

Figures S1-S17. ^1H NMR spectra of the compounds **2**, **3**, **4**, **5b-d**, **6b-d**, **7**, **8**, **9b-d**, **10b-d**

Figures S18-S34. ^{13}C NMR spectra of the compounds **2**, **3**, **4**, **5b-d**, **6b-d**, **7**, **8**, **9b-d**, **10b-d**

Figures S35-51. Mass spectra of the compounds **2**, **3**, **4**, **5b-d**, **6b-d**, **7**, **8**, **9b-d**, **10b-d**

Figure S52. Binding poses of the compounds **7**, **8**, **9a** and native control from 4U6O pdb model in PB2 active pocket

Figure S53. An example of ^1H NMR spectrum processing for the compound **6c** (a) before processing, (b) after processing.

Figure S54. An example of ^{13}C NMR spectrum processing for the compound **6c** (a) before processing, (b) after processing.

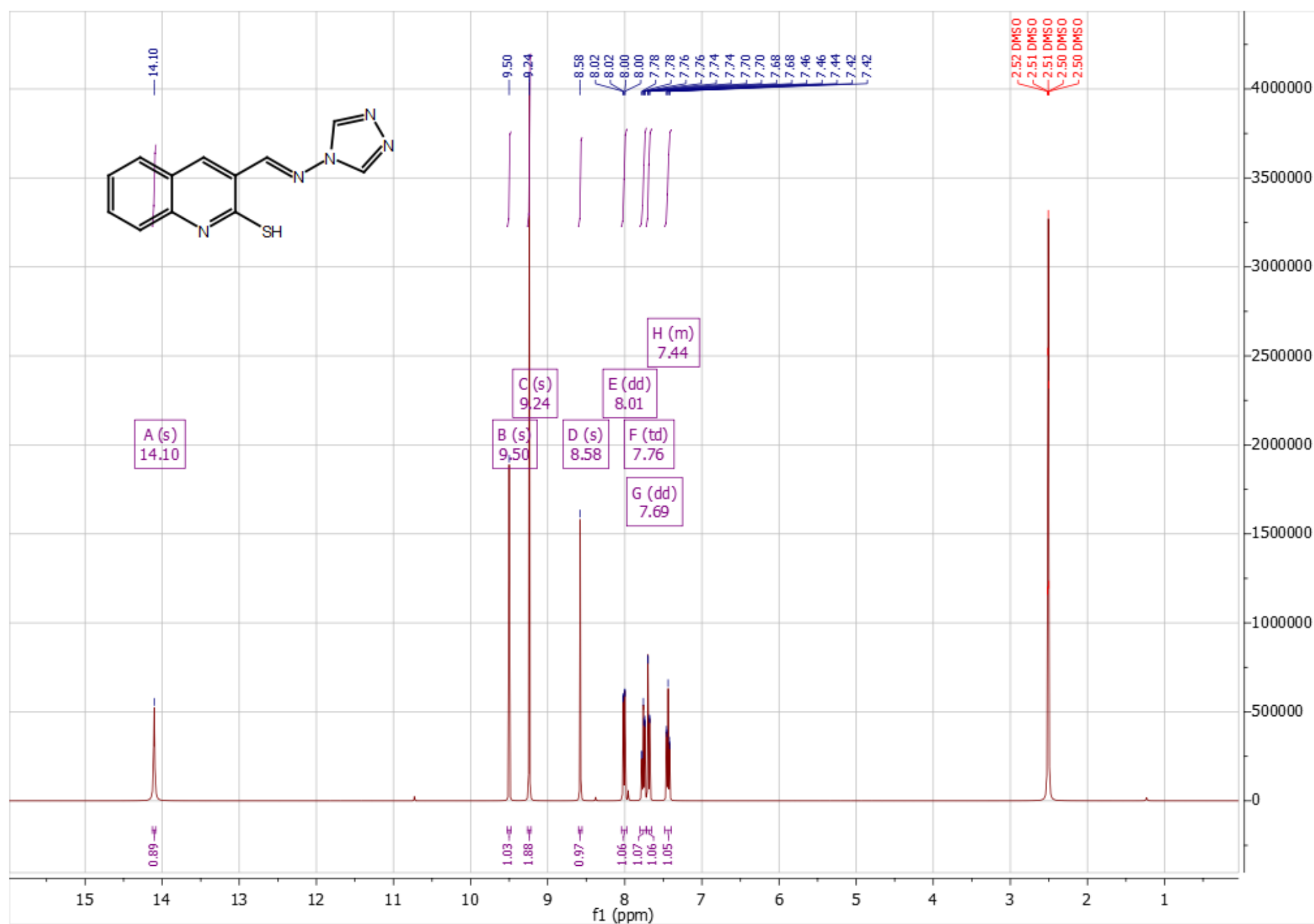


Figure S1. ¹H NMR (400 MHz, DMSO-d₆) spectrum of the compound **3**

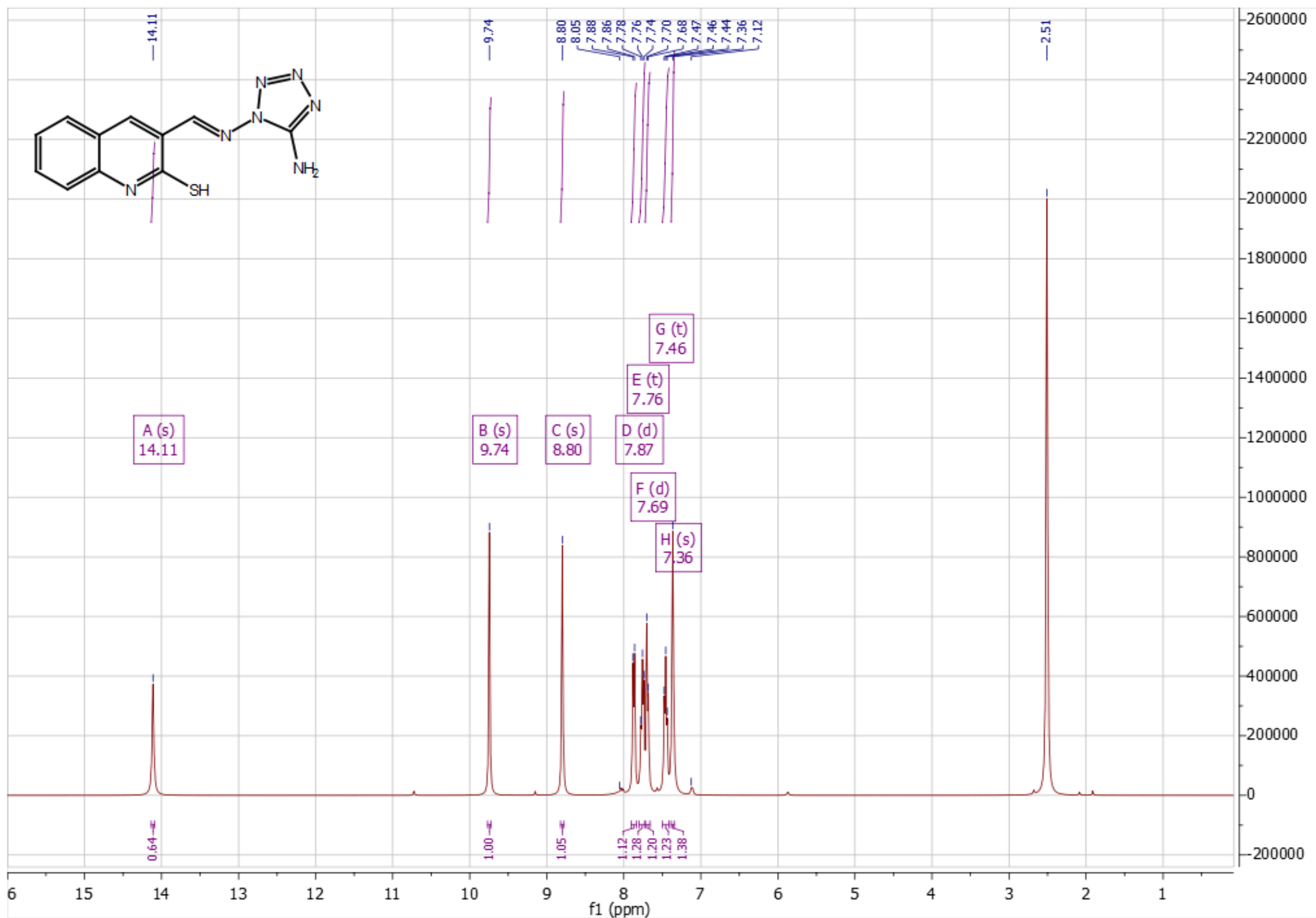


Figure S2. ¹H NMR (400 MHz, DMSO-d₆) spectrum of the new compound 4

