

## Supporting Information

### High selectivity and significant cytotoxicity of rare earth naphthalene dicarboxylate complexes on non-small cell lung cancer cells

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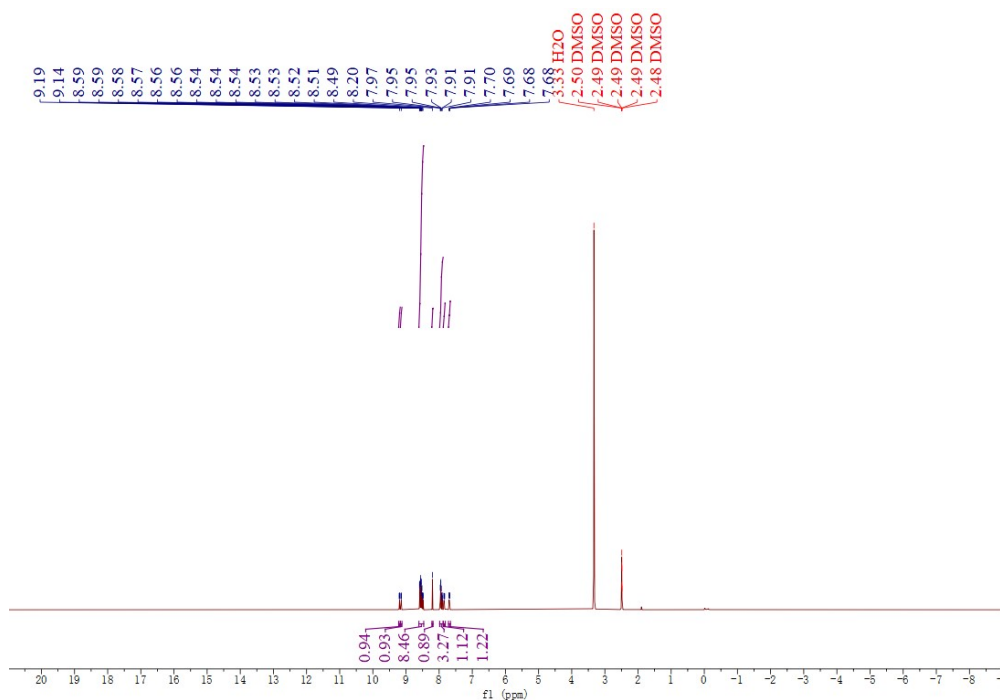
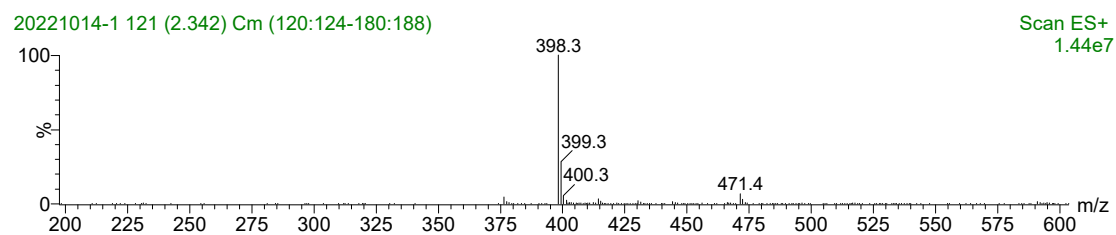


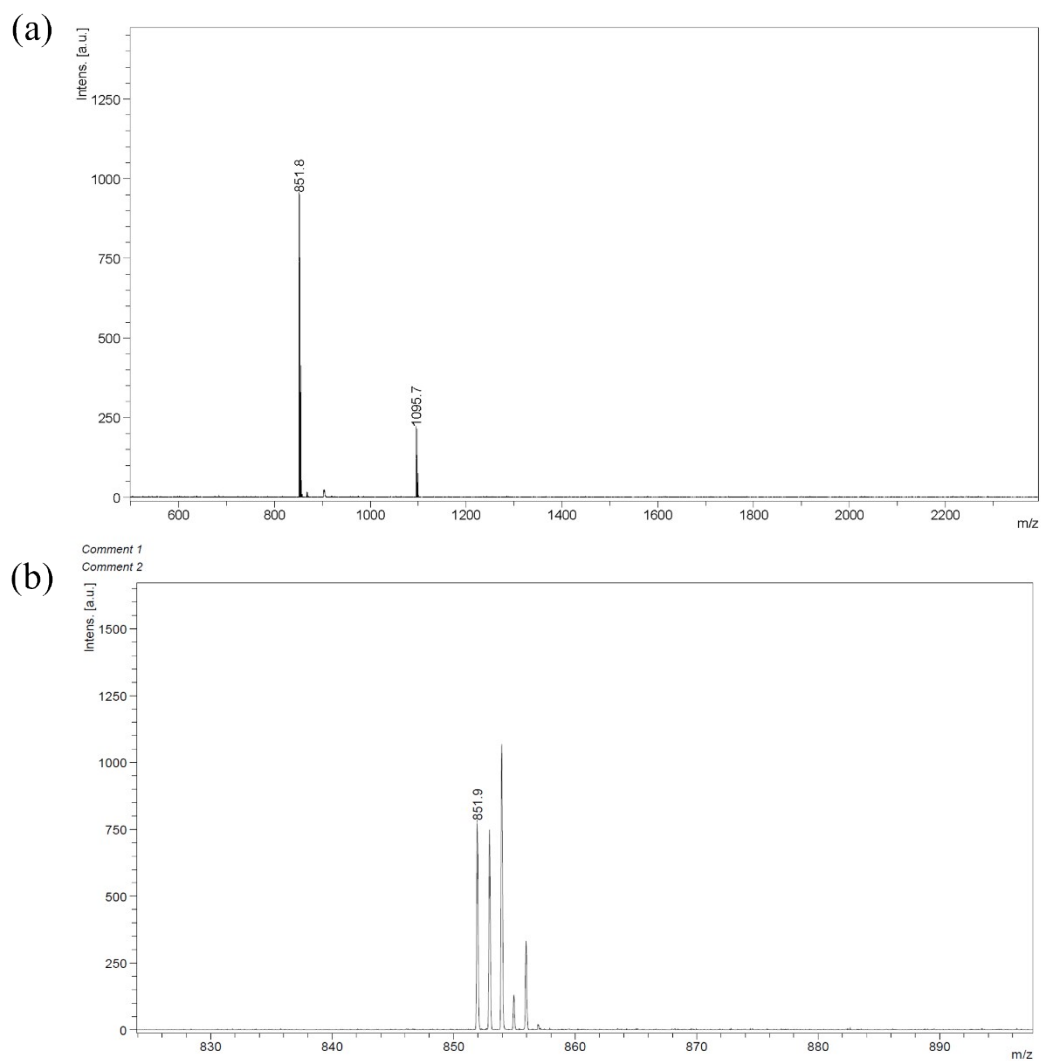
Figure S1. <sup>1</sup>H NMR spectrum of NI-Phen.

