

Supplementary Information

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- Figure S56** ^{13}C NMR spectrum of compound **8** in CDCl_3
- Table S1** NMR spectroscopic data for compounds **6–8** in CDCl_3

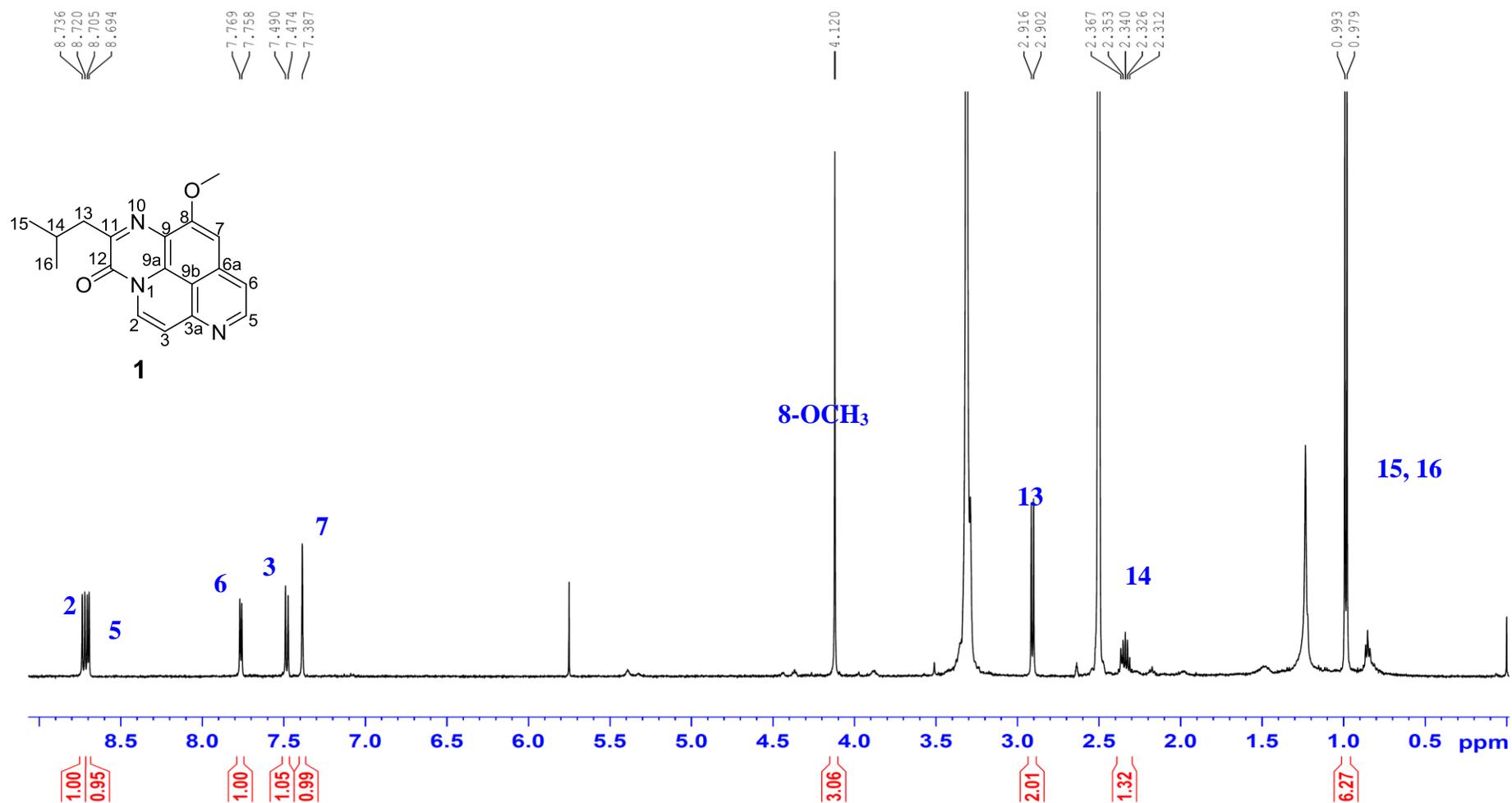
Figure S1. ¹H NMR spectrum of compound 1 in DMSO-*d*₆.

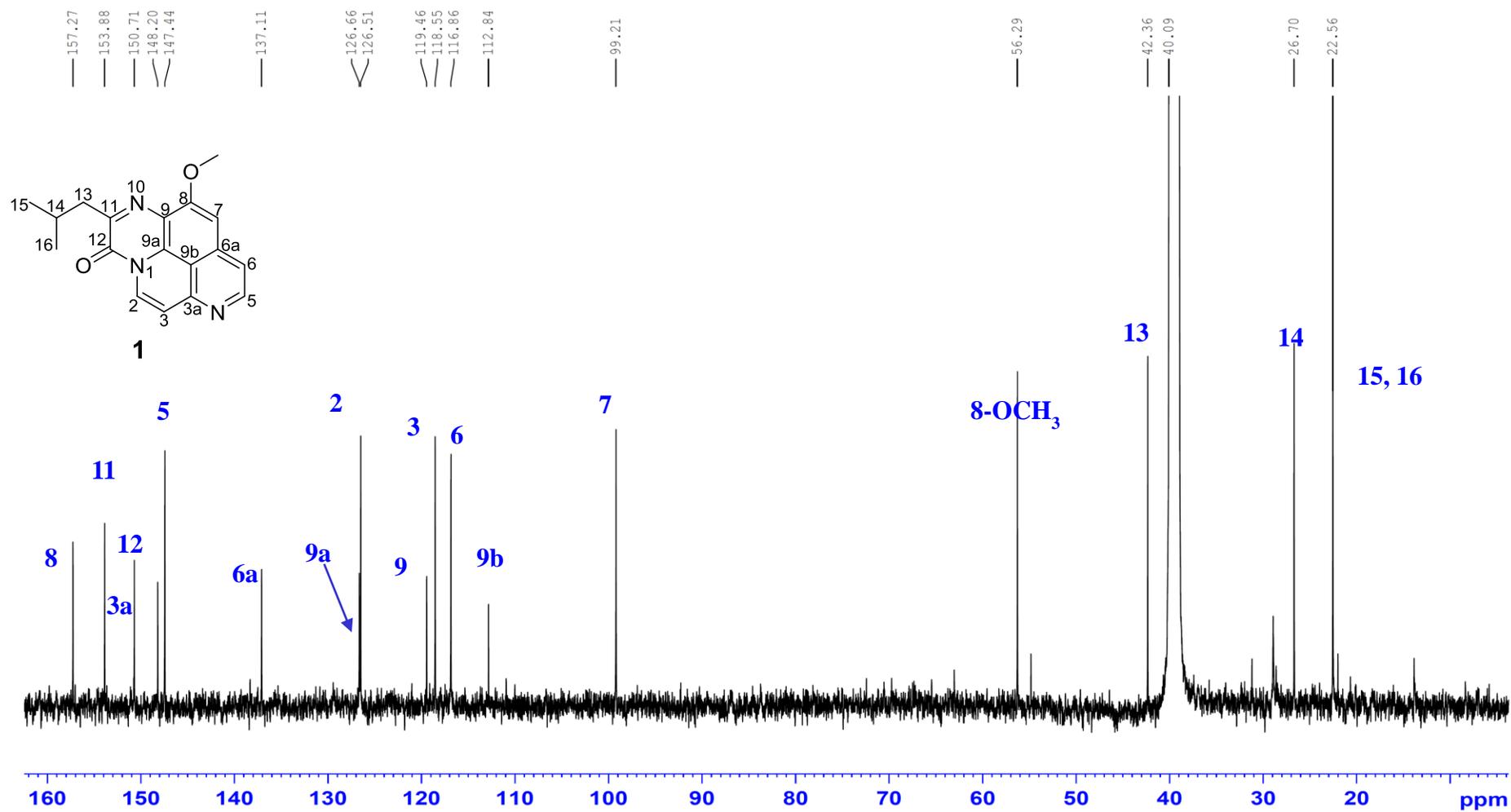
Figure S2. ^{13}C NMR spectrum of compound 1 in $\text{DMSO-}d_6$.

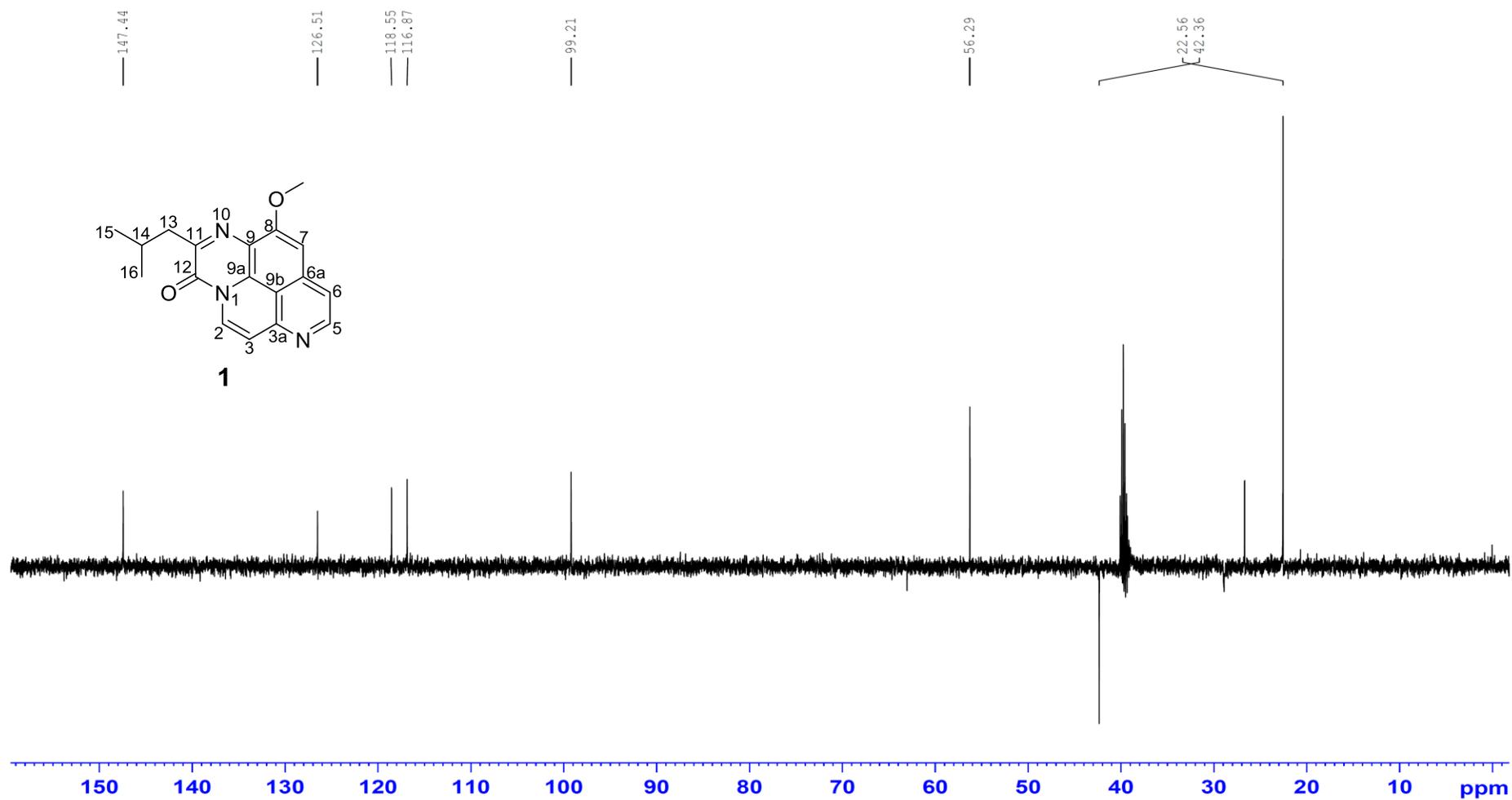
Figure S3. DEPT135 Spectrum of compound 1 in DMSO-*d*₆.

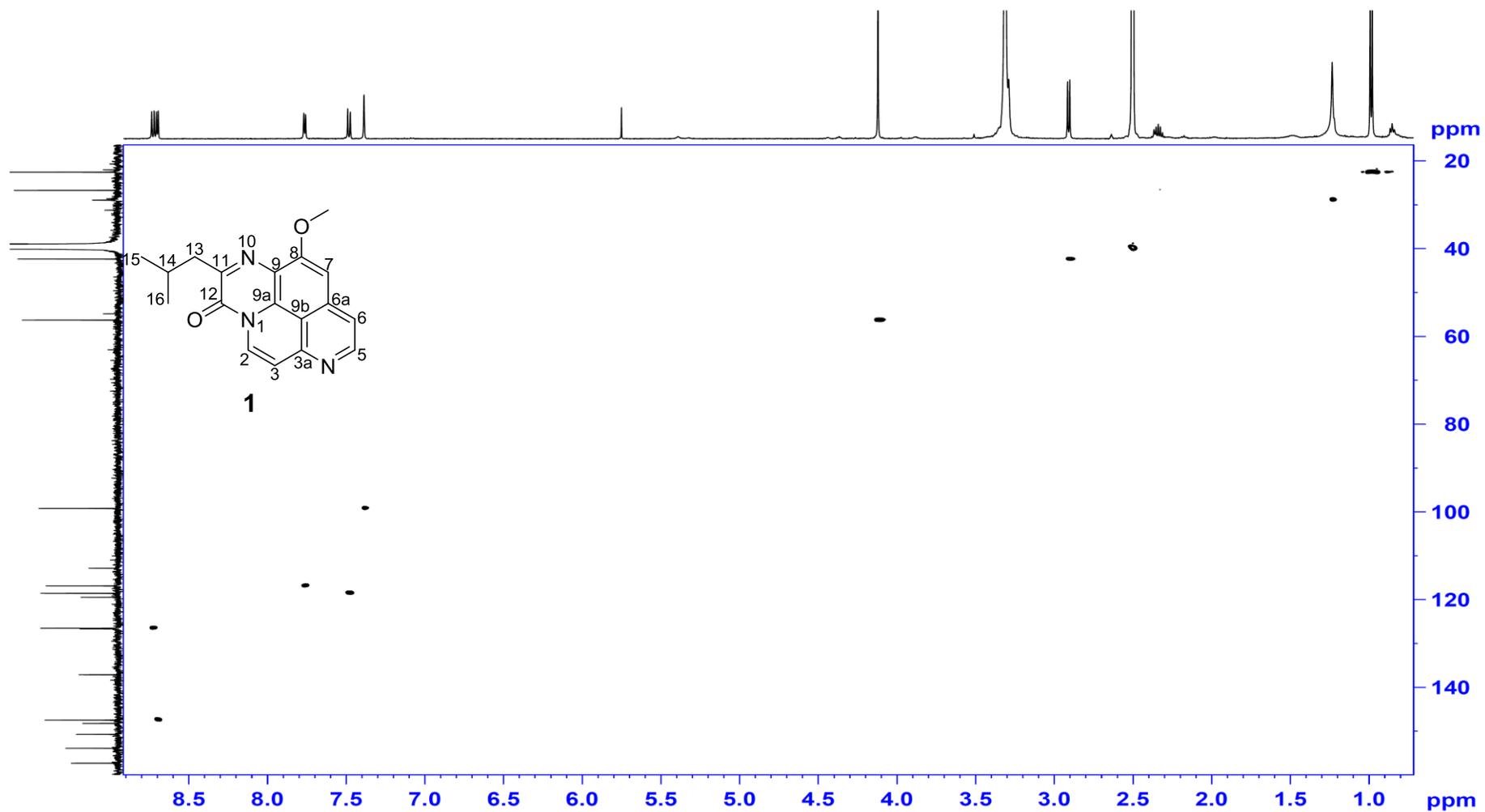
Figure S4. HSQC spectrum of compound 1 in DMSO-*d*₆.

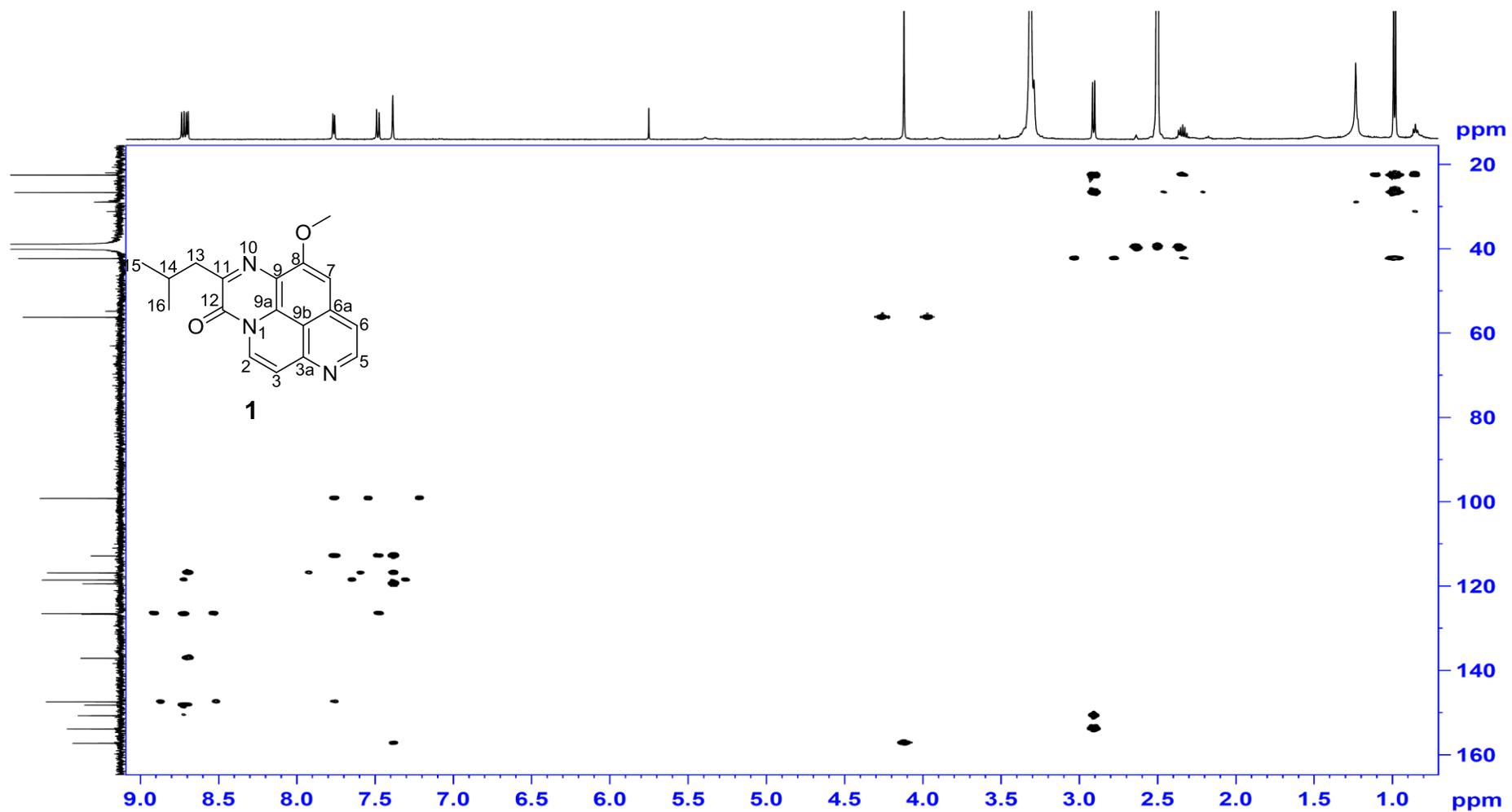
Figure S5. HMBC spectrum of compound 1 in DMSO-*d*₆.

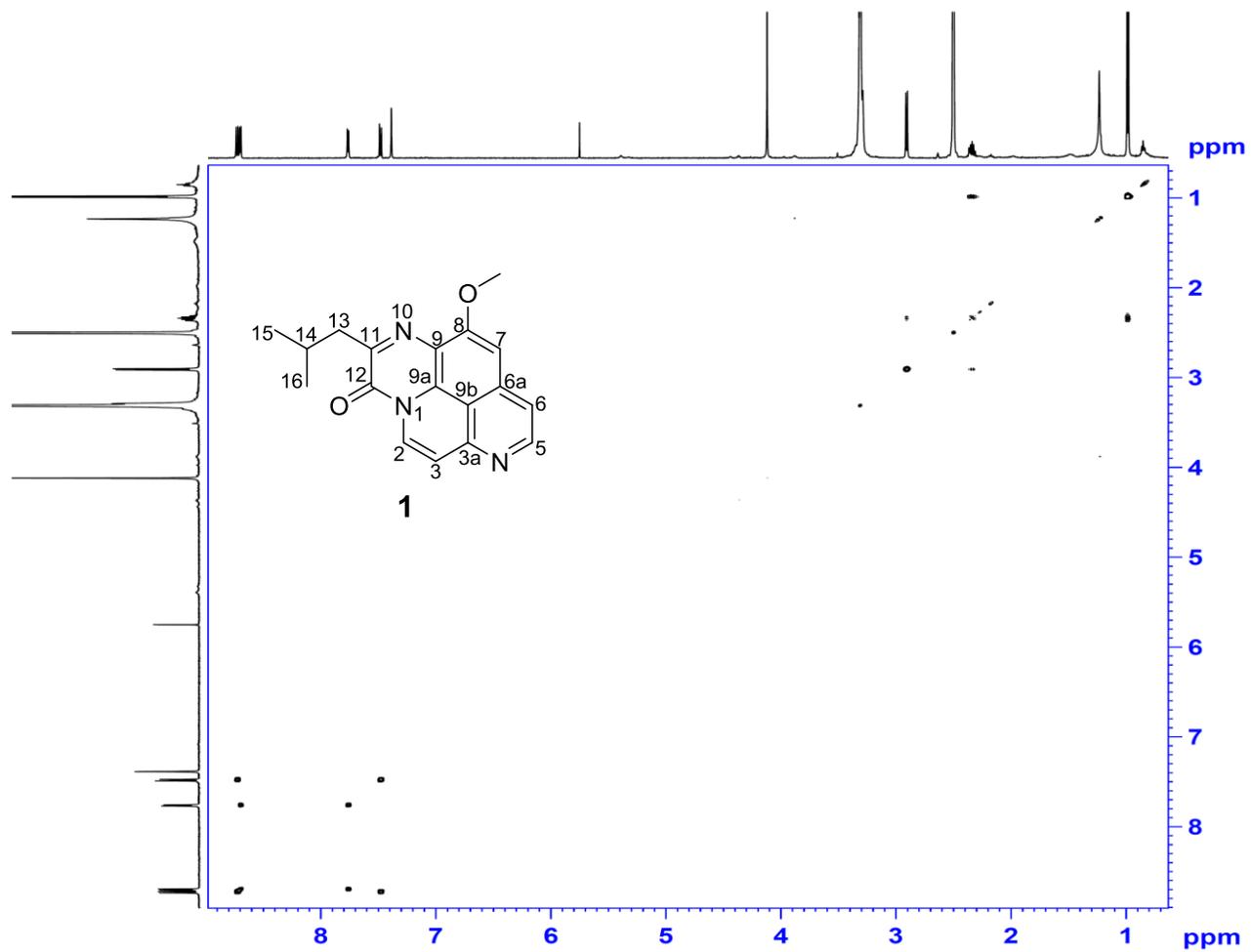
Figure S6. ^1H - ^1H COSY spectrum of compound **1** in $\text{DMSO-}d_6$.

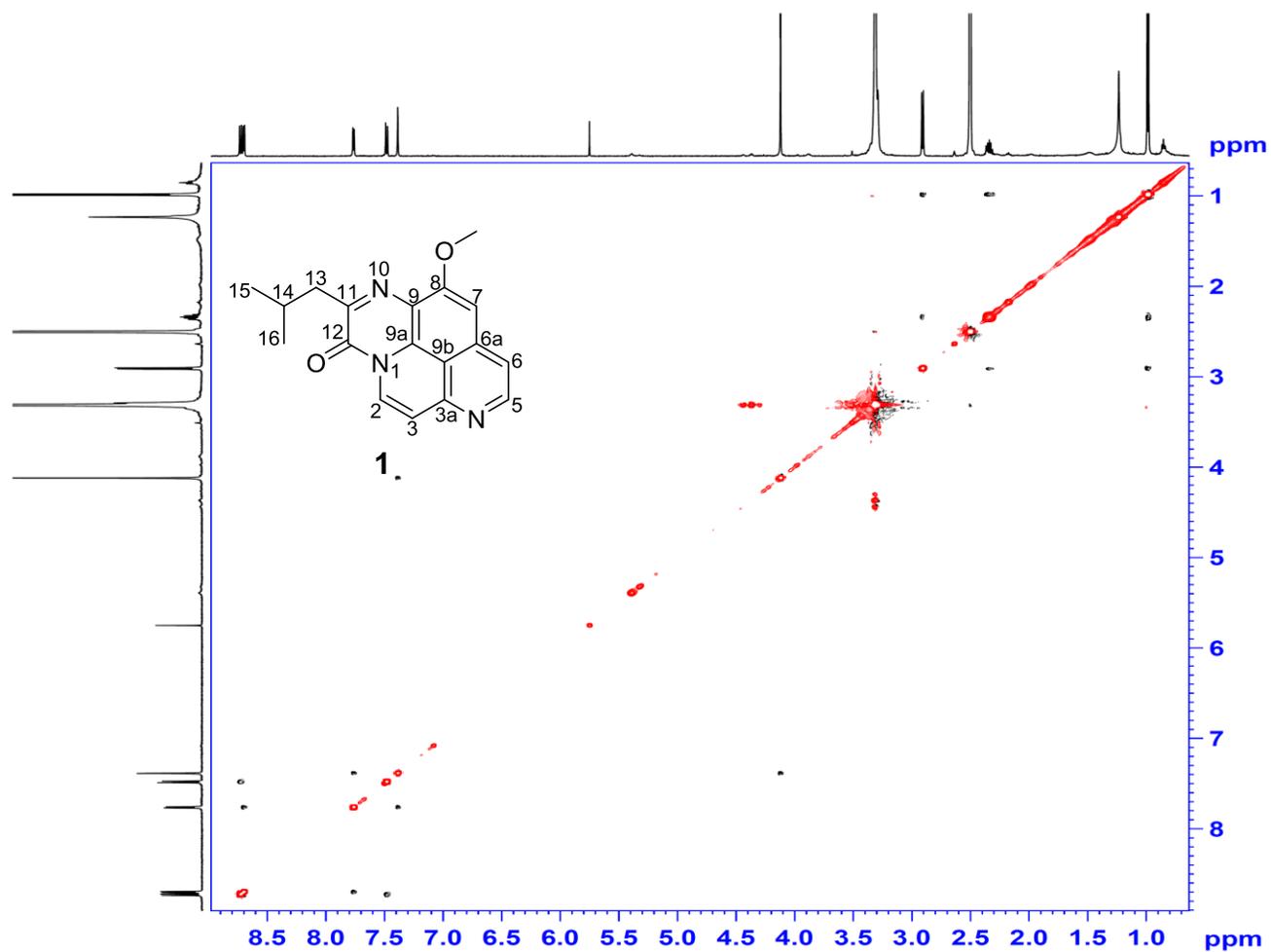
Figure S7. NOESY spectrum of compound 1 in DMSO-*d*₆.

