Supplementary Data

Design and Synthesis of Novel Indole Ethylamine Derivatives as a Lipid Metabolism Regulator Targeting PPARα/CPT1 in AML12 Cells

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content

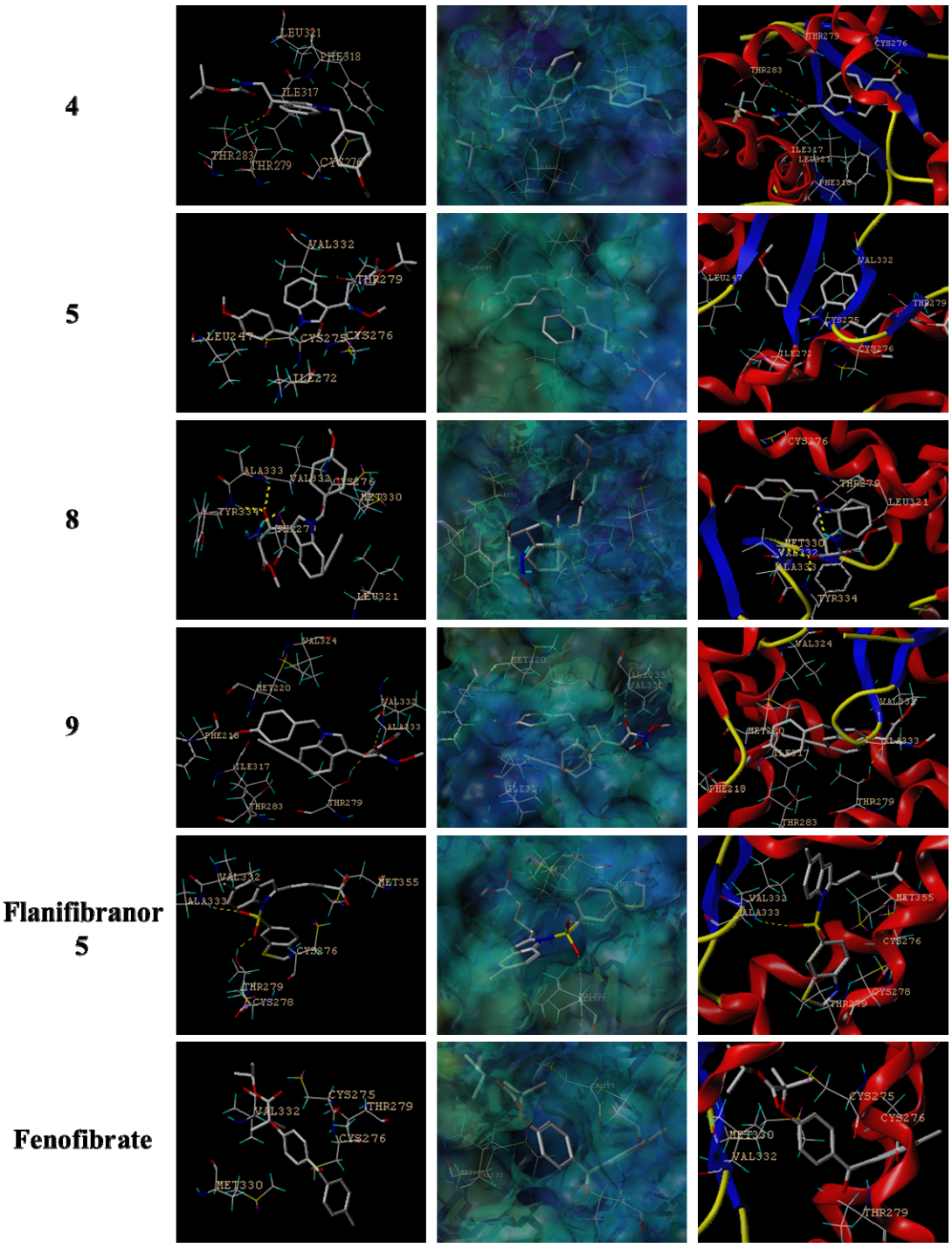

Figure S1. Novel indole-derived structures (**4**, **5**, **8**, **9**), fenofibrate and flanifibranor 5 have comparable high binding affinities to PPARα.

tert-butyl (2-(1-(4-methoxybenzyl)-1H-indol-3-yl)-2-oxoethyl)carbamate of (3)

