

(3+2) Cycloaddition of *N*-benzylazomethine methylide with 4-arylidene-1*H*-imidazole-5(4*H*)-ones

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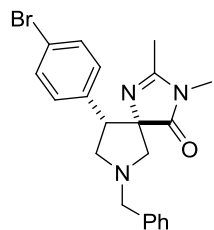
⁴ *A.N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences,
28 Vavilova St., Moscow 119991, Russia*

SUPPLEMENTARY INFORMATION

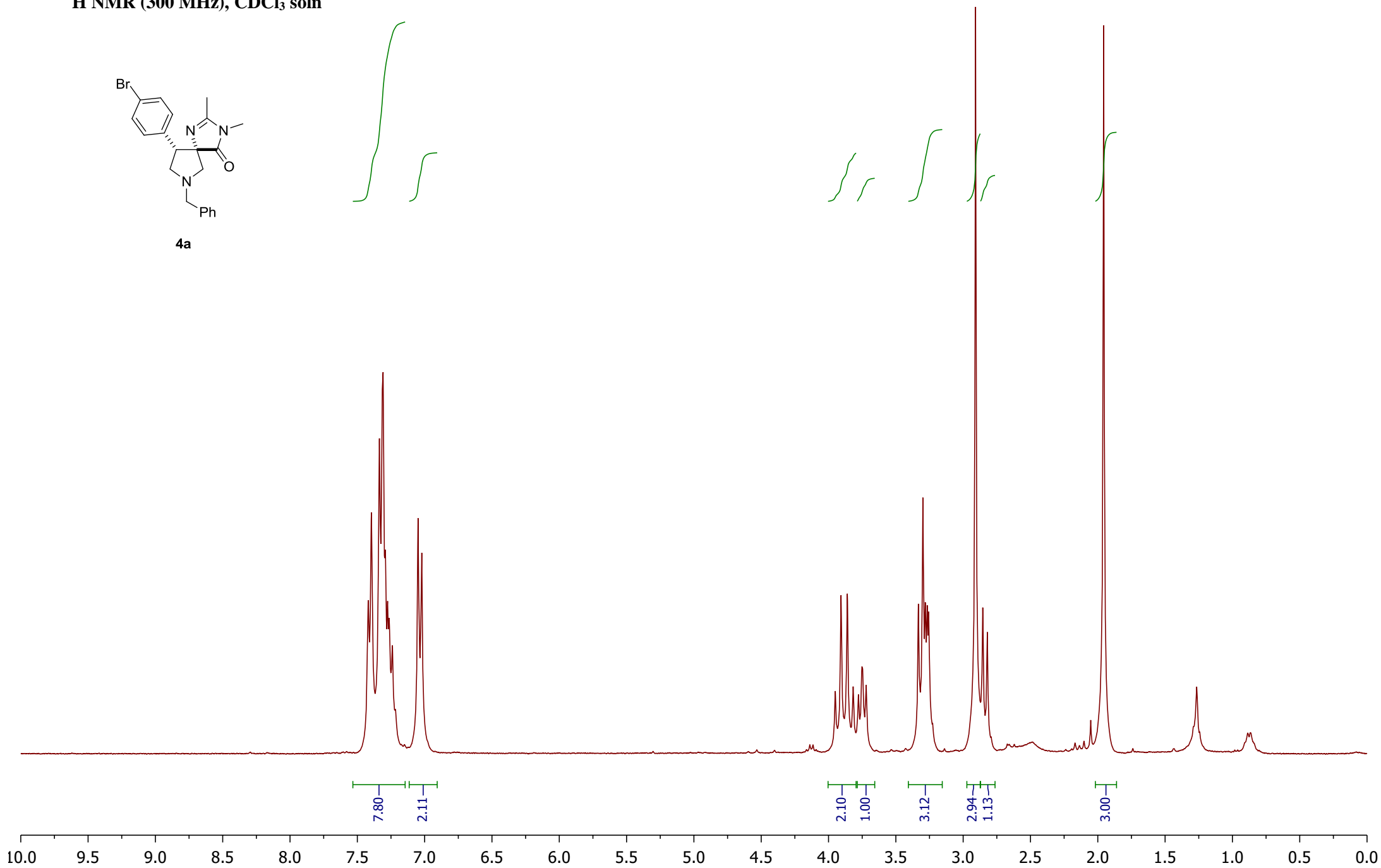
Результаты рентгеноструктурного анализа для соединения 4f