Figure S8. IR spectrum of compound 1.

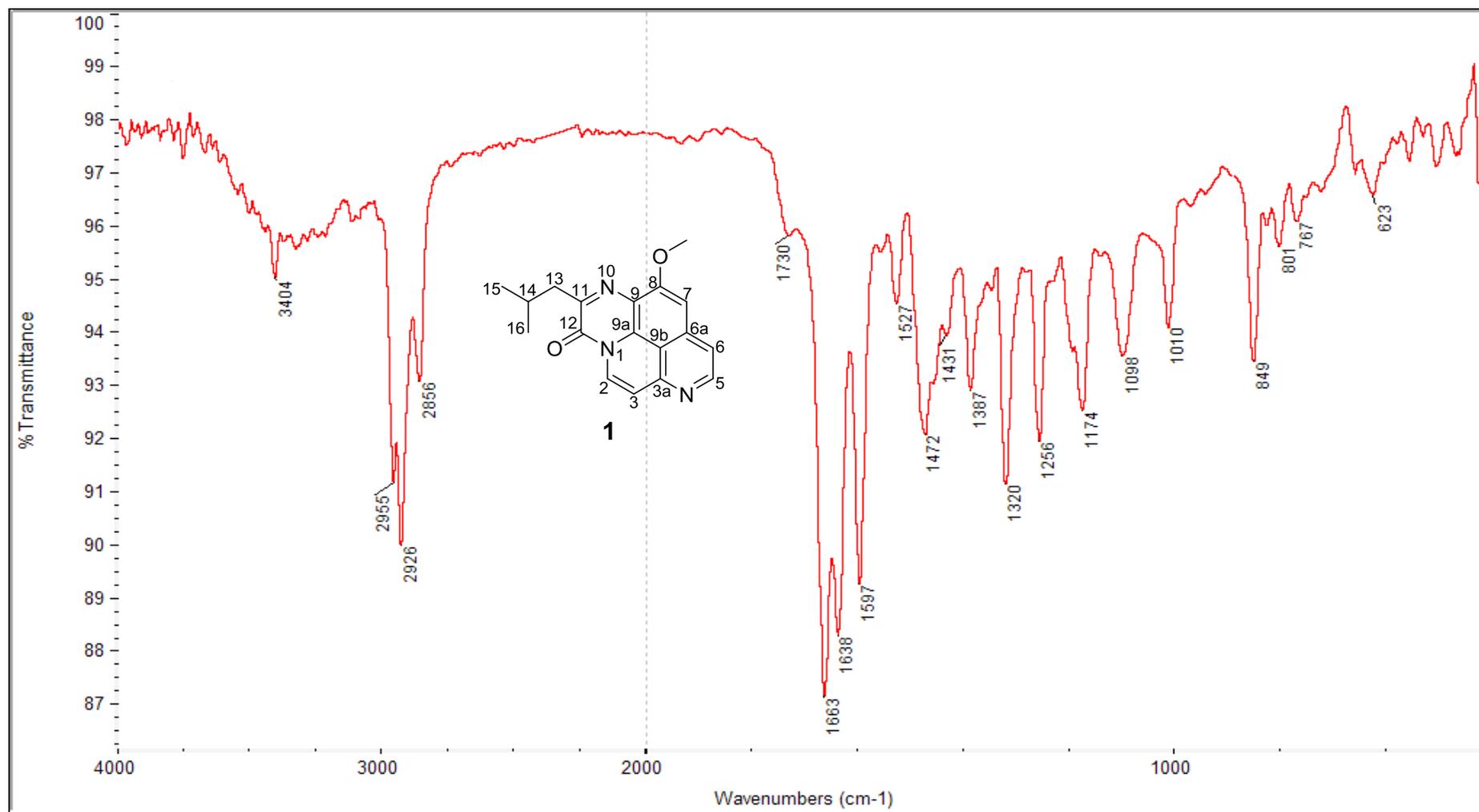


Figure S9. HRESIMS of compound 1.

Elemental Composition Report

Page 1

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 Selected filters: None

Monoisotopic Mass, Even Electron Ions

8 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass),

Elements Used:

C: 5-20 H: 5-25 N: 1-3 O: 1-2 Na: 1-1

SIPI

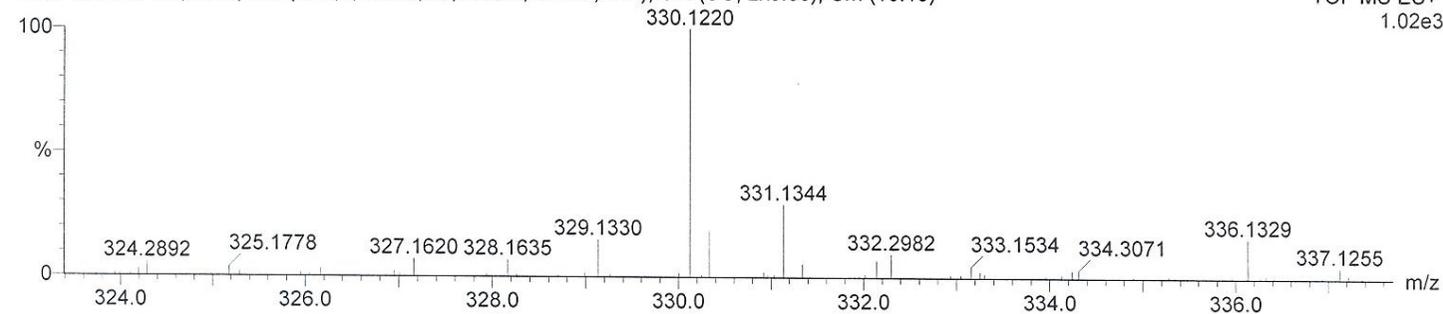
M.W=307

Q-ToF micro
 YA019

22-Jul-2014,15:21:17

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TOF MS ES+
 1.02e3



Minimum: 60.00
 Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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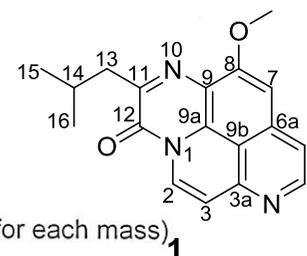


Figure S10. UV spectrum of compound 1.

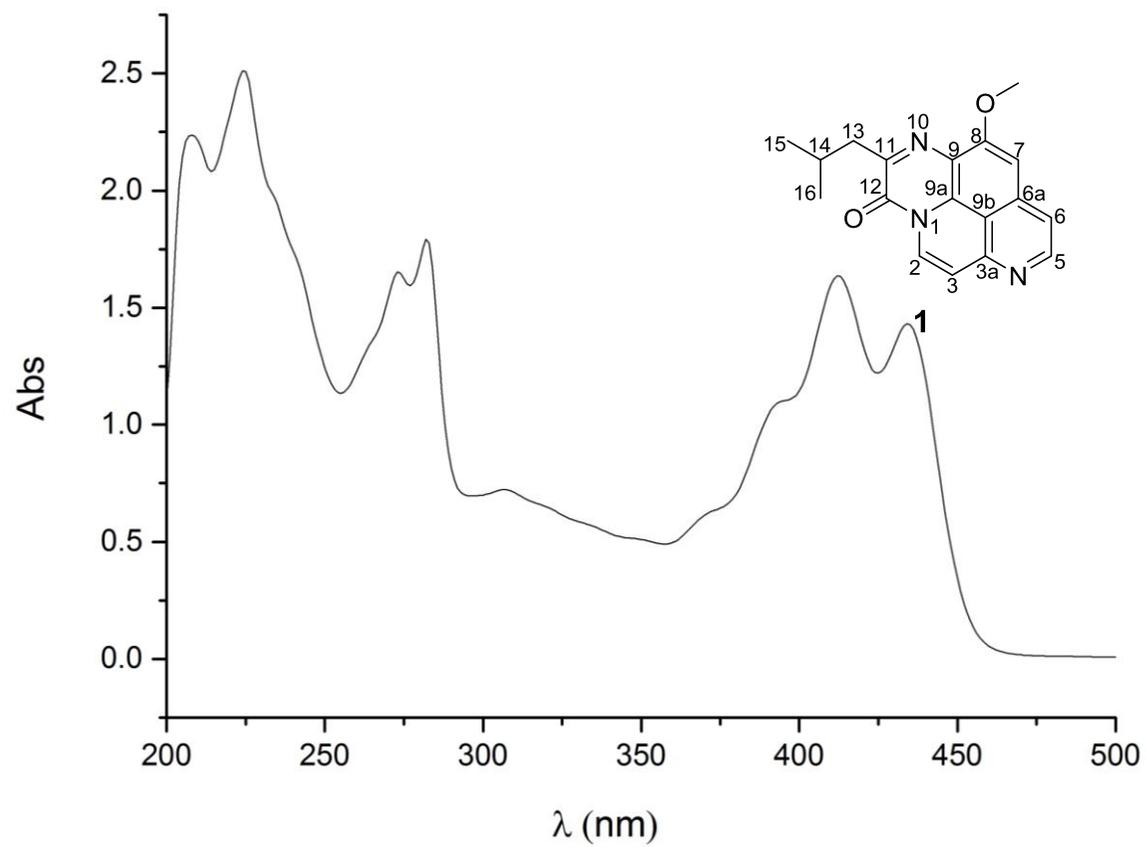


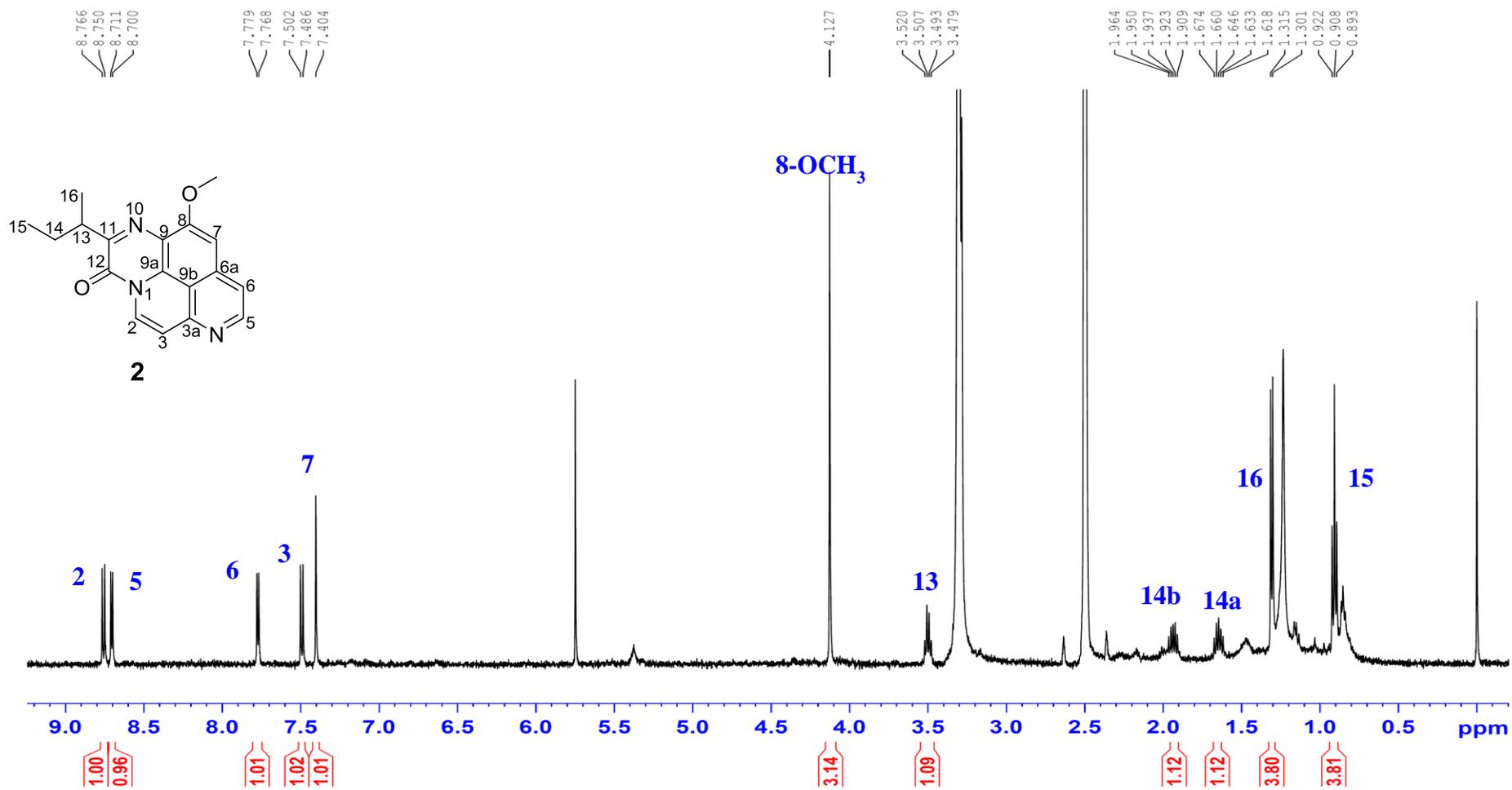
Figure S11. ^1H NMR spectrum of compound **2** in $\text{DMSO-}d_6$.

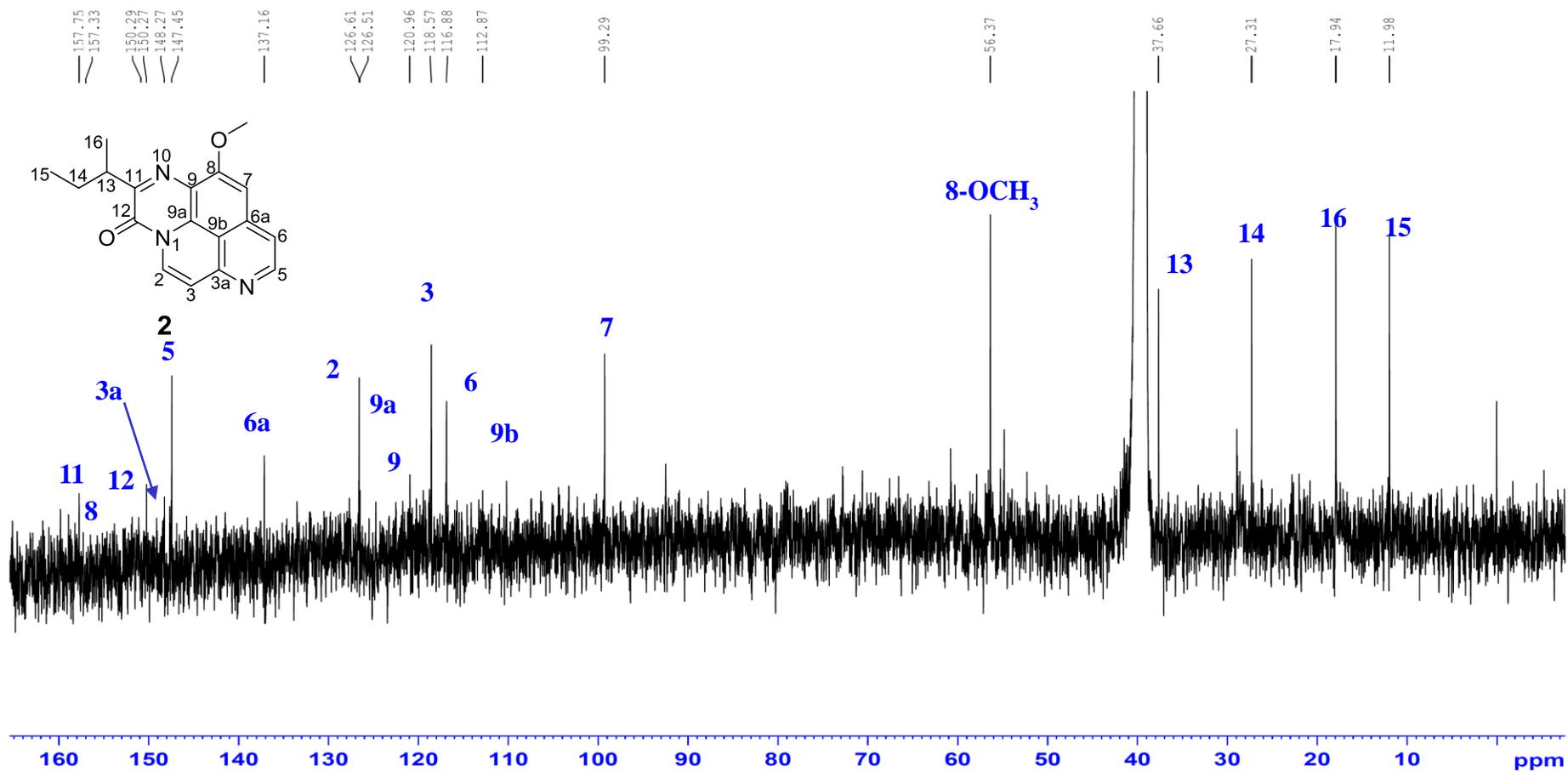
Figure S12. ^{13}C NMR spectrum of compound 2 in $\text{DMSO-}d_6$.

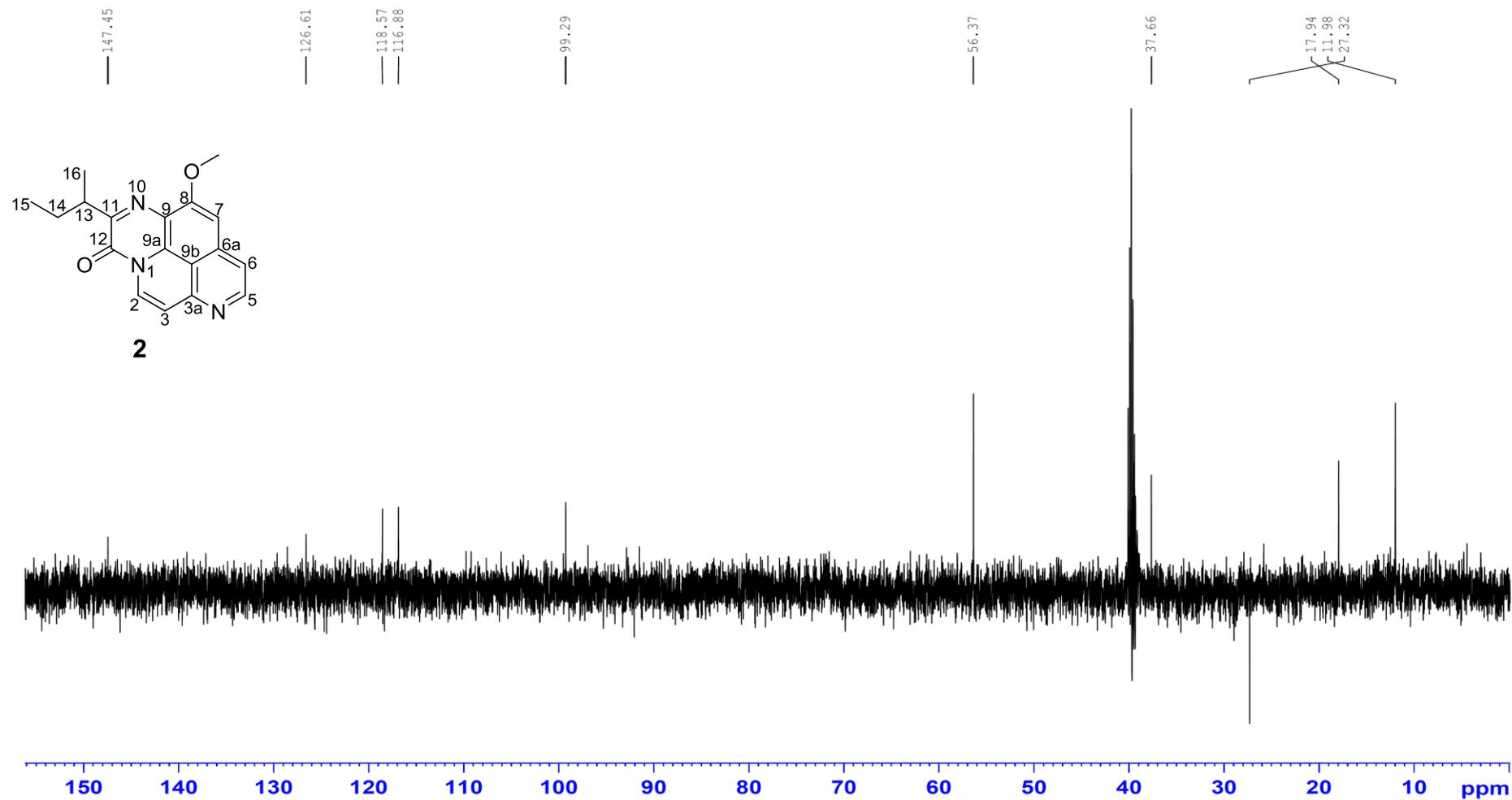
Figure S13. DEPT135 Spectrum of compound 2 in DMSO-*d*₆.

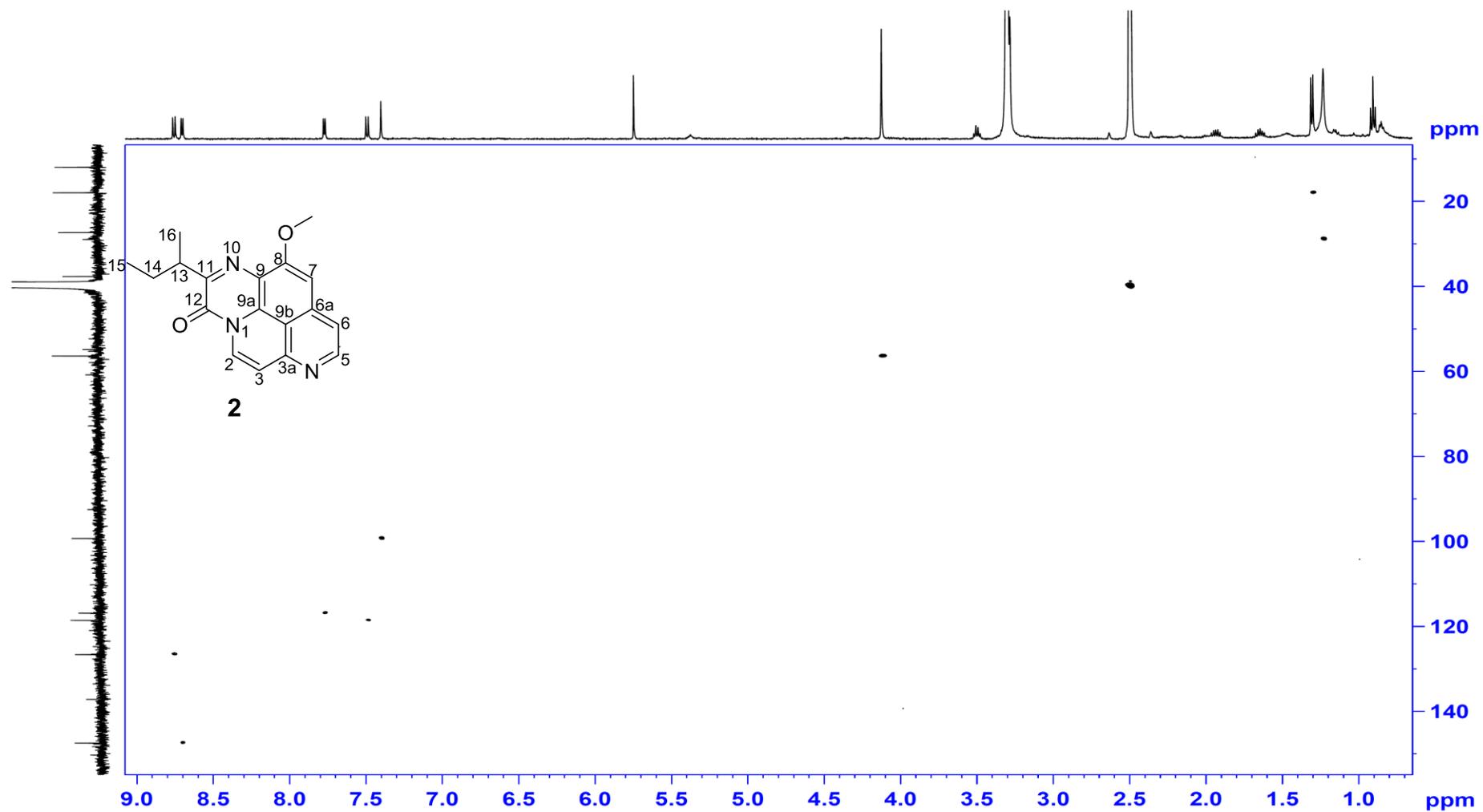
Figure S14. HSQC spectrum of compound 2 in DMSO-*d*₆.