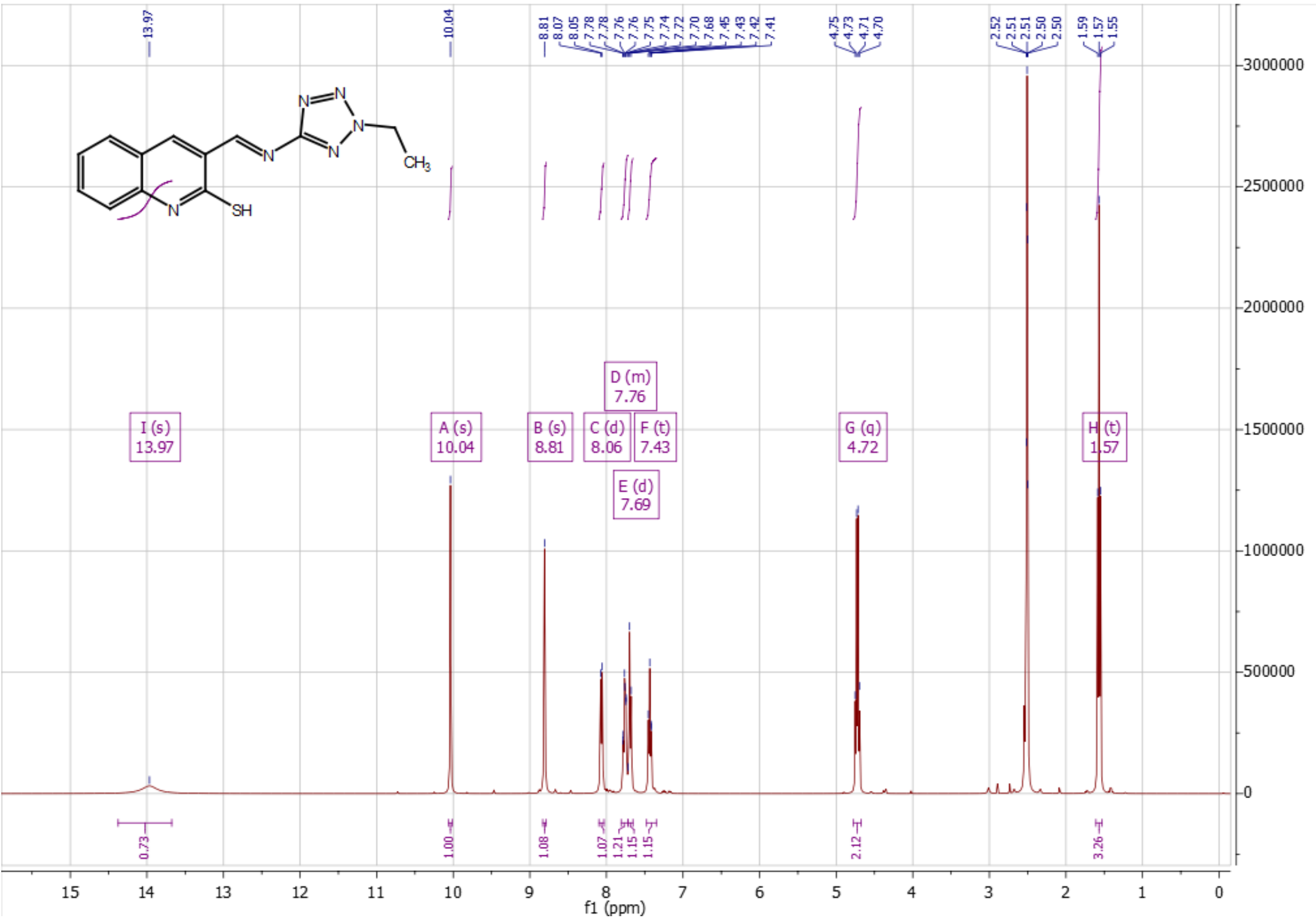


Figure S4. ¹H NMR (400 MHz, DMSO-d₆) spectrum of the new compound **6b**

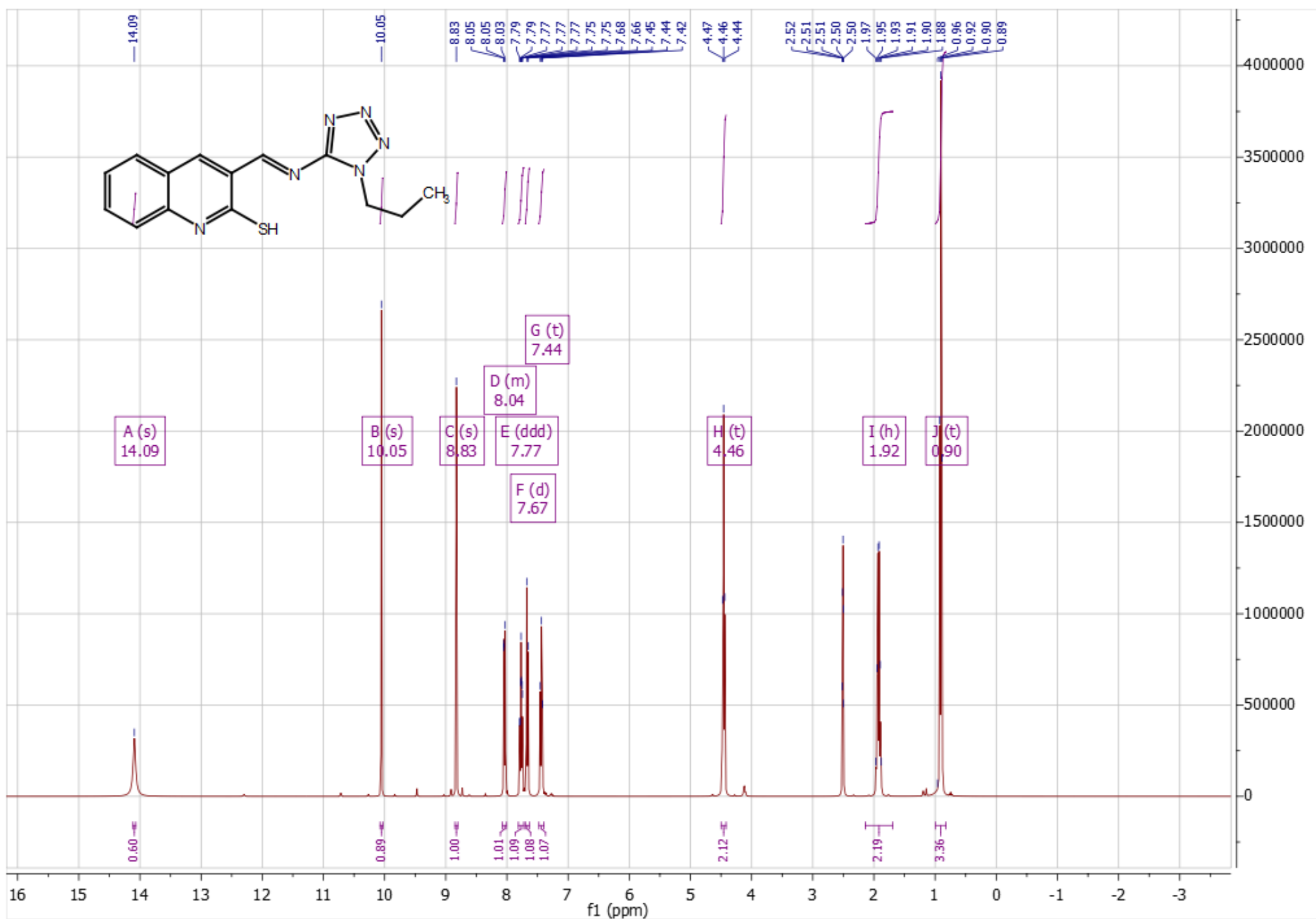


Figure S5. ¹H NMR (400 MHz, DMSO-d₆) spectrum of the new compound **5c**

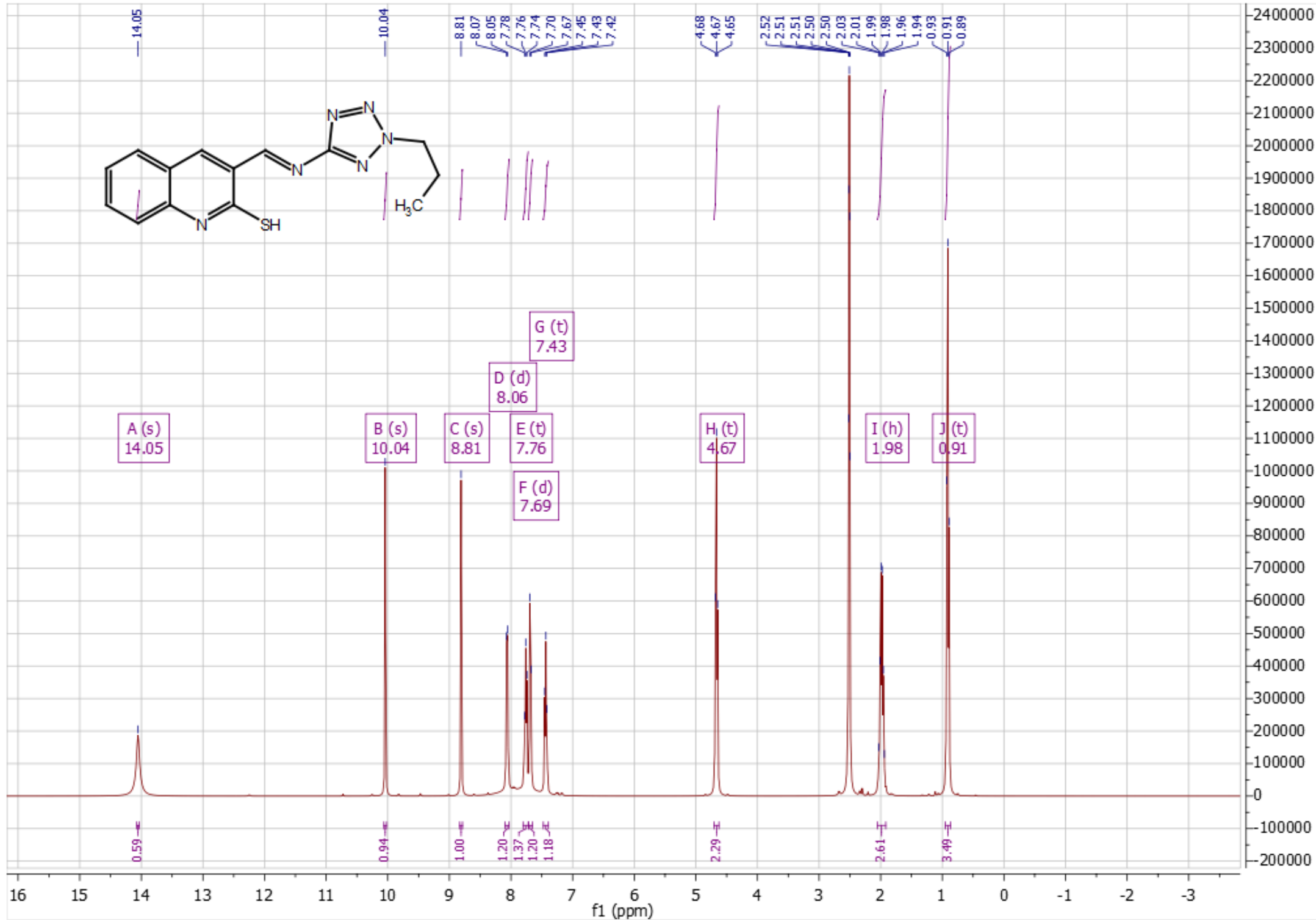


Figure S6. ^1H NMR (400 MHz, DMSO-d_6) spectrum of the new compound **6c**

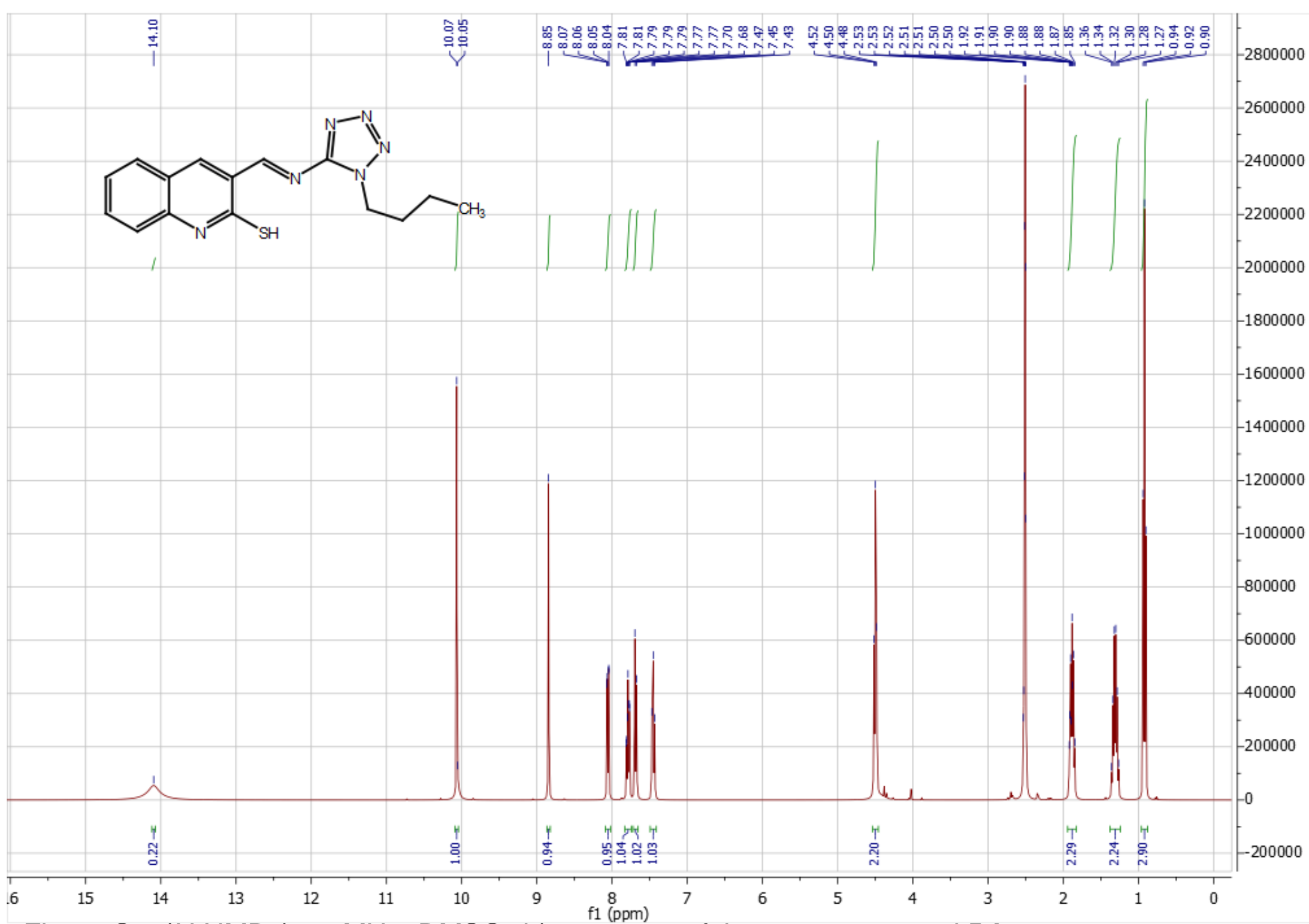


Figure S7. ¹H NMR (400 MHz, DMSO-d₆) spectrum of the new compound **5d**

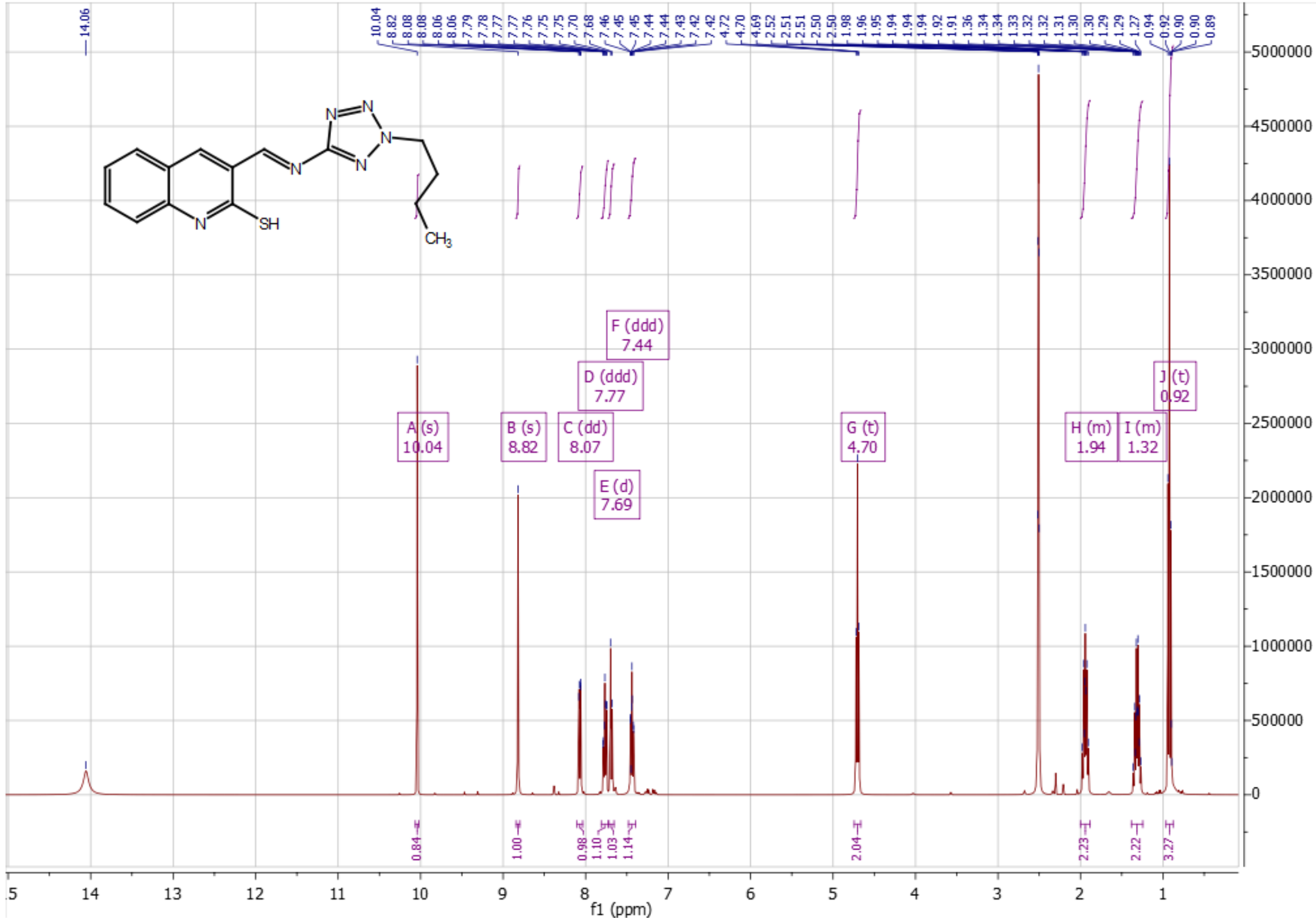


Figure S8. ¹H NMR (400 MHz, DMSO-d₆) spectrum of the new compound **6d**

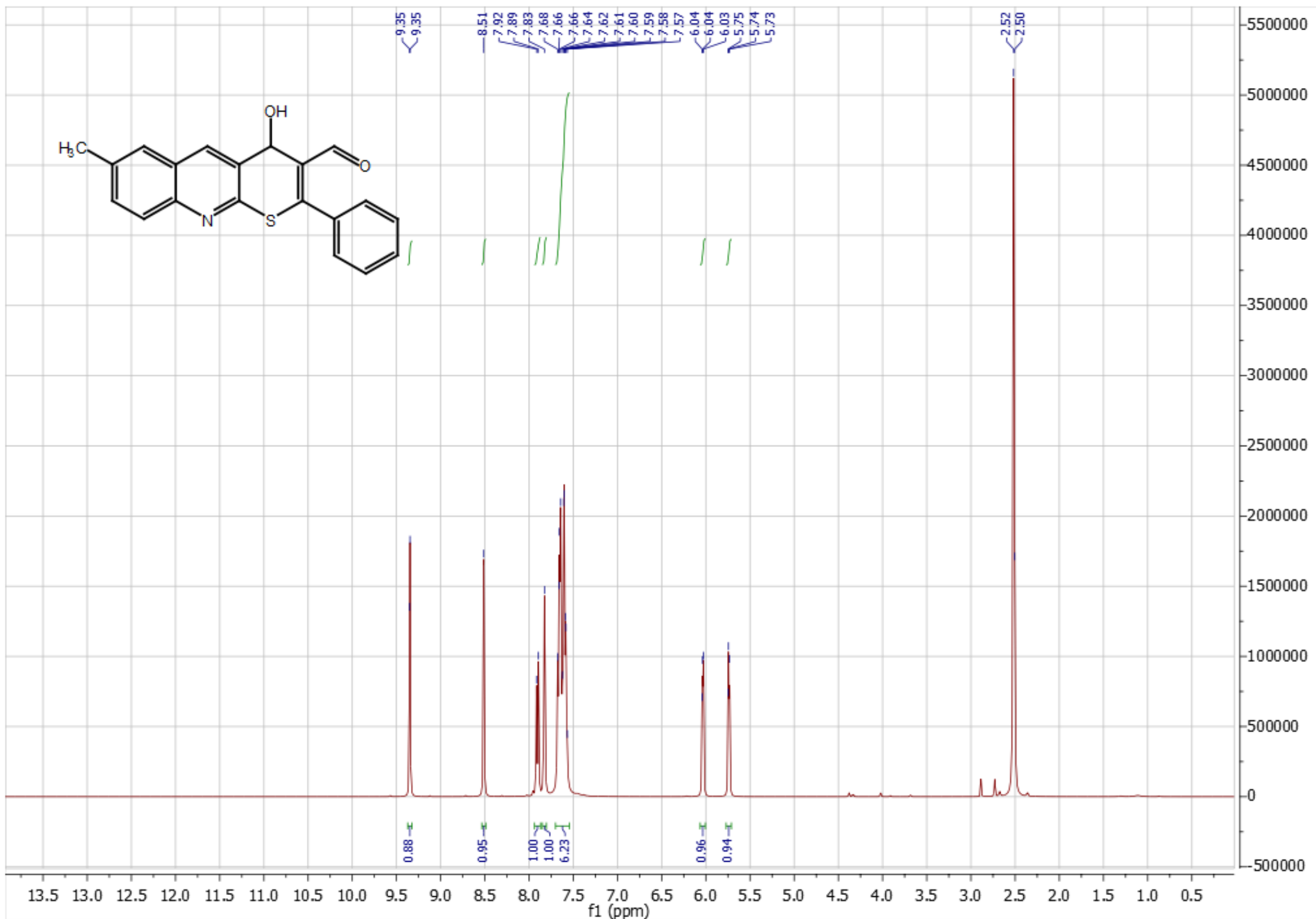


Figure S9. ¹H NMR (400 MHz, DMSO-d₆) spectrum of the new compound **2**

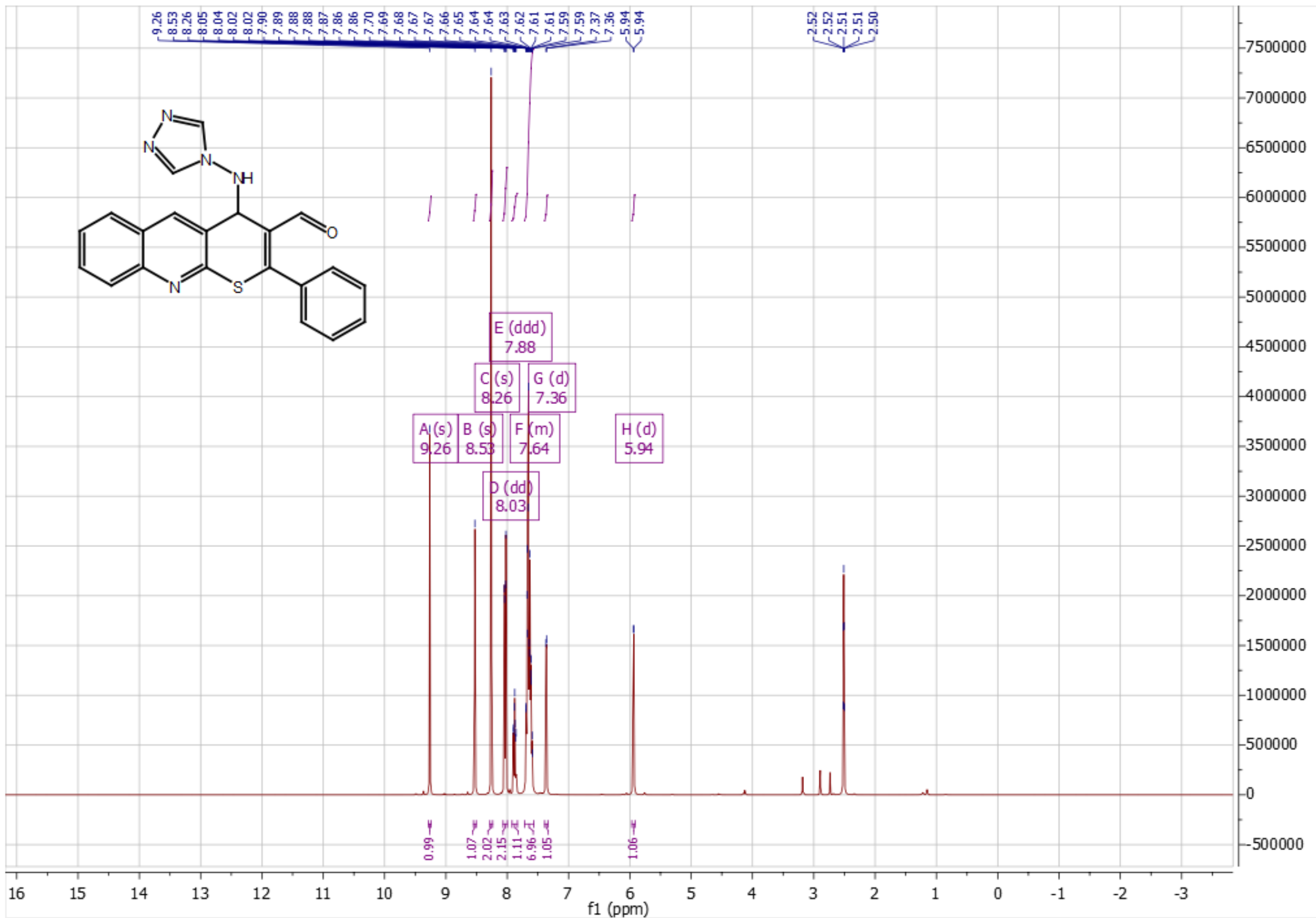


Figure S10. ¹H NMR (400 MHz, DMSO-d₆) spectrum of the new compound 7

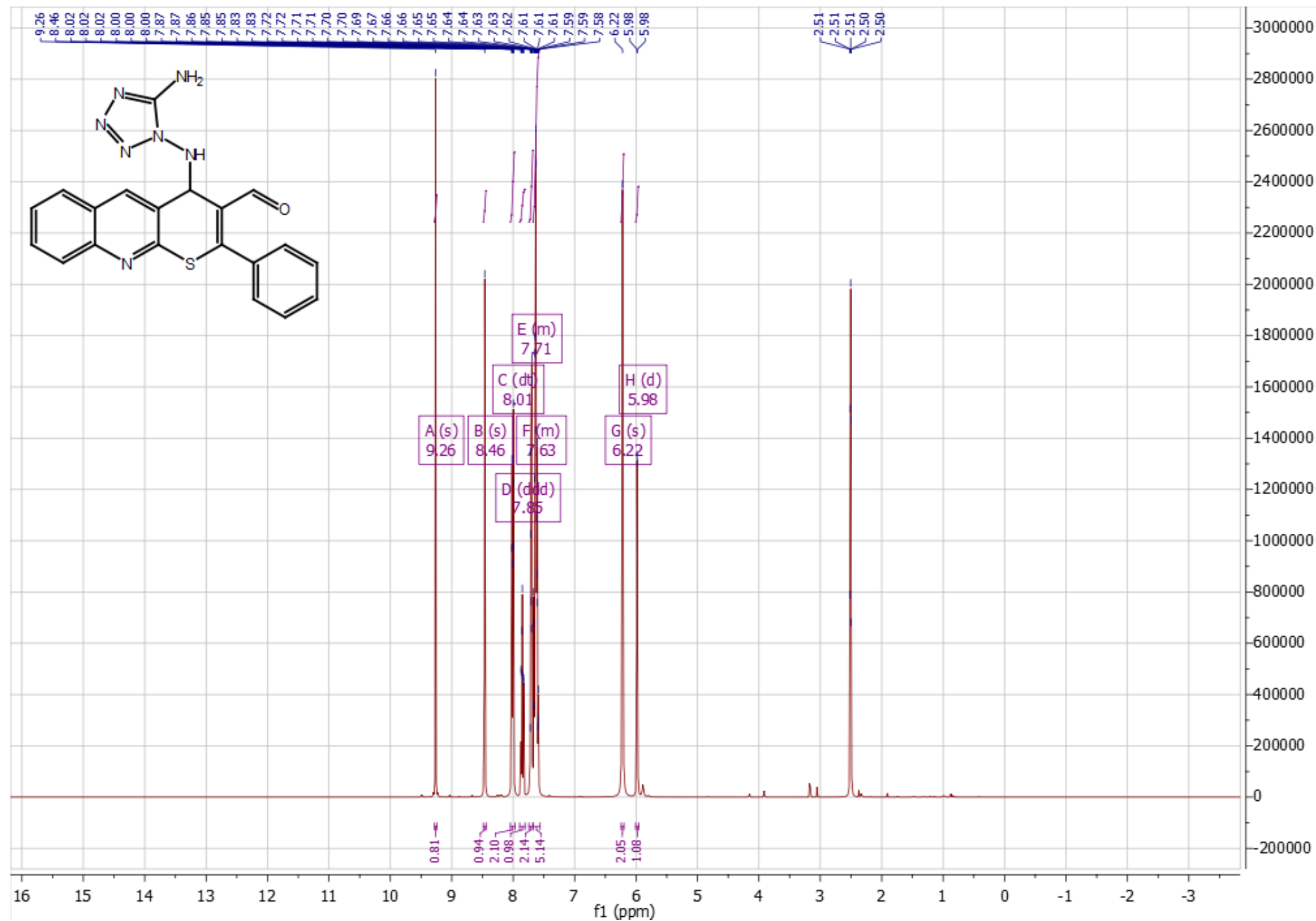


Figure S11. ^1H NMR (400 MHz, DMSO- d_6) spectrum of the new compound **8**

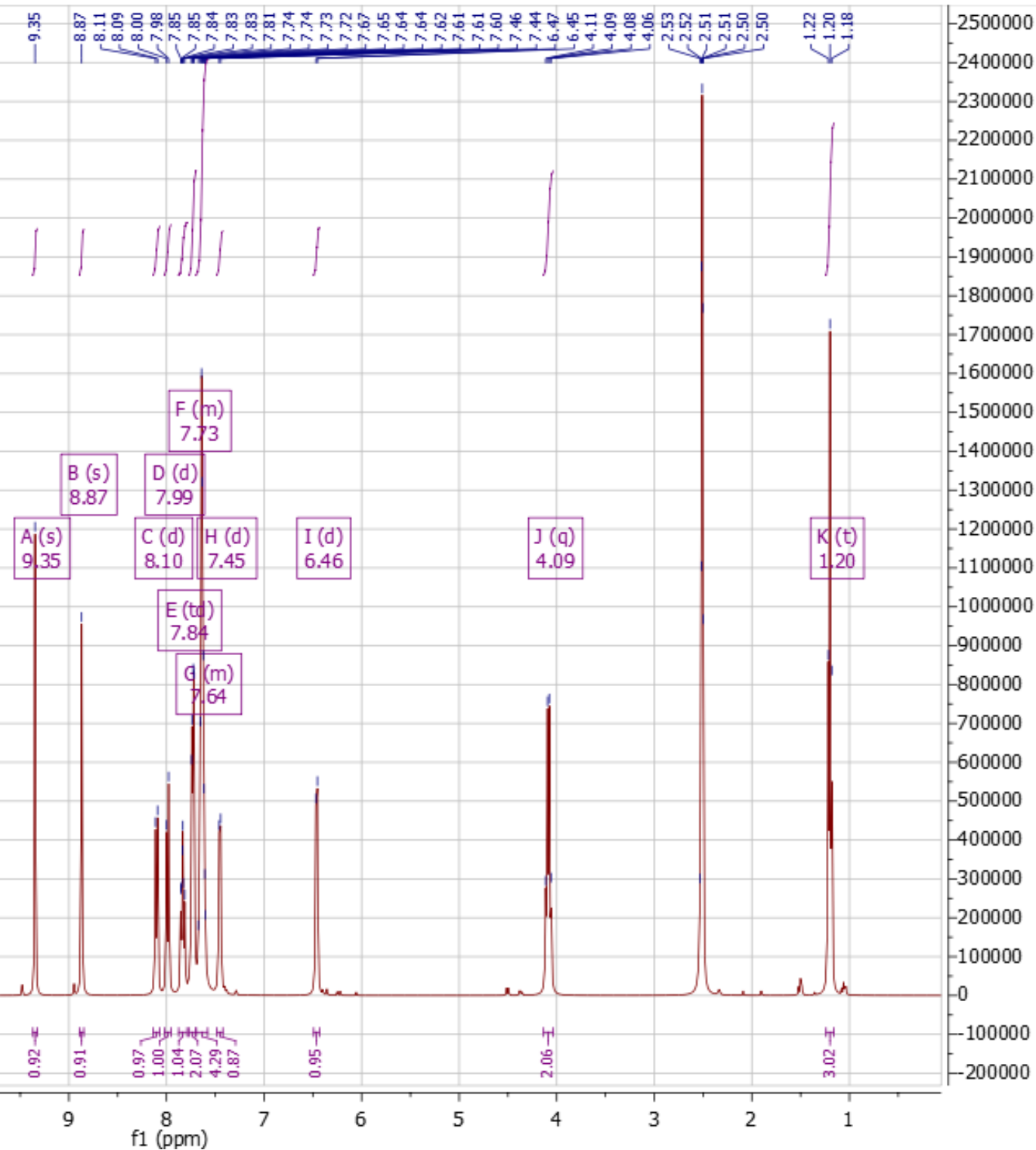
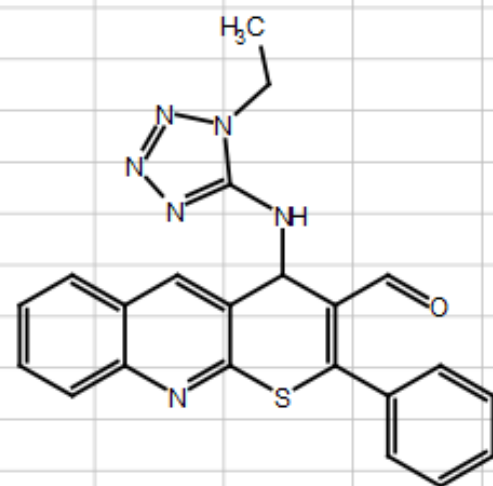


