

Supporting Information
for
Chiral Ruthenium(II) Complex as Potent Radiosensitizer of ^{125}I
through DNA-Damage-Mediated Apoptosis

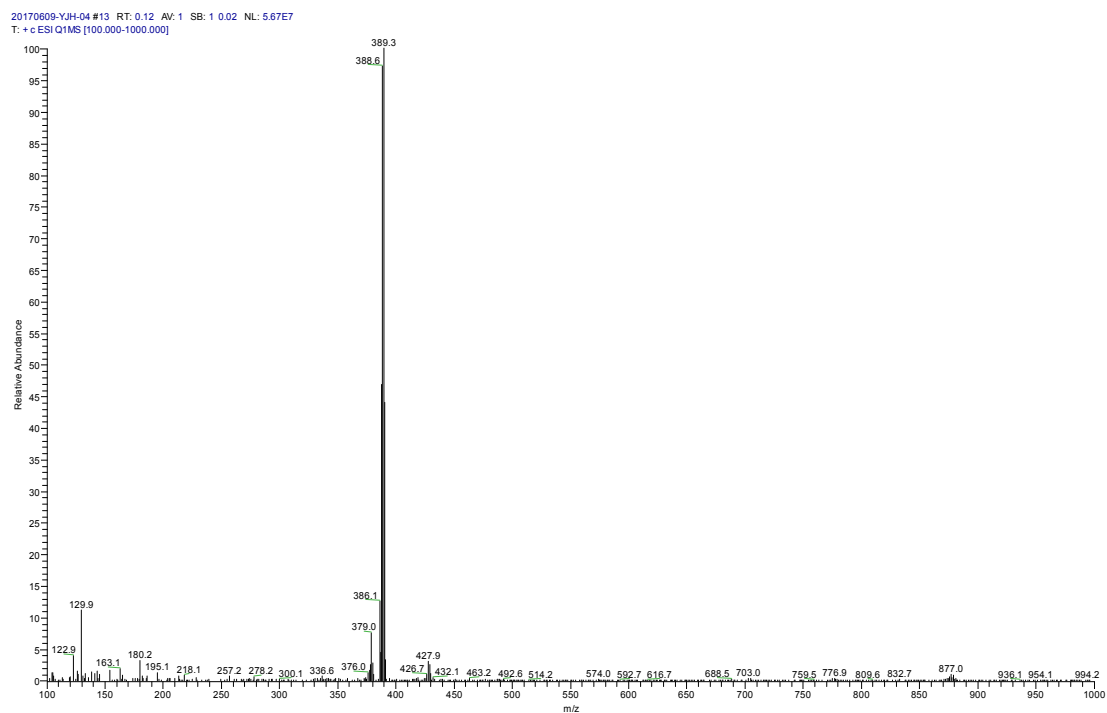
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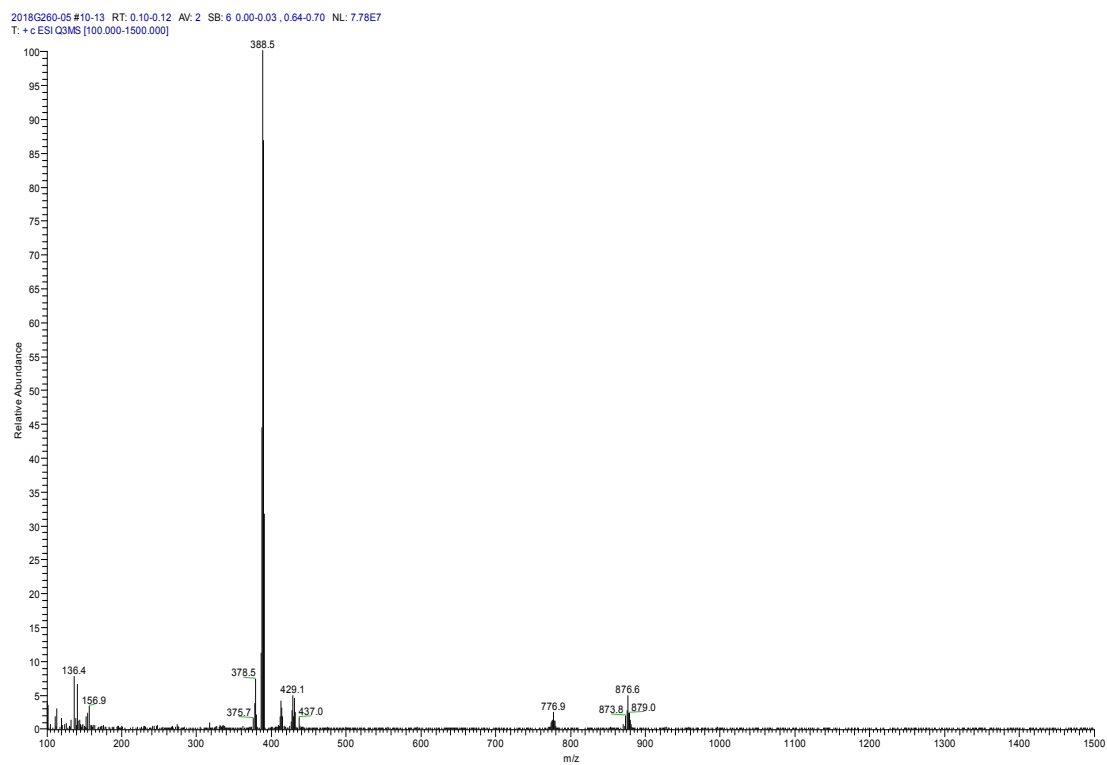
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A