Название образца	akn006
Брутто формула	$C_{22}H_{22}F_3N_3O_2$
Молекулярная масса	417.431
T, K	120
Пространственная группа	C2/c
Z	8
a, Å	26.6231(7)
b, Å	6.2832(2)
c, Å	24.5590(6)
α , °	90
β , °	99.0130(10)
γ , °	90
V, Å ³	4057.46(19)
$d_{\text{выч}}$, г·см ⁻³	1.367
μ , см ⁻¹	9.1
F(000)	1744
$2\theta_{\text{max}}$, °	135
Число измеренных отражений	25006
Число независимых отражений	3966
Число отражений с $I > 2\sigma(I)$	3682
Количество уточняемых параметров	359
R1	0.0410
wR2	0.1135
GOF	1.052
Остаточная электронная плотность, е·Å ⁻³ ($d_{\text{min}}/d_{\text{max}}$)	0.272/-0.303

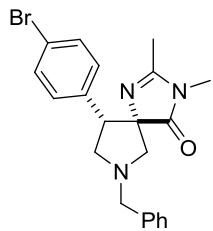
¹H NMR (300 MHz), CDCl₃ soln



4a

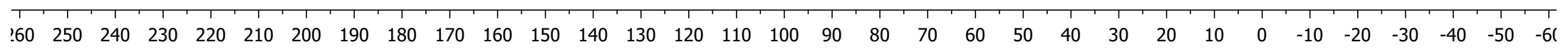


¹³C NMR (75 MHz), CDCl₃ soln

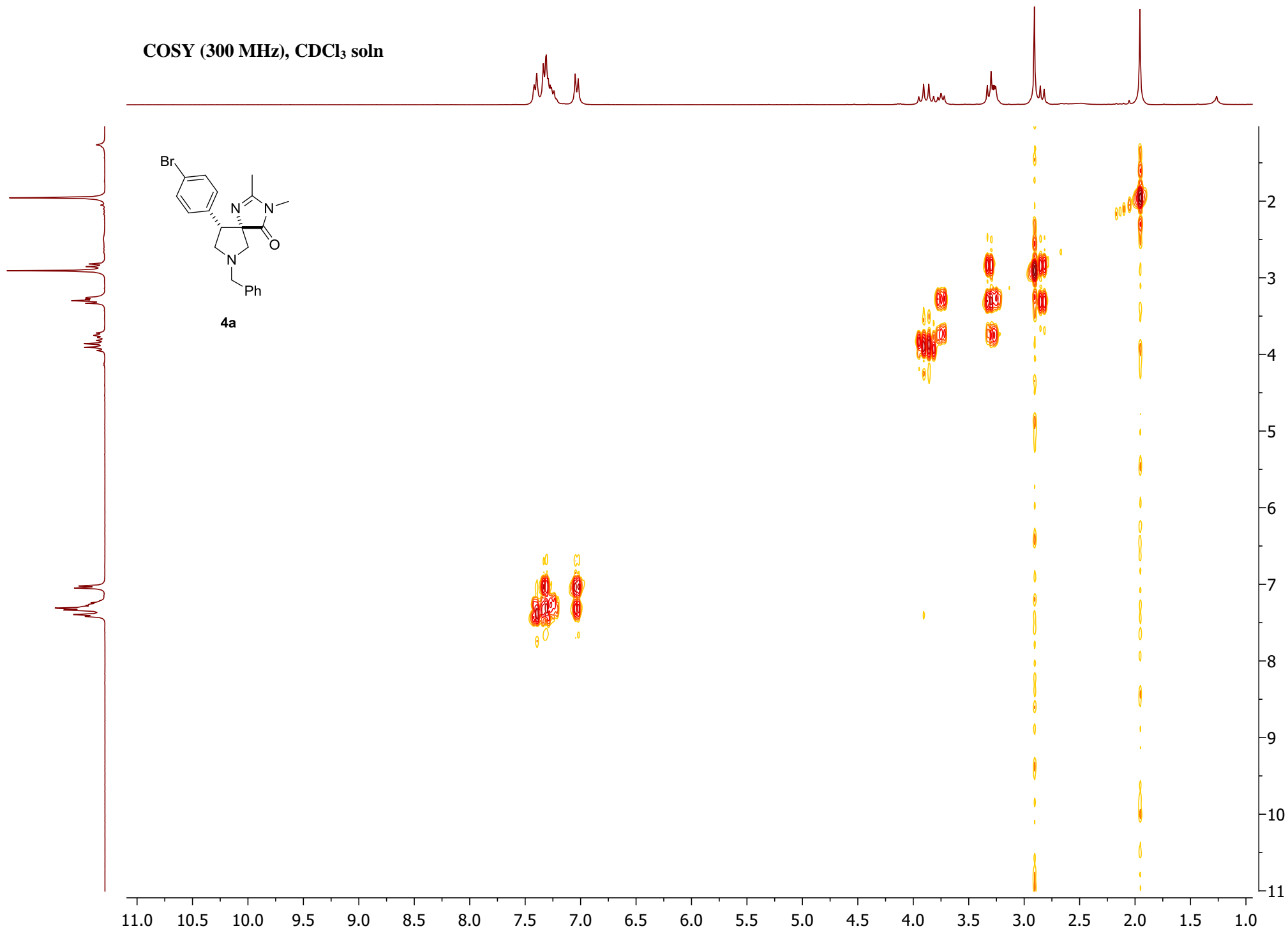


4a

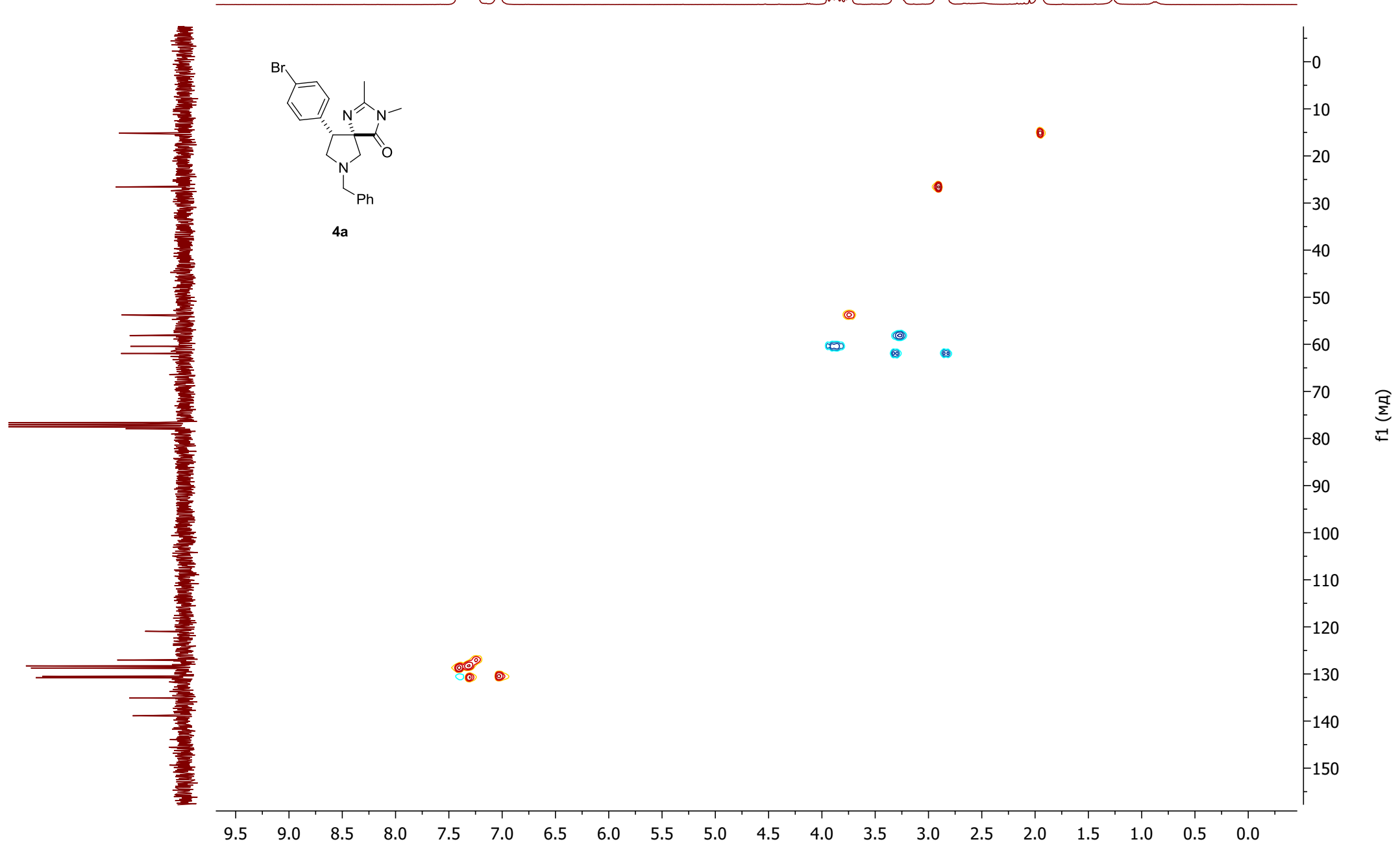
183.24
159.78
138.98
138.98
135.19
130.87
130.59
128.84
128.38
127.14
121.04
78.03
62.05
60.54
58.22
53.88
26.69
15.27