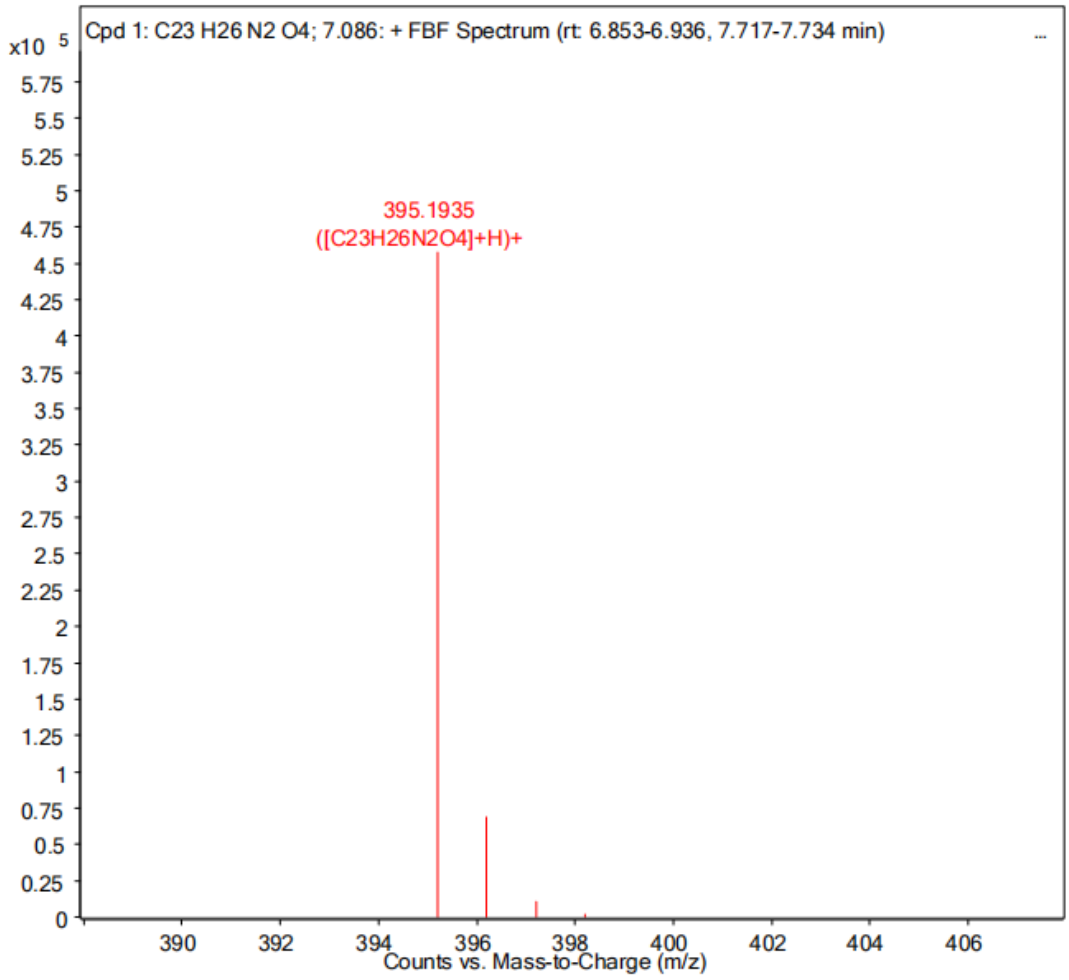

Figure S2. The HRESIMS spectrum of **3**

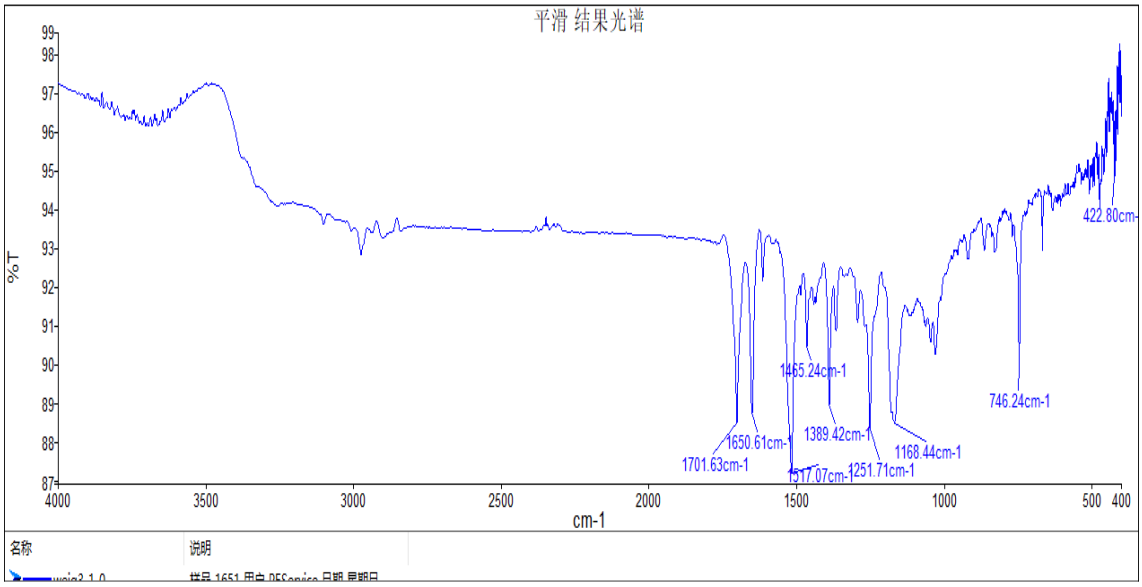

Figure S3. IR (KBr) Spectrum of compound **3**

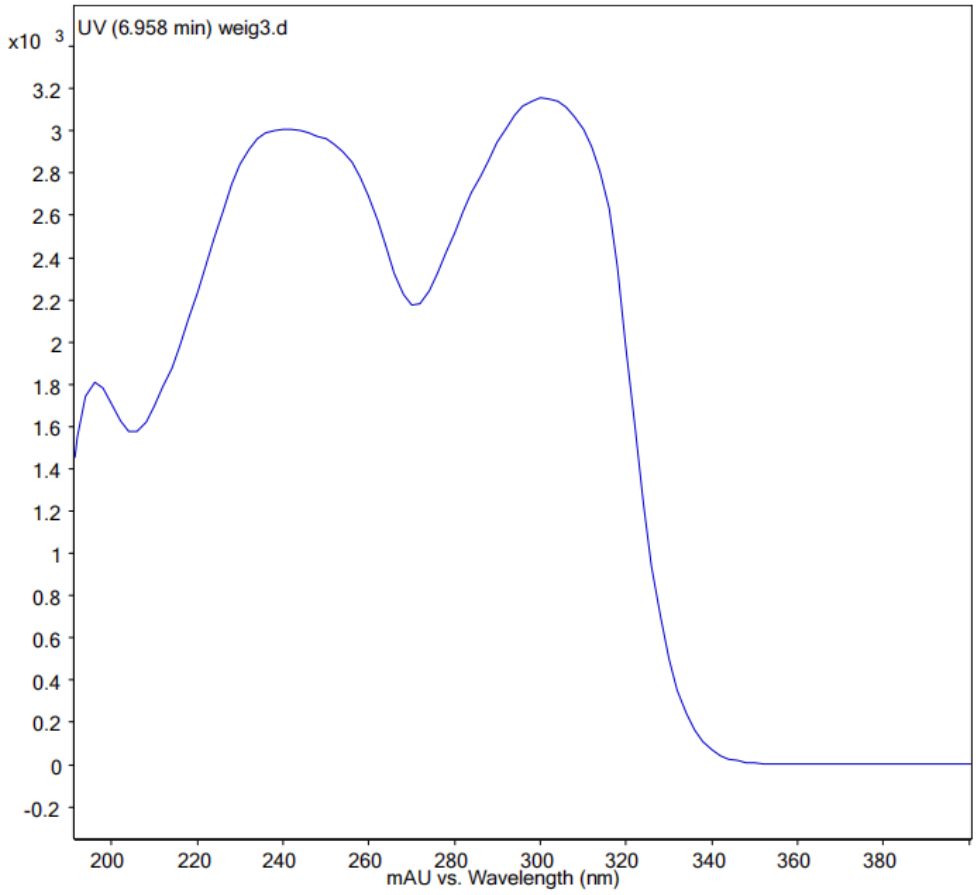

Figure S4. The UV spectrum of **3** (MeOH)

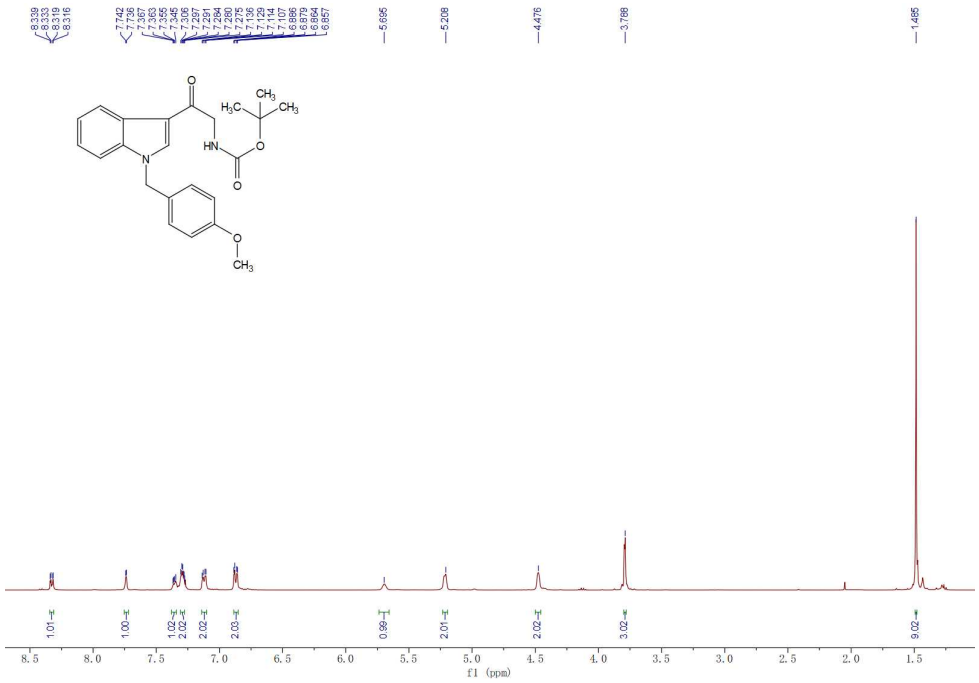

Figure S5. The ^{1}H NMR spectrum (400 MHz, chloroform-*d*) of **3**

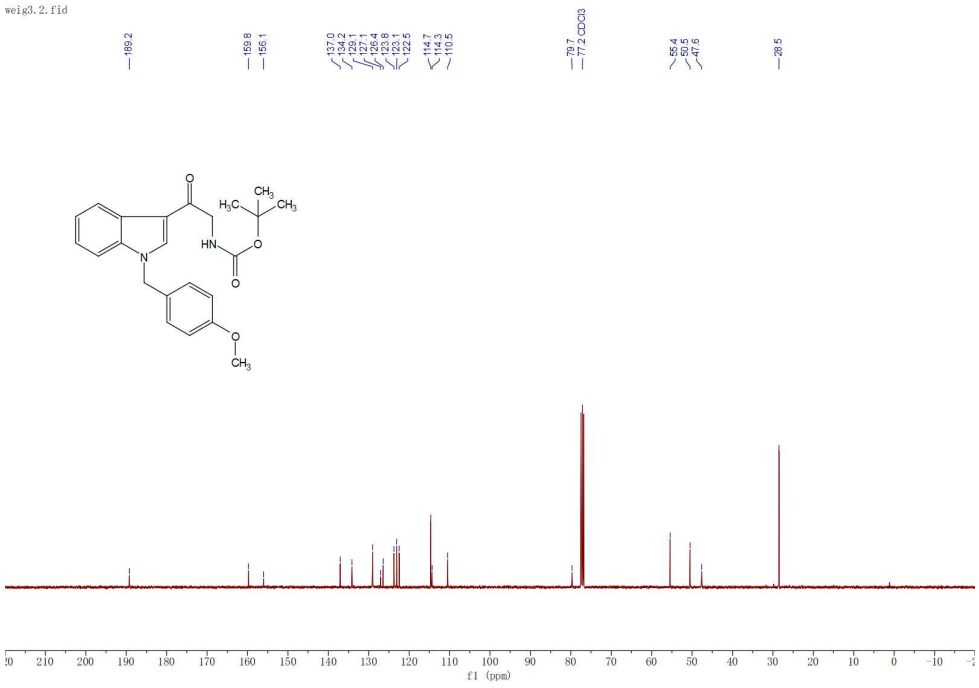

Figure S6. The ^{13}C NMR spectrum (400 MHz, chloroform-*d*) of **3**

tert-butyl (2-hydroxy-2-(1-(4-methoxybenzyl)-1H-indol-3-yl)ethyl)carbamate (4)

