

## Electronic Supplementary Information

### **A molecular switch with varying gated photochromism**

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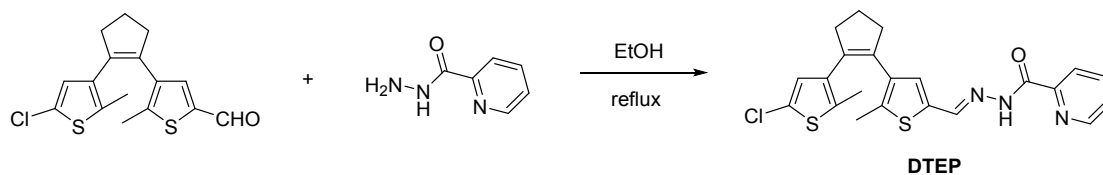
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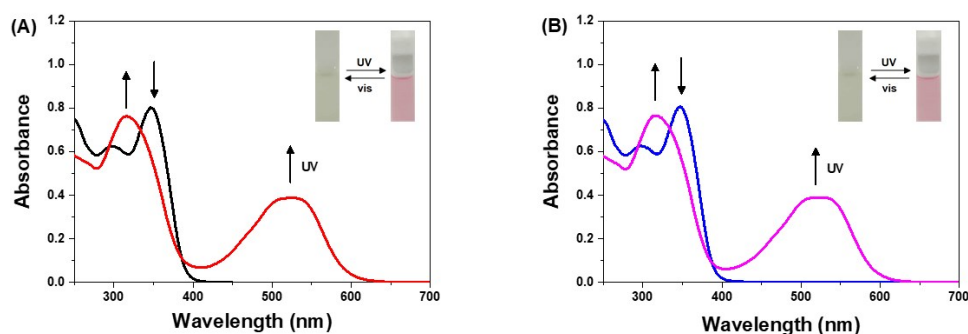
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## Supplementary scheme and figures

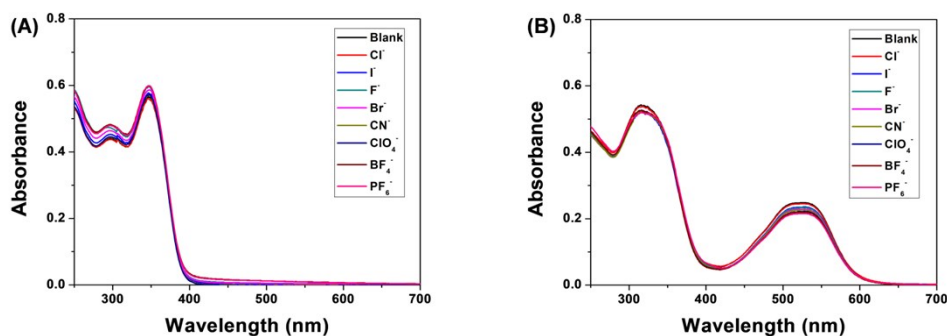


**Scheme S1.** Synthesis route of compound **DTEP**.

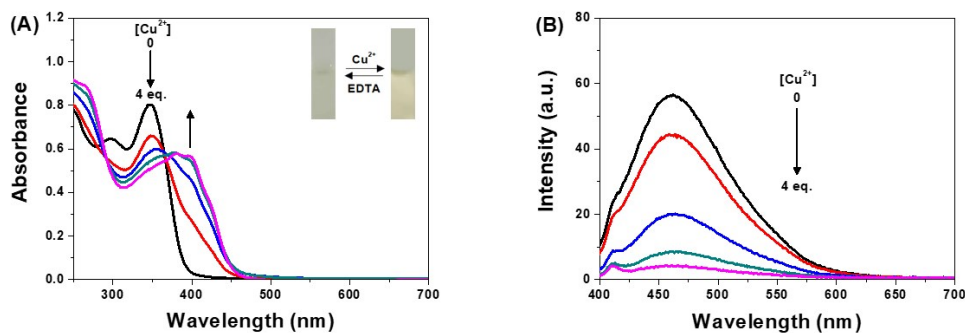


**Figure S1.** The UV-vis absorption spectral changes of compound **DTEP** (10  $\mu\text{M}$ ) upon alternative irradiation with UV and visible light in MeOH solution at 25 $^{\circ}\text{C}$ : **(A)** the original solution; **(B)** the solution heated at 338 K for 48 h.

