

Supporting Information for

Design and Synthesis of Biotinylated Bivalent Carboline Derivatives

as Potent Anti-tumor Agents

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TableS1. Effect of compound **6** on the *in vivo* tumor growth of S180 mice.

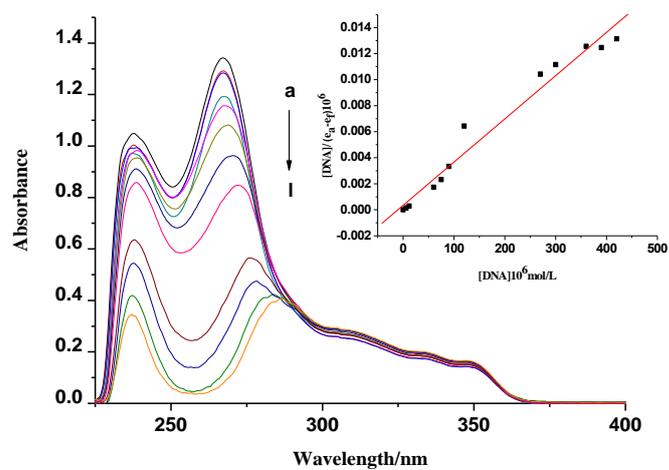
Compound	Tumor weight (mean \pm SD g)	Dose (μ mol/kg)
NS	2.088 \pm 0.471	/
Dox	0.618 \pm 0.170 ^a	2
Compound 2	1.313 \pm 0.256 ^a	8
Compound 5	1.091 \pm 0.321 ^{a, b}	2
Compound 6	0.931 \pm 0.202 ^{a, c, d}	0.2

^a Compared to NS $P < 0.01$.

^b Compared to Compound **2** $P > 0.05$.

^c Compared to Compound **5** $P > 0.05$.

^d Compared to Compound **2** $P < 0.01$.



FigureS1. UV/vis spectra of **6** in the presence of increasing amounts of CT-DNA ($0 \sim 4.2 \times 10^{-4}$ M).

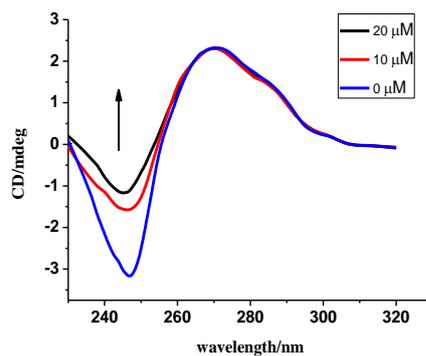


Figure S2. CD spectra of CT-DNA (100 μM) at increasing concentrations of **6** (0, 10, 20 μM) in Tris-HCl buffer (pH = 7.40, C = 0.1 M).



Figure S3. The shade of orange color of complex faded with an increase in the molar ratio of compound **6** to avidin (from left to right, $[\mathbf{6}]/[\text{avidin}] = 0, 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0, 10.0$, respectively.).

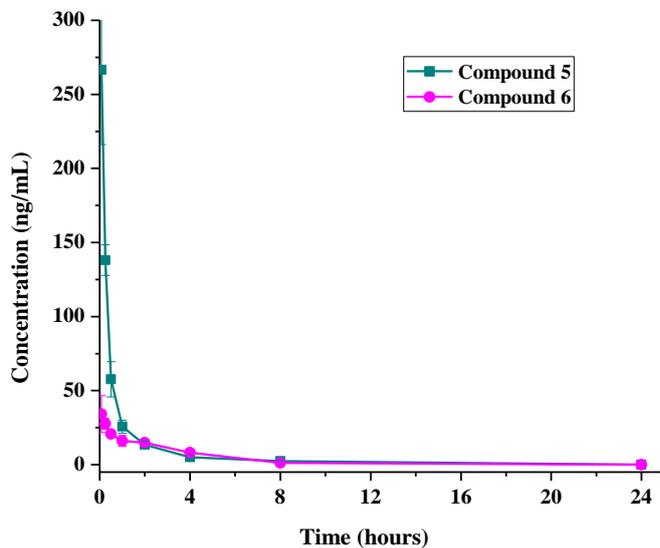


Figure S4. Pharmacokinetic analysis of **5** and **6** in S180 tumor bearing mice.