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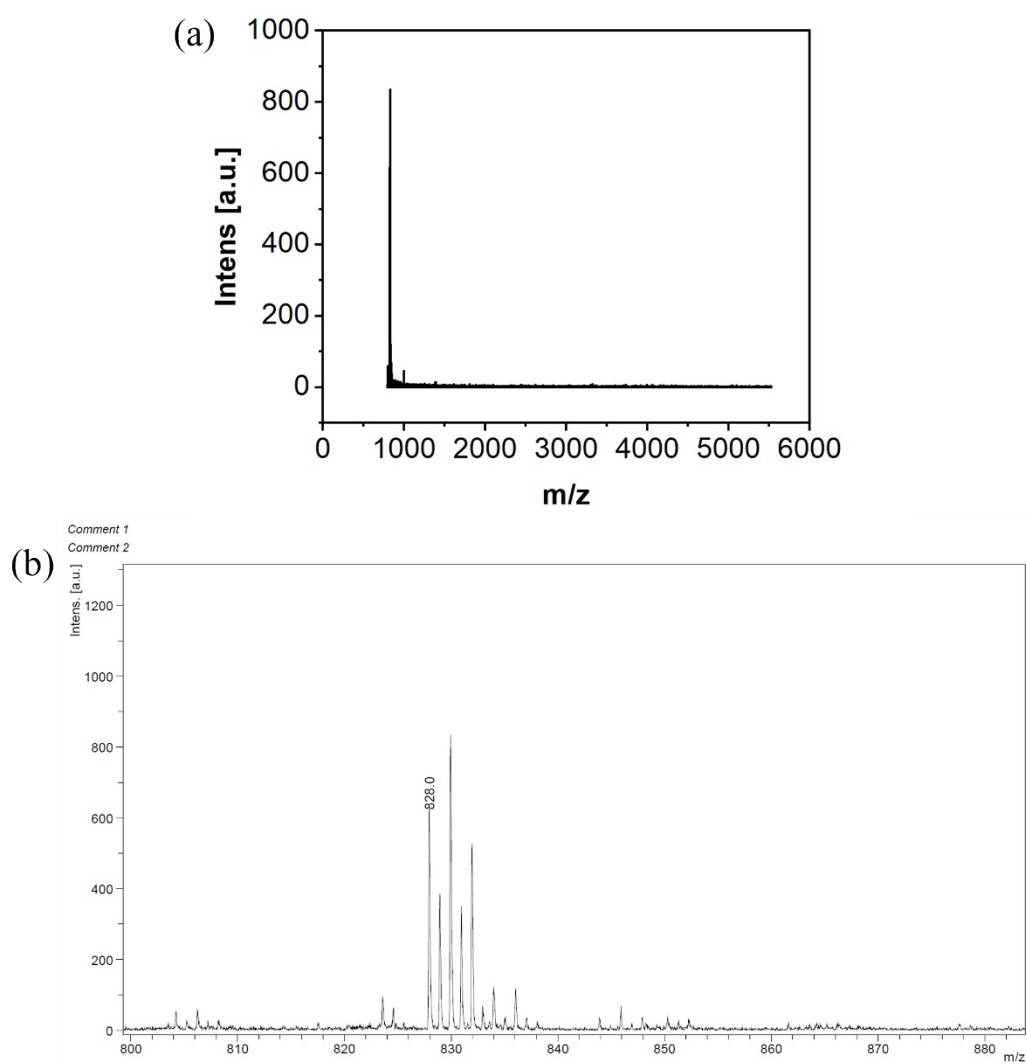
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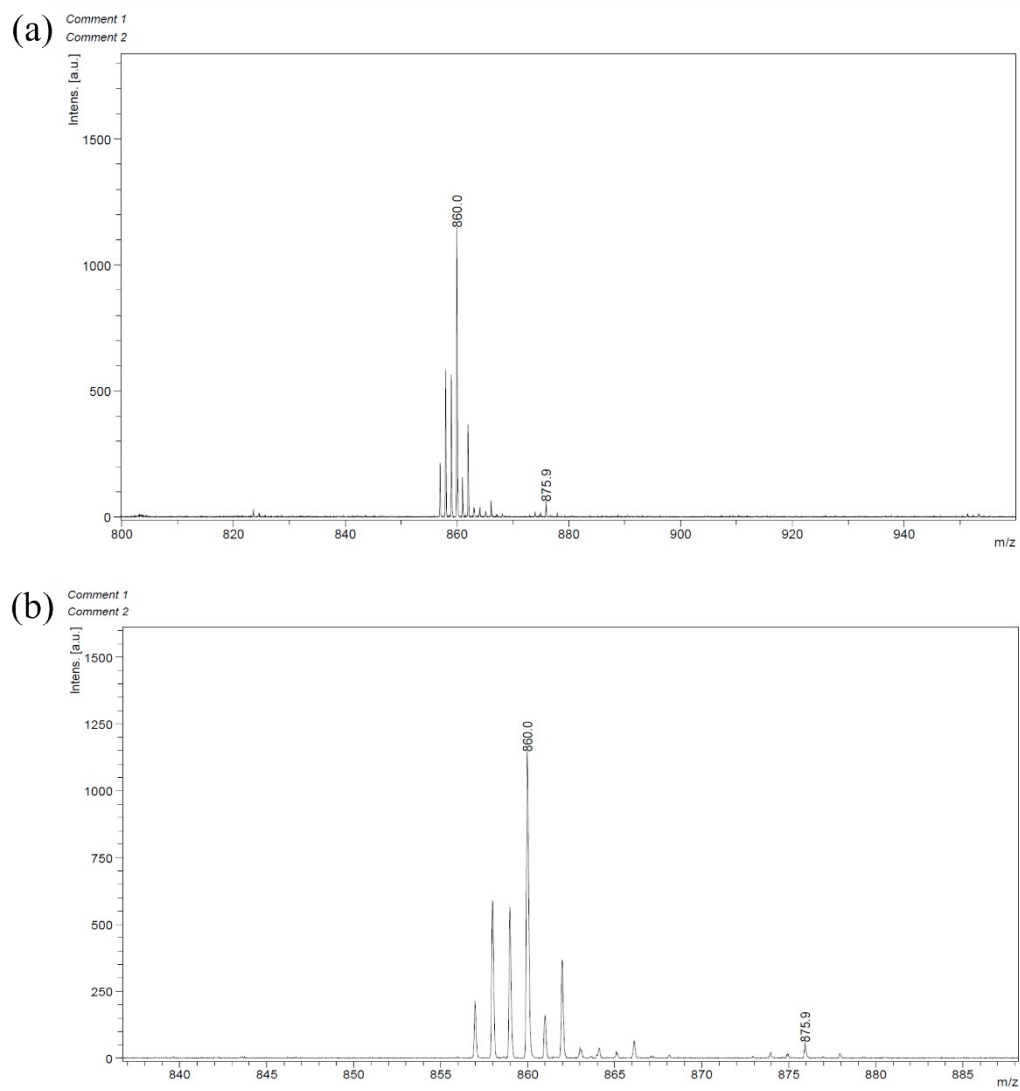
**Figure S2.** ESI-MS spectrum of NI-Phen.



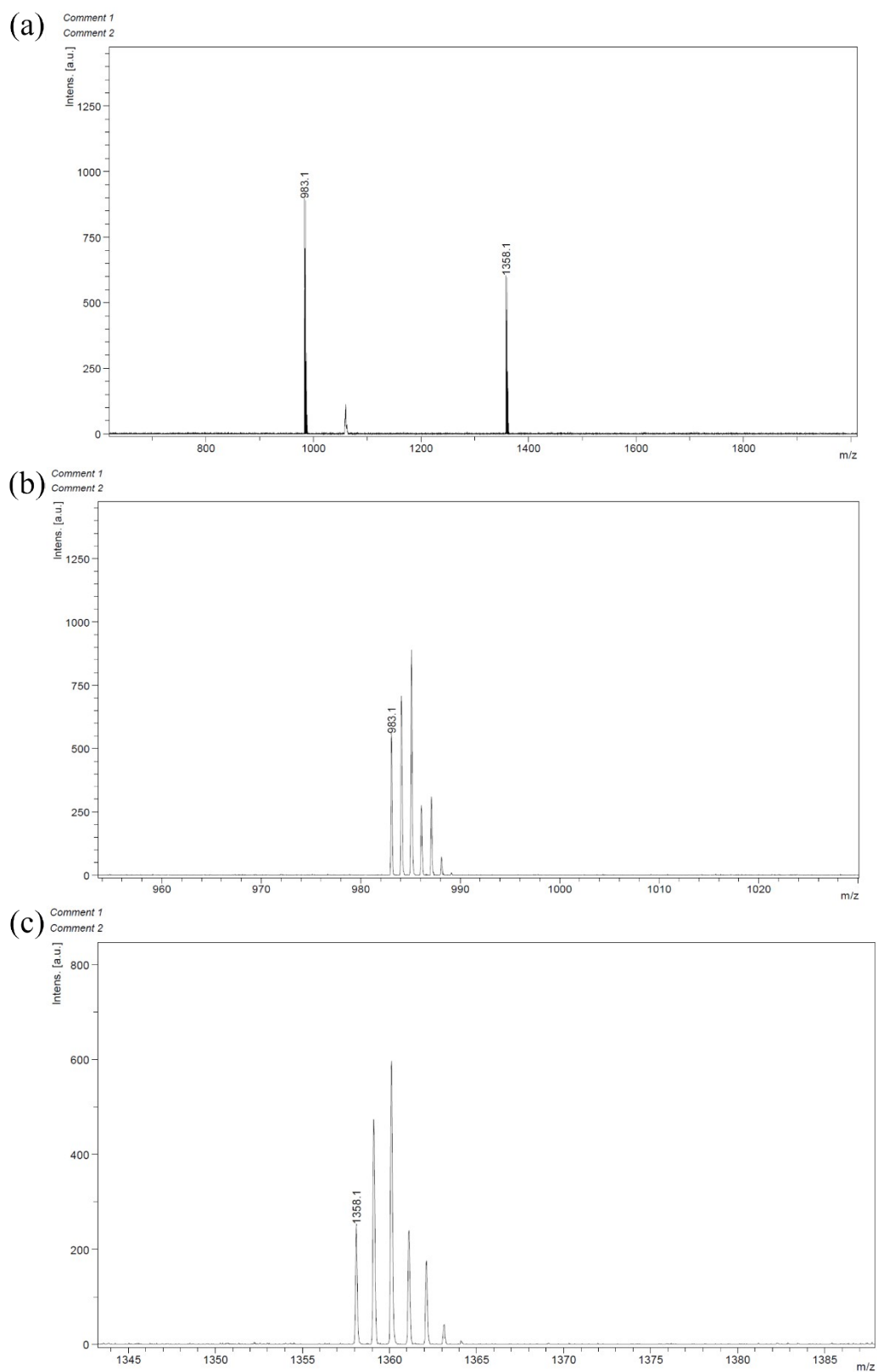
**Figure S3.** (a) MALDI-TOF-MS spectrum of  $\text{Er}(\text{TTA})_3\text{H}_2\text{O}$ . (b) Magnified MALDI-TOF-MS spectrum of  $\text{Er}(\text{TTA})_3\text{H}_2\text{O}$ .