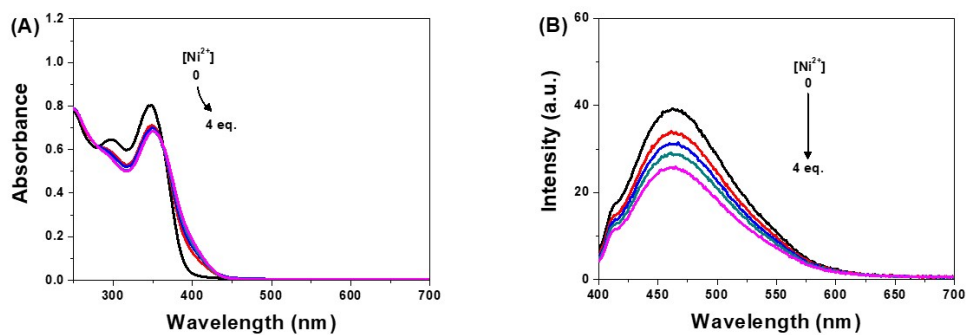
The irradiated solution still exhibited the similar photochromic behaviors in comparison with the original solution, indicating that compound **DTEP** possessed the good thermal stability.



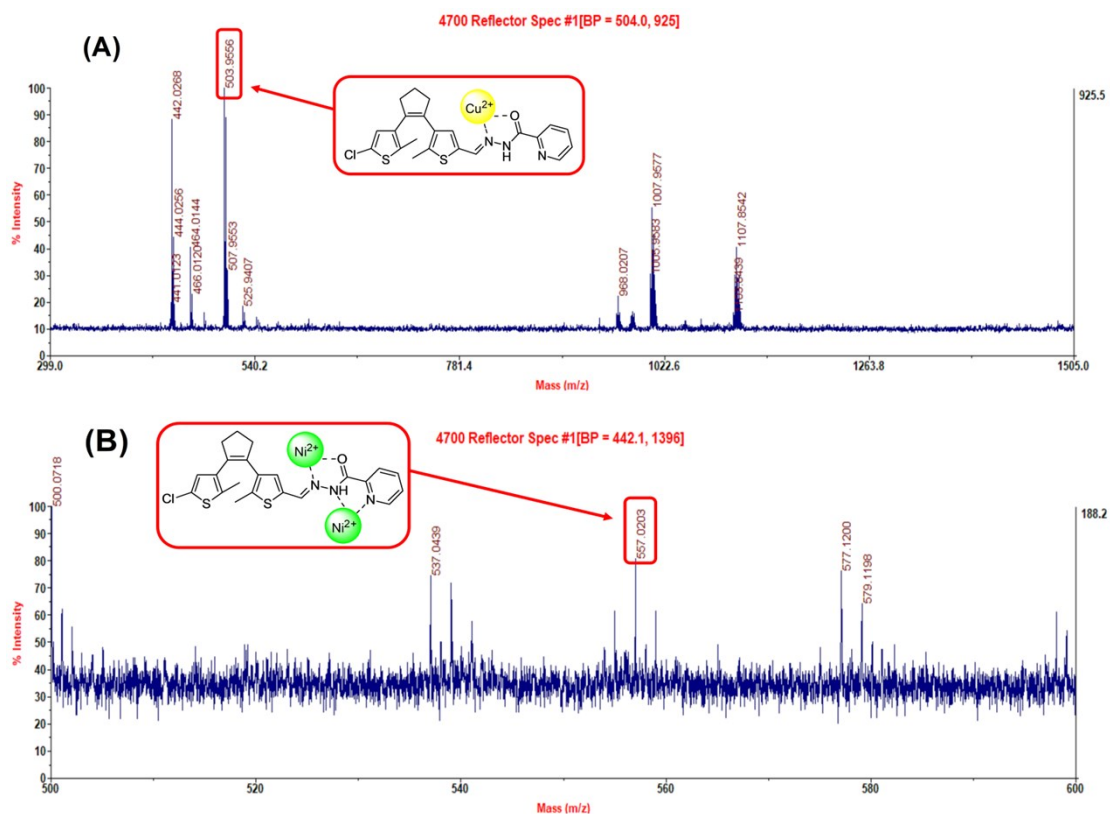
**Figure S2.** The UV-vis absorption changes of **(A)** compound **DTEP** (10  $\mu\text{M}$ ) and **(B)** its photostationary state with various anions (40  $\mu\text{M}$ ) in MeOH solution at 25  $^{\circ}\text{C}$ .



