

SUPPORTING INFORMATION

Design, synthesis, and molecular docking studies of chroman-4-one linked thiosemicarbazide derivatives as inhibitors of KatG and anti-Mycobacterium tuberculosis agents

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Zai-Chang Yang: yangzaichangzm@163.com (Zai-Chang Yang)

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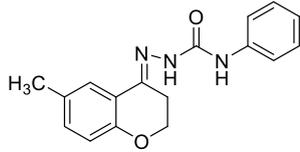
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Molecular docking results

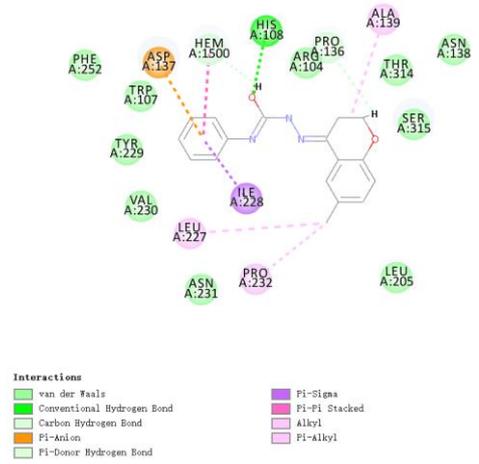
Figure S1. Results of molecular docking of compounds with KatG

Serial Number	Compound	Lib Dock Score	2D Diagram
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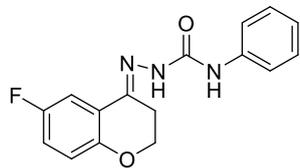
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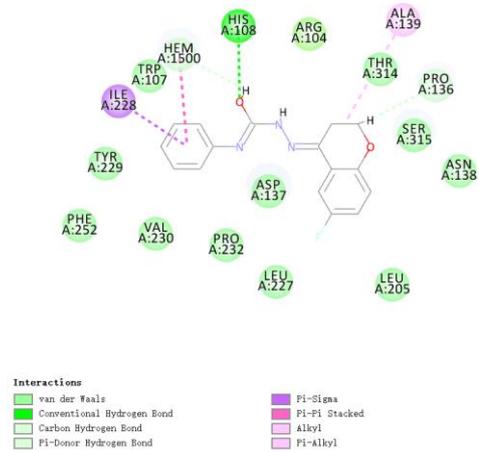
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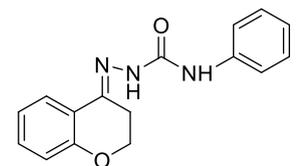
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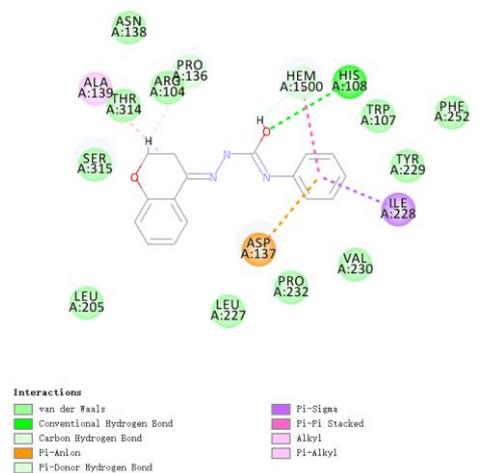
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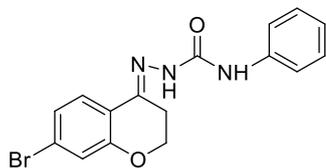
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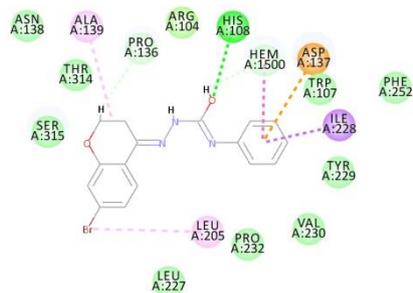
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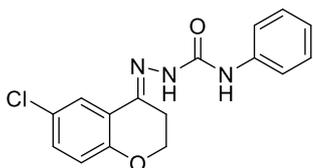
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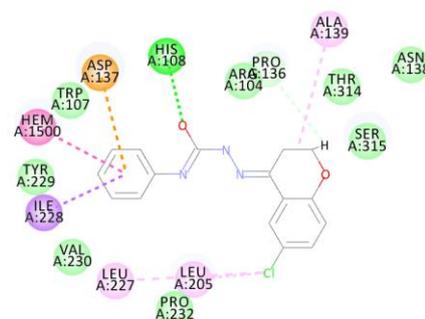
Interactions

- van der Waals
- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- PI-Anion
- PI-Donor Hydrogen Bond
- PI-Sigma
- PI-Pi Stacked
- Alkyl
- PI-Alkyl

e



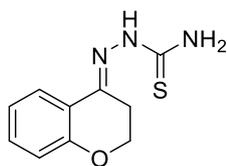
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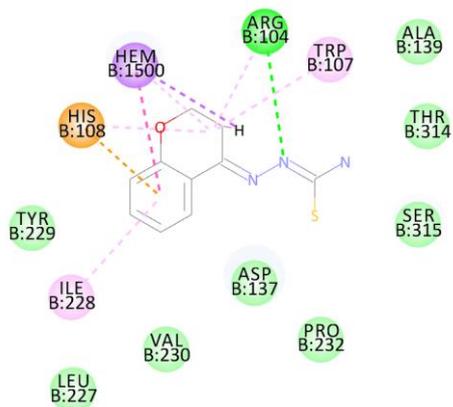
Interactions

- van der Waals
- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- PI-Anion
- PI-Sigma
- PI-Pi Stacked
- Alkyl
- PI-Alkyl

f



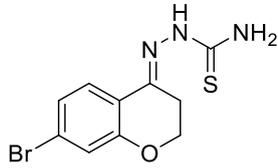
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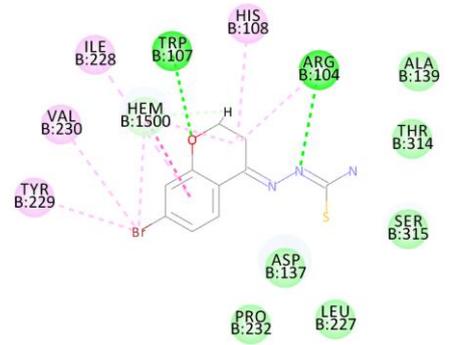
Interactions

- van der Waals
- Conventional Hydrogen Bond
- PI-Cation
- PI-Sigma
- PI-Pi Stacked
- Alkyl
- PI-Alkyl

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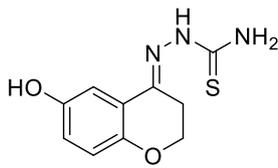


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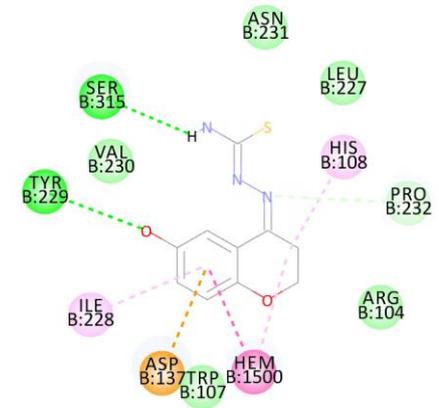


Interactions
van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Pi-Pi Stacked
Alkyl
Pi-Alkyl

h

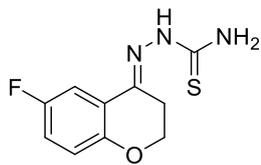


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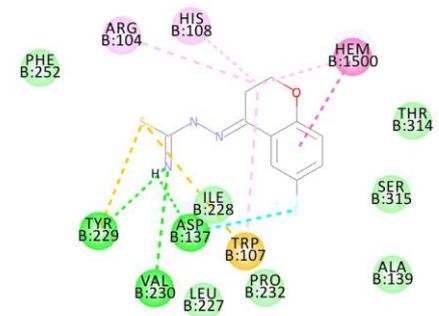


Interactions
van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Pi-Pi Stacked
Alkyl
Pi-Alkyl
Pi-Anion

i

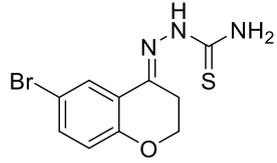


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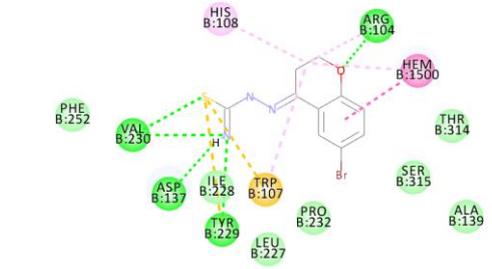


Interactions
van der Waals
Conventional Hydrogen Bond
Halogen (Fluorine)
Pi-Sulfur
Pi-Pi Stacked
Alkyl
Pi-Alkyl

g

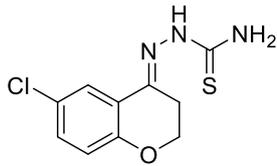


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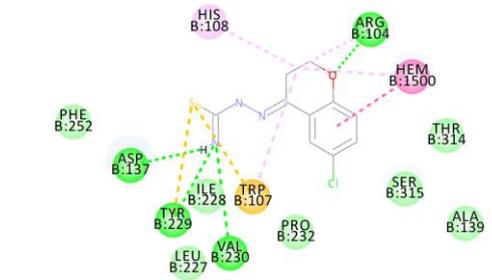


Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Sulfur
Pi-Pi Stacked
Alkyl
Pi-Alkyl

k

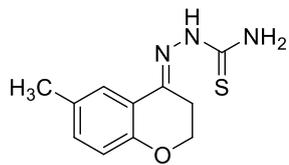


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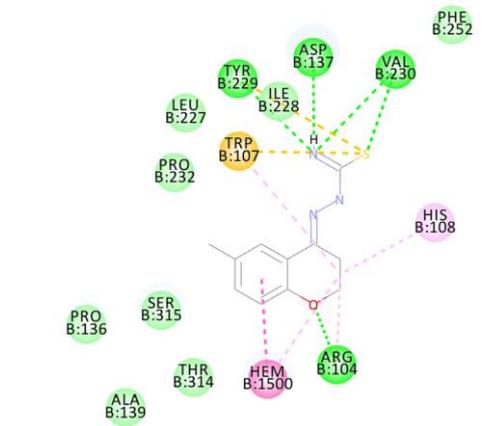


Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Sulfur
Pi-Pi Stacked
Alkyl
Pi-Alkyl

l

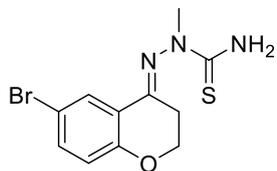


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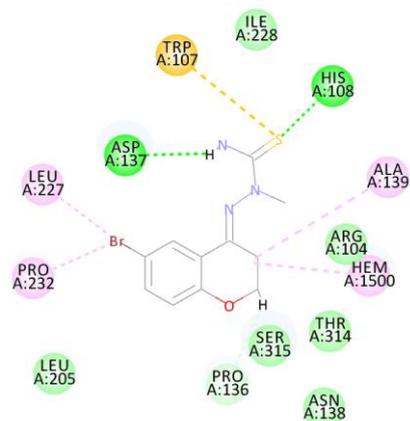


Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Sulfur
Pi-Pi Stacked
Alkyl
Pi-Alkyl

m

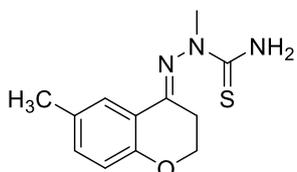


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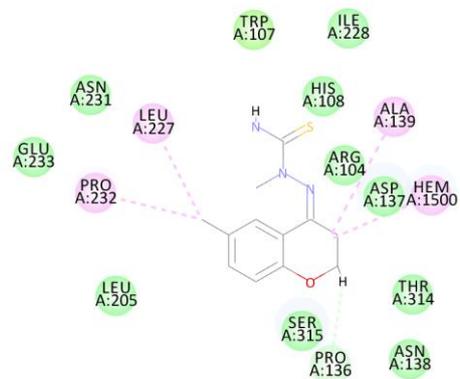


Interactions
van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Pi-Sulfur
Alkyl

n

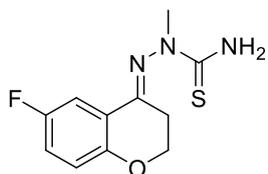


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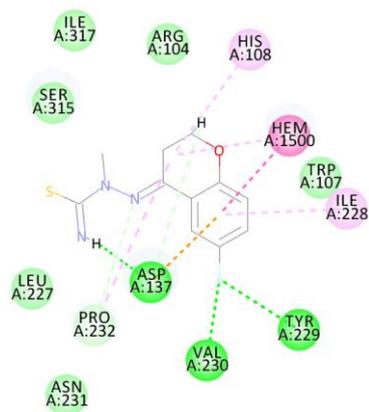


Interactions
van der Waals
Carbon Hydrogen Bond
Alkyl

o

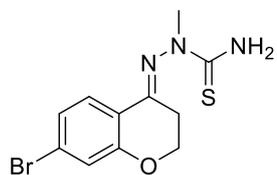


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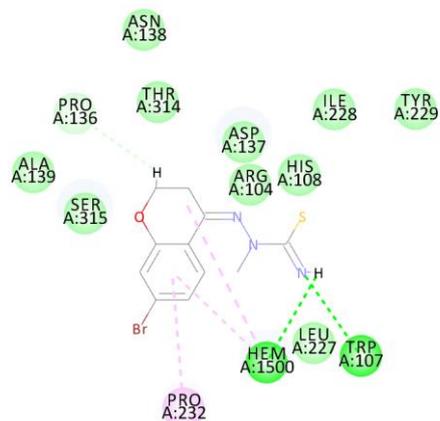


Interactions
van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Halogen (Fluorine)
Pi-Anion
Pi-Pi Stacked
Alkyl
Pi-Alkyl

p

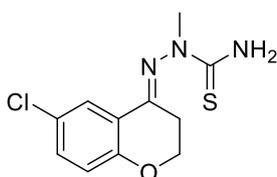


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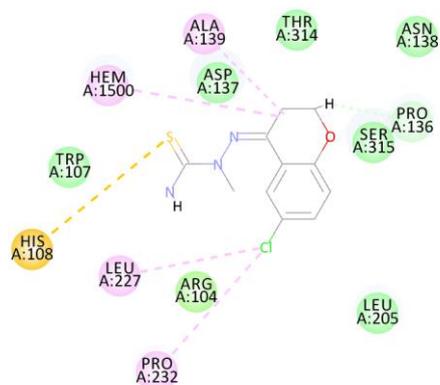


Interactions
van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Alkyl
Pi-Alkyl

q

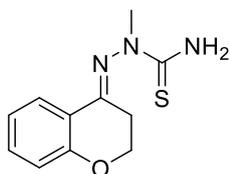


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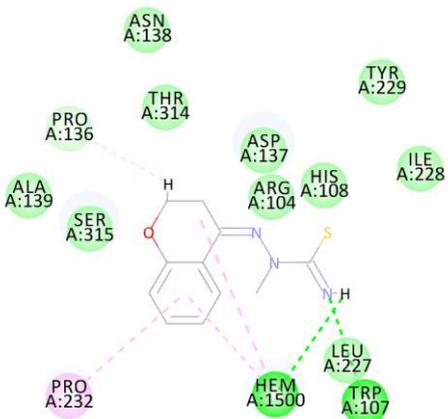


Interactions
van der Waals
Carbon Hydrogen Bond
Pi-Sulfur
Alkyl

r

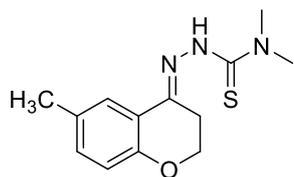


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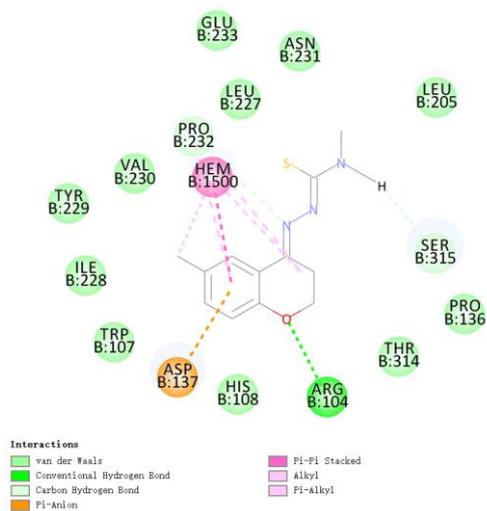


Interactions
van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Alkyl
Pi-Alkyl

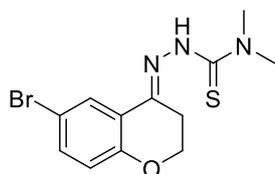
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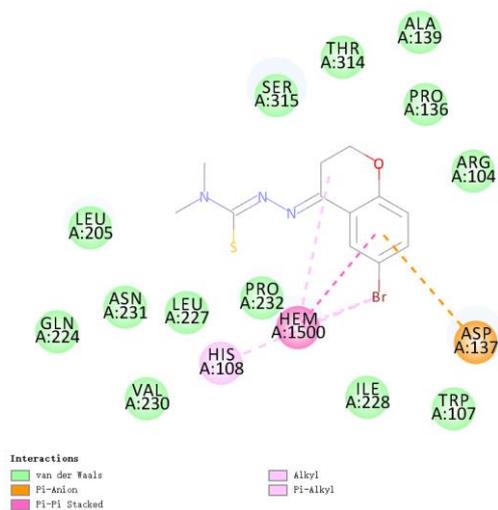
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86.3805



