

# **Discovery of Novel 3-Hydroxyquinazoline-2,4(1*H*,3*H*)-dione Derivatives: A Series of Metal Ion Chelators with Potent Anti-HCV Activities**

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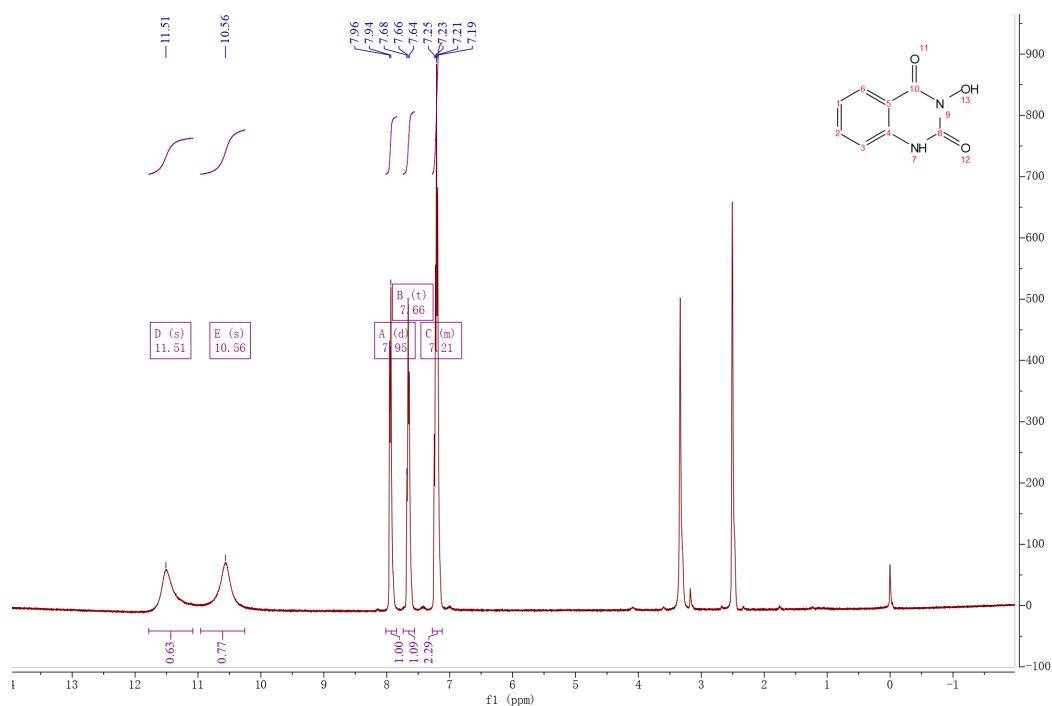
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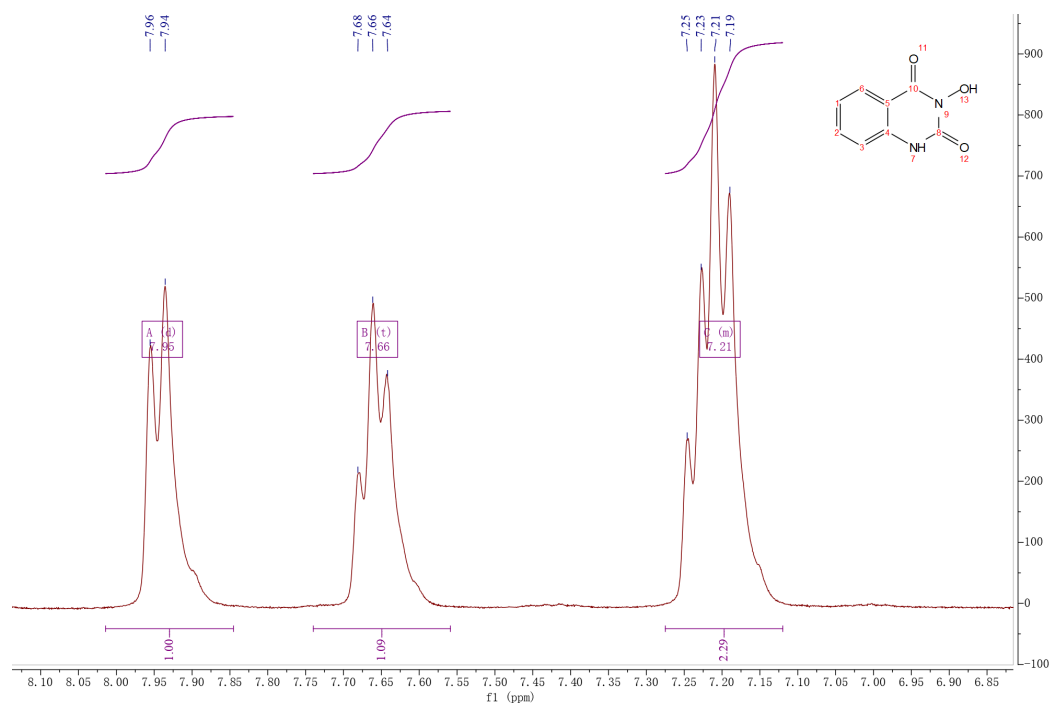


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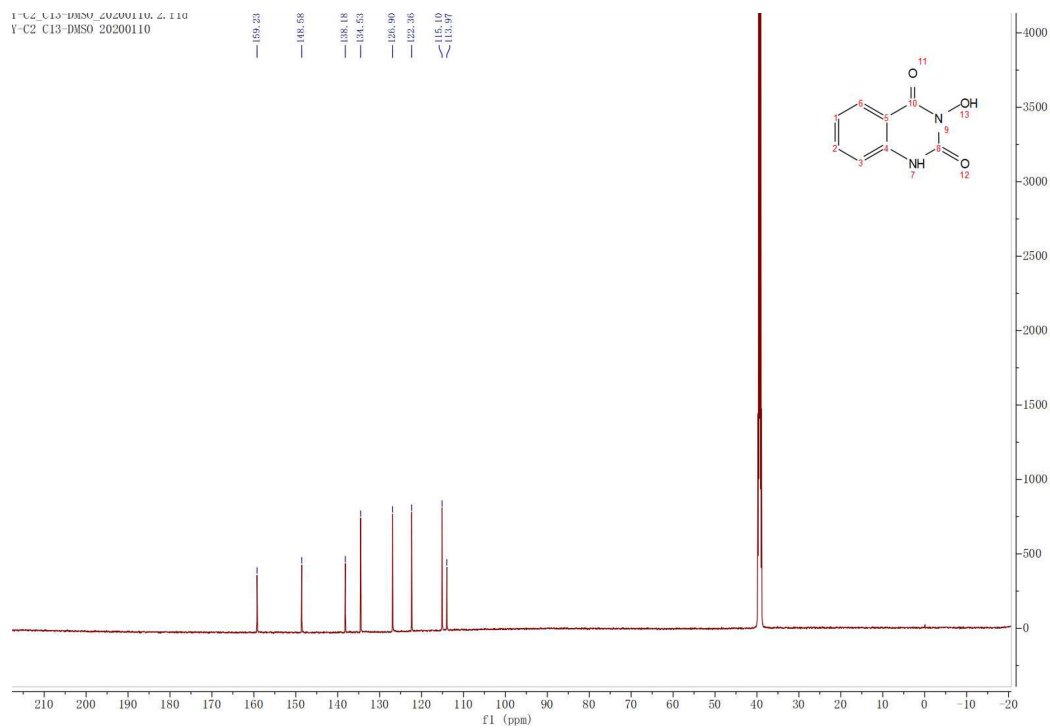
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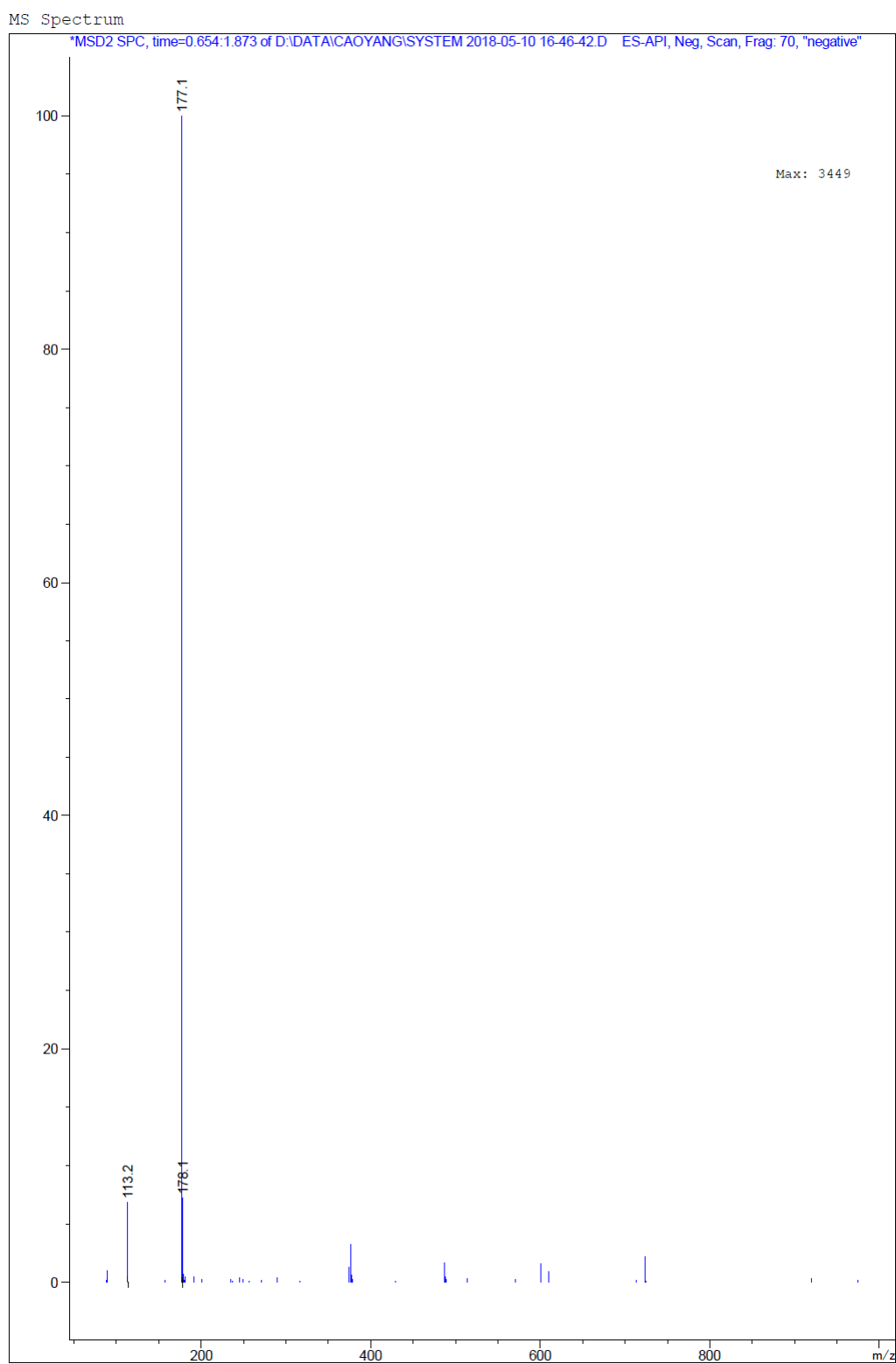
**Figure S1.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10a**



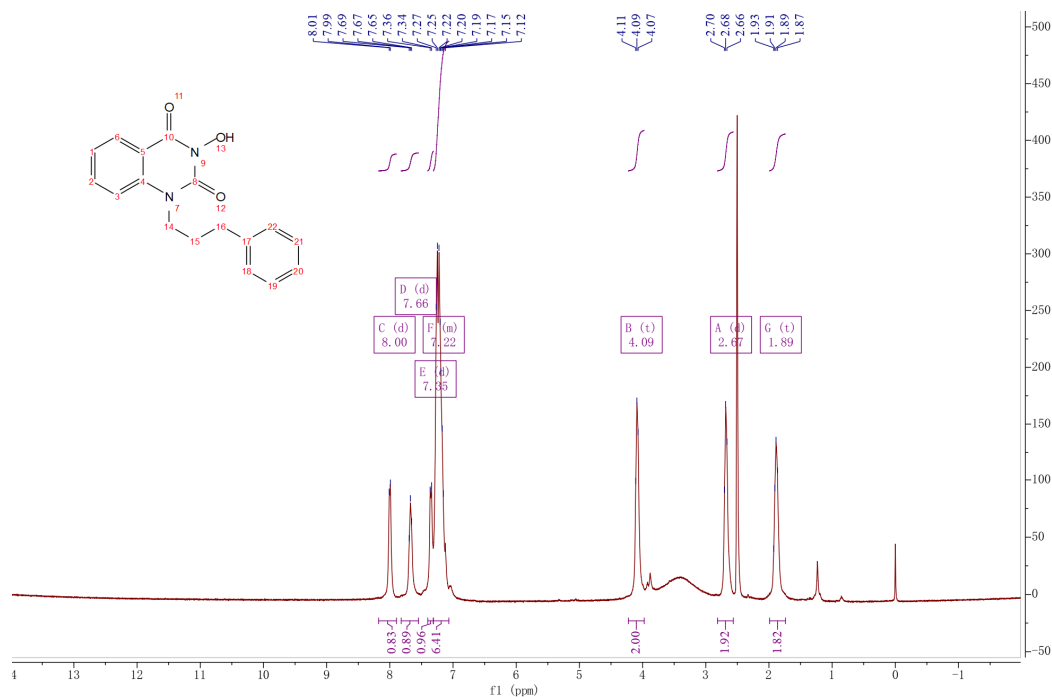
**Figure S2.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **10a**



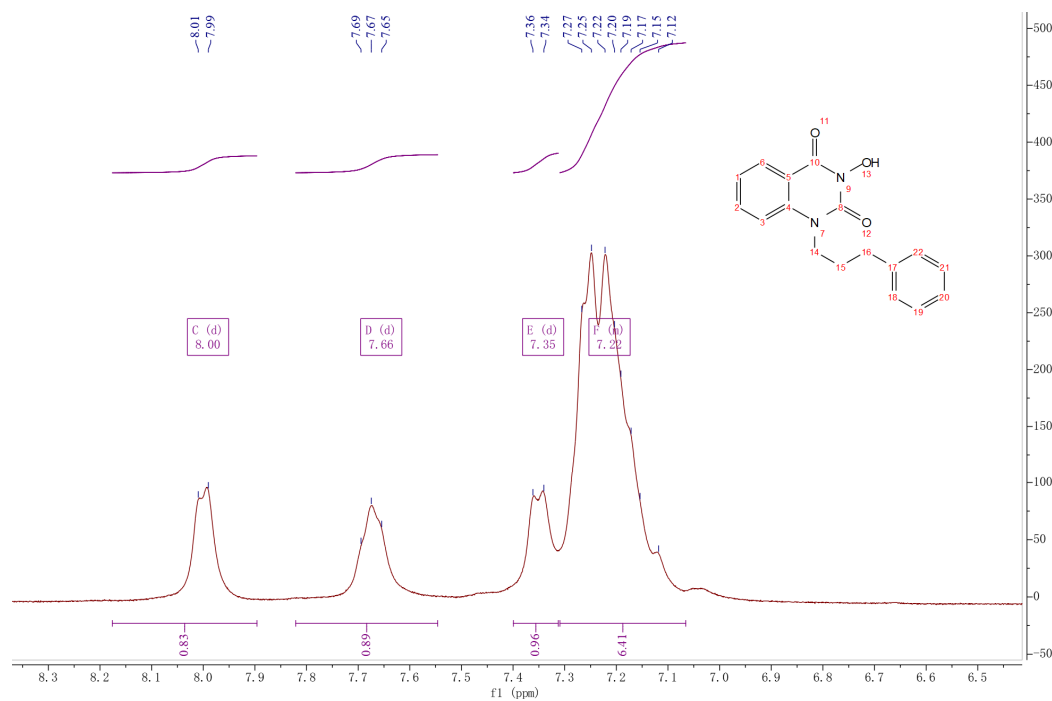
**Figure S3.** <sup>13</sup>C NMR (151 MHz, DMSO-*d*<sub>6</sub>) spectrum of **10a**



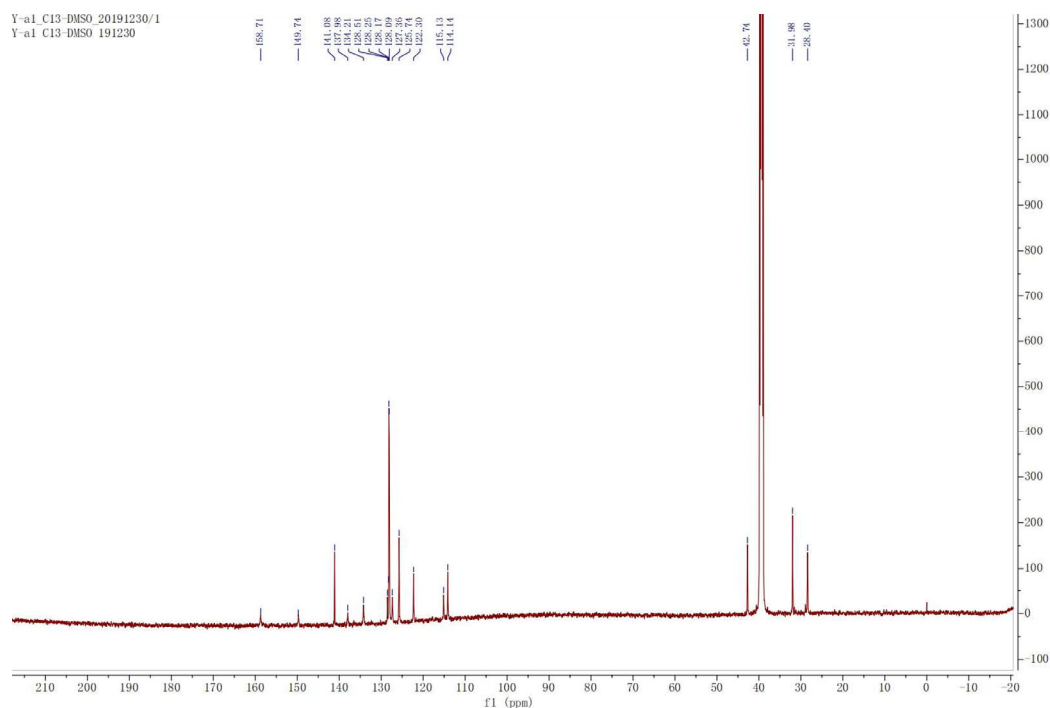
**Figure S4.** Mass spectrum (negative ionization) of **10a**



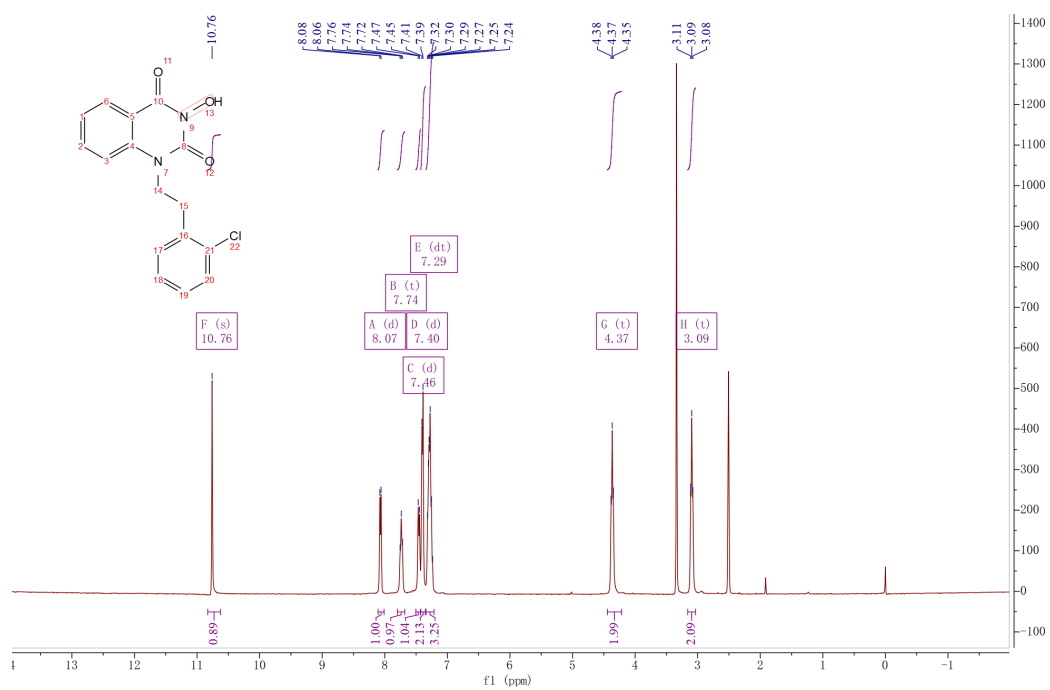
**Figure S5.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10b**



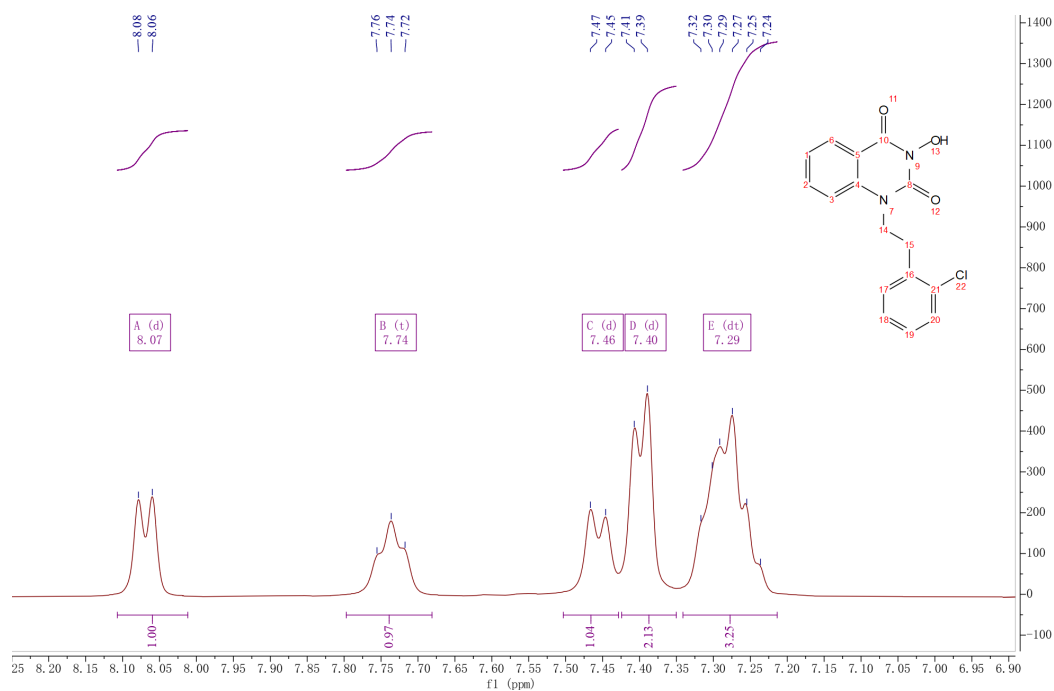
**Figure S6.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **10b**



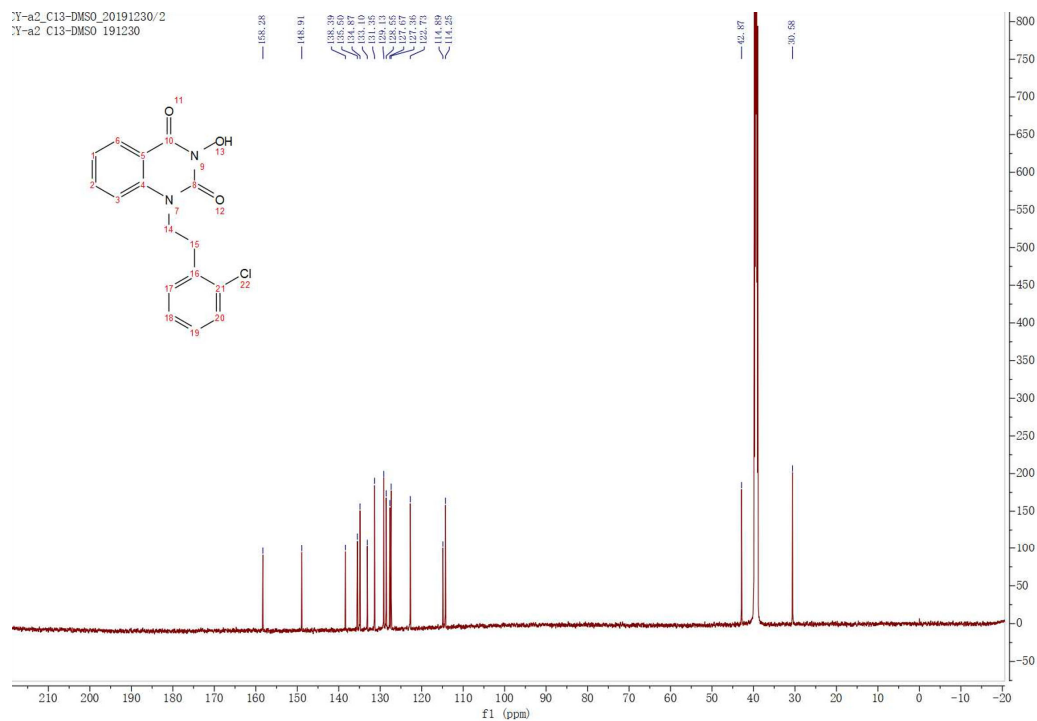
**Figure S7.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10b**



**Figure S8.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10c**

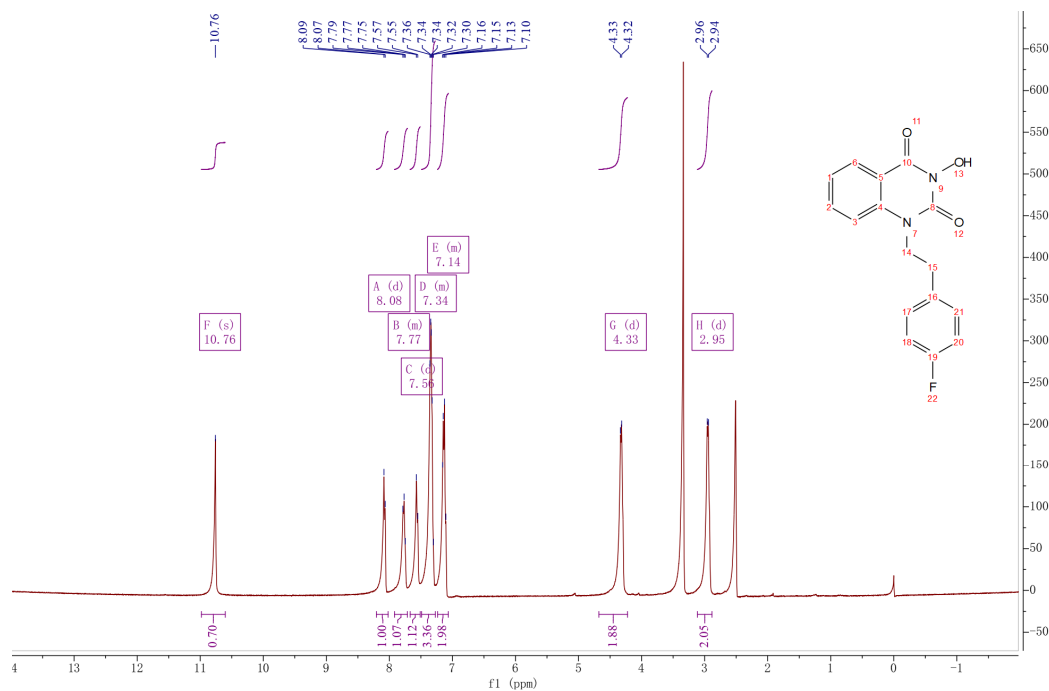


**Figure S9.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **10c**

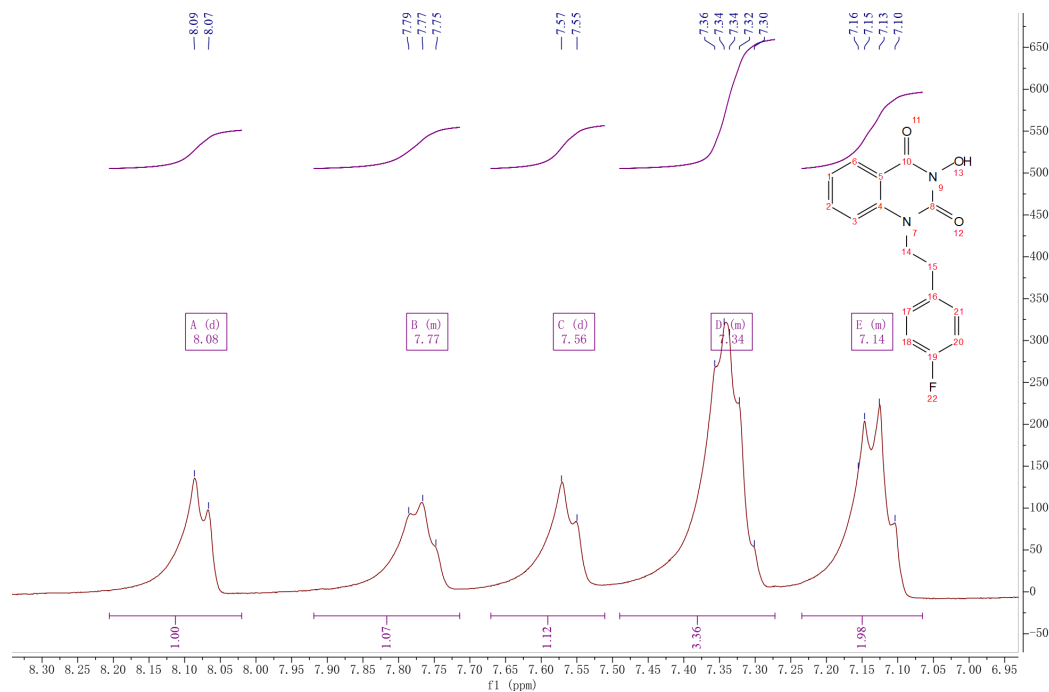


**Figure S10.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10c**

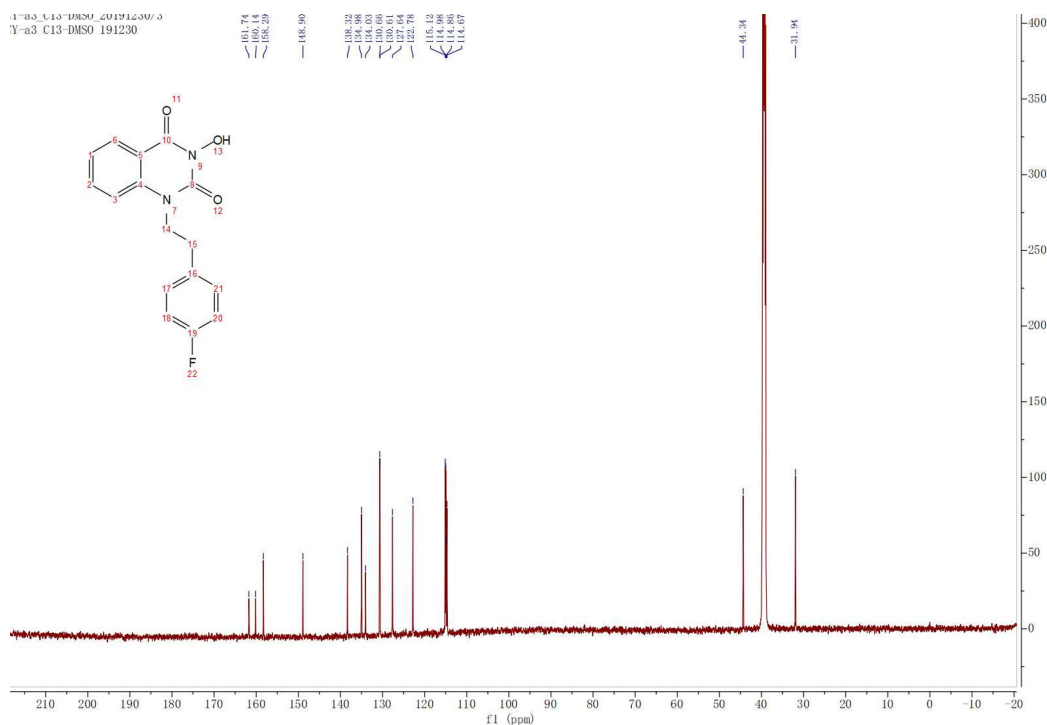




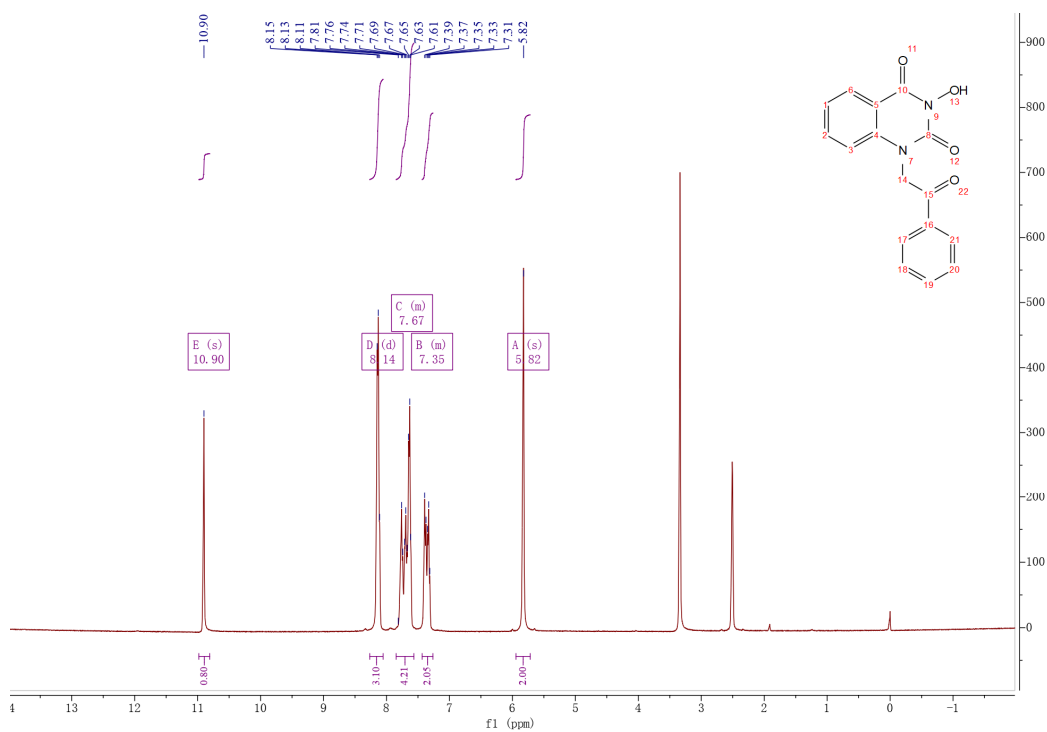
**Figure S11.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10d**



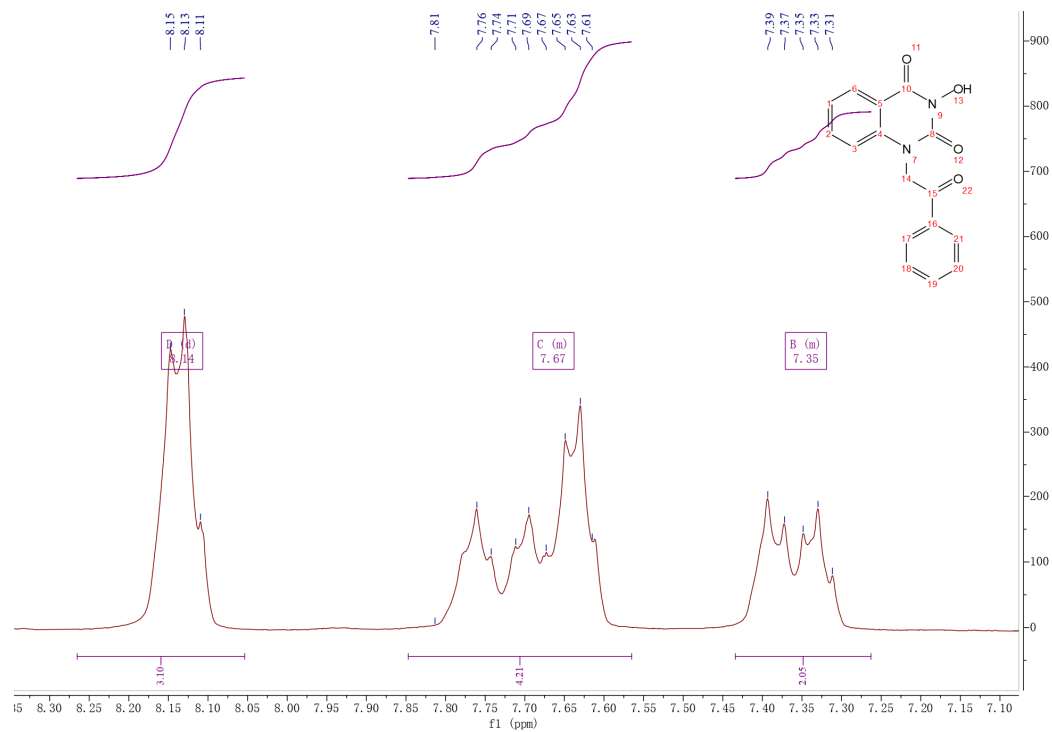
**Figure S12.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **10d**



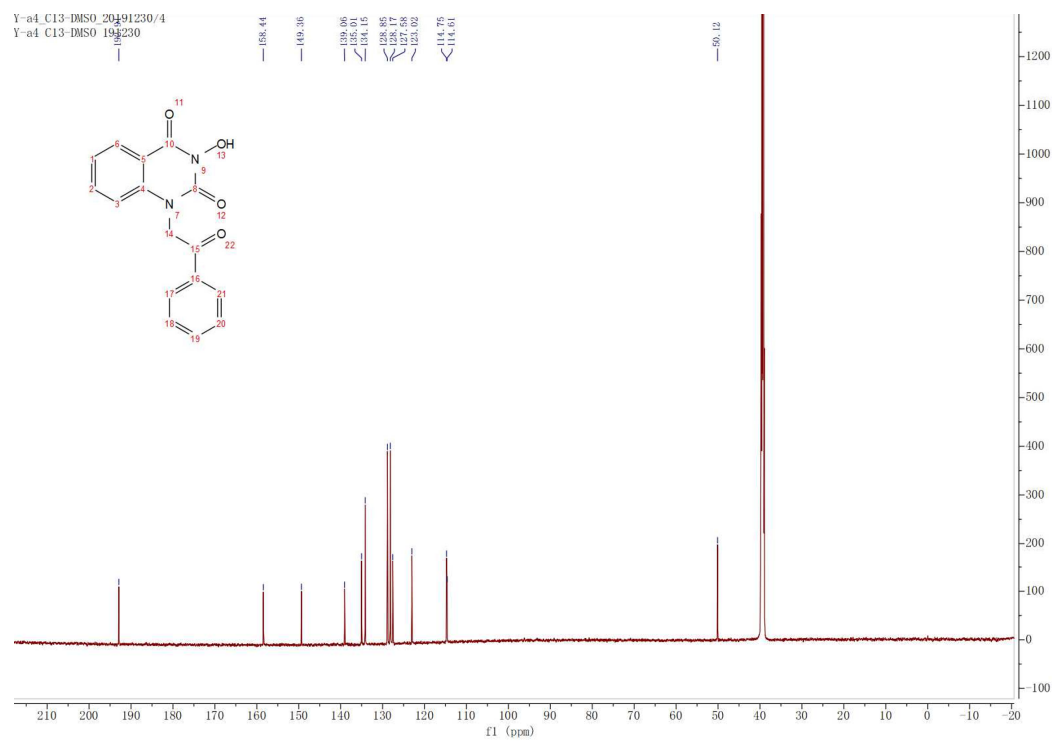
**Figure S13.** <sup>13</sup>C NMR (151 MHz, DMSO-*d*<sub>6</sub>) spectrum of **10d**



**Figure S14.** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of **10e**



**Figure S15.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **10e**



**Figure S16.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10e**

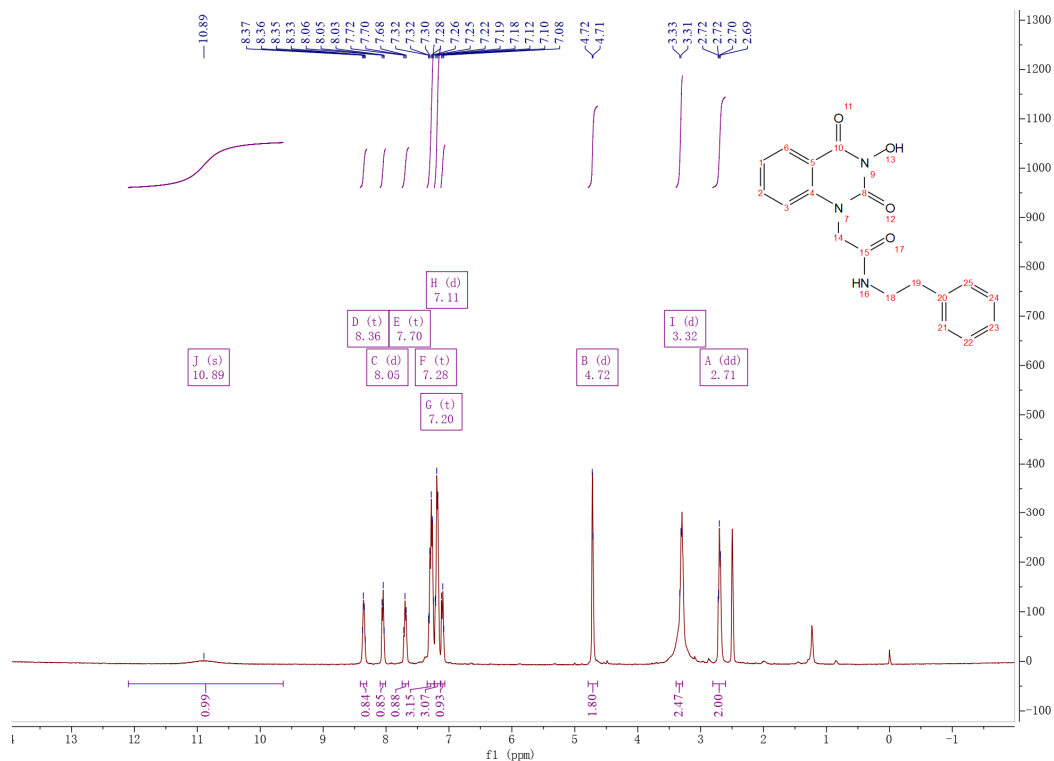


Figure S17.  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10f**

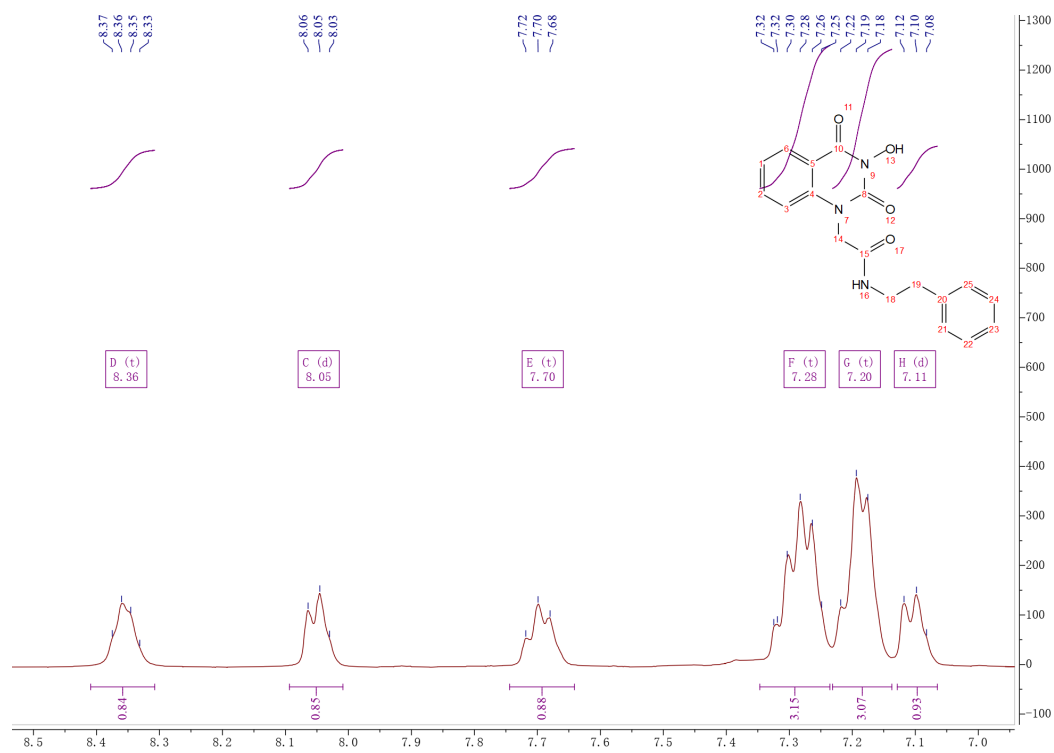
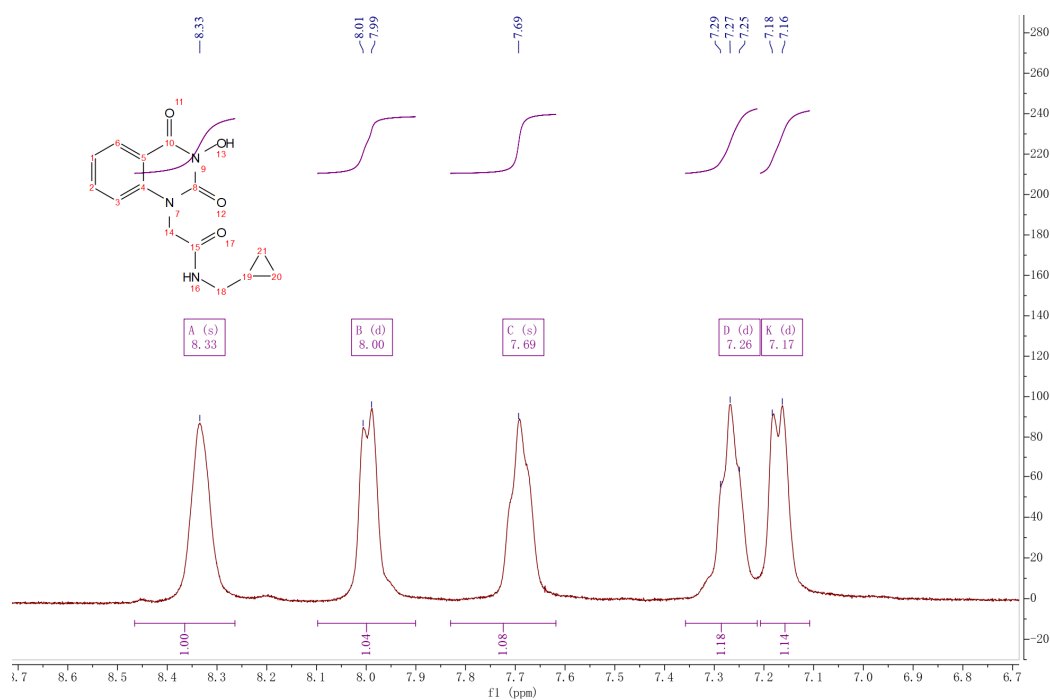


Figure S18. Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **10f**

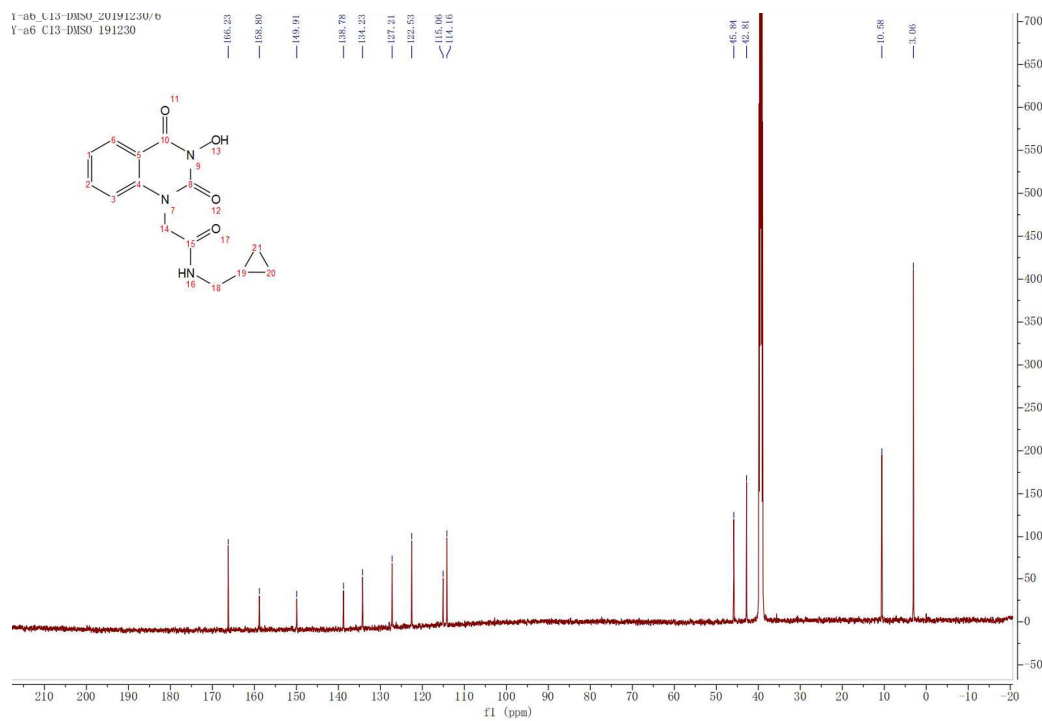
Chemical structure of compound 10 is shown in the top left. The <sup>1</sup>H NMR spectrum (DMSO-d<sub>6</sub>) is displayed below, with peaks labeled A through J and their corresponding chemical shifts and integrations.

Label	Chemical Shift (ppm)	Multiplicity	Integration
A	8.33	s	1.00
B	8.00	d	1.04
C	7.69	s	1.08
D	7.26	d	1.18
E	4.73	s	1.14
F	2.97	s	2.37
G	2.50	s	1.73
H	0.88	s	1.07
I	0.38	d	2.00
J	0.13	s	2.03

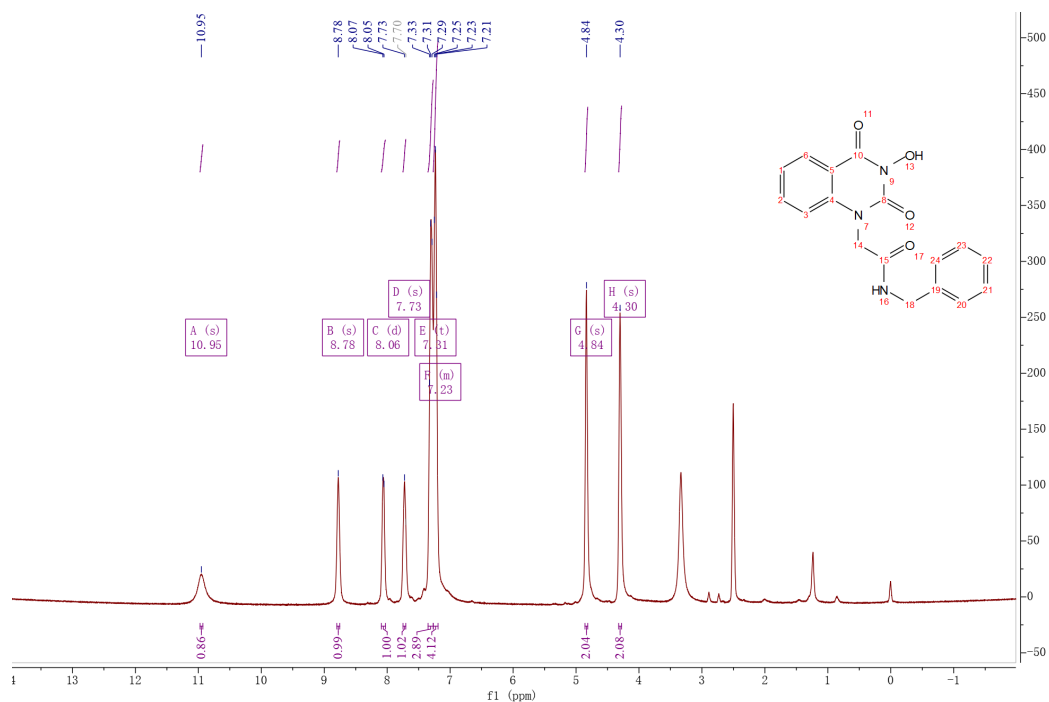
**Figure S20.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10g**



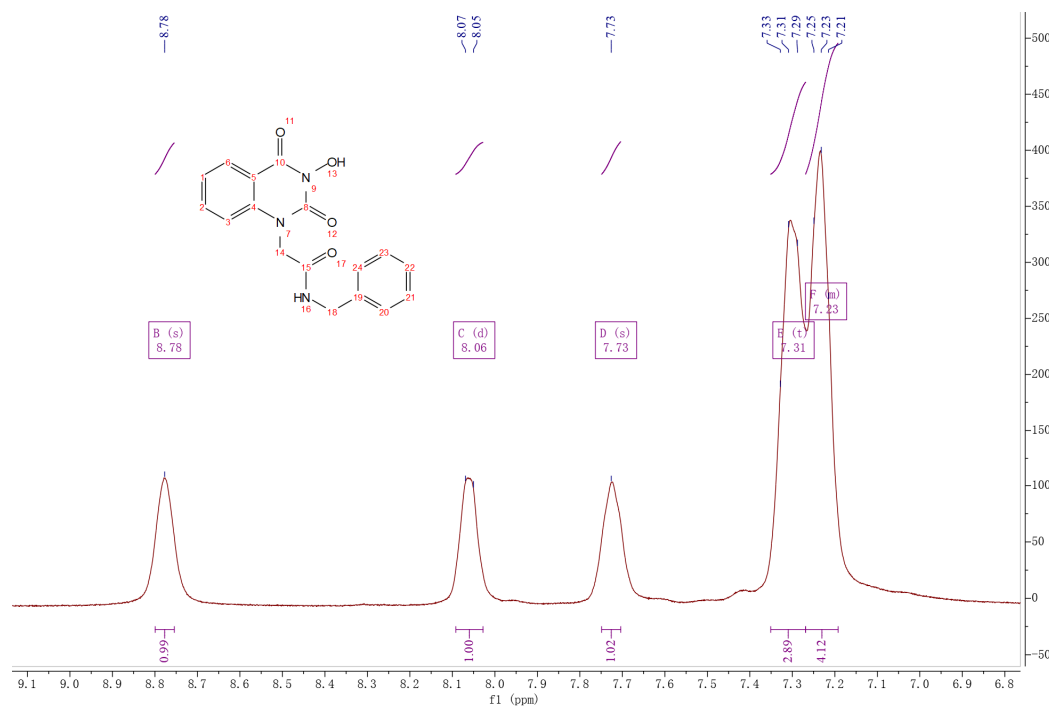
**Figure S21.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **10g**



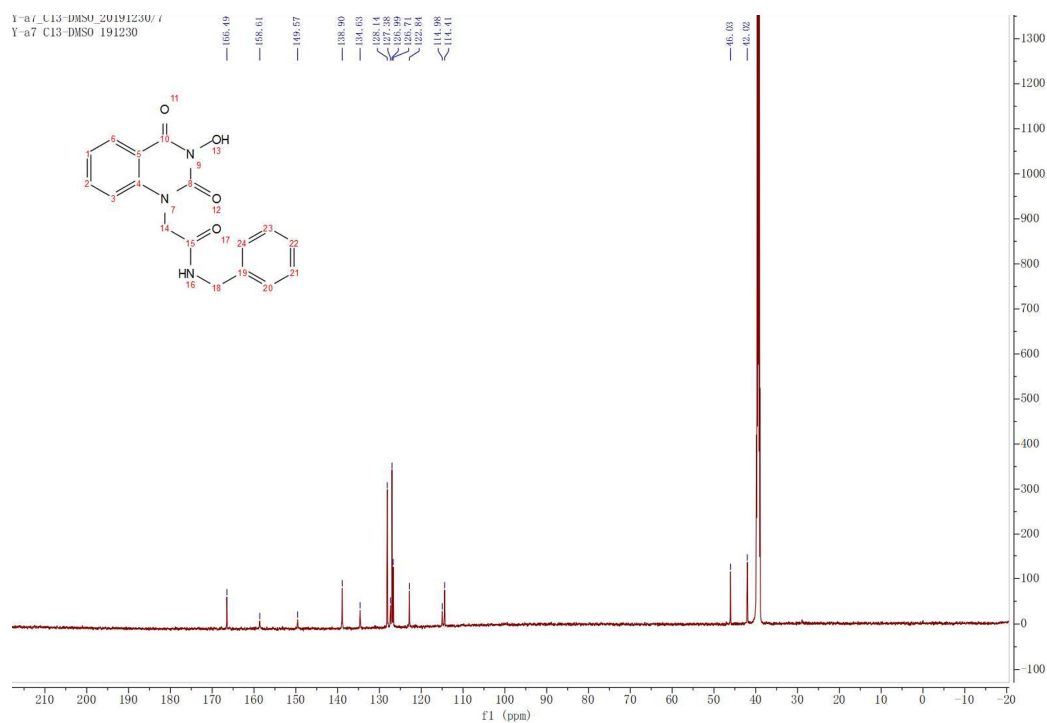
**Figure S22.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10g**



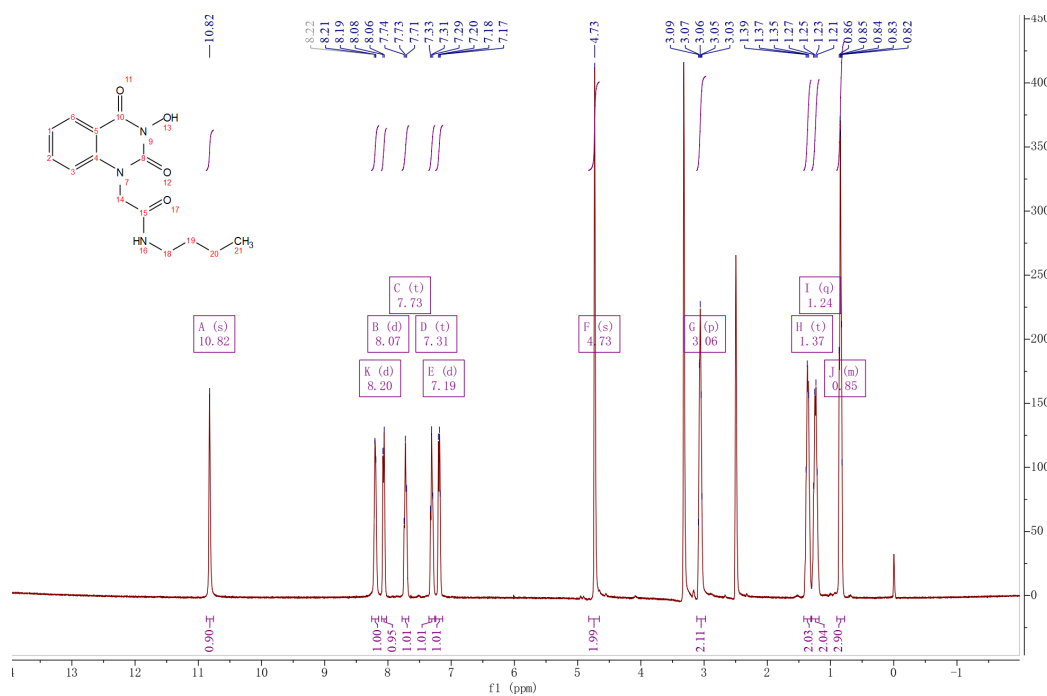
**Figure S23.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10h**



