

Design, synthesis, and evaluation of 1,4-naphthoquinone-chromene hybrids as potential anti-K562 and A549 agents

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Supporting Information

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1. X-Ray crystal data for compound 4am

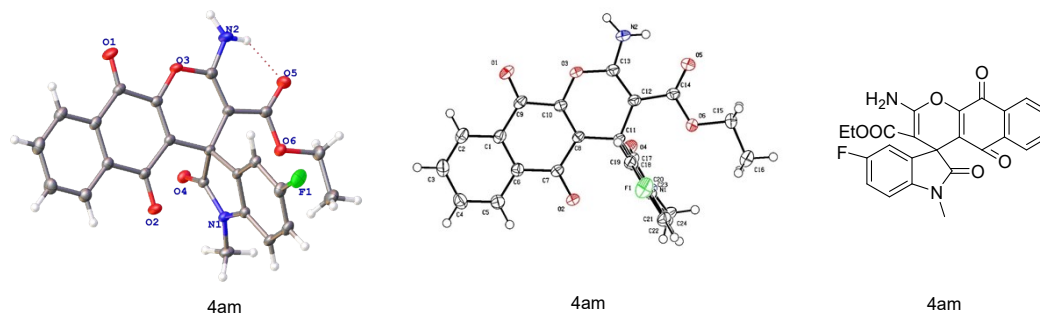


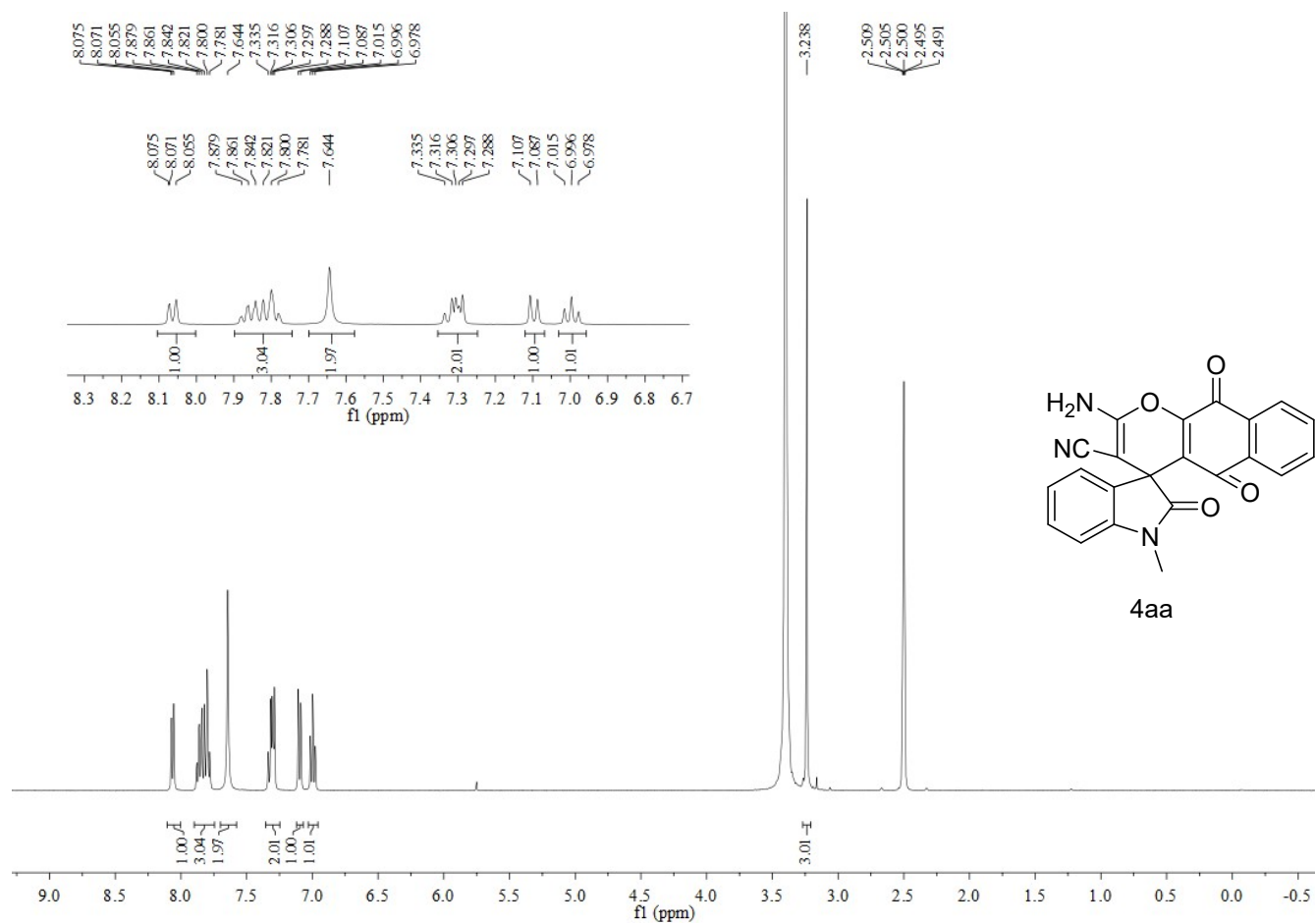
Table 1 Crystal data and structure refinement for 4am

Identification code	yes-21
Empirical formula	C ₂₄ H ₁₇ FN ₂ O ₆
Formula weight	448.39
Temperature/K	149.99(10)
Crystal system	triclinic
Space group	P-1
<i>a</i> /Å	8.7150(8)
<i>b</i> /Å	10.4907(8)
<i>c</i> /Å	12.3492(6)
α/°	92.135(5)
β/°	101.797(6)
γ/°	108.263(7)
Volume/Å ³	1043.27(14)
<i>Z</i>	2
ρ _{calc} /cm ³	1.427
μ/mm ⁻¹	0.927
<i>F</i> (000)	464.0
Crystal size/mm ³	0.16 × 0.13 × 0.11
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	7.356 to 147.674
Index ranges	-10 ≤ <i>h</i> ≤ 9, -10 ≤ <i>k</i> ≤ 13, -15 ≤ <i>l</i> ≤ 15
Reflections collected	6860
Independent reflections	4079 [R _{int} = 0.0186, R _{sigma} = 0.0232]
Data/restraints/parameters	4079/0/305
Goodness-of-fit on <i>F</i> ²	1.013
Final <i>R</i> indexes [<i>I</i> > 2σ (<i>I</i>)]	R ₁ = 0.0400, wR ₂ = 0.1075
Final <i>R</i> indexes [all data]	R ₁ = 0.0422, wR ₂ = 0.1098
Largest diff. peak/hole / e Å ⁻³	0.22/-0.27

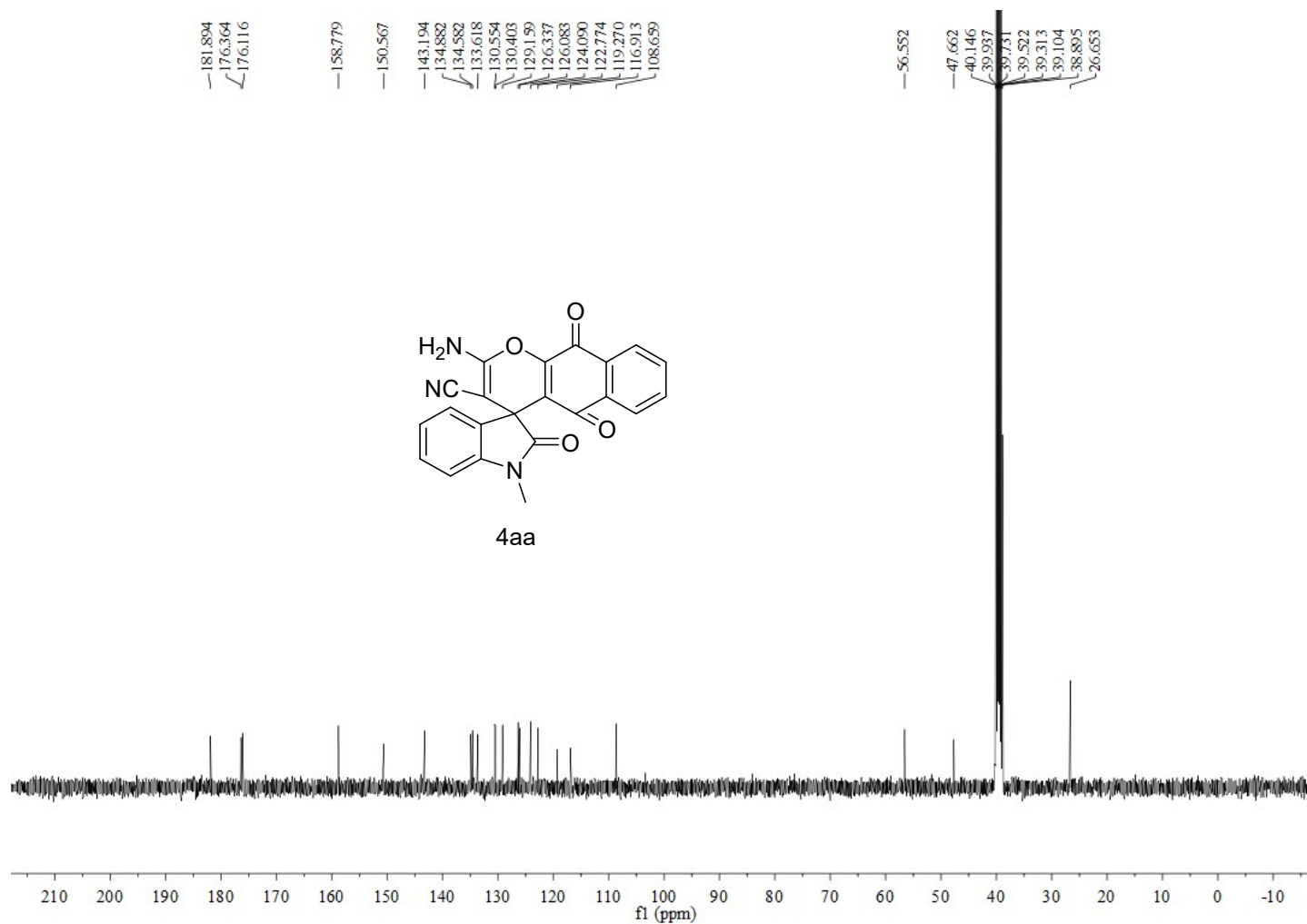
Crystal structure determination of 4am

Crystal Data for $C_{24}H_{17}FN_2O_6$ ($M=448.39$ g/mol): triclinic, space group P-1 (no. 2), $a = 8.7150(8)$ Å, $b = 10.4907(8)$ Å, $c = 12.3492(6)$ Å, $\alpha = 92.135(5)^\circ$, $\beta = 101.797(6)^\circ$, $\gamma = 108.263(7)^\circ$, $V = 1043.27(14)$ Å³, $Z = 2$, $T = 149.99(10)$ K, $\mu(\text{Cu K}\alpha) = 0.927$ mm⁻¹, $D_{\text{calc}} = 1.427$ g/cm³, 6860 reflections measured ($7.356^\circ \leq 2\Theta \leq 147.674^\circ$), 4079 unique ($R_{\text{int}} = 0.0186$, $R_{\text{sigma}} = 0.0232$) which were used in all calculations. The final R_1 was 0.0400 ($I > 2\sigma(I)$) and wR_2 was 0.1098 (all data).

2. The copies of ^1H NMR and ^{13}C NMR spectra for compounds 4



^1H NMR of Compound **4aa** (400 MHz, $\text{DMSO-}d_6$)

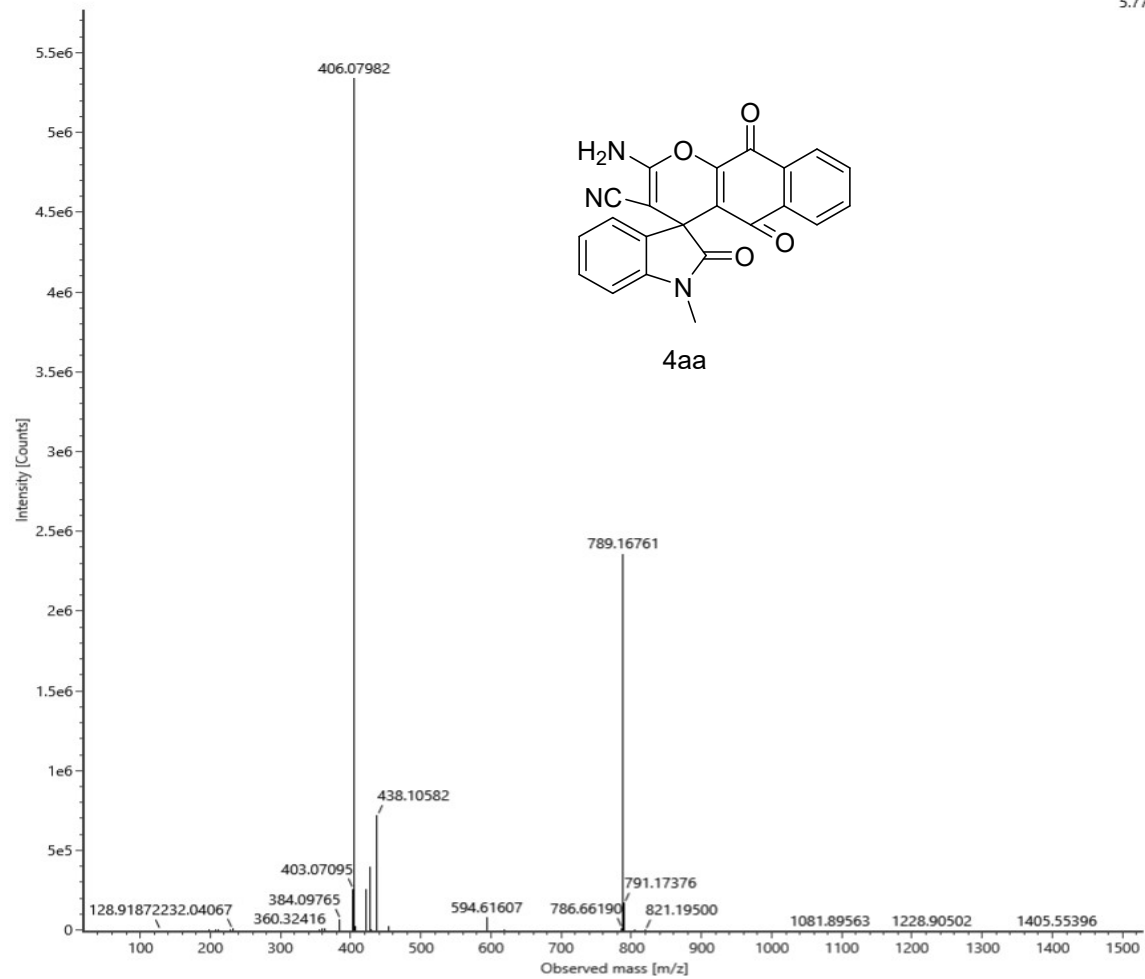


¹³C NMR of Compound **4aa** (101 MHz, DMSO-*d*₆)

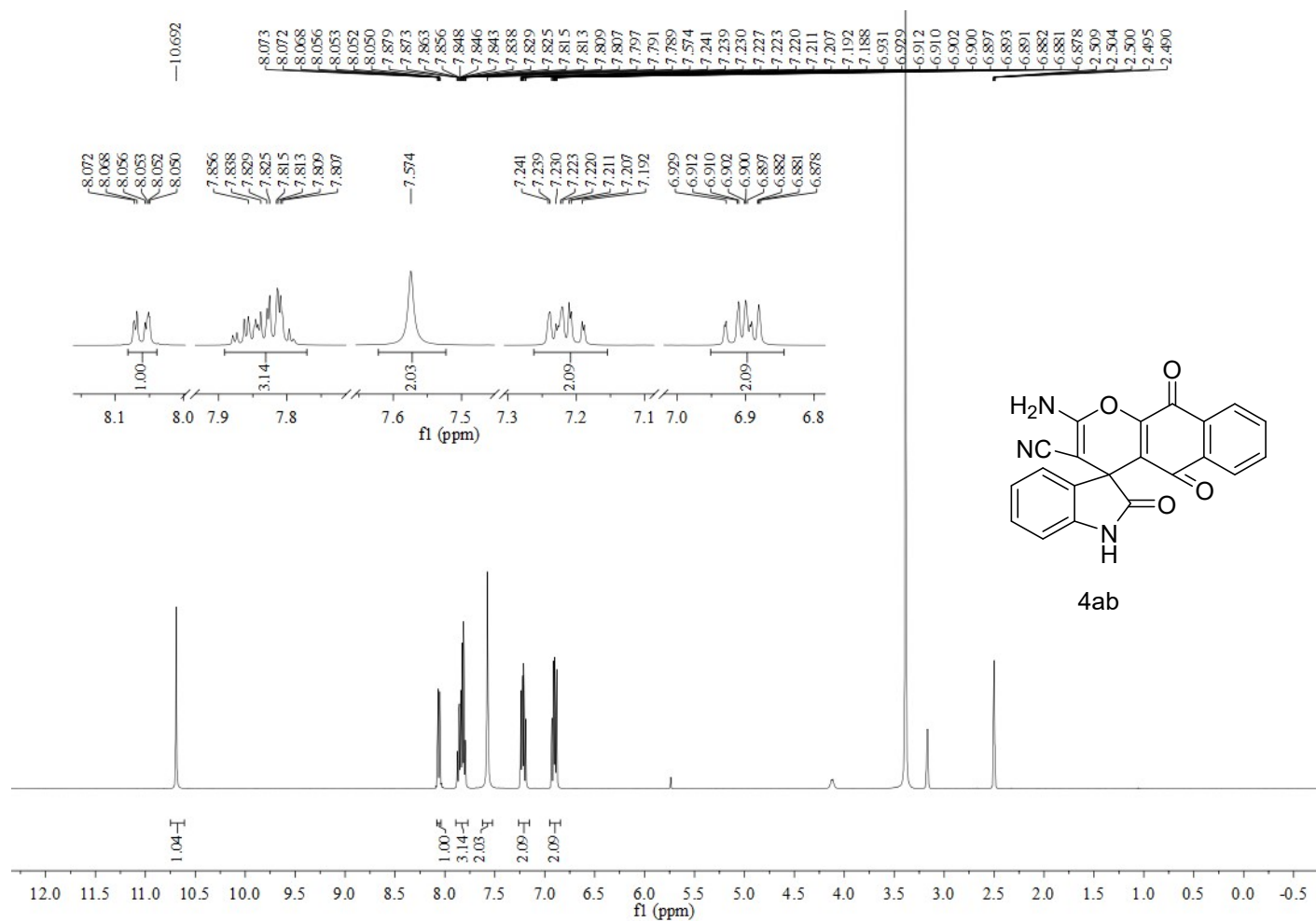
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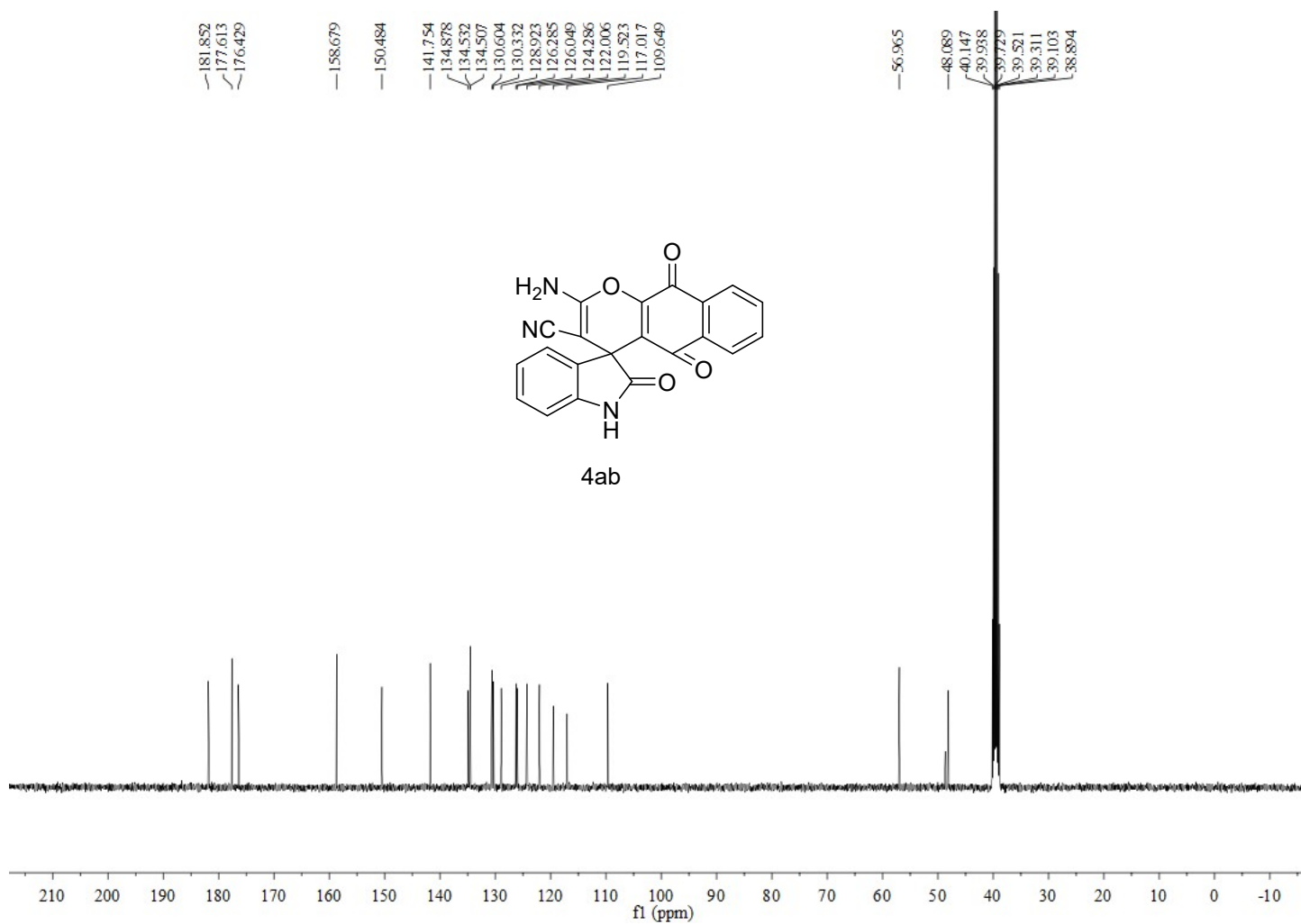
5.77e6



HRMS of Compound 4aa



$^1\text{H NMR}$ of Compound **4ab** (400 MHz, $\text{DMSO-}d_6$)

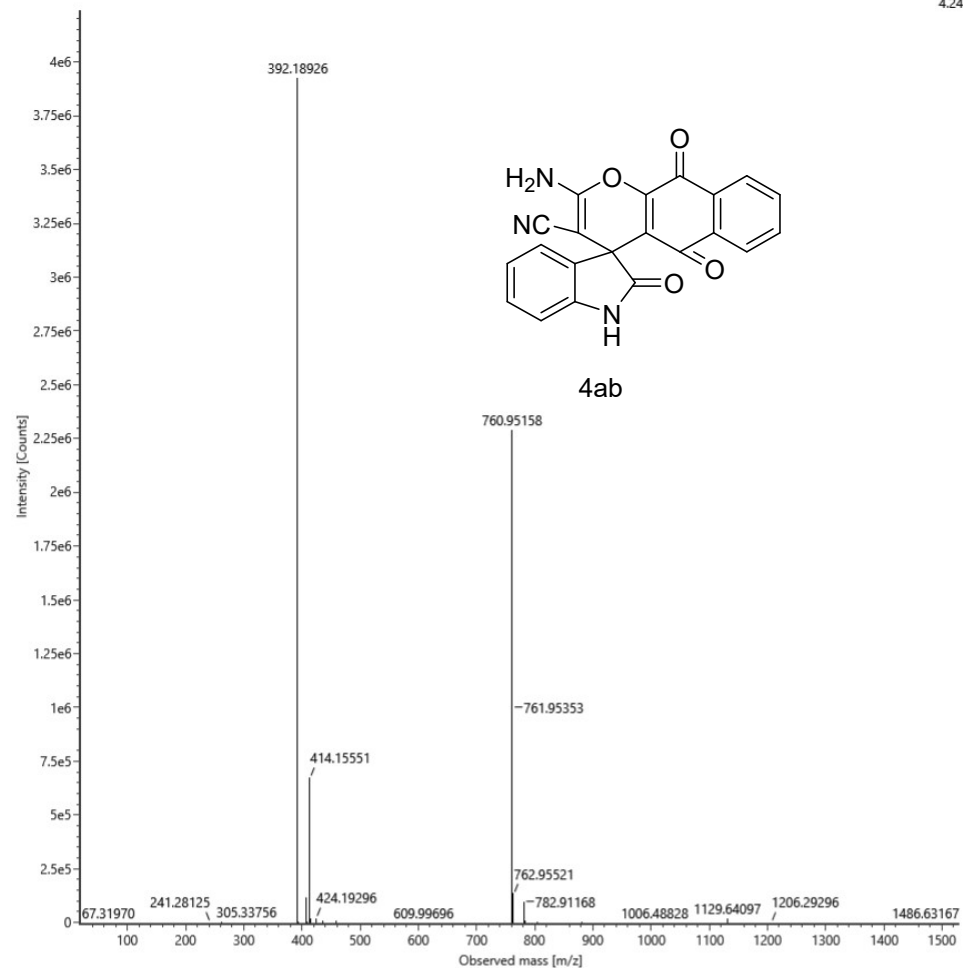


¹³C NMR of Compound **4ab** (101 MHz, DMSO-*d*₆)

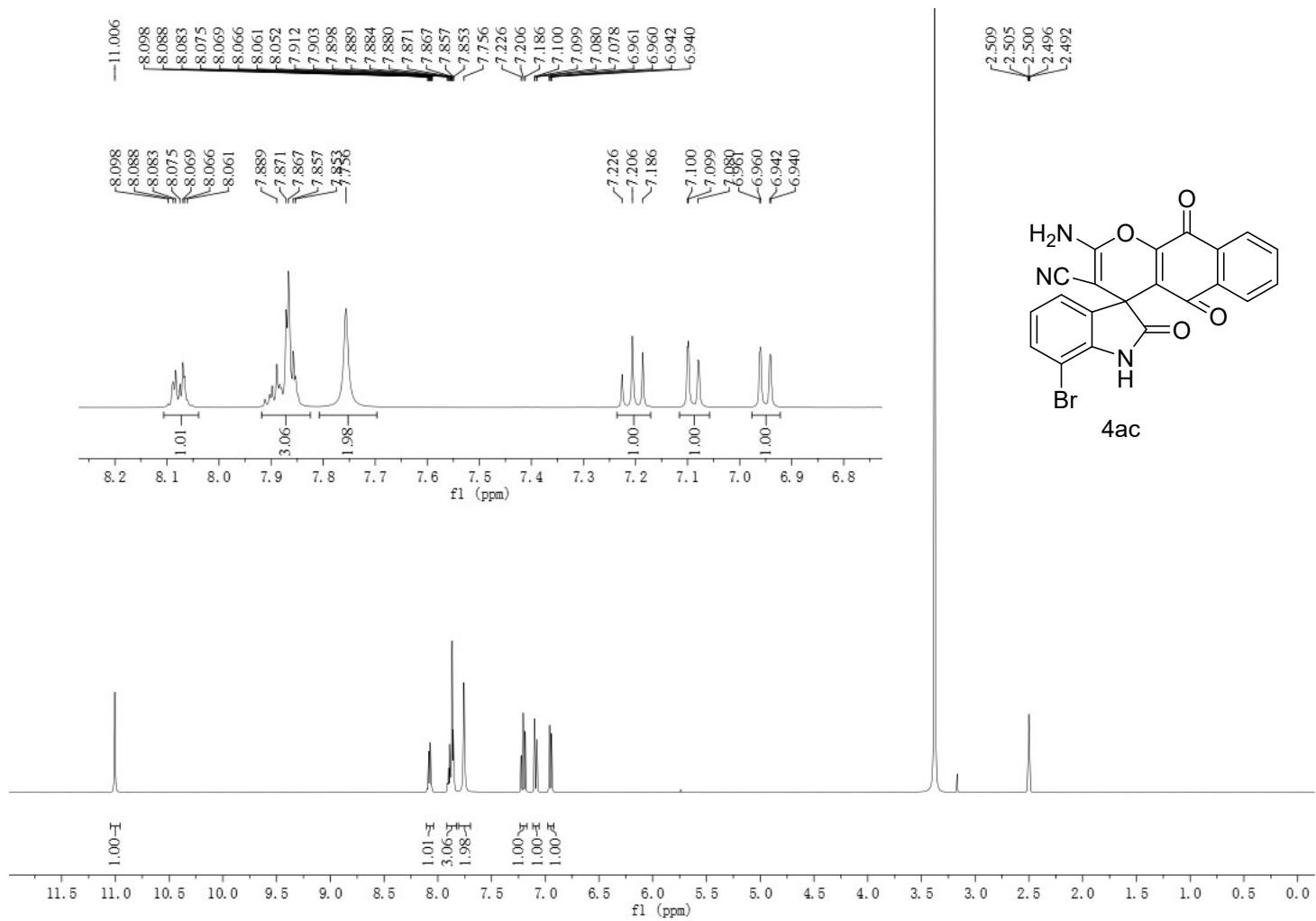
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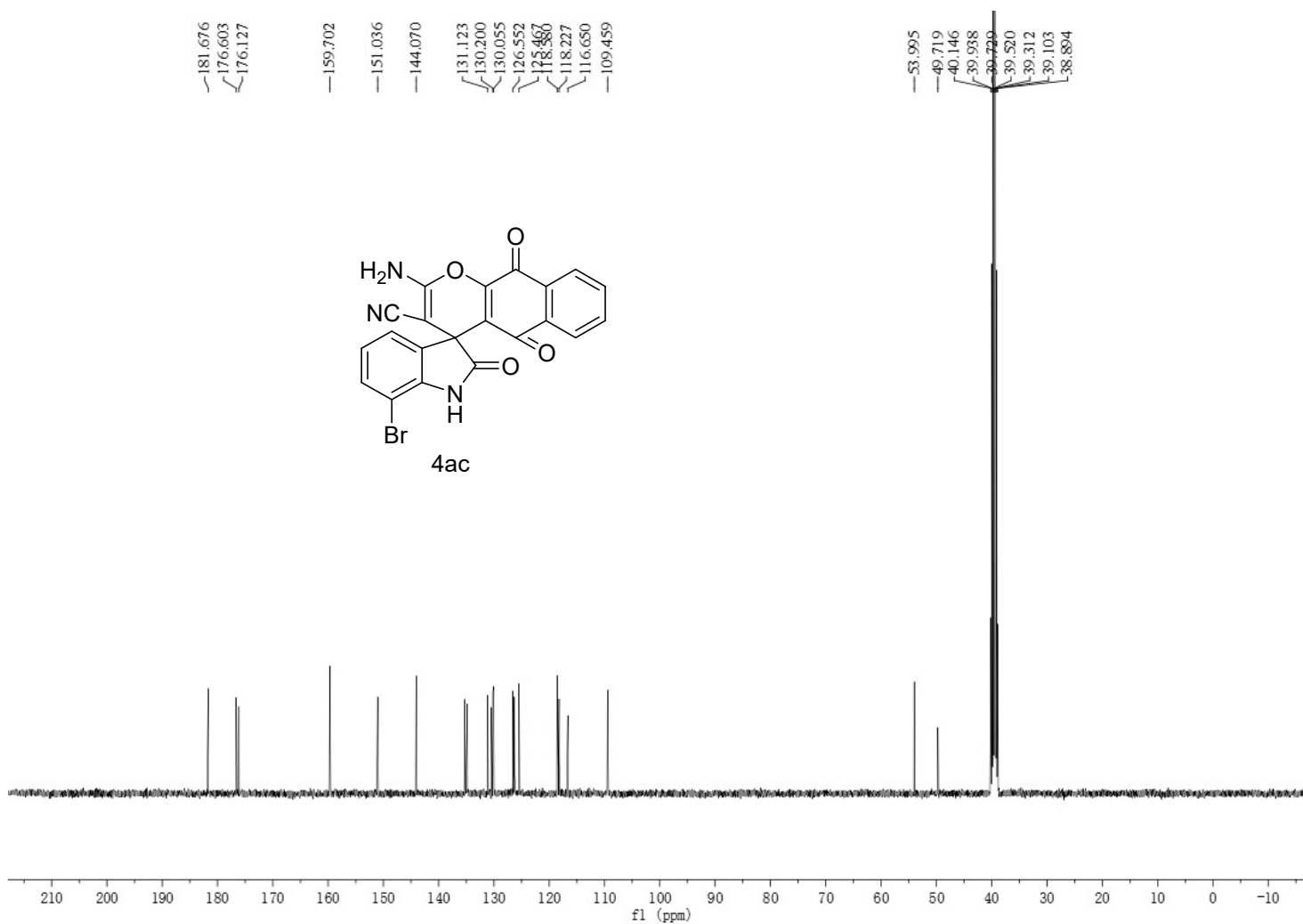
4.24e6



HRMS of Compound 4ab



¹H NMR of Compound 4ac (400 MHz, DMSO-*d*₆)

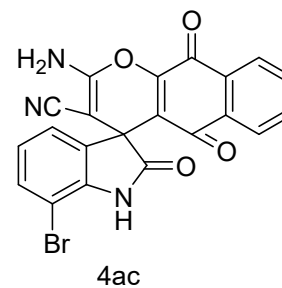
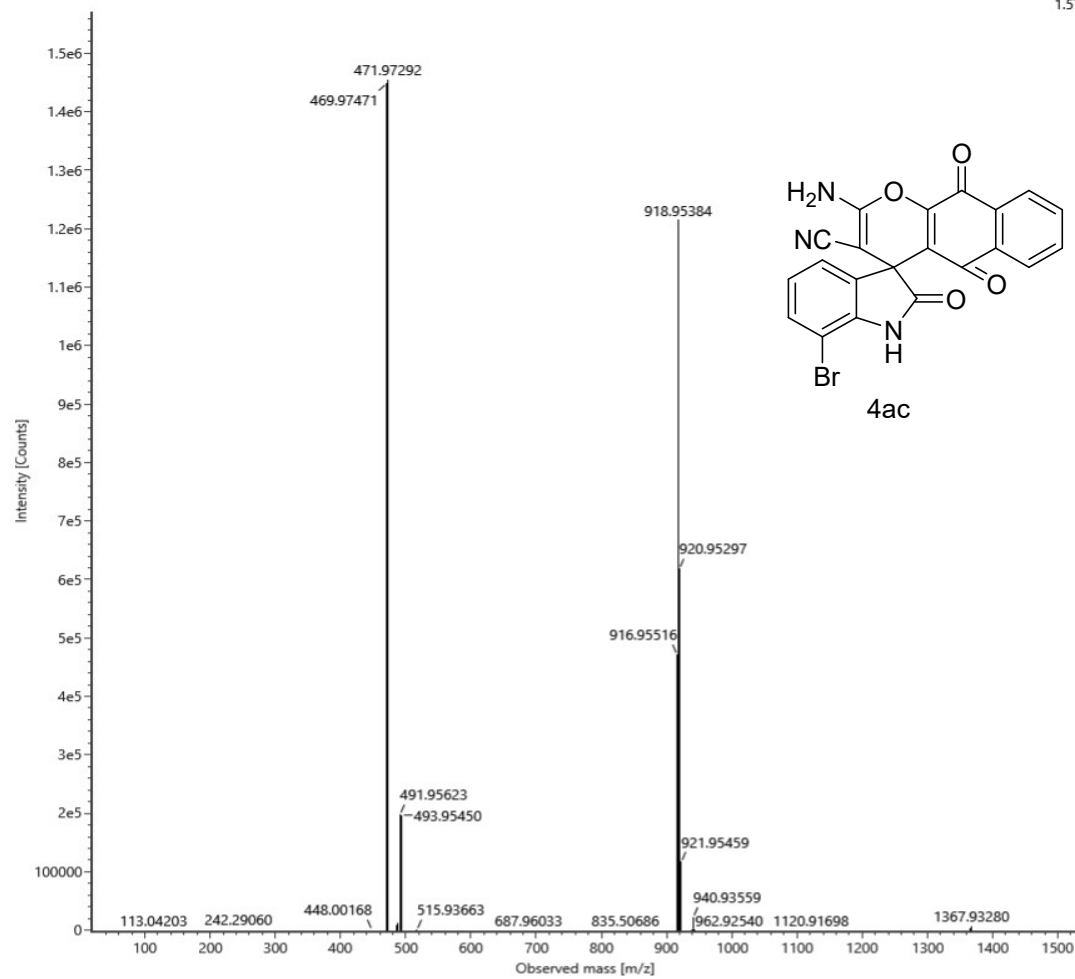


¹³C NMR of Compound **4ac** (101 MHz, DMSO-*d*₆)

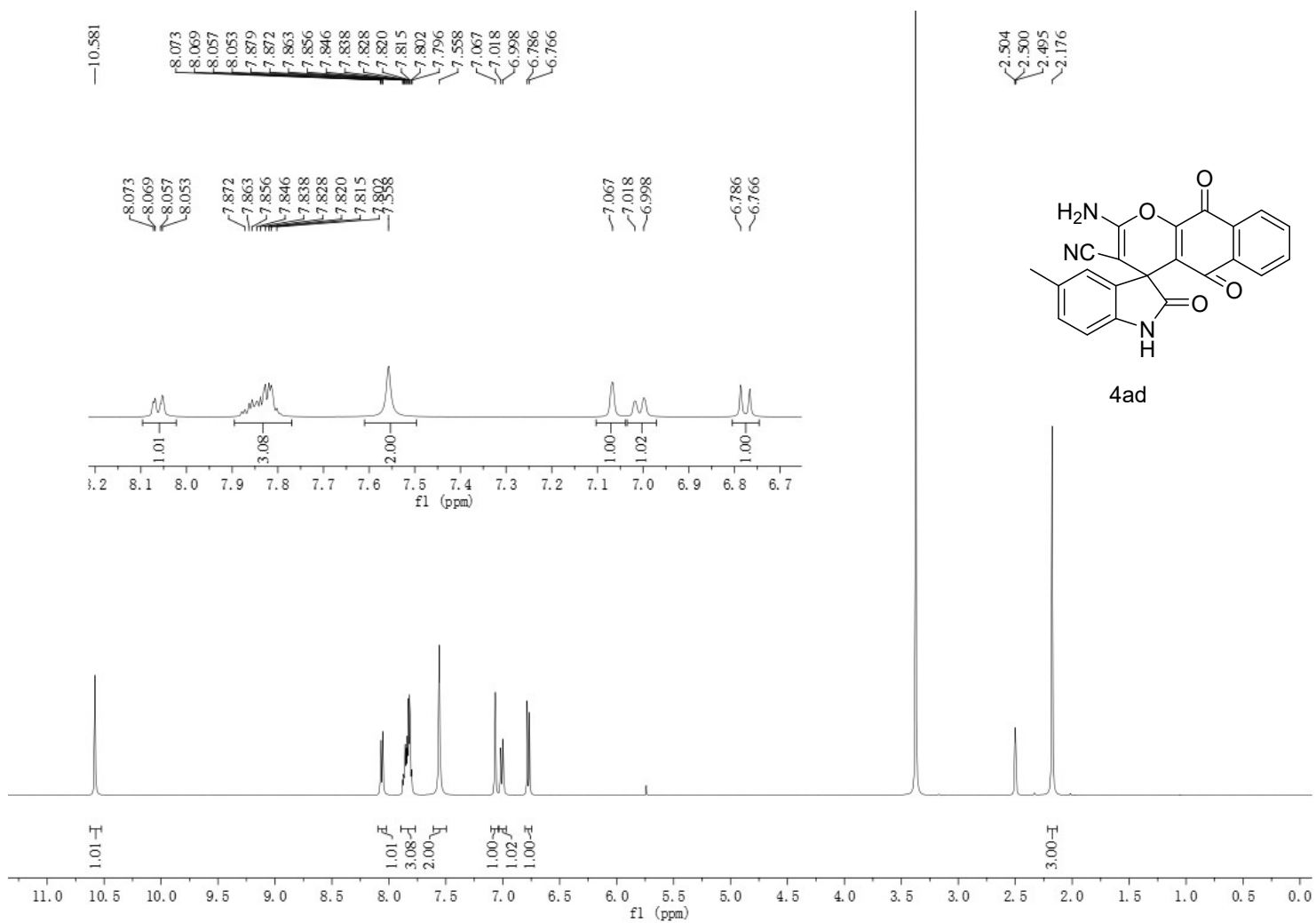
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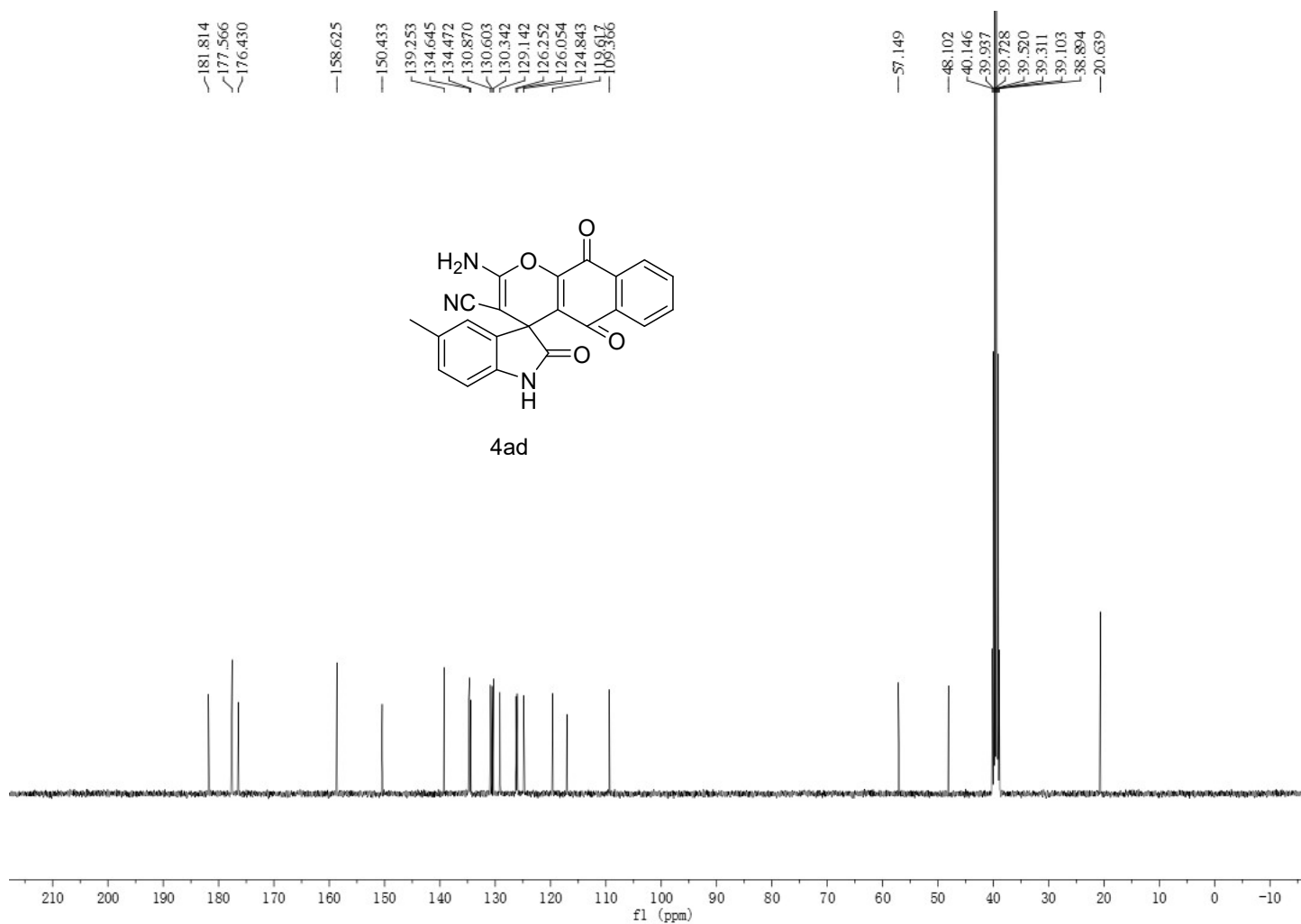
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1.57e6