NMR Spectra and HRMS spectra of compounds

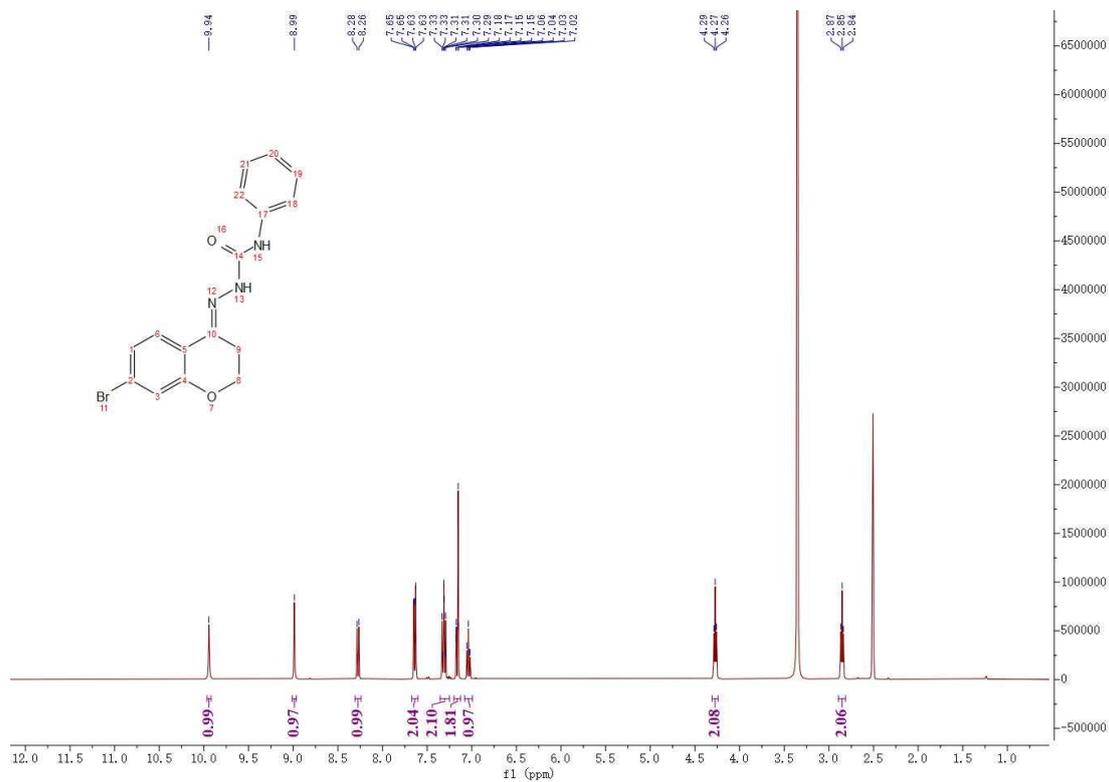


Figure S2. ¹H NMR Spectrum of Compound 3a

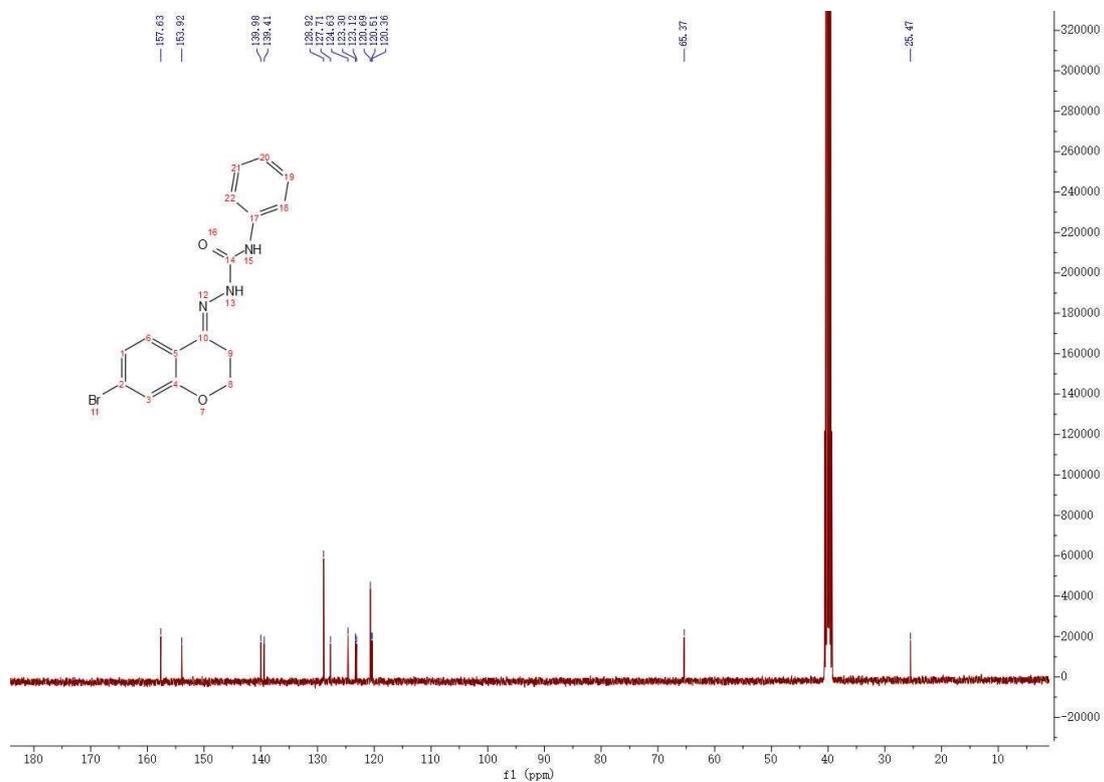


Figure S3. ¹³C NMR Spectrum of Compound 3a

Item name: 3a
Item description:

Channel name: 1: Average Time 0.1046 min : TOF MS (50-1500) ESI+ : Centroided : Combined

9.73e6

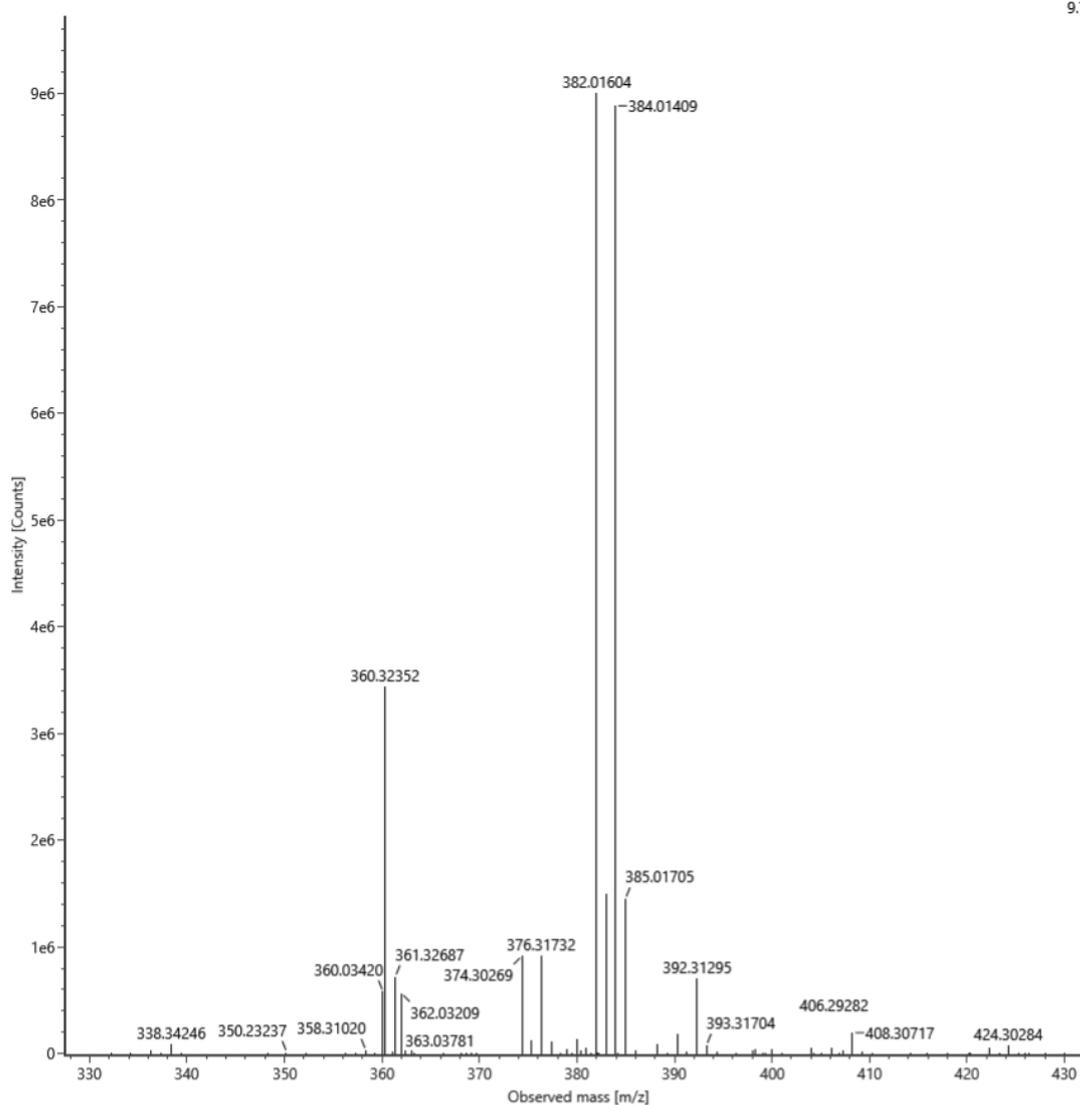


Figure S4. HRMS Spectrogram of Compound **3a**

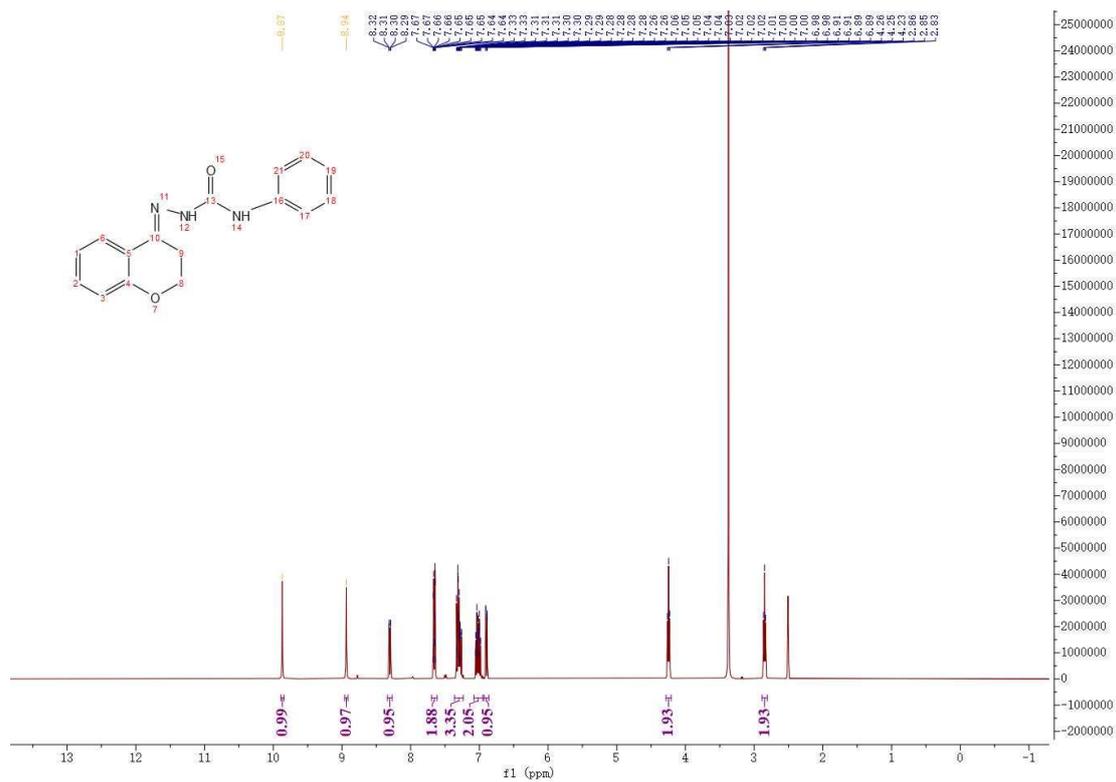


Figure S5. ^1H NMR Spectrum of Compound **3b**

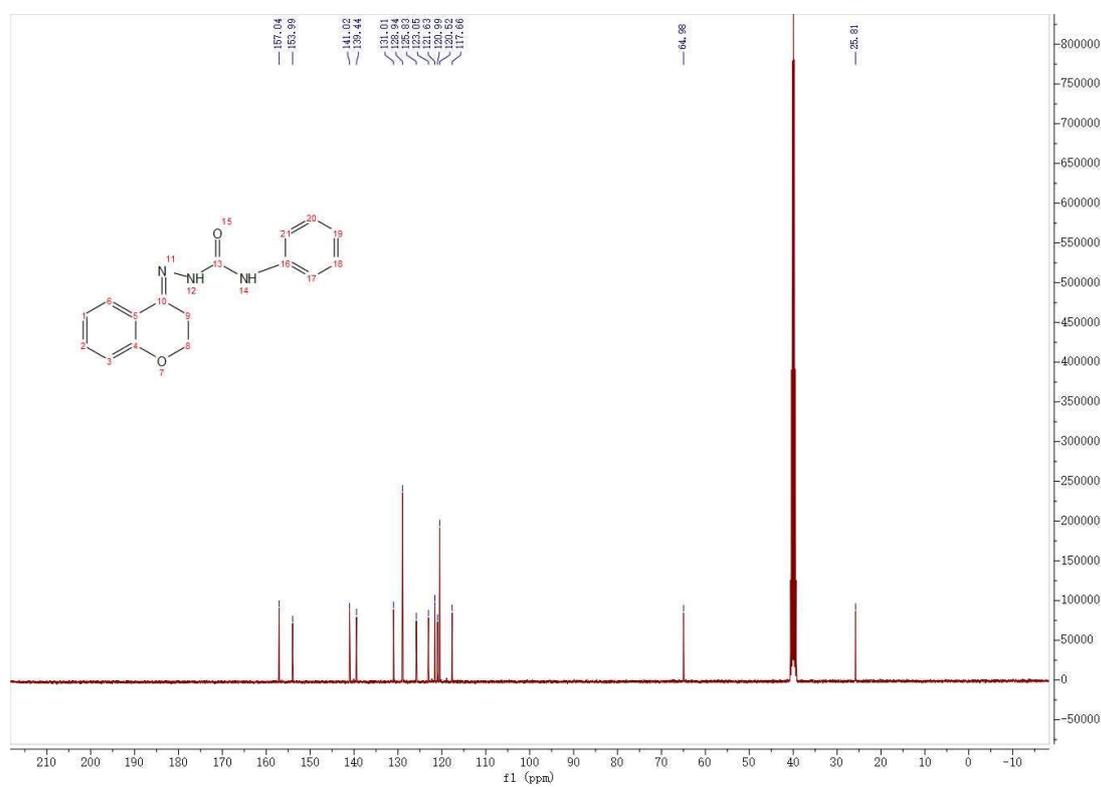


Figure S6. ^{13}C NMR Spectrum of Compound **3b**

Item name: 3b
Item description:

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

3.98e7

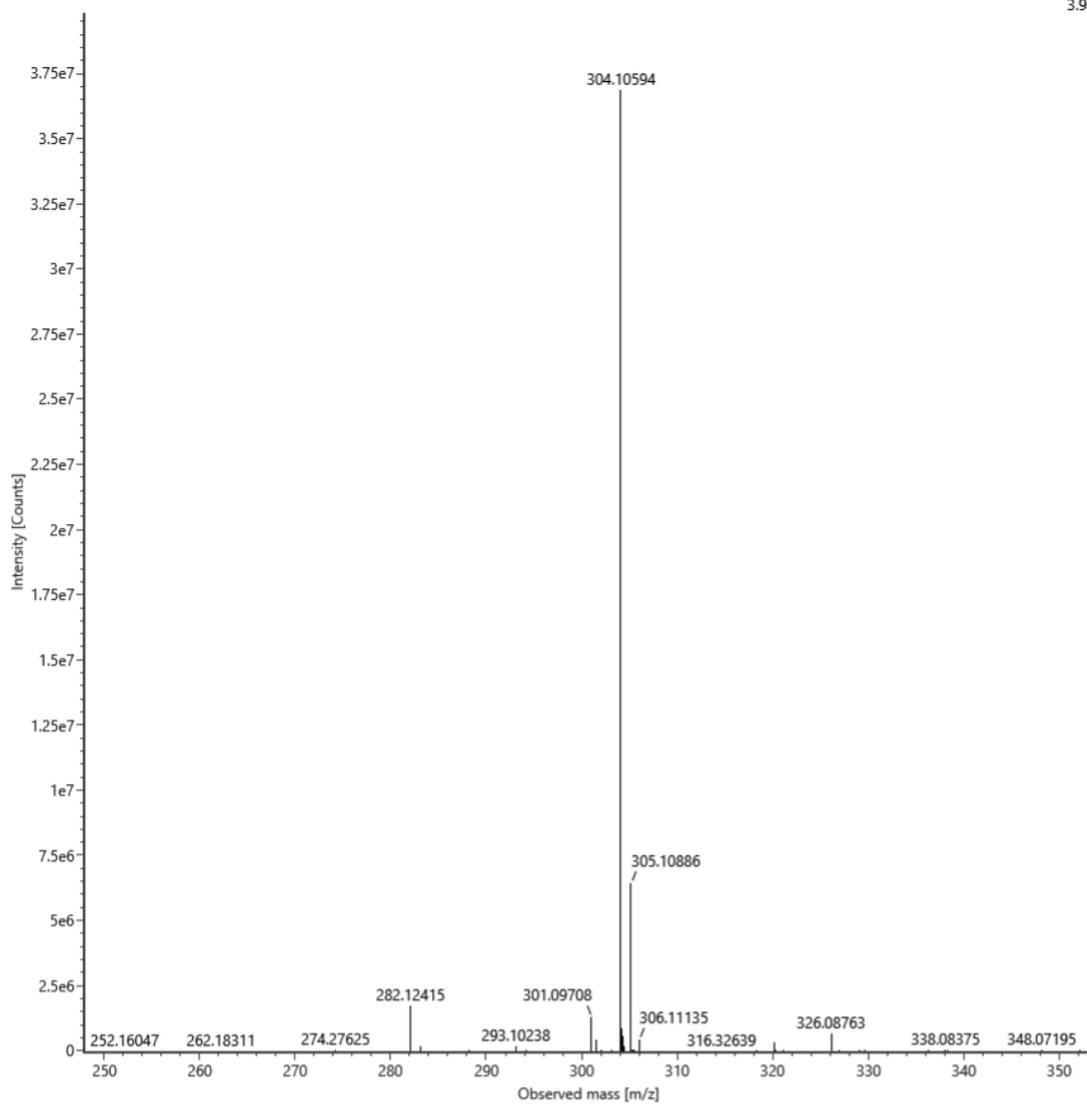


Figure S7. HRMS Spectrogram of Compound **3b**

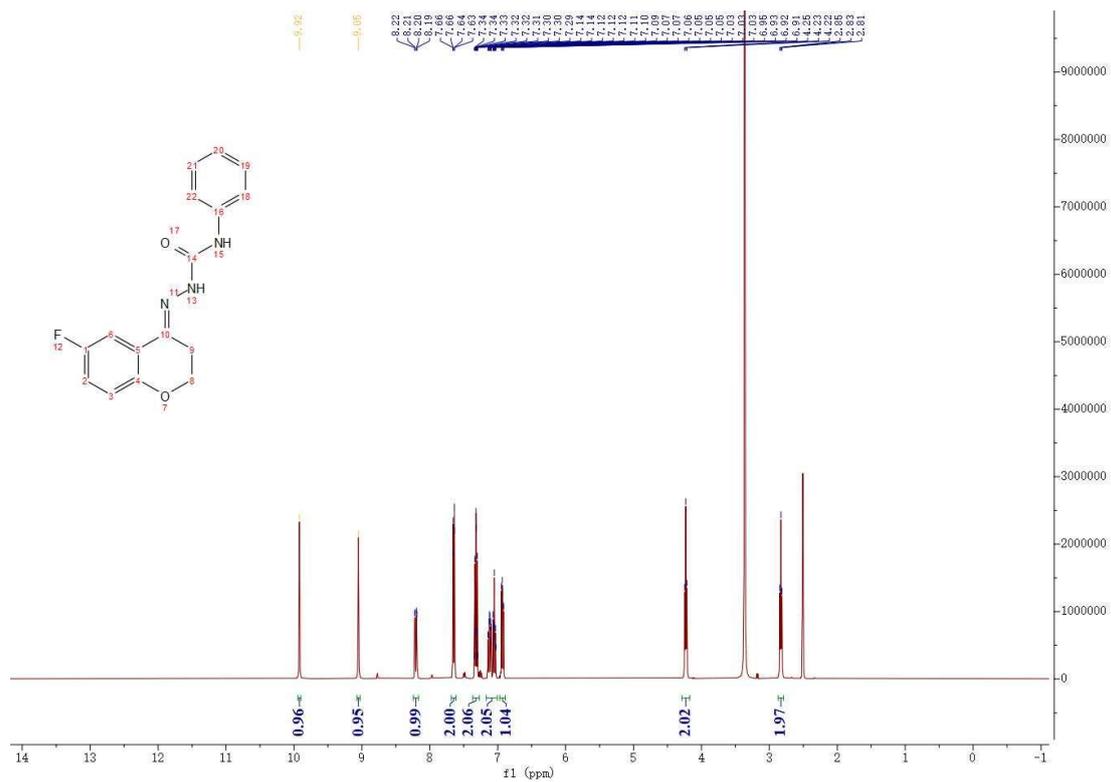


Figure S8. ^1H NMR Spectrum of Compound 3c

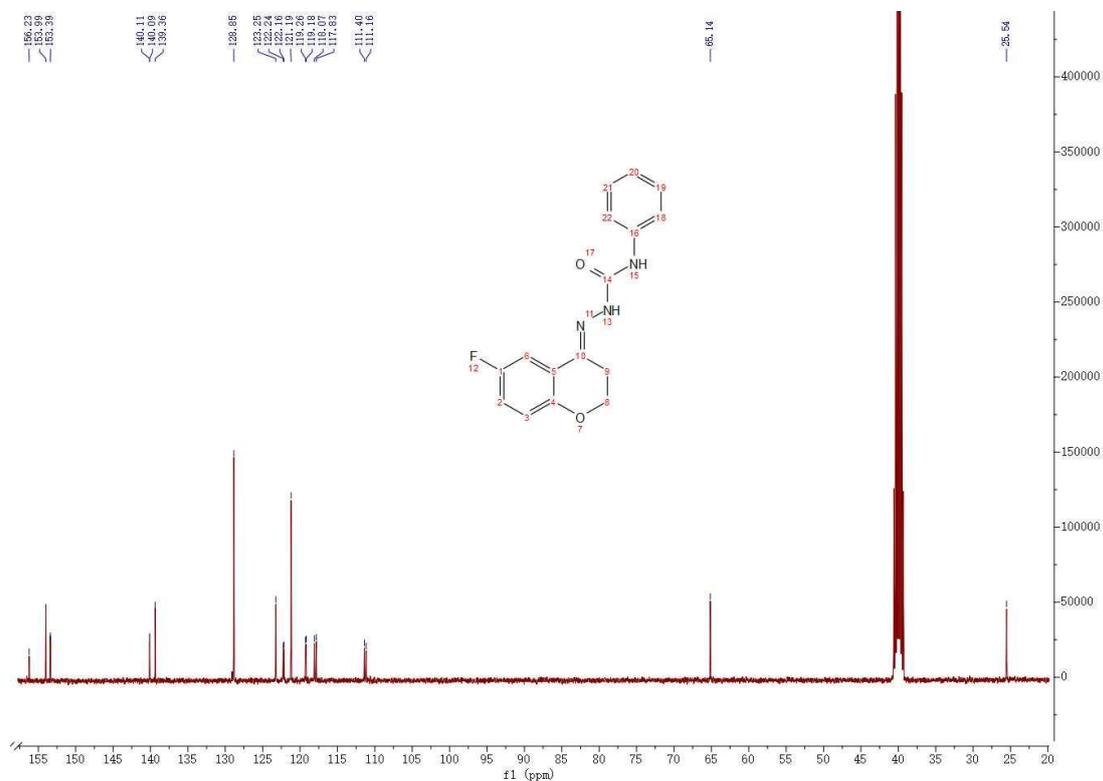


Figure S9. ^{13}C NMR Spectrum of Compound 3c

Item name: 3c
Item description:

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

2.5e7

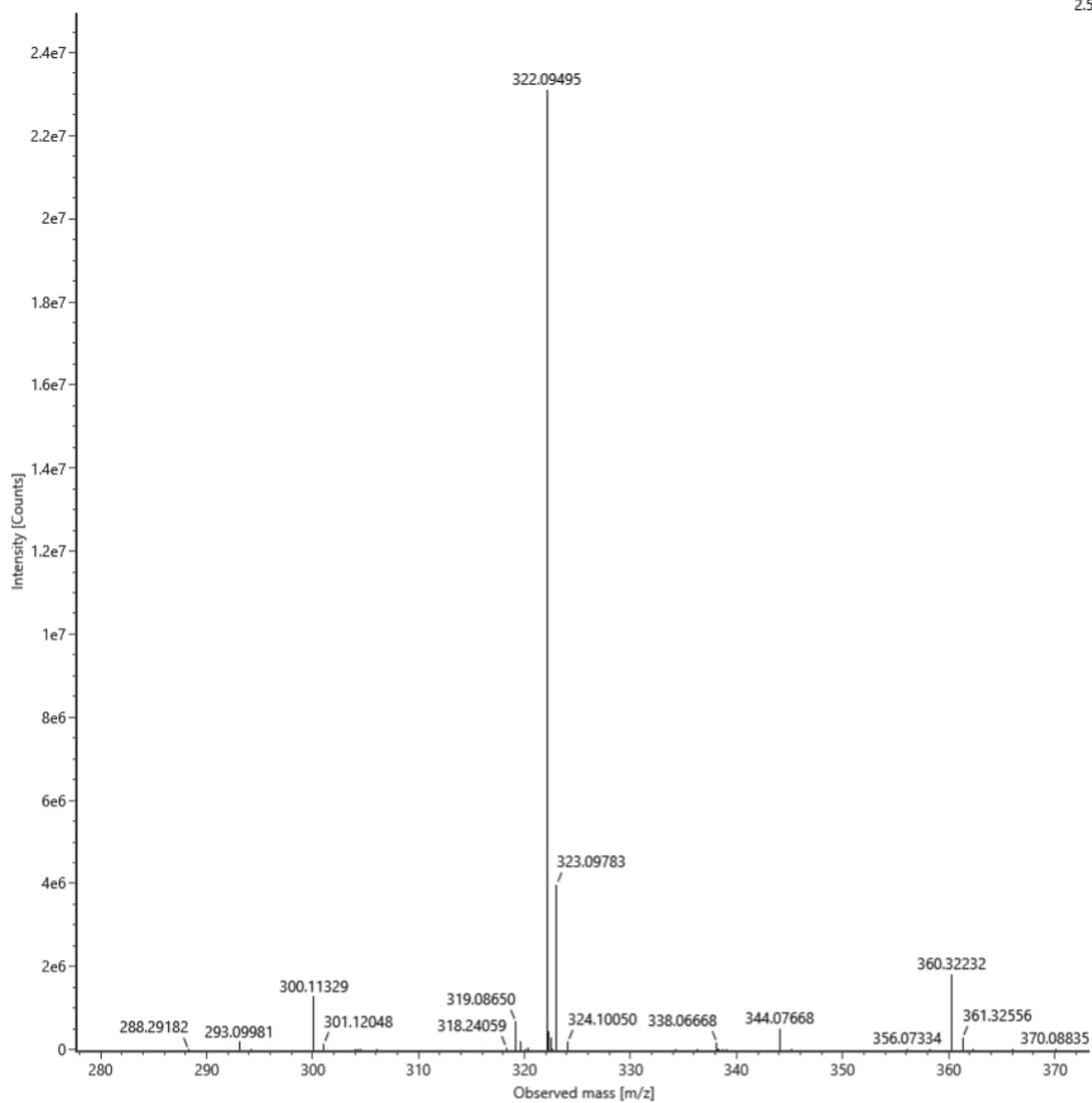


Figure S10. HRMS Spectrogram of Compound **3c**

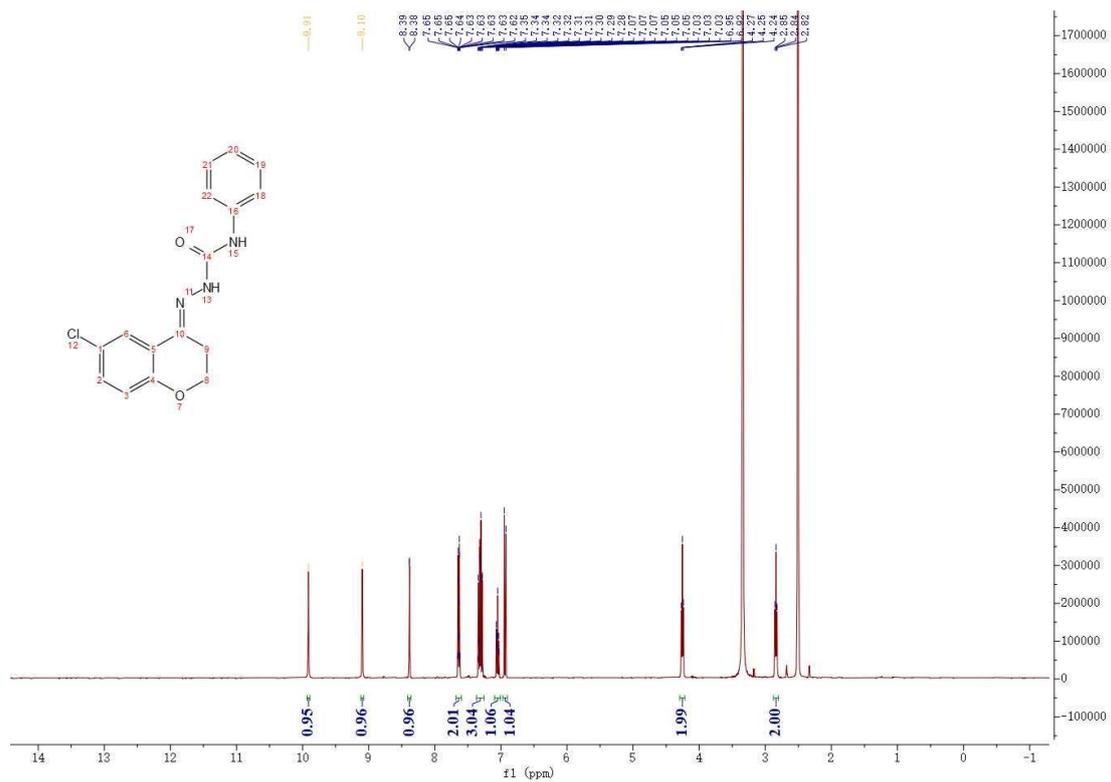


Figure S11. ¹H NMR Spectrum of Compound 3d

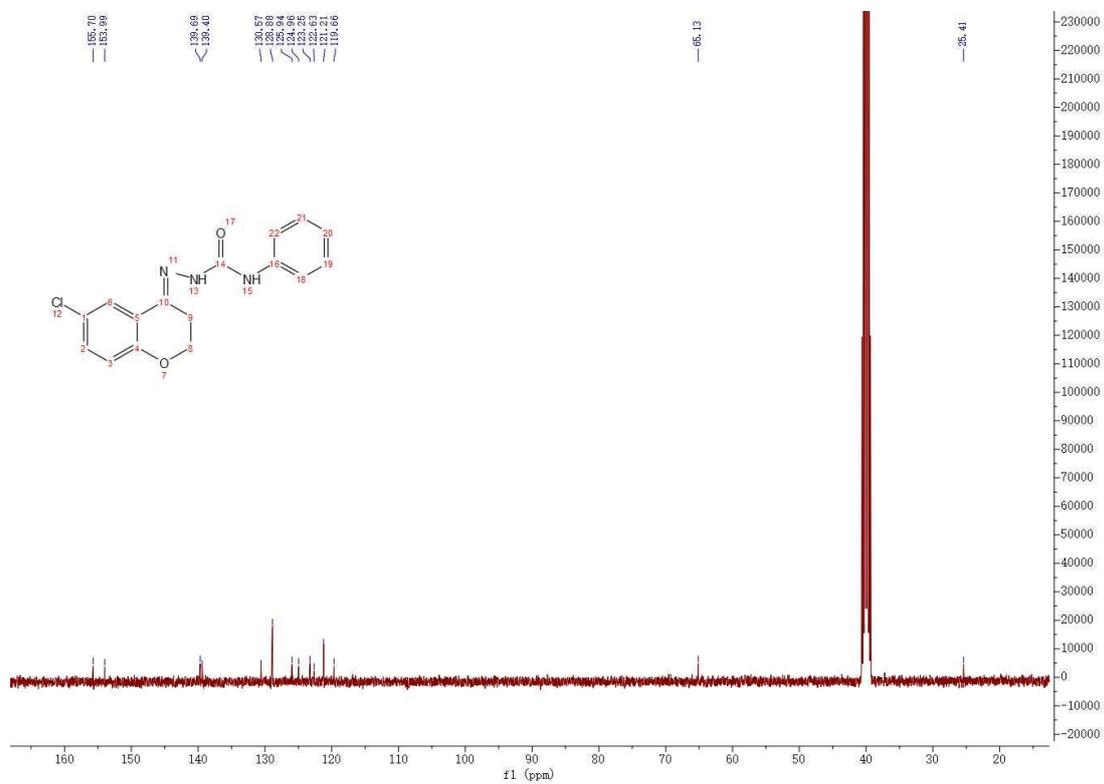


Figure S12. ¹³C NMR Spectrum of Compound 3d

Item name: 3d
Item description:

Channel name: 1: Average Time 0.1132 min : TOF MS (50-1500) ESI+ : Centroided : Combined