**Figure S24.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **10h**

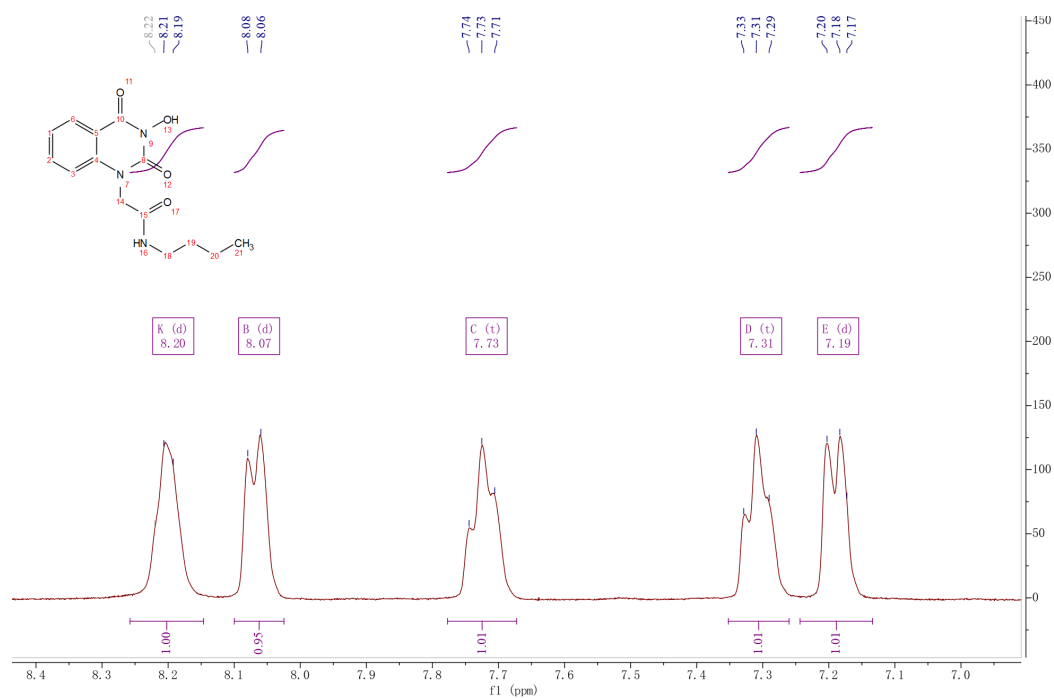


**Figure S25.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10h**

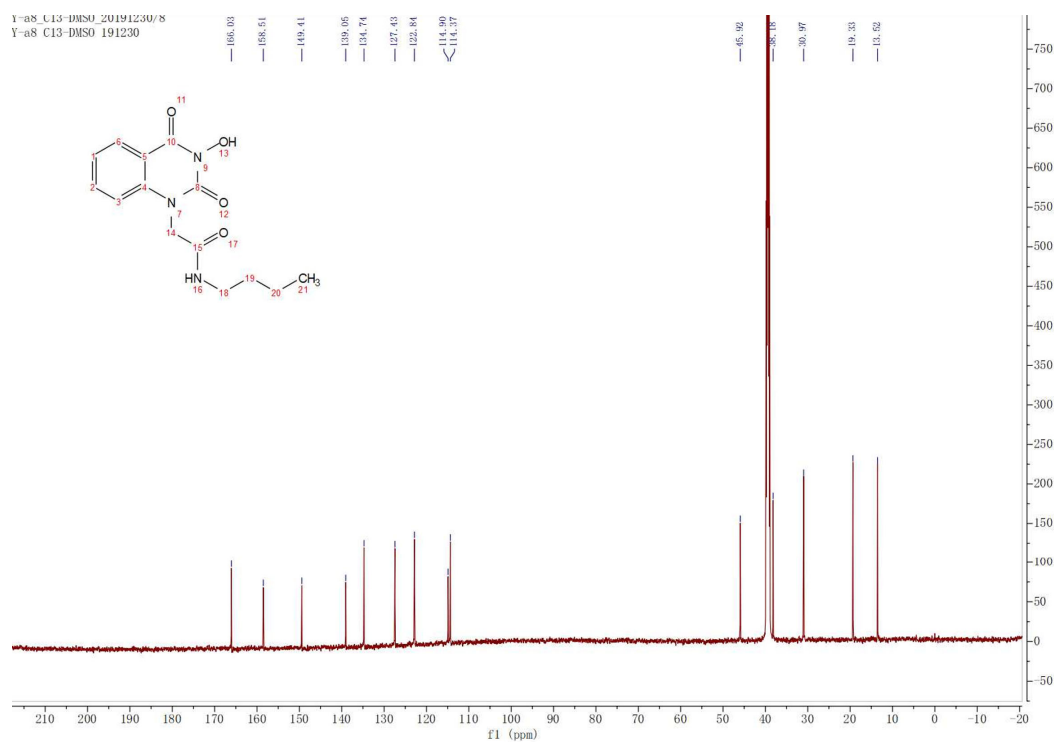


**Figure S26.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10i**

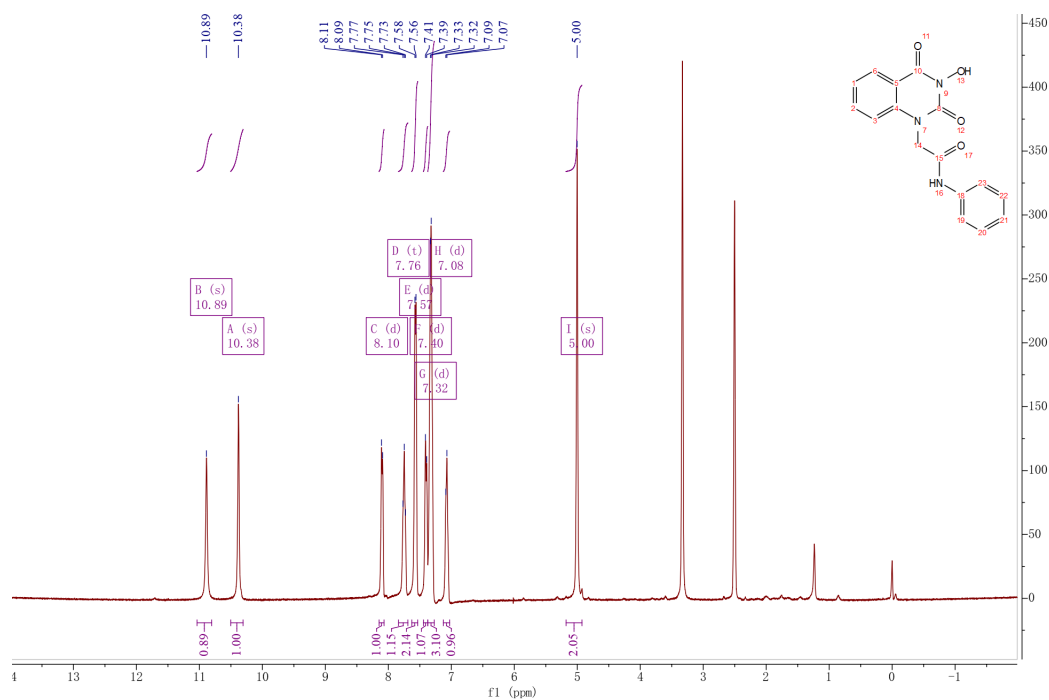




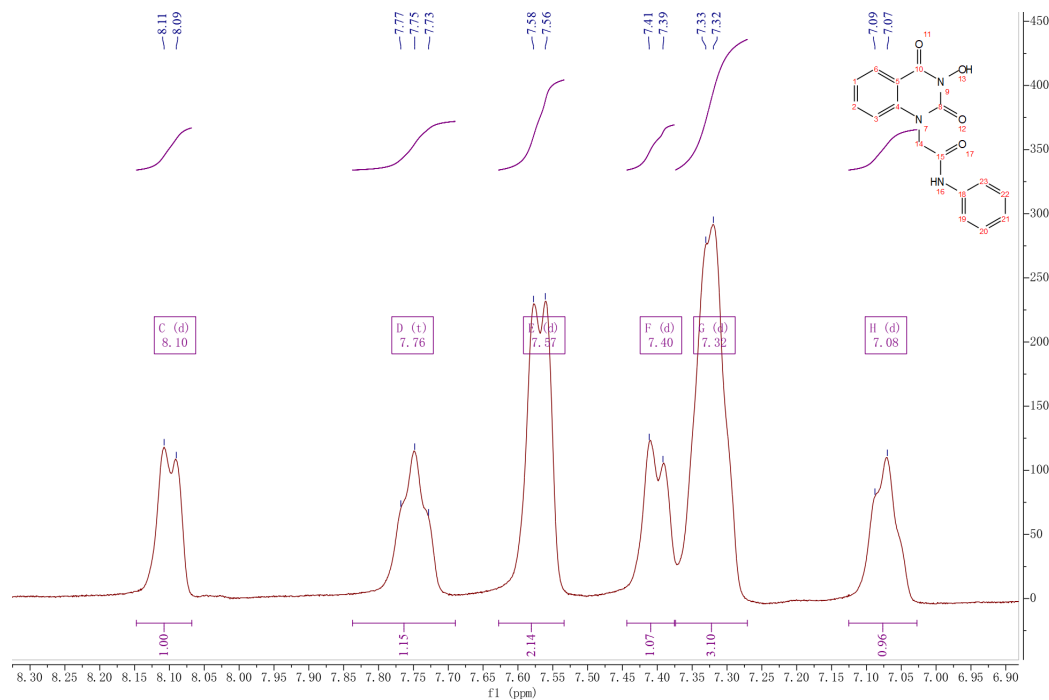
**Figure S27.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **10i**



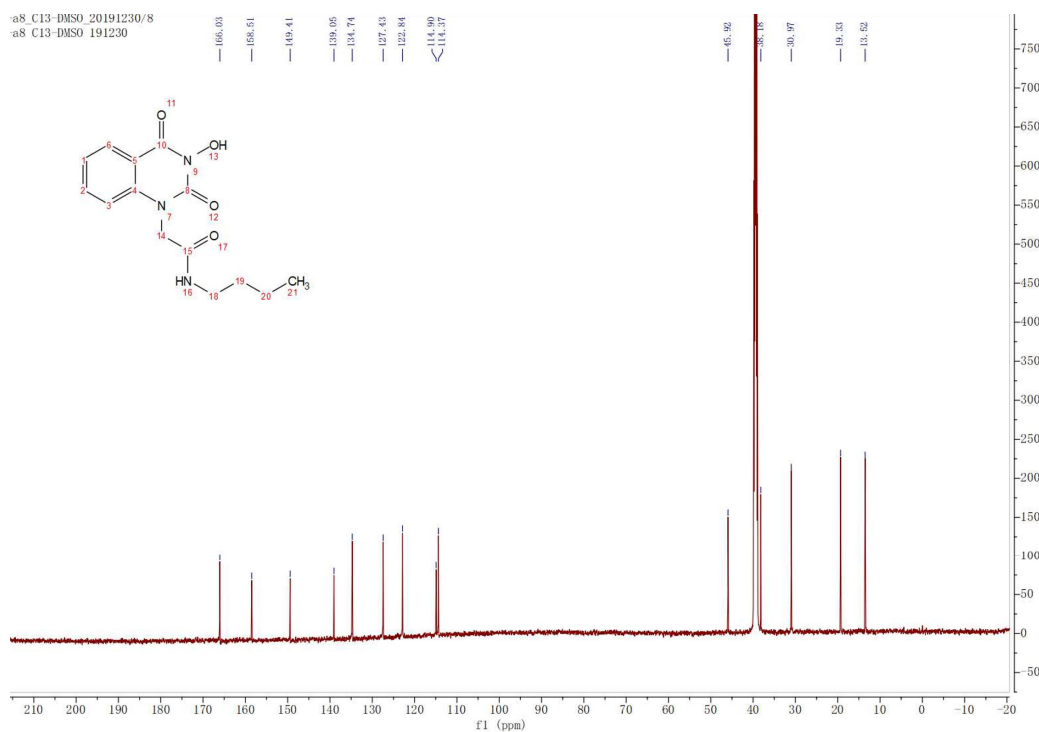
**Figure S28.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10i**



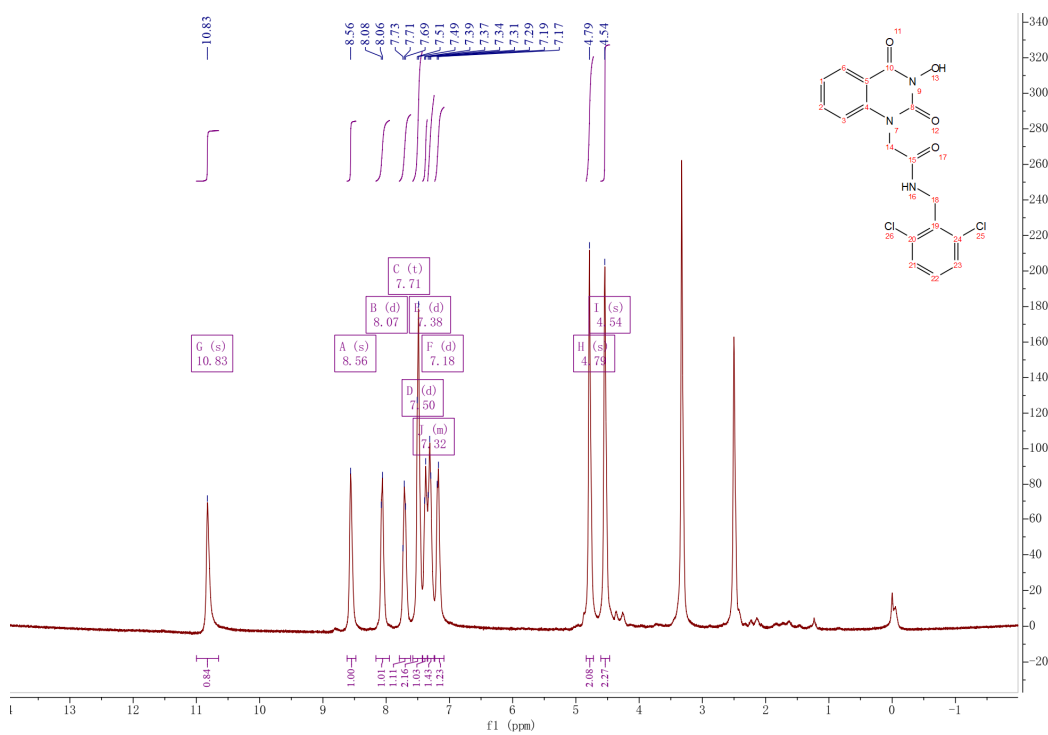
**Figure S29.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10j**



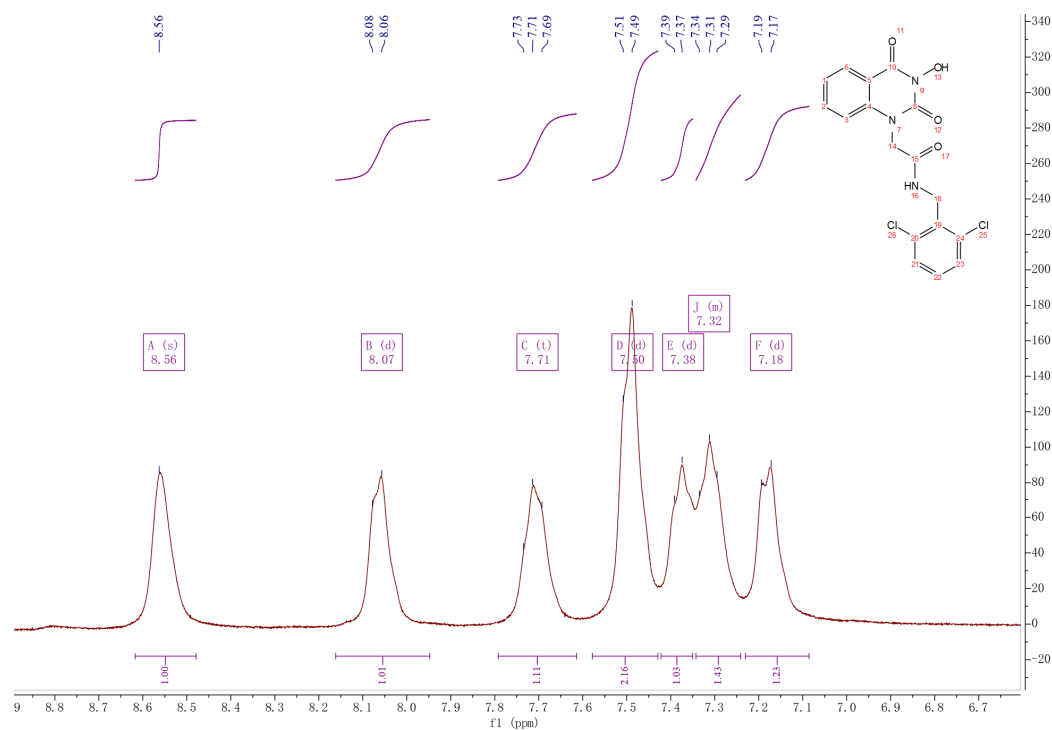
**Figure S30.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **10j**



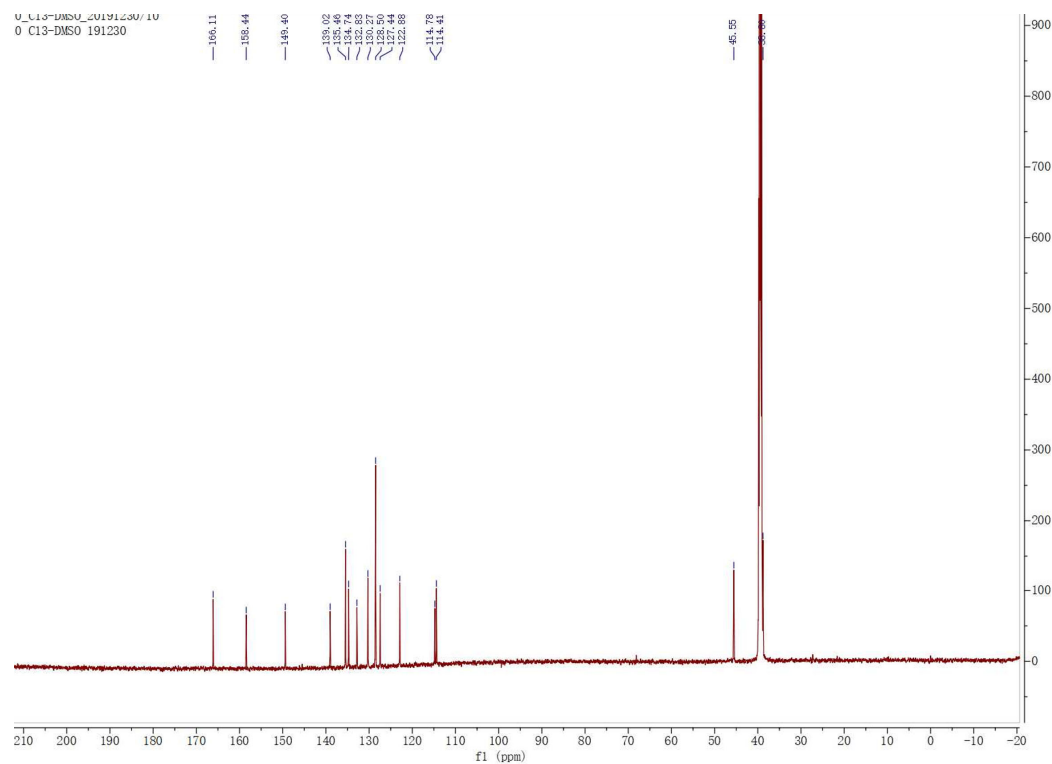
**Figure S31.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10j**



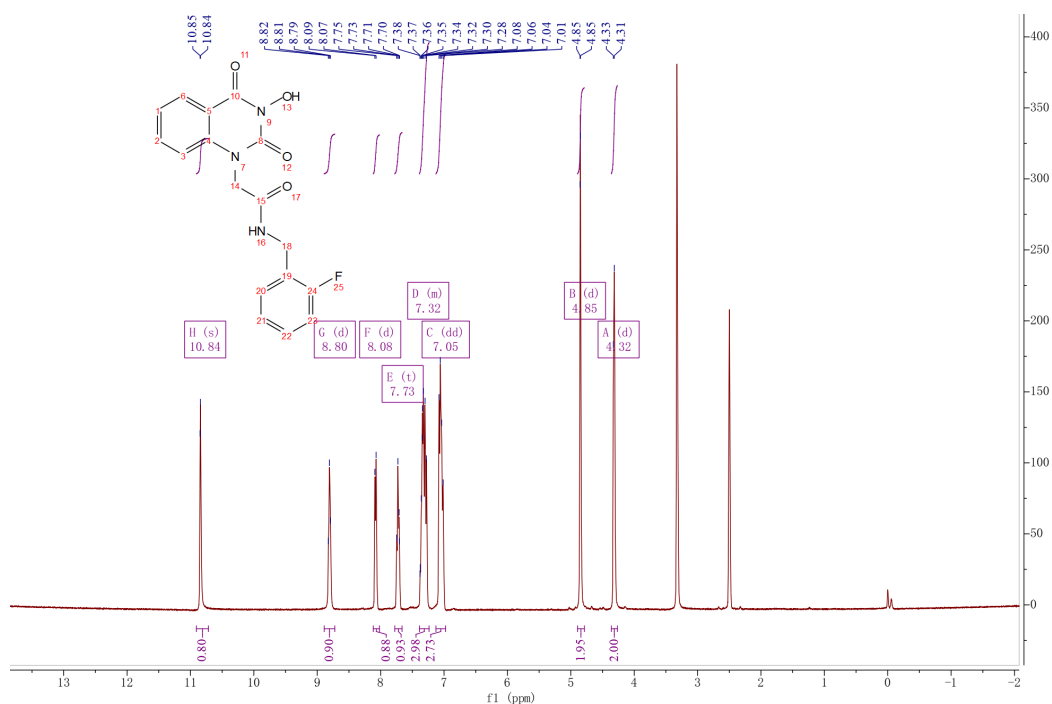
**Figure S32.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10k**



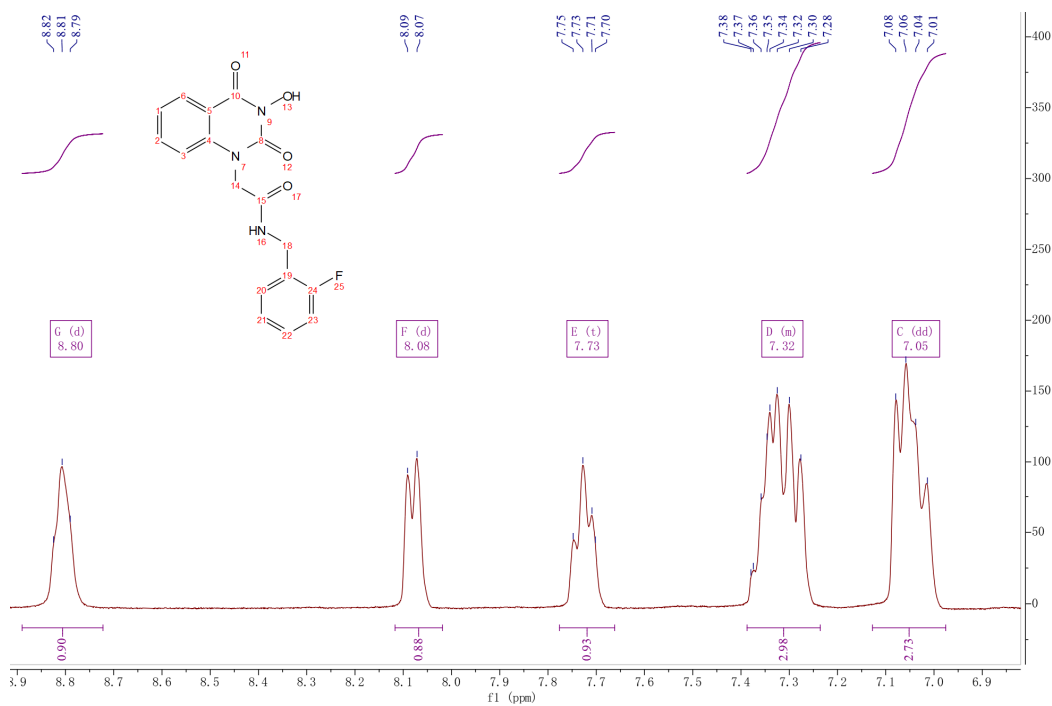
**Figure S33.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **10k**



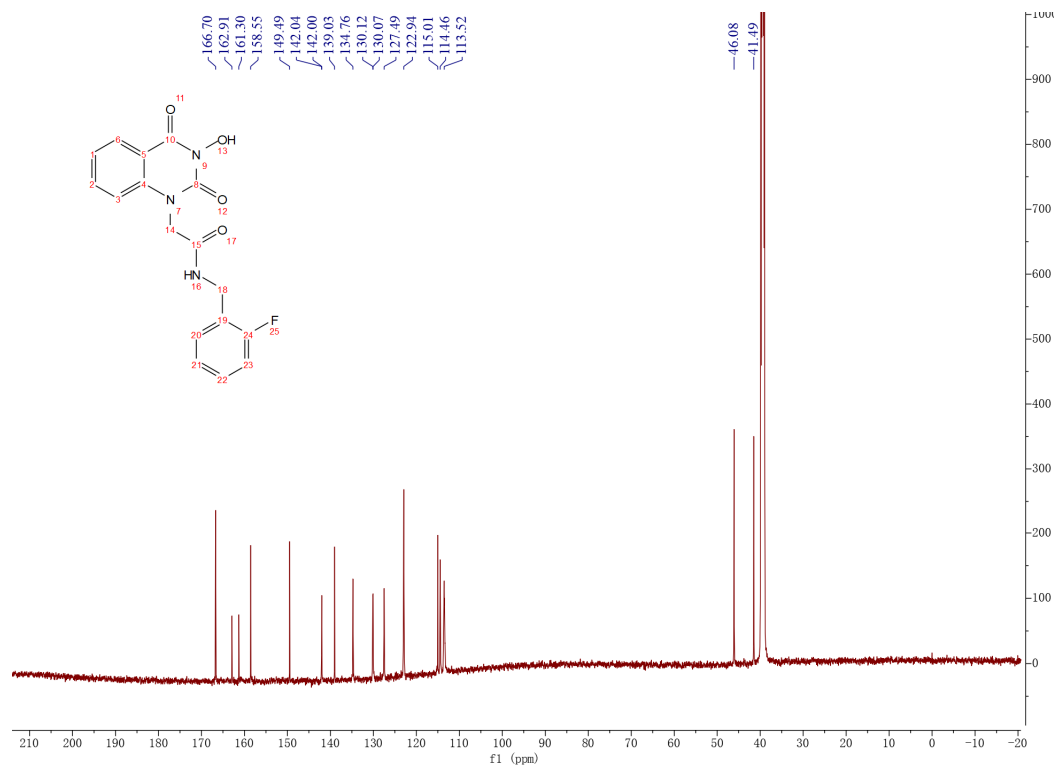
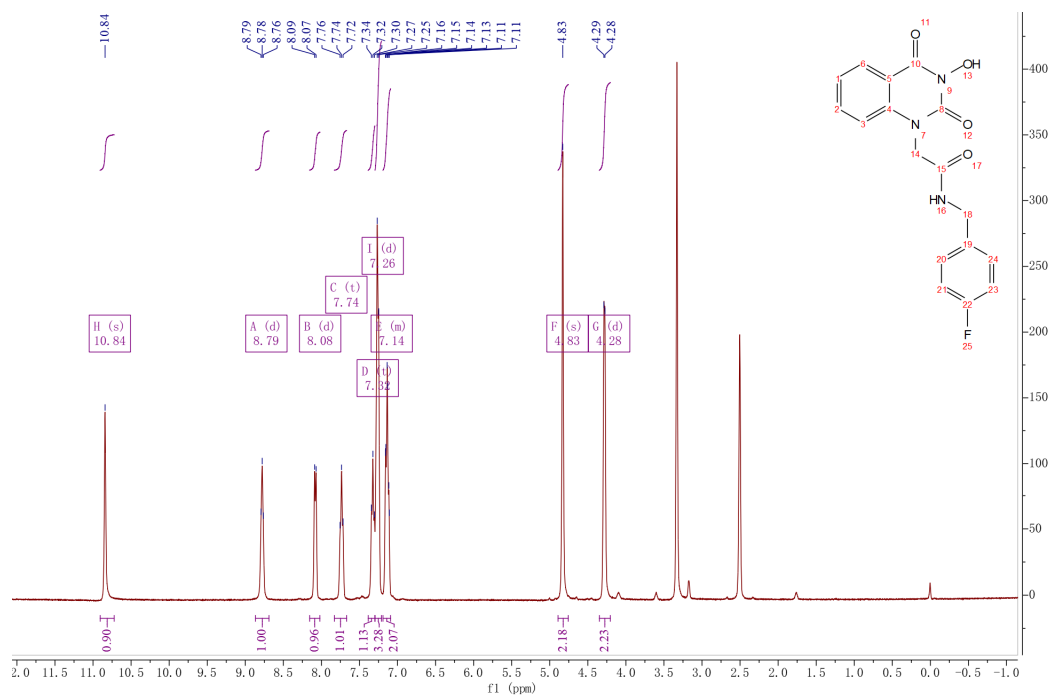
**Figure S34.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10k**

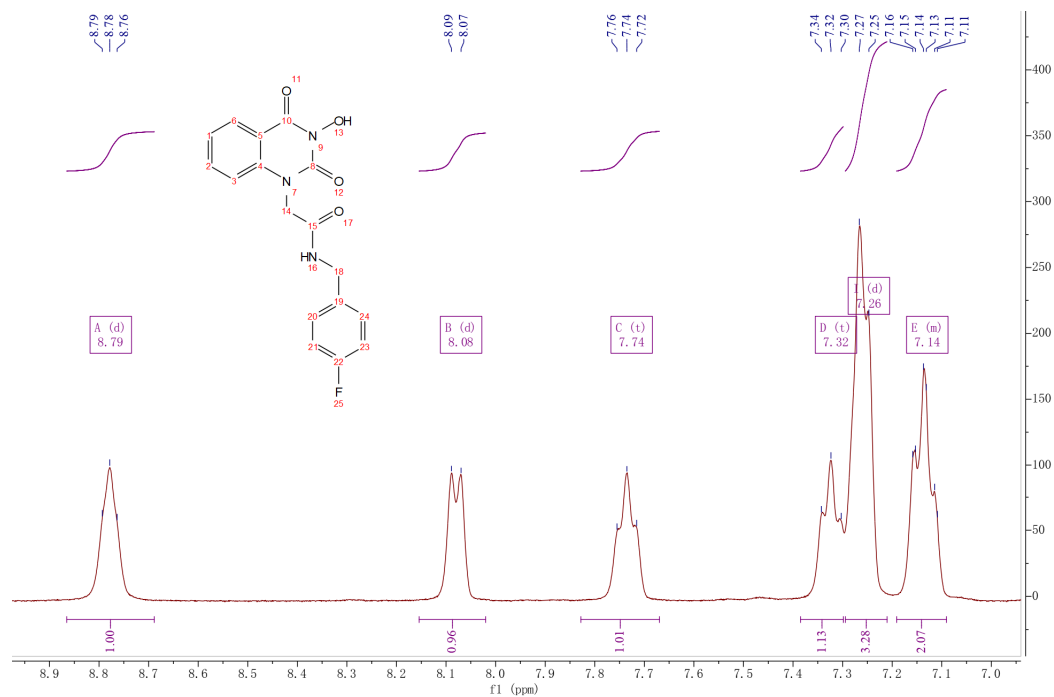


**Figure S35.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **101**

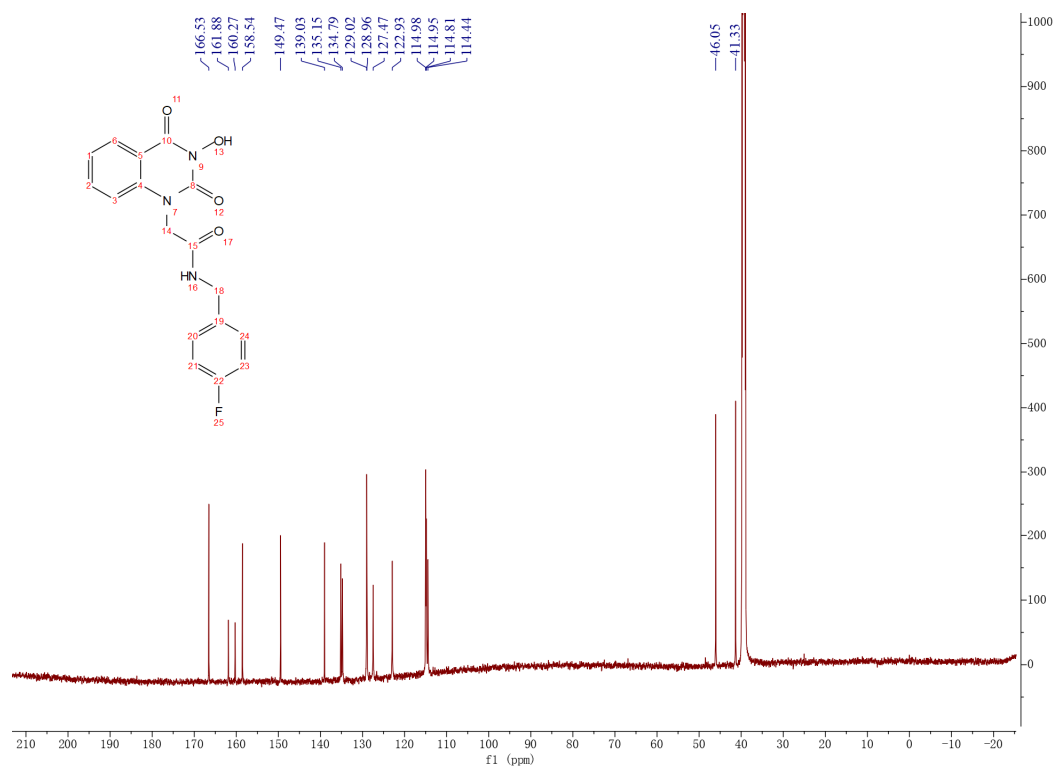


**Figure S36.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **101**

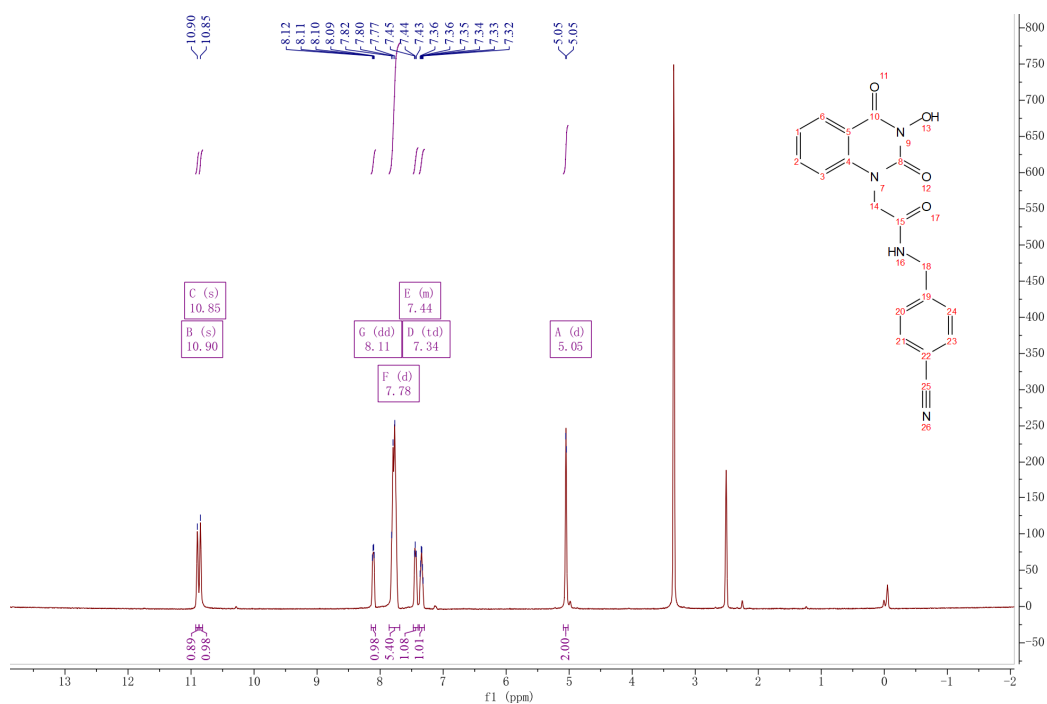
Figure S37.  $^{13}\text{C}$  NMR (151 MHz, DMSO- $d_6$ ) spectrum of 10lFigure S38.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ) spectrum of 10m



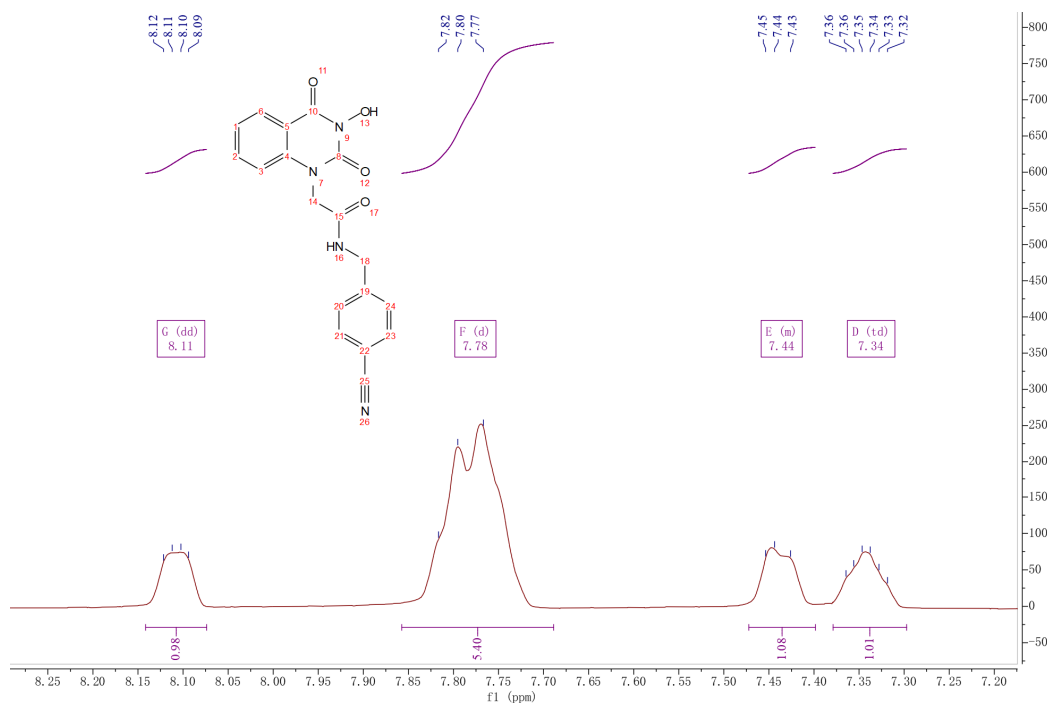
**Figure S39.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **10m**



**Figure S40.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10m**

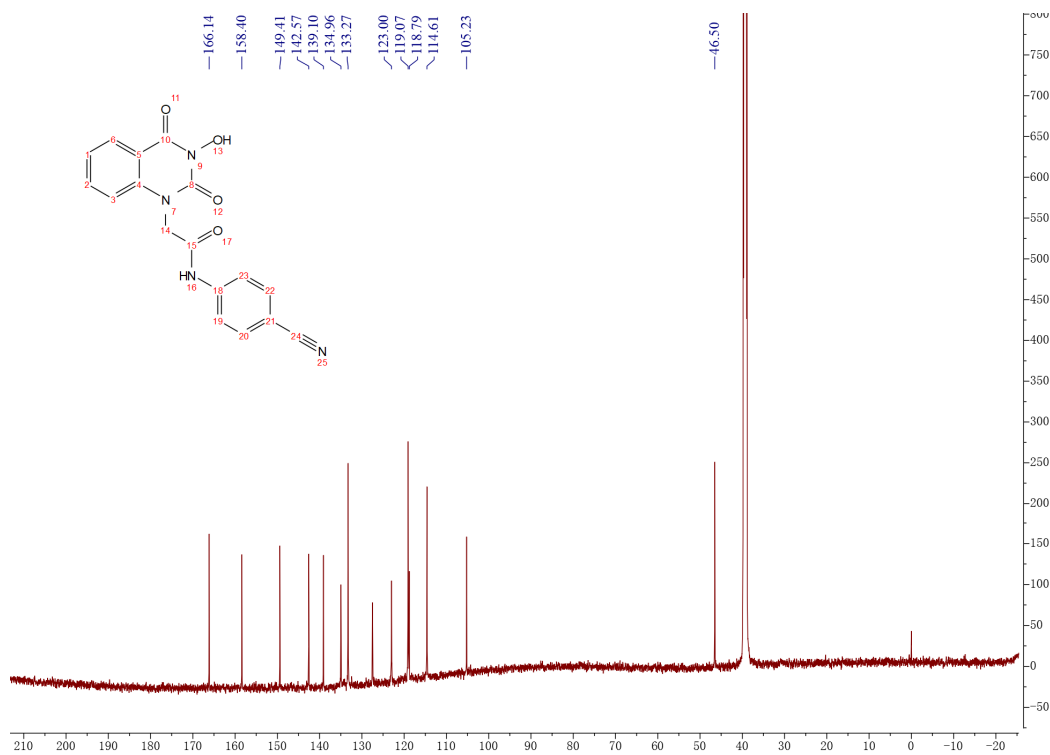


**Figure S41.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10n**

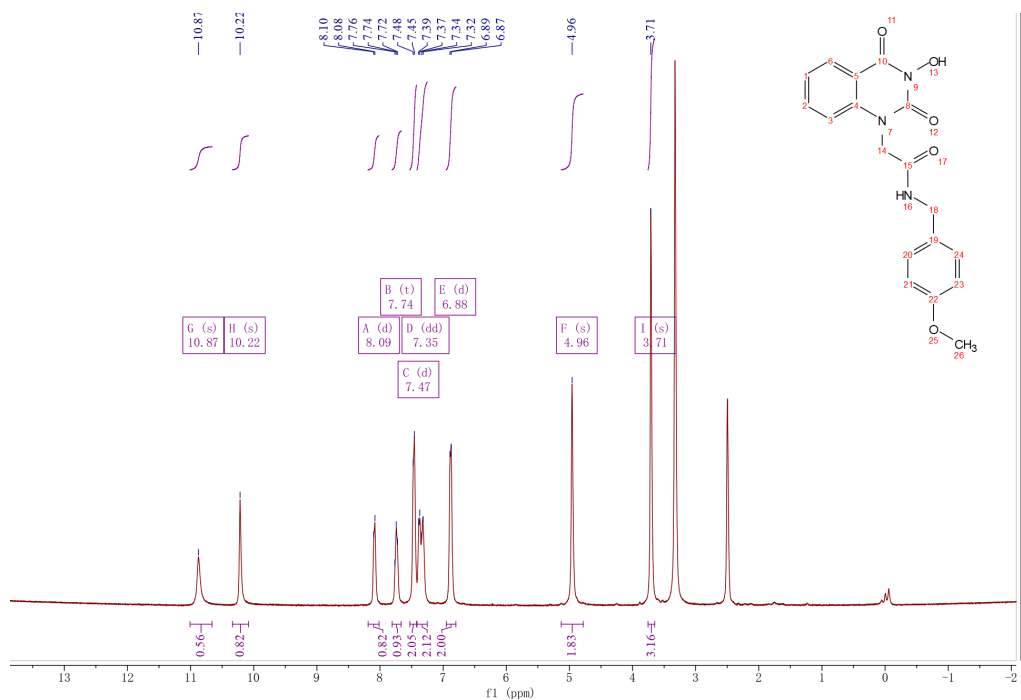


**Figure S42.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **10n**

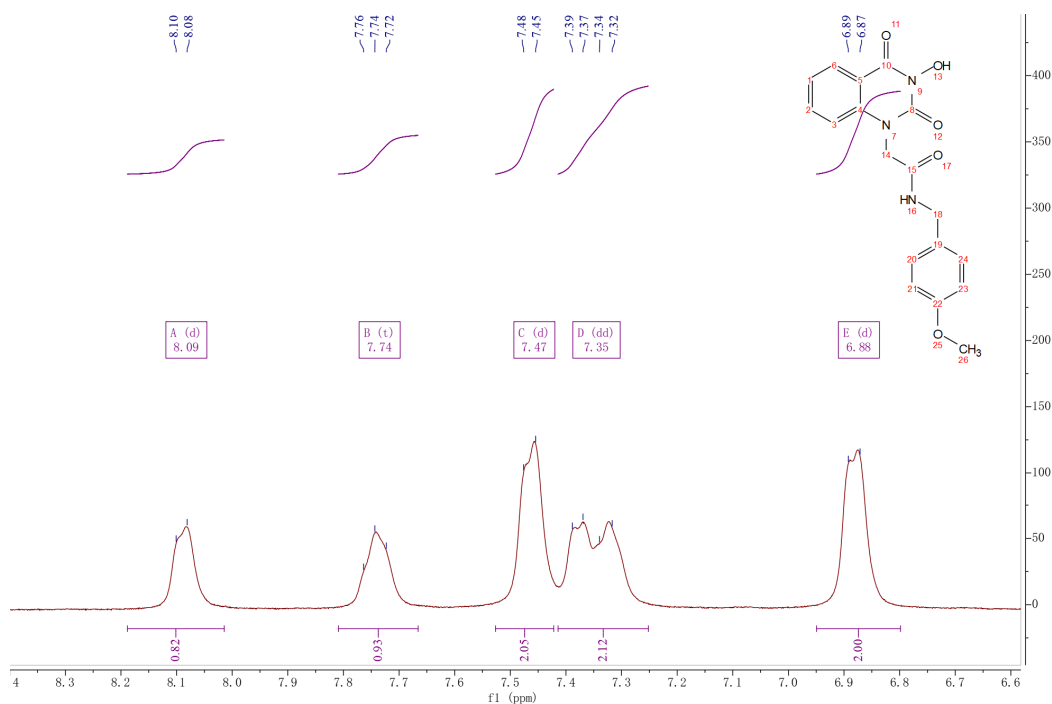




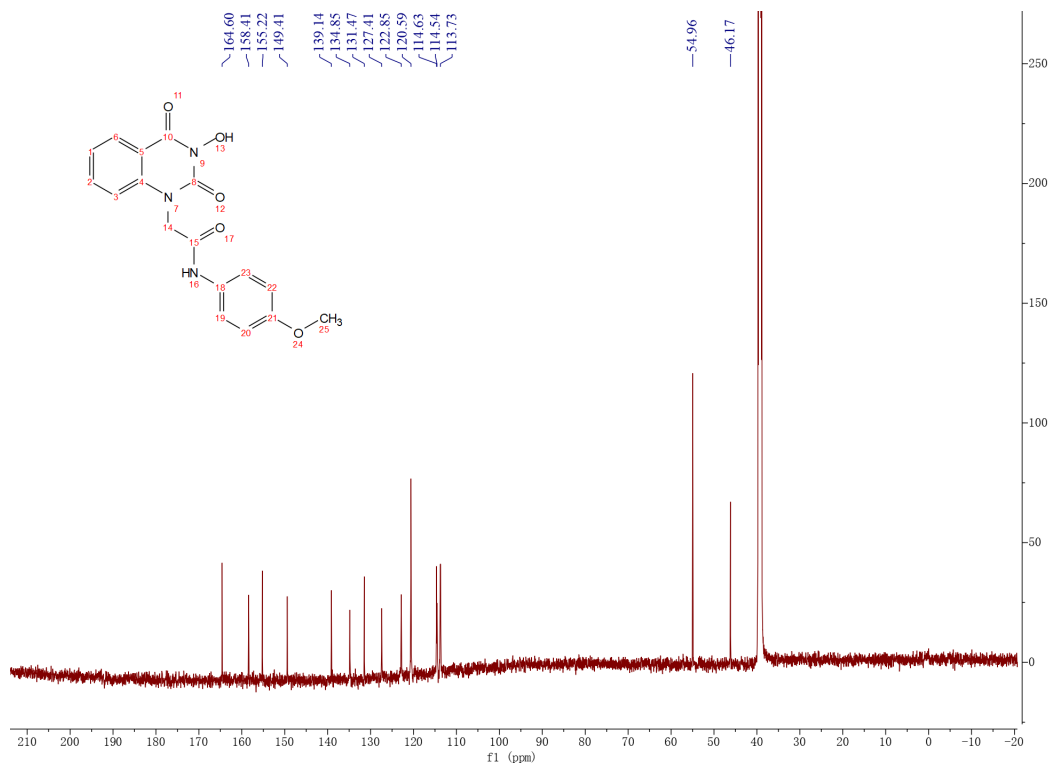
**Figure S43.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10n**



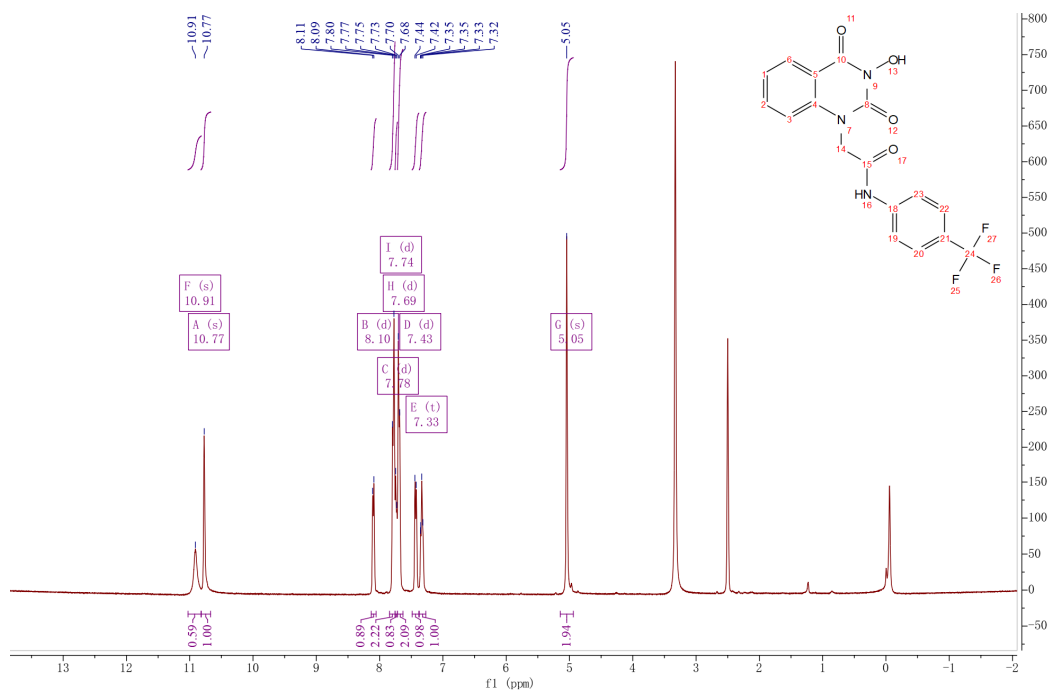
**Figure S44.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10o**



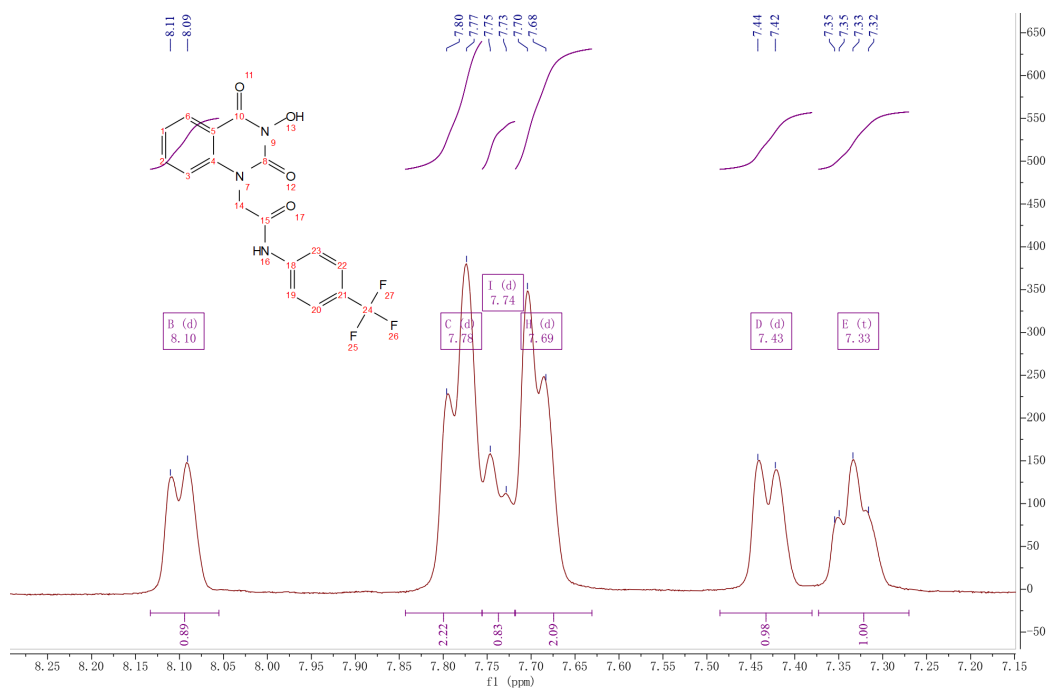
**Figure S45.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **10o**



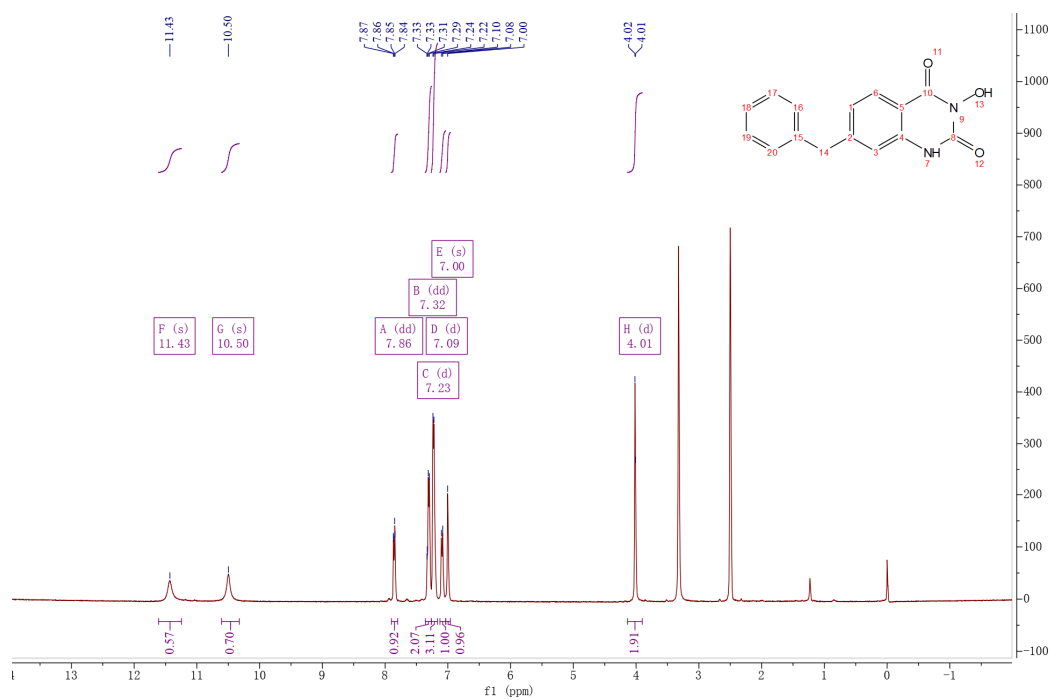
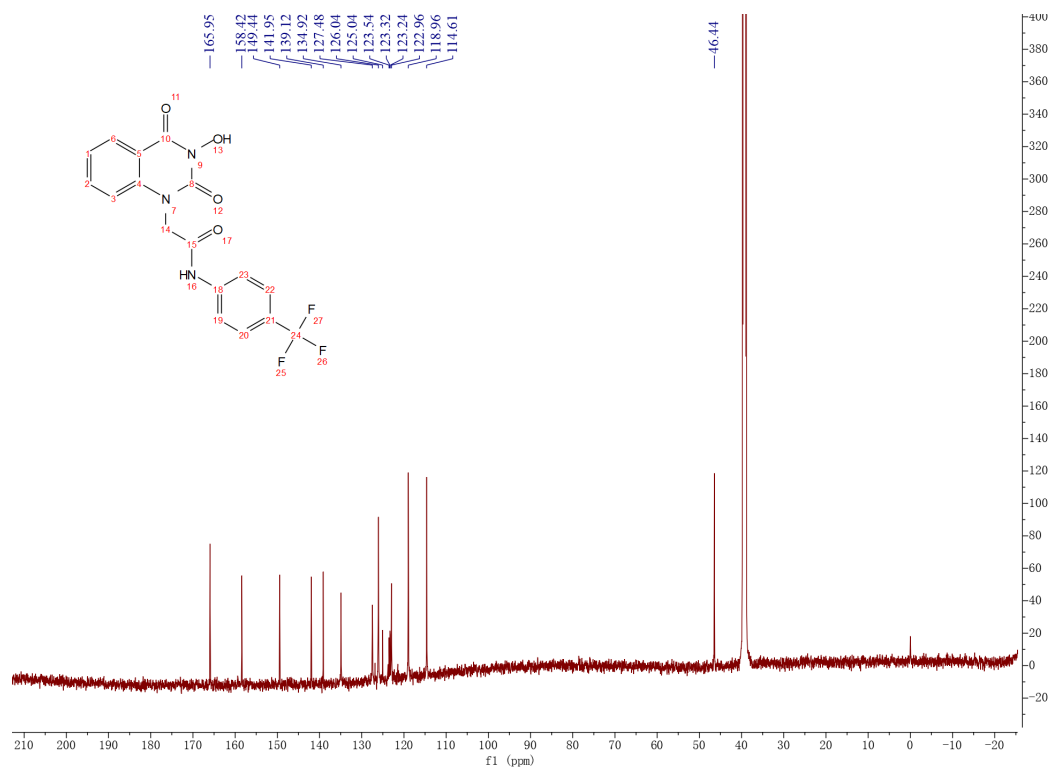
**Figure S46.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10o**