B

Figure S1. The ESI-MS spectra of LR042 (A) and DR042 (B)

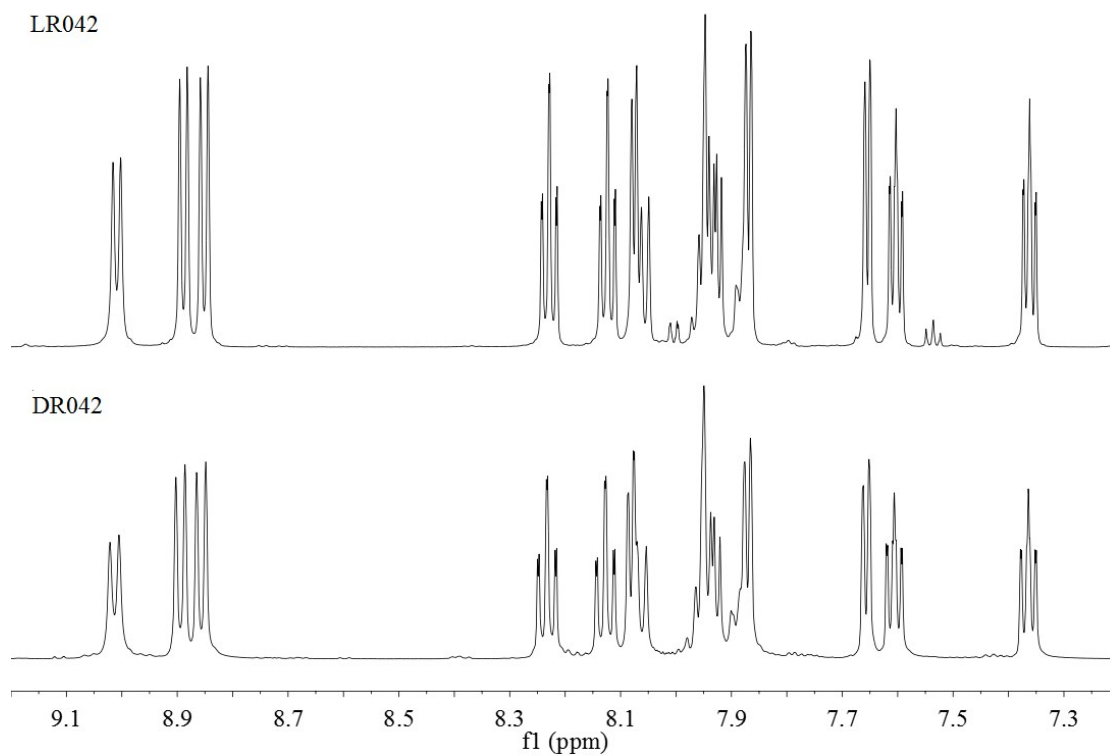


Figure S2. The ¹H NMR spectra of LR042 (upper) and DR042 (lower)