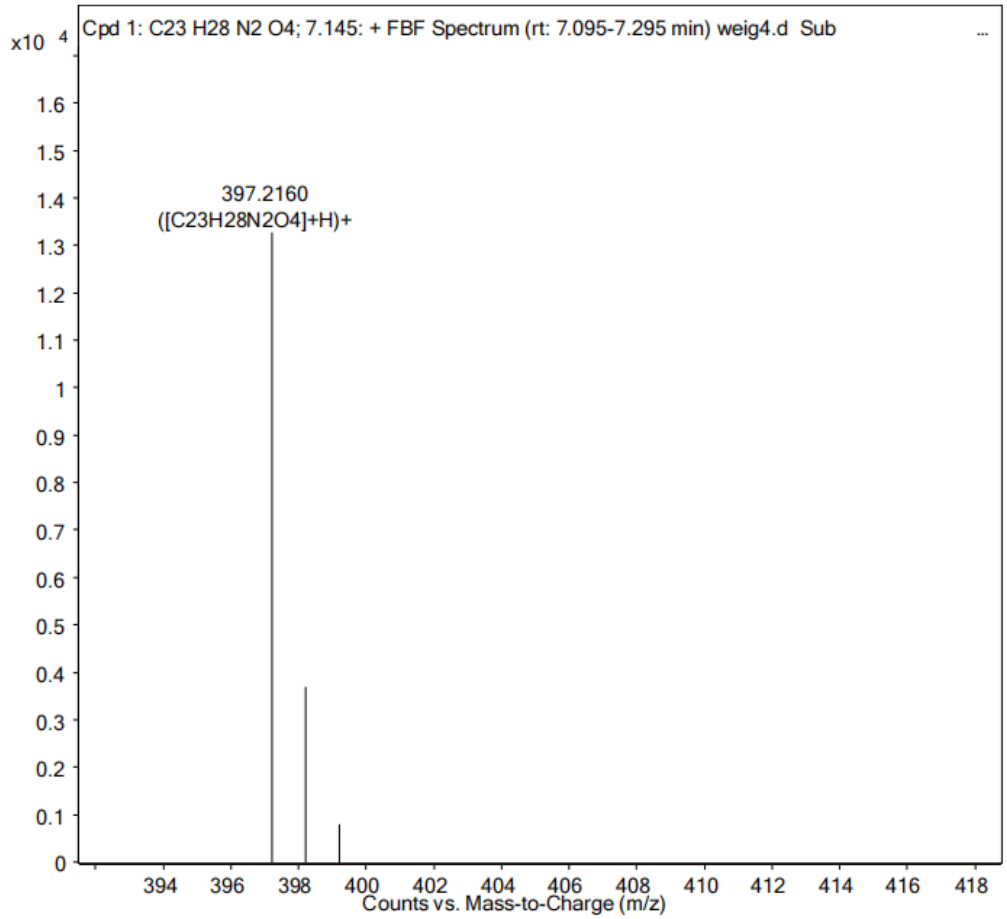

Figure S7. The HRESIMS spectrum of **4**

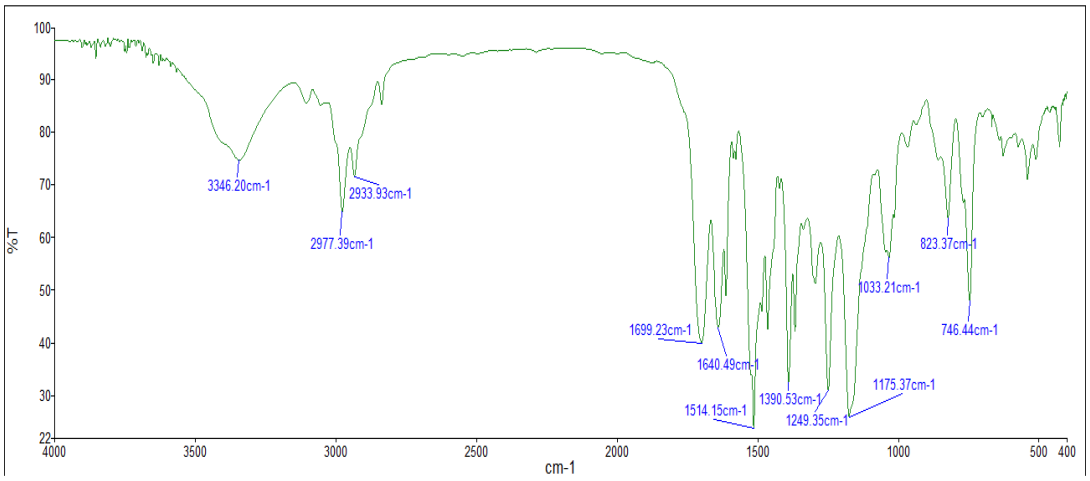

Figure S8. IR (KBr) spectrum of compound **4**

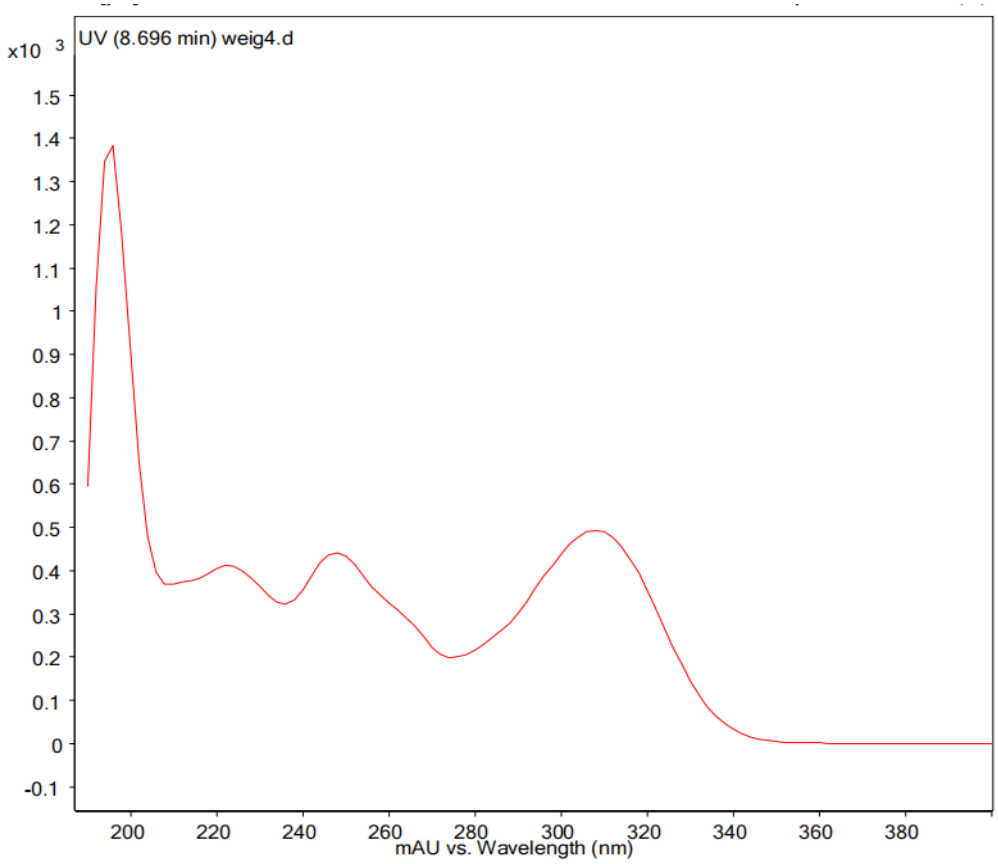

Figure S9. The UV spectrum of **4** (MeOH)

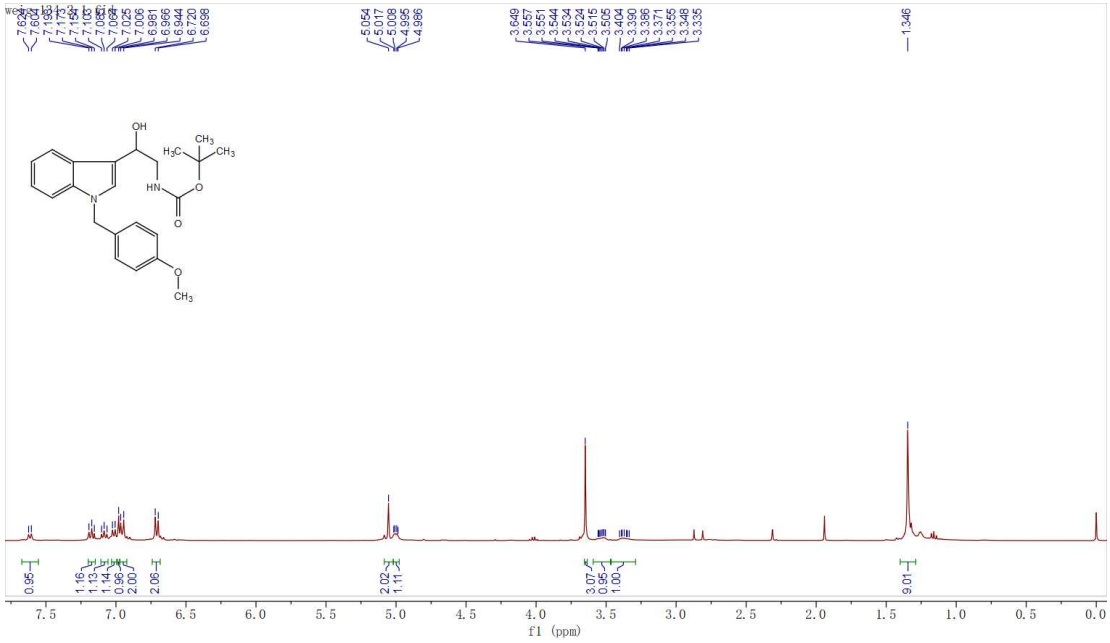

Figure S10. The ^{1}H NMR spectrum (400 MHz, chloroform-*d*) of **4**

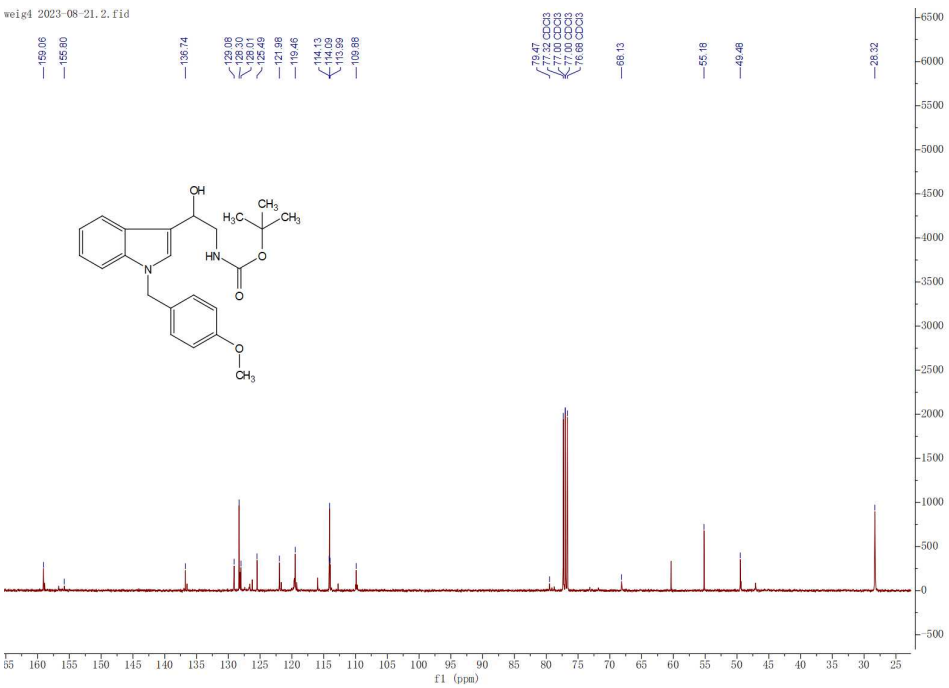

Figure S11. The ^{13}C NMR spectrum (400 MHz, chloroform-*d*) of **4**

tert-butyl(2-(methoxyamino)-2-(1-(4-methoxybenzyl)-1H-indol-3-yl)ethyl)carbamate (5)