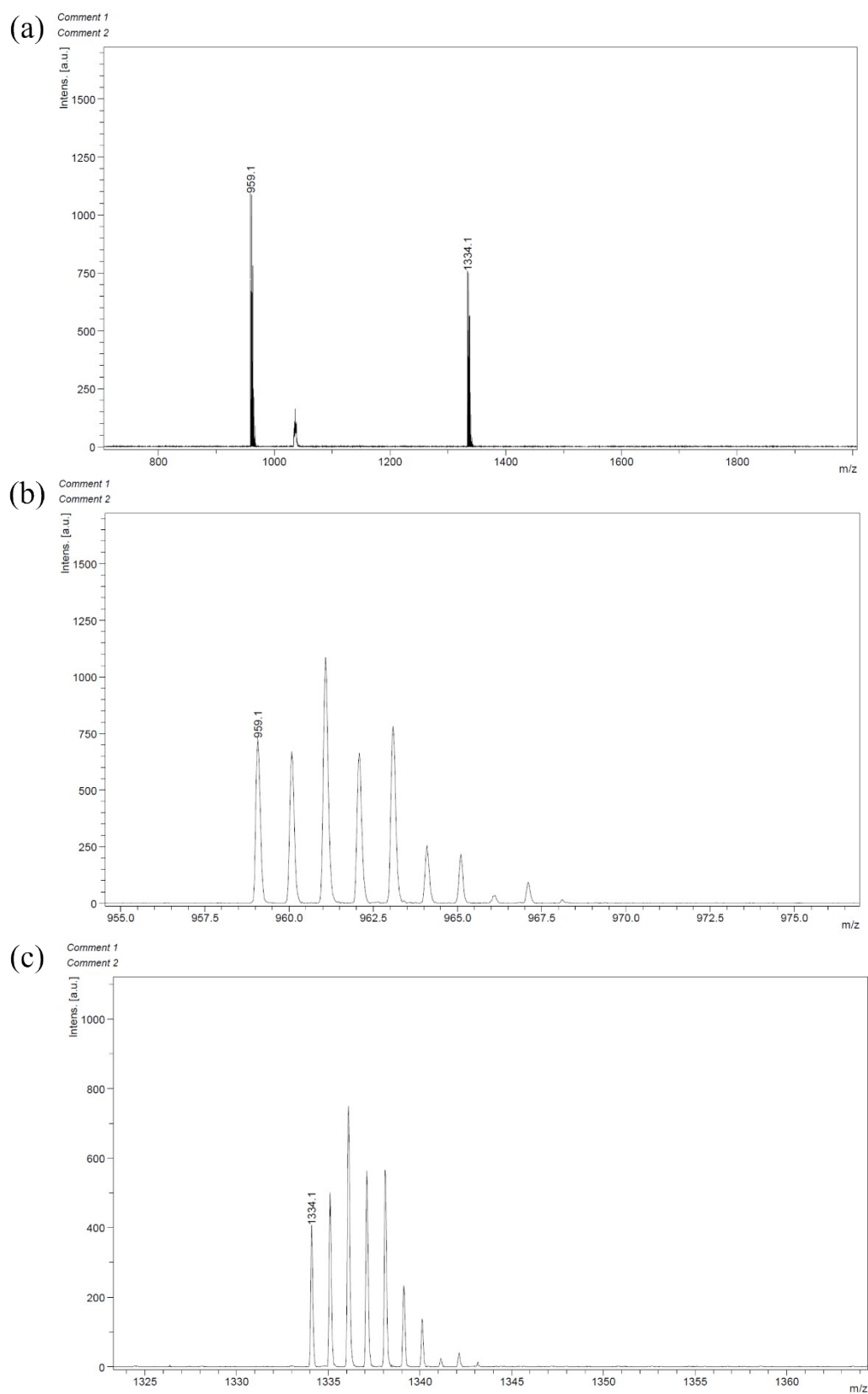
**Figure S4.** (a) MALDI-TOF-MS spectrum of  $\text{Nd}(\text{TTA})_3 \cdot 2\text{H}_2\text{O}$ . (b) Magnified MALDI-TOF-MS spectrum of  $\text{Nd}(\text{TTA})_3 \cdot 2\text{H}_2\text{O}$ .



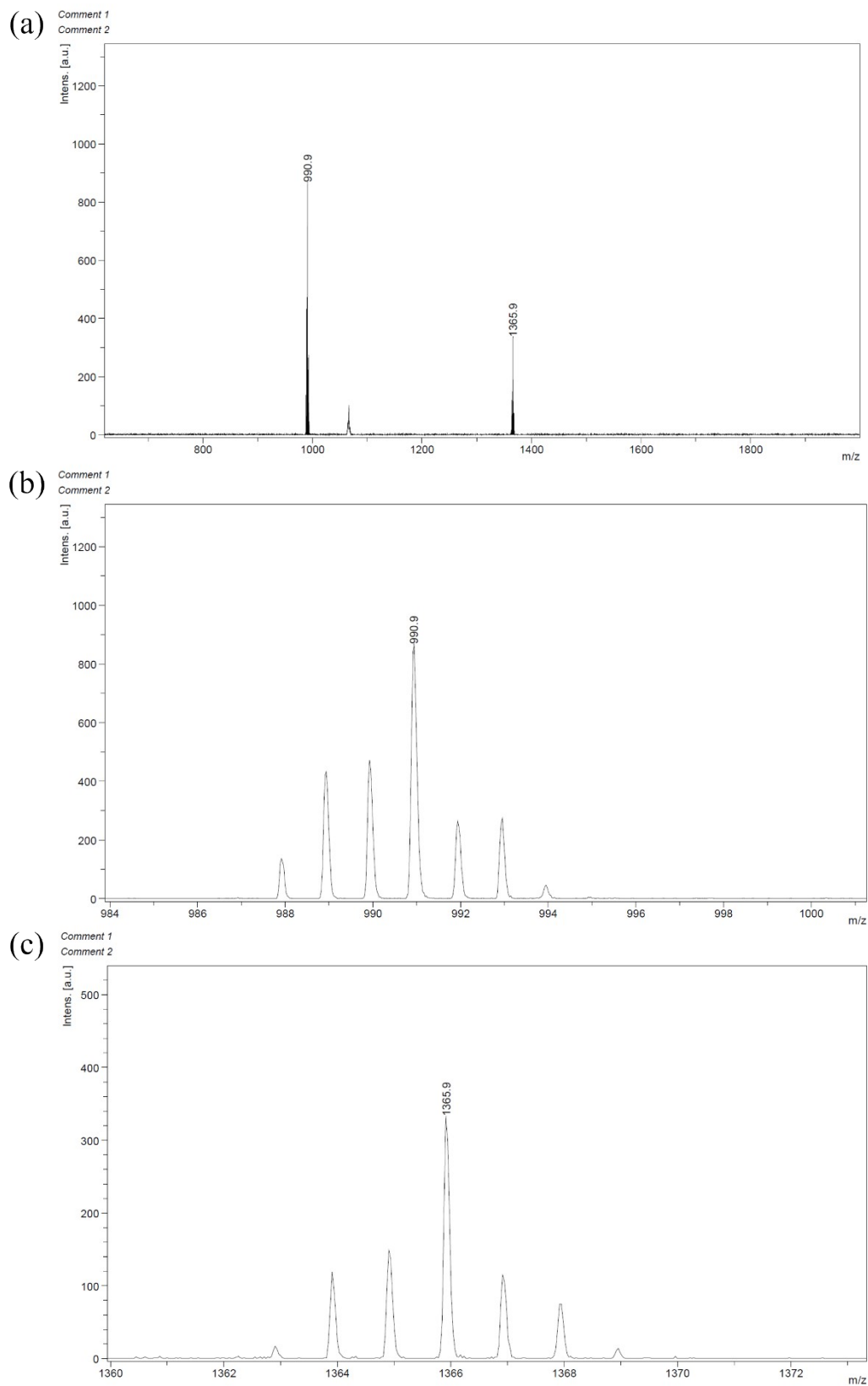
**Figure S5.** (a) MALDI-TOF-MS spectrum of  $\text{Yb}(\text{TTA})_3 \cdot 2\text{H}_2\text{O}$ . (b) Magnified MALDI-TOF-MS spectrum of  $\text{Yb}(\text{TTA})_3 \cdot 2\text{H}_2\text{O}$ .



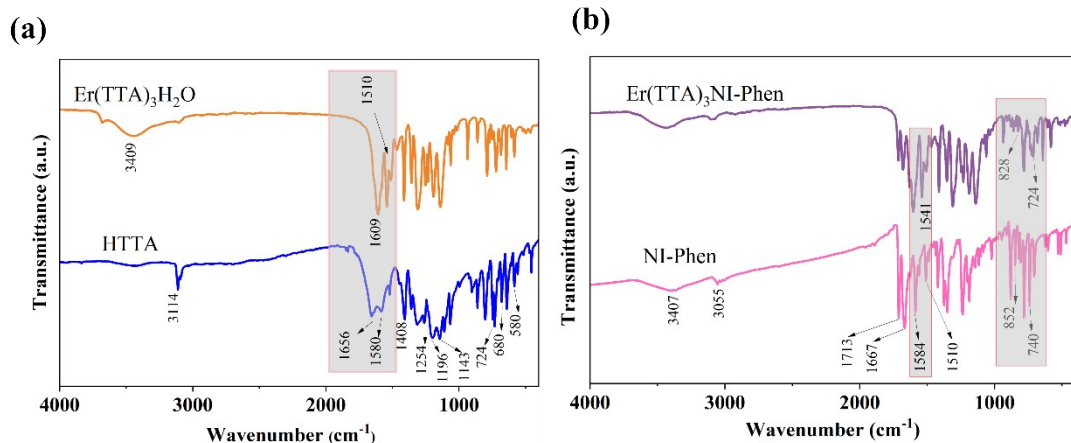
**Figure S6.** (a) MALDI-TOF-MS spectrum of  $\text{Er}(\text{TTA})_3\text{NI-Phen}$ . (b, c) Magnified MALDI-TOF-MS spectrum of  $\text{Er}(\text{TTA})_3\text{NI-Phen}$ .