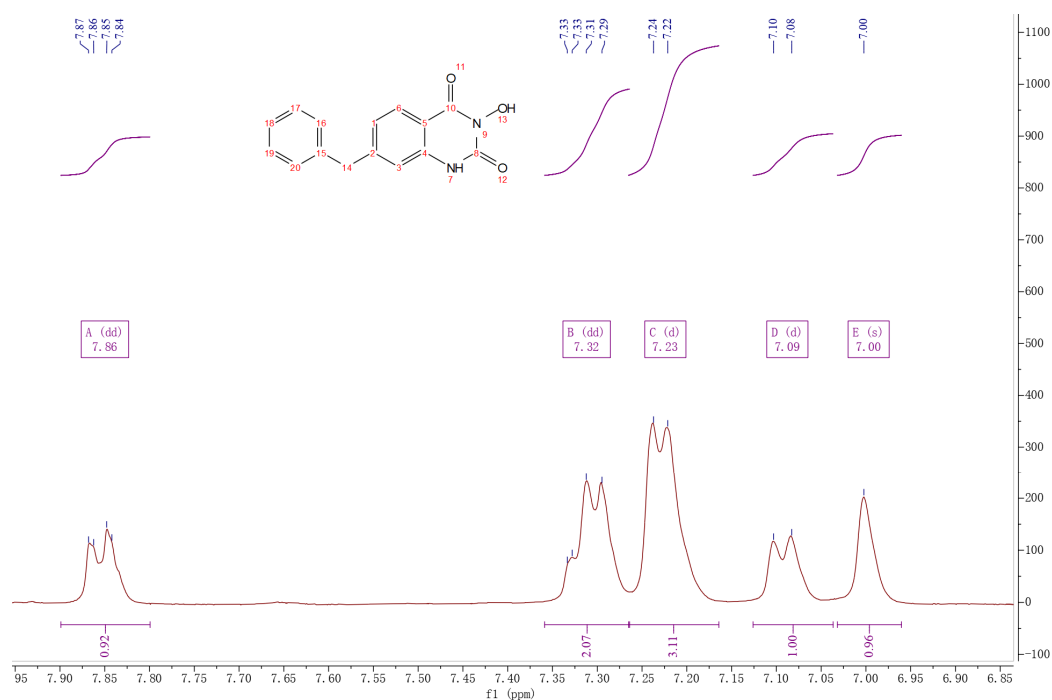


**Figure S47.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10p**

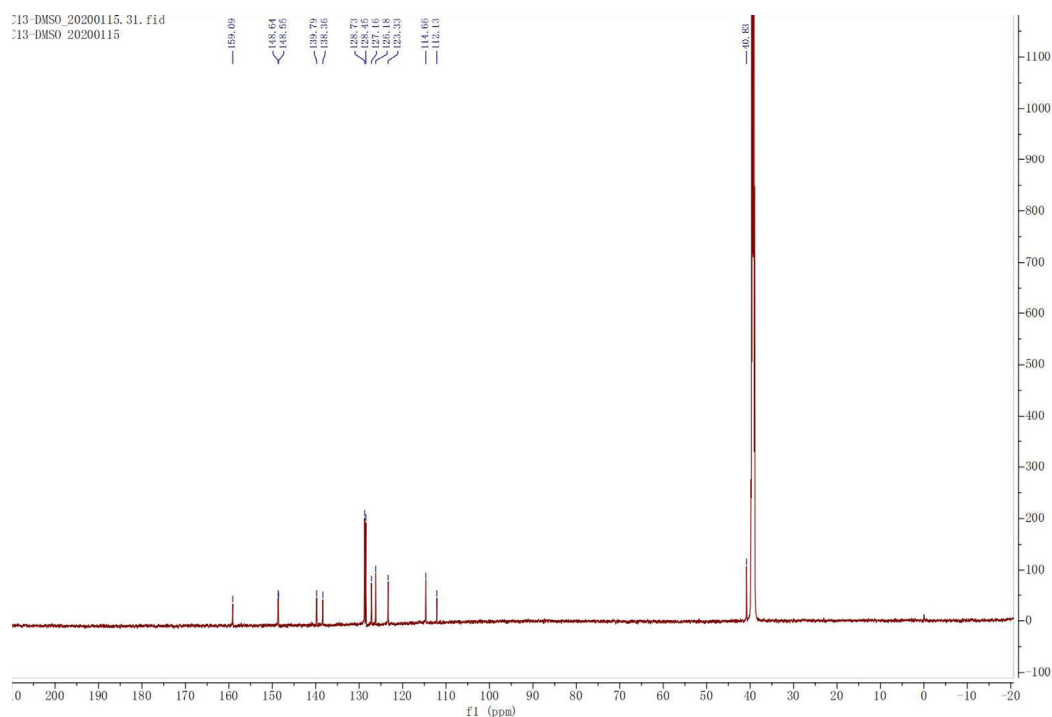


**Figure S48.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **10p**

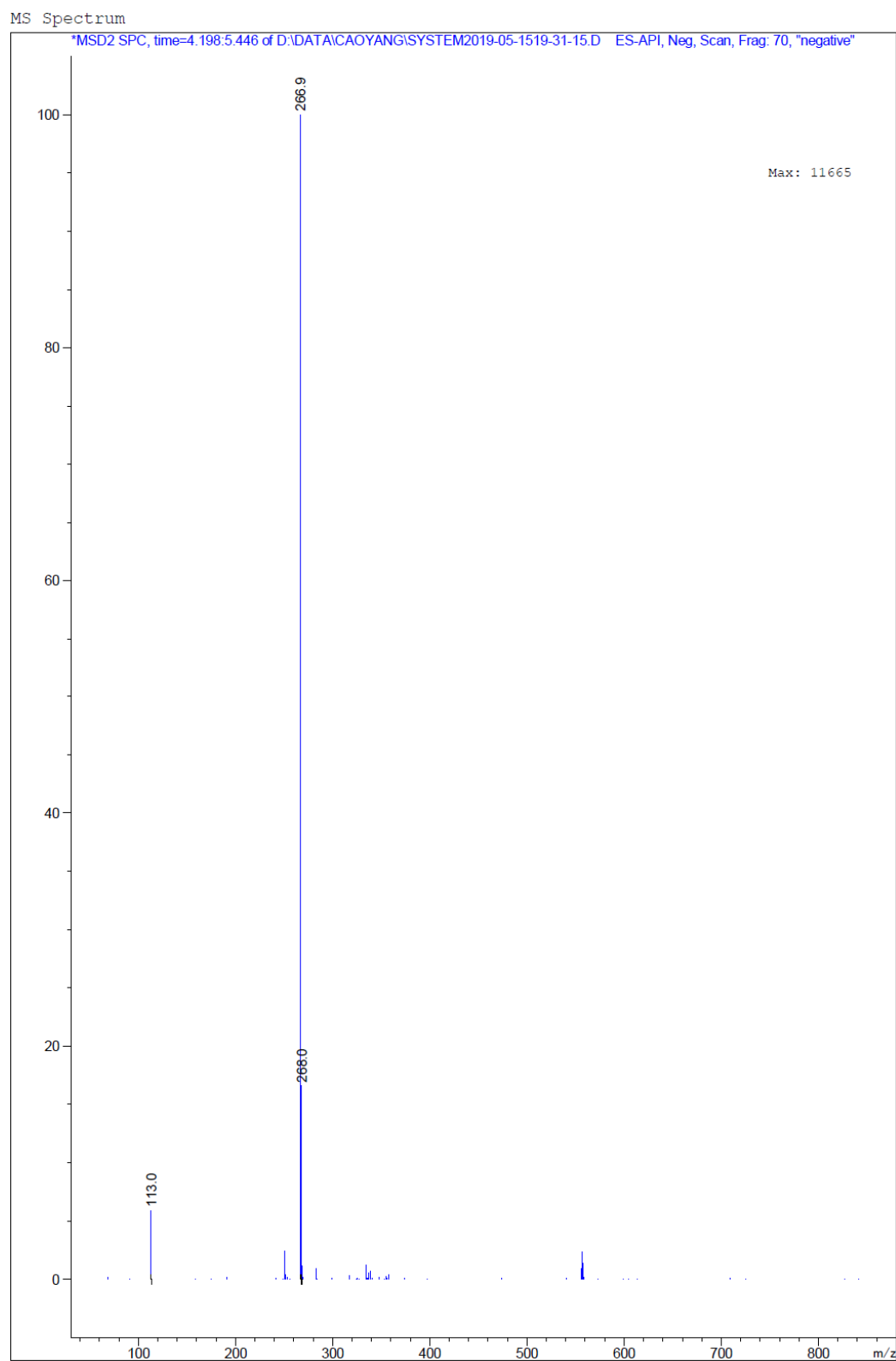




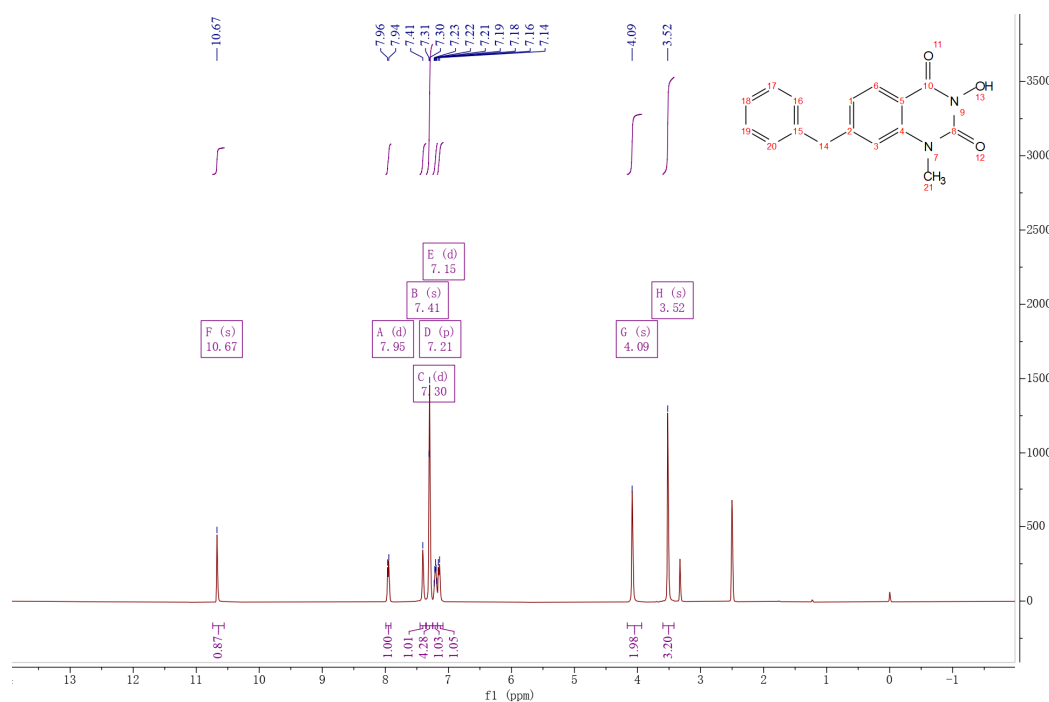
**Figure S51.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **18a**



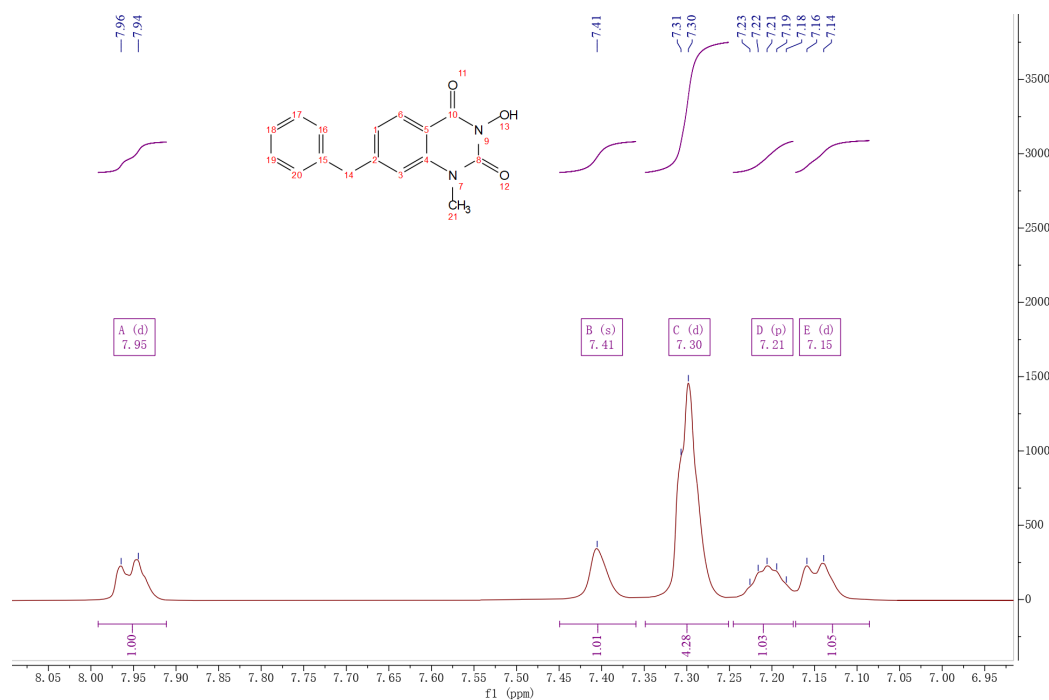
**Figure S52.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **18a**



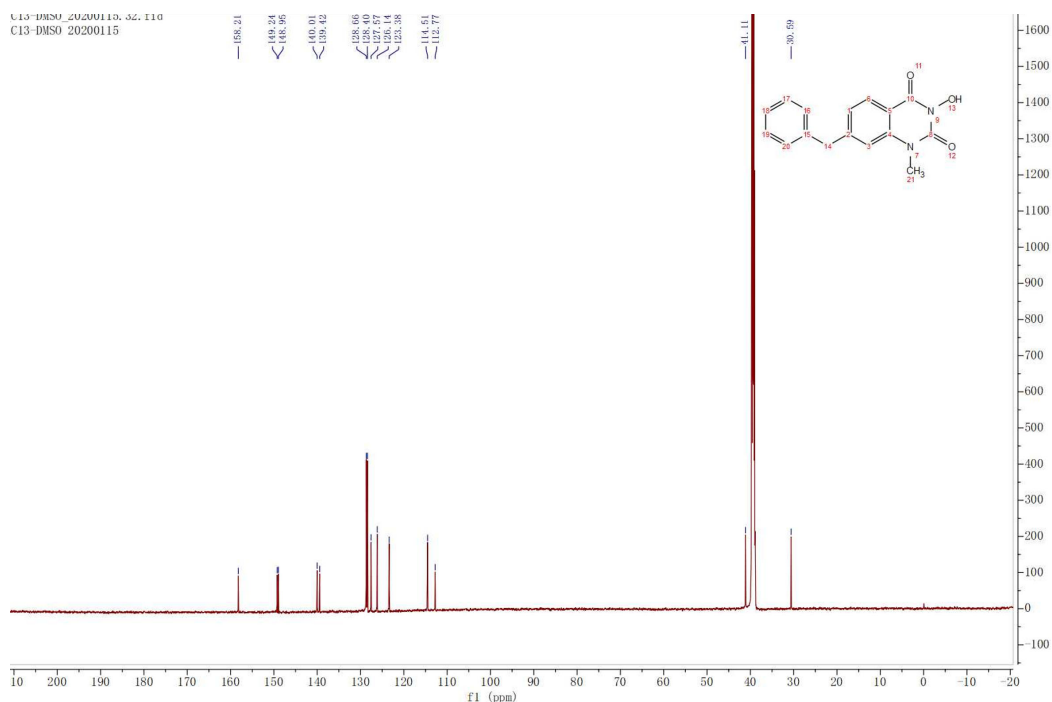
**Figure S53.** Mass spectrum (negative ionization) of **18a**



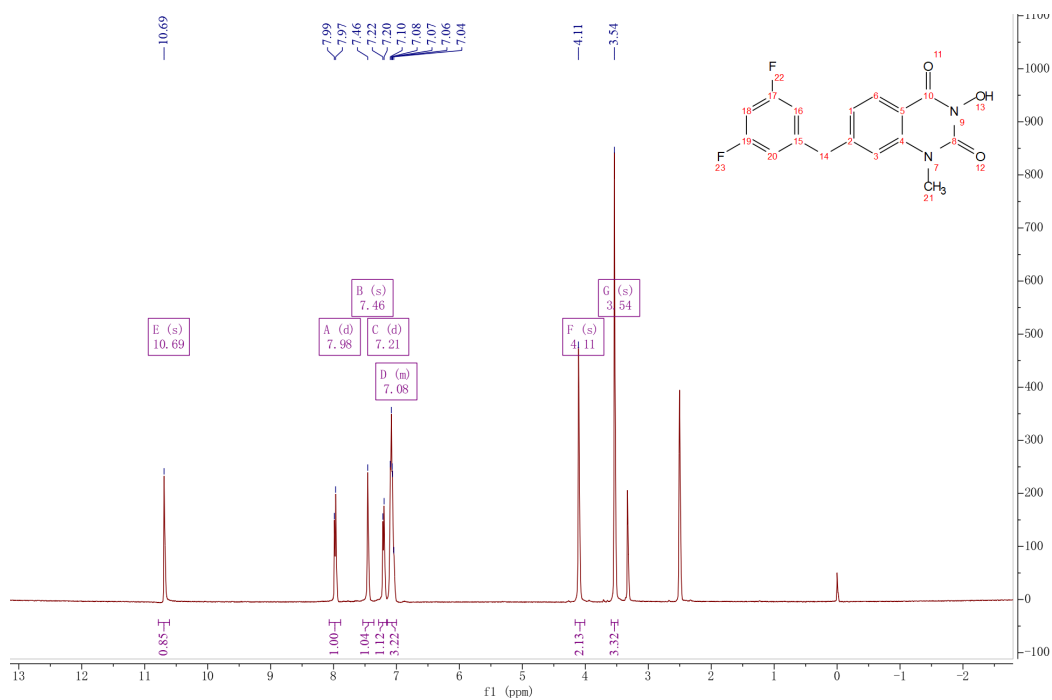
**Figure S54.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **18b**



**Figure S55.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **18b**

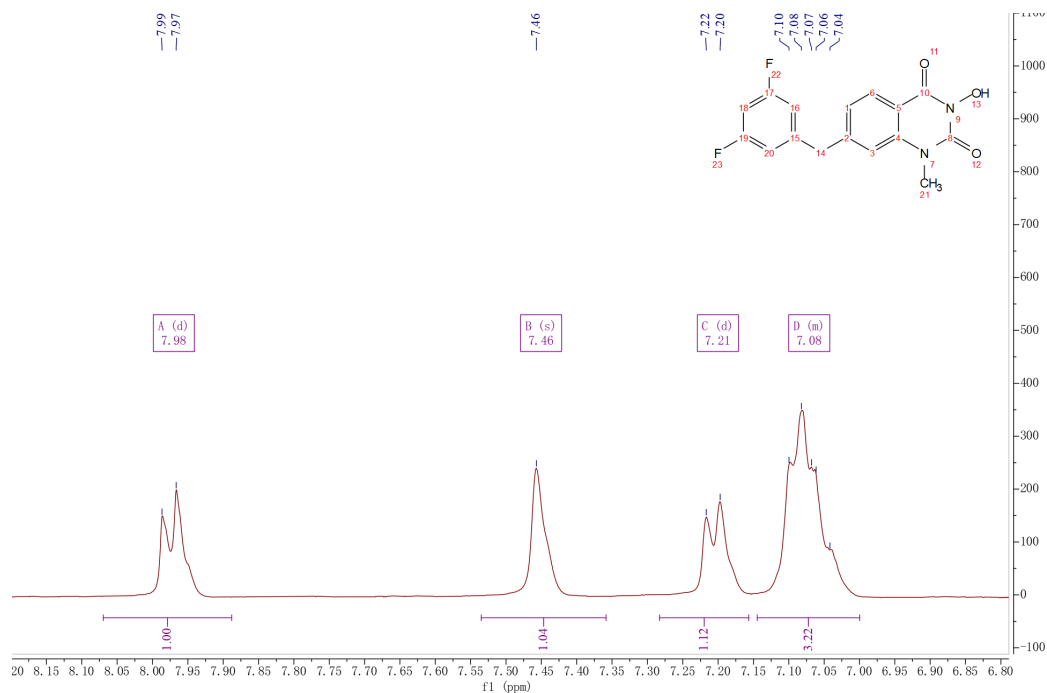


**Figure S56.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **18b**

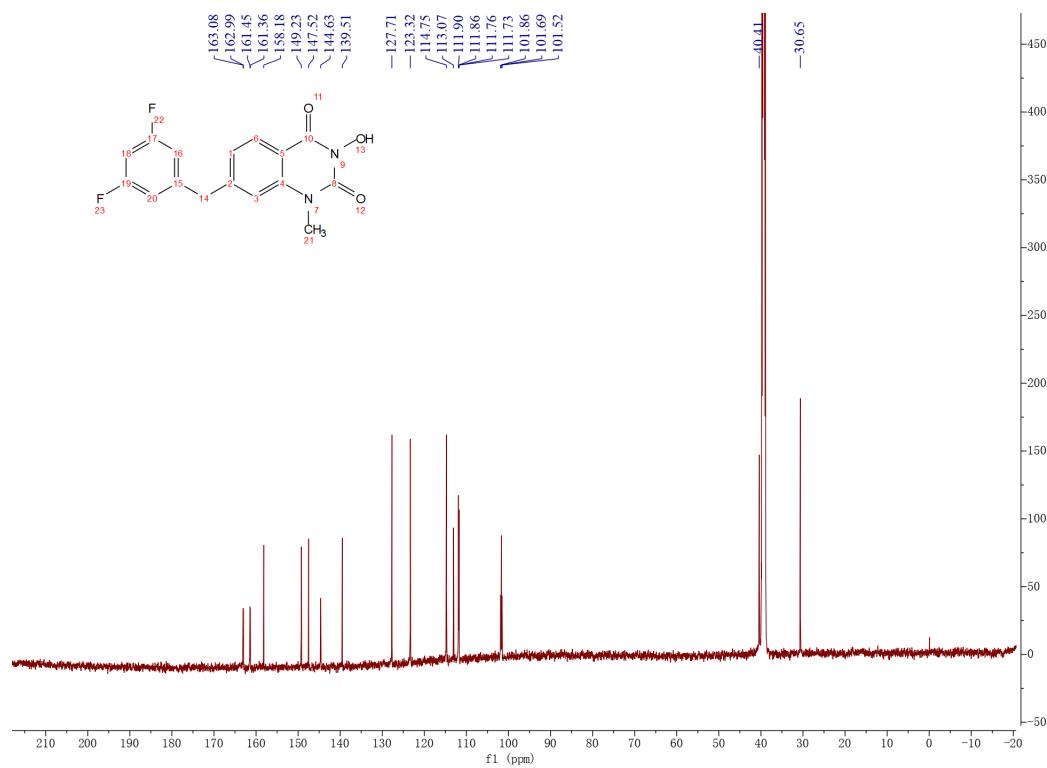


**Figure S57.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **18c**

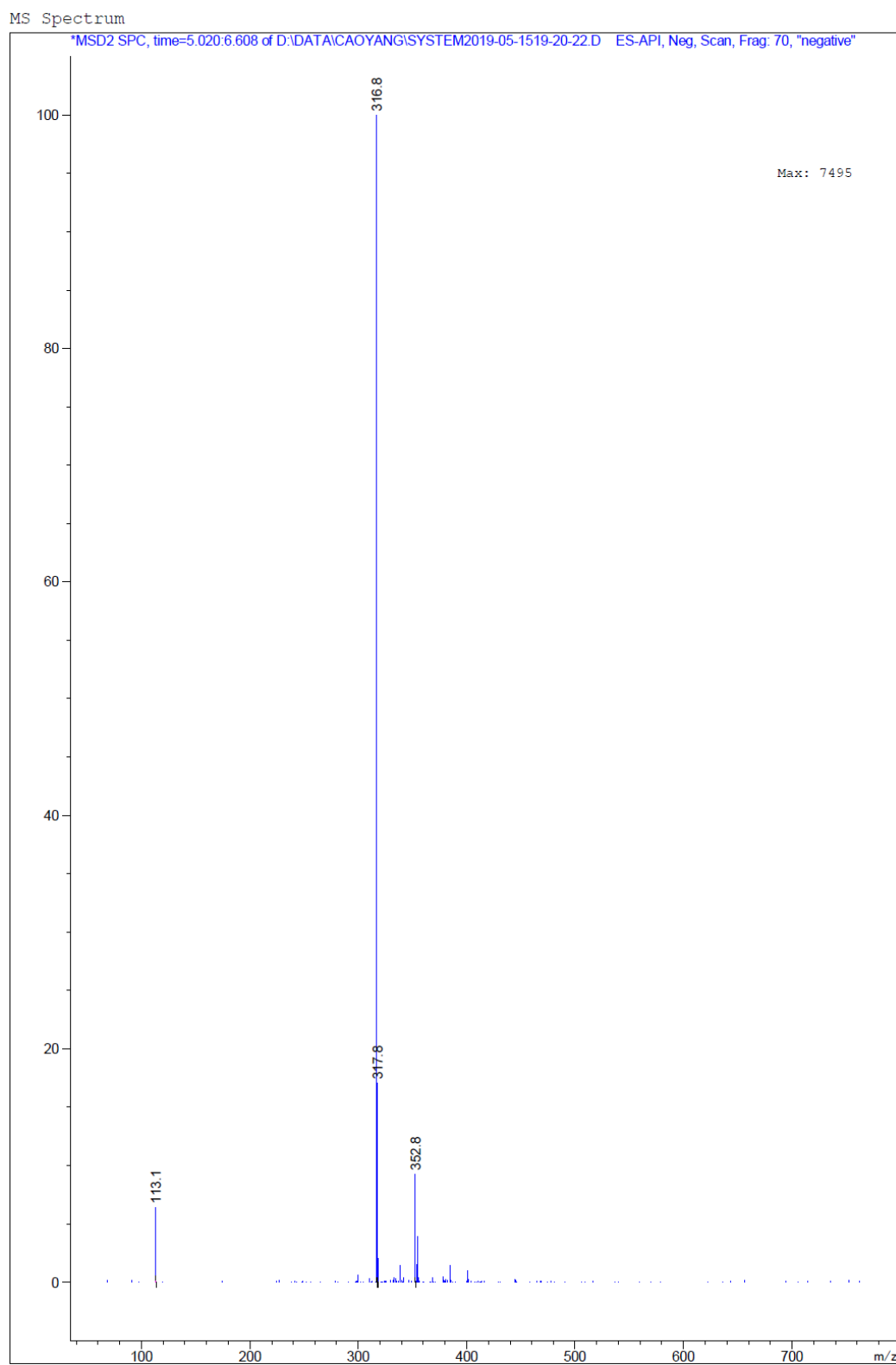




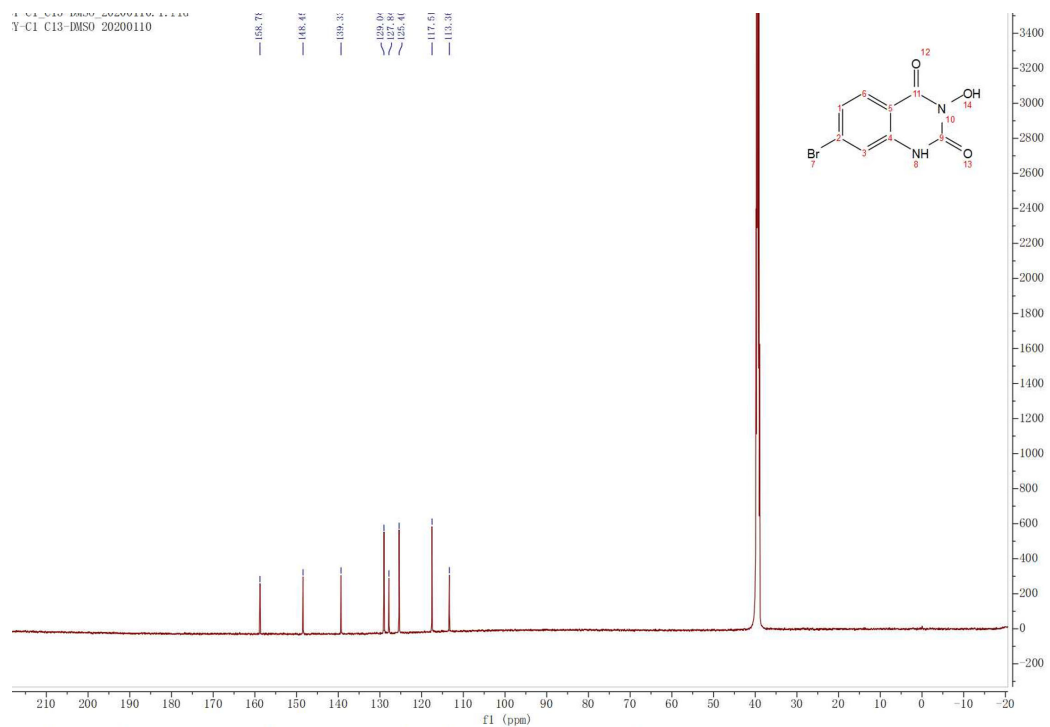
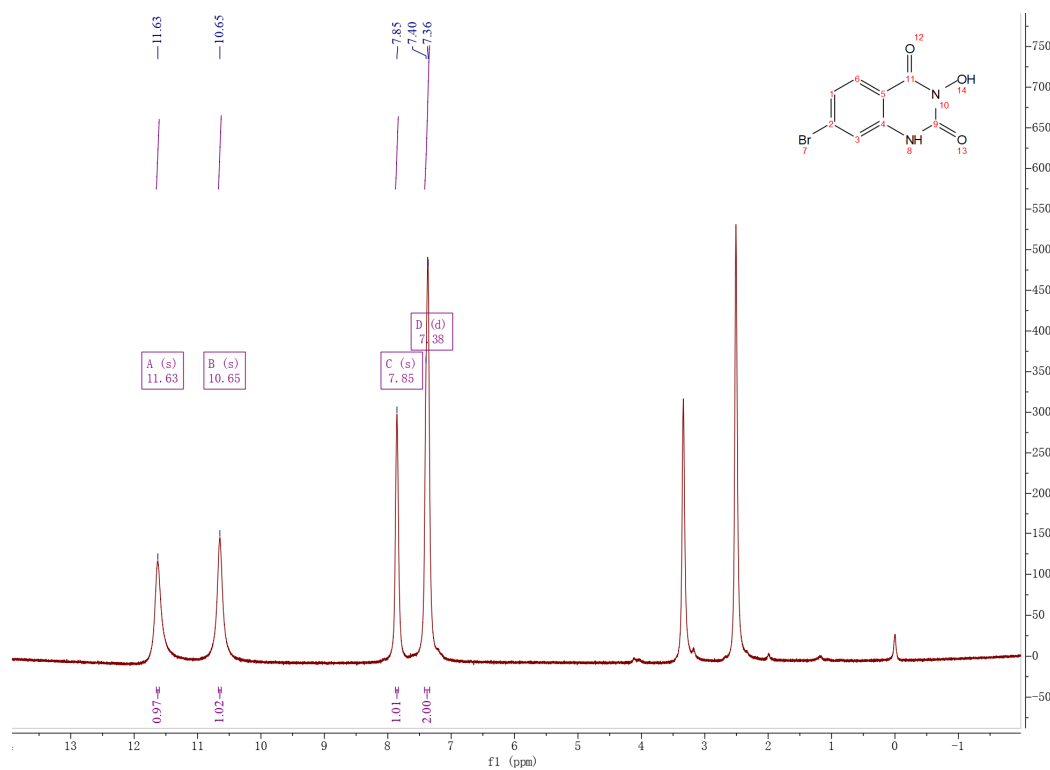
**Figure S58.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **18c**

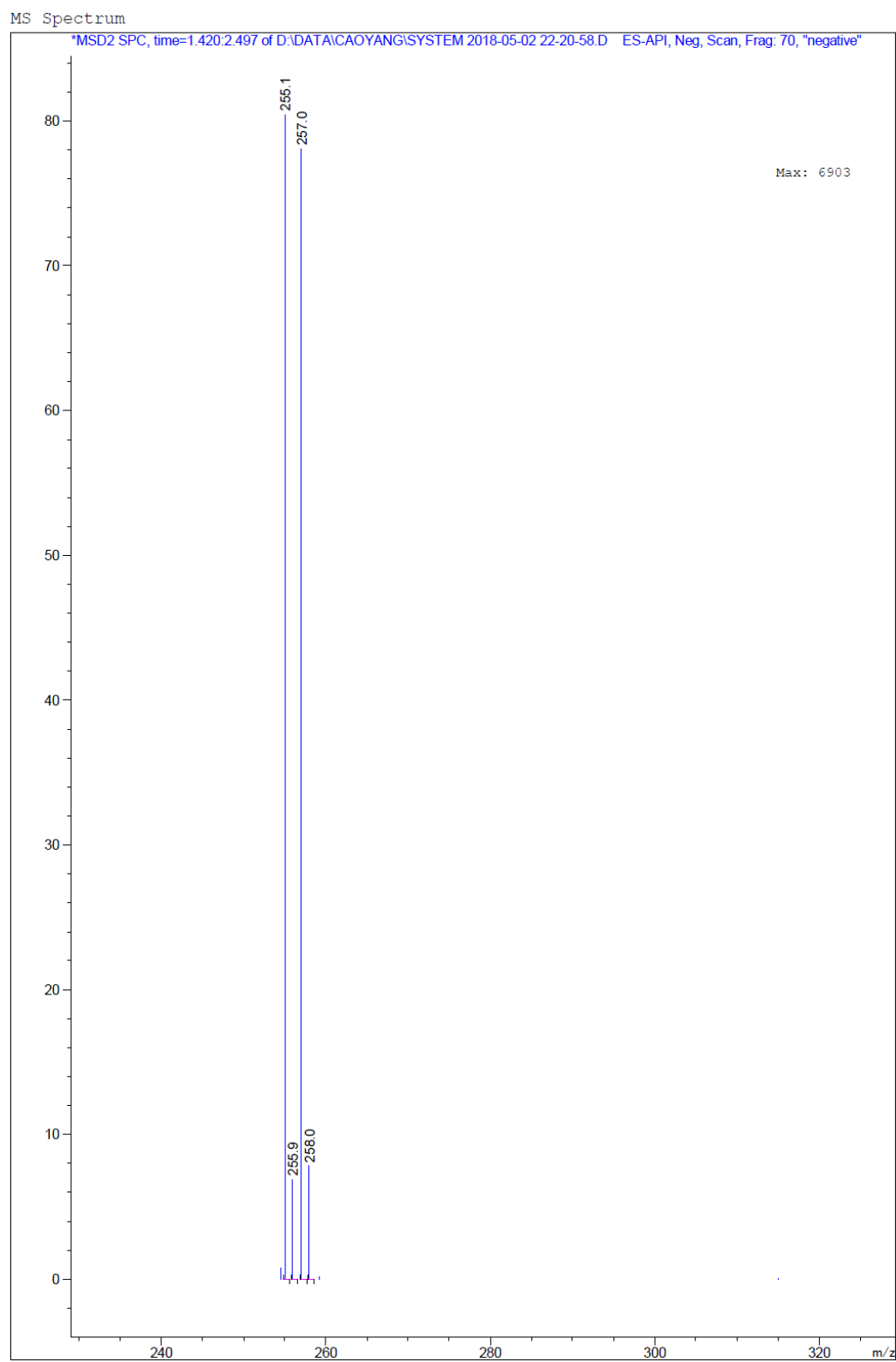


**Figure S59.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **18c**

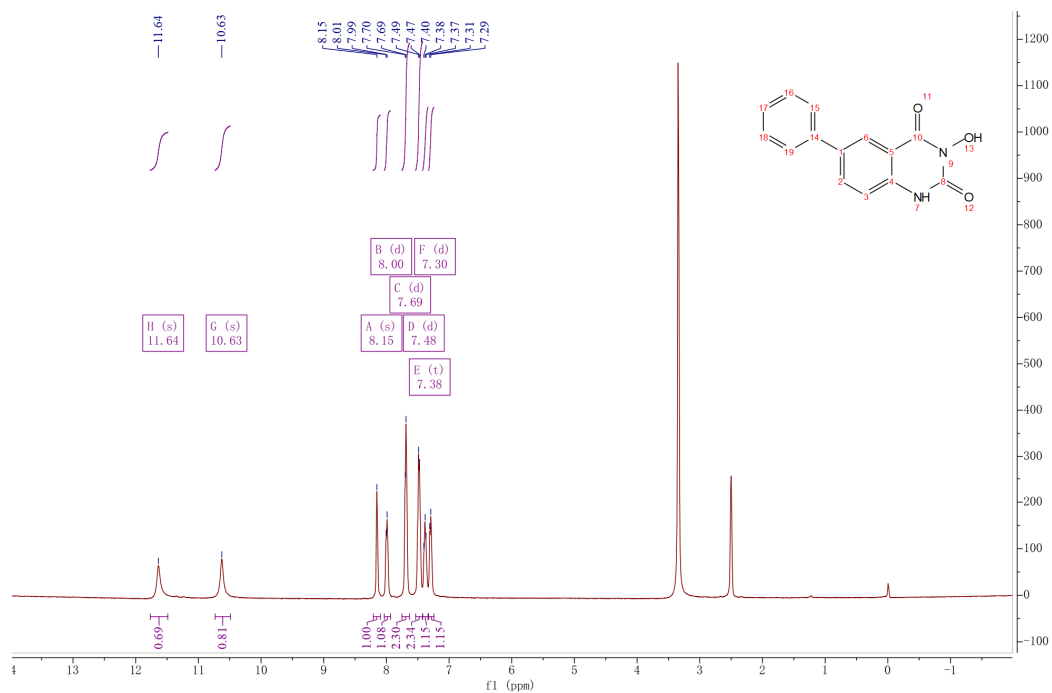


**Figure S60.** Mass spectrum (negative ionization) of **18c**

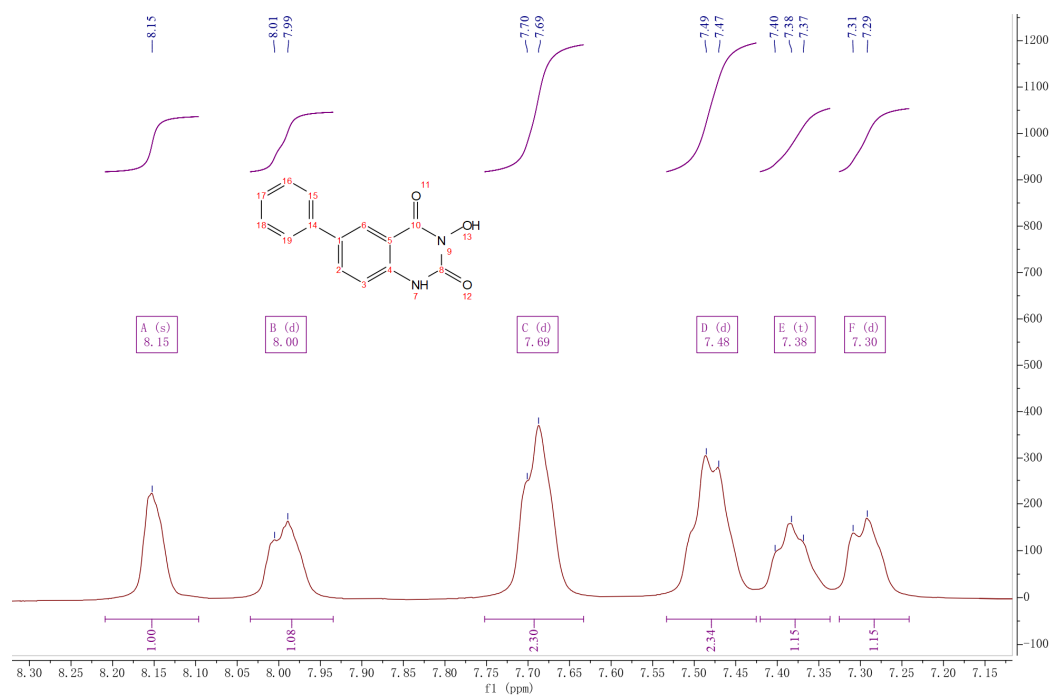




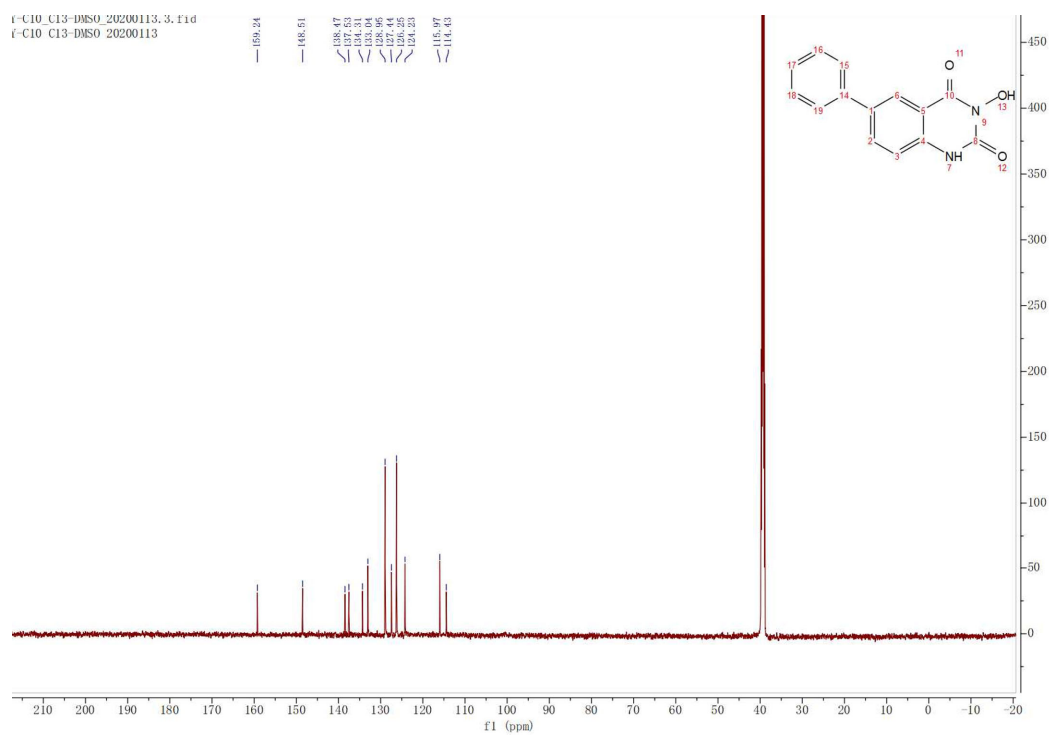
**Figure S63.** Mass spectrum (negative ionization) of **19**



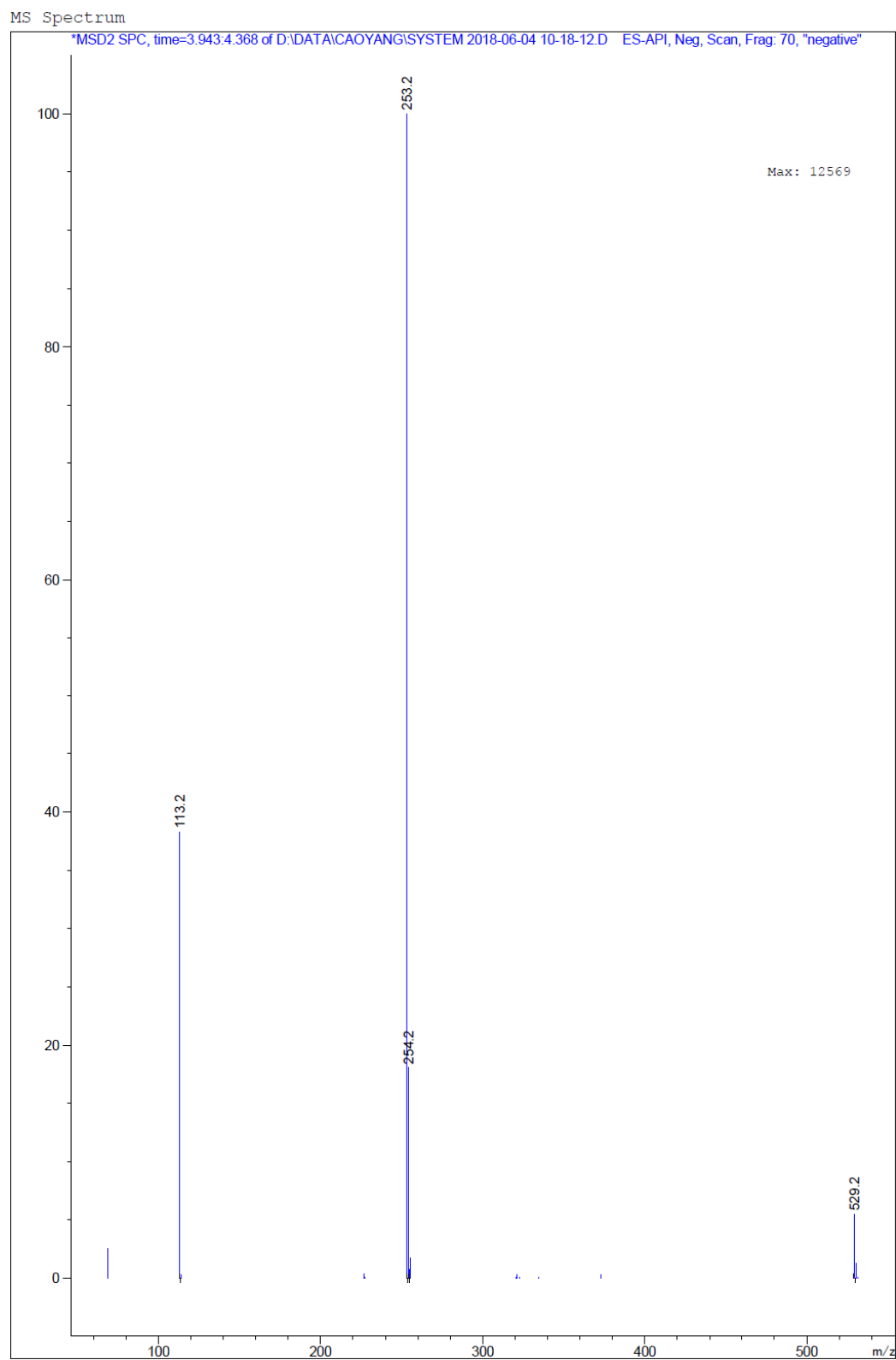
**Figure S64.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21a**



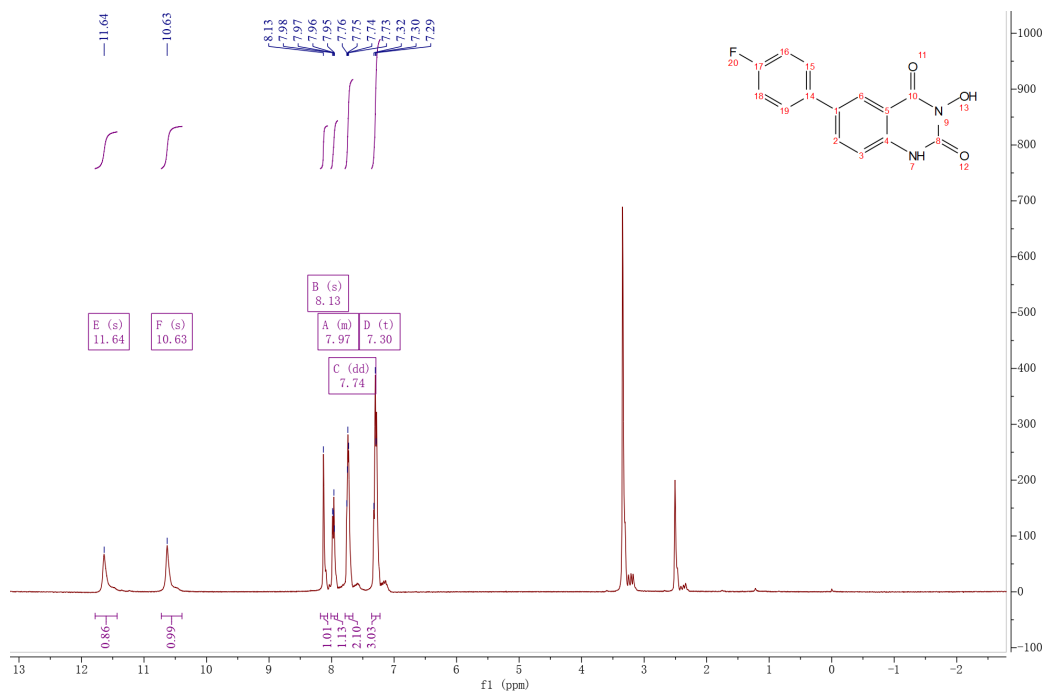
**Figure S65.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21a**



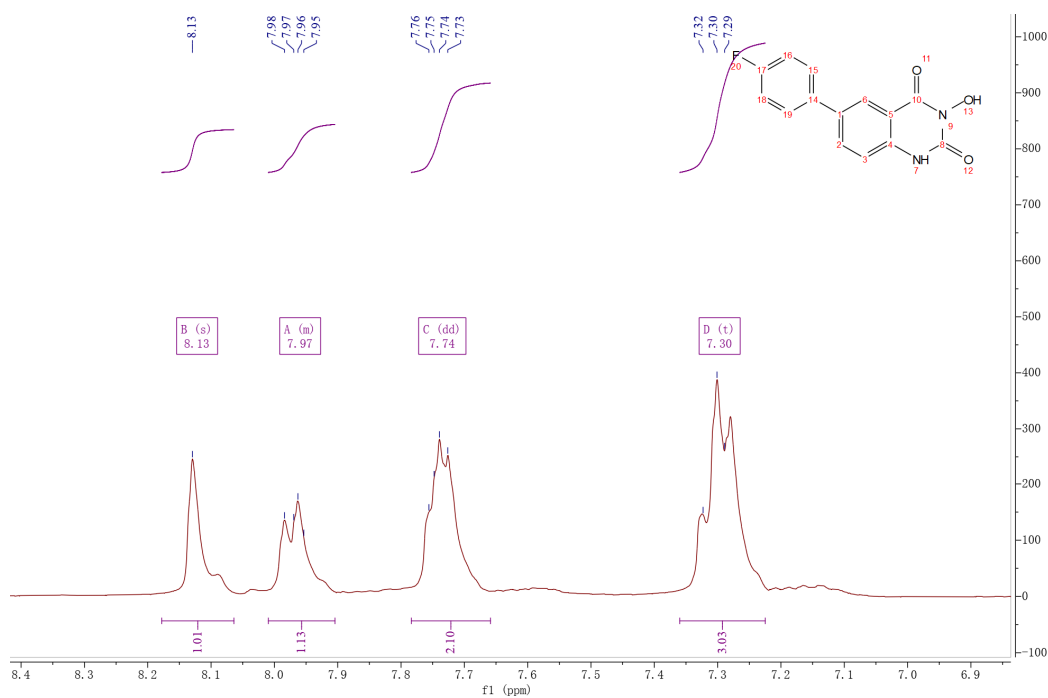
**Figure S66.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21a**



**Figure S67.** Mass spectrum (negative ionization) of **21a**

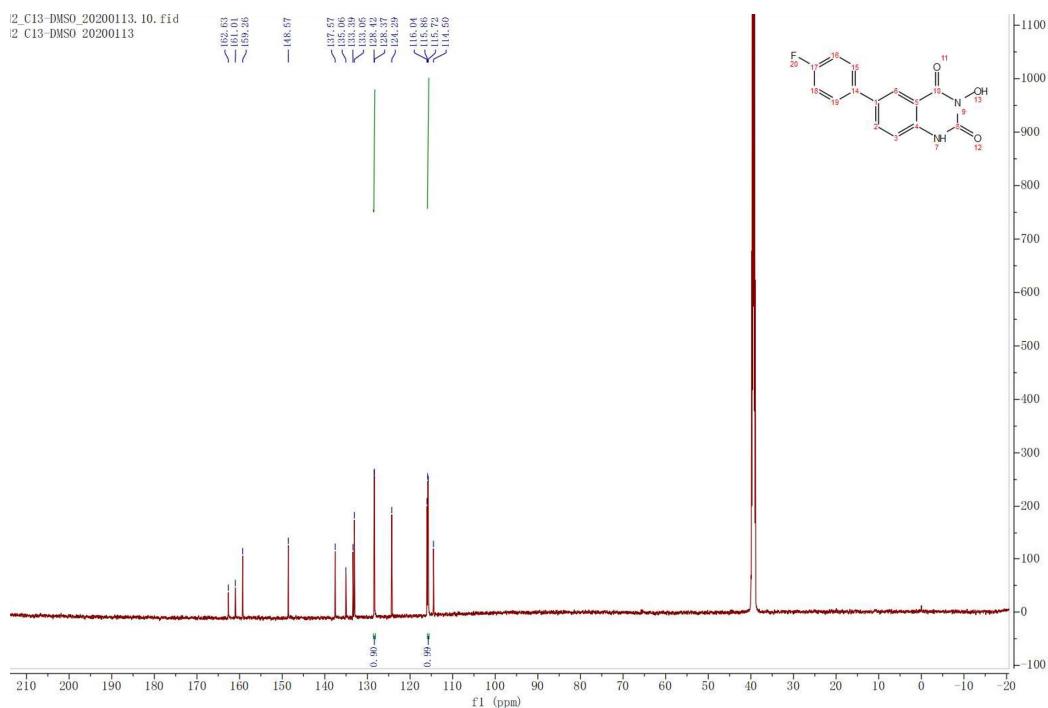


**Figure S68.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21b**

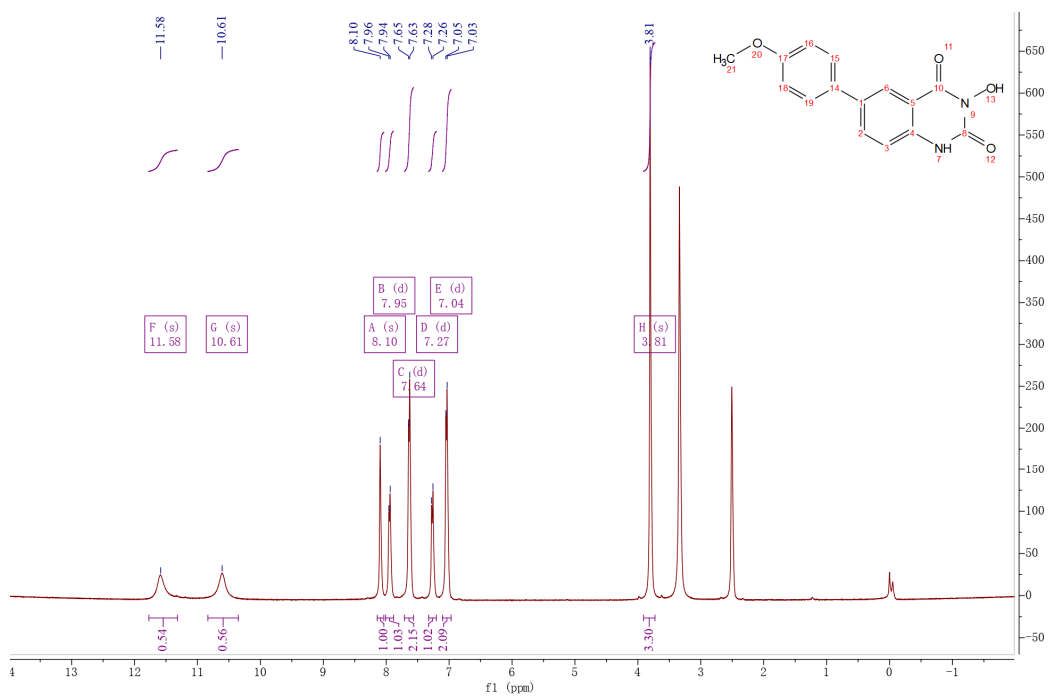


**Figure S69.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21b**

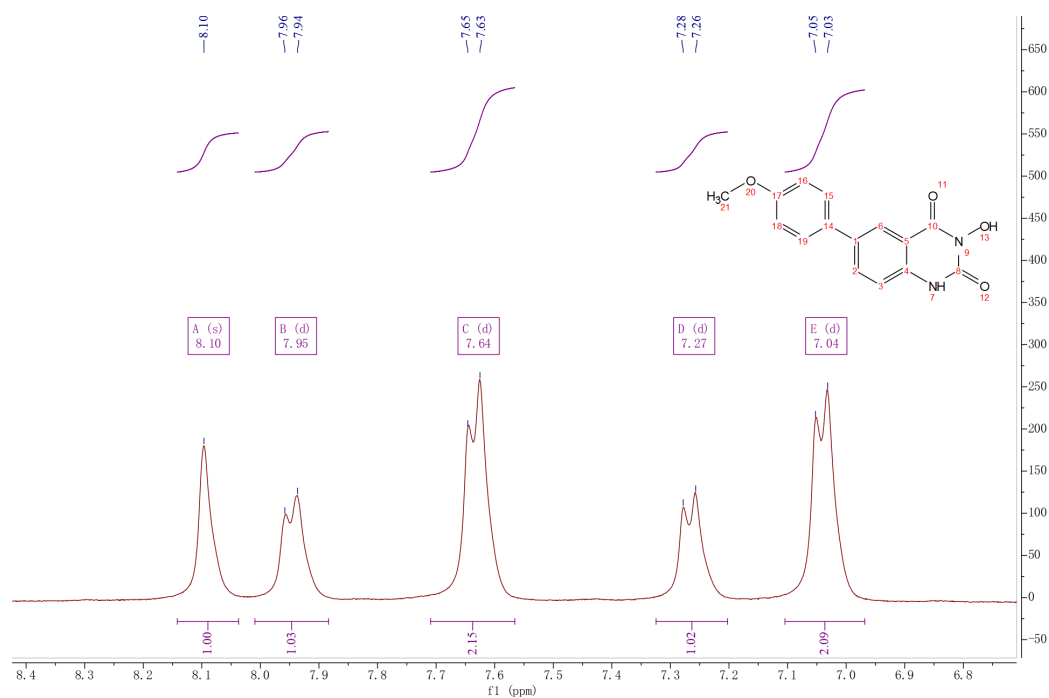




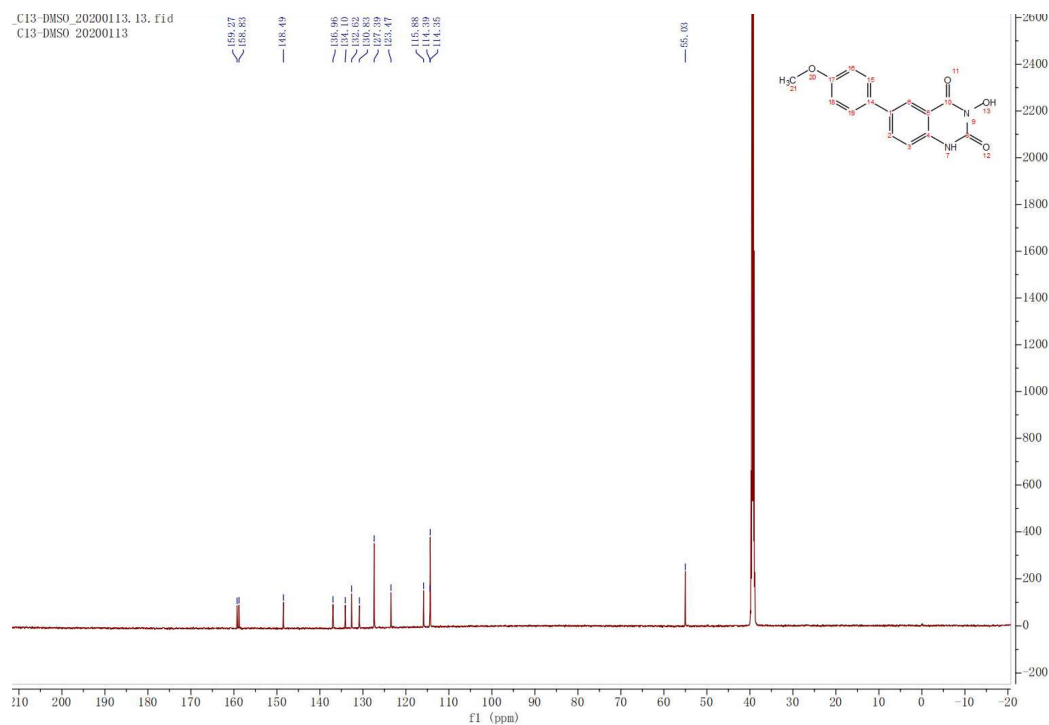
**Figure S70.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21b**