7.48e6

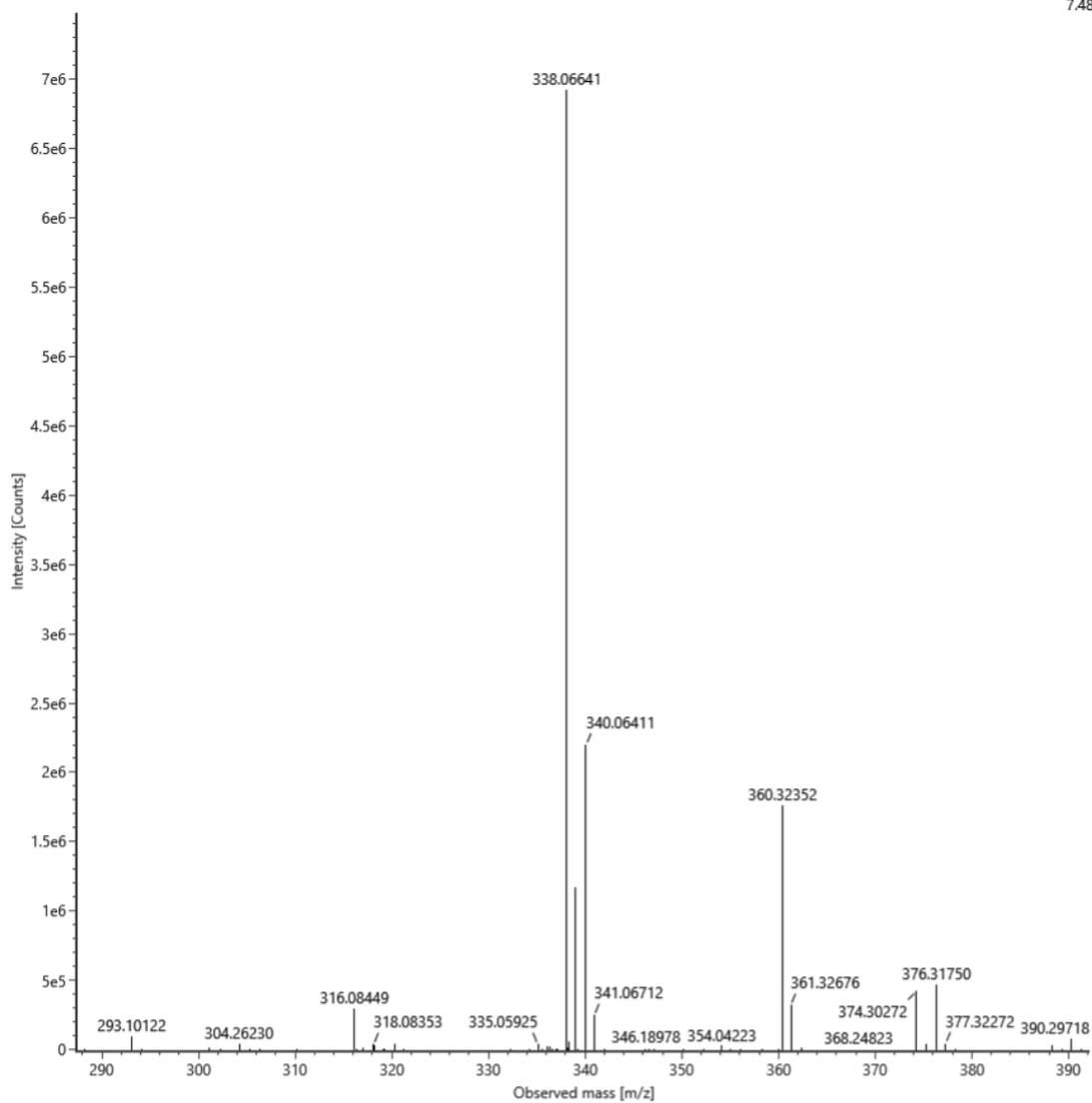
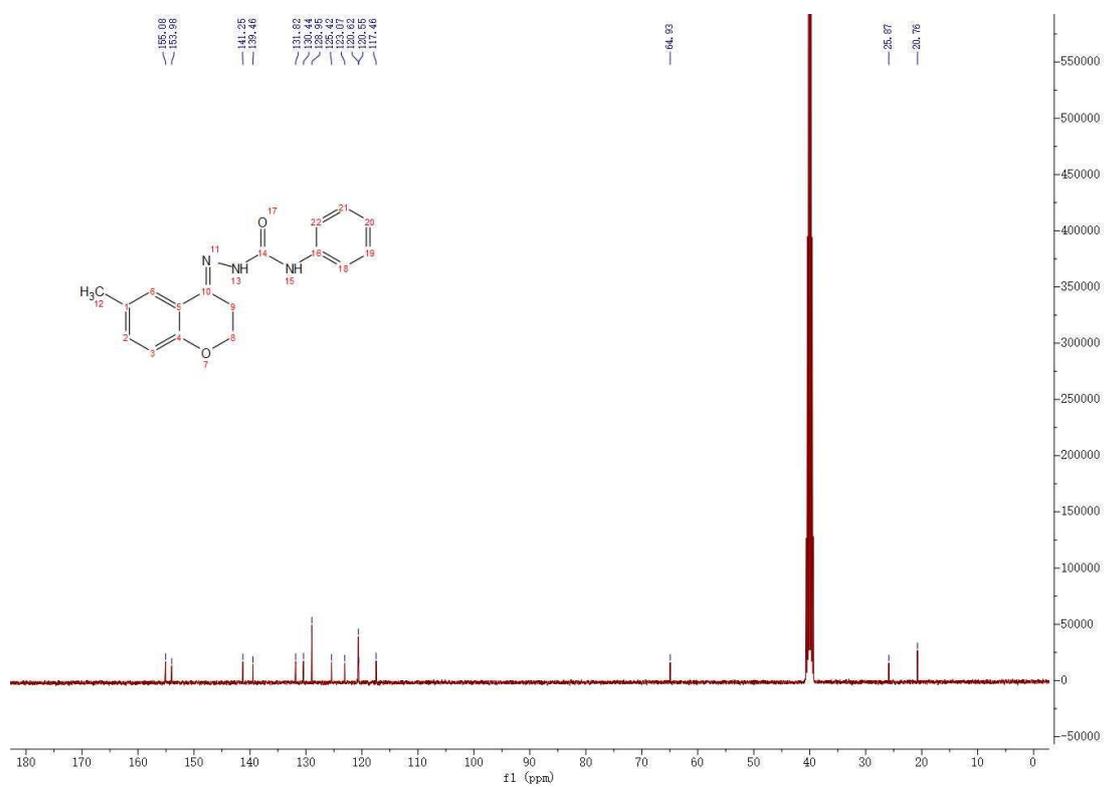
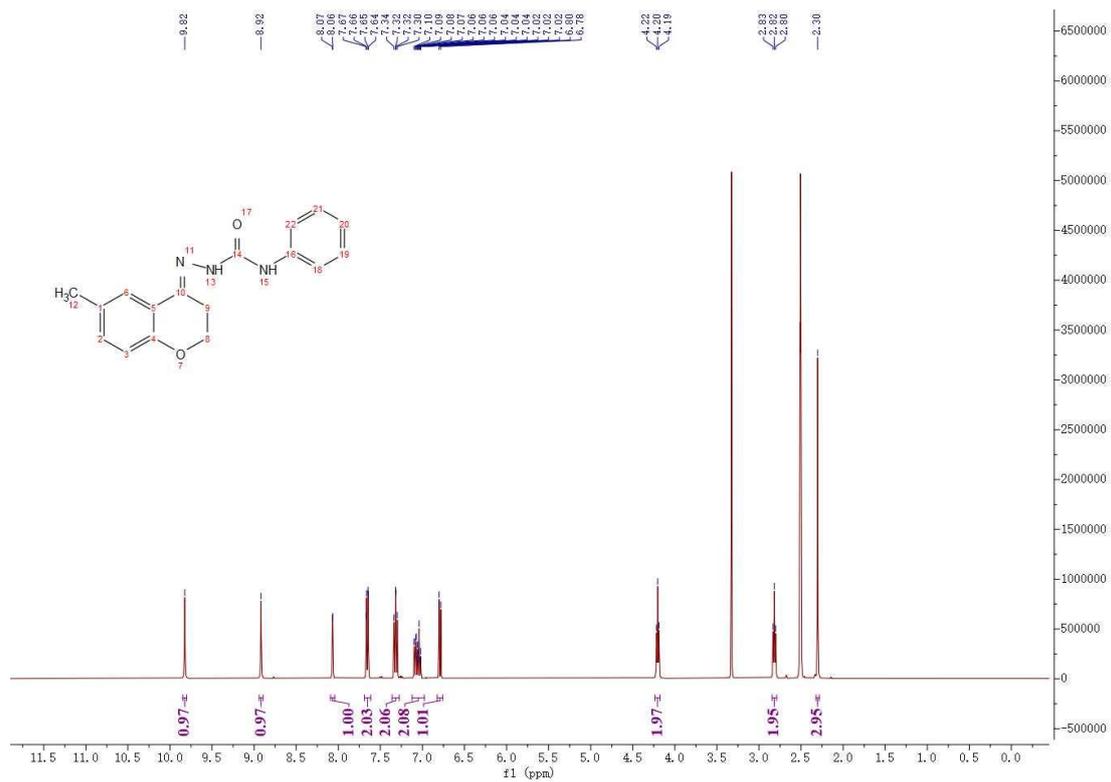


Figure S13. HRMS Spectrogram of Compound **3d**



Item name: 3e
Item description:

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

3.25e7

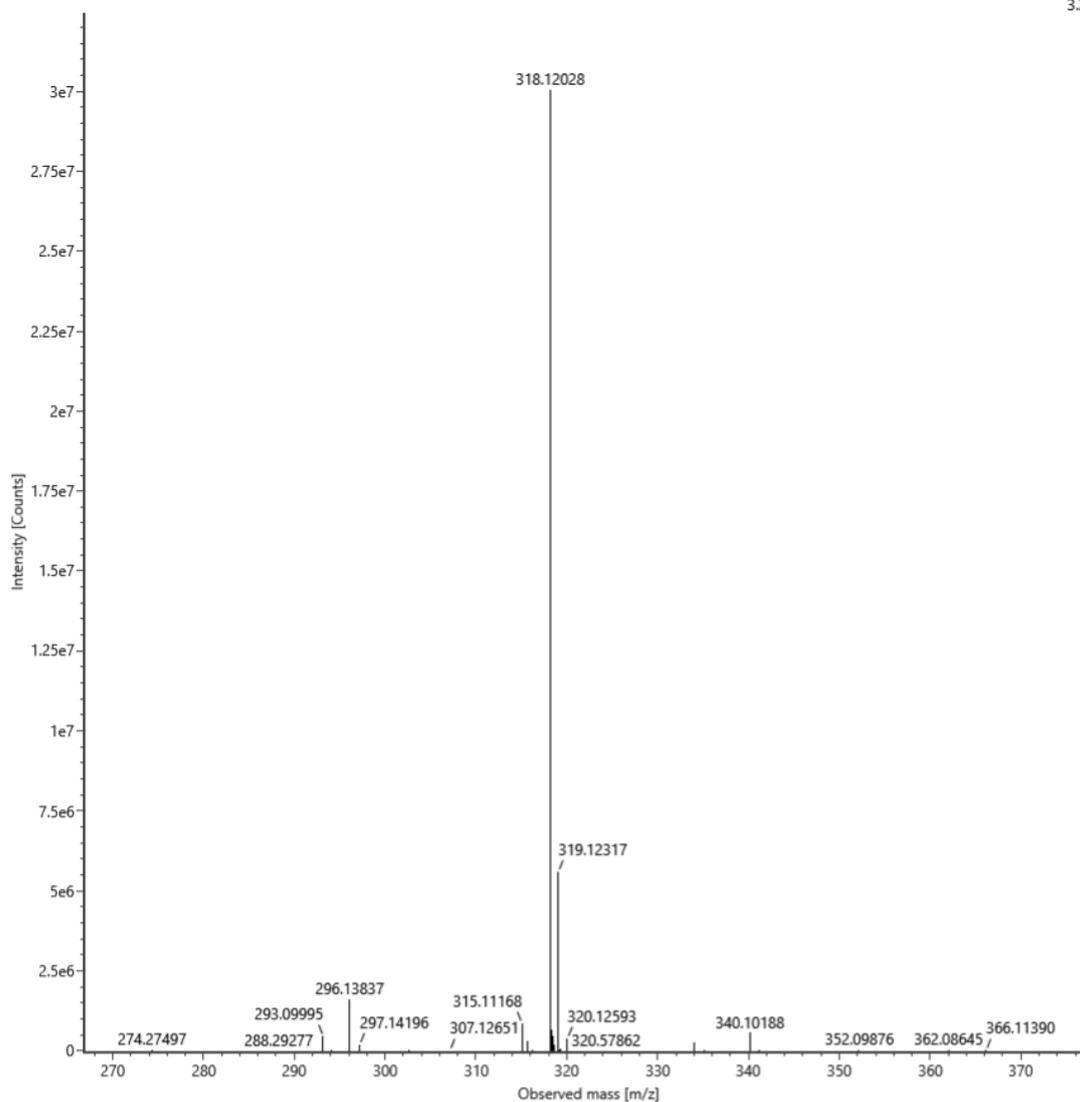
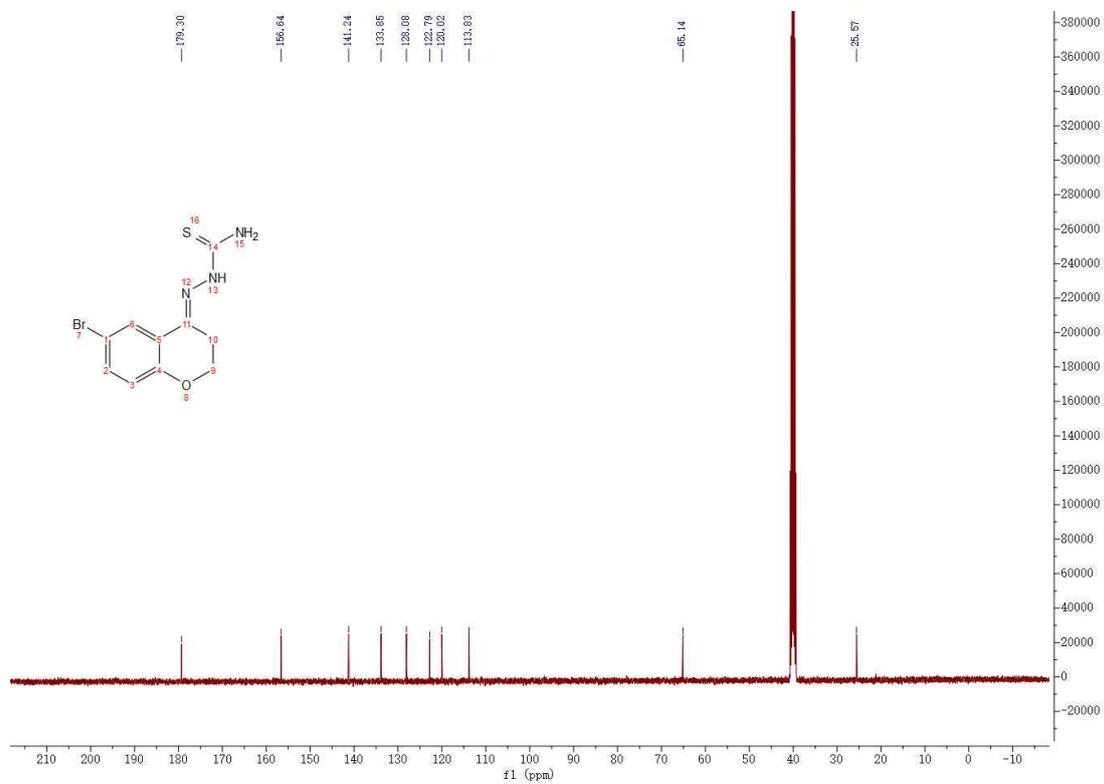
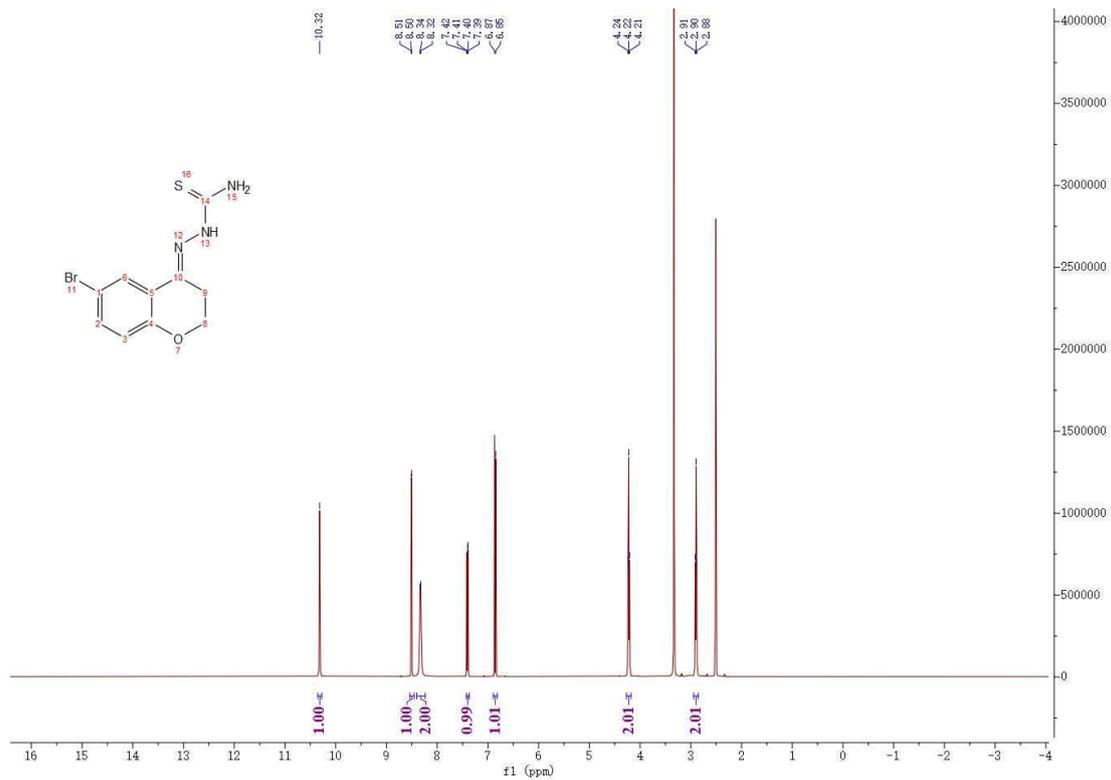
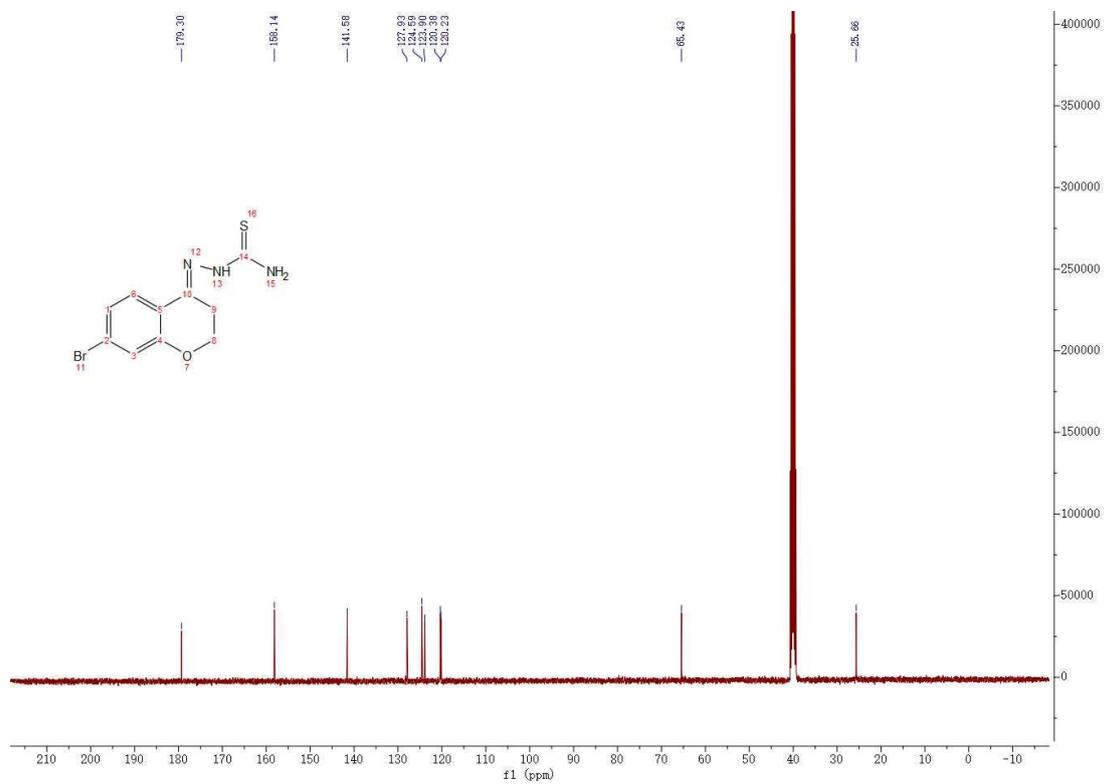
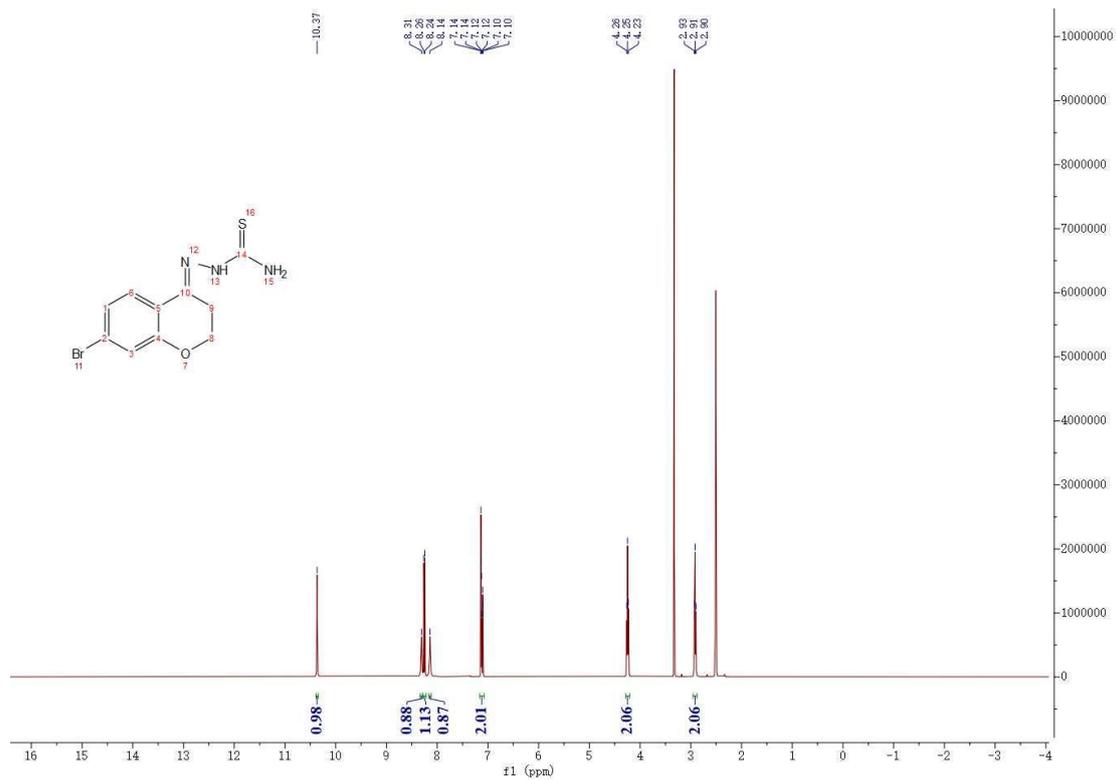