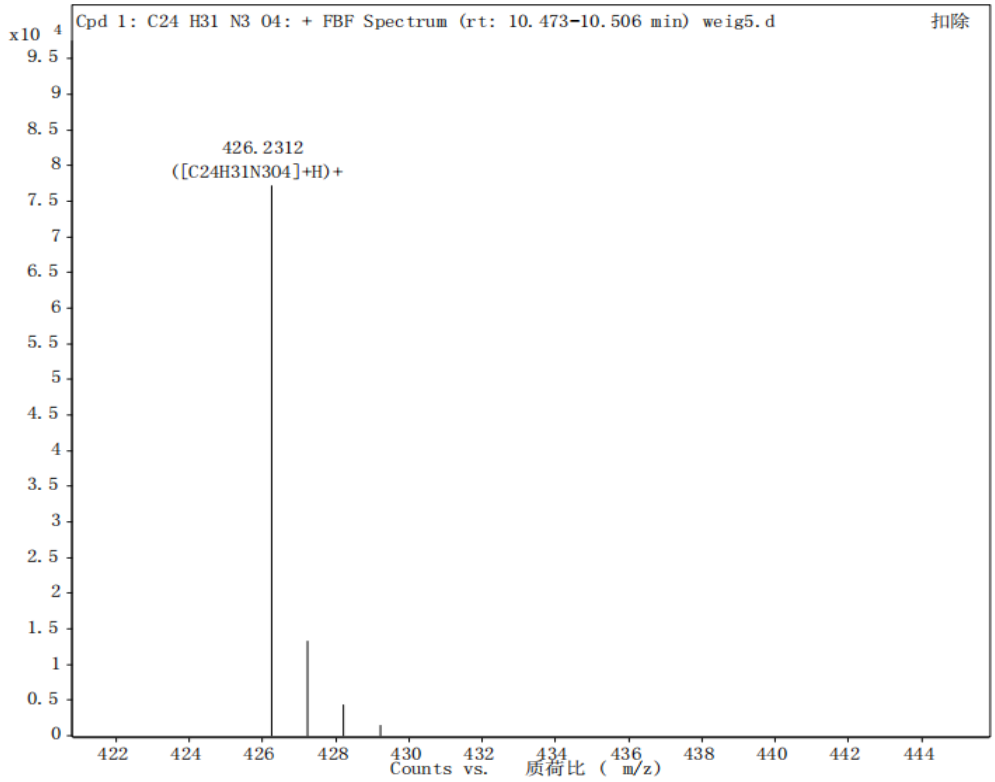

Figure S12. The HRESIMS spectrum of **5**

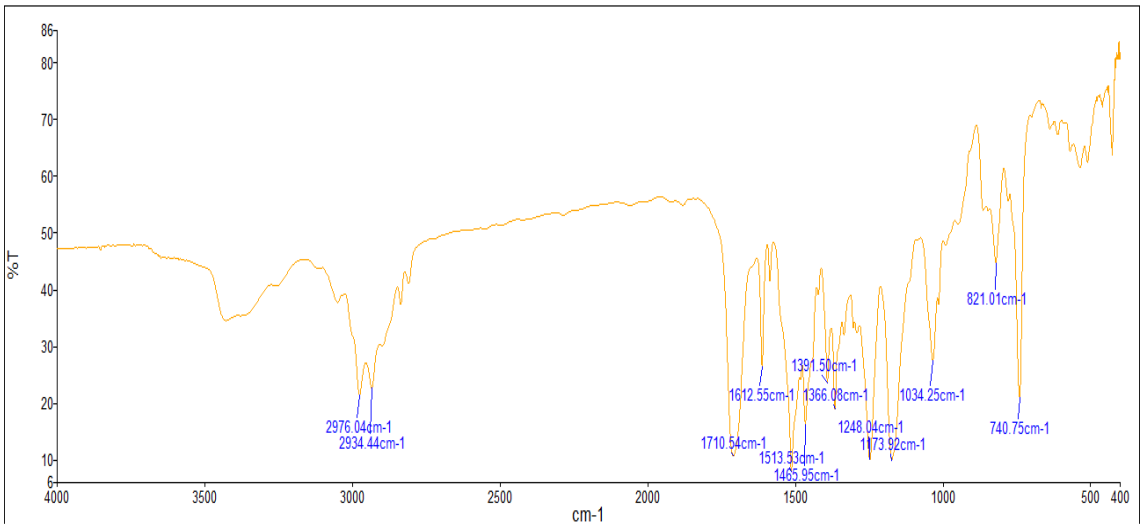

Figure S13. IR (KBr) spectrum of compound **5**

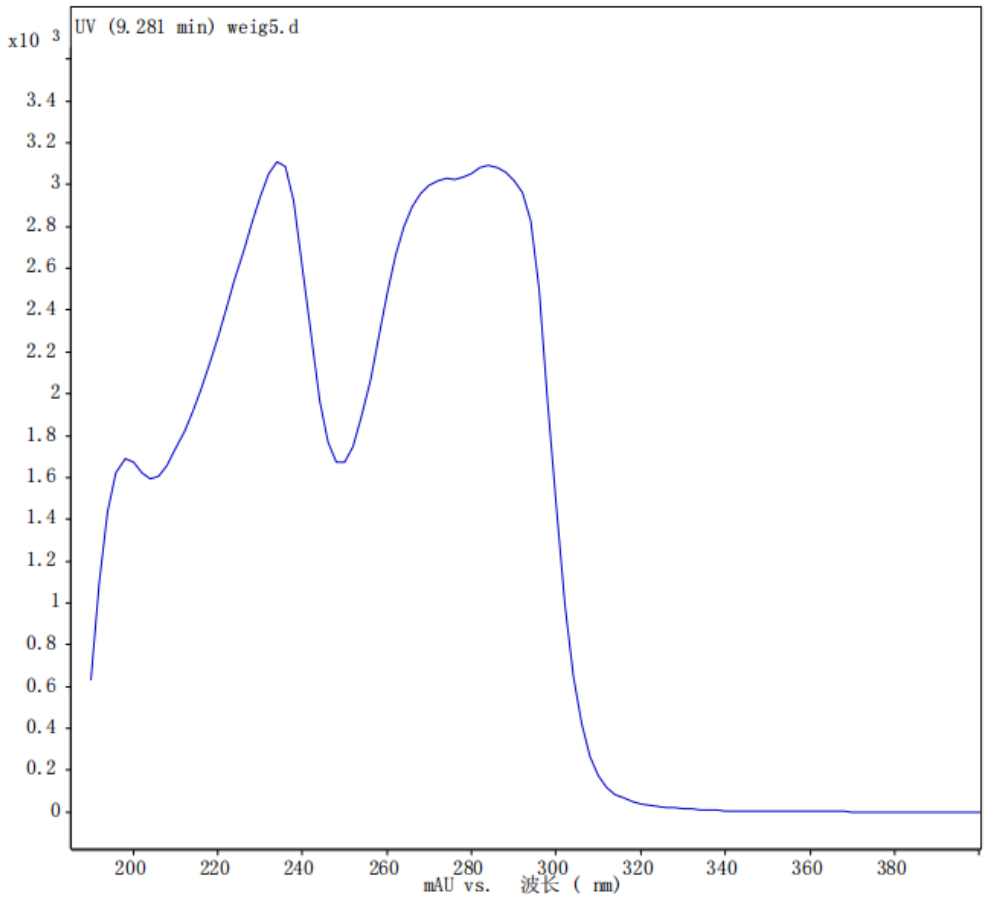

Figure S14. The UV spectrum of **5** (MeOH)

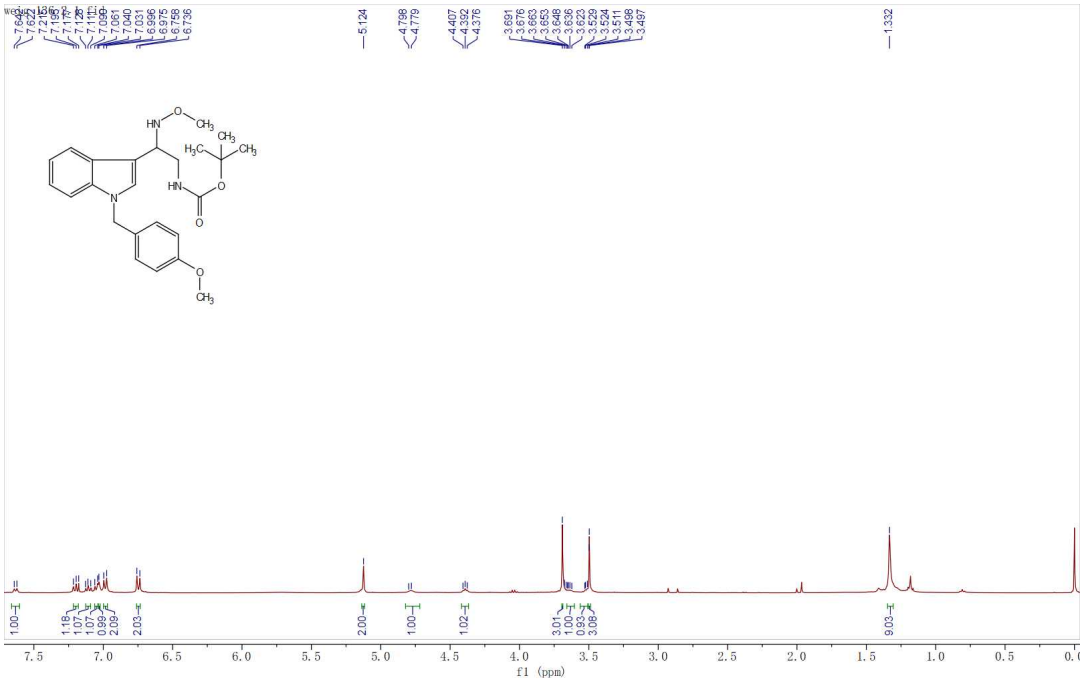

Figure S15. The ^{1}H NMR spectrum (400 MHz, chloroform-*d*) of **5**

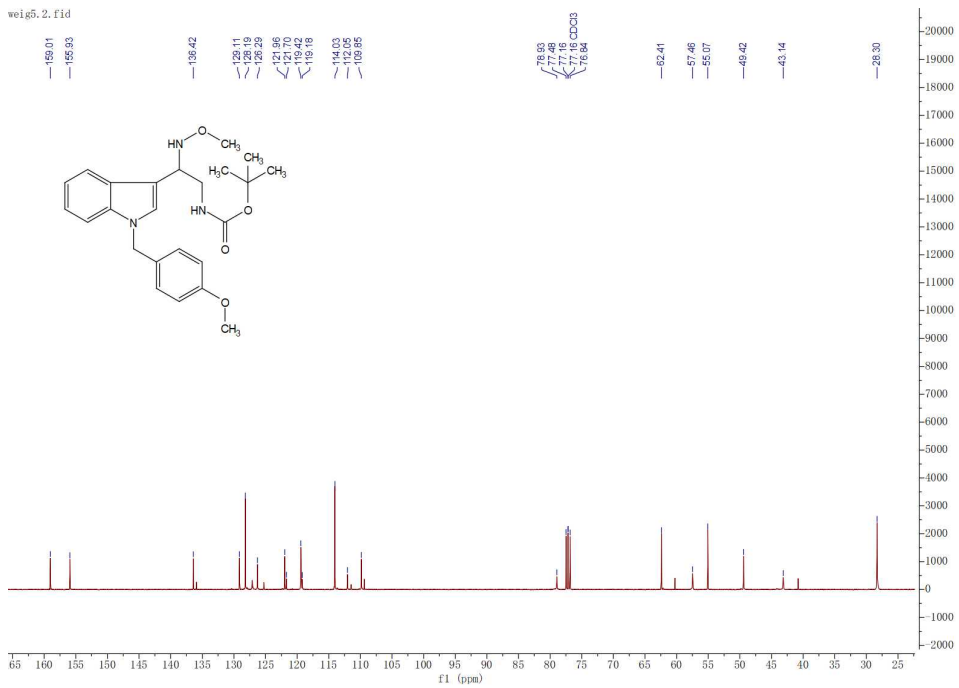

Figure S16. The ^{13}C NMR spectrum (400 MHz, chloroform-*d*) of **5**

6-bromo-1-(4-methoxybenzyl)-1H-indole (6)

