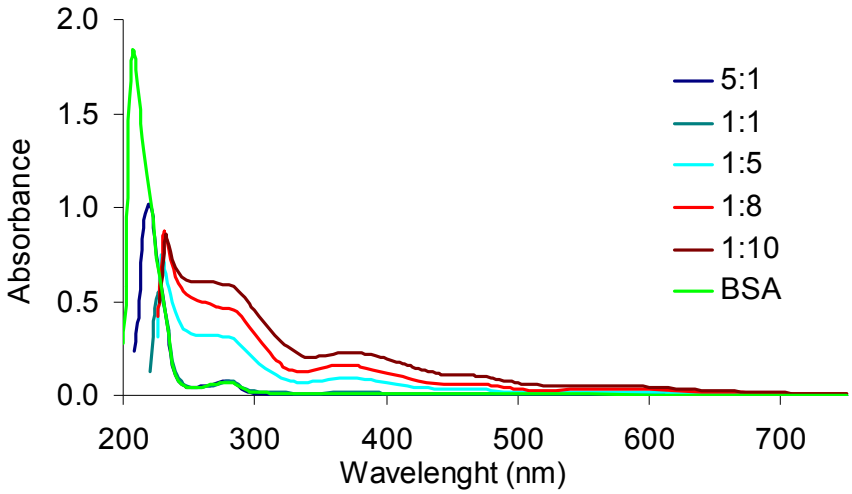

Figure S3. UV-visible spectra of $[Ru(ESDT)_3]$ in phosphate buffered saline with BSA / 0.5 % (v/v) dimethyl sulfoxide at room temperature, $c_{BSA} = 1.4 \cdot 10^{-6}$ mol·dm^{-3}, with different BSA:complex ratios.

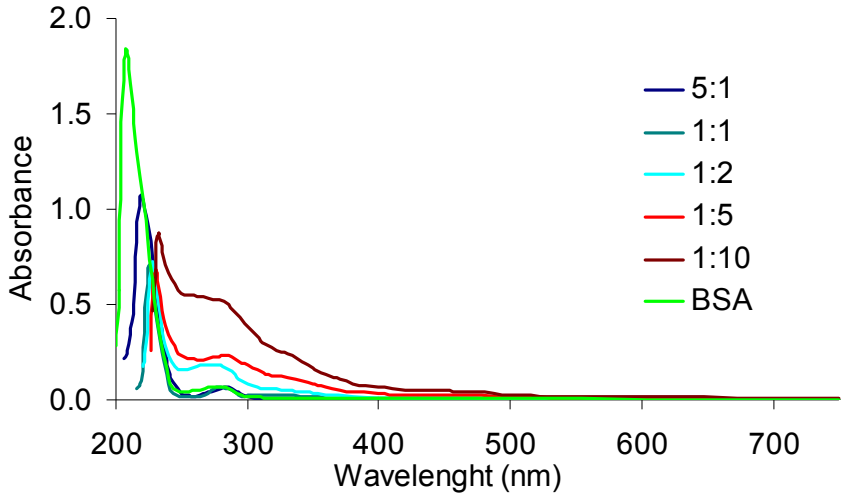

Figure S4. UV-visible spectra of α-$[Ru_2(ESDT)_5]Cl$ in phosphate buffered saline with BSA / 0.5 % (v/v) dimethyl sulfoxide at room temperature, $c_{BSA} = 1.4 \cdot 10^{-6}$ mol·dm^{-3}, with different BSA:complex ratios.

