

Supporting Information
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Supporting information

Synthesis of Angularly Fused (Homo)triquinane Type Hydantoins as Precursors of Bicyclic α -Prolines

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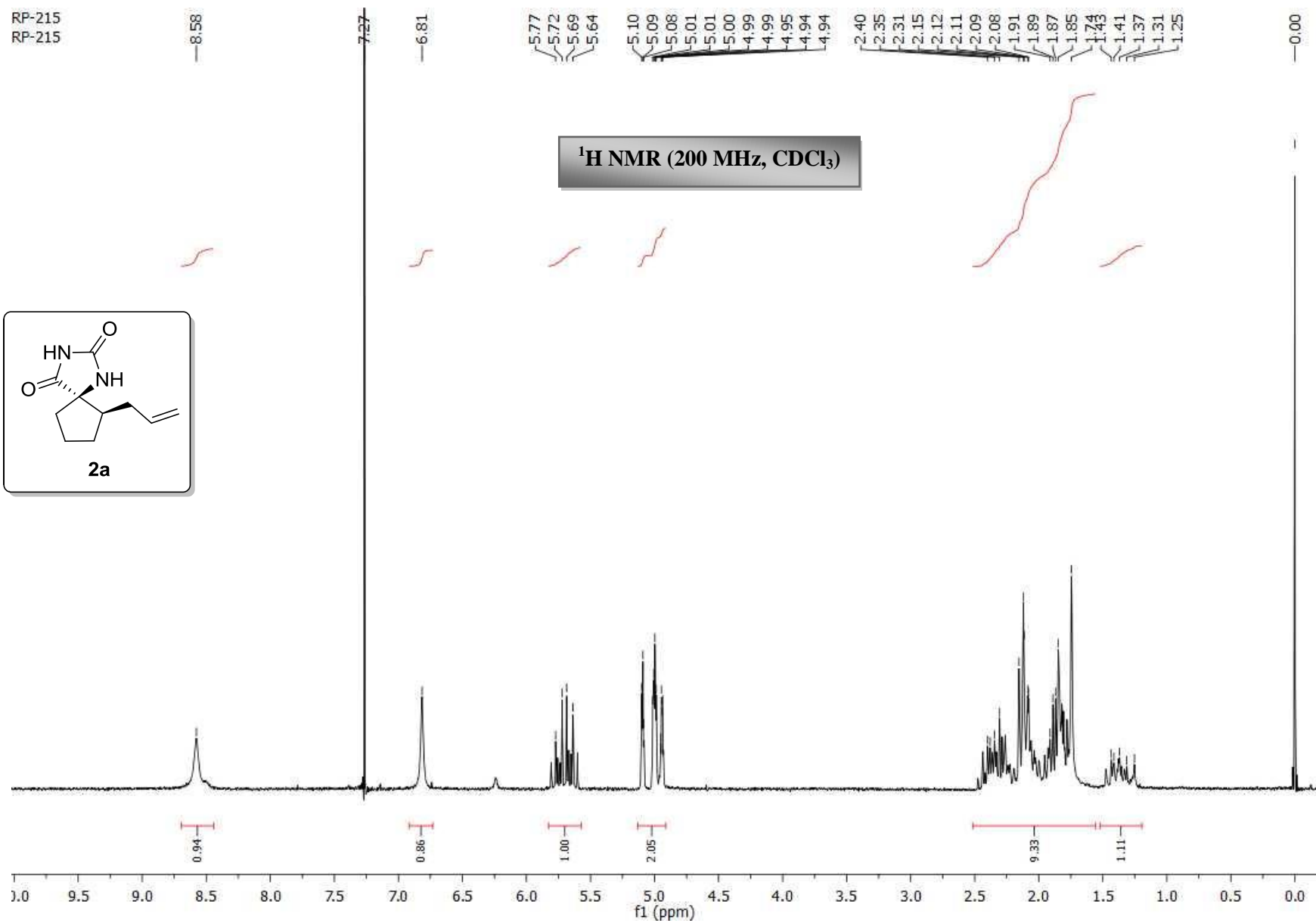
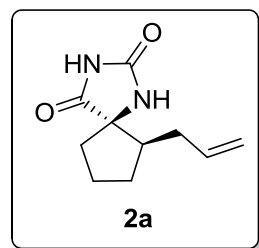
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Table S1. Crucial Correlations Observed in NOESY and HMBC Spectra