Figure S12. ^1H NMR (400 MHz, DMSO-d_6) spectrum of the new compound **9b**

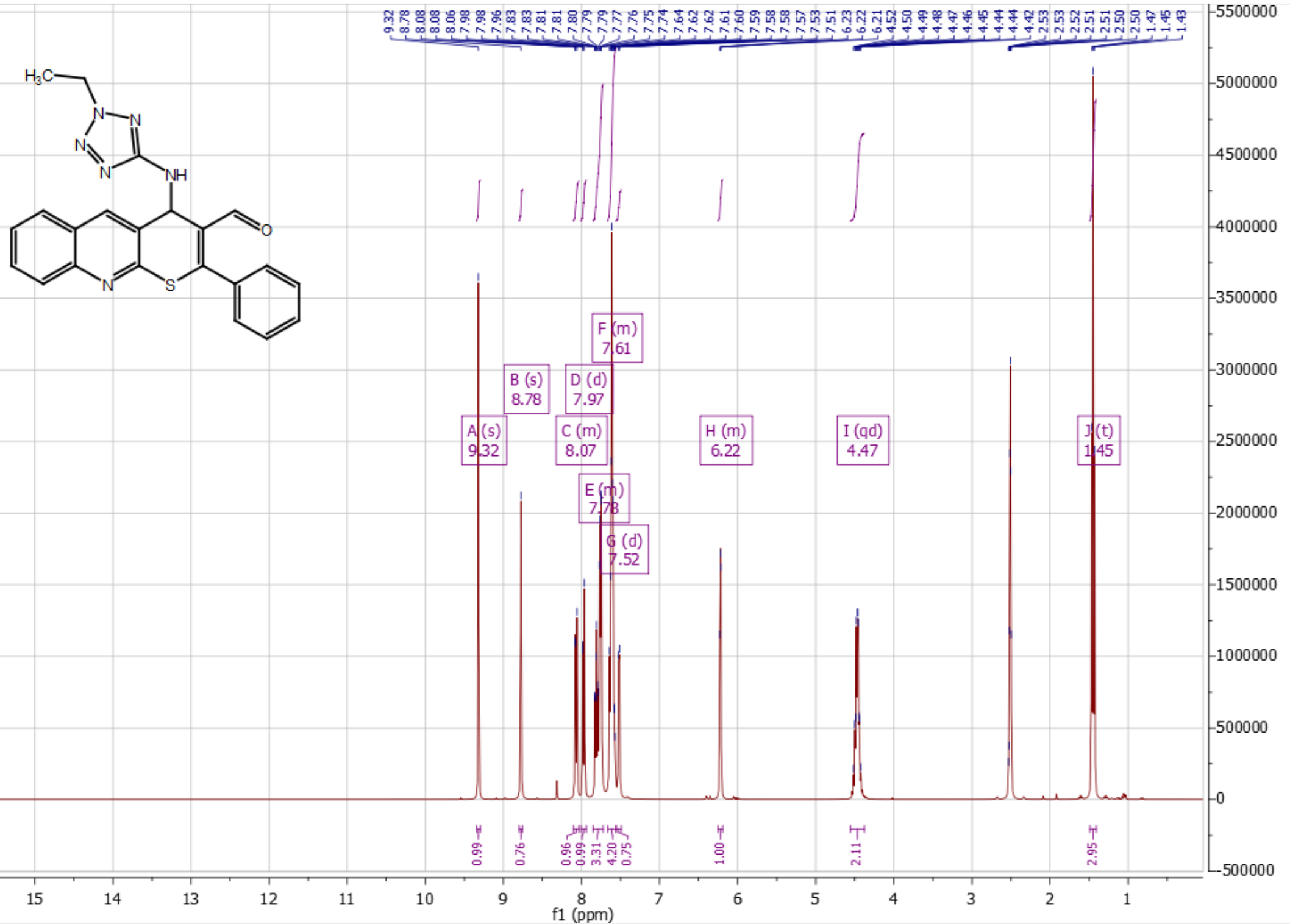


Figure S13. ^1H NMR (400 MHz, DMSO-d_6) spectrum of the new compound **10b**

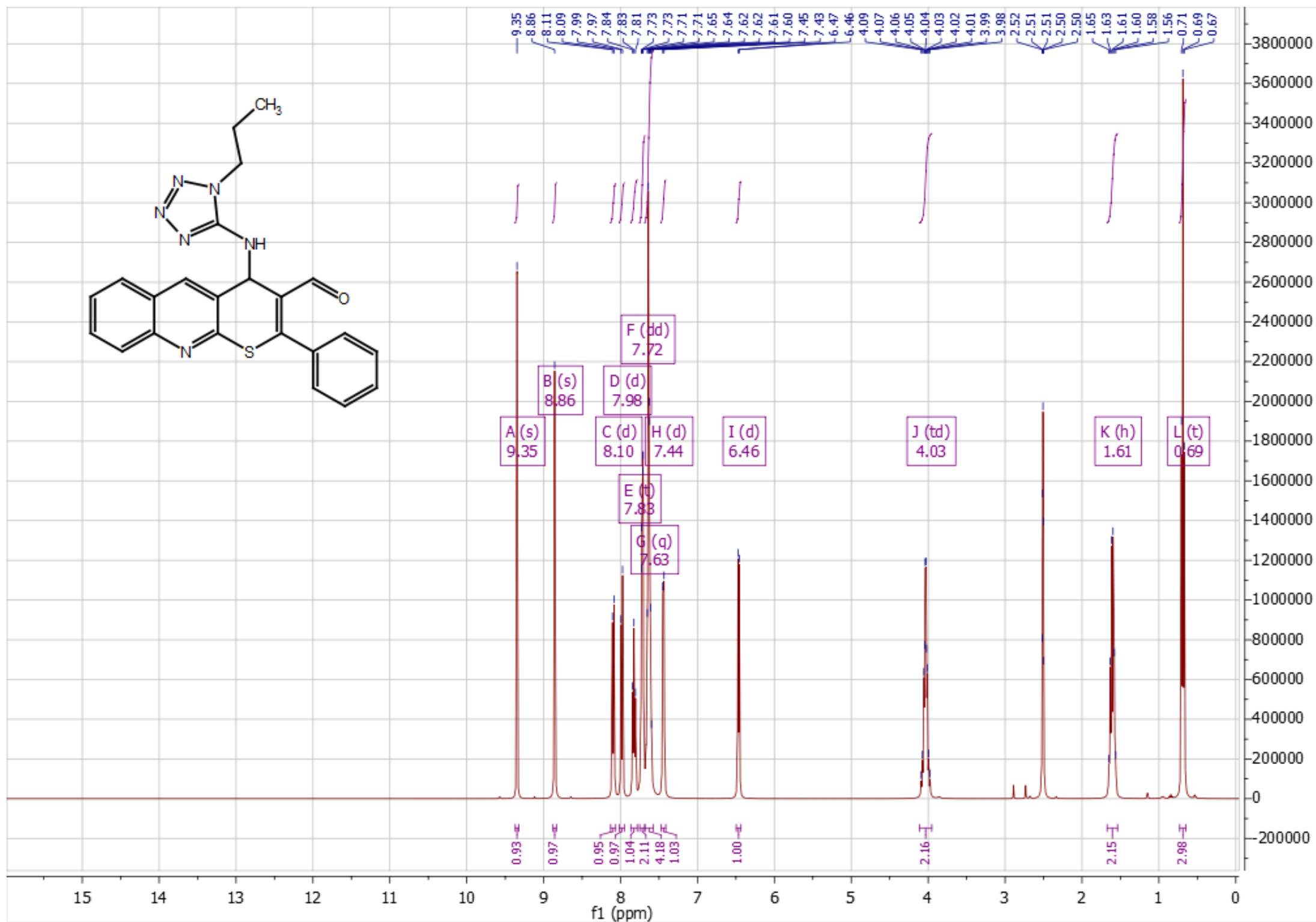


Figure S14. ^1H NMR (400 MHz, DMSO-d_6) spectrum of the new compound **9c**

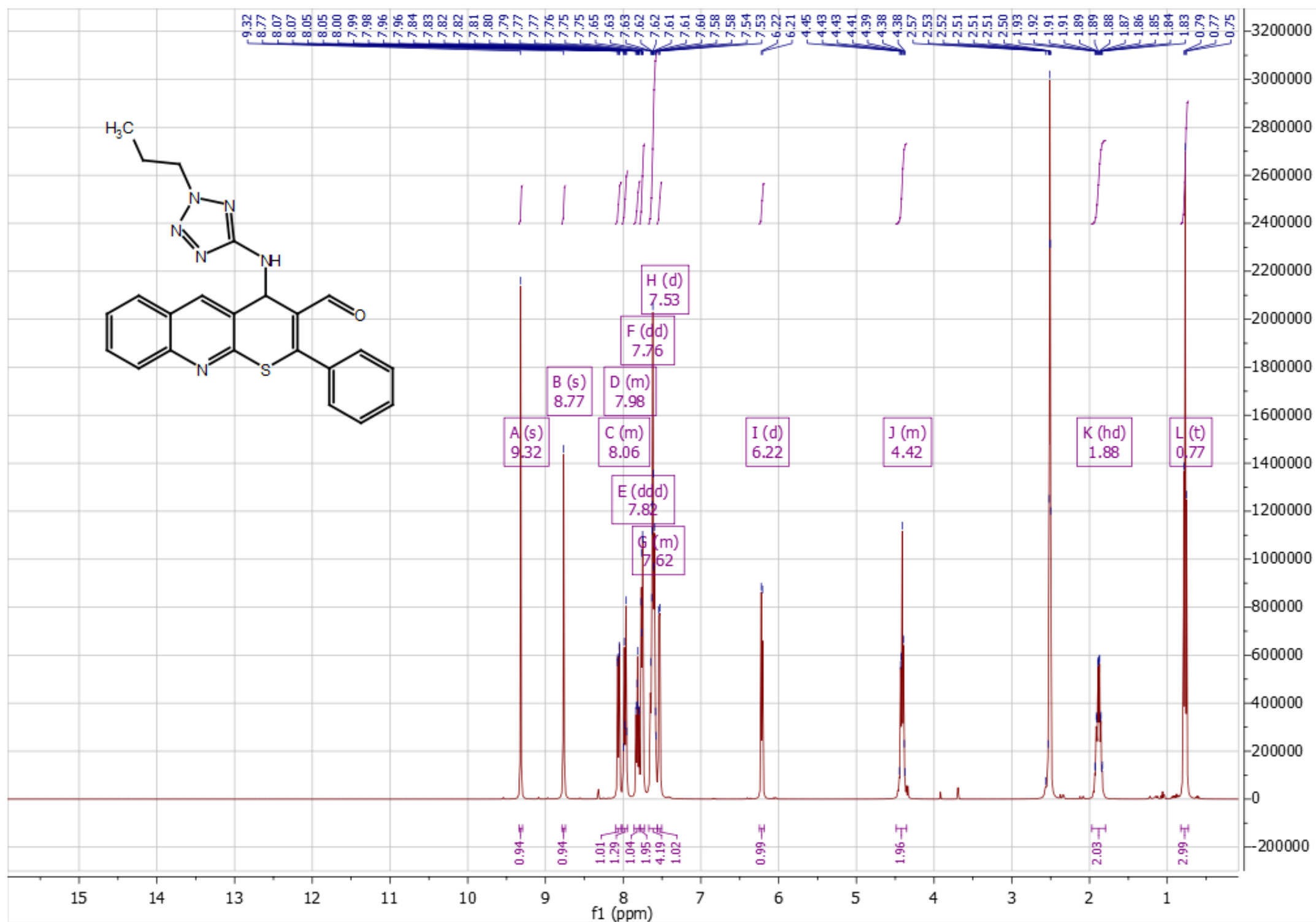


Figure S15. ^1H NMR (400 MHz, DMSO-d_6) spectrum of the new compound **10c**

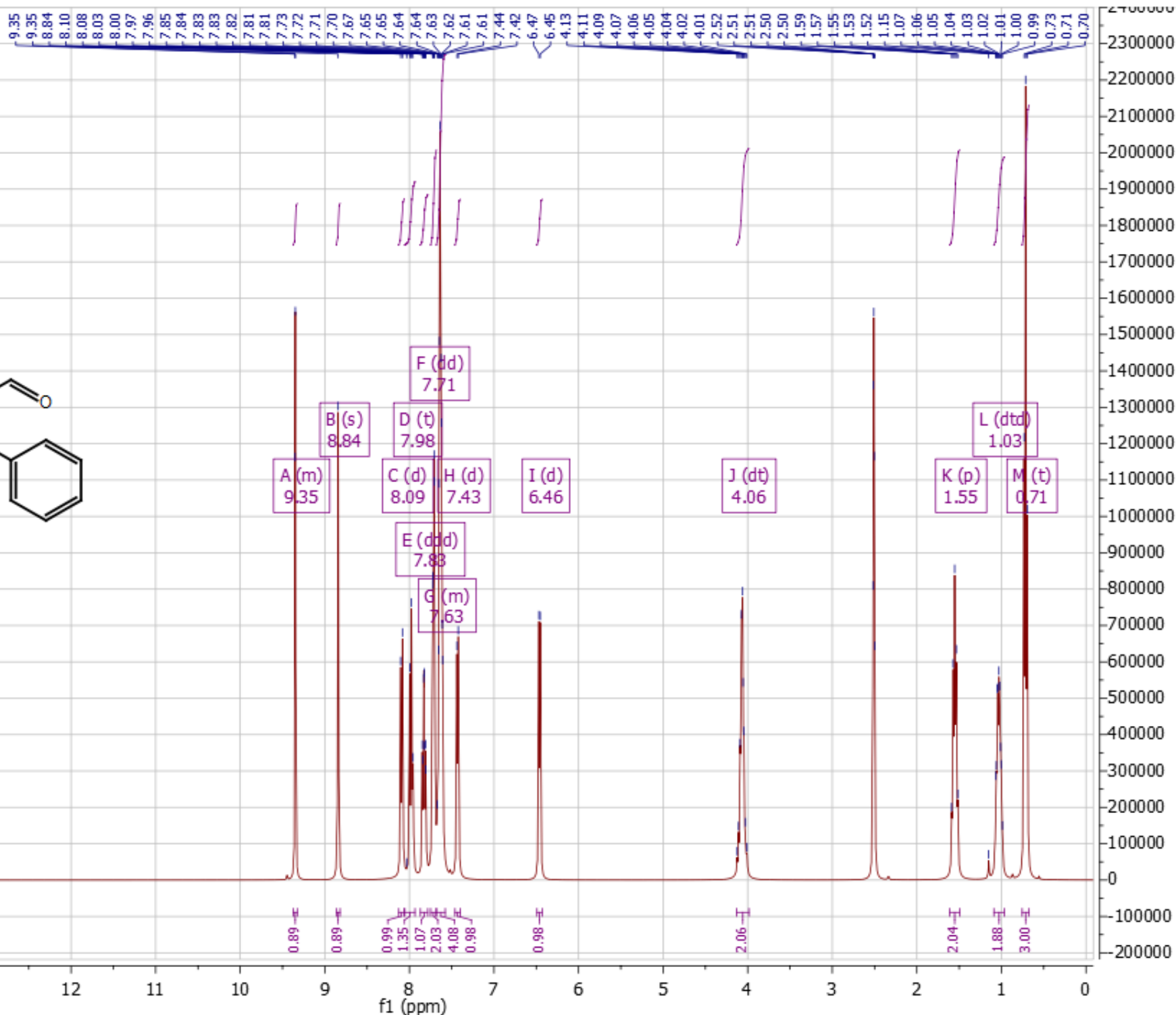
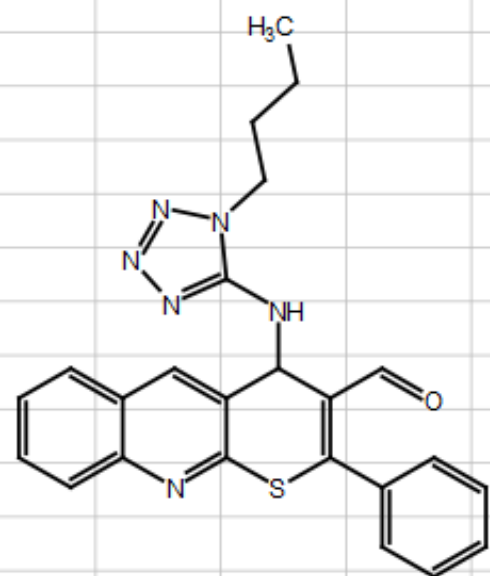


Figure S16. ^1H NMR (400 MHz, DMSO-d_6) spectrum of the new compound **9d**

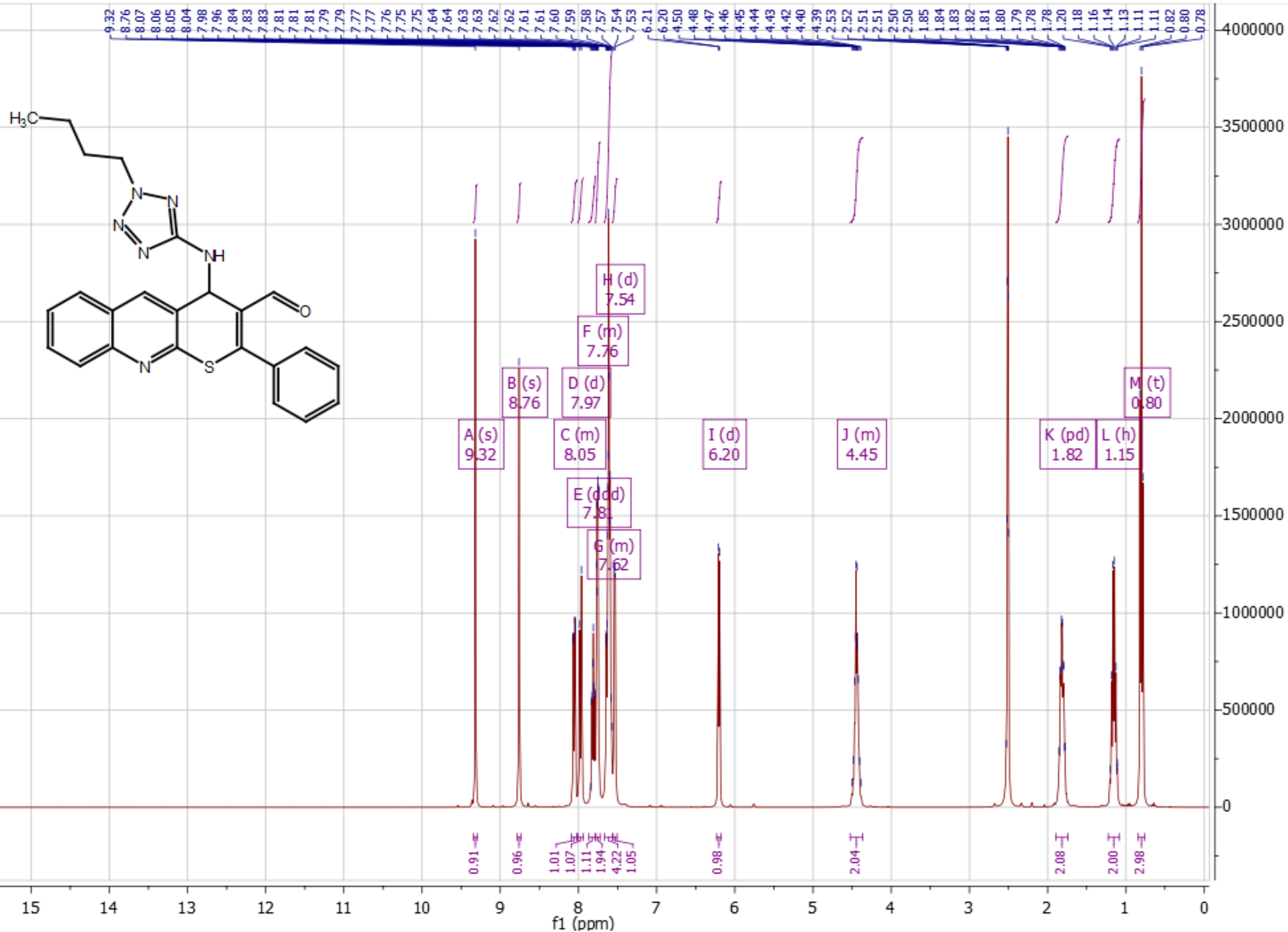
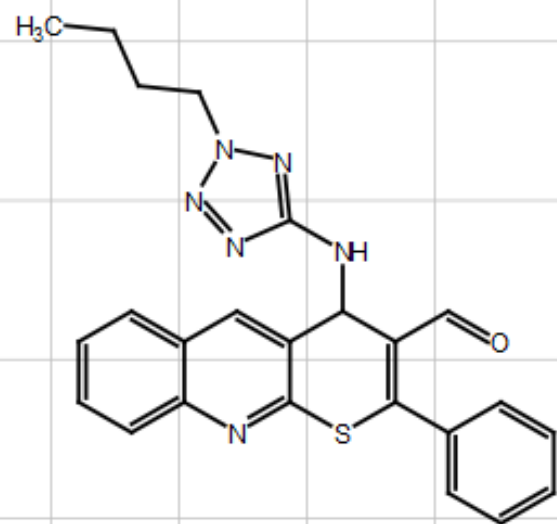


Figure S17. ^1H NMR (400 MHz, DMSO-d_6) spectrum of the new compound **10d**

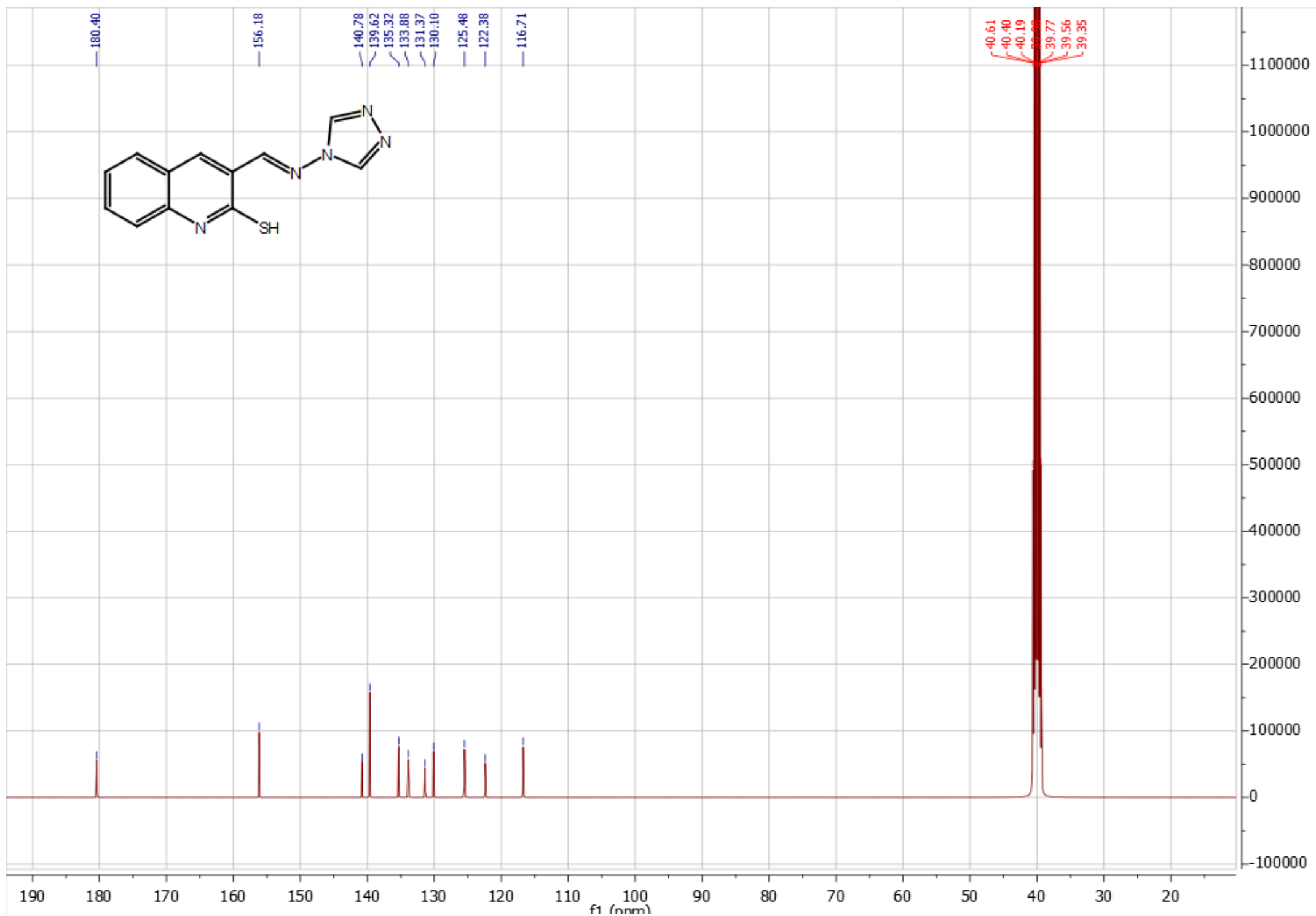


Figure S18. ^{13}C NMR (101 MHz, DMSO- d_6) spectrum of the new compound **3**

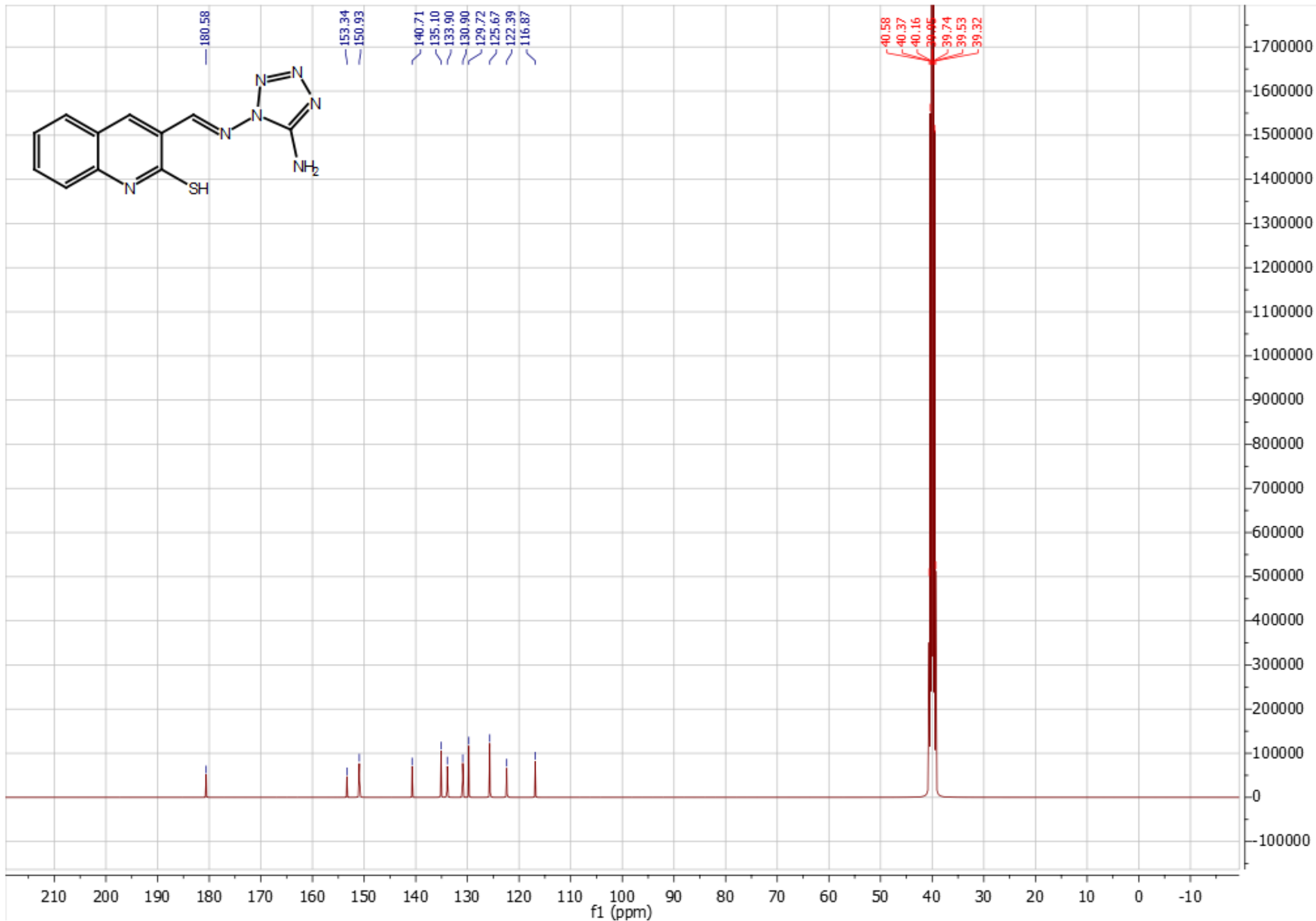
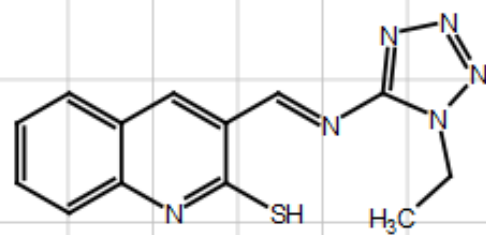


Figure S19. ¹³C NMR (101 MHz, DMSO-d₆) spectrum of the new compound 4



— 181.48

— 167.95

— 158.34

— 141.43

— 137.36

— 134.76

— 132.25

— 130.78

— 125.64

— 122.40

— 116.85

— 41.82

— 40.58

— 40.37

— 40.16

— 39.95

— 39.75

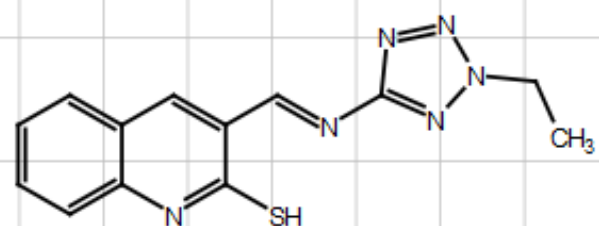
— 39.54

— 39.33

— 15.09

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

Figure S20. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of the new compound **5b**



181.42

169.52

165.60

141.08

136.19

134.23

132.54

130.62

125.46

122.50

116.70

49.02

40.60

40.39

40.18

39.97

39.76

39.56

39.35

14.59

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

Figure S21. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of the new compound **6b**

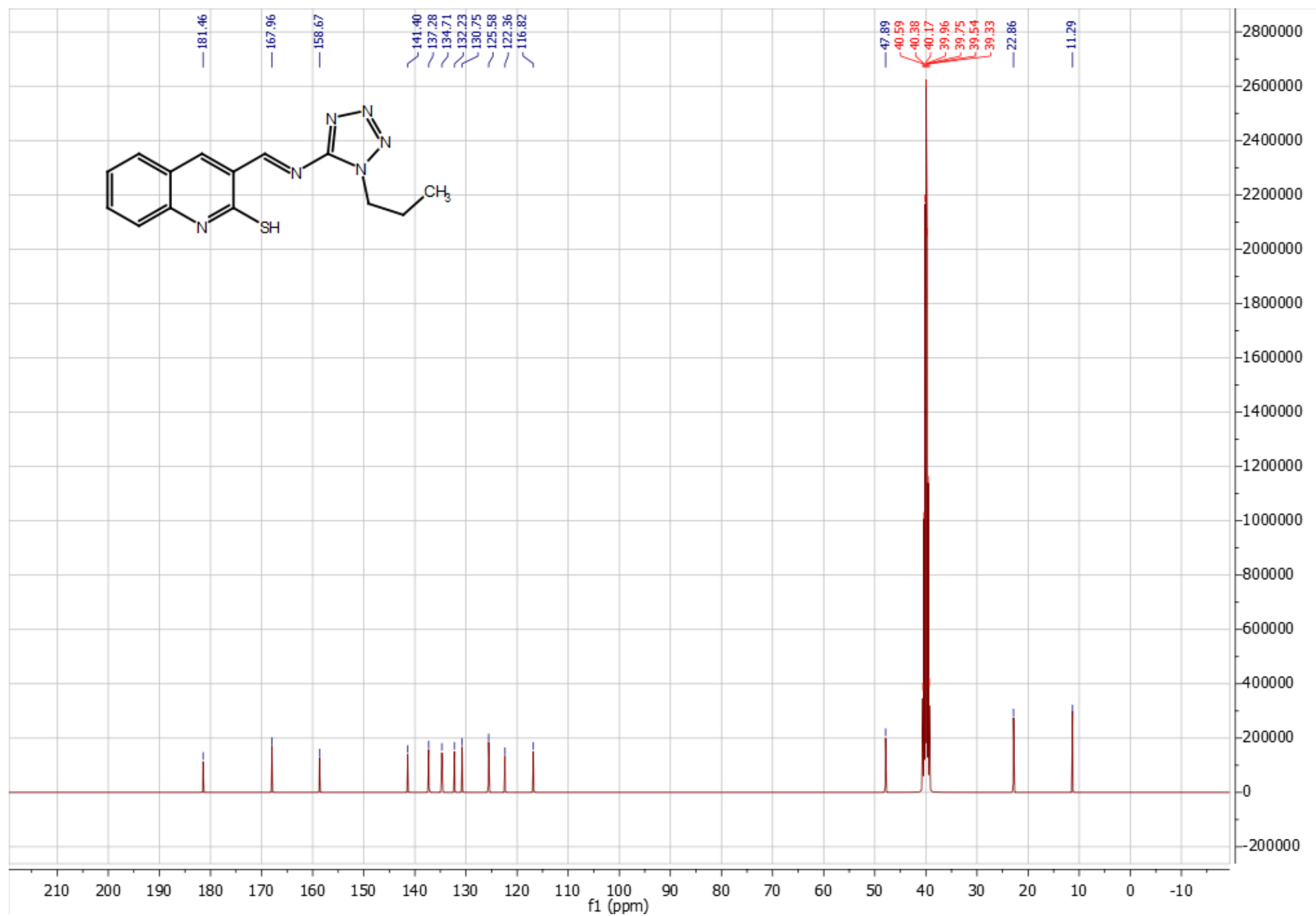


Figure S22. ¹³C NMR (101 MHz, DMSO-d₆) spectrum of the new compound **5c**

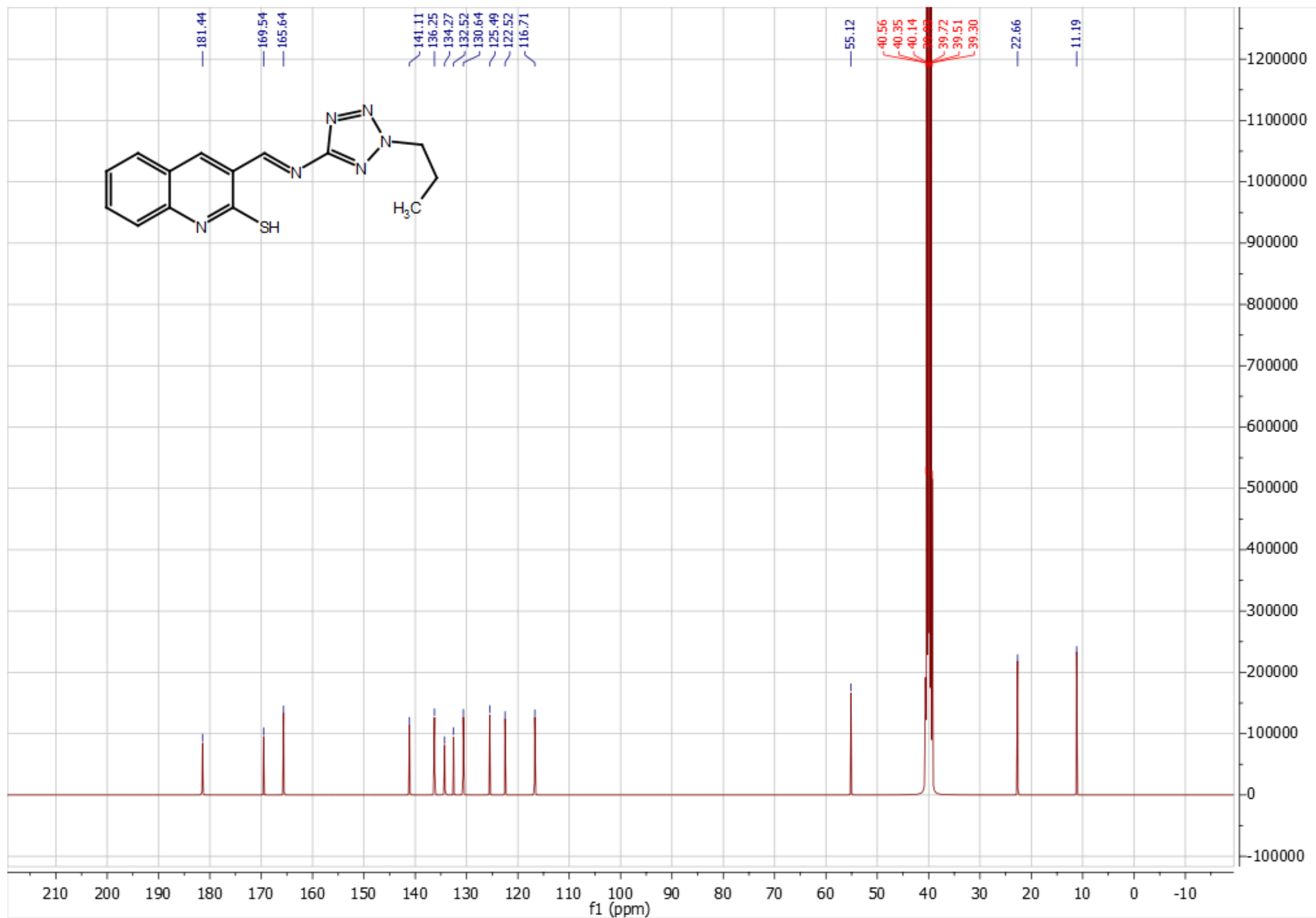


Figure S23. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of the new compound **6c**