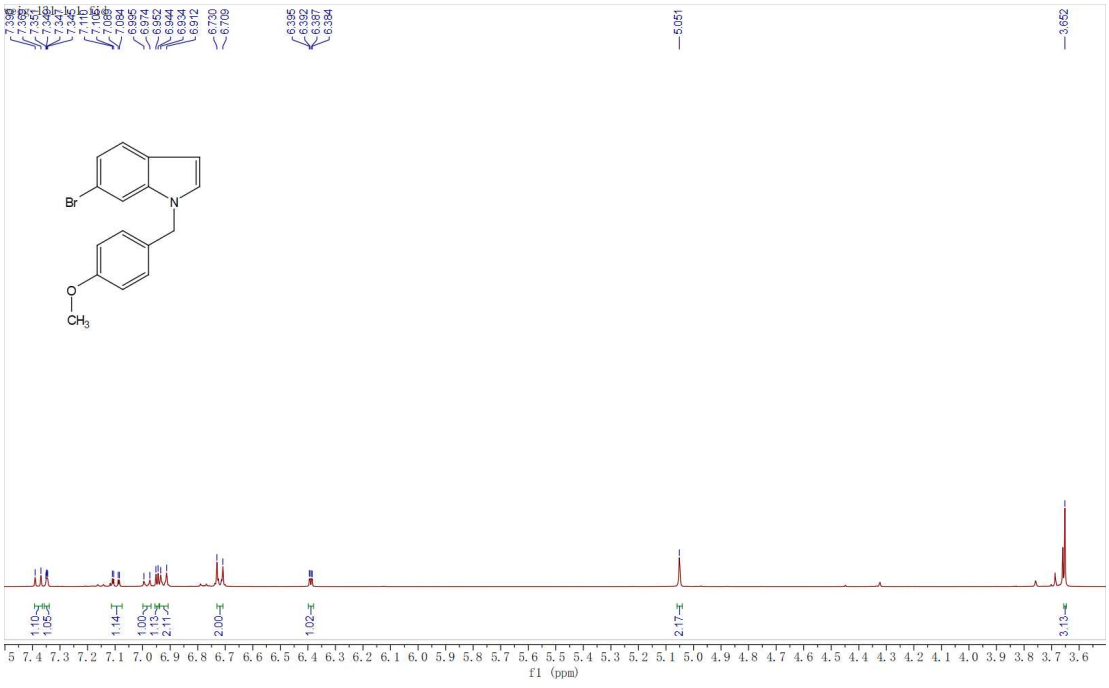

Figure S17. The ^{1}H NMR spectrum (400 MHz, chloroform-*d*) of **6**

methyl 3-(6-bromo-1-(4-methoxybenzyl)-1H-indol-3-yl)-3-oxopropanoate (7).

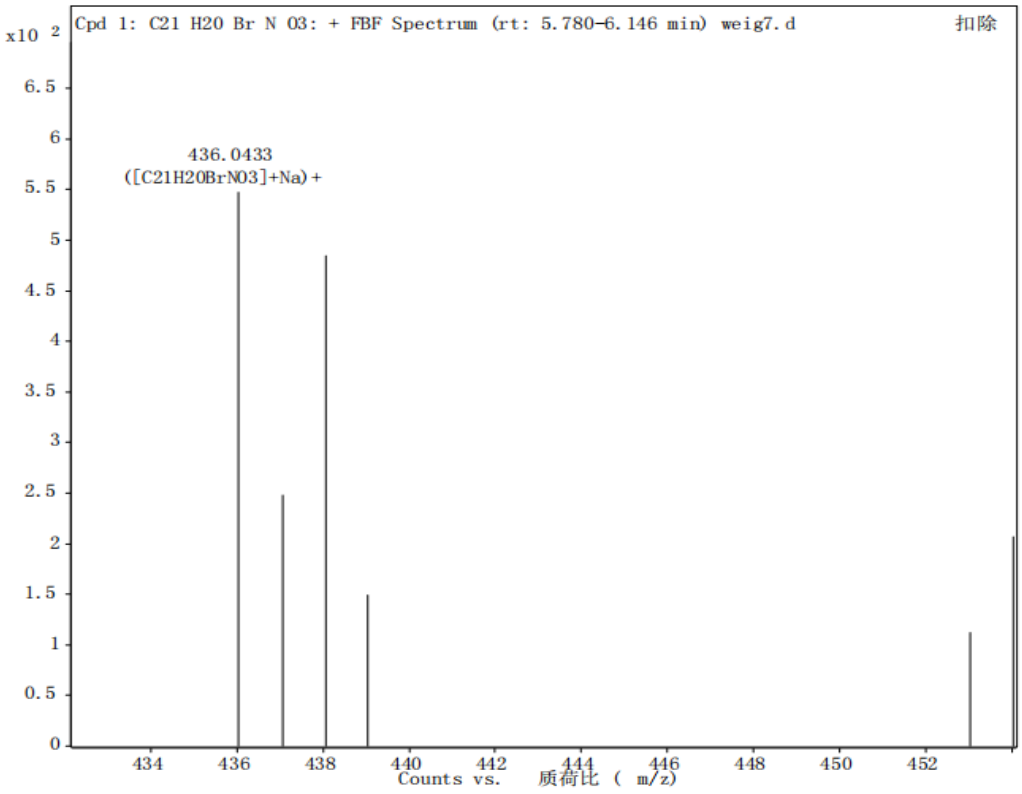

Figure S18. The HRESIMS spectrum of **7**

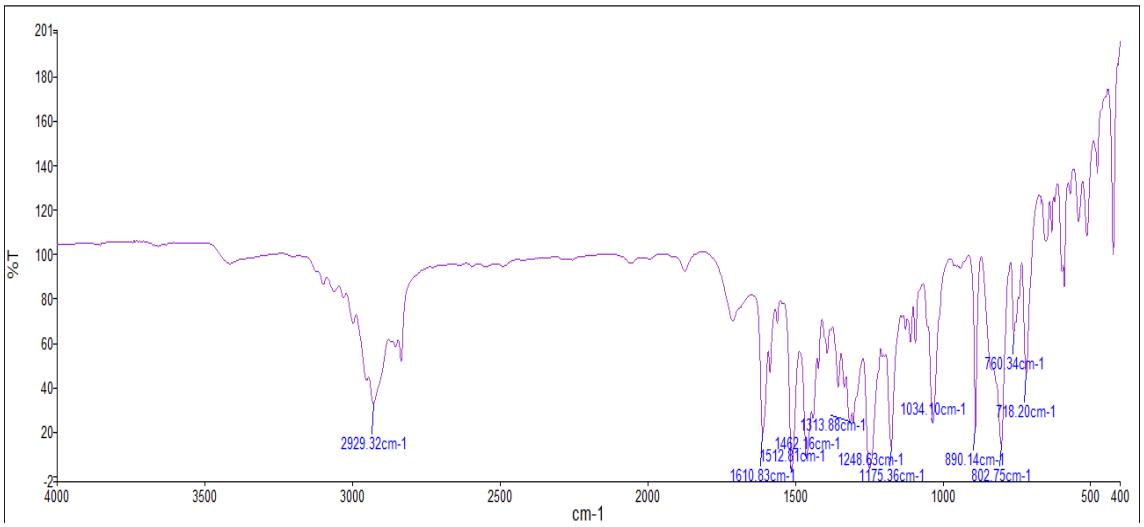

Figure S19. IR (KBr) spectrum of compound **7**

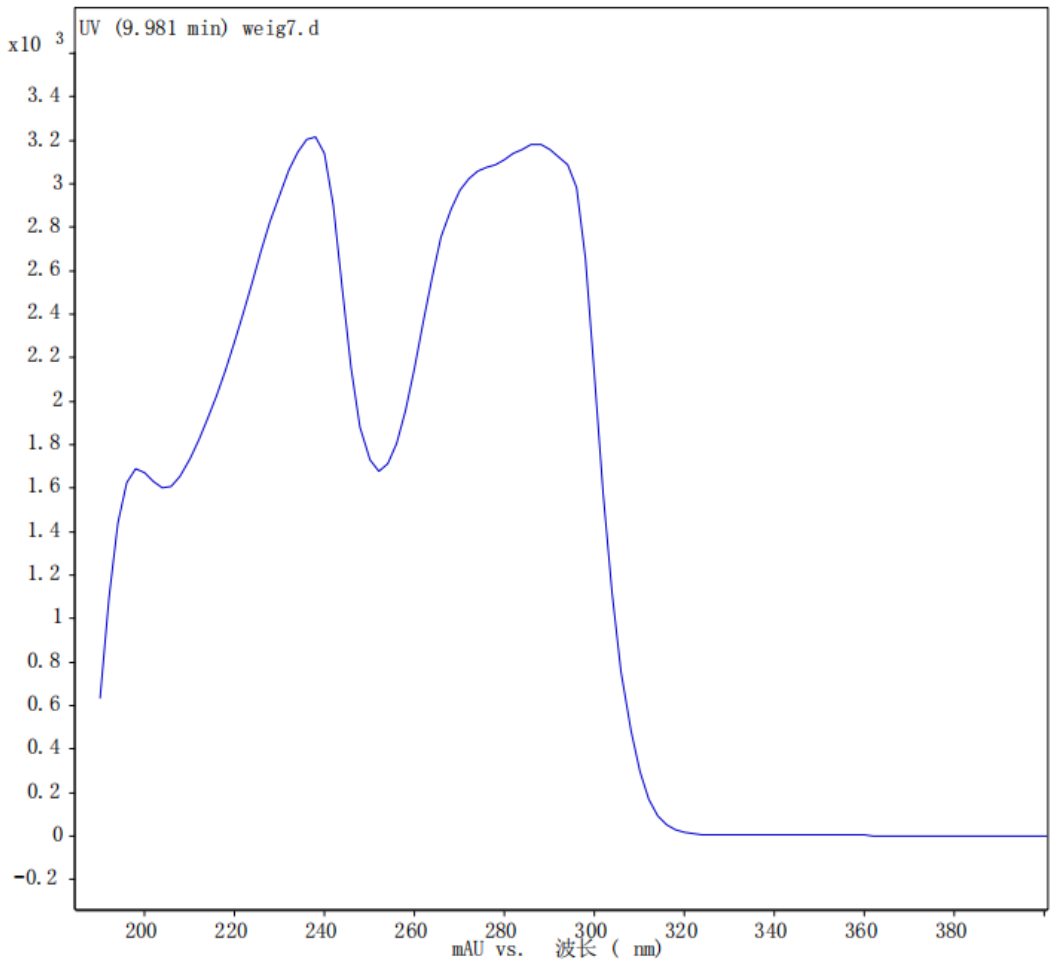

Figure S20. The UV spectrum of **7** (MeOH)