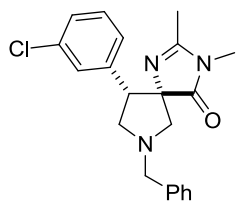
COSY (300 MHz), CDCl₃ soln



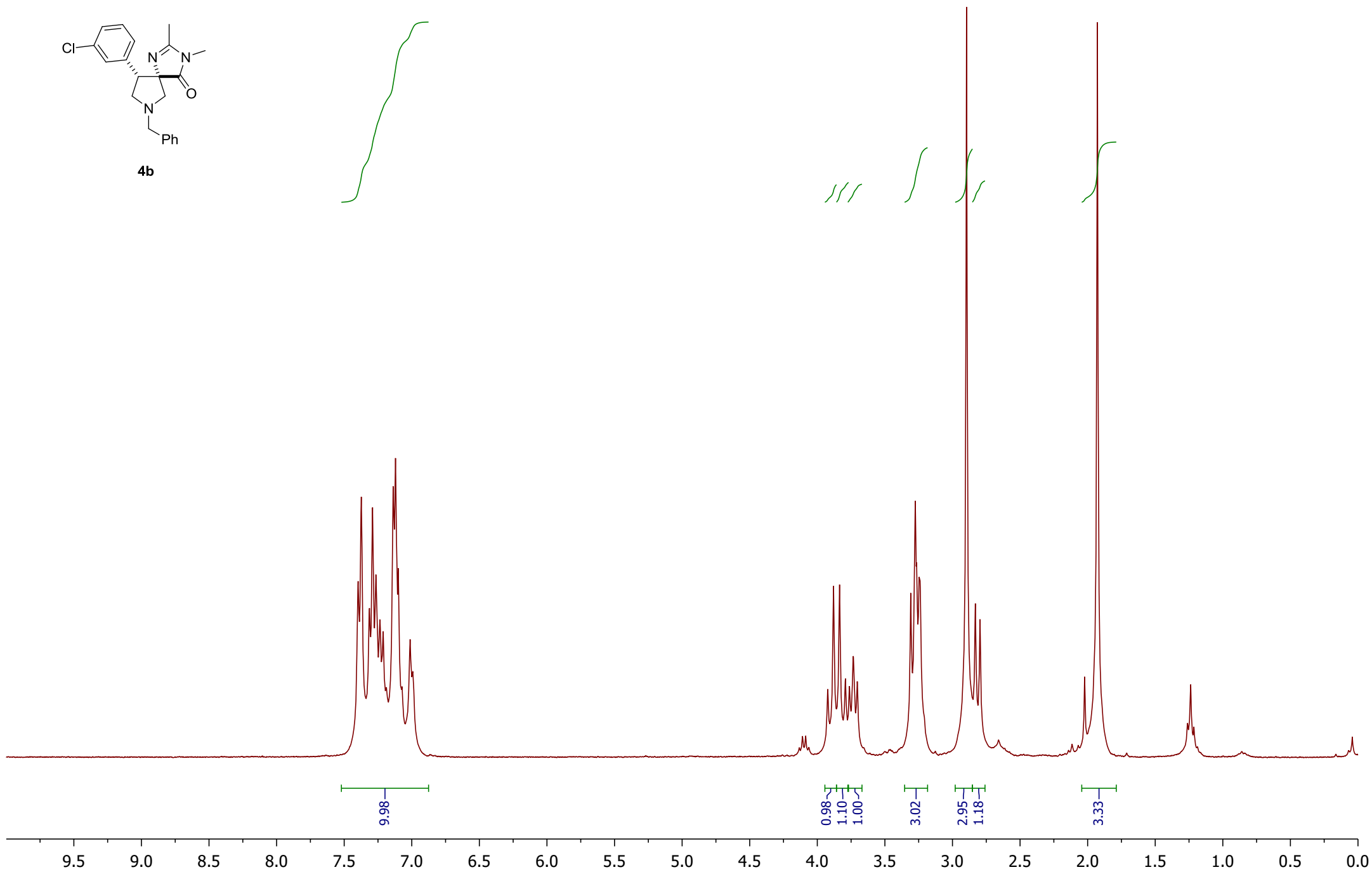
HSQC (300 MHz), CDCl₃ soln



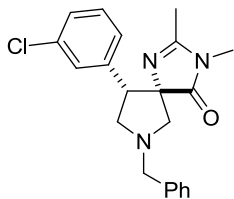
¹H NMR (300 MHz), CDCl₃ soln



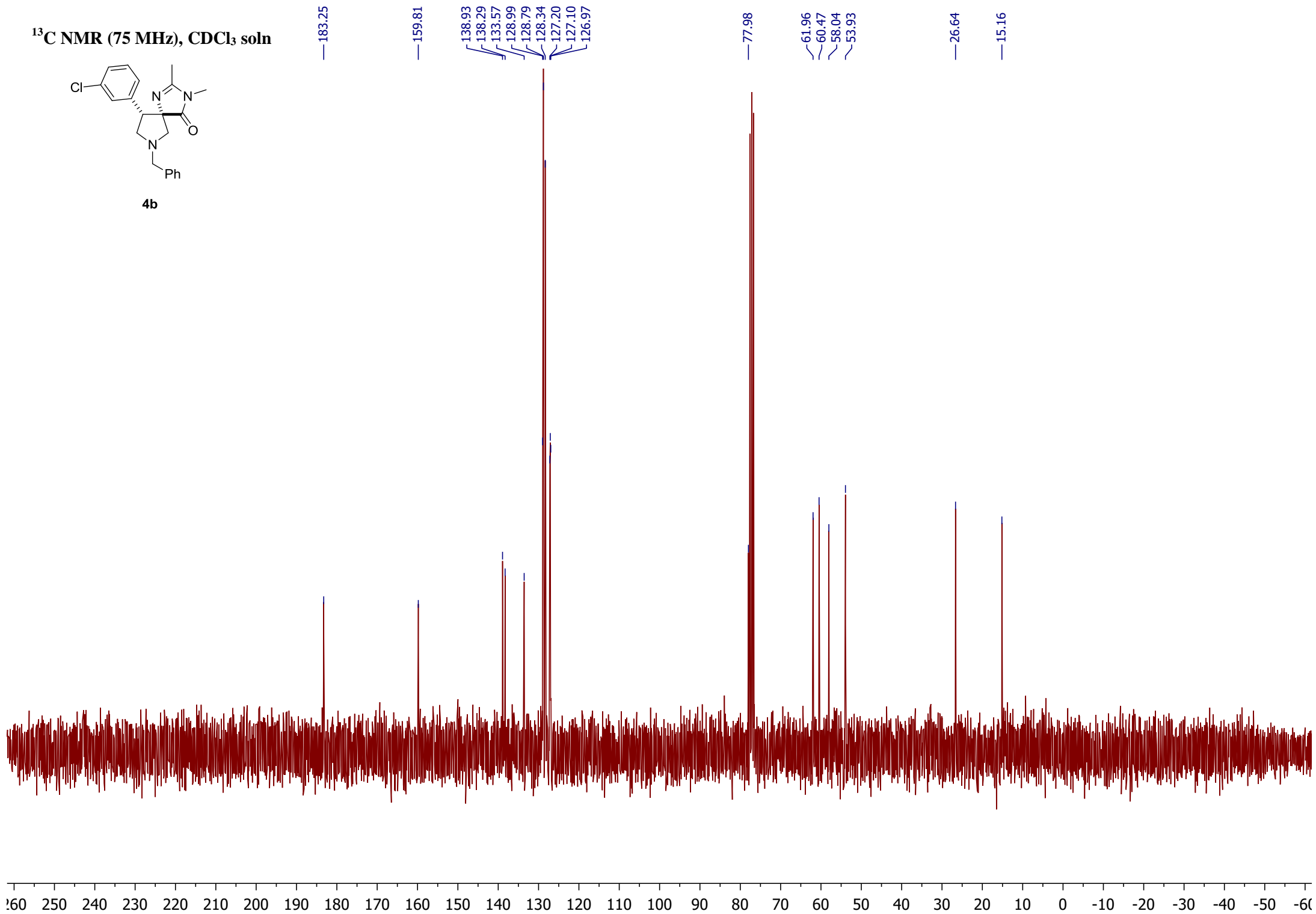
4b



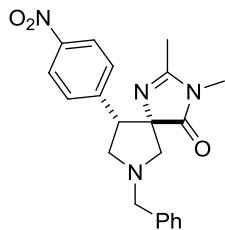
¹³C NMR (75 MHz), CDCl₃ soln



4b



¹H NMR (300 MHz), CDCl₃ soln



4c



2.00

7.58

3.06

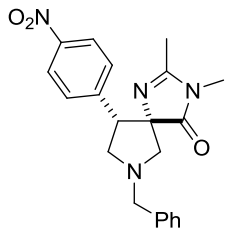
3.06

4.06

3.09

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¹³C NMR (75 MHz), CDCl₃ soln