HRMS of Compound 4ac



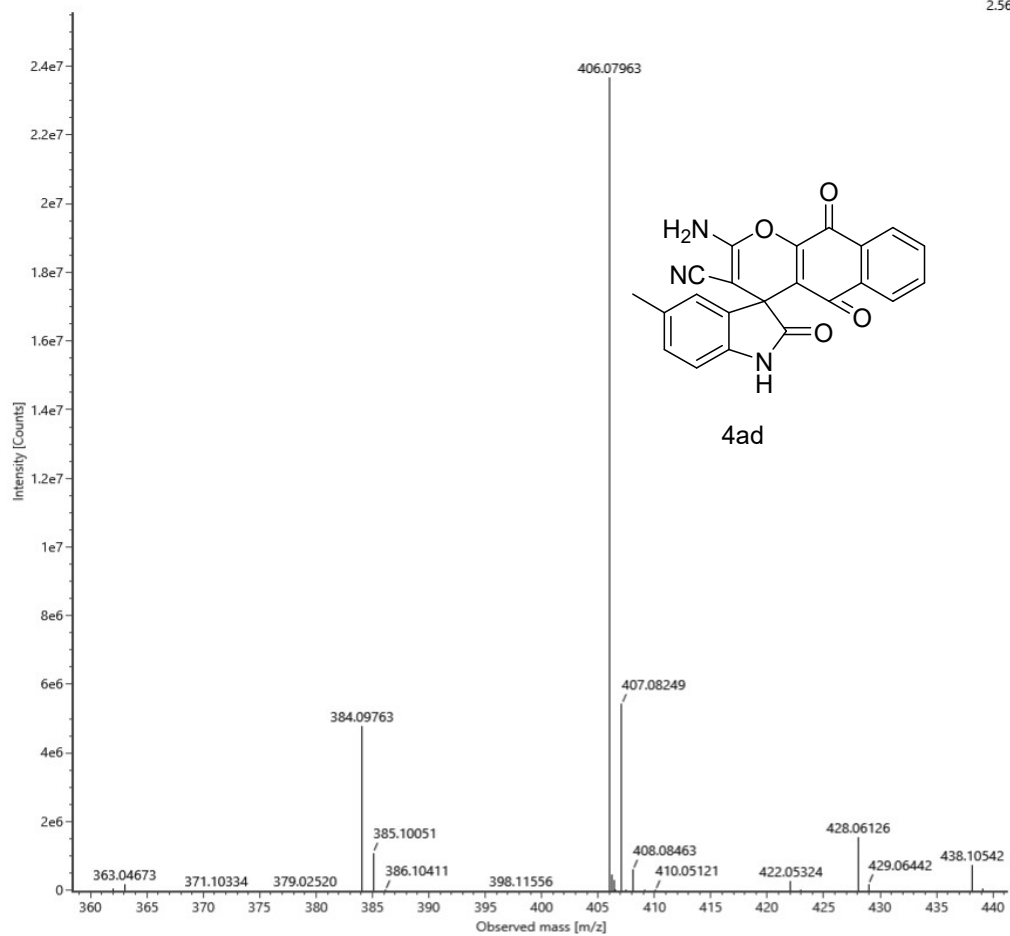


¹³C NMR of Compound **4ad** (101 MHz, DMSO-*d*₆)

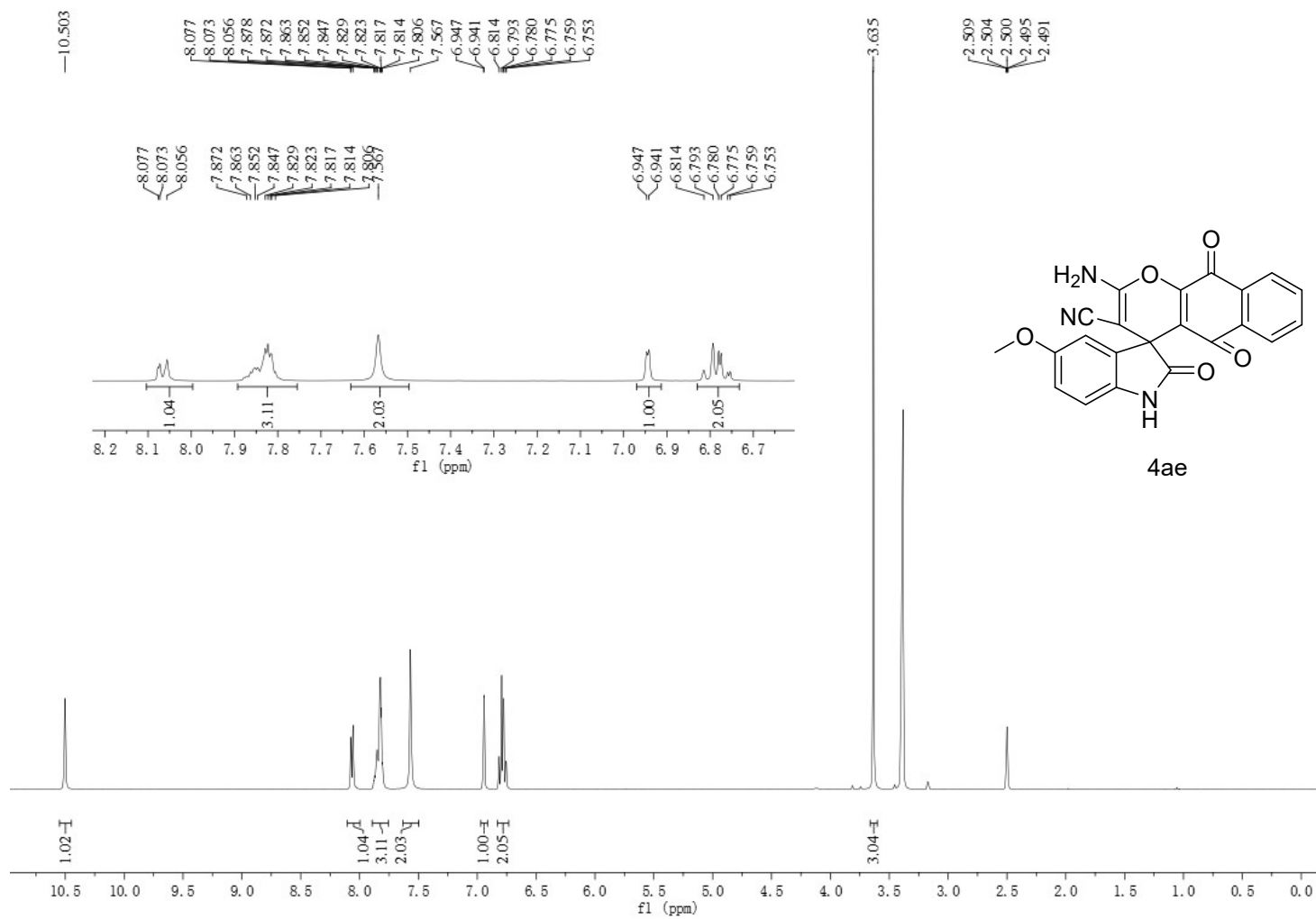
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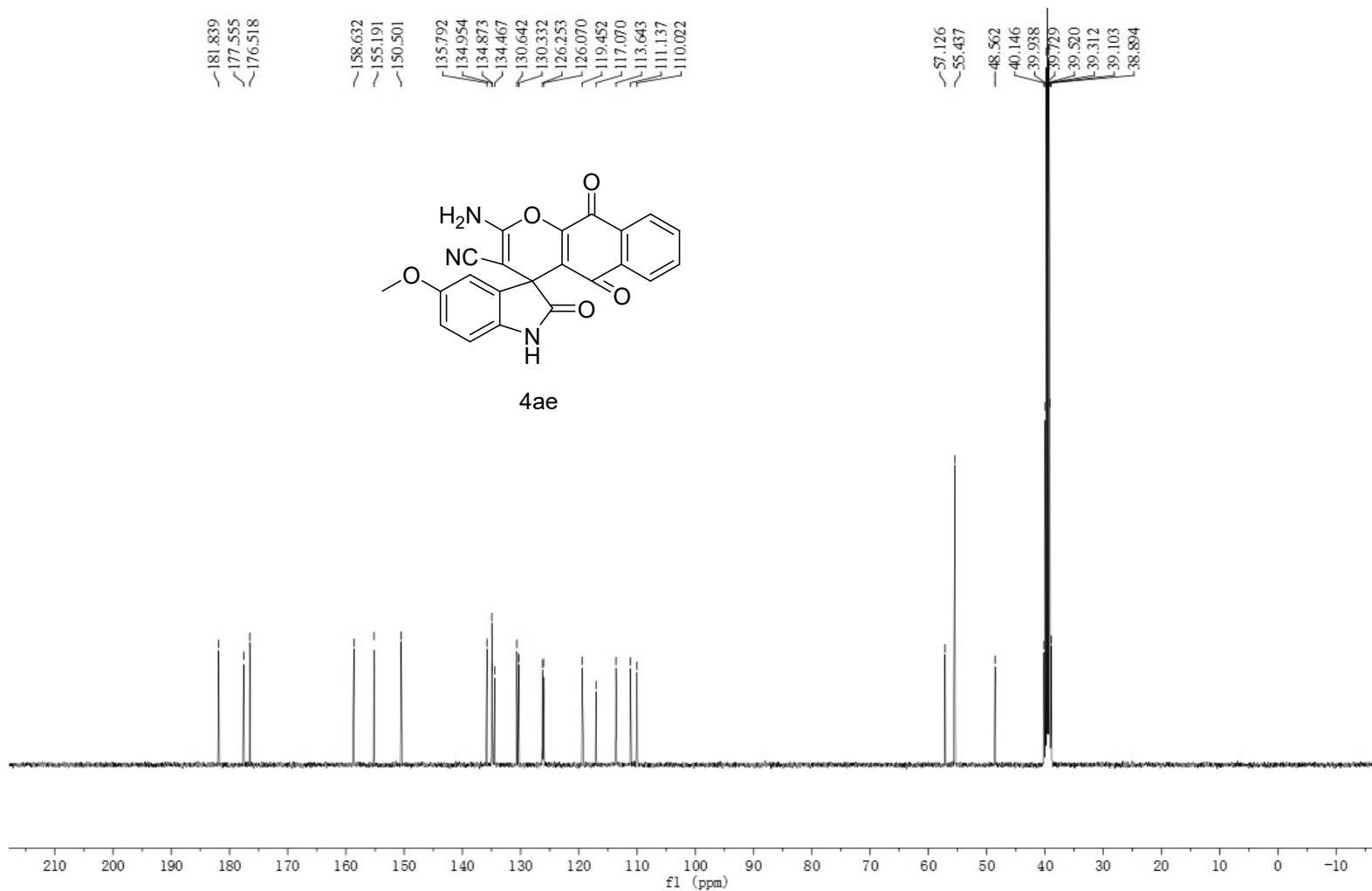
2.56e7



HRMS of Compound **4ad**



¹H NMR of Compound **4ae** (400 MHz, DMSO-*d*₆)

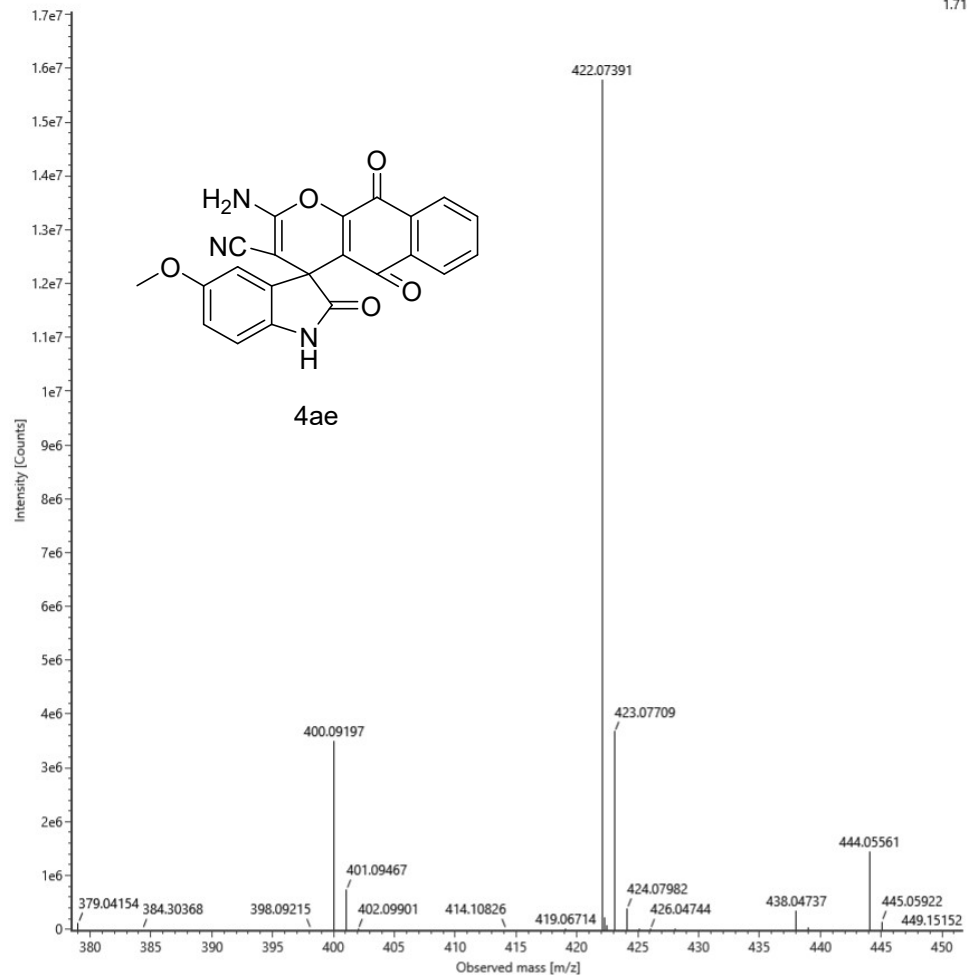


¹³C NMR of Compound **4ae** (101 MHz, DMSO-*d*₆)

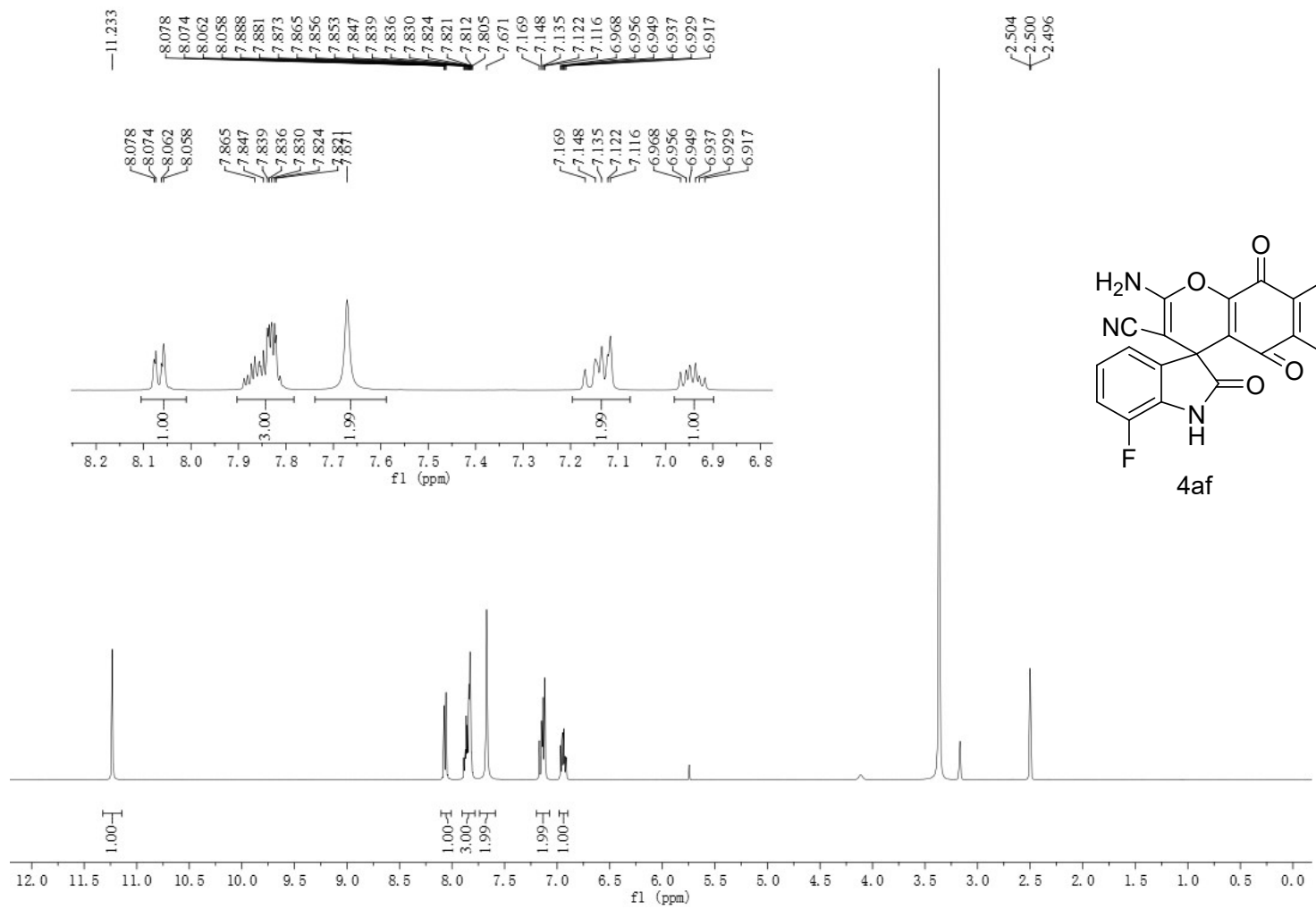
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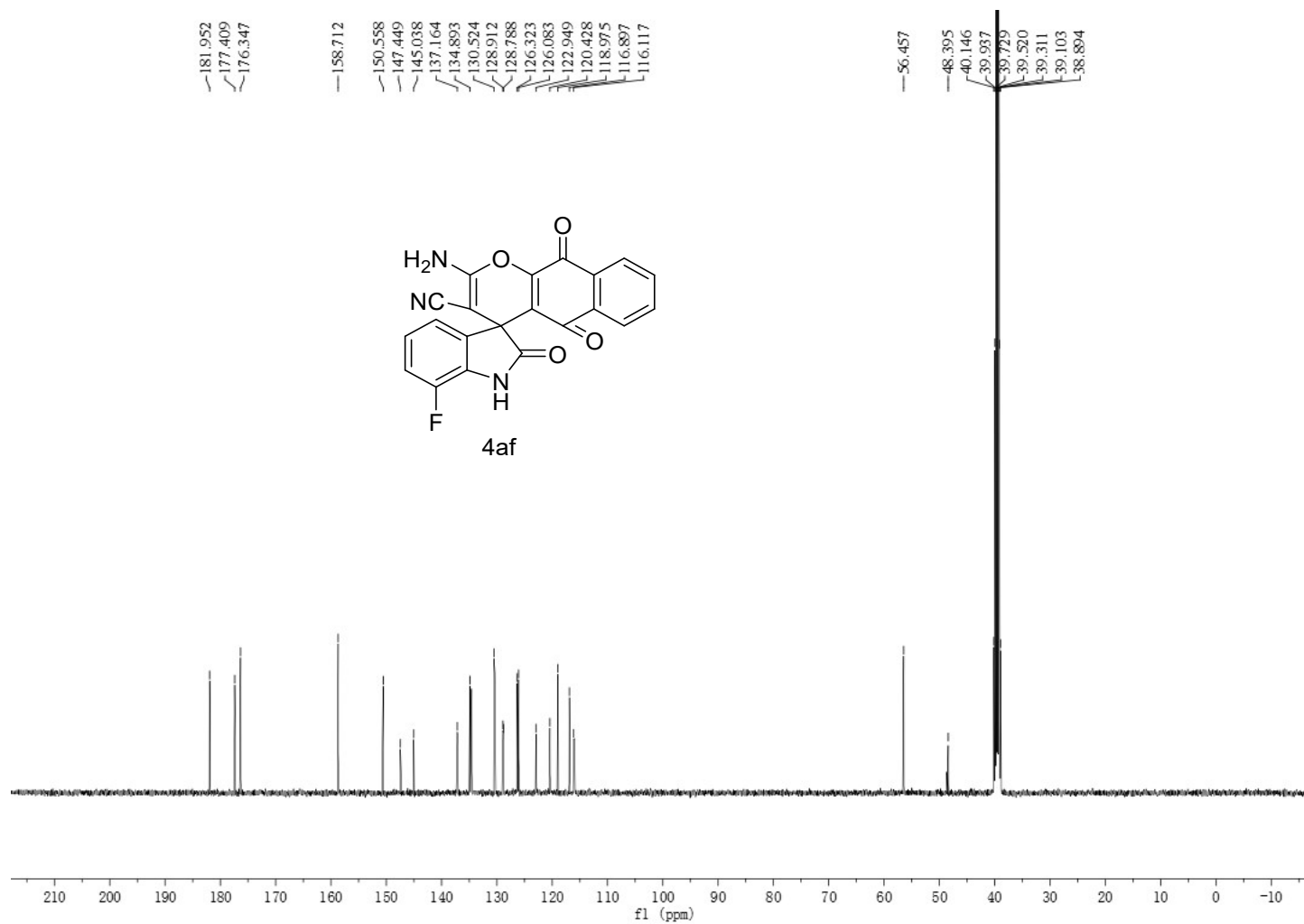
1.71e7



HRMS of Compound 4ae



¹H NMR of Compound **4af** (400 MHz, DMSO-*d*₆)

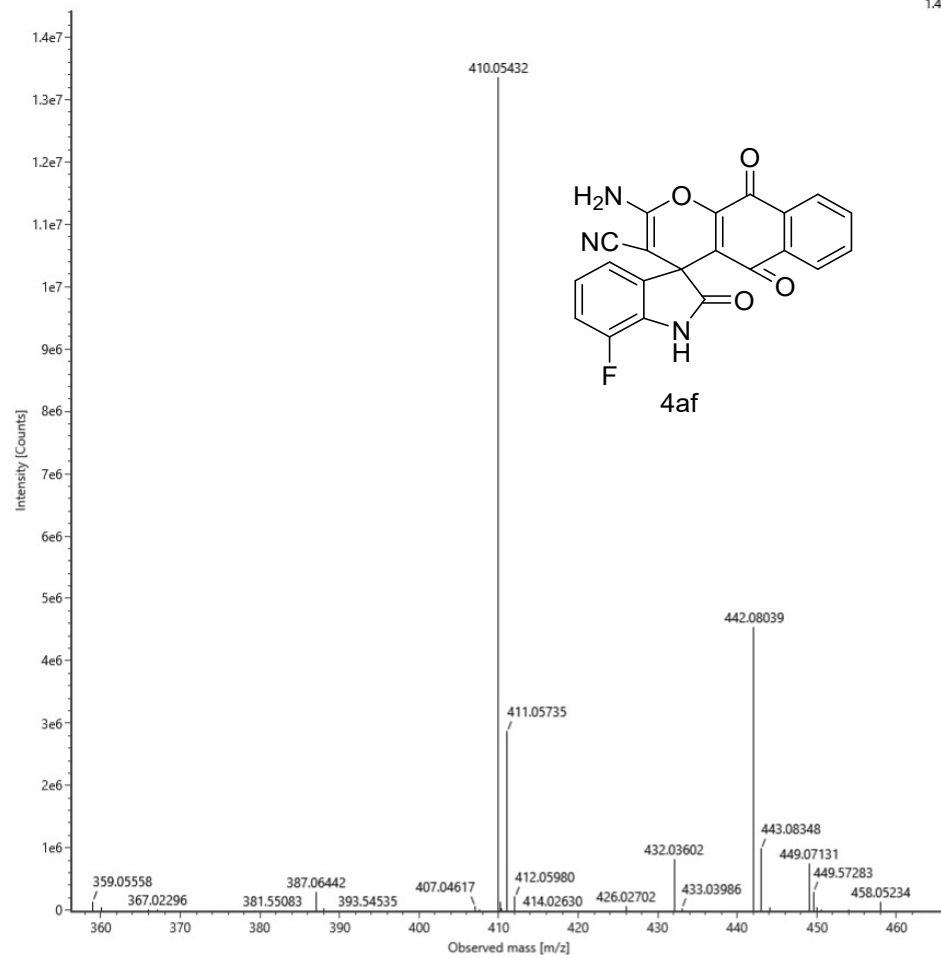


¹³C NMR of Compound **4af** (101 MHz, DMSO-*d*₆)

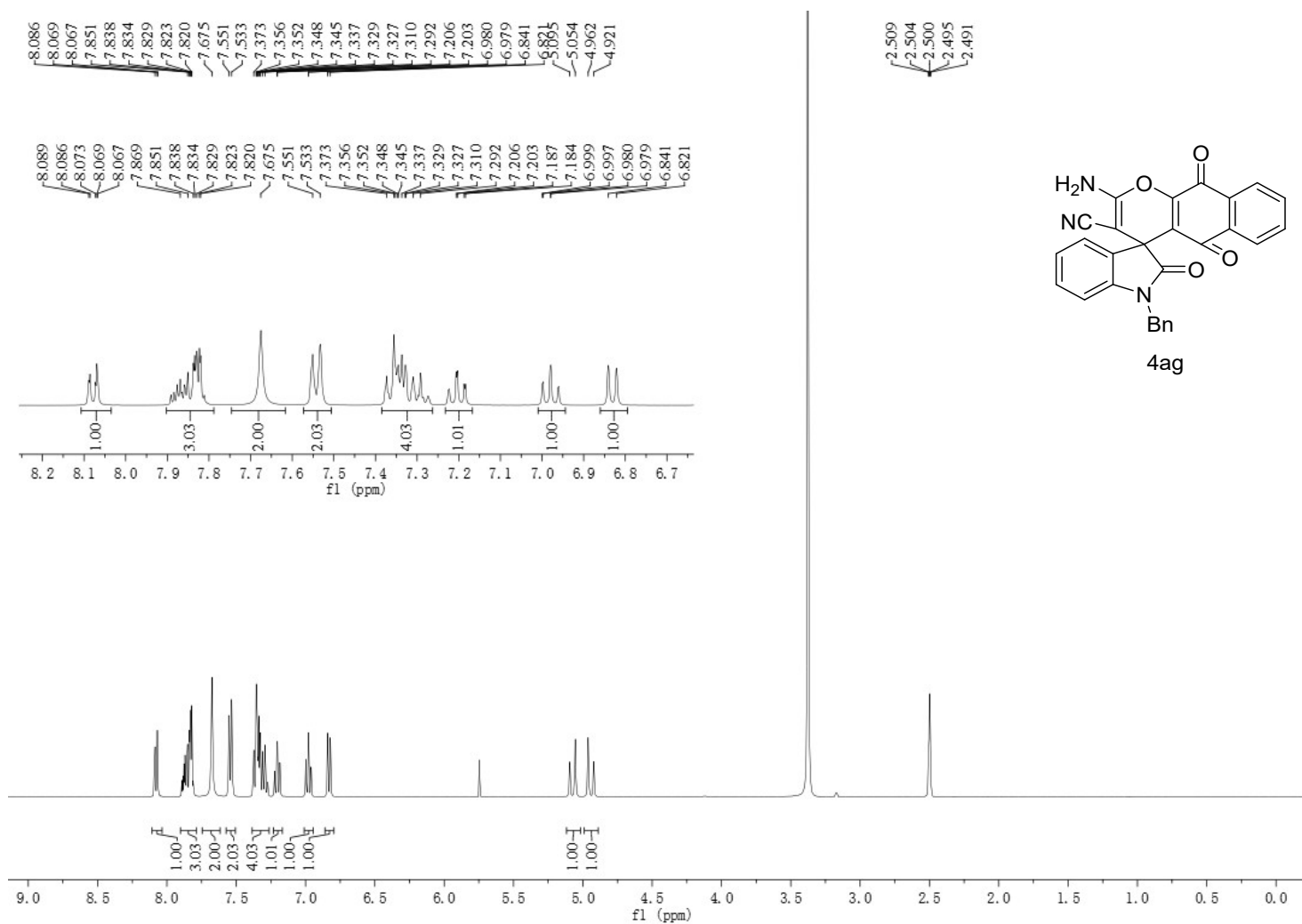
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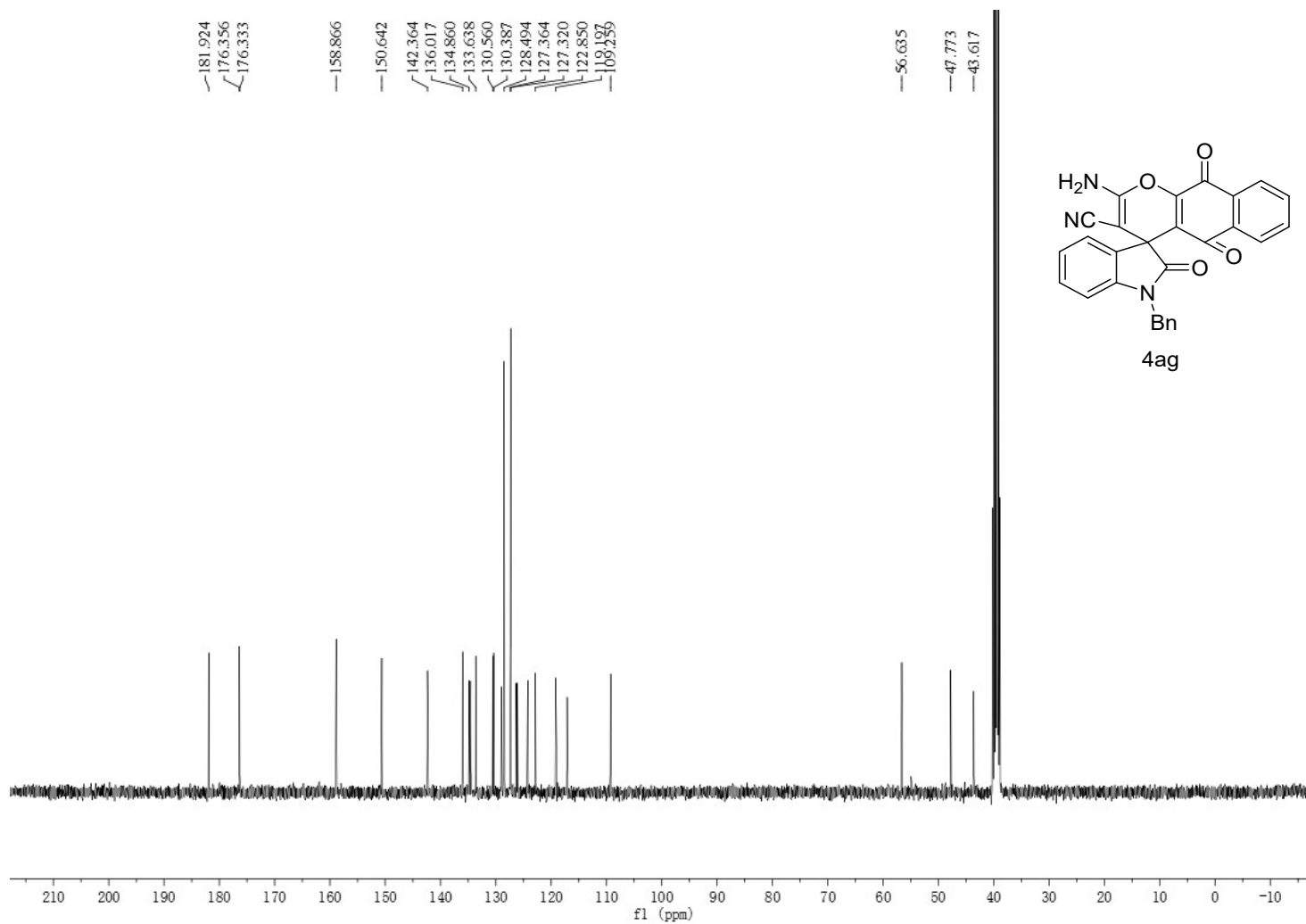
1.44e7



HRMS of Compound **4af**



¹H NMR of Compound 4ag (400 MHz, DMSO-*d*₆)

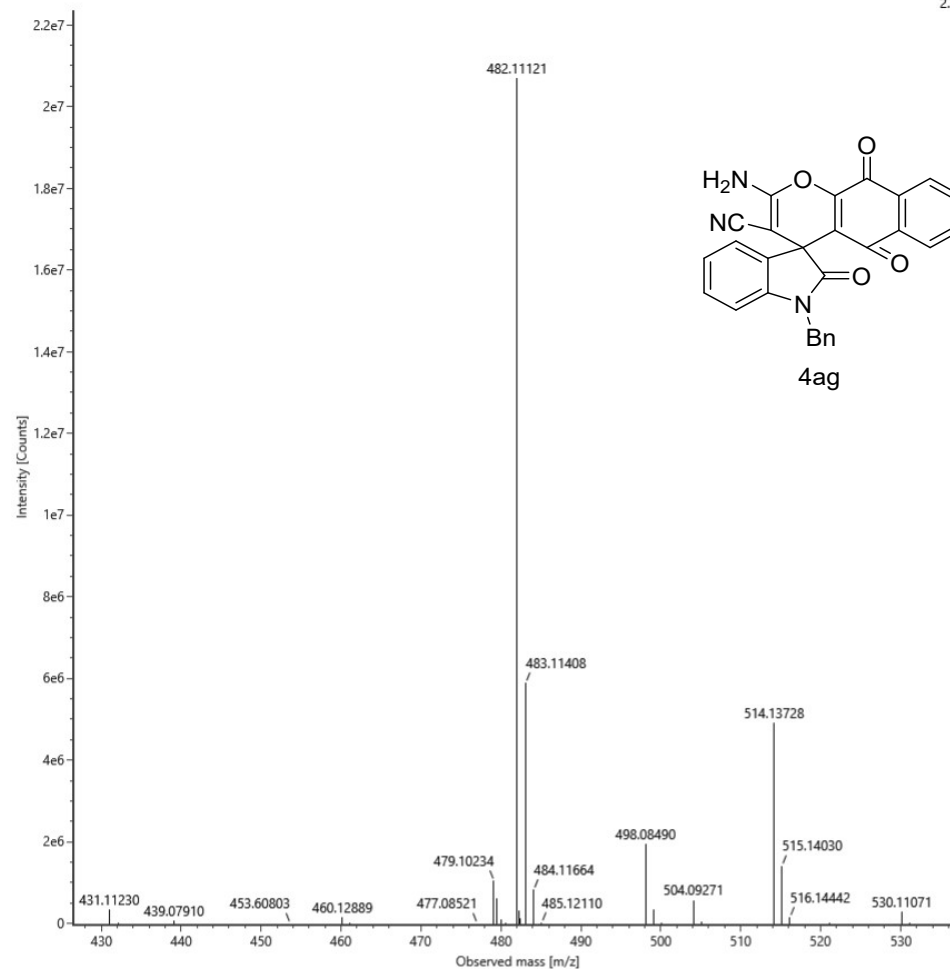


¹³C NMR of Compound **4ag** (101 MHz, DMSO-*d*₆)

Item name: Yes-10
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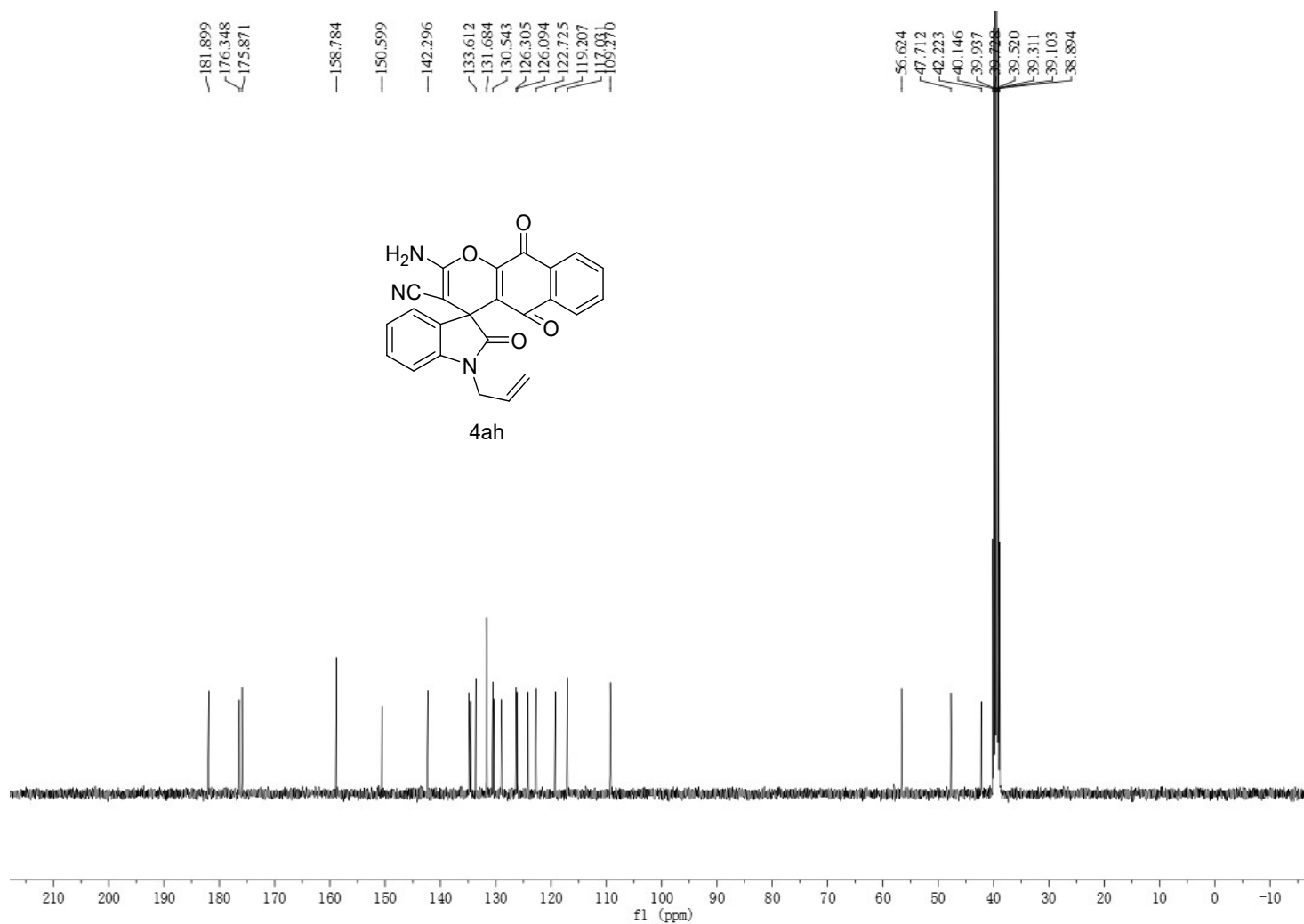
2.24e7



HRMS of Compound **4ag**



¹H NMR of Compound **4ah** (400 MHz, DMSO-*d*₆)