		Compound				
		rac-(5 <i>R</i> ,6 <i>aS</i> ,9 <i>aS</i>)- 3a	rac-(5 <i>S</i> ,6 <i>aS</i> ,9 <i>aS</i>)- 3a	rac-(5 <i>R</i> ,6 <i>aS</i> ,9 <i>aS</i>)- 3b	rac-(5 <i>R</i> ,6 <i>aS</i> ,9 <i>aS</i>)- 3c	rac-(5 <i>S</i> ,6 <i>aS</i> ,9 <i>aS</i>)- 3c
NOE correlations	H(9) α \leftrightarrow H(5) α	H(9) α \leftrightarrow CH ₂ ^{Se}	H(8) α \leftrightarrow H(5) α	H(6a) β \leftrightarrow CH ₂ ^{Se}	H(8) α \leftrightarrow H(10) α	
	H(6a) β \leftrightarrow H(8) β	H(6) α \leftrightarrow CH ₂ ^{Se}	H(8) α \leftrightarrow H(6) α	H(6a) β \leftrightarrow H(9) β	H(8) α \leftrightarrow H(6) α	
		H(6a) β \leftrightarrow H(8) β	H(10) α \leftrightarrow H(5) α	CH ₃ \leftrightarrow CH ₂ ^{Se}	CH ₃ \leftrightarrow CH ₂ ^{Se}	
		H(6a) β \leftrightarrow H(5) β	H(6) β \leftrightarrow CH ₂ ^{Se}	CH ₃ \leftrightarrow H(10) α	H(6) β \leftrightarrow CH ₂ ^{Se}	
			H(6a) β \leftrightarrow CH ₂ ^{Se}	H(6) β \leftrightarrow CH ₂ ^{Se}	H(6a) β \leftrightarrow H(9) β	
				H(8) α \leftrightarrow H(10) α	H(6a) β \leftrightarrow CH ₃	
				H(8) α \leftrightarrow H(6) α		
HMBC correlations	CH ₂ ^{Se} \leftrightarrow C(6)	CH ₂ ^{Se} \leftrightarrow C(6)	CH ₂ ^{Se} \leftrightarrow C(6)	CH ₂ ^{Se} \leftrightarrow C(6)	CH ₂ ^{Se} \leftrightarrow C(6)	
	CH ₂ ^{Se} \leftrightarrow C(5)	CH ₂ ^{Se} \leftrightarrow C(5)	CH ₂ ^{Se} \leftrightarrow C(5)	CH ₂ ^{Se} \leftrightarrow C(5)	CH ₂ ^{Se} \leftrightarrow C(5)	
	H(5) \leftrightarrow CH ₂ ^{Se}	H(5) \leftrightarrow CH ₂ ^{Se}	H(5) \leftrightarrow C(6)	CH ₂ ^{Se} \leftrightarrow CH ₃	CH ₂ ^{Se} \leftrightarrow CH ₃	
	H(5) \leftrightarrow C(3)	H(5) \leftrightarrow C(6)	H(6) \leftrightarrow C(5)	CH ₃ \leftrightarrow C(6)	CH ₃ \leftrightarrow CH ₂ ^{Se}	
	H(6) \leftrightarrow C(9)	H(5) \leftrightarrow C(6a)	H(6) \leftrightarrow C(6a)	CH ₃ \leftrightarrow C(5)	CH ₃ \leftrightarrow C(6)	
	H(6) \leftrightarrow C(9a)	H(5) \leftrightarrow C(9a)	H(6) \leftrightarrow CH ₂ ^{Se}	CH ₃ \leftrightarrow CH ₂ ^{Se}	CH ₃ \leftrightarrow C(5)	
	H(6) \leftrightarrow C(6a)	H(5) \leftrightarrow C(3)	H(6) \leftrightarrow C(10)	H(6) \leftrightarrow C(6a)	H(6) \leftrightarrow C(5)	