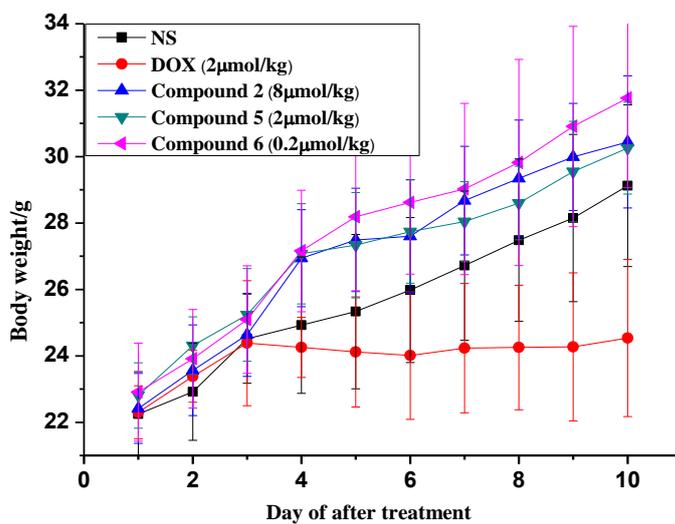


Figure S5. Effect of compound **6** on the body weight of S180 mice, $n = 10$.

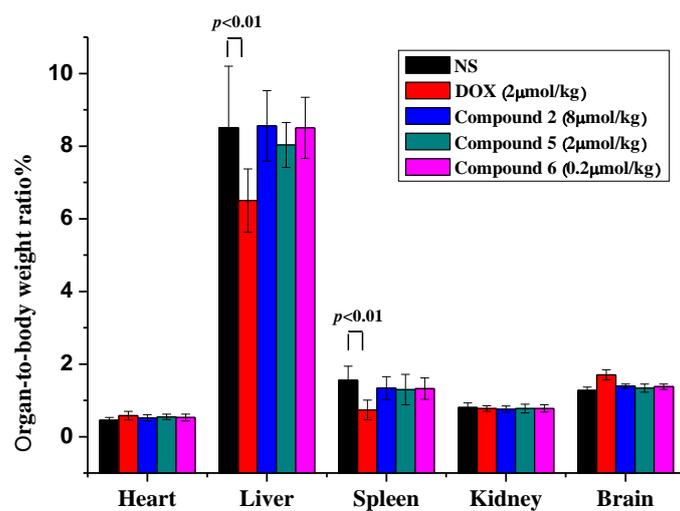


Figure S6. Effect of compound **6** on organ-to-body weight ratio of S180 mice, $n = 10$.