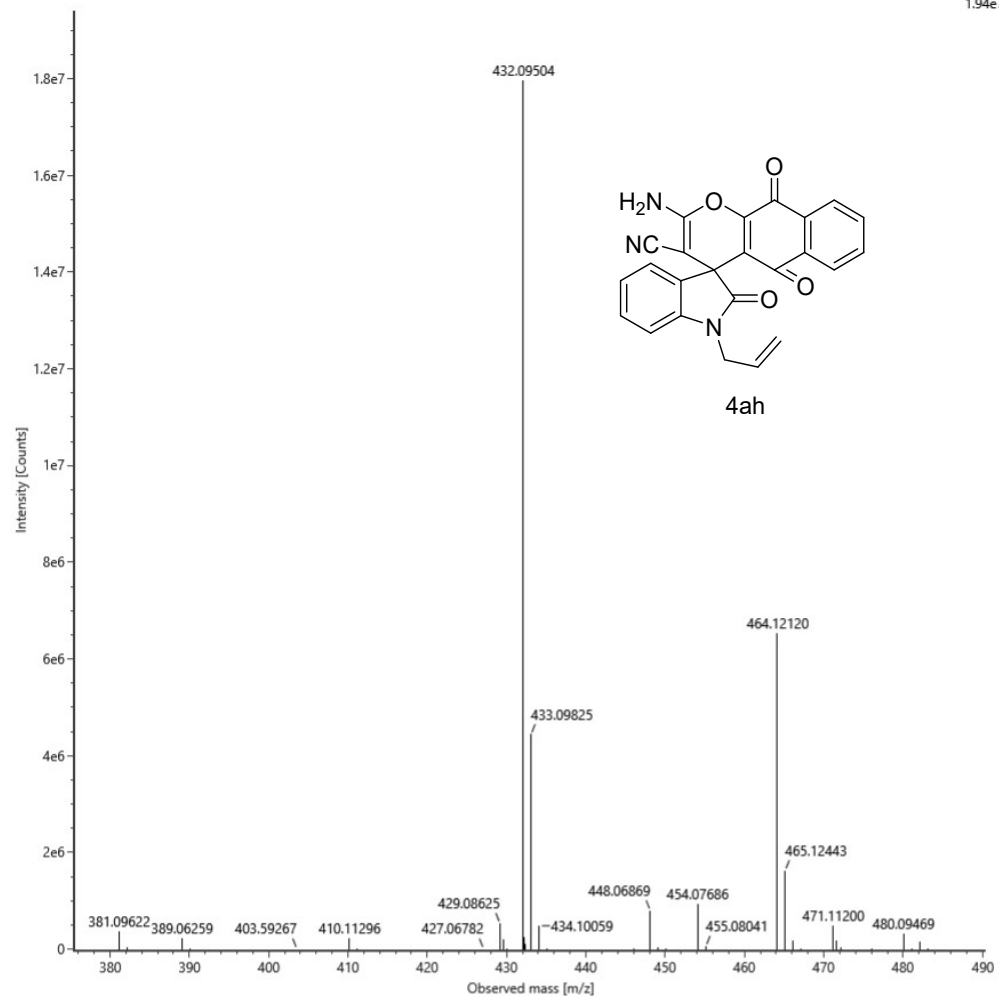


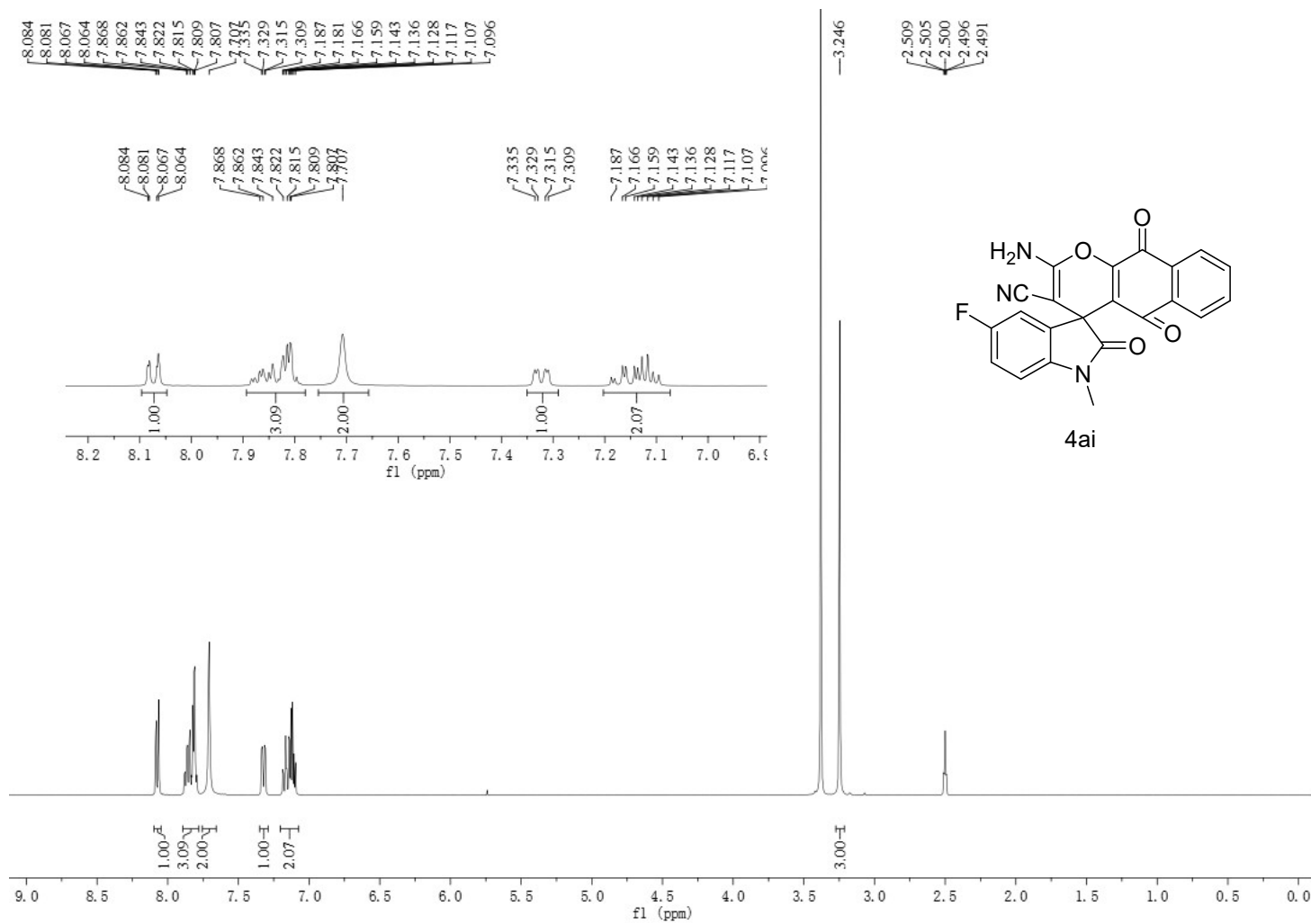
¹³C NMR of Compound **4ah** (101 MHz, DMSO-*d*₆)

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Item description:

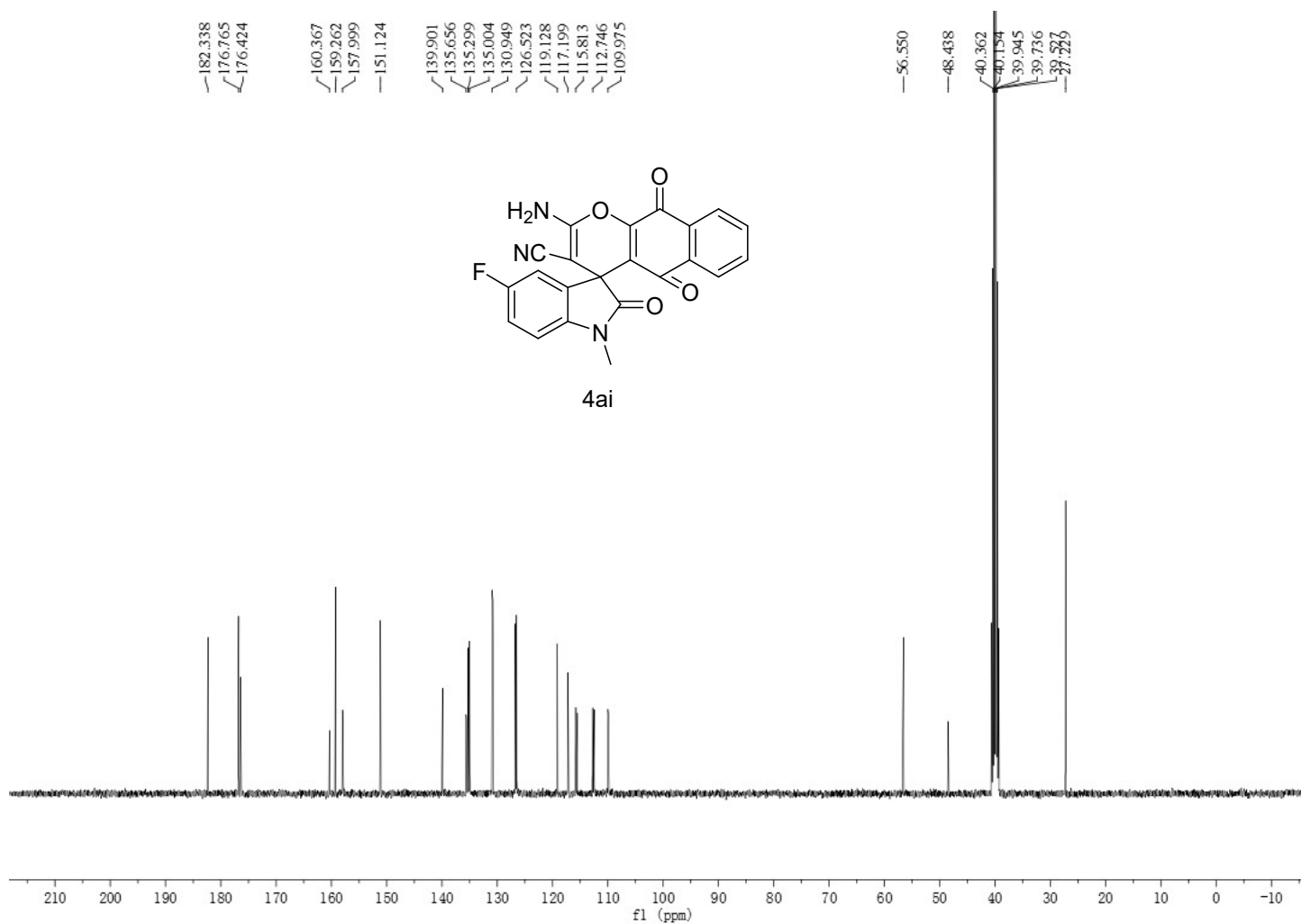
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1.94e7





¹H NMR of Compound 4ai (400 MHz, DMSO-*d*₆)

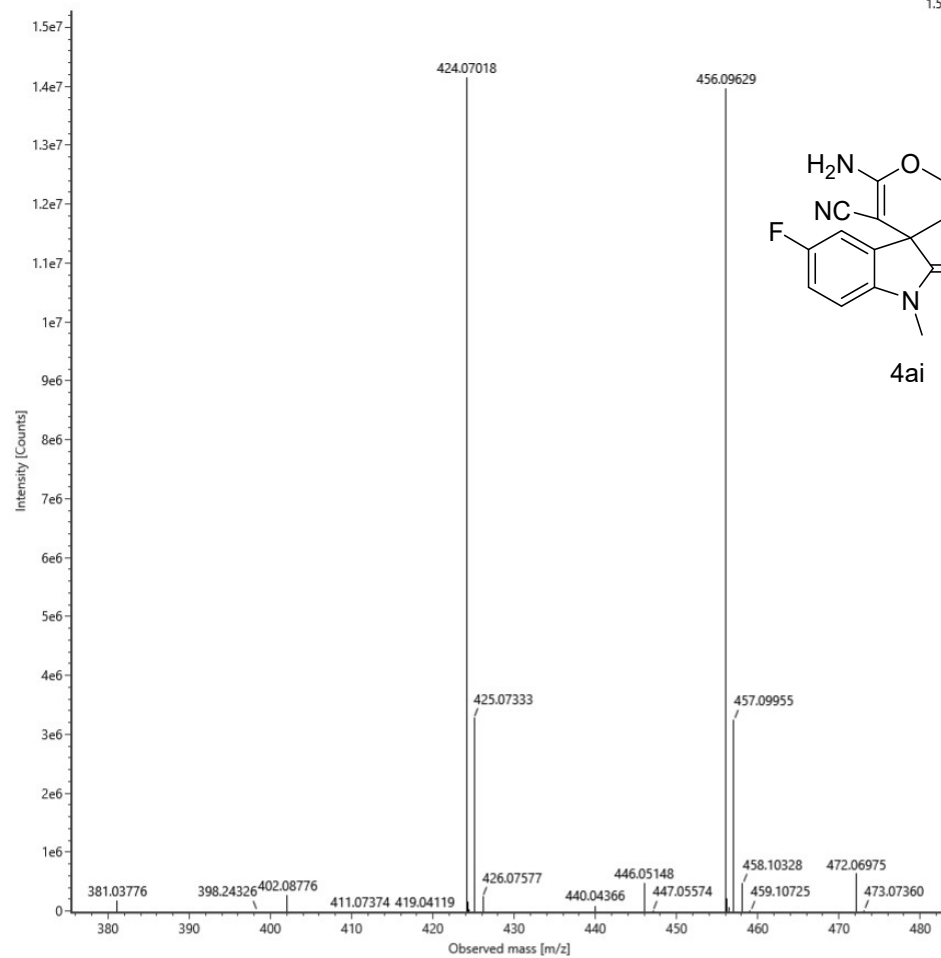


¹³C NMR of Compound **4ai** (101 MHz, DMSO-*d*₆)

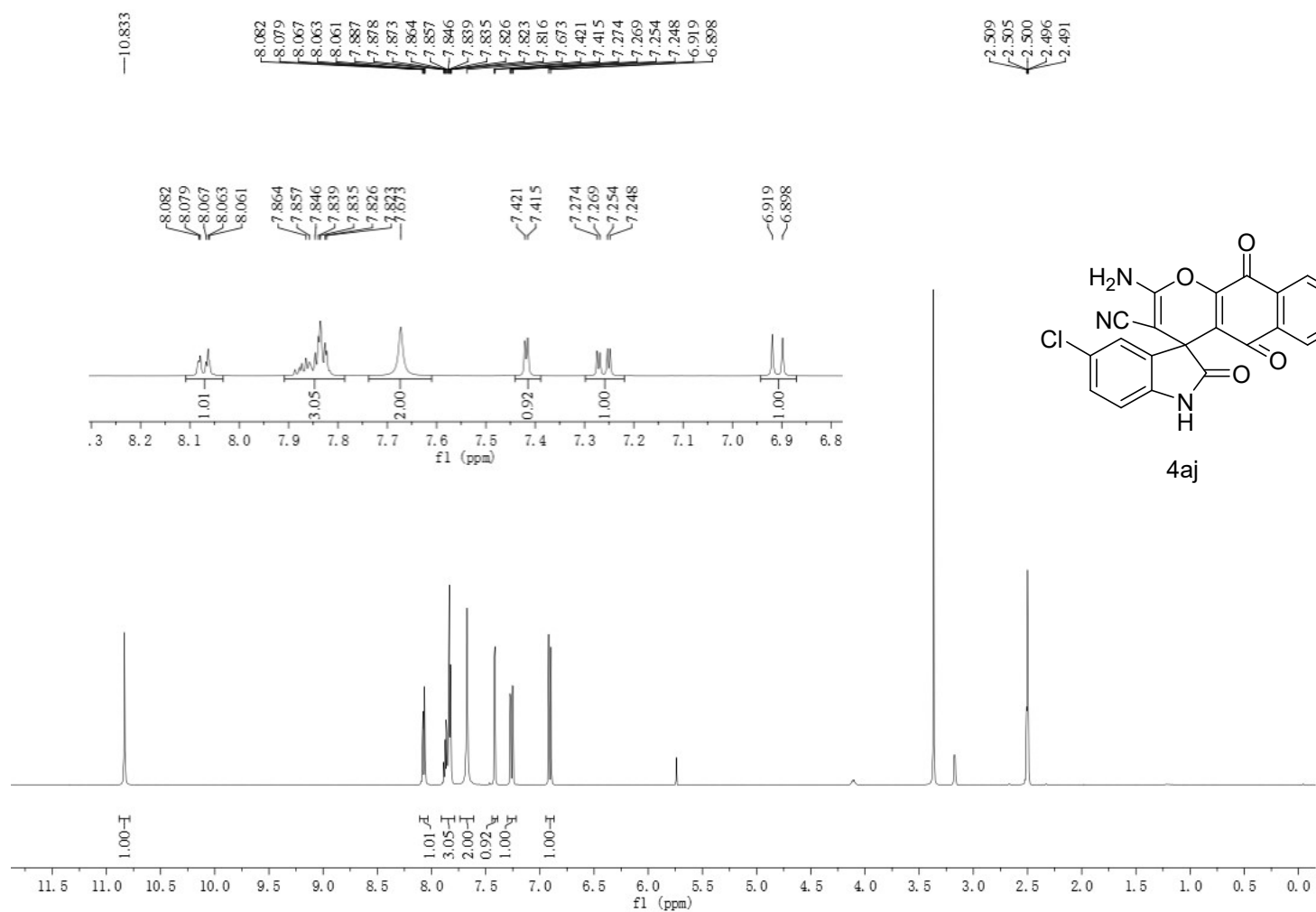
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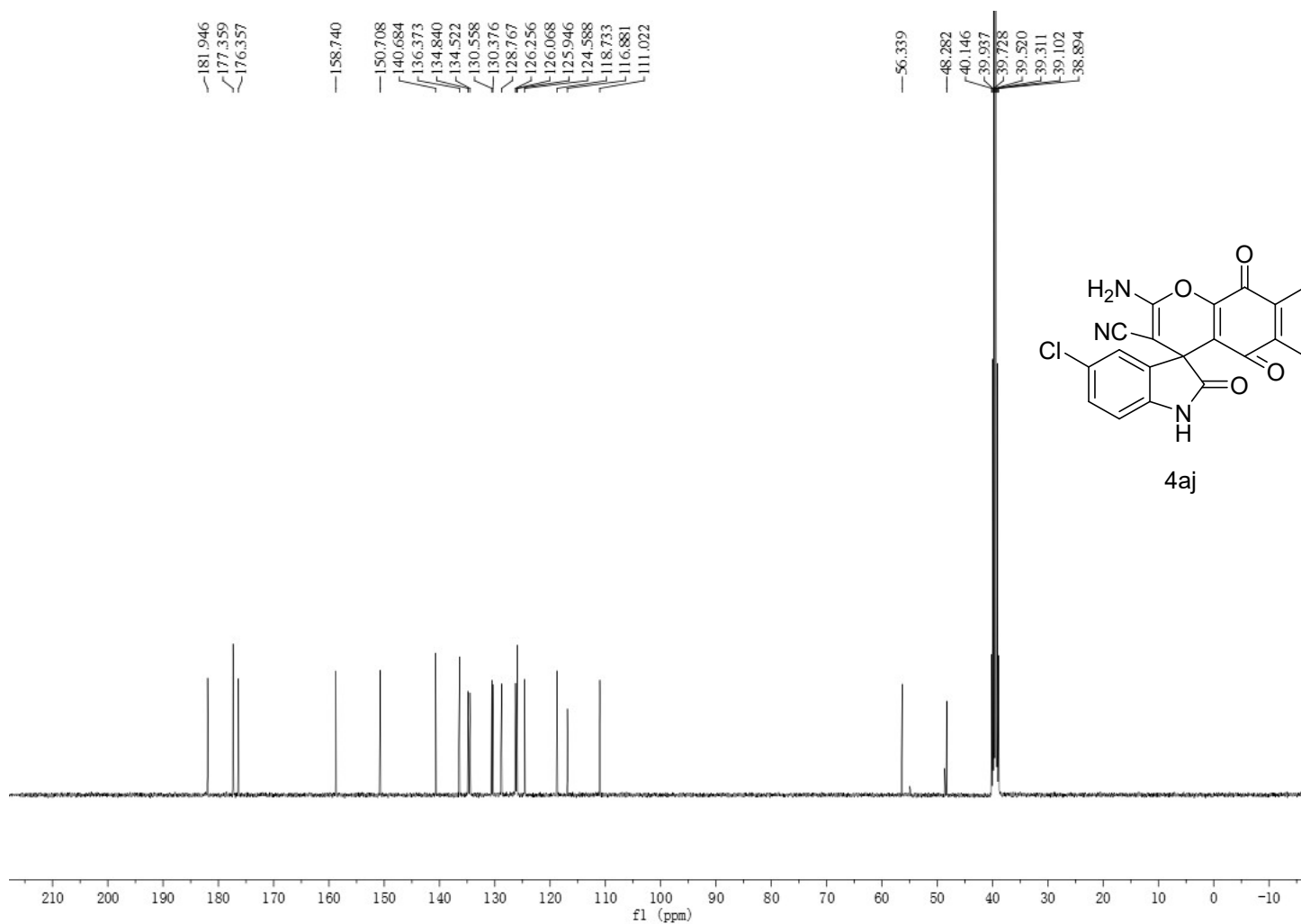
1.53e7



HRMS of Compound 4ai



¹H NMR of Compound 4aj (400 MHz, DMSO-*d*₆)

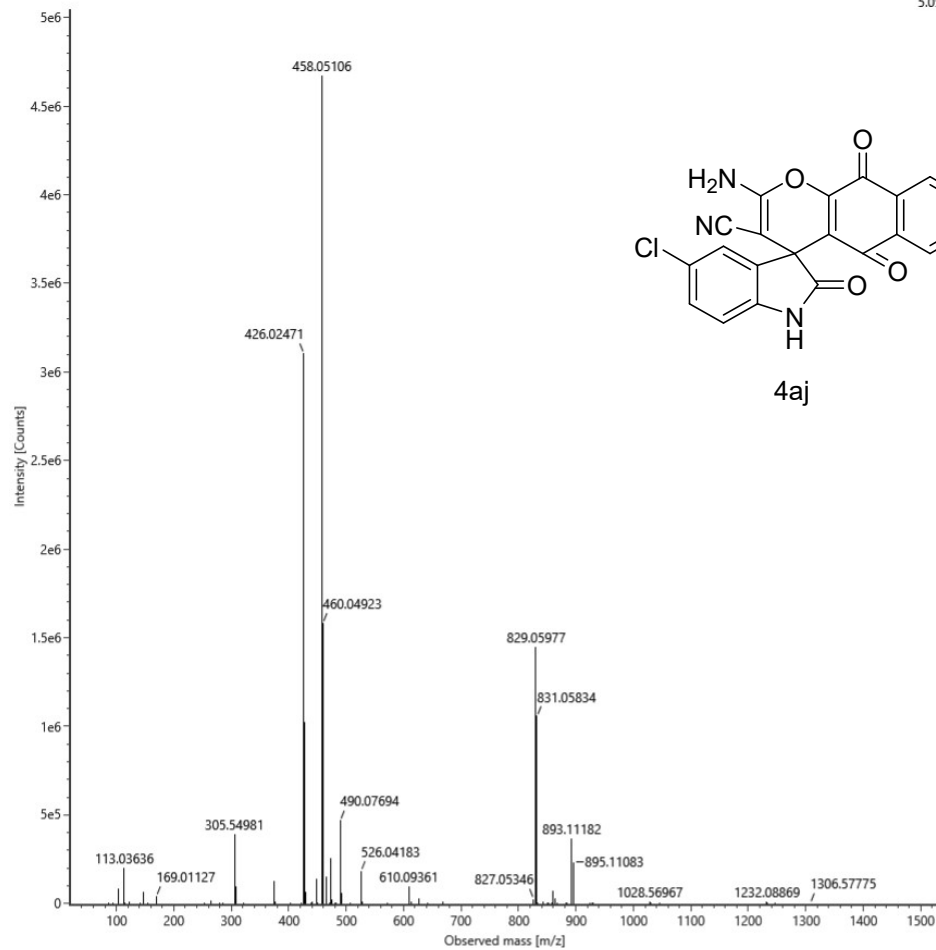


¹³C NMR of Compound **4aj** (101 MHz, DMSO-*d*₆)

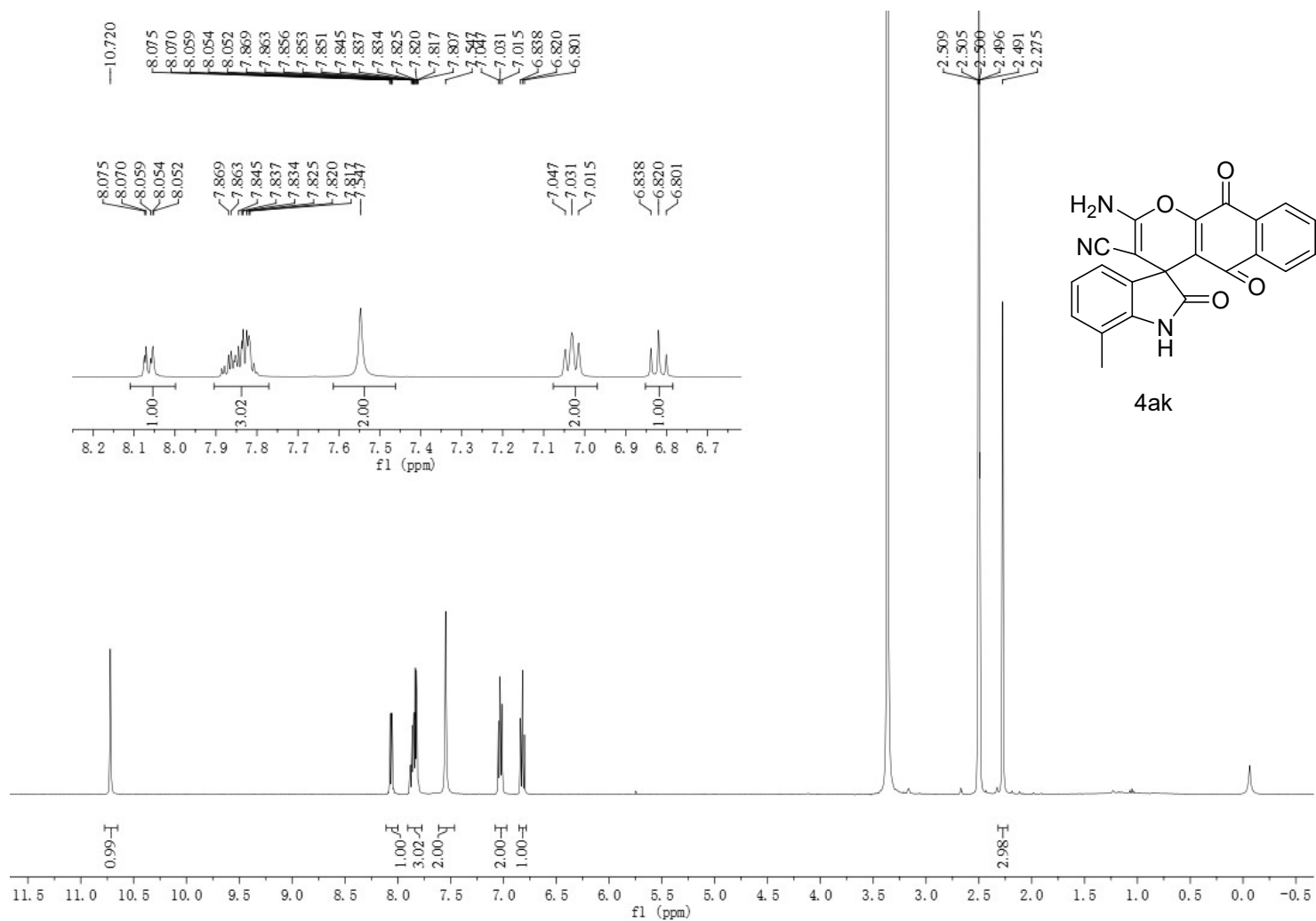
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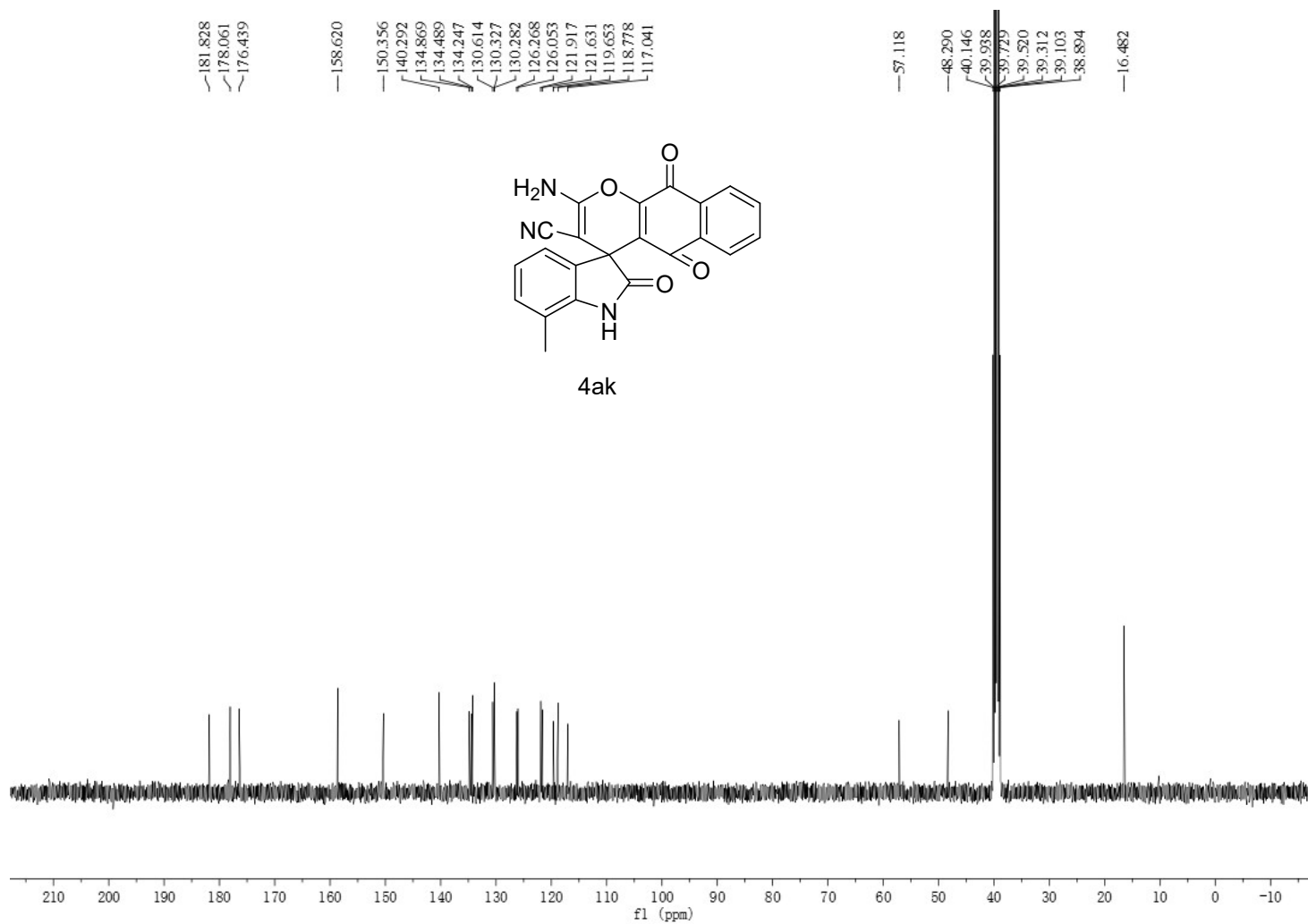
5.05e6



HRMS of Compound 4aj



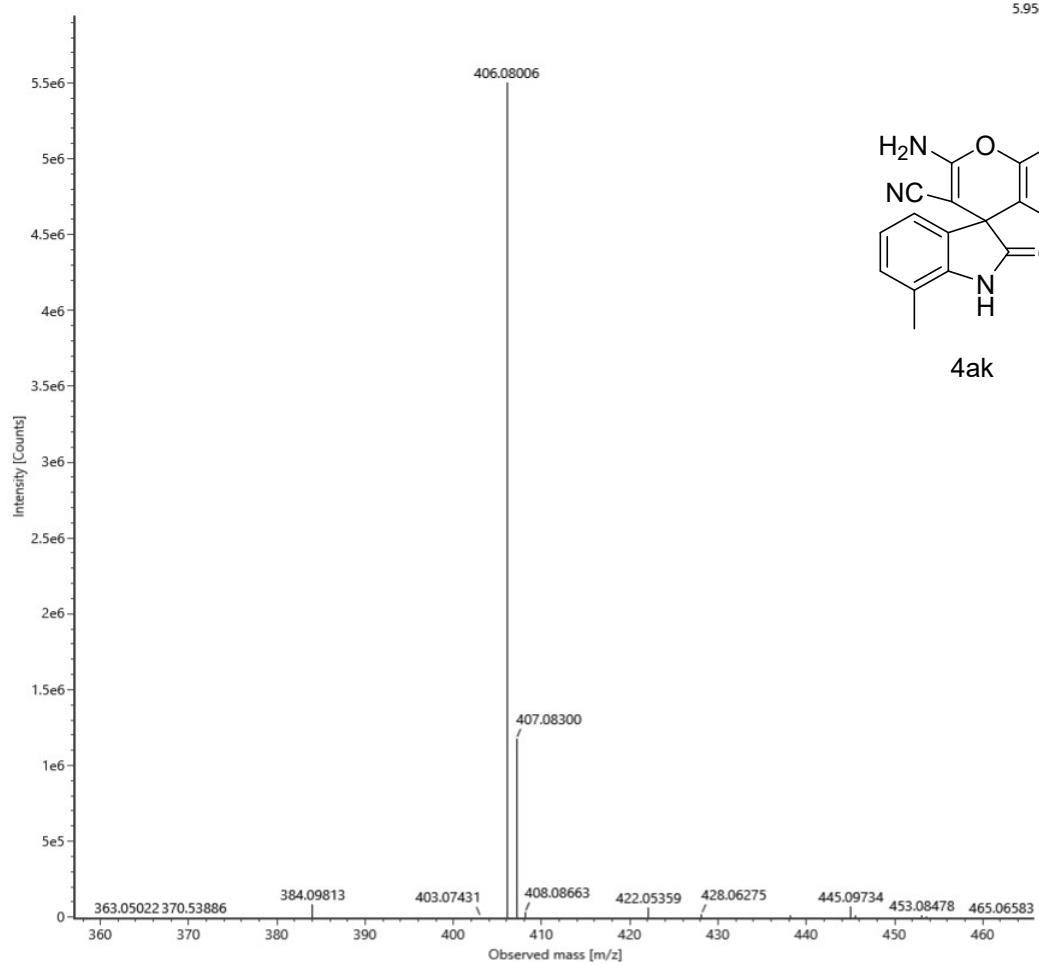
¹H NMR of Compound **4ak** (400 MHz, DMSO-*d*₆)



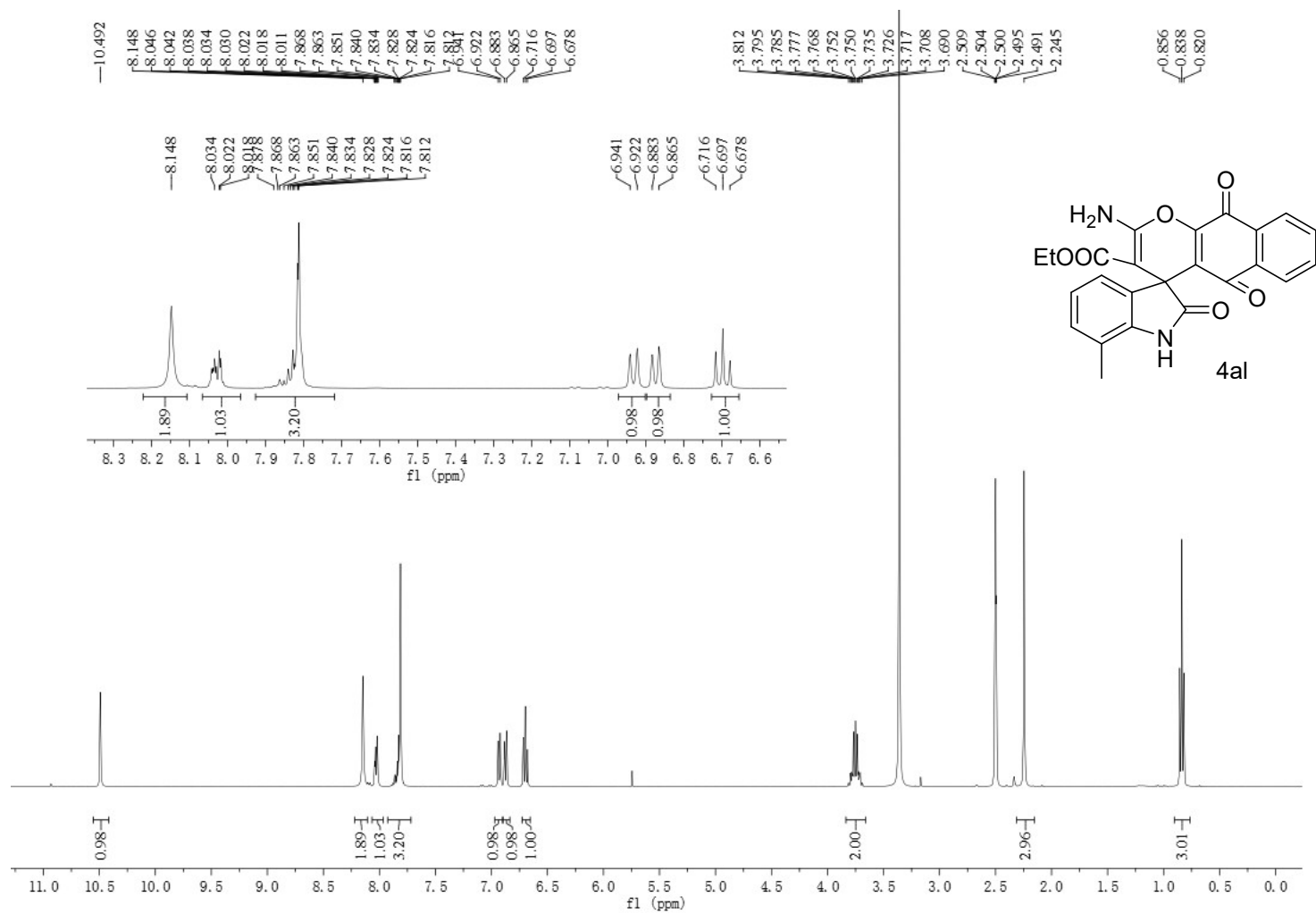
¹³C NMR of Compound **4ak** (101 MHz, DMSO-*d*₆)

Item name: Yes-17
Item description:

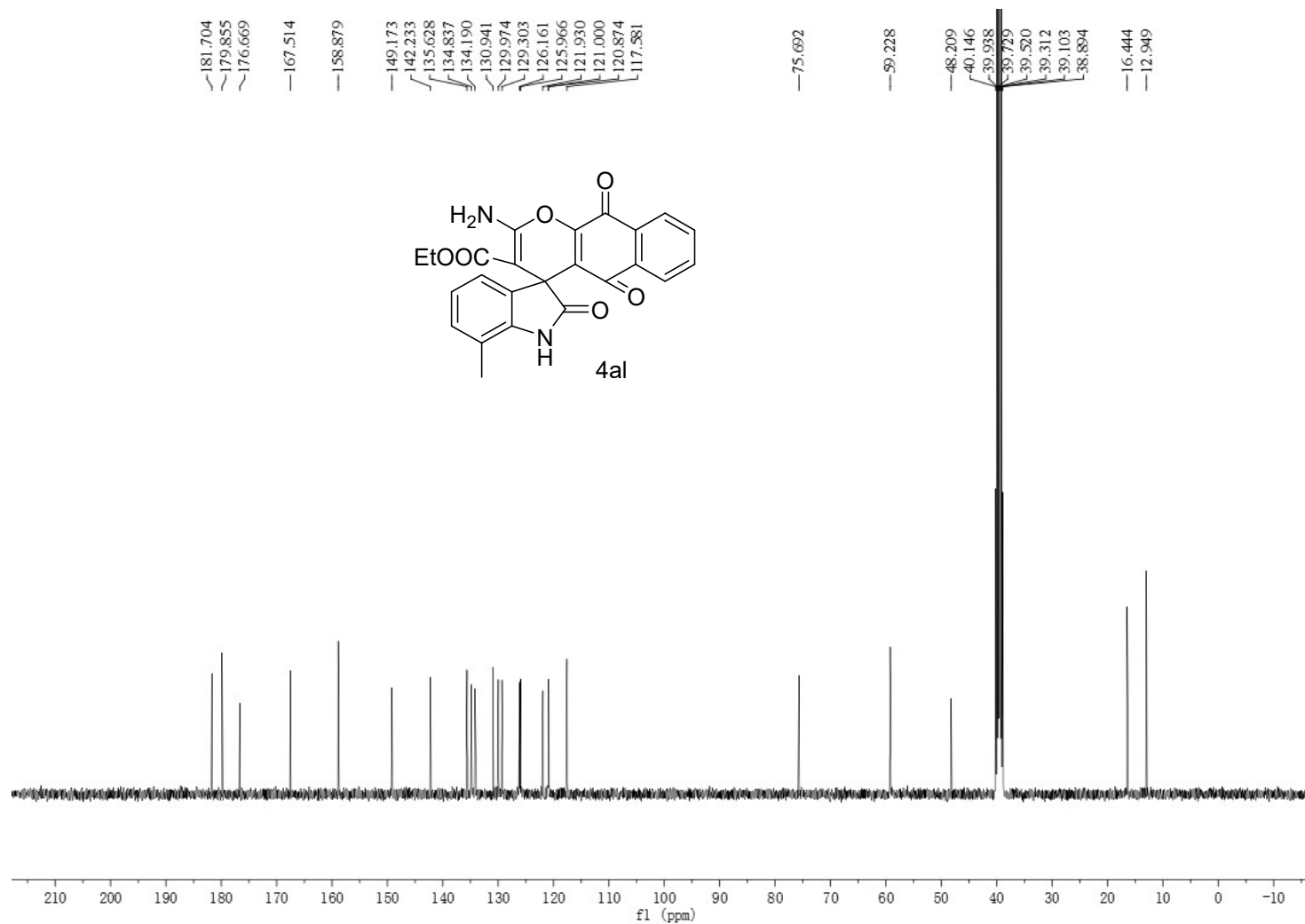
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HRMS of Compound **4ak**



¹H NMR of Compound **4al** (400 MHz, DMSO-*d*₆)