	H(6a) \leftrightarrow C(1)	H(6) \leftrightarrow C(7)	H(6) \leftrightarrow C(10a)	H(6) \leftrightarrow CH ₃	H(6) \leftrightarrow C(6a)	
	H(6a) \leftrightarrow C(5)	H(6) \leftrightarrow CH ₂ ^{Se}	H(6) \leftrightarrow C(10)	H(6) \leftrightarrow C(7)	H(6) \leftrightarrow C(5)	
	H(6a) \leftrightarrow C(8)	H(6) \leftrightarrow C(6a)	H(6a) \leftrightarrow C(5)	H(6) \leftrightarrow CH ₂ ^{Se}	H(6a) \leftrightarrow C(1)	
	H(7) \leftrightarrow C(8)	H(6) \leftrightarrow C(5)	H(6a) \leftrightarrow C(6)	H(6) \leftrightarrow C(5)	H(6a) \leftrightarrow C(5)	
	H(7) \leftrightarrow C(9)	H(6) \leftrightarrow C(9a)	H(6a) \leftrightarrow CH ₂ ^{Se}	H(6) \leftrightarrow C(10a)	H(6a) \leftrightarrow C(6)	
	H(7) \leftrightarrow C(6a)	H(6a) \leftrightarrow C(8)	H(6a) \leftrightarrow C(10a)	H(6a) \leftrightarrow C(8)	H(6a) \leftrightarrow C(7)	
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	H(8) \leftrightarrow C(6a)	H(7) \leftrightarrow C(6)	H(7) \leftrightarrow C(1)	H(6a) \leftrightarrow C(1)		
	H(8) \leftrightarrow C(7)	H(7) \leftrightarrow C(6a)	H(8) \leftrightarrow C(9)	H(7) \leftrightarrow C(6)		
	H(8) \leftrightarrow C(9a)	H(7) \leftrightarrow C(9a)	H(9) \leftrightarrow C(8)	H(7) \leftrightarrow C(8)		
	H(9) \leftrightarrow C(8)	H(8) \leftrightarrow C(6)	H(9) \leftrightarrow C(10a)	H(9) \leftrightarrow C(8)		
	H(9) \leftrightarrow C(7)	H(8) \leftrightarrow C(7)	H(9) \leftrightarrow C(1)	H(9) \leftrightarrow C(10a)		
	H(9) \leftrightarrow C(6a)	H(8) \leftrightarrow C(9)	H(10) \leftrightarrow C(1)	H(9) \leftrightarrow C(1)		
	H(9) \leftrightarrow C(6)	H(8) \leftrightarrow C(1)	H(10) \leftrightarrow C(6a)	H(9) \leftrightarrow C(10)		
	H(9) \leftrightarrow C(9a)	H(9) \leftrightarrow C(1)	H(10) \leftrightarrow C(10a)	H(10) \leftrightarrow C(1)		
		H(9) \leftrightarrow C(8)		H(10) \leftrightarrow C(6a)		
		H(9) \leftrightarrow C(7)		H(10) \leftrightarrow C(10a)		
		H(9) \leftrightarrow C(6a)		H(10) \leftrightarrow C(8)		
		H(9) \leftrightarrow C(9a)				

