SUPPORTING INFORMATION

Metal-Coumarin Derivatives as Promising Photosensitizers: Unlocking Their Cancer Phototherapy Potential

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Table S1. Absorption maxima (λ_{abs}), molar extinction coefficients (ε), singlet oxygen quantum yields (Φ_{Δ}), light conditions used for photocytotoxicity studies, and biological activity under normoxic and hypoxic conditions of metal-coumarin complexes.

Complex	$\lambda_{abs\ max}$/nm (solvent/ ε, $M^{-1}cm^{-1}$)	Light	Φ_{Δ} (solvent)	TOF, h^{-1} [NADH]	Cell line	Condition	IC_{50} Light, μM	IC_{50} Dark, μM	PI	ref
Ir1	305 (PBS/40000)	520 nm (5.4 J/cm²)	-	-	HeLa	Normoxia	32.7± 4.9	95.2± 6.4	2.9	34, 38
						Hypoxia	31.5± 3.3	101± 10	3.2	
					A2780cisR	Normoxia	1.5 ± 0.4	>250	>167	
						Hypoxia	11 ± 2	>250	>23	
Ir2	308 (PBS/43000)	520 nm (5.4 J/cm²)	<0.01 (PBS)	-	A2780cisR	Normoxia	3.5 ± 0.4	>250	>71	38
		620 nm (6.7 J/cm²)	-		A2780cisR	Normoxia	9 ± 2	>250	>28	
Ir-COUPY-1	550 (PBS/17000)	520 nm (5.4 J/cm²)	<0.01 (PBS)	-	HeLa	Normoxia	2.51 ± 0.32	213 ± 14	85	34, 38
						Hypoxia	219 ± 6	2.77± 0.20	79	
					A2780cisR	Normoxia	0.70 ± 0.06	>250	>357	
						Hypoxia	3.8 ± 0.3	>250	>66	
		620 nm (6.7 J/cm²)	-	179	A2780cisR	Normoxia	0.71 ± 0.02	>250	>352	
						Hypoxia	1.6 ± 0.2	>250	>156	
Ir-COUPY-2	436 (PBS/17000)	520 nm (5.4 J/cm²)	<0.01 (PBS)	-	HeLa	Normoxia	18 ± 2	>100	>6	37
						Hypoxia	-	-	-	
					A2780cisR	Normoxia	61 ± 8	>250	>4.1	
						Hypoxia	31 ± 7	>250	>8.1	
Ir-COUPY-3	575 (PBS/13000)	520 nm (5.4 J/cm²)	<0.01 (PBS)	-	HeLa	Normoxia	45 ± 4	>100	>2.2	37, 38
						Hypoxia	-	-	-	
					A2780cisR	Normoxia	1.04 ± 0.02	>250	>240	
						Hypoxia	8 ± 1	>250	>31	
		620 nm (6.7 J/cm²)	-	164	A2780cisR	Normoxia	1.2 ± 0.1	>250	>208	
						Hypoxia	5 ± 1	>250	>50	
Ir-COUPY-4	550	520 nm (5.4 J/cm²)	<0.01 (PBS)	-	HeLa	Normoxia	2.0 ± 0.4	>100	>50	37
						Hypoxia	-	-	-	
					A2780cisR	Normoxia	1.1 ± 0.2	>250	>227	
						Hypoxia	1.9 ± 0.2	>250	>131	
Ir-COUPY-5	541 (PBS/20000)	520 nm (5.4 J/cm²)	<0.01 (PBS)	-	HeLa	Normoxia	9.3 ± 0.8	>100	>11	37
						Hypoxia	-	-	-	
					A2780cisR	Normoxia	0.93 ± 0.04	>250	>268	