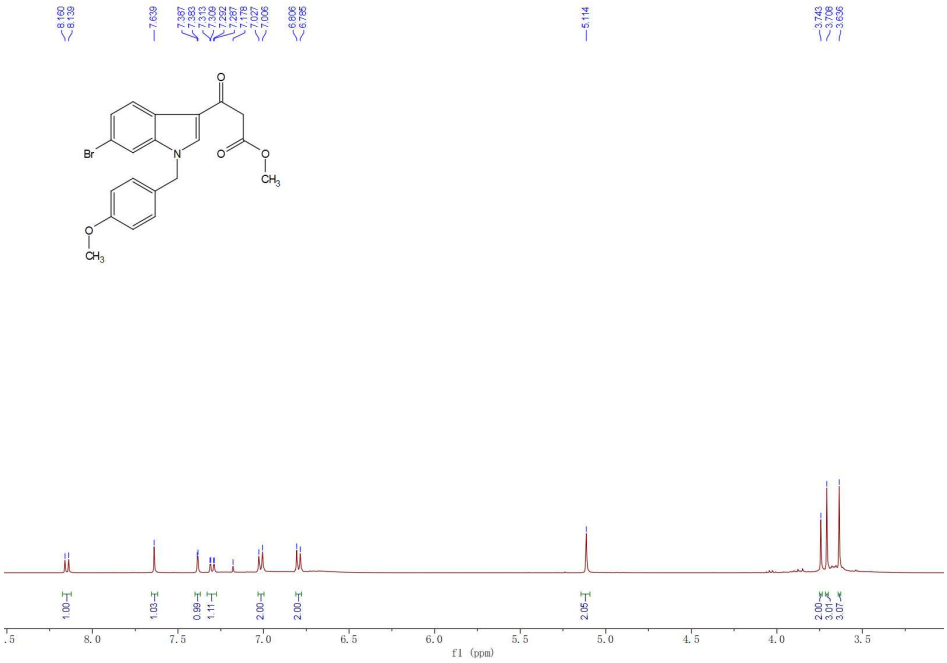

Figure S21. The ^{1}H NMR spectrum (400 MHz, chloroform-*d*) of **7**

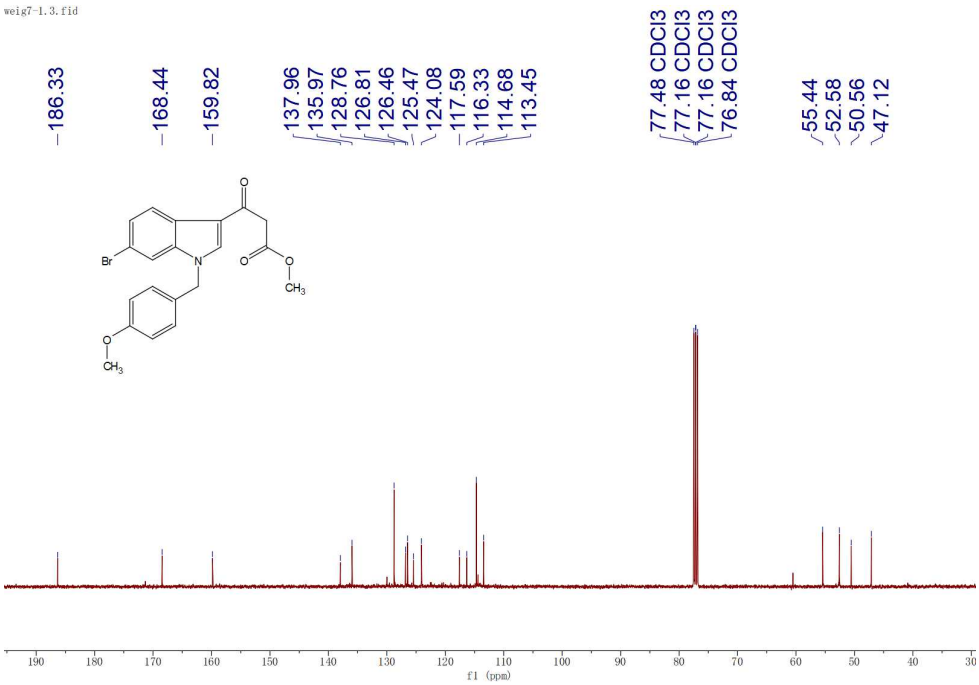

Figure S22. The ^{13}C NMR spectrum (400 MHz, chloroform-*d*) of **7**

methyl-3-(6-bromo-1-(4-methoxybenzyl)-1H-indol-3-yl)-2-diazo-3-oxopropanoate (8)

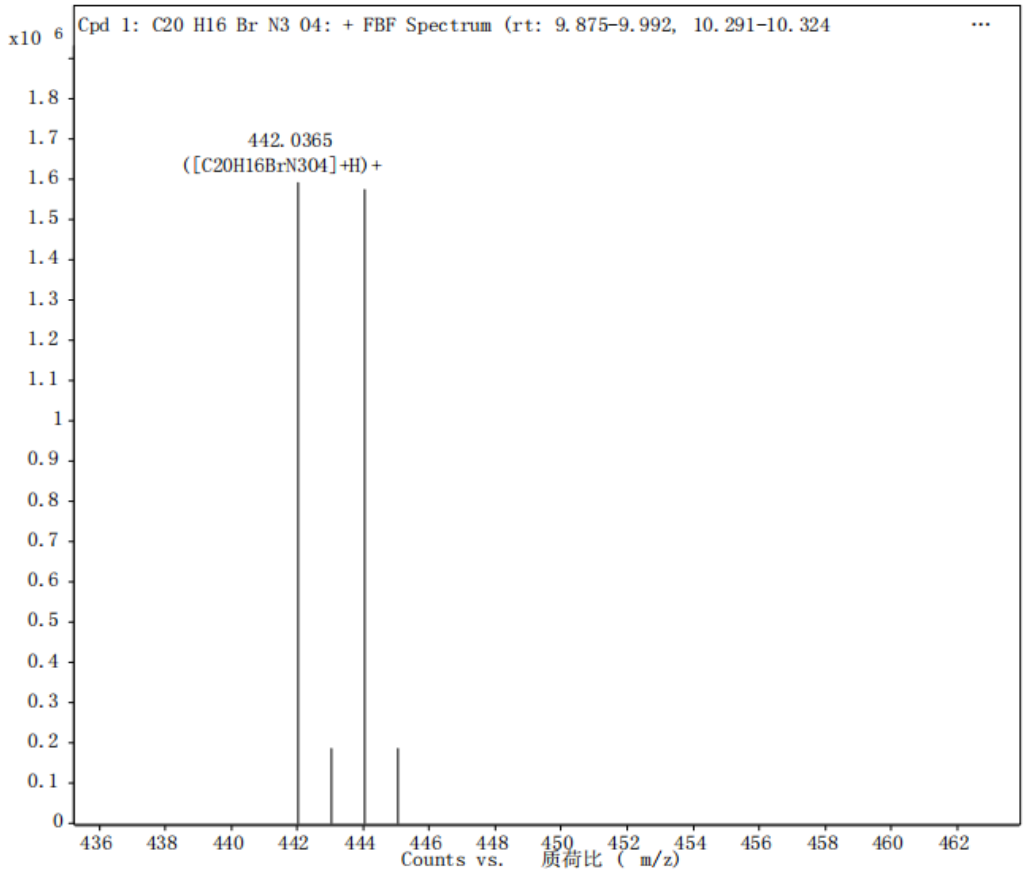

Figure S23. The HRESIMS spectrum of **8**

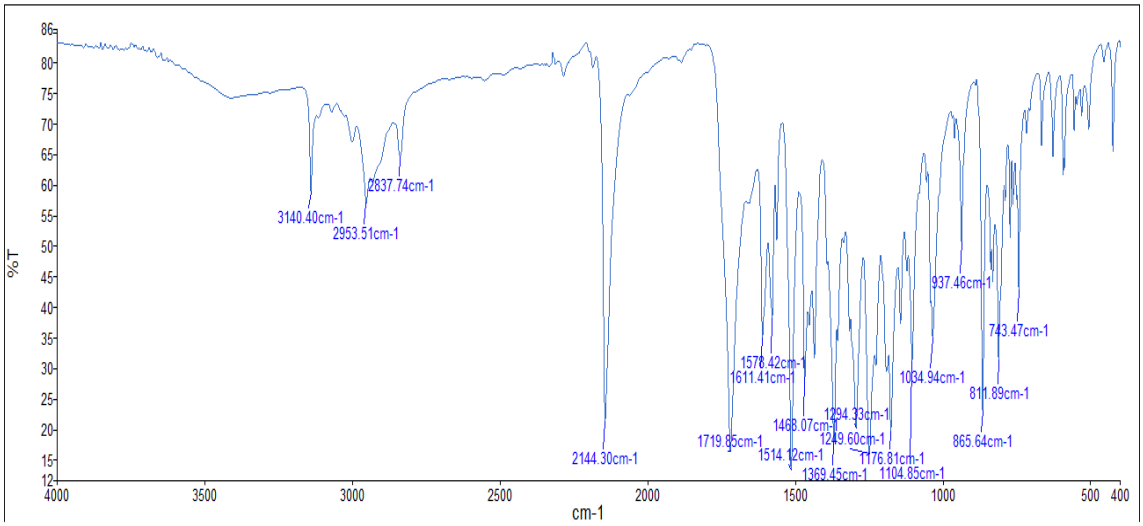

Figure S24. IR (KBr) Spectrum of compound **8**

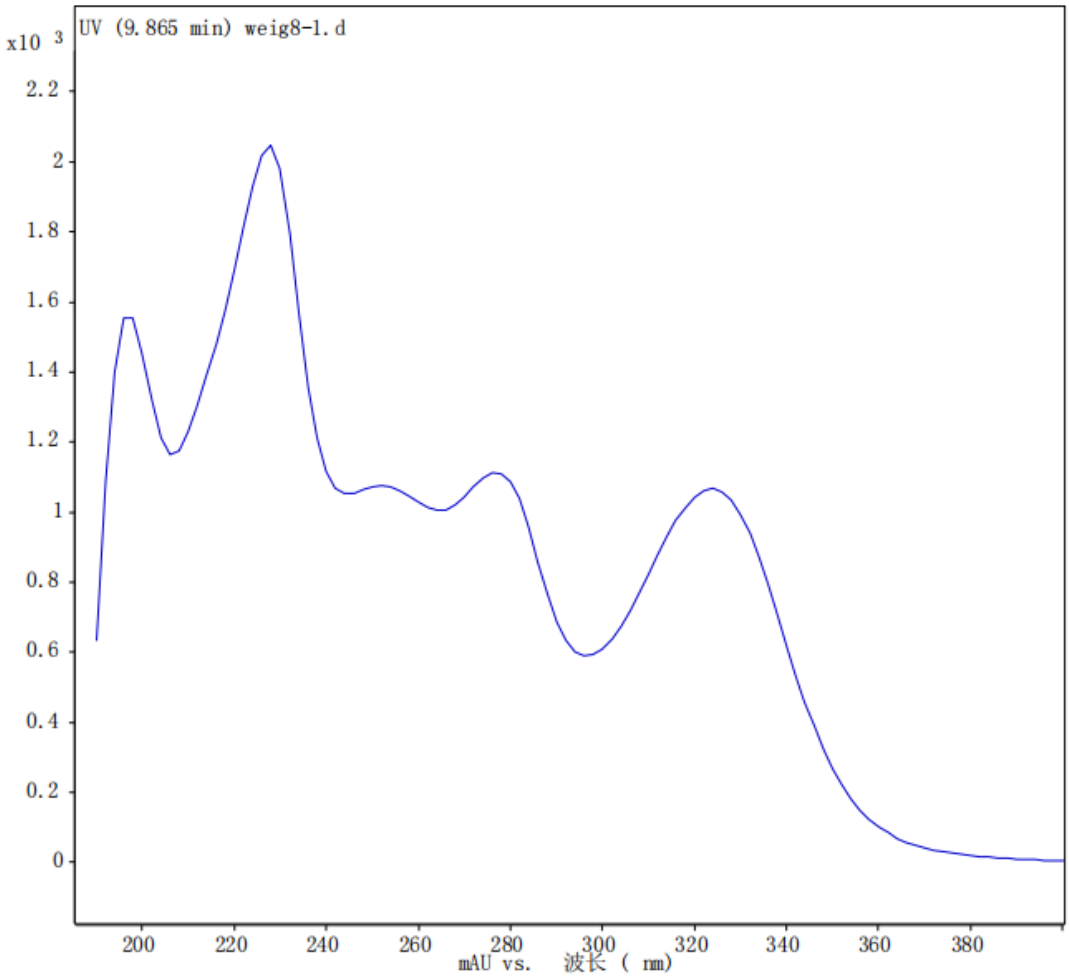

Figure S25. The UV spectrum of **8** (MeOH)