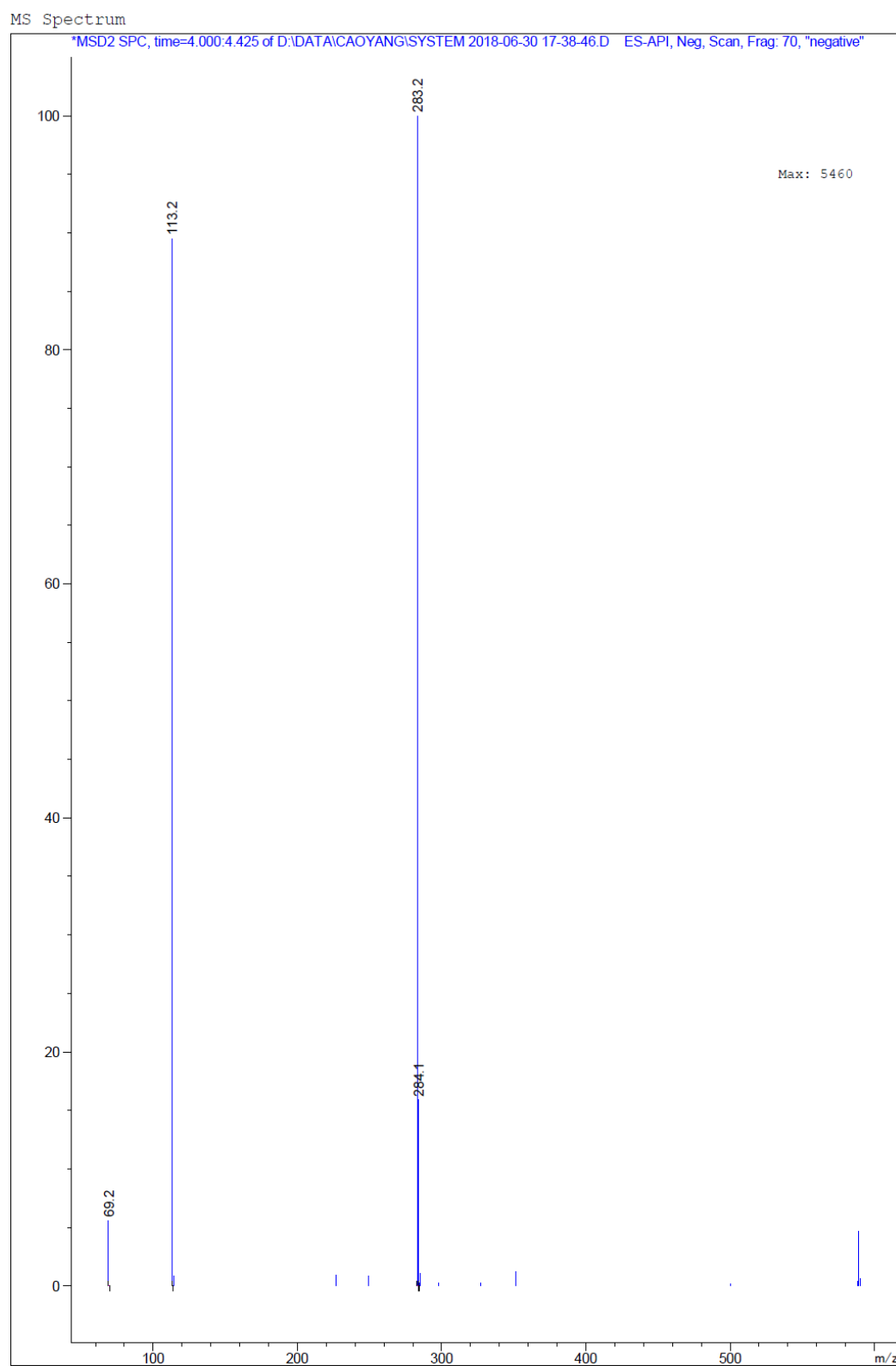
**Figure S71.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21c**



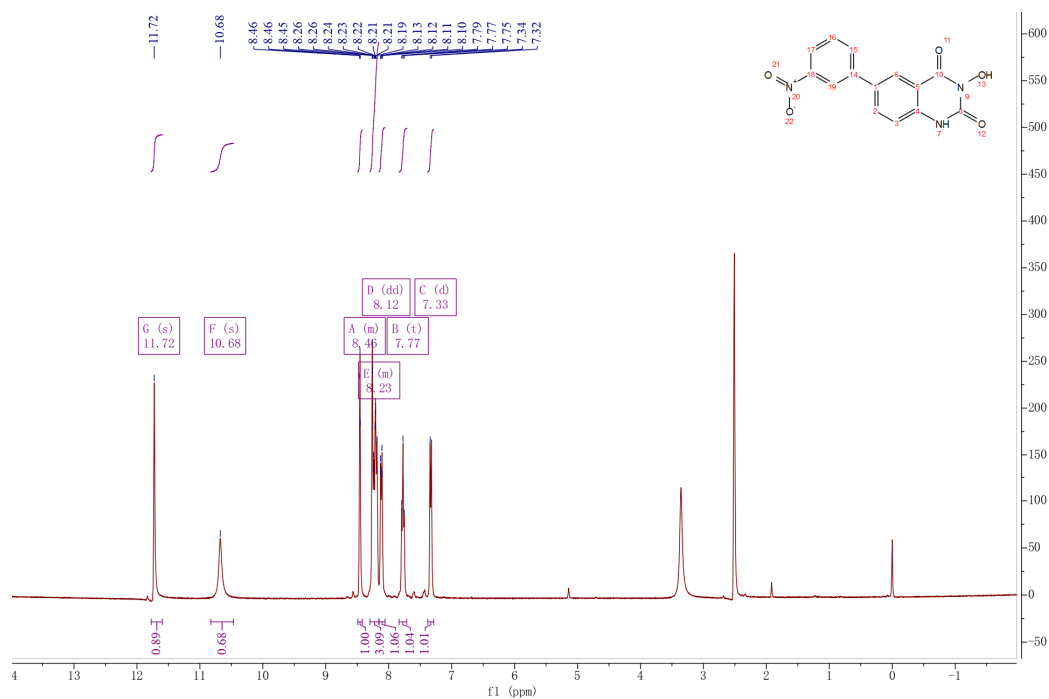
**Figure S72.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21c**



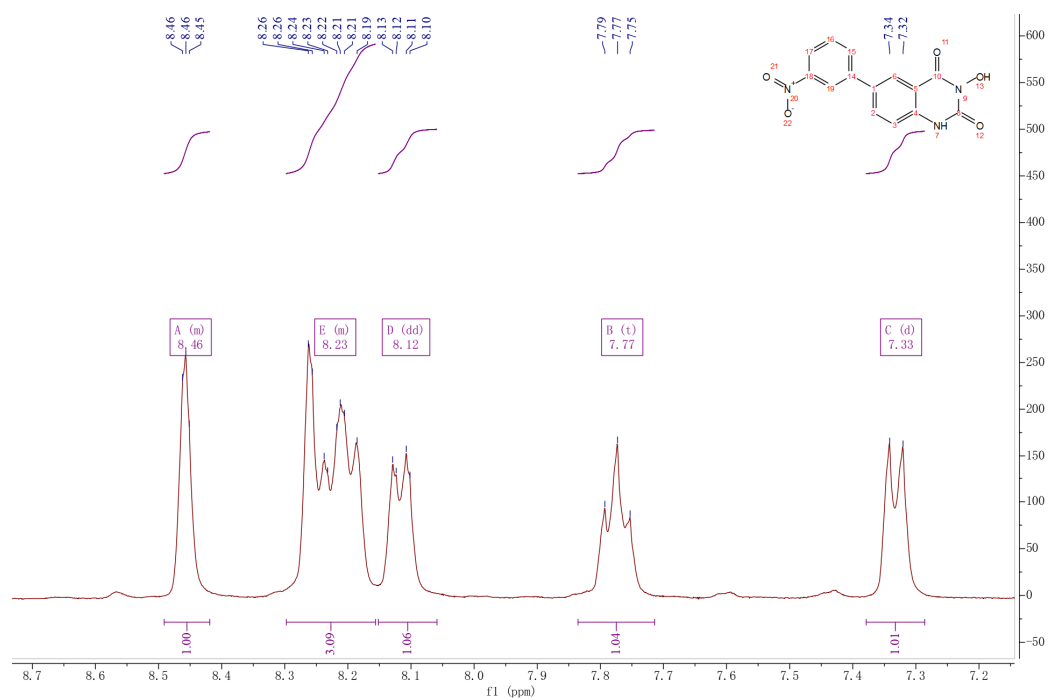
**Figure S73.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21c**



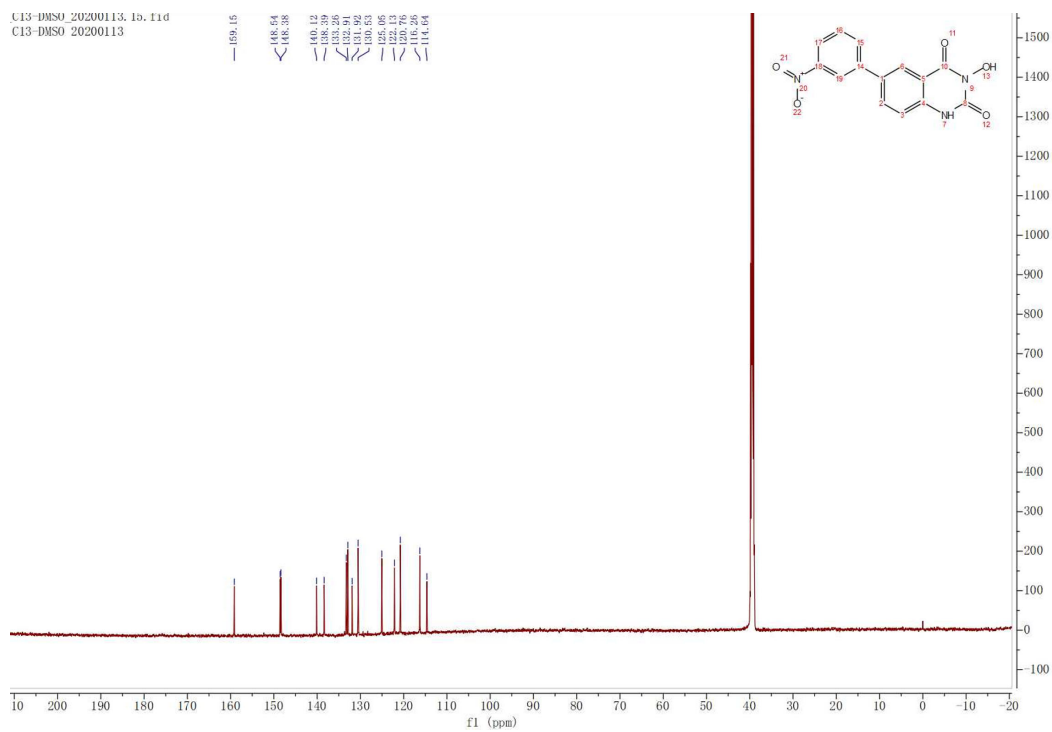
**Figure S74.** Mass spectrum (negative ionization) of **21c**



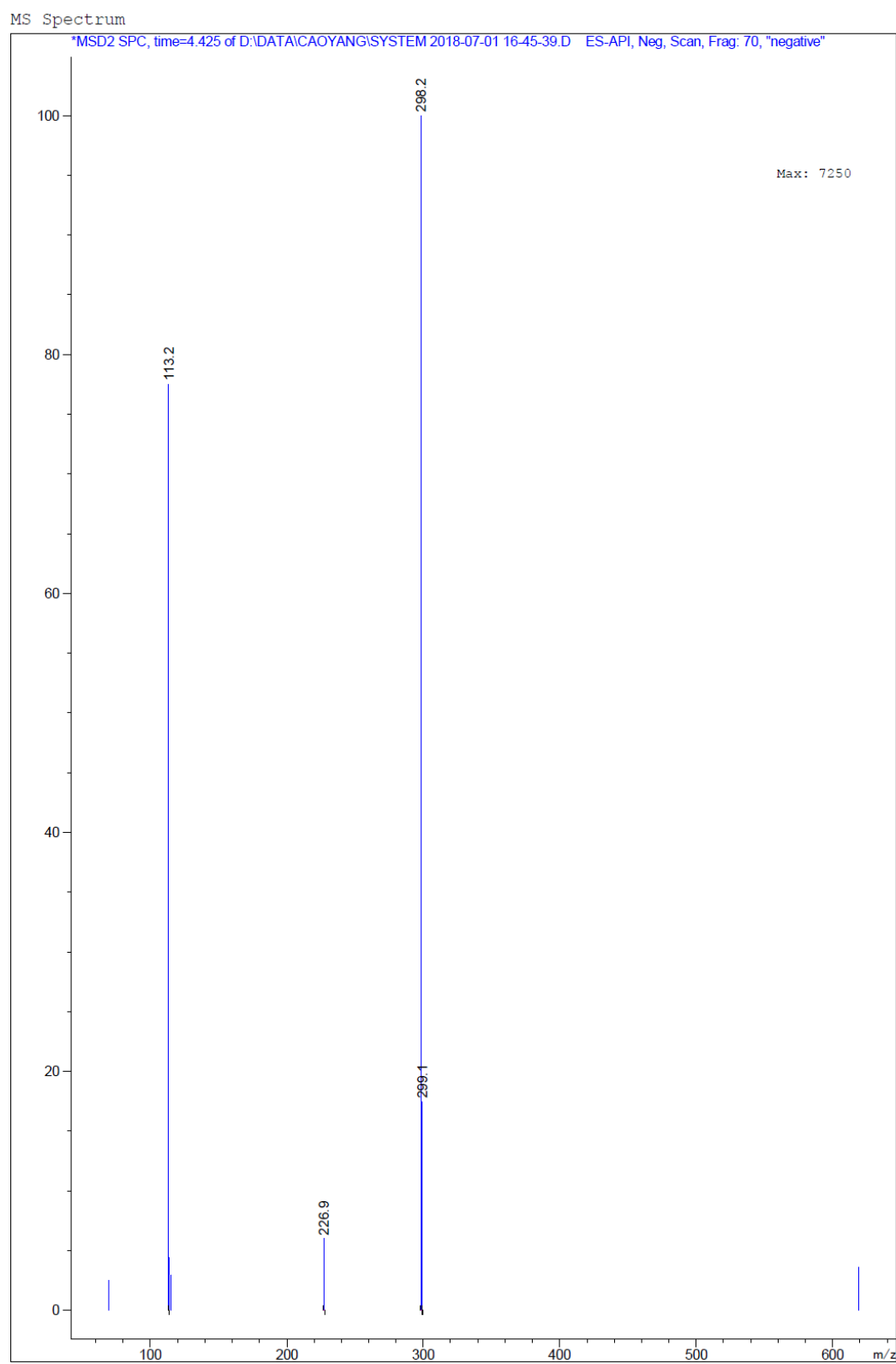
**Figure S75.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21d**



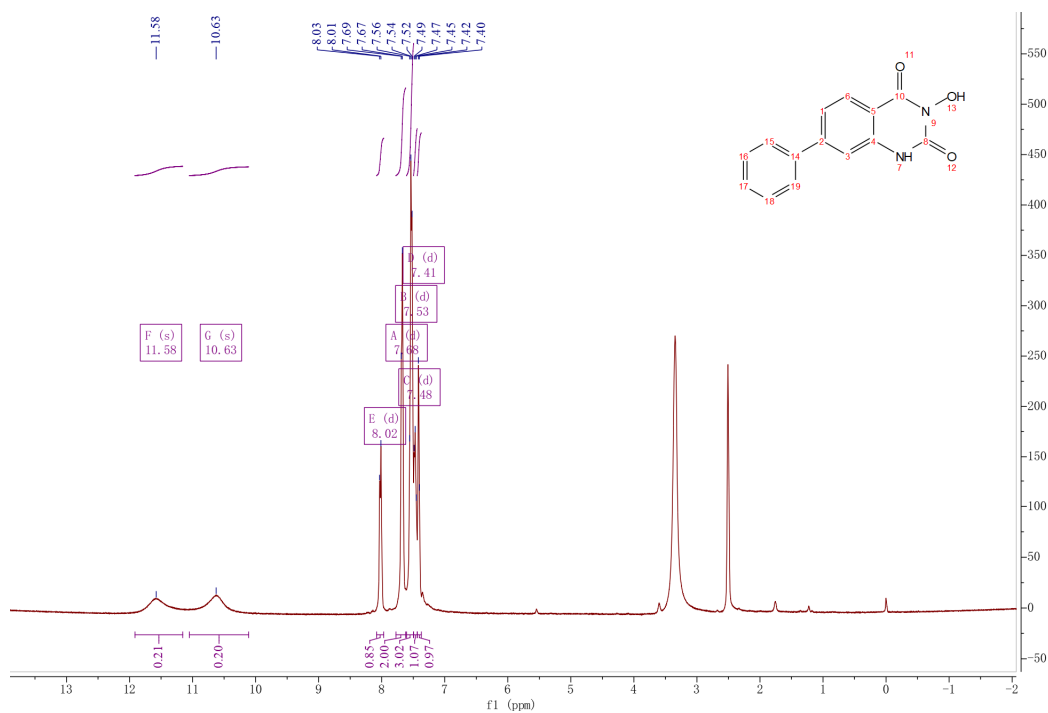
**Figure S76.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21d**



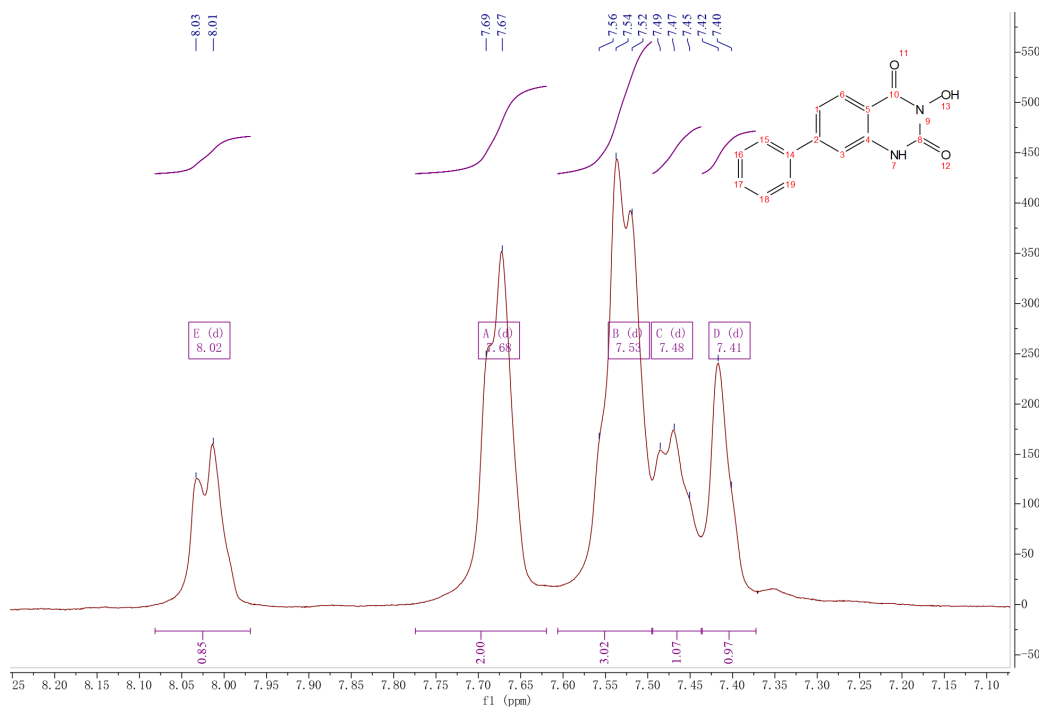
**Figure S77.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21d**



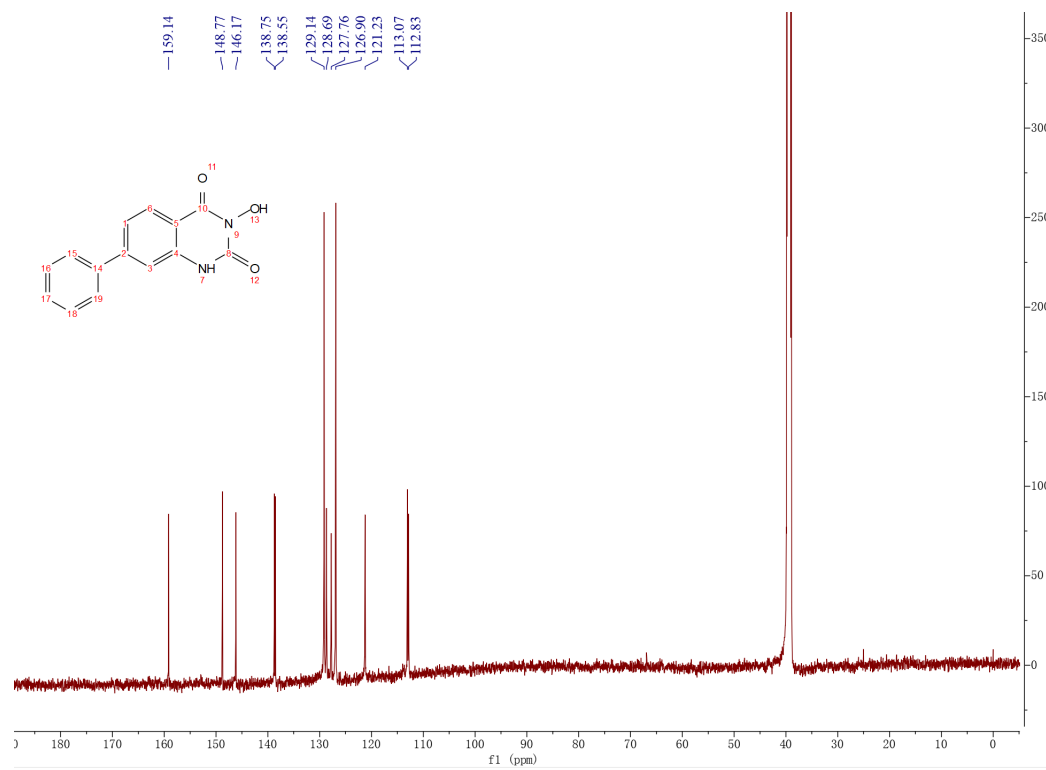
**Figure S78.** Mass spectrum (negative ionization) of **21d**



**Figure S79.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21e**

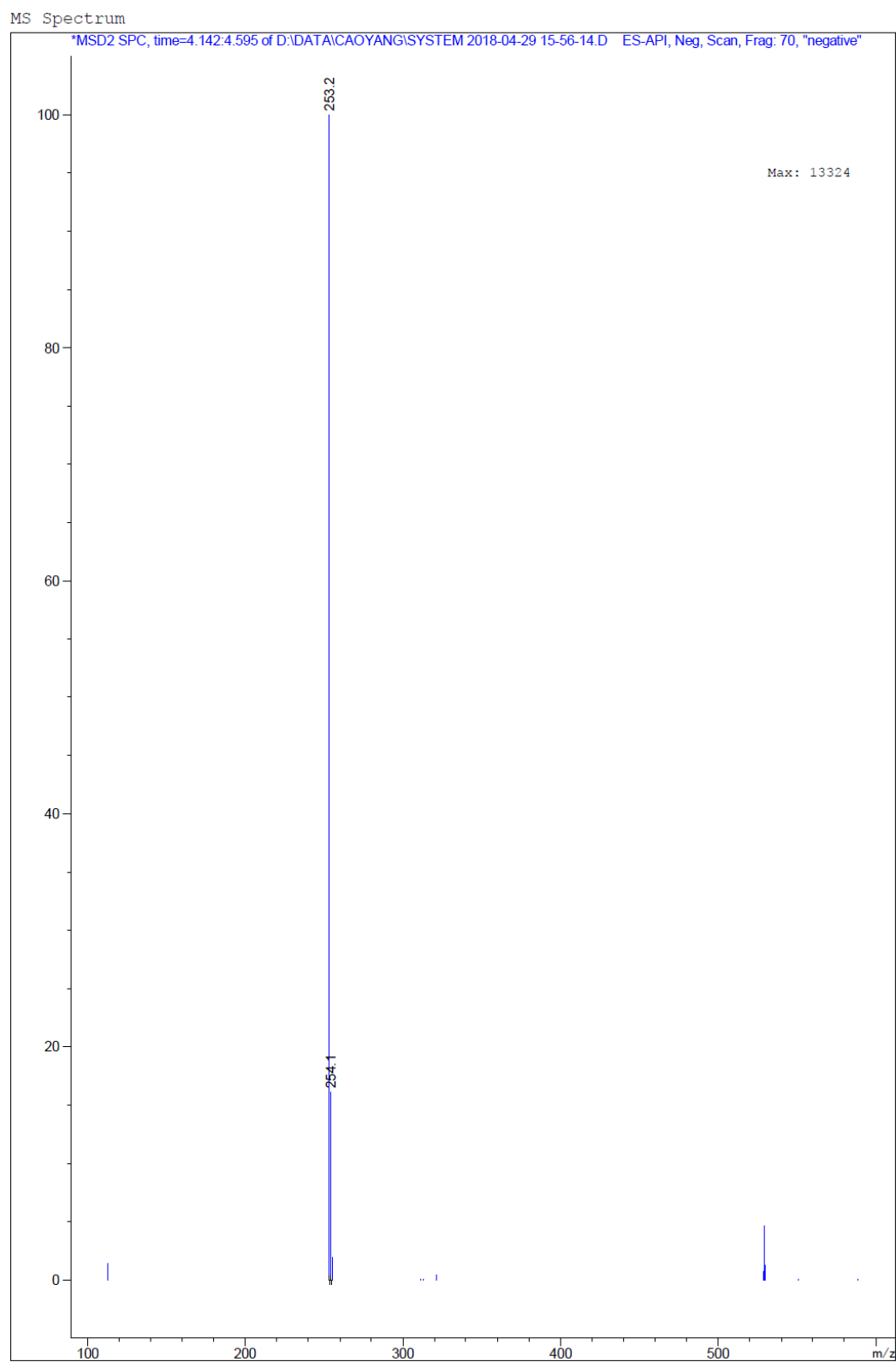


**Figure S80.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21e**

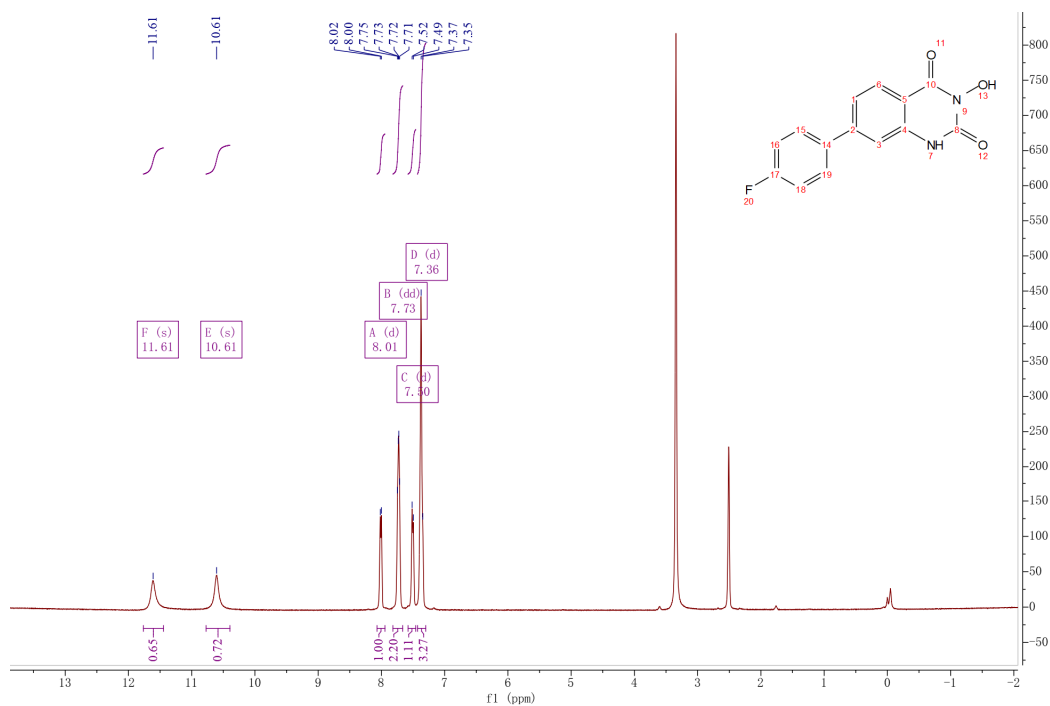


**Figure S81.** <sup>13</sup>C NMR (151 MHz, DMSO-*d*<sub>6</sub>) spectrum of **21e**

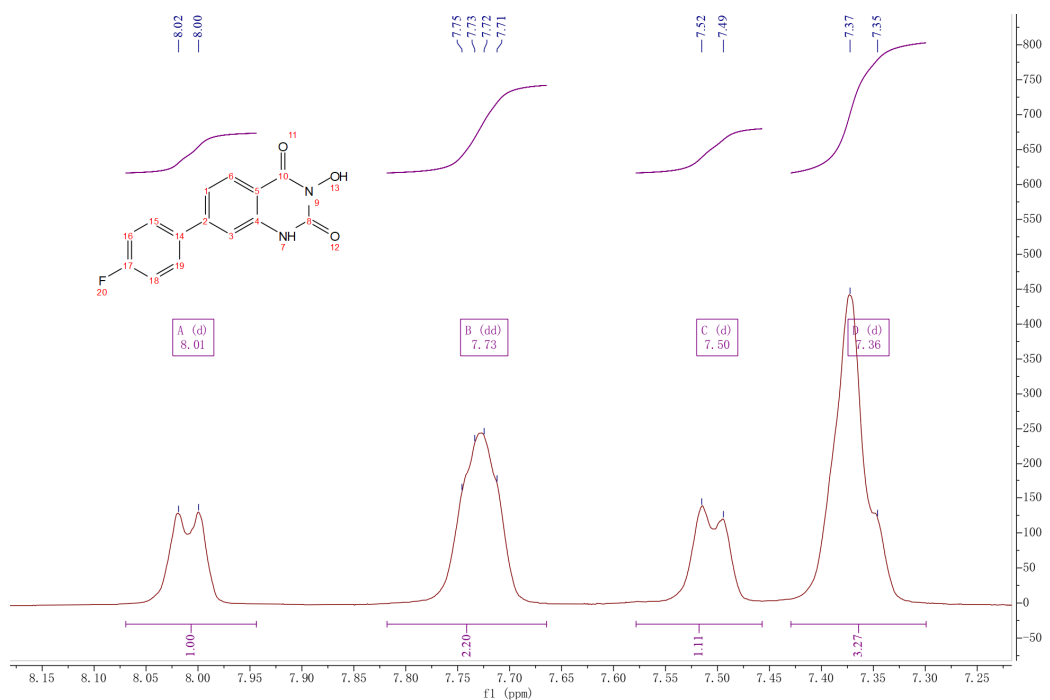




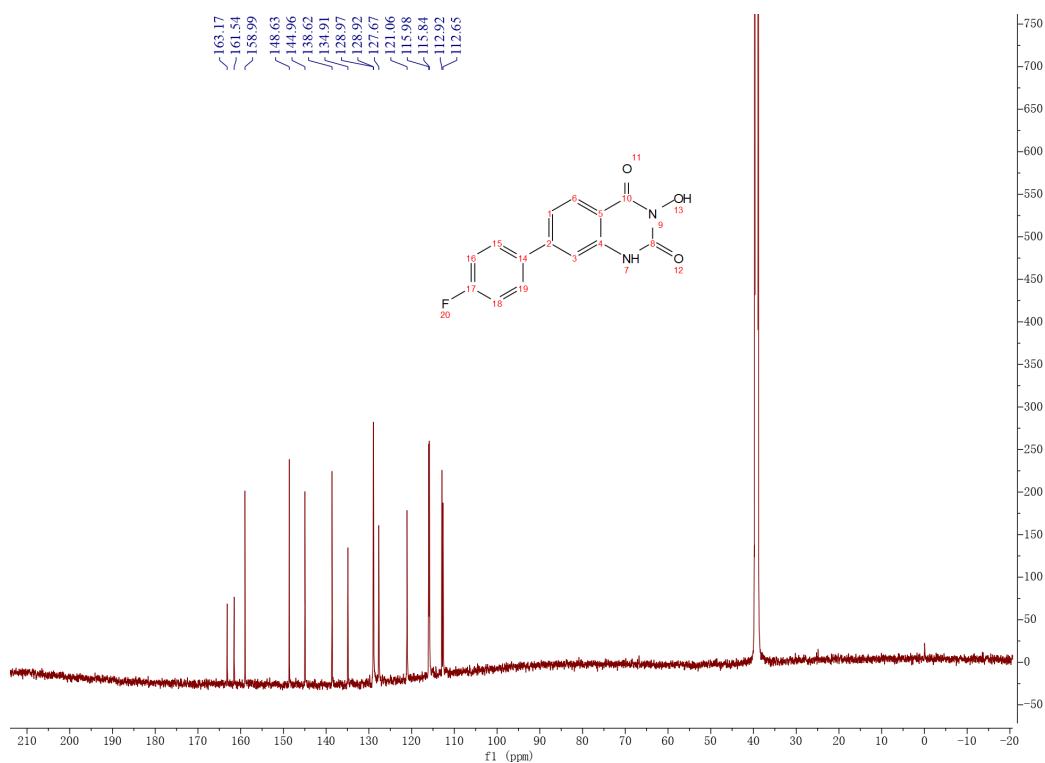
**Figure S82.** Mass spectrum (negative ionization) of **21e**



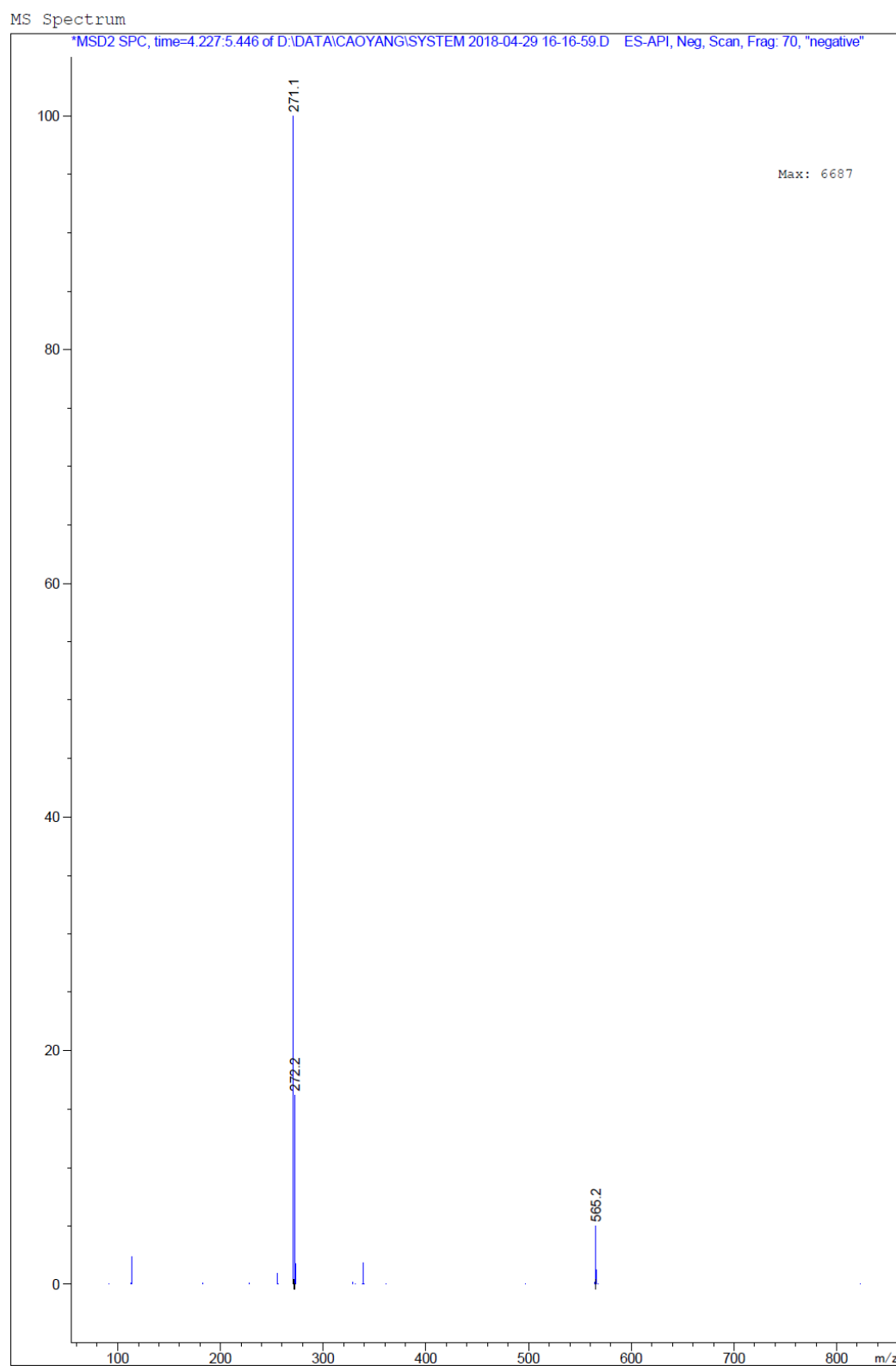
**Figure S83.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21f**



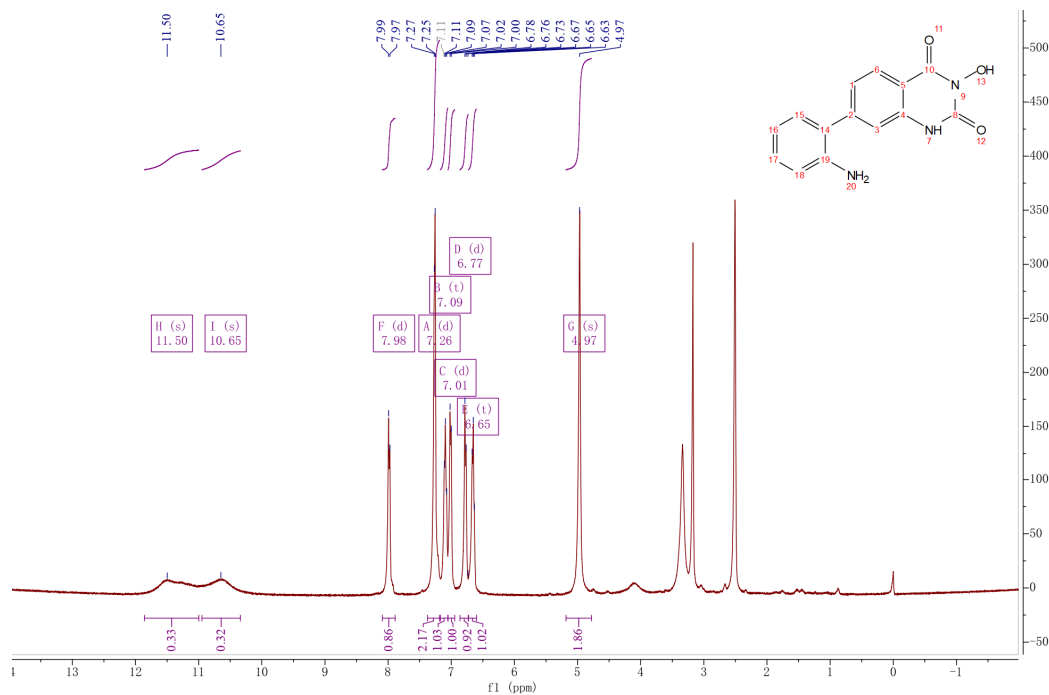
**Figure S84.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21f**



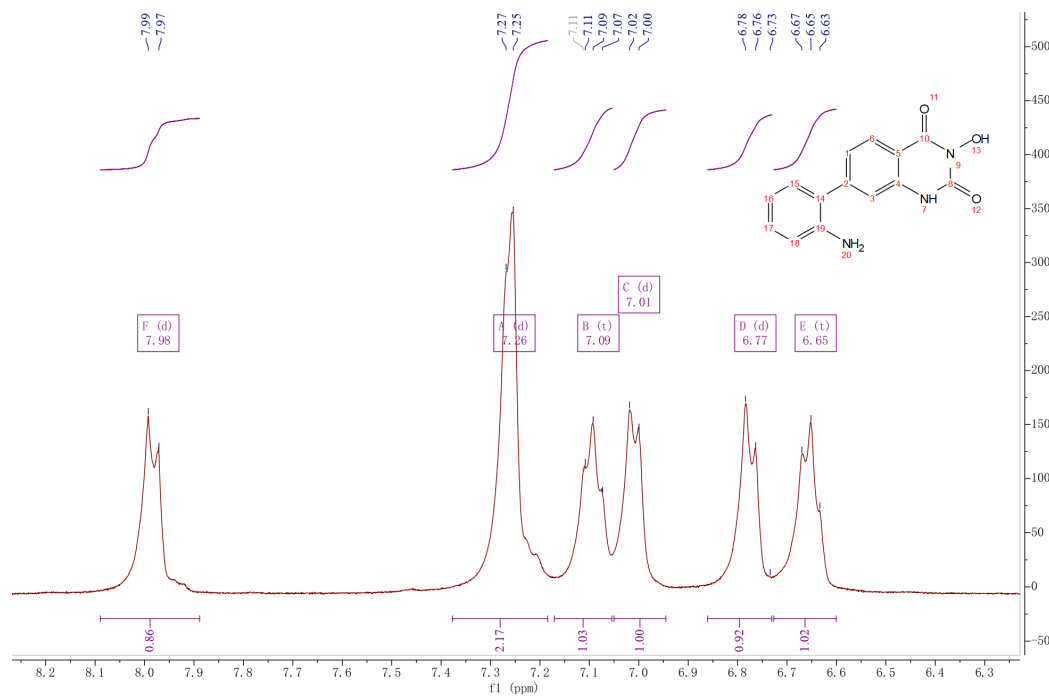
**Figure S85.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21f**



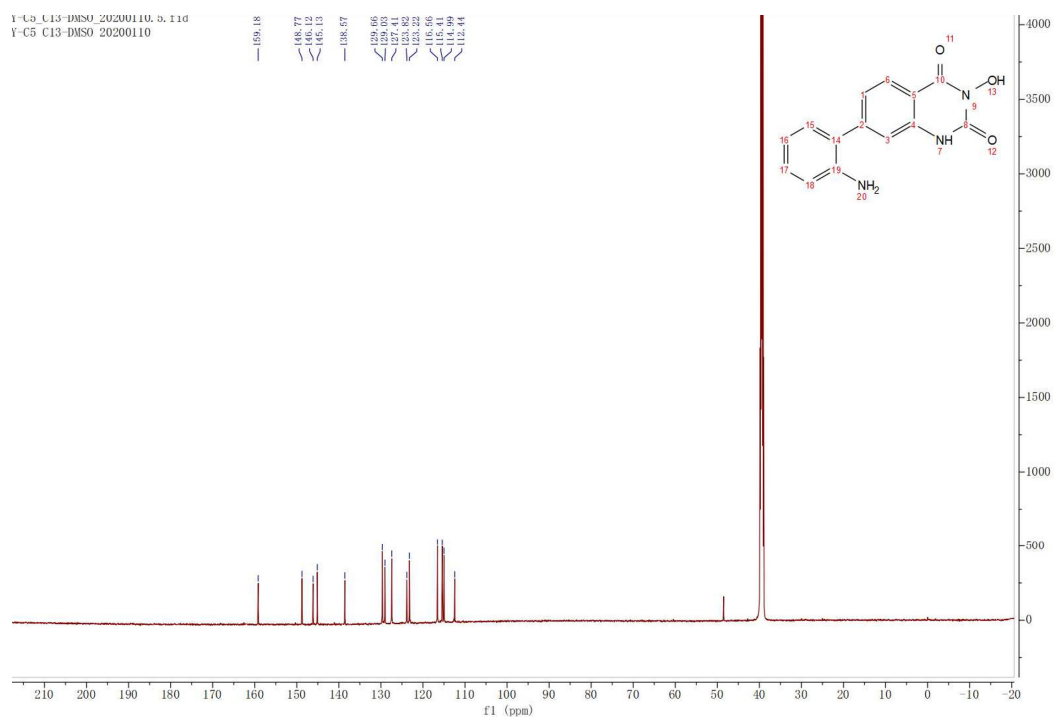
**Figure S86.** Mass spectrum (negative ionization) of **21f**



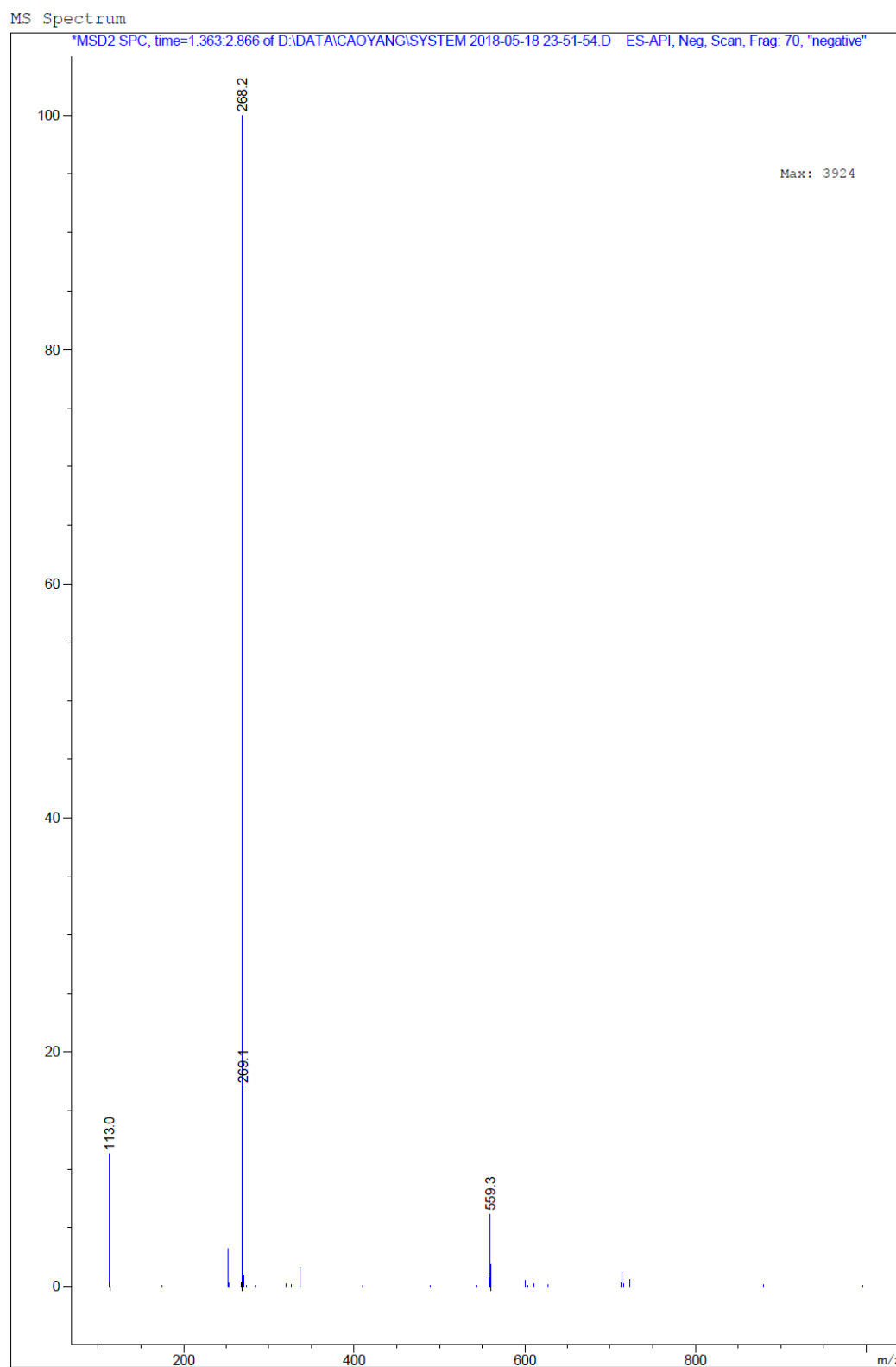
**Figure S87.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21g**



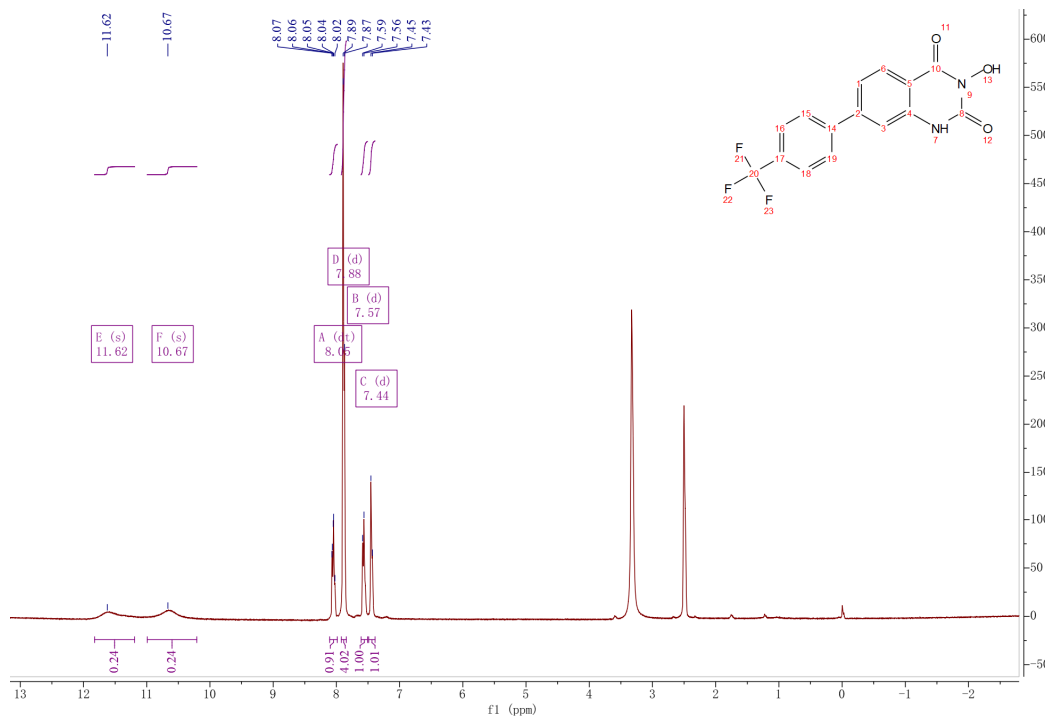
**Figure S88.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21g**



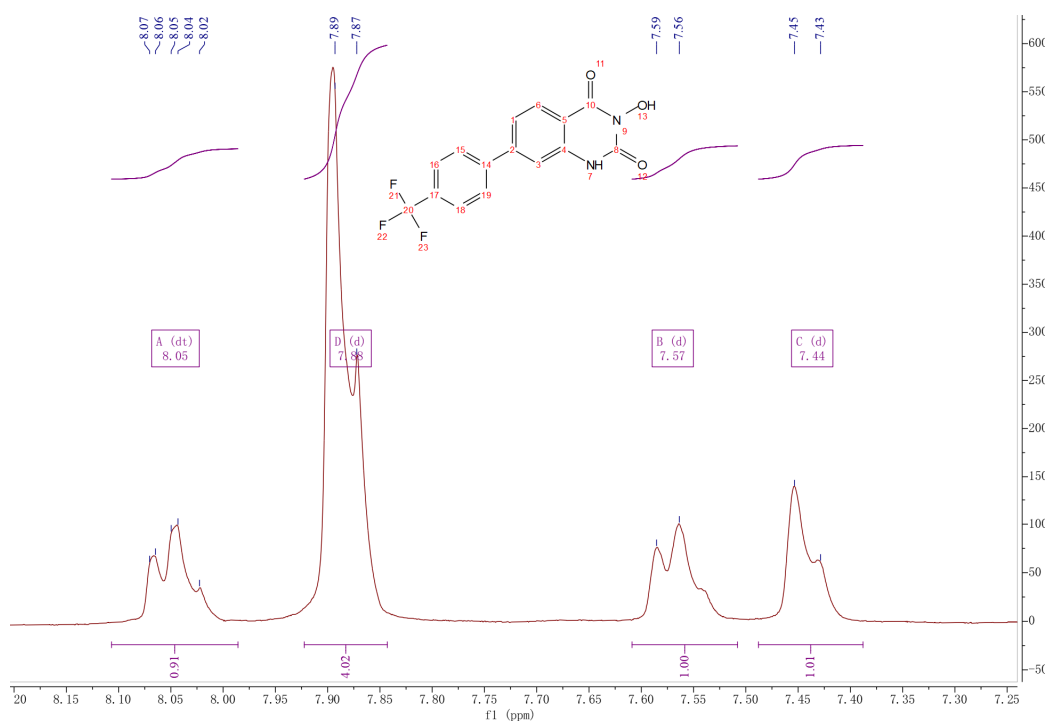
**Figure S89.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO-}d_6$ ) spectrum of **21g**



**Figure S90.** Mass spectrum (negative ionization) of **21g**

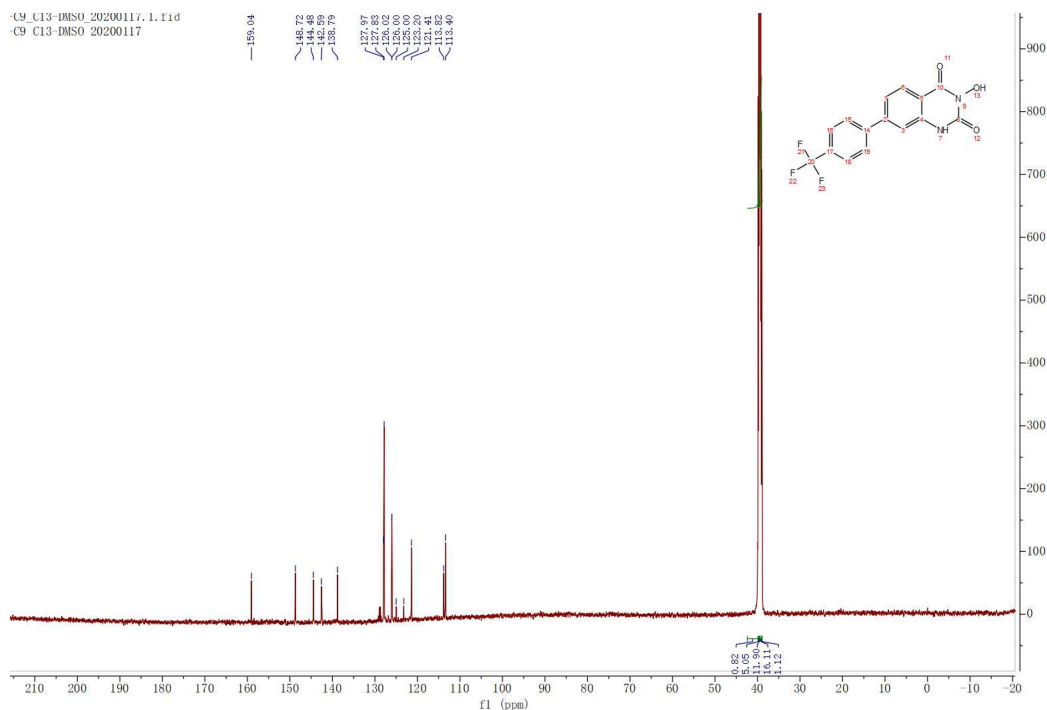


**Figure S91.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21h**

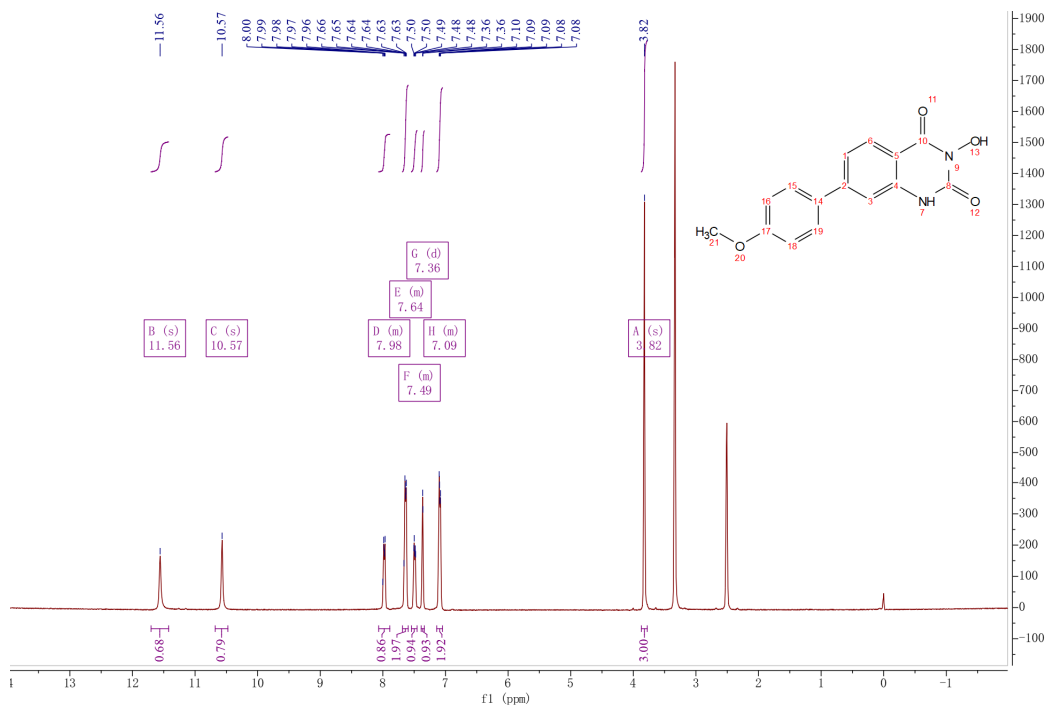


**Figure S92.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21h**

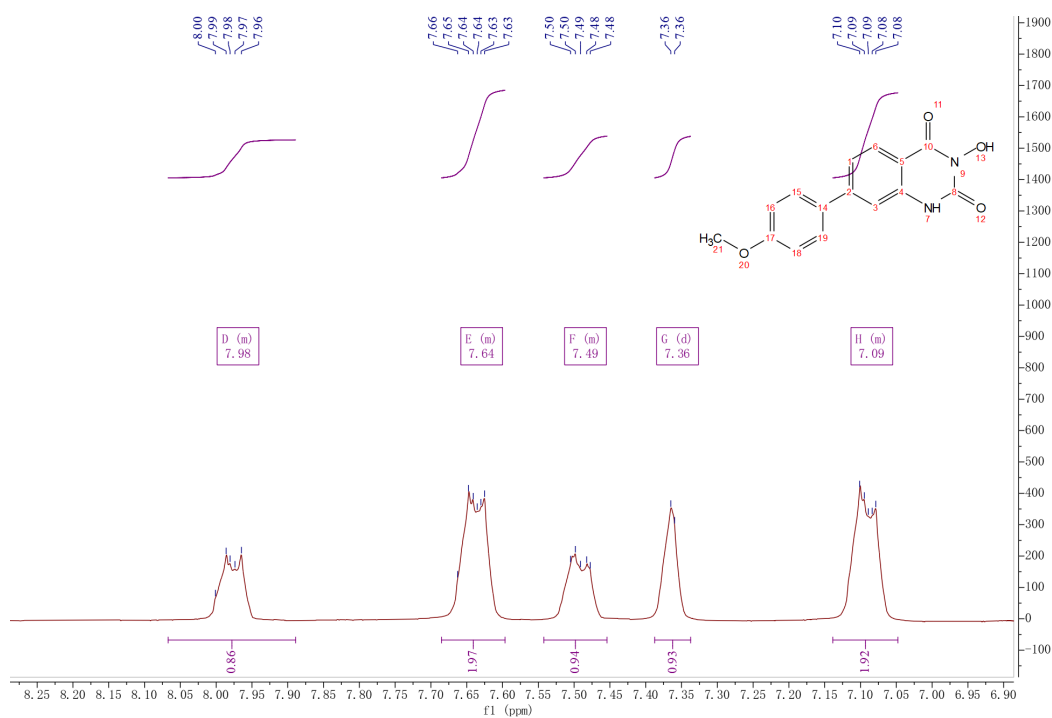




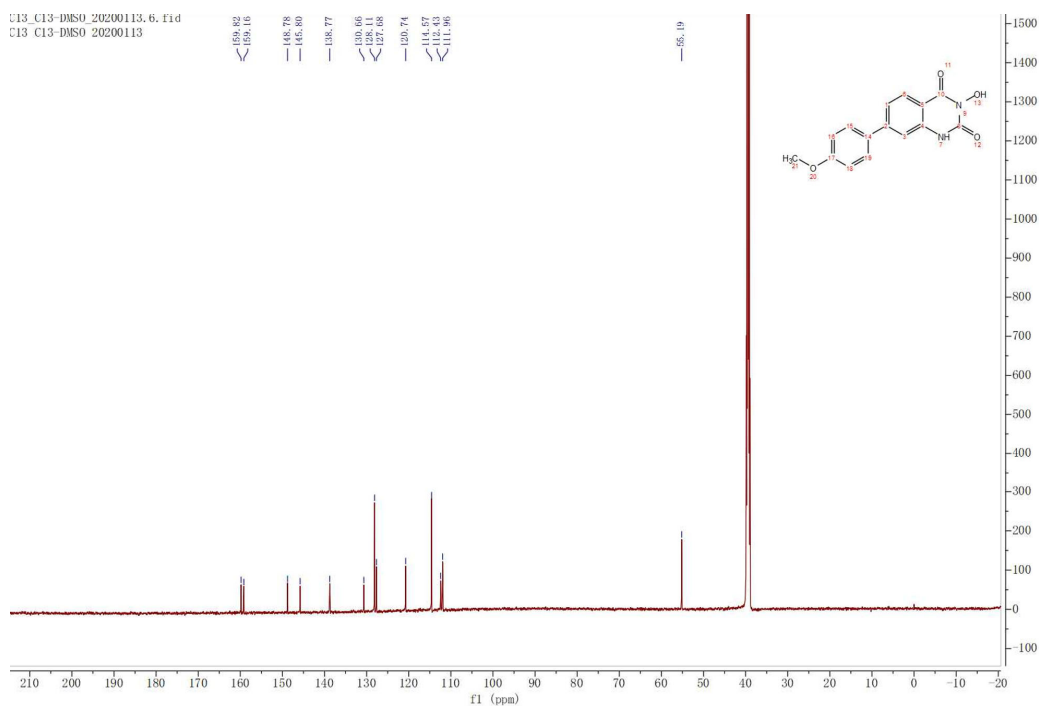
**Figure S93.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO-}d_6$ ) spectrum of **21h**