**Figure S3.** UV-vis absorption (A) and fluorescence changes (B) of compound **DTEP** (10 μM) with the addition of Cu<sup>2+</sup> (0-40 μM) in MeOH solution at 25° C.  $\lambda_{\text{ex}} = 365$  nm, slits: 5 nm/ 5 nm. Inset: the corresponding photographic images upon irradiation with UV and visible light.



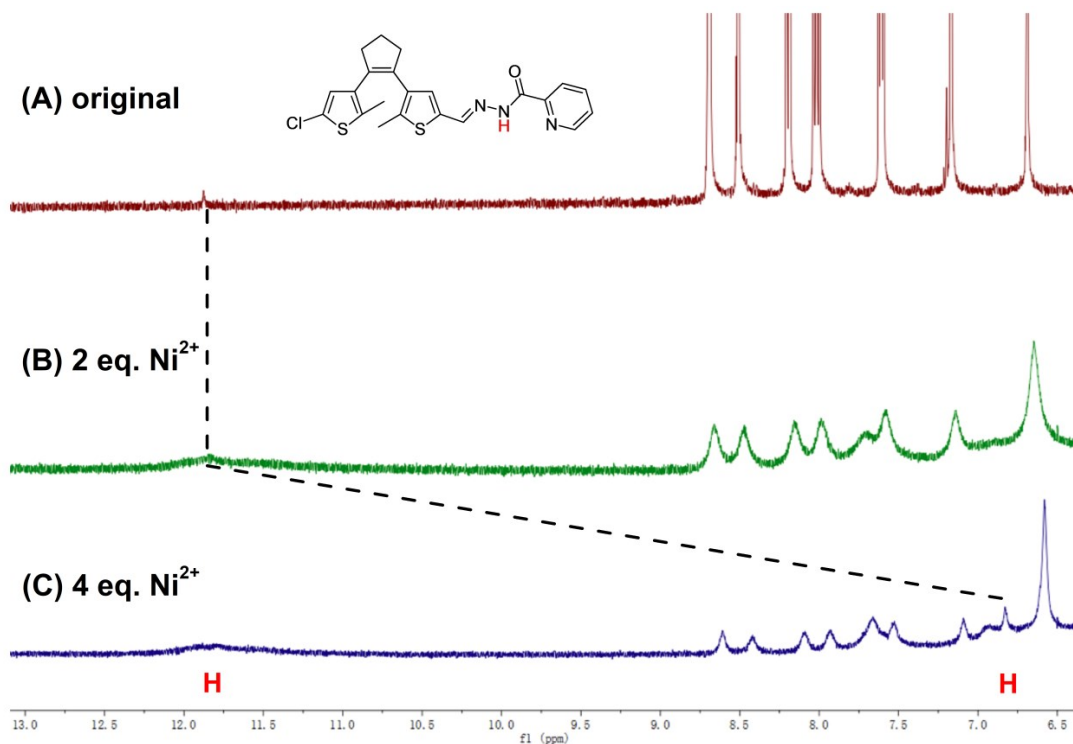
**Figure S4.** UV-vis absorption (A) and fluorescence changes (B) of compound **DTEP** (10 μM) with the addition of Ni<sup>2+</sup> (0-40 μM) in MeOH solution at 25° C.  $\lambda_{\text{ex}} = 365$  nm, slits: 5 nm/ 5 nm.