Figure S16. HRMS Spectrogram of Compound **3e**





Item name: 4g
Item description:

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

6.34e5

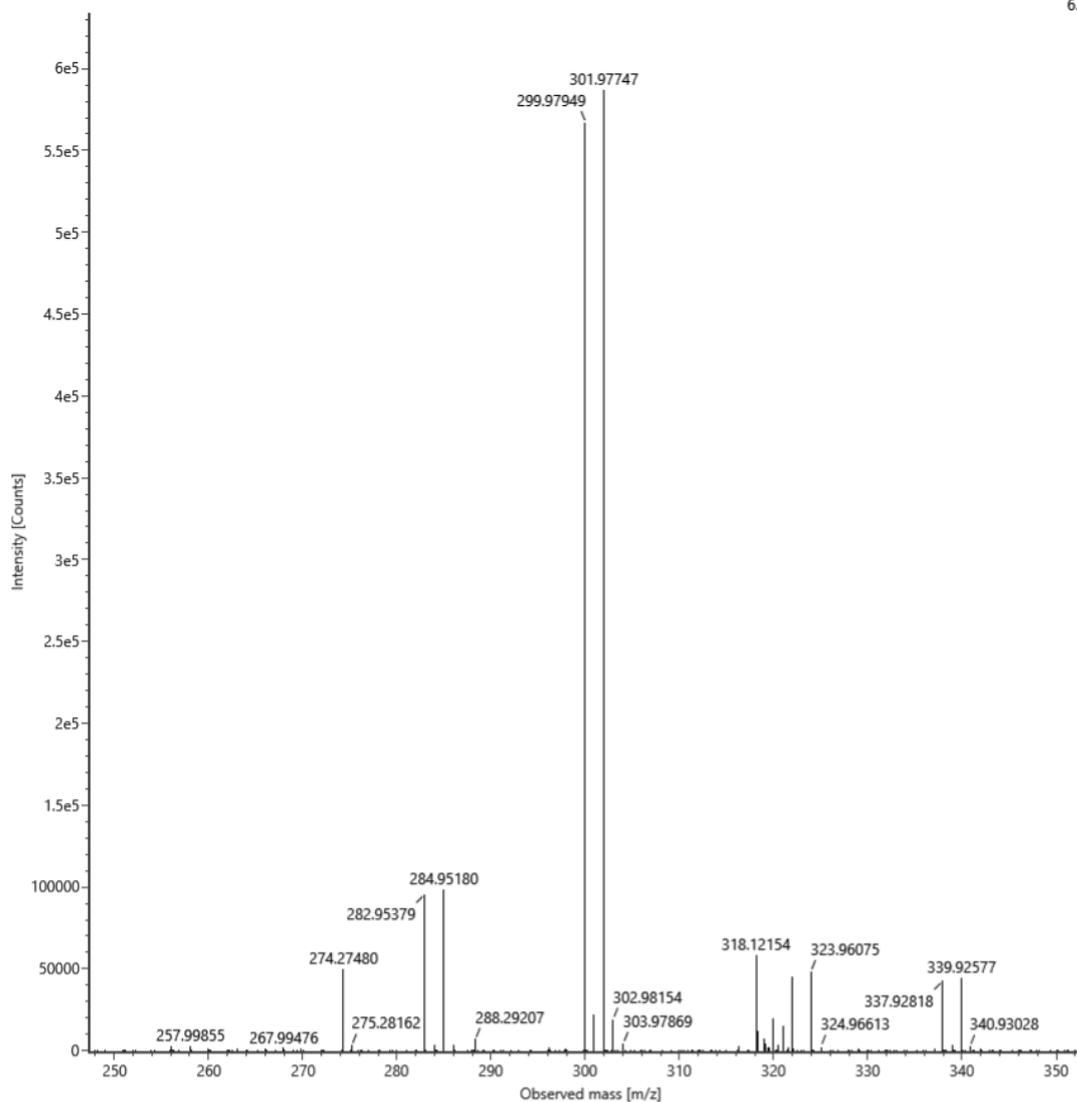
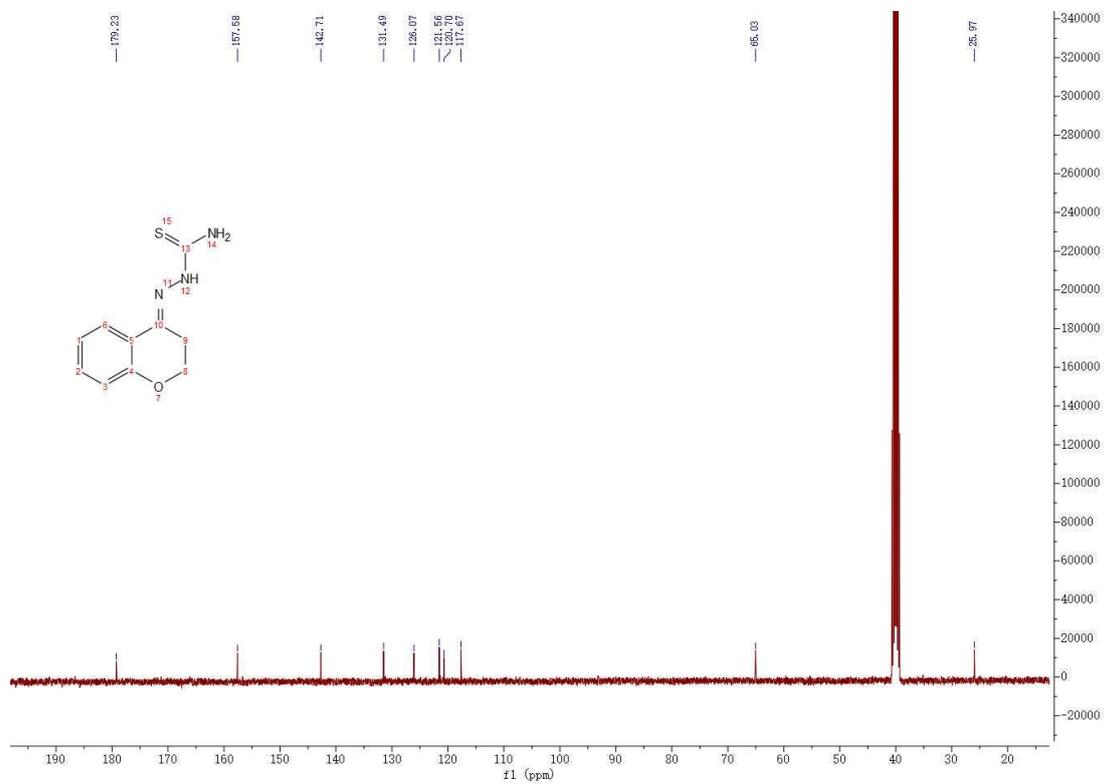
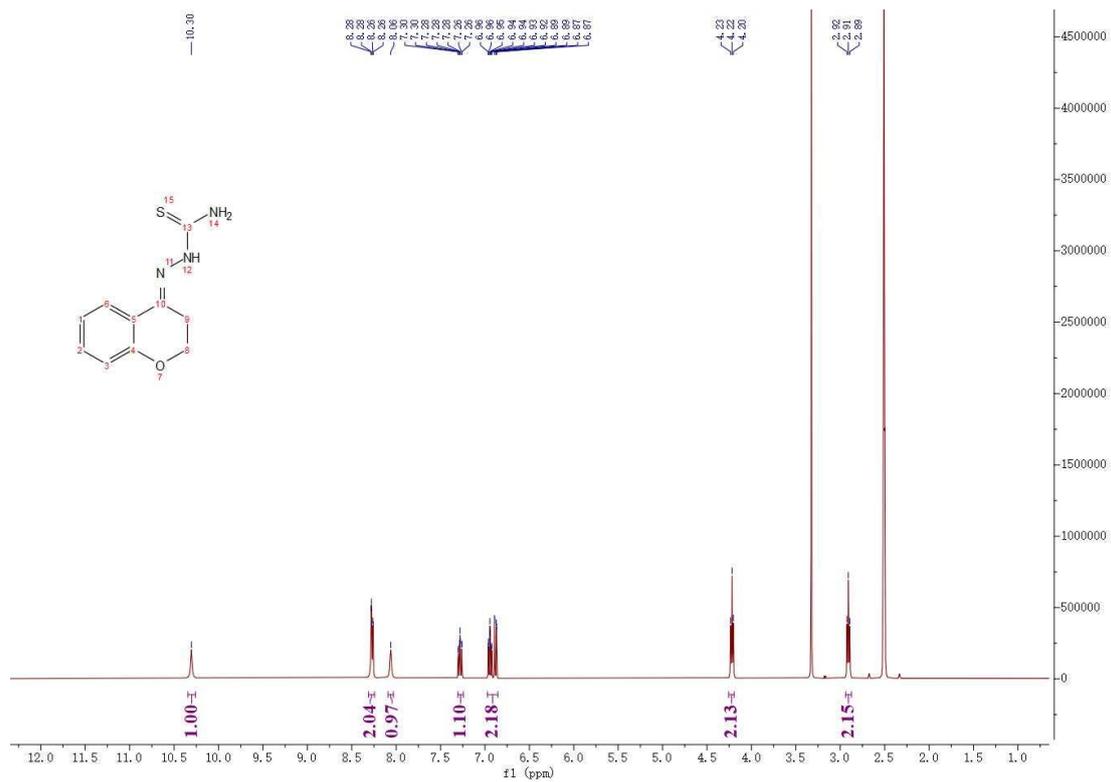
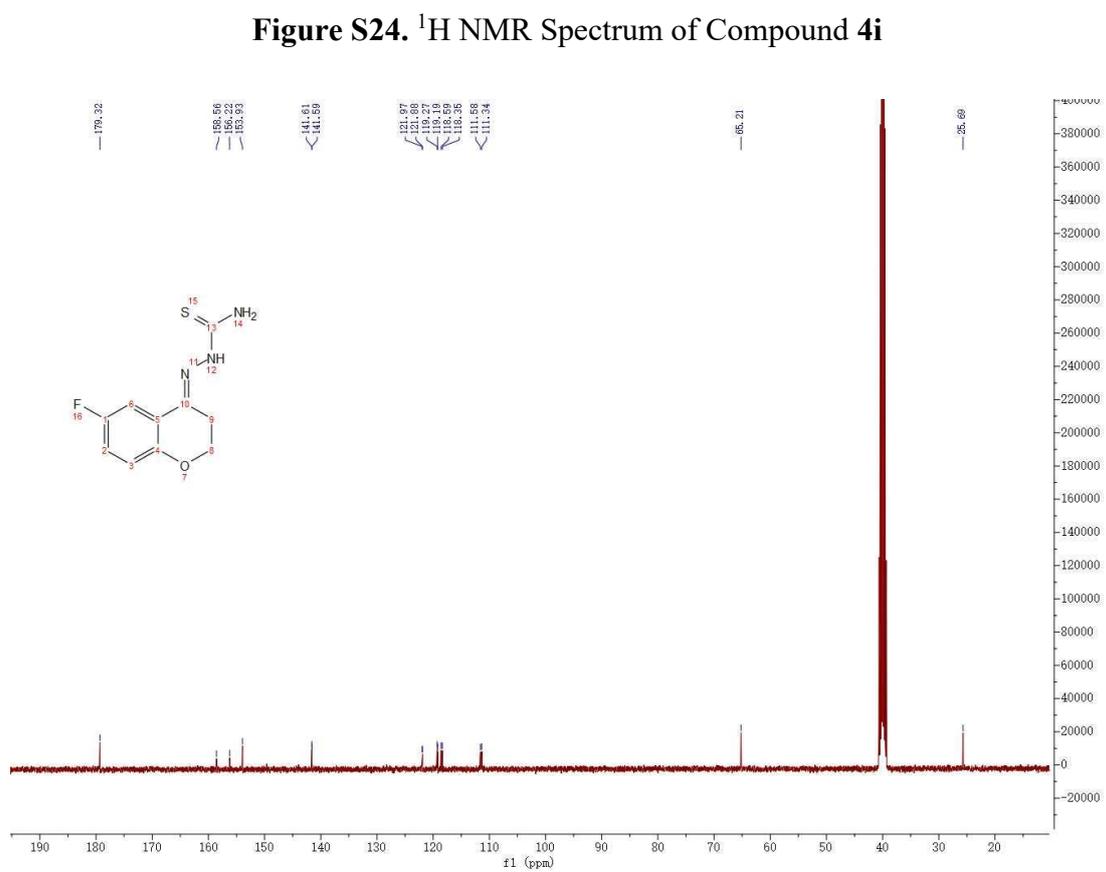
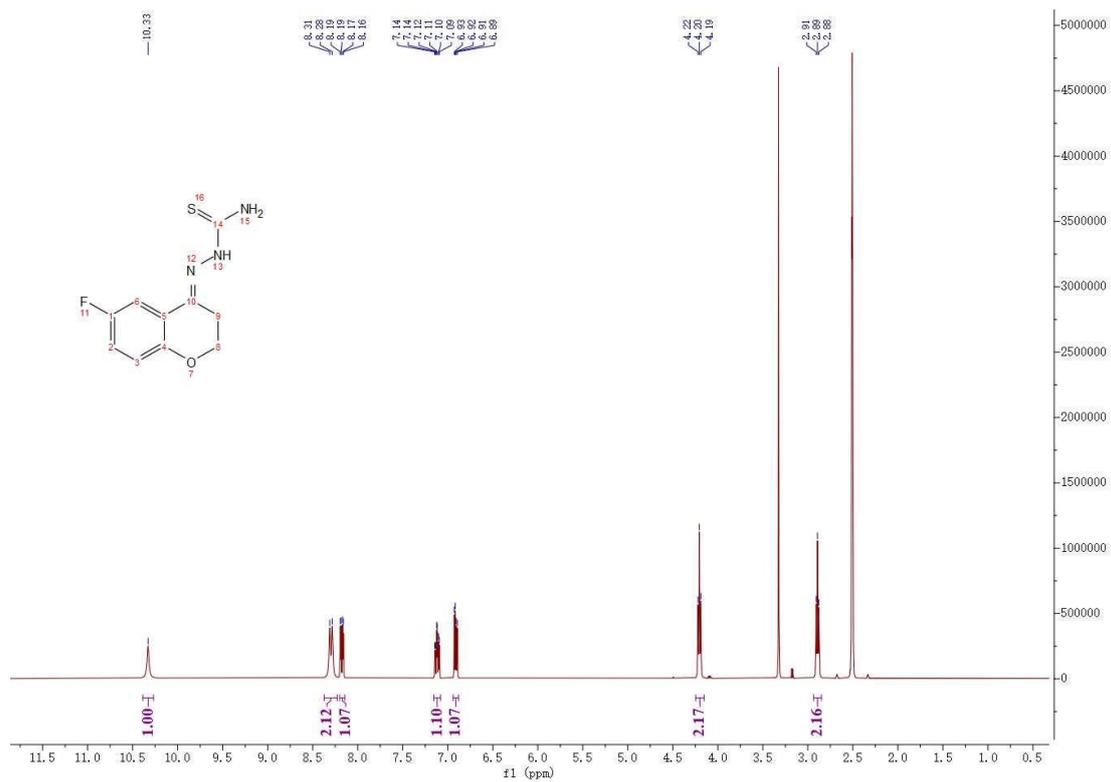