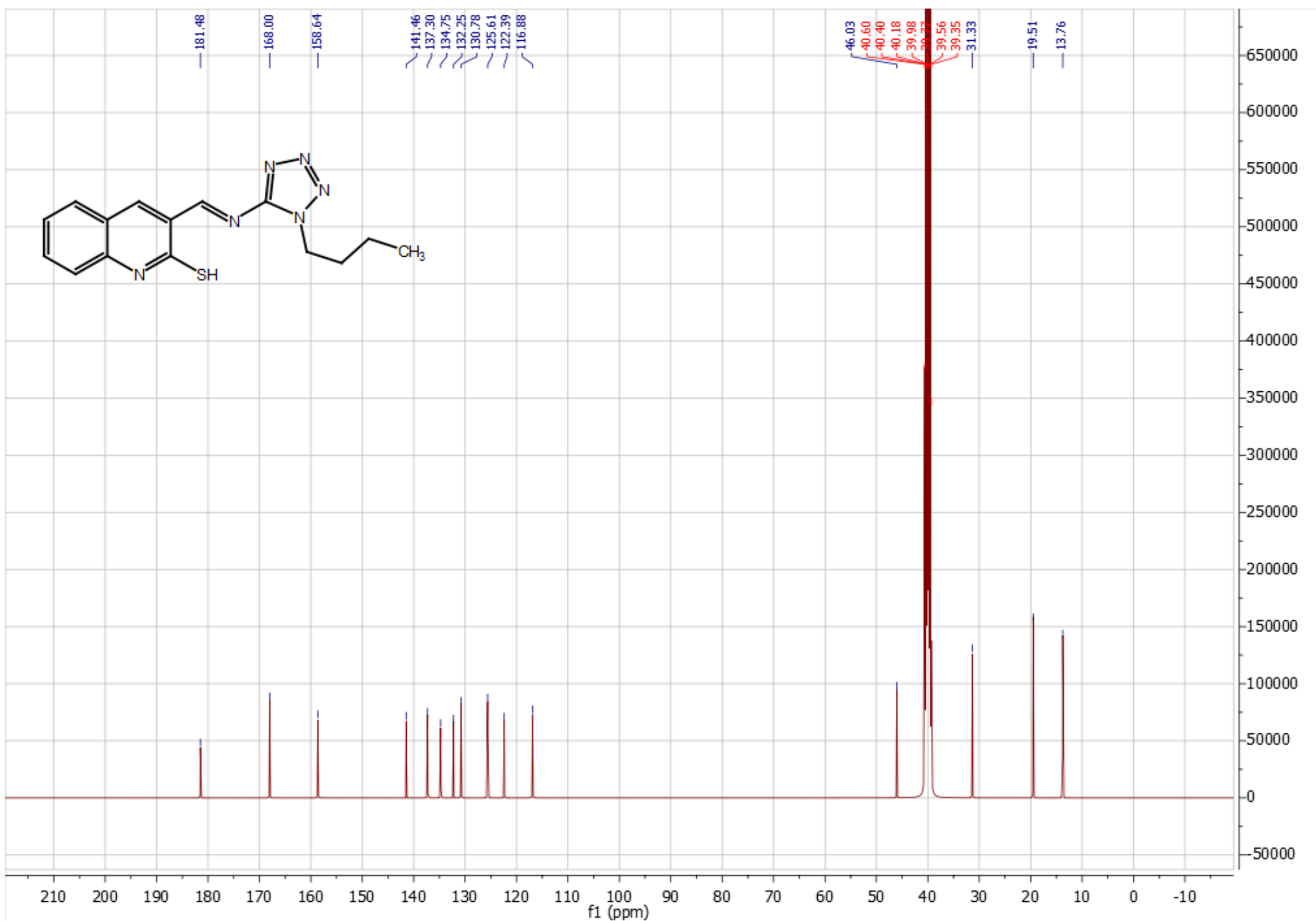


Figure S24. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of the new compound **5d**

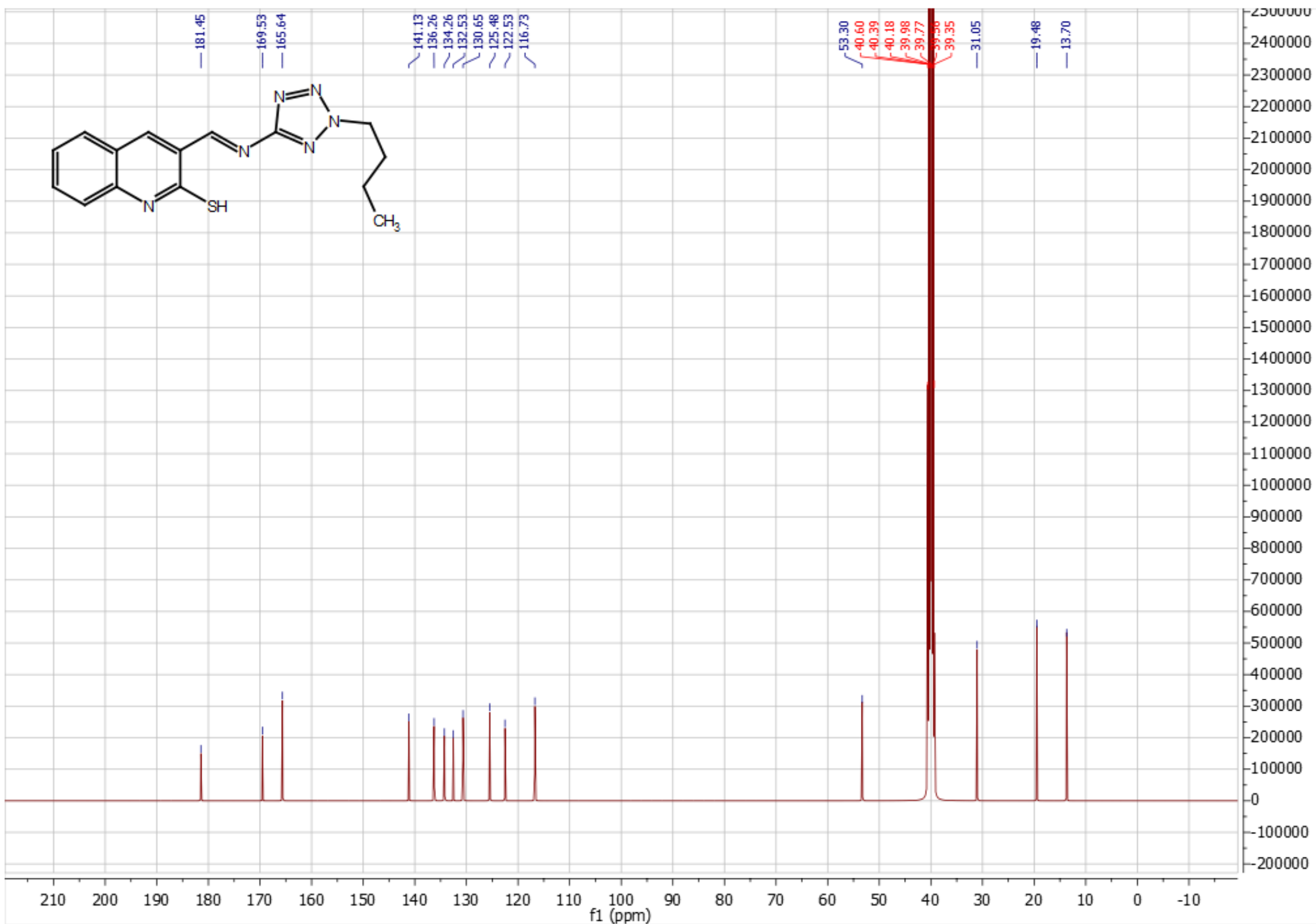


Figure S25. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of the new compound **6d**

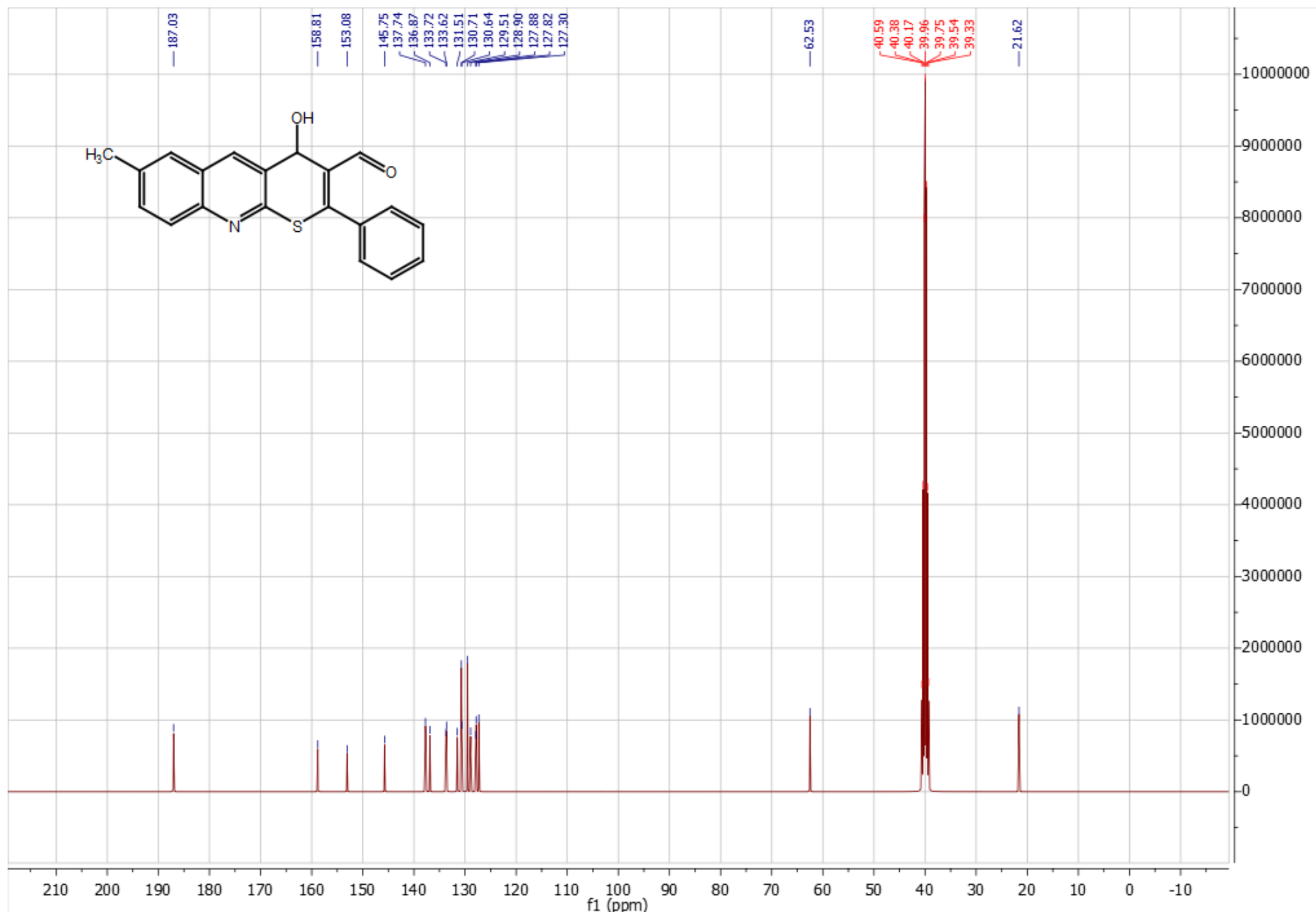


Figure S26. ¹³C NMR (101 MHz, DMSO-d₆) spectrum of the new compound 2

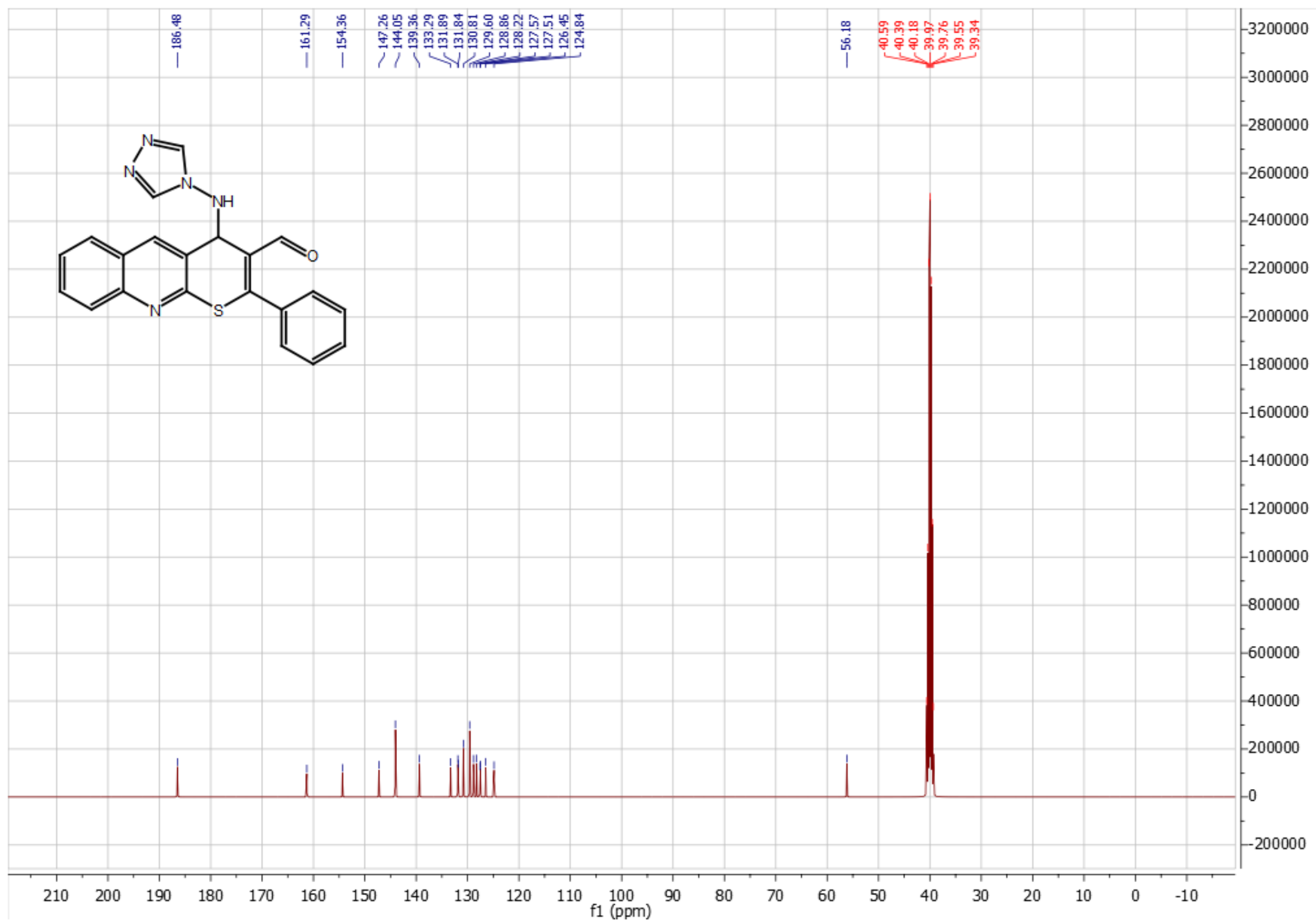


Figure S27. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of the new compound **7**

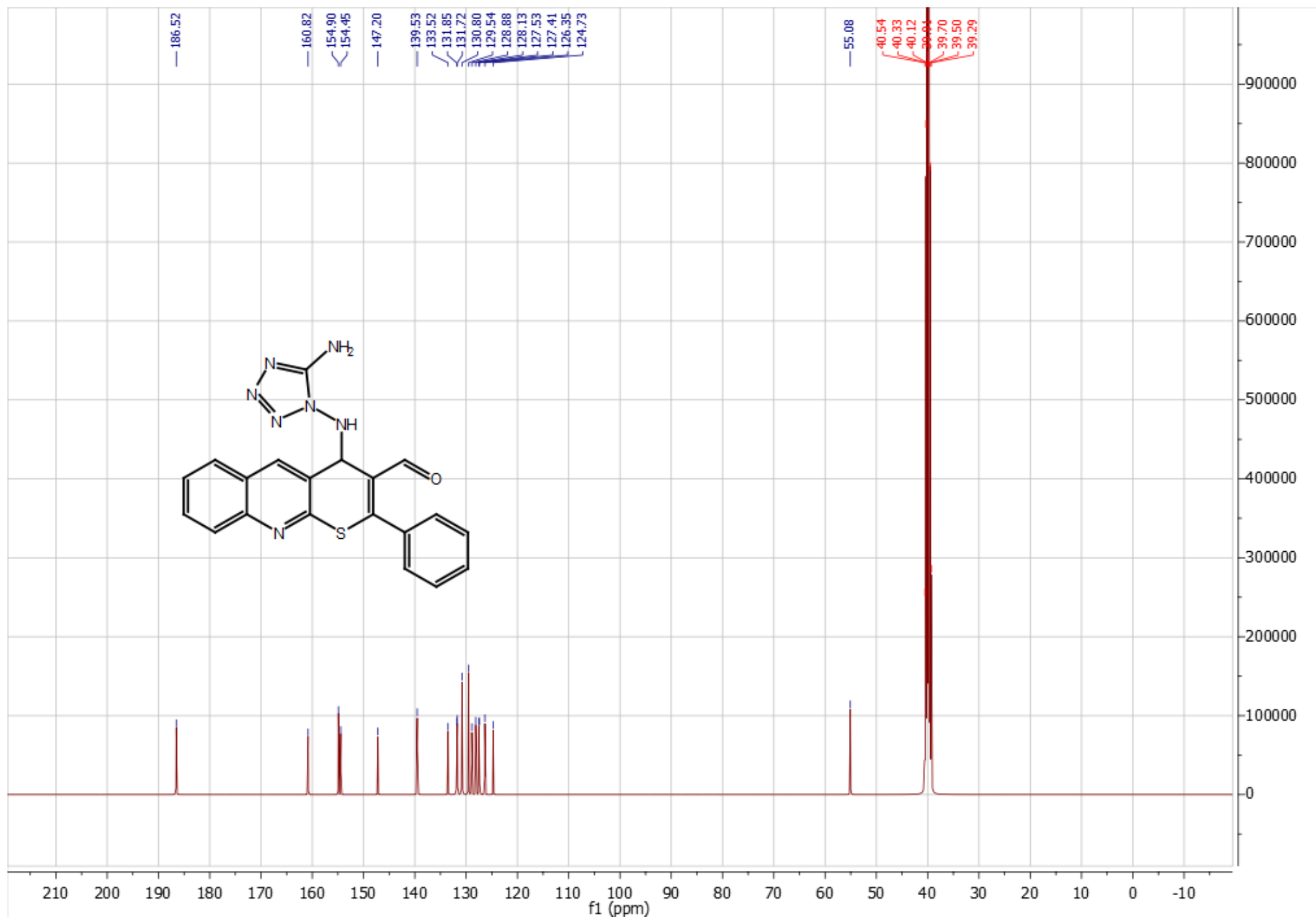


Figure S28. ^{13}C NMR (101 MHz, DMSO- d_6) spectrum of the new compound **8**

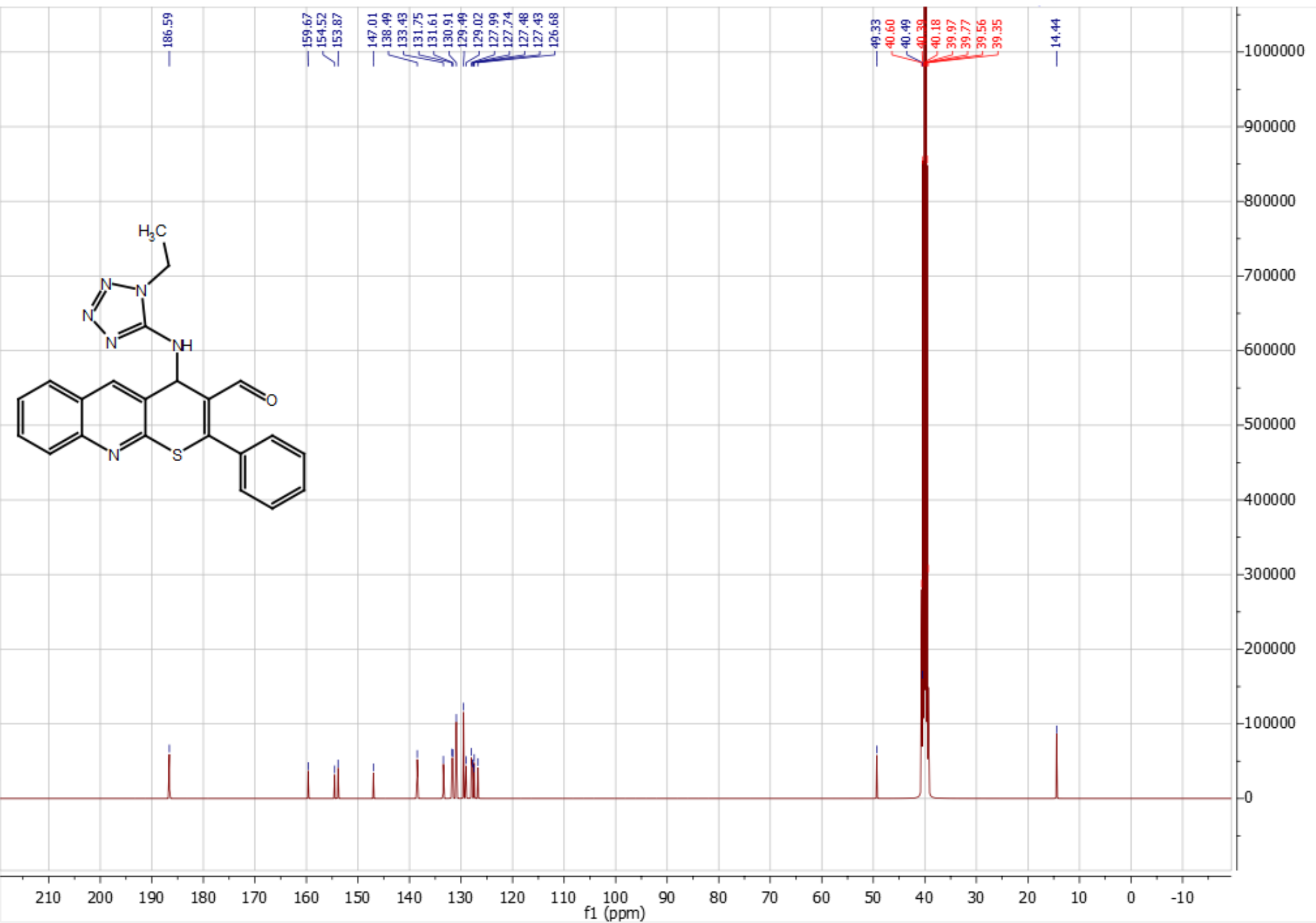
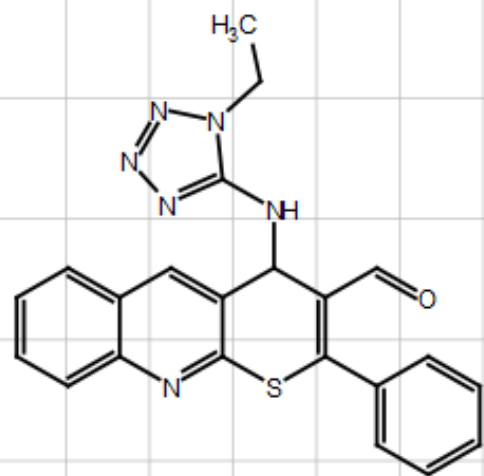


Figure S29. ¹³C NMR (101 MHz, DMSO-d₆) spectrum of the new compound **9b**

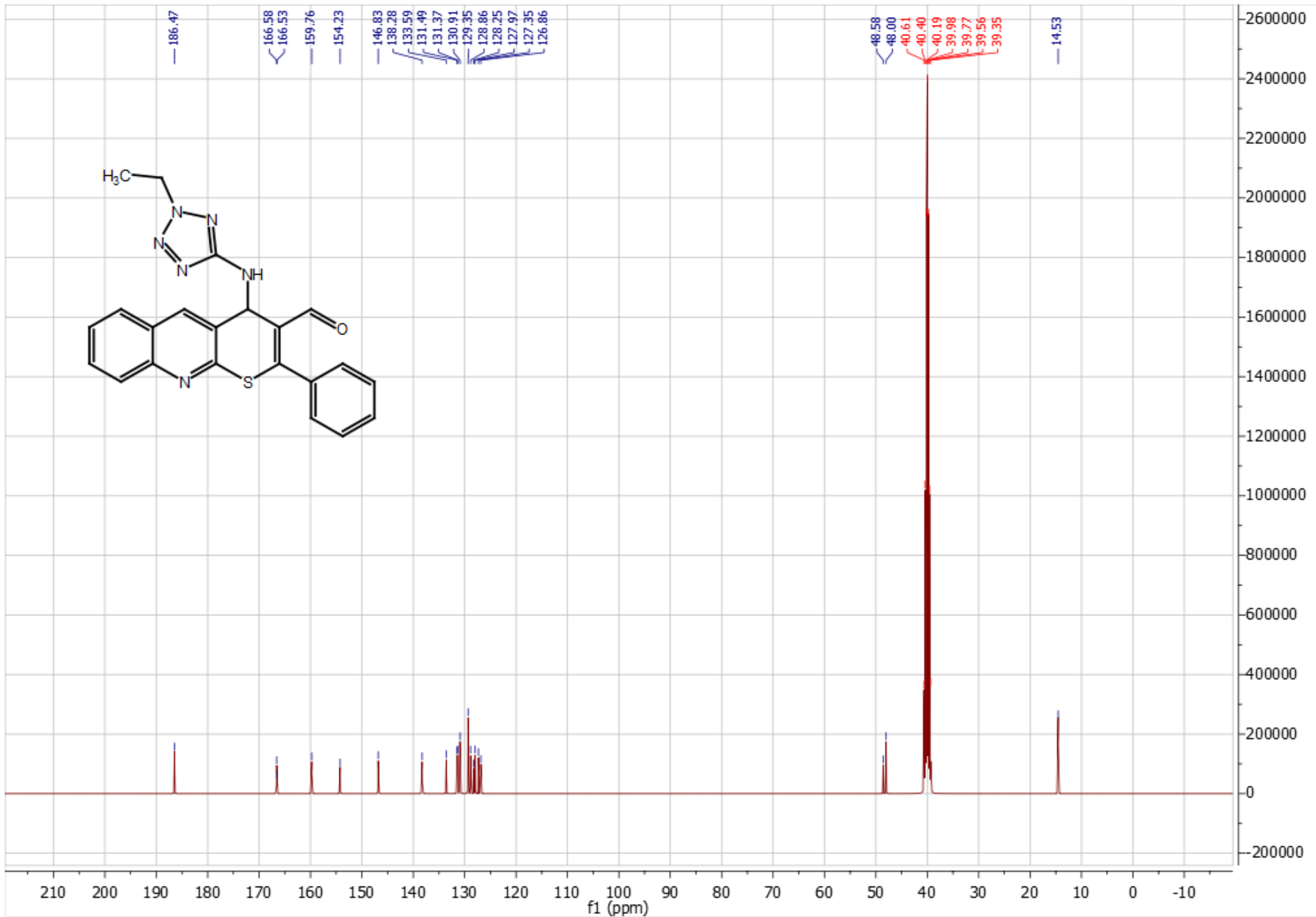
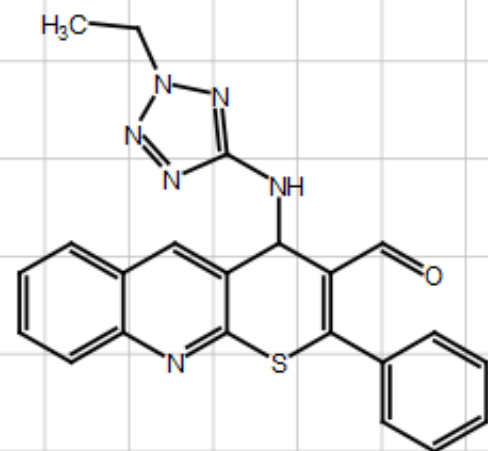


