

Supplement Material

A novel isaindigotone derivative displays better anti-proliferation activities and induces apoptosis in gastric cancer cells

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The chemical atlas data of BLG26.

¹H NMR, ¹³C NMR, HRESIMS and HPLC Spectra of BLG26

BLG26 displays antiproliferative activity against SMMC-7721, PANC-1 and HCT116 cells.

BLG26 can get into AGS and HGC27 cells.

The yield was 69%. The m.p. was 231-233°C. Then, the NMR and ESI mass

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spectrometry were analysed. ^1H NMR (400 MHz, Chloroform-*d*) δ : 7.76 (d, J = 12.9 Hz, 1H), 7.61 (d, J = 3.1 Hz, 1H), 7.32 - 7.24 (m, 1H), 7.23 - 7.12 (m, 2H), 7.08 (d, J = 7.8 Hz, 1H), 4.20 (t, J = 7.1 Hz, 2H), 3.24 (t, J = 4.8 Hz, 4H), 3.17 (d, J = 9.8 Hz, 2H), 2.56 (t, J = 4.9 Hz, 4H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ : 159.11, 154.14 (d, J = 44.5 Hz), 151.88, 150.65 (d, J = 12.7 Hz), 148.16 (d, J = 16.1 Hz), 146.51, 145.35 (d, J = 10.0 Hz), 131.67, 126.89, 125.27, 117.06, 116.89, 116.73, 114.17 (d, J = 3.6 Hz), 113.51 (d, J = 8.4 Hz), 111.04 (d, J = 23.7 Hz), 53.89, 48.91 (d, J = 4.7 Hz), 45.09, 42.93, 24.38. Purity 99.5% by HPLC. HRESIMS-ESI m/z : calcd for $\text{C}_{23}\text{H}_{21}\text{F}_3\text{N}_4\text{O}[\text{M}+\text{H}]^+$: 427.1667; found: 427.1769.

Figure S1. ^1H NMR spectra of BLG26.

Figure S2. ^{13}C NMR spectra of BLG26.

Figure S3. HRESIMS spectra of BLG26.

Figure S4. HPLC spectra of BLG26.

Figure S5. BLG26 displays anti-proliferative activity against SMMC-7721, PANC-1 and HCT116 cells. (A) BLG26 suppresses the growth of SMMC-7721 cells at 48 h. (B) BLG26 suppresses the growth of HCT116 cells at 48 h. (C) BLG26 suppresses the growth of PANC-1 cells at 48 h.

Figure S6. BLG26 can get into AGS and HGC27 cells. (A) Excitation spectrum of BLG26. (B) Emission spectrum of BLG26. (C) Treated AGS cells and HGC27 cells showed fluorescence.

Figure S1.