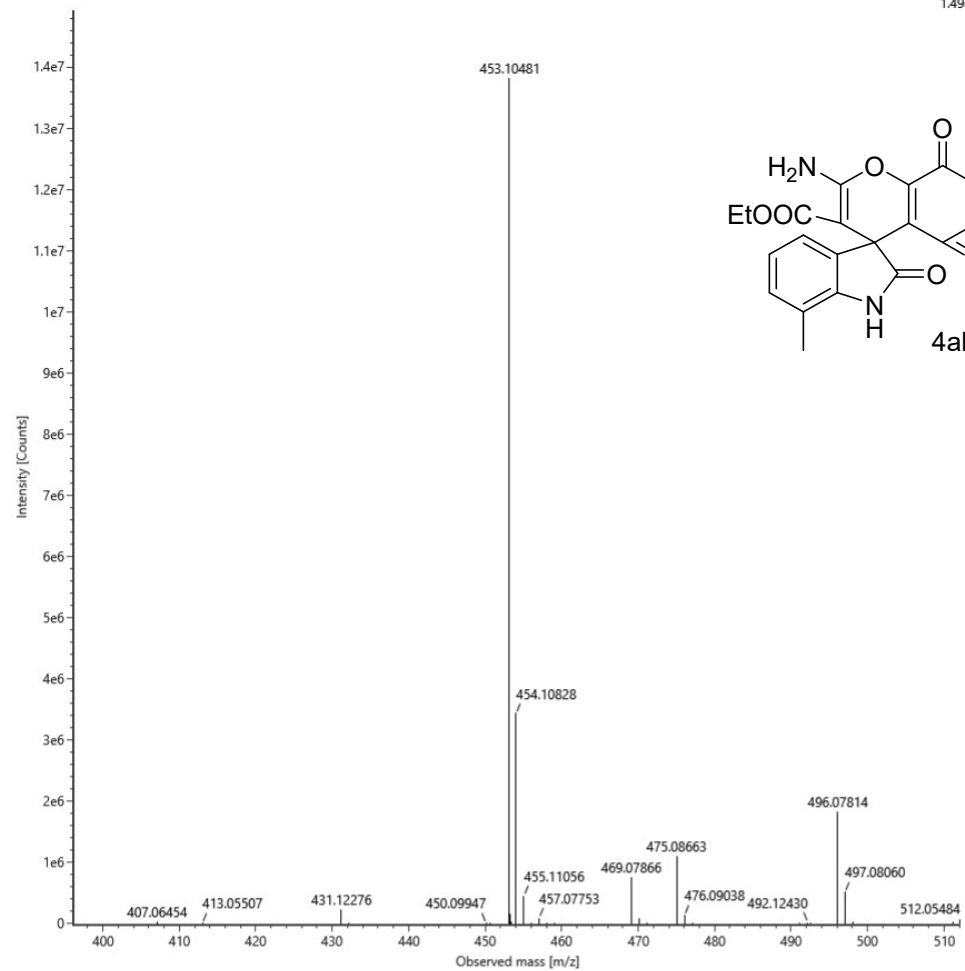


¹³C NMR of Compound **4al** (101 MHz, DMSO-*d*₆)

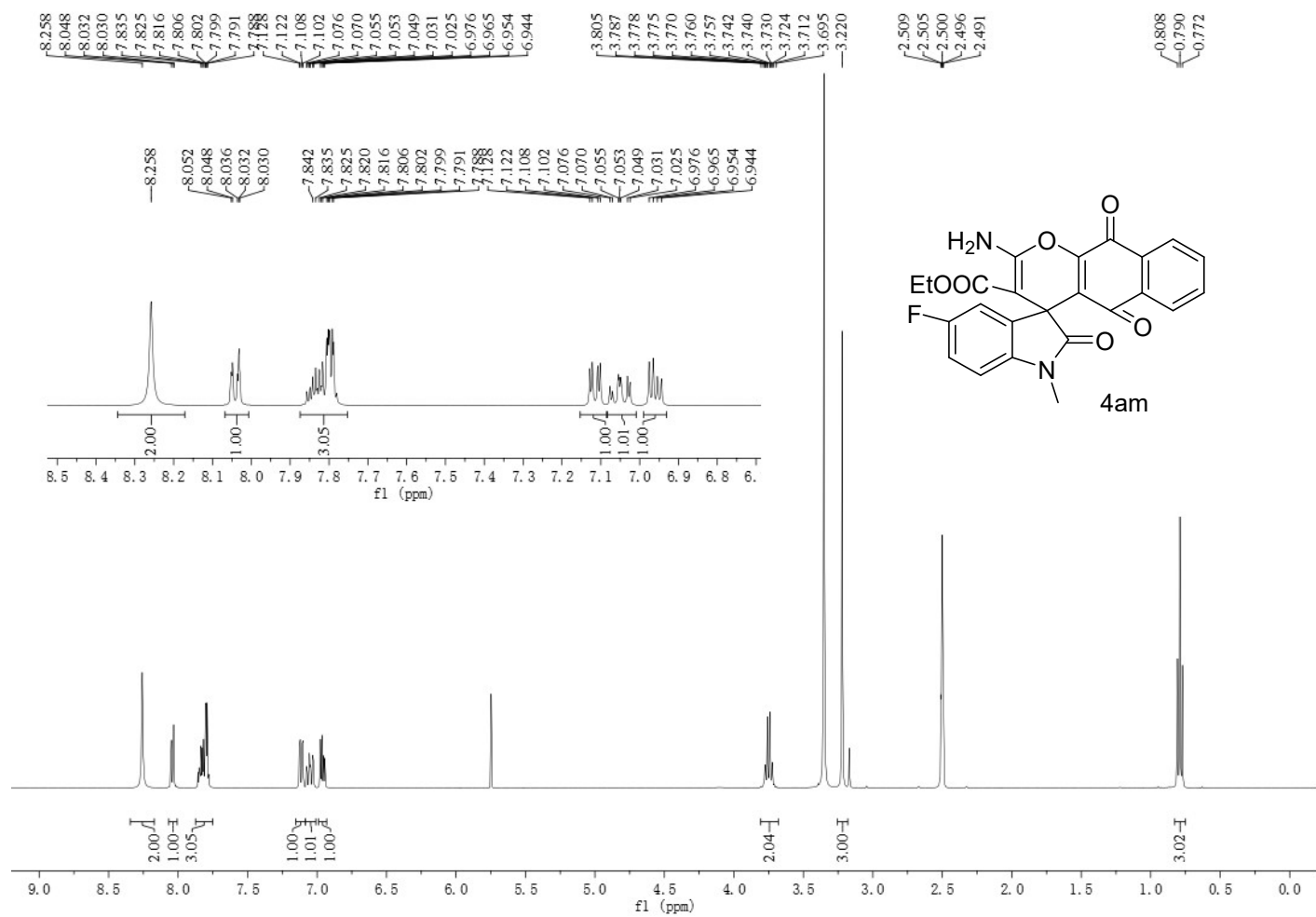
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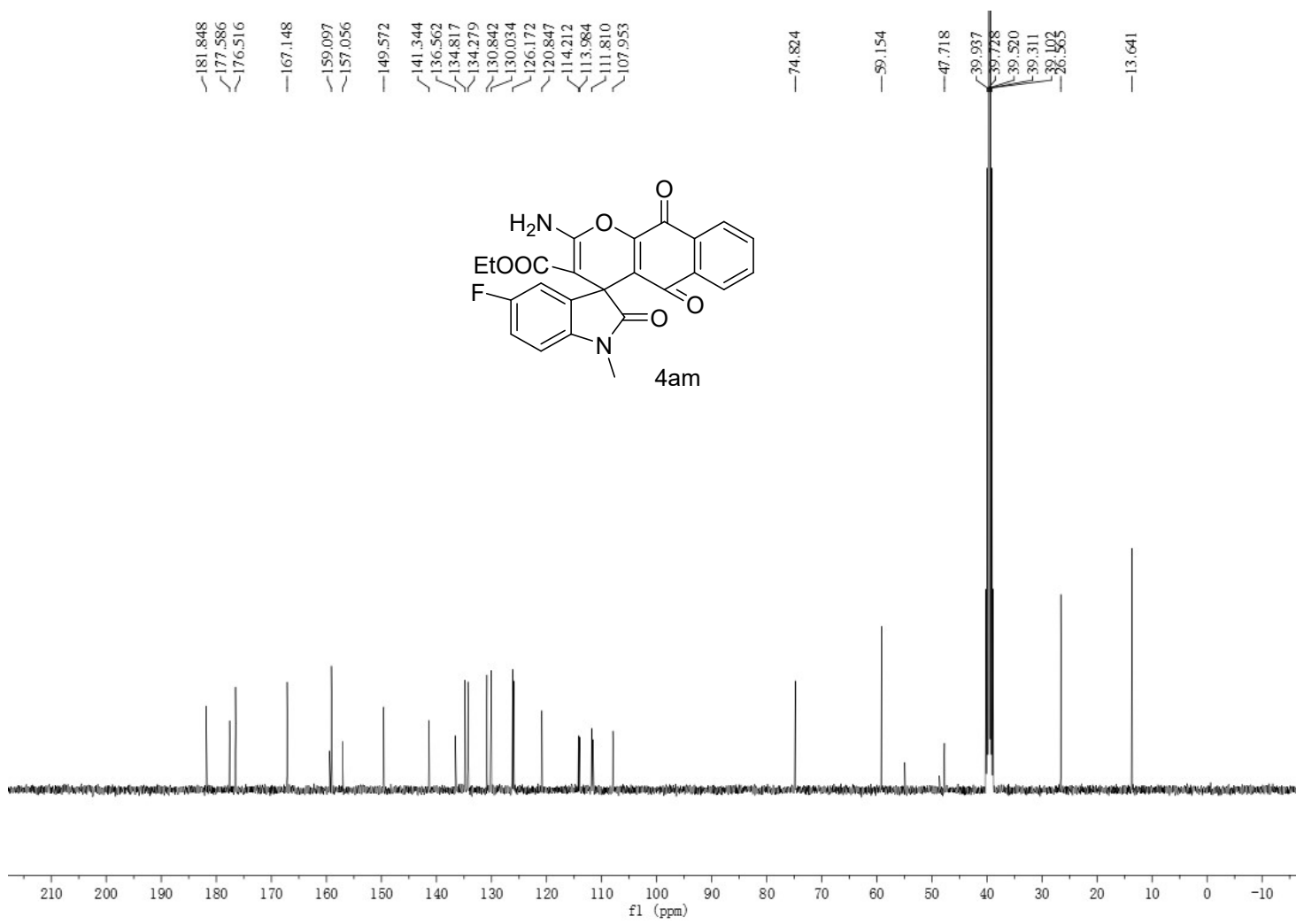
1.49e7



HRMS of Compound 4al



^1H NMR of Compound **4am** (400 MHz, $\text{DMSO-}d_6$)

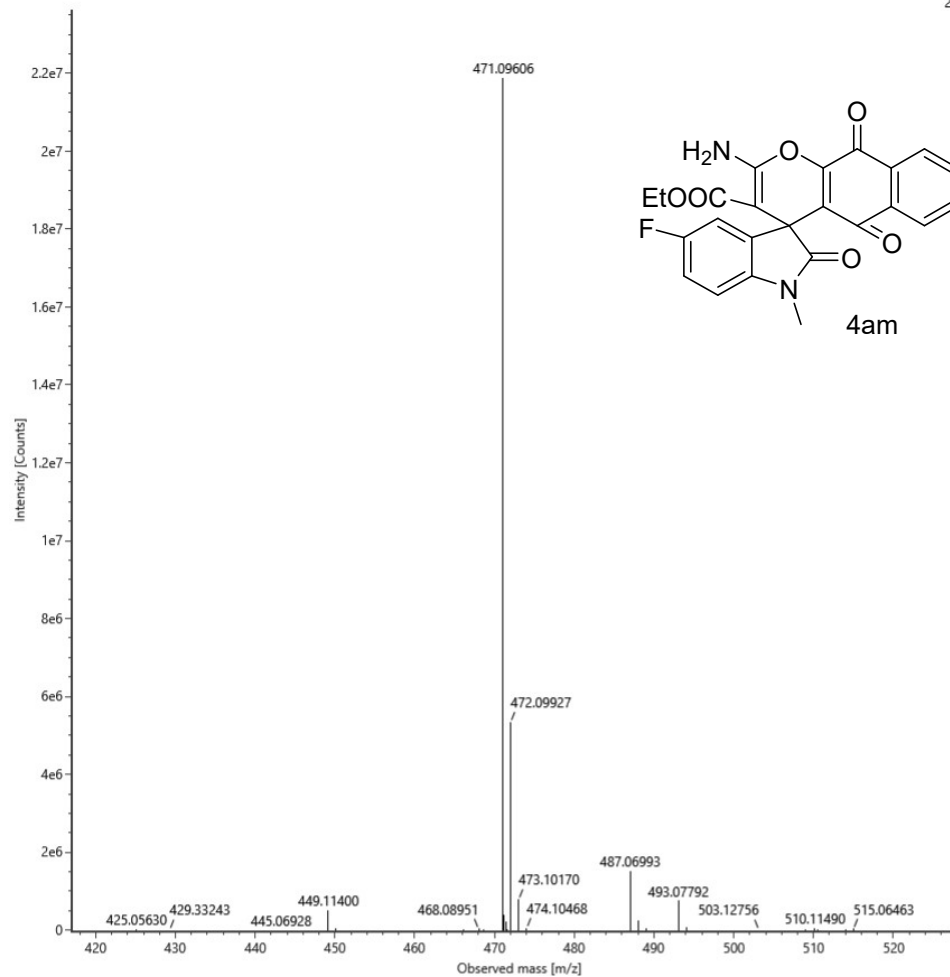


¹³C NMR of Compound **4am** (101 MHz, DMSO-*d*₆)

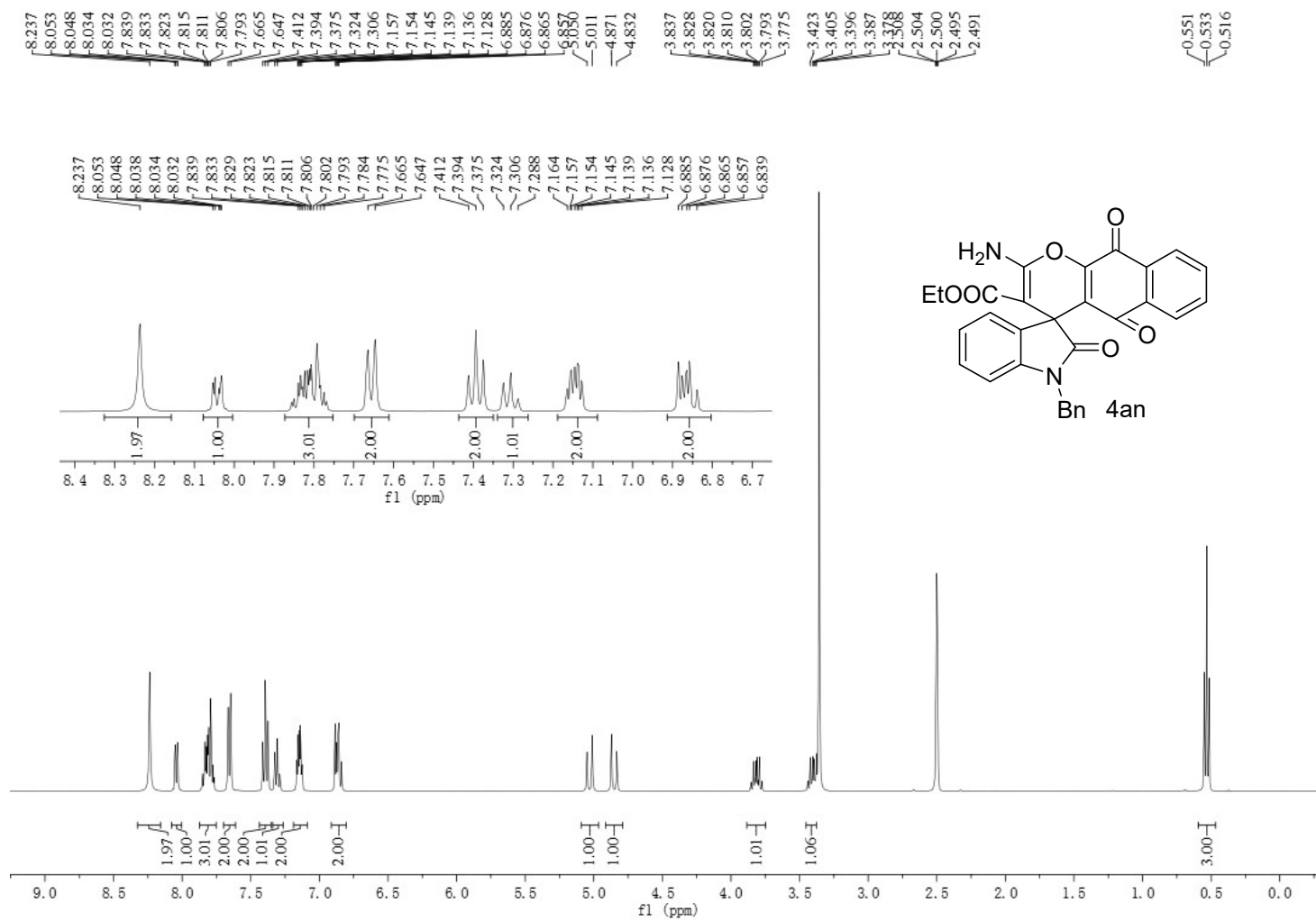
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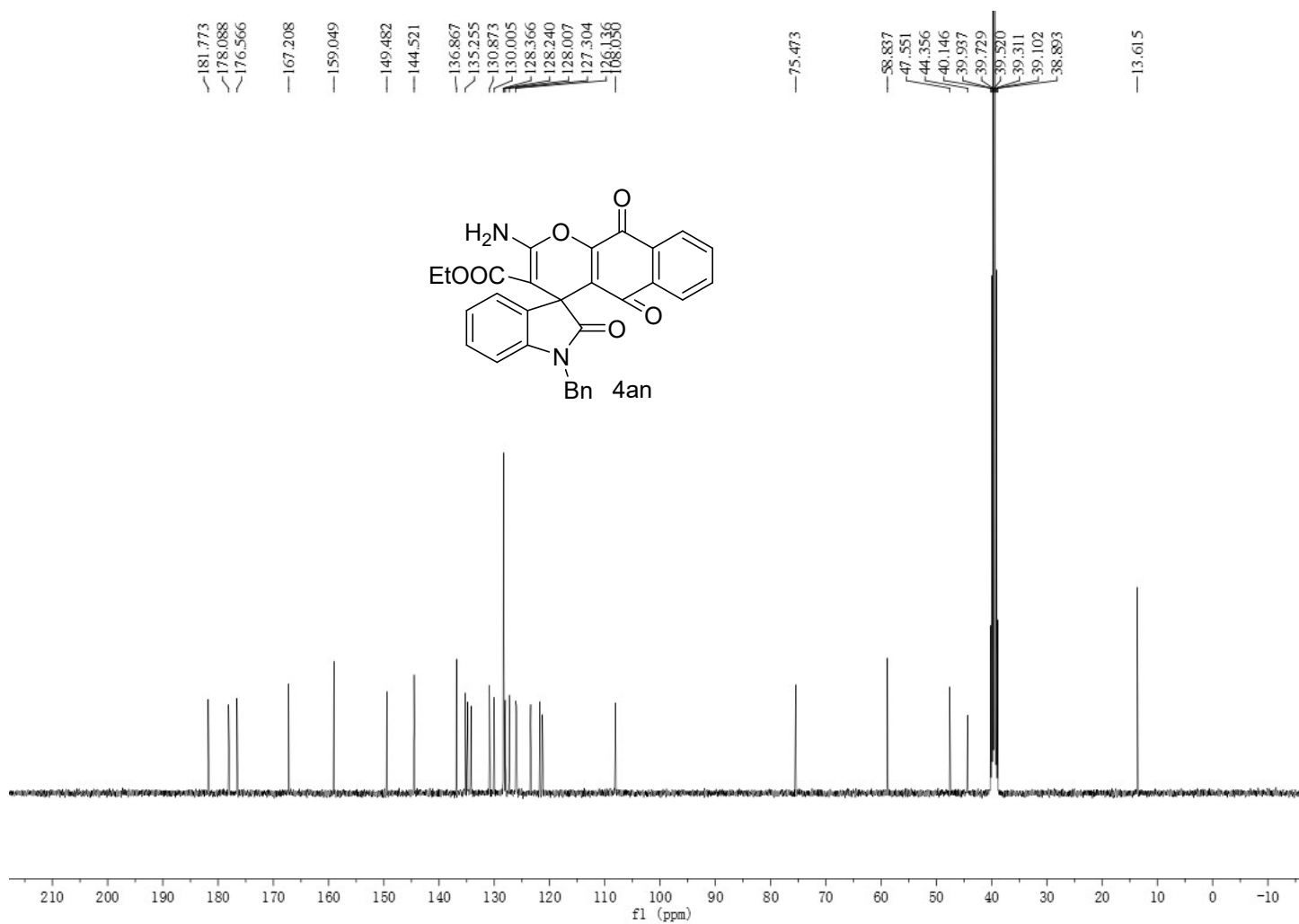
2.36e7



HRMS of Compound **4am**



¹H NMR of Compound **4an** (400 MHz, DMSO-*d*₆)

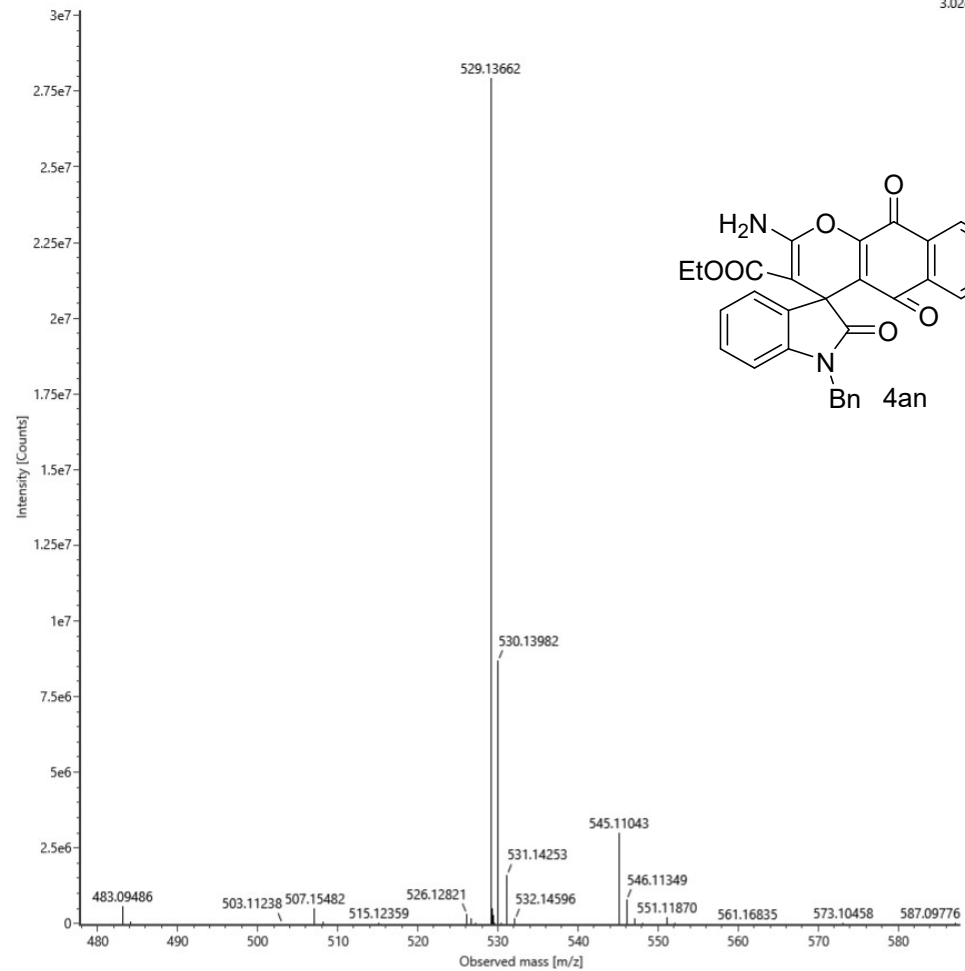


¹³C NMR of Compound **4an** (101 MHz, DMSO-*d*₆)

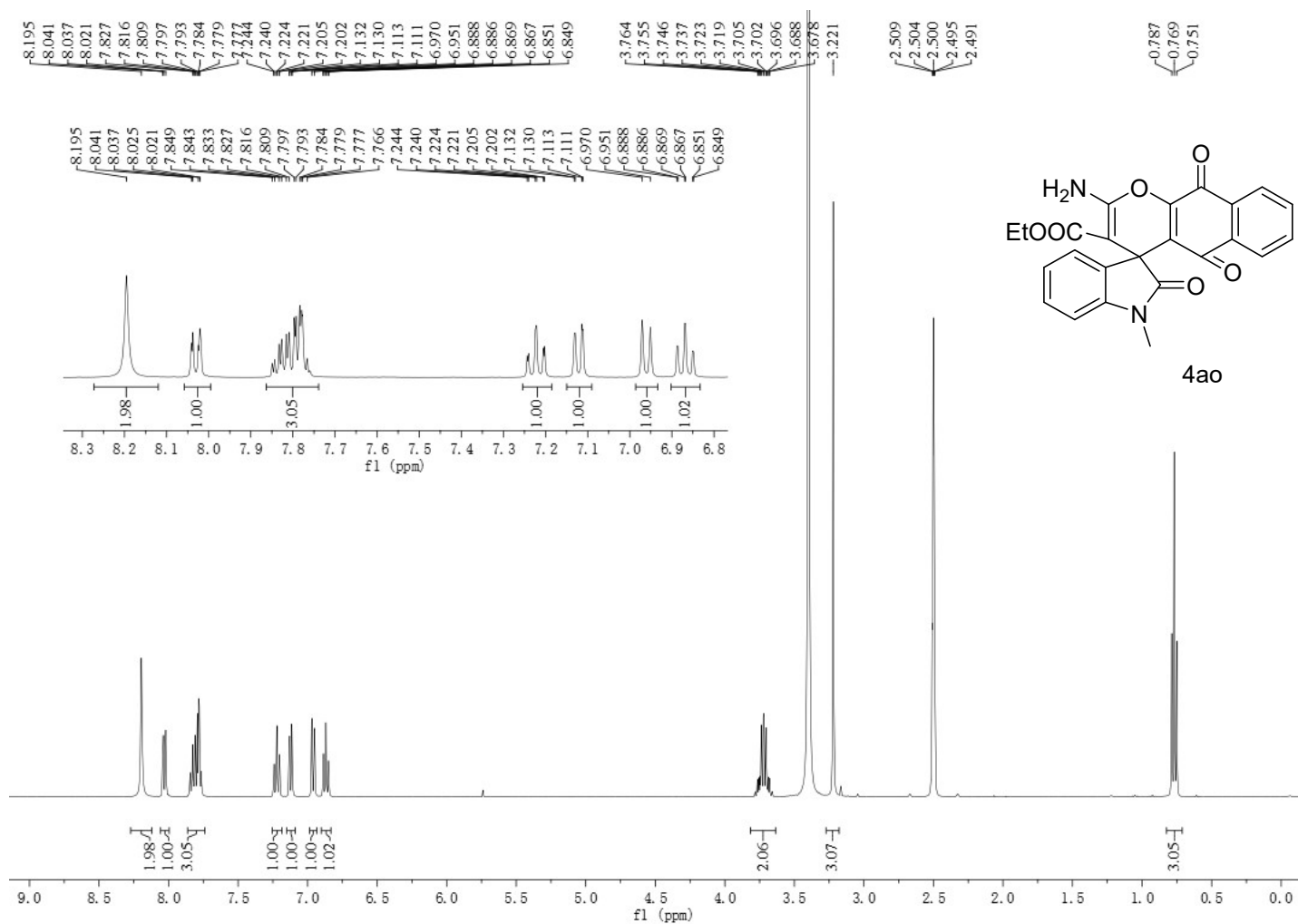
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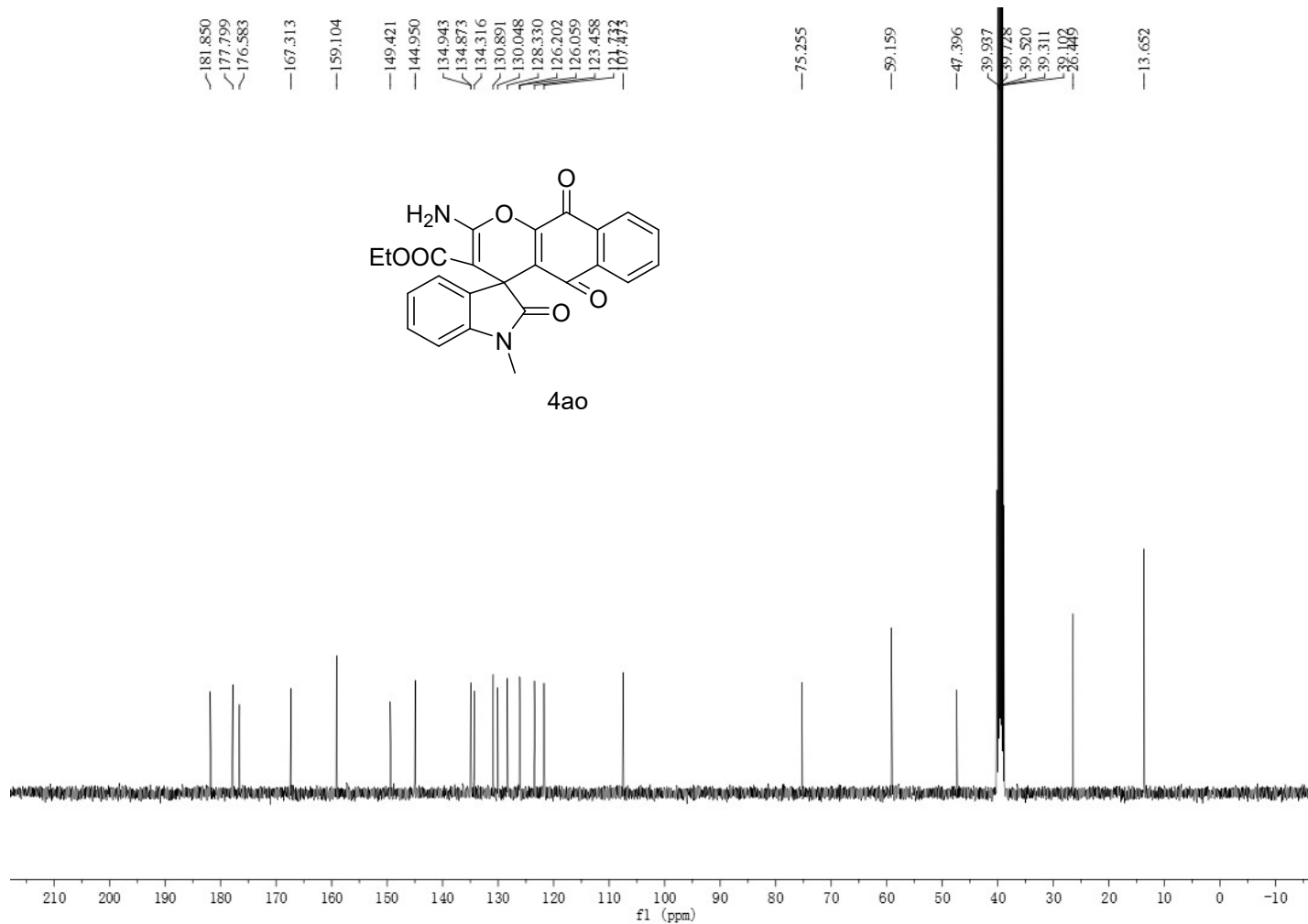
3.02e7



HRMS of Compound 4an



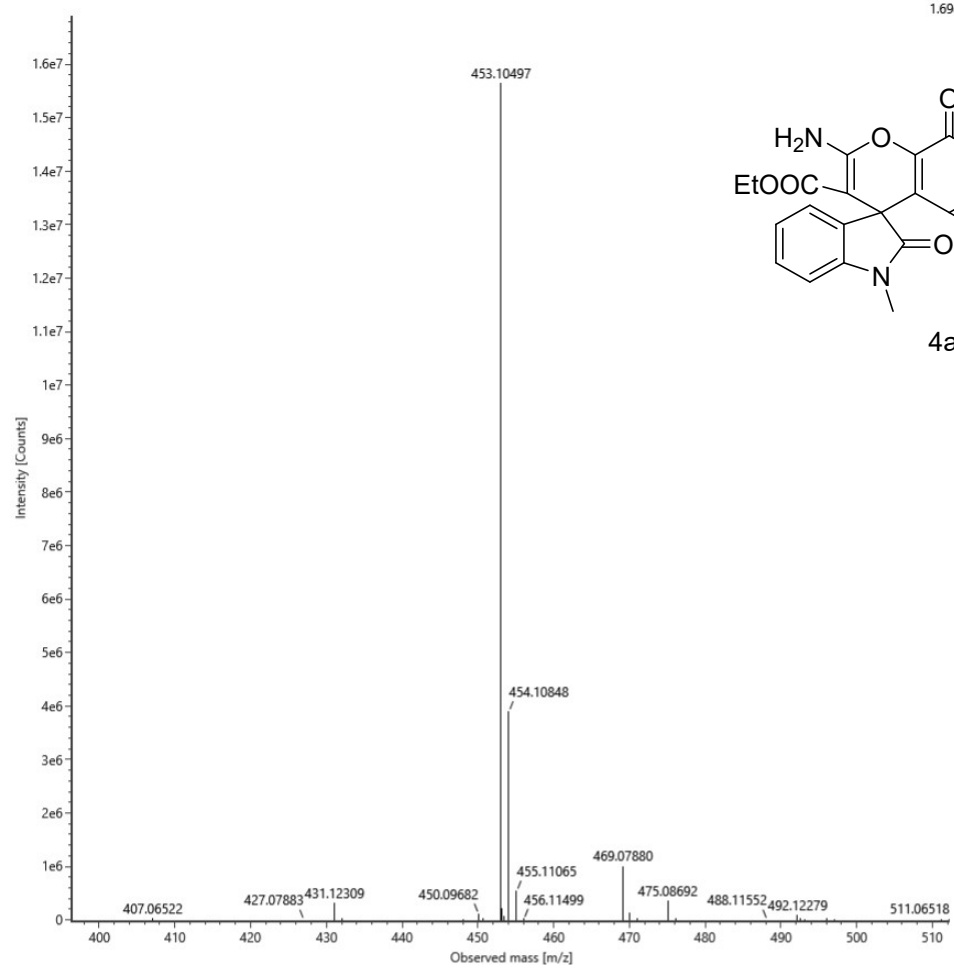
¹H NMR of Compound **4ao** (400 MHz, DMSO-*d*₆)



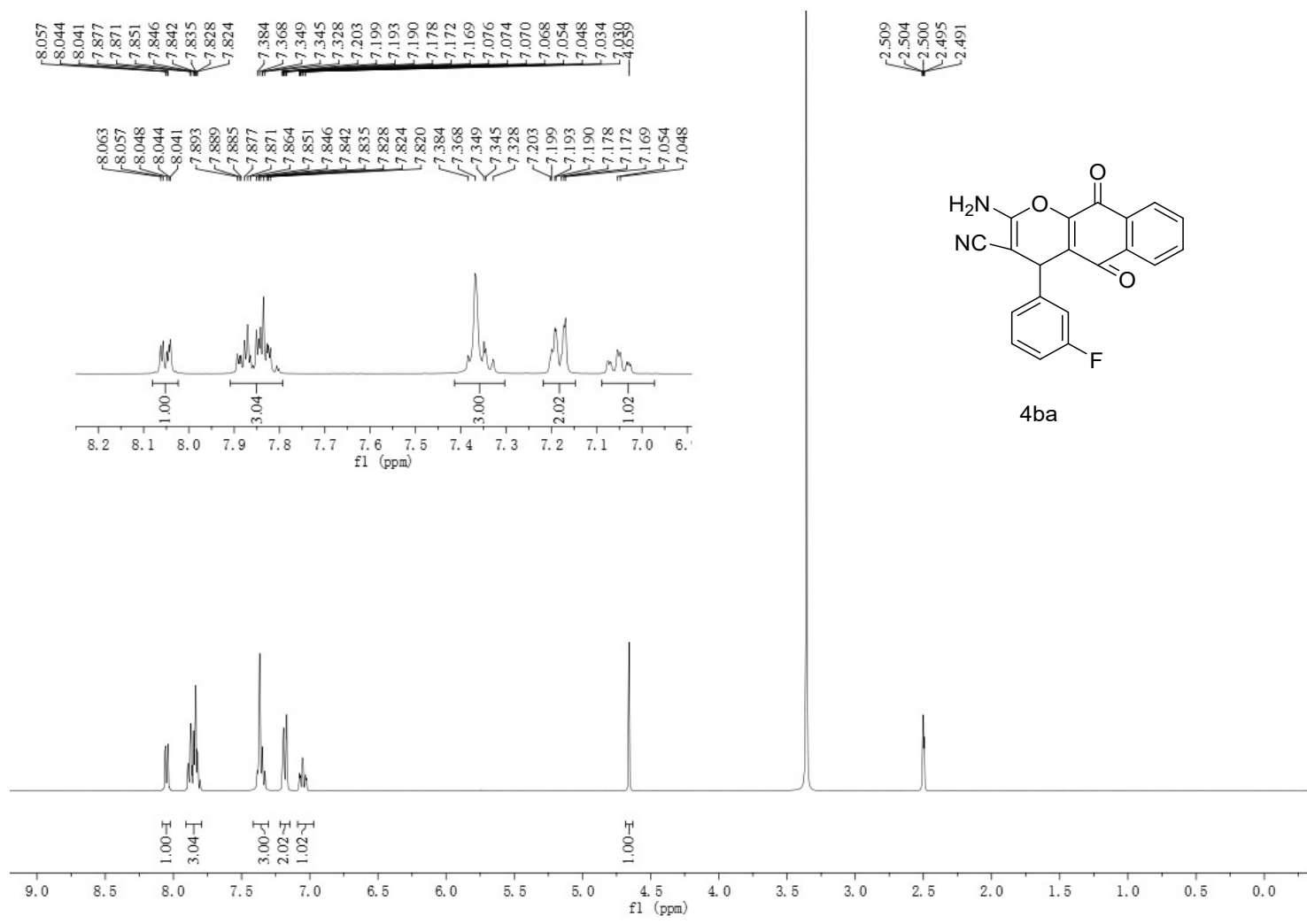
¹³C NMR of Compound **4ao** (101 MHz, DMSO-*d*₆)

Item name: Yes-23
Item description:

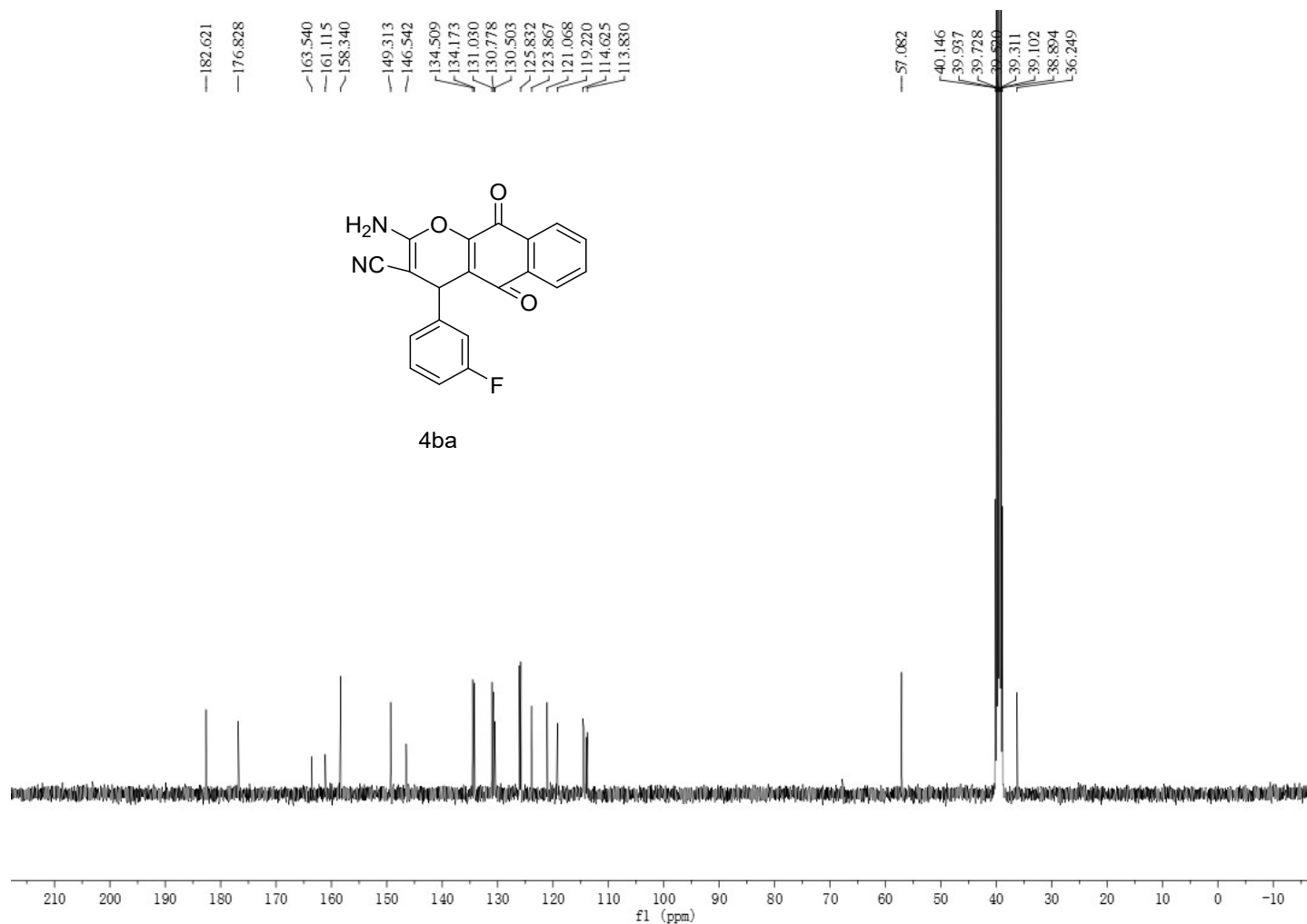
Channel name: 1: Average Time 0.1217 min : TOF MS (50-1500) ESI+ : Centroided : Combined



HRMS of Compound **4ao**



¹H NMR of Compound **4ba** (400 MHz, DMSO-*d*₆)