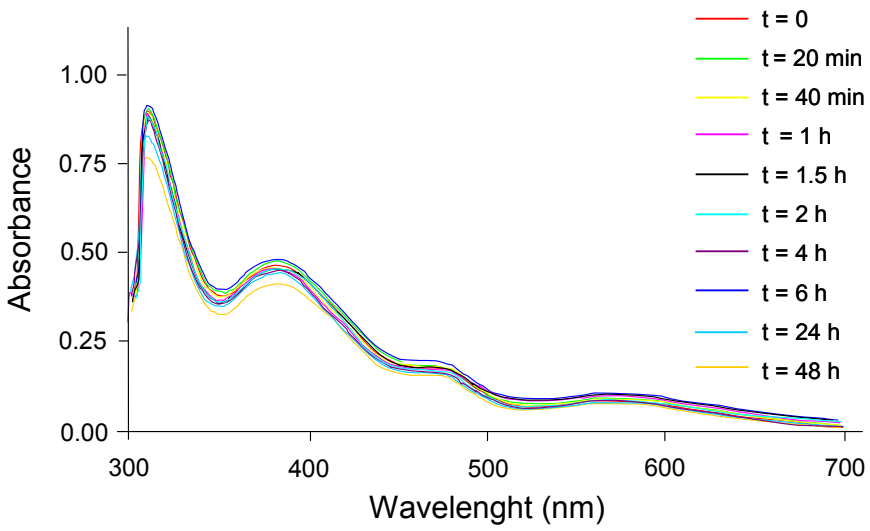

Figure S5. UV-visible spectra of $[Ru(ESDT)_3]$ in phosphate buffered saline with BSA at room temperature, $c_{BSA} = 1.4 \cdot 10^{-4}$ mol·dm^{-3}, BSA:complex 5:1, followed for 48 h.

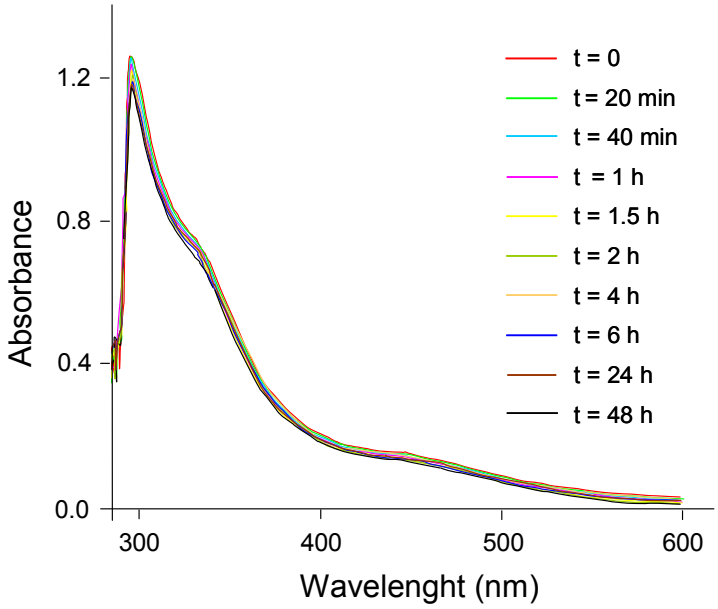

Figure S6. UV-visible spectra of α-$[Ru_2(ESDT)_5]Cl$ in phosphate buffered saline with BSA at room temperature, $c_{BSA} = 1.4 \cdot 10^{-4}$ mol·dm^{-3}, BSA:complex 5:1, followed for 48 h.