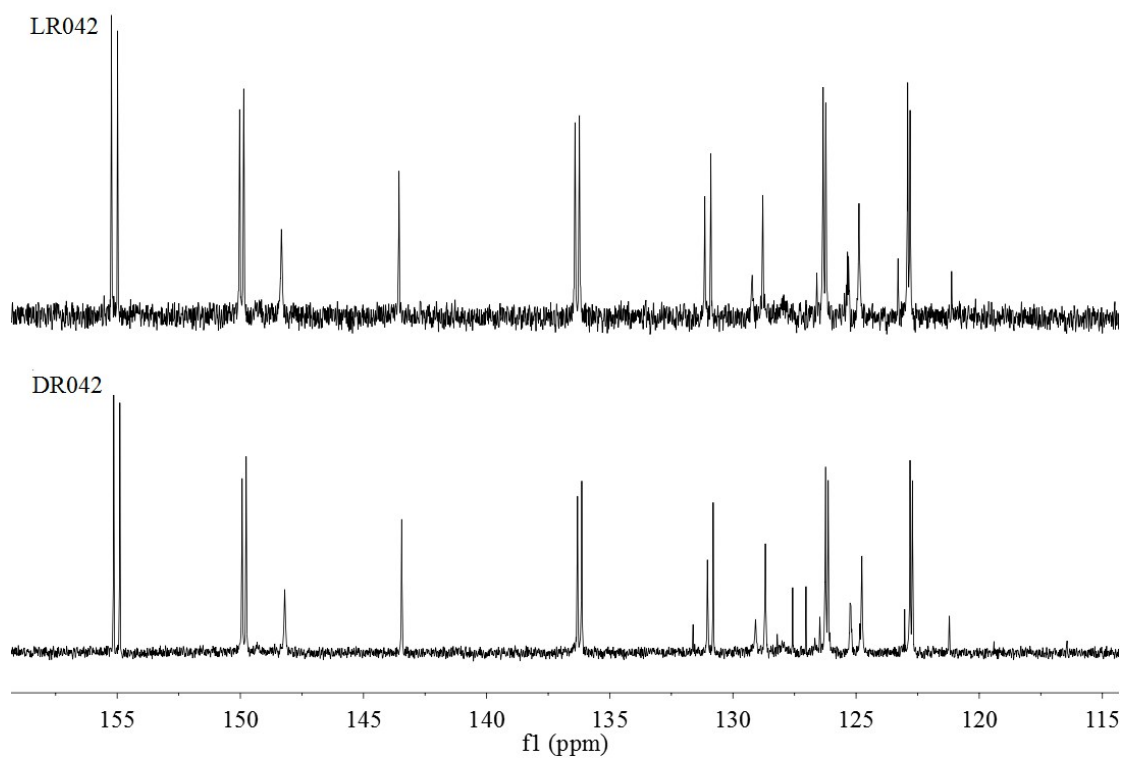
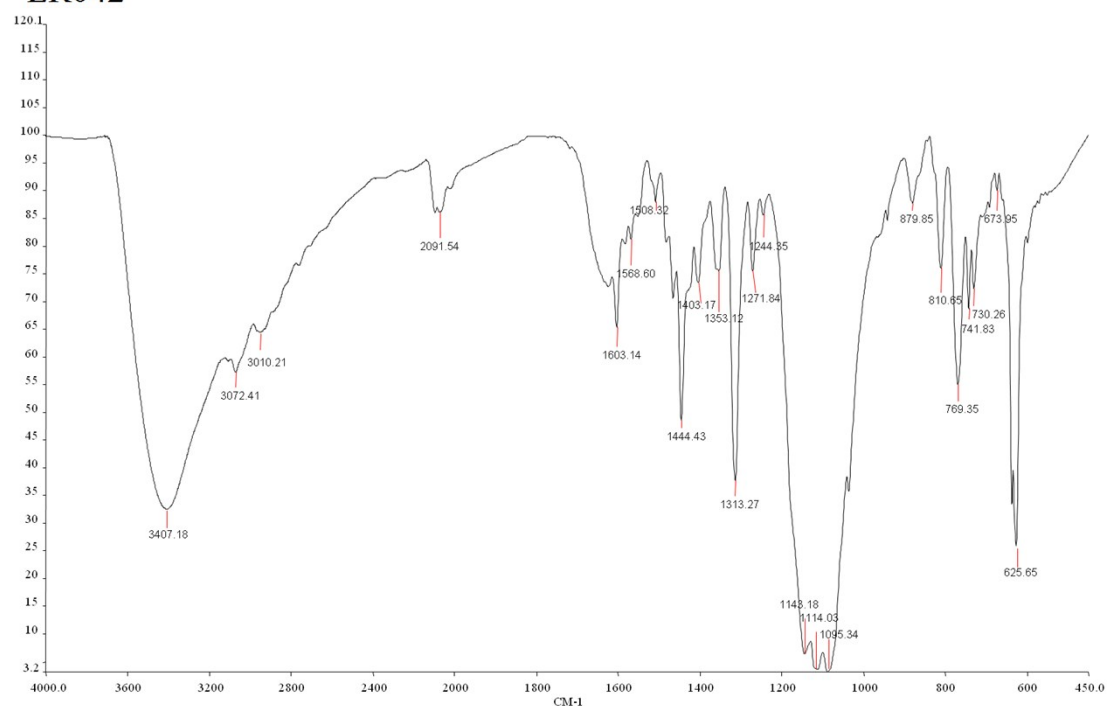