4c

— 183.11

— 160.20

— 147.06

— 144.63

— 138.75

— 129.73

— 128.82

— 128.44

— 127.25

— 123.00

— 77.98

— 62.41

— 60.34

— 58.36

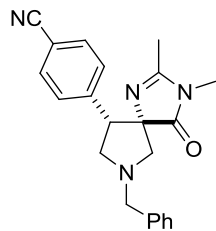
— 53.71

— 26.78

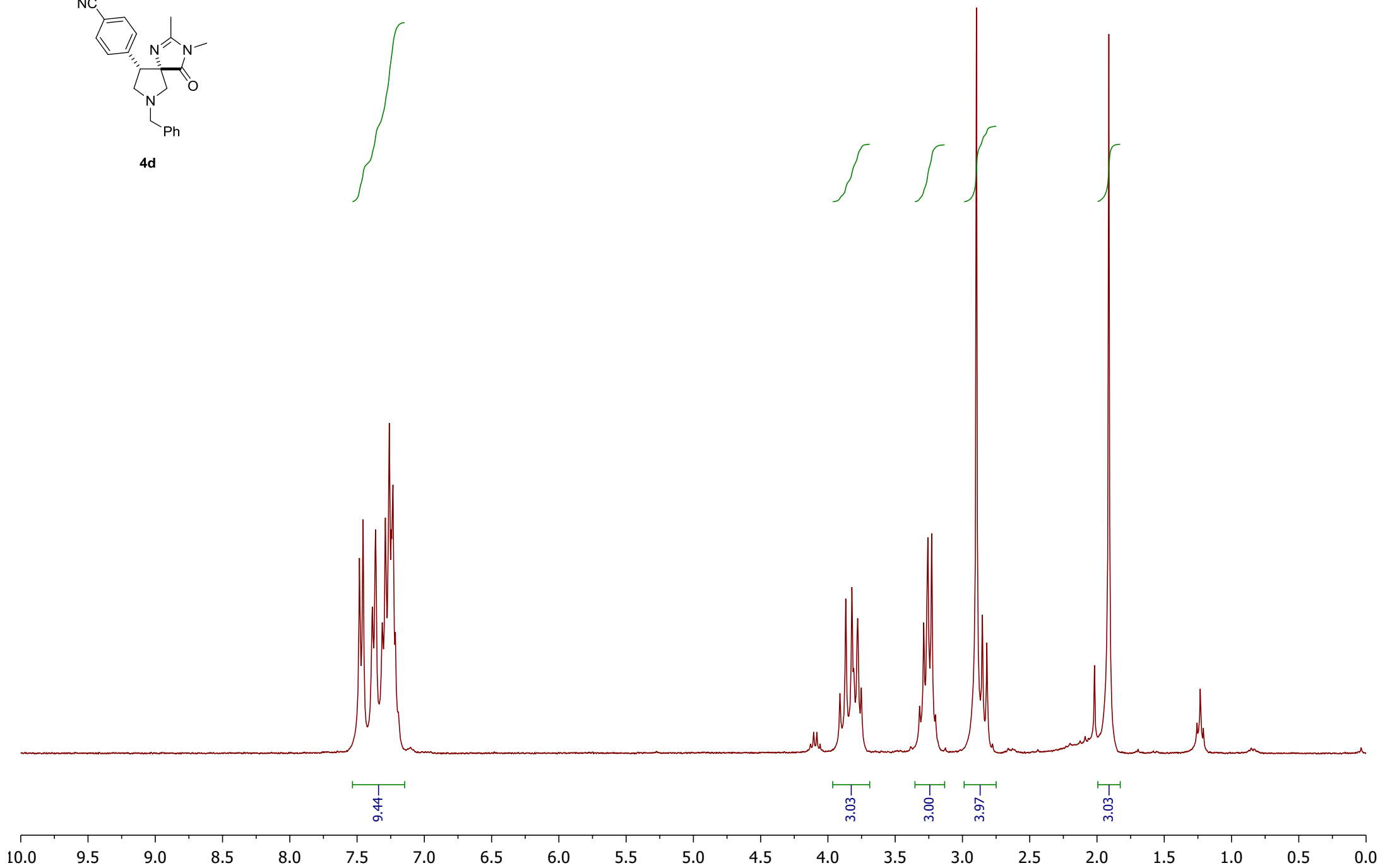
— 15.30

160 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60

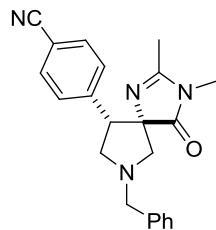
¹H NMR (300 MHz), CDCl₃ soln



4d



¹³C NMR (75 MHz), CDCl₃ soln



4d

— 183.12

— 160.08

142.37

138.77

131.59

129.62

128.82

128.42

127.22

— 118.95

— 110.89

— 77.98

62.30

60.37

58.16

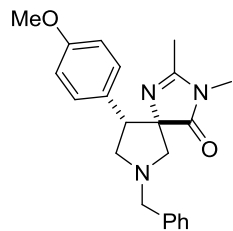