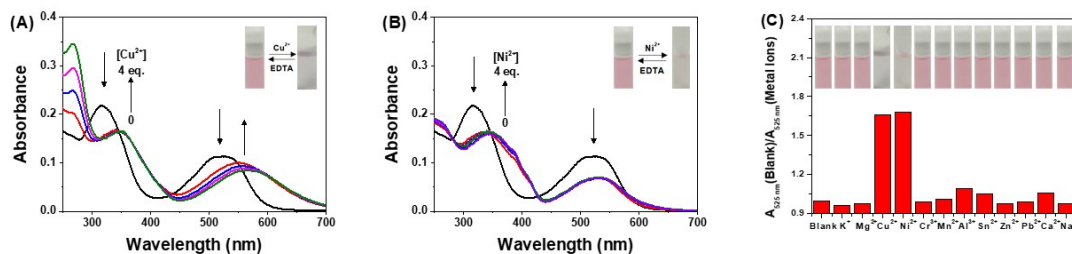
**Figure S5.** MS (MALDI-TOF) of compound **DTEP** (10  $\mu\text{M}$ ) with  $\text{Cu}^{2+}$  (**A**) and  $\text{Ni}^{2+}$  (**B**) ions (40  $\mu\text{M}$ ) in MeOH solution at 25  $^{\circ}\text{C}$ .

When 4.0 equiv. of  $\text{Cu}^{2+}$  ions was added to the **DTEP** solution, a new peak appeared at  $m/z$  503.9556 (Figure S4A) that was attributed to the [**DTEP**+ $\text{Cu}^{2+}$ ] adduct (the calculated value was 504.0121), suggesting the complex of **DTEP** and  $\text{Cu}^{2+}$  ions with a binding stoichiometry of 1:1.

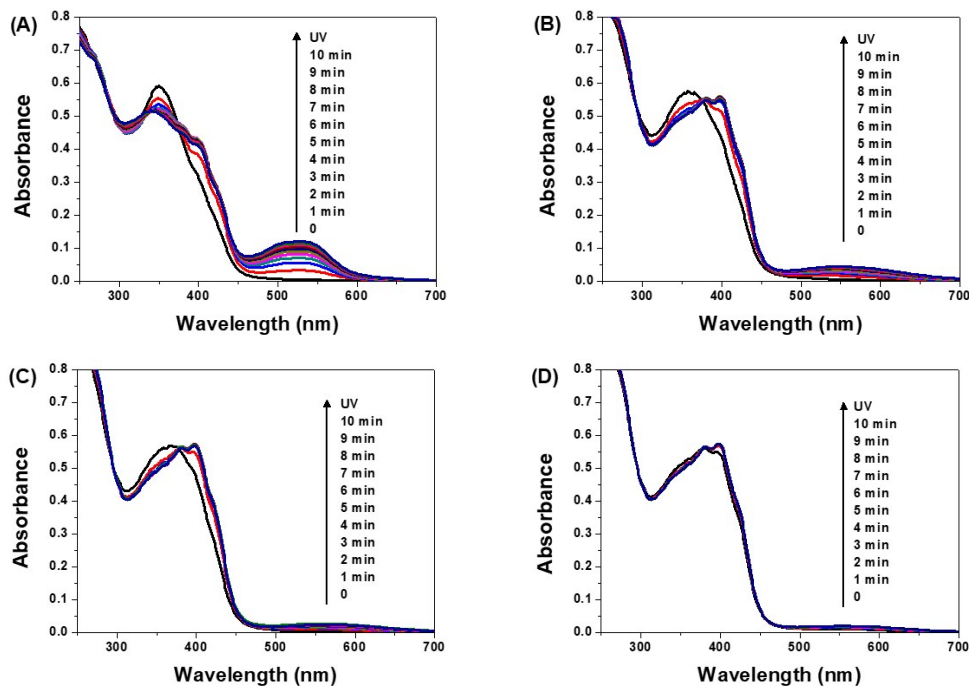
When 4.0 equiv. of  $\text{Ni}^{2+}$  ions was added to the **DTEP** solution, a new peak appeared at  $m/z$  557.0203 (Figure S4B) that was attributed to the [ $\text{Ni}^{2+}$ +**DTEP**+ $\text{Ni}^{2+}$ ] adduct (the calculated value was 556.9421), suggesting the complex of **DTEP** and  $\text{Ni}^{2+}$  ions with a binding stoichiometry of 1:2.