Figure S3. The ¹³C NMR spectra of LR042 (upper) and DR042 (lower)

LR042



DR042

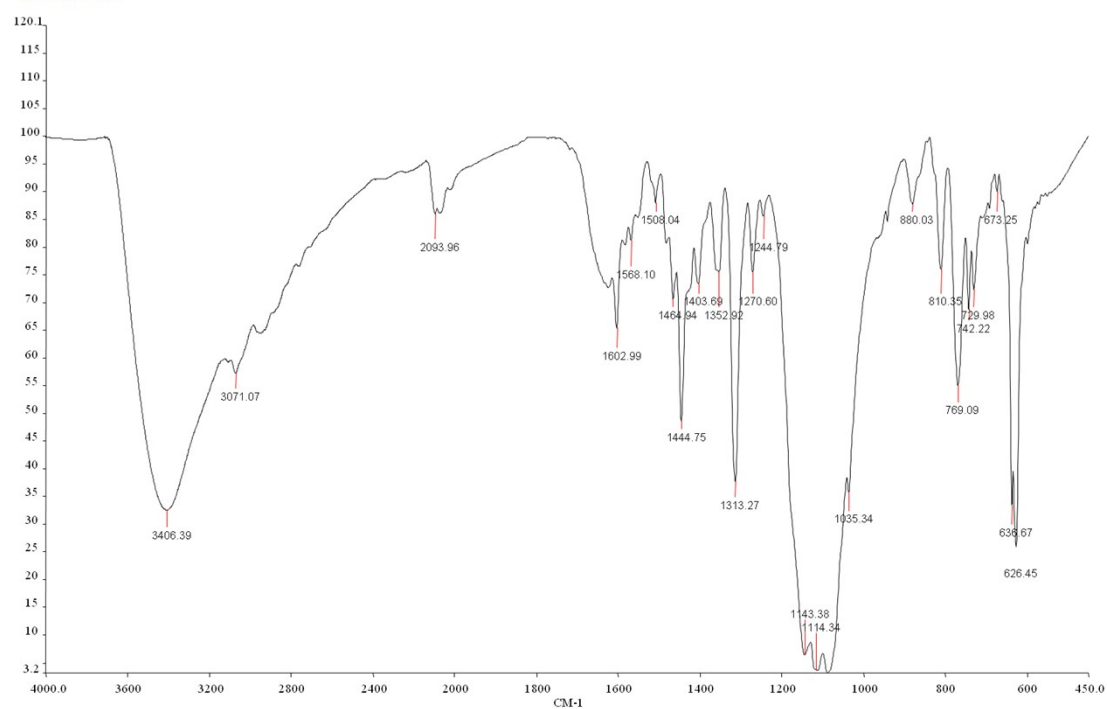