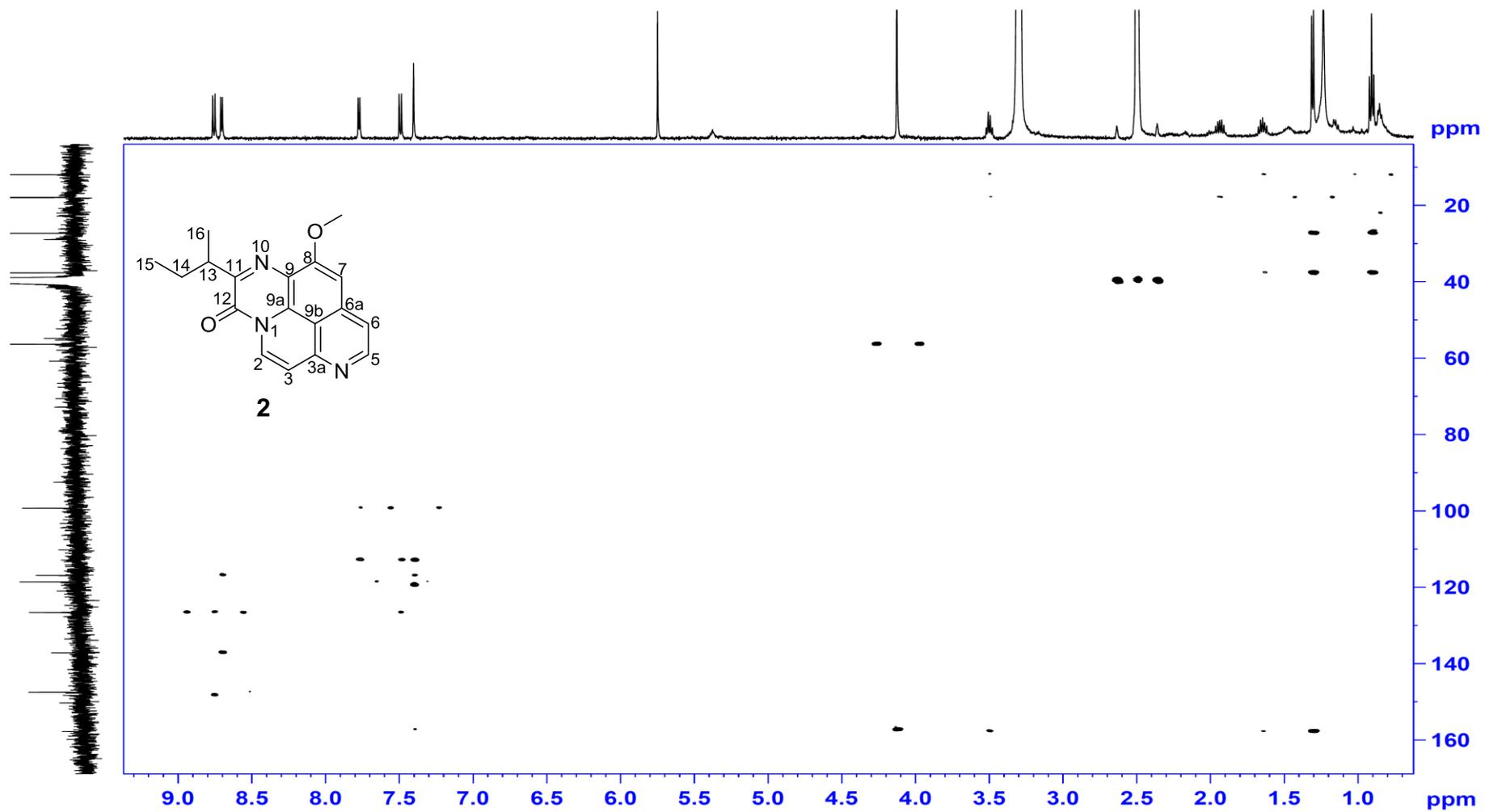
Figure S15. HMBC spectrum of compound 2 in DMSO-*d*₆.

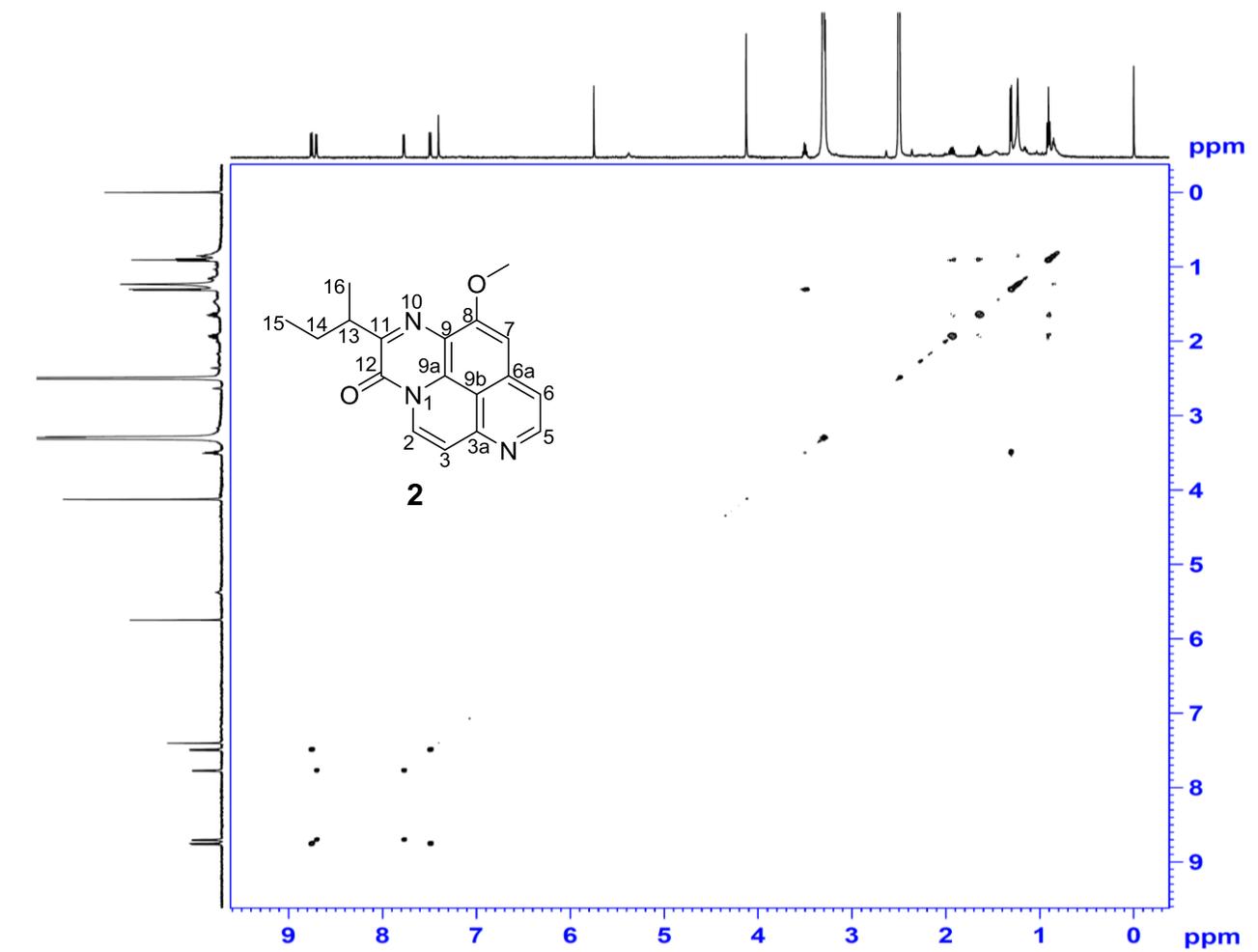
Figure S16. ^1H - ^1H COSY spectrum of compound **2** in $\text{DMSO-}d_6$.

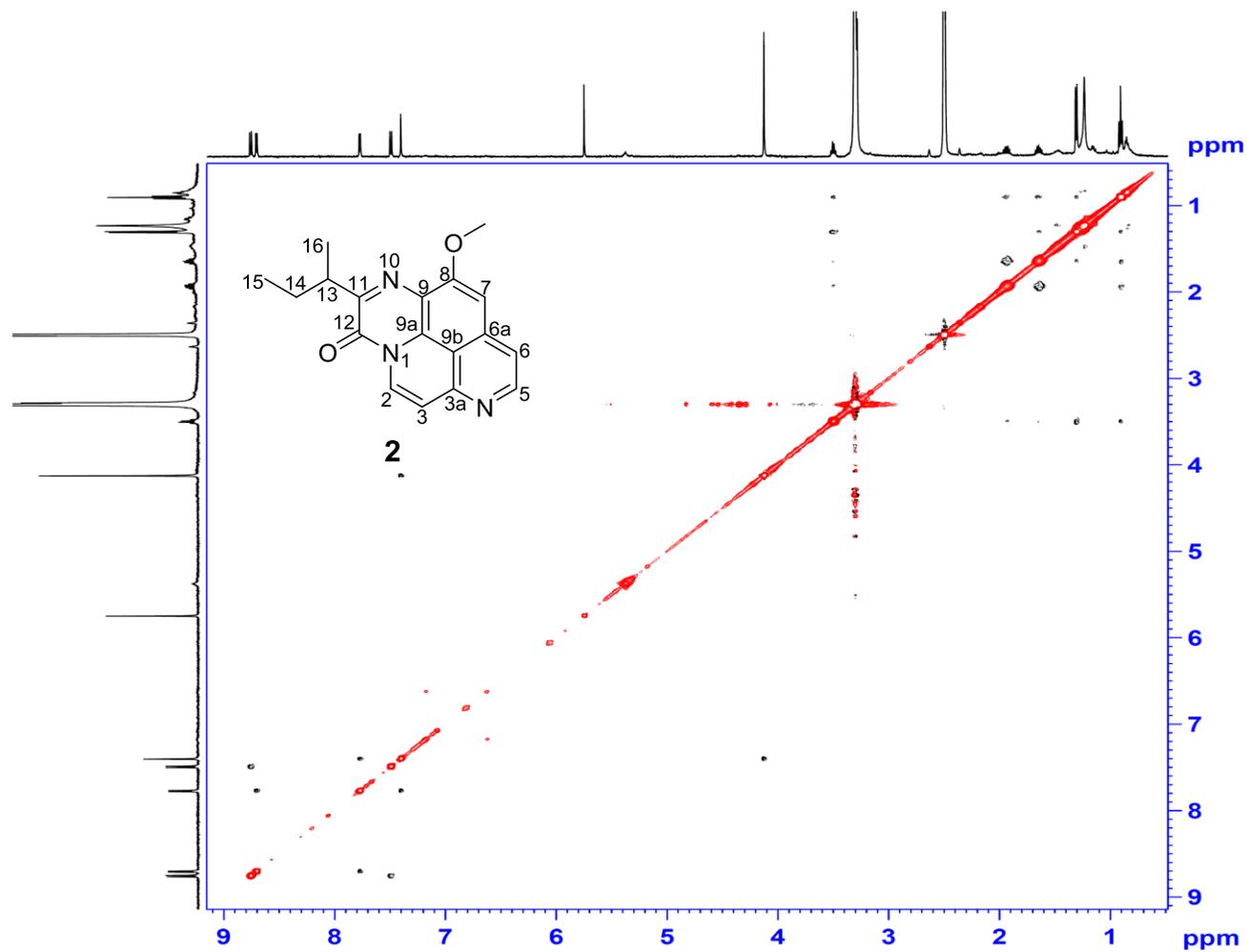
Figure S17. NOESY spectrum of compound 2 in DMSO-*d*₆.

Figure S18. IR spectrum of compound 2.

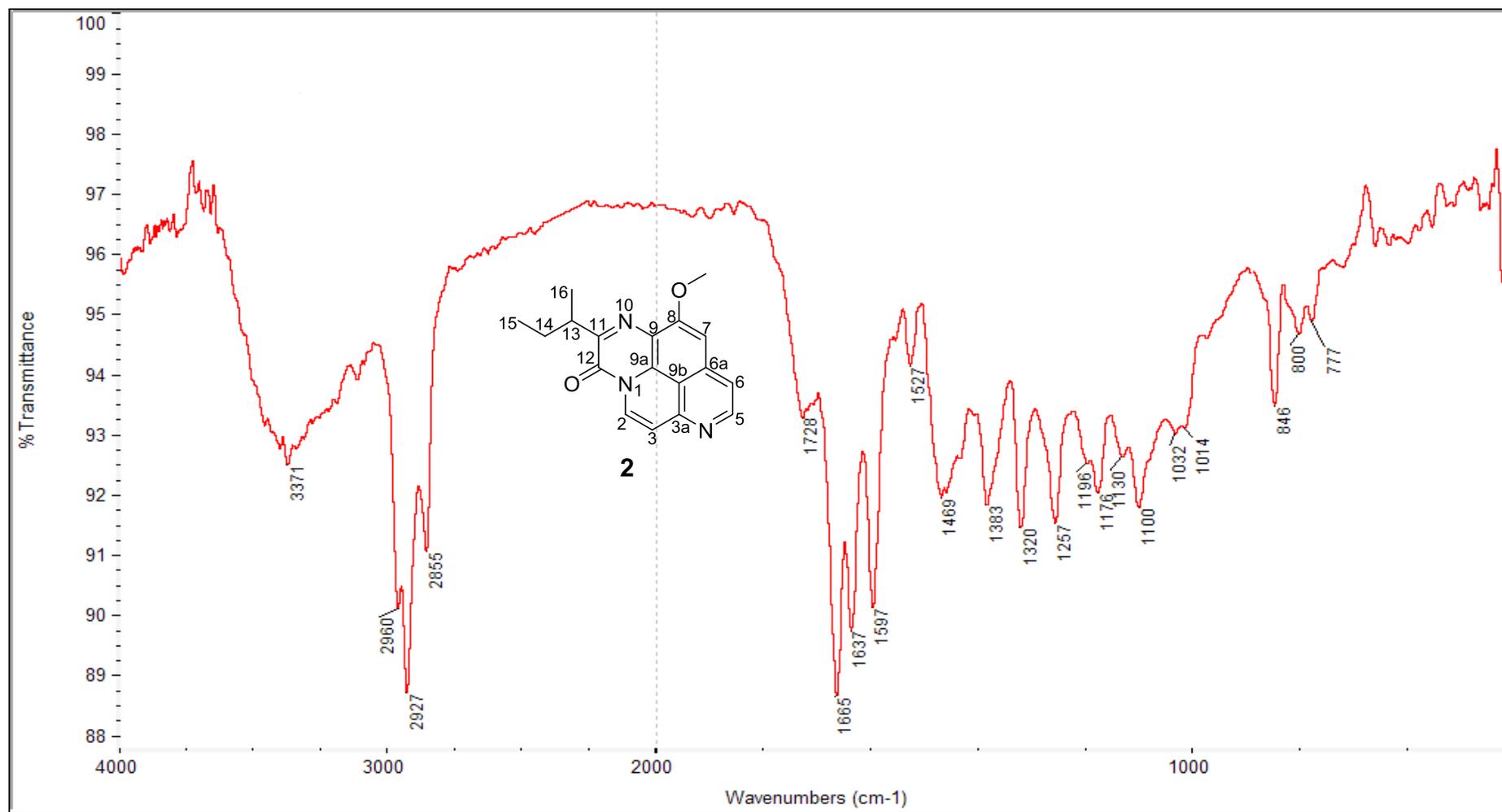


Figure S19. HRESIMS of compound 2.

Elemental Composition Report

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 Selected filters: None

Monoisotopic Mass, Even Electron Ions

8 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 5-20 H: 5-25 N: 1-3 O: 1-2

SIPI

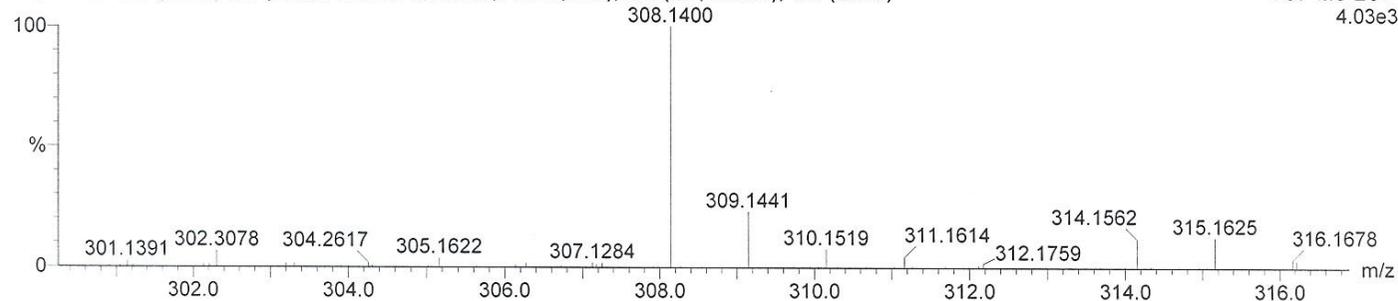
M.W=307

Q-ToF micro
 YA019

22-Jul-2014, 15:27:52

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TOF MS ES+
 4.03e3



Minimum: 60.00
 Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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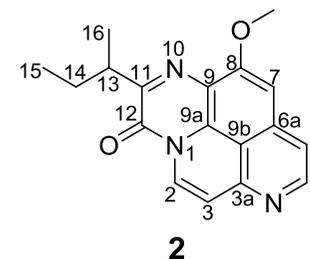


Figure S20. UV spectrum of compound 2.

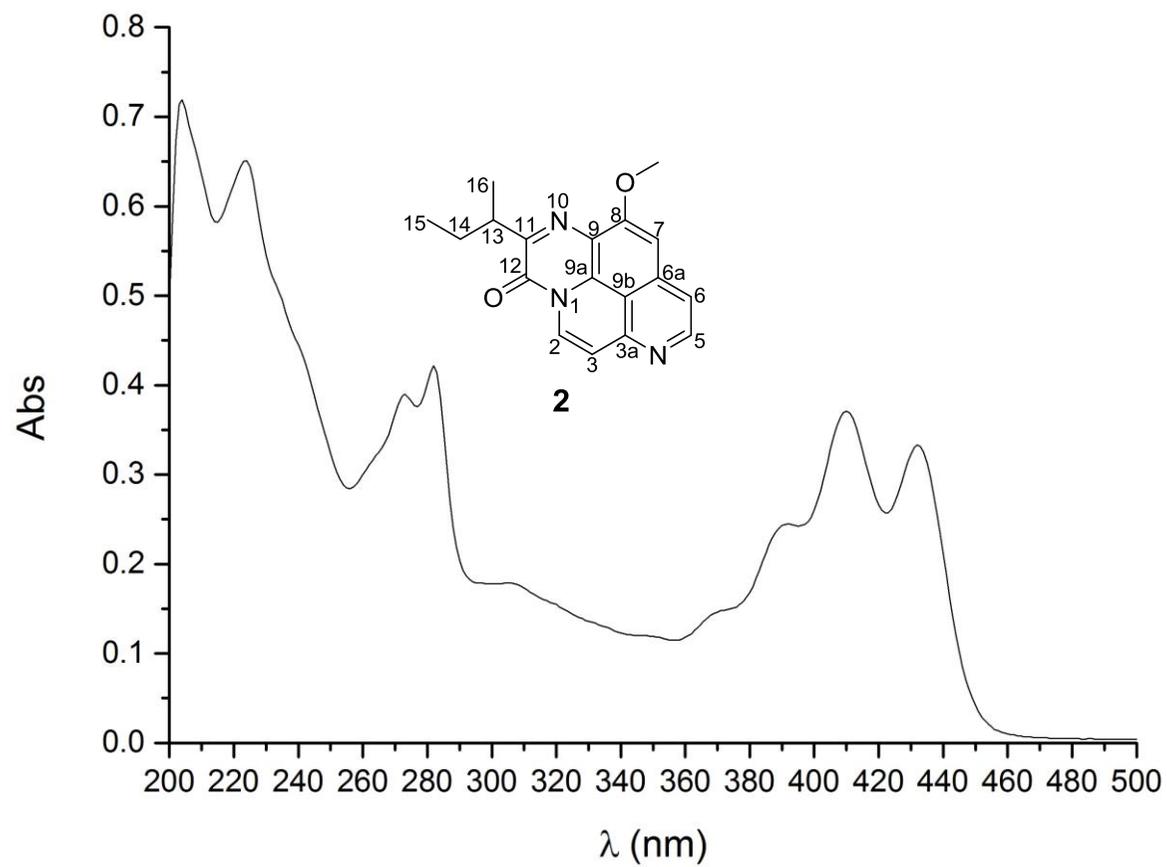


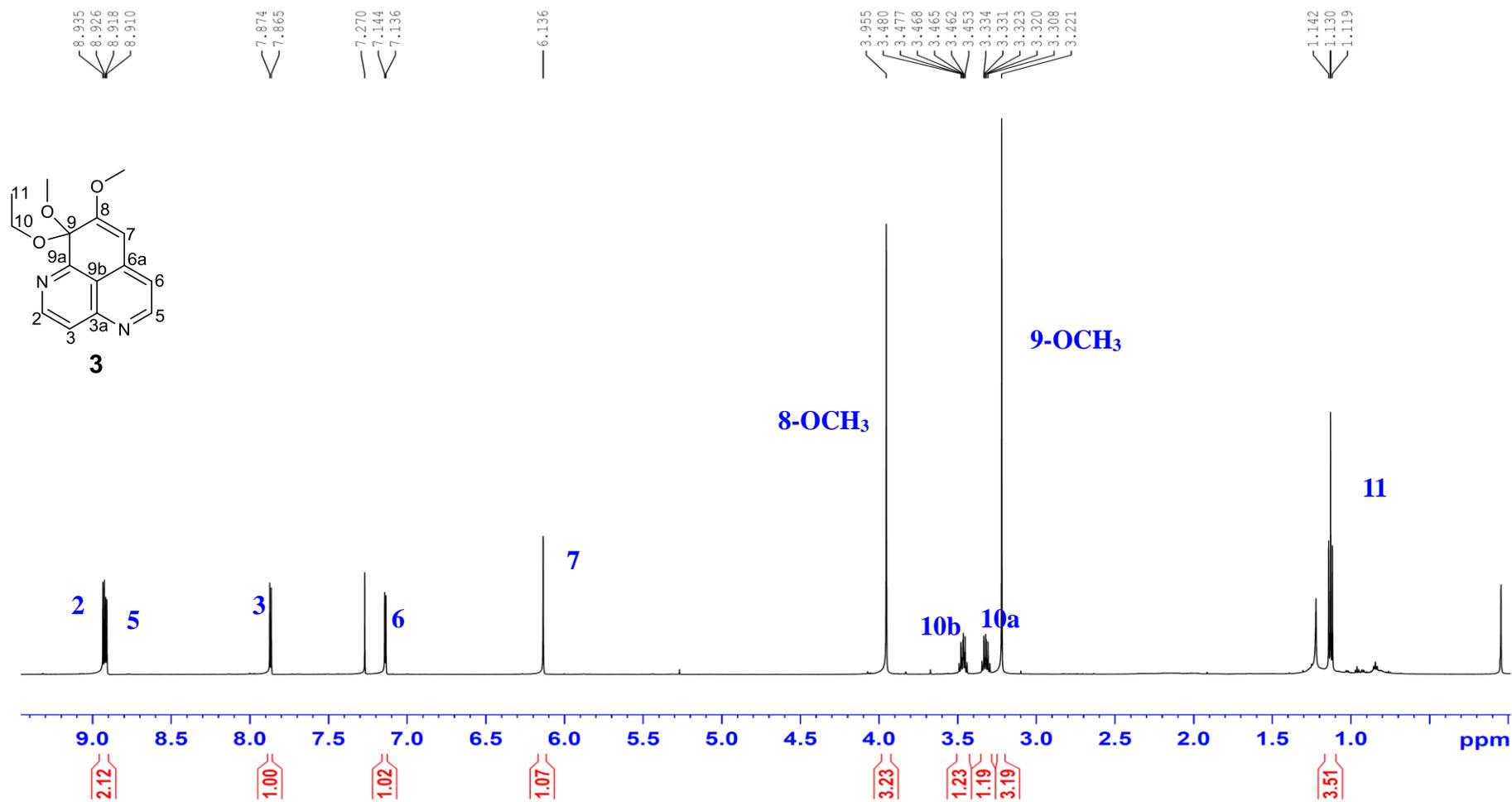
Figure S21. ^1H NMR spectrum of compound **3** in CDCl_3 .