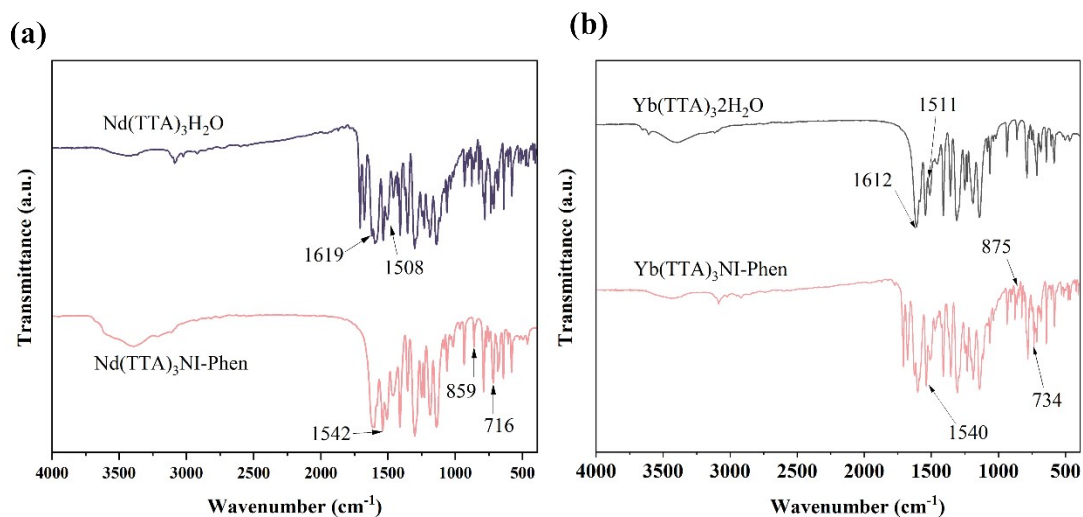
**Figure S7.** (a) MALDI-TOF-MS spectrum of  $\text{Nd}(\text{TTA})_3\text{NI-Phen}$ . (b, c) Magnified MALDI-TOF-MS spectrum of  $\text{Nd}(\text{TTA})_3\text{NI-Phen}$ .



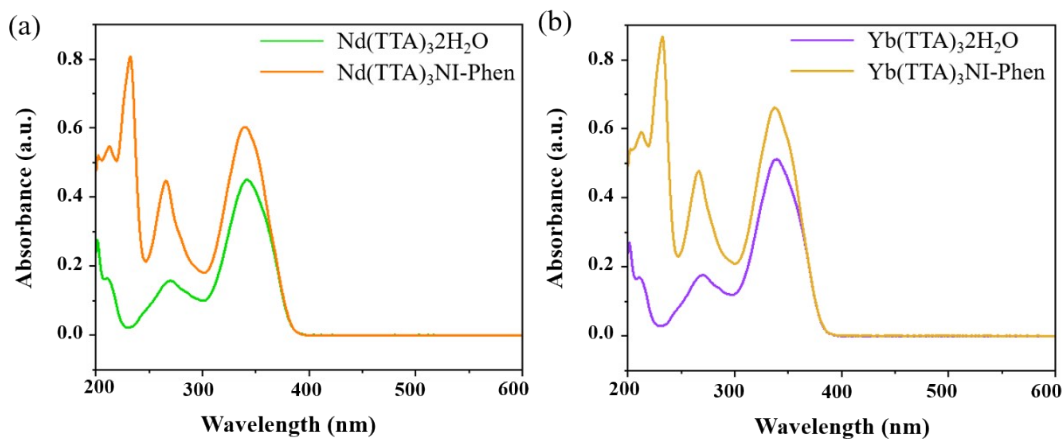
**Figure S8.** (a) MALDI-TOF-MS spectrum of  $\text{Yb}(\text{TTA})_3\text{NI-Phen}$ . (b, c) Magnified MALDI-TOF-MS spectrum of  $\text{Yb}(\text{TTA})_3\text{NI-Phen}$ .



**Figure S9.** FT-IR spectra of (a):  $\text{Er}(\text{TTA})_3\text{H}_2\text{O}$  and HTTA. (b):  $\text{Er}(\text{TTA})_3\text{NI-Phen}$  and NI-Phen.



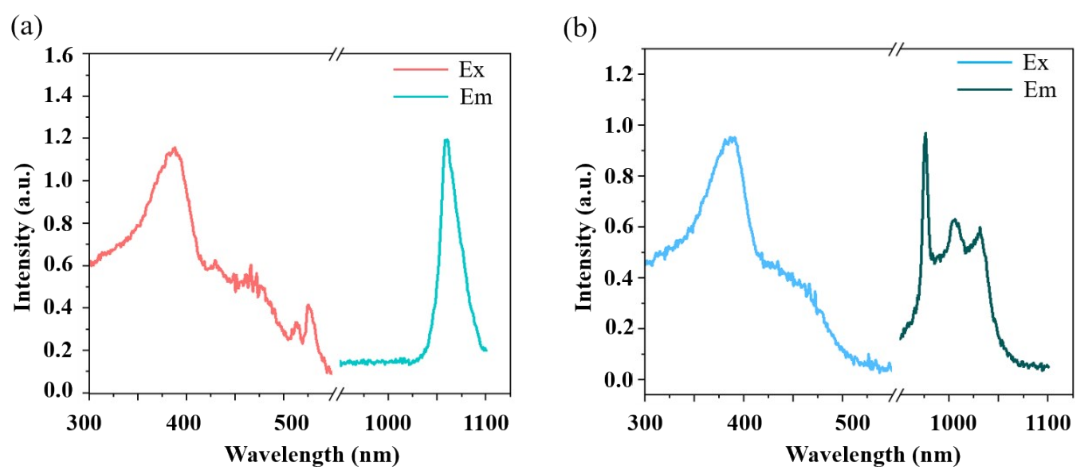
**Figure S10.** FT-IR spectra of (a):  $\text{Nd}(\text{TTA})_32\text{H}_2\text{O}$  and  $\text{Nd}(\text{TTA})_3\text{NI-Phen}$ , (b):  $\text{Yb}(\text{TTA})_32\text{H}_2\text{O}$  and  $\text{Yb}(\text{TTA})_3\text{NI-Phen}$ .



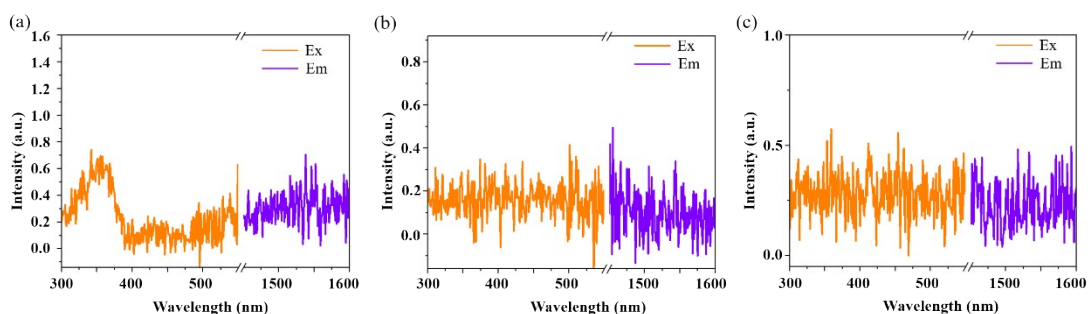
**Figure S11.** UV-vis spectra of  $\text{Ln}(\text{TTA})_32\text{H}_2\text{O}$  and  $\text{Ln}(\text{TTA})_3\text{NI-Phen}$  in anhydrous ethanol



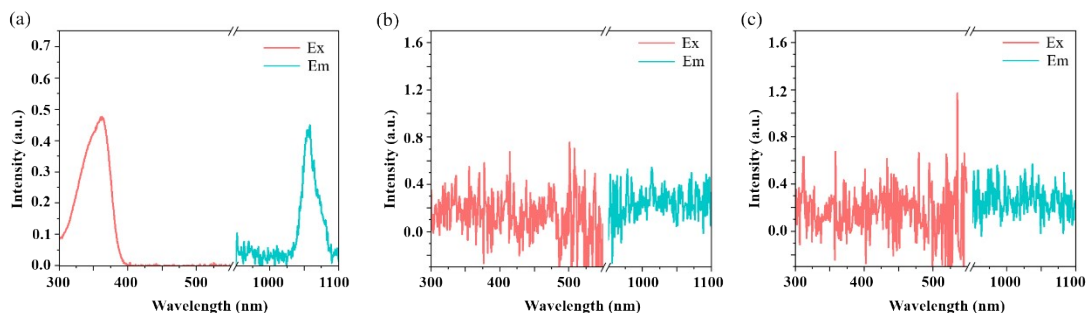
( $1 \times 10^{-5}$  mol/L) at room temperature. (a): Nd(TTA)<sub>3</sub>2H<sub>2</sub>O and Nd(TTA)<sub>3</sub>NI-Phen, (b): Yb(TTA)<sub>3</sub>2H<sub>2</sub>O and Yb(TTA)<sub>3</sub>NI-Phen.



**Figure S12.** Fluorescence spectroscopy of Ln(TTA)<sub>3</sub>NI-Phen powder at room temperature. (a): Nd(TTA)<sub>3</sub>NI-Phen ( $\lambda_{\text{ex}}=388$  nm,  $\lambda_{\text{em}}=1058$  nm). (b): Yb(TTA)<sub>3</sub>NI-Phen ( $\lambda_{\text{ex}}=386$  nm,  $\lambda_{\text{em}}=976$  nm).