						Hypoxia	1.7 ± 0.3	>250	>147	
Ir-COUPY-6	544 (PBS/22000)	520 nm (5.4 J/cm^2)	-	-	A2780cisR	Normoxia	1.9 ± 0.3	>250	>134	38
		620 nm (6.7 J/cm^2)	<0.01 (PBS)	152	A2780cisR	Normoxia	1.2 ± 0.2	>250	>208	
						Hypoxia	1.4 ± 0.5	>250	>179	
Ru1	561 (ACN/17000)	620 nm (6.7 J/cm^2)	-	-	HeLa	Normoxia	0.11 ± 0.03	7 ± 1	63	36
					HT-29	Normoxia	0.18 ± 0.08	2.4 ± 0.4	39	
		740 nm (12.6 J/cm^2)	-	-	HT-29	Normoxia	0.5± 0.03	2.4 ± 0.4	5	
						Hypoxia	1.5± 0.4	11 ± 3	7	
Ru-COUPY	623 (ACN/36000)	620 nm (6.7 J/cm^2)	-	-	HeLa	Normoxia	2.9 ± 0.3	>300	>103	36
					HT-29	Normoxia	3.1 ± 0.1	>300	>97	
		740 nm (12.6 J/cm^2)	-		HT-29	Normoxia	7.1 ± 0.3	>300	>42	
						Hypoxia	7.1 ± 0.3	>300	>23	
Pt1	480 (PBS/-)	880 nm (0.4 W/cm^2; 80 min)	-	-	LCSCs	Normoxia	3.5 ± 0.3	> 50	>14	69
						Hypoxia	3.7 ± 0.4	> 50	>13	
					A549	Normoxia	4.2 ± 0.3	> 50	>12	
						Hypoxia	4.0 ± 0.5	> 50	>12	
					A549R	Normoxia	3.8 ± 0.5	> 50	>13	
						Hypoxia	4.1 ± 0.4	> 50	>12	
					A2780cisR	Normoxia	2.7 ± 0.3	> 50	>19	
						Hypoxia	2.8 ± 0.4	> 50	>18	
Pt2	480 (PBS/-)	880 nm (0.4 W/cm^2; 80 min)	-	-	LCSCs	Normoxia	5.1 ± 0.4	> 50	>10	
						Hypoxia	5.2 ± 0.5	> 50	>10	
					A549	Normoxia	6.7 ± 0.8	> 50	>7	
						Hypoxia	7.2 ± 0.7	> 50	>7	
					A549R	Normoxia	6.9 ± 0.7	> 50	>7	
						Hypoxia	7.3 ± 1.0	> 50	>7	
					A2780cisR	Normoxia	4.0 ± 0.5	> 50	>13	
						Hypoxia	4.3 ± 0.6	> 50	>12	
Pt3	298 (RPMI/ 31660)	465 nm (4.8 mW/cm^2 ; 60 min)	-	-	A2780	Normoxia	2.9 ± 0.2	>100	>34	72
					A549		7.8 ± 0.1	>100	>13	
					MRC5		-	>100	-	

Pt4	306 (RPMI/ 30650)	465 nm (4.8 mW/cm^2; 60 min)	-	-	A2780	Normoxia	0.11 ± 0.02	1.9 ± 0.1	>17	
					A549		2.6 ± 0.3	>50	>19	
					MRC5		-	>50	-	
Pt5	-	450 nm (8 mW cm^2; 60 min)	-	-	HCT116 p53$^{+/+}$	Normoxia	0.9 ± 0.2	47.1 ± 5.9	52	74
					HCT116 p53$^{-/-}$		1.3 ± 0.3	80.6 ± 7.1	62	
					A549R		4.0 ± 0.5	114.6 ± 7.7	29	
Ir3	480 (H_2O/48000)	465 nm (11.7 J/cm^2)	-	1097.8	HeLa	Normoxia	0.3	12.8	43	76
					B16		1.3	>100	77	
					A431		0.02	1.8	90	
					NP69		1.0	14.3	14	
		525 nm (29.56 J/cm^2)		1014.6	HeLa	Normoxia	0.4	12.4	32	
					A431		0.1	1.8	18	
Ir4	480 (H_2O /34000)	465 nm (11.7 J/cm^2)	-	1060.4	HeLa	Normoxia	0.03	23.8	793	
					B16		1.1	37.7	34	
					A431		0.01	3.8	380	
					NP69		0.5	11.9	24	
		525 nm (29.56 J/cm^2)		896.2	HeLa	Normoxia	0.1	23.8	238	
					A431		0.01	3.8	380	
Ir5	470 (H_2O /48000)	465 nm (11.7 J/cm^2)	-	1357.2	HeLa	Normoxia	0.1	2.3	23	
					B16		0.4	9.8	25	
					A431		0.003	0.1	33	
					NP69		0.4	1.1	3	
		525 nm (29.56 J/cm^2)		1338.2	HeLa	Normoxia	0.3	2.3	8	