RP-215
RP-215



RP-215c
RP-215

—177.70

—157.06

—135.70

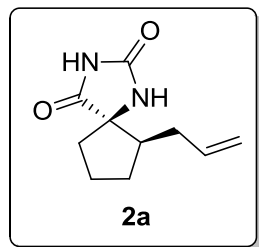
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77.63
77.00
76.36
71.96

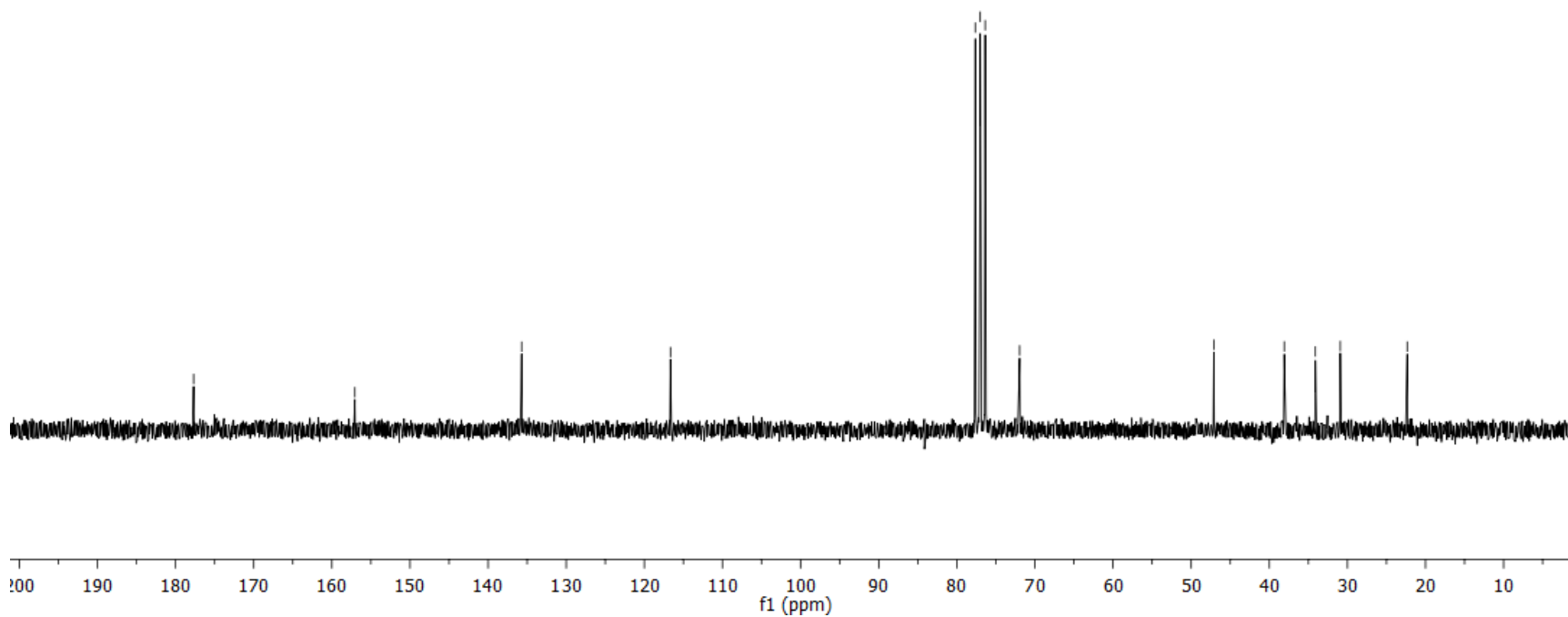
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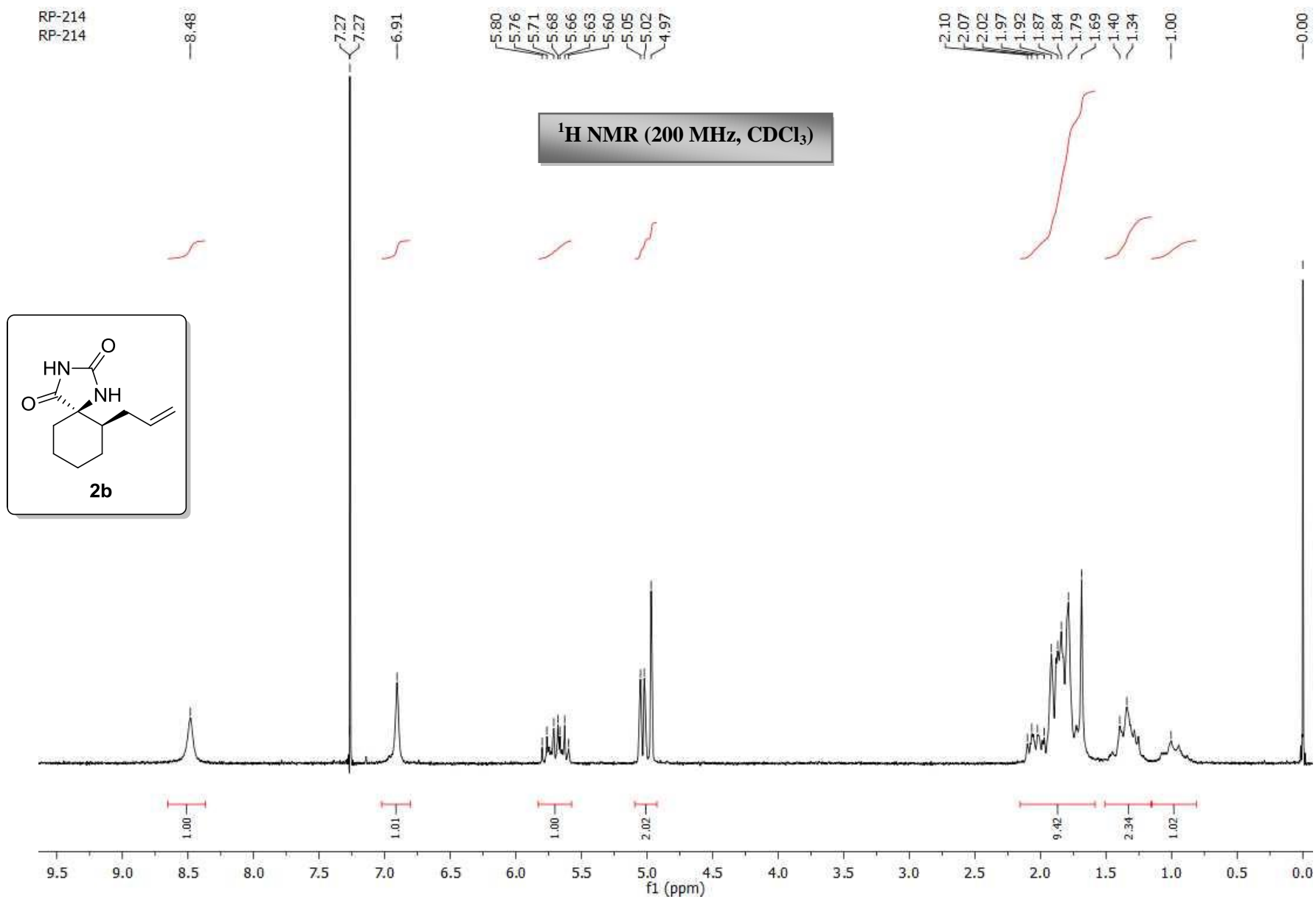
38.08
34.10
30.92