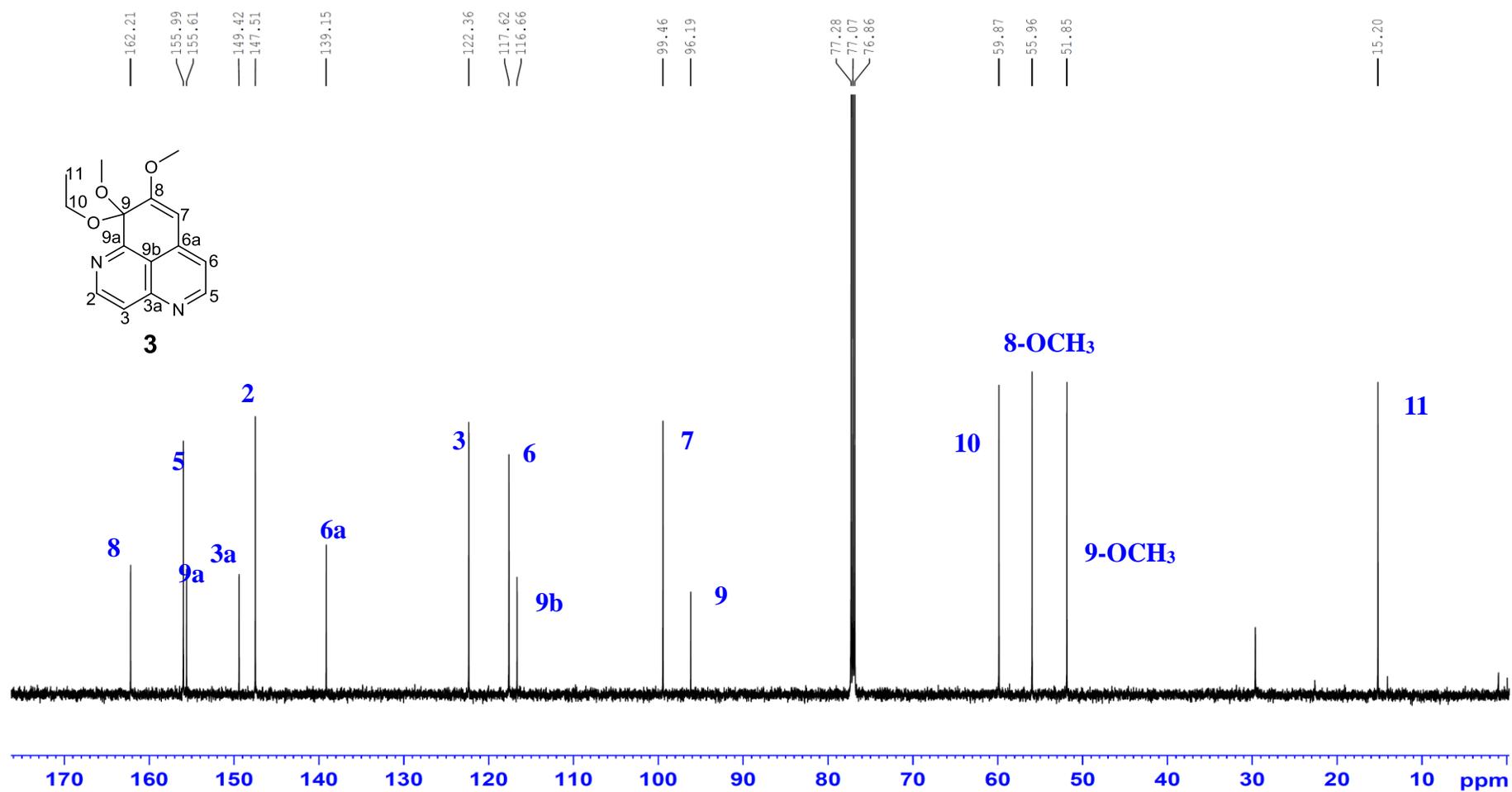
Figure S22. ^{13}C NMR spectrum of compound **3** in CDCl_3 .

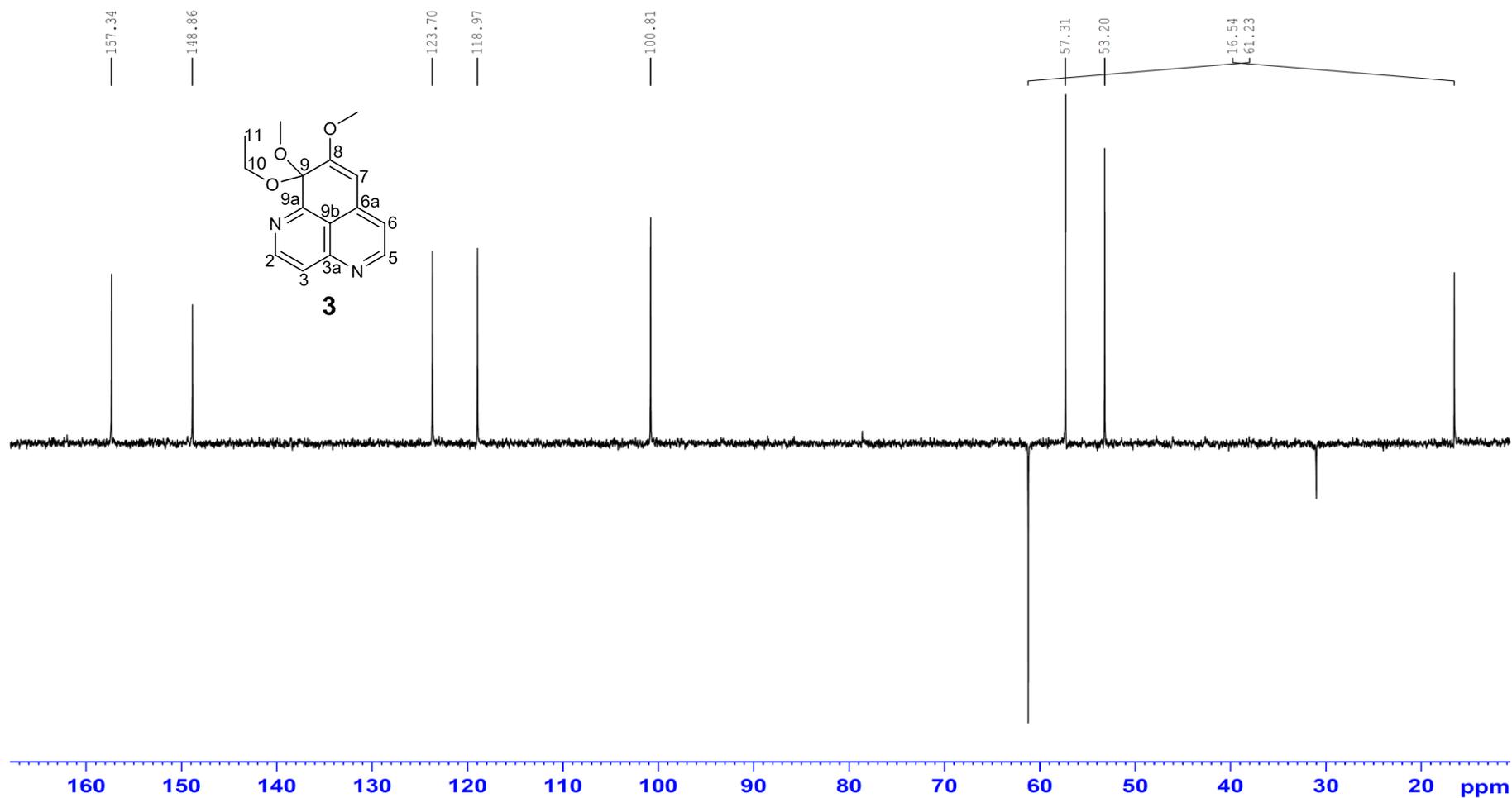
Figure S23. DEPT135 Spectrum of compound **3** in CDCl₃.

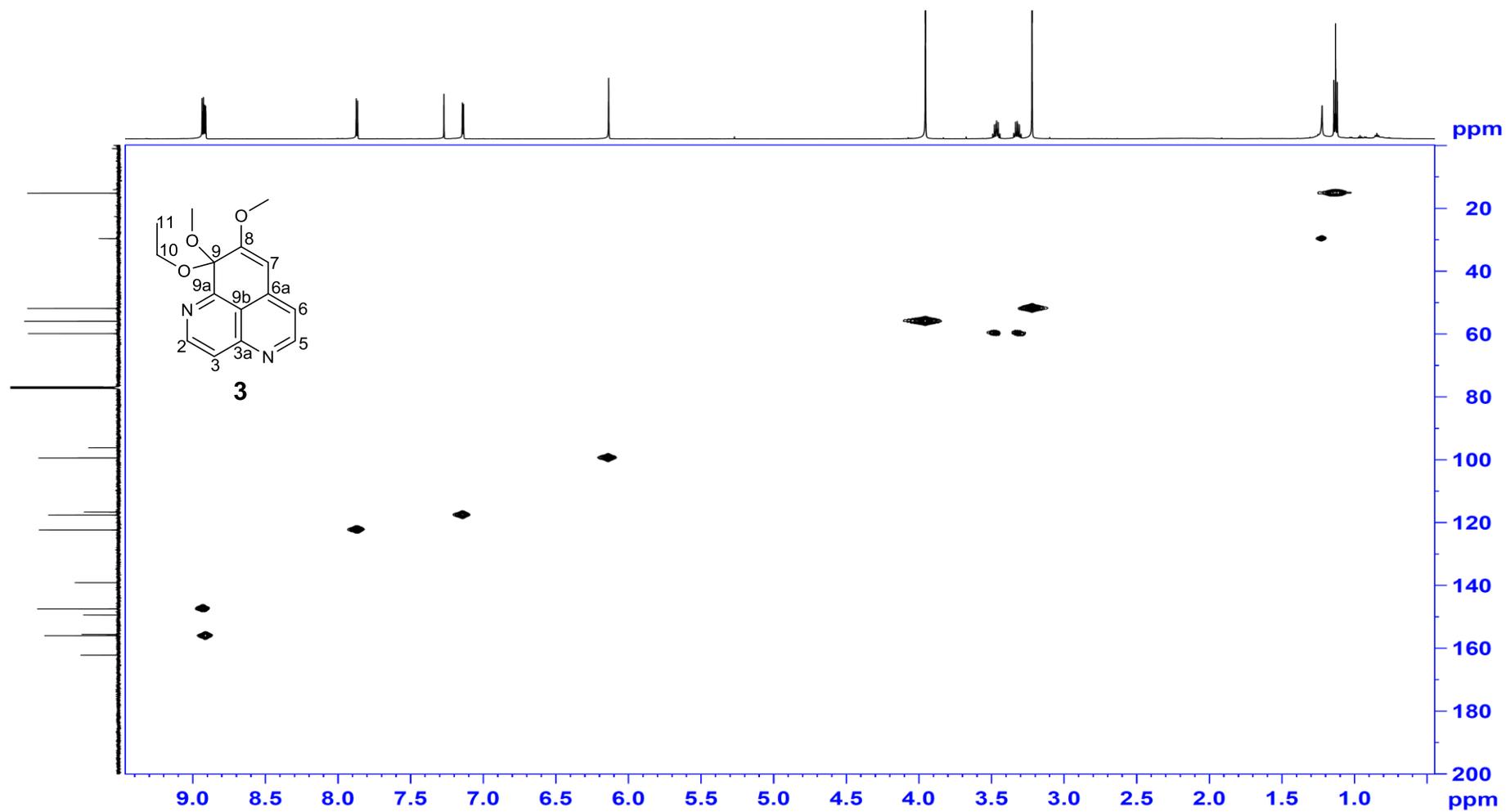
Figure S24. HSQC spectrum of compound 3 in CDCl₃.

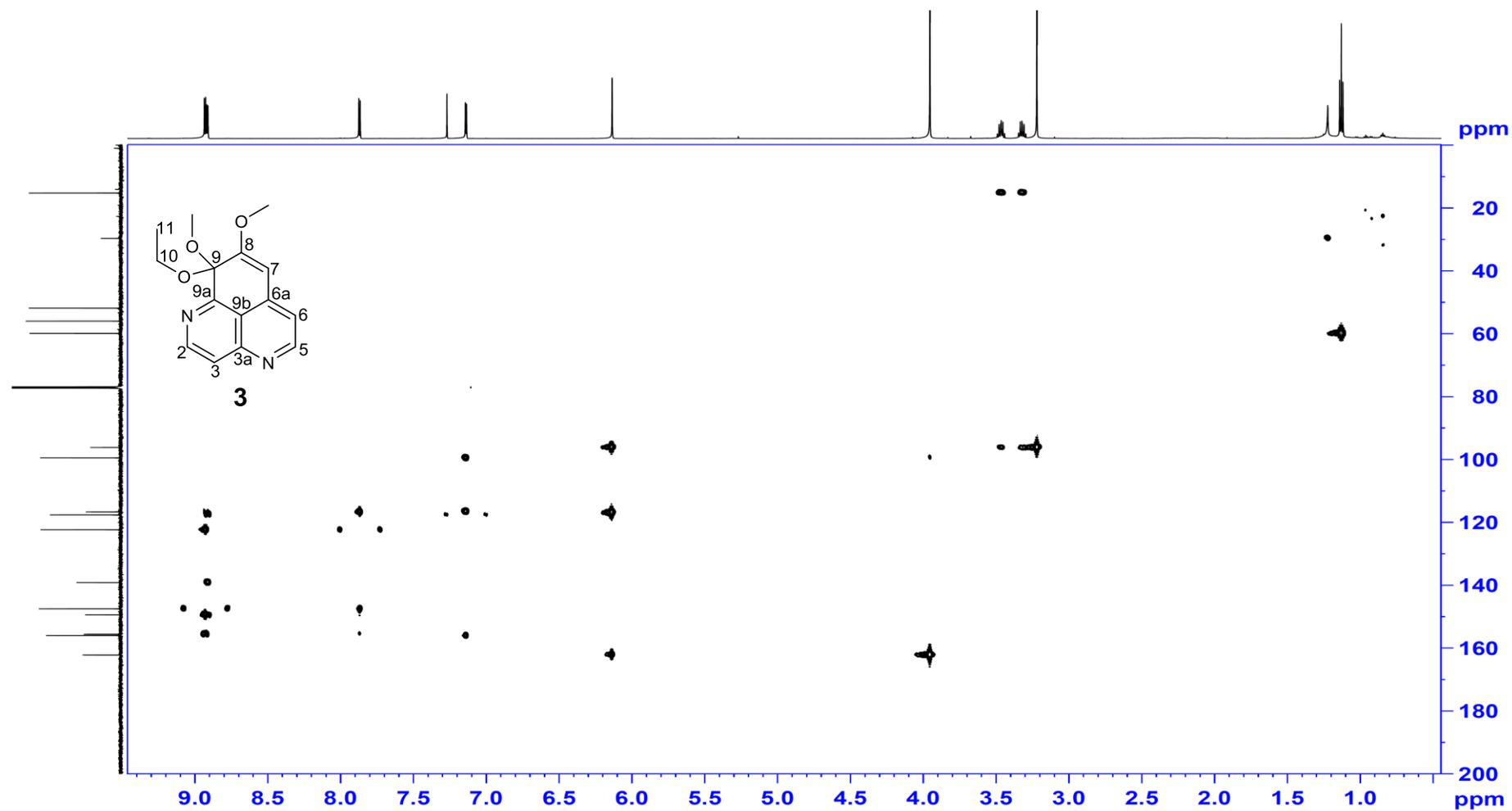
Figure S25. HMBC spectrum of compound 3 in CDCl₃.

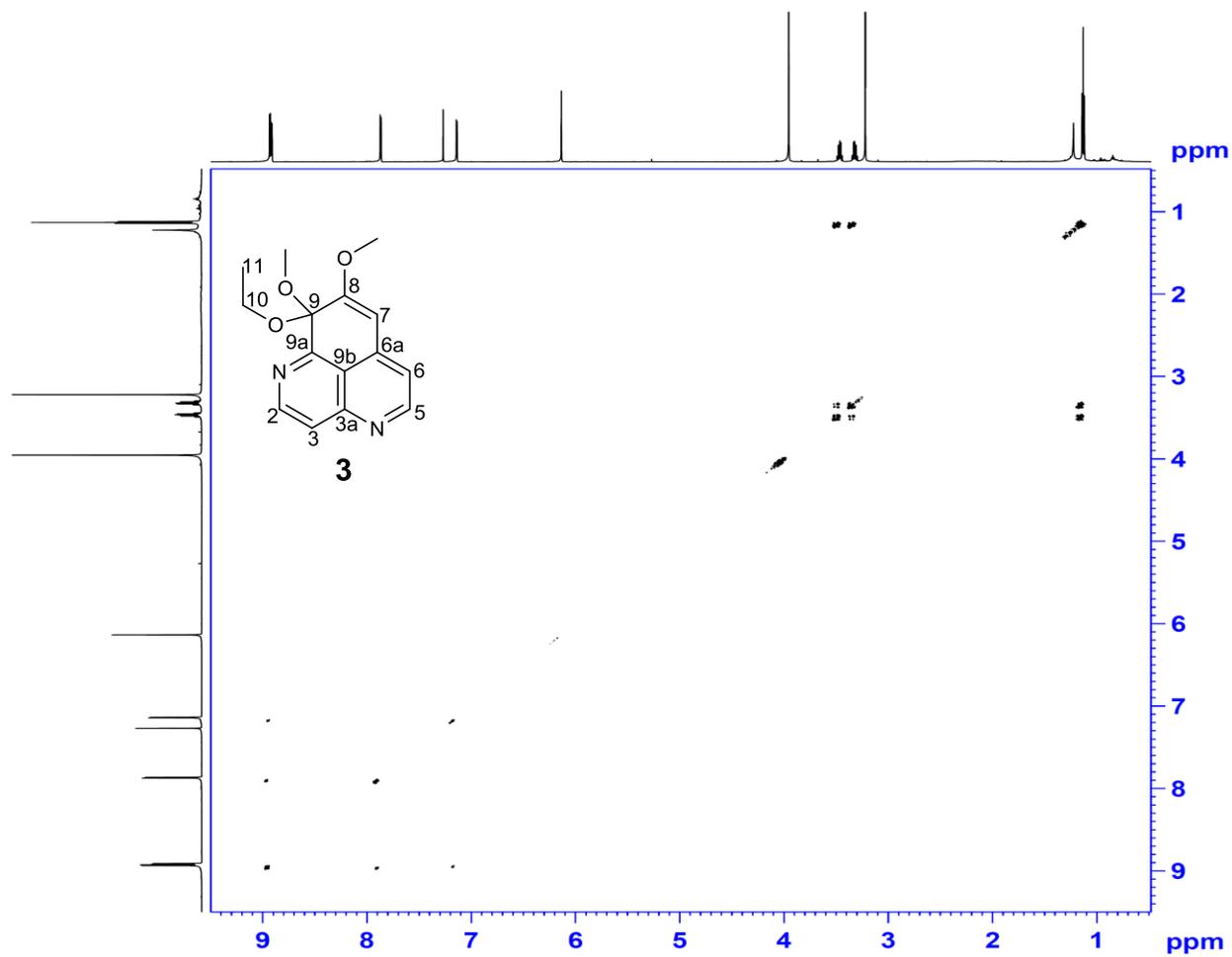
Figure S26. ^1H - ^1H COSY spectrum of compound **3** in CDCl_3 .

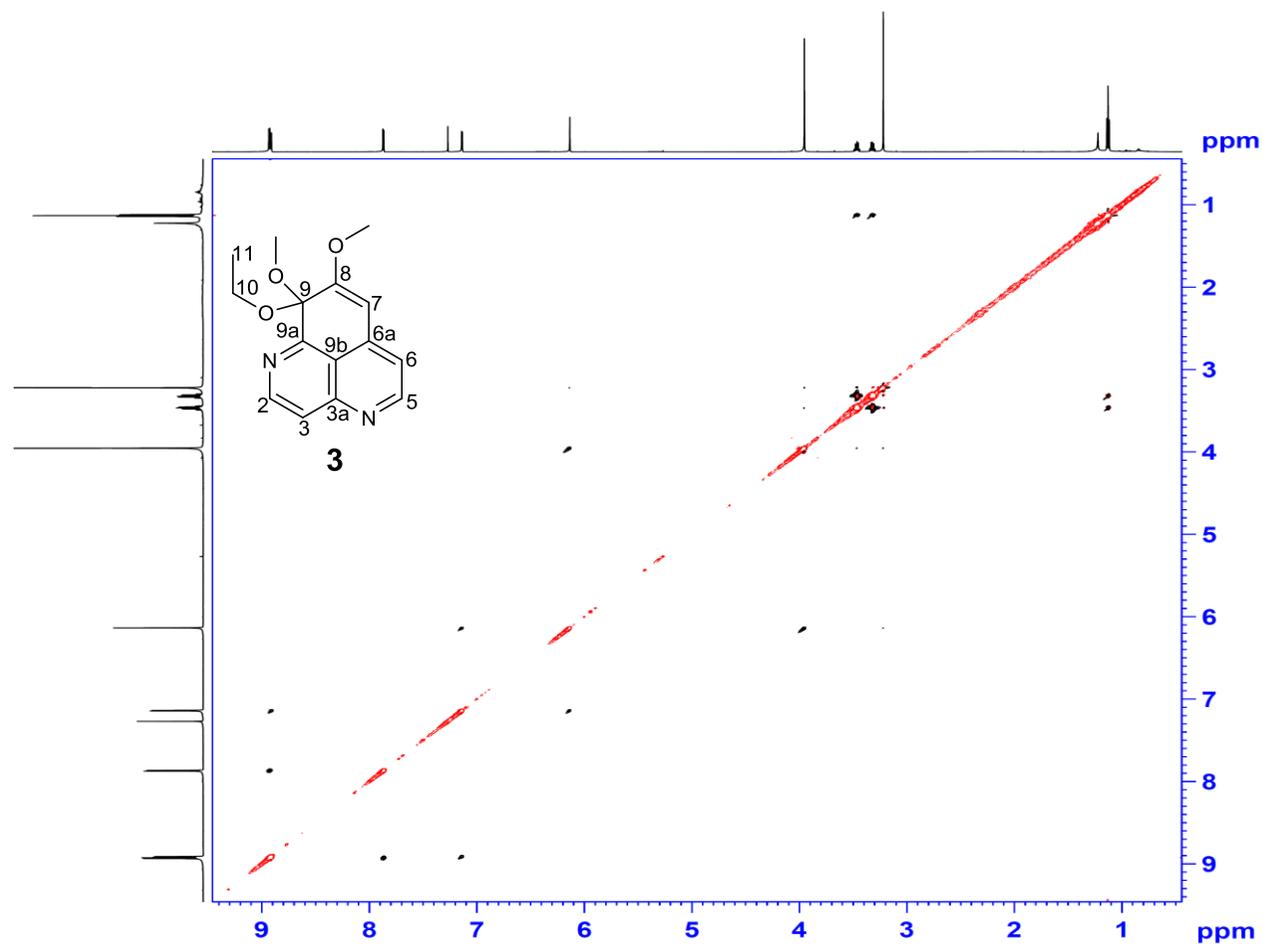
Figure S27. NOESY spectrum of compound **3** in CDCl₃.

Figure S28. IR spectrum of compound 3.

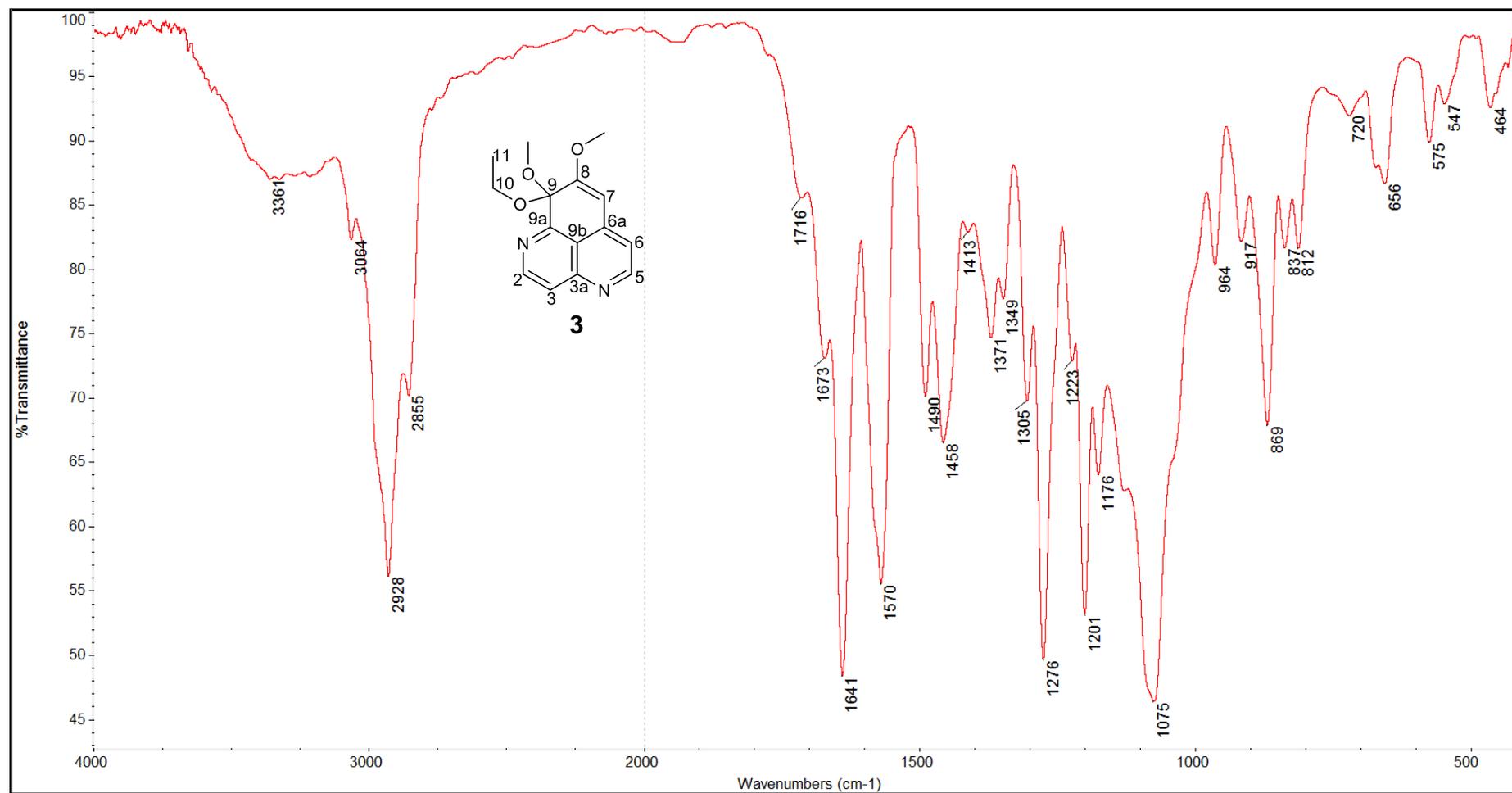


Figure S29. HRESIMS of compound 3.