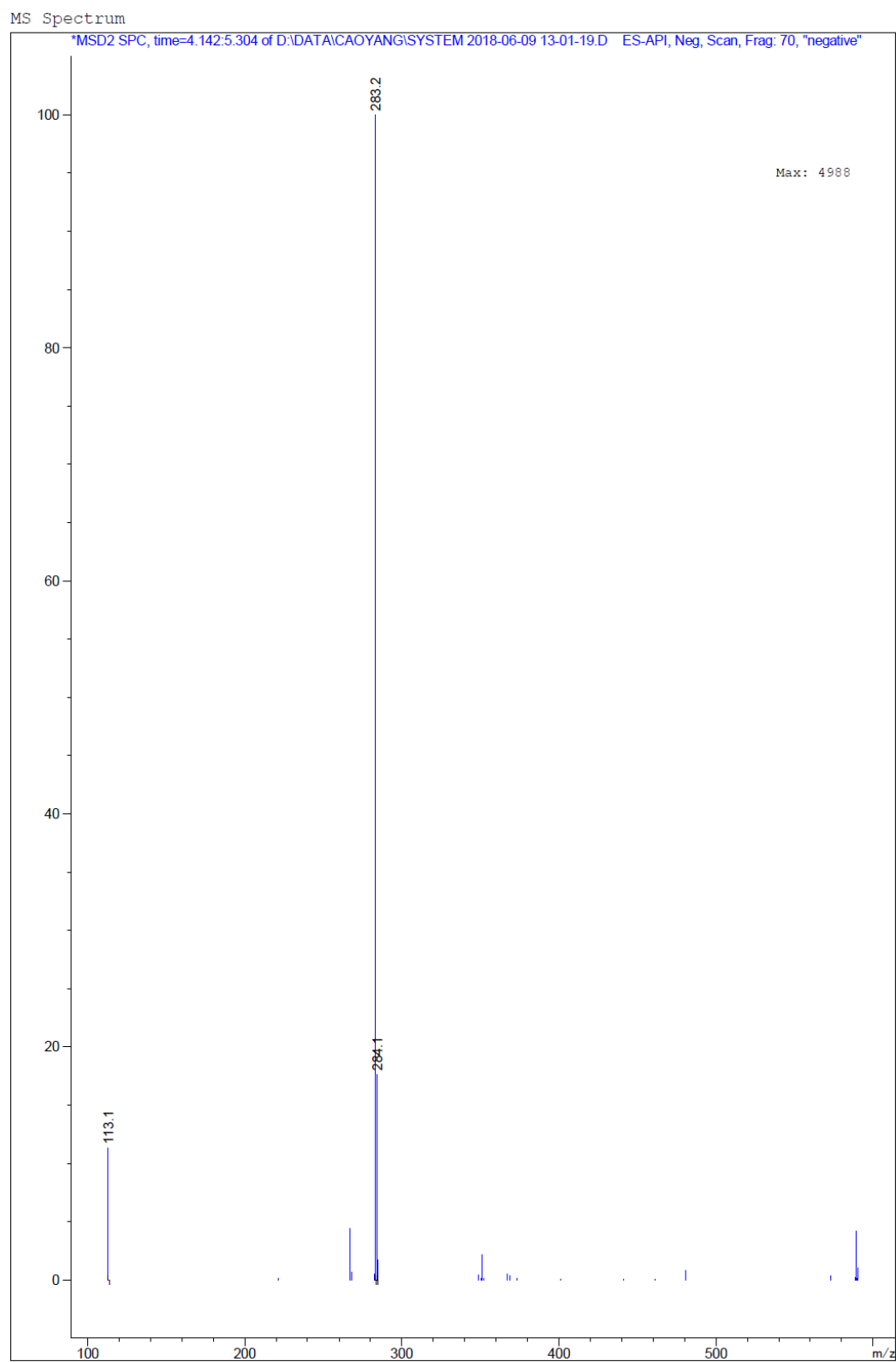
**Figure S94.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) spectrum of **21i**



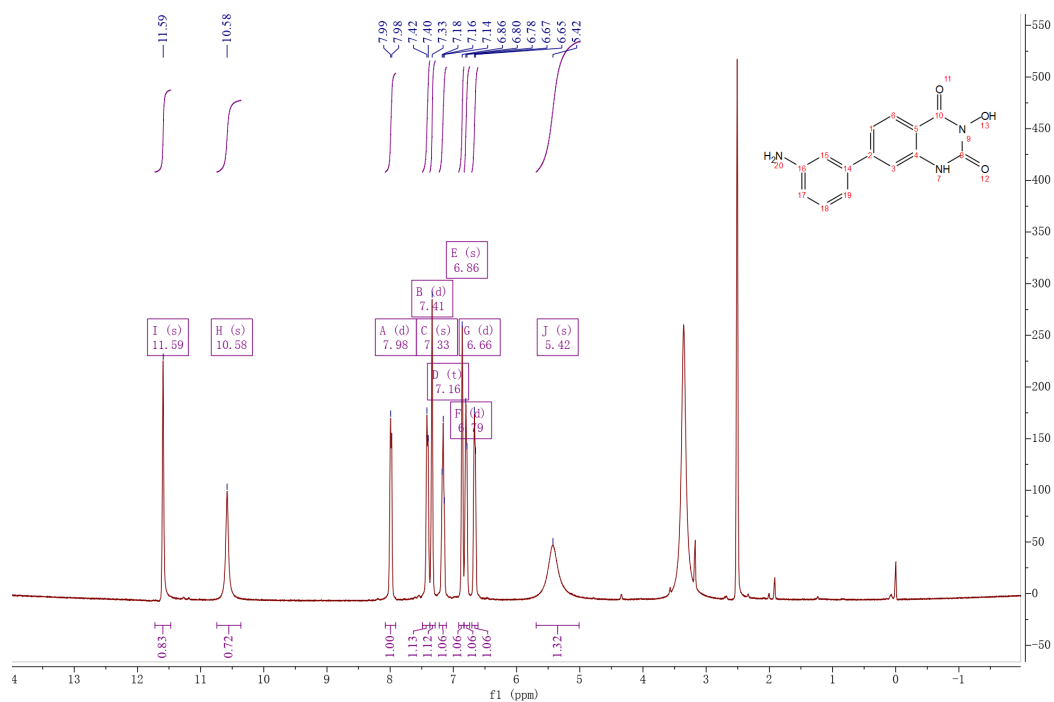
**Figure S95.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21i**



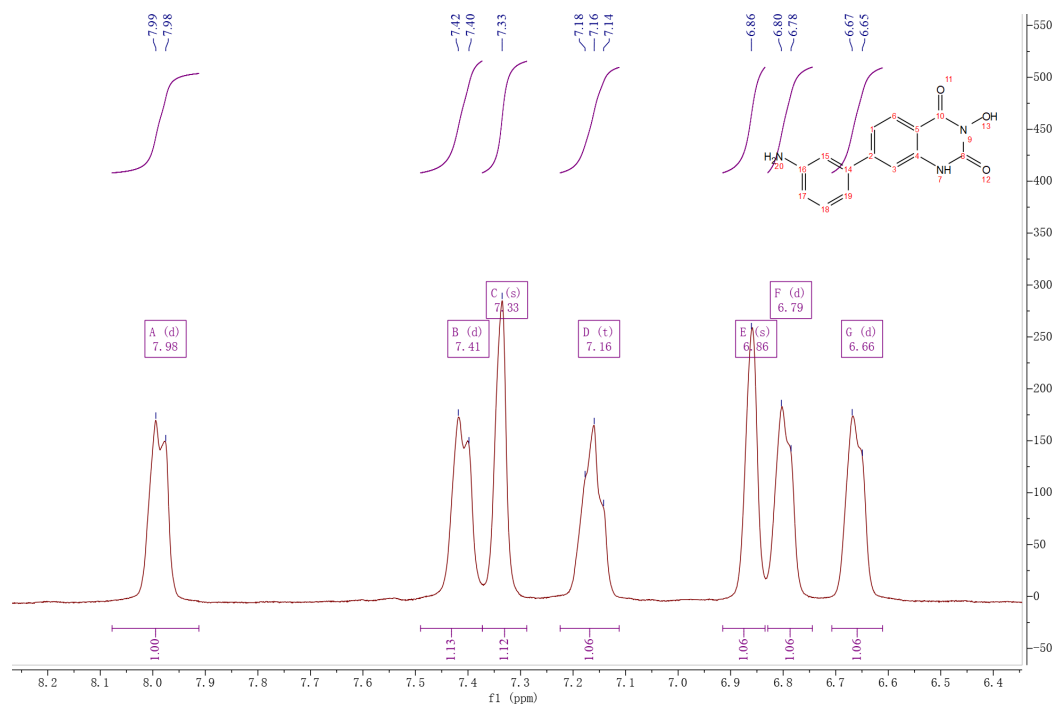
**Figure S96.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21i**



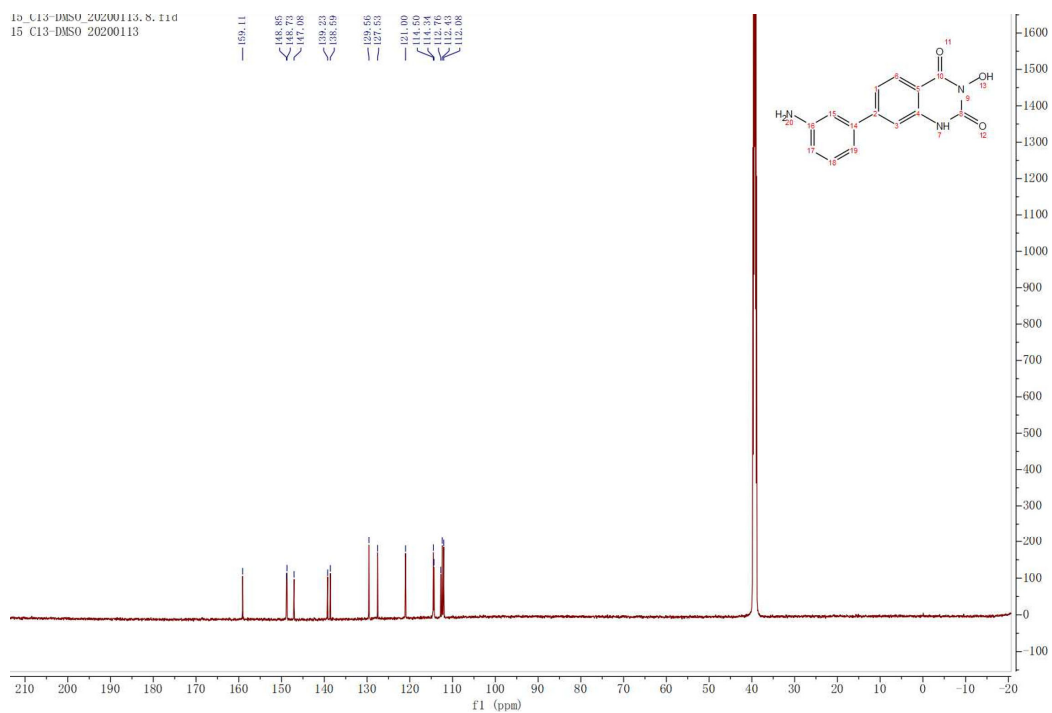
**Figure S97.** Mass spectrum (negative ionization) of **21i**



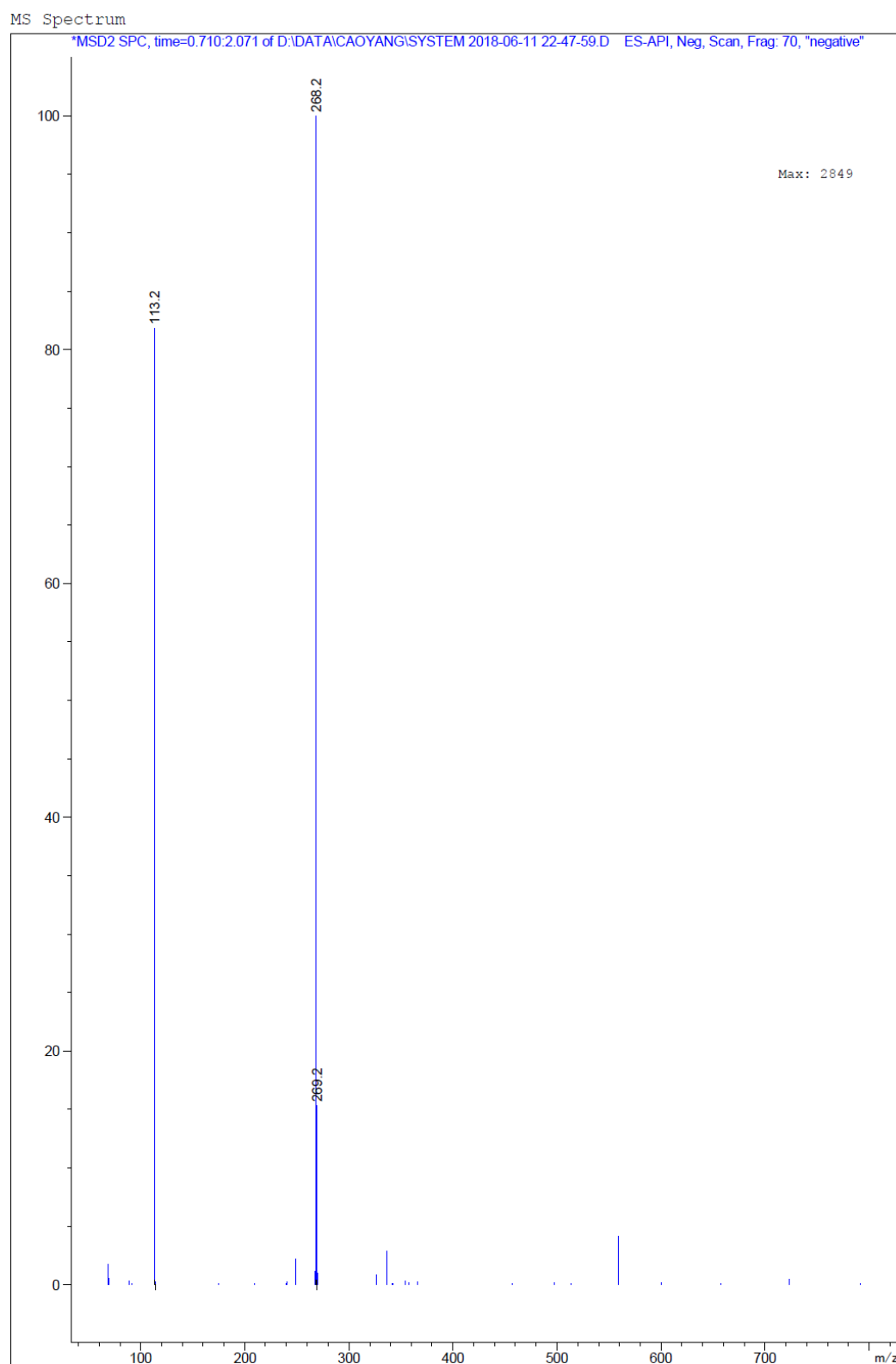
**Figure S98.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21j**



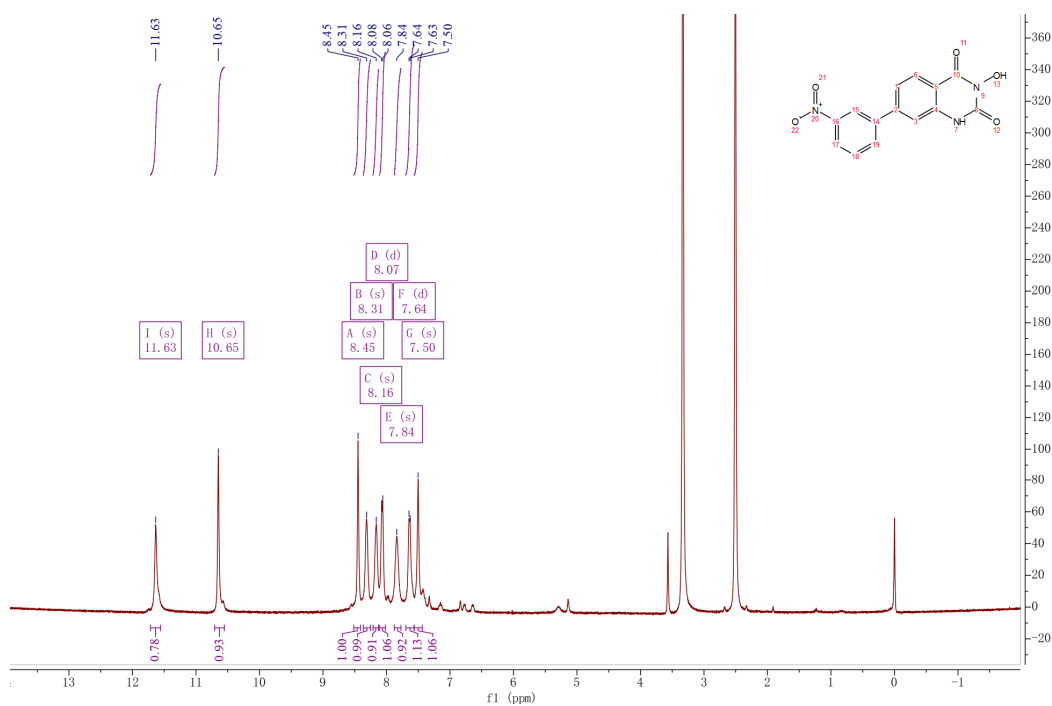
**Figure S99.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21j**



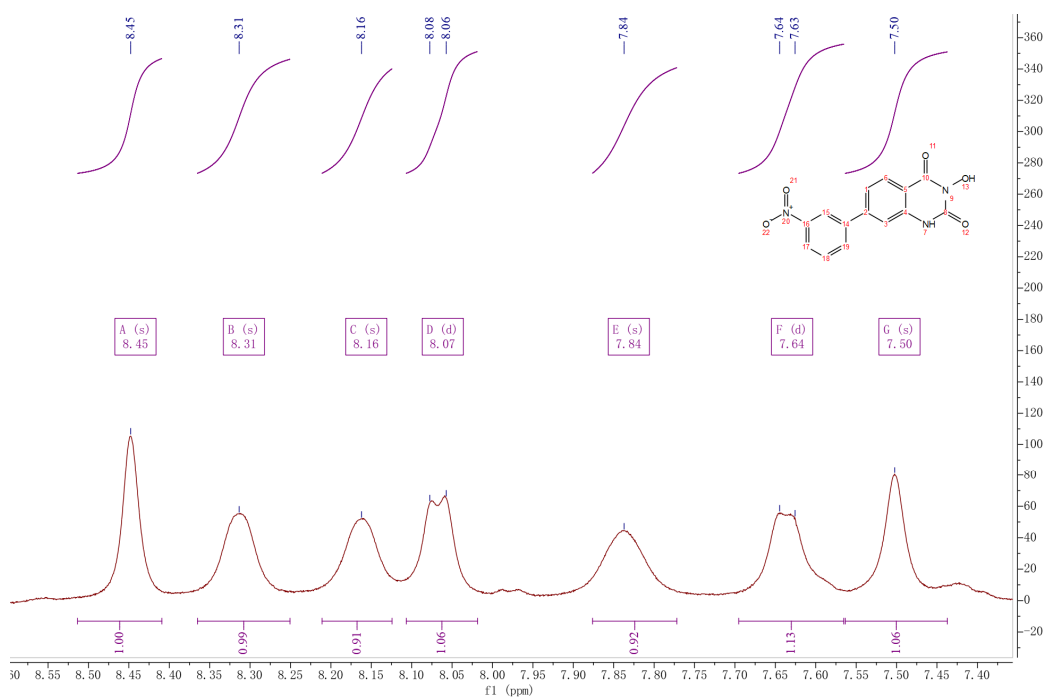
**Figure S100.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21j**



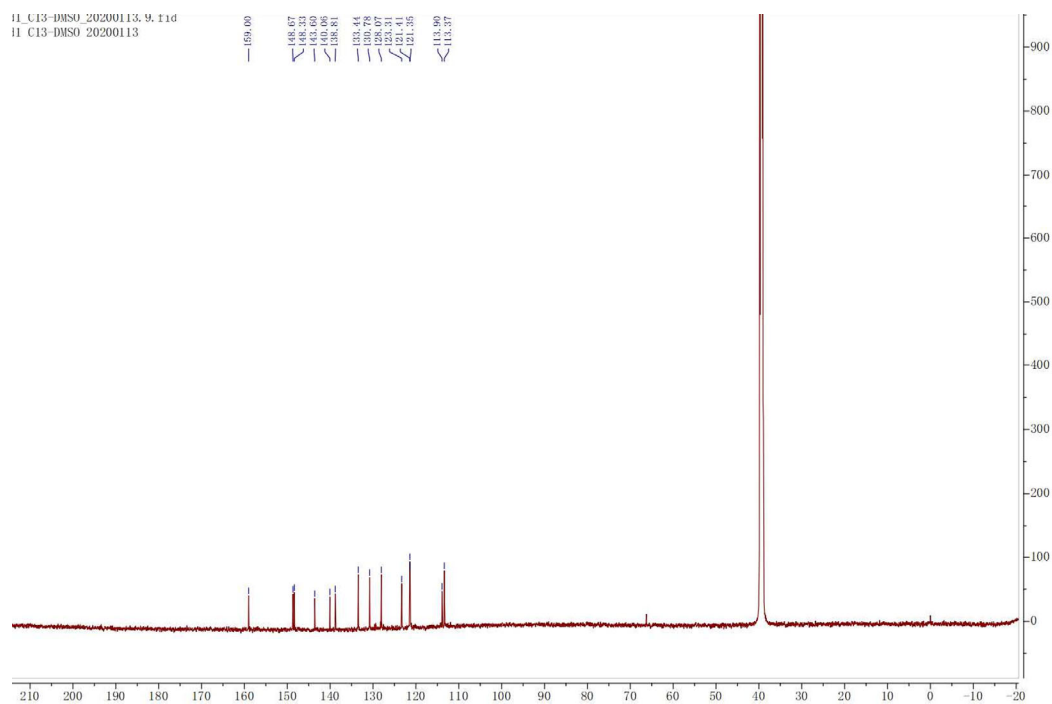
**Figure S101.** Mass spectrum (negative ionization) of **21j**



**Figure S102.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21k**

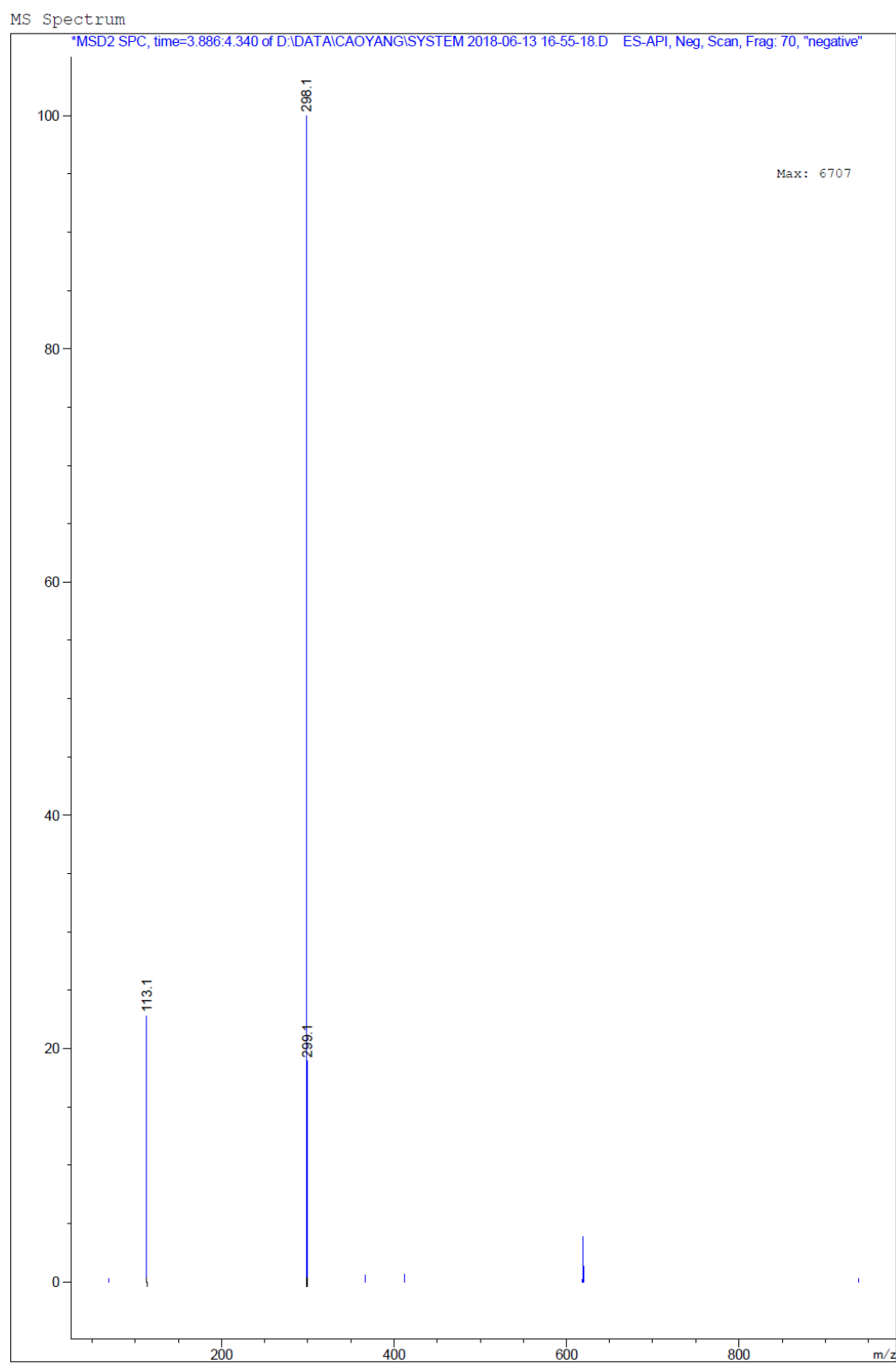


**Figure S103.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21k**

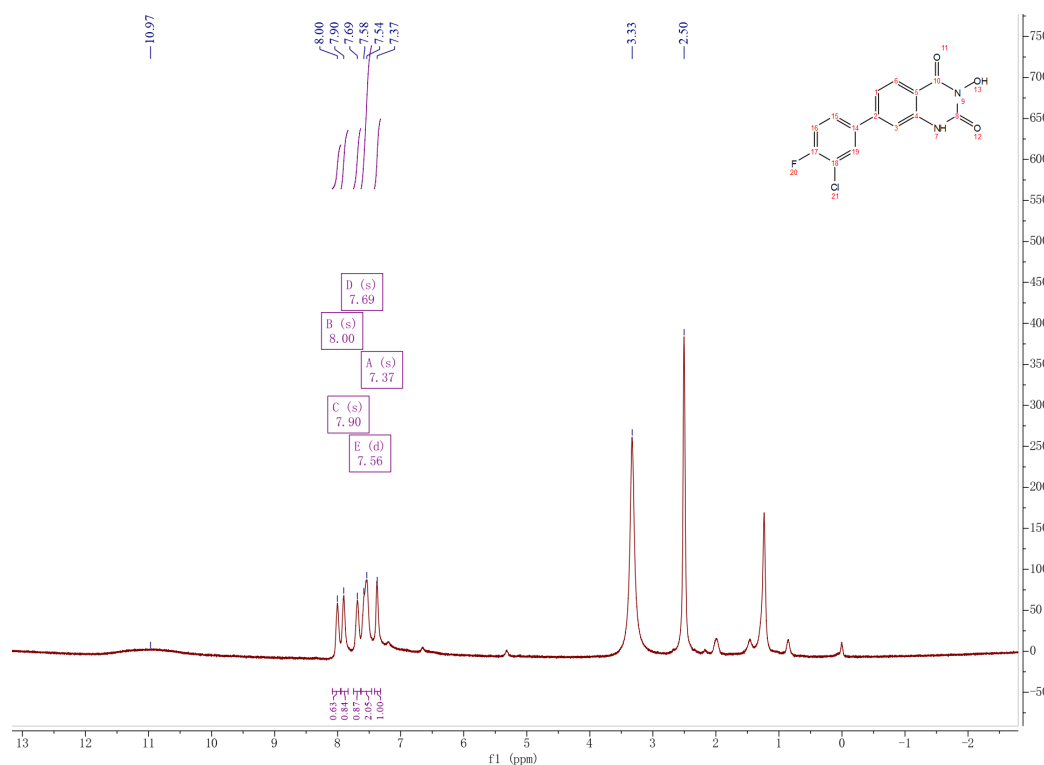


**Figure S104.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO-}d_6$ ) spectrum of **21k**

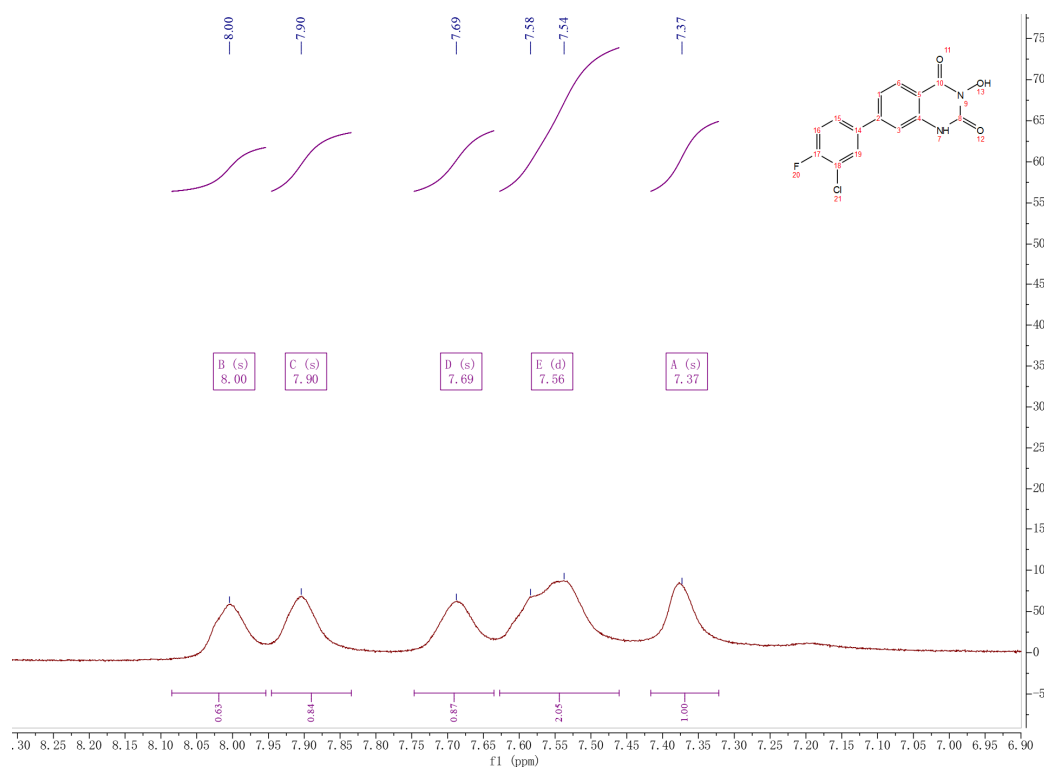




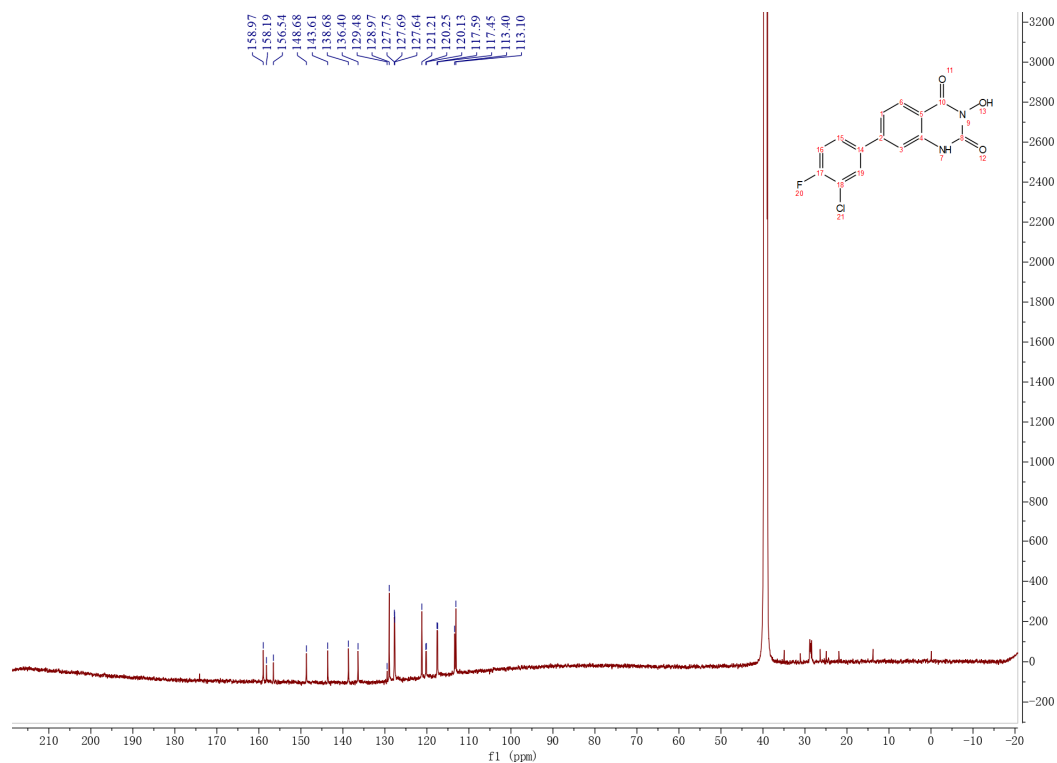
**Figure S105.** Mass spectrum (negative ionization) of **21k**



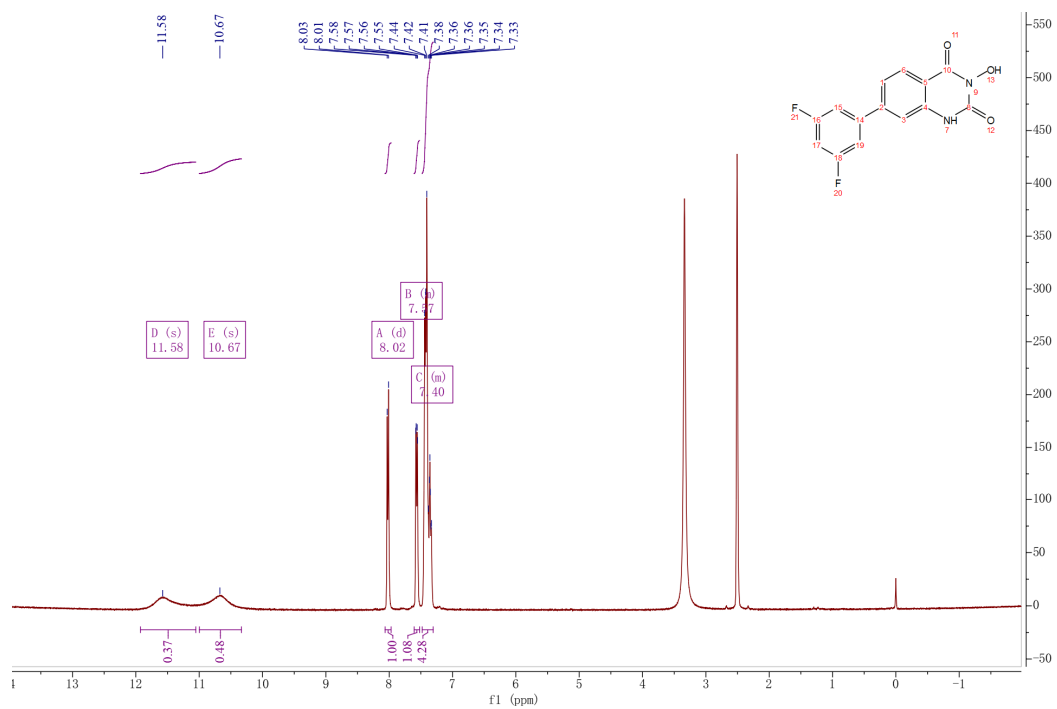
**Figure S106.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **211**



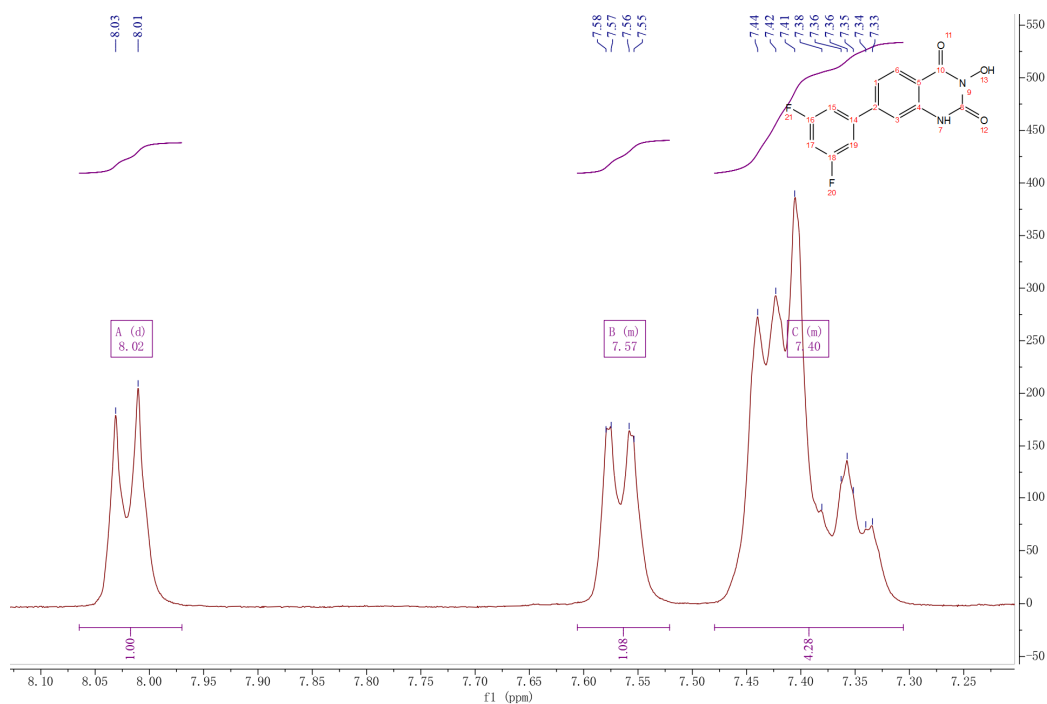
**Figure S107.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **211**



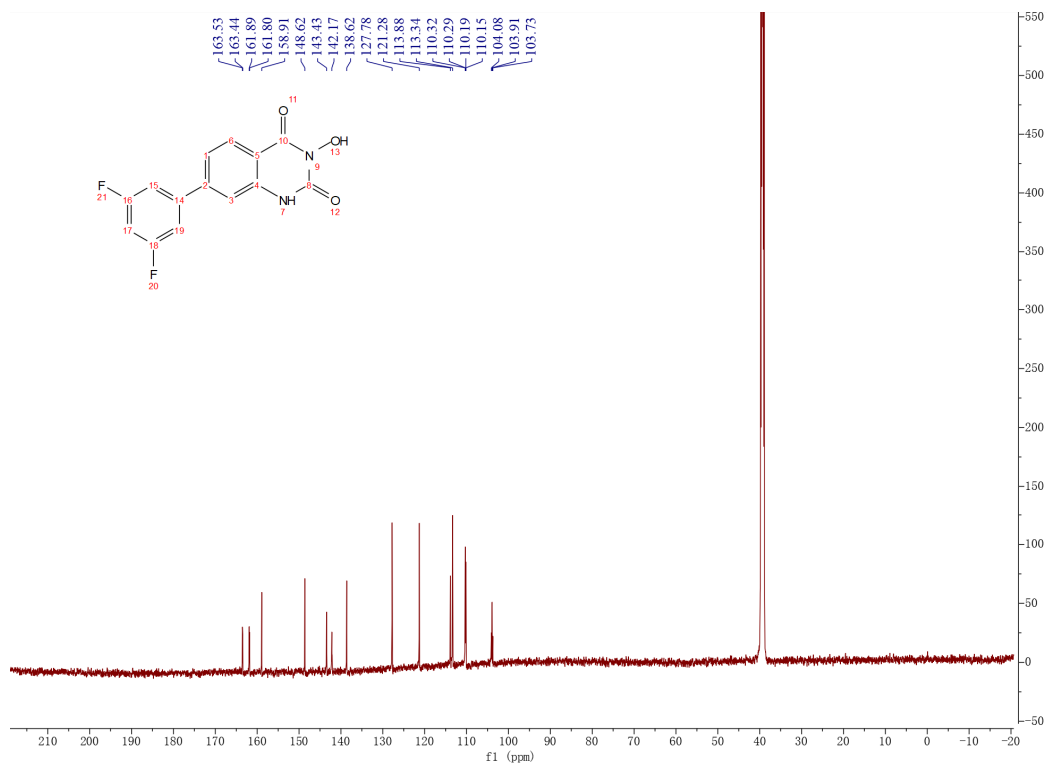
**Figure S108.** <sup>13</sup>C NMR (151 MHz, DMSO-*d*<sub>6</sub>) spectrum of **21l**



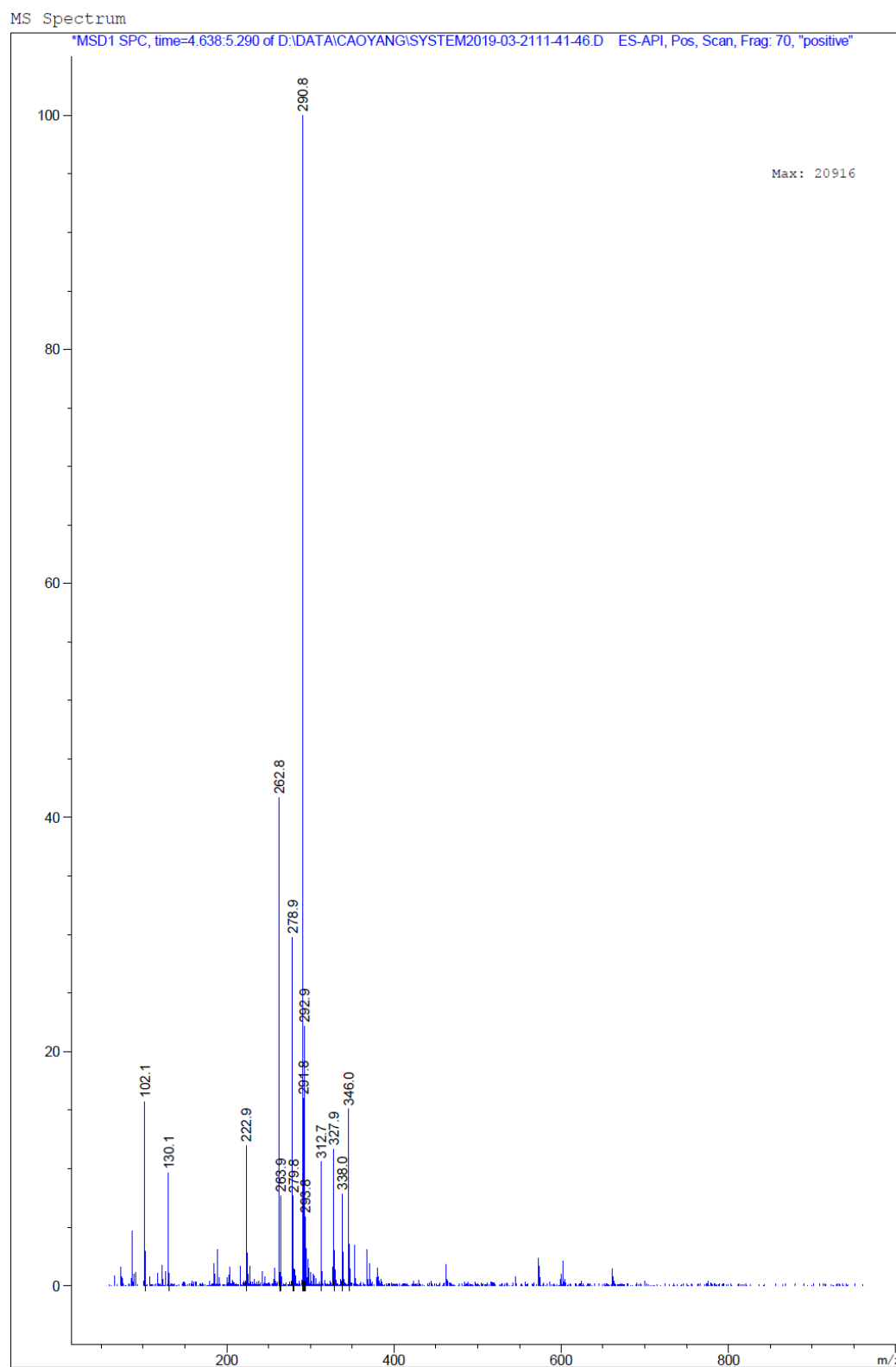
**Figure S109.** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of **21m**



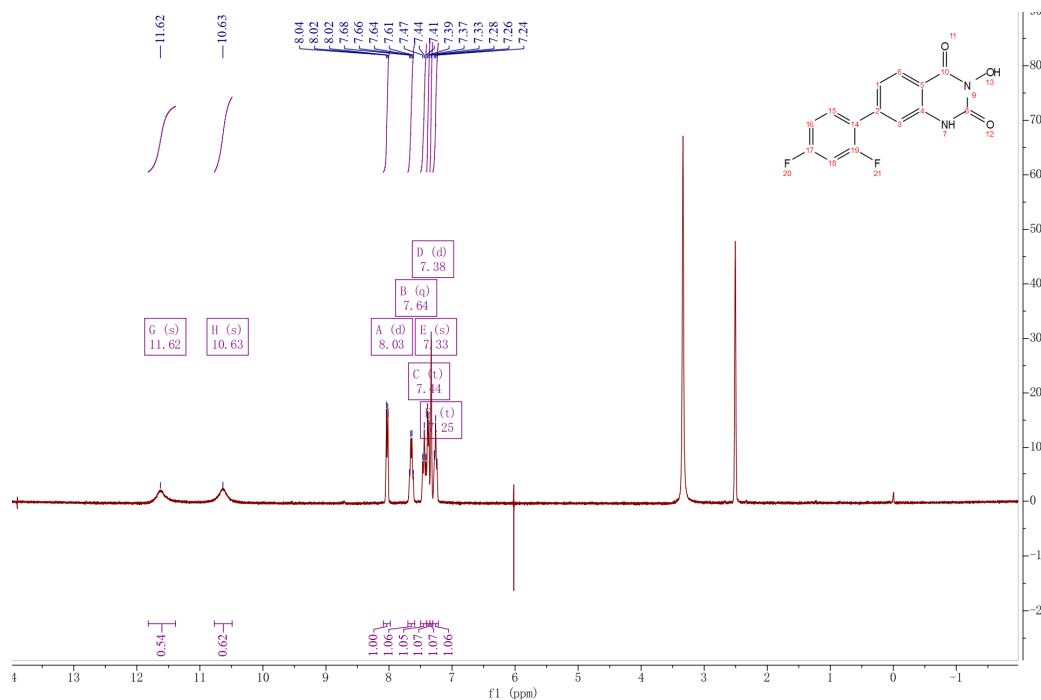
**Figure S110.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21m**



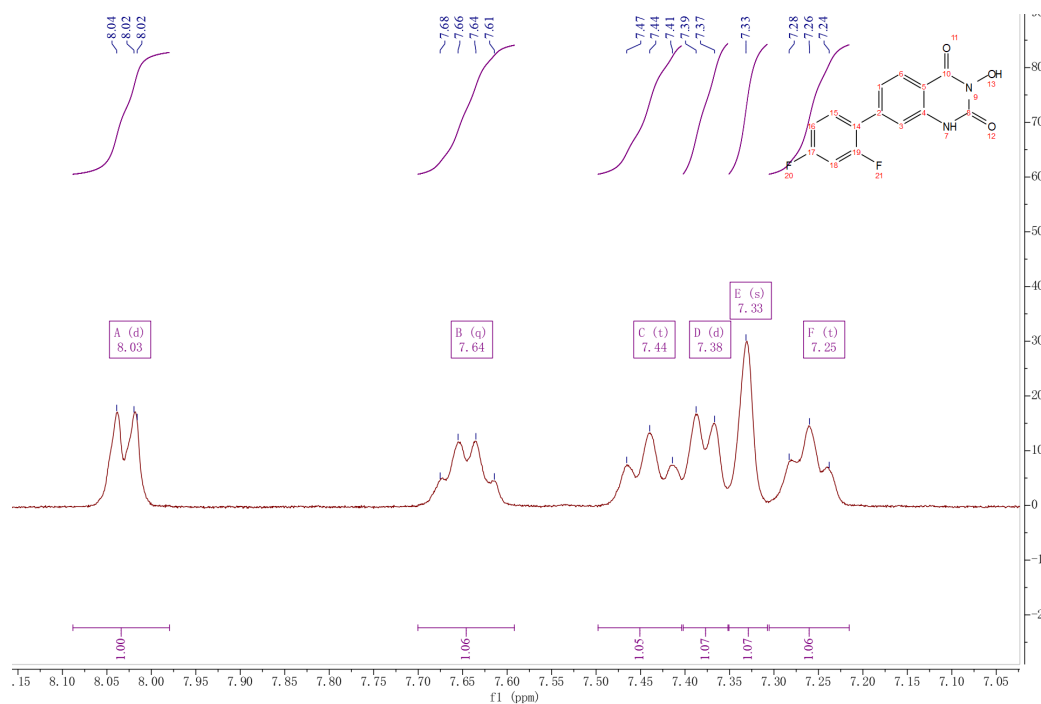
**Figure S111.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21m**



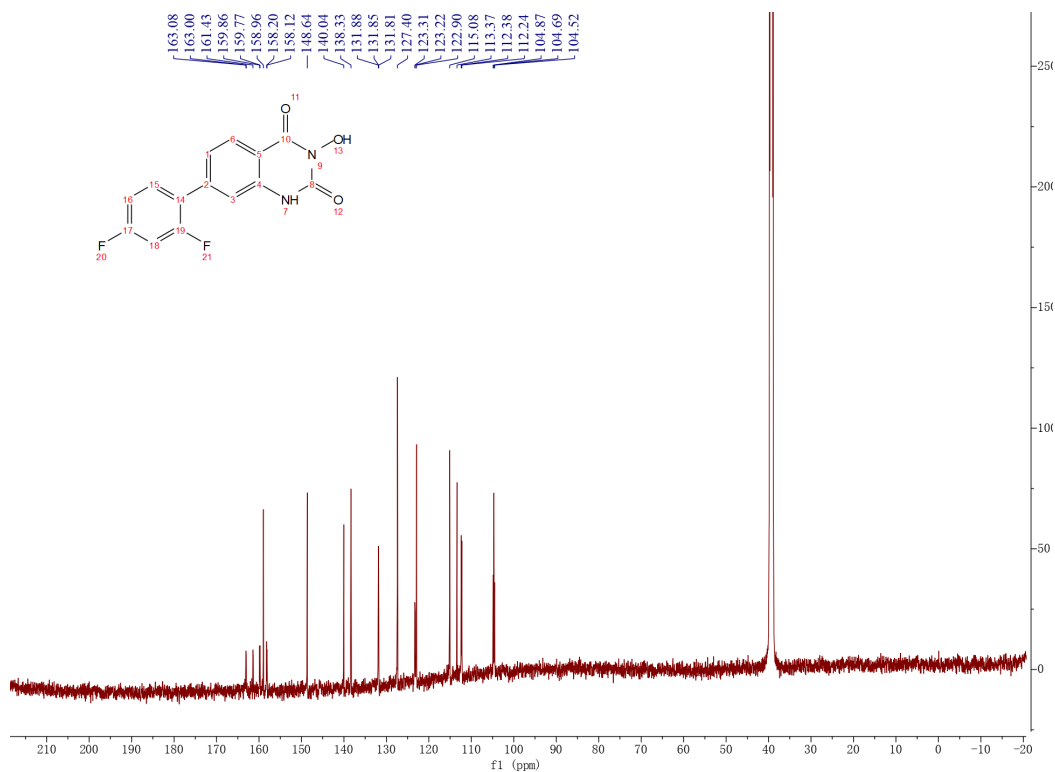
**Figure S112.** Mass spectrum (positive ionization) of **21m**



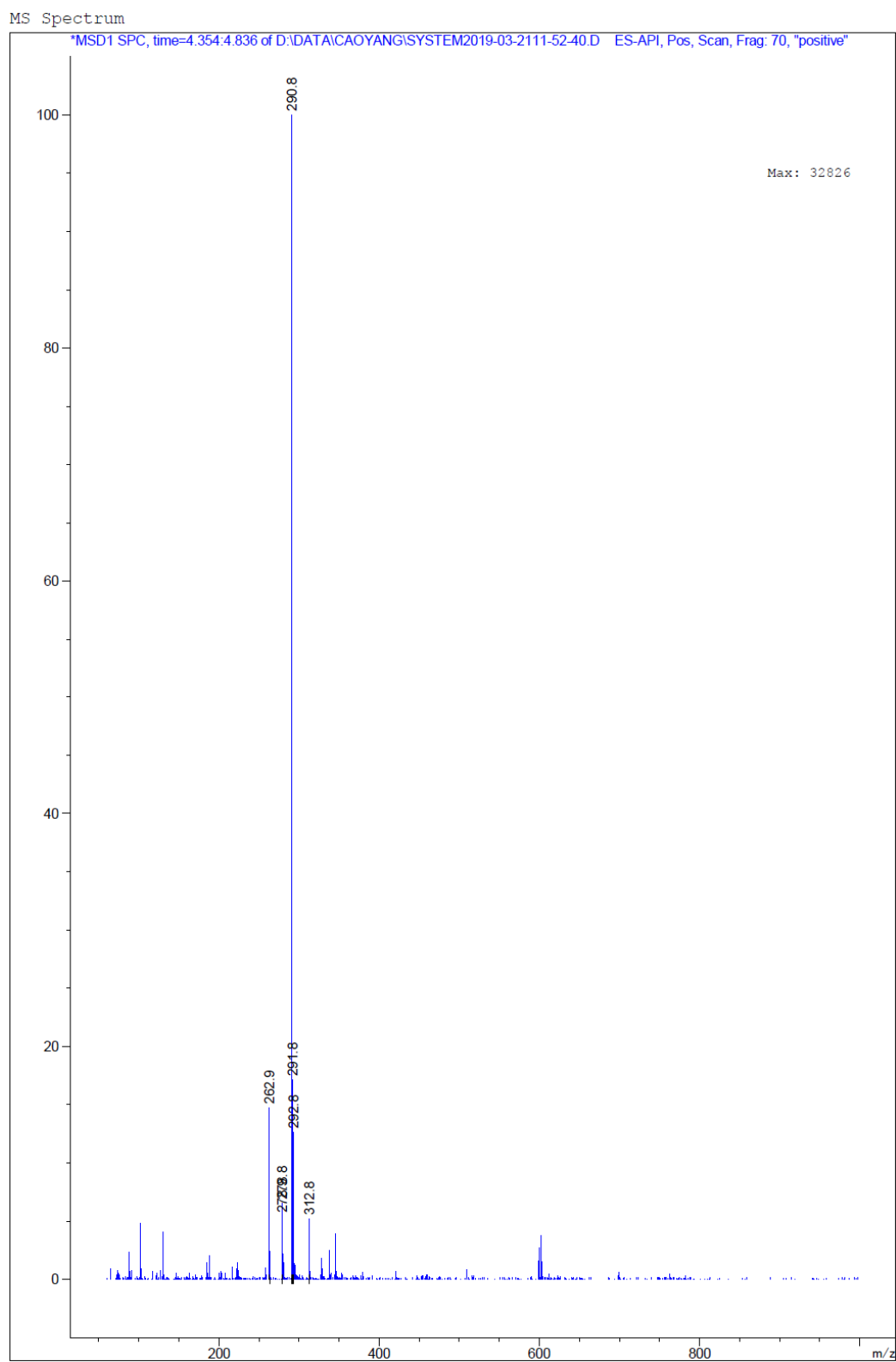
**Figure S113.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21n**