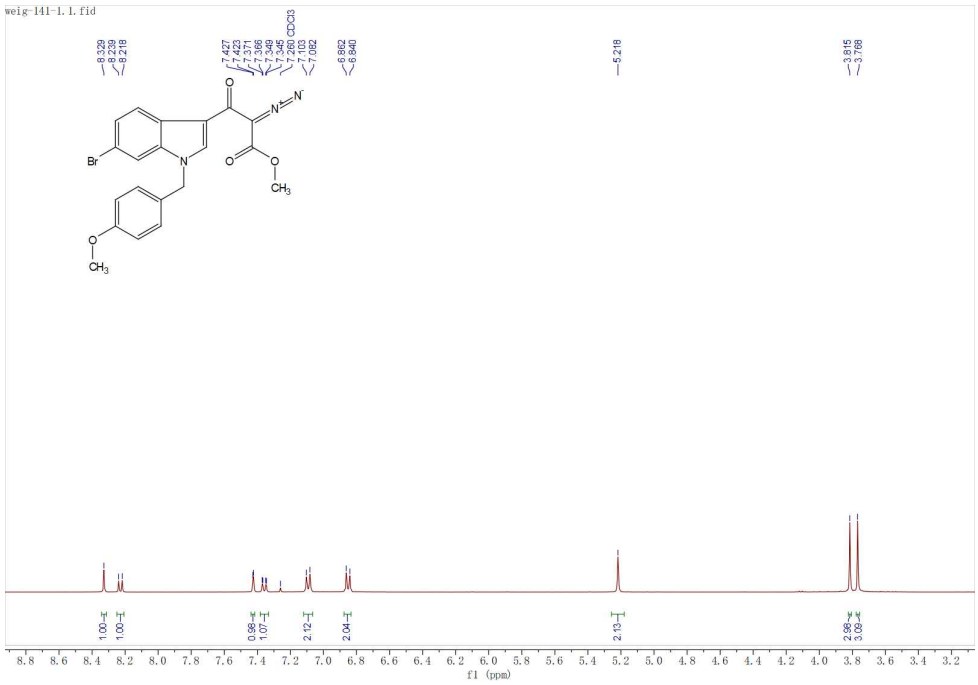

Figure S26. The ^{1}H NMR spectrum (400 MHz, chloroform-*d*) of **8**

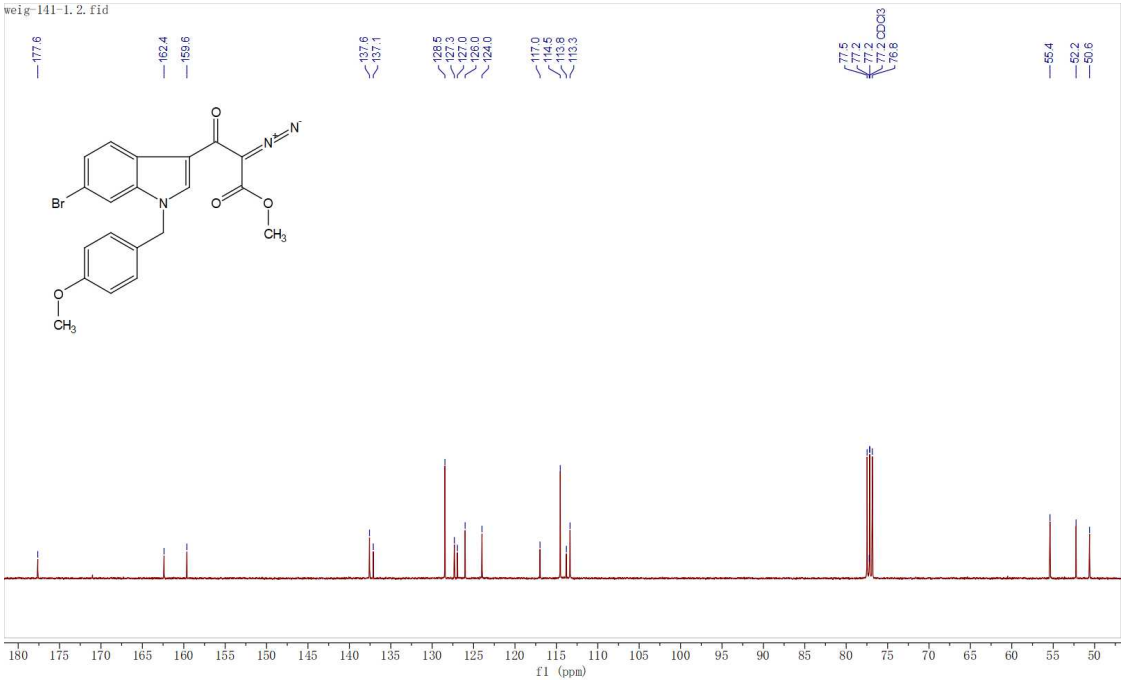

Figure S27. The ^{13}C NMR spectrum (400 MHz, chloroform-*d*) of **8**

Methyl-2-(6-bromo-1-(4-methoxybenzyl)-1H-indol-3-yl)-3-(methoxyamino)-3-oxo propanoate (9)