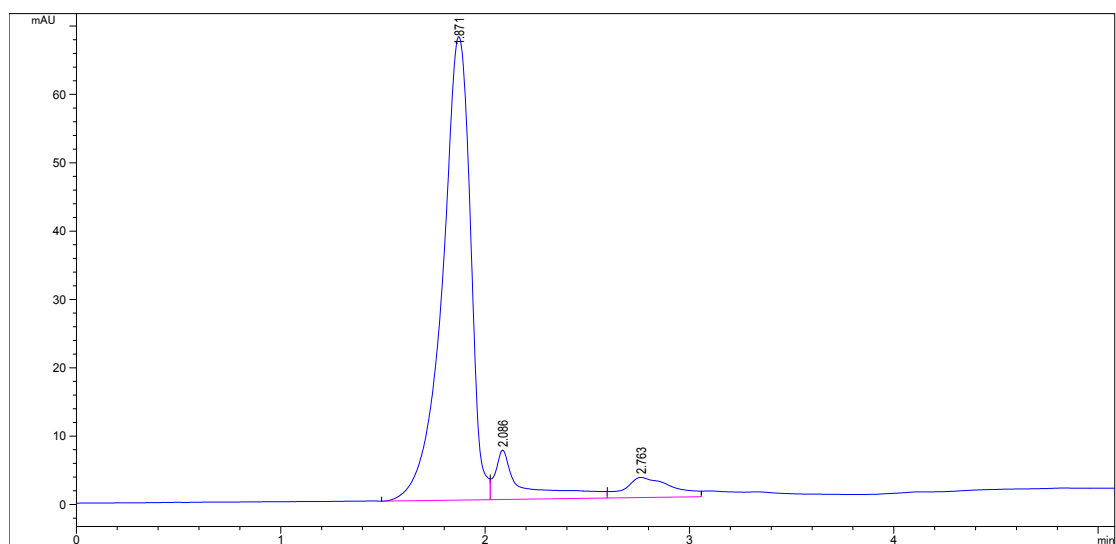
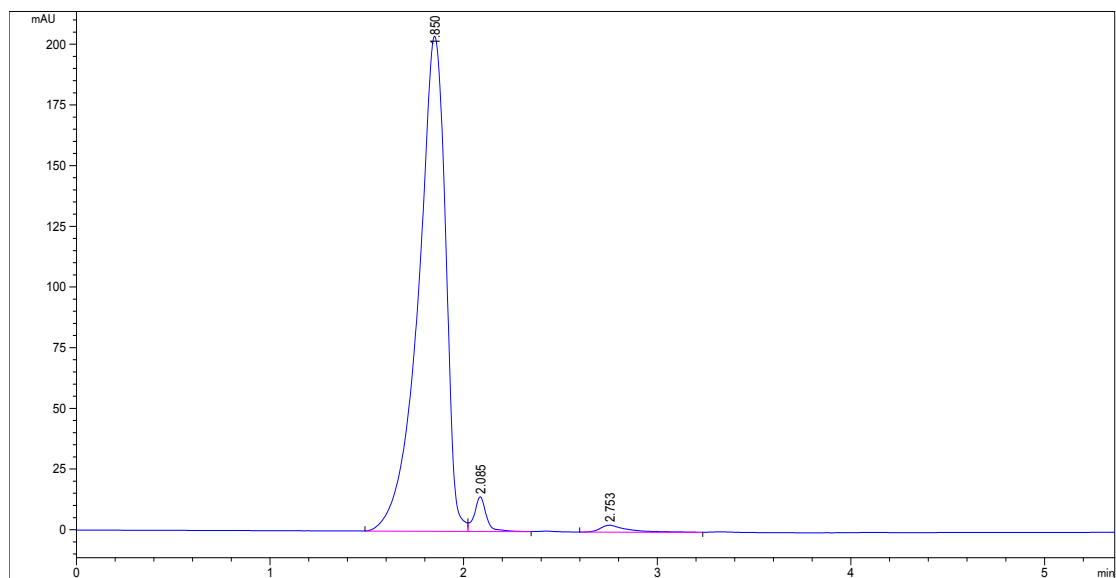