—22.34



¹³C NMR (50 MHz, CDCl₃)





RP-214c
RP-214

—177.30

—157.14

—135.43

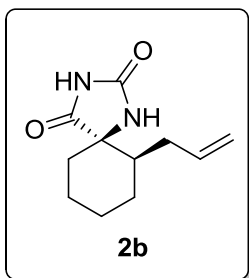
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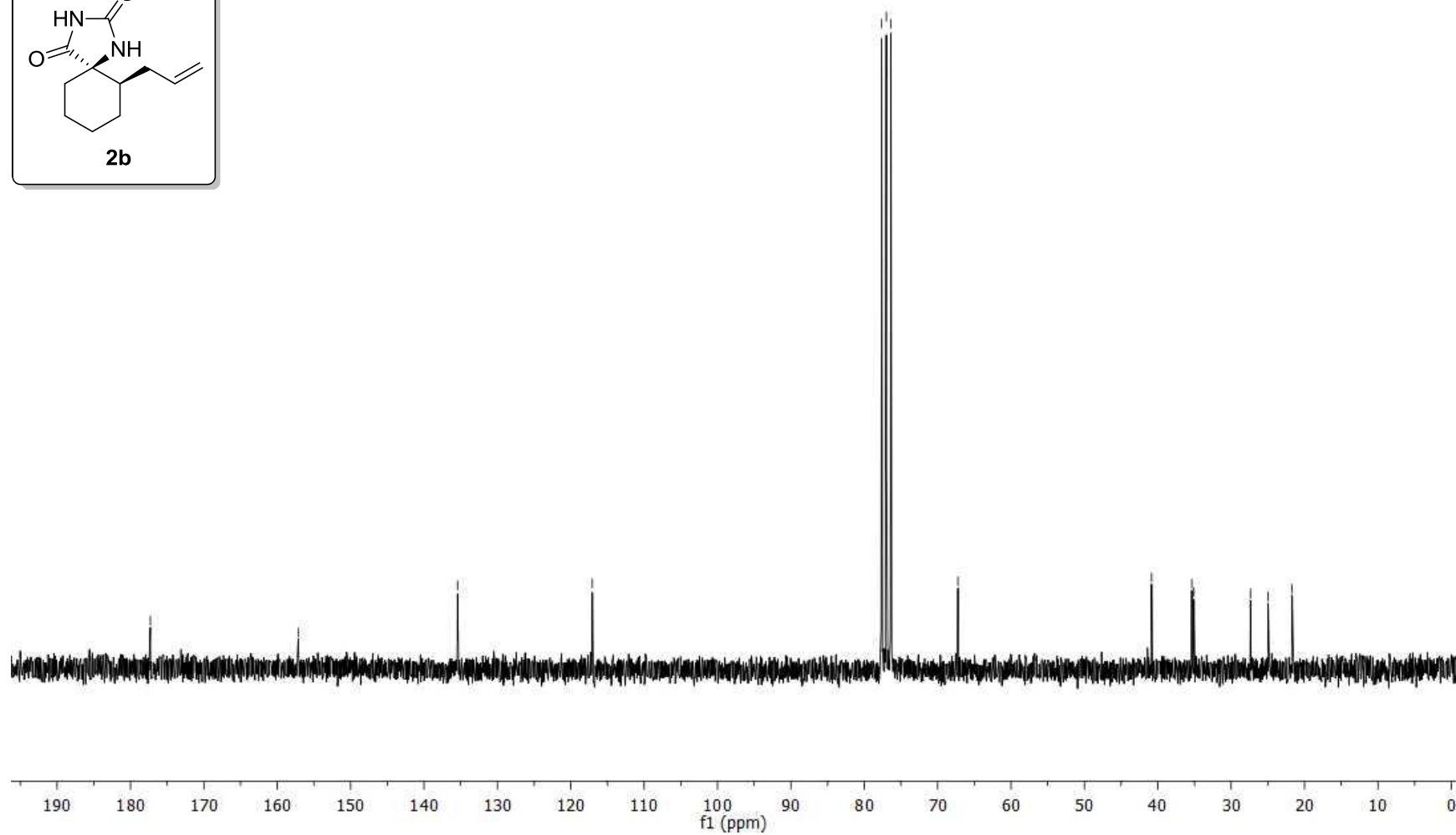