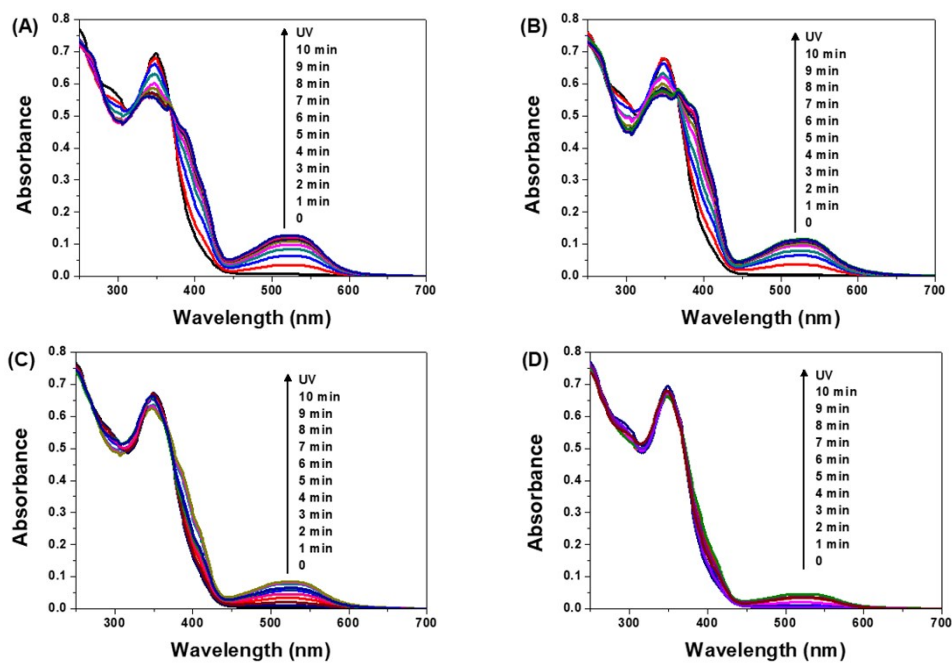
**Figure S6.**  $^1\text{H}$  NMR titration of compound **DTEP** ( $10\ \mu\text{M}$ ) with  $\text{Ni}^{2+}$  ions ( $0$ - $40\ \mu\text{M}$ ) in  $\text{CD}_3\text{OD}$  solution at  $25\ ^\circ\text{C}$ .



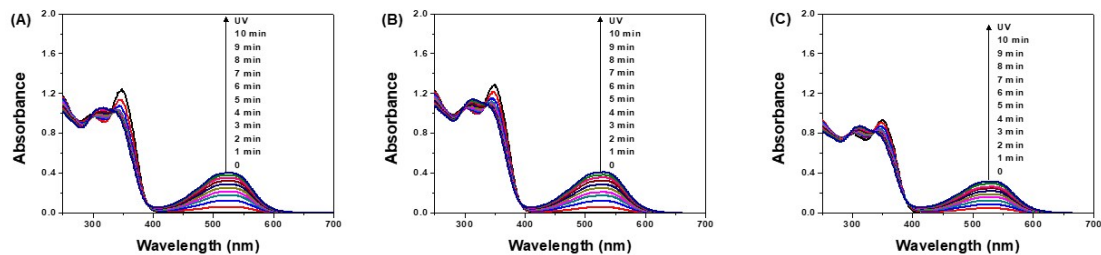
**Figure S7.** The UV-vis absorption changes of compound **DTEP** ( $10\ \mu\text{M}$ ) in the photostationary state upon the titration of (A)  $\text{Cu}^{2+}$  ( $0$ - $40\ \mu\text{M}$ ) and (B)  $\text{Ni}^{2+}$  ( $0$ - $40\ \mu\text{M}$ ) in  $\text{MeOH}$  solution at  $25\ ^\circ\text{C}$ . (C) The ratio of absorbance at  $525\ \text{nm}$  of compound **DTEP** ( $10\ \mu\text{M}$ ) at photostationary state without and with various metal ions ( $40\ \mu\text{M}$ ) in  $\text{MeOH}$  solution at  $25\ ^\circ\text{C}$ . Inset: the corresponding photographic images of compound **DTEP** in the photostationary state with various metal ions.