**Figure S114.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21n**

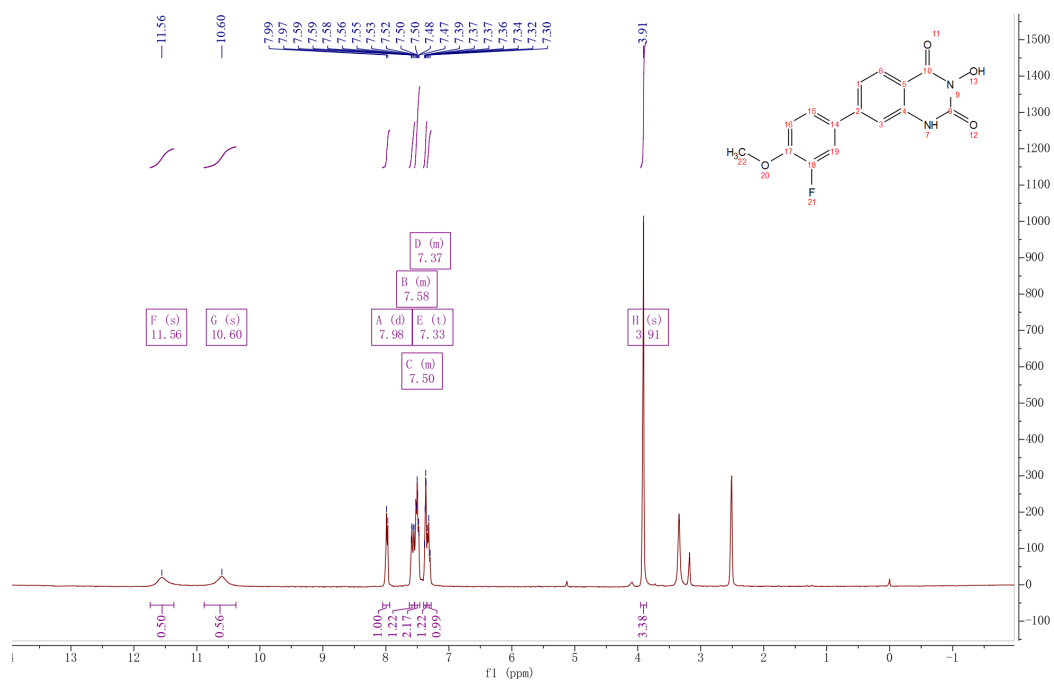


**Figure S115.**  $^{13}\text{C}$  NMR (151 MHz, DMSO- $d_6$ ) spectrum of **21n**

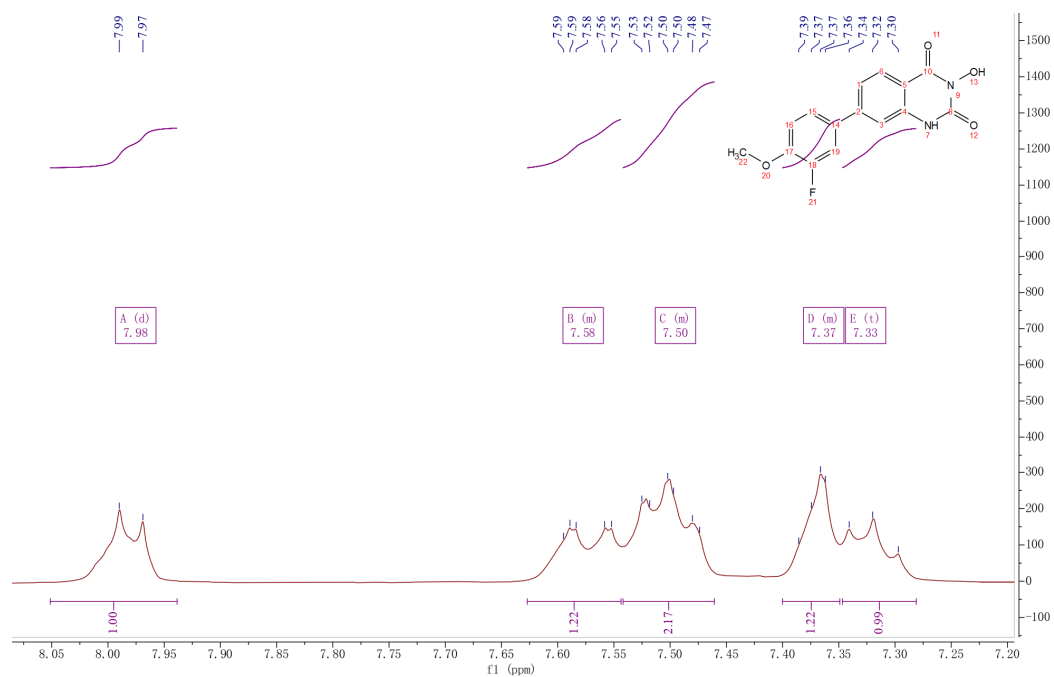


**Figure S116.** Mass spectrum (positive ionization) of **21n**

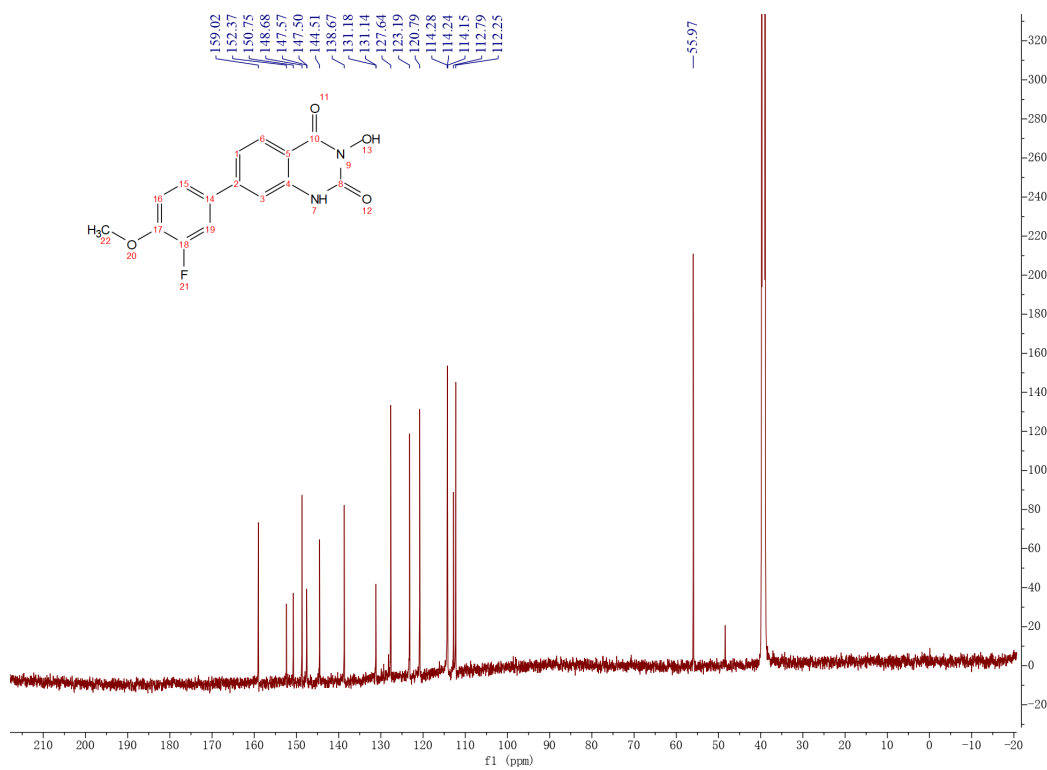




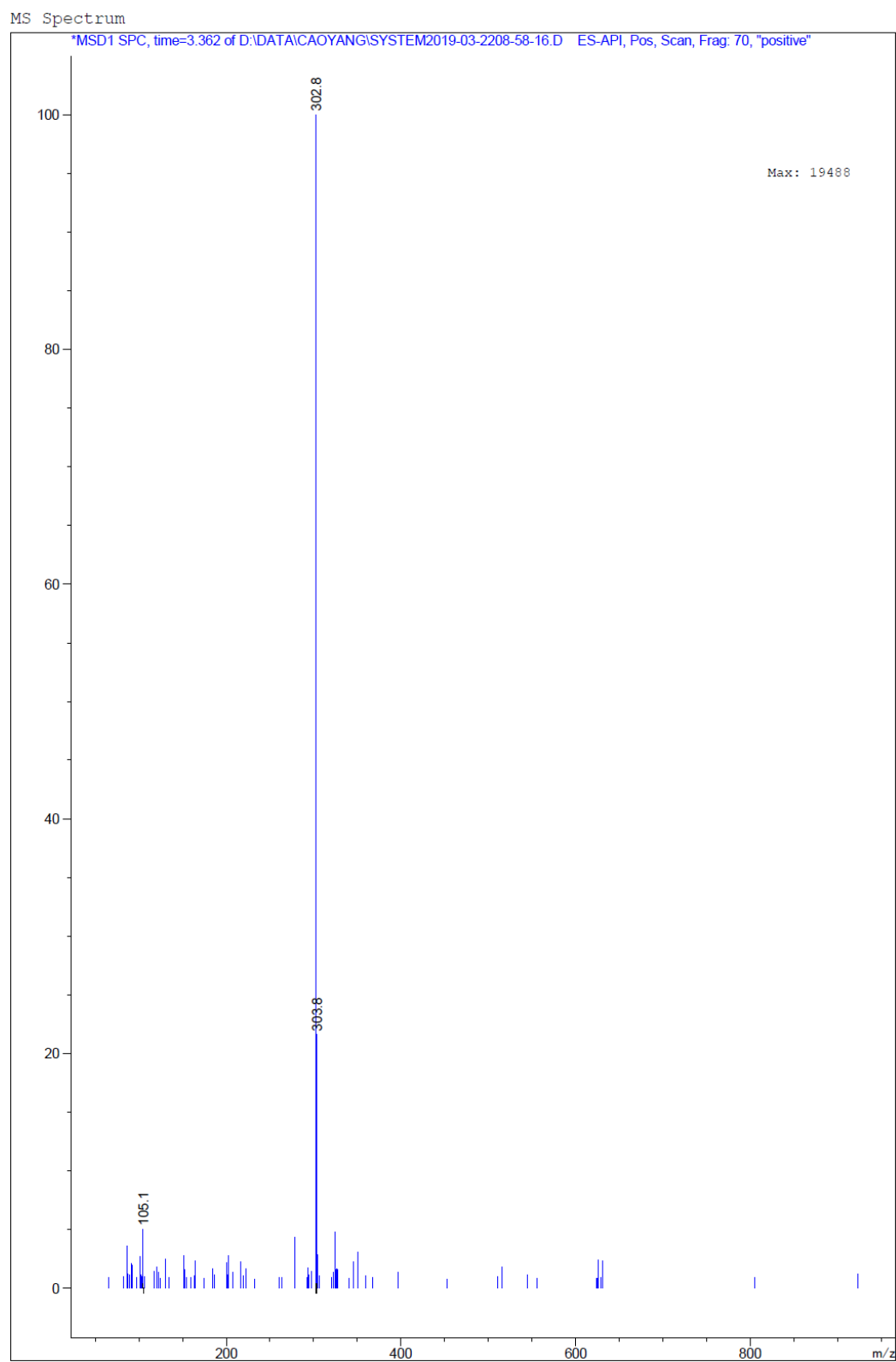
**Figure S117.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21o**



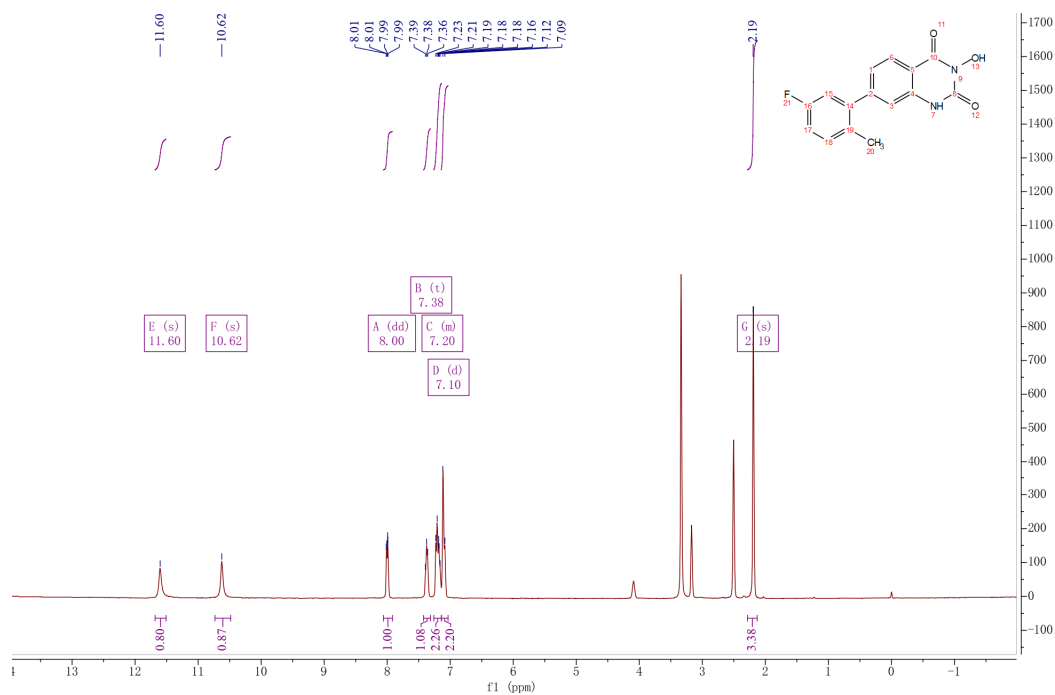
**Figure S118.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21o**



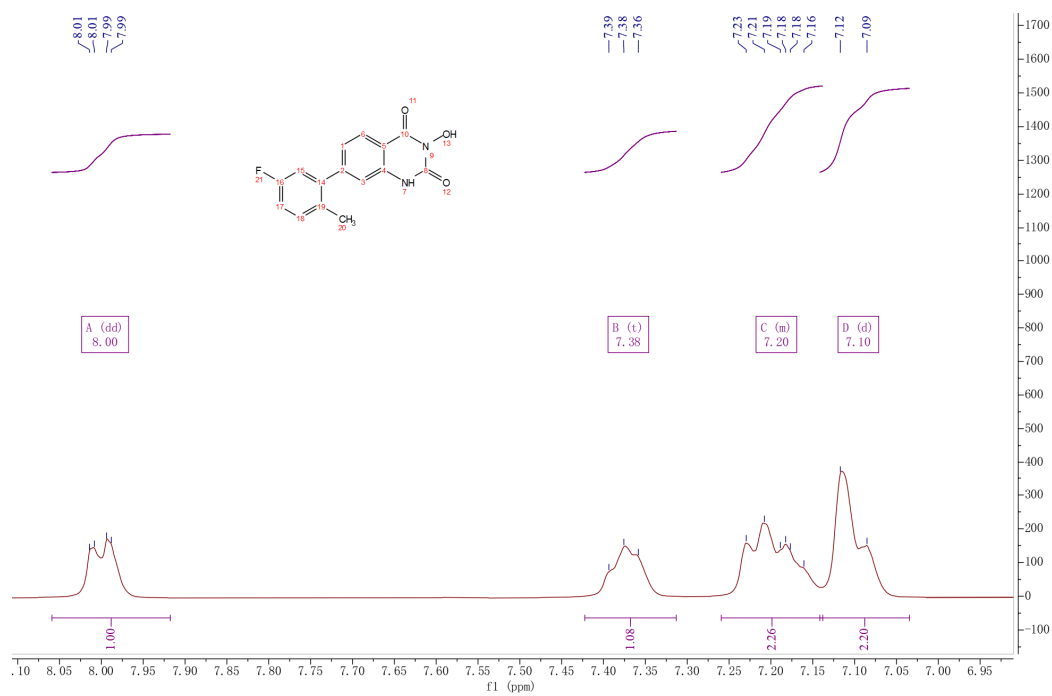
**Figure S119.** <sup>13</sup>C NMR (151 MHz, DMSO-*d*<sub>6</sub>) spectrum of **21o**



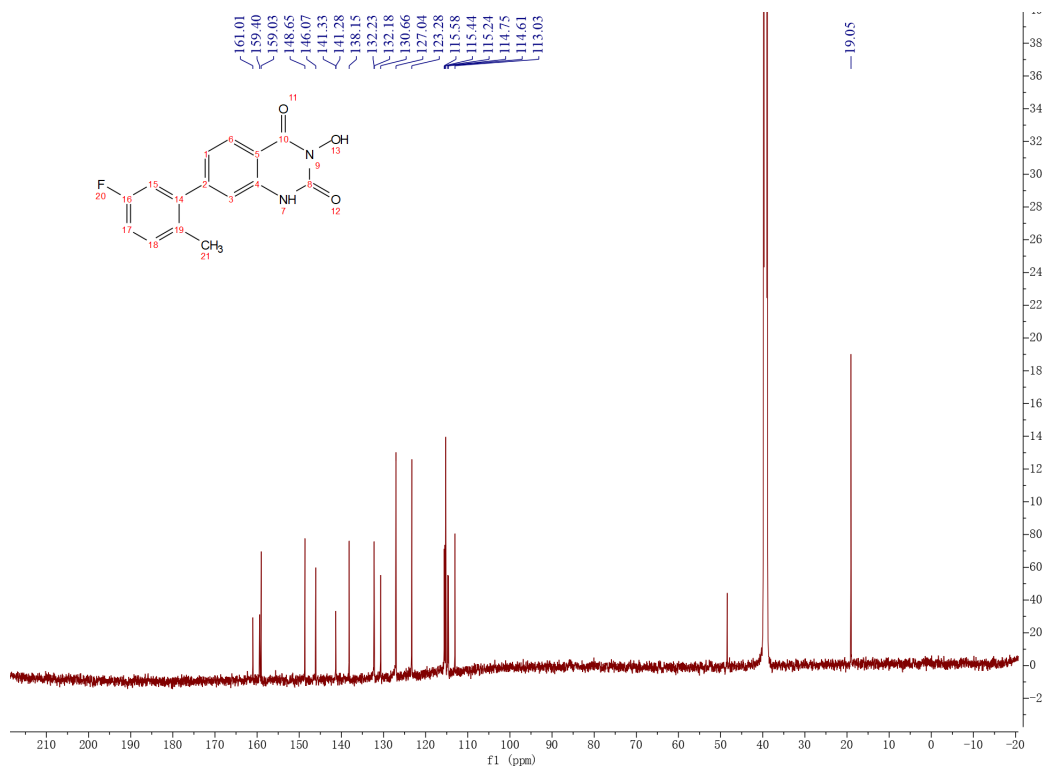
**Figure S120.** Mass spectrum (positive ionization) of **21o**



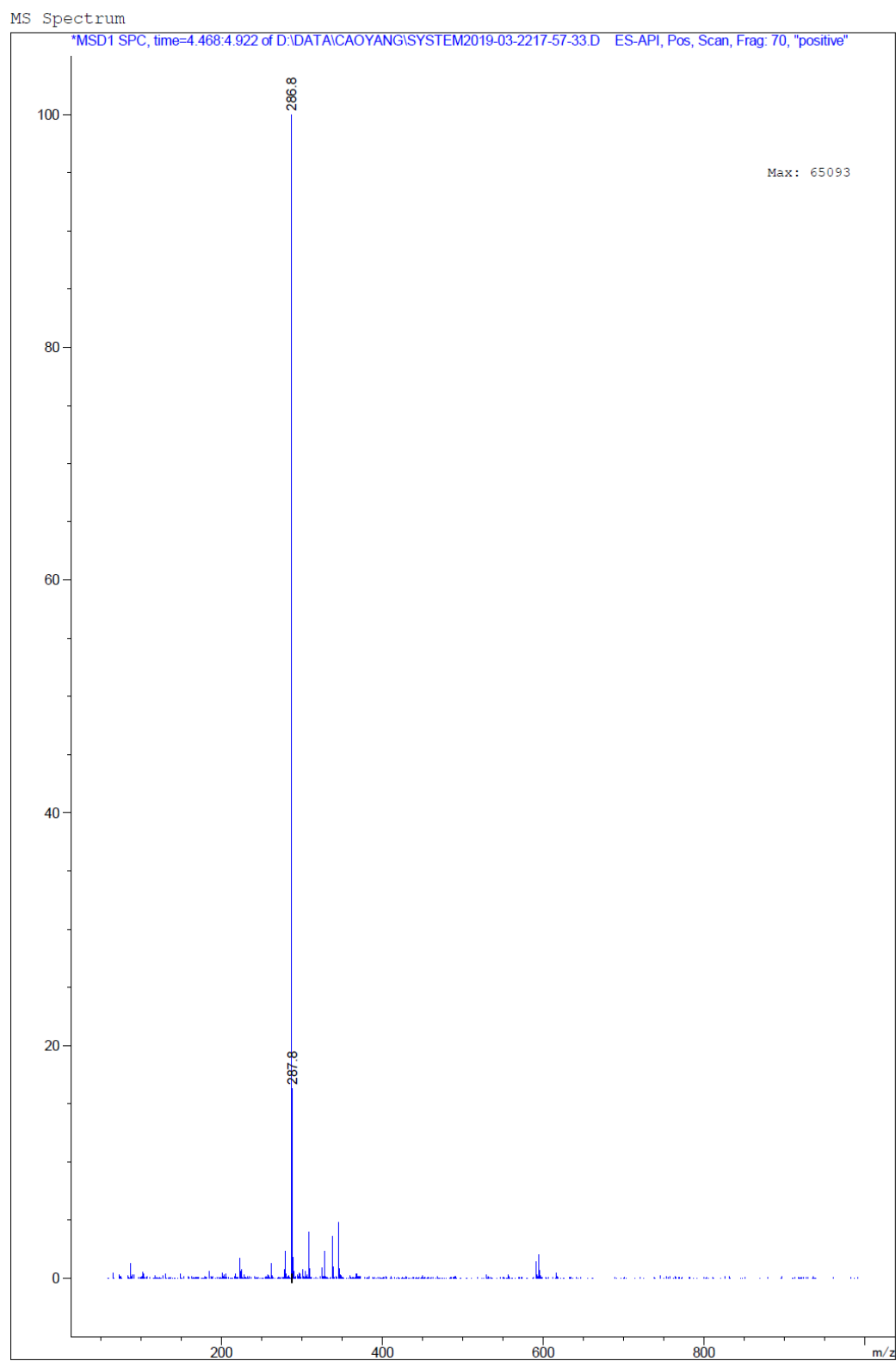
**Figure S121.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21p**



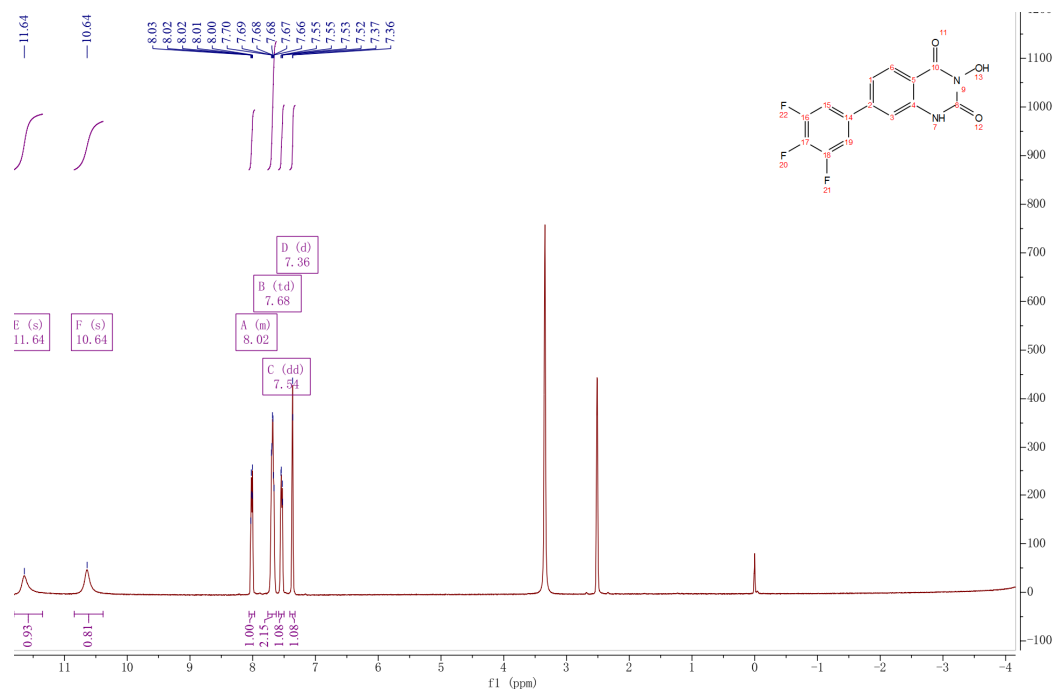
**Figure S122.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21p**



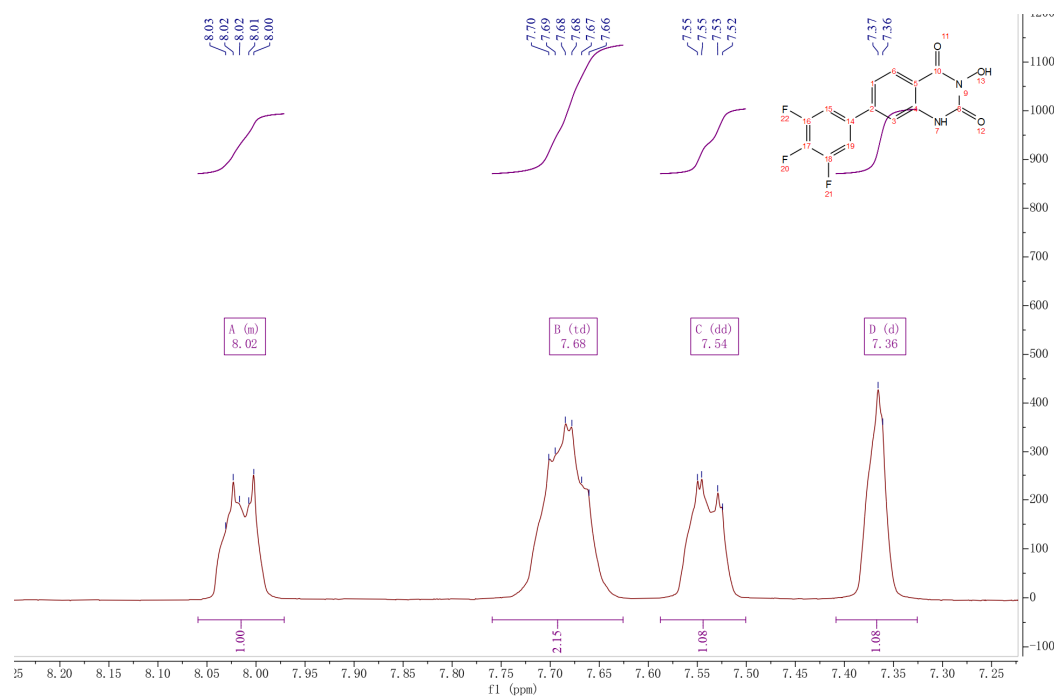
**Figure S123.**  $^{13}\text{C}$  NMR (151 MHz, DMSO- $d_6$ ) spectrum of **21p**



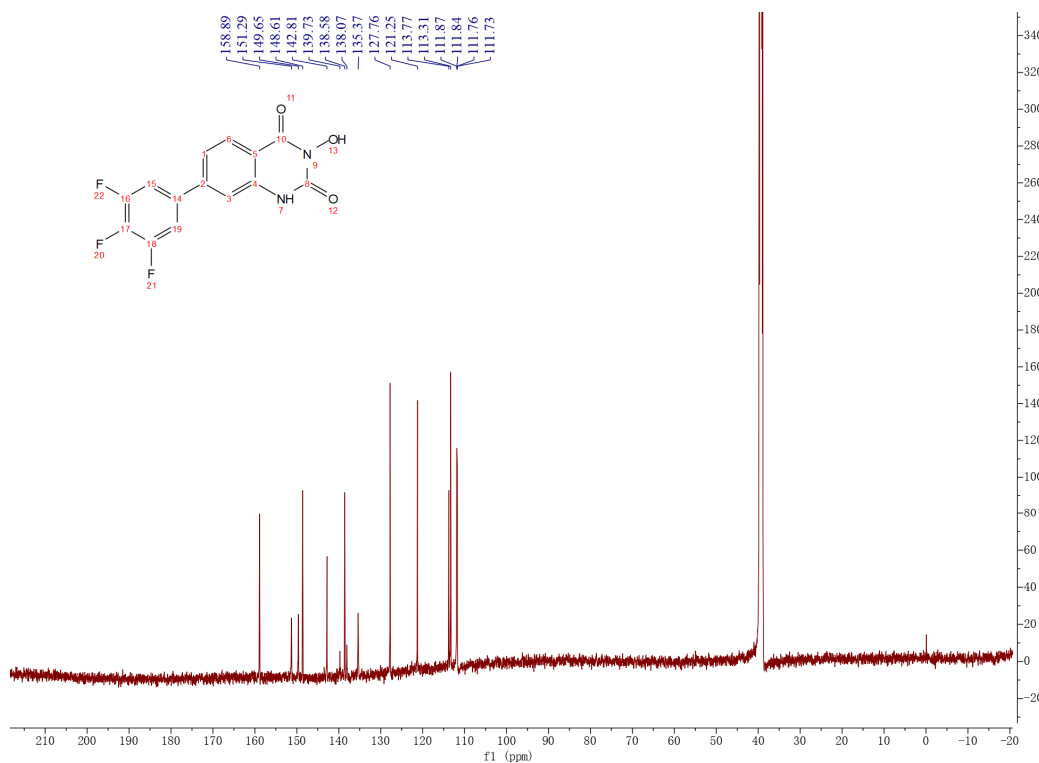
**Figure S124.** Mass spectrum (positive ionization) of **21p**



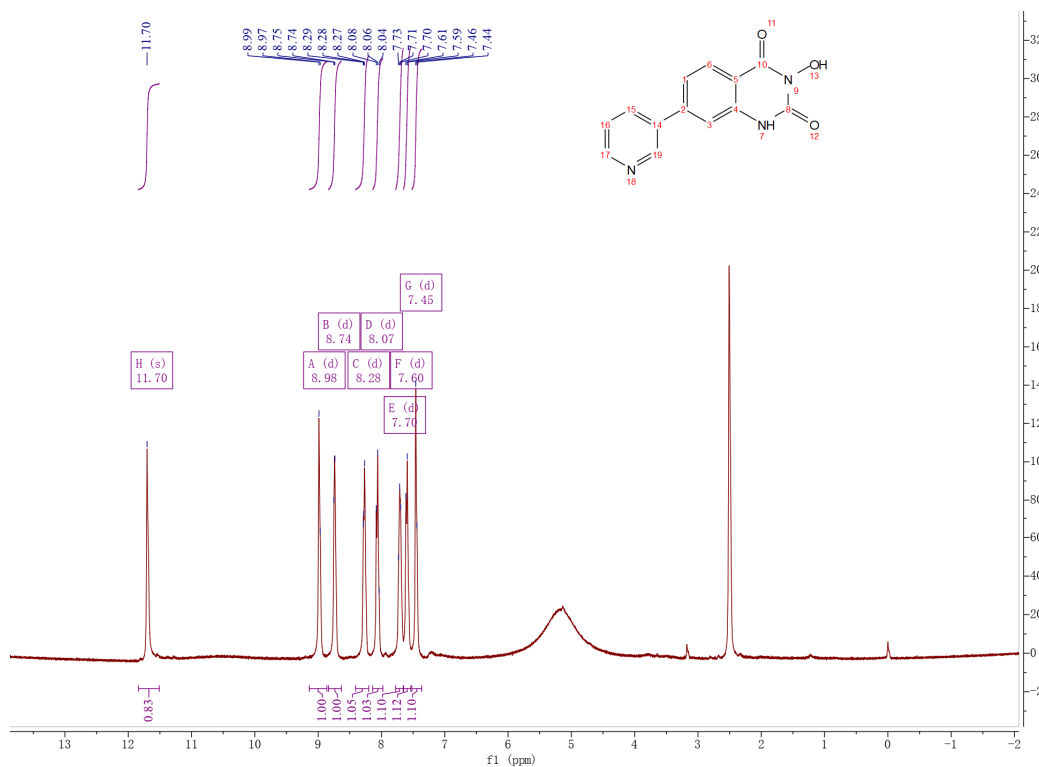
**Figure S125.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21q**



**Figure S126.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21q**

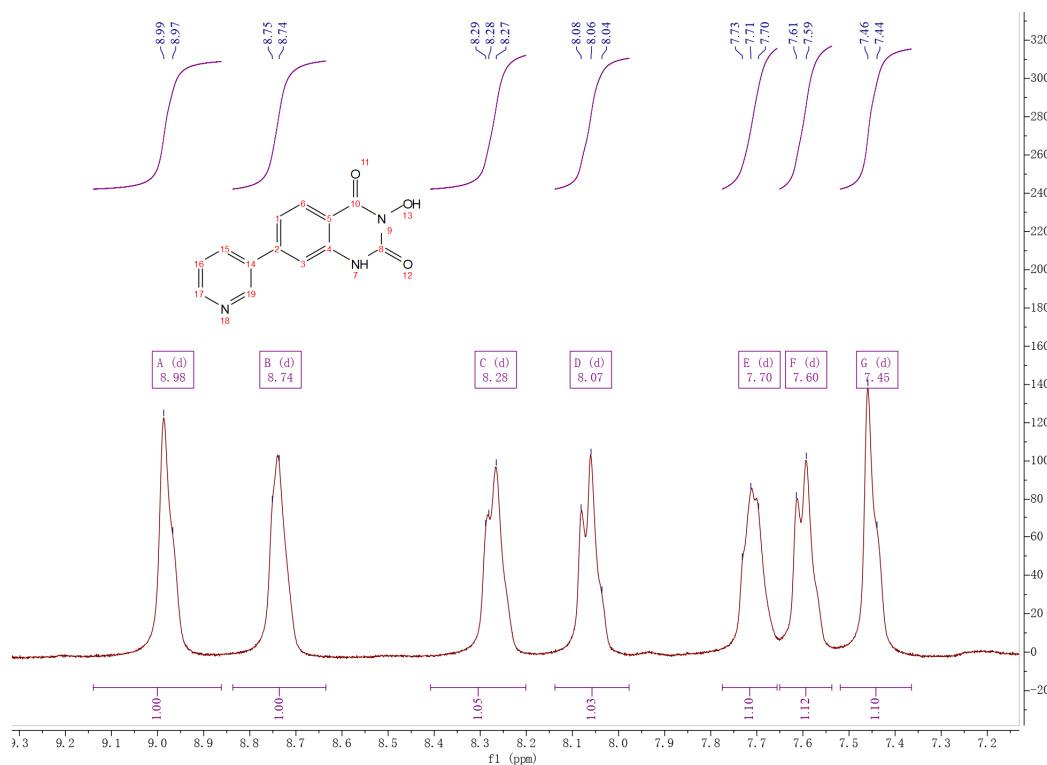


**Figure S127.**  $^{13}\text{C}$  NMR (151 MHz, DMSO- $d_6$ ) spectrum of **21q**

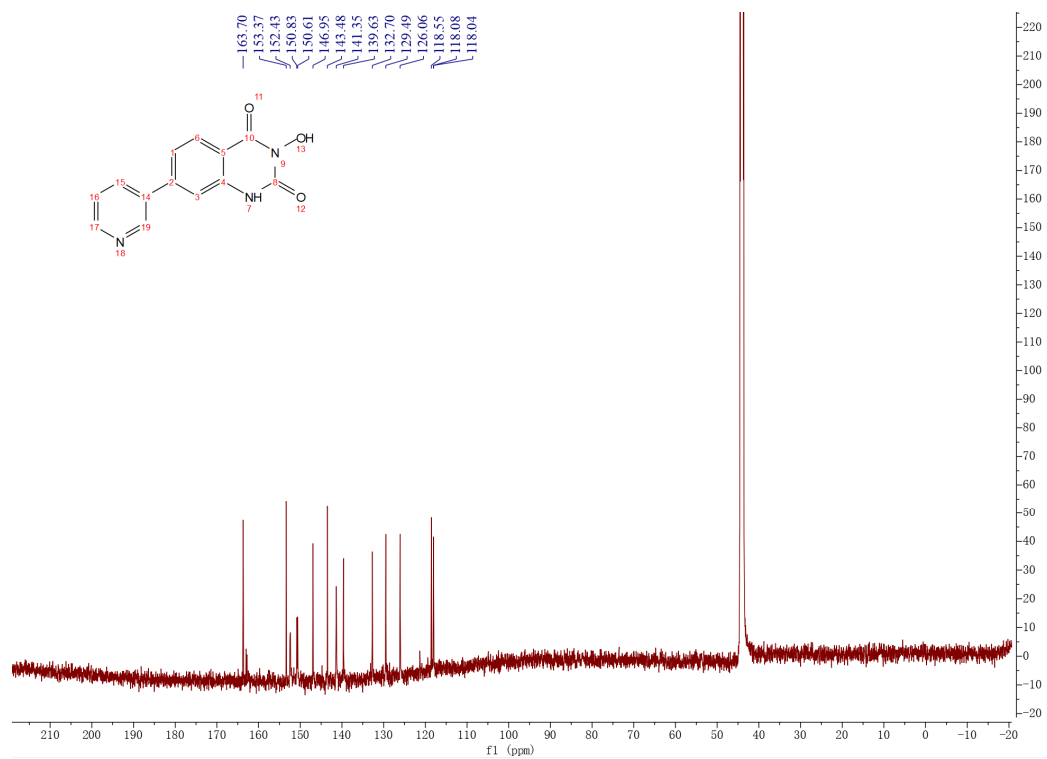


**Figure S128.**  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ) spectrum of **21r**

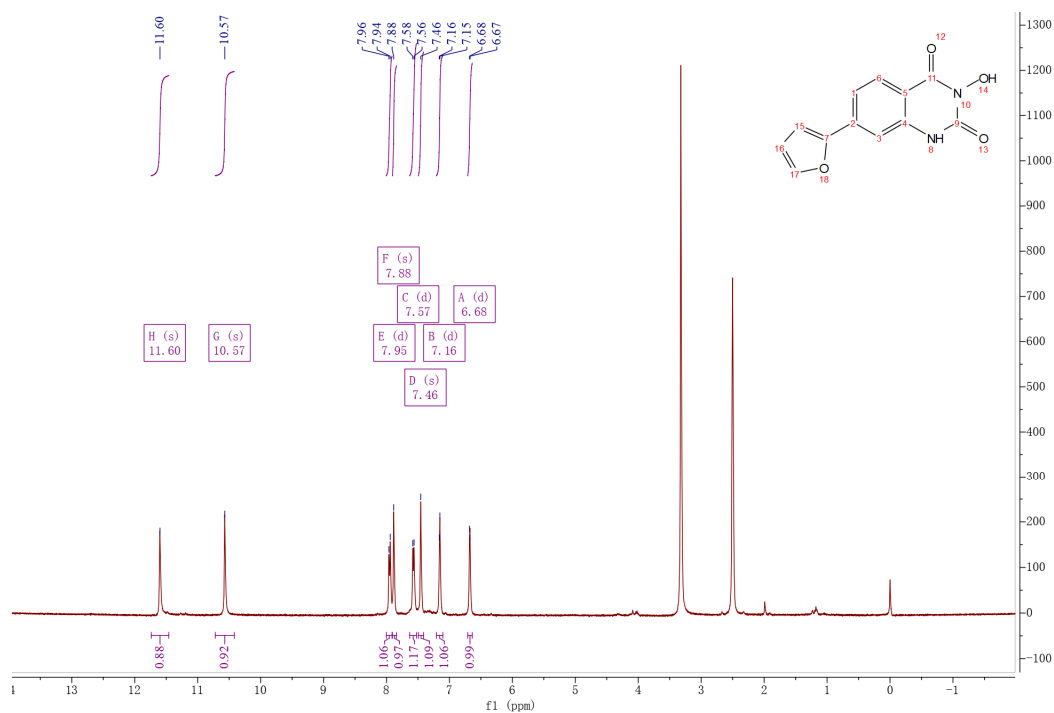




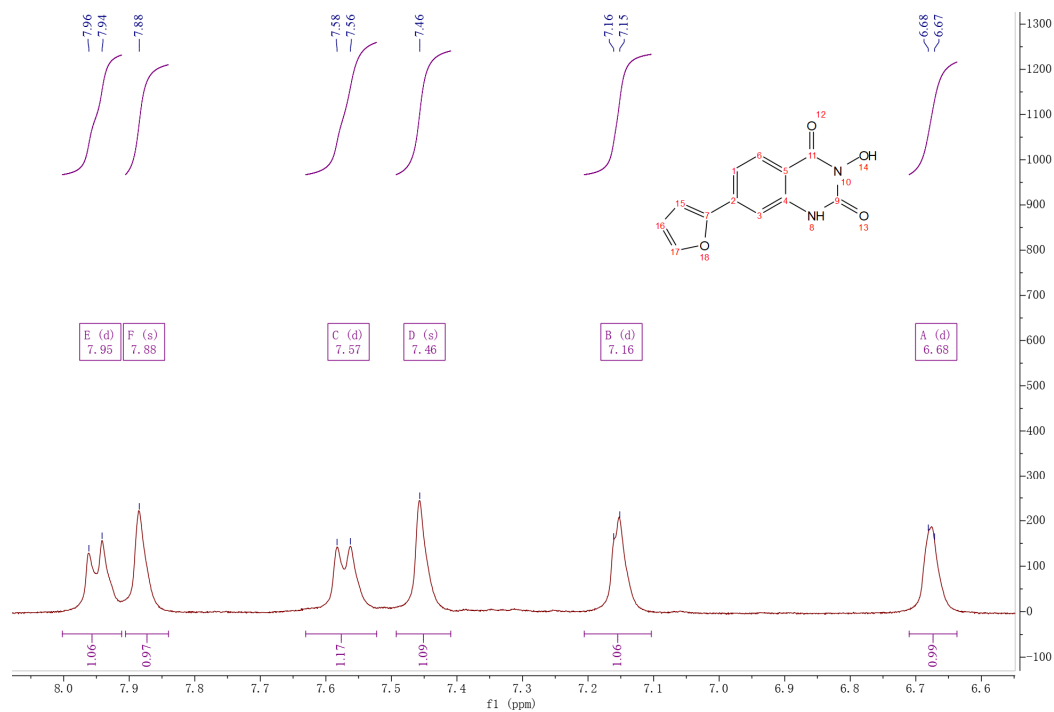
**Figure S129.** Magnified  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ) spectrum fragments of **21r**



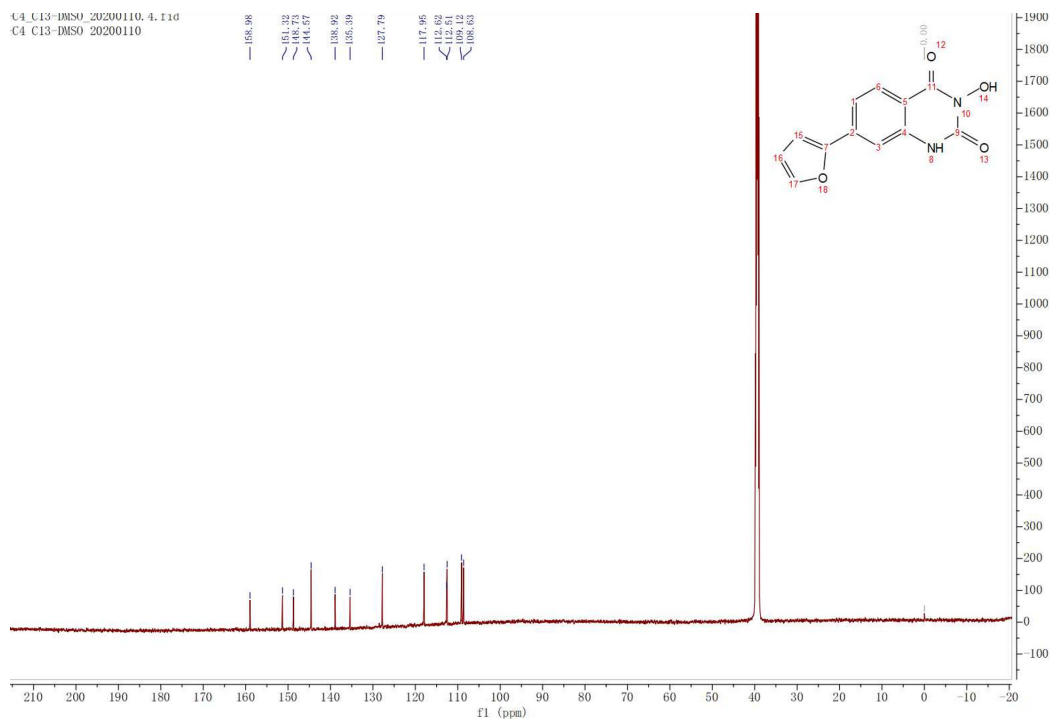
**Figure S130.**  $^{13}\text{C}$  NMR (151 MHz, DMSO- $d_6$ ) spectrum of **21r**



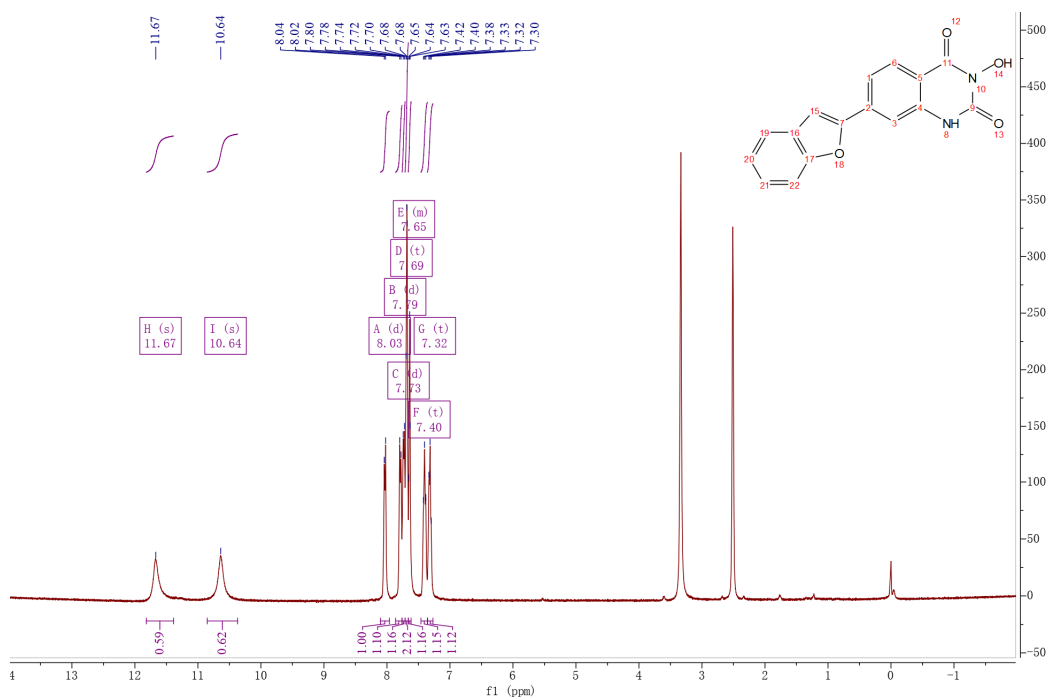
**Figure S131.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21s**



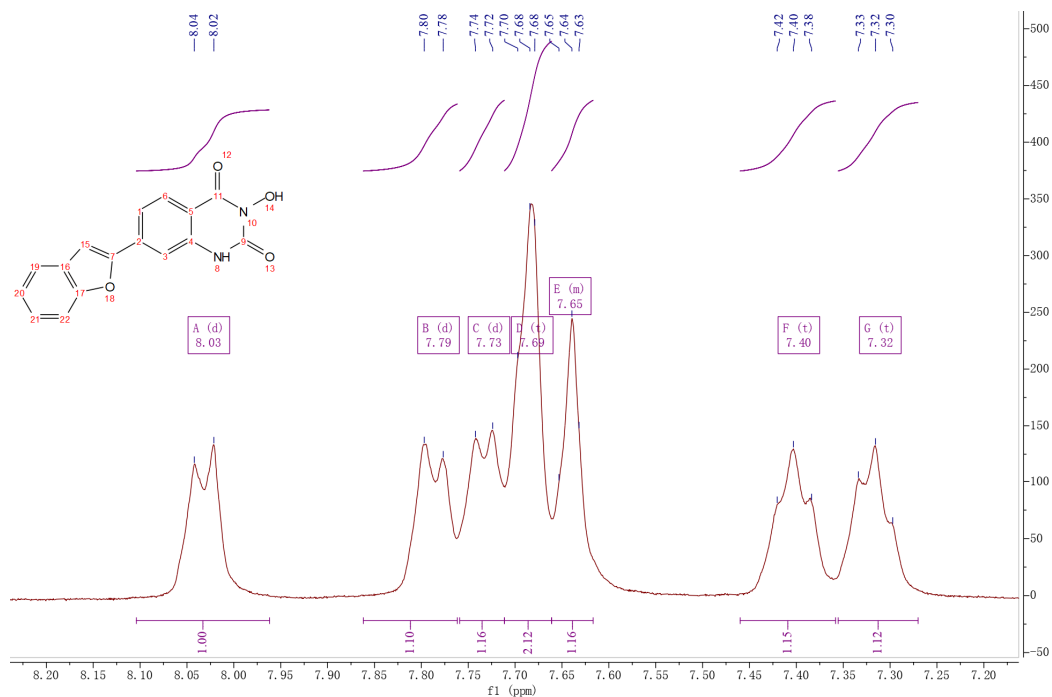
**Figure S132.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21s**



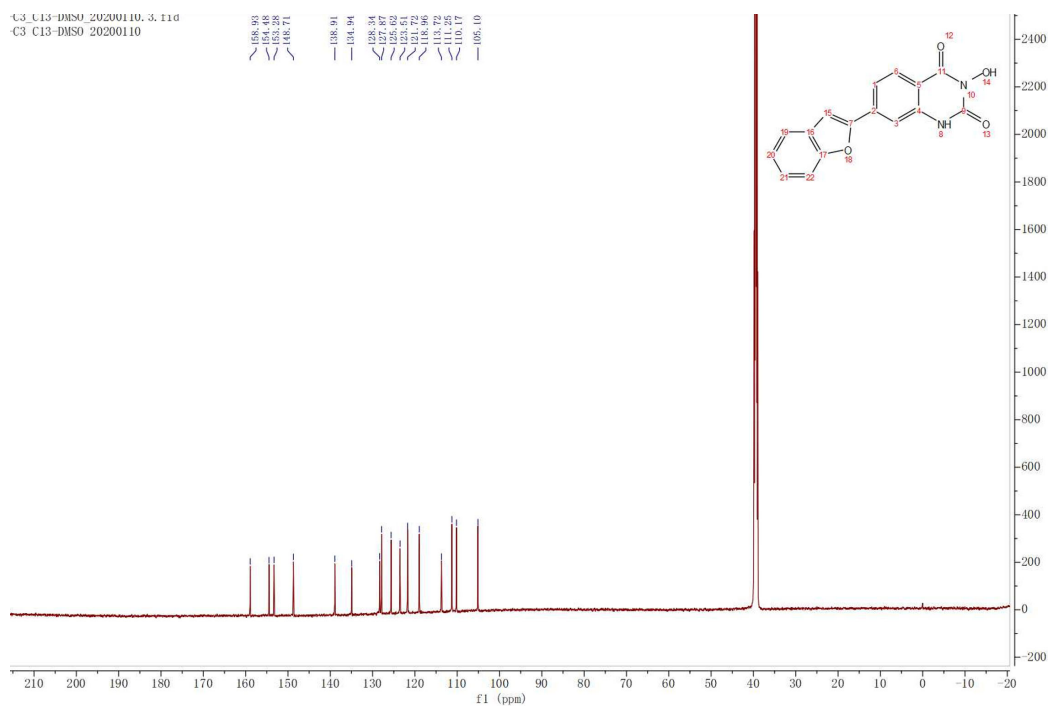
**Figure S133.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21s**



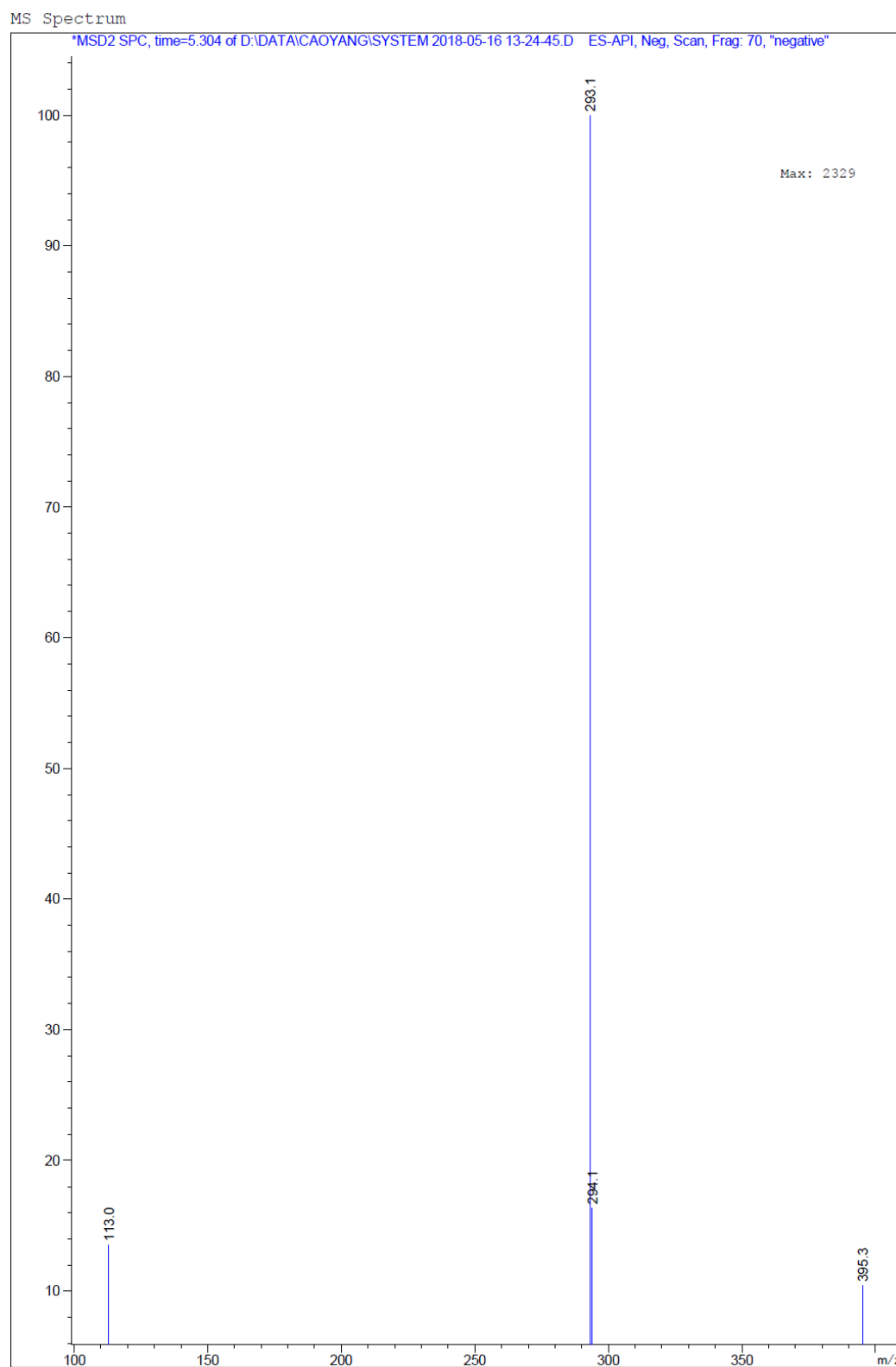
**Figure S134.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21t**



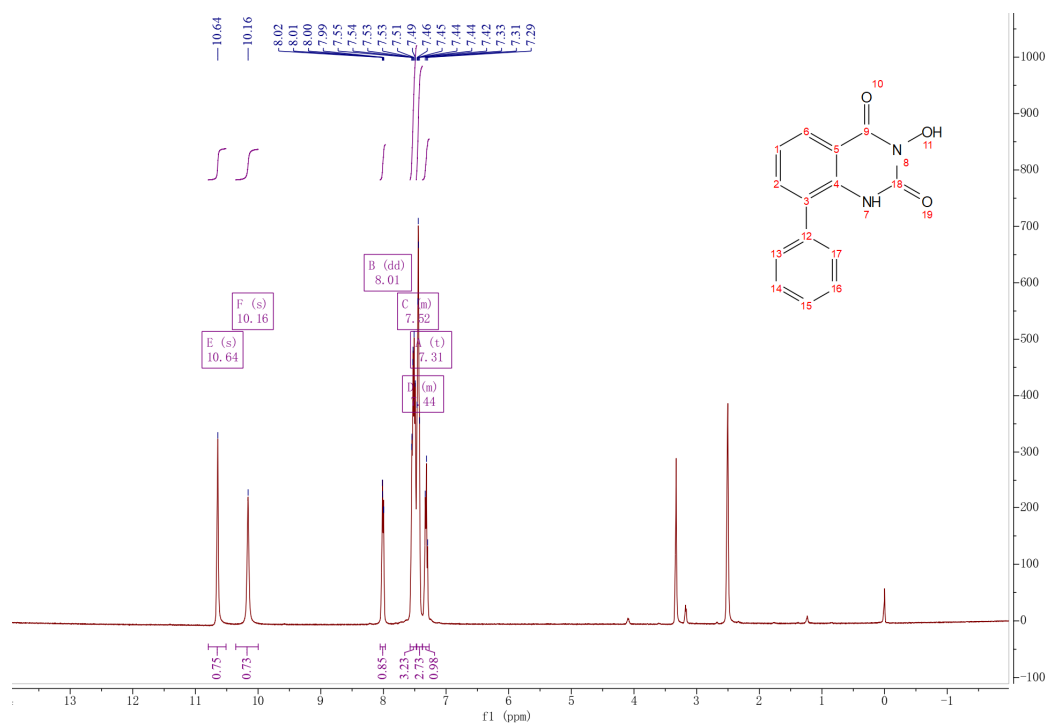
**Figure S135.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21t**



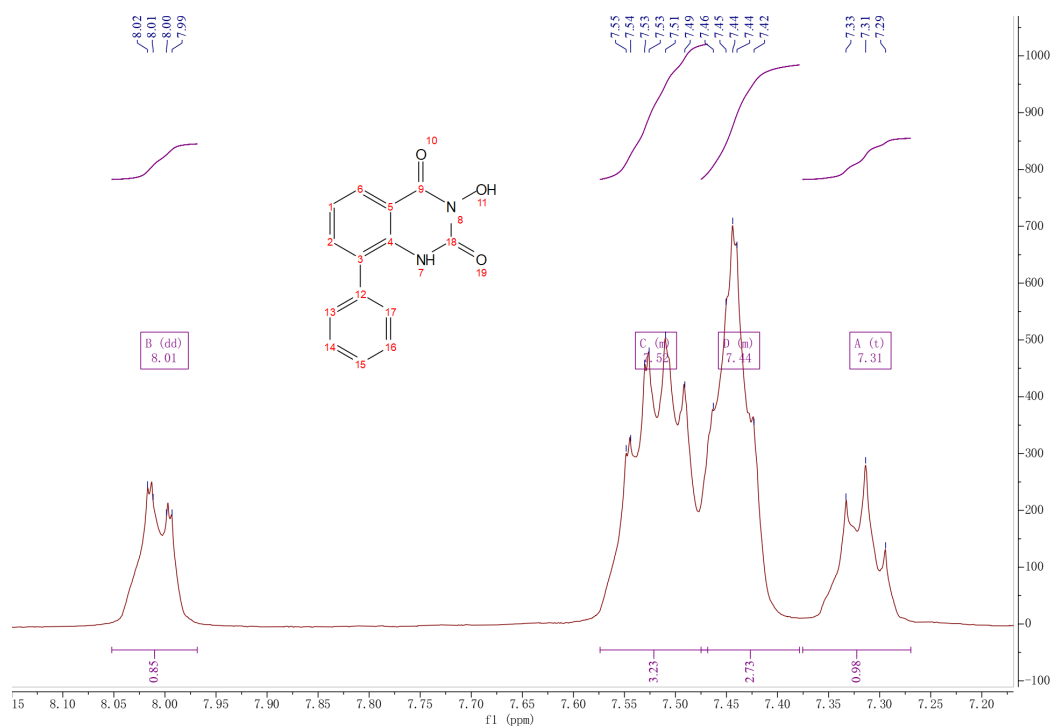
**Figure S136.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21t**