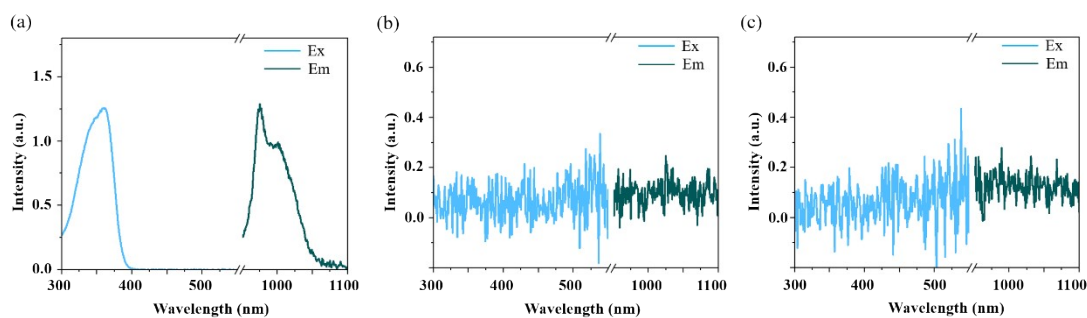


**Figure S13.** Fluorescence spectroscopy of Er(TTA)<sub>3</sub>NI-Phen ( $1 \times 10^{-5}$  mol/L) in DMSO (a), RPMI1640 (b) and DMEM (c) at room temperature.



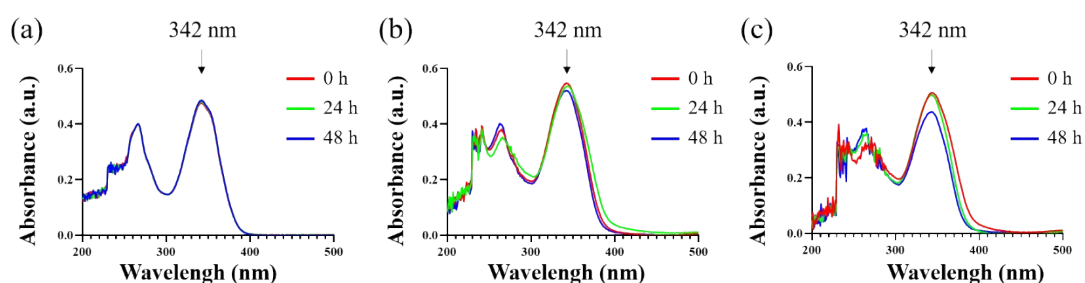
**Figure S14.** Fluorescence spectroscopy of Nd(TTA)<sub>3</sub>NI-Phen ( $1 \times 10^{-5}$  mol/L) in DMSO (a),

RPMI1640 (b) and DMEM (c) at room temperature ( $\lambda_{\text{ex}}=362$  nm,  $\lambda_{\text{em}}=1058$  nm).



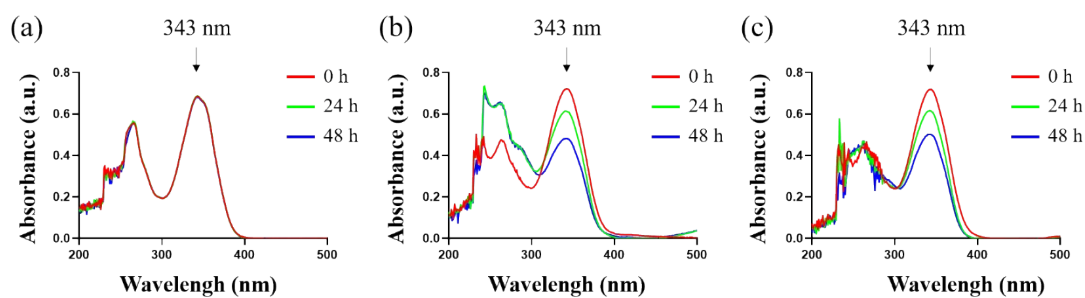
**Figure S15.** Fluorescence spectroscopy of Yb(TTA)<sub>3</sub>NI-Phen ( $1 \times 10^{-5}$  mol/L) in DMSO (a),

RPMI1640 (b) and DMEM (c) at room temperature ( $\lambda_{\text{ex}}=360$  nm,  $\lambda_{\text{em}}=976$  nm).



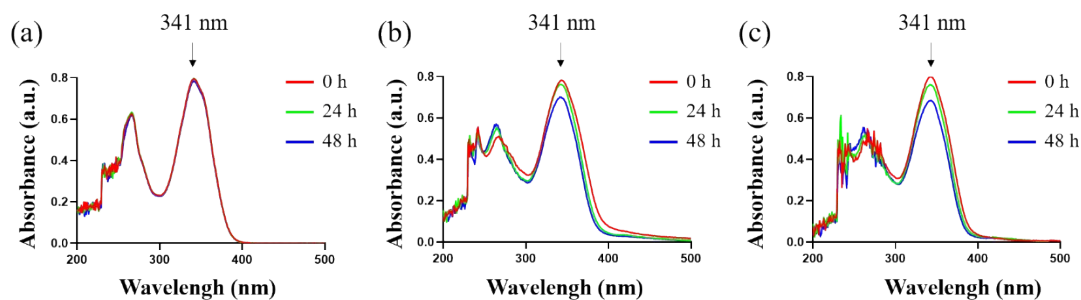
**Figure S16.** UV-vis spectra of Er(TTA)<sub>3</sub>NI-Phen ( $1 \times 10^{-5}$  mol/L) in DMSO (a), RPMI1640 (b)

and DMEM (c) at various time intervals (0-48 hours).

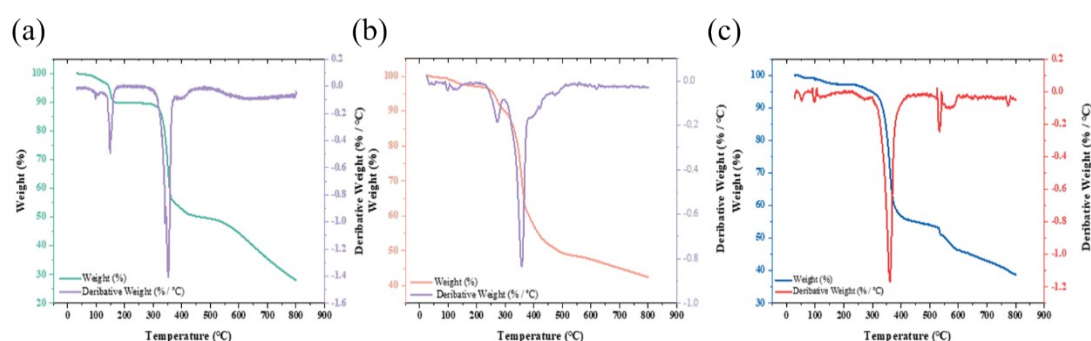


**Figure S17.** UV-vis spectra of Nd(TTA)<sub>3</sub>NI-Phen ( $1 \times 10^{-5}$  mol/L) in DMSO (a), RPMI1640 (b)

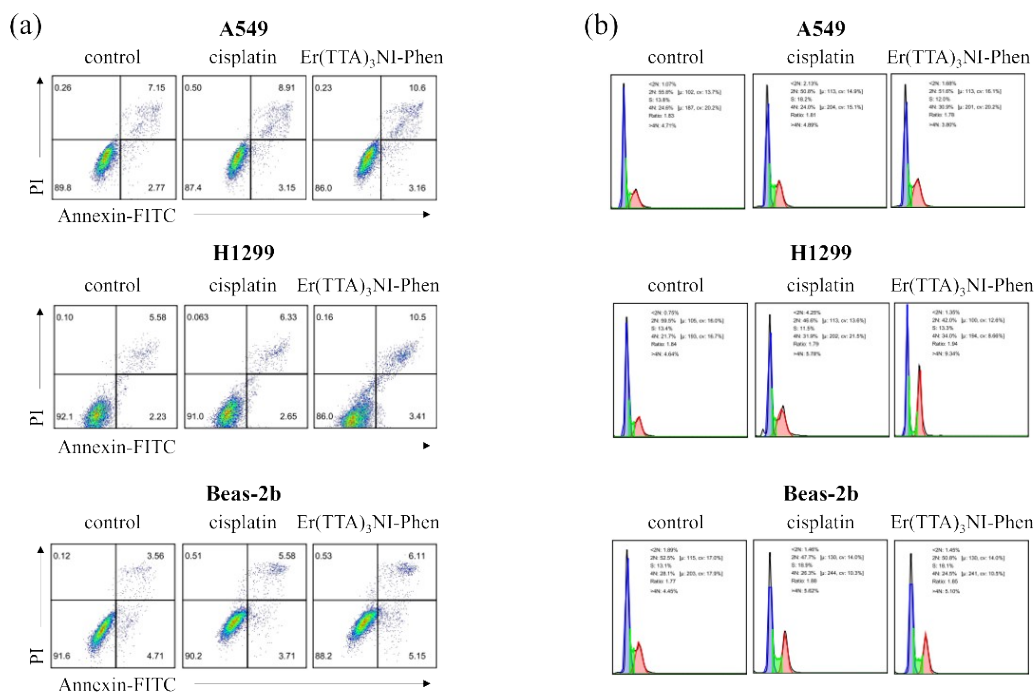
and DMEM (c) at various time intervals (0-48 hours).



**Figure S18.** UV-vis spectra of Yb(TTA)<sub>3</sub>NI-Phen ( $1 \times 10^{-5}$  mol/L) in DMSO (a), RPMI1640 (b) and DMEM (c) at various time intervals (0-48 hours).