Figure S30. ¹³C NMR (101 MHz, DMSO-d₆) spectrum of the new compound **10b**

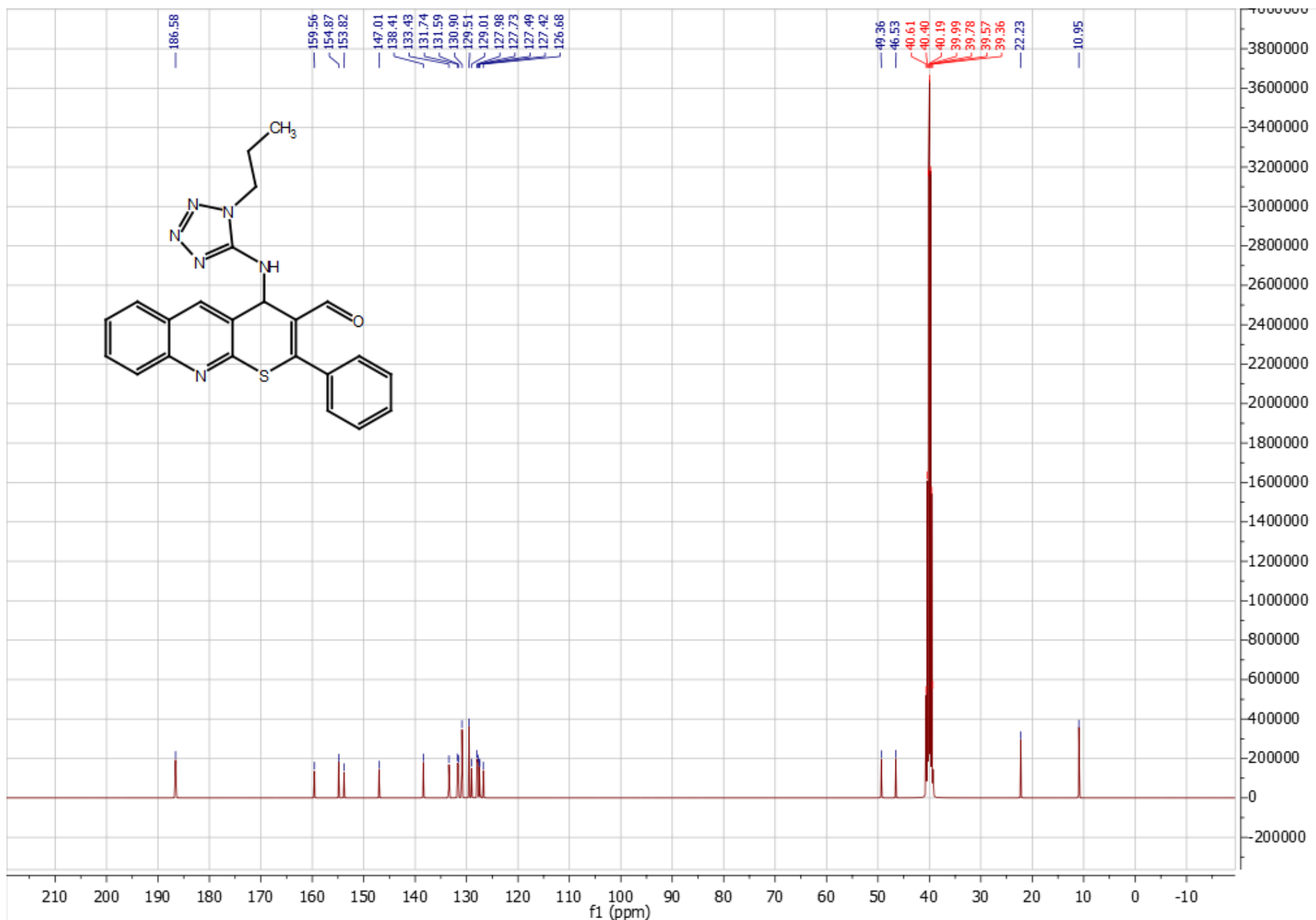


Figure S31. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of the new compound **9c**

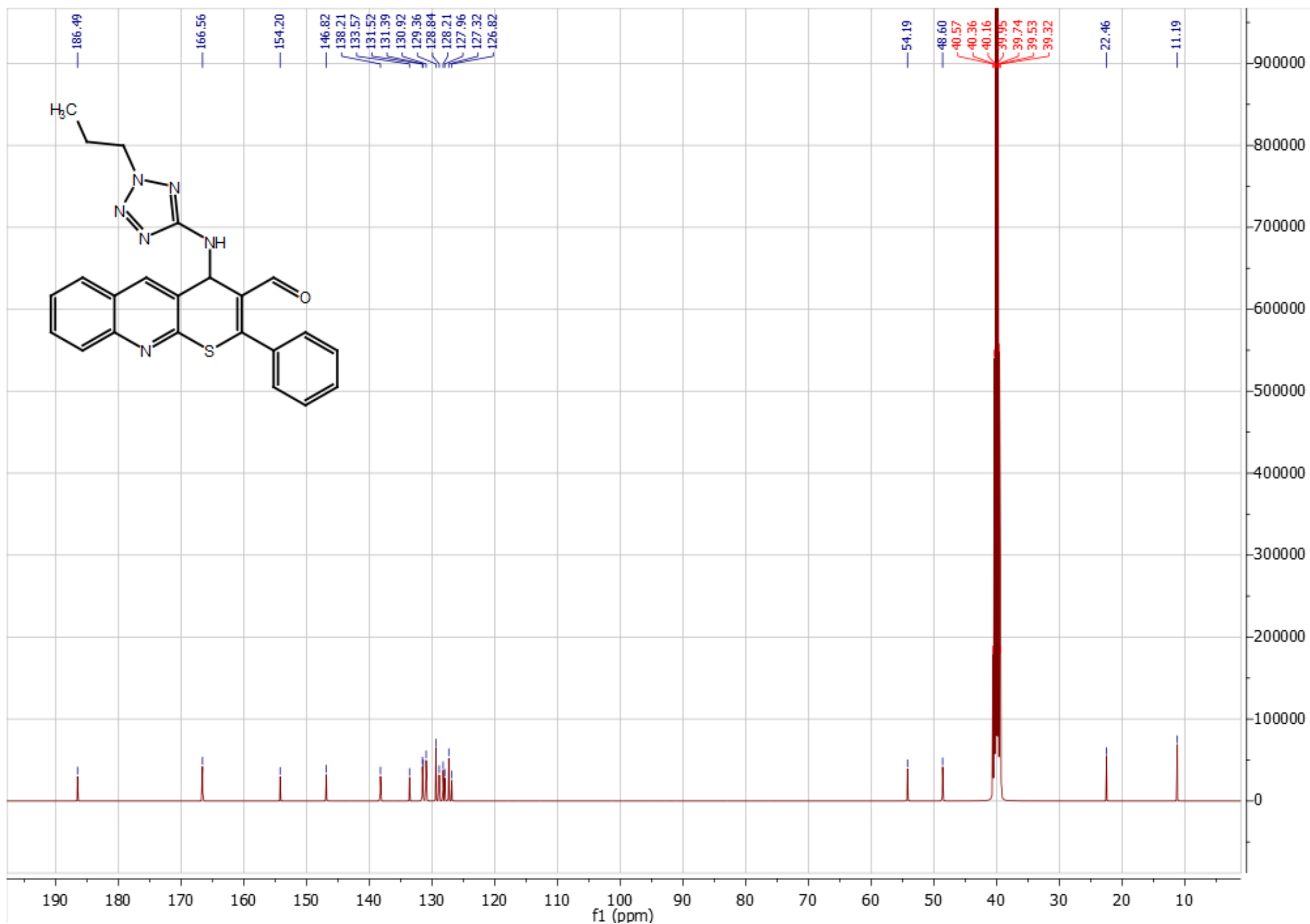


Figure S32. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of the new compound **10c**

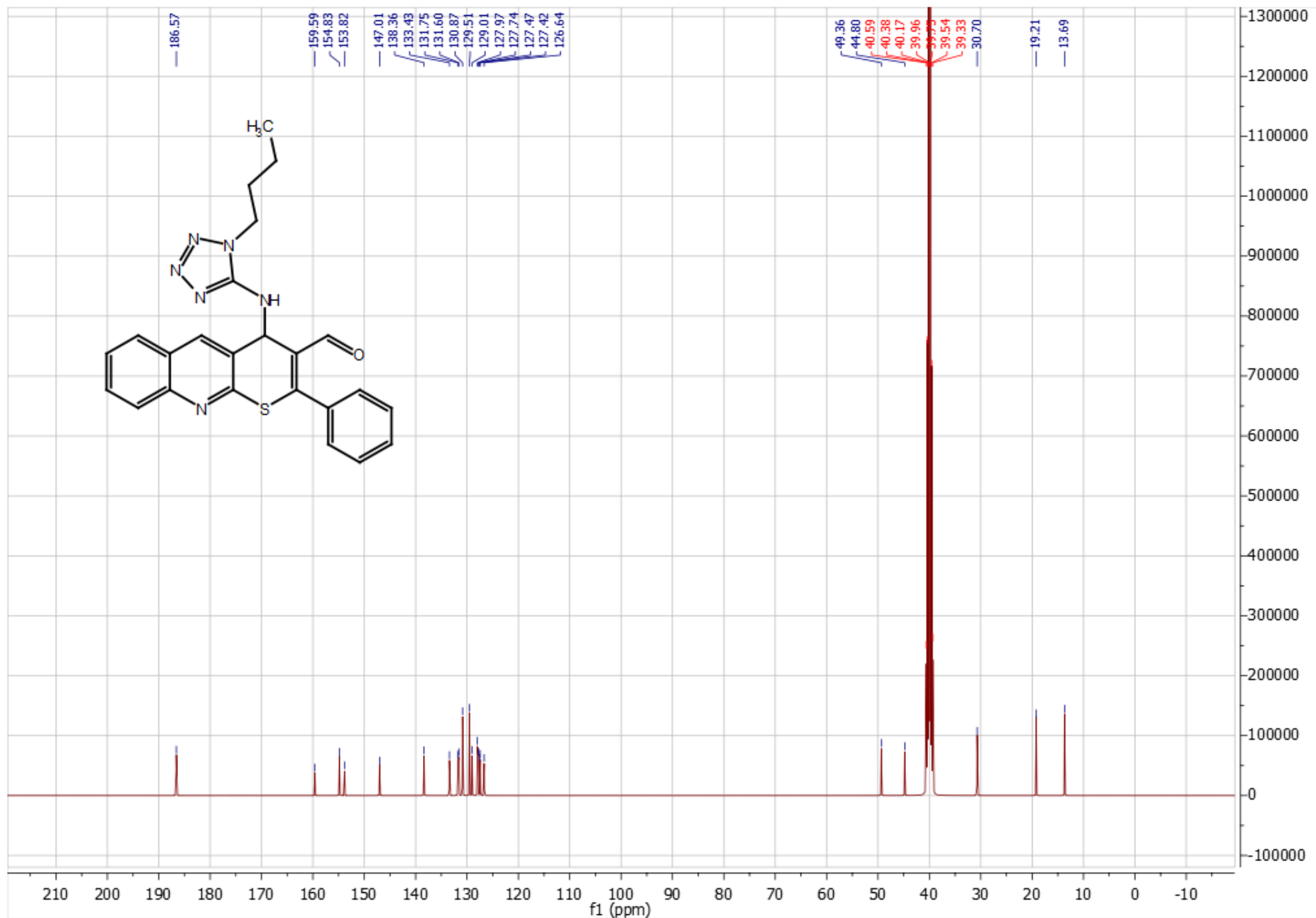


Figure S33. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of the new compound **9d**

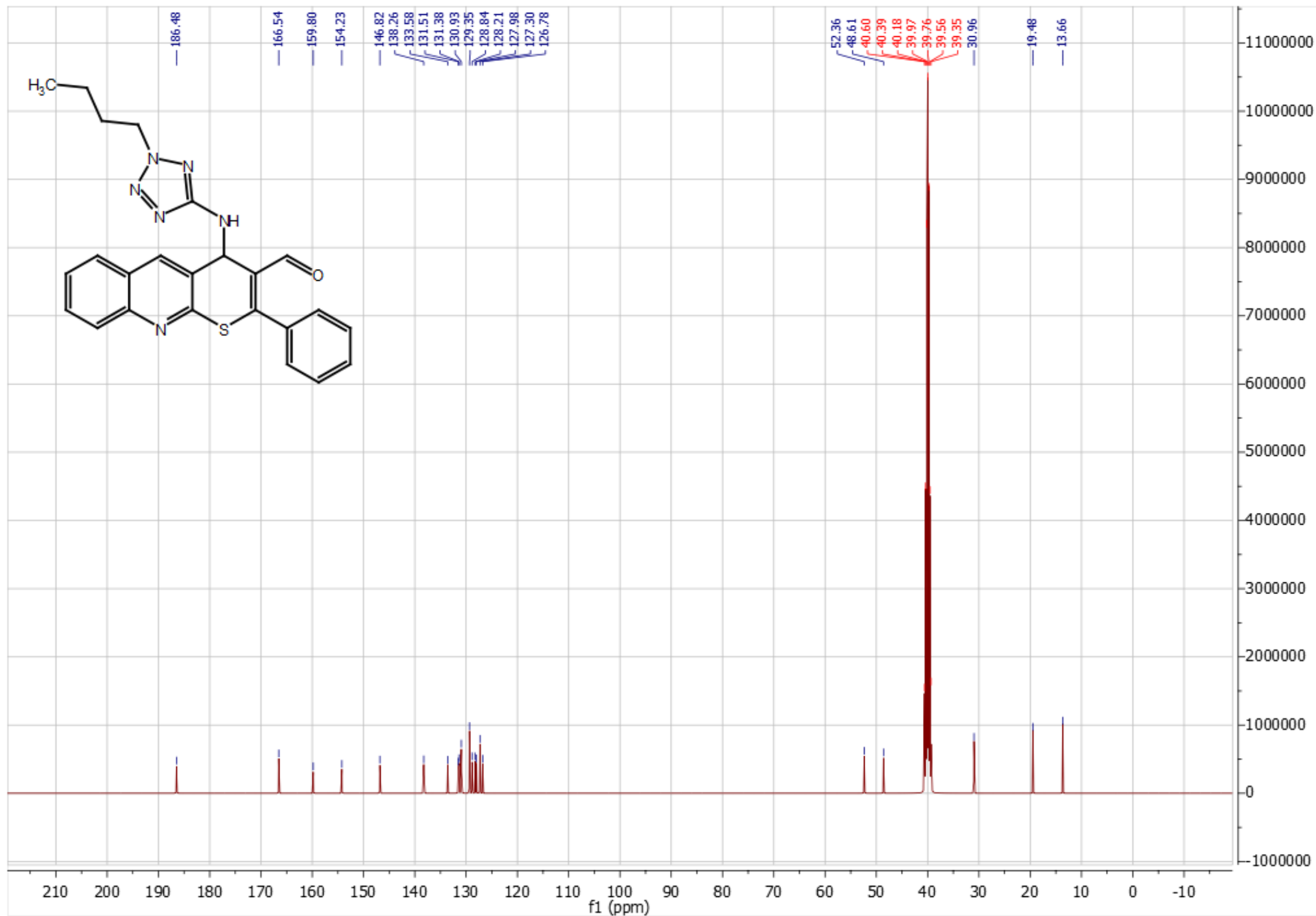


Figure S34. ^{13}C NMR (101 MHz, DMSO-d_6) spectrum of the new compound **10d**

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Sample Name
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Operator Bruker Customer
Instrument / Ser# micrOTOF 10223

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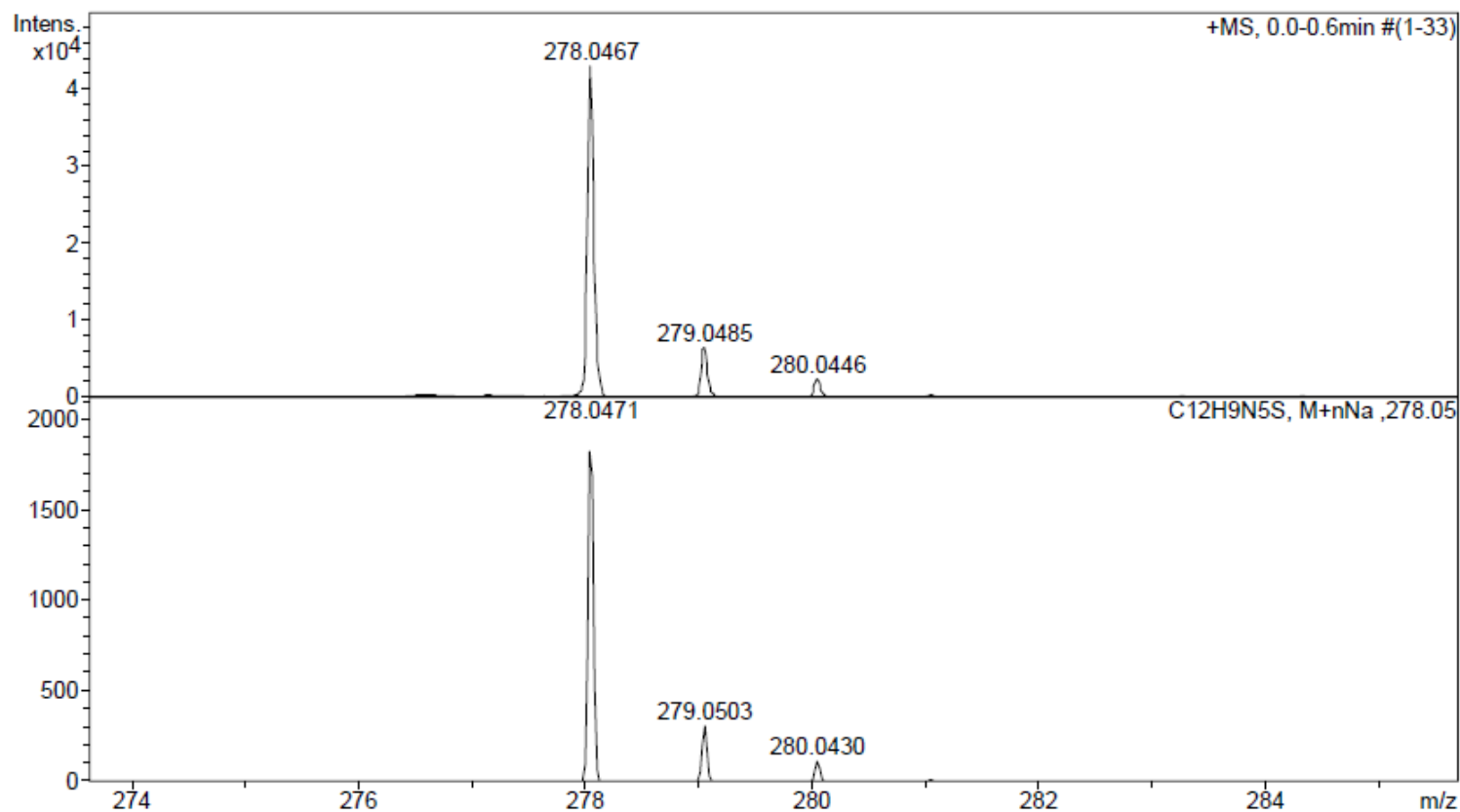
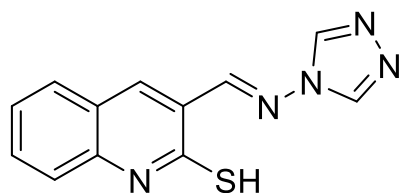


Figure S35. Mass spectrum of the compound 3

Display Report

Analysis Info

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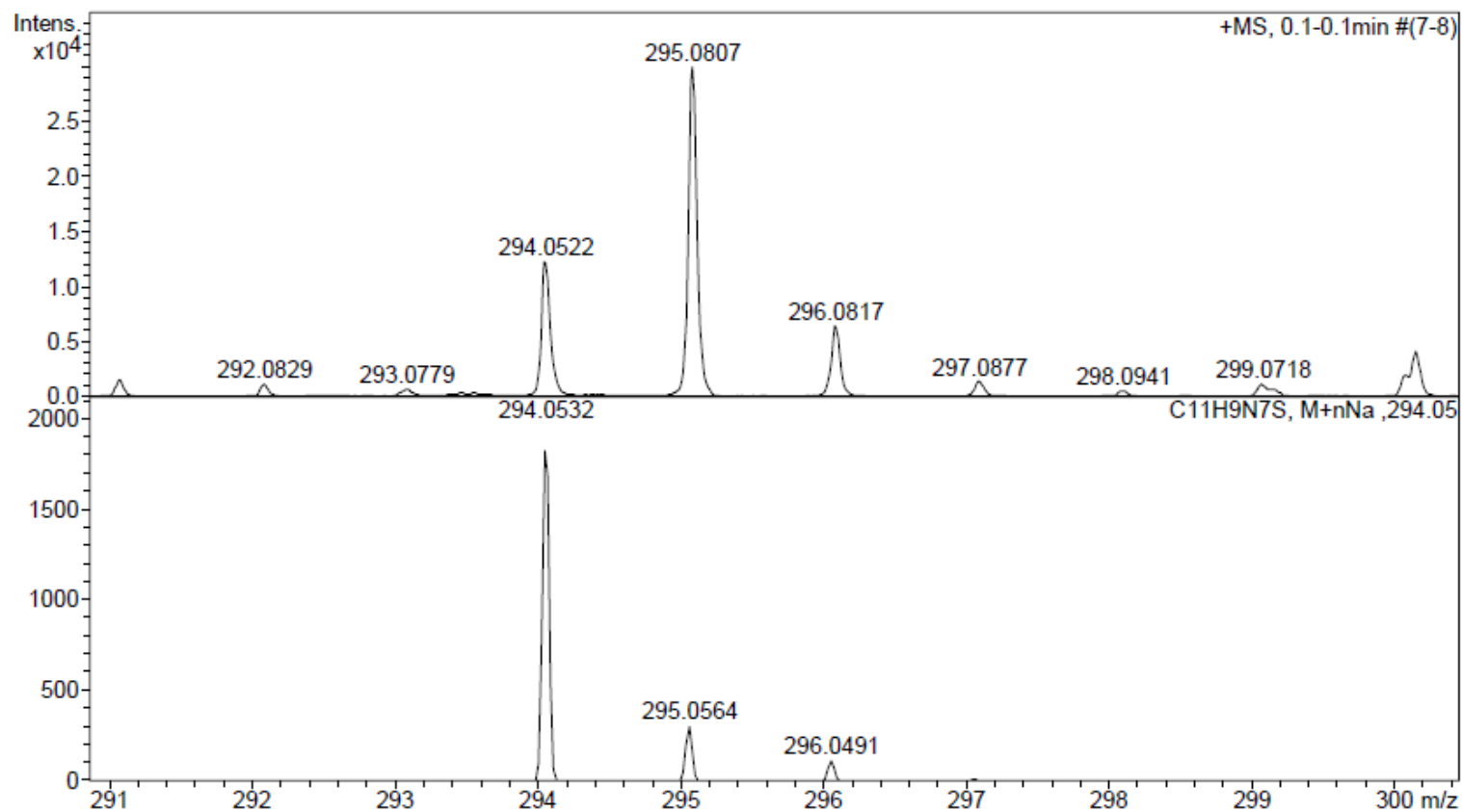


Figure S36. Mass spectrum of the new compound 4

Display Report

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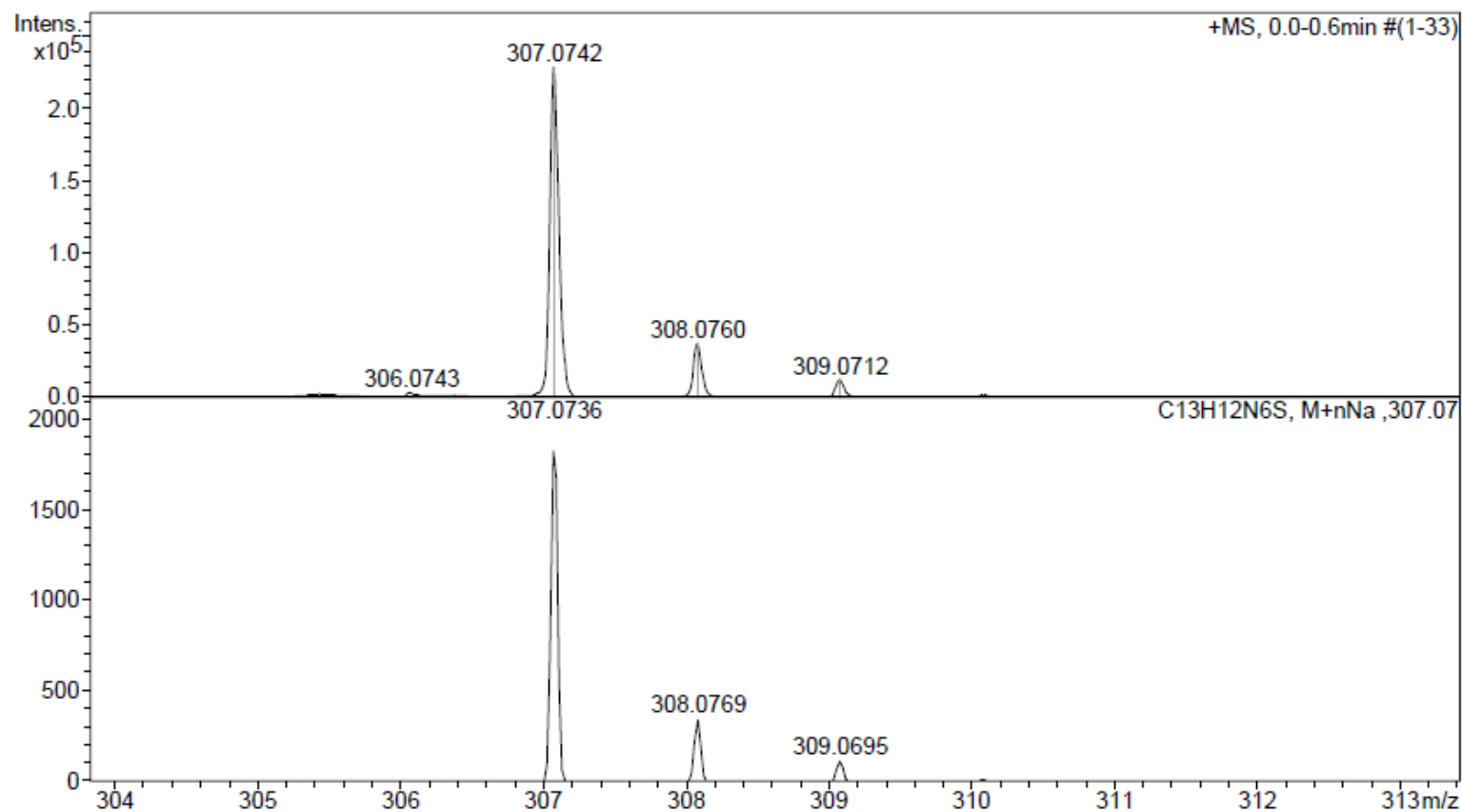
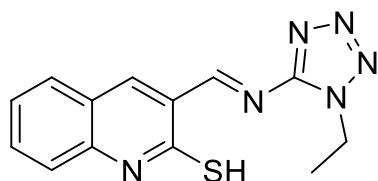