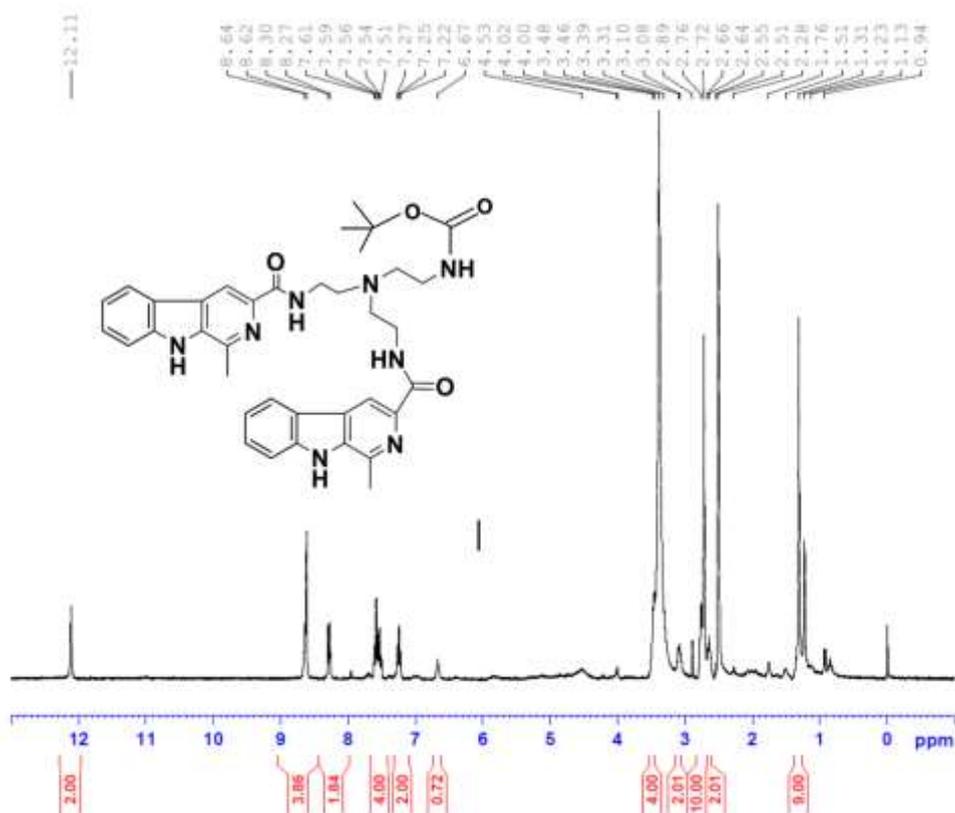


Figure S7. ^1H NMR spectrum (300 MHz) of **4** in $\text{DMSO-}d_6$.

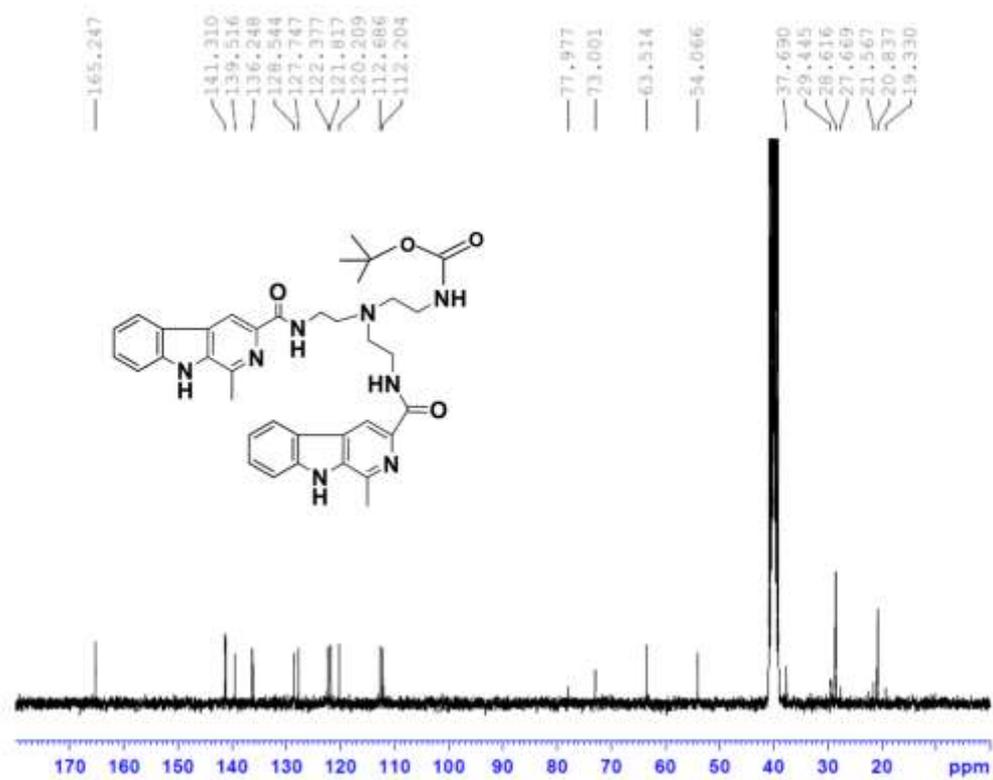


Figure S8. ^{13}C NMR spectrum (75 MHz) of **4** in $\text{DMSO-}d_6$.