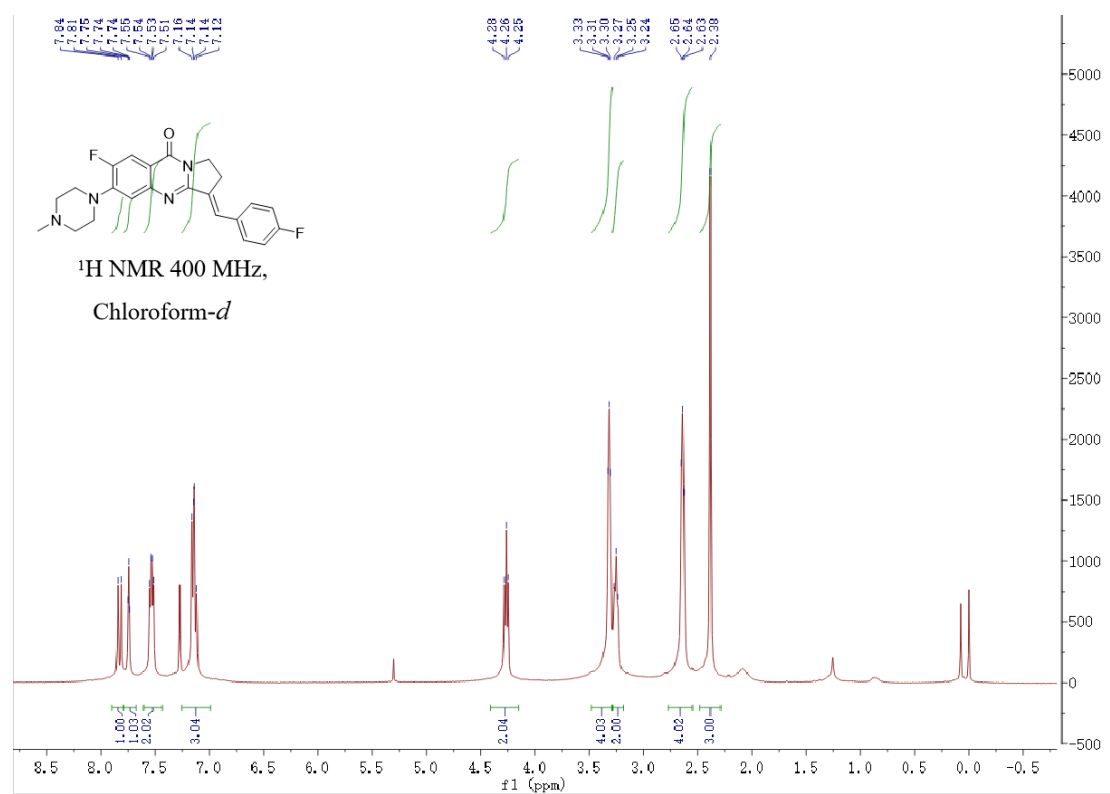
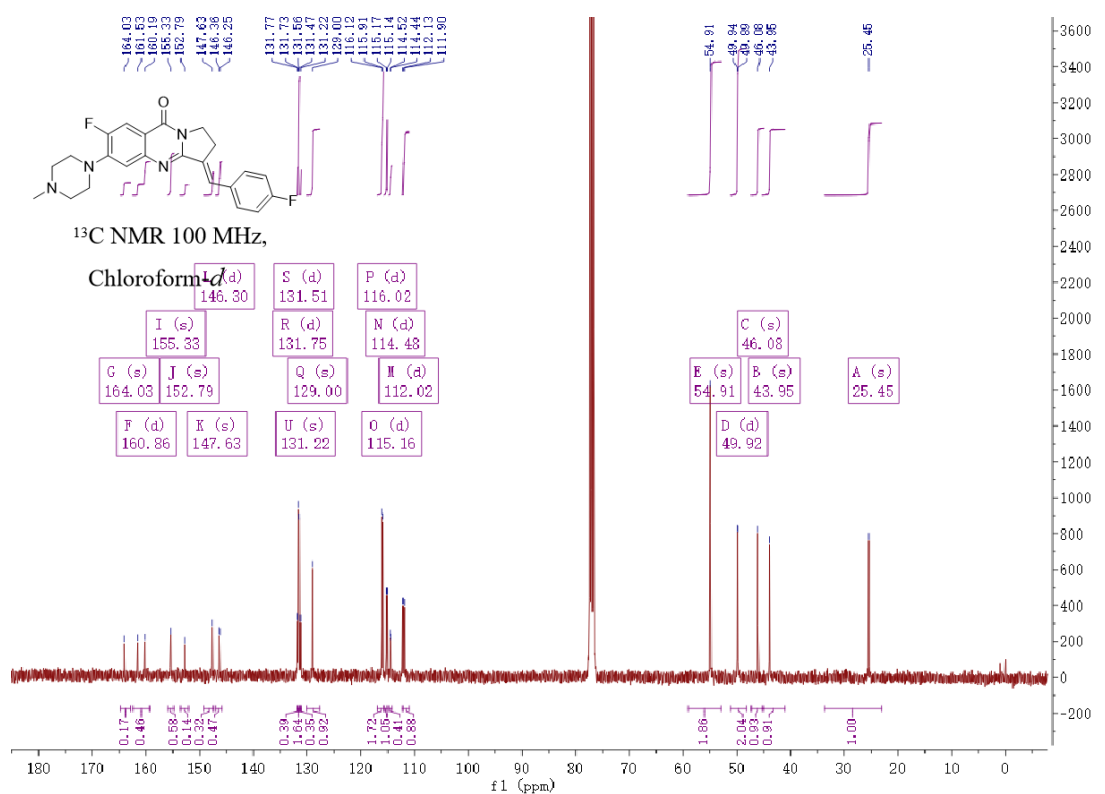


Figure S2.