Figure S21. HRMS Spectrogram of Compound **4g**





Item name: 4i
Item description:

Channel name: 1: Average Time 0.1377 min : TOF MS (50-1500) ESI+ : Centroided : Combined

1.7e6

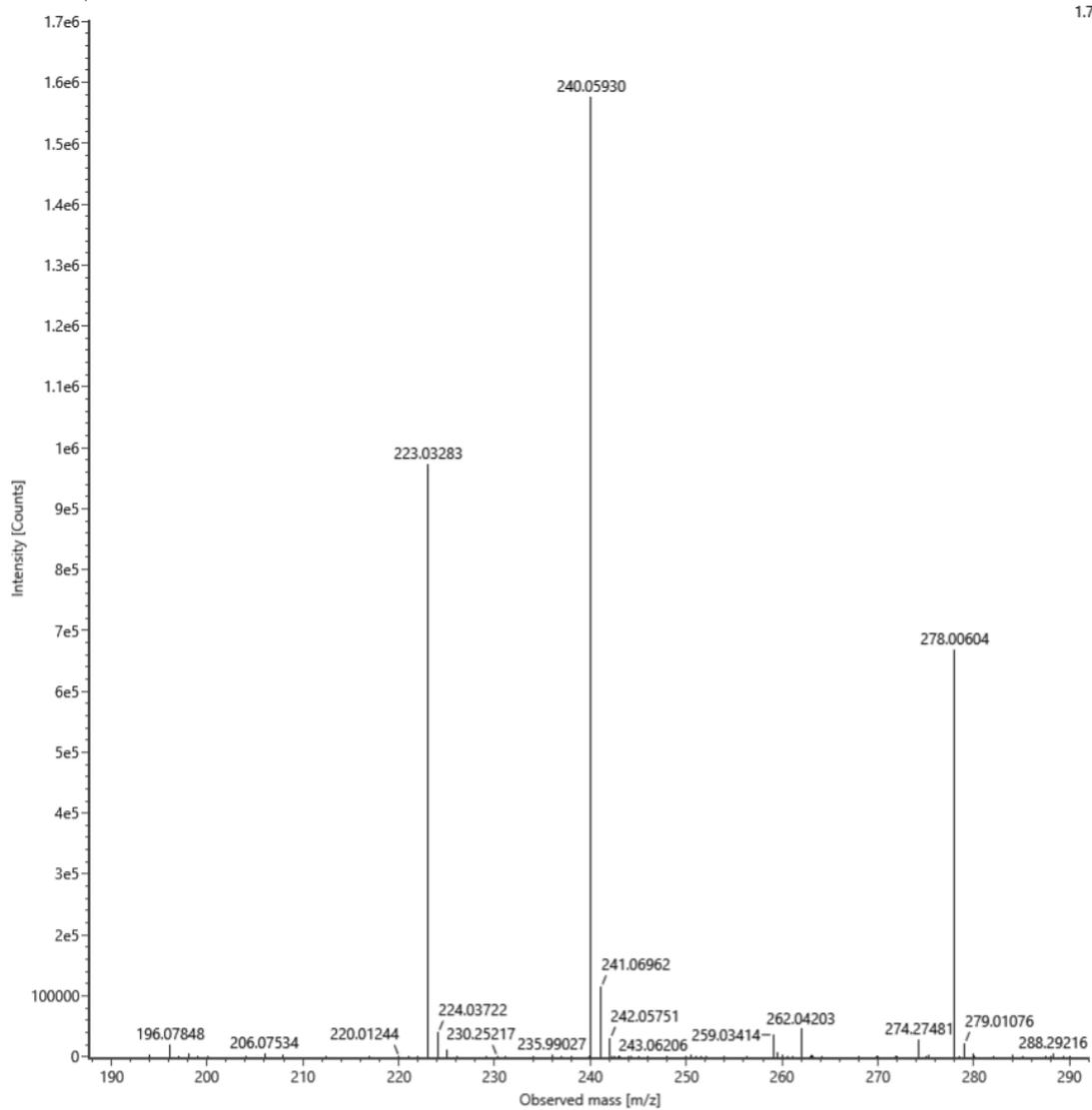


Figure S26. HRMS Spectrogram of Compound **4i**

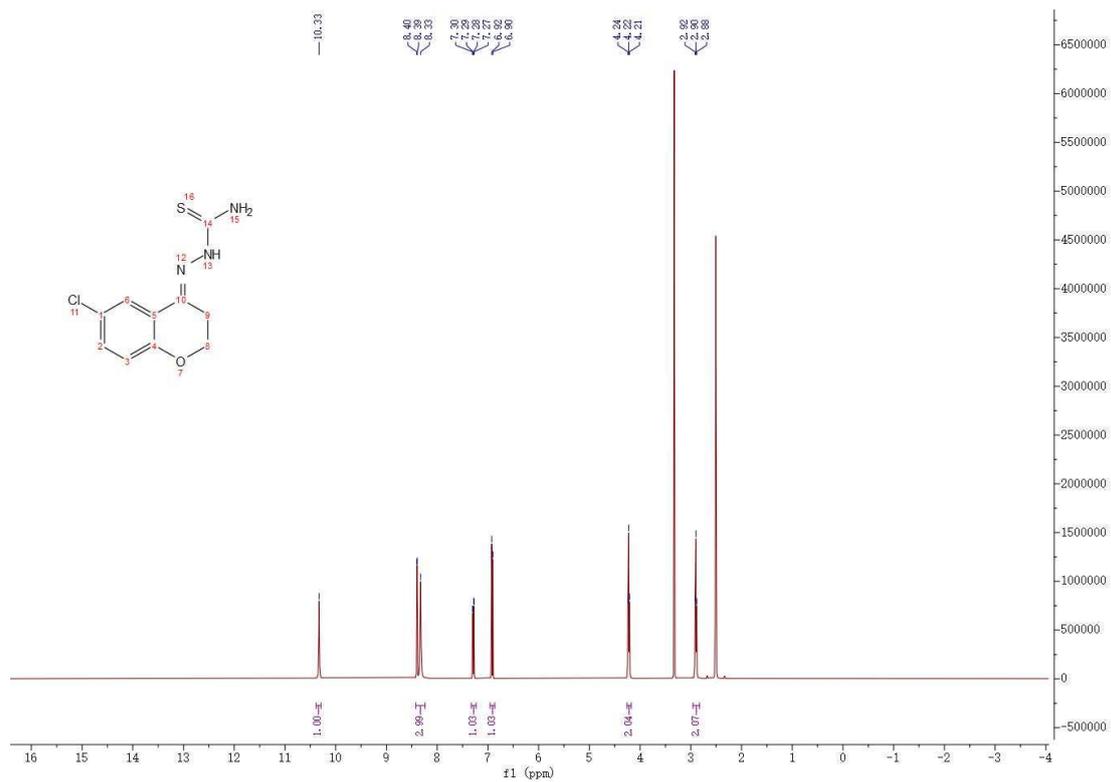


Figure S27. ¹H NMR Spectrum of Compound 4j

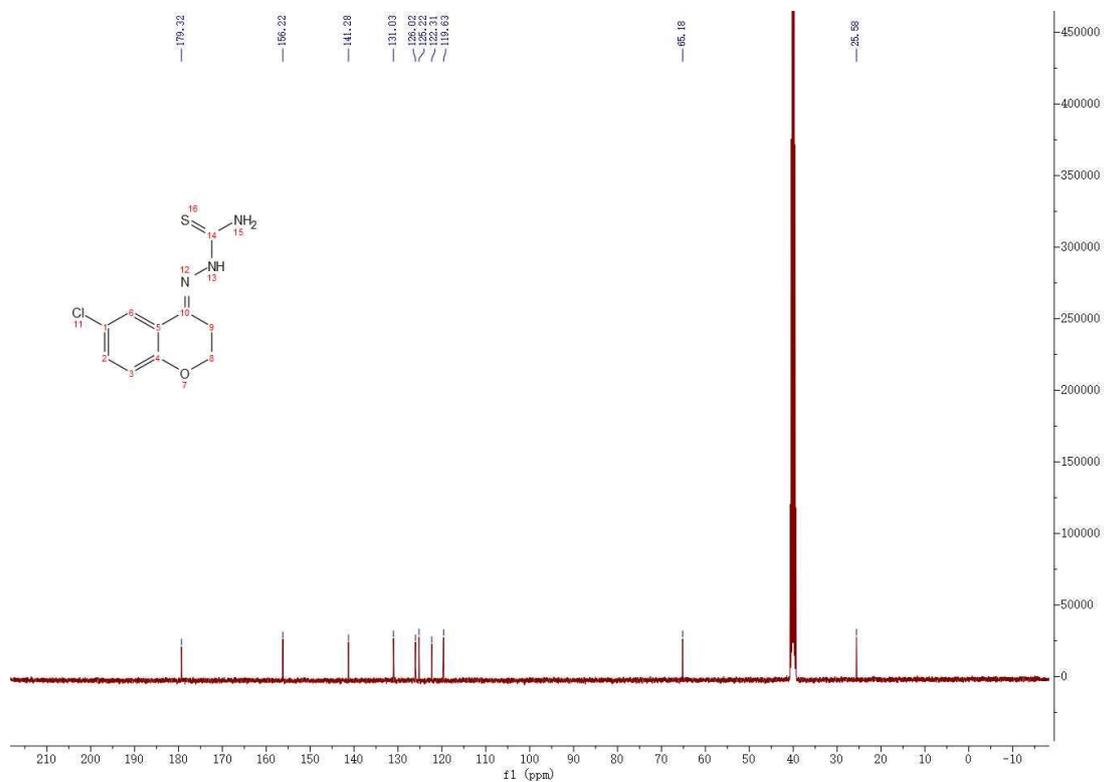


Figure S28. ¹³C NMR Spectrum of Compound 4j

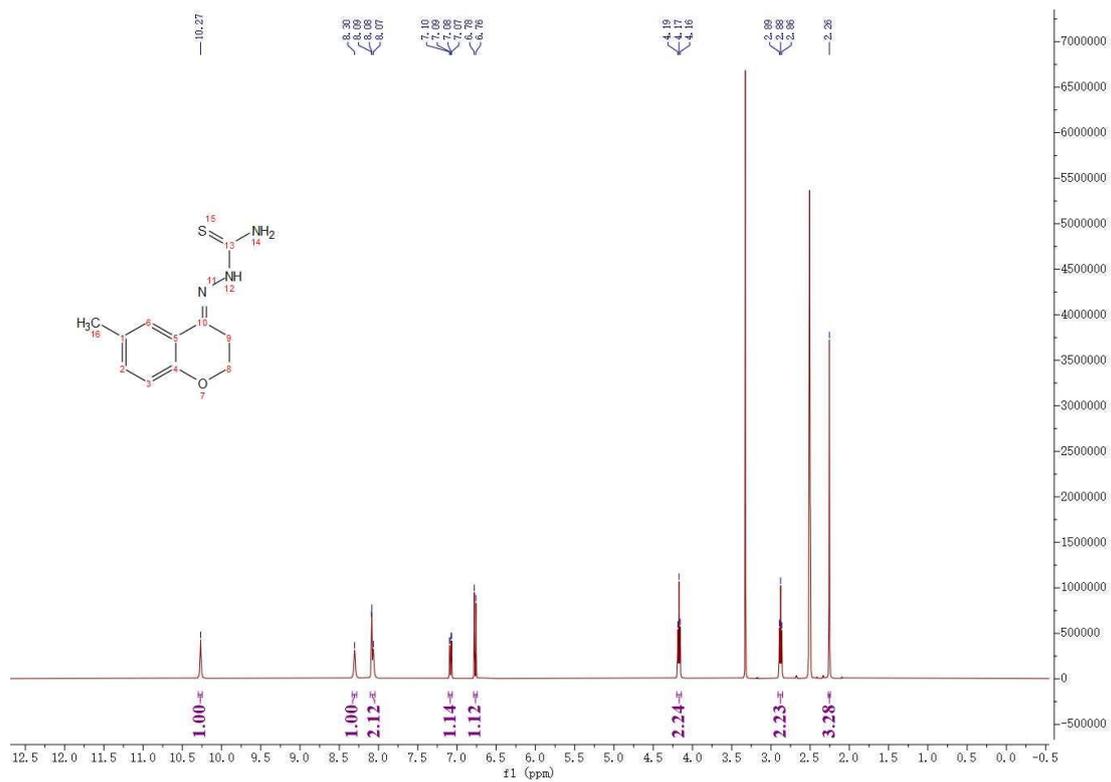


Figure S29. ^1H NMR Spectrum of Compound 4k