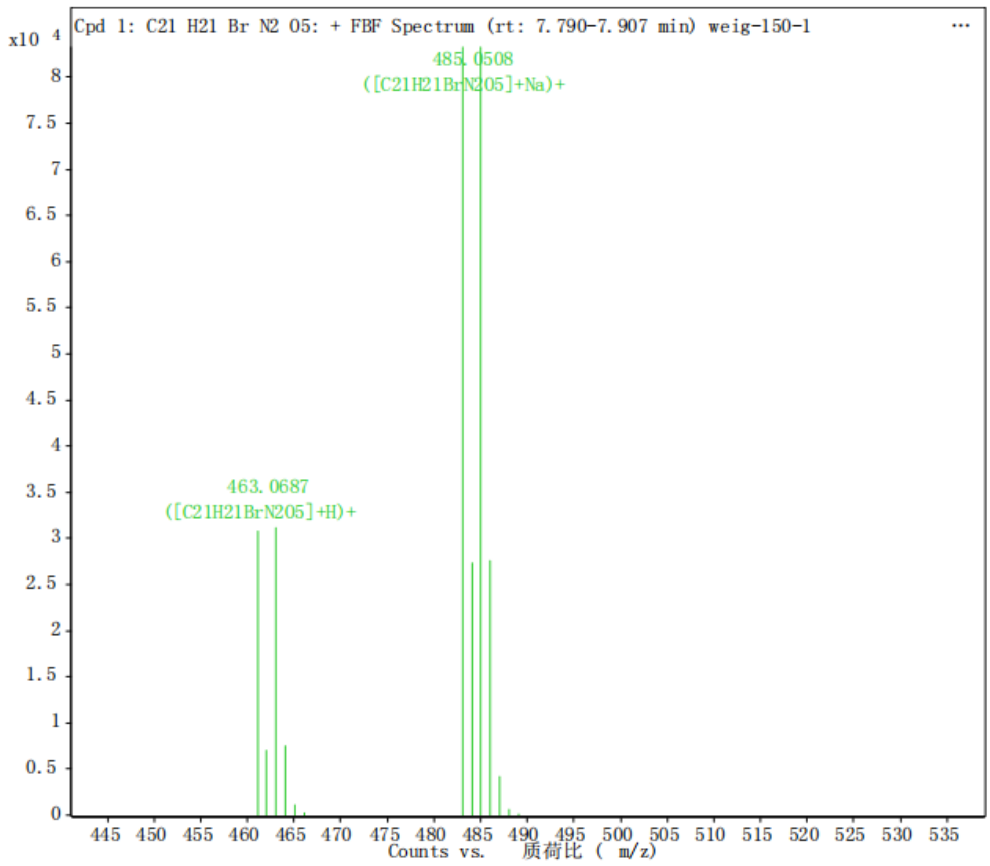

Figure S28. The HRESIMS spectrum of **9**

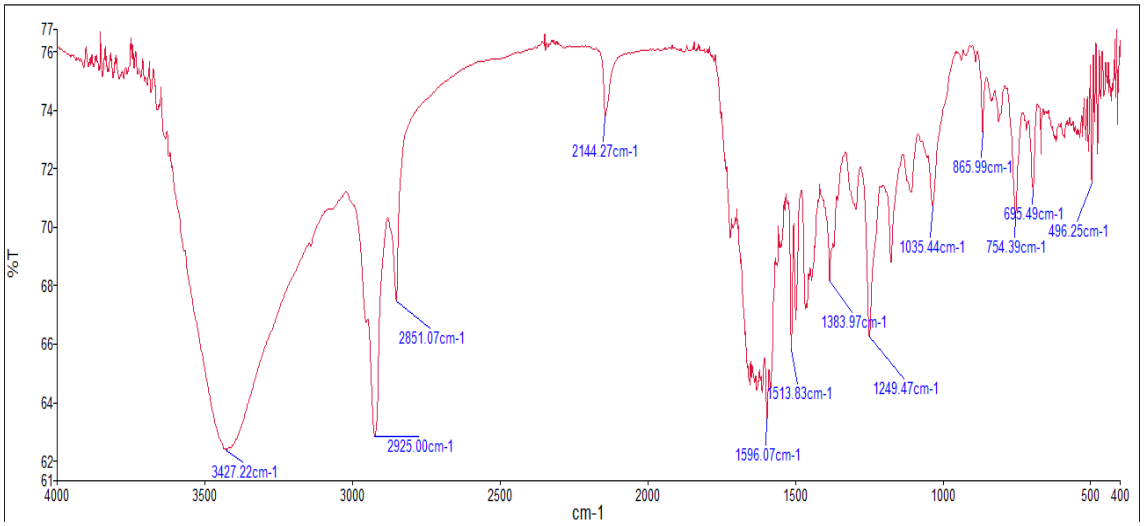

Figure S29. IR (KBr) spectrum of compound **9**

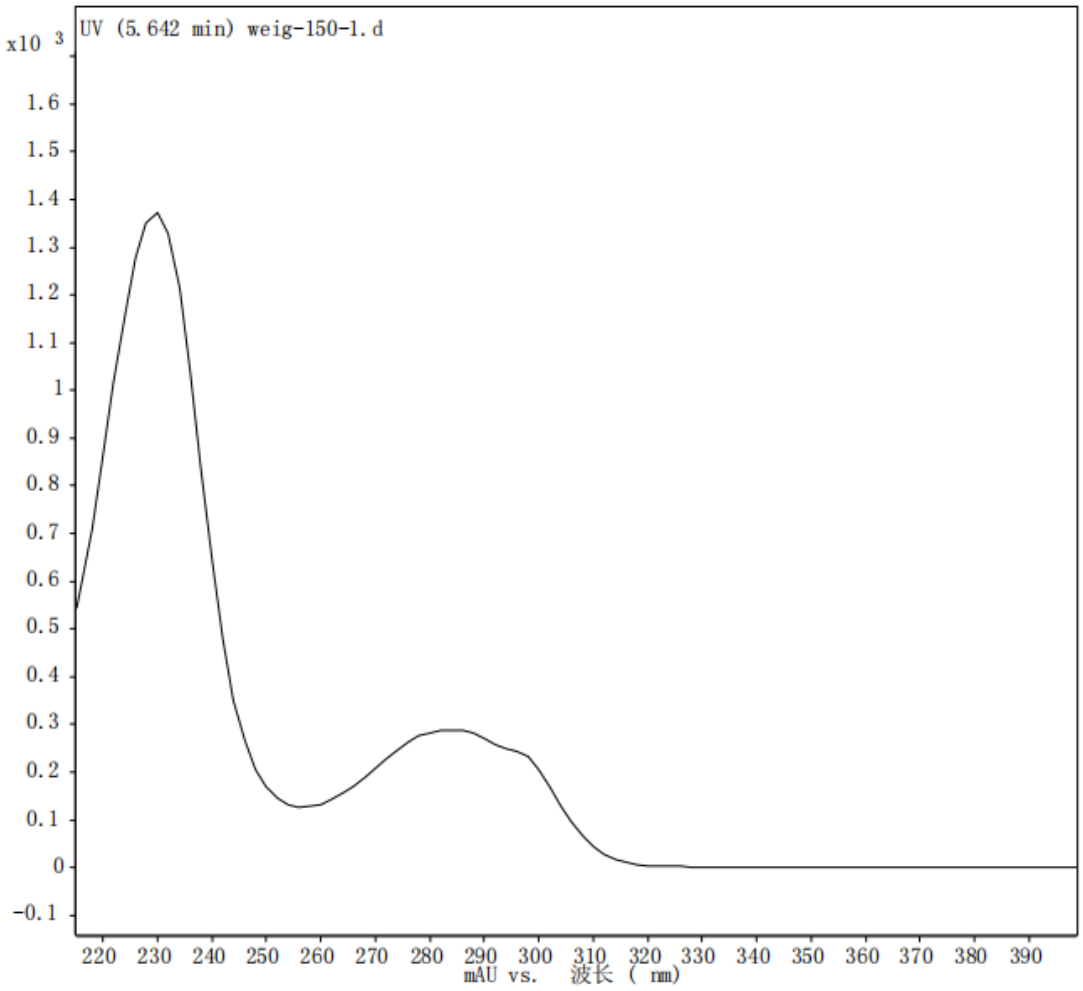

Figure S30. The UV spectrum of **9**

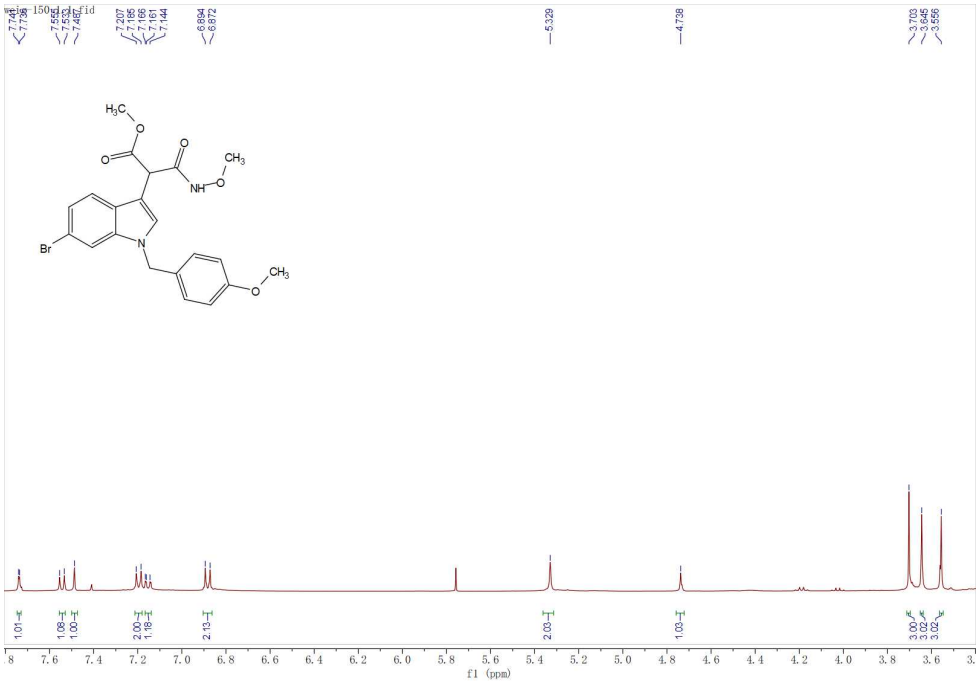

Figure S31. The ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of **9**

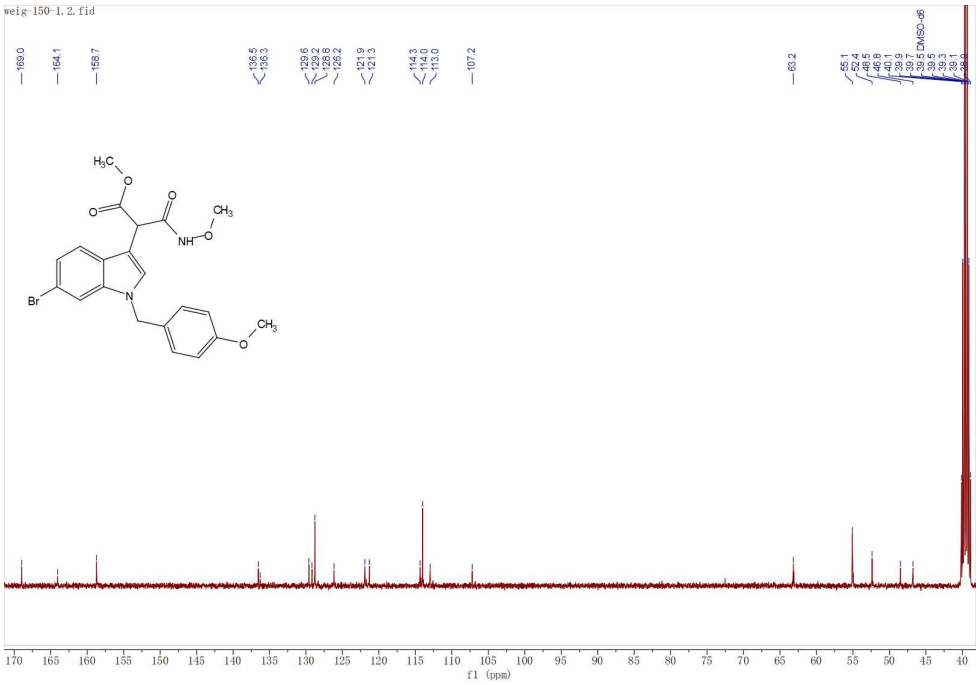

Figure S32. The ^{13}C NMR spectrum (400 MHz, DMSO-d_6) of **9**

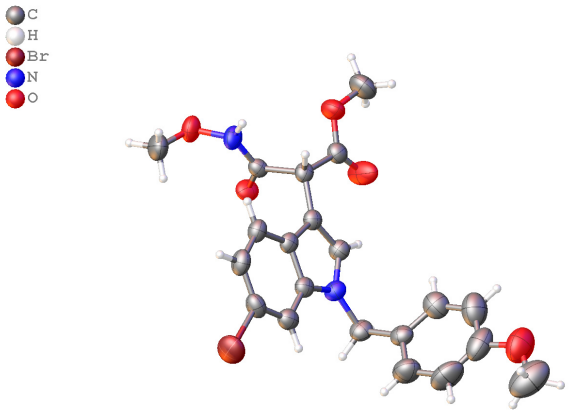

Figure S33. X-ray molecular structure of **9**

Table S1. The crystallographic data of **9**

Identification code	9
Empirical formula	$C_{21}H_{21}BrN_2O_5$
Formula weight	461.31
Temperature/K	295.01 (2)
Crystal system	orthorhombic
Space group	Pbca
a/Å	9.74420(10)
b/Å	8.63240(10)
c/Å	48.4549(6)
α/°	90
β/°	90
γ/°	90
VolμMe/Å^3	4075.82(4)
Z	8
ρ_{calc}g/cm^3	1.504
μ/mm^{-1}	3.056
F (000)	1888.0
Crystal size/mm^3	N/A × N/A × N/A
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.298 to 151.422
Index ranges	-12 ≤ h ≤ 12, -10 ≤ k ≤ 10, -60 ≤ l ≤ 21
Reflections collected	14792
Independent reflections	4074 [Rint = 0.0255, Rsigma = 0.0202]
Data/restraints/parameters	4074/0/265
Goodness-of-fit on F^2	1.139
Final R indexes [I>=2σ (I)]	R1 = 0.0699, wR2 = 0.1834
Final R indexes [all data]	R1 = 0.0790, wR2 = 0.1885
Largest diff. peak/hole / e Å^{-3}	0.80/-0.45