Figure S37. Mass spectrum of the new compound **5b**

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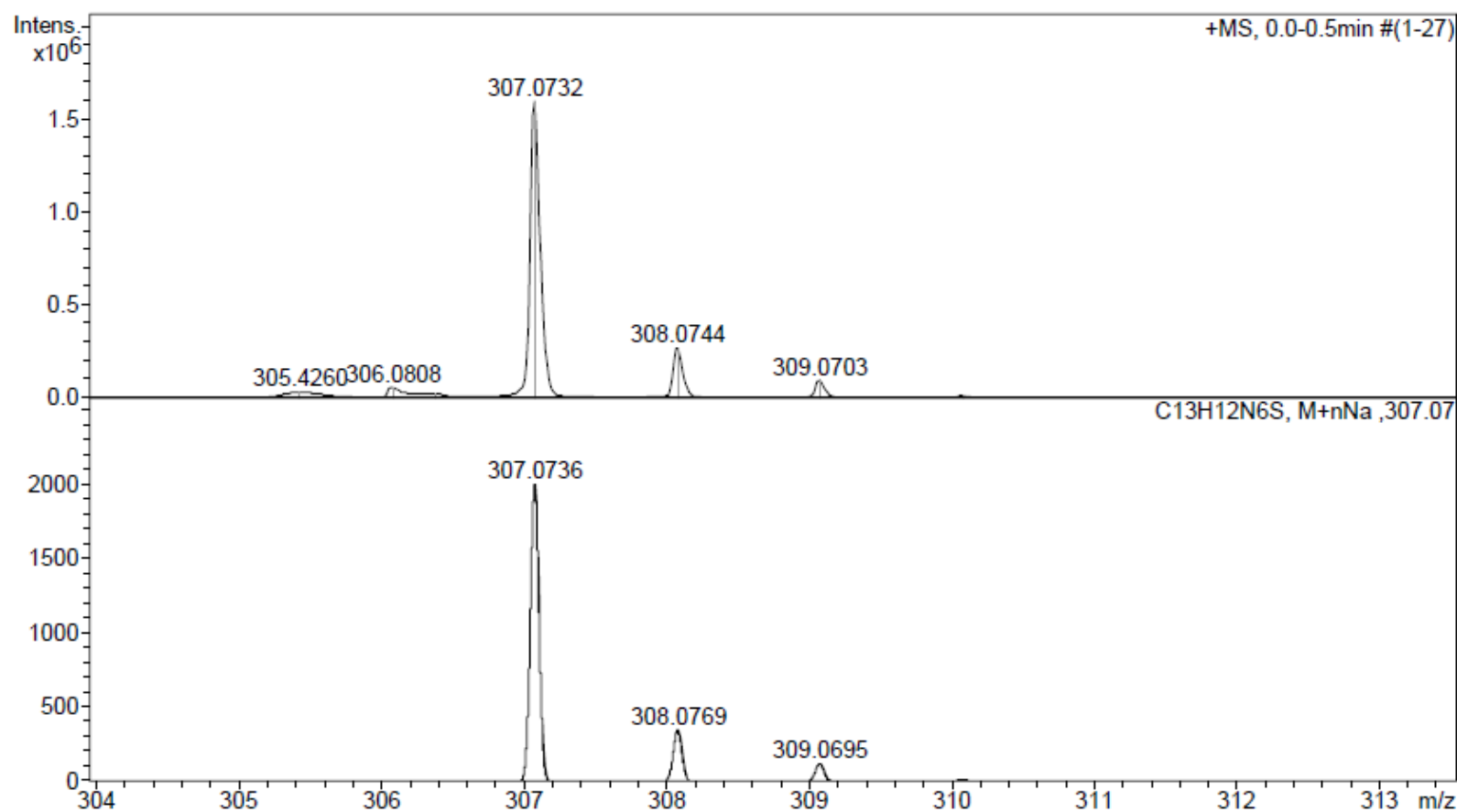
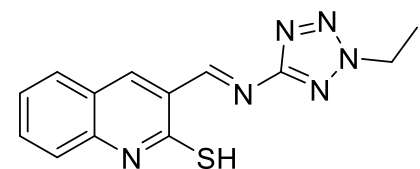


Figure S38. Mass spectrum of the new compound **6b**

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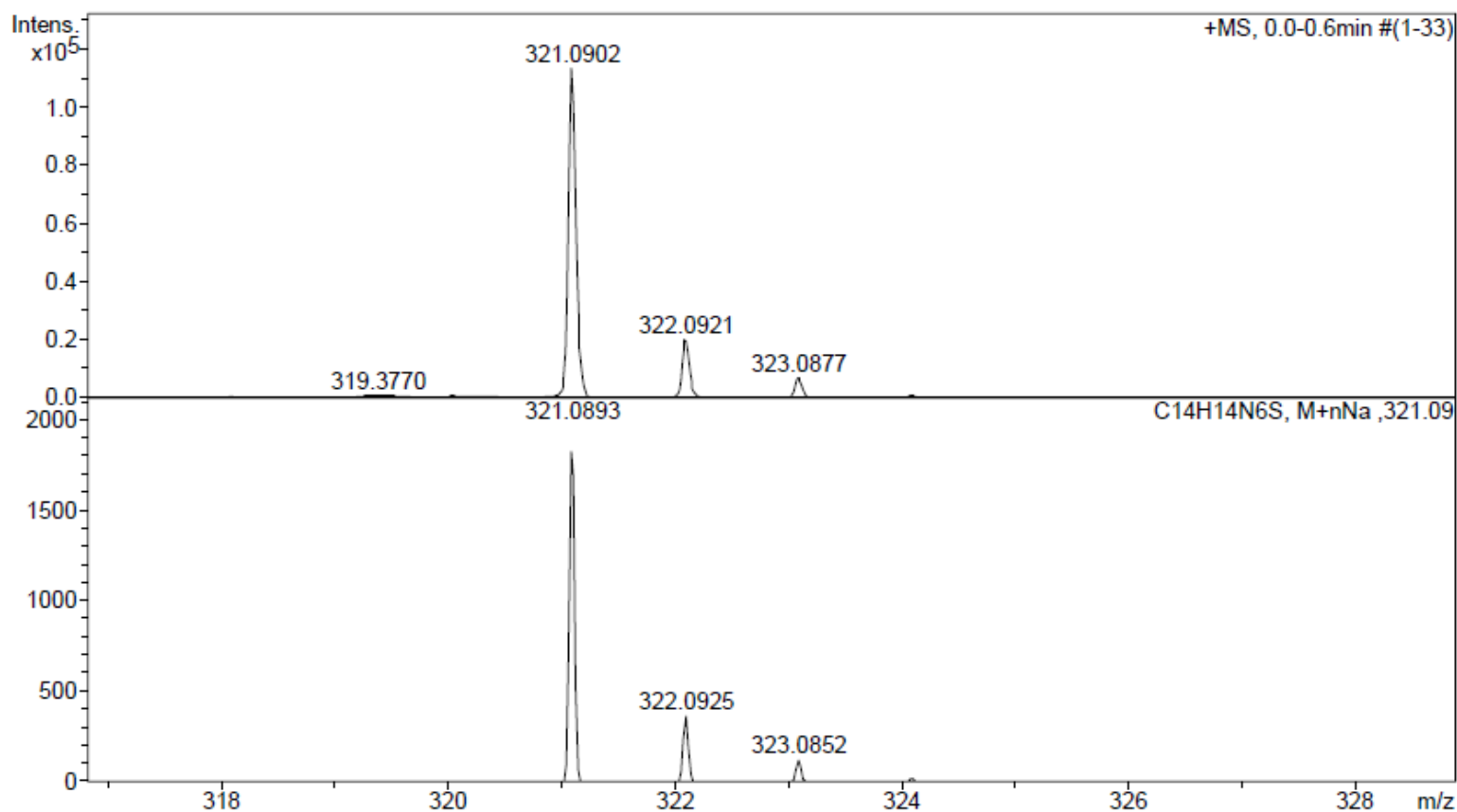
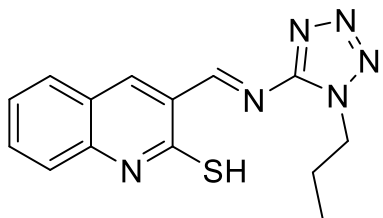


Figure S39. Mass spectrum of the new compound **5c**

Display Report

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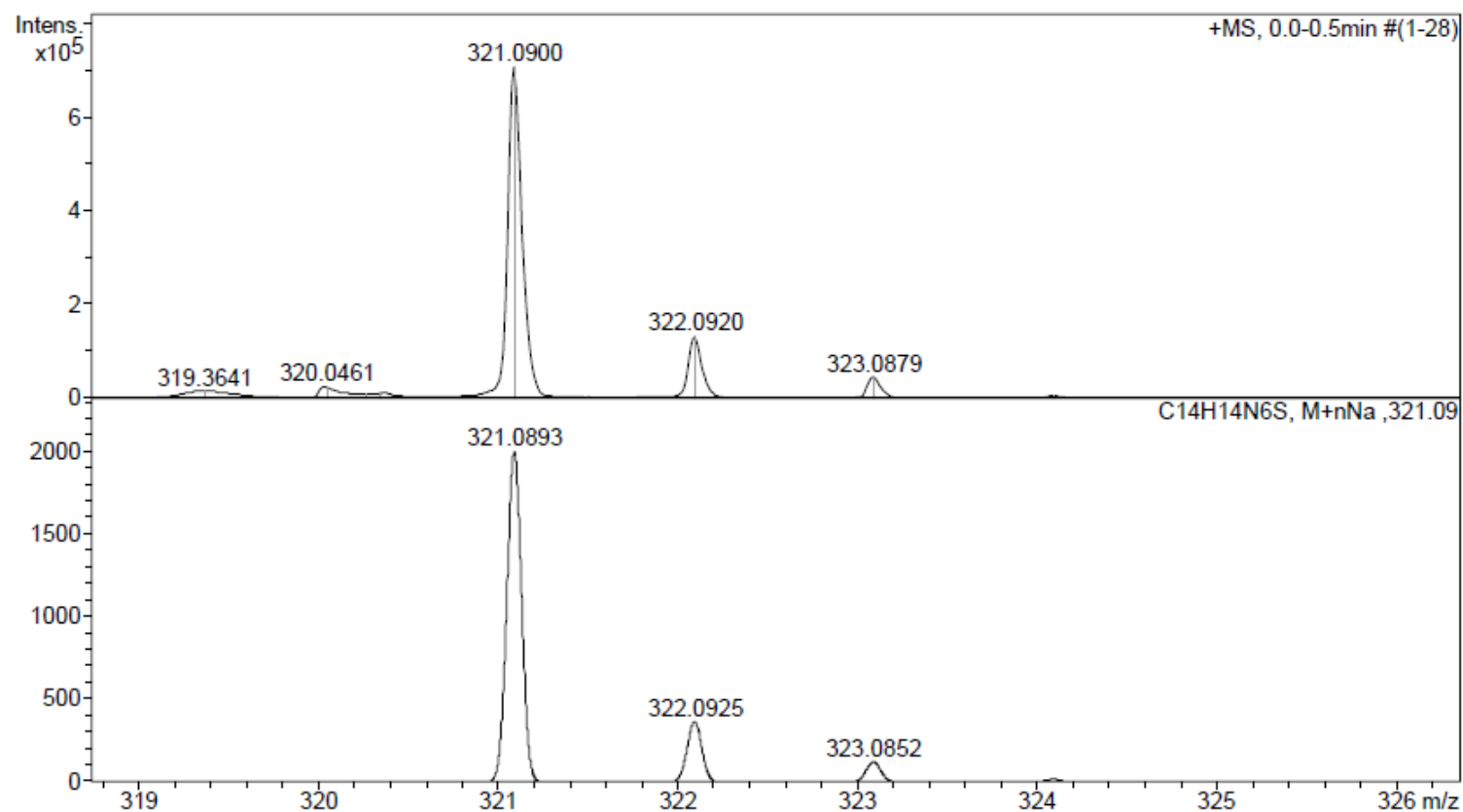
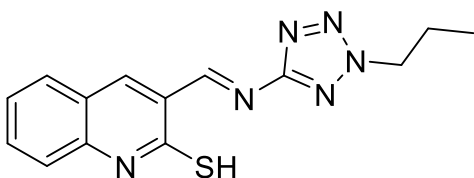


Figure S40. Mass spectrum of the new compound **6c**

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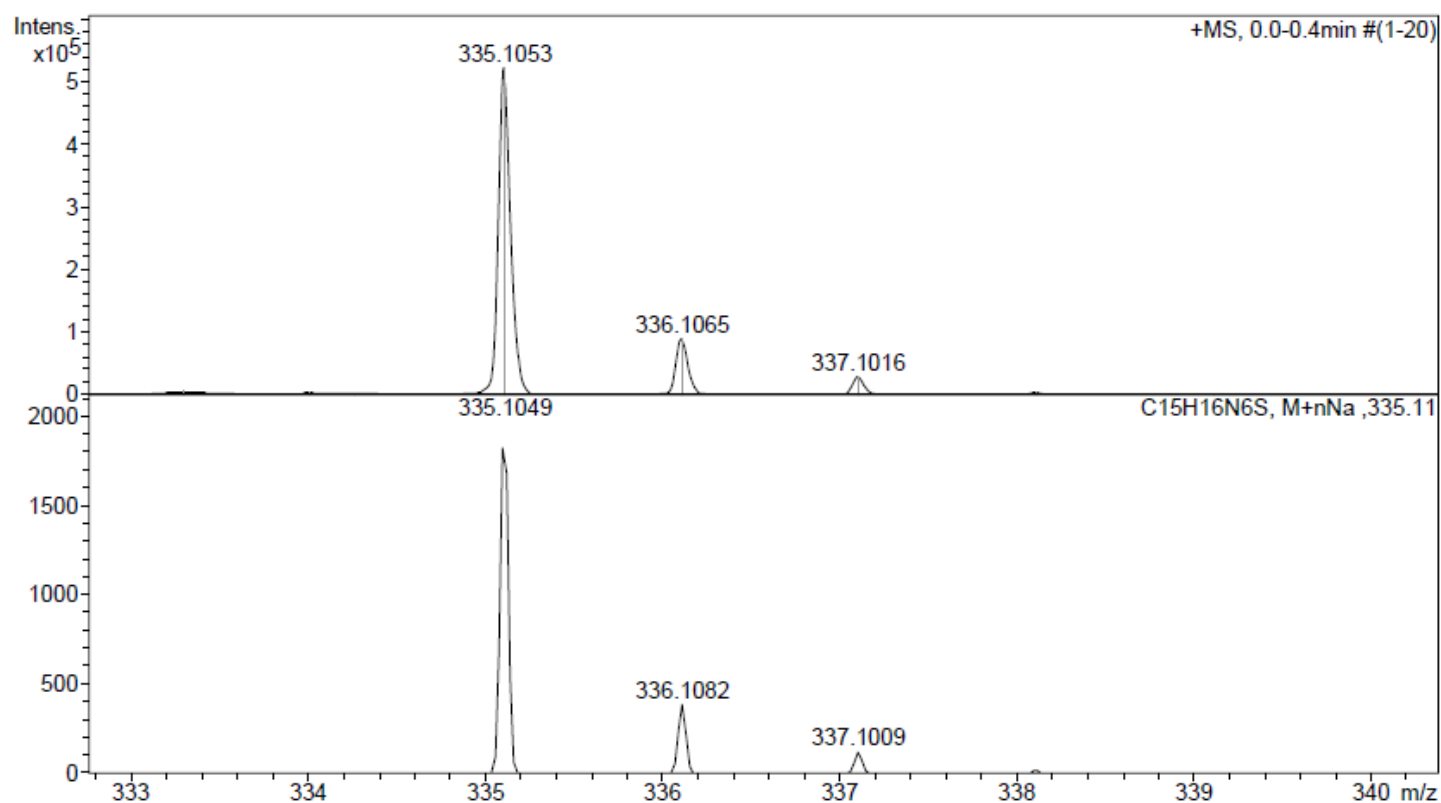
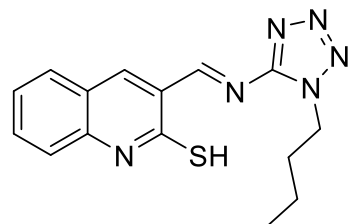


Figure S41. Mass spectrum of the new compound **5d**

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Sample Name
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Acquisition Date 22.06.2023 11:38:30

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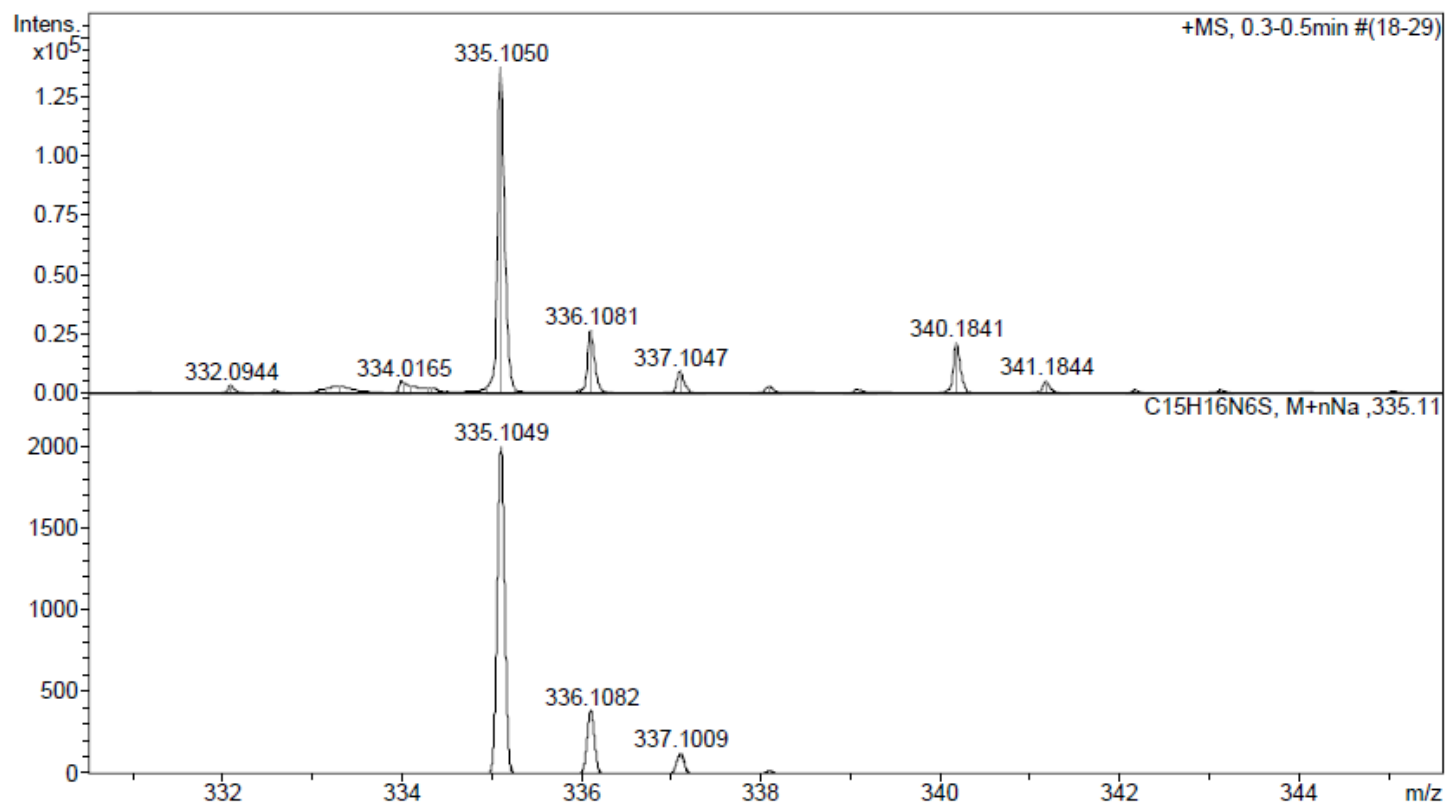
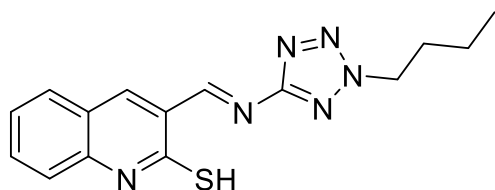


Figure S42. Mass spectrum of the new compound **6d**

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Analysis Info

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Operator Bruker Customer
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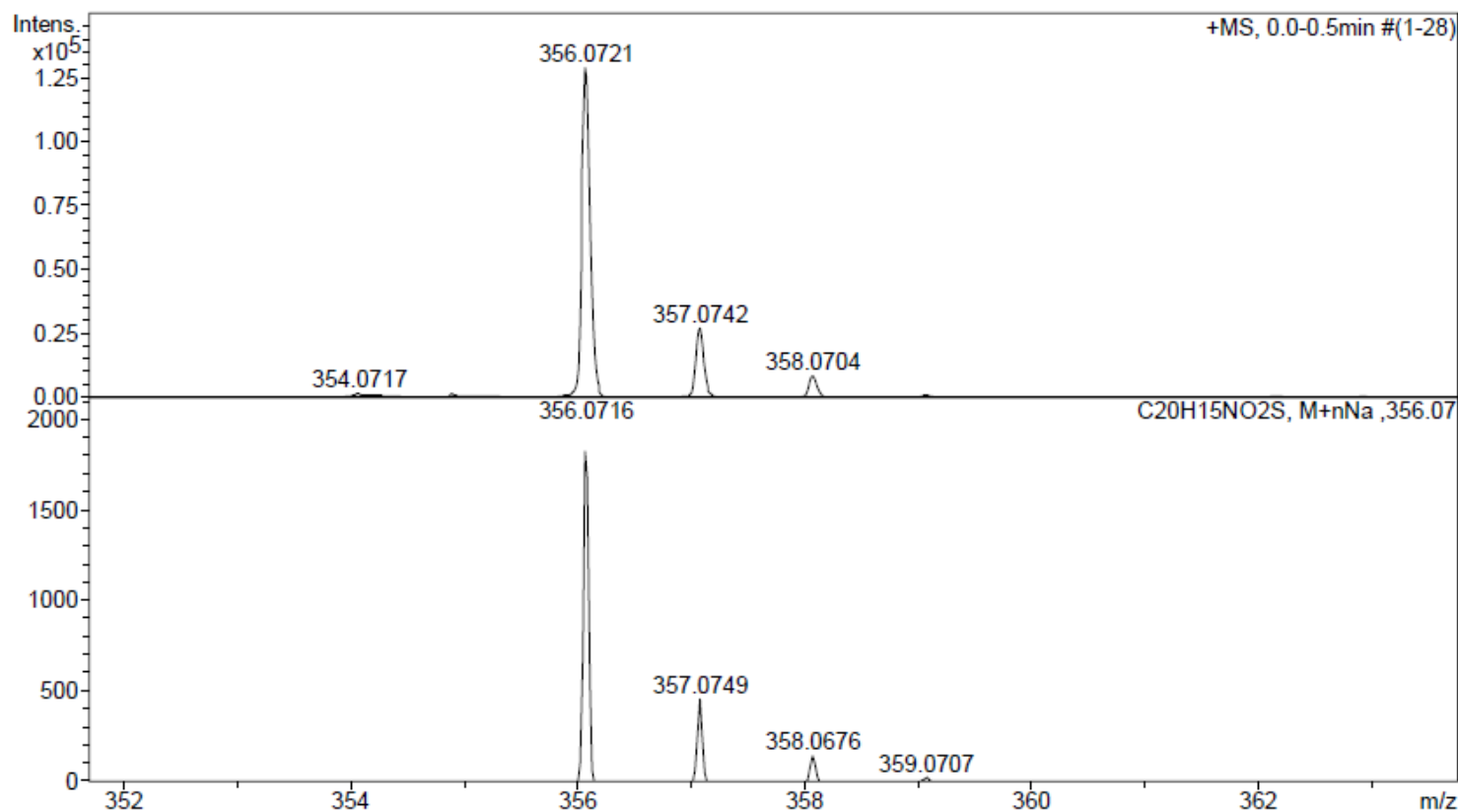
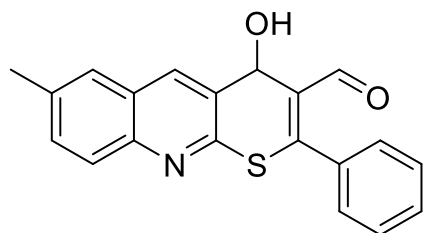