Elemental Composition Report

Multiple Mass Analysis: 2 mass(es) processed

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Selected filters: None

Monoisotopic Mass, Even Electron Ions

28 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

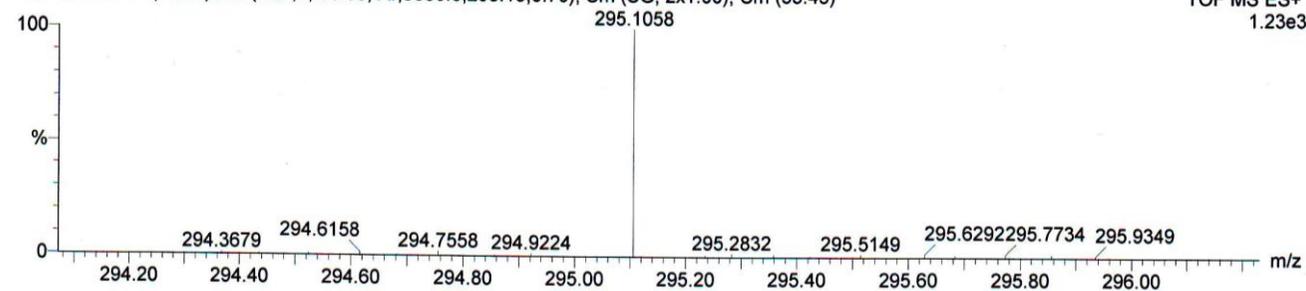
Elements Used:

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SIPI

M.W.=272

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Minimum: 85.00
Maximum: 100.00

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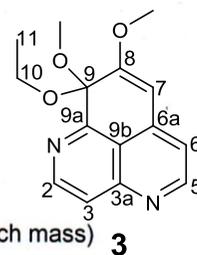


Figure S30. UV spectrum of compound 3.

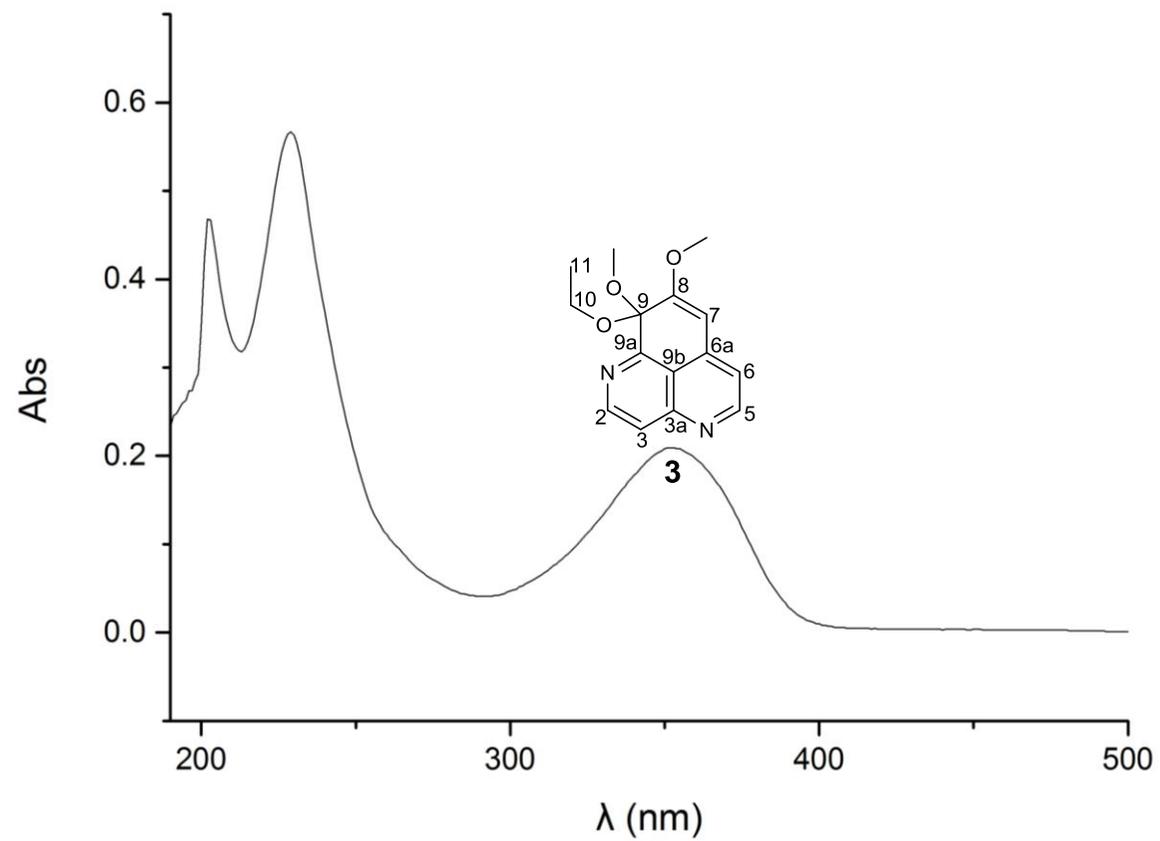


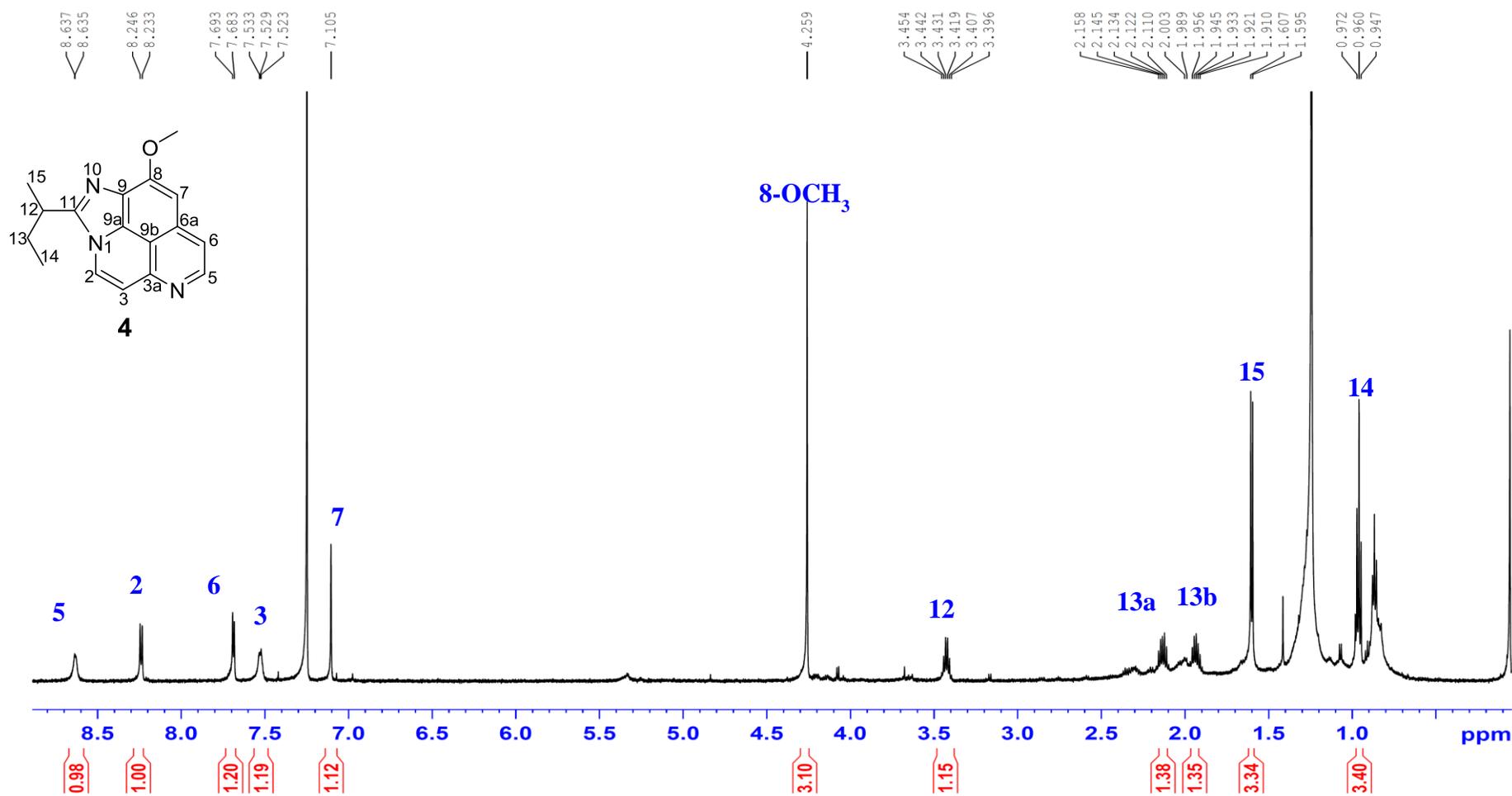
Figure S31. ¹H NMR spectrum of compound 4 in CDCl₃.

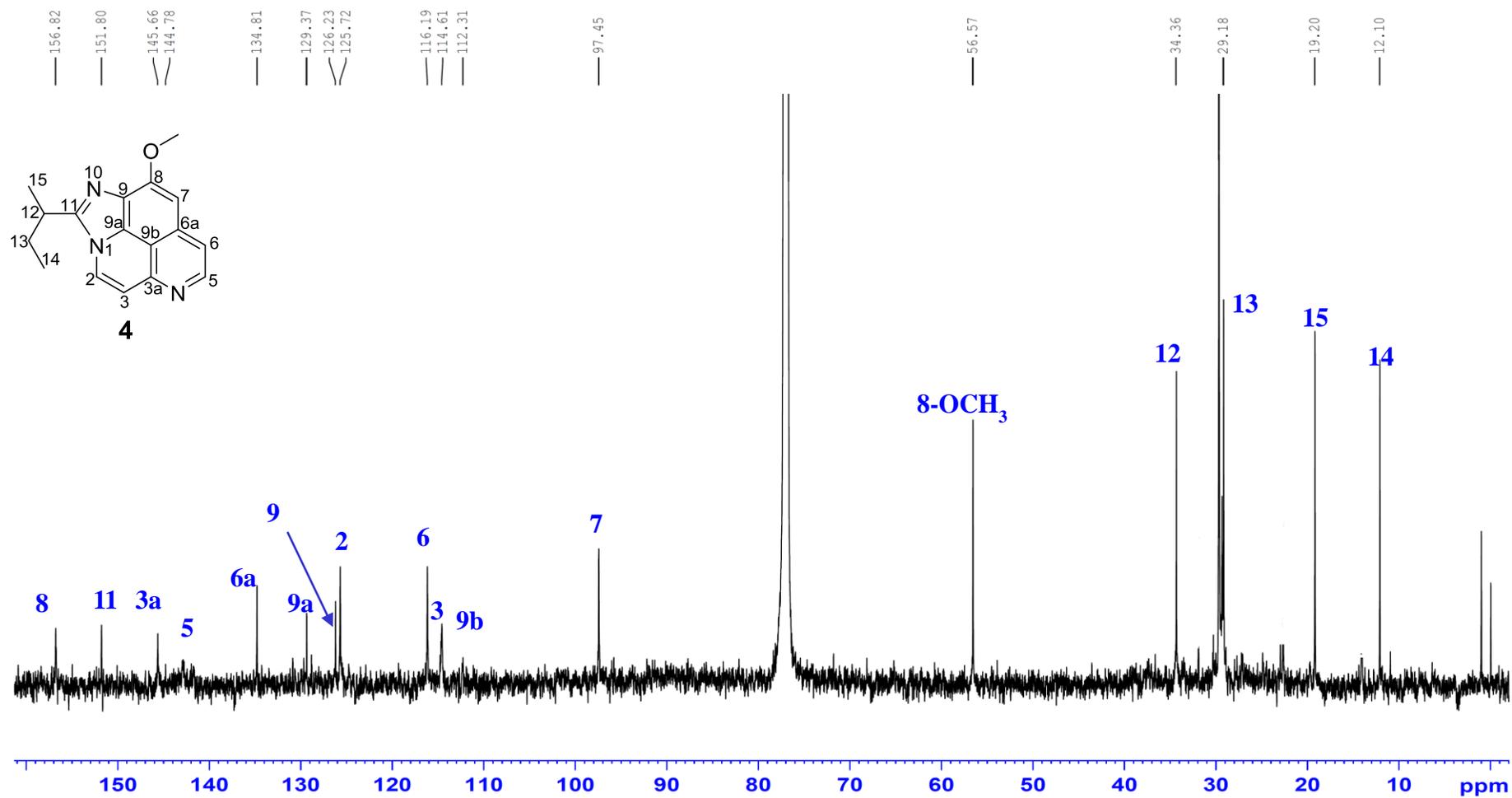
Figure S32. ^{13}C NMR spectrum of compound **4** in CDCl_3 .

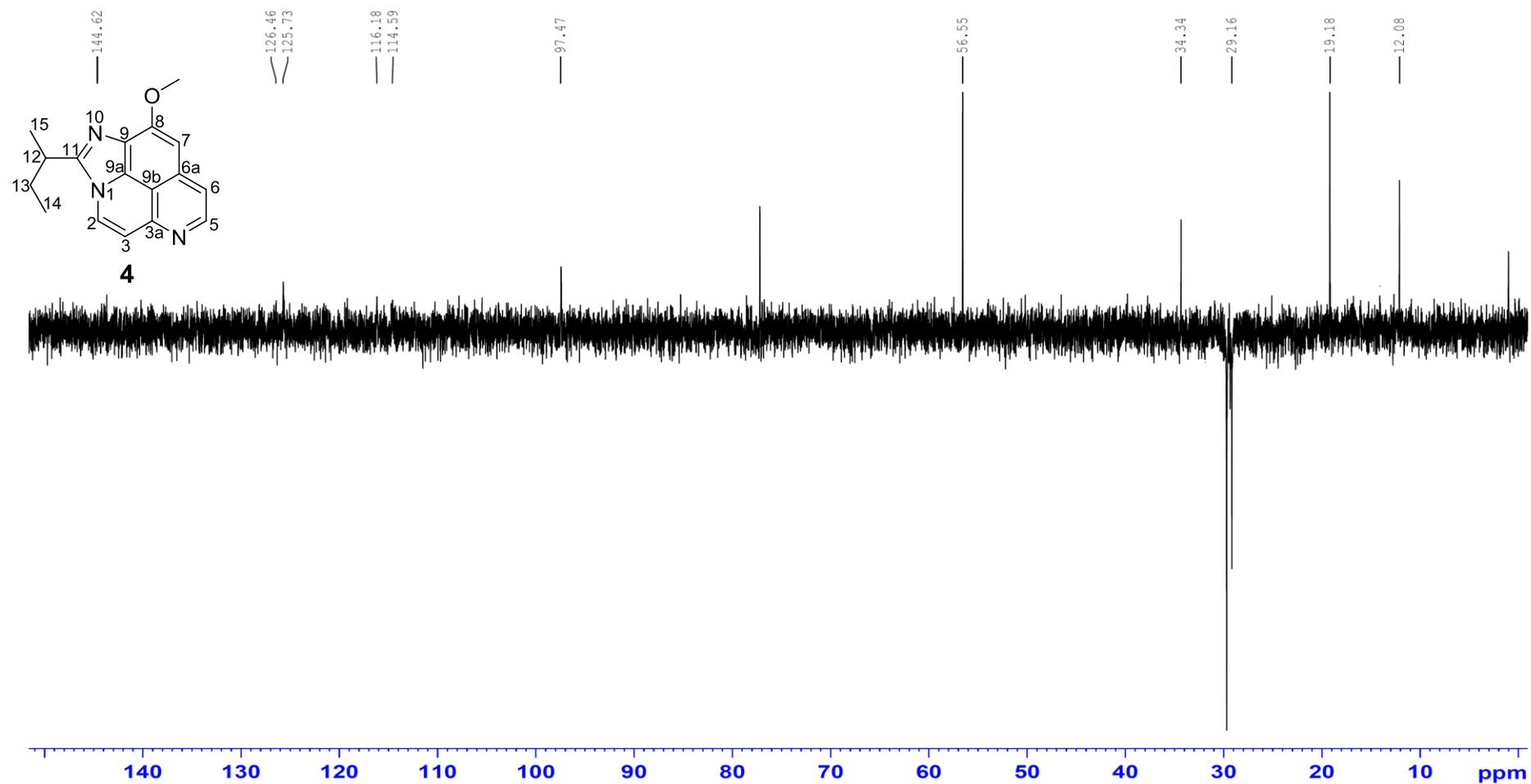
Figure S33. DEPT135 Spectrum of compound **4** in CDCl₃.

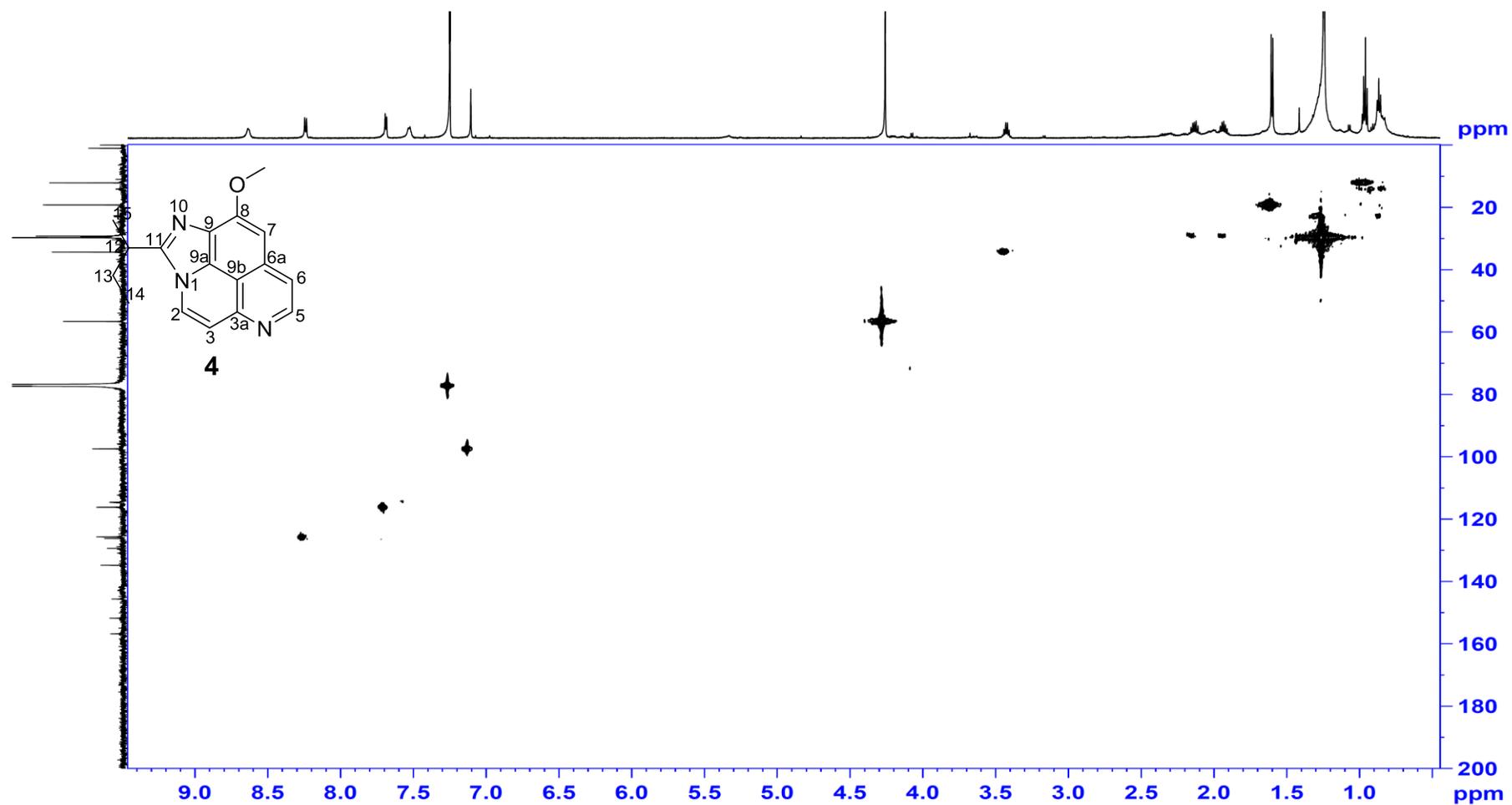
Figure S34. HSQC spectrum of compound 4 in CDCl₃.

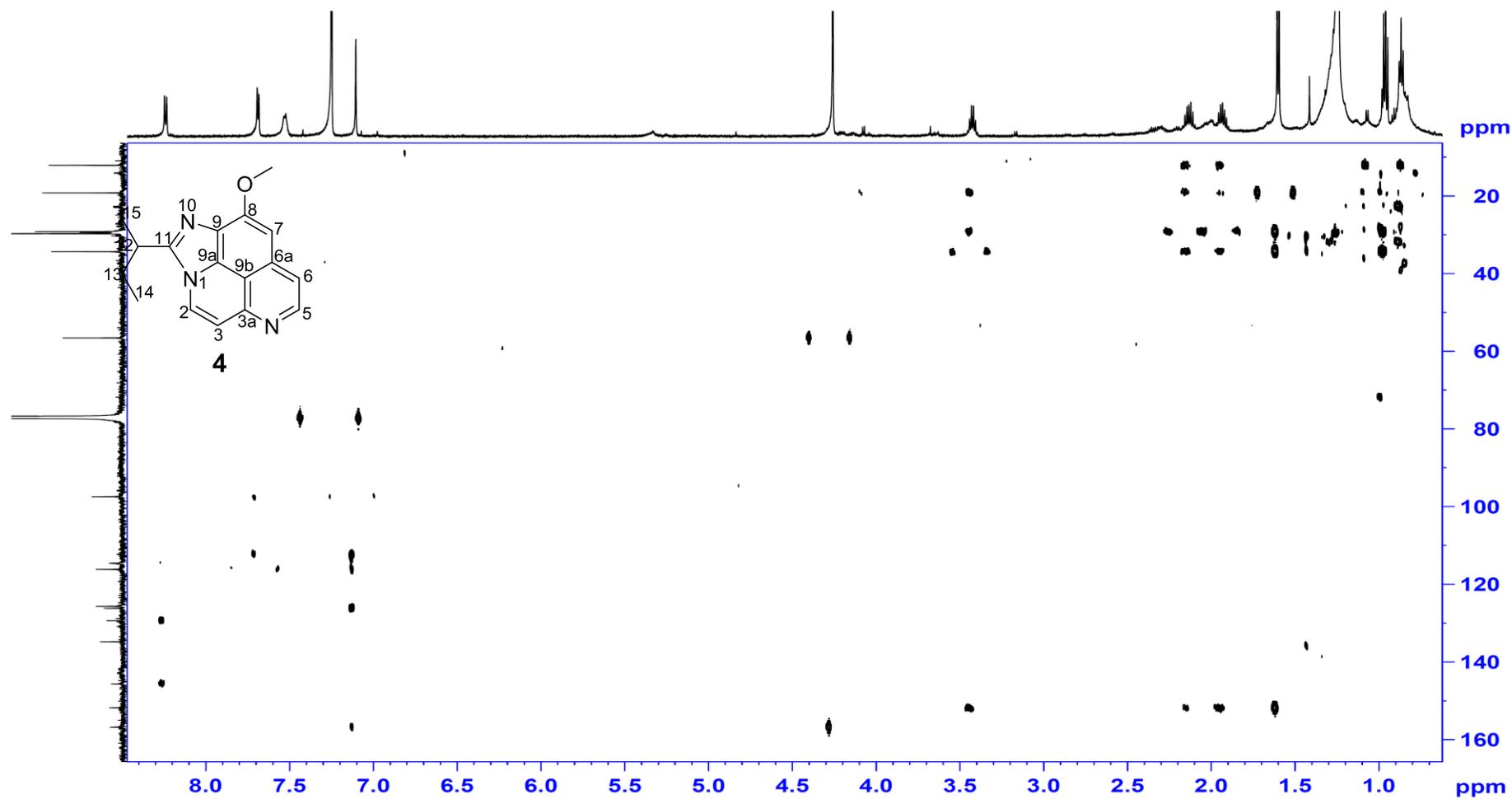
Figure S35. HMBC spectrum of compound 4 in CDCl₃.