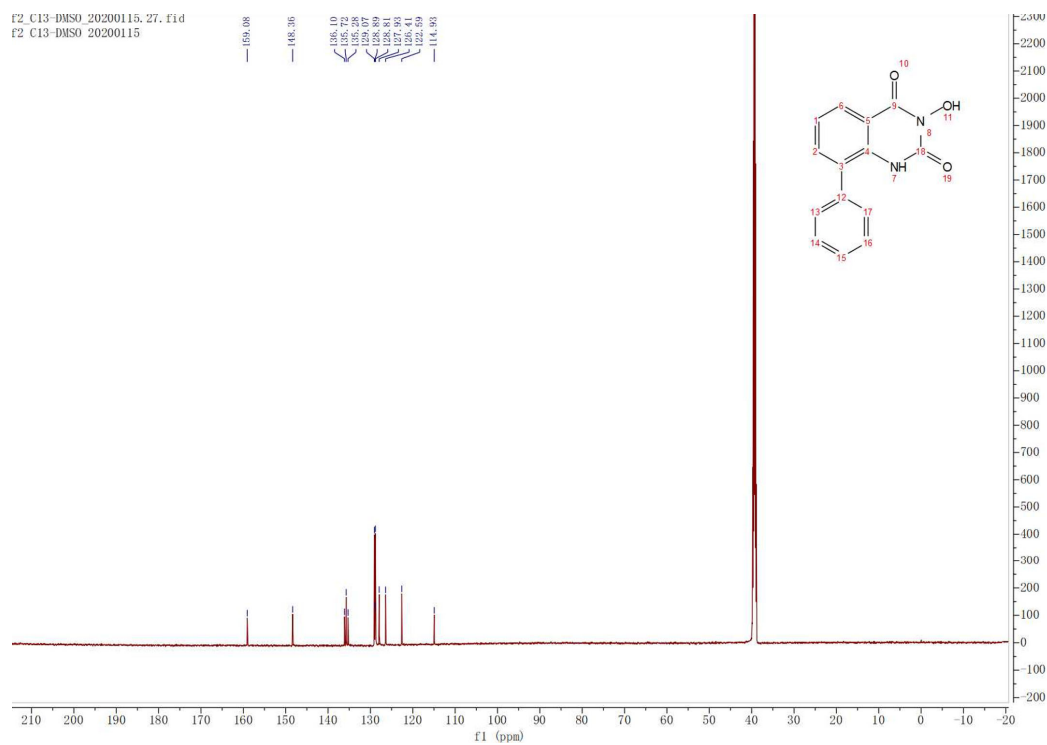
**Figure S137.** Mass spectrum (negative ionization) of **21t**



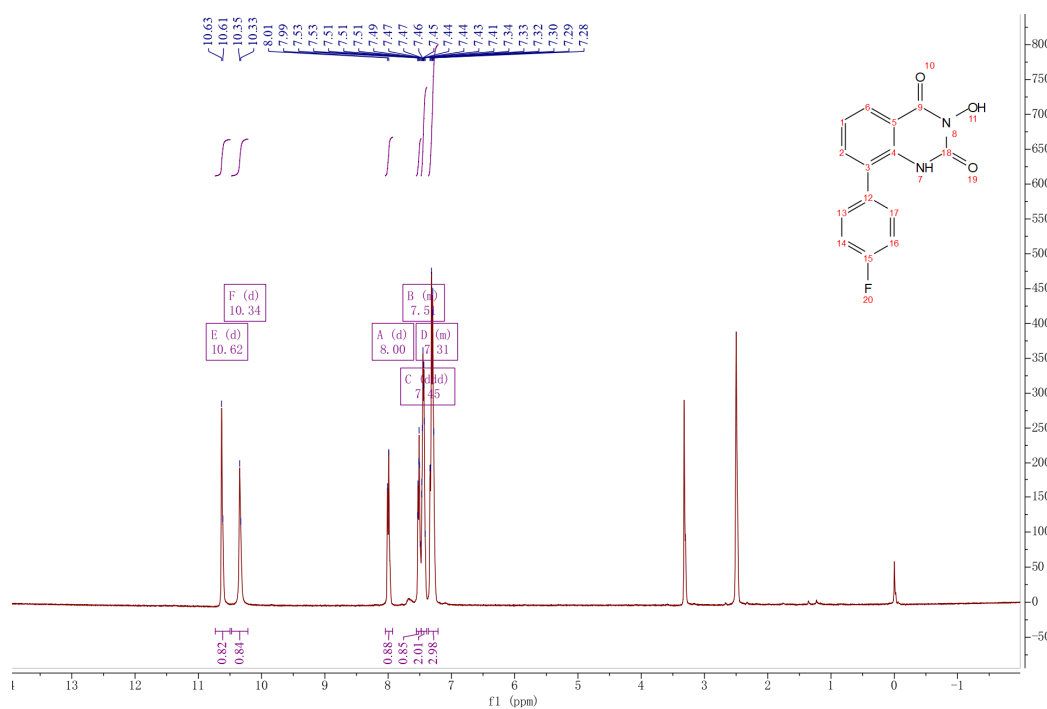
**Figure S138.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21u**



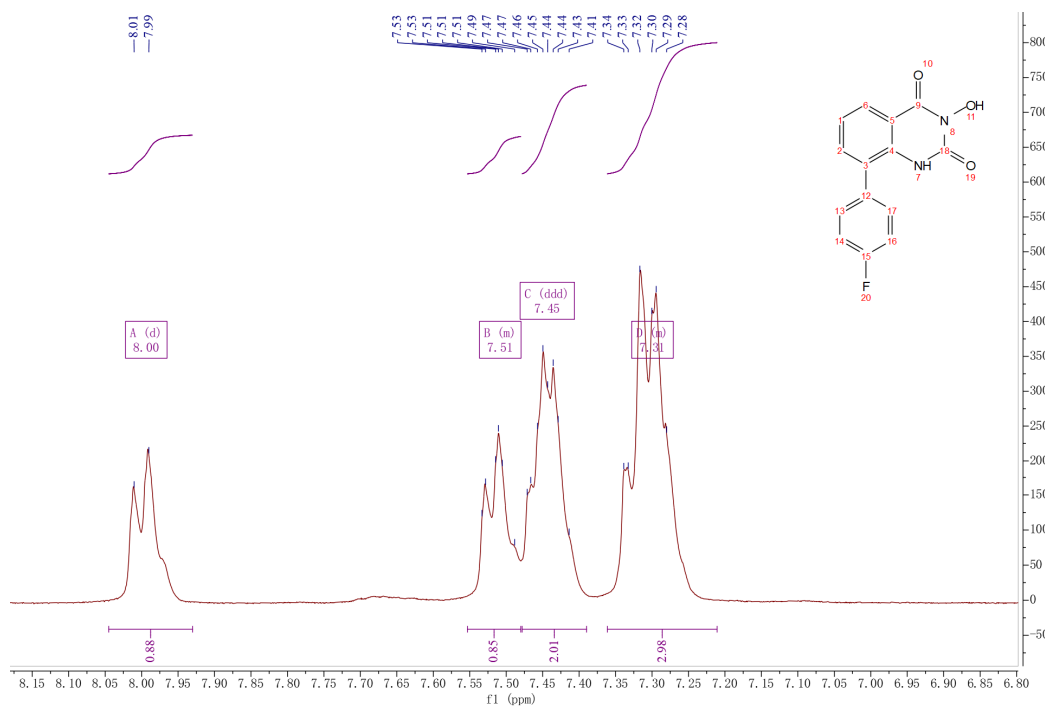
**Figure S139.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21u**



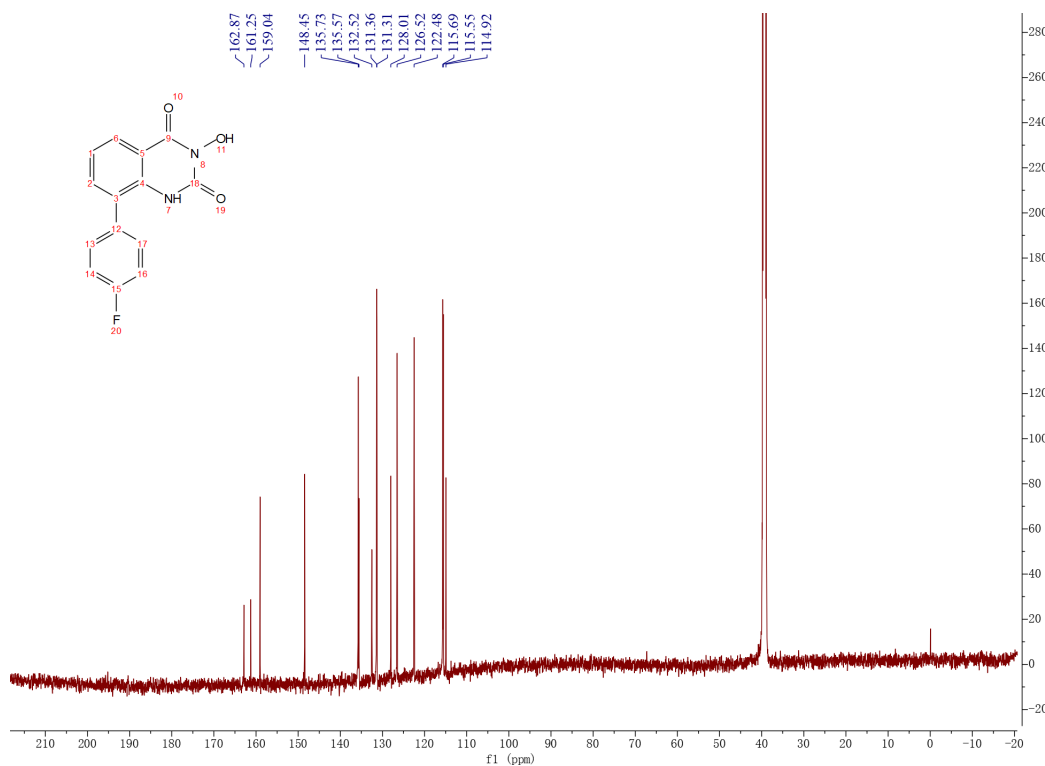
**Figure S140.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21u**



**Figure S141.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21v**

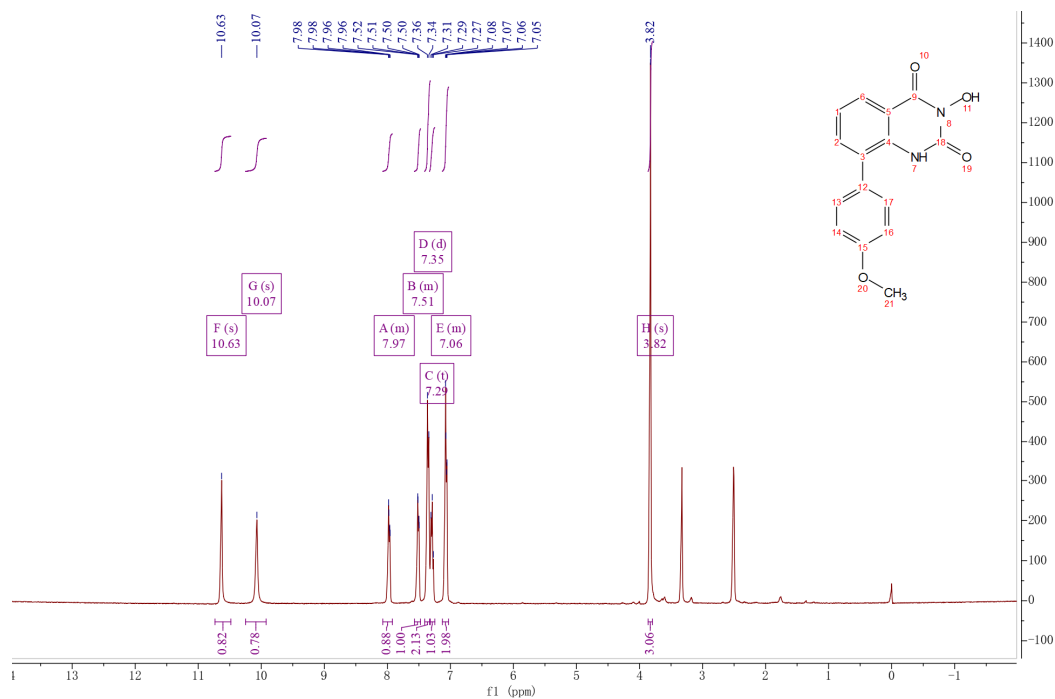


**Figure S142.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21v**

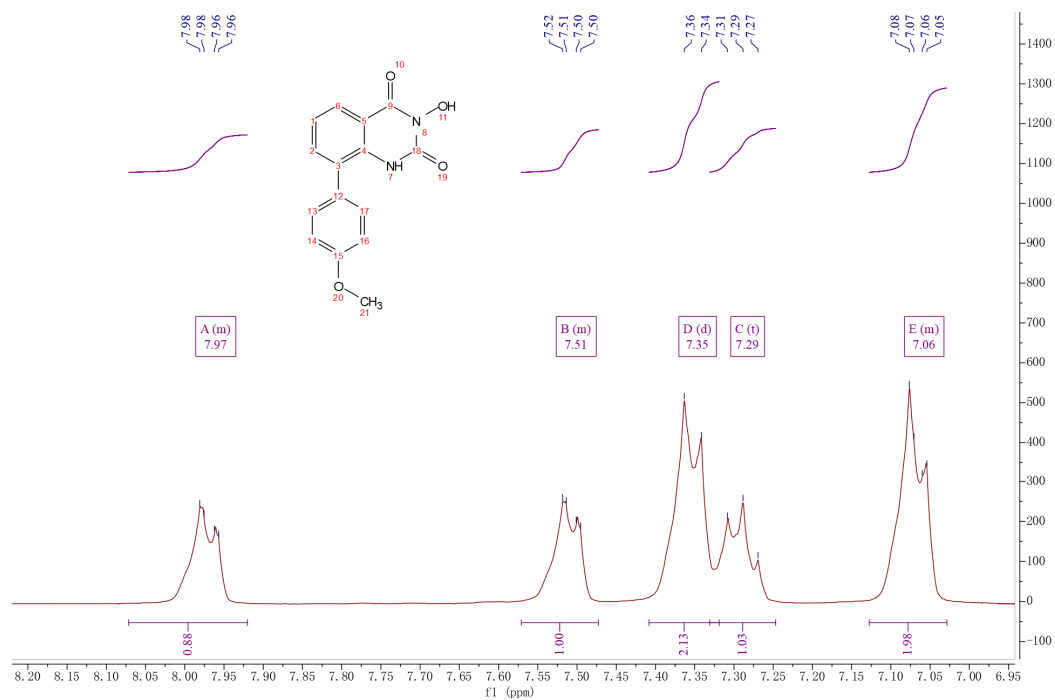


**Figure S143.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21v**

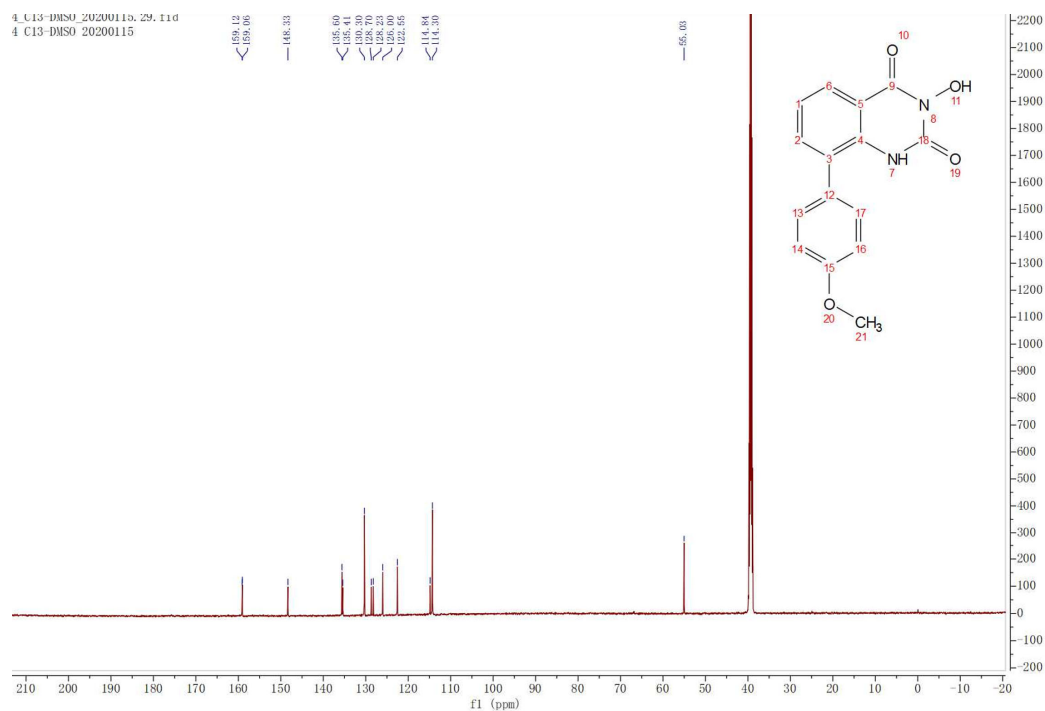




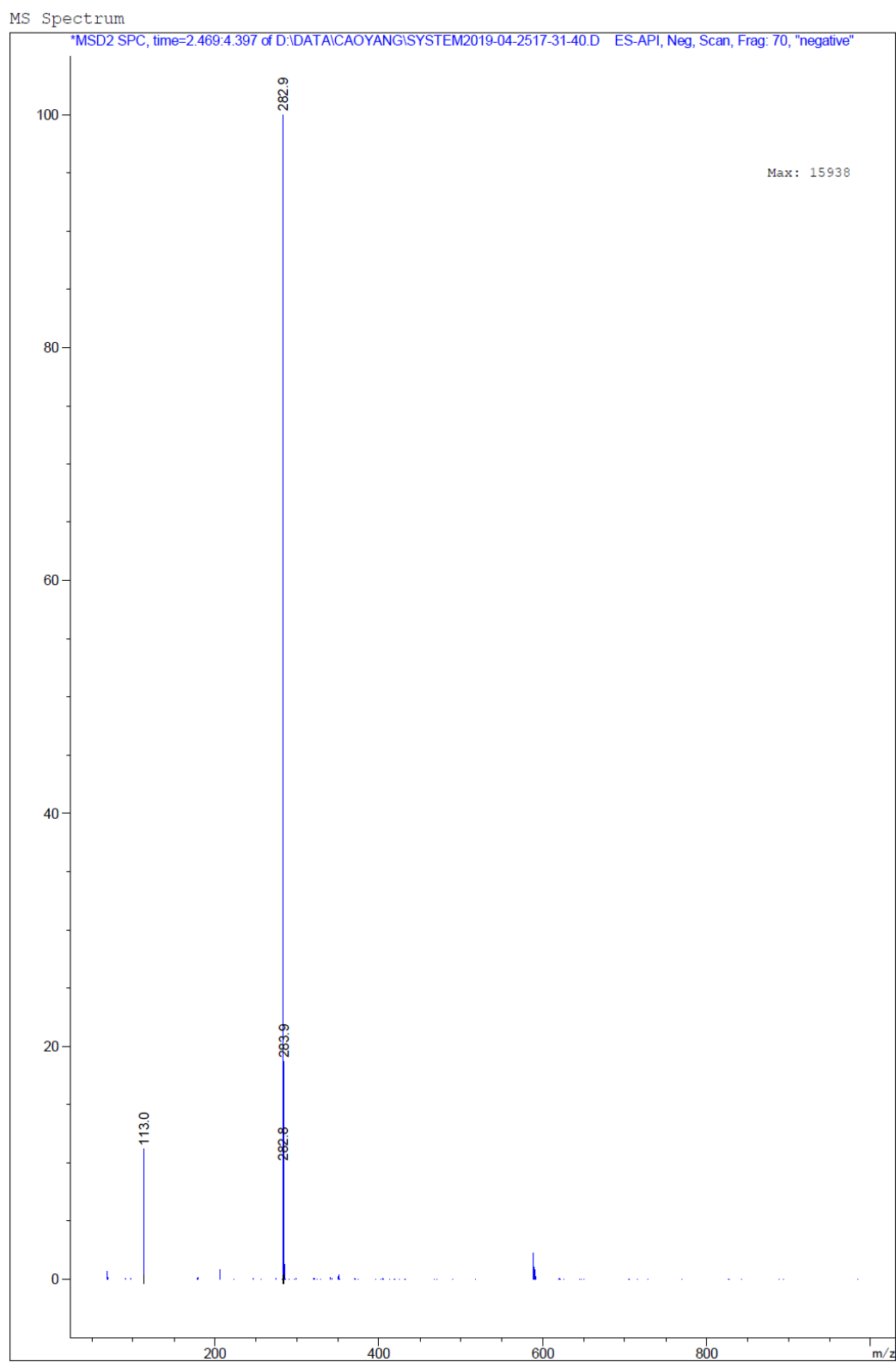
**Figure S144.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21w**



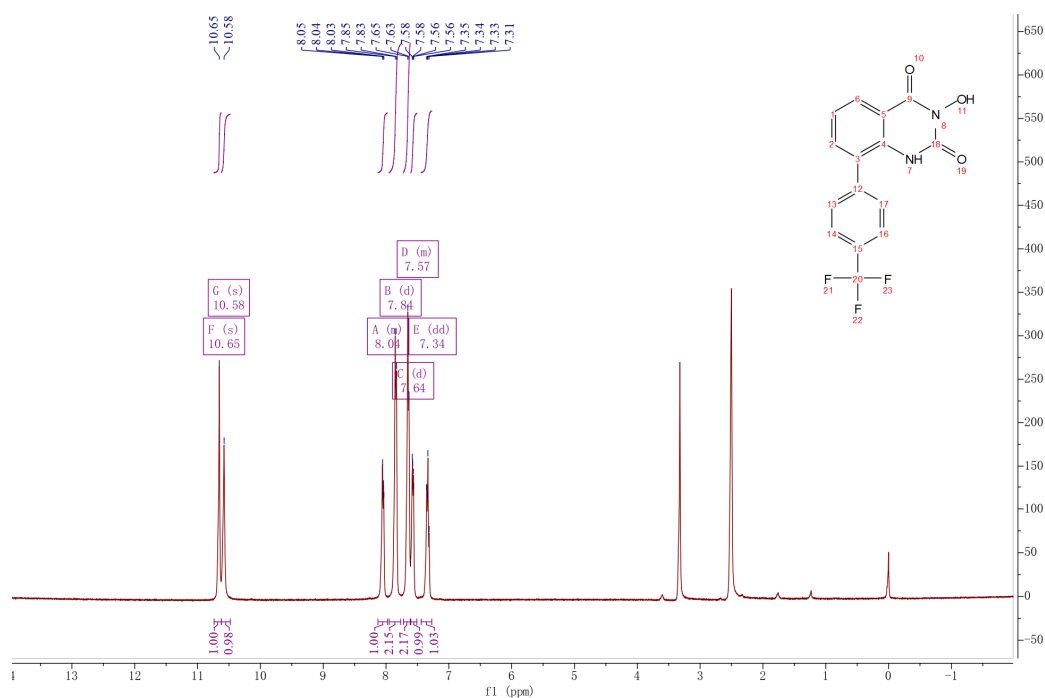
**Figure S145.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21w**



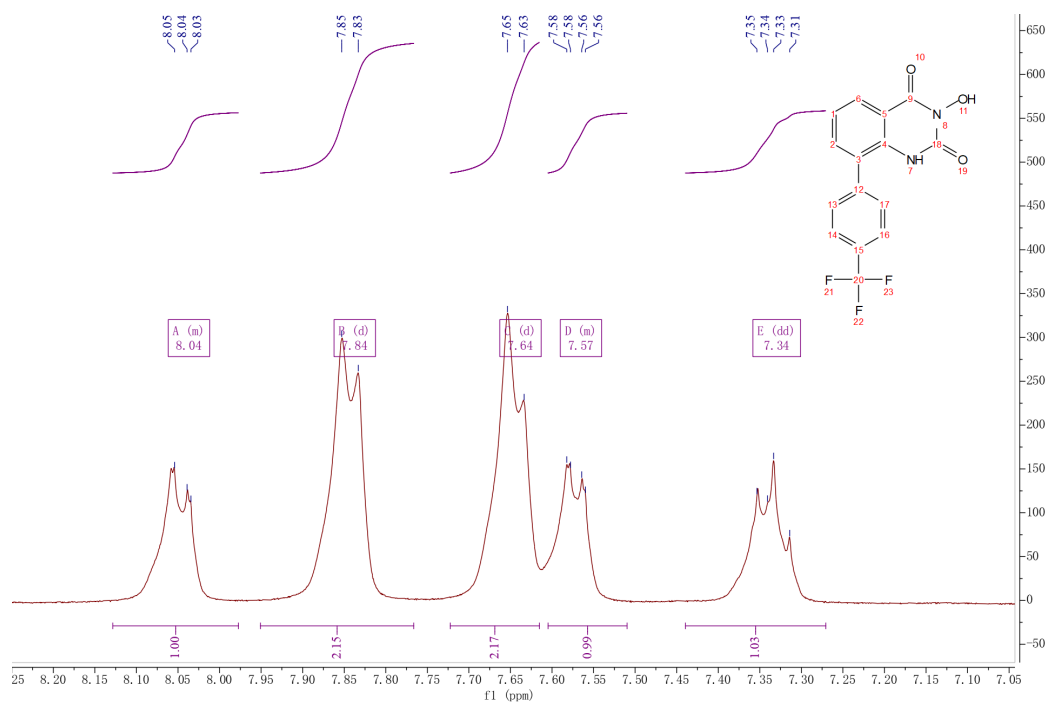
**Figure S146.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21w**



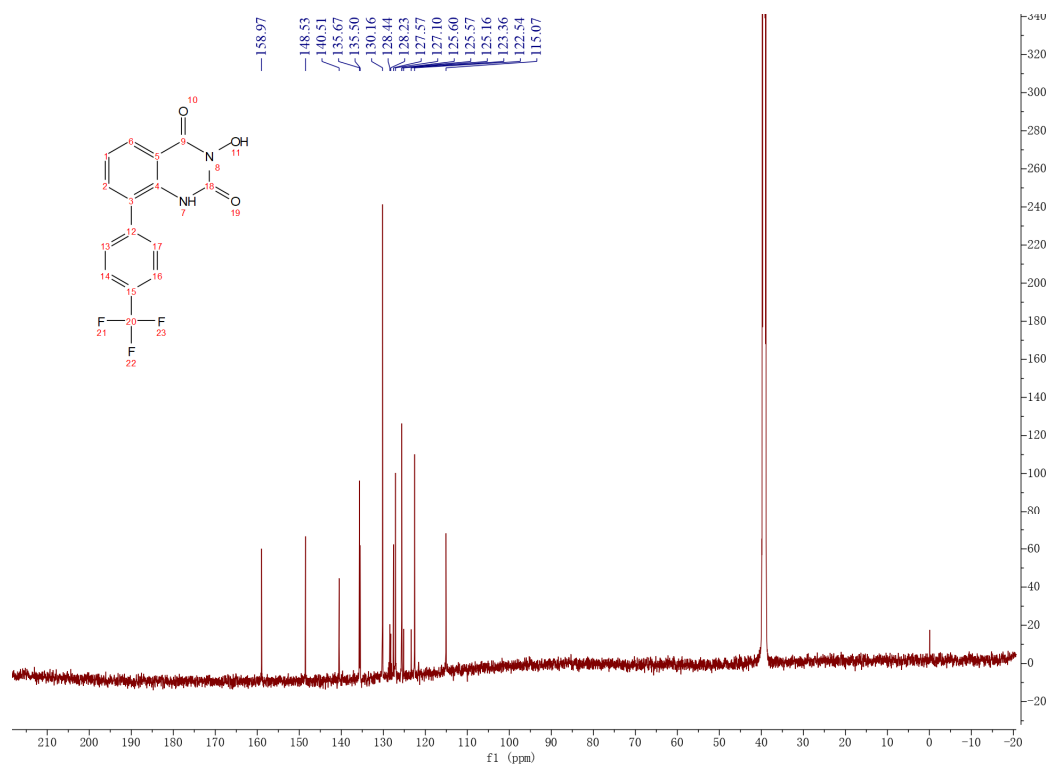
**Figure S147.** Mass spectrum (negative ionization) of **21w**



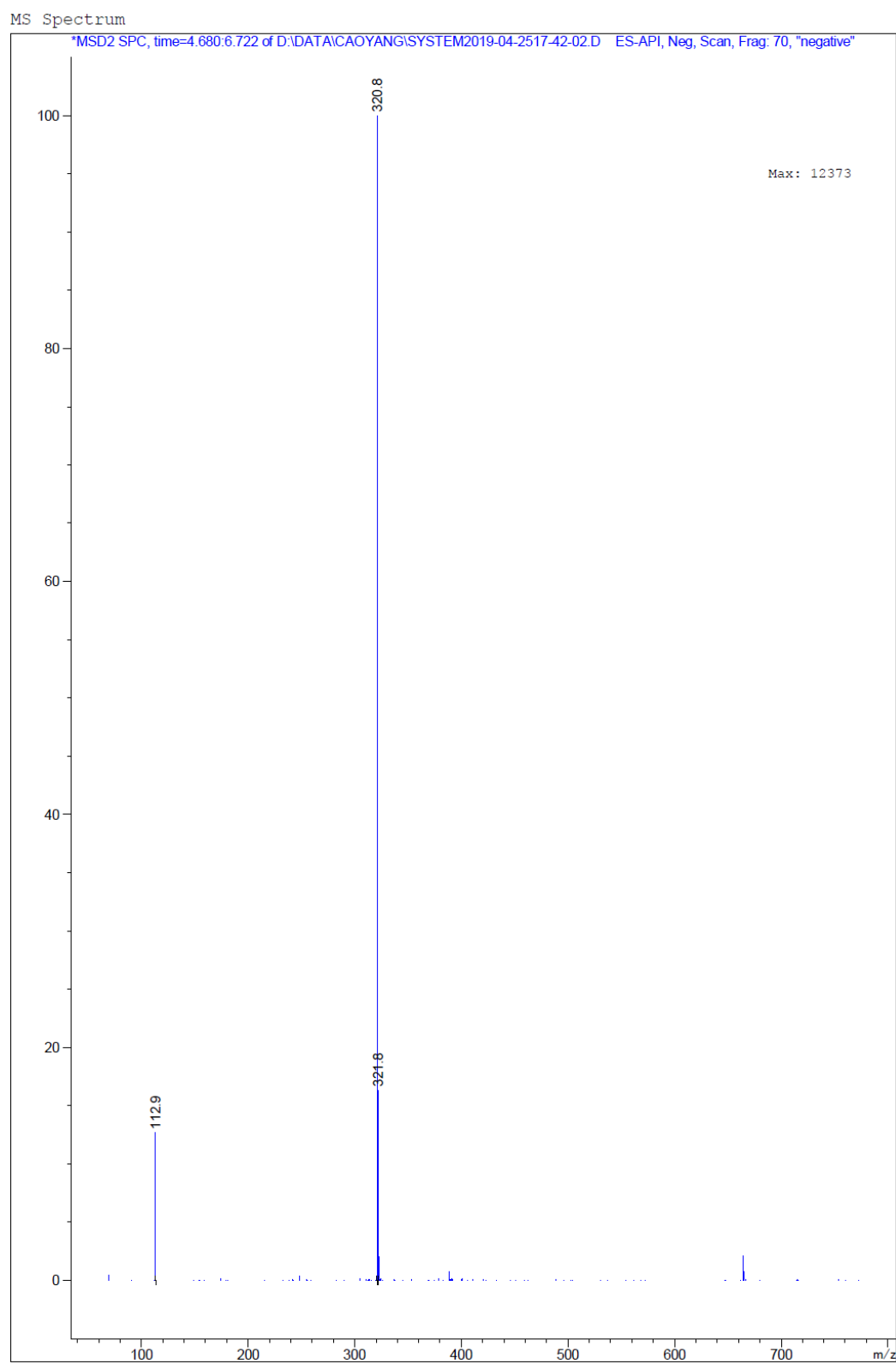
**Figure S148.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **21x**



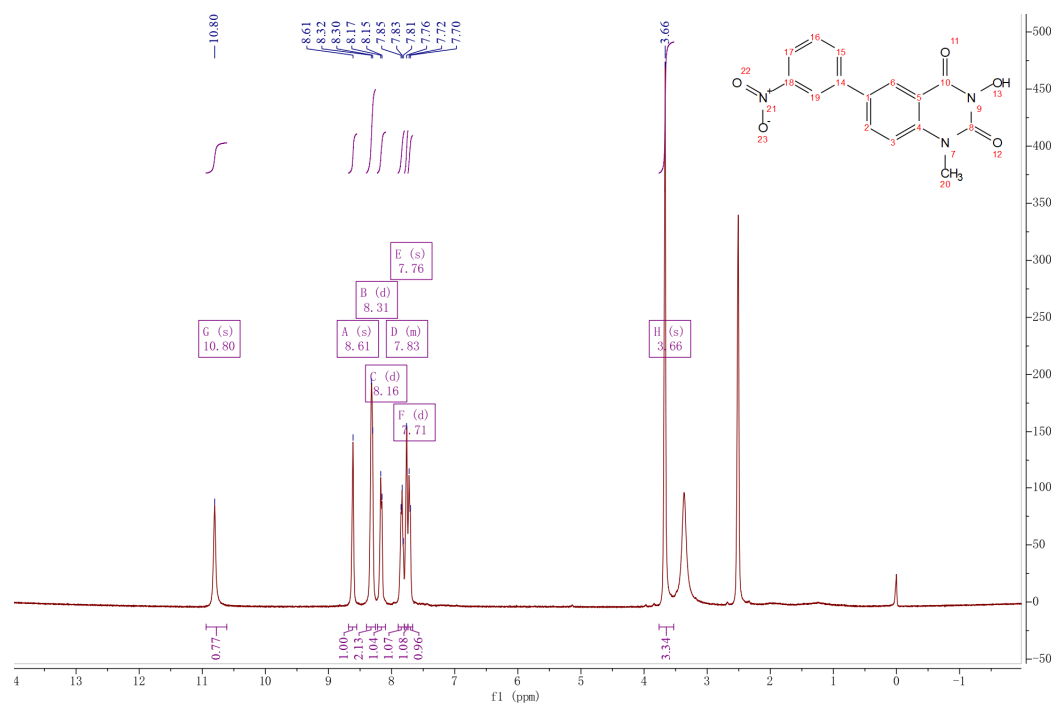
**Figure S149.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **21x**



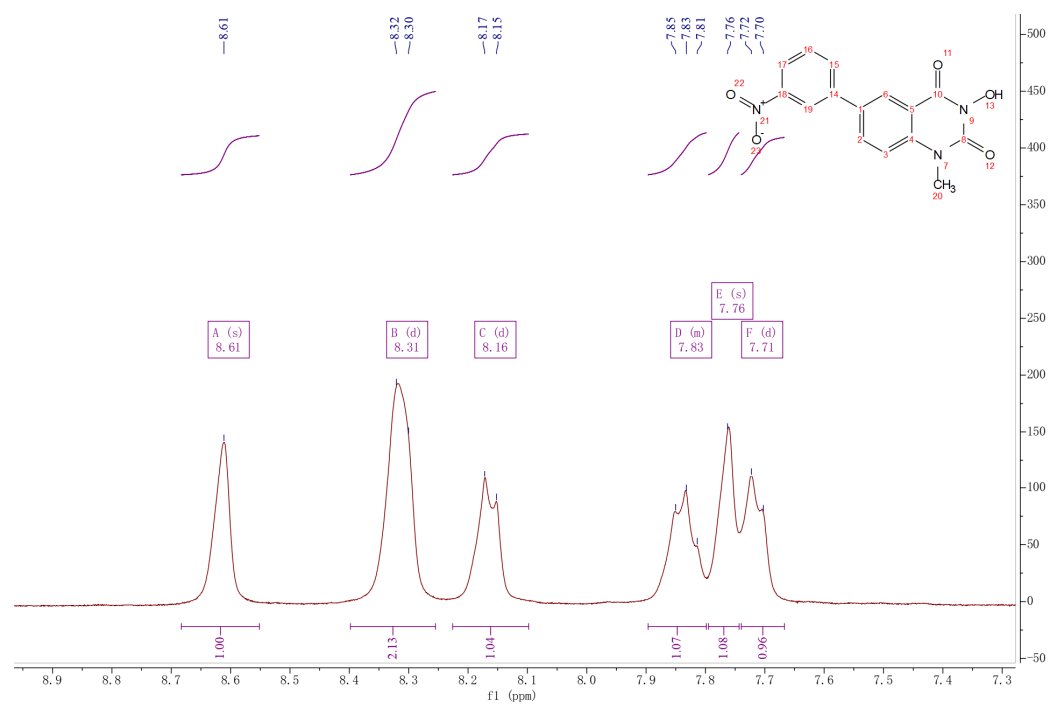
**Figure S150.**  $^{13}\text{C}$  NMR (151 MHz, DMSO- $d_6$ ) spectrum of **21x**



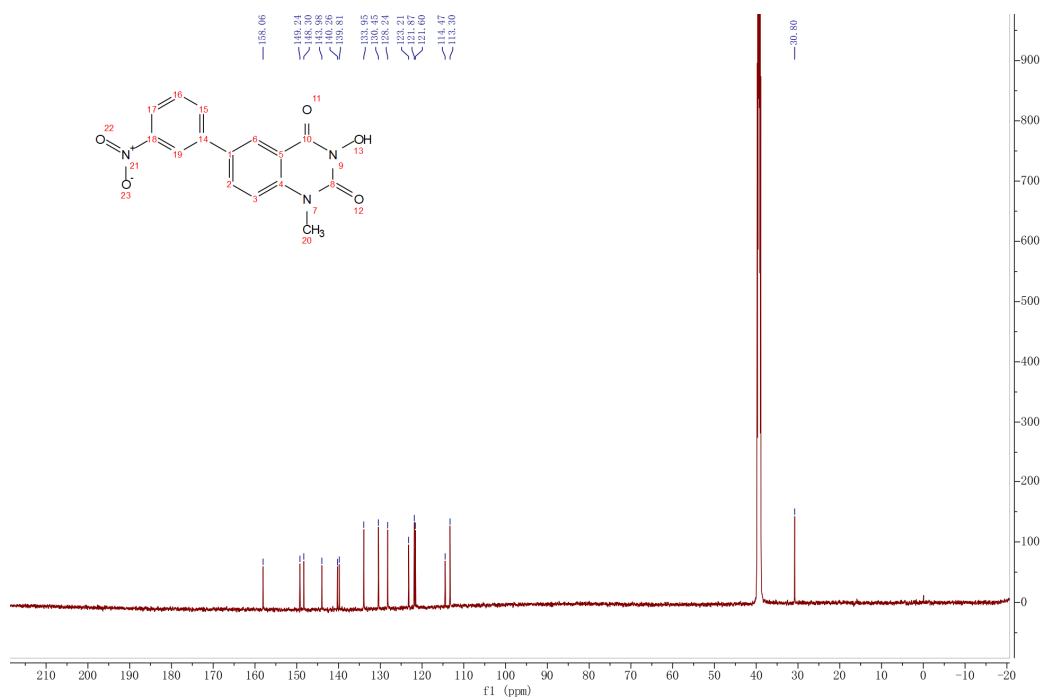
**Figure S151.** Mass spectrum (negative ionization) of **21x**



**Figure S152.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **23a**

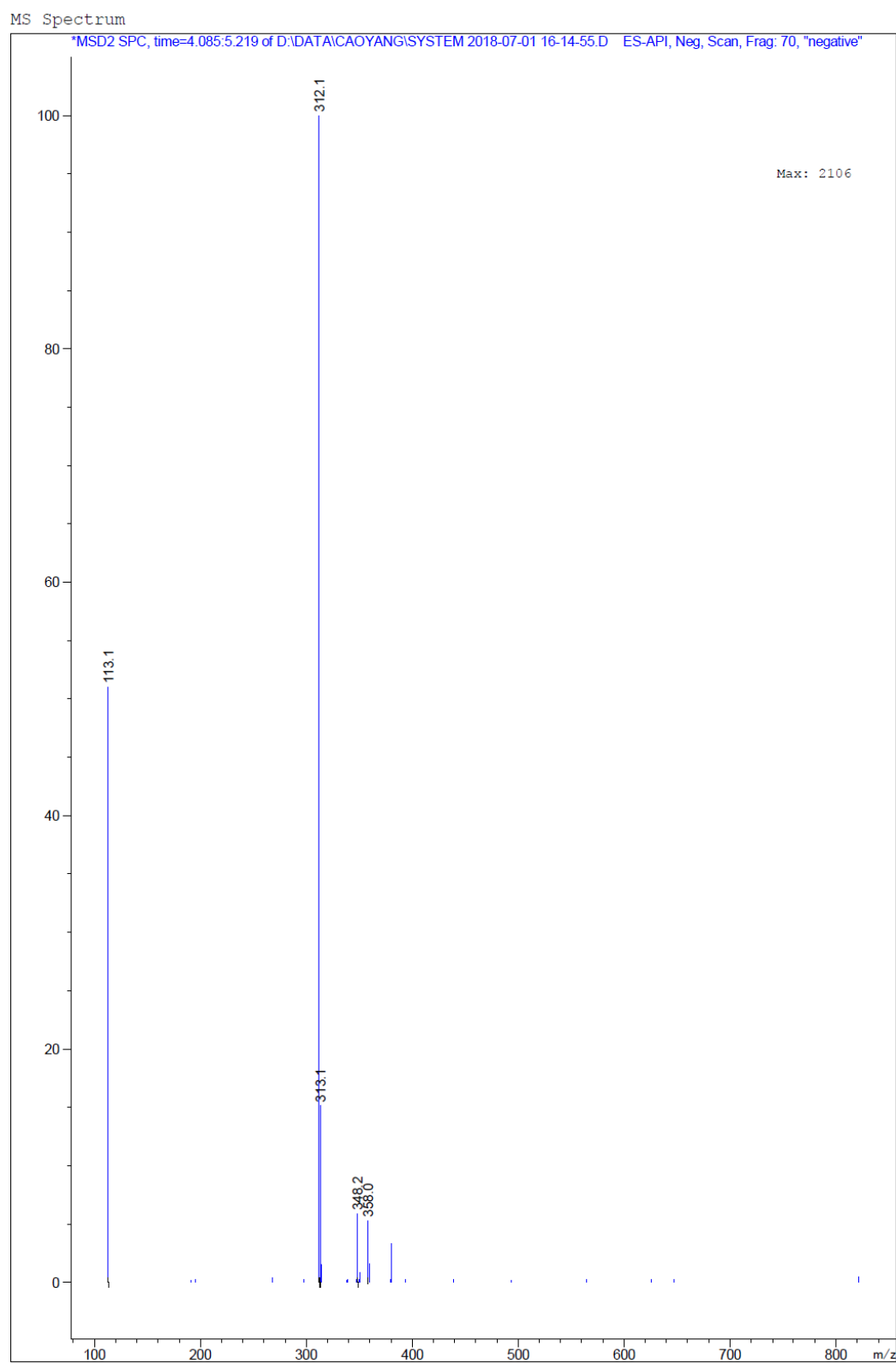


**Figure S153.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **23a**

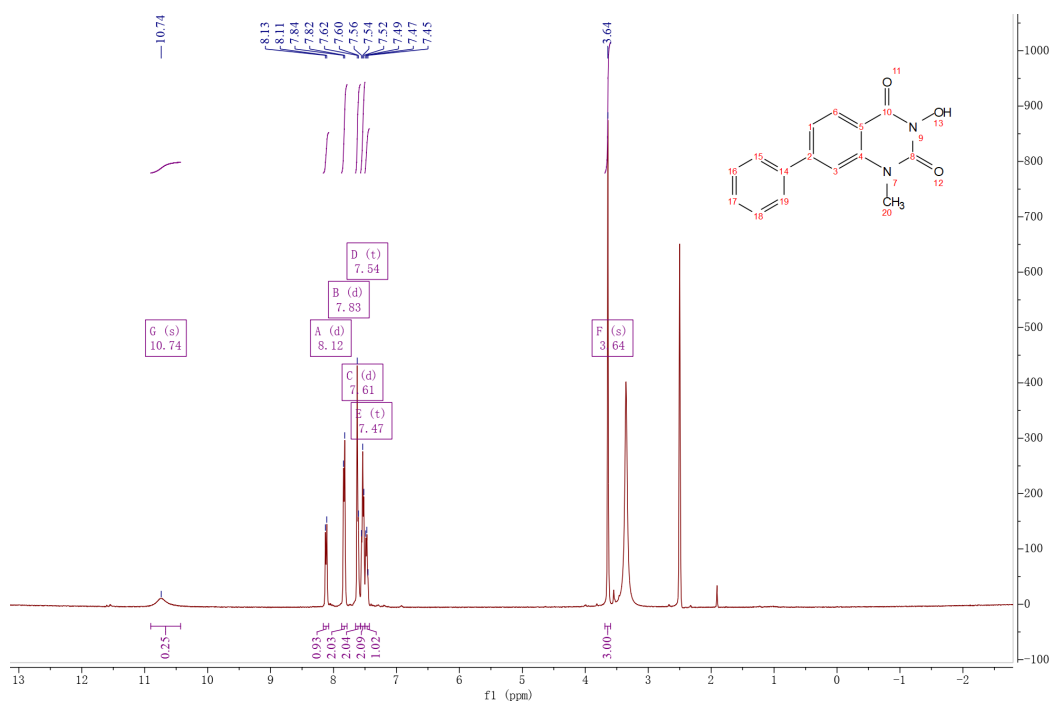


**Figure S154.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO-}d_6$ ) spectrum of **23a**

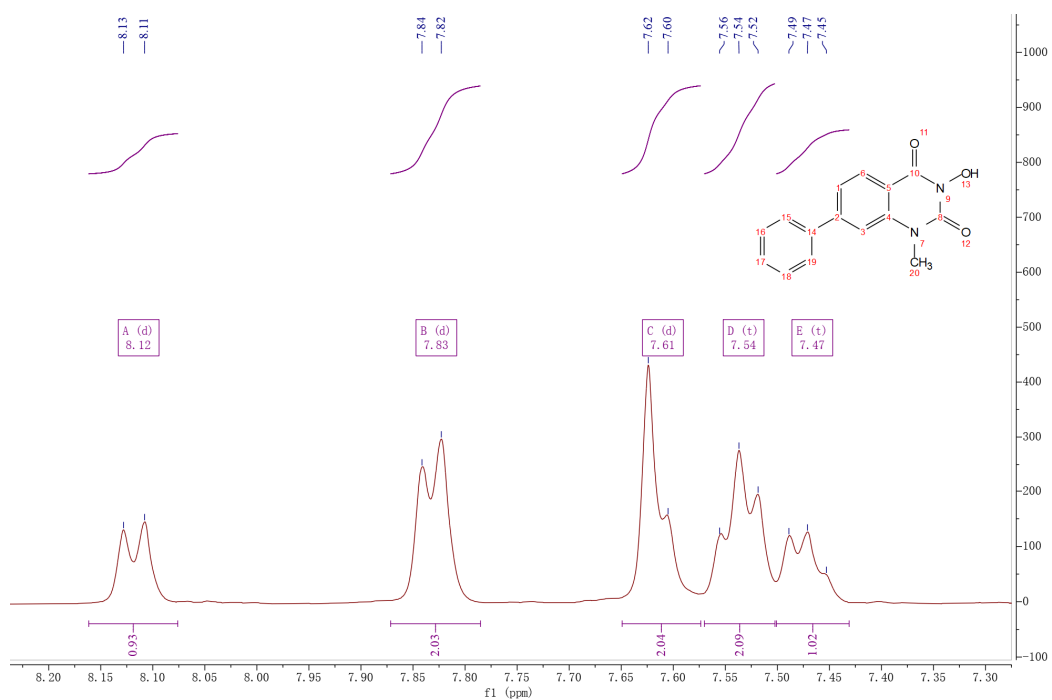




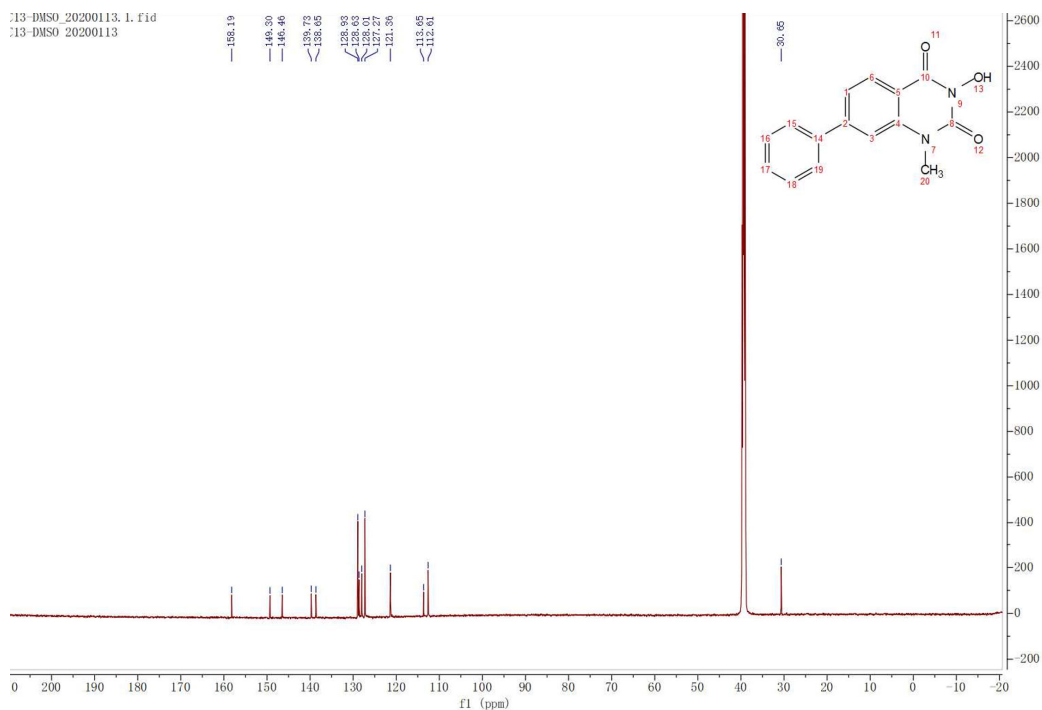
**Figure S155.** Mass spectrum (negative ionization) of **23a**



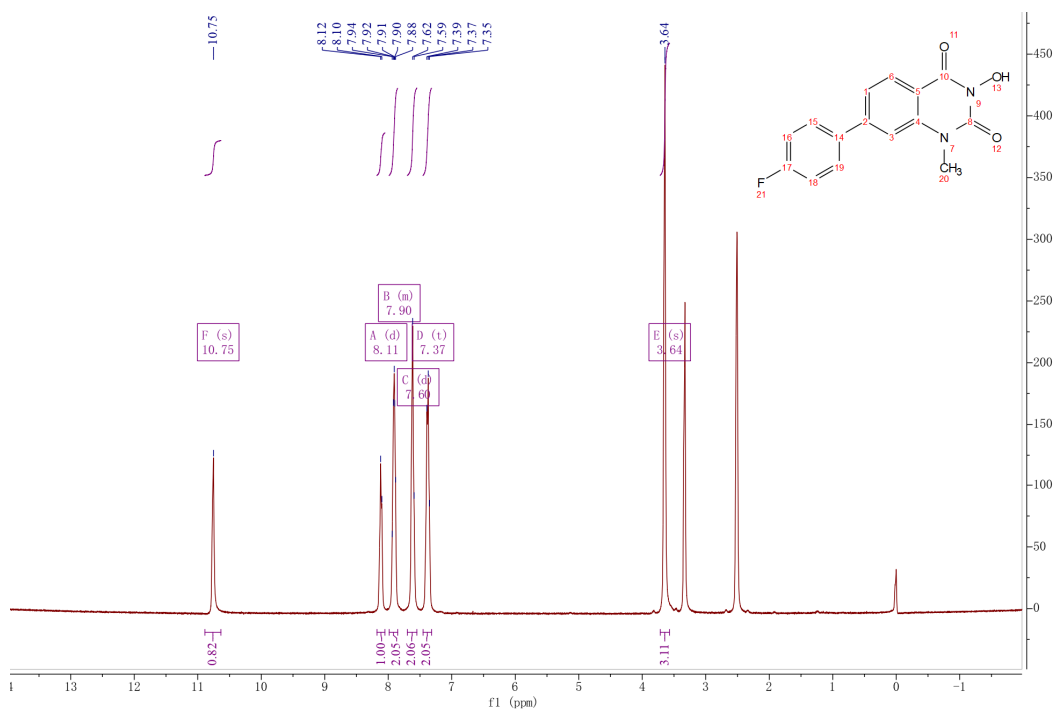
**Figure S156.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **23b**



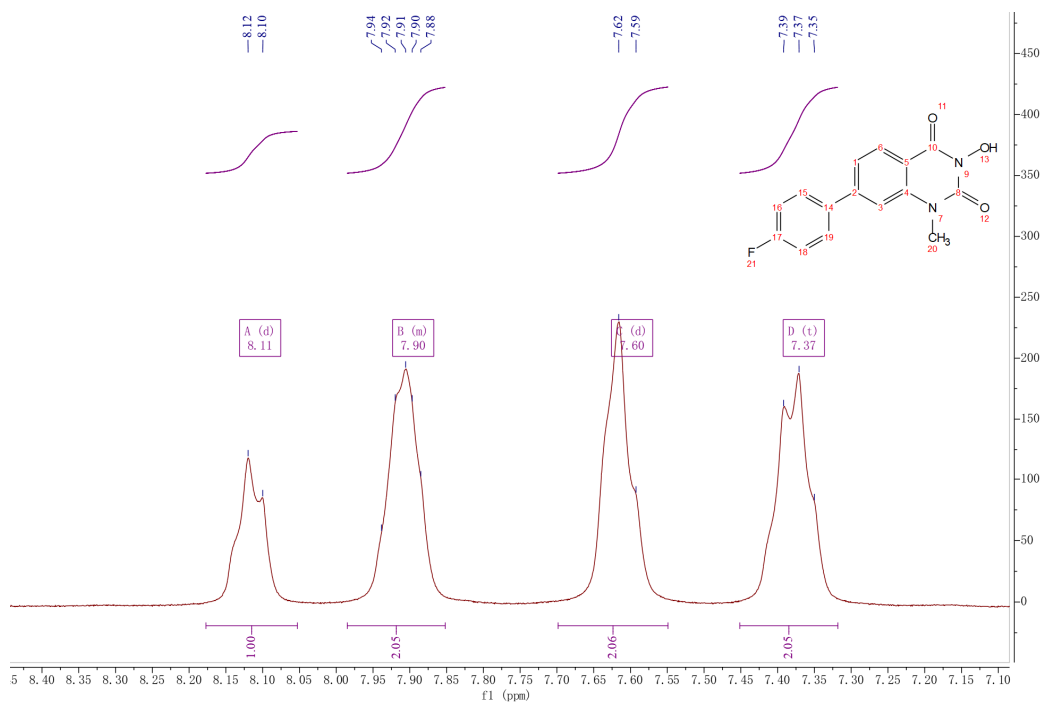
**Figure S157.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **23b**



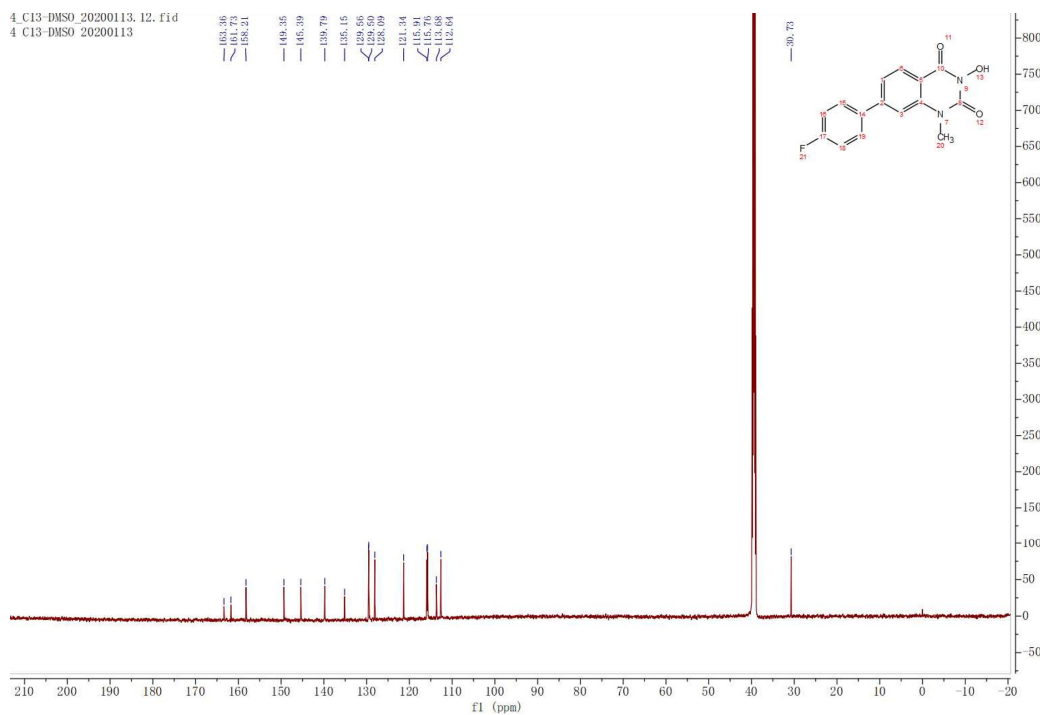
**Figure S158.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **23b**



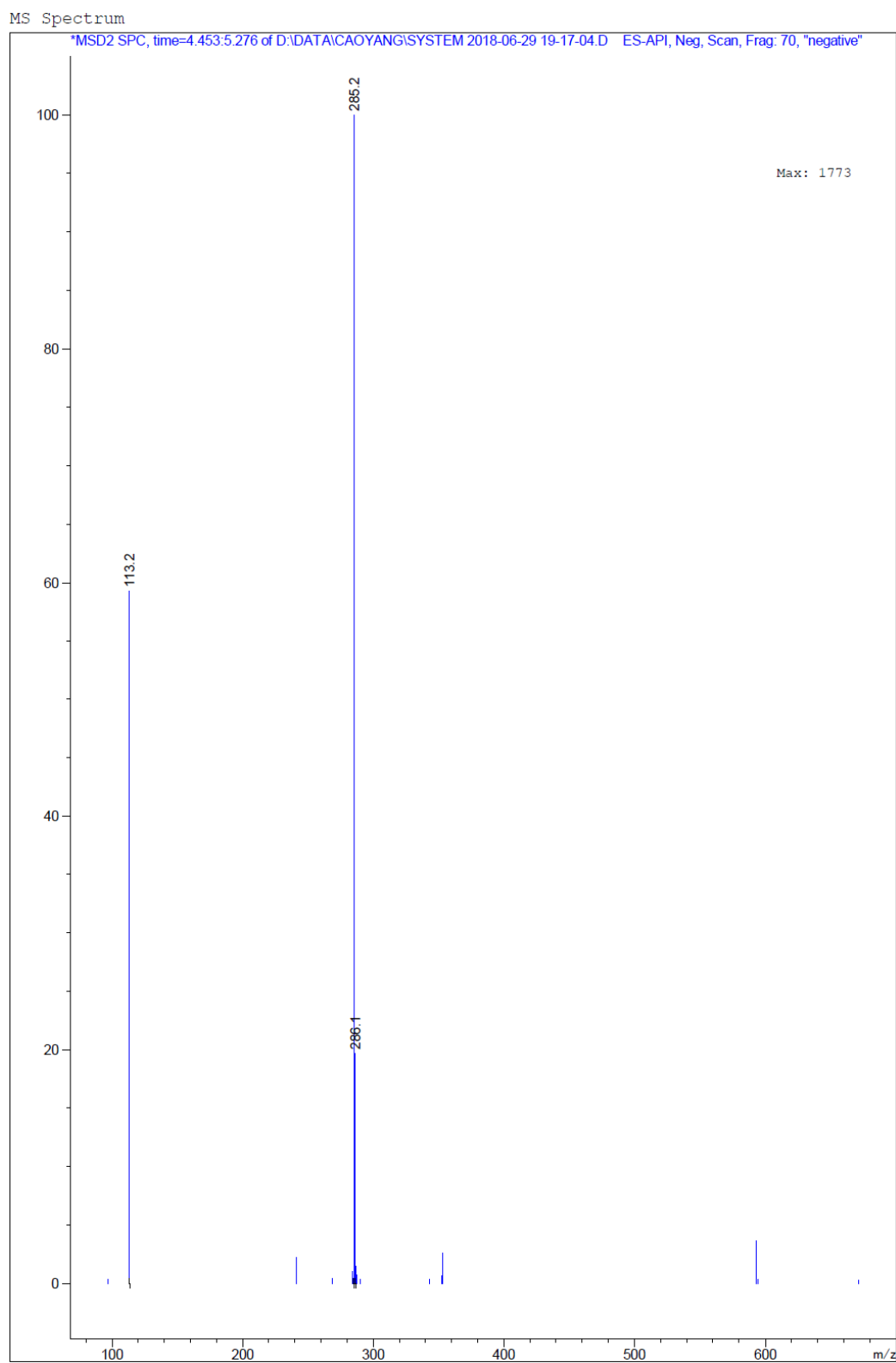
**Figure S159.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **23c**