Display Report

Analysis Info
Analysis Name: D:\Data\zhengyi\2019072301.d
Method: tune_low_neg20151023.m
Sample Name: sy
Comment:
Acquisition Date: 7/23/2019 2:17:39 PM
Operator: Q-TOF
Instrument: micrOTOF-Q 138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.3 Bar
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Scan End	3000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste

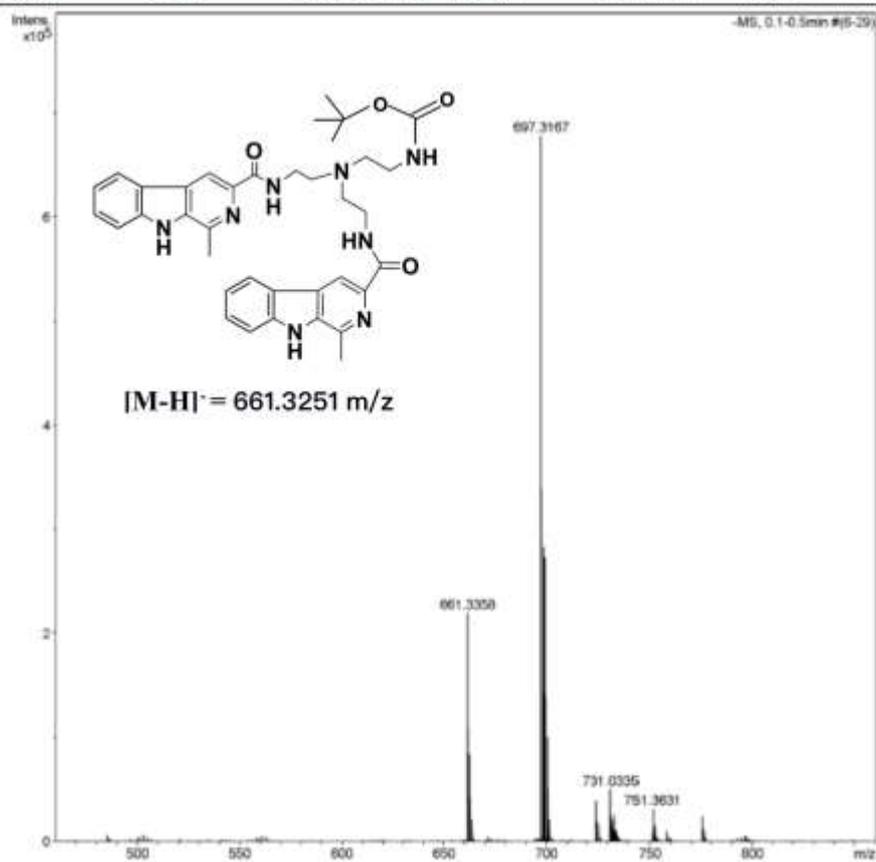


Figure S9. ESI-MS spectrum of 4.