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—40.84
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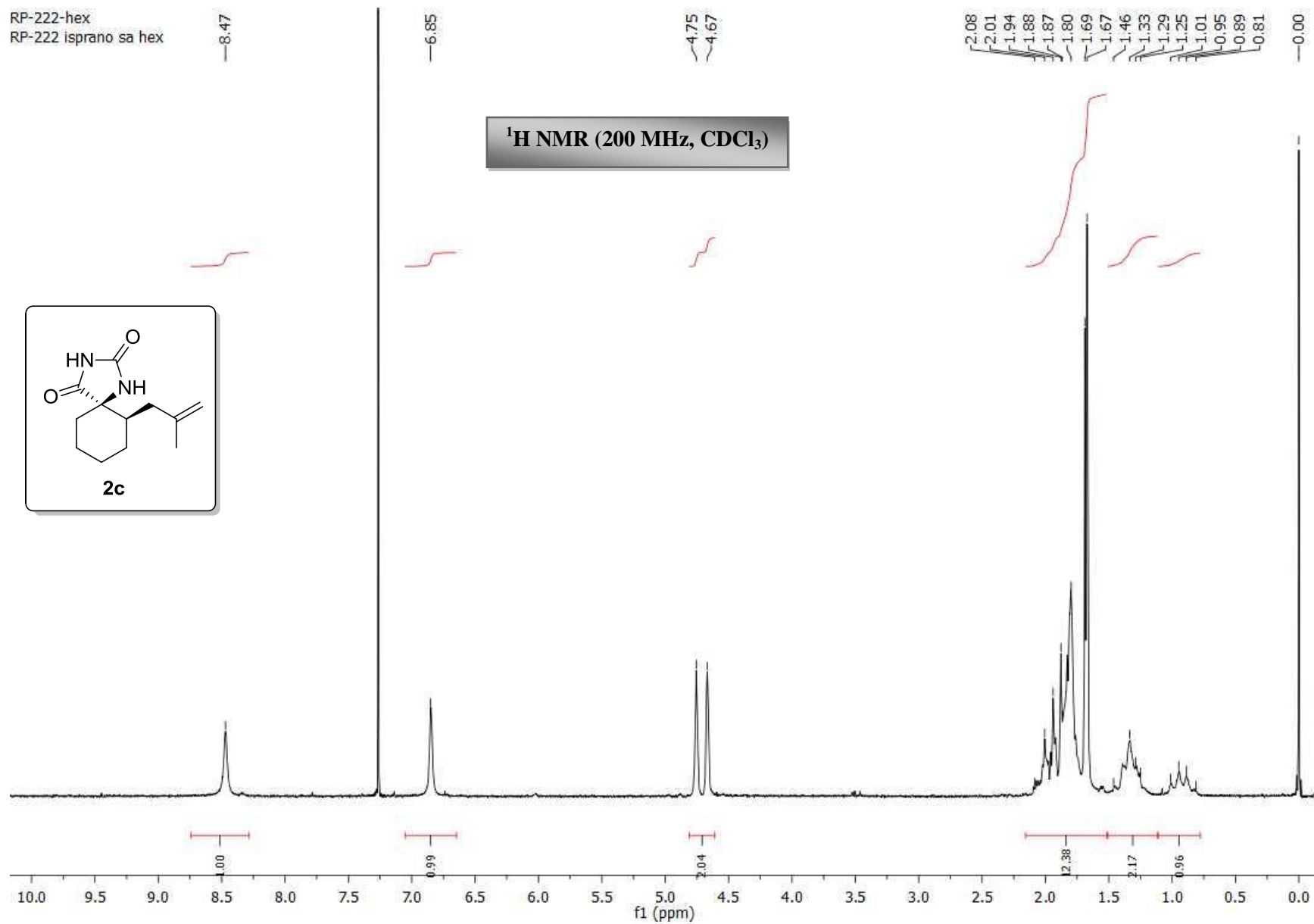
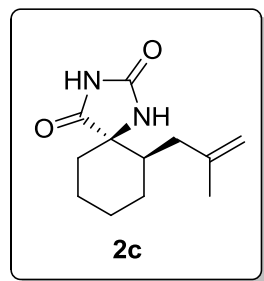
—27.37
—24.96
—21.69