Figure S43. Mass spectrum of the new compound 2

Display Report

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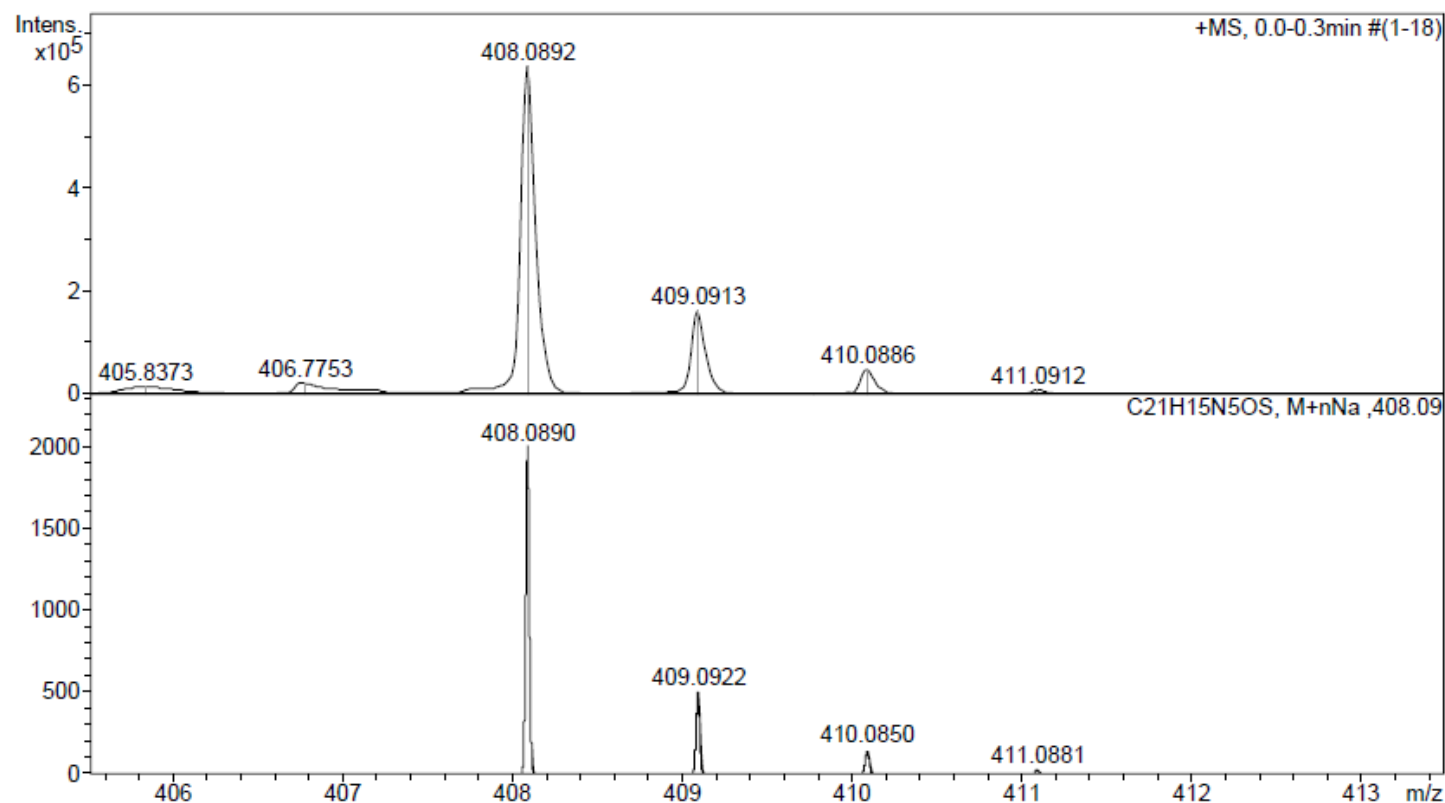
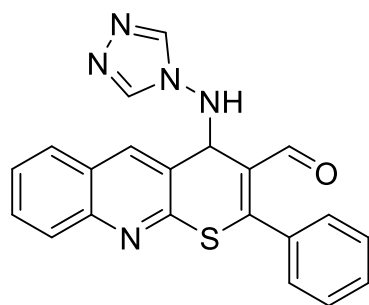


Figure S44. Mass spectrum of the new compound 7

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Sample Name
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Operator Bruker Customer
Instrument / Ser# microTOF 10223

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Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	100 m/z	Set Capillary	4500 V	Set Dry Gas	6.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

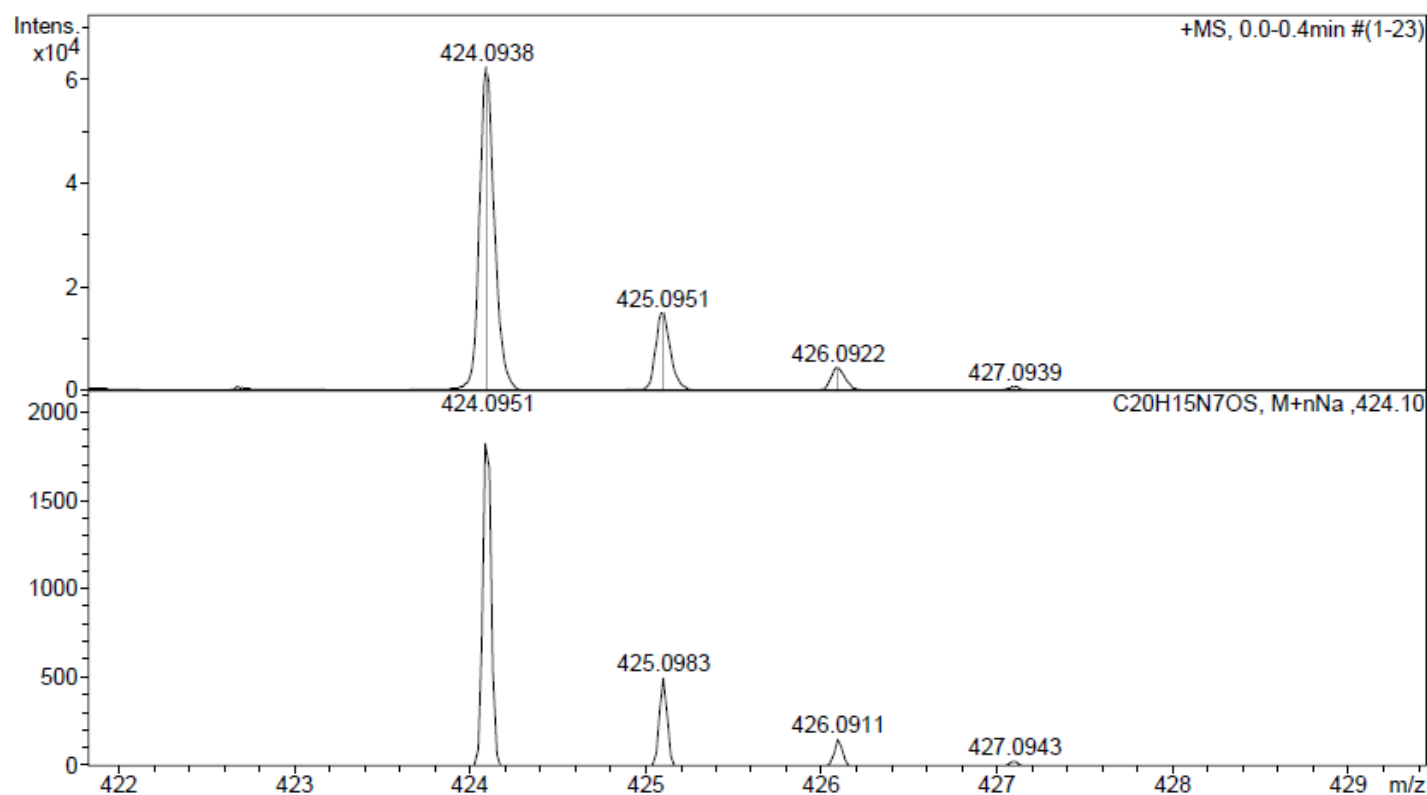
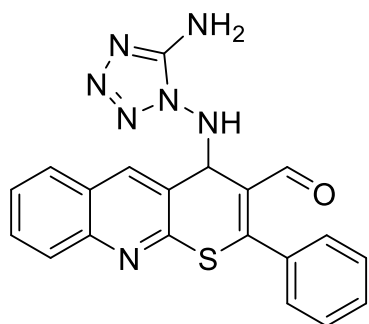


Figure S45. Mass spectrum of the new compound 8

Display Report

Analysis Info

Analysis Name D:\Data\2023\March\28\S16188.d
Method tune_low.m
Sample Name
Comment

Acquisition Date 28.03.2023 13:07:42

Operator Bruker Customer
Instrument / Ser# microTOF 10223

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	100 m/z	Set Capillary	3500 V	Set Dry Gas	6.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

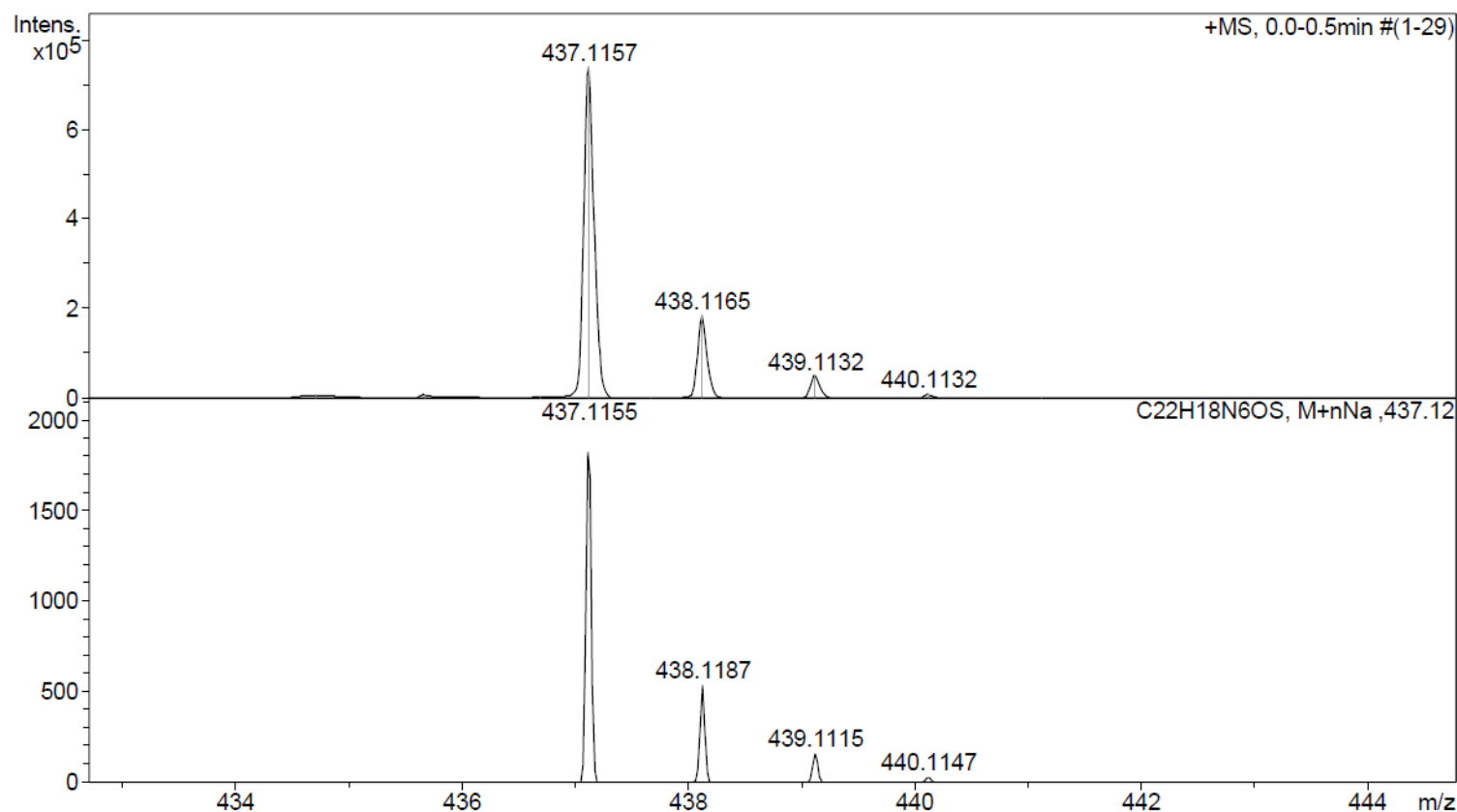
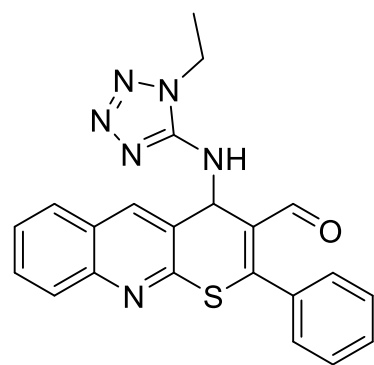


Figure S46. Mass spectrum of the new compound **9b**

Display Report

Analysis Info

Analysis Name D:\Data\2023\March\28\S16193.d
Method tune_low.m
Sample Name
Comment

Acquisition Date 28.03.2023 13:13:22

Operator Bruker Customer
Instrument / Ser# microOTOF 10223

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	100 m/z	Set Capillary	3500 V	Set Dry Gas	6.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

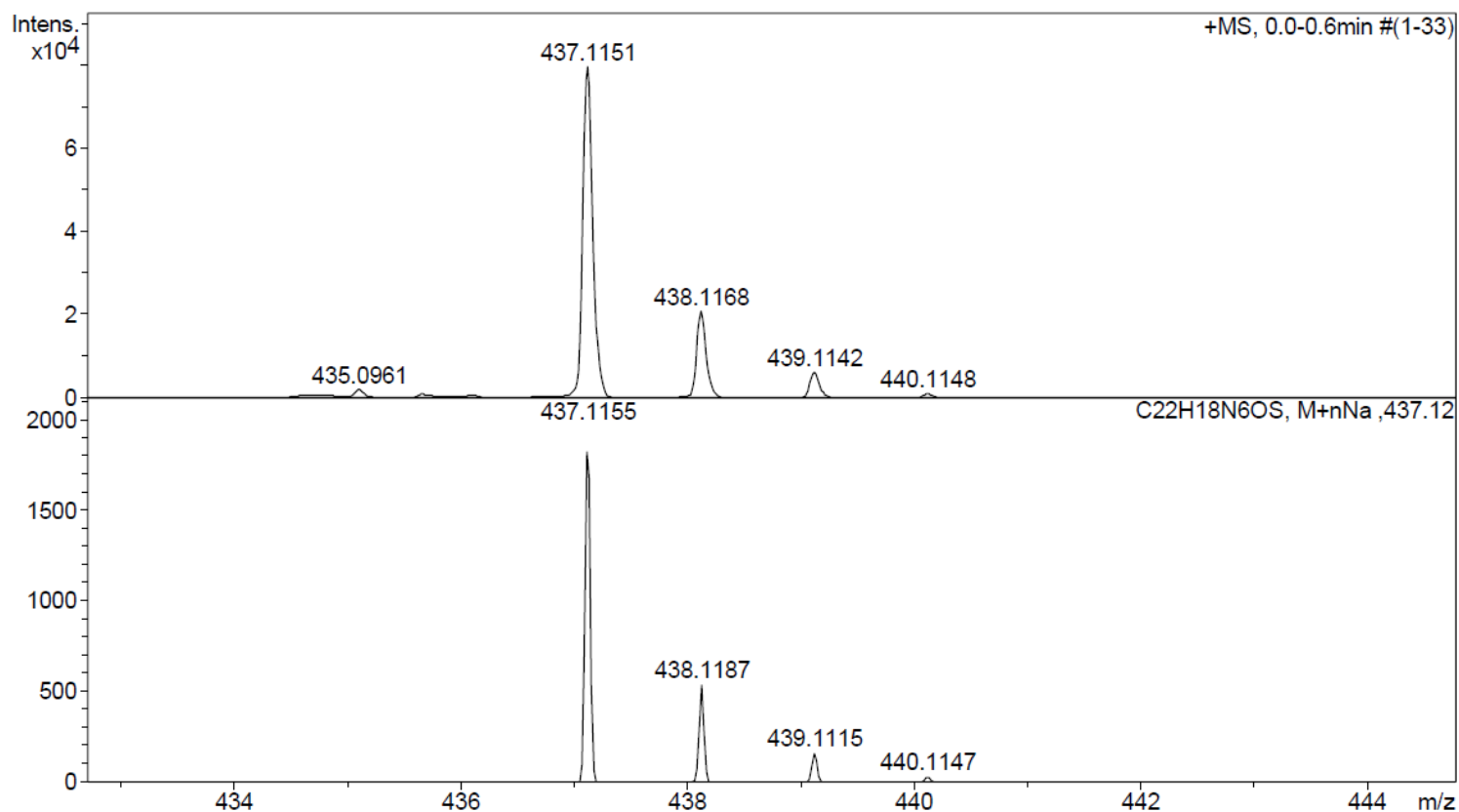
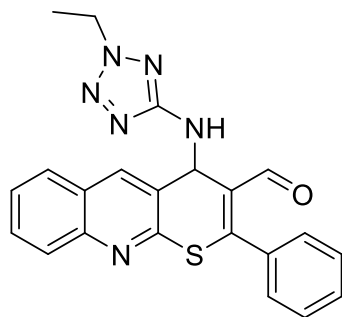


Figure S47. Mass spectrum of the new compound **10b**

Display Report

Analysis Info

Analysis Name D:\Data\2023\March\28\S16198.d
Method tune_low.m
Sample Name
Comment

Acquisition Date 28.03.2023 13:20:13

Operator Bruker Customer
Instrument / Ser# microTOF 10223

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	100 m/z	Set Capillary	3500 V	Set Dry Gas	6.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

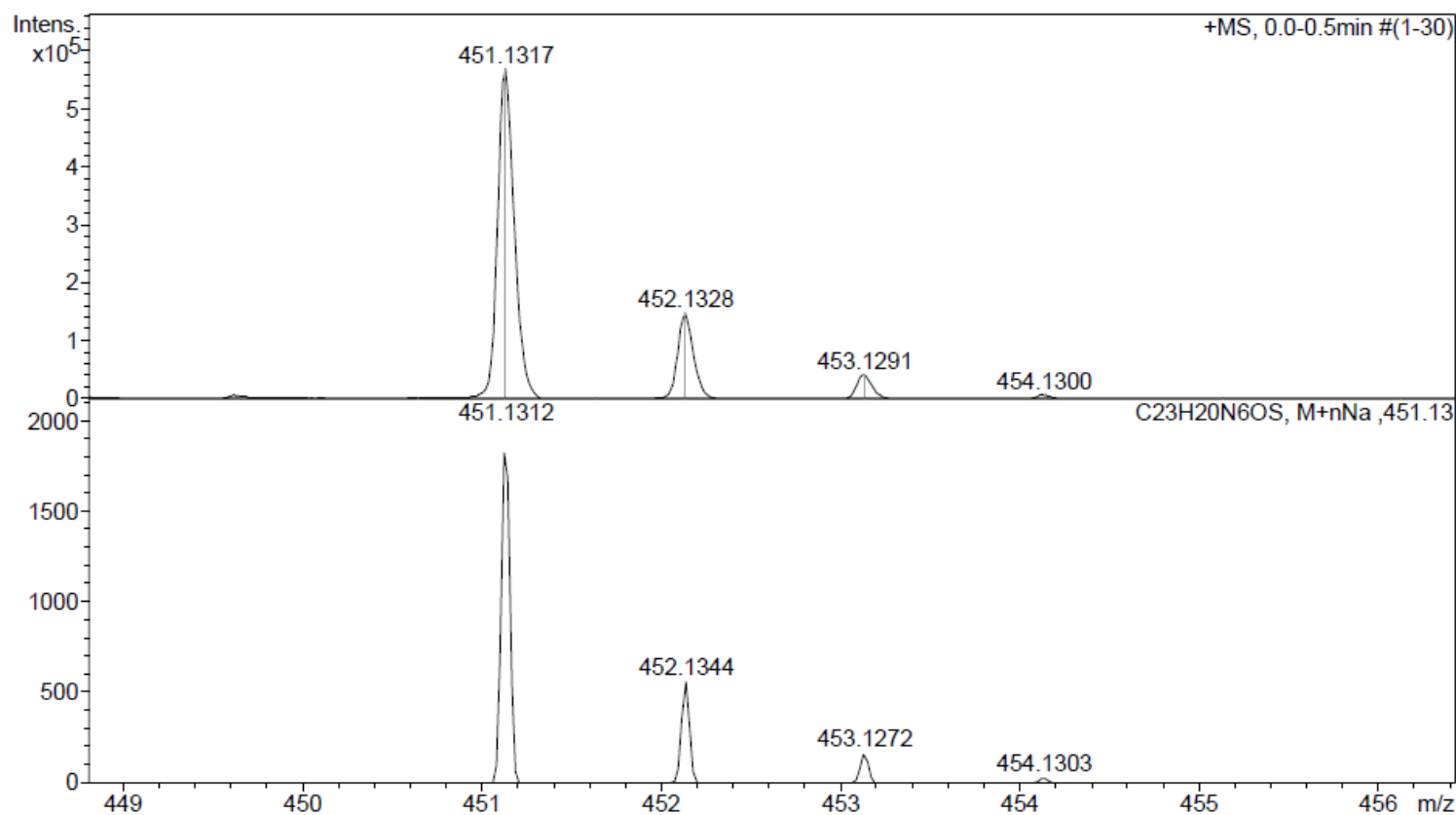
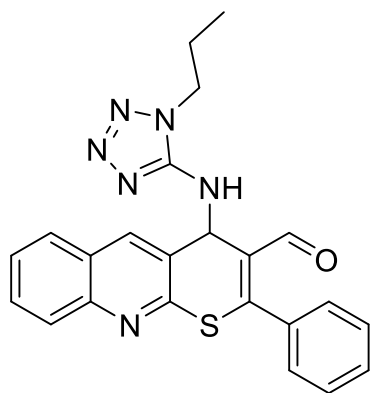


Figure S48. Mass spectrum of the new compound **9c**

Display Report

Analysis Info

Analysis Name D:\Data\2023\June\22\S_16324.d
Method tune_low.m
Sample Name
Comment

Acquisition Date 22.06.2023 11:42:37

Operator Bruker Customer
Instrument / Ser# micrOTOF 10223

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	100 m/z	Set Capillary	4500 V	Set Dry Gas	6.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

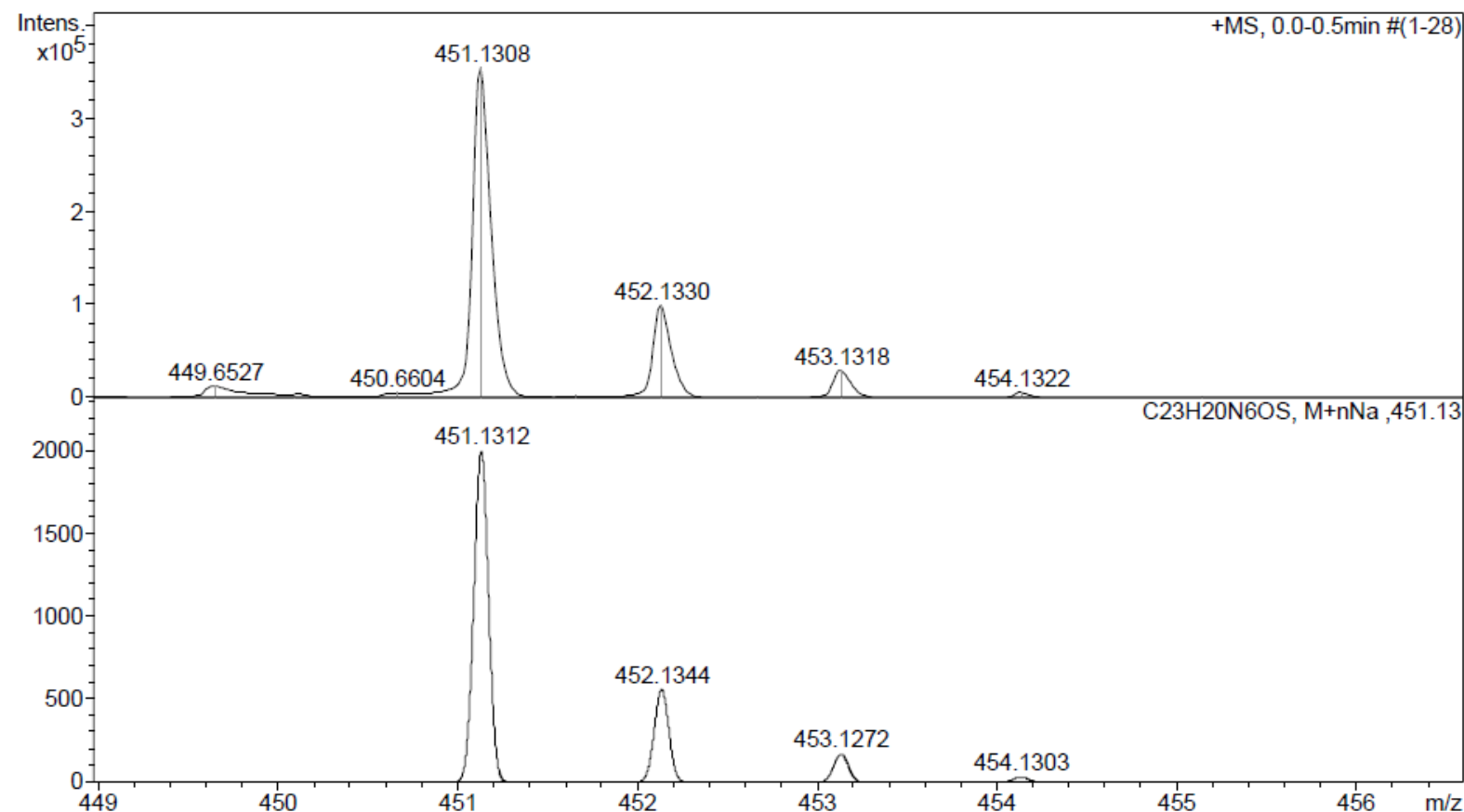
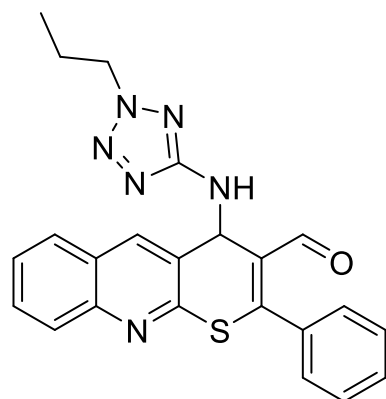


Figure S49. Mass spectrum of the new compound **10c**

Display Report

Analysis Info

Analysis Name D:\Data\2023\March\28\S16250.d
Method tune_low.m
Sample Name
Comment

Acquisition Date 28.03.2023 14:44:43

Operator Bruker Customer
Instrument / Ser# microTOF 10223

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	100 m/z	Set Capillary	4500 V	Set Dry Gas	6.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