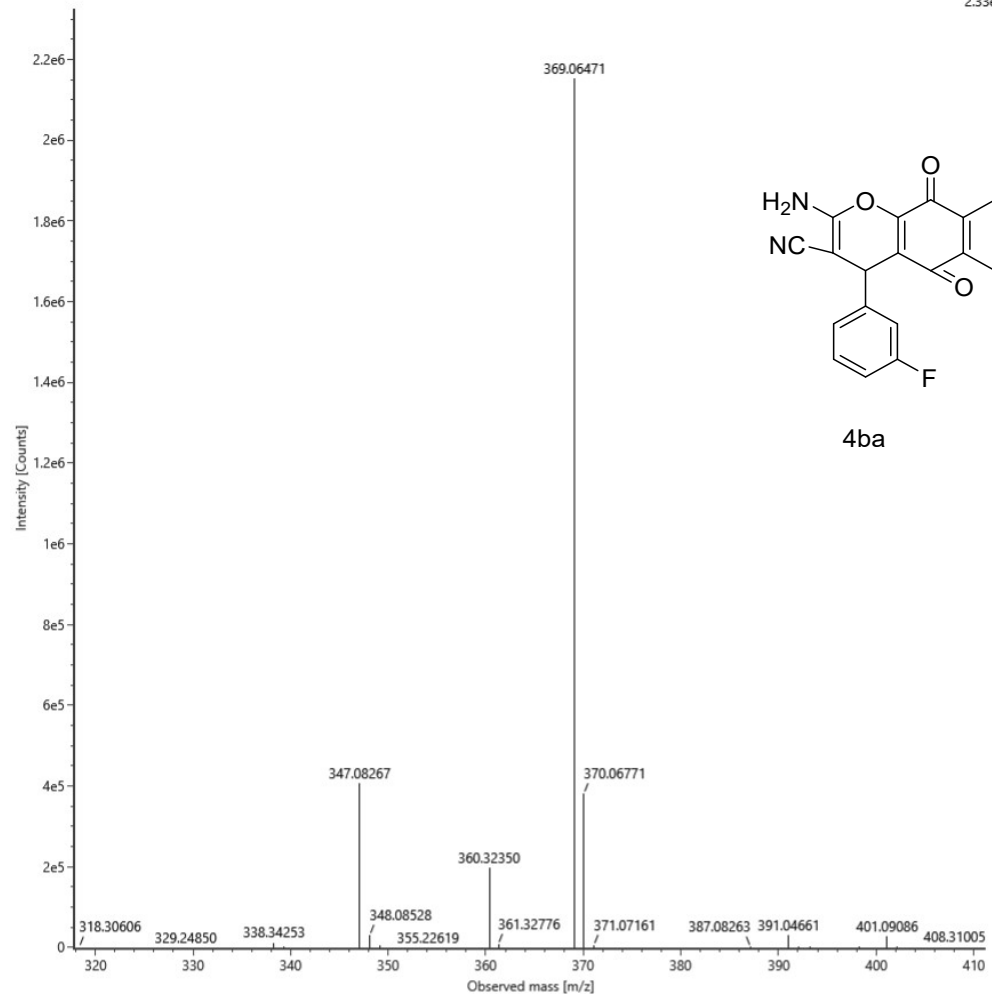


¹³C NMR of Compound **4ba** (101 MHz, DMSO-*d*₆)

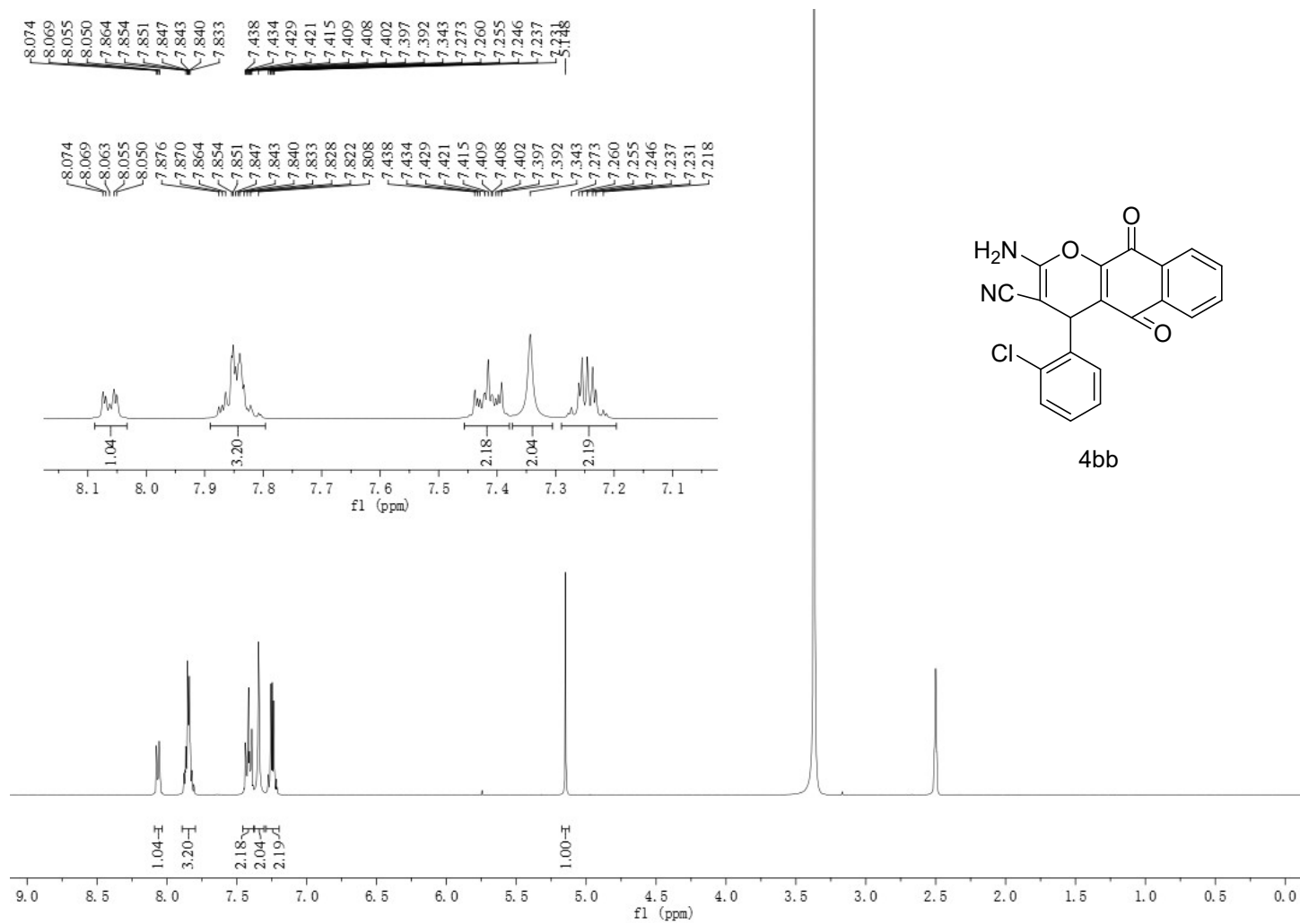
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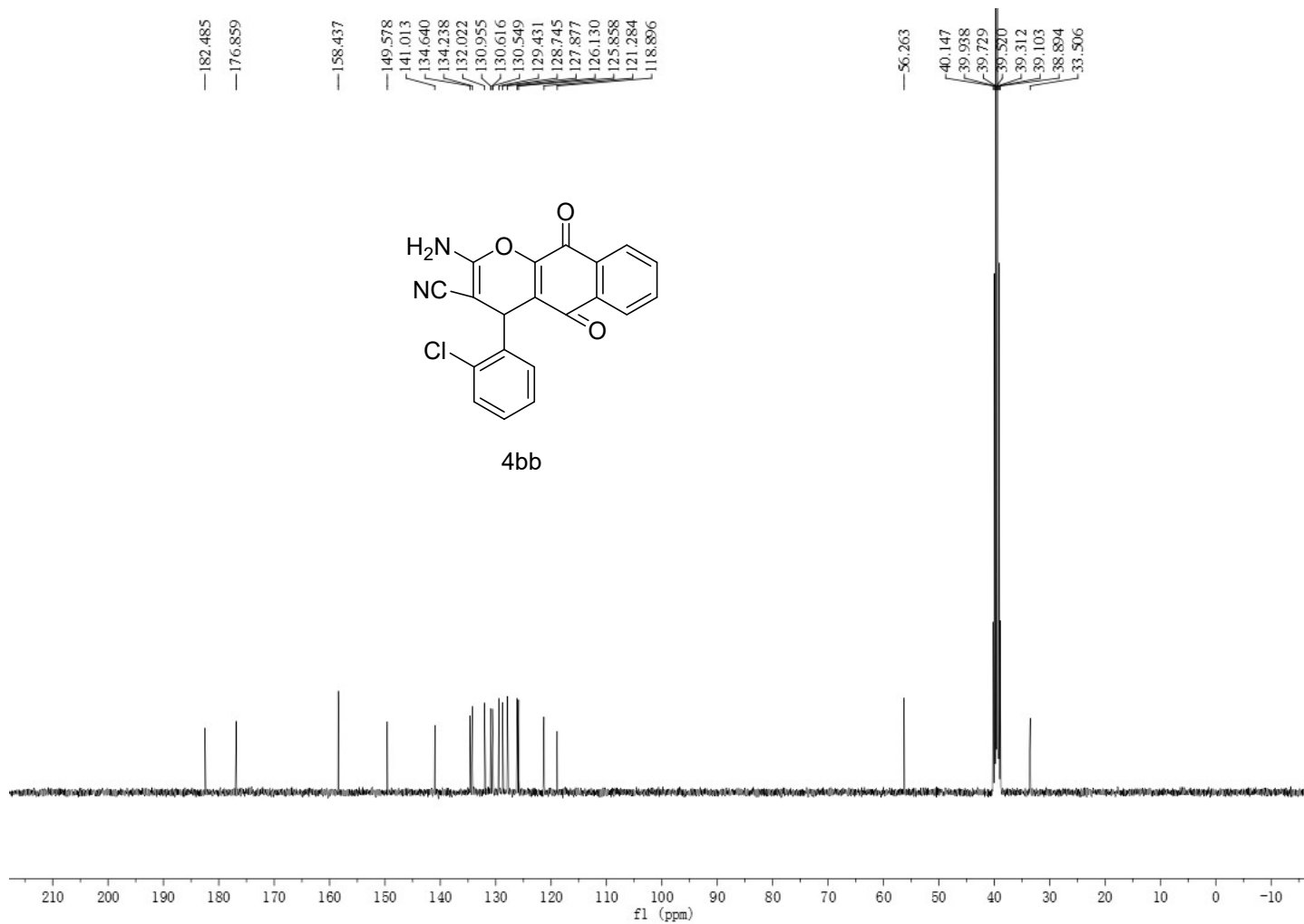
2.33e6



HRMS of Compound **4ba**



¹H NMR of Compound **4bb** (400 MHz, DMSO-*d*₆)

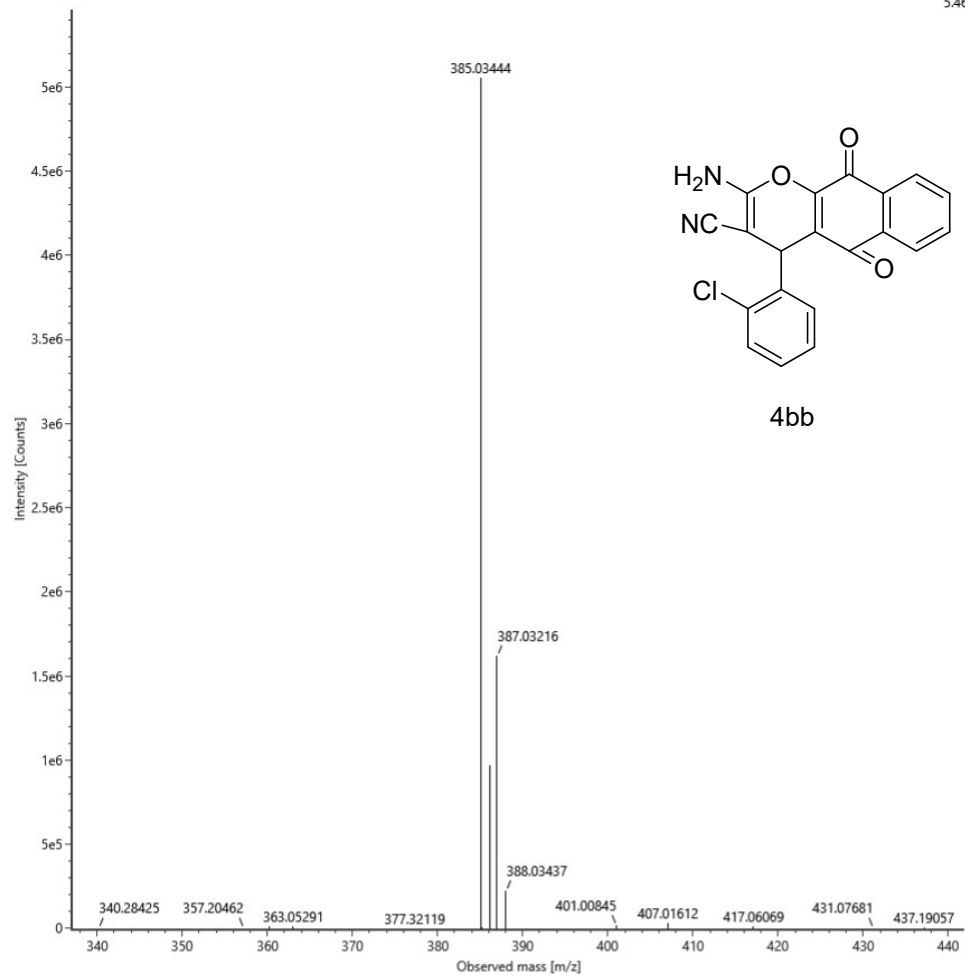


¹³C NMR of Compound **4bb** (101 MHz, DMSO-*d*₆)

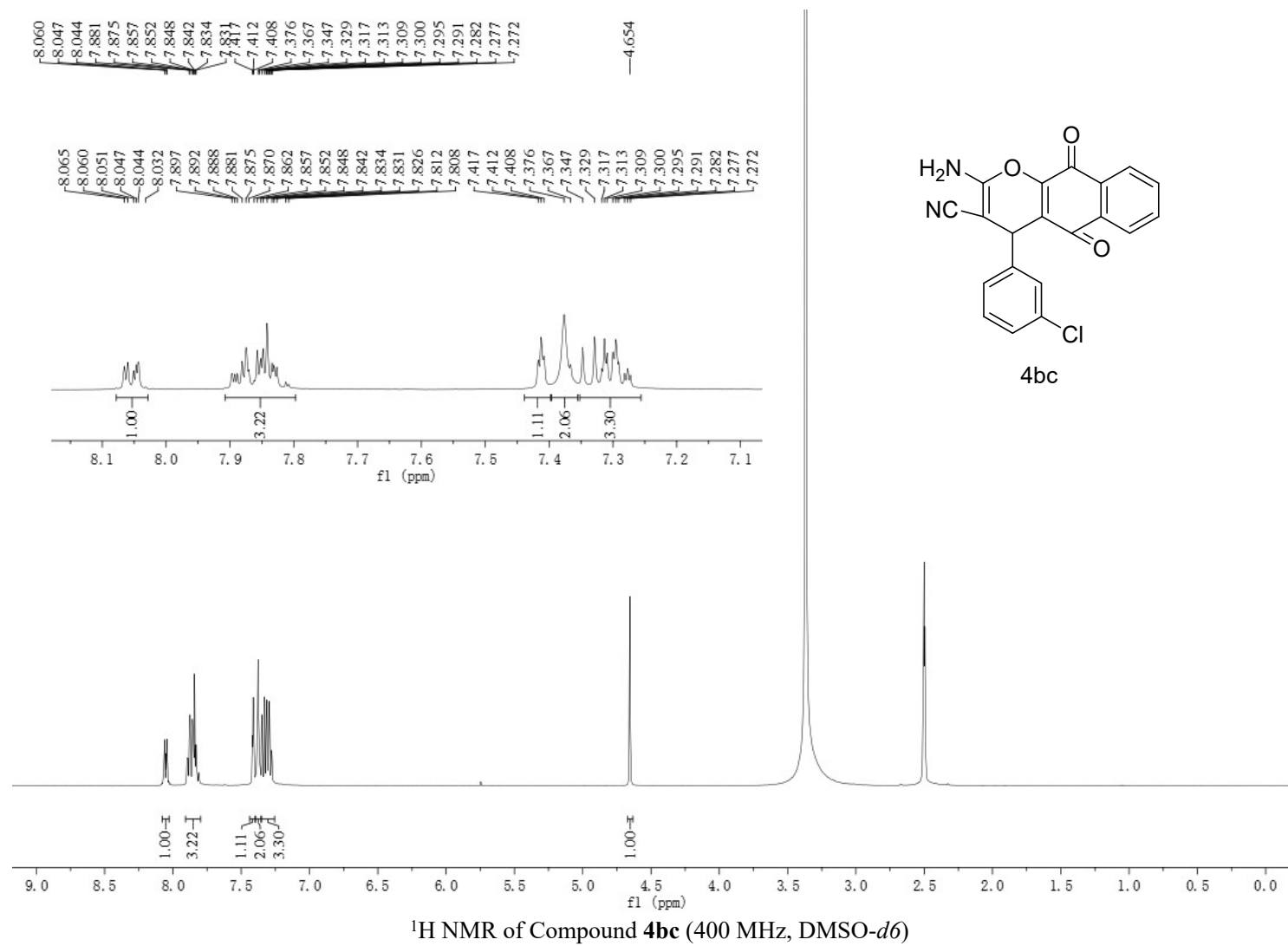
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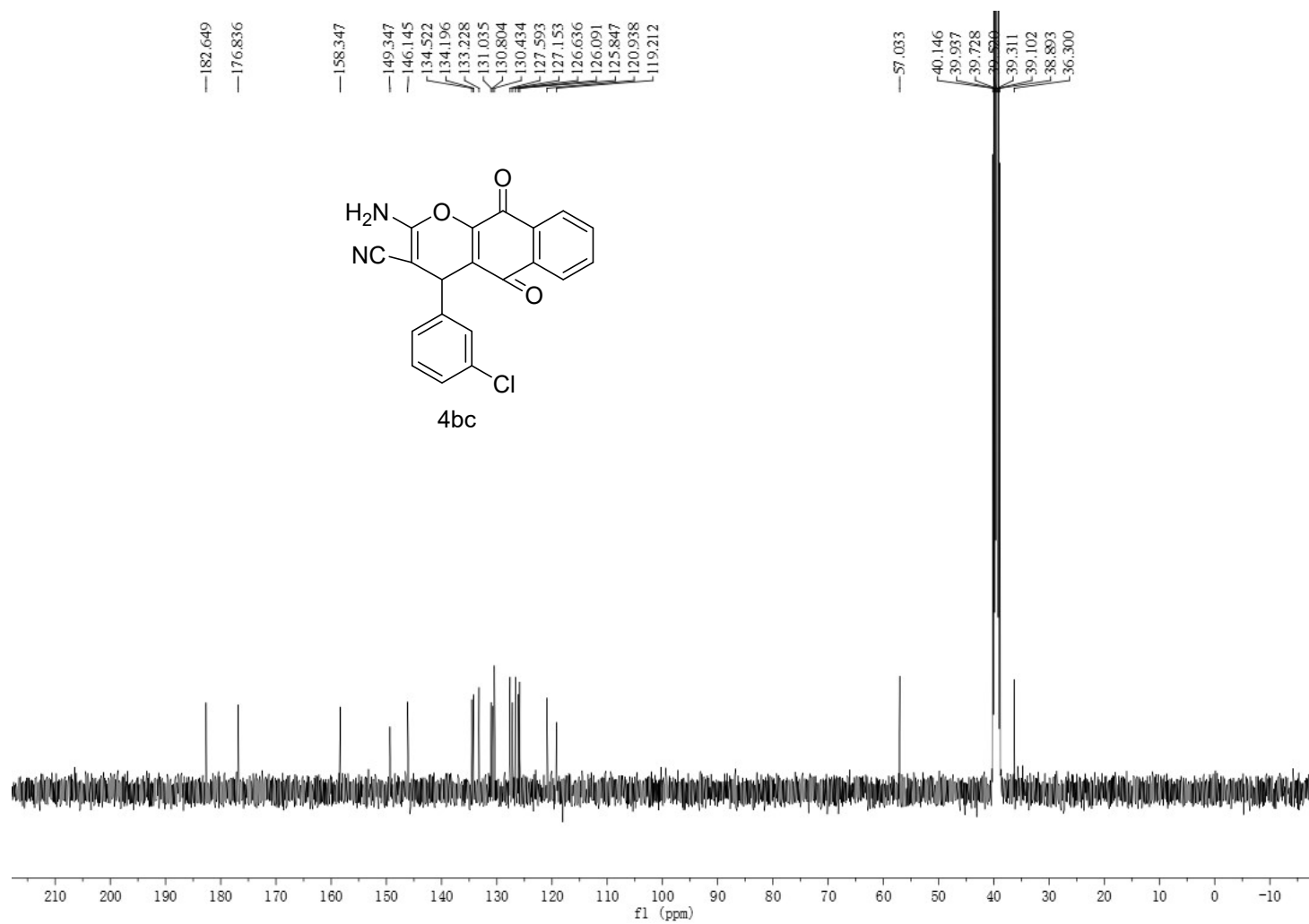
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5.46e6



HRMS of Compound **4bb**



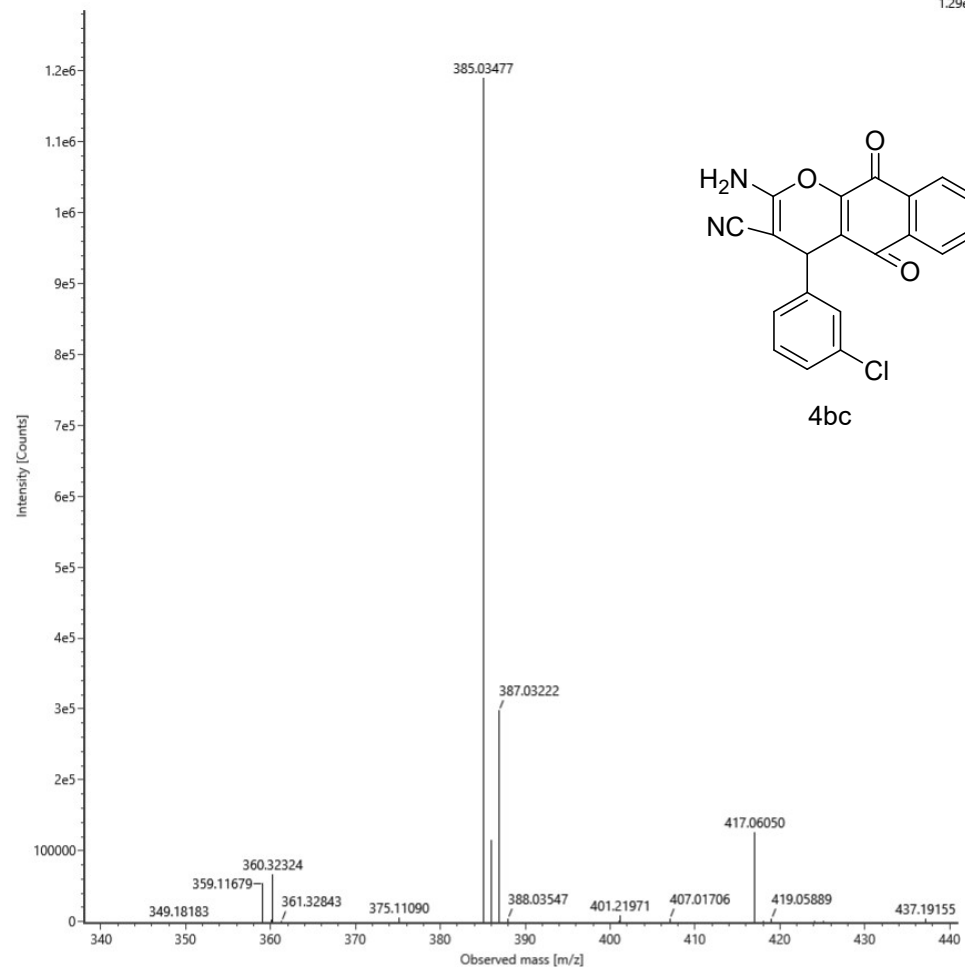


¹³C NMR of Compound **4bc** (101 MHz, DMSO-*d*₆)

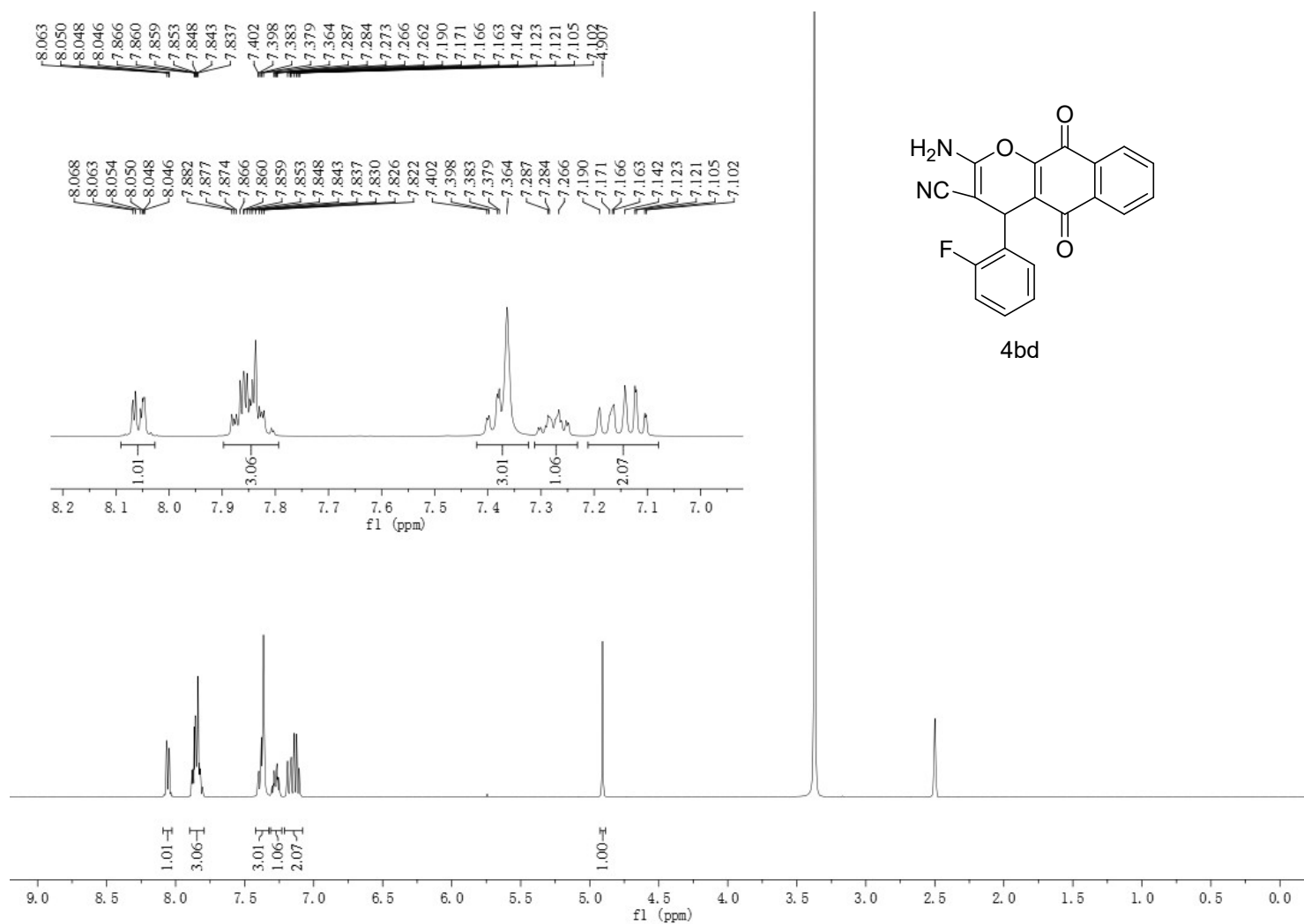
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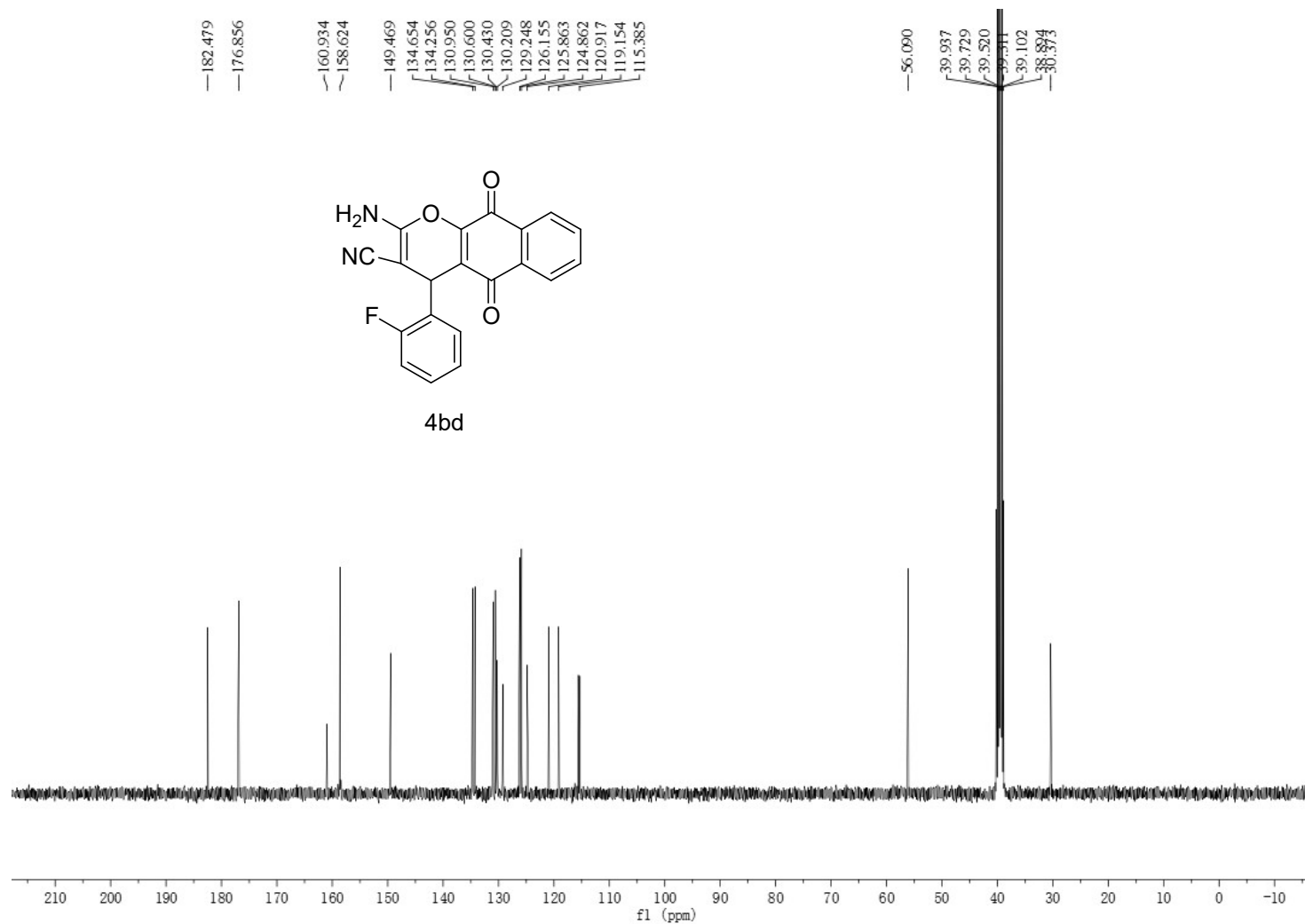
1.29e6



HRMS of Compound **4bc**



¹H NMR of Compound **4bd** (400 MHz, DMSO-*d*₆)

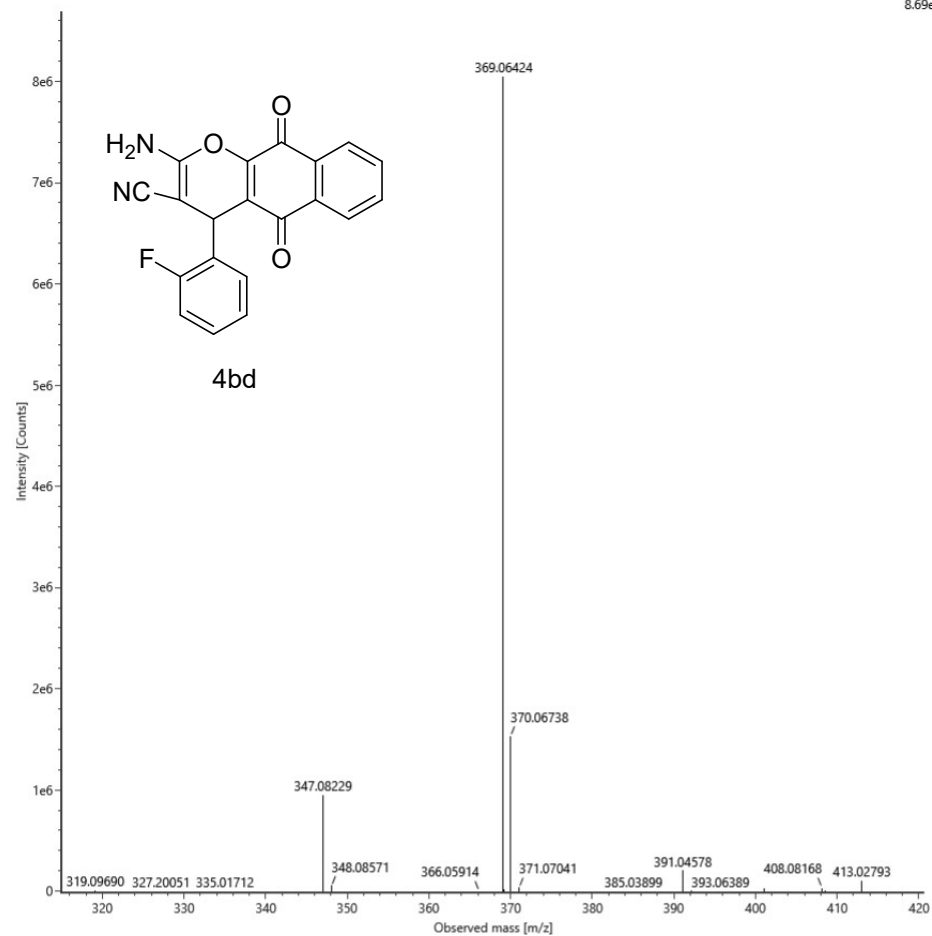


¹³C NMR of Compound **4bd** (101 MHz, DMSO-*d*₆)

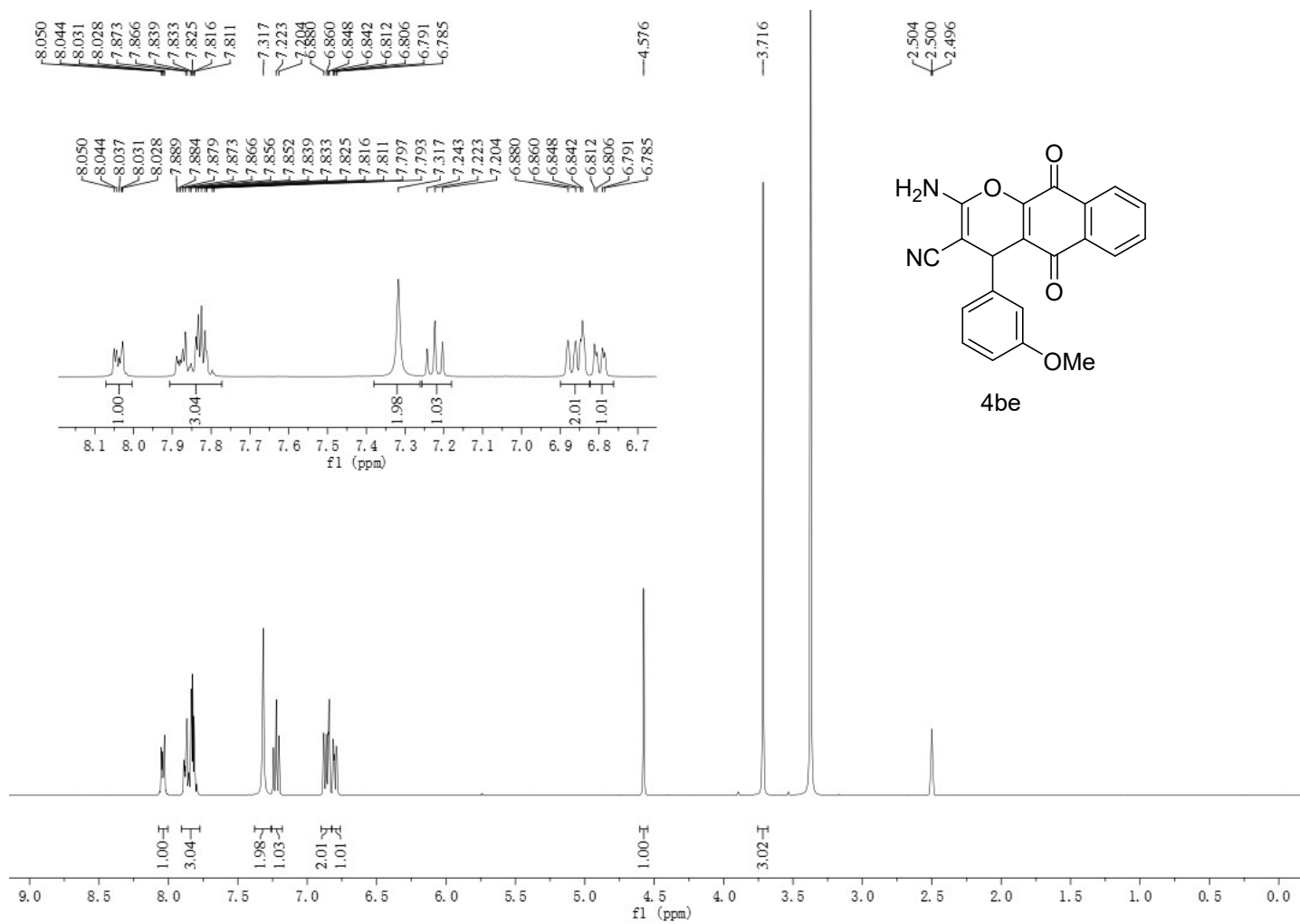
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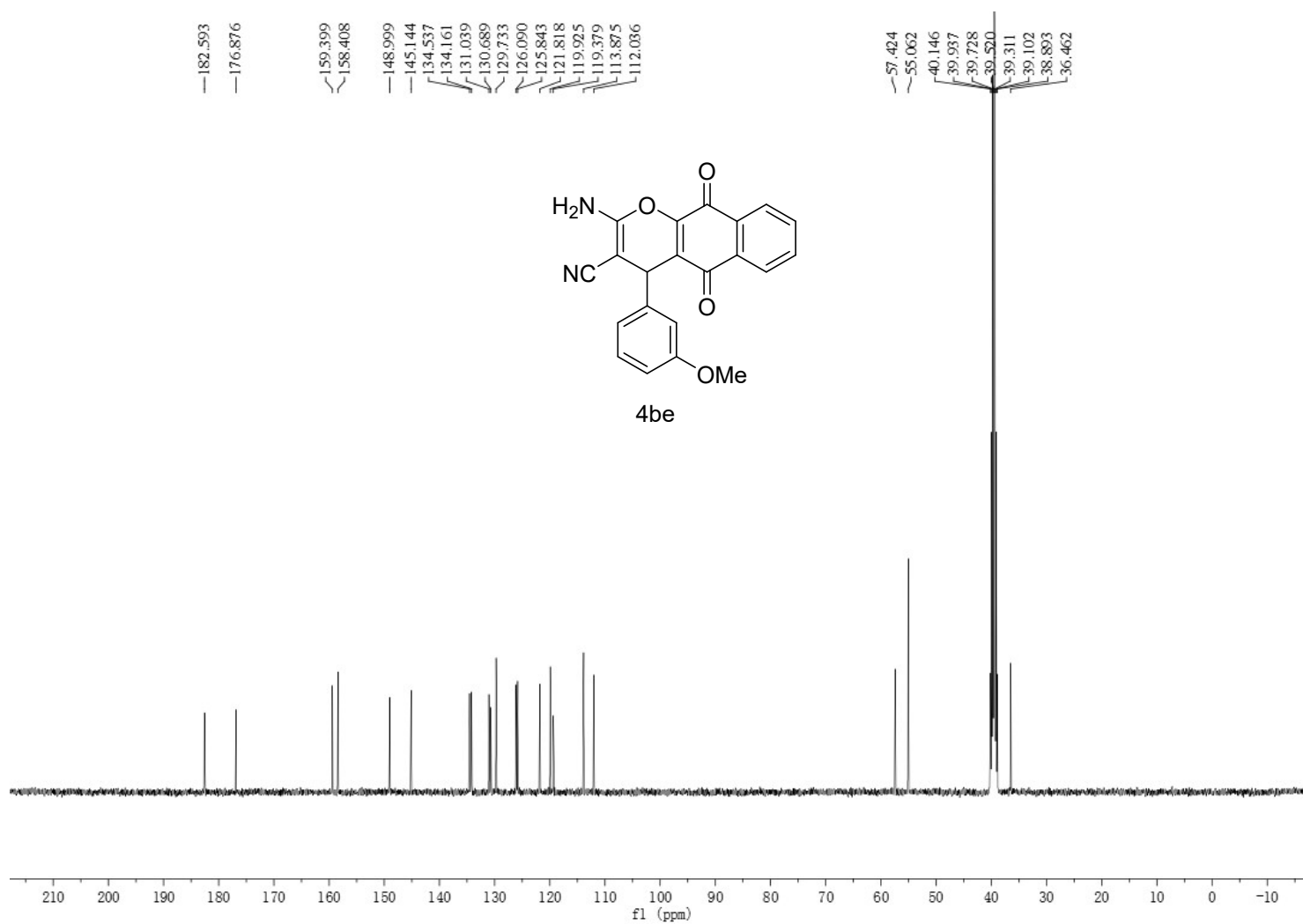
8.69e6



HRMS of Compound **4bd**



¹H NMR of Compound **4be** (400 MHz, DMSO-*d*₆)