¹³C NMR (50 MHz, CDCl₃)



RP-222-hex
RP-222 isprano sa hex



RP-222-ispranosHex
RP-222 isprano sa hex

—177.16

—157.08

—142.22

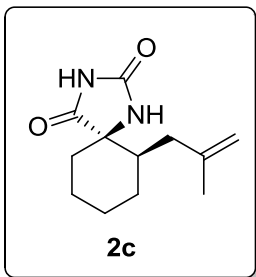
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76.36

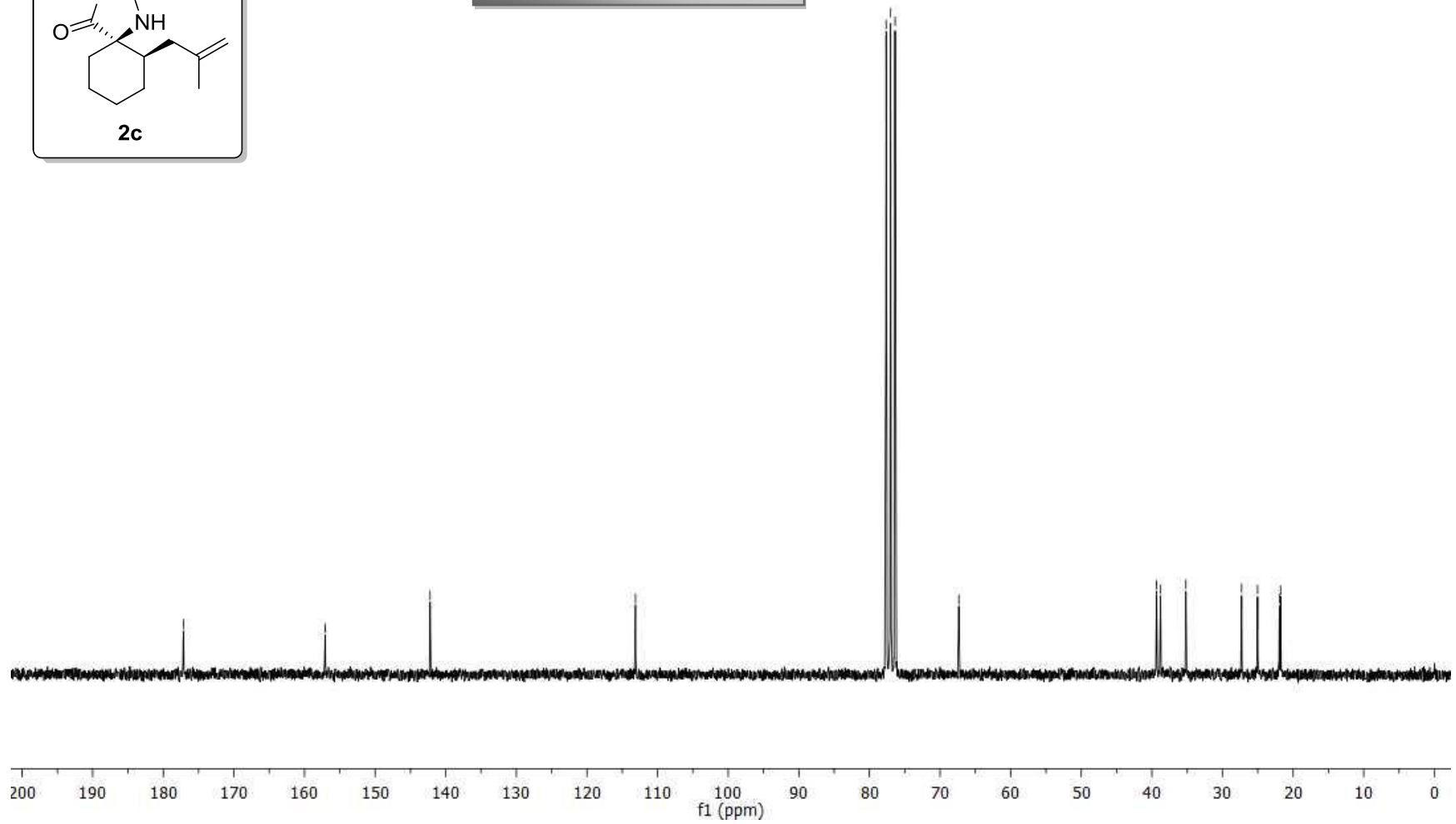
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