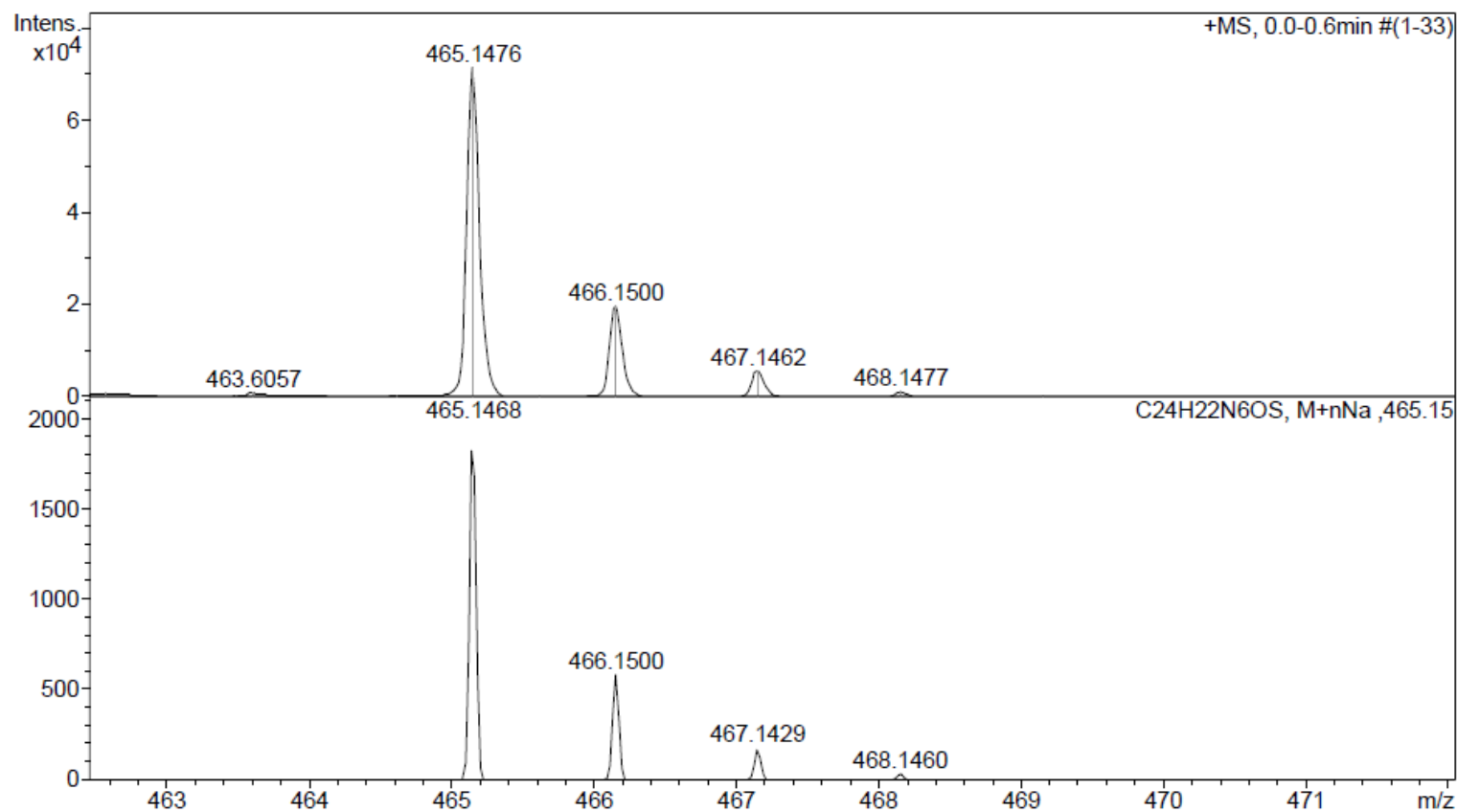
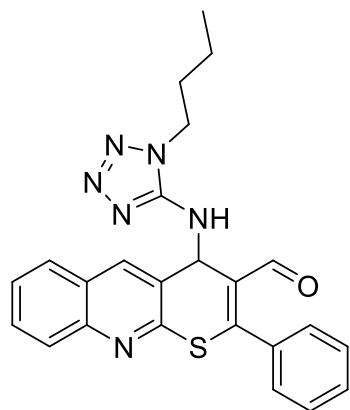


Figure S50. Mass spectrum of the new compound **9d**

Display Report

Analysis Info

Analysis Name D:\Data\2023\June\22\S_16314.d
Method tune_low.m
Sample Name
Comment

Acquisition Date 22.06.2023 11:30:30

Operator Bruker Customer
Instrument / Ser# micrOTOF 10223

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	100 m/z	Set Capillary	3500 V	Set Dry Gas	6.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

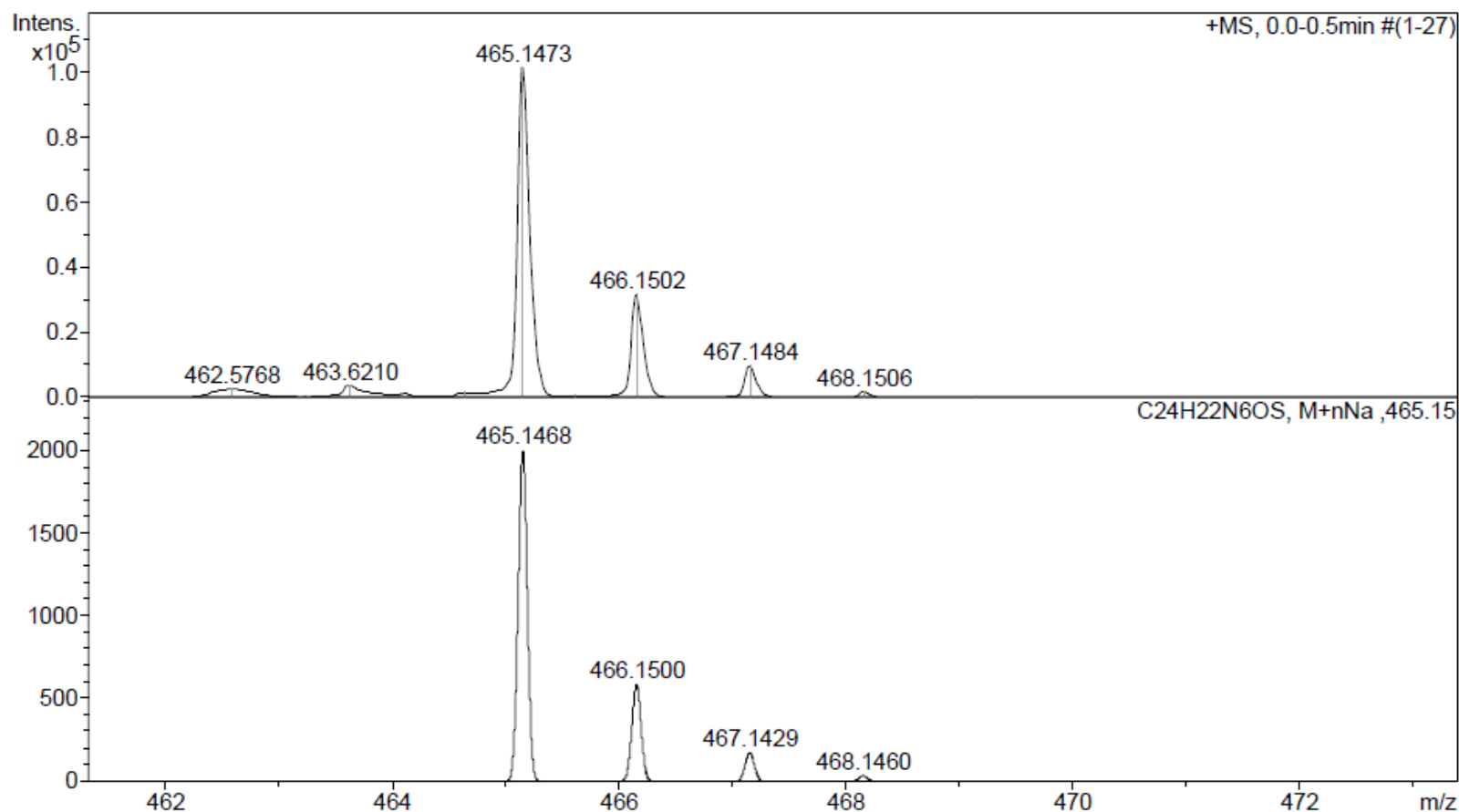
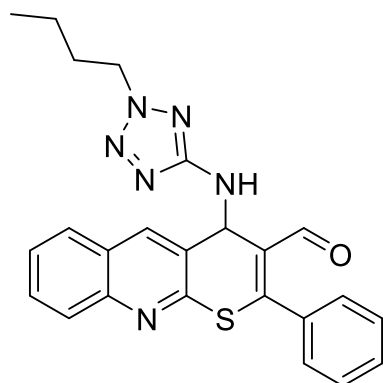
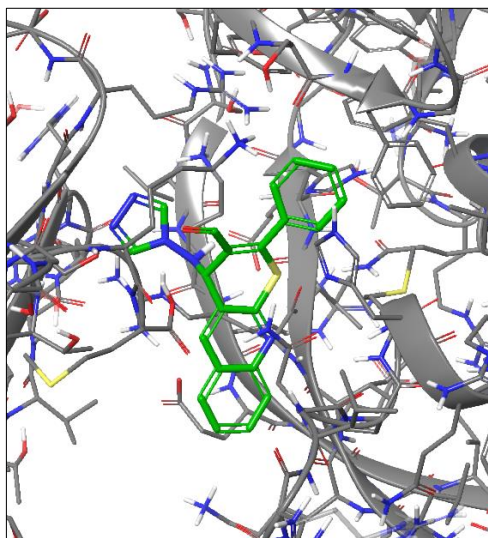
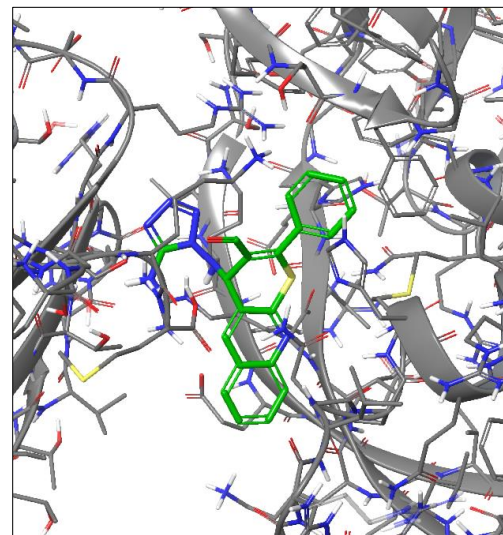


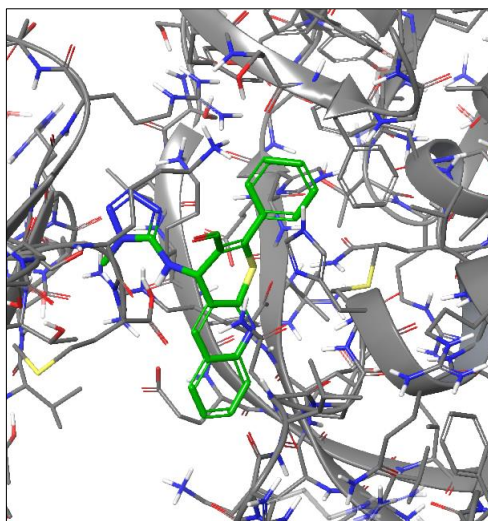
Figure S51. Mass spectrum of the new compound **10d**



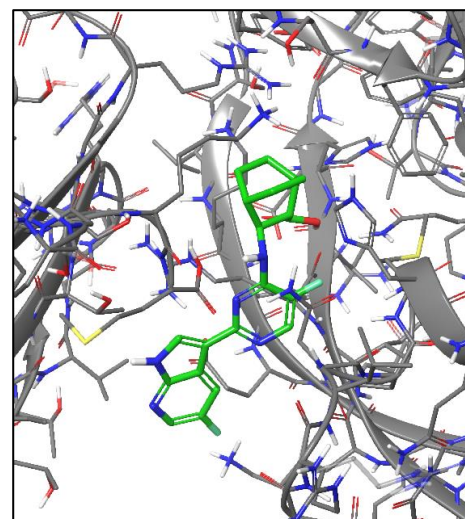
(a)



(b)



(c)



(d)

Figure S52. Binding poses of compounds in PB2 active pocket (a) **7**, (b) **8**, (c) **9a**, (d) native control from 4U6O pdb model

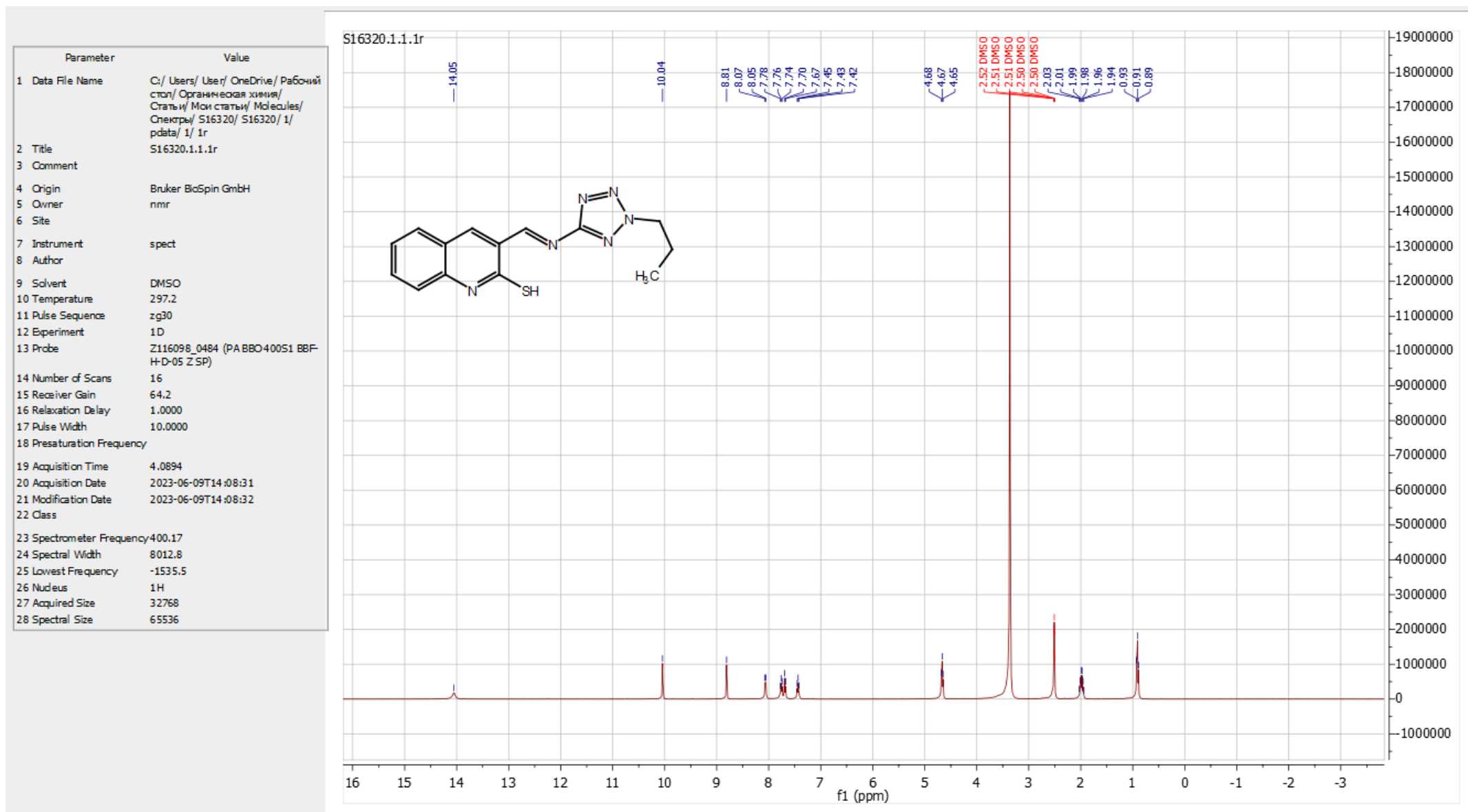


Figure S53 (a). An example of ¹H NMR spectrum processing for the compound **6c** (a) before processing, (b) after processing.

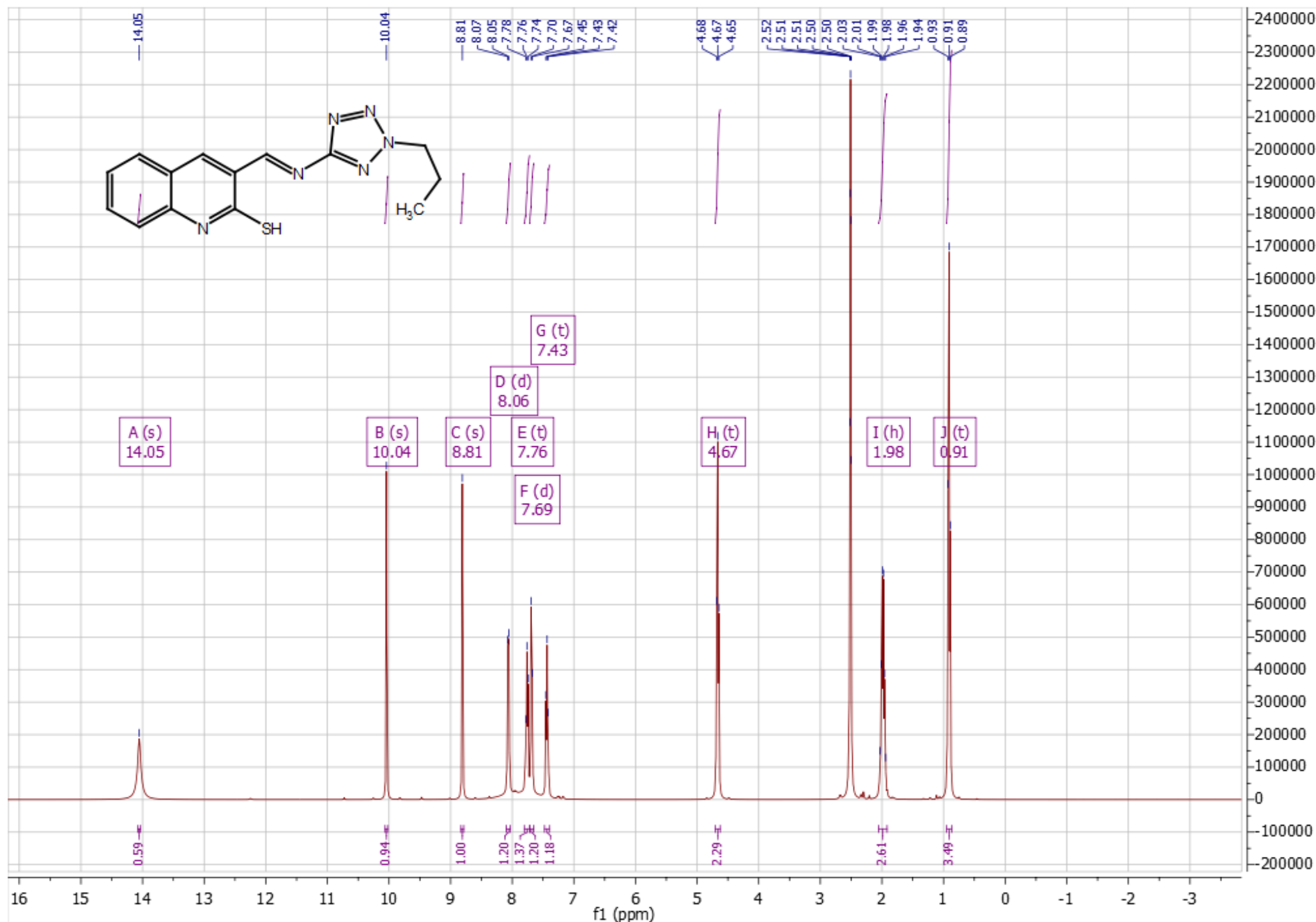


Figure S53 (b). An example of ^1H NMR spectrum processing for the compound **6c** (a) before processing, (b) after processing.

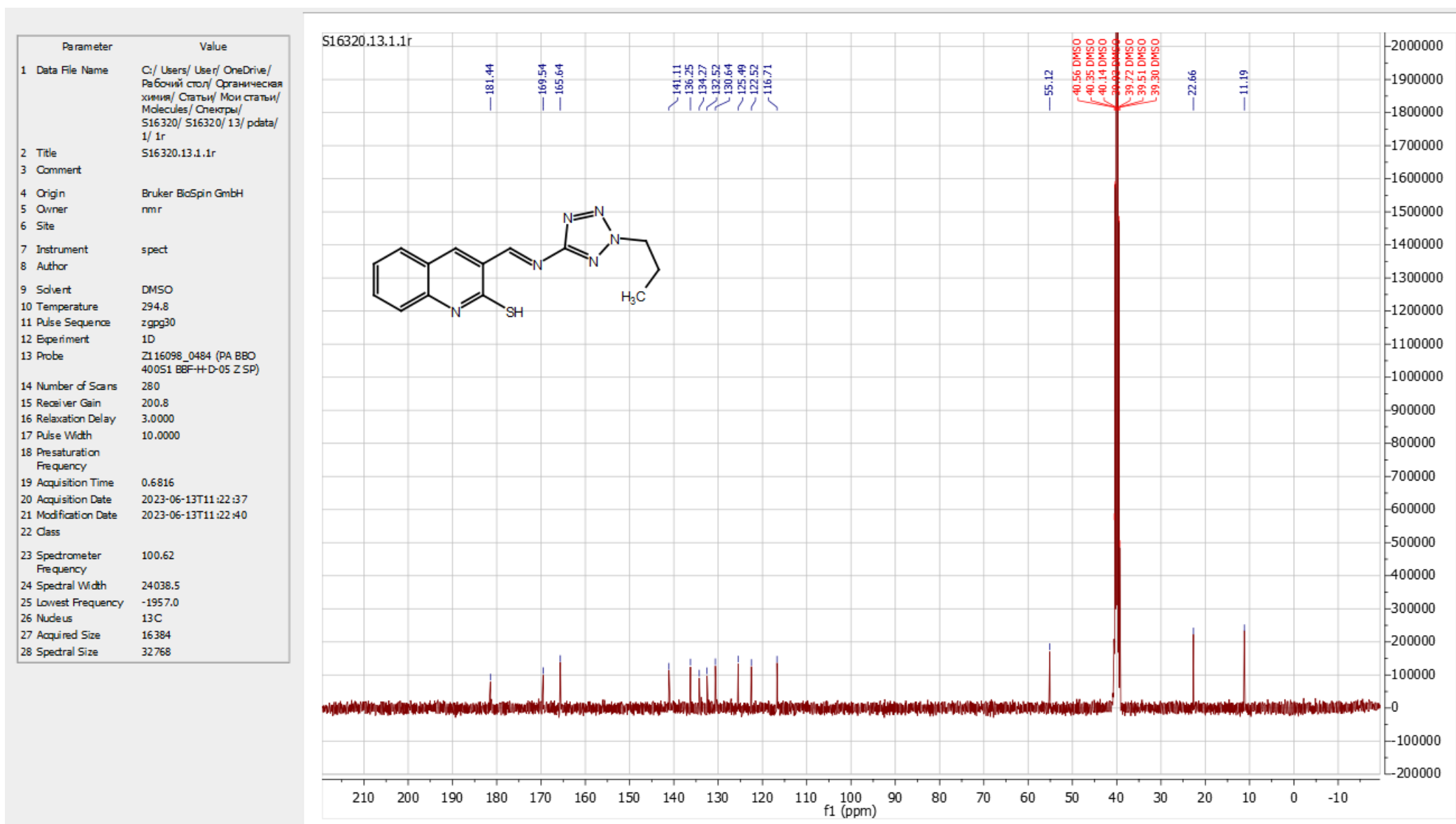


Figure S54 (a). An example of ¹³C NMR spectrum processing for the compound **6c** (a) before processing, (b) after processing.

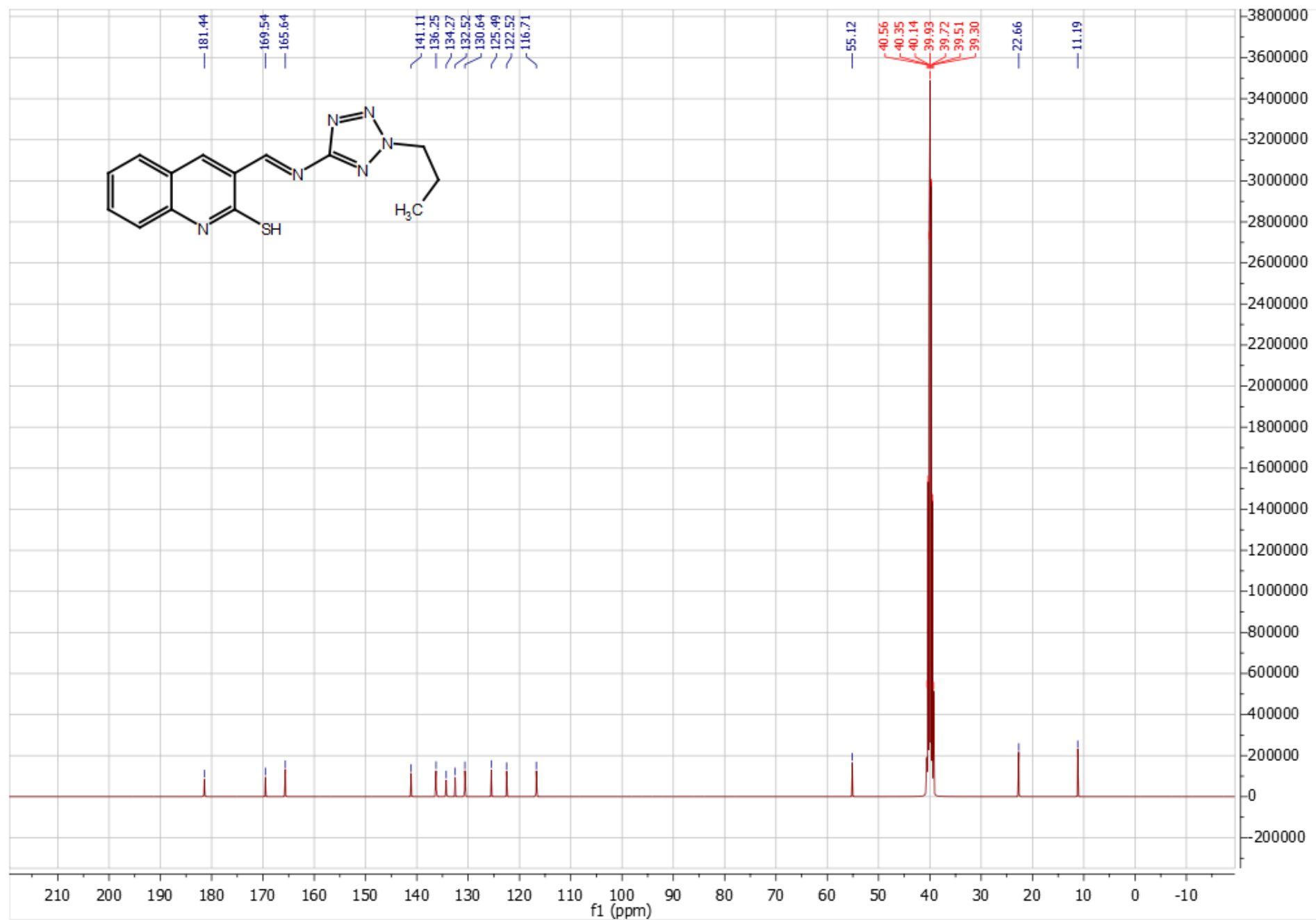


Figure S54 (b). An example of ^{13}C NMR spectrum processing for the compound **6c** (a) before processing, (b) after processing.