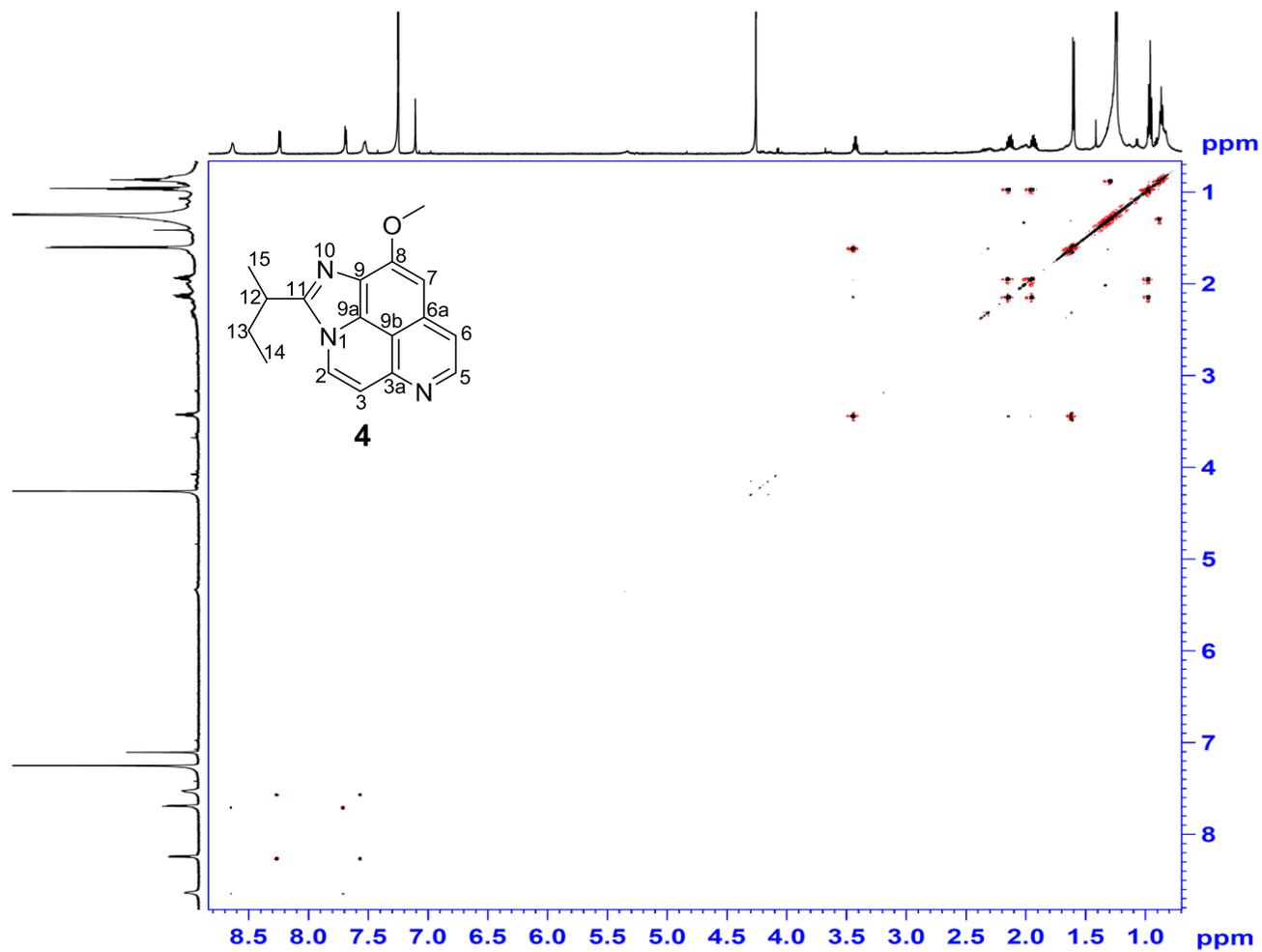
Figure S36. ^1H - ^1H COSY spectrum of compound **4** in CDCl_3 .

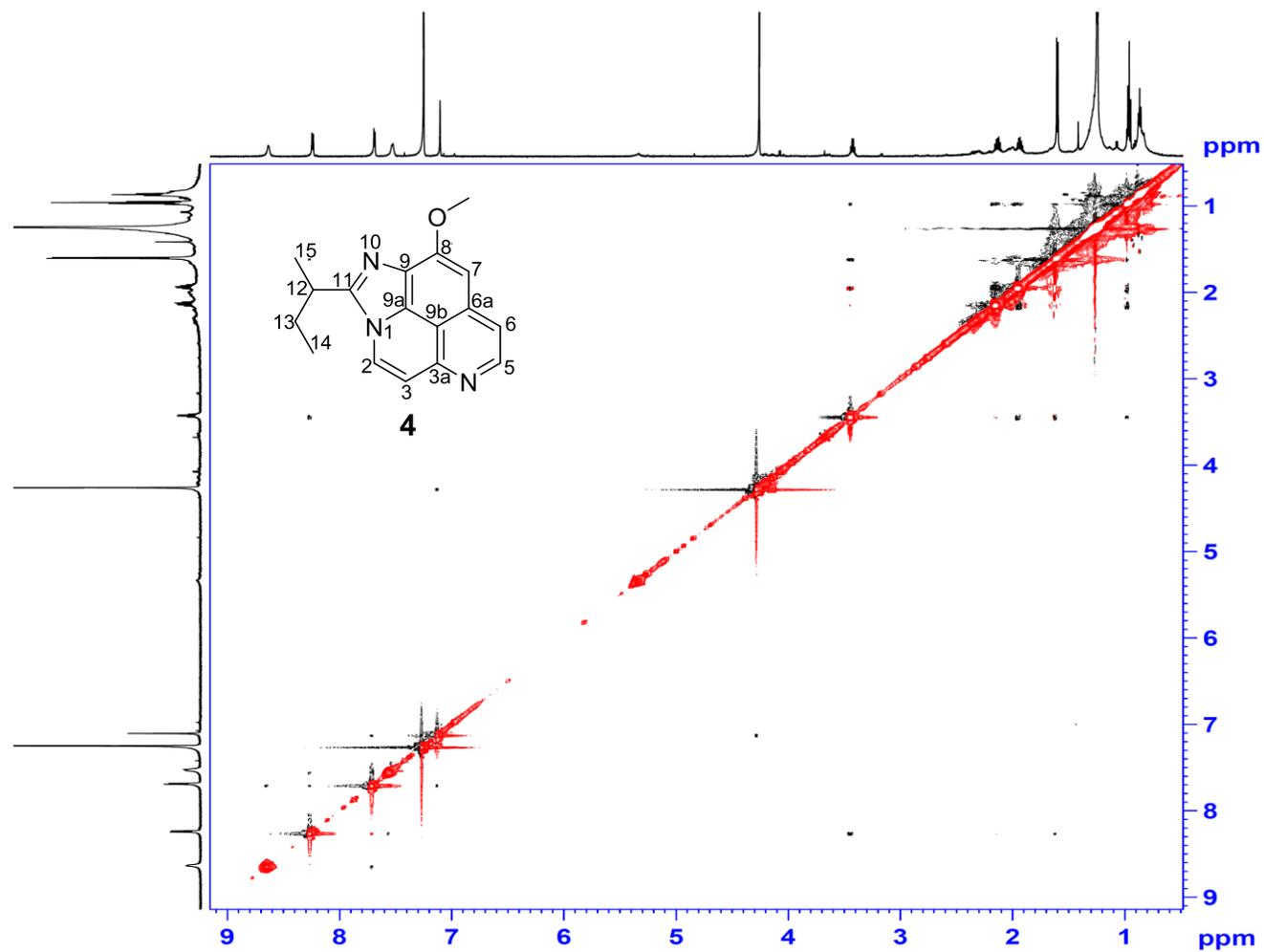
Figure S37. NOESY spectrum of compound 4 in CDCl₃.

Figure S38. IR spectrum of compound 4.

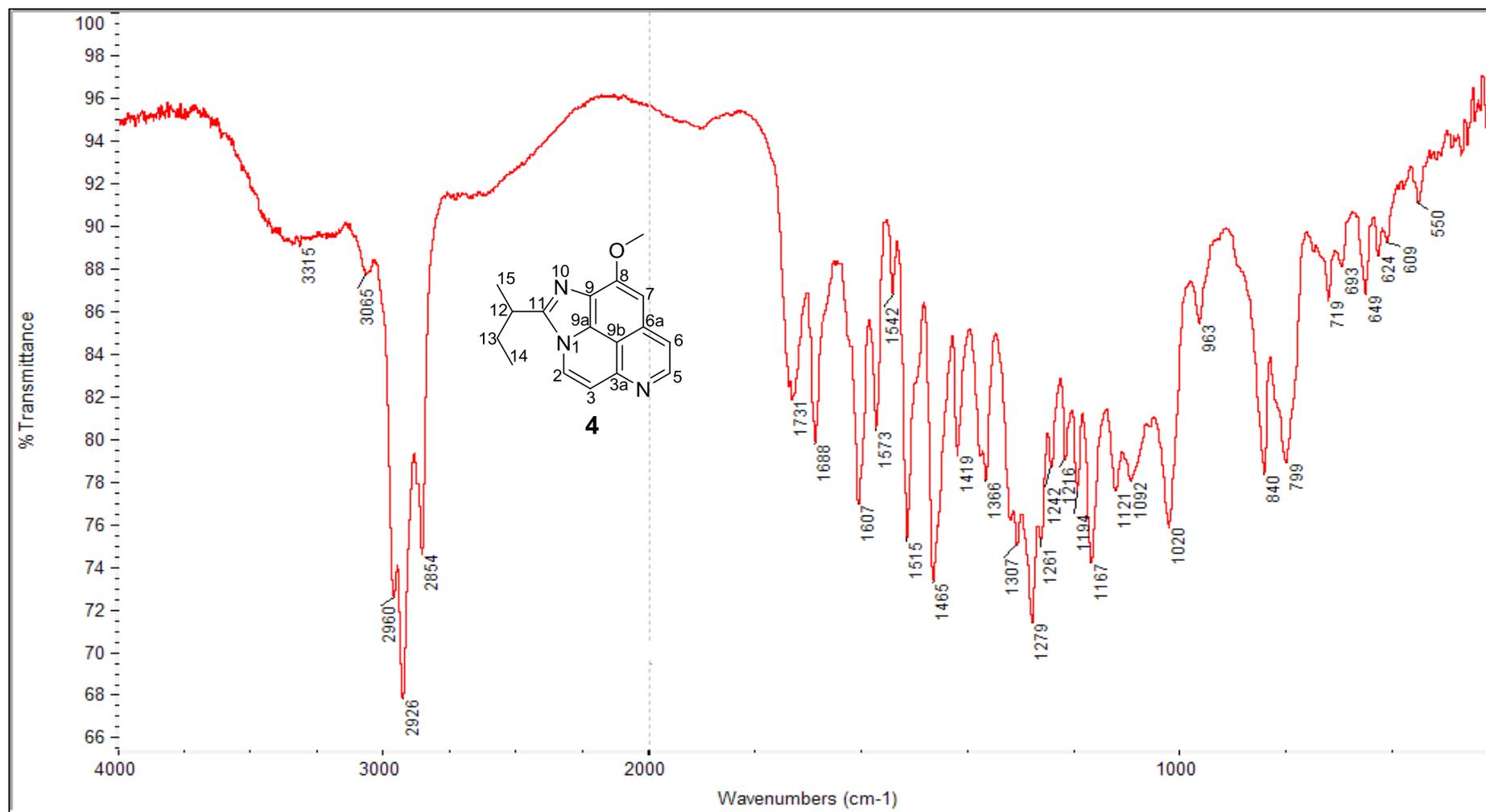


Figure S39. HRESIMS of compound 4.

Elemental Composition Report

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
 Selected filters: None

Monoisotopic Mass, Even Electron Ions

12 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

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SIPI

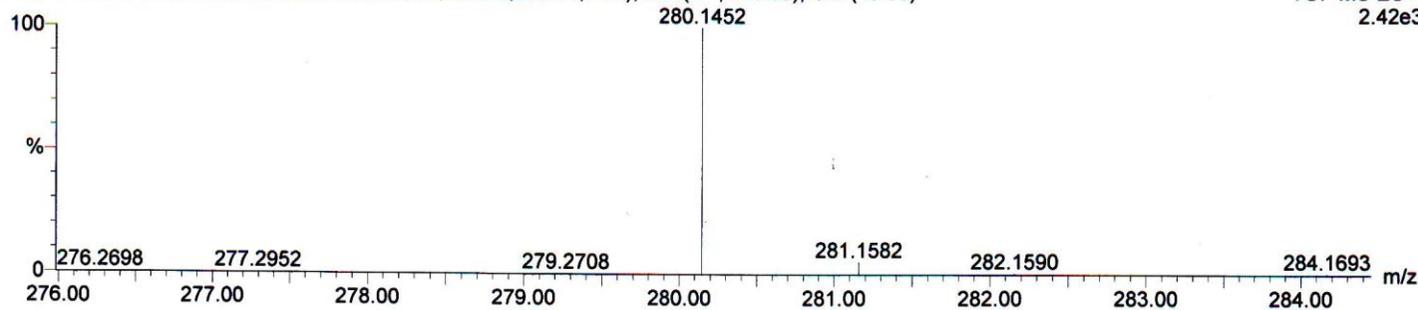
M.W.=279

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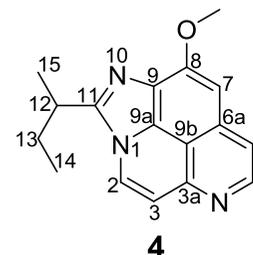
Q-Tof micro
 YA019

31-Oct-2013,15:52:17

TOF MS ES+
 2.42e3



Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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Figure S40. UV spectrum of compound 4.

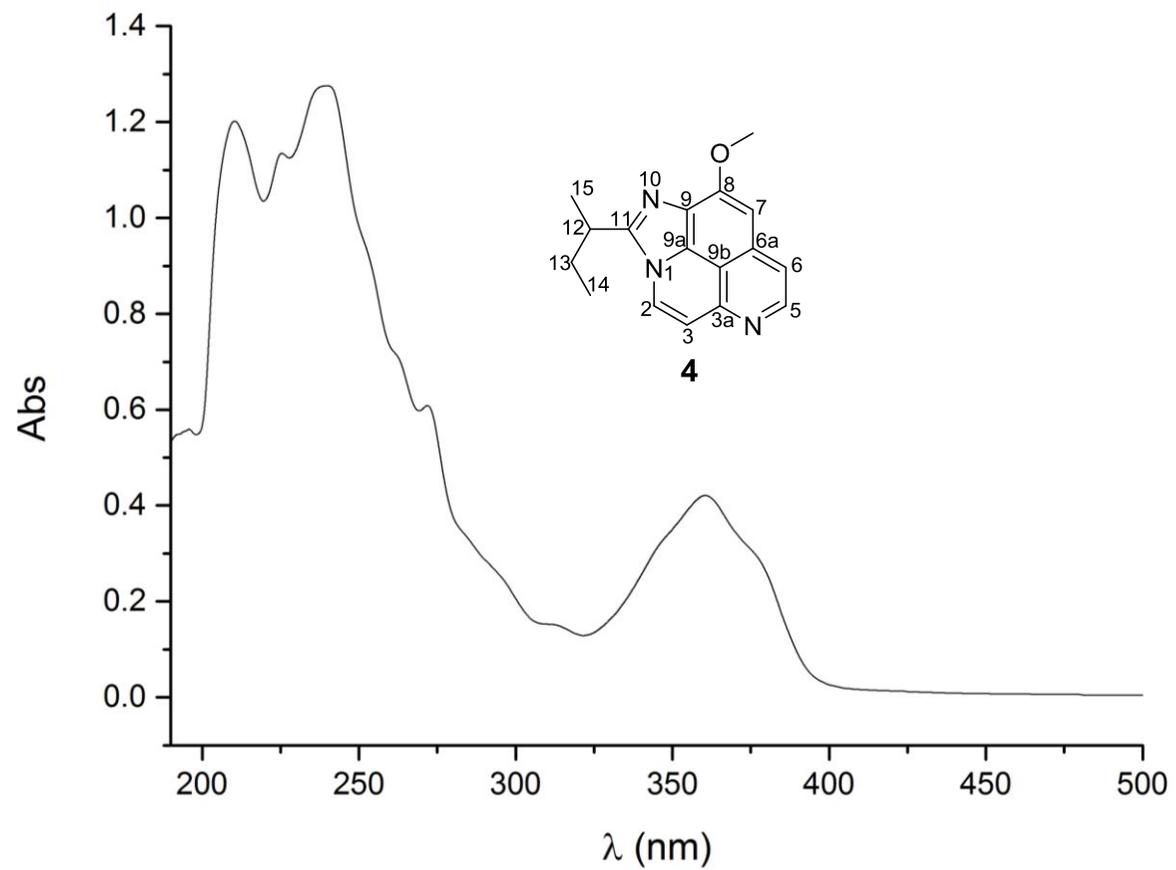


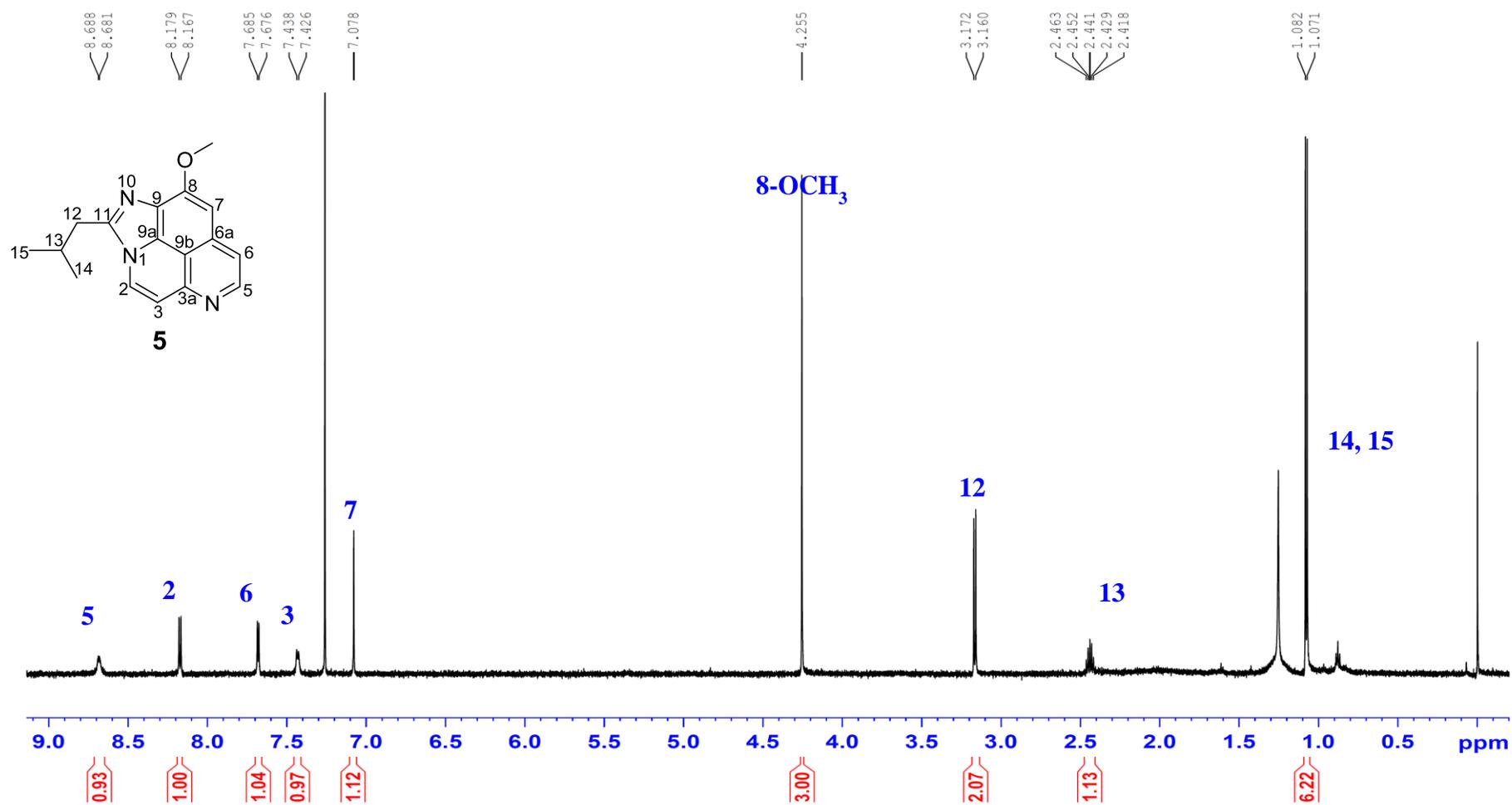
Figure S41. ¹H NMR spectrum of compound **5** in CDCl₃.

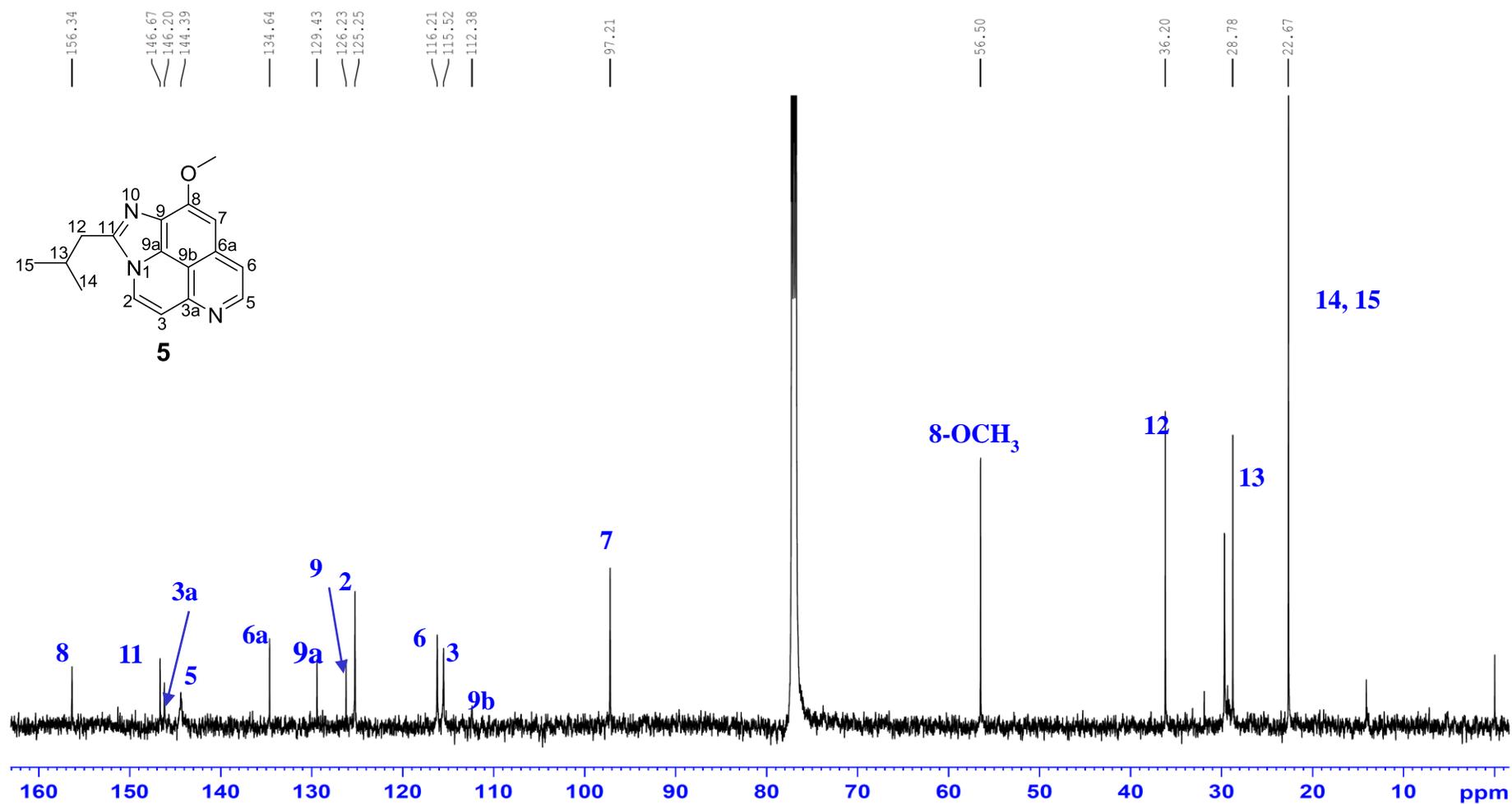
Figure S42. ^{13}C NMR spectrum of compound **5** in CDCl_3 .

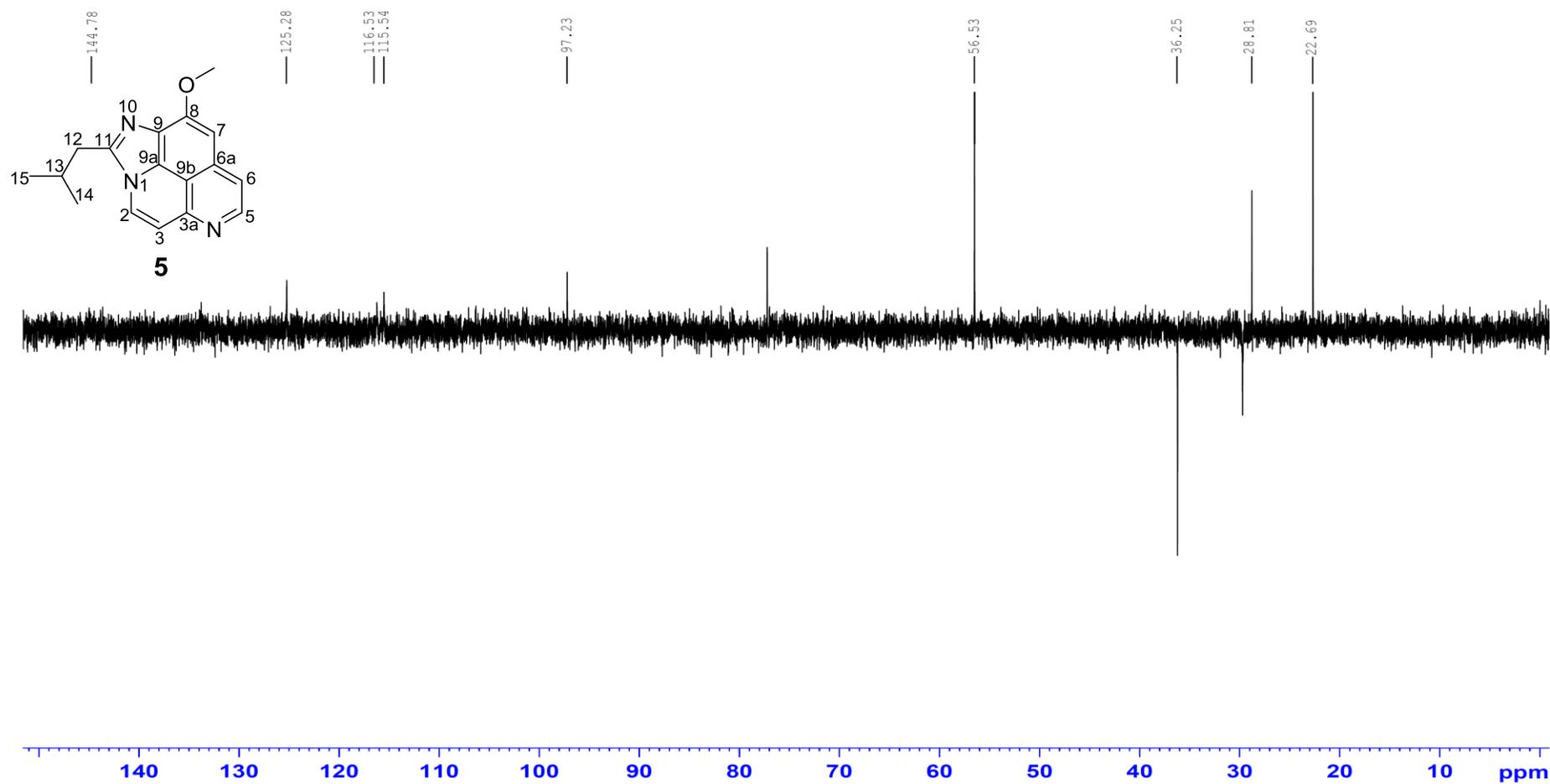
Figure S43. DEPT135 Spectrum of compound **5** in CDCl₃.