Figure S5. The IR spectra of LR042 (upper) and DR042 (lower)



A

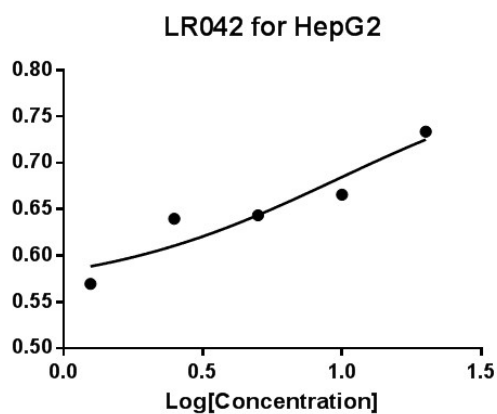


B

Figure S6. The HPLC purity analysis for LR042 (A) and DR042 (B). The eluent is MeOH:CH₃CN=1:1 for 10 min.

Table S1. Inhibitory effect (IC₅₀, μM) of DR042 and ¹²⁵I on human cancer cells after 72 h of treatment.

Comp.	IC ₅₀ (μM)			
	HepG2	SW480	A549	HaCaT
DR042	>20	>20	>20	>20
DR042 with ¹²⁵I	>20	>20	>20	>20

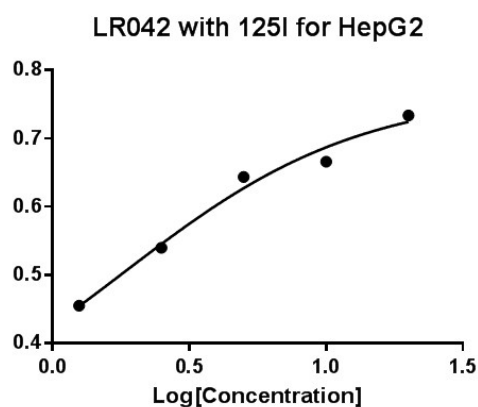


A

Nonlin fit		A
		Inhibitory rate
		Y
1	log(inhibitor) vs. response (three parameters)	
2	Best-fit values	
3	Bottom	0.8044
4	Top	0.5601
5	LogIC50	0.9835
6	IC50	9.627
7	Span	-0.2443
8	Std. Error	
9	Bottom	0.1370
10	Top	0.05307
11	LogIC50	0.7149
12	Span	0.1056
13	95% Confidence Intervals	
14	Bottom	0.2148 to 1.394
15	Top	0.3318 to 0.7885
16	LogIC50	-2.093 to 4.060
17	IC50	0.008078 to 11474
18	Span	-0.6985 to 0.2100
19	Goodness of Fit	
20	Degrees of Freedom	2
21	R square	0.8820
22	Absolute Sum of Squares	0.001637
23	Sy.x	0.02861

B

Figure S7. The fitting curve (A) and calculating results (B) of LR042 treated with HepG2 cells