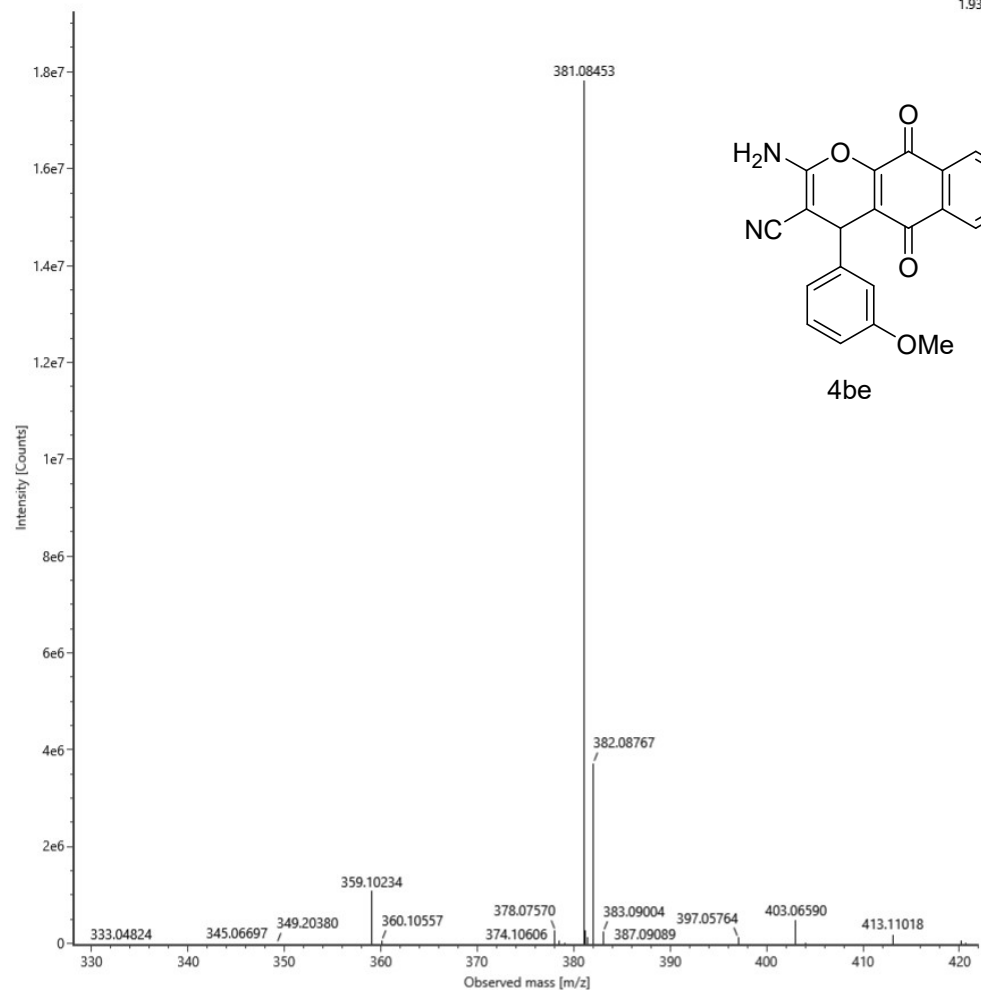


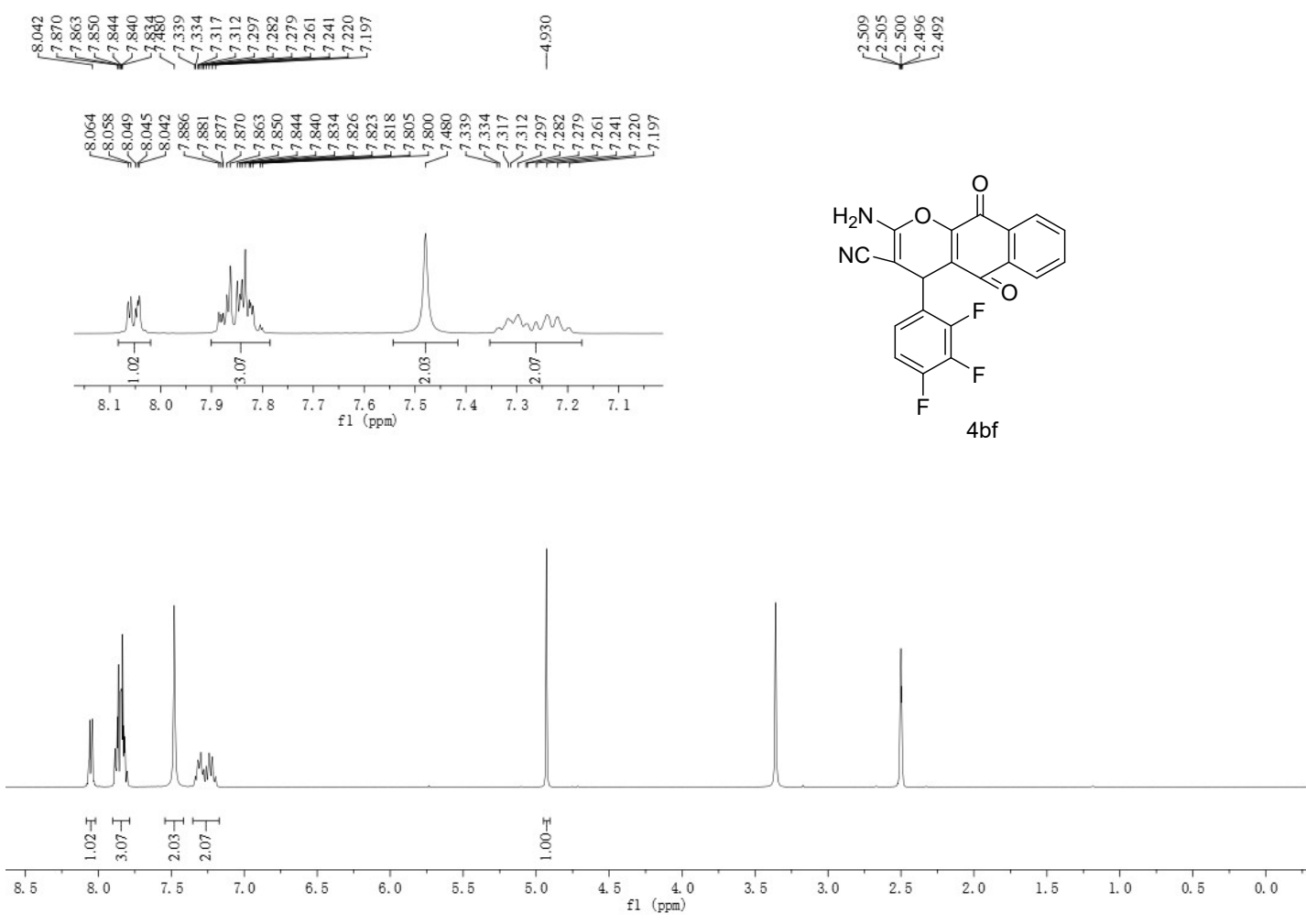
¹³C NMR of Compound **4be** (101 MHz, DMSO-*d*₆)

Item name: TAF-7
Item description:

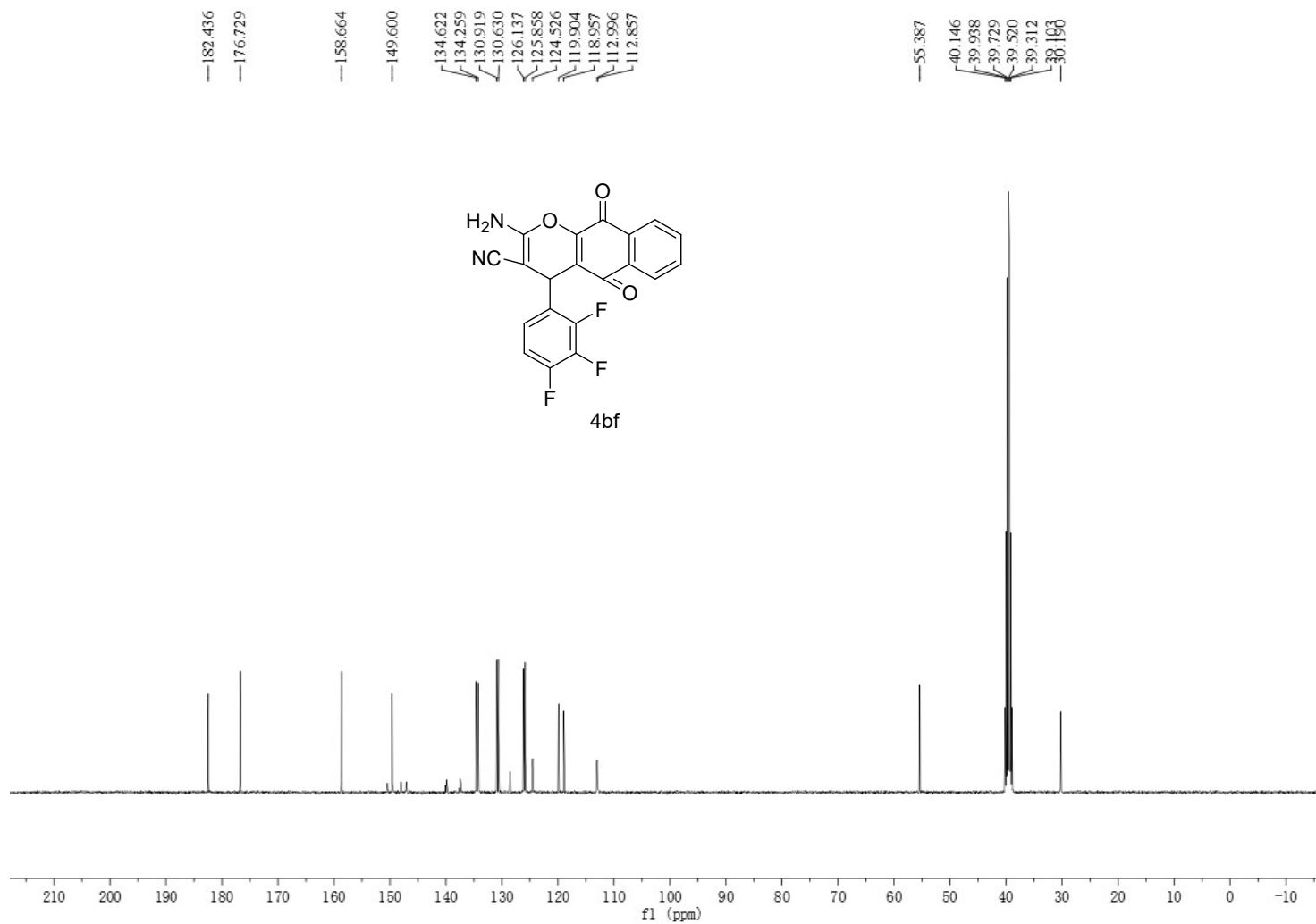
Channel name: 1: Average Time 0.1174 min : TOF MS (50-1500) ESI+ : Centroided : Combined

1.93e7





¹H NMR of Compound **4bf** (400 MHz, DMSO-*d*₆)

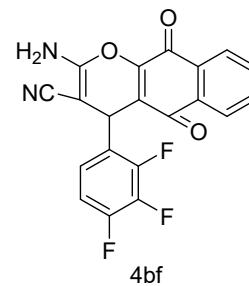
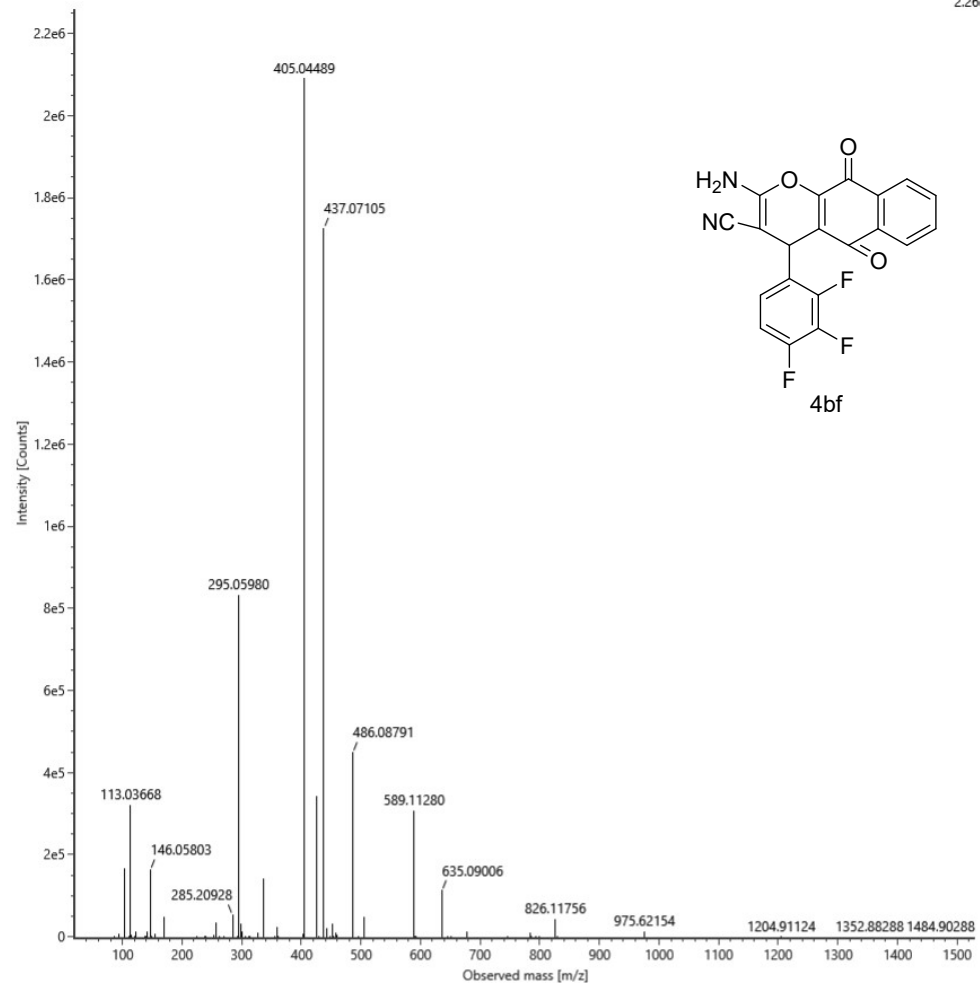


¹³C NMR of Compound **4bf** (101 MHz, DMSO-*d*₆)

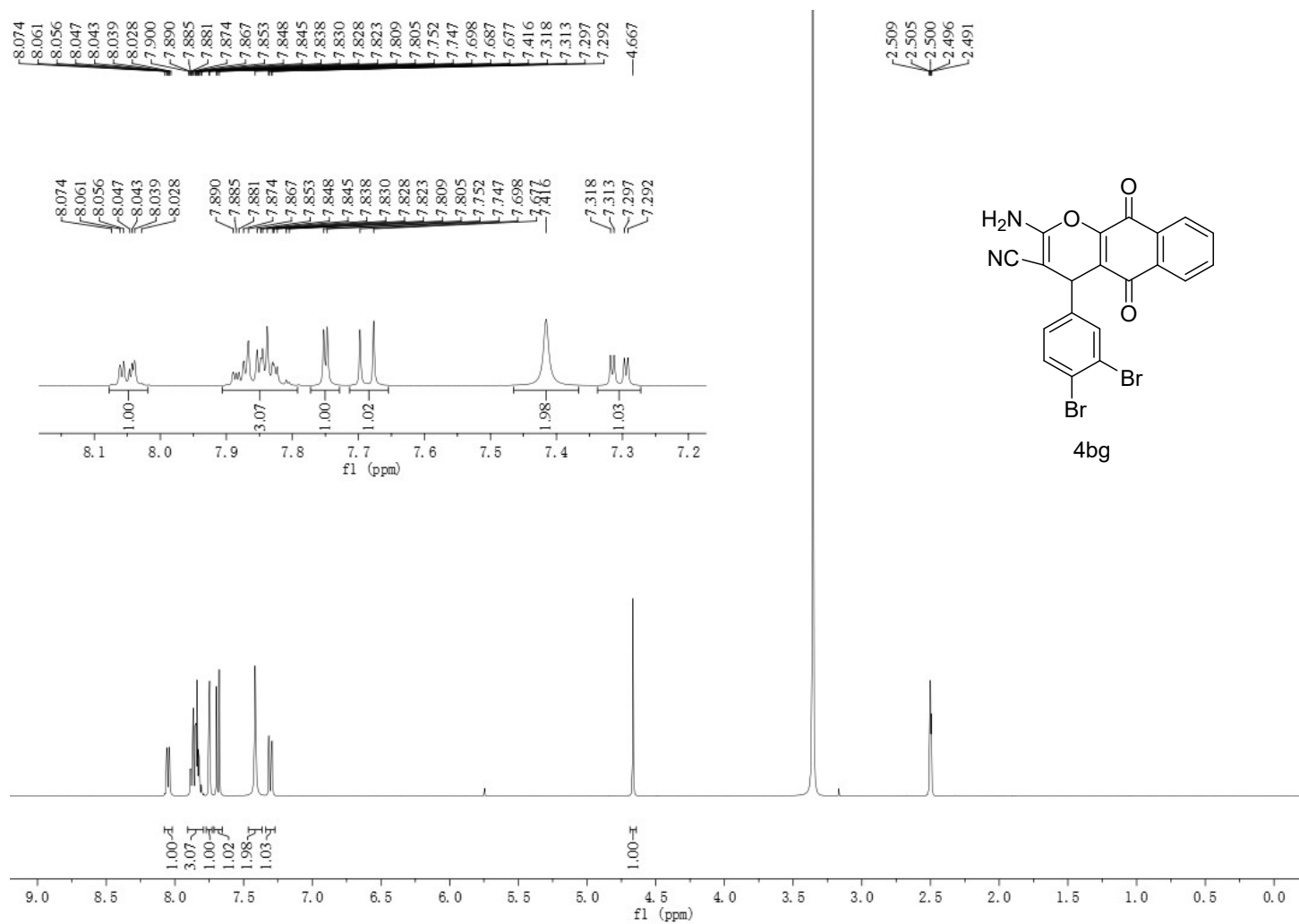
Item name: TAF-9
Item description:

Channel name: 1: Average Time 0.1462 min : TOF MS (50-1500) ESI+ : Centroided : Combined

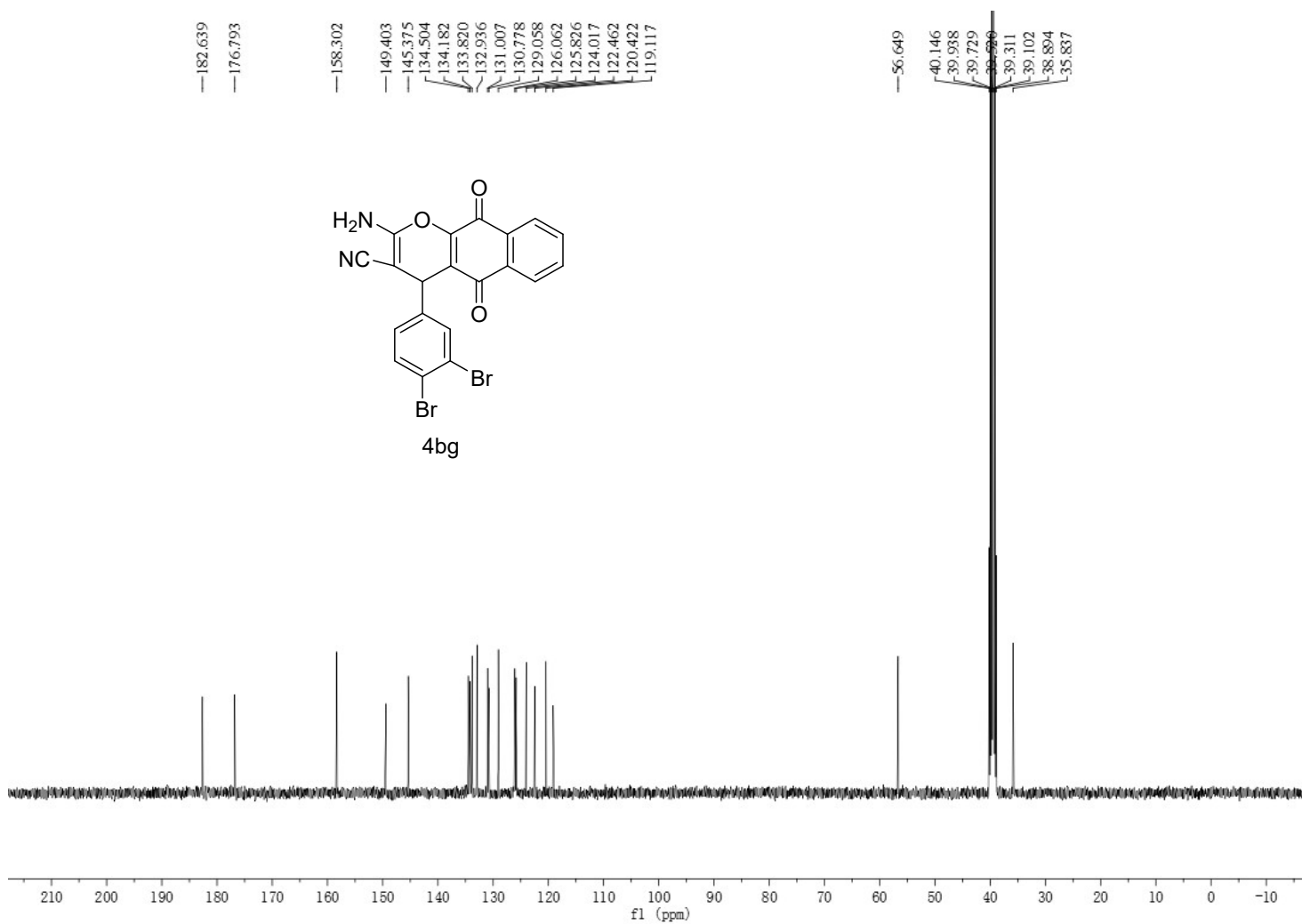
2.26e6



HRMS of Compound 4bf



¹H NMR of Compound **4bg** (400 MHz, DMSO-*d*₆)

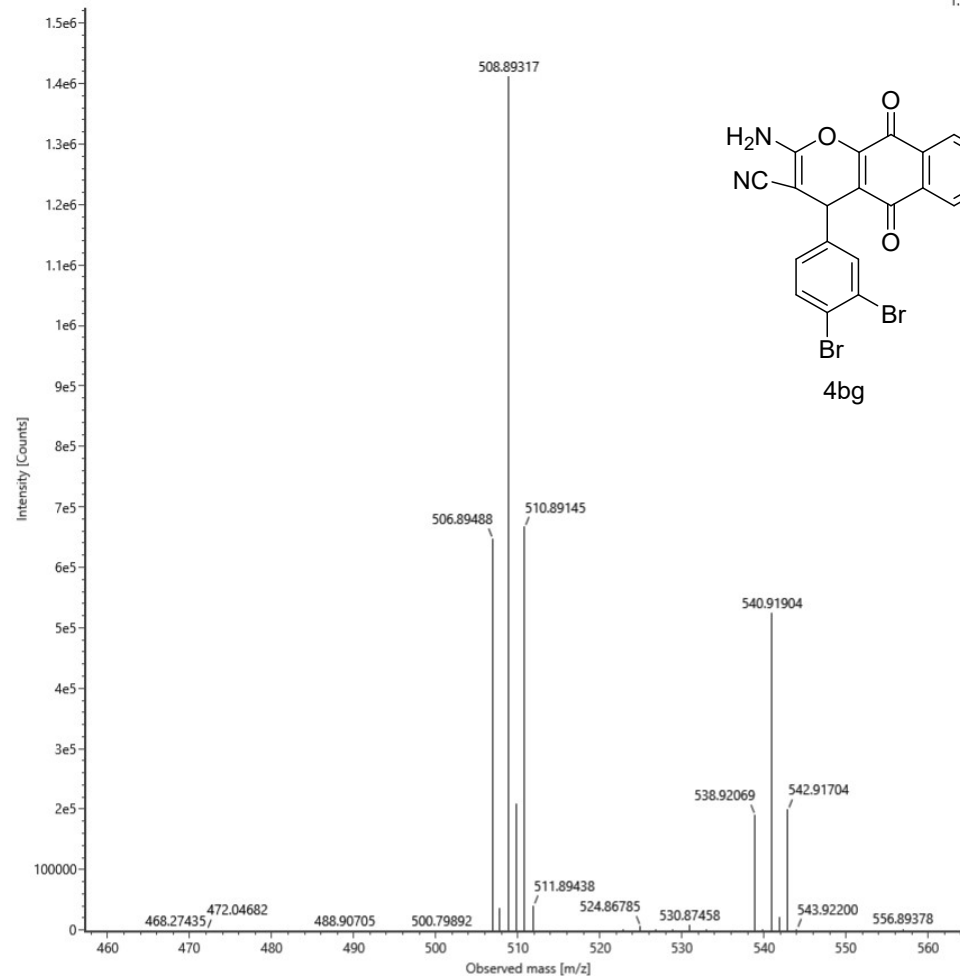


¹³C NMR of Compound **4bg** (101 MHz, DMSO-*d*₆)

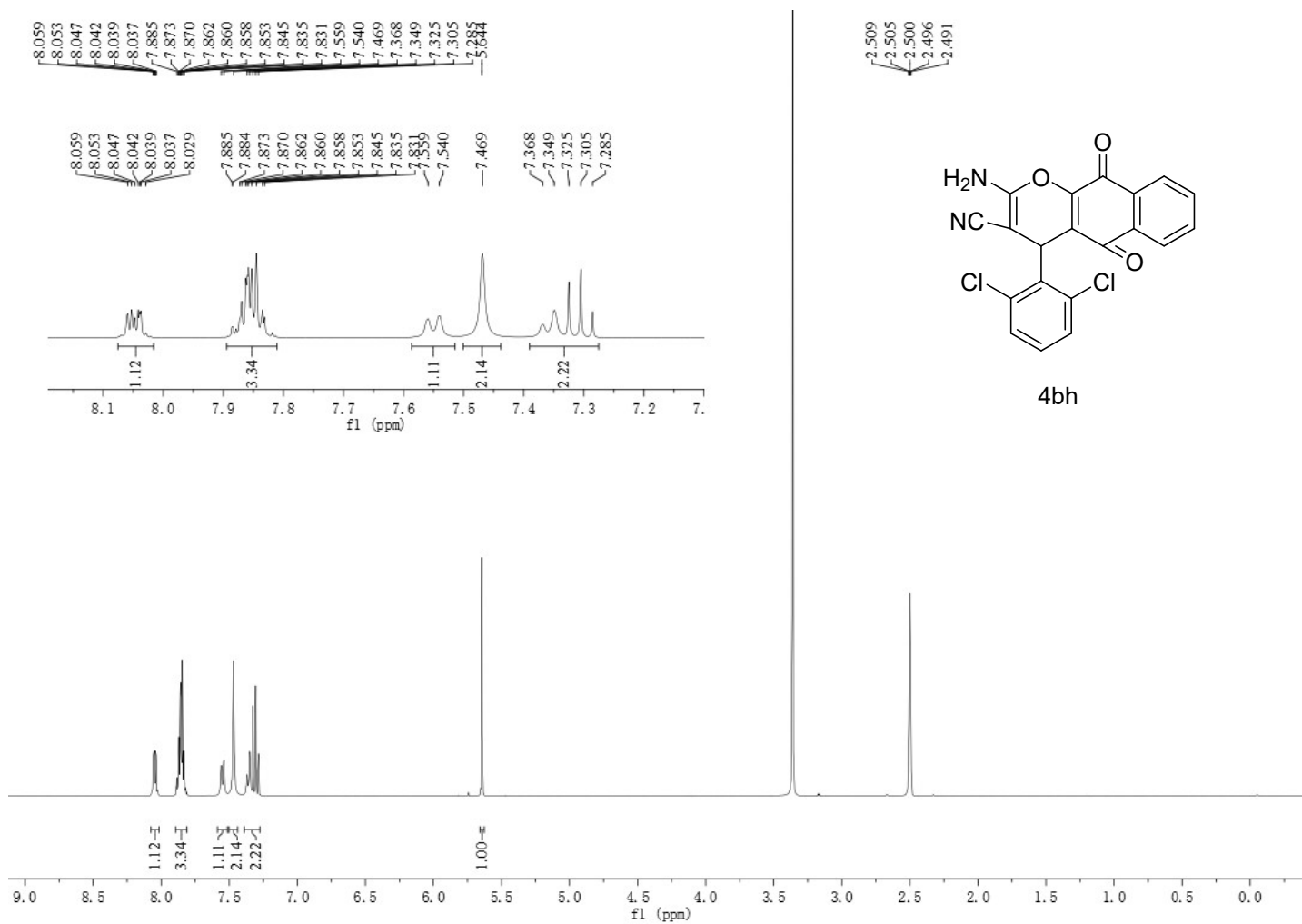
Item name: TAF-11
Item description:

Channel name: 1: Average Time 0.1217 min : TOF MS (50-1500) ESI+ : Centroided : Combined

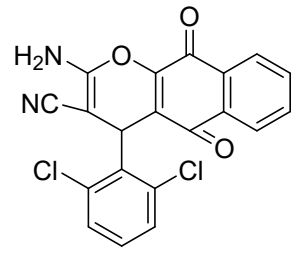
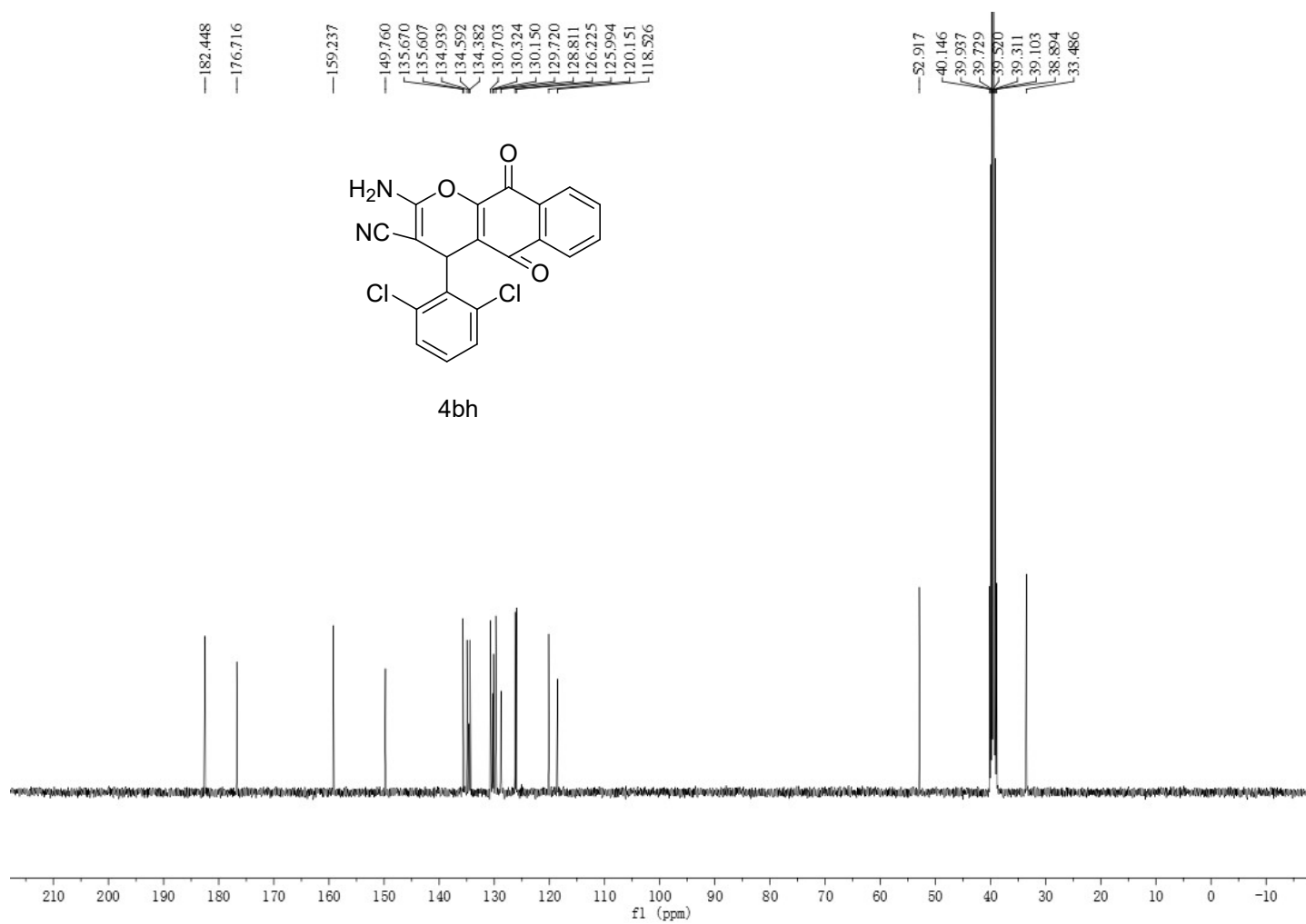
1.53e6



HRMS of Compound **4bg**



^1H NMR of Compound **4bh** (400 MHz, $\text{DMSO-}d_6$)



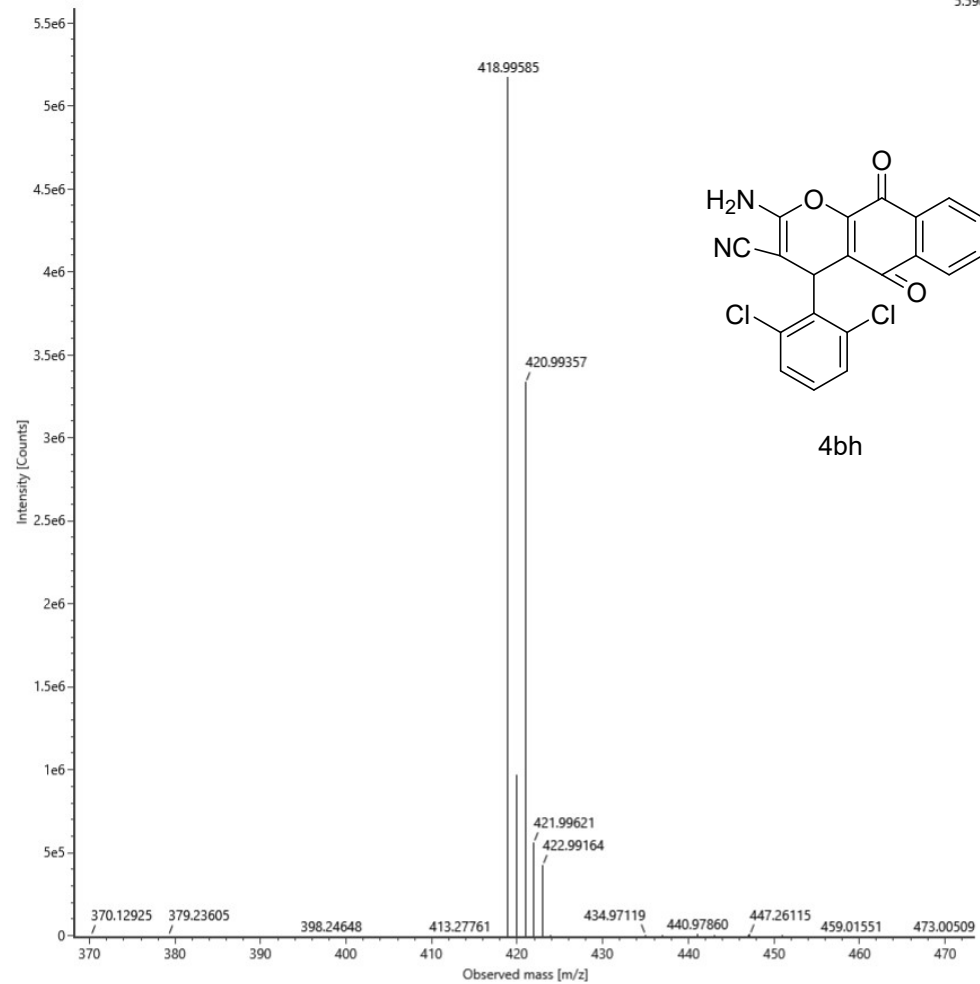
4bh

¹³C NMR of Compound **4bh** (101 MHz, DMSO-*d*₆)

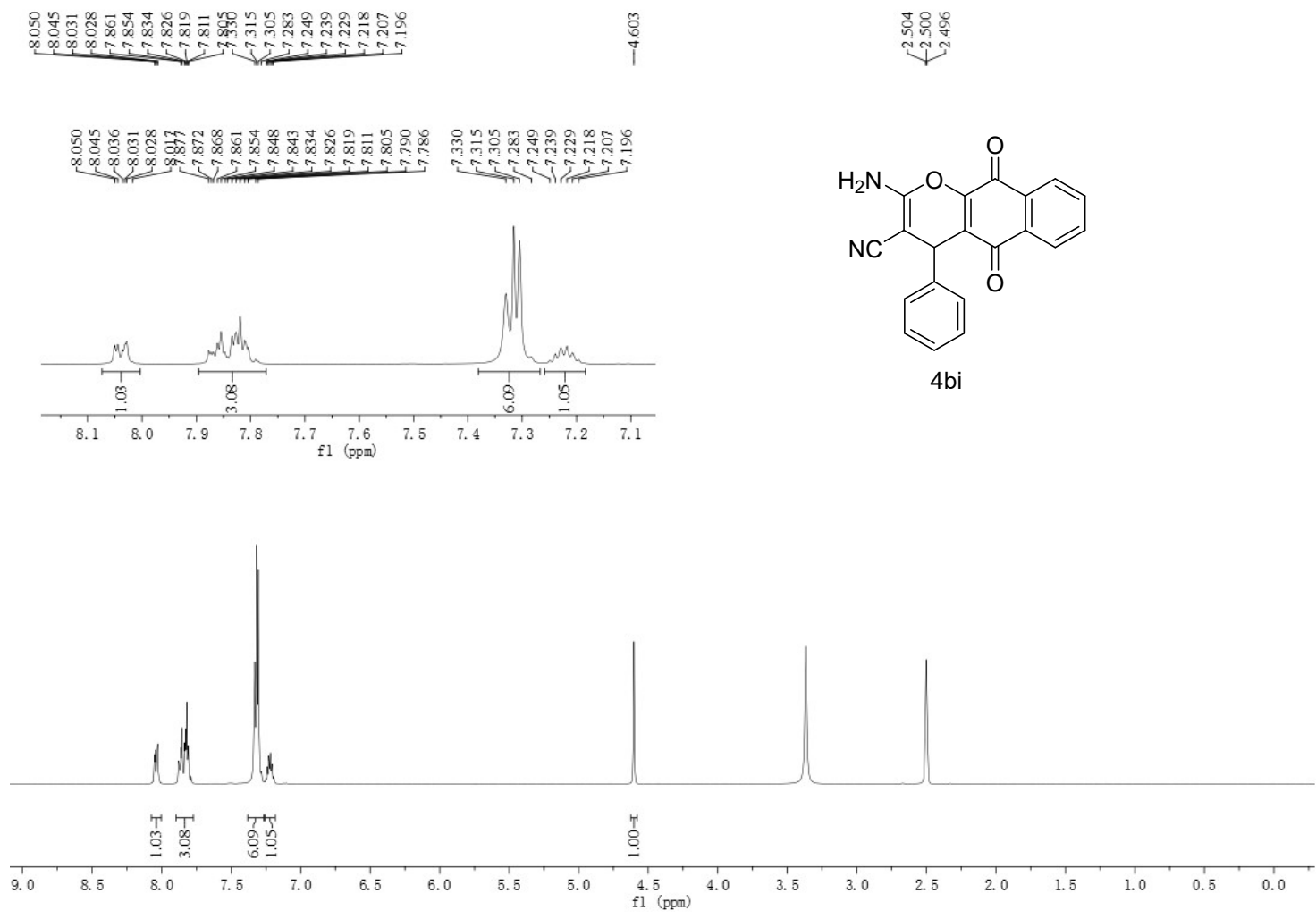
Item name: TAF-15
Item description:

Channel name: 1: Average Time 0.1217 min : TOF MS (50-1500) ESI+ : Centroided : Combined

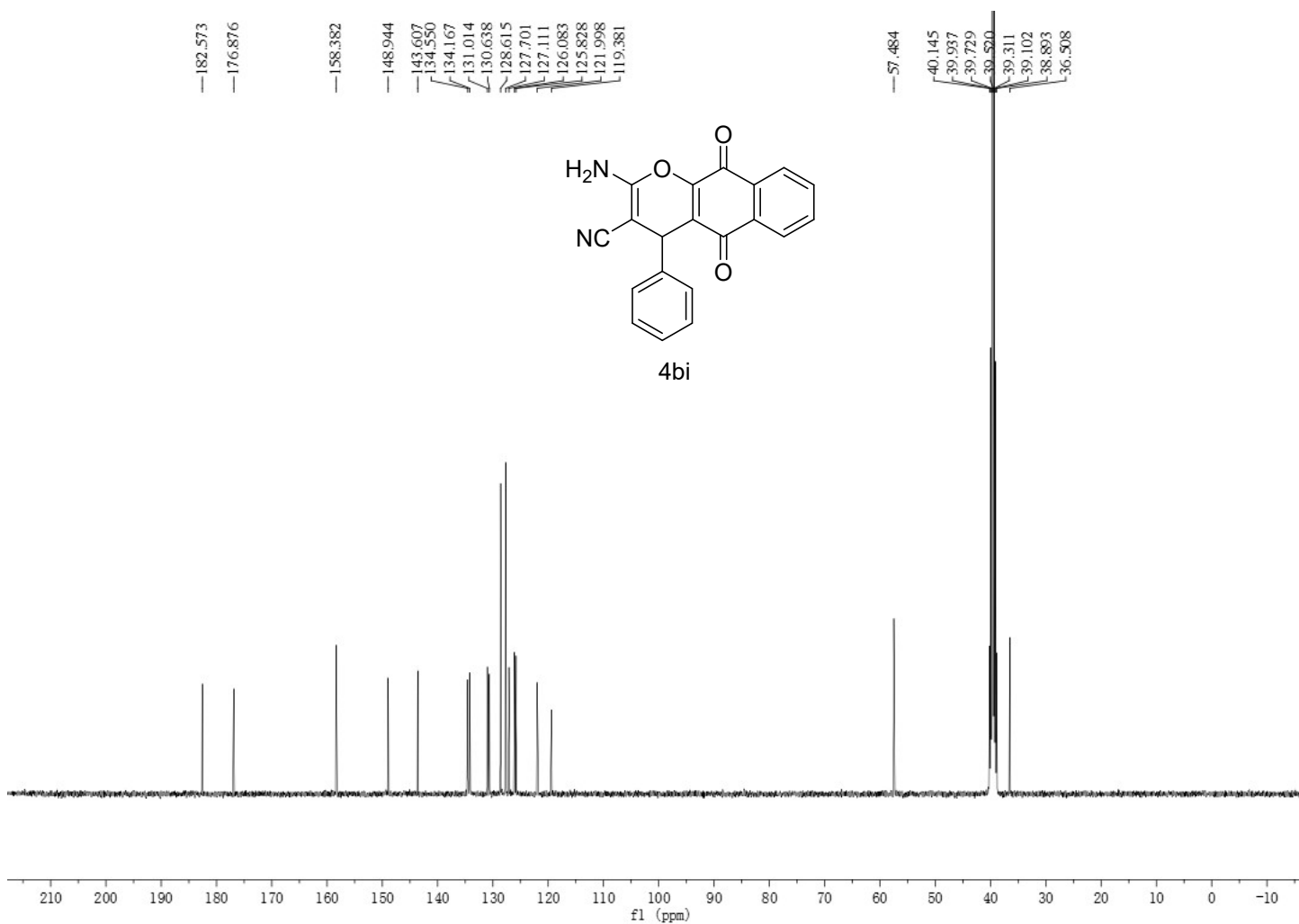
5.59e6



HRMS of Compound **4bh**



¹H NMR of Compound **4bi** (400 MHz, DMSO-*d*₆)