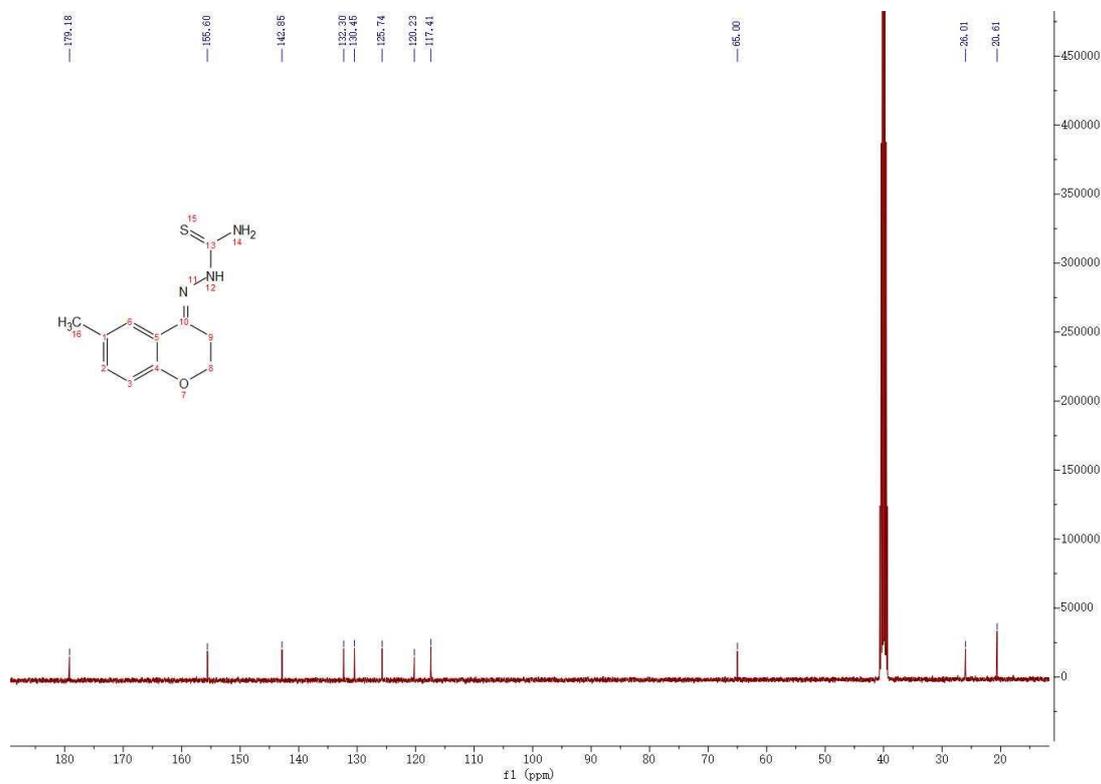
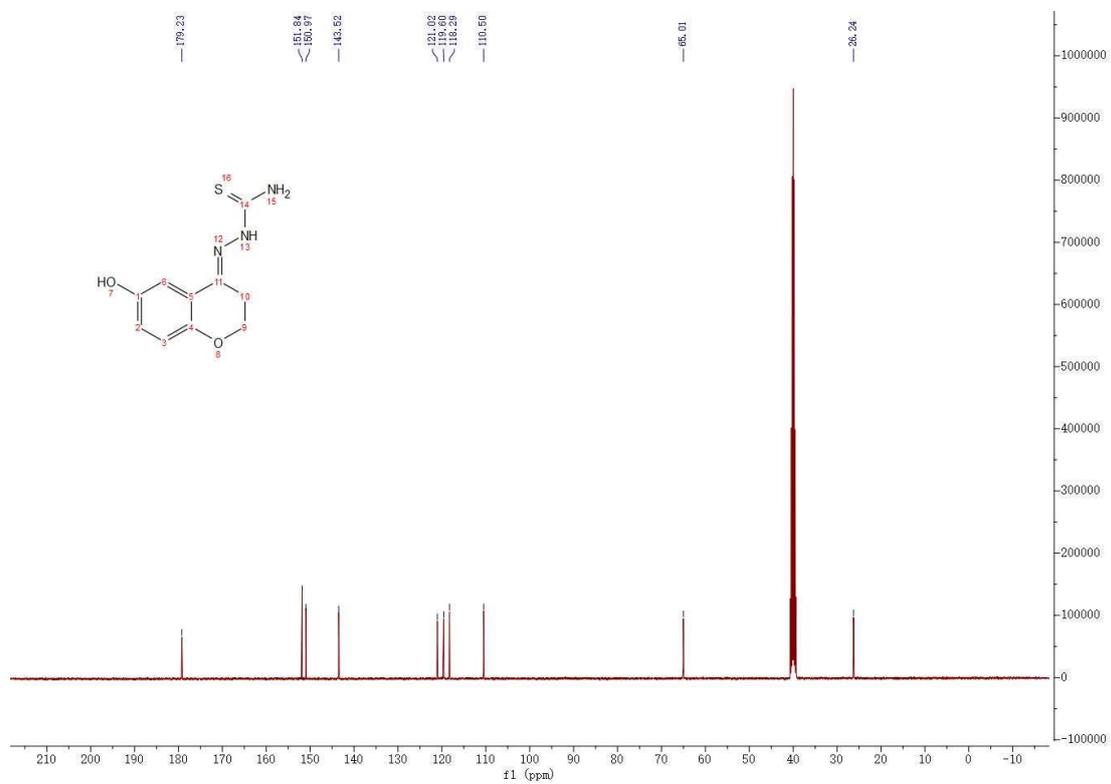
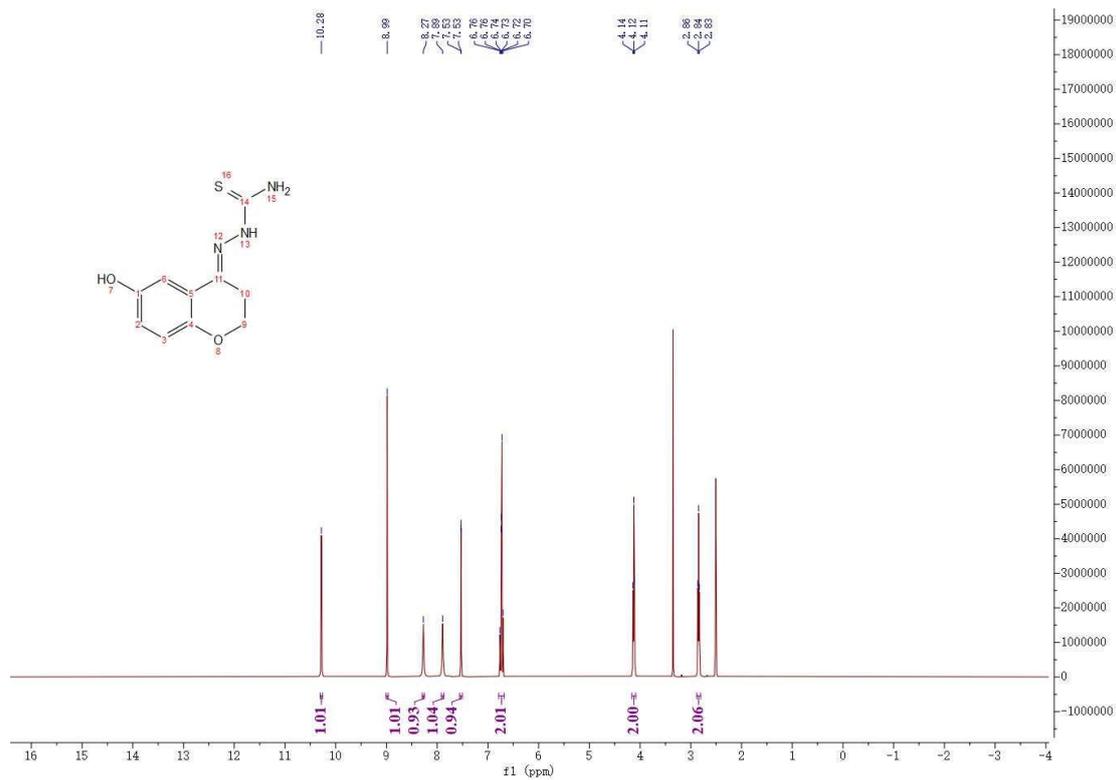


Figure S30. ^{13}C NMR Spectrum of Compound 4k



Item name: 4l
Item description:

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

1.47e6

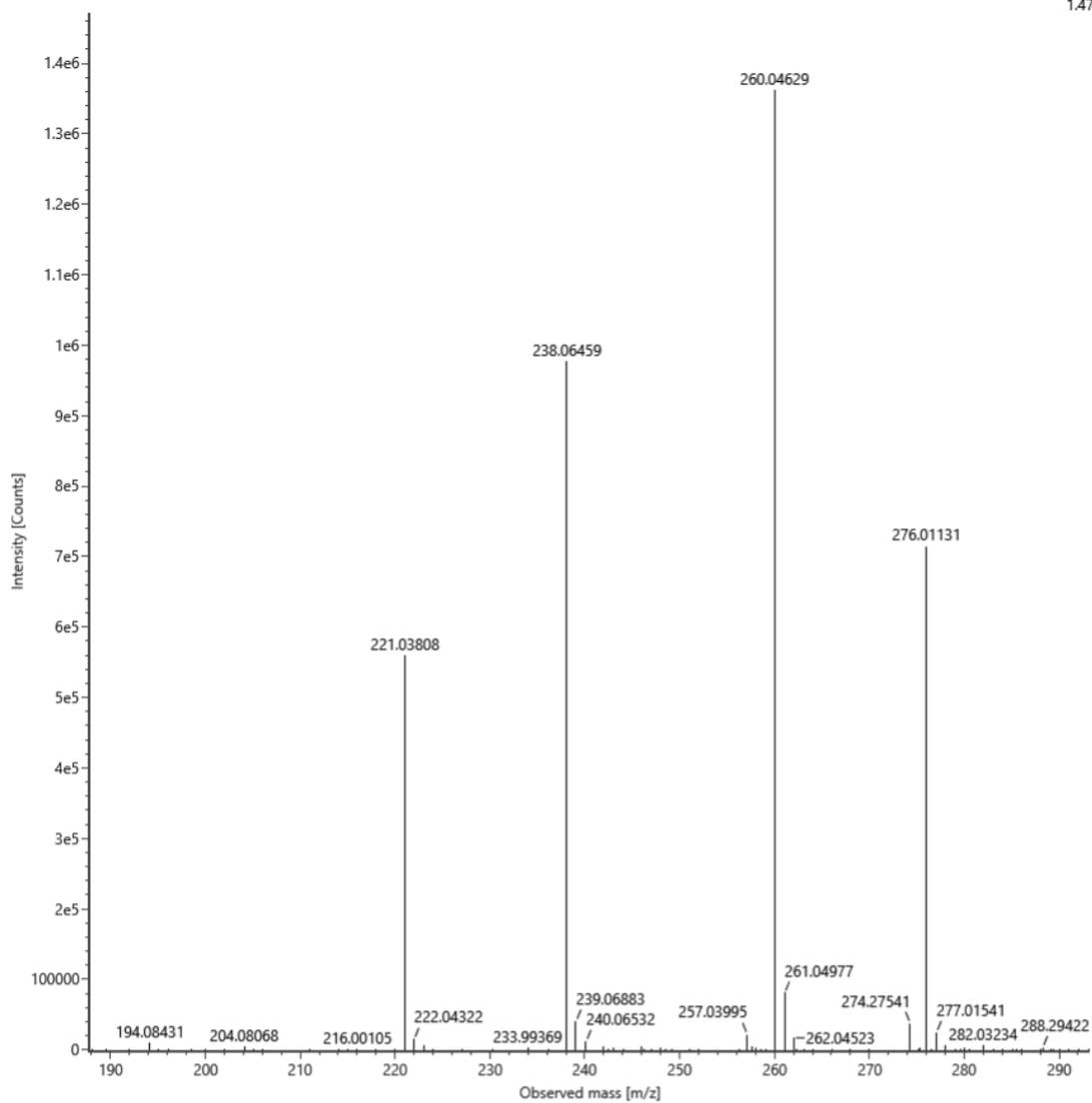


Figure S33. HRMS Spectrogram of Compound 4l

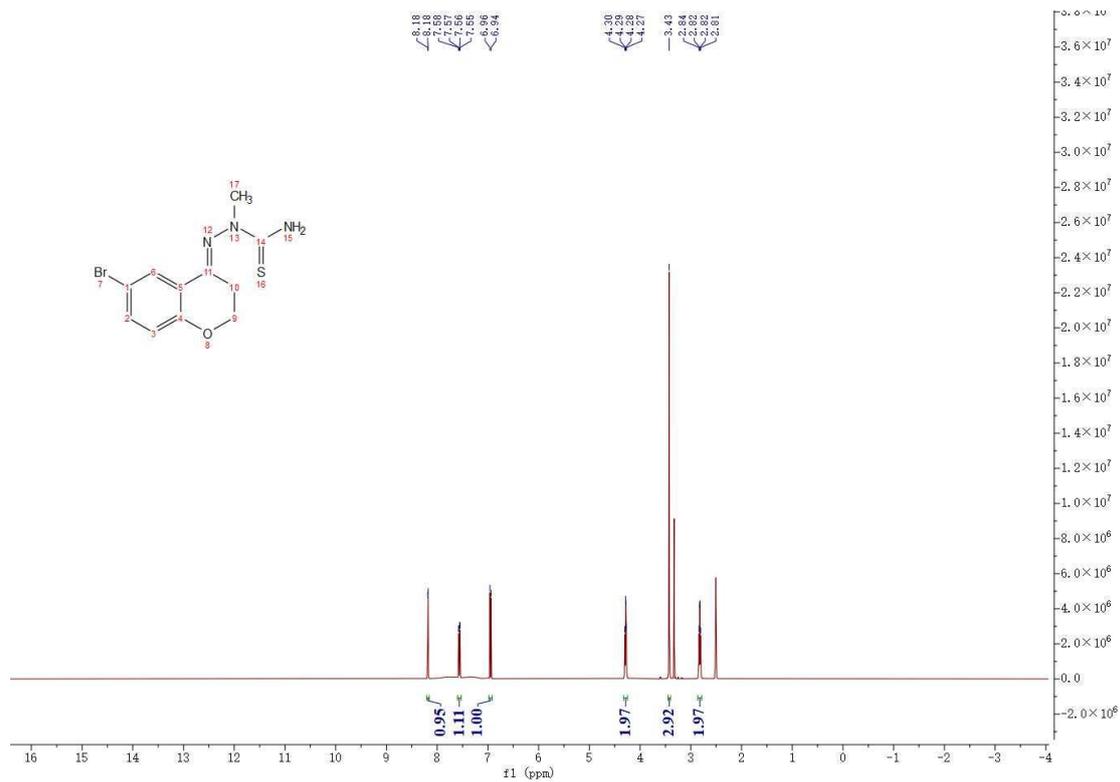


Figure S34. ¹H NMR Spectrum of Compound 4m

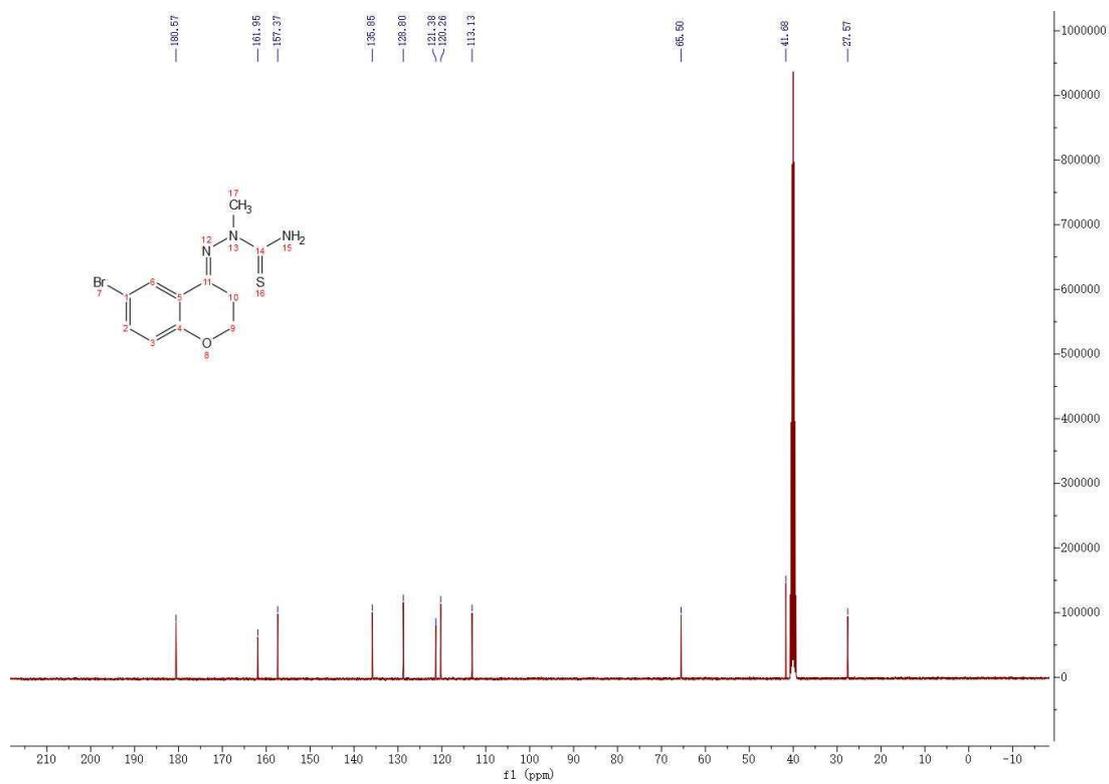


Figure S35. ¹³C NMR Spectrum of Compound 4m

Item name: 4m
Item description:

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

6.21e6

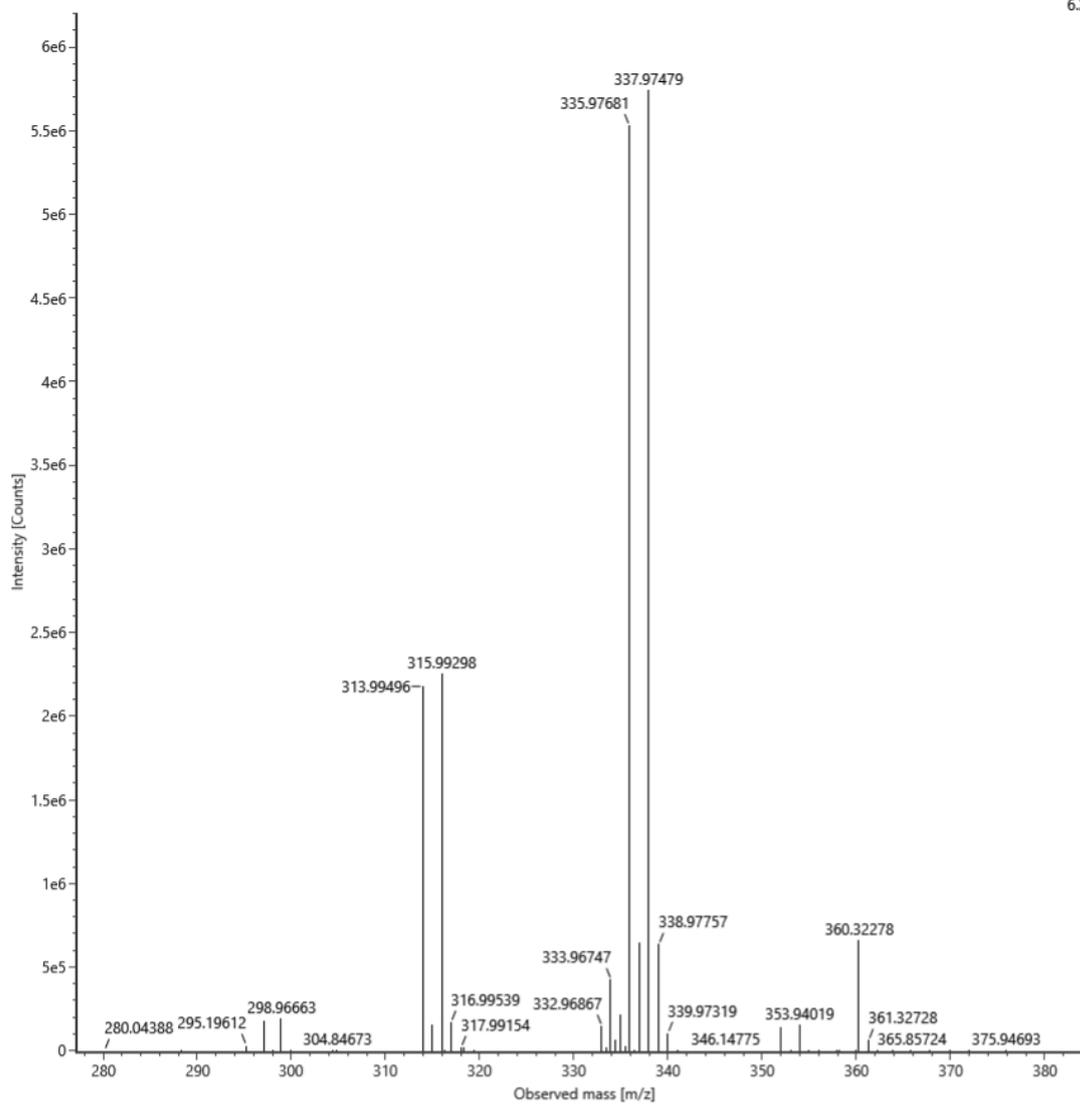


Figure S36. HRMS Spectrogram of Compound **4m**

IR Spectra of compounds 3a-e and 4g, i, l, m

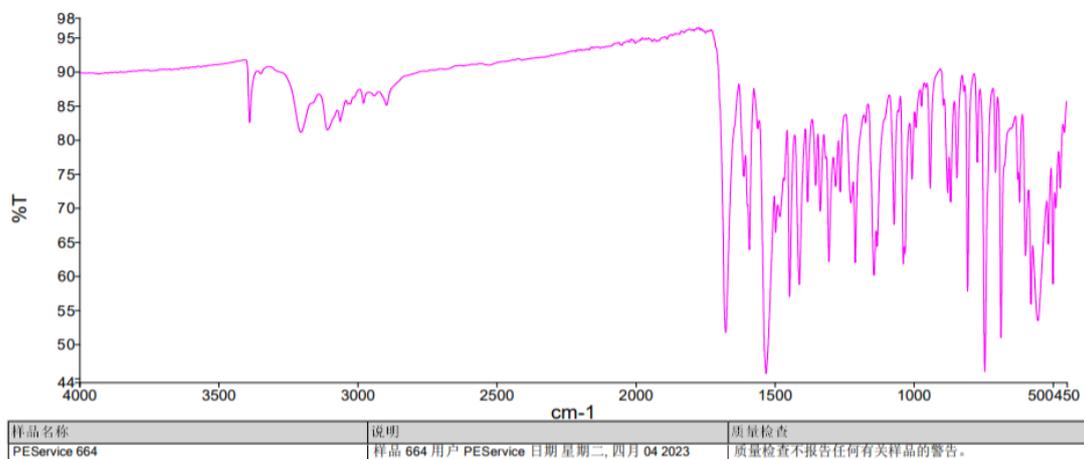


Figure S37. IR Spectra of compound 3a

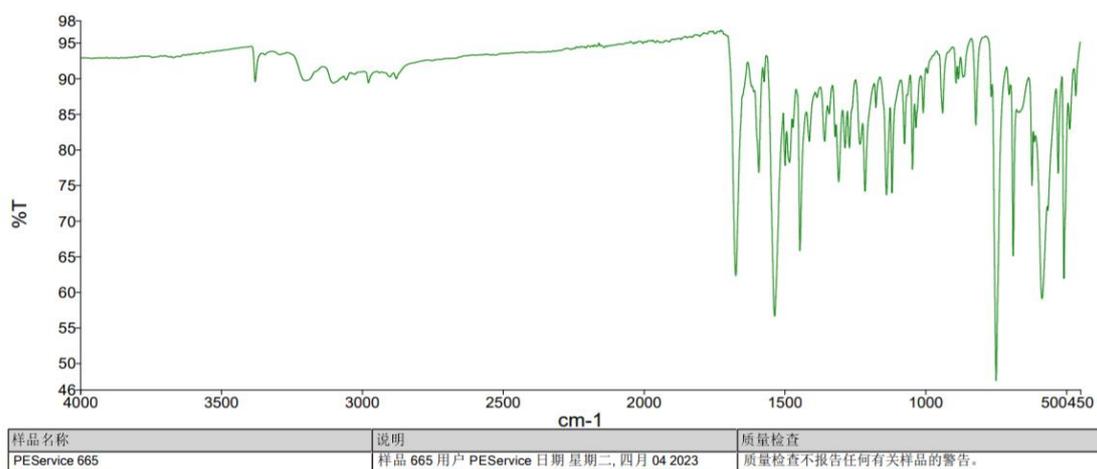


Figure S38. IR Spectra of compound 3b

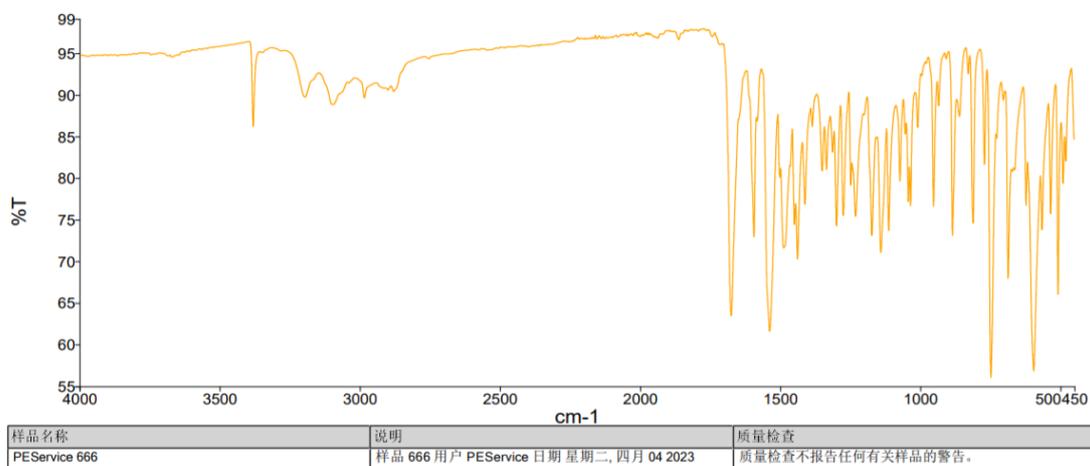


Figure S39. IR Spectra of compound 3c

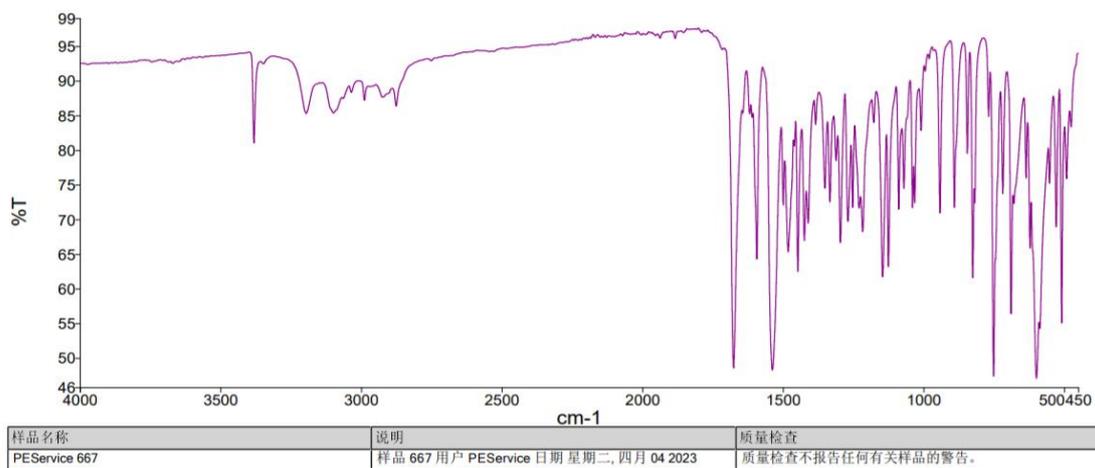


Figure S40. IR Spectra of compound **3d**

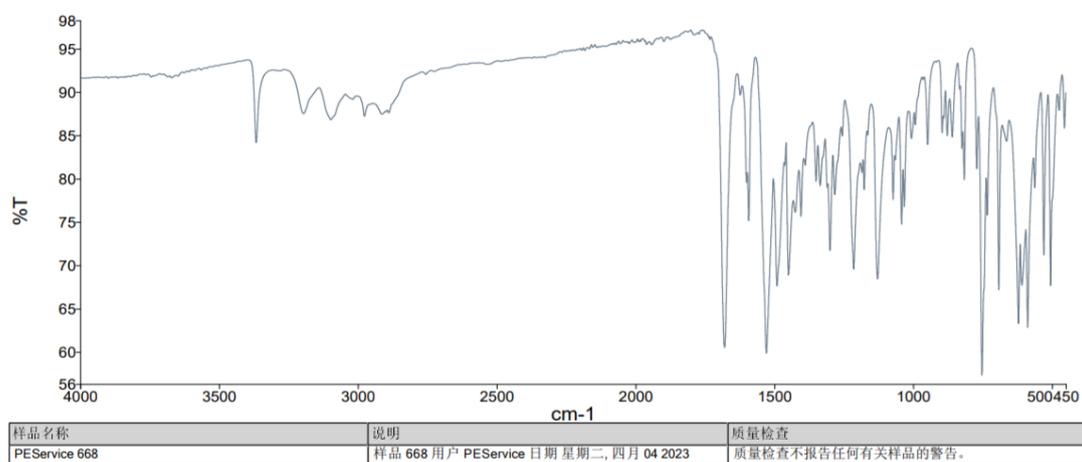


Figure S41. IR Spectra of compound **3e**

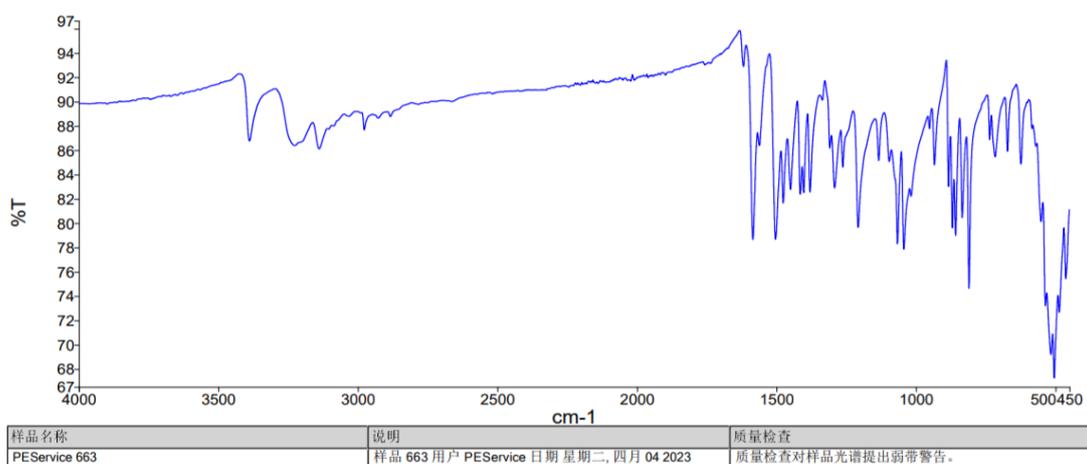


Figure S42. IR Spectra of compound **4g**

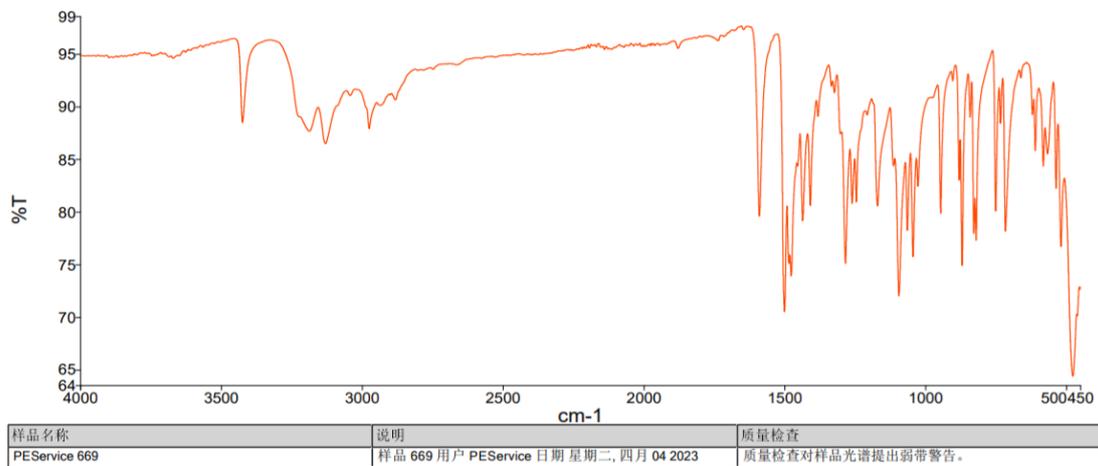


Figure S43. IR Spectra of compound 4i

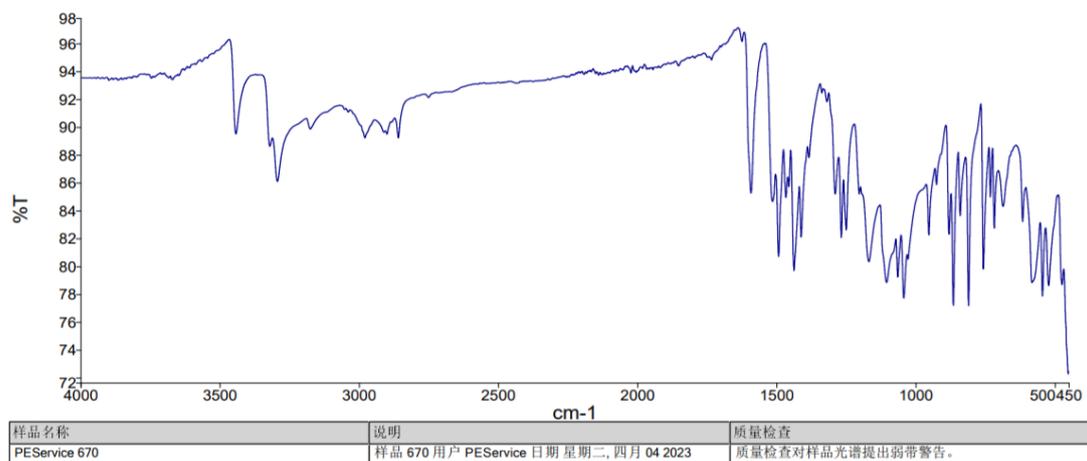


Figure S44. IR Spectra of compound 4l

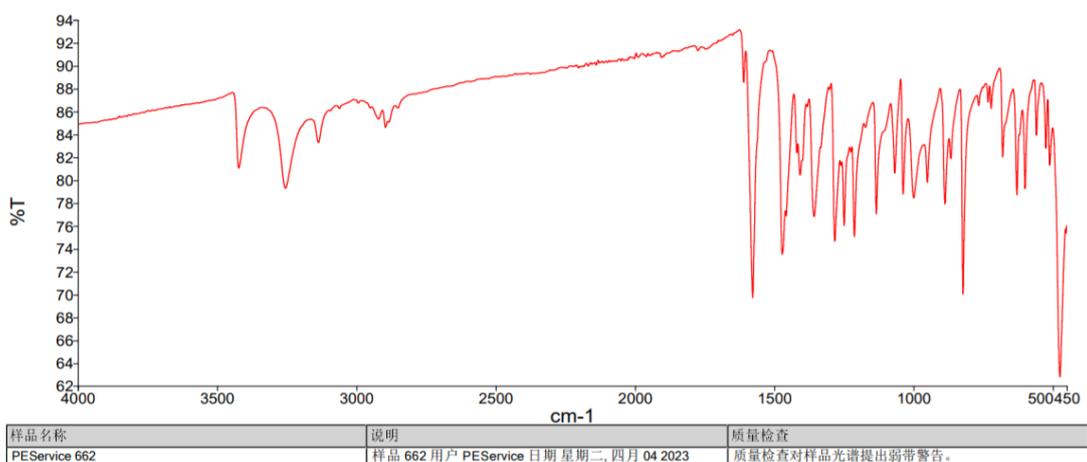


Figure S45. IR Spectra of compound 4m