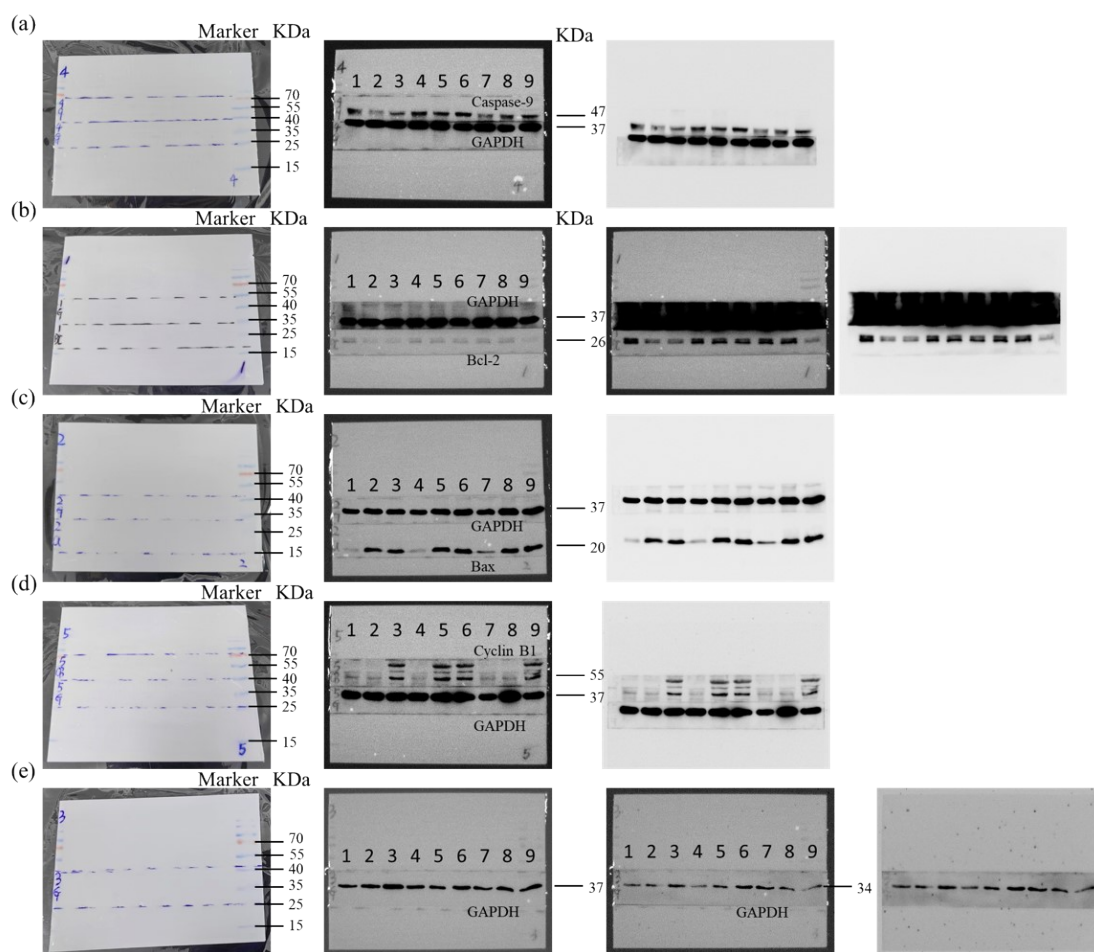


**Figure S19.** TGA curves of Er(TTA)<sub>3</sub>NI-Phen (a), Nd(TTA)<sub>3</sub>NI-Phen (b) and Yb(TTA)<sub>3</sub>NI-Phen (c) in nitrogen.



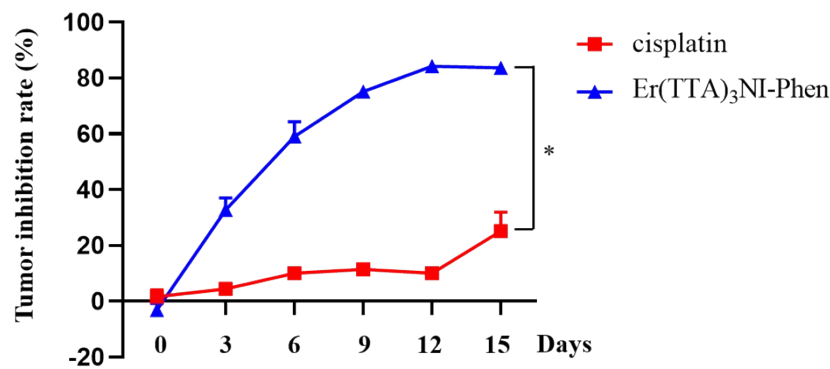
**Figure S20.** Cells apoptosis (a) and cells cycle (b) induced by cisplatin ( $5 \mu\text{M}$ ) and Er(TTA)<sub>3</sub>NI-

Phen (1  $\mu$ M). control group: equal volume DMSO.

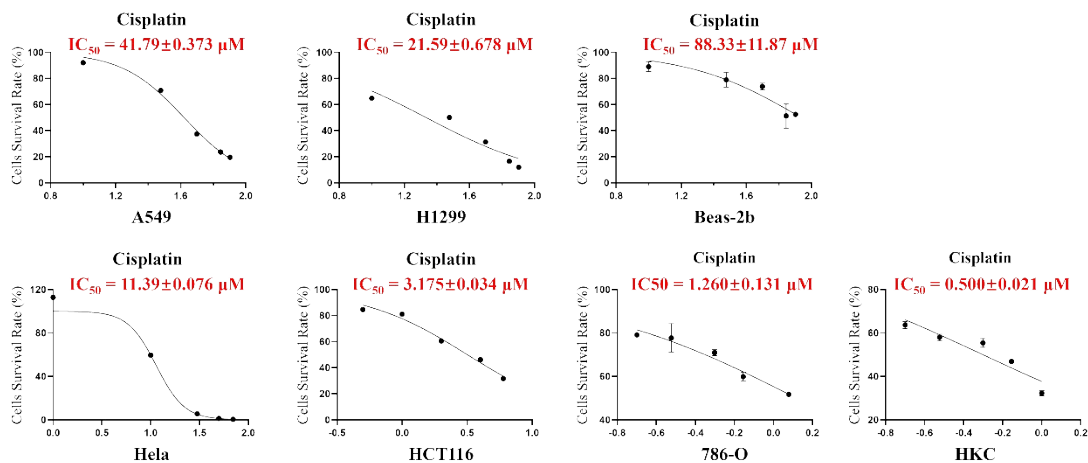


**Figure S21.** Raw data associated with the WB data provided in Fig. 8 (d). (a): Caspase-9 protein.

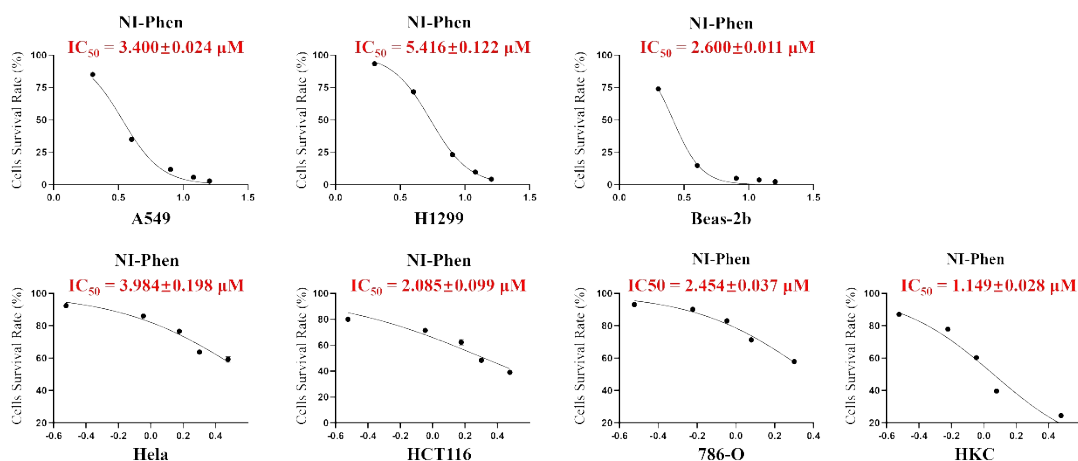
(b): Bcl-2 protein. (c): Bax protein. (d): Cyclin B1 protein. (e): *p*-CDK1 protein. The *p*-CDK1 protein and GAPDH protein are very similar in size, and markers cannot accurately separate the two proteins. So first, stain the GAPDH protein imprint with GAPDH antibody, then wash it off with eluent, and re-incubate *p*-CDK1 antibody on the same band to stain *p*-CDK1 protein. Lane 1, 2, 3: A549 cells treated with DMSO, cisplatin, Er(TTA)<sub>3</sub>NI-Phen. Lane 4, 5, 6: H1299 cells treated with DMSO, cisplatin, Er(TTA)<sub>3</sub>NI-Phen. Lane 7, 8, 9: Beas-2b cells treated with DMSO, cisplatin, Er(TTA)<sub>3</sub>NI-Phen.



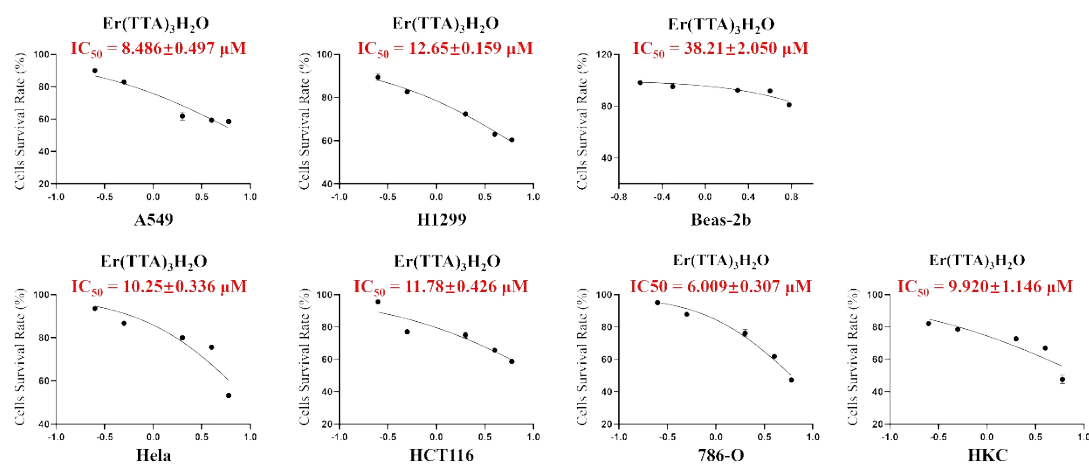
**Figure S22.** Tumor inhibition rates of mice injected with cisplatin and Er(TTA)<sub>3</sub>NI-Phen. Value graphed as means  $\pm$  SD (n=5). \* $P$ <0.05 vs cisplatin.