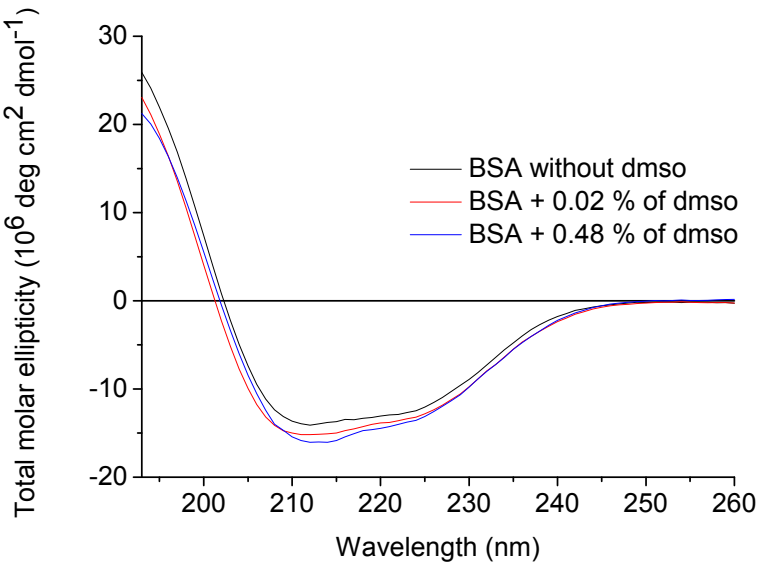

Figure S7. CD spectra of BSA in phosphate buffered saline with dimethyl sulfoxide (dmso) at room temperature, $c_{BSA} = 1.4 \cdot 10^{-6}$ mol·dm^{-3}.

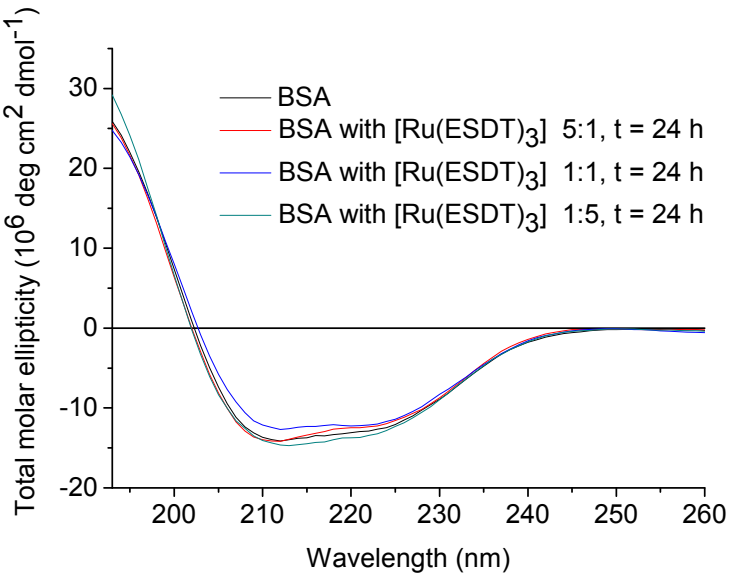

Figure S8. CD spectra of BSA in phosphate buffered saline with [Ru(ESDT)$_3$] at room temperature, 24 h after the admixture, $c_{BSA} = 1.4 \cdot 10^{-6}$ mol·dm^{-3}.

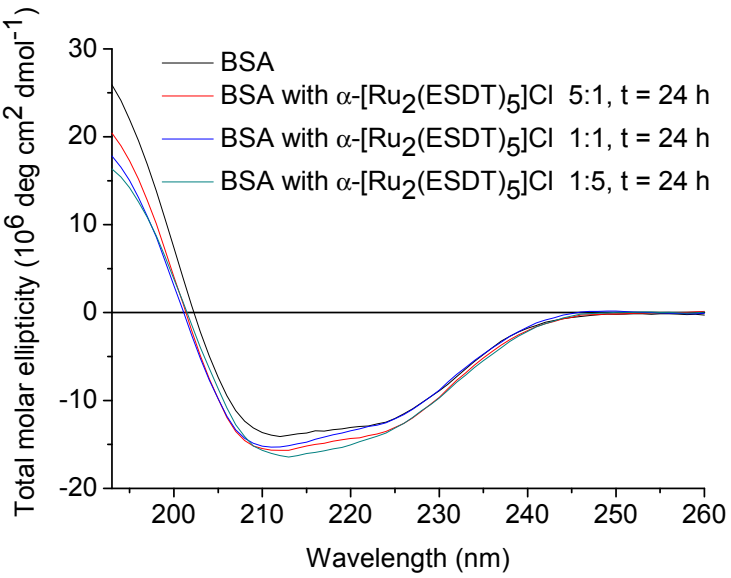

Figure S9. CD spectra of BSA in phosphate buffered saline with α-$[Ru_2(ESDT)_5]Cl$ at room temperature, 24 h after the admixture, $c_{BSA} = 1.4 \cdot 10^{-6}$ mol·dm^{-3}.