					A431		0.01	0.1	10	
Ir6	484 (PBS/-)	465 nm (11.7 J/cm^2)	0.90 (PBS)	354.8	-	-	-	-	-	77
Ir7	484 (PBS/-)		0.14 (PBS)	48.0	A549	Normoxia	5.4	>200	>37	
					A549R		1.6	>200	>125	
					HepG2		4.9	>200	>41	
					HepG2-SR		0.4	63.8	159	
					CT-26		2.6	>200	>77	
Ir8	488 (H_2O /-)	465 nm (11.7 J/cm^2)	-	-	HeLa	Normoxia	0.2 ± 0.0	0.7 ± 0.0	3.5	78
Ir9	488 (H_2O /-)		0.23 (H_2O)	414.2	HeLa		0.08 ± 0.0	26.7±0.7	333. 8	
					A549		0.2 ± 0.0	55.0±0.3	275. 0	
					B16		0.002 ± 0.0	0.8±0.03	400.0	
Ir10	500 (DMSO:H_2O, 1:9/-)	400-700 nm (10 J/cm^2)	0.24 (PBS, 0.5% DMSO)	841.4	A549	Normoxia	0.9 ± 0.1	43.2 ± 1.7	44.1	79
					HeLa		1.6 ± 0.1	44.4 ± 2.1	27.8	
					A549	Hypoxia	0.9 ± 0.3	45.9 ± 3.2	16.3	
Ir11	480 (DMSO:H_2O, 1:9/-)		0.26 PBS, 0.5% DMSO)	1003.7	A549	Normoxia	0.6 ± 0.1	41.2 ± 1.5	71. 0	
					HeLa		0.9 ± 0.1	43.7 ± 1.8	47.0	
					A549	Hypoxia	0.7 ± 0.1	42.1 ± 2.7	30.2	
Ir12	-	400-700 nm (5 J/cm^2)	0.03 (PBS, 0.5% DMSO)	969.0	MCF-7	Normoxia	22.1 ±1.9	23.5 ±2.7	1.1	80
					HeLa		23.12 ±1.4	>25	>1.1	
					HEK-293		>25	>25	-	
Ir13	-		0.05 (PBS, 0.5% DMSO)	1084.0	MCF-7	Normoxia	0.3 ± 0.1	0.6 ± 0.1	2.0	
					HeLa		7.0 ± 0.2	7.0 ± 0.2	1.9	
					HEK-293		7.9± 0.4	13.4 ± 1.3	-	
Fe1	720 (DMF:PBS, 1:9/2000)	400-700 nm (10 J/cm^2)	-	-	MCF-7	Normoxia	3.2 ± 0.8	>50	>16	81
					HeLa		7.4 ± 1.0	>50	>7	
					HaCaT		5.1 ± 1.1	>50	>10	
		600-720 nm, 50 J/cm^2)	-	-	MCF-7		8.8 ± 1.3	>50	>6	
					HeLa		15.3 ± 1.1	>50	>3	
					HaCaT		11.8 ± 1.7	>50	>4	
Co1	~402 (DMF:PBS, 1:9/-)	400-700 nm (10 J/cm^2)	-	-	HeLa	Normoxia	20.1 ± 0.2	>50	>2.5	82
					MCF-7		17.2 ± 0.2	>50	>3	
Co2	~402		-	-	HeLa	Normoxia	10.0 ± 0.1	>50	>5.0	

	(DMF:PBS, 1:9/-)				MCF-7		8.8 ± 0.1	>50	>6	
Co3	~402 (DMF:PBS, 1:9/-)		-	-	HeLa	Normoxia	1.6 ± 0.1	>50	>32	
					MCF-7		1.1 ± 0.1	>50	>46	
Co4	-	808 nm; (1.0 W/cm^2; 5 min)	-	-	A549	Normoxia	15.20 ± 1.33	18.26 ± 1.2	1.2	83
Co5	-		0.13 (dmso)	-	A549	Normoxia	10.0 ± 1.23	14.11 ± 1.1	1.4	
Ru2	562 (ACN,35500)	400–800 nm (30 mW/cm^2; 10 min)	0.184 (-)	-	-	-	-	-	-	91
Ru3	471 nm (ACN/ 63300)	450 nm (30 min)	0.67 (CH_2Cl_2:MeOH , 9:1)	-	-	-	-	-	-	92
Ru4	421nm (ACN/ 66300)	450 nm (30 min)	0.42 (CH_2Cl_2:MeOH , 9:1)	-	-	-	-	-	-	
SCV42	555 (ACN/25000)	540 nm (9.0 J/ cm^2)	0.33 (ACN)	-	CT-26	Normoxia	0.0082 ± 0.0006	>250	>30487	39
						Hypoxia	0.035 ± 0.005	>250	>7143	
		645 nm (9.0 J/ cm^2)	-	-	CT-26	Normoxia	0.048 ± 0.003	>250	>5208	
						Hypoxia	0.920 ± 0.09	>250	>272	
SCV49	571 (ACN/20000)	540 nm (9.0 J/ cm^2)	0.12 (ACN)	-	CT-26	Normoxia	0.025 ± 0.002	>250	>10000	39
						Hypoxia	0.086 ± 0.011	>250	>2907	
		645 nm (9.0 J/ cm^2)	-	-	CT-26	Normoxia	0.0074 ± 0.0006	>250	>33783	
						Hypoxia	0.076 ± 0.008	>250	>3290	
		670 nm (13.5 J/ cm^2)	-	-	CT-26	Normoxia	0.036 ± 0.003	>250	>6944	39
						Hypoxia	0.074 ± 0.005	>250	>3378	
		740 nm (12.6 J/ cm^2)	-	-	CT-26	Normoxia	0.76 ± 0.06	>250	>329	
						Hypoxia	9.56 ± 2.15	>250	>26	