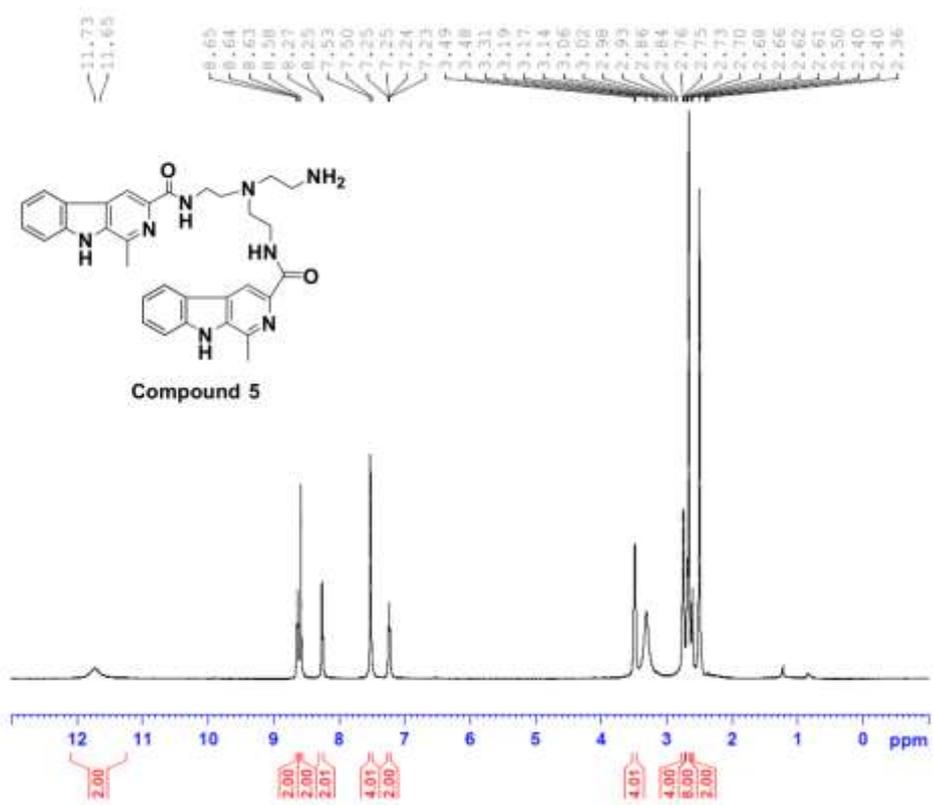


Figure S10. ¹H NMR spectrum (500 MHz) of **5** in DMSO-*d*₆.

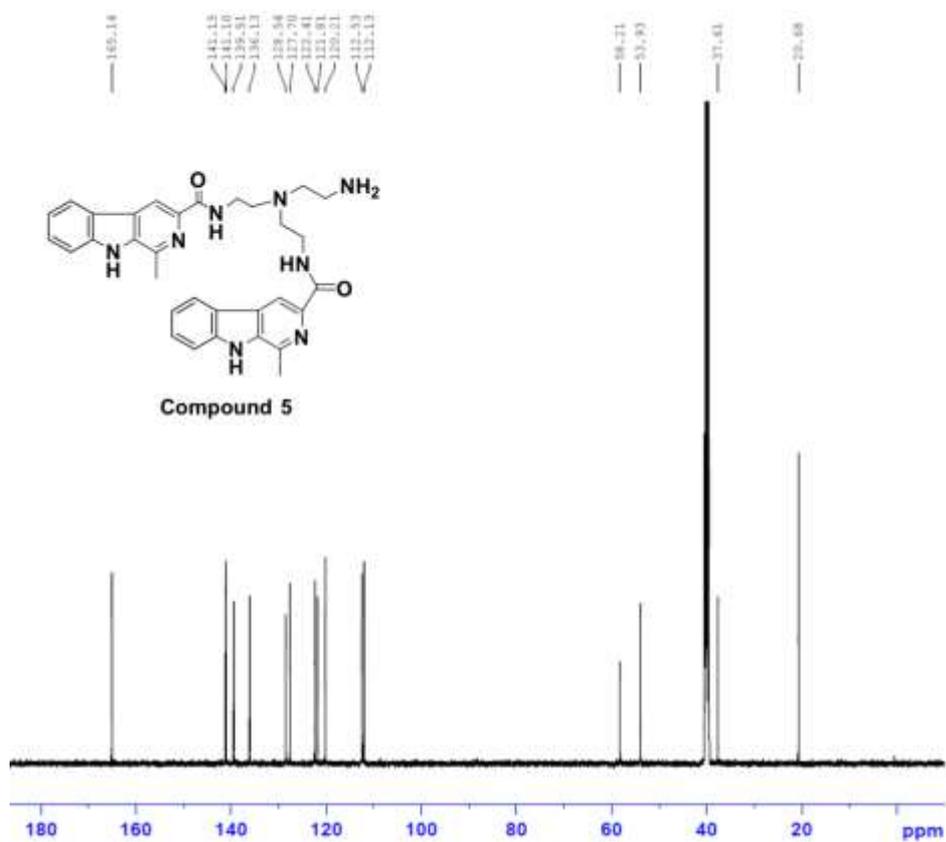


Figure S11. ¹³C NMR spectrum (125 MHz) of **5** in DMSO-d₆.