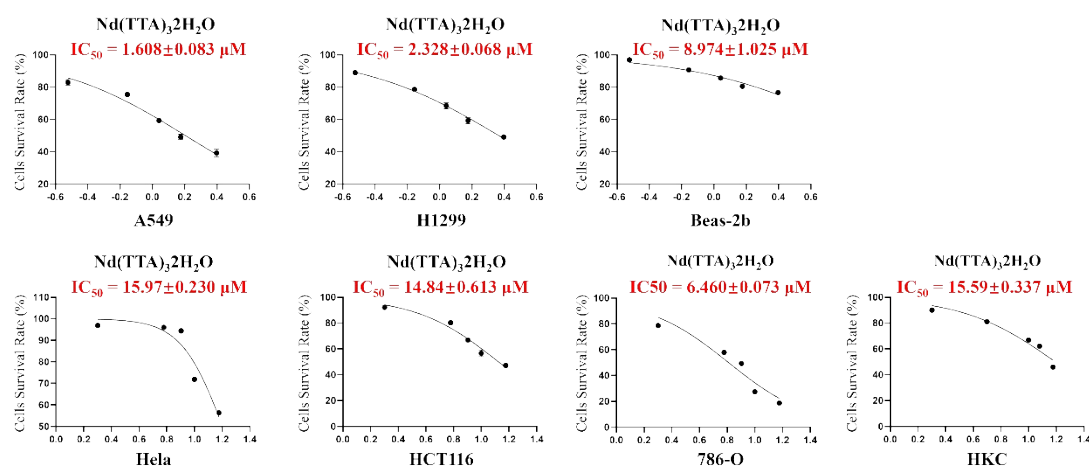
**Figure S23.** The curve fits of dose survival curves on cisplatin against seven cells.



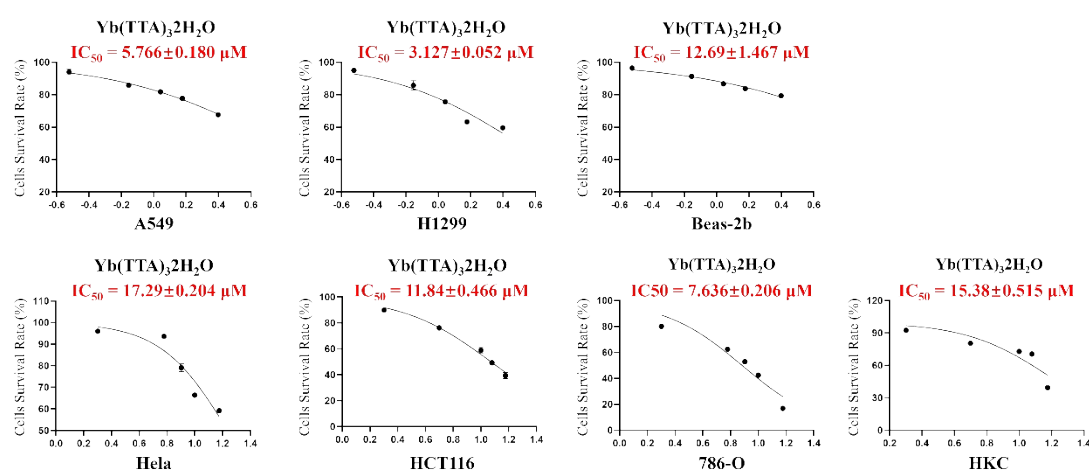
**Figure S24.** The curve fits of dose survival curves on NI-Phen against seven cells.



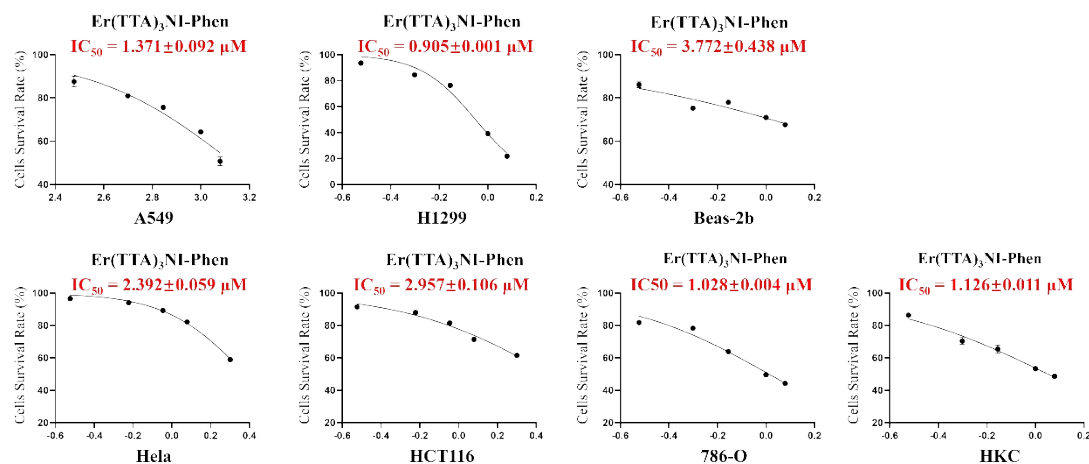
**Figure S25.** The curve fits of dose survival curves on  $\text{Er}(\text{TTA})_3\text{H}_2\text{O}$  against seven cells.



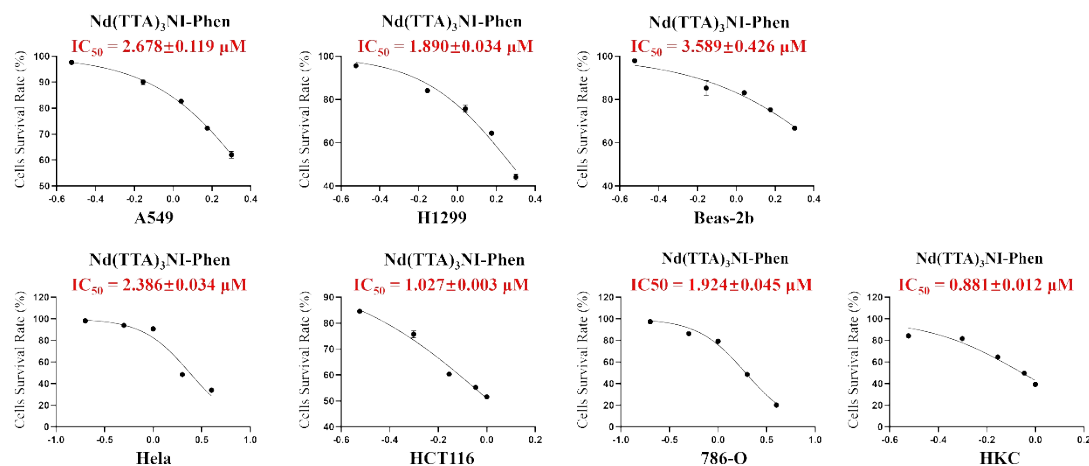
**Figure S26.** The curve fits of dose survival curves on  $\text{Nd}(\text{TTA})_32\text{H}_2\text{O}$  against seven cells.



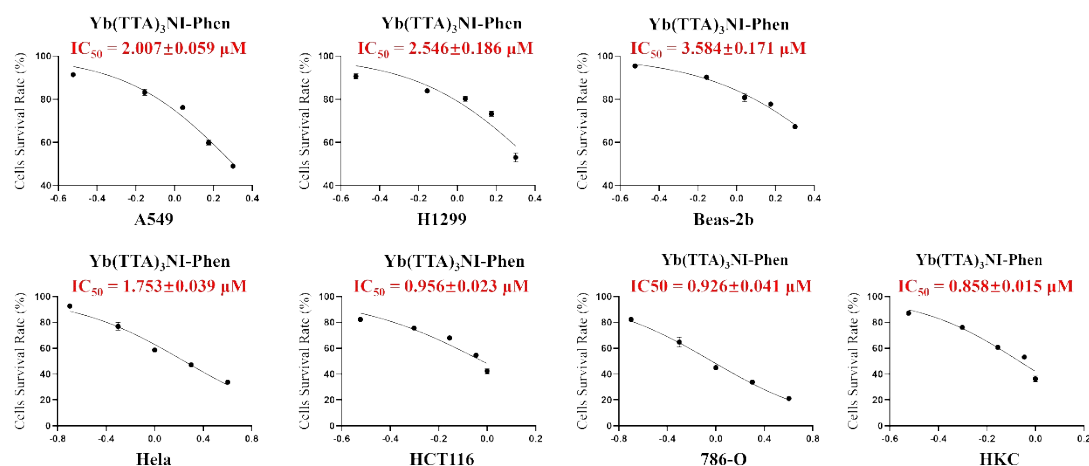
**Figure S27.** The curve fits of dose survival curves on  $\text{Yb}(\text{TTA})_32\text{H}_2\text{O}$  against seven cells.