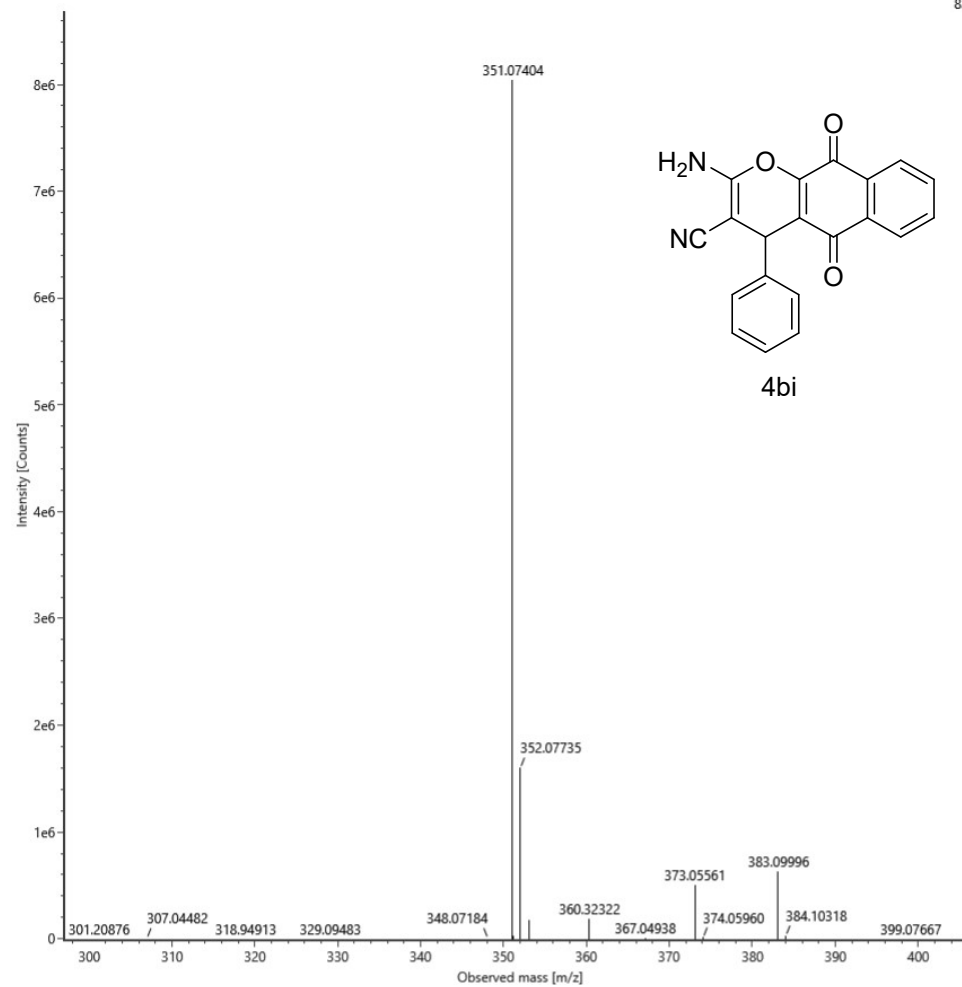


^{13}C NMR of Compound **4bi** (101 MHz, DMSO-*d*₆)

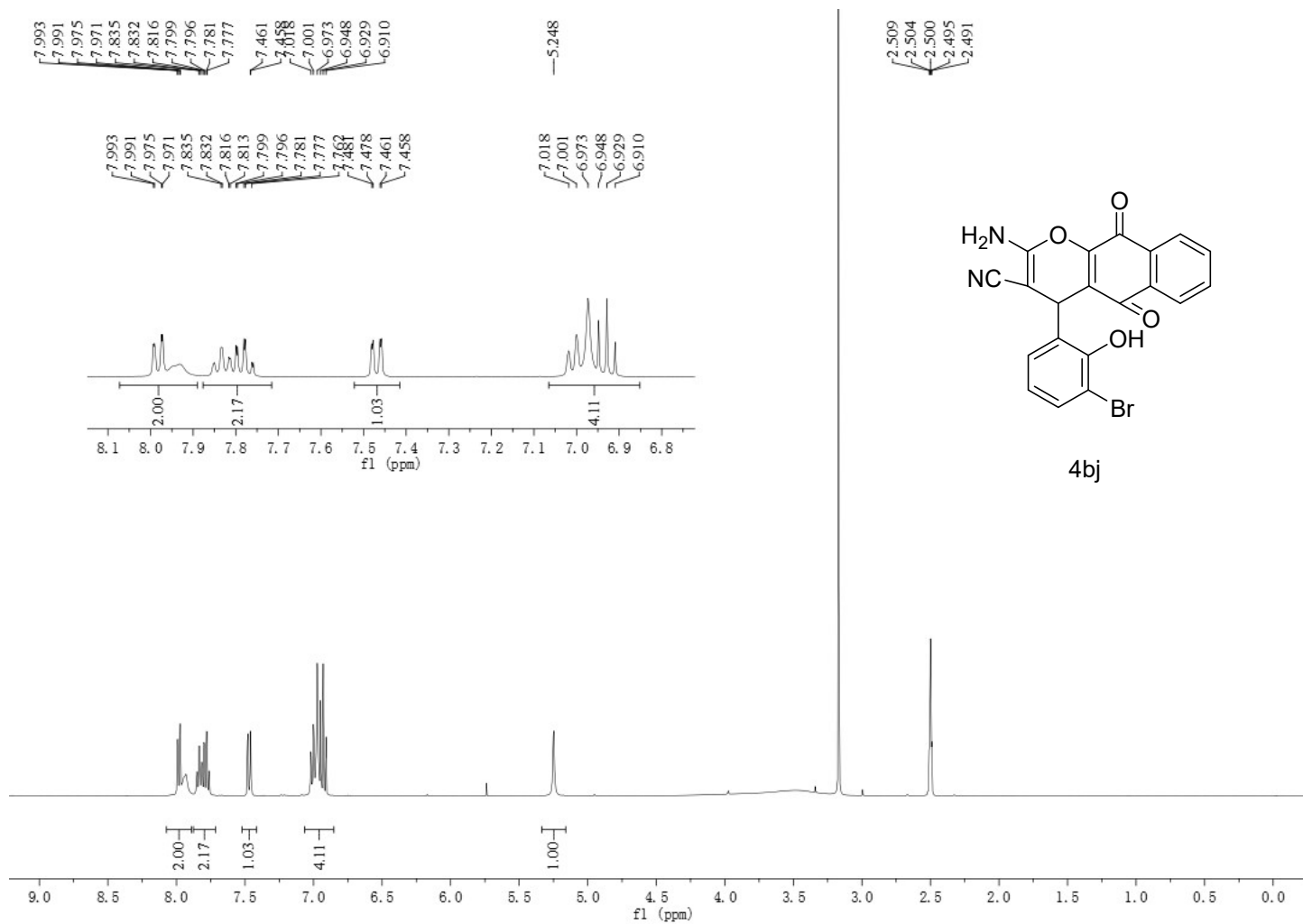
Item name: TAF-16
Item description:

Channel name: 1: Average Time 0.1003 min : TOF MS (50-1500) ESI+ : Centroided : Combined

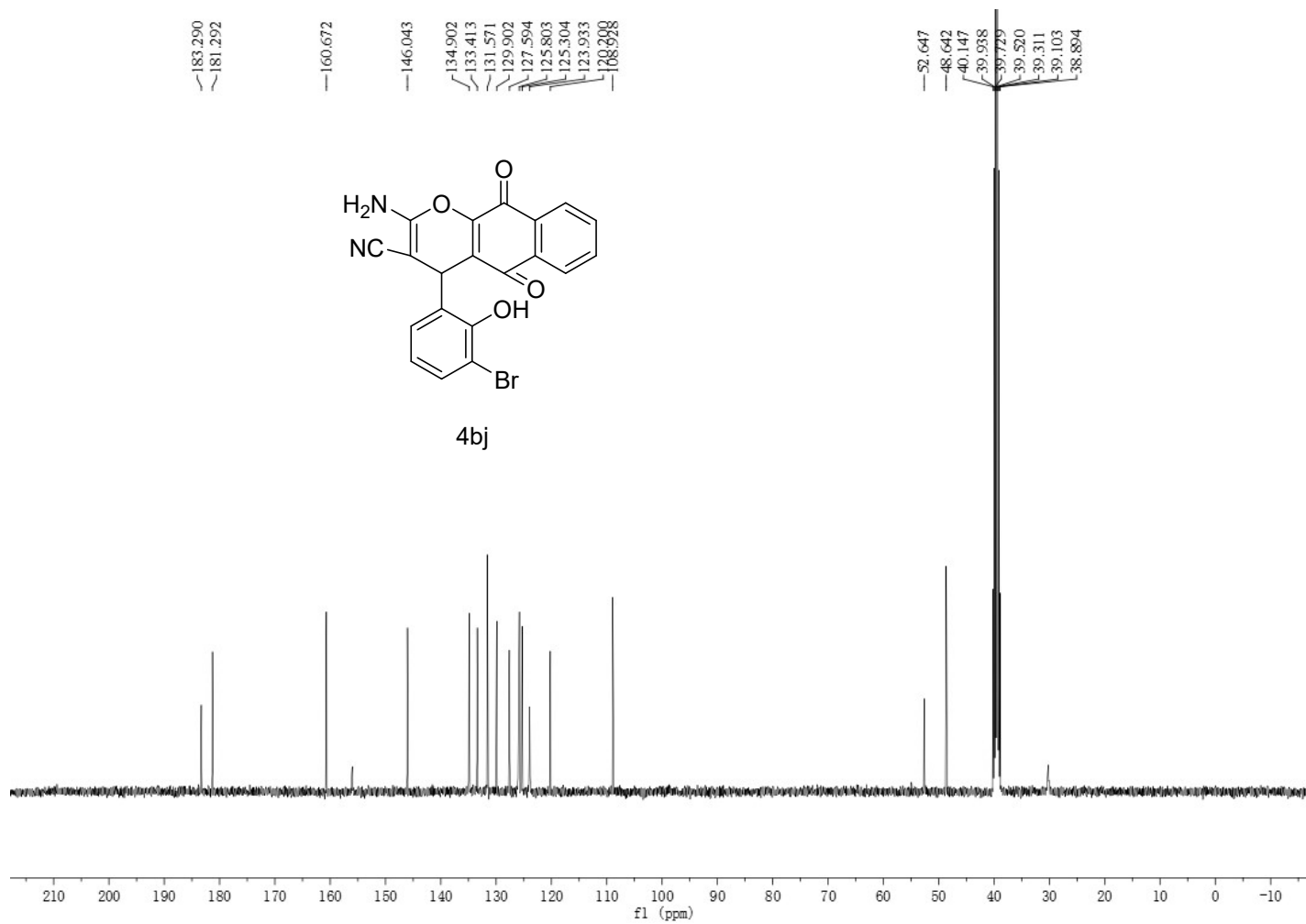
8.69e6



HRMS of Compound **4bi**



¹H NMR of Compound **4bj** (400 MHz, DMSO-*d*₆)

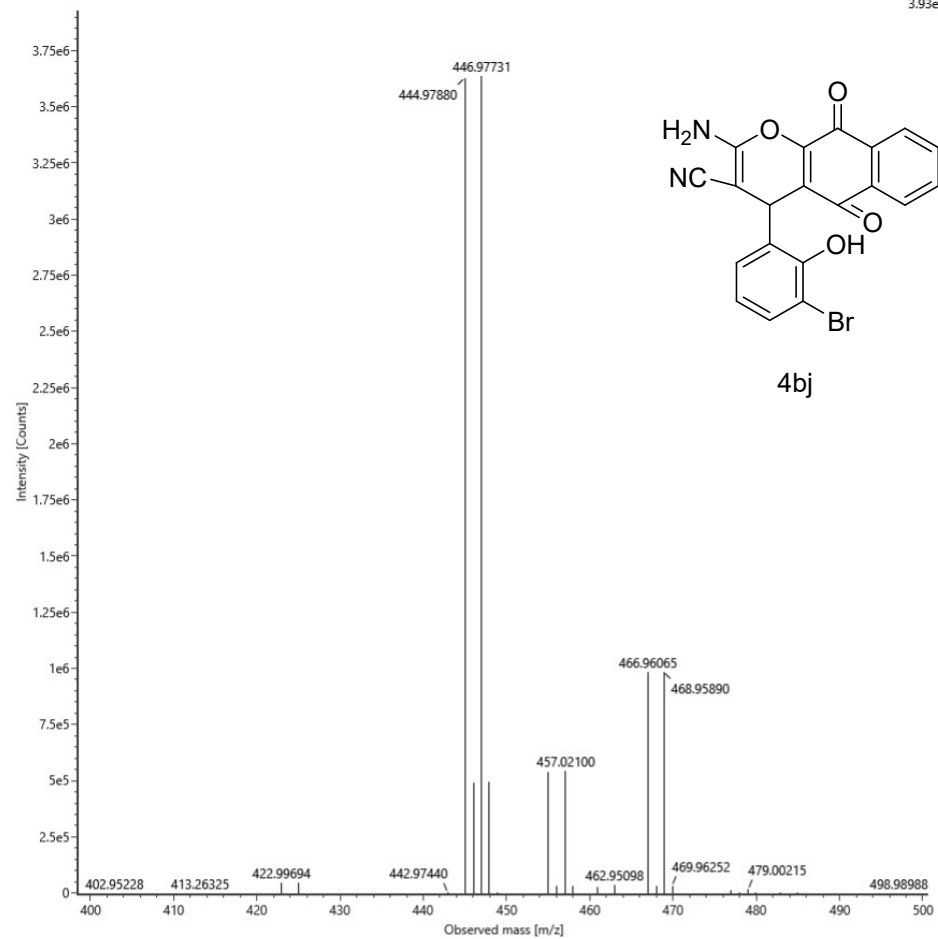


¹³C NMR of Compound **4bj** (101 MHz, DMSO-*d*₆)

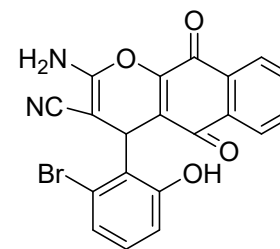
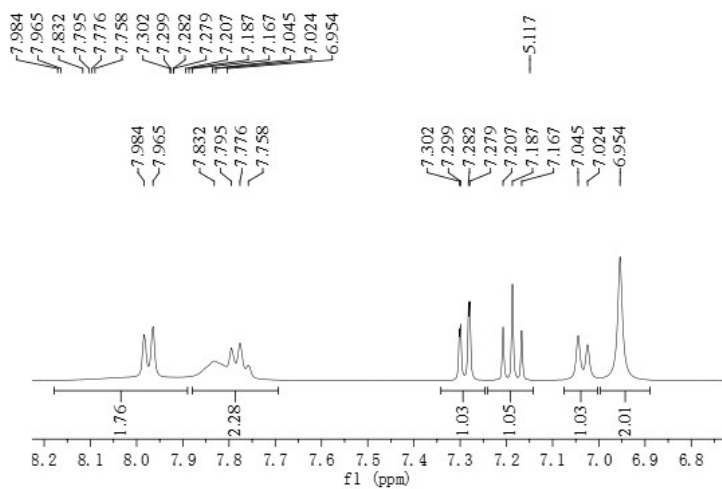
Item name: TAF-18
Item description:

Channel name: 1: Average Time 0.1806 min : TOF MS (50-1500) ESI+ : Centroided : Combined

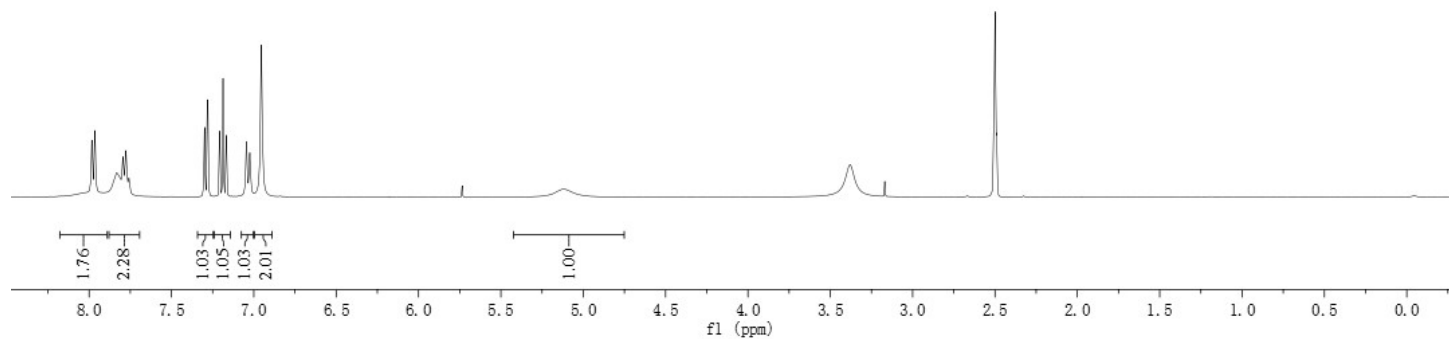
3.93e6



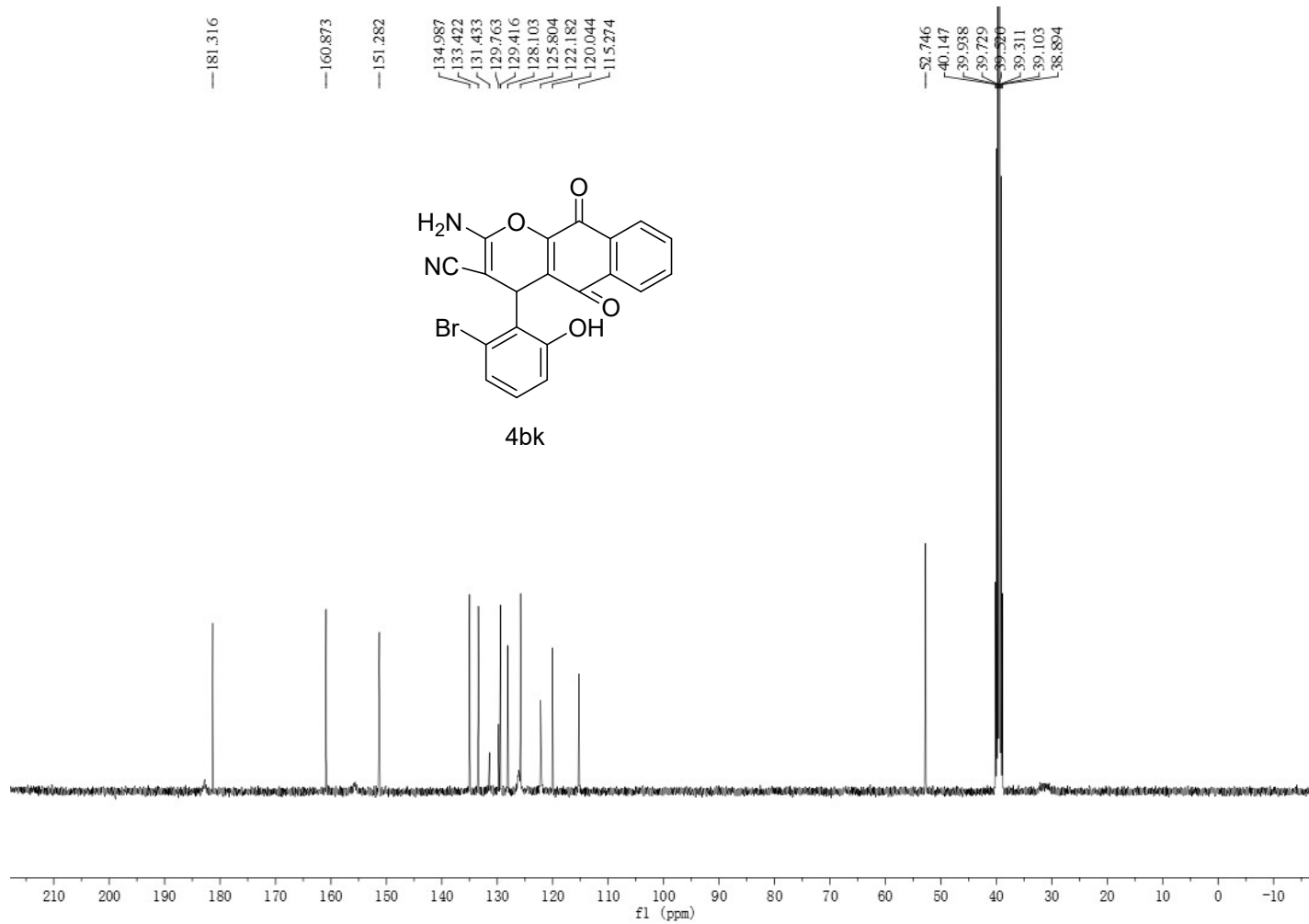
HRMS of Compound **4bj**



4bk



¹H NMR of Compound **4bk** (400 MHz, DMSO-*d*₆)

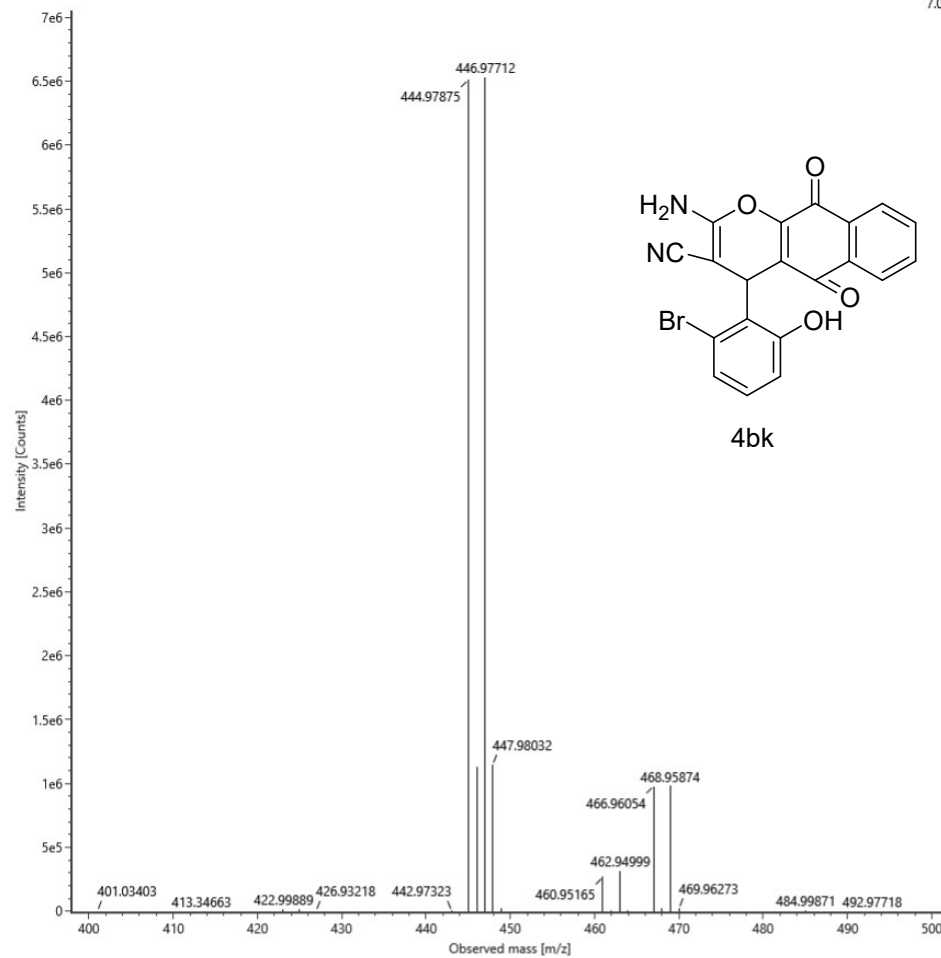


¹³C NMR of Compound **4bk** (101 MHz, DMSO-*d*₆)

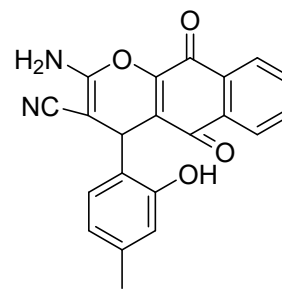
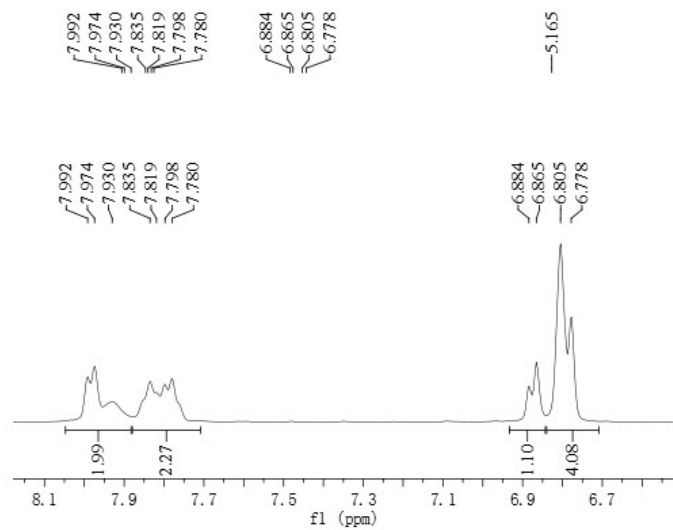
Item name: TAF-19
Item description:

Channel name: 1: Average Time 0.1334 min : TOF MS (50-1500) ESI+ : Centroided : Combined

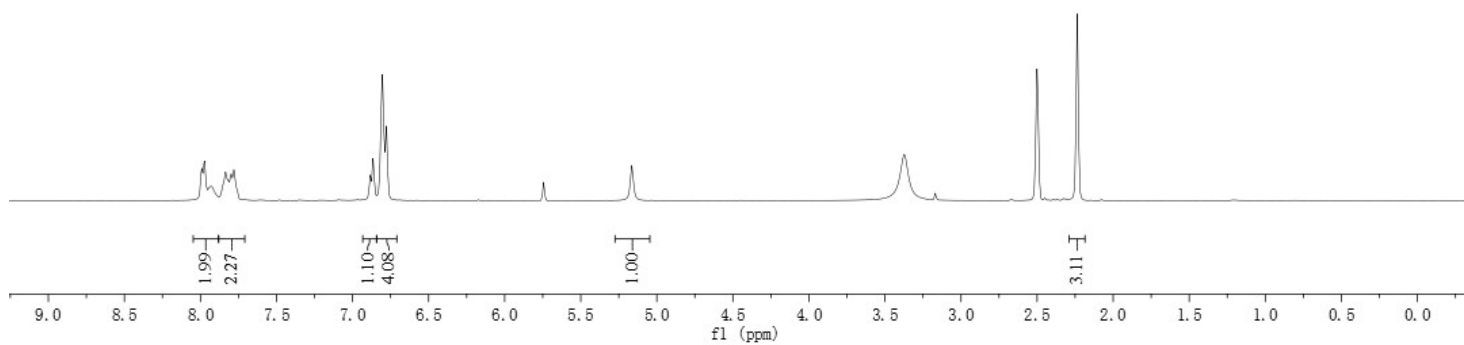
7.06e6



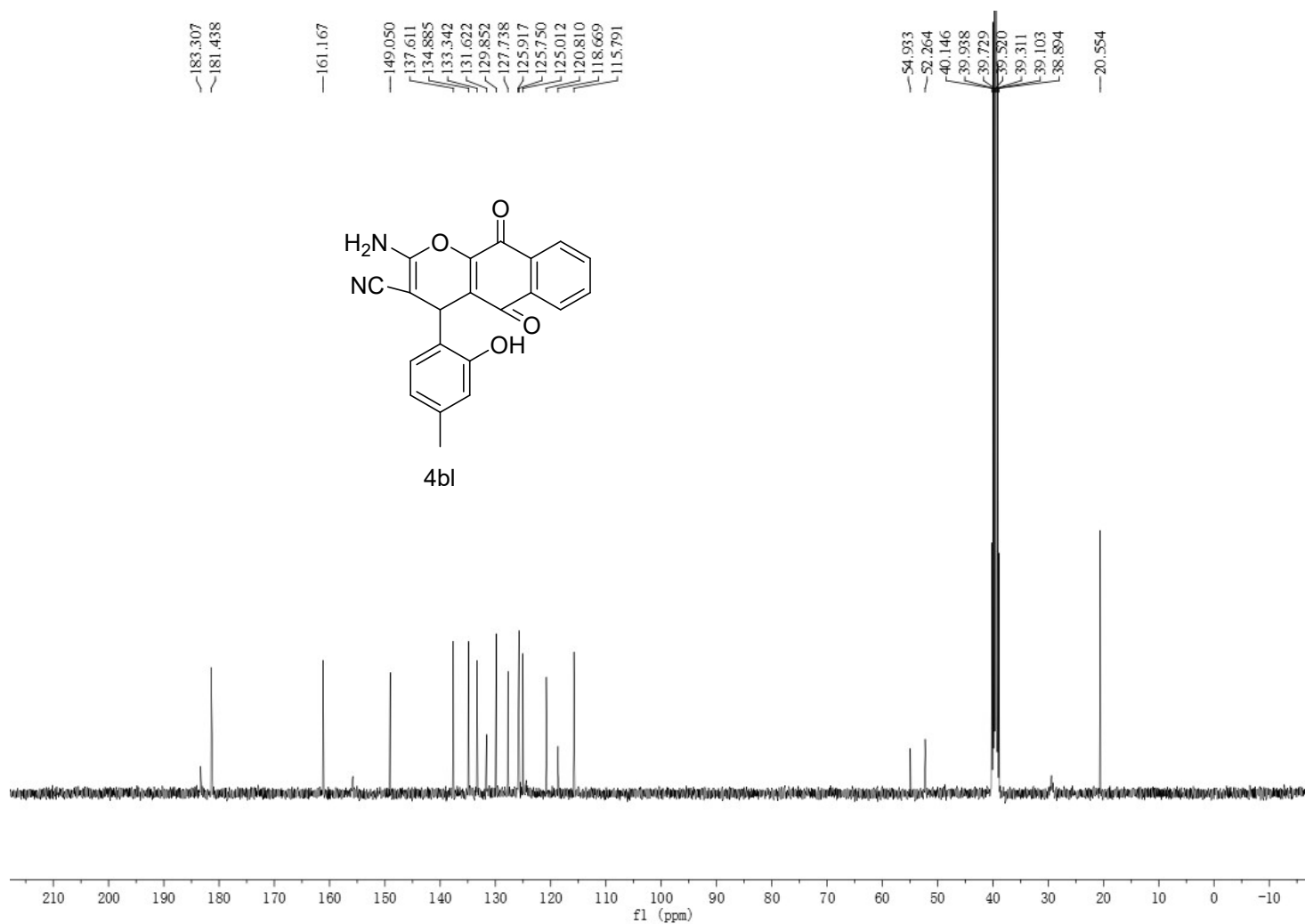
HRMS of Compound **4bk**



4bl



^1H NMR of Compound **4bl** (400 MHz, $\text{DMSO-}d_6$)

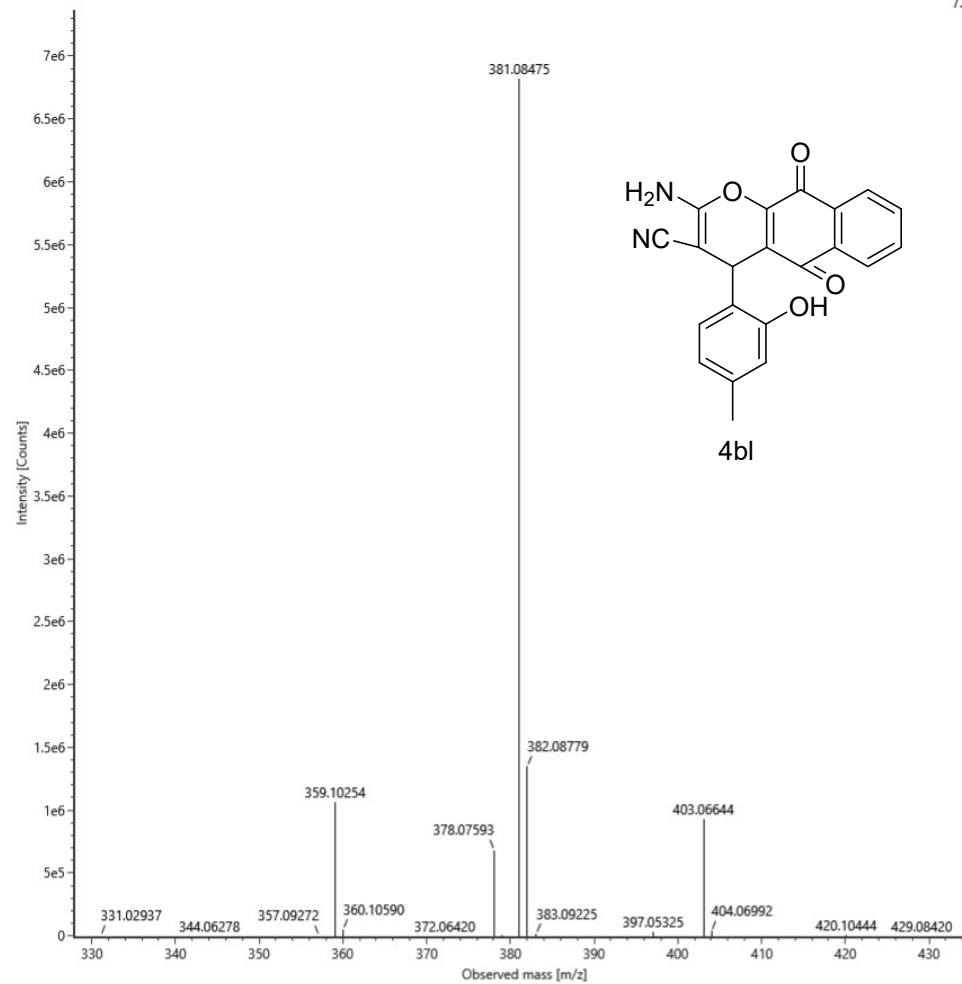


¹³C NMR of Compound **4bl** (101 MHz, DMSO-*d*₆)

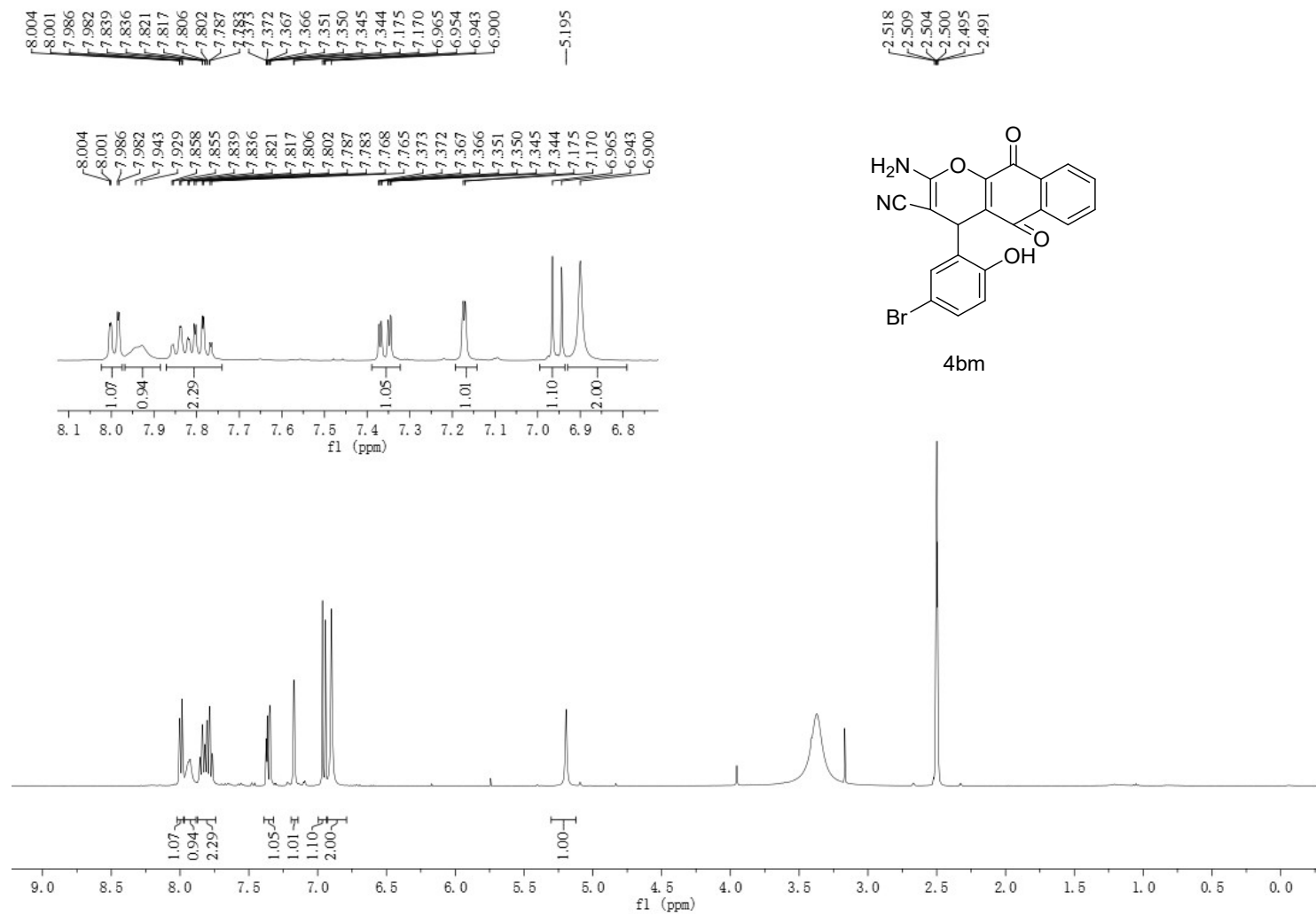
Item name: TAF-20
Item description:

Channel name: 1: Average Time 0.1217 min : TOF MS (50-1500) ESI+ : Centroided : Combined

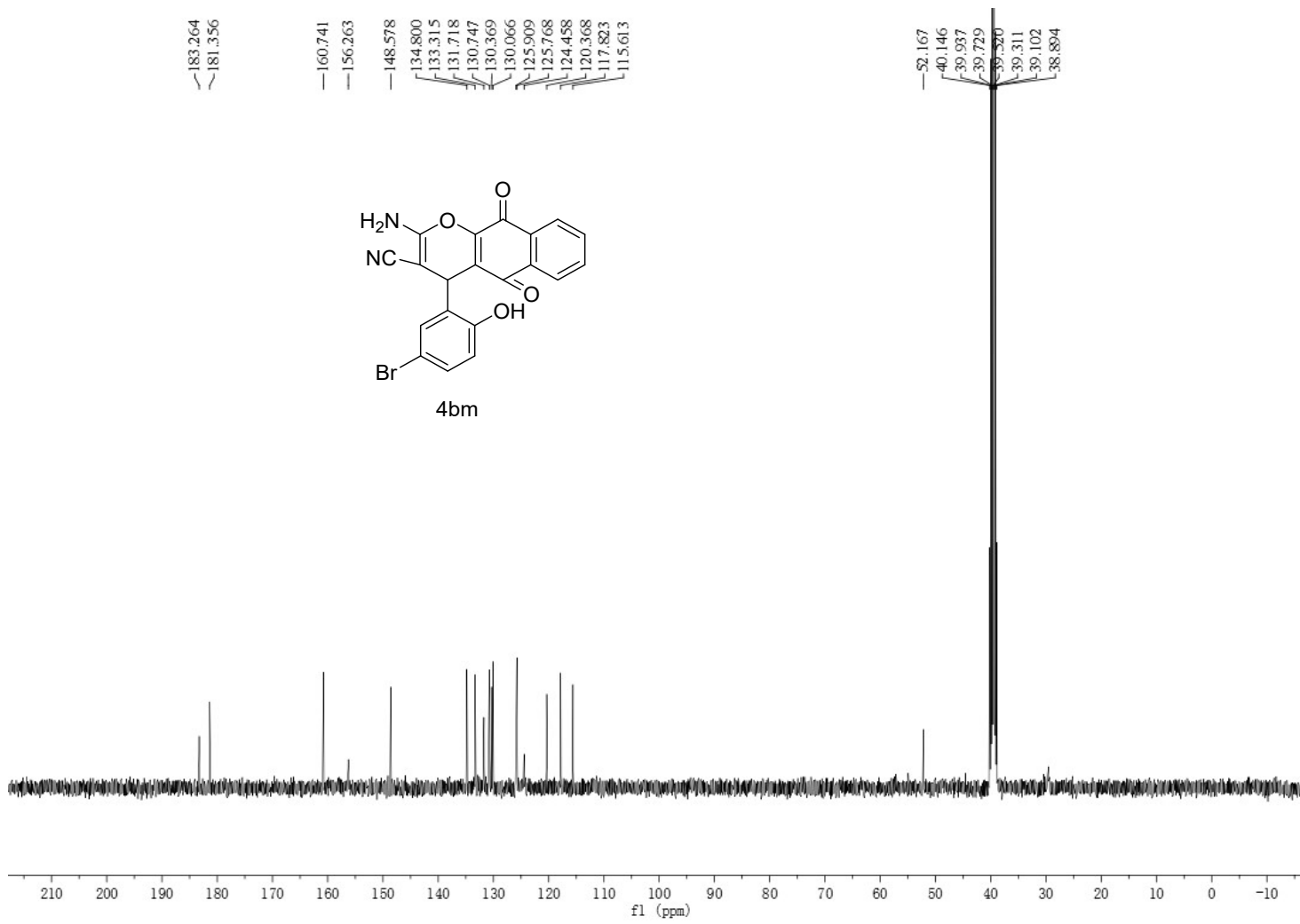
7.37e6



HRMS of Compound **4bl**



¹H NMR of Compound **4bm** (400 MHz, DMSO-d6)