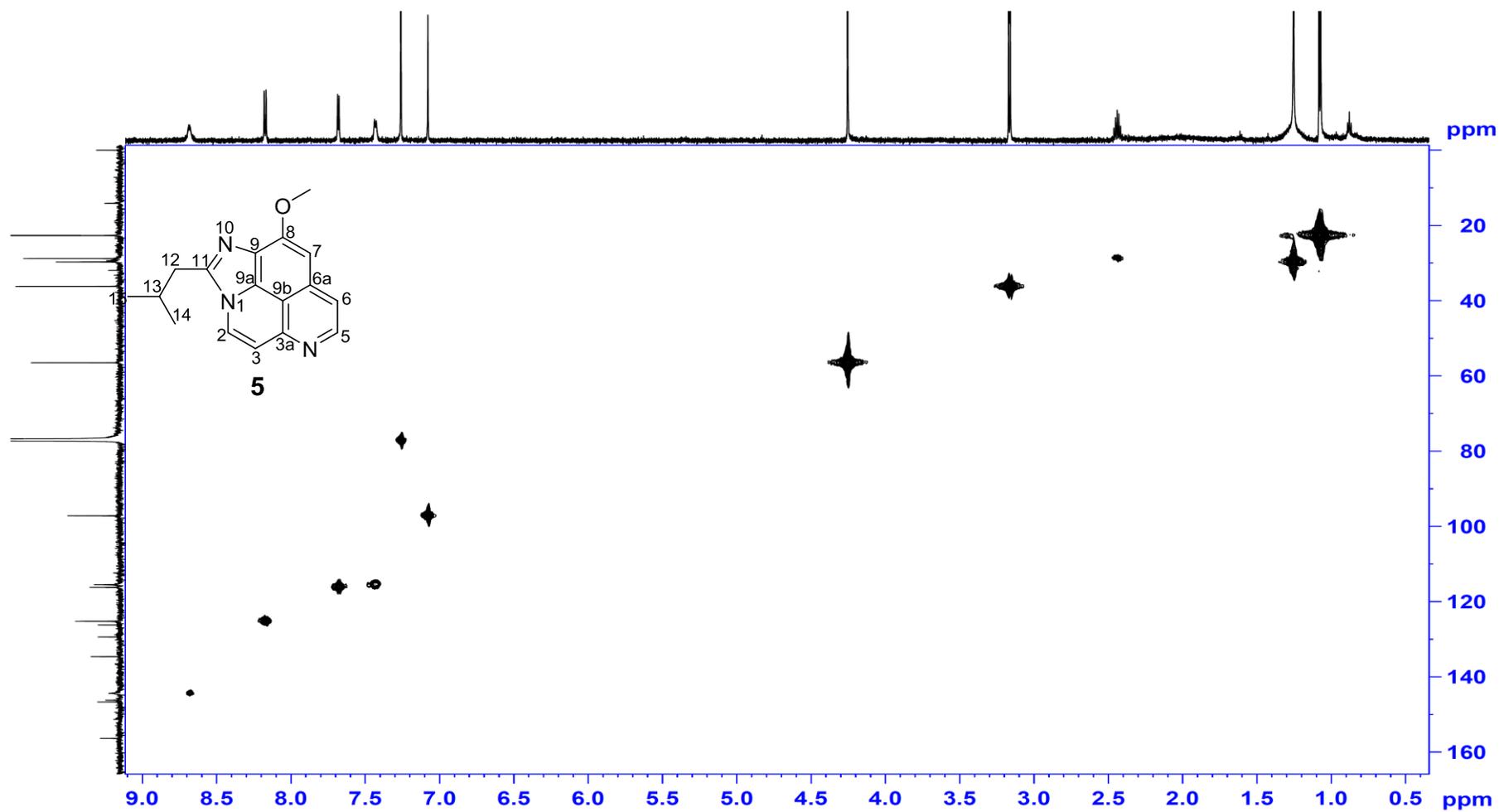
Figure S44. HSQC spectrum of compound **5** in CDCl₃.

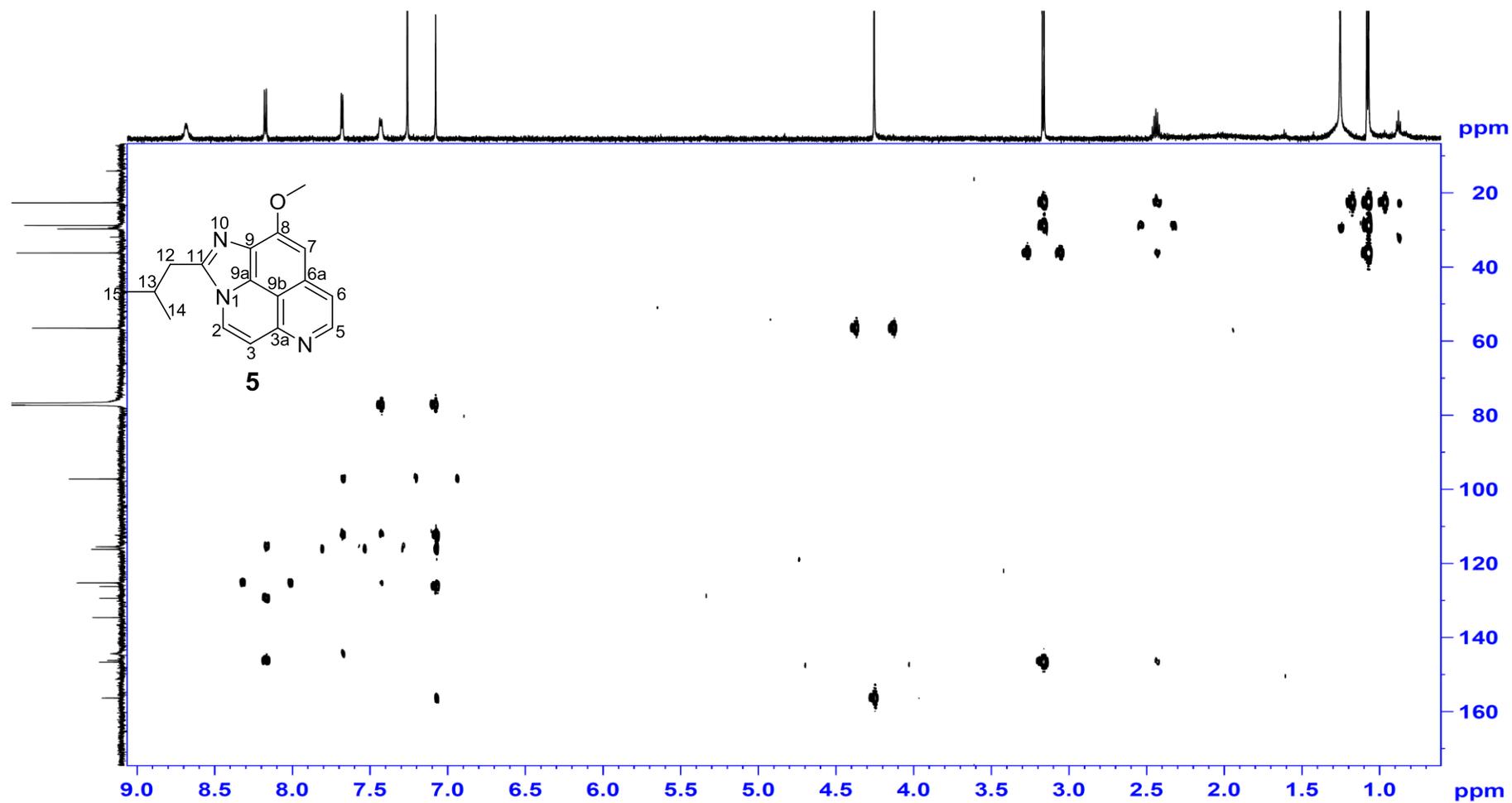
Figure S45. HMBC spectrum of compound 5 in CDCl₃.

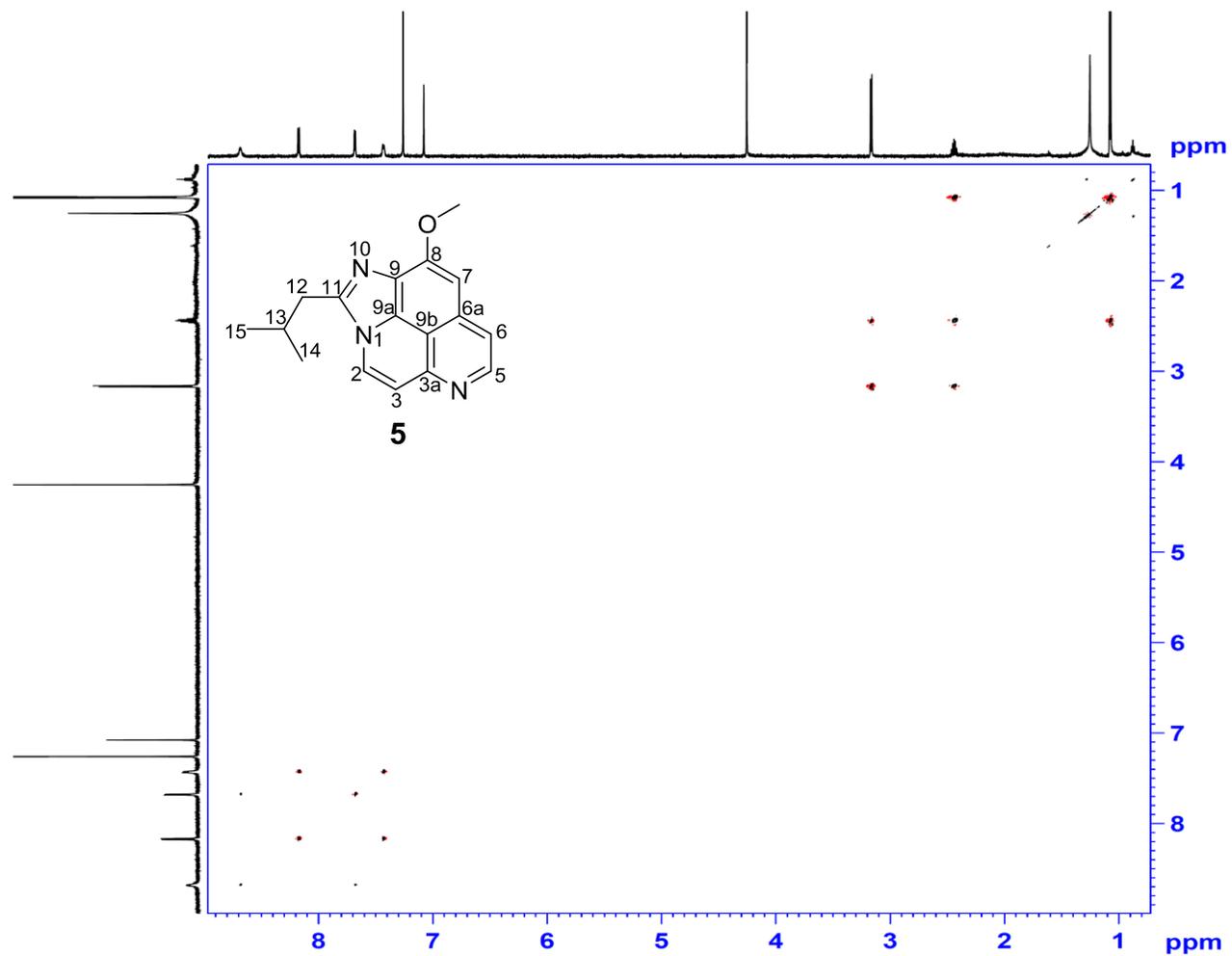
Figure S46. ^1H - ^1H COSY spectrum of compound **5** in CDCl_3 .

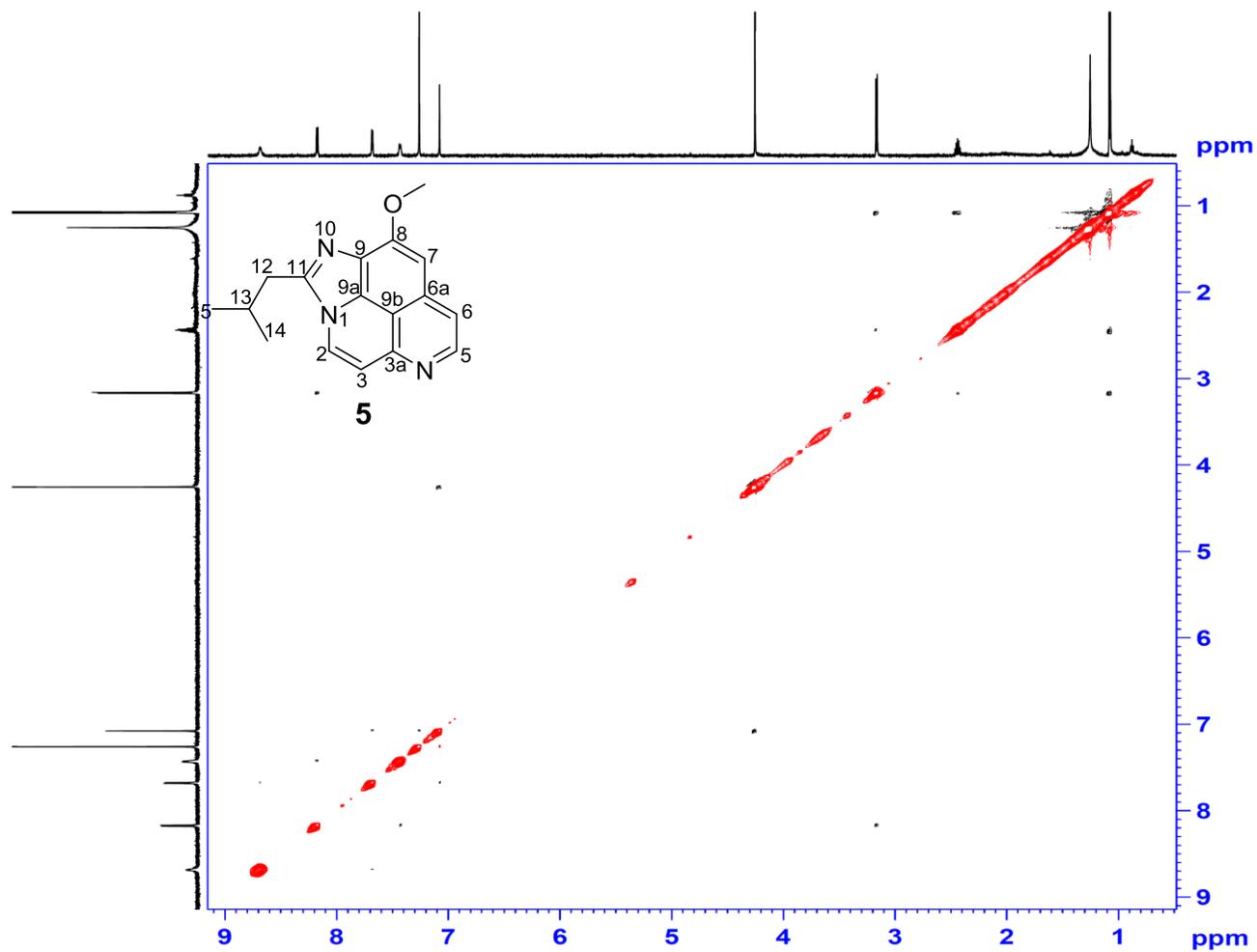
Figure S47. NOESY spectrum of compound **5** in CDCl₃.

Figure S48. IR spectrum of compound 5.

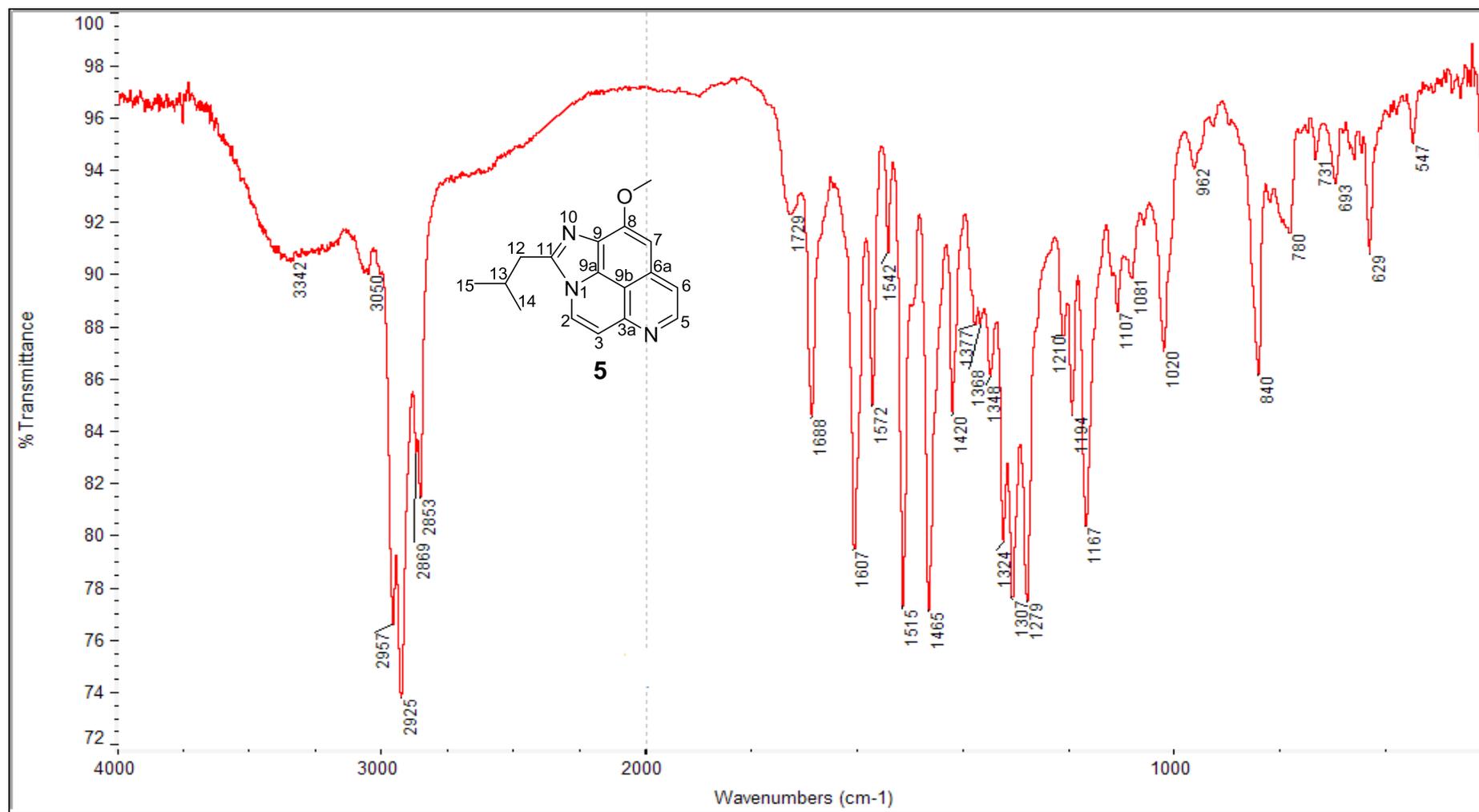
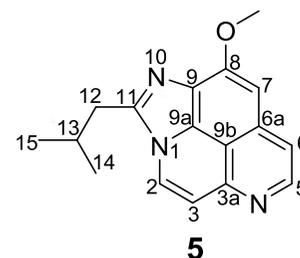


Figure S49. HRESIMS of compound 5.

Elemental Composition Report

Page 1

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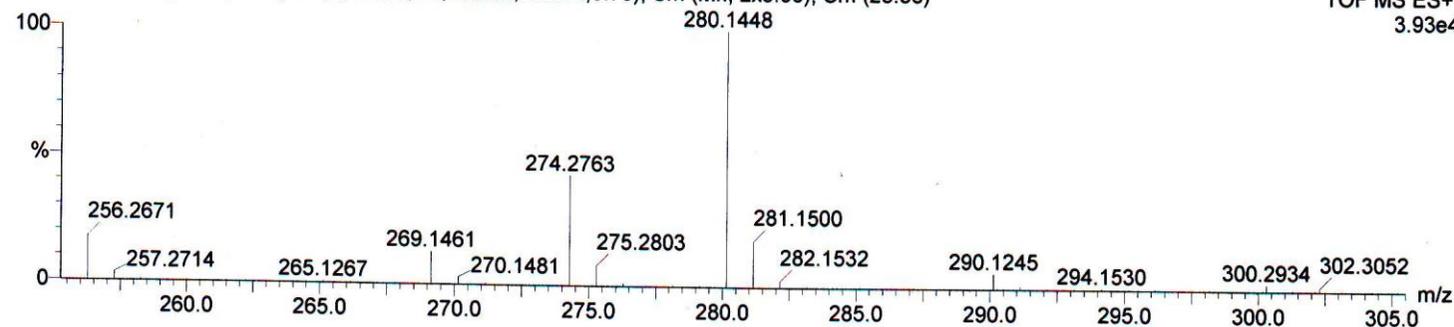
Monoisotopic Mass, Even Electron Ions
 5 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:
 C: 5-20 H: 5-20 N: 1-3 O: 1-1

SIPI
 M.W.=279
 Q-ToF micro YA019
 WQ14-004H 23 (0.794) AM (Cen,4, 80.00, Ar,5000.0,268.14,0.70); Sm (Mn, 2x3.00); Cm (23:38)

03-Jan-2014,14:41:48

TOF MS ES+
 3.93e4



Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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Figure S50. UV spectrum of compound 5.