Generic Display Report

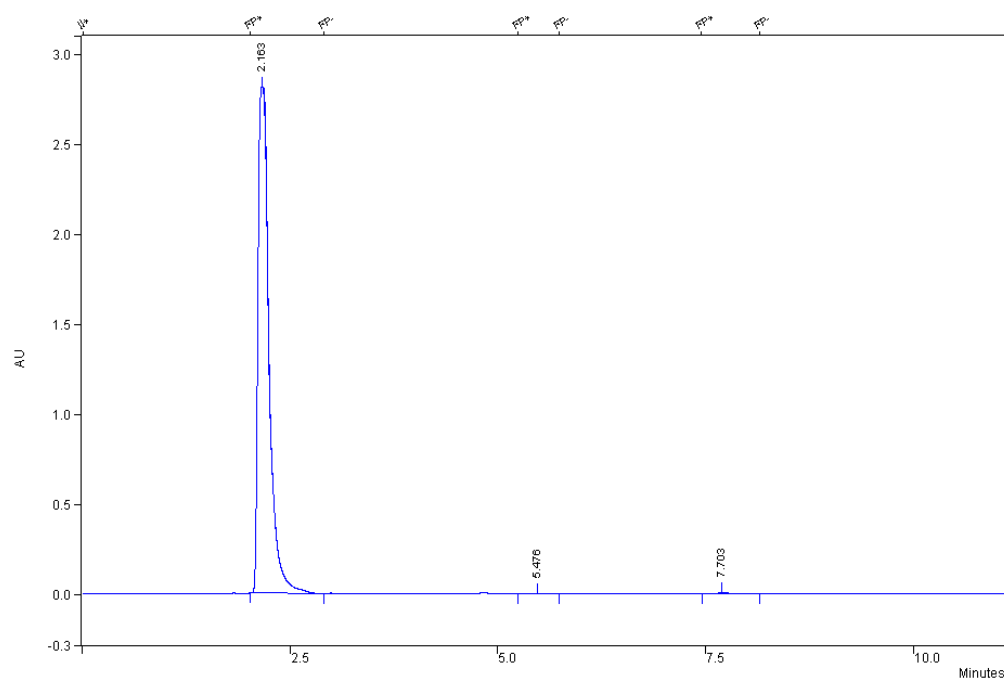
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Sample Name	YANGCHENGJIE210519_5	Instrument	micrOTOF
Comment			

Mass spectrum plot showing intensity (x10⁶) versus m/z. The x-axis ranges from 100 to 800 m/z. The y-axis ranges from 0.0 to 1.5 x10⁶. A major peak is labeled at m/z 409.1659. A minor peak is labeled at m/z 205.0996. The plot is titled "+MS, 0.1-0.9min #8-51, -Peak Bkgrnd".

m/z	Intensity (x10 ⁶)
205.0996	~0.1
409.1659	~1.6

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Figure S4.



Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1		99.5622	2.163	0.000	260839888	BB	7.9	
2		0.1514	5.476	0.000	396529	BB	12.2	
3		0.2864	7.703	0.000	750338	BB	15.1	
Totals:		100.0000		0.000	261986755			

Figure S5.

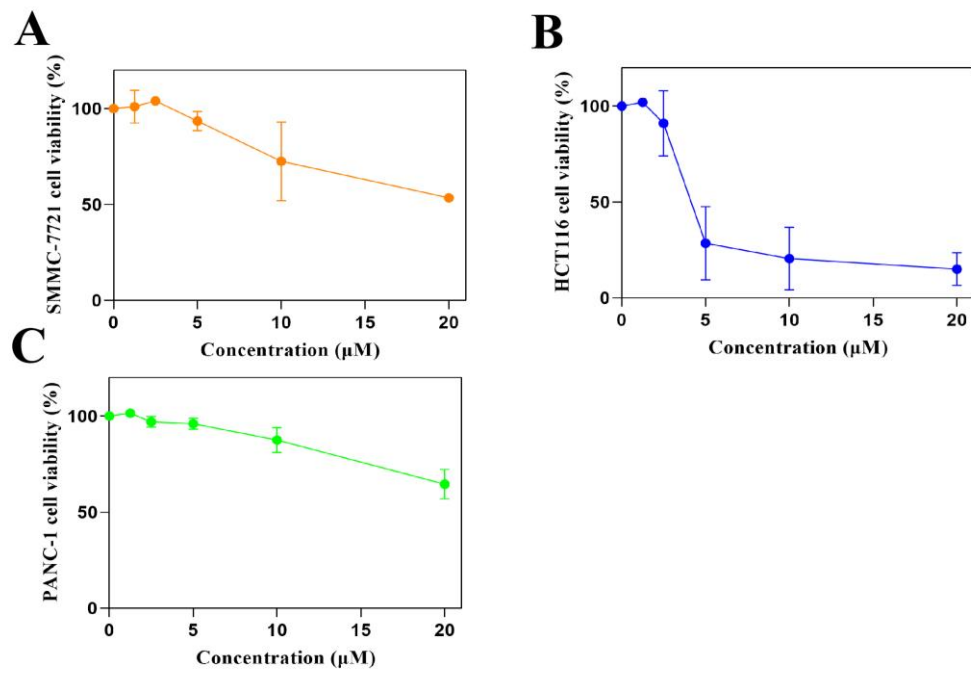


Figure S6.