54.01

— 26.75

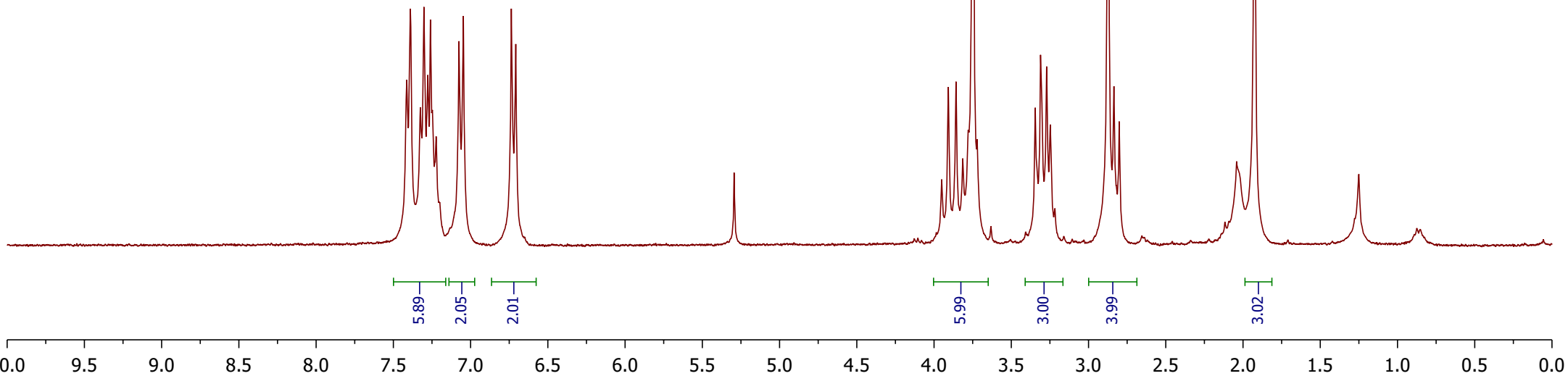
— 15.25

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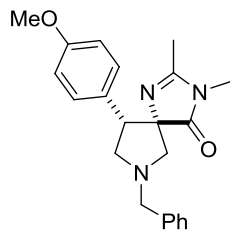
¹H NMR (300 MHz), CDCl₃ soln



4e



¹³C NMR (75 MHz), CDCl₃ soln



4e

—183.51

—159.44

—158.62

—139.20

—129.90

—128.88

—128.37

—127.89

—127.08

—113.11

—78.40

—61.83

—60.71

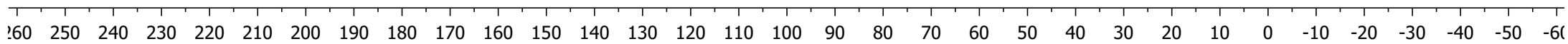
—58.39

—55.29

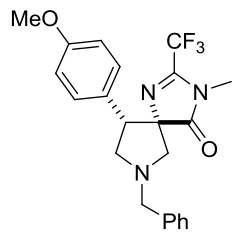
—54.16

—26.65

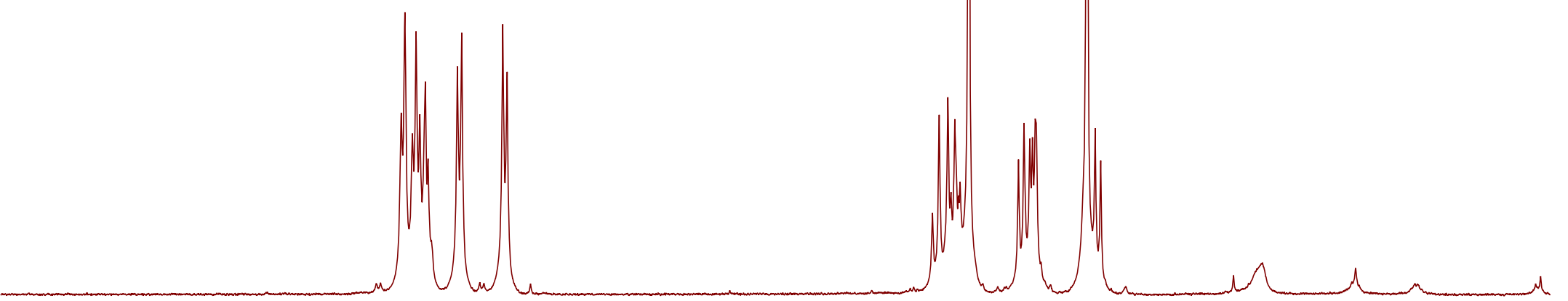
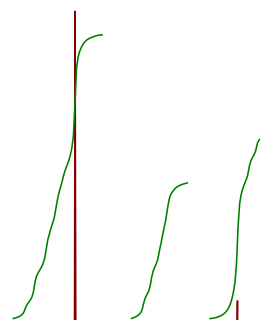
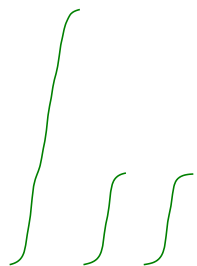
—15.24