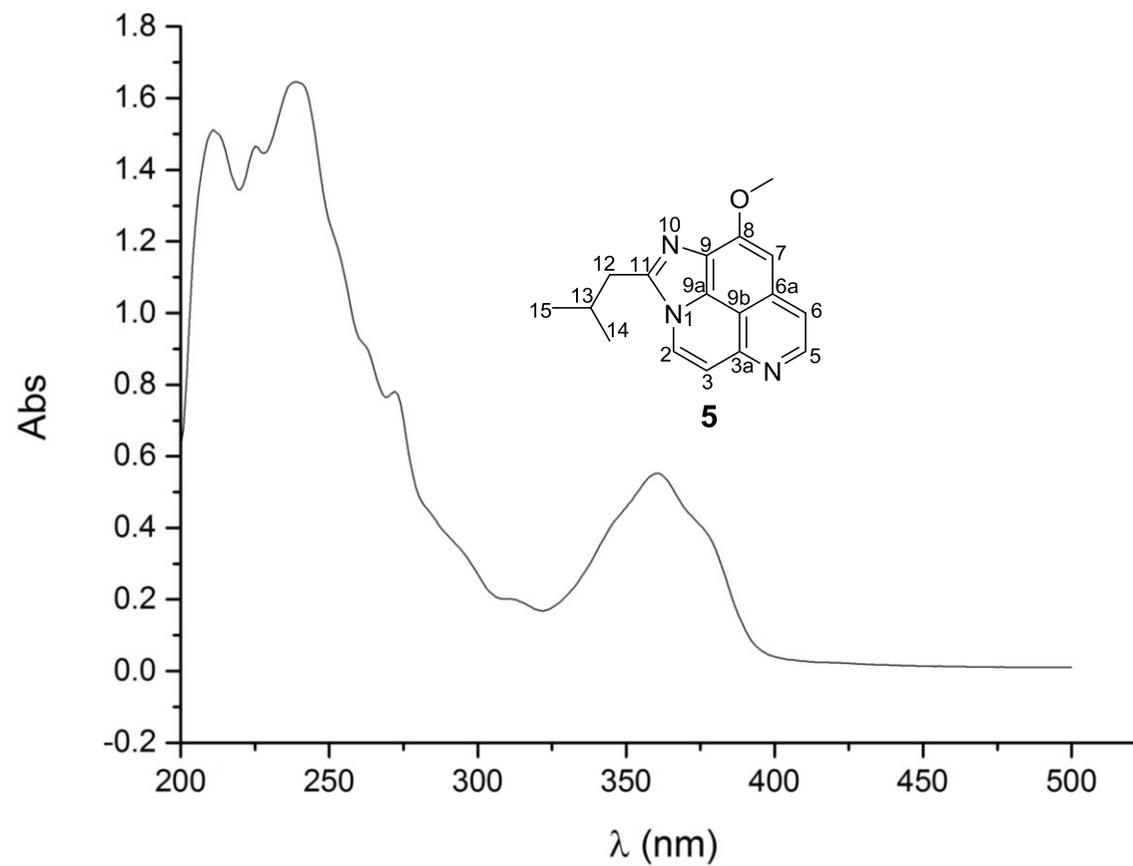


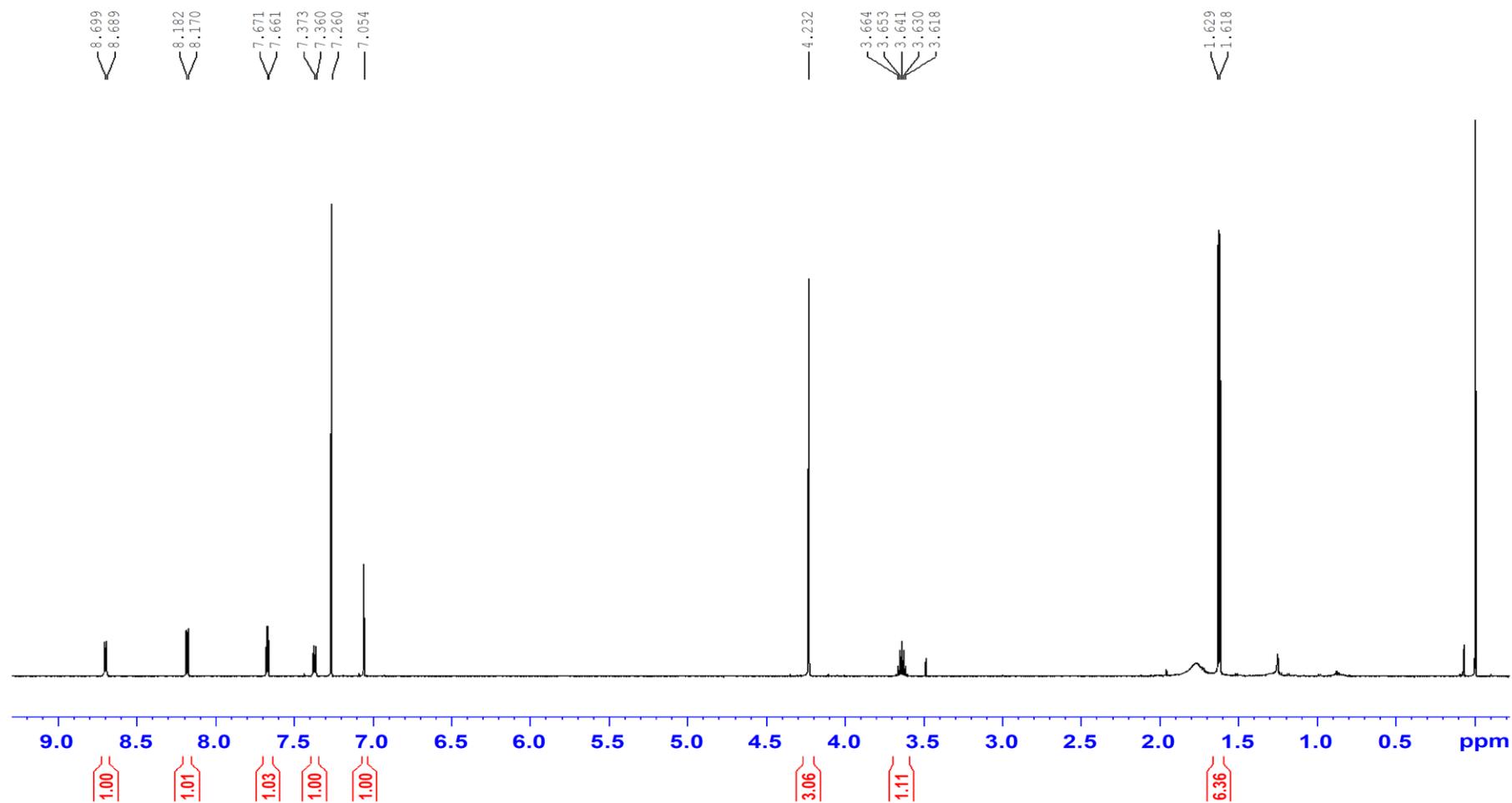
Figure S51. ^1H NMR spectrum of compound **6** in CDCl_3 .

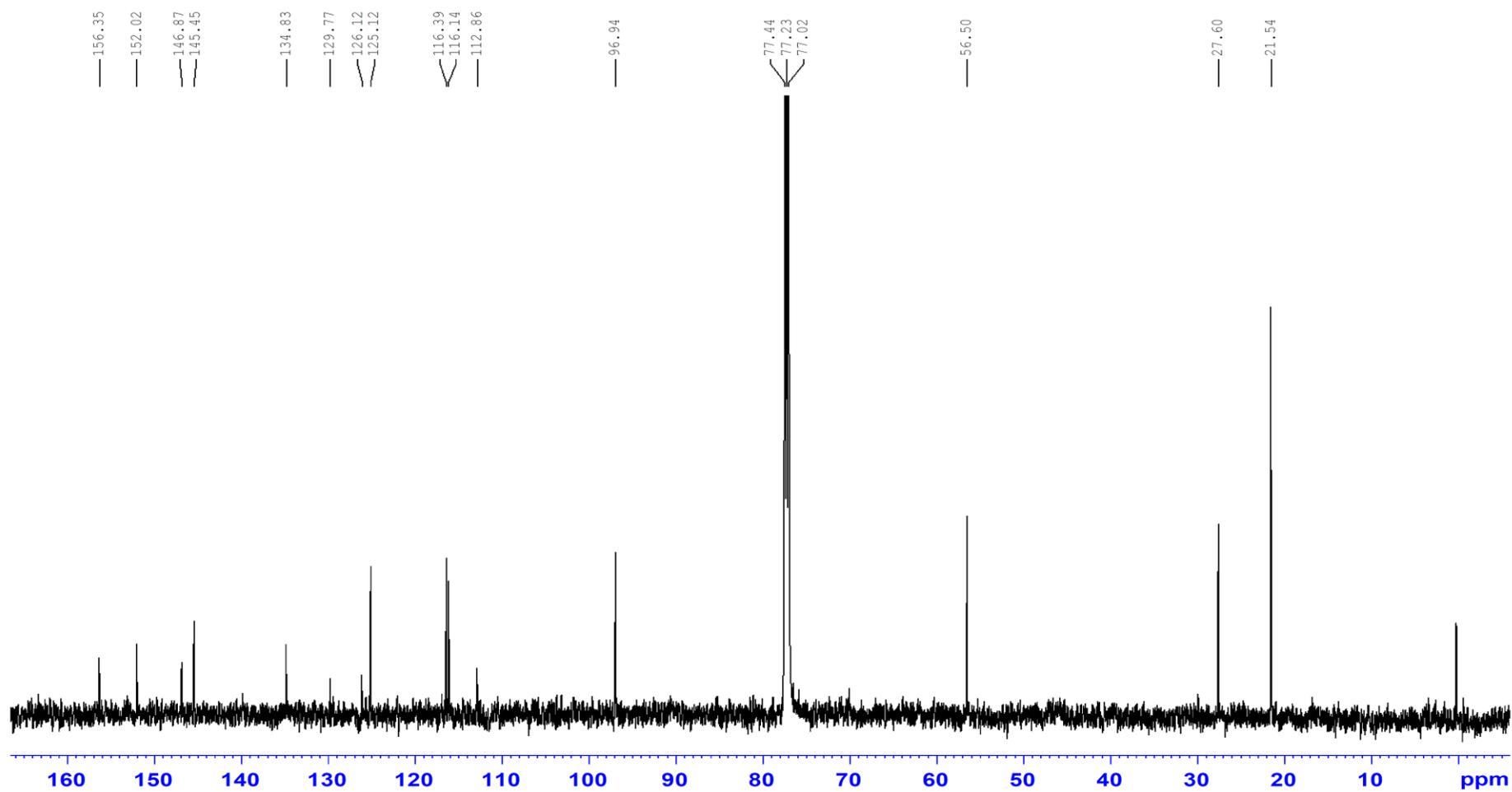
Figure S52. ^{13}C NMR spectrum of compound **6** in CDCl_3 .

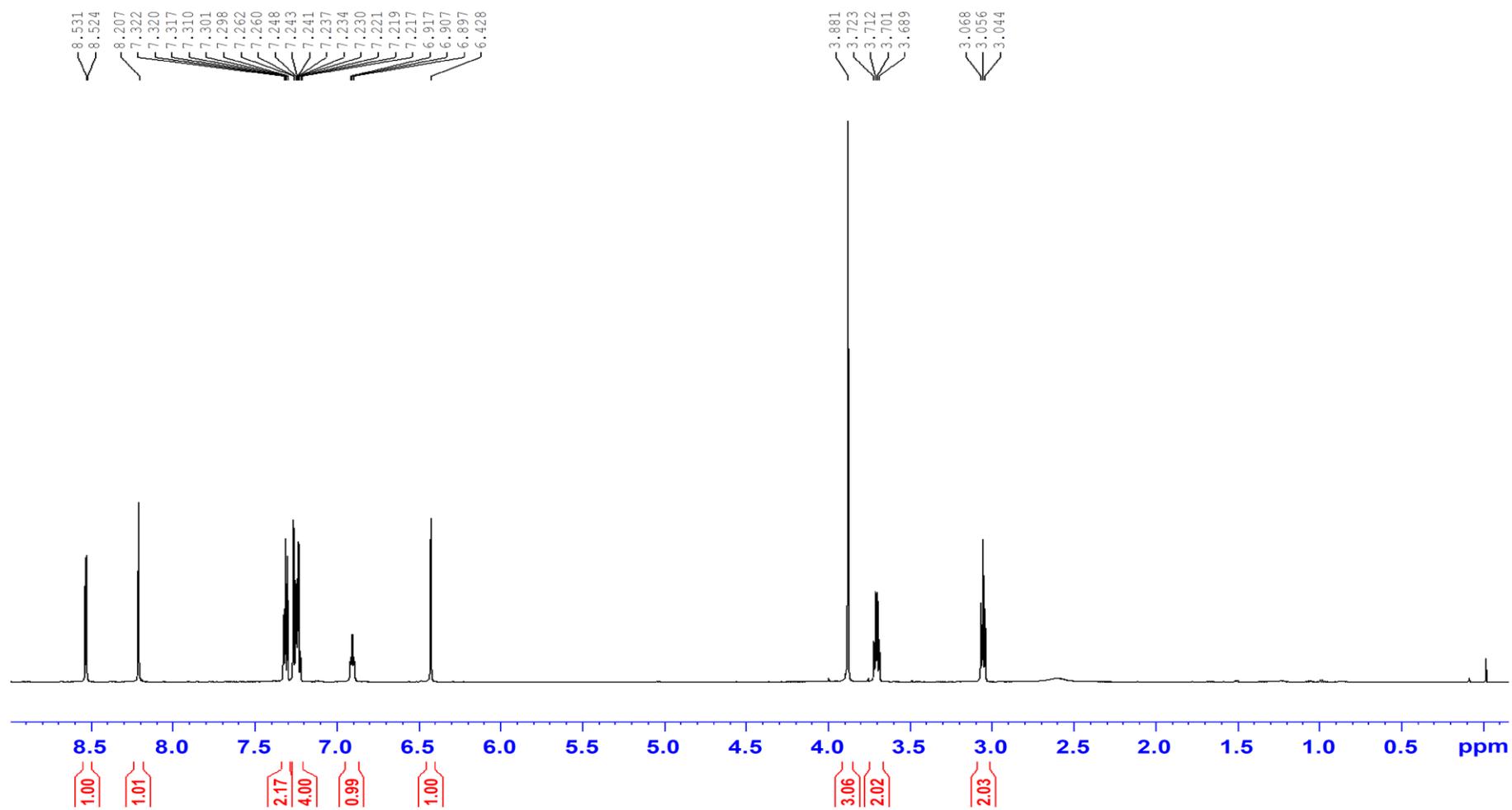
Figure S53. ^1H NMR spectrum of compound **7** in CDCl_3 .

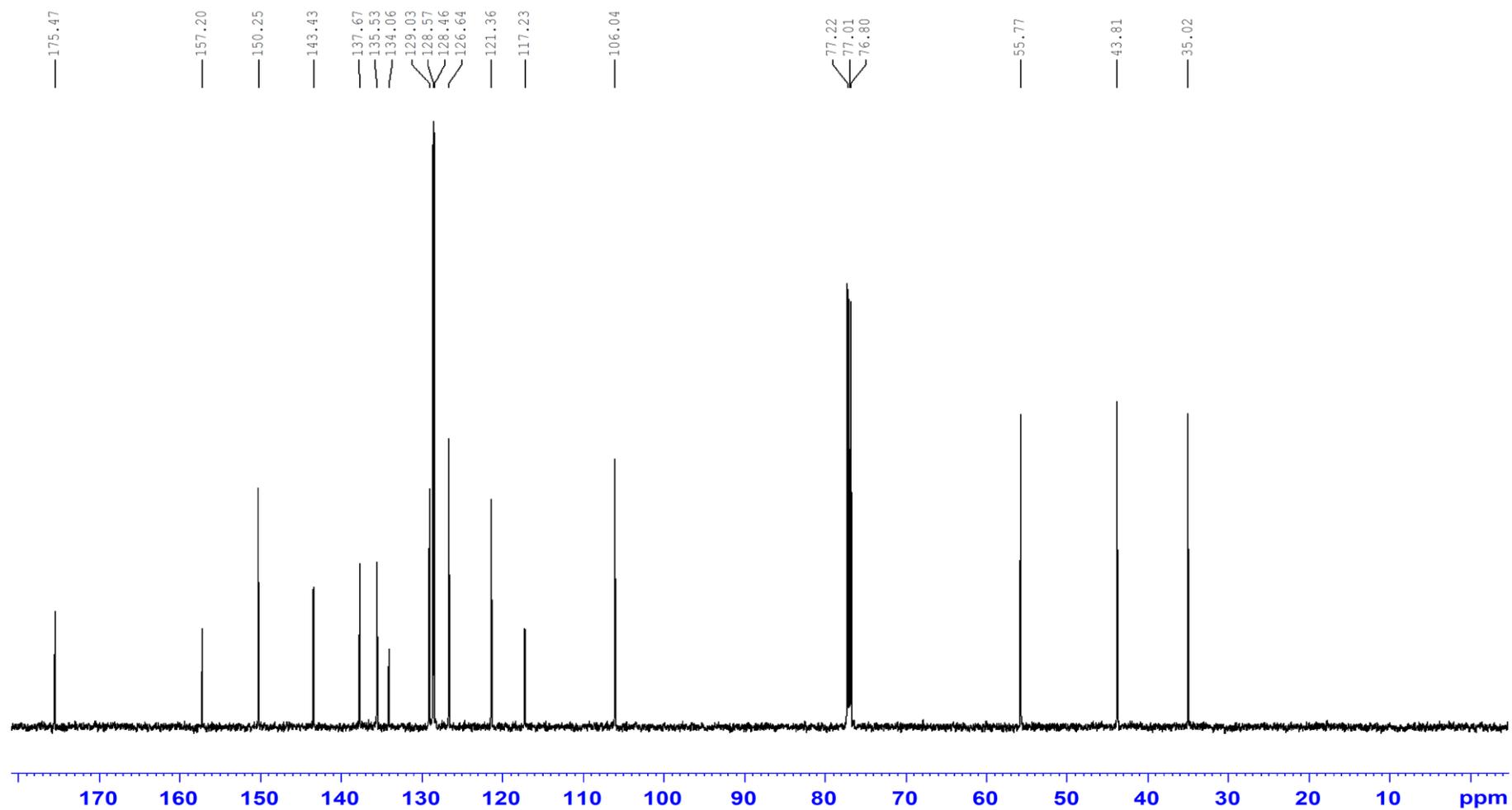
Figure S54. ^{13}C NMR spectrum of compound 7 in CDCl_3 .

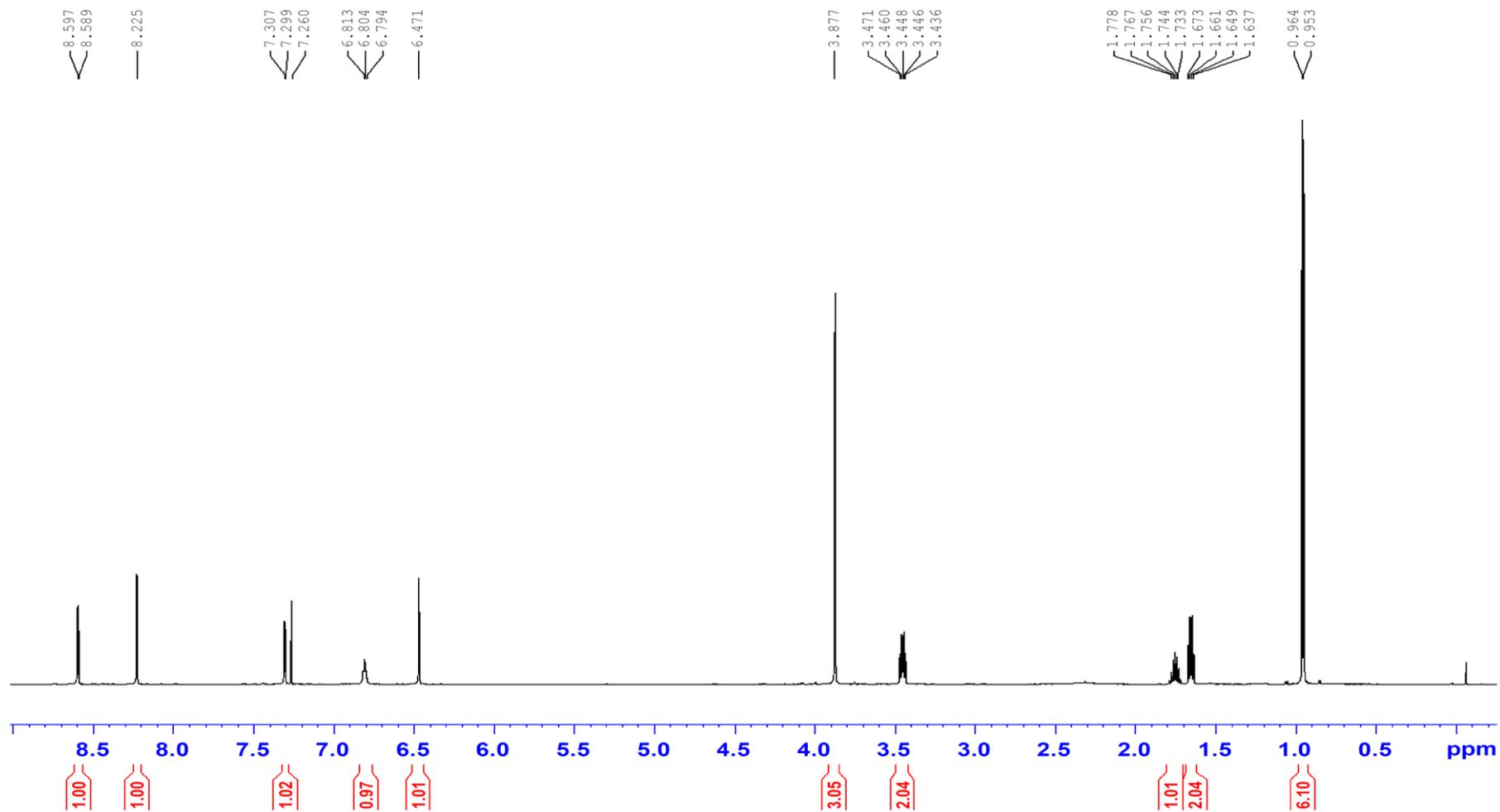
Figure S55. ^1H NMR spectrum of compound **8** in CDCl_3 .

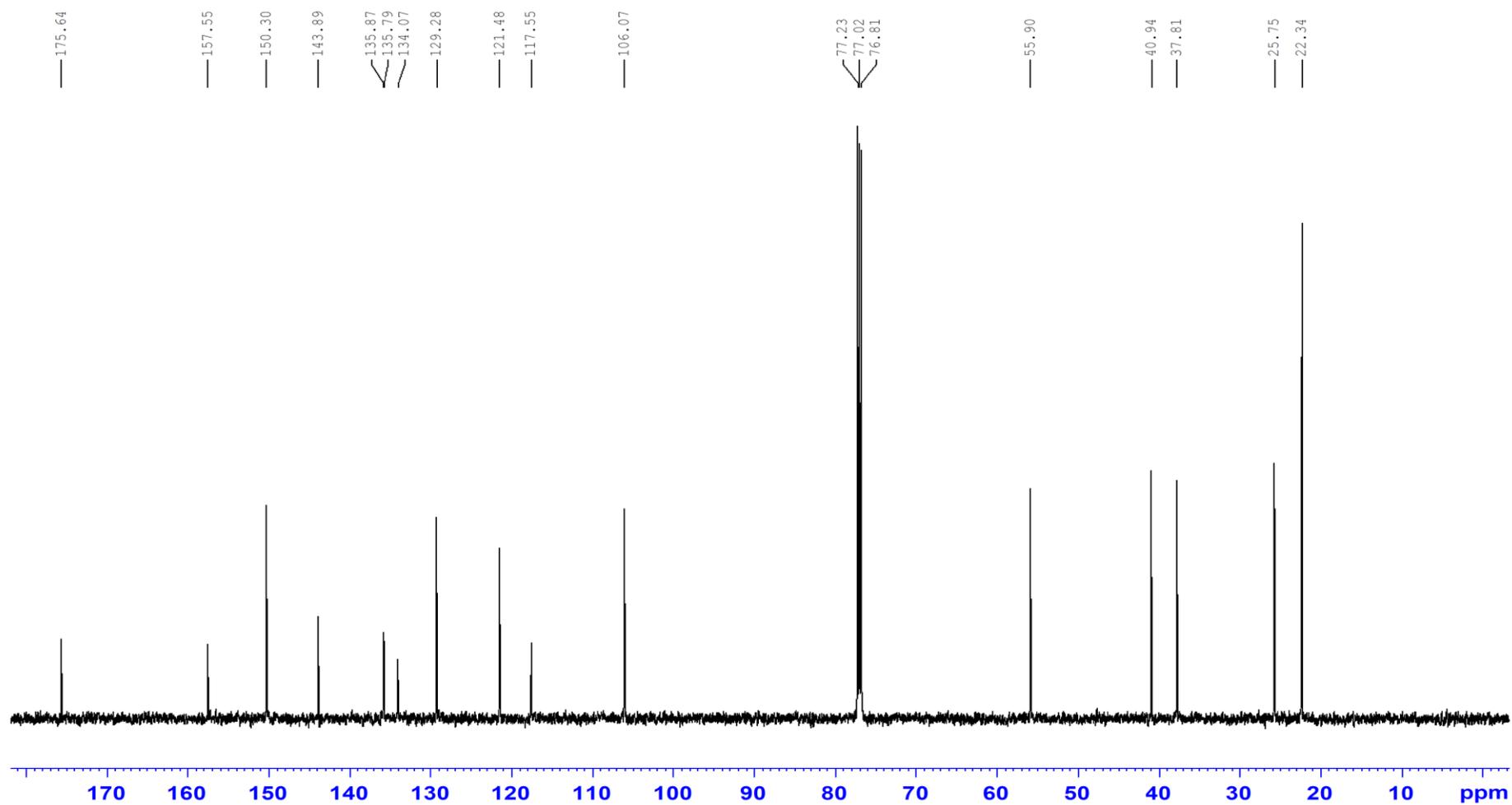
Figure S56. ^{13}C NMR spectrum of compound **8** in CDCl_3 .

Table S1. NMR Spectroscopic Data for Compounds 6–8 in CDCl₃.

Position	6 ^a		7 ^a		8 ^a	
	δ_C	δ_H , mult. (J in Hz)	δ_C	δ_H , mult. (J in Hz)	δ_C	δ_H , mult. (J in Hz)
2	125.1, CH	8.69, d, (6.0)	129.0, CH	8.21, s	129.3, CH	8.22, s
3	116.1, CH	7.37, d, (7.2)	143.4, qC		143.9, qC	
3a	146.9, qC		135.5, qC		135.8, qC	
5	145.4, CH	8.17, d, (7.2)	150.3, CH	8.53, d, (4.2)	150.3, CH	8.59, d, (4.2)
6	116.4, CH	7.67, d, (6.0)	121.4, CH	7.32, d, (4.2)	121.5, CH	7.30, d, (4.2)
6a	134.8, qC		135.5, qC		135.8, qC	
7	96.9, CH	7.05, s	106.1, CH	6.43, s	106.1, CH	6.47, s
8	156.4, qC		157.2, qC		157.6, qC	
9	126.1, qC		175.5, qC		175.6, qC	
9a	129.8, qC		134.1, qC		134.1, qC	
9b	112.9, qC		117.2, qC		117.6, qC	
8-OCH ₃	56.5, CH ₃	4.23, s	55.8, CH ₃	3.88, s	55.9, CH ₃	3.88, s
11	152.0, qC					
12	27.6, CH	3.64, m				
13	21.5, CH ₃	1.62, d, (7.2)				
14	21.5, CH ₃	1.62, d, (7.2)				
1'				6.91, t, (6.0)		6.80, t, (6.0)
2'			43.8, CH ₂	3.70, q, (13.8, 7.2)	40.9, CH ₂	3.45, m
3'			35.0, CH ₂	3.06, t, (7.2)	37.8, CH ₂	1.65, q, (13.0, 7.2)
4'			137.7, qC		25.8, CH	1.75, m
5'			128.5, CH	7.23, m	22.3, CH ₃	0.96, d, (6.6)
6'			128.6, CH	7.30, m	22.3, CH ₃	0.96, d, (6.6)
7'			126.6, CH	7.23, m		
8'			128.6, CH	7.30, m		
9'			128.5, CH	7.23, m		

^a Measured at 600 MHz (¹H) and 150 MHz (¹³C).