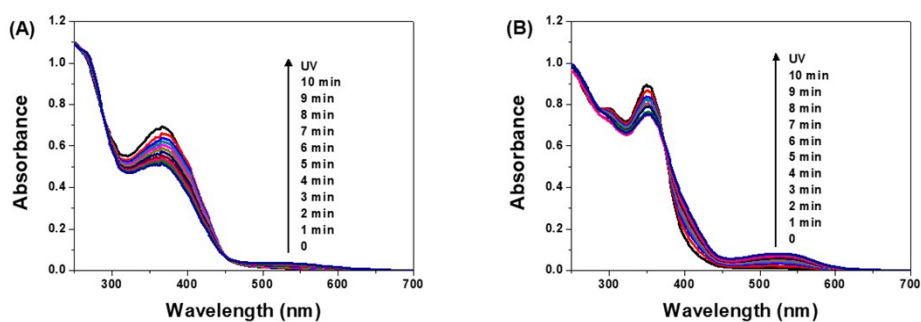
**Figure S8.** UV-vis absorption spectral changes of compound **DTEP** (10  $\mu\text{M}$ ) with different amounts of  $\text{Cu}^{2+}$  upon irradiation with 365 nm light in MeOH solution at 25  $^{\circ}\text{C}$ : **(A)** 1 equiv.; **(B)** 2 equiv.; **(C)** 3 equiv. and **(D)** 4 equiv.



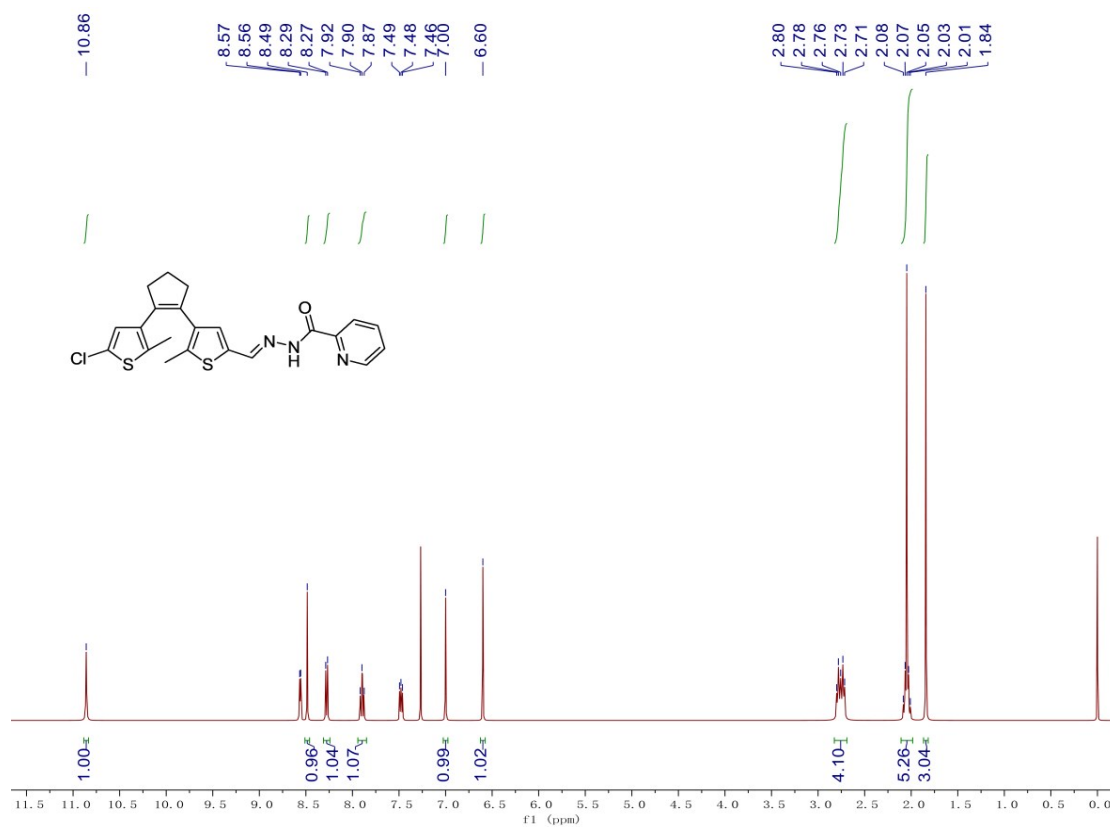
**Figure S9.** UV-vis absorption spectral changes of compound **DTEP** (10  $\mu\text{M}$ ) with different amounts of  $\text{Ni}^{2+}$  upon irradiation with 365 nm light in MeOH solution at 25  $^{\circ}\text{C}$ : **(A)** 1 equiv.; **(B)** 2 equiv.; **(C)** 3 equiv. and **(D)** 4 equiv.