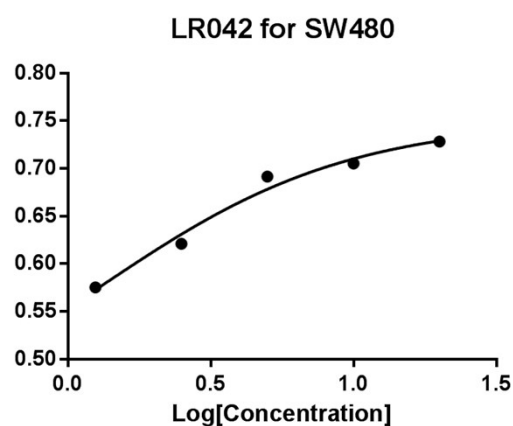


A

Nonlin fit		A
		Data Set-A
		Y
1	log(inhibitor) vs. response (three parameters)	
2	Best-fit values	
3	Bottom	0.7681
4	Top	0.2380
5	LogIC50	0.2583
6	IC50	1.813
7	Span	-0.5301
8	Std. Error	
9	Bottom	0.03258
10	Top	0.1449
11	LogIC50	0.2848
12	Span	0.1234
13	95% Confidence Intervals	
14	Bottom	0.6279 to 0.9083
15	Top	-0.3853 to 0.8614
16	LogIC50	-0.9672 to 1.484
17	IC50	0.1078 to 30.46
18	Span	-1.061 to 0.0008156
19	Goodness of Fit	
20	Degrees of Freedom	2
21	R square	0.9828
22	Absolute Sum of Squares	0.0008343
23	Sy.x	0.02042

B

Figure S8. The fitting curve (A) and calculating results (B) of LR042 with ¹²⁵I treated with HepG2 cells

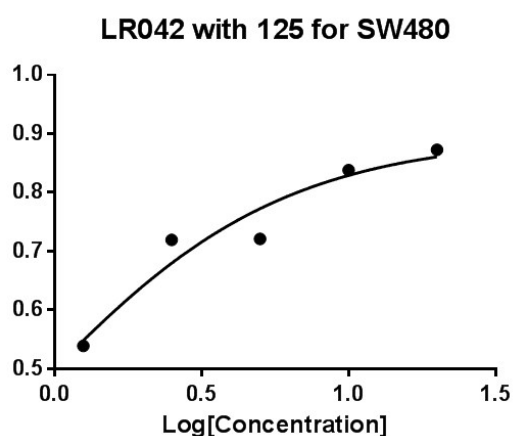


A

Nonlin fit		A
		Inhibitory rate
	Y	
1	log(inhibitor) vs. response (three parameters)	
2	Best-fit values	
3	Bottom	0.7501
4	Top	0.4028
5	LogIC50	0.1163
6	IC50	1.307
7	Span	-0.3473
8	Std. Error	
9	Bottom	0.01778
10	Top	0.1325
11	LogIC50	0.3377
12	Span	0.1202
13	95% Confidence Intervals	
14	Bottom	0.6736 to 0.8266
15	Top	-0.1673 to 0.9729
16	LogIC50	-1.337 to 1.569
17	IC50	0.04605 to 37.10
18	Span	-0.8644 to 0.1697
19	Goodness of Fit	
20	Degrees of Freedom	2
21	R square	0.9811
22	Absolute Sum of Squares	0.0003073
23	Sy.x	0.01240
24		

B

Figure S9. The fitting curve (A) and calculating results (B) of LR042 treated with SW480 cells