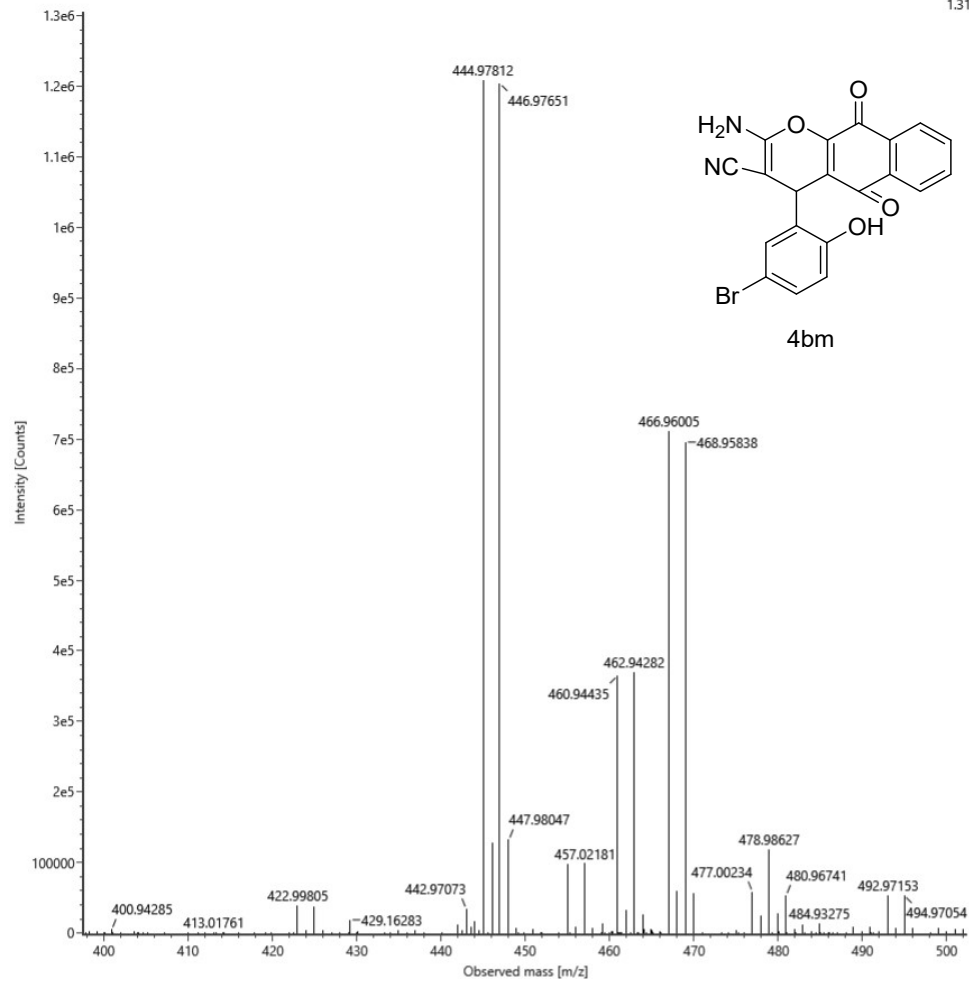


¹³C NMR of Compound **4bm** (101 MHz, DMSO-*d*₆)

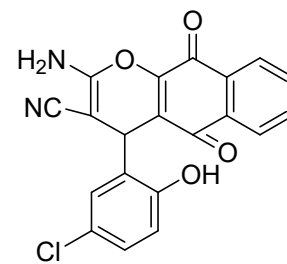
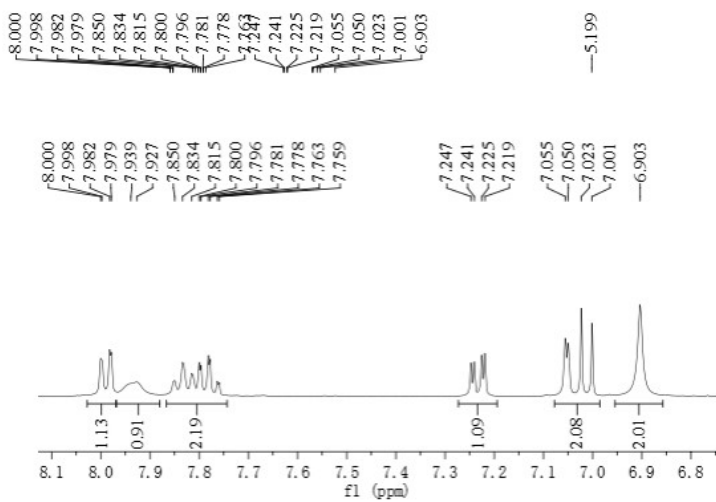
Item name: TAF-21
Item description:

Channel name: 1: Average Time 0.1089 min : TOF MS (50-1500) ESI+ : Centroided : Combined

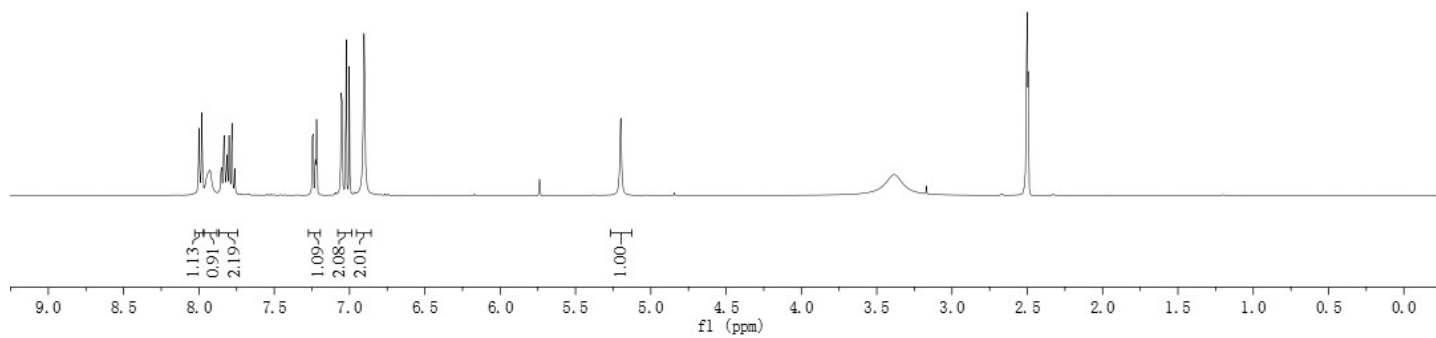
1.31e6



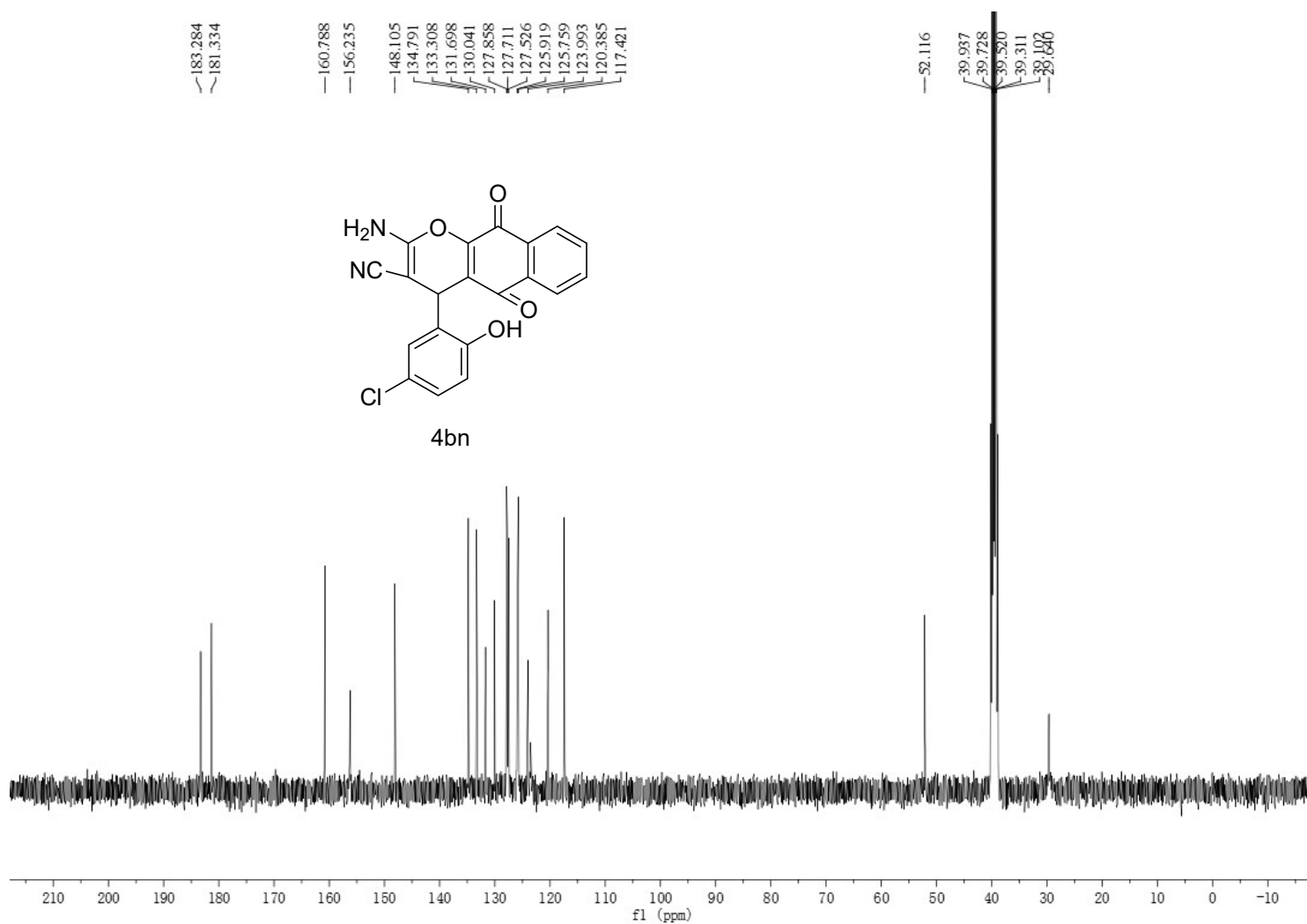
HRMS of Compound 4bm



4bn



¹H NMR of Compound **4bn** (400 MHz, DMSO-*d*₆)

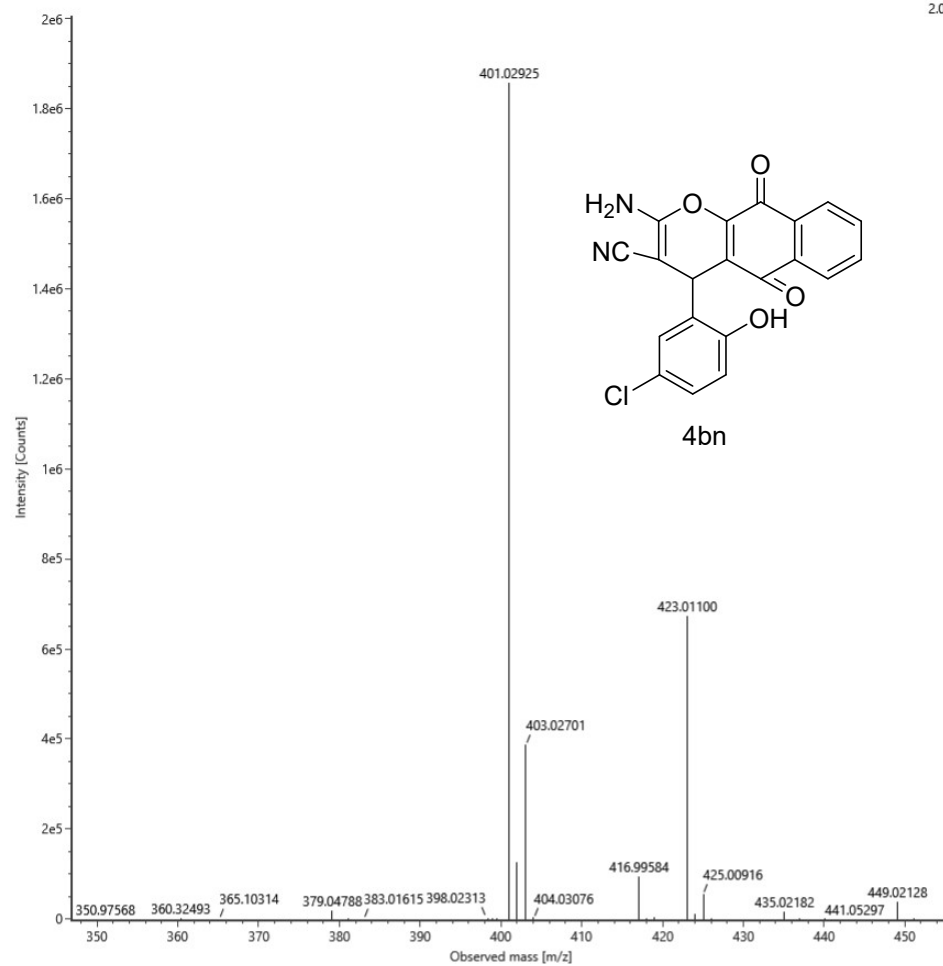


¹³C NMR of Compound **4bn** (101 MHz, DMSO-*d*₆)

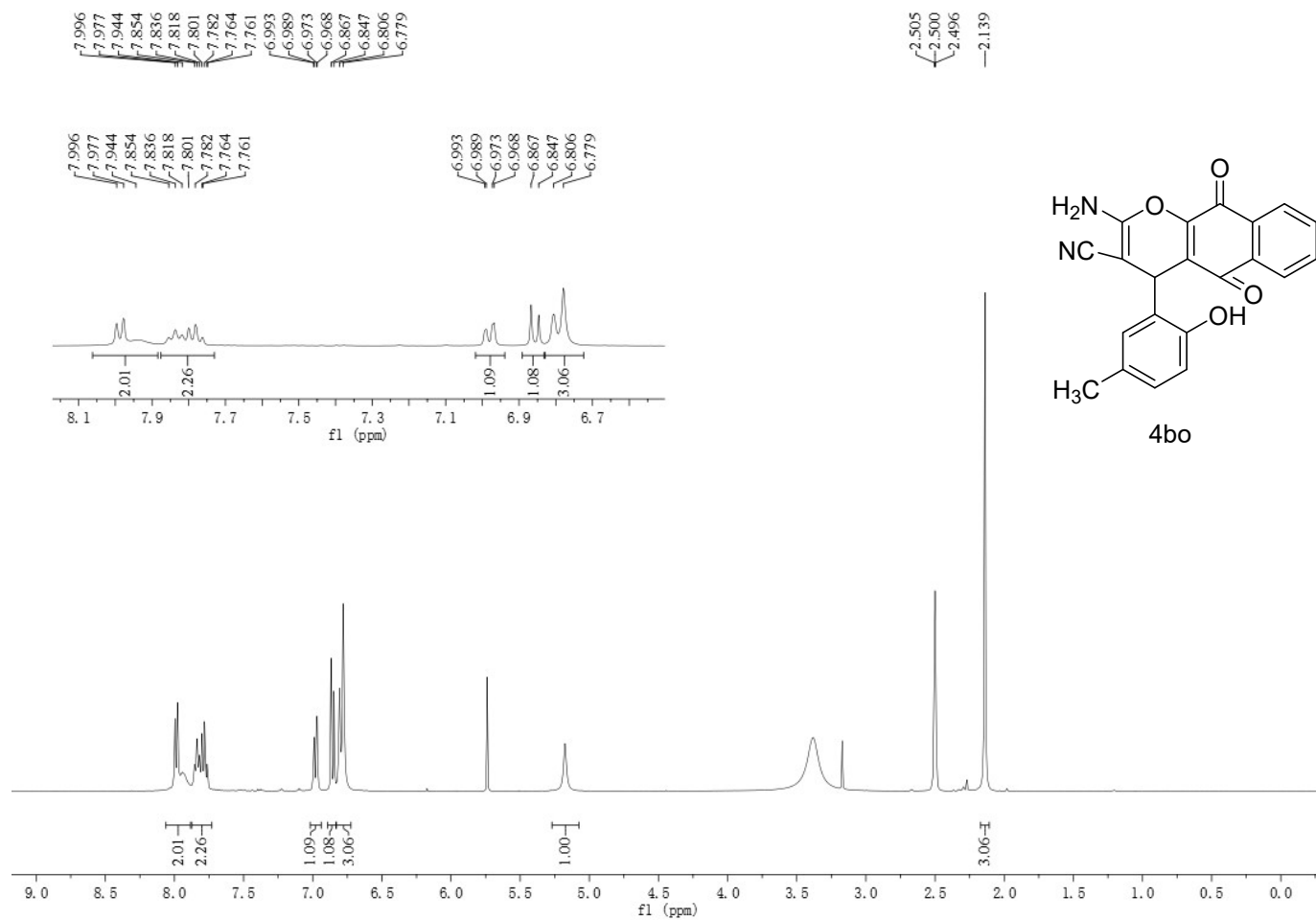
Item name: TAF-25
Item description:

Channel name: 1: Average Time 0.1174 min : TOF MS (50-1500) ESI+ : Centroided : Combined

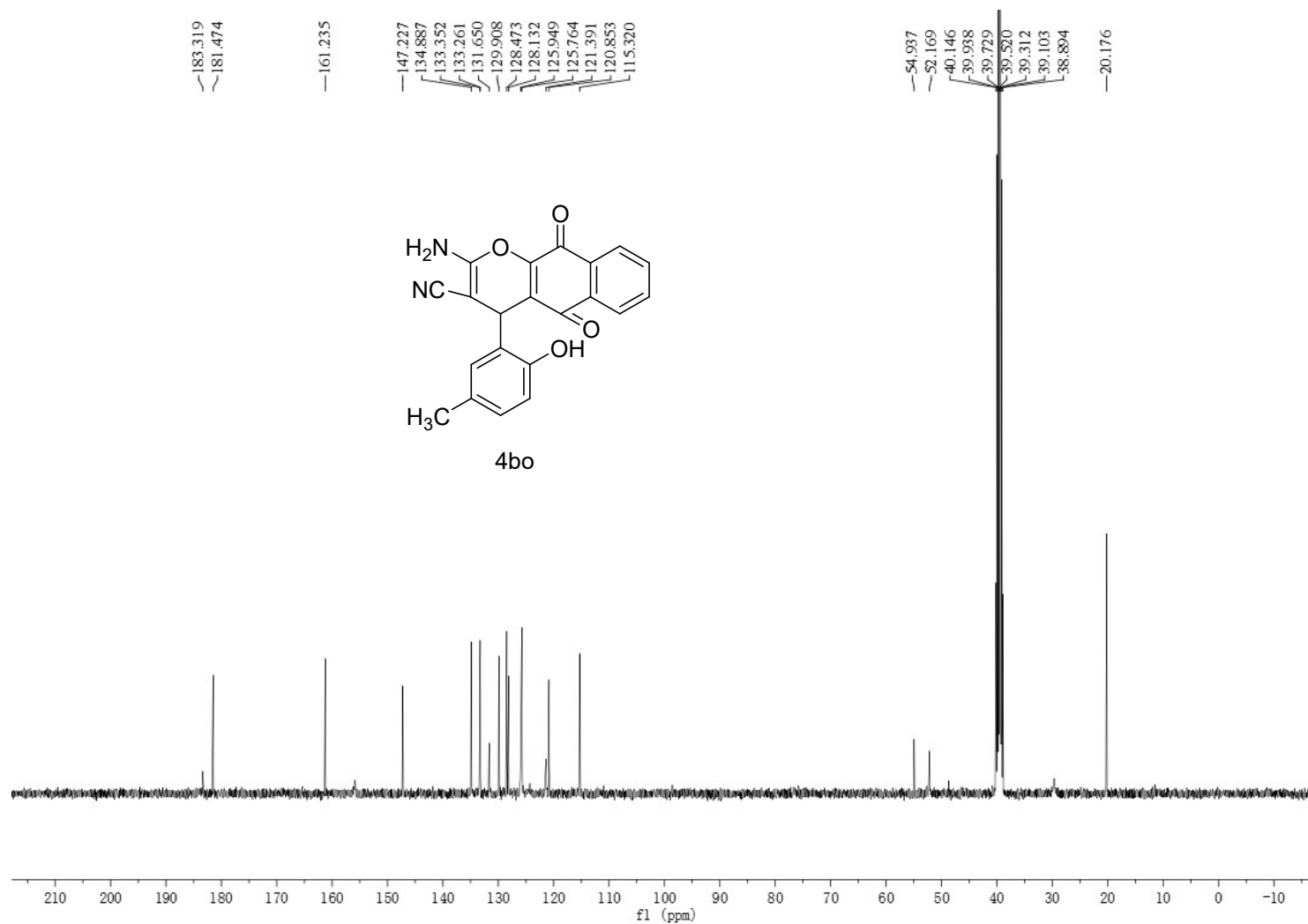
2.01e6



HRMS of Compound **4bn**



¹H NMR of Compound **4bo** (400 MHz, DMSO-*d*₆)

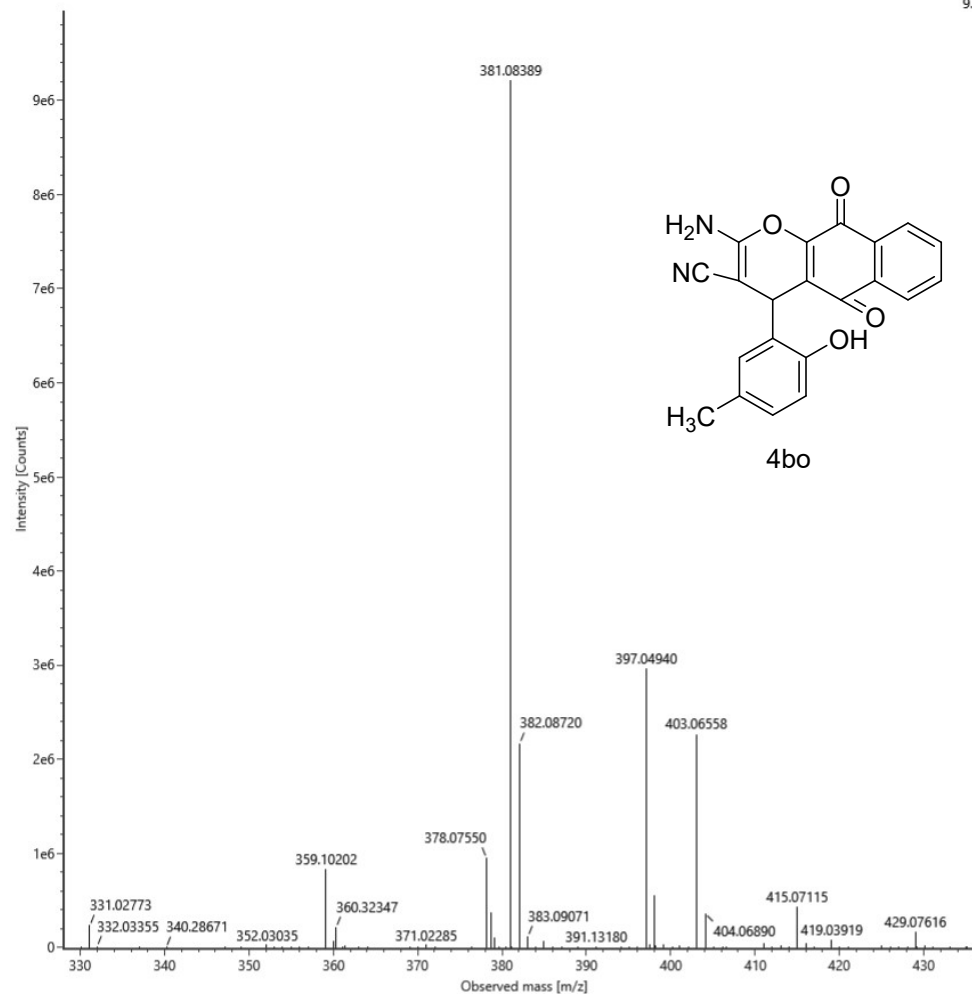


¹³C NMR of Compound **4bo** (101 MHz, DMSO-*d*₆)

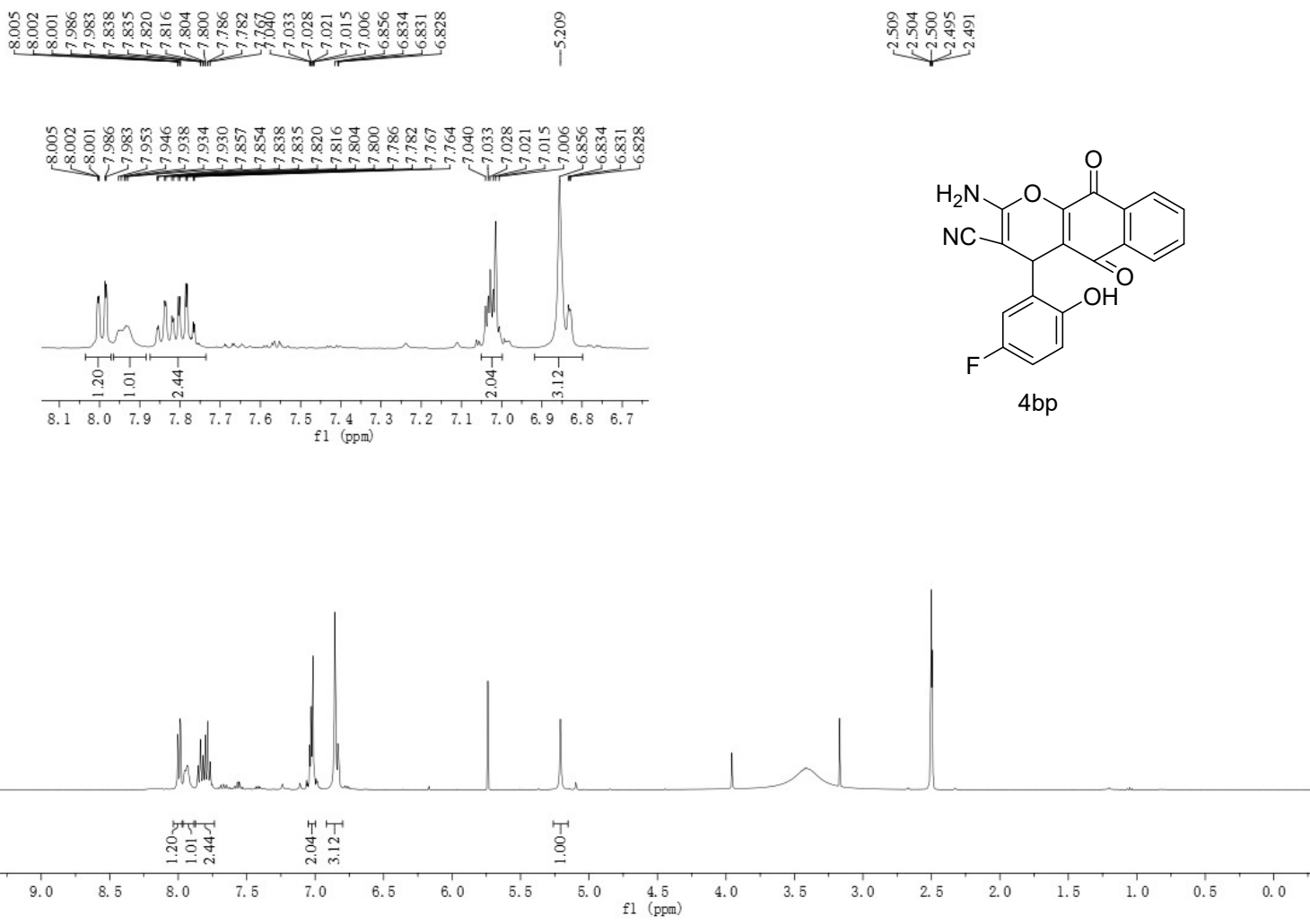
Item name: TAF-22
Item description:

Channel name: 1: Average Time 0.1131 min : TOF MS (50-1500) ESI+ : Centroided : Combined

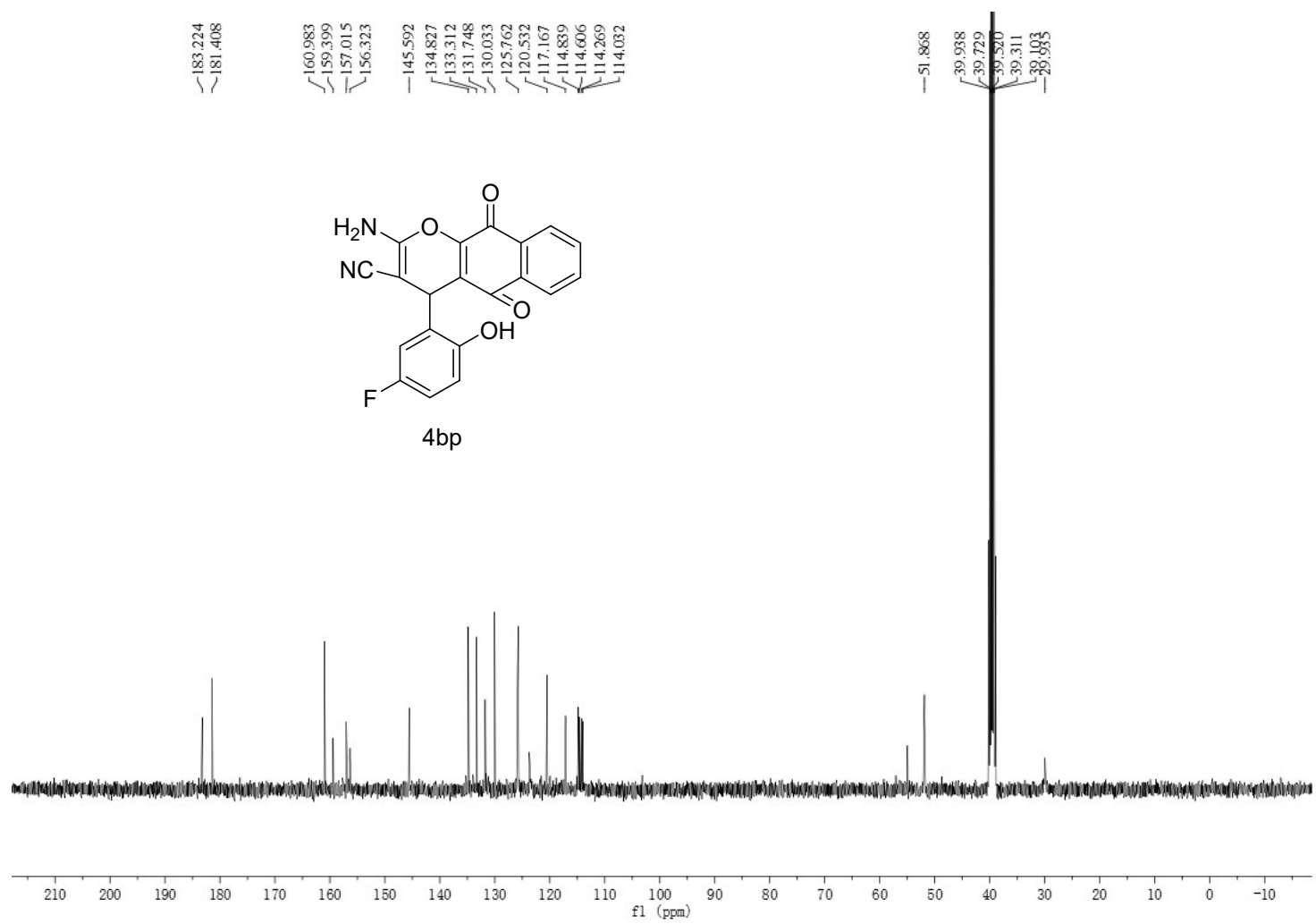
9.96e6



HRMS of Compound **4bo**



¹H NMR of Compound **4bp** (400 MHz, DMSO-*d*₆)

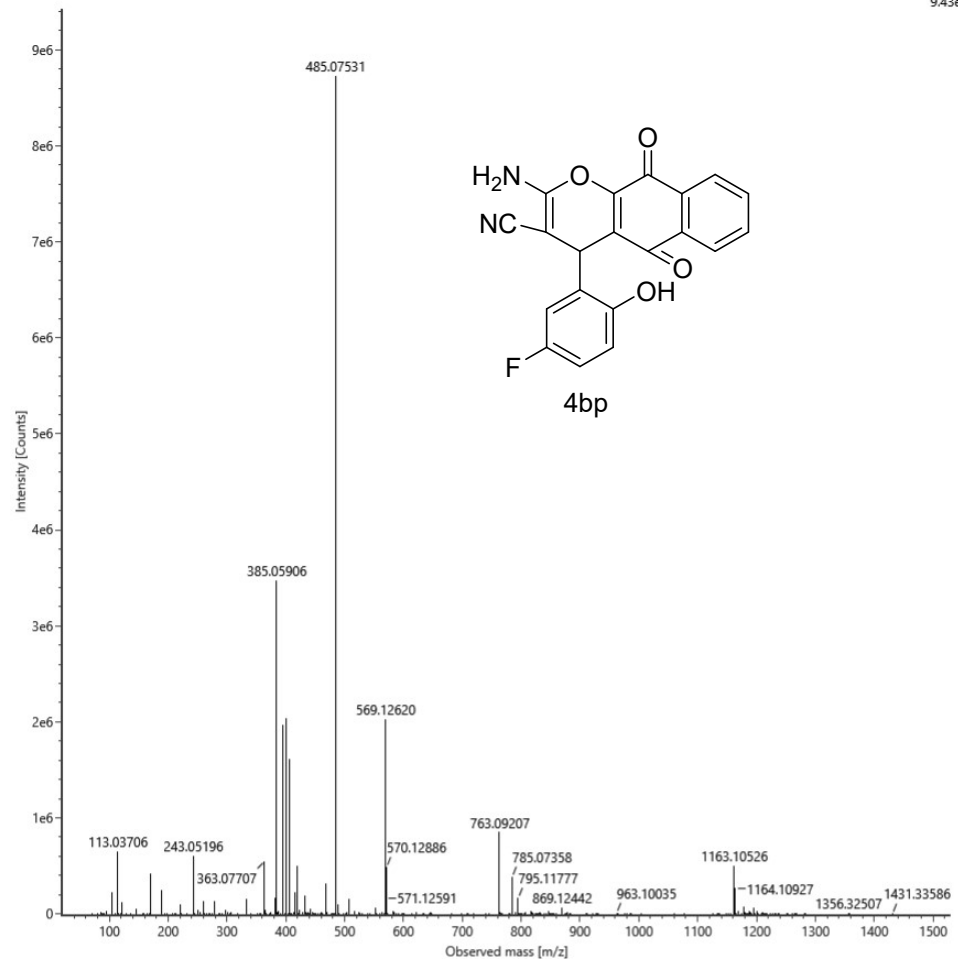


¹³C NMR of Compound **4bp** (101 MHz, DMSO-*d*₆)

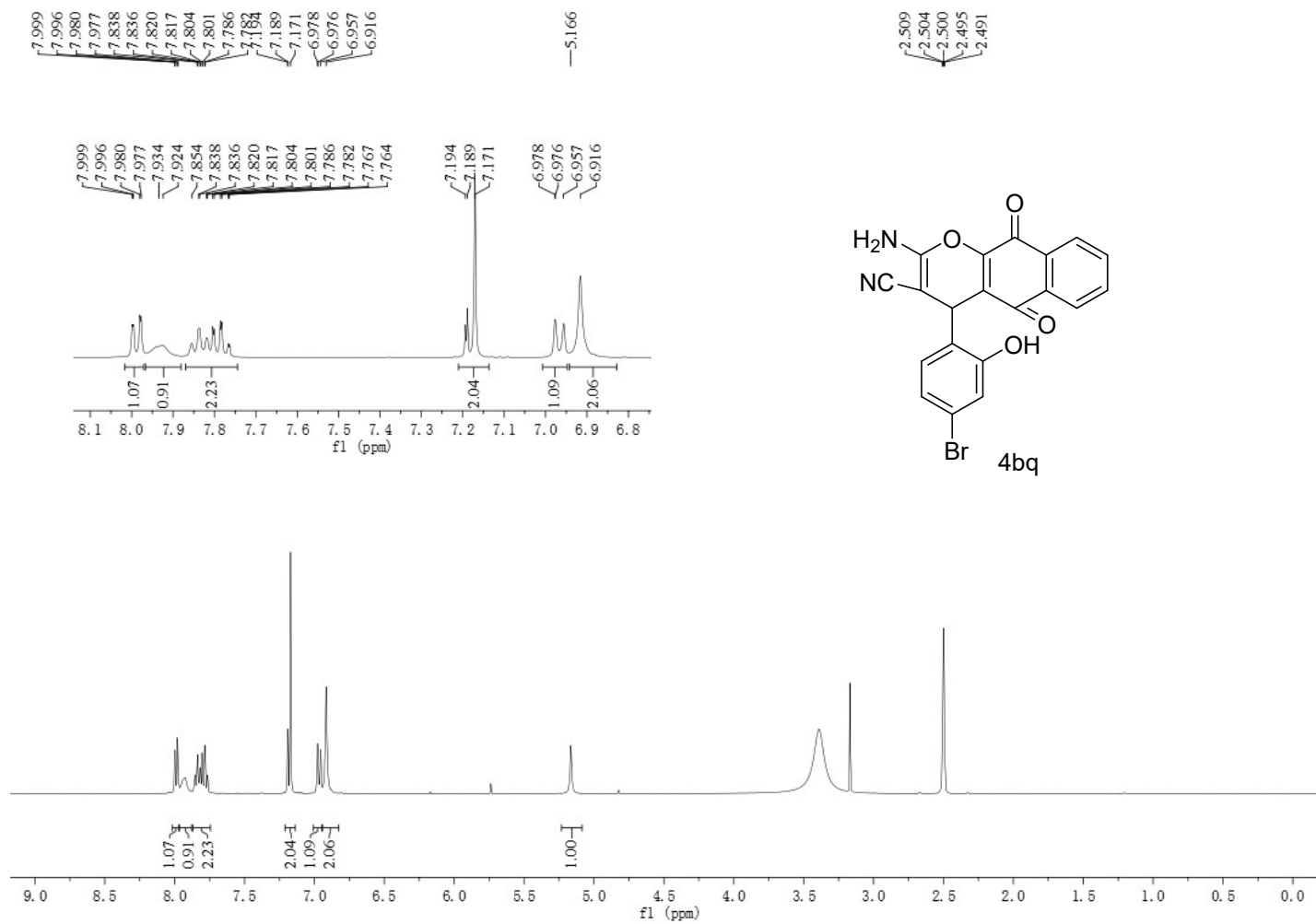
Item name: TAF-23
Item description:

Channel name: 1: Average Time 0.1089 min : TOF MS (50-1500) ESI+ : Centroided : Combined

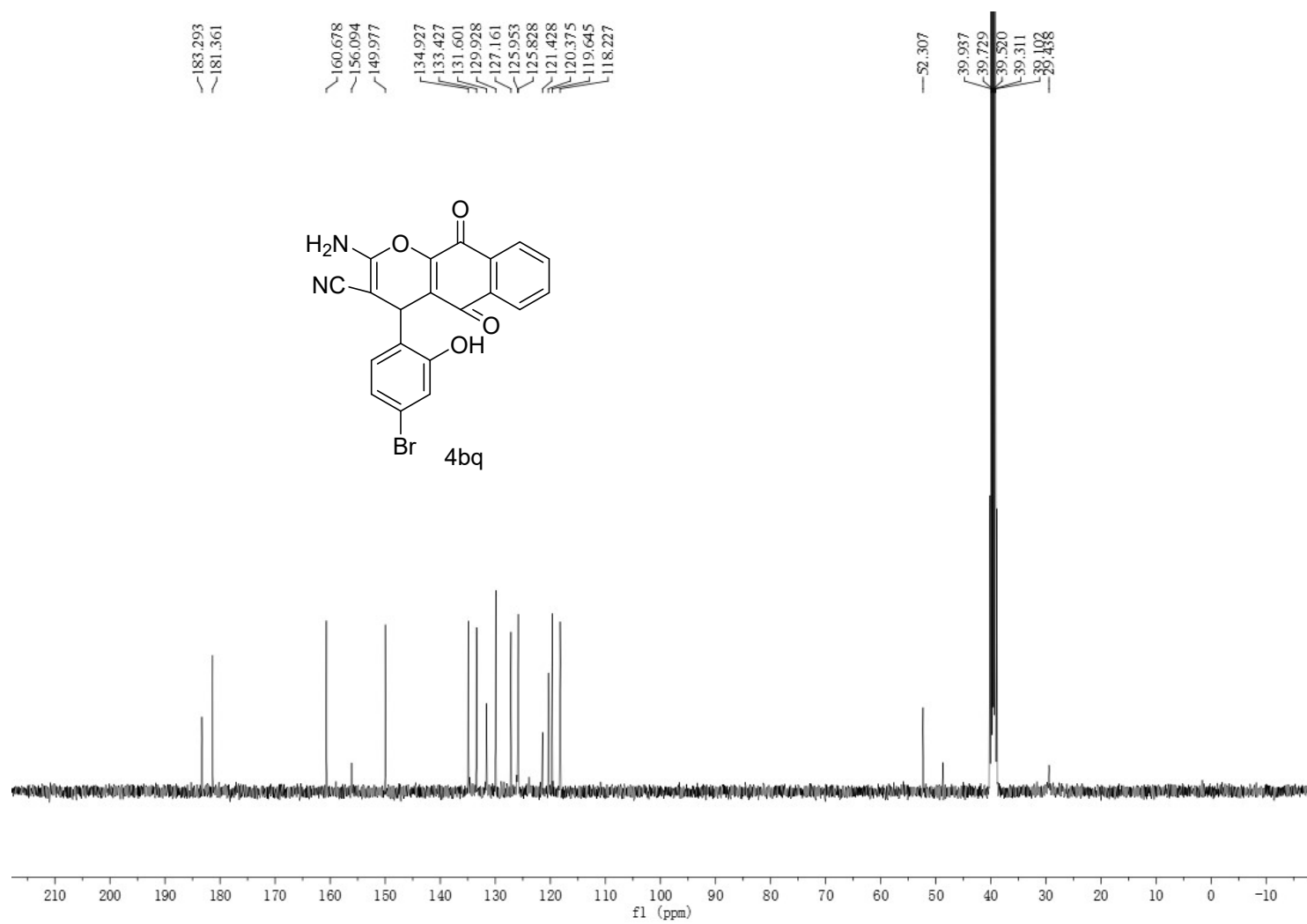
9.43e6



HRMS of Compound 4bp



^1H NMR of Compound **4bq** (400 MHz, $\text{DMSO-}d_6$)



¹³C NMR of Compound **4bq** (101 MHz, DMSO-*d*₆)

Item name: TAF-27
Item description:

Channel name: 1: Average Time 0.1420 min : TOF MS (50-1500) ESI+ : Centroided : Combined

3.32e6