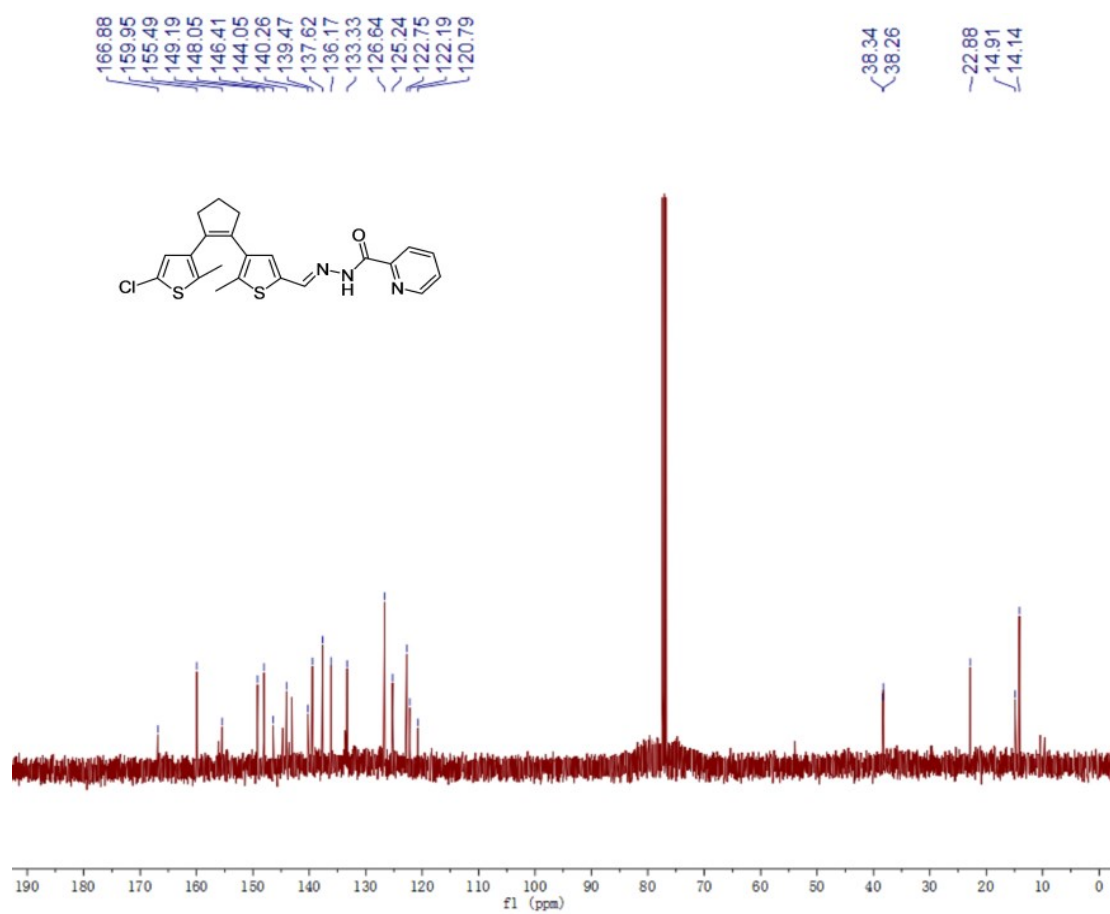
**Figure S10.** UV-vis absorption spectral changes of compound **DTEP** ( $10\ \mu\text{M}$ ) with different proportion of water upon irradiation with 365 nm light in MeOH- $\text{H}_2\text{O}$  solution at  $25\ ^\circ\text{C}$ : **(A)** 9: 1, v/v.; **(B)** 7: 3, v/v and **(C)** 5: 5, v/v.



**Figure S11.** UV-vis absorption spectral changes of compound **DTEP** ( $10\ \mu\text{M}$ ) with **(A)**  $\text{Cu}^{2+}$  ( $40\ \mu\text{M}$ ) and **(B)**  $\text{Ni}^{2+}$  ( $40\ \mu\text{M}$ ) upon irradiation with 365 nm light in MeOH- $\text{H}_2\text{O}$  (5: 5, v/v) solution at  $25\ ^\circ\text{C}$ .



**Figure S12.** <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) spectrum of compound DTEP.



**Figure S13.** <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz) spectrum of compound DTEP.



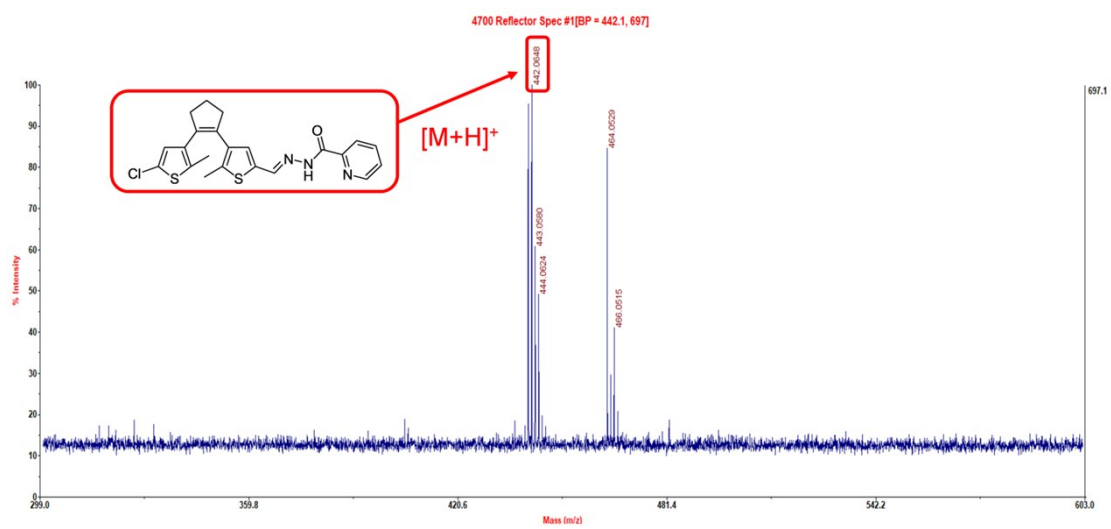


Figure S14. MS (MALDI-TOF) of compound DTEP.