¹H NMR (300 MHz), CDCl₃ soln



4f

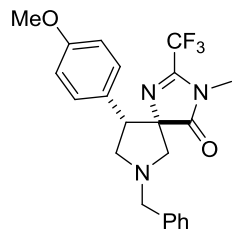


5.63
2.02
2.00

6.26
3.00
4.04

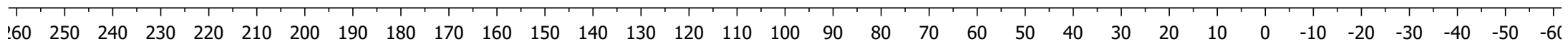
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¹³C NMR (75 MHz), CDCl₃ soln

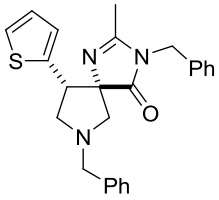


4f

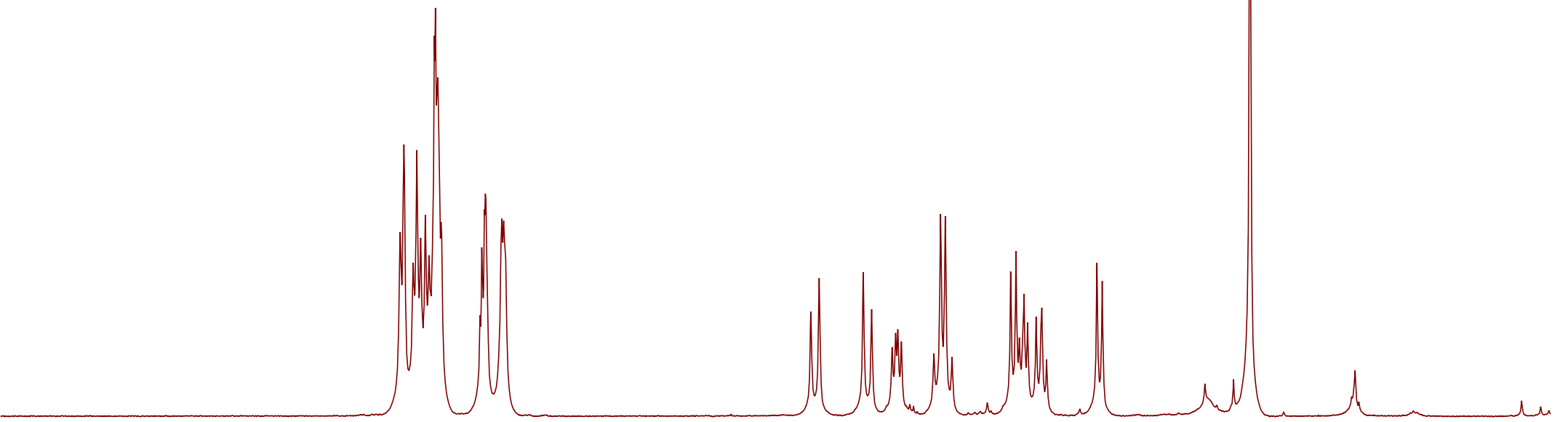
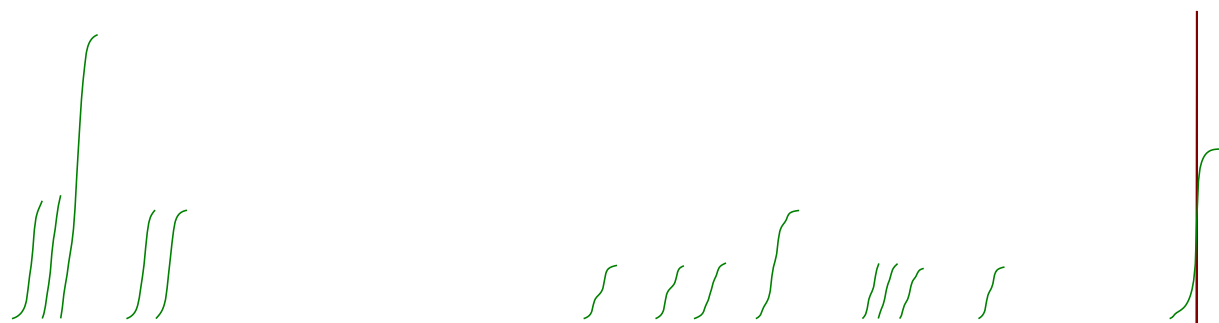
— 182.20
— 159.05
— 151.43
— 150.91
— 150.39
— 149.88
— 138.91
— 129.72
— 128.71
— 128.38
— 127.15
— 125.98
— 122.23
— 118.61
— 114.97
— 113.28
— 111.33
— 79.55
— 60.87
— 60.51
— 58.08
— 55.45
— 55.22
— 27.09
— 27.06



¹H NMR (300 MHz), CDCl₃ soln

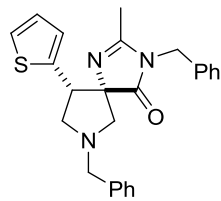


4g



10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

¹³C NMR (75 MHz), CDCl₃ soln



4g