**Figure S28.** The curve fits of dose survival curves on  $\text{Er}(\text{TTA})_3\text{NI-Phen}$  against seven cells.

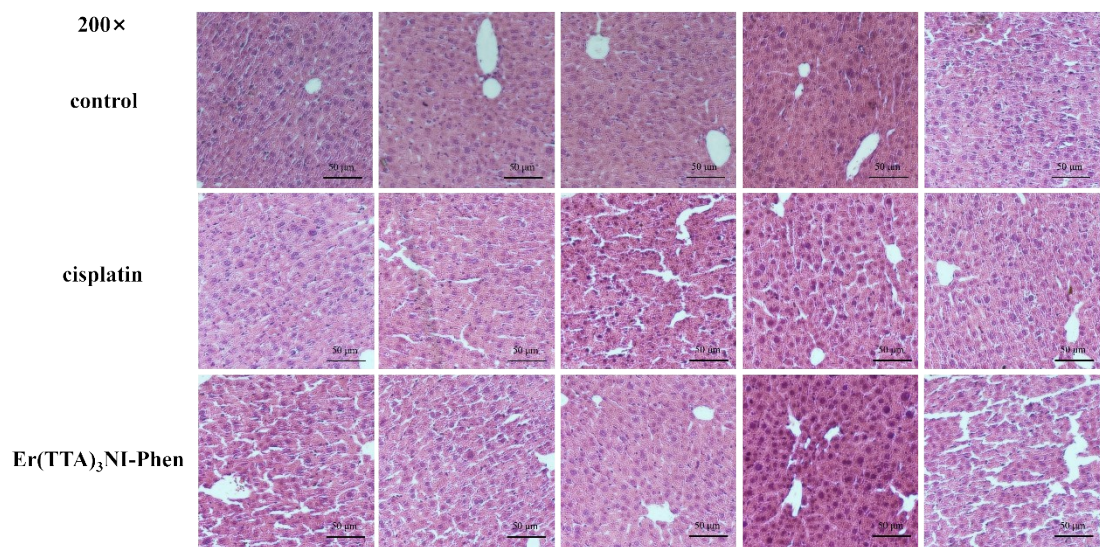


**Figure S29.** The curve fits of dose survival curves on  $\text{Nd}(\text{TTA})_3\text{NI-Phen}$  against seven cells.

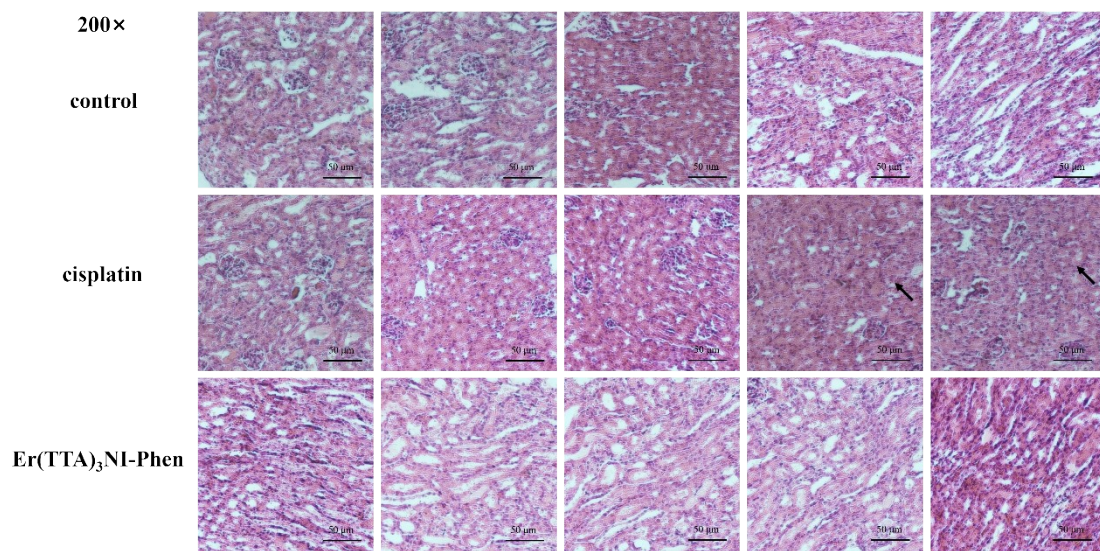


**Figure S30.** The curve fits of dose survival curves on  $\text{Yb}(\text{TTA})_3\text{NI-Phen}$  against seven cells.





**Figure S31.** HE staining images of liver tissues from each group. The magnification is 200 times, and each group consists of liver tissue from 5 mice.



**Figure S32.** HE staining images of kidney tissues in each group. The magnification is 200 times, and each group consists of kidney tissue from 5 mice. The black arrow marked the disappearance of normal glomerular structure and renal interstitial edema.

**Table S1.** The 95% Confidence Interval of Hill Slope and IC<sub>50</sub> value in Table 1.

Groups	95% CI <sup>a</sup>	A549	H1299	Beas-2b
cisplatin	Hill Slope	-3.103 to -1.642	-2.285 to -0.429	-3.161 to -0.408



	IC <sub>50</sub>	36.40 to 46.99	7.349 to 36.21	62.32 to 304.3
	Hill Slope	-4.878 to -1.922	-3.256 to -2.636	-5.823 to -2.710
NI-Phen	IC <sub>50</sub>	2.909 to 3.975	5.172 to 5.669	2.332 to 2.910
	Hill Slope	-0.944 to -0.234	-0.631 to -0.403	-6.433 to -0.094
Er(TTA) <sub>3</sub> H <sub>2</sub> O	IC <sub>50</sub>	4.180 to 67.92	8.994 to 20.80	7.416 to infinity
	Hill Slope	-1.554 to -0.686	-1.211 to -0.859	-1.315 to -0.520
Nd(TTA) <sub>3</sub> 2H <sub>2</sub> O	IC <sub>50</sub>	1.288 to 2.174	2.066 to 2.702	4.981 to 32.80
	Hill Slope	-1.057 to -0.752	-1.839 to -0.529	-1.072 to -0.567
Yb(TTA) <sub>3</sub> 2H <sub>2</sub> O	IC <sub>50</sub>	4.661 to 7.648	2.145 to 8.796	7.390 to 31.50
	Hill Slope	-2.471 to -0.797	-6.579 to -2.248	-1.233 to -0.191
Er(TTA) <sub>3</sub> NI-Phen	IC <sub>50</sub>	1.093 to 2.268	0.786 to 1.003	1.803 to 246.1
	Hill Slope	-1.884 to -1.529	-3.034 to -1.178	-2.013 to -0.735
Nd(TTA) <sub>3</sub> NI-Phen	IC <sub>50</sub>	2.510 to 2.869	1.631 to 2.452	2.529 to 7.471
	Hill Slope	-2.497 to -0.930	-3.951 to -0.367	-1.828 to -0.900
Yb(TTA) <sub>3</sub> NI-Phen	IC <sub>50</sub>	1.671 to 2.855	1.757 to 22.52	2.763 to 5.645

<sup>a</sup> The 95% Confidence Interval (95% CI) represents a 95% confidence level that the interval contains the true range of Hill Slope and IC<sub>50</sub> value.

**Table S2.** The 95% Confidence Interval of Hill Slope and IC<sub>50</sub> value in Table 2.

Groups	95% CI <sup>a</sup>	Hela	HCT116	786-O	HKC
cisplatin	Hill Slope	-infinity to -1.303	-1.458 to -0.769	-1.111 to -0.491	-1.295 to -0.216
	IC <sub>50</sub>	7.535 to 16.75	2.545 to 4.079	0.974 to 2.351	0.301 to 0.933

Ni-Phen	Hill Slope	-1.833 to -0.590	-1.662 to -0.406	-2.041 to -0.974	-3.087 to -0.749
	IC <sub>50</sub>	2.869 to 8.813	1.459 to 4.055	1.990 to 3.596	0.834 to 1.760
Er(TTA) <sub>3</sub> H <sub>2</sub> O	Hill Slope	-3.882 to -0.142	-1.315 to -0.125	-1.504 to -0.610	-1.283 to -0.041
	IC <sub>50</sub>	4.760 to 9404	4.783 to 7444	4.550 to 9.669	3.421 to infinity
Nd(TTA) <sub>3</sub> 2H <sub>2</sub> O	Hill Slope	-6.088 to -1.036	-2.229 to -0.880	-3.898 to -0.590	-2.668 to -0.615
	IC <sub>50</sub>	12.90 to 34.59	11.07 to 18.40	3.809 to 9.171	12.08 to 29.29
Yb(TTA) <sub>3</sub> 2H <sub>2</sub> O	Hill Slope	-3.551 to -0.591	-1.875 to -0.987	-4.172 to -0.531	-12.35 to -0.049
	IC <sub>50</sub>	12.77 to 64.54	10.35 to 13.86	4.620 to 11.41	9.721 to infinity
Er(TTA) <sub>3</sub> Ni-Phen	Hill Slope	-2.679 to -1.669	-1.621 to -0.764	-2.126 to -0.920	-1.640 to -0.912
	IC <sub>50</sub>	2.154 to 2.783	2.252 to 4.960	0.876 to 1.320	0.981 to 1.377
Nd(TTA) <sub>3</sub> Ni-Phen	Hill Slope	-3.970 to -0.810	-1.874 to -1.017	-2.505 to -1.260	-4.302 to -1.035
	IC <sub>50</sub>	1.616 to 4.241	0.911 to 1.236	1.606 to 2.318	0.745 to 1.193
Yb(TTA) <sub>3</sub> Ni-Phen	Hill Slope	-1.284 to -0.662	-3.329 to -0.638	-1.138 to 0.774	-3.538 to -1.100
	IC <sub>50</sub>	1.331 to 2.429	0.768 to 1.731	0.783 to 1.093	0.731 to 1.098

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