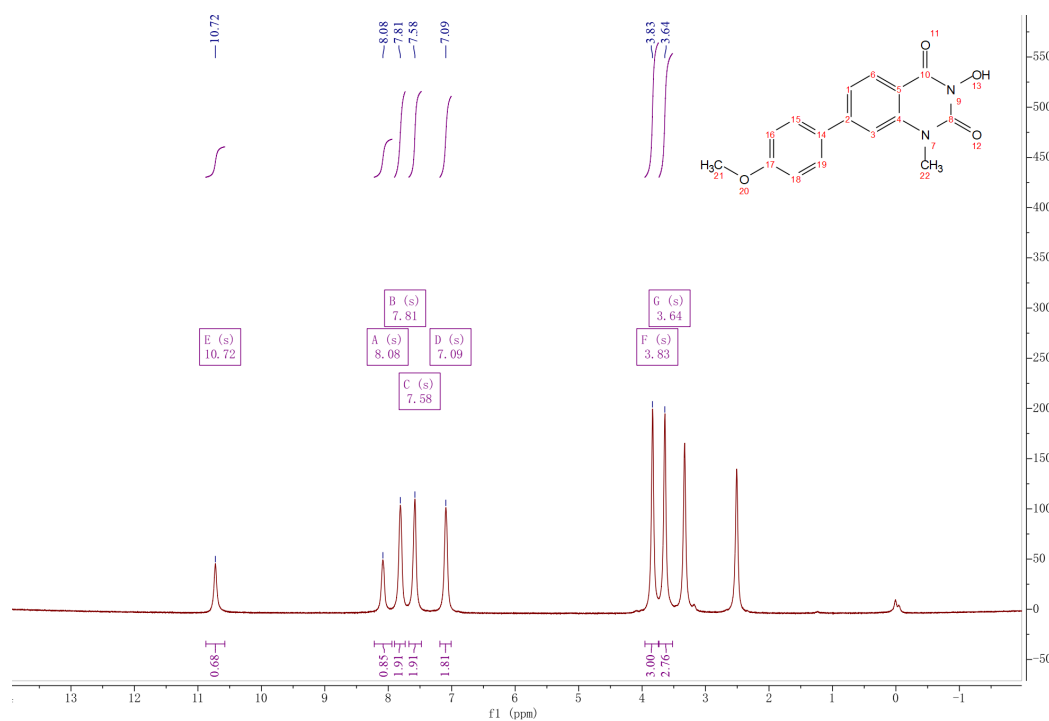
**Figure S160.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **23c**



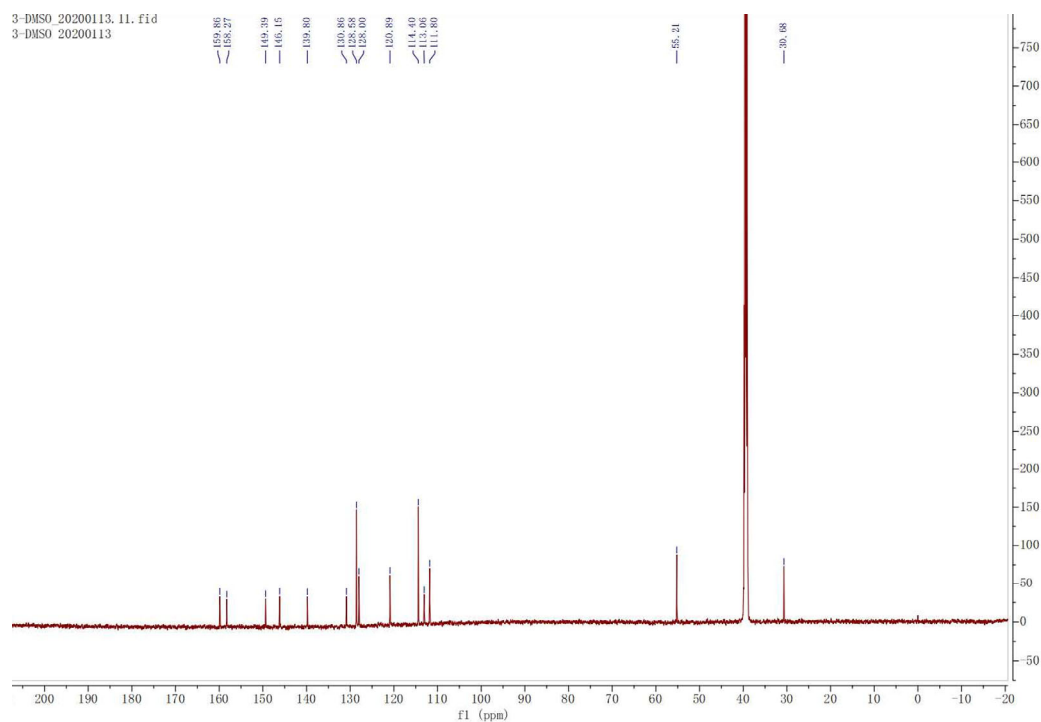
**Figure S161.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **23c**



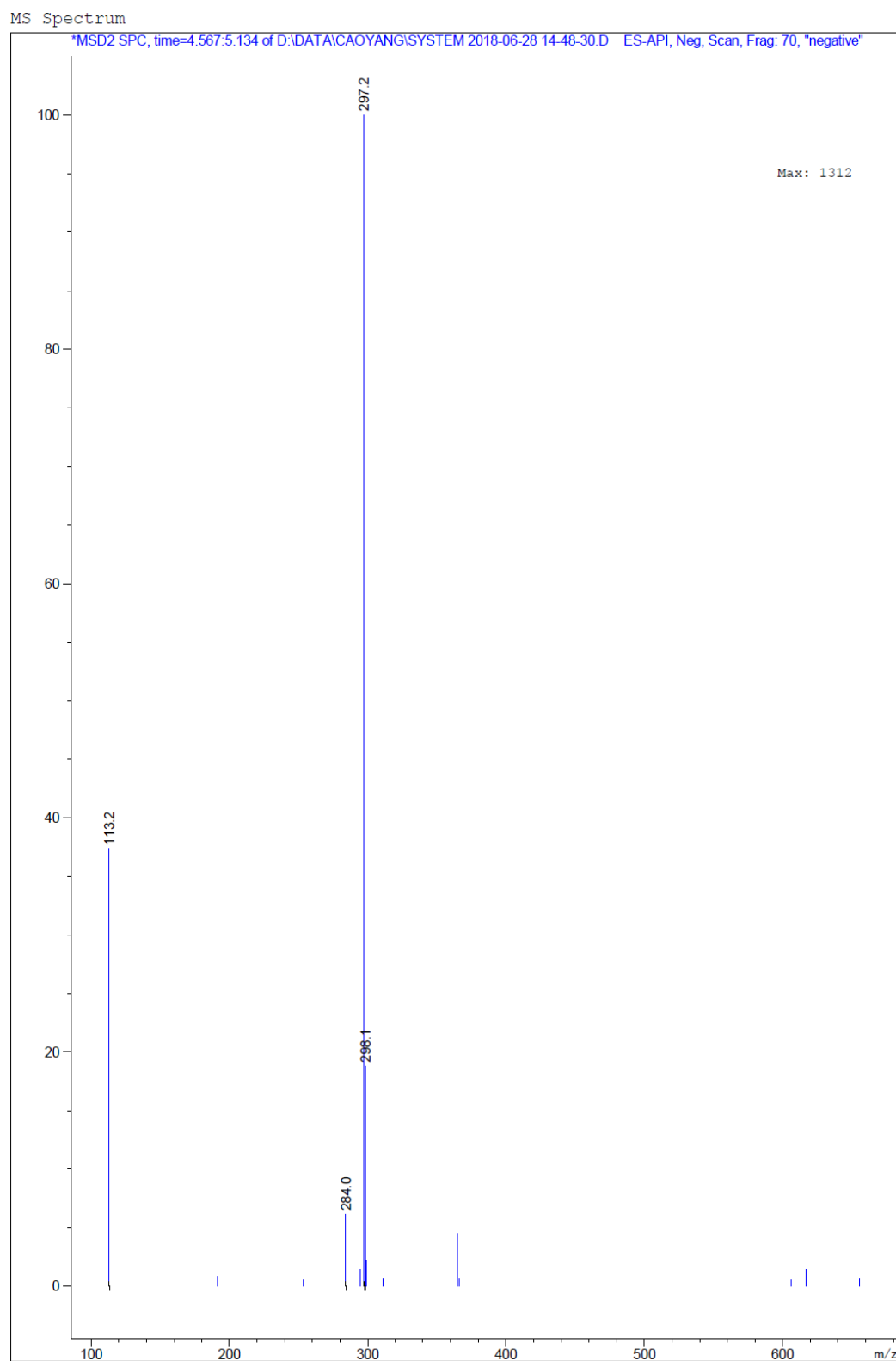
**Figure S162.** Mass spectrum (negative ionization) of **23c**



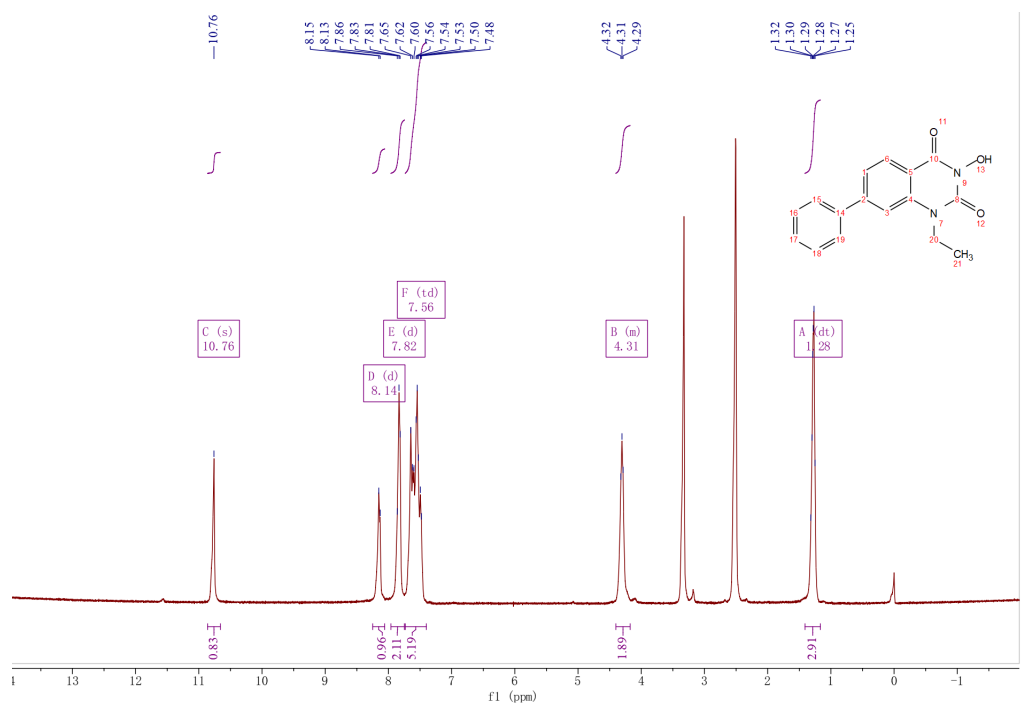
**Figure S163.** <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of **23d**



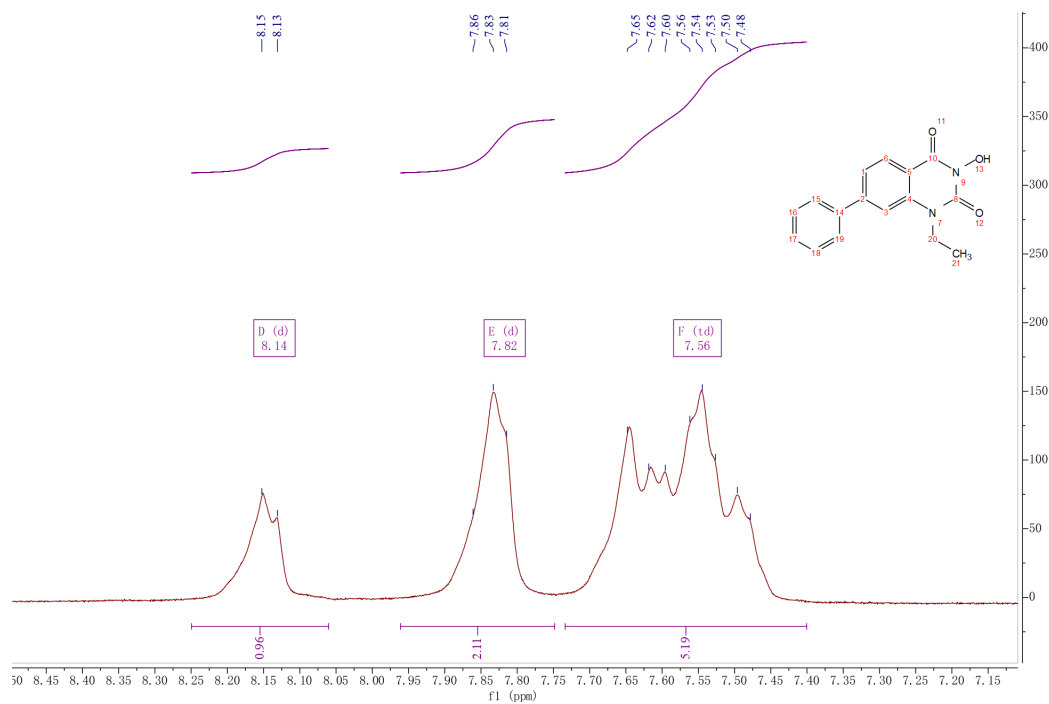
**Figure S164.** <sup>13</sup>C NMR (151 MHz, DMSO-*d*<sub>6</sub>) spectrum of **23d**



**Figure S165.** Mass spectrum (negative ionization) of **23d**

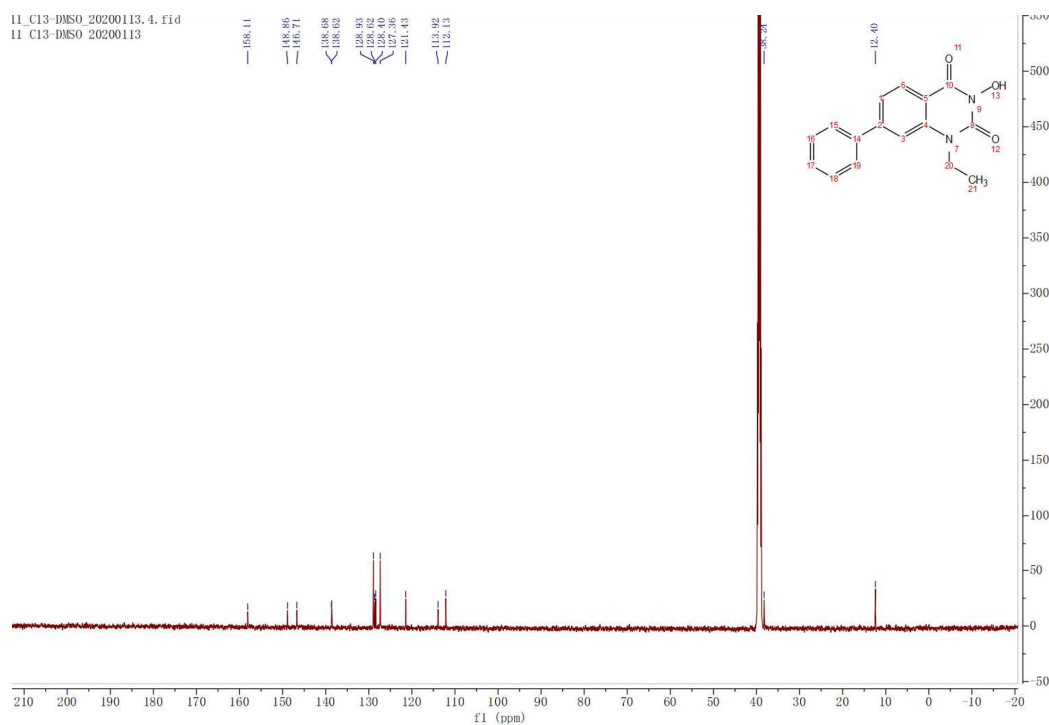


**Figure S166.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **23e**

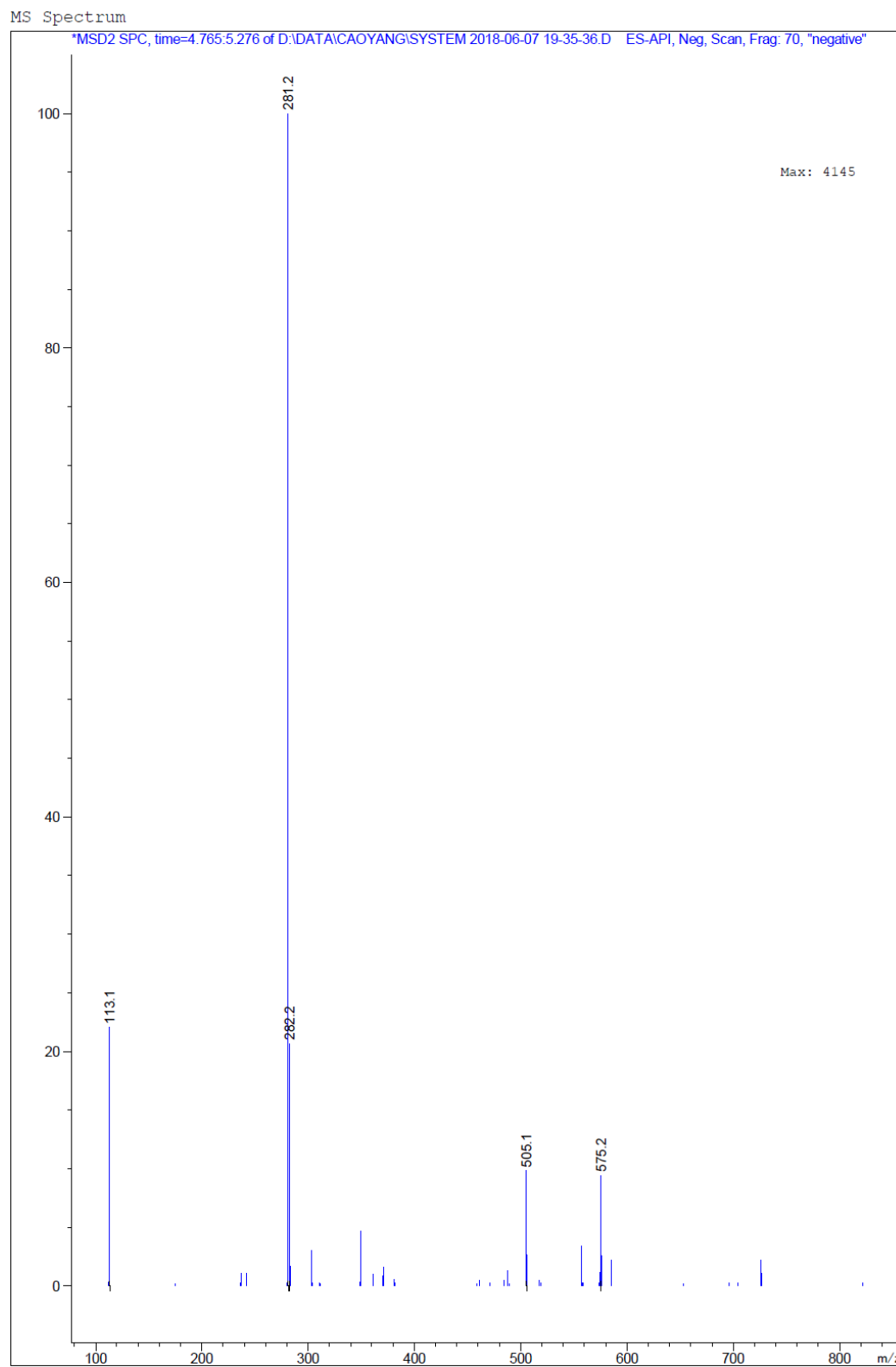


**Figure S167.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **23e**

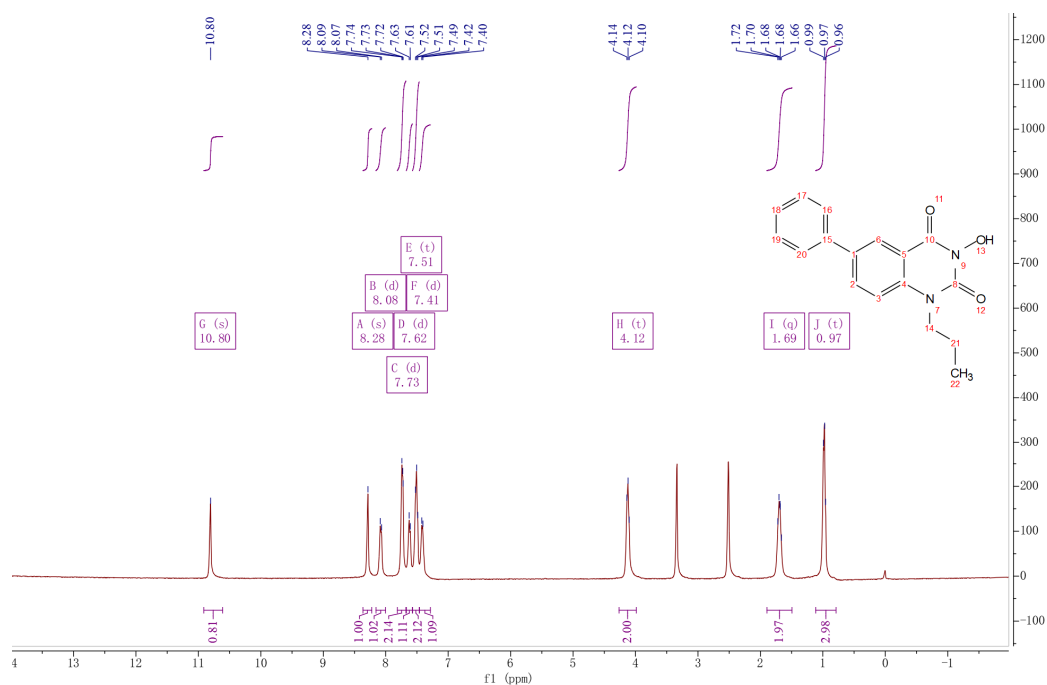




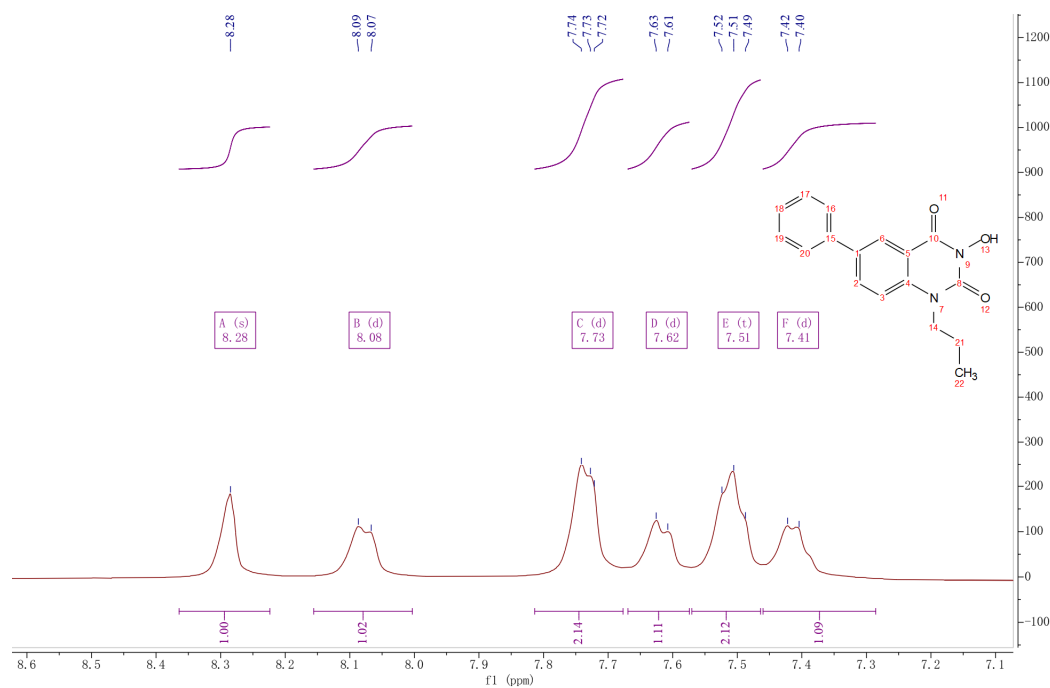
**Figure S168.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO-}d_6$ ) spectrum of **23e**



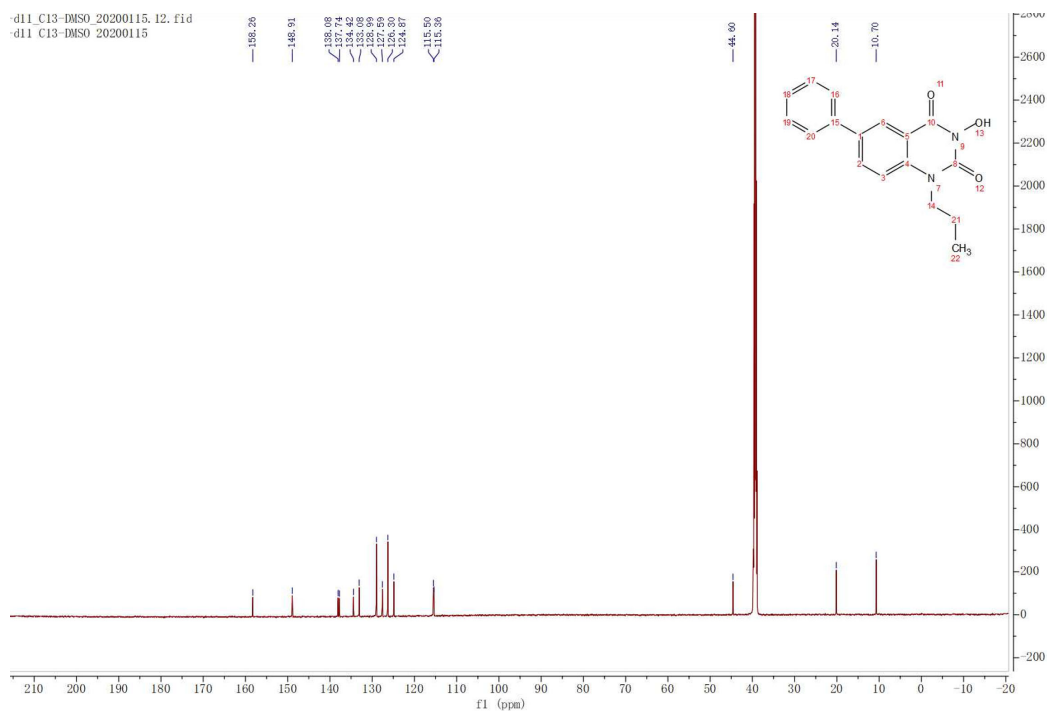
**Figure S169.** Mass spectrum (negative ionization) of **23e**



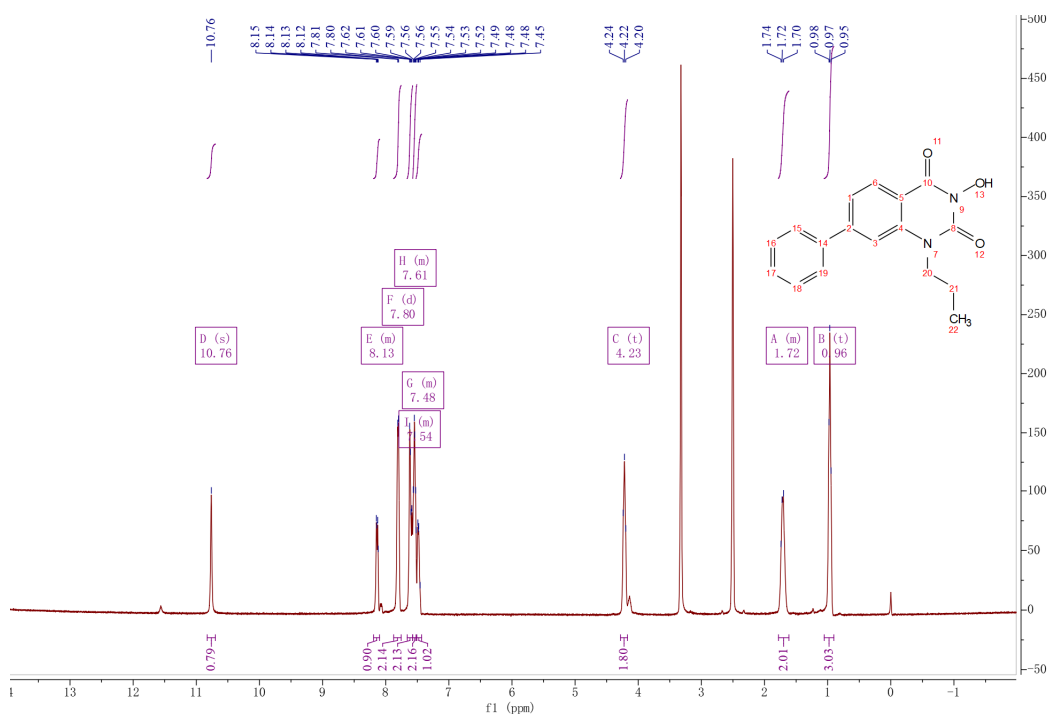
**Figure S170.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **23f**



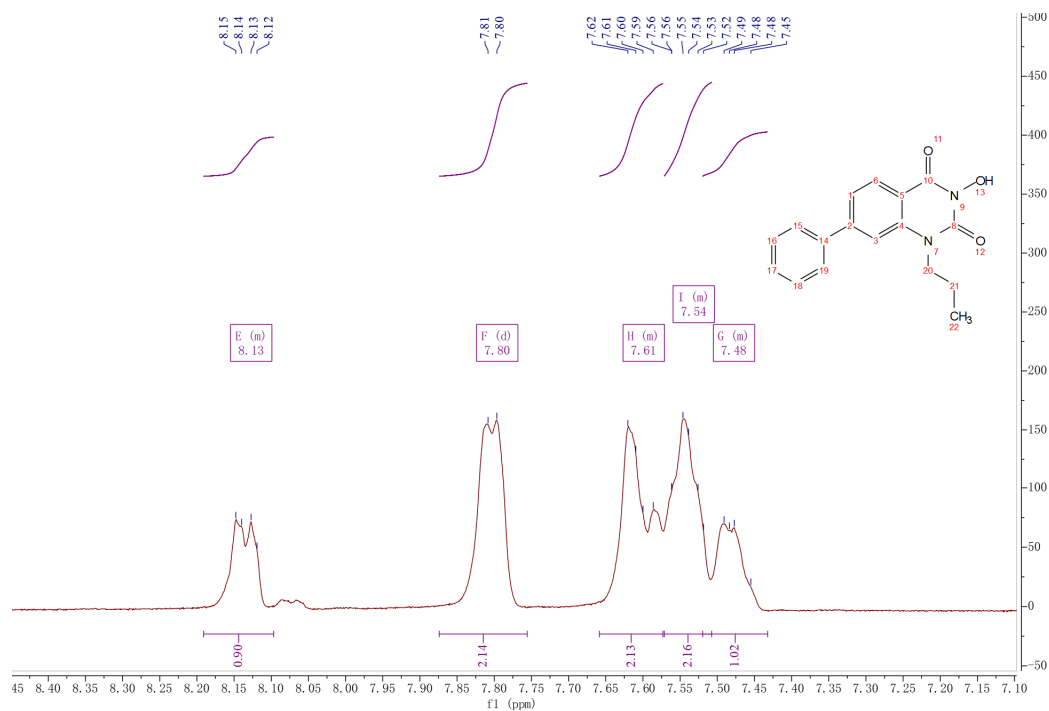
**Figure S171.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **23f**



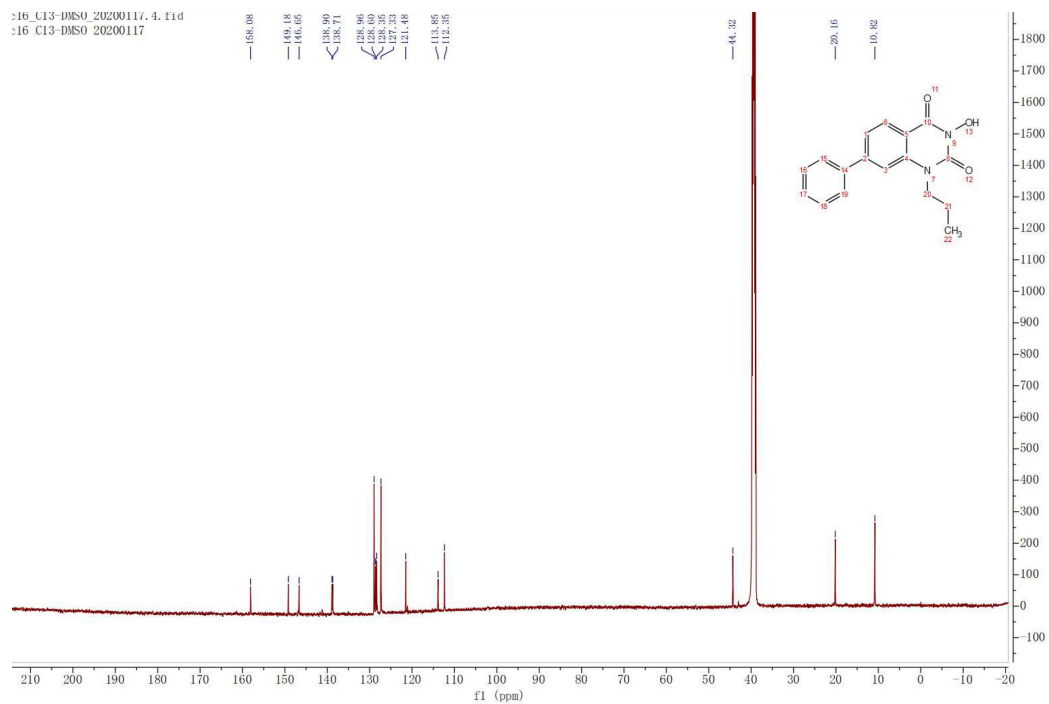
**Figure S172.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **23f**



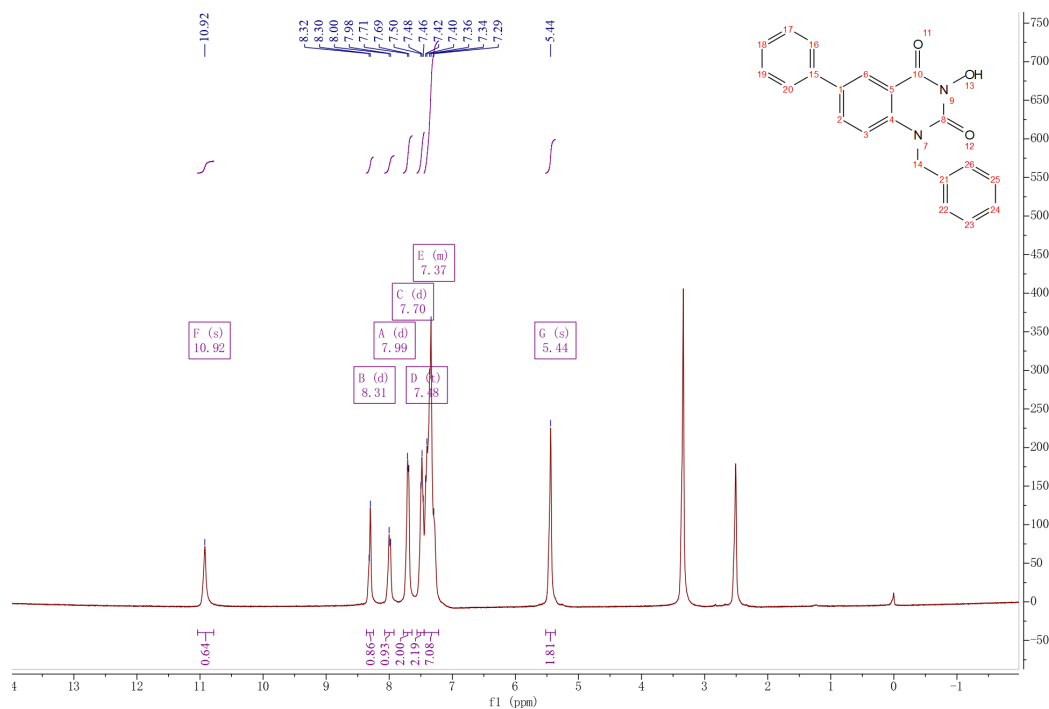
**Figure S173.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **23g**



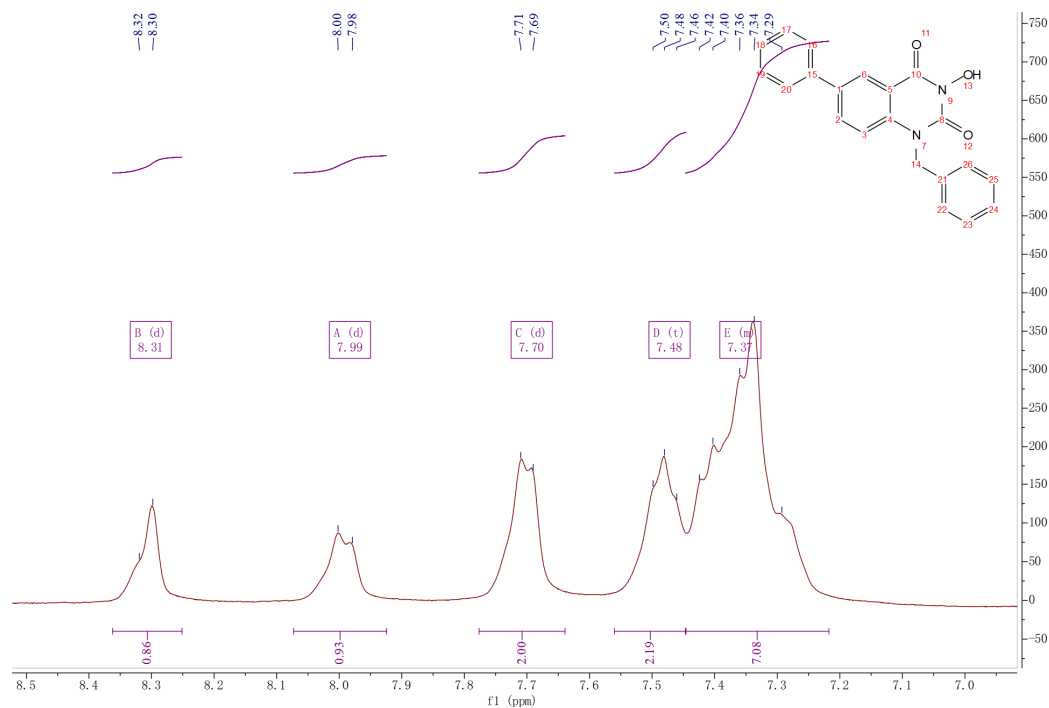
**Figure S174.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **23g**



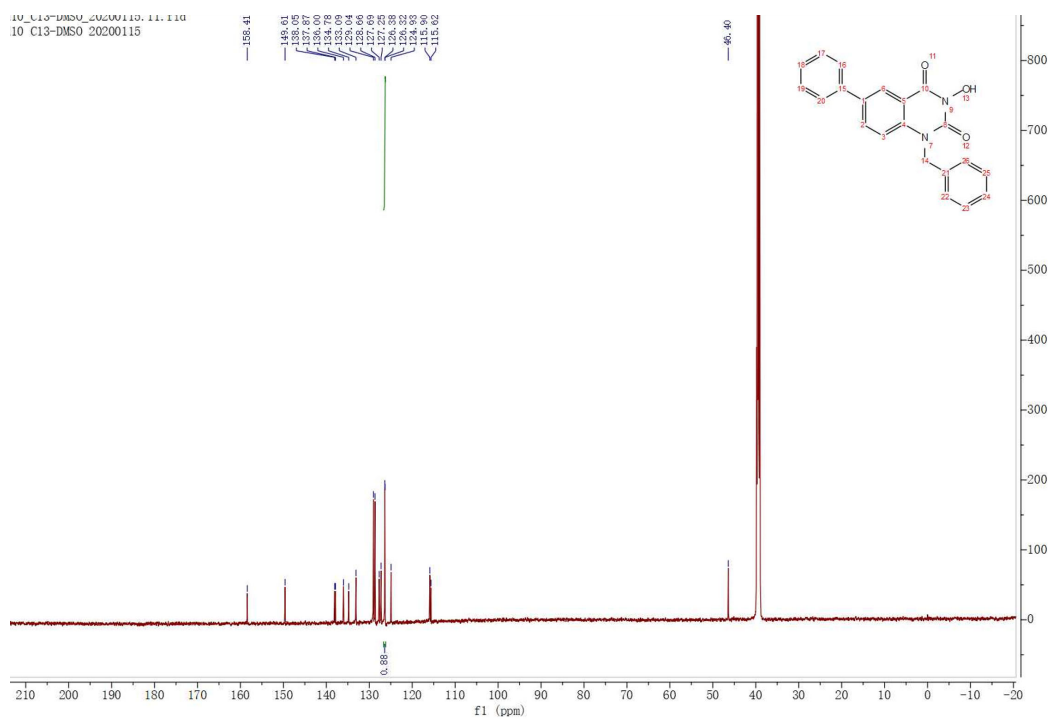
**Figure S175.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **23g**



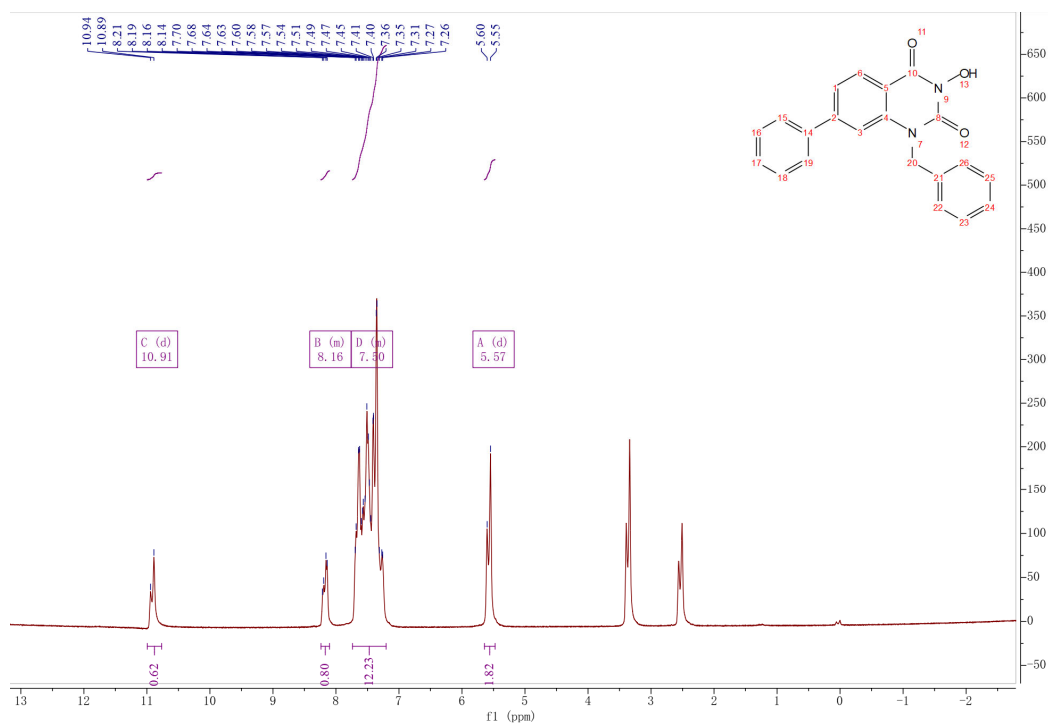
**Figure S176.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **23h**



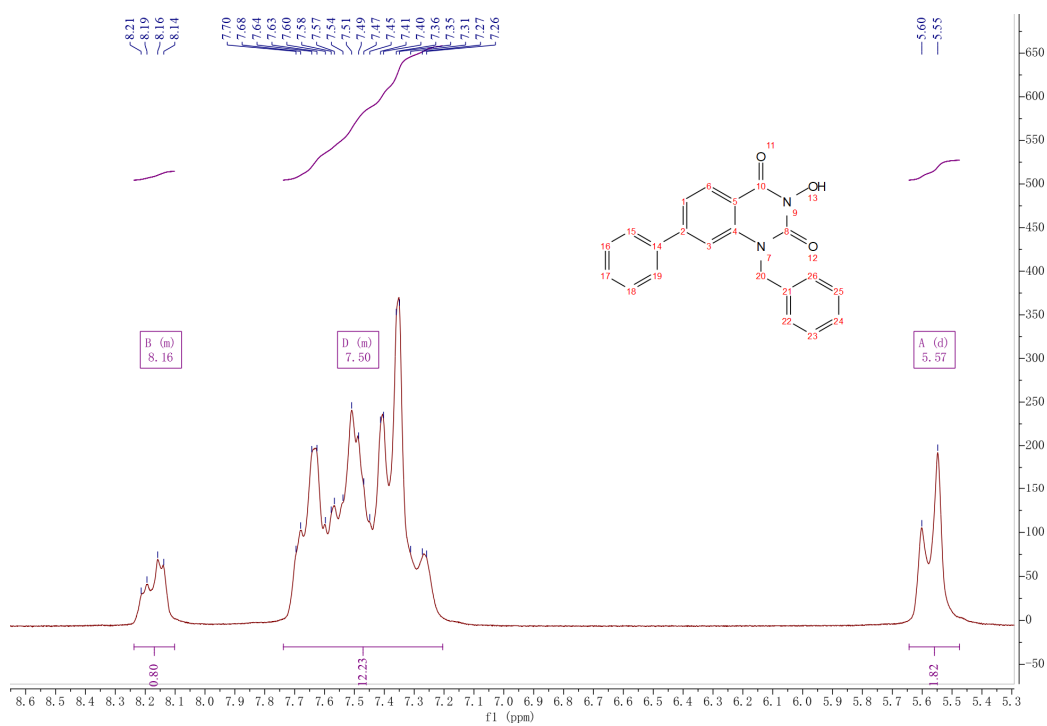
**Figure S177.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **23h**



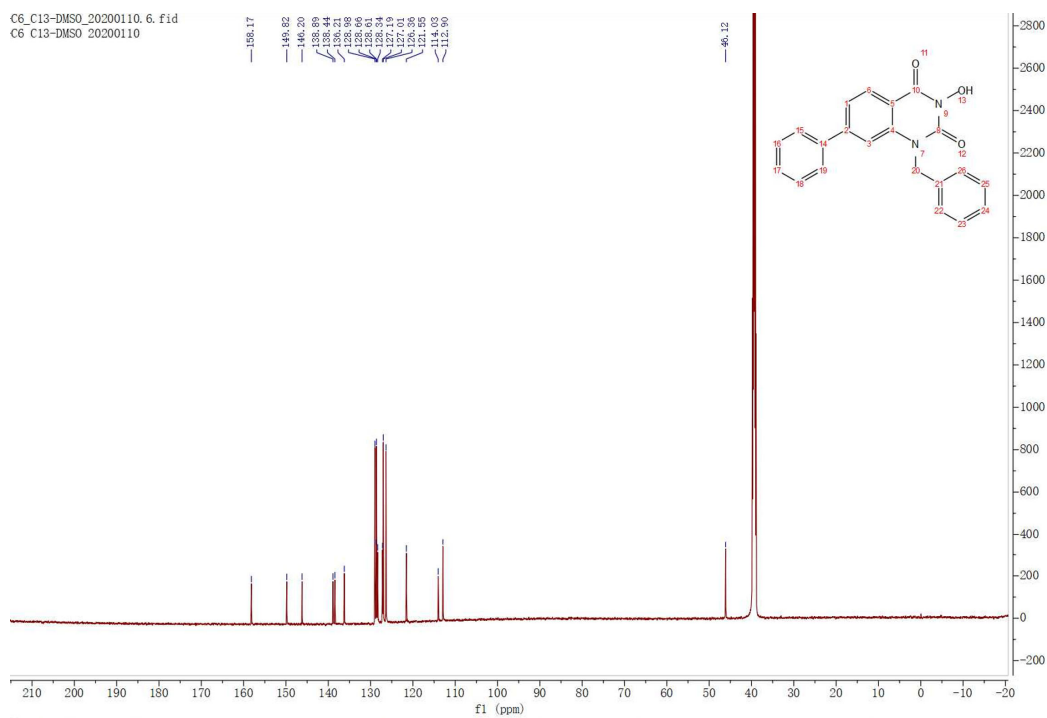
**Figure S178.**  $^{13}\text{C}$  NMR (151 MHz, DMSO- $d_6$ ) spectrum of **23h**



**Figure S179.**  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ) spectrum of **23i**

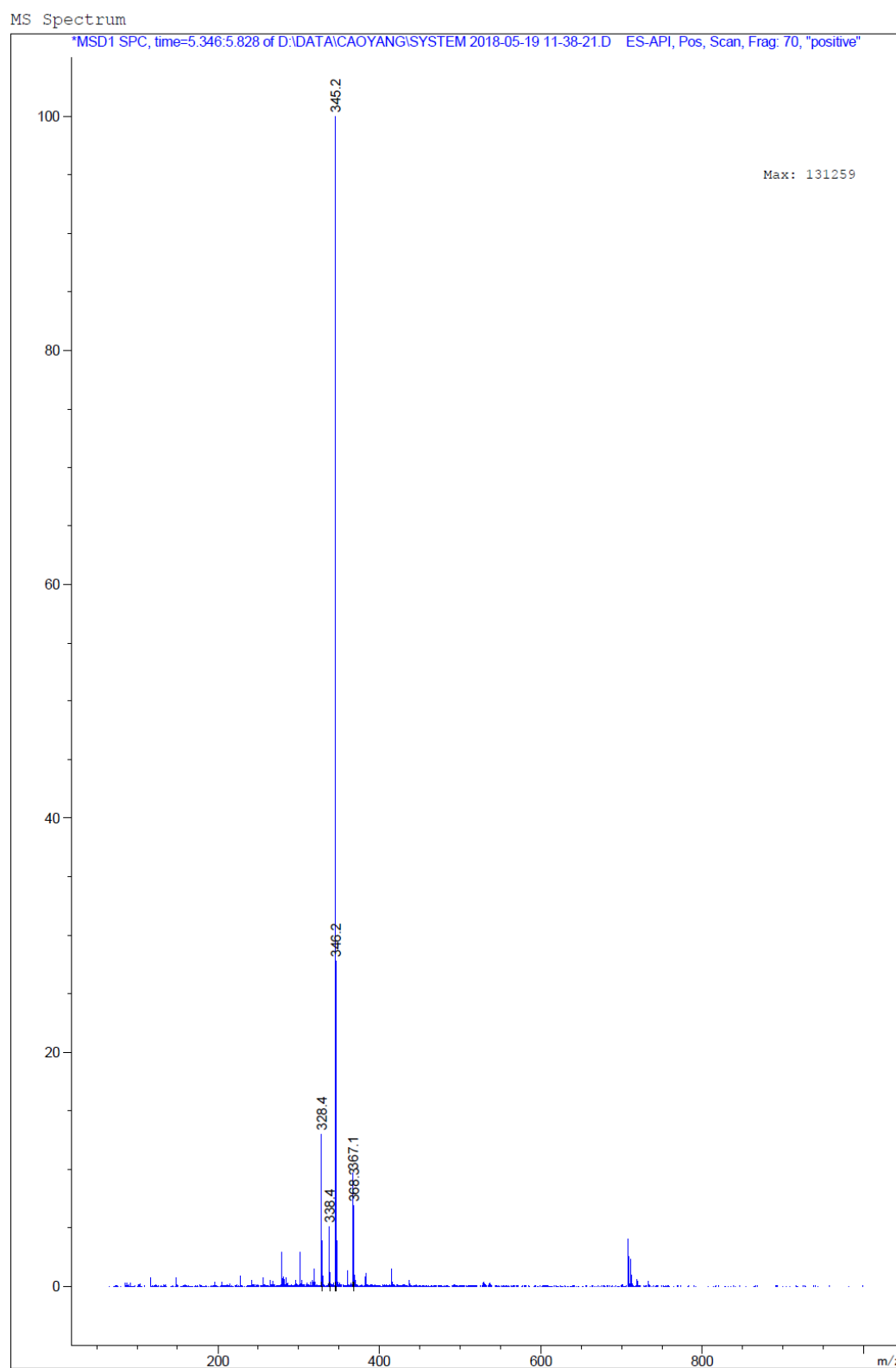


**Figure S180.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **23i**

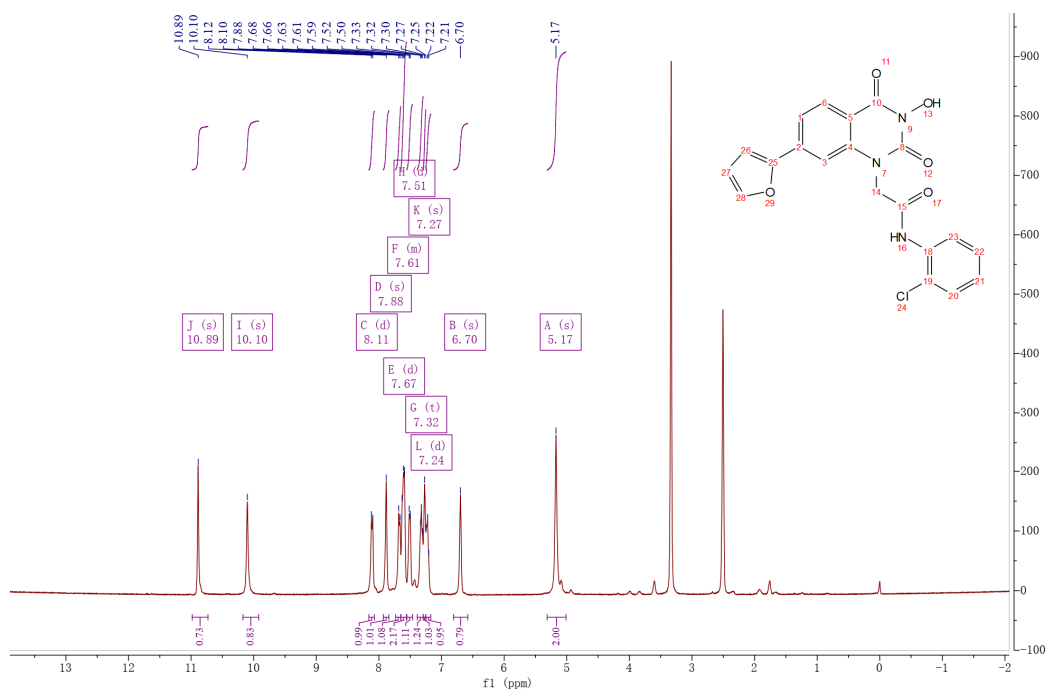


**Figure S181.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **23i**

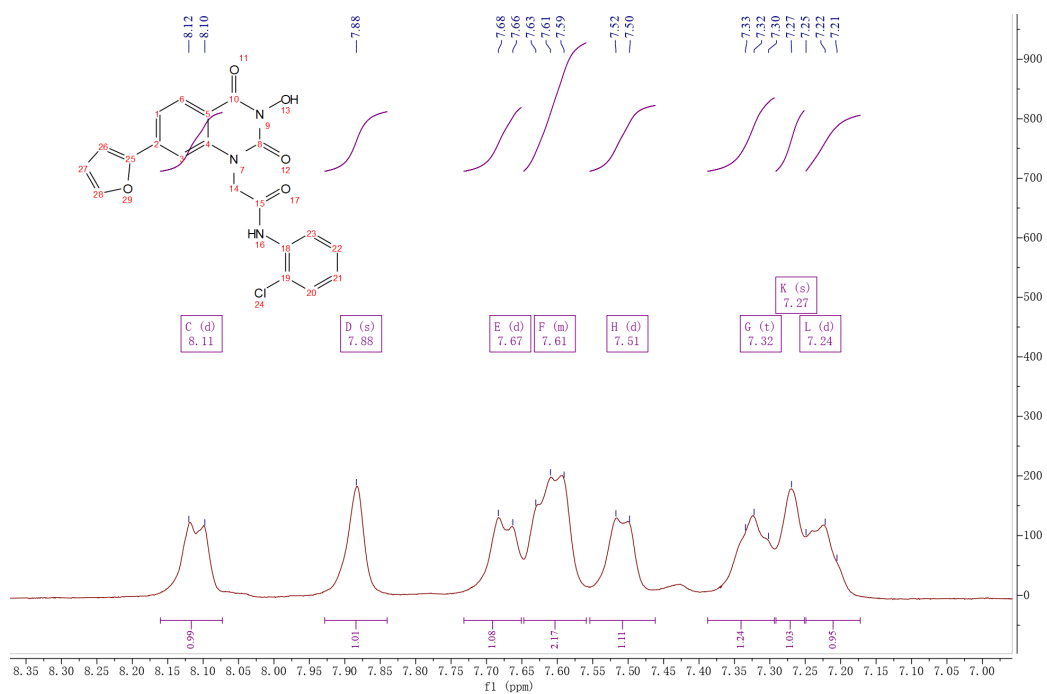




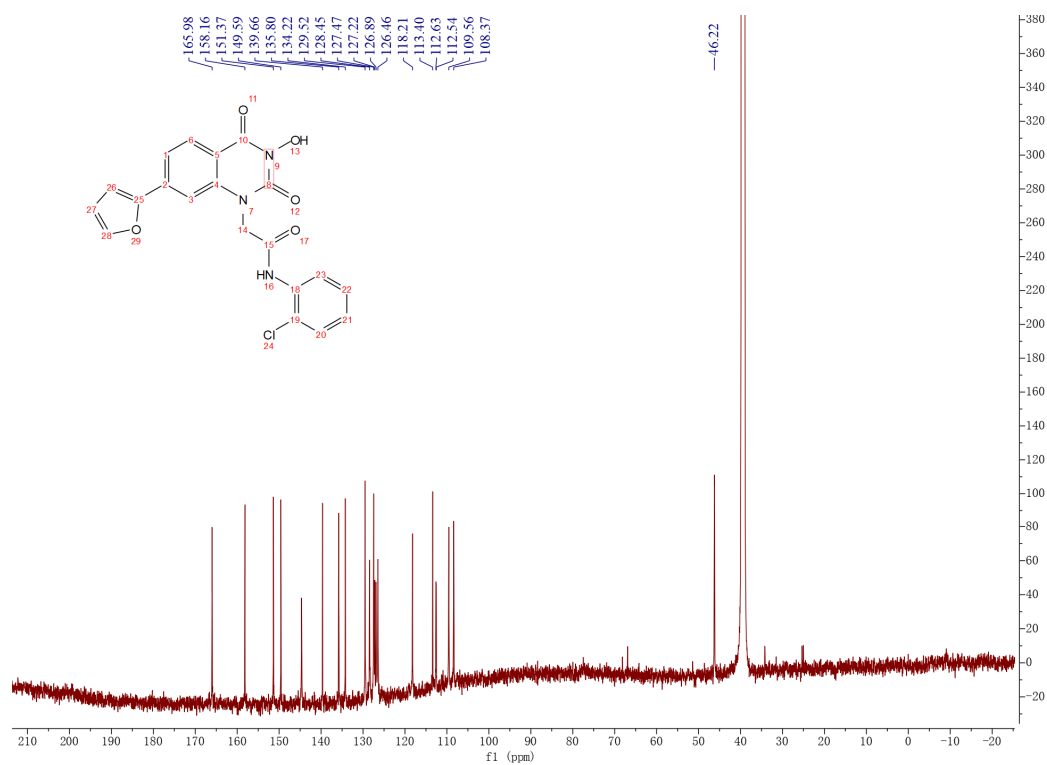
**Figure S182.** Mass spectrum (positive ionization) of **23i**



**Figure S183.**  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum of **23j**



**Figure S184.** Magnified  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ) spectrum fragments of **23j**



**Figure S185.**  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **23j**