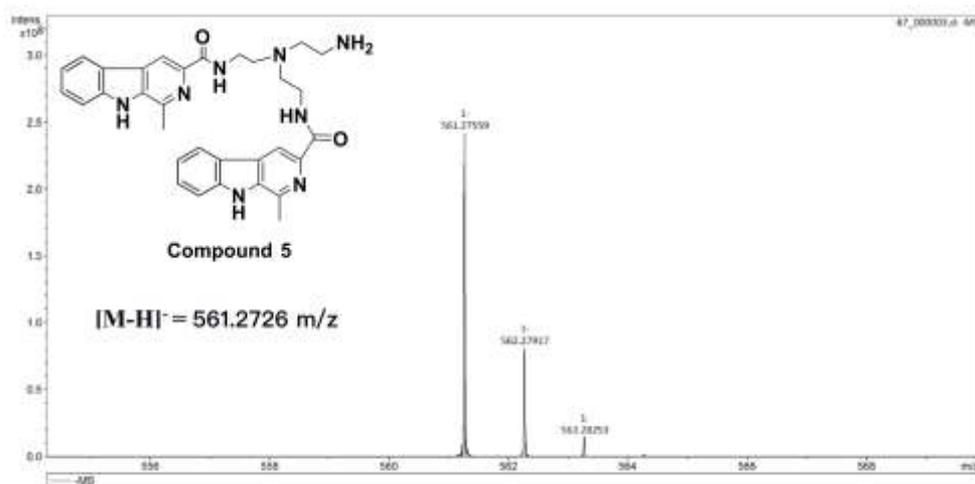


Figure S12. HR-MS spectrum of **5**.

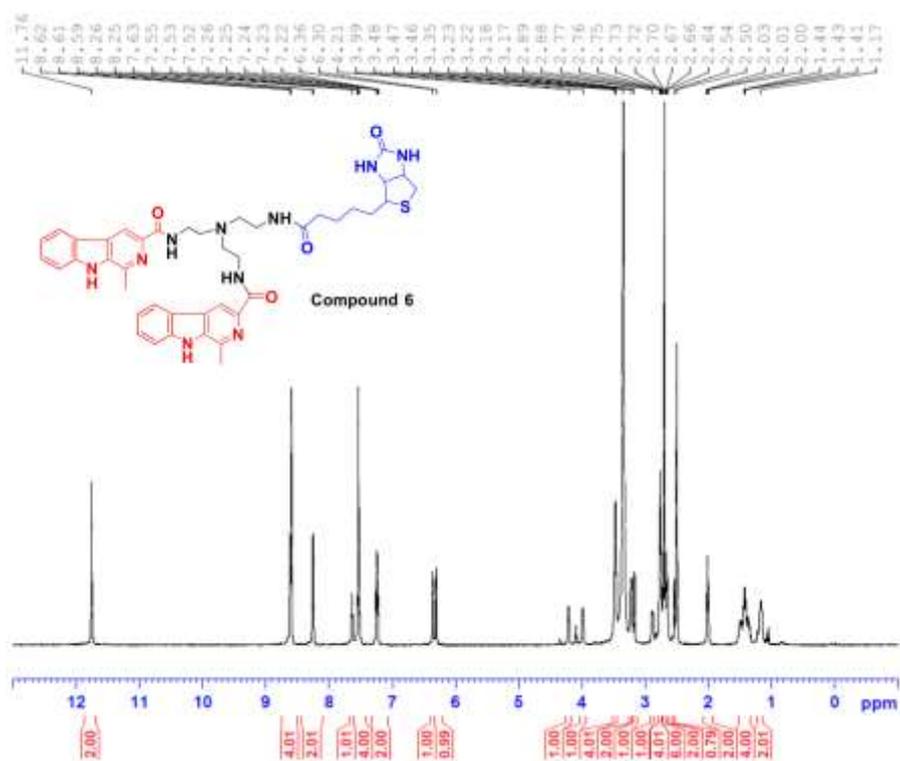


Figure S13. ^1H NMR spectrum (500 MHz) of **6** in $\text{DMSO-}d_6$.