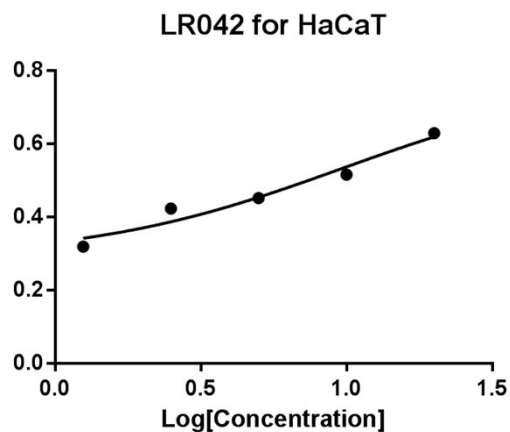


A

Nonlin fit		A
		Inhibitory rate
	Y	
1	log(inhibitor) vs. response (three parameters)	
2	Best-fit values	
3	Bottom	0.8947
4	Top	0.0001982
5	LogIC50	-0.1019
6	IC50	0.7909
7	Span	-0.8945
8	Std. Error	
9	Bottom	0.06079
10	Top	1.048
11	LogIC50	0.8393
12	Span	1.004
13	95% Confidence Intervals	
14	Bottom	0.6331 to 1.156
15	Top	-4.510 to 4.510
16	LogIC50	-3.713 to 3.510
17	IC50	0.0001935 to 3232
18	Span	-5.215 to 3.426
19	Goodness of Fit	
20	Degrees of Freedom	2
21	R square	0.9337
22	Absolute Sum of Squares	0.004543
23	Sy.x	0.04766
24		

B

Figure S10. The fitting curve (A) and calculating results (B) of LR042 with ¹²⁵I treated with SW480 cells

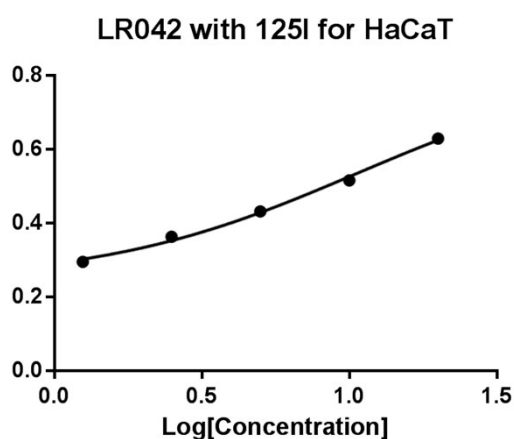


A

Nonlin fit		A	
		Inhibitory rate	T
		Y	
1	log(inhibitor) vs. response (three parameters)		
2	Best-fit values		
3	Bottom	0.7792	
4	Top	0.2844	
5	LogIC50	0.9847	
6	IC50	9.653	
7	Span	-0.4948	
8	Std. Error		
9	Bottom	0.1645	
10	Top	0.06346	
11	LogIC50	0.4230	
12	Span	0.1268	
13	95% Confidence Intervals		
14	Bottom	0.07136 to 1.487	
15	Top	0.01135 to 0.5575	
16	LogIC50	-0.8354 to 2.805	
17	IC50	0.1461 to 637.8	
18	Span	-1.041 to 0.05092	
19	Goodness of Fit		
20	Degrees of Freedom	2	
21	R square	0.9553	
22	Absolute Sum of Squares	0.002347	
23	Sy.x	0.03426	

B

Figure S11. The fitting curve (A) and calculating results (B) of LR042 treated with HaCaT cells.



A

Nonlin fit		A	
		Inhibitory rate	T
		Y	
1	log(inhibitor) vs. response (three parameters)		
2	Best-fit values		
3	Bottom	0.8279	
4	Top	0.2396	
5	LogIC50	1.026	
6	IC50	10.61	
7	Span	-0.5883	
8	Std. Error		
9	Bottom	0.06387	
10	Top	0.02140	
11	LogIC50	0.1307	
12	Span	0.05070	
13	95% Confidence Intervals		
14	Bottom	0.5531 to 1.103	
15	Top	0.1476 to 0.3317	
16	LogIC50	0.4633 to 1.588	
17	IC50	2.906 to 38.75	
18	Span	-0.8064 to -0.3701	
19	Goodness of Fit		
20	Degrees of Freedom	2	
21	R square	0.9957	
22	Absolute Sum of Squares	0.0002911	
23	Sy.x	0.01206	

B

Figure S12. The fitting curve (A) and calculating results (B) of LR042 with ¹²⁵I treated with HaCaT cells