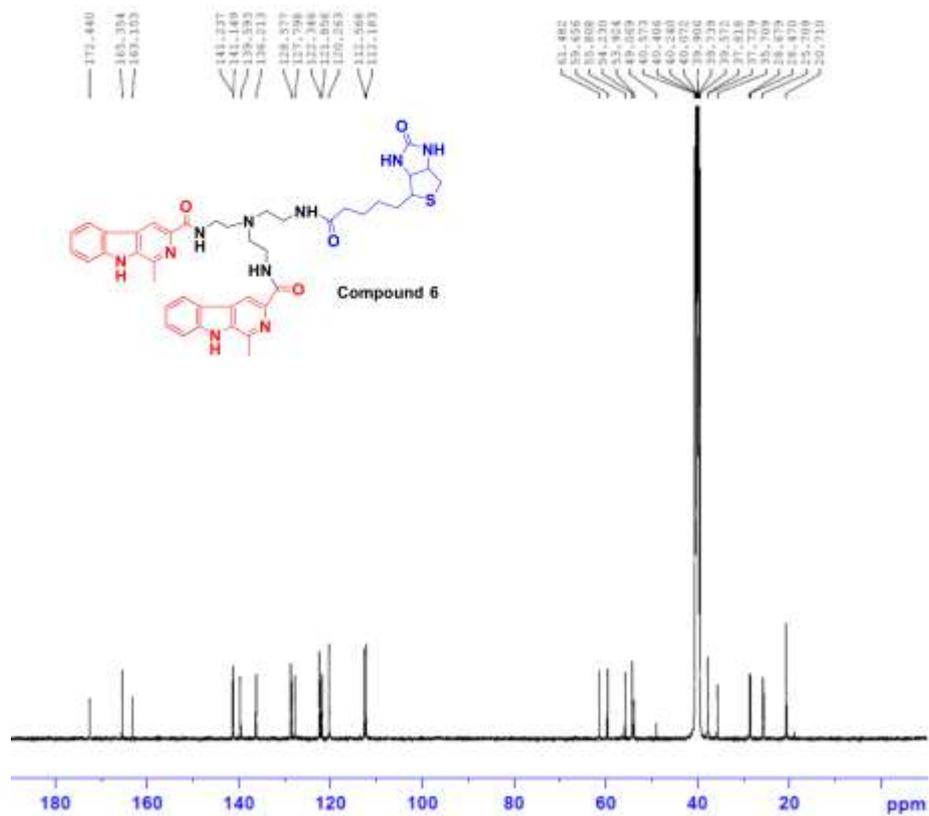


Figure S14. ^{13}C NMR spectrum (125 MHz) of **6** in $\text{DMSO-}d_6$.

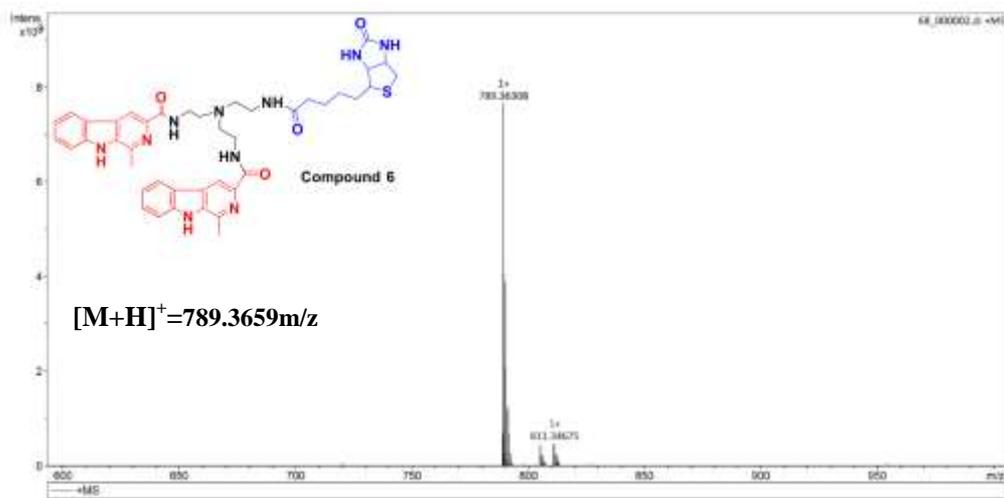


Figure S15. HR-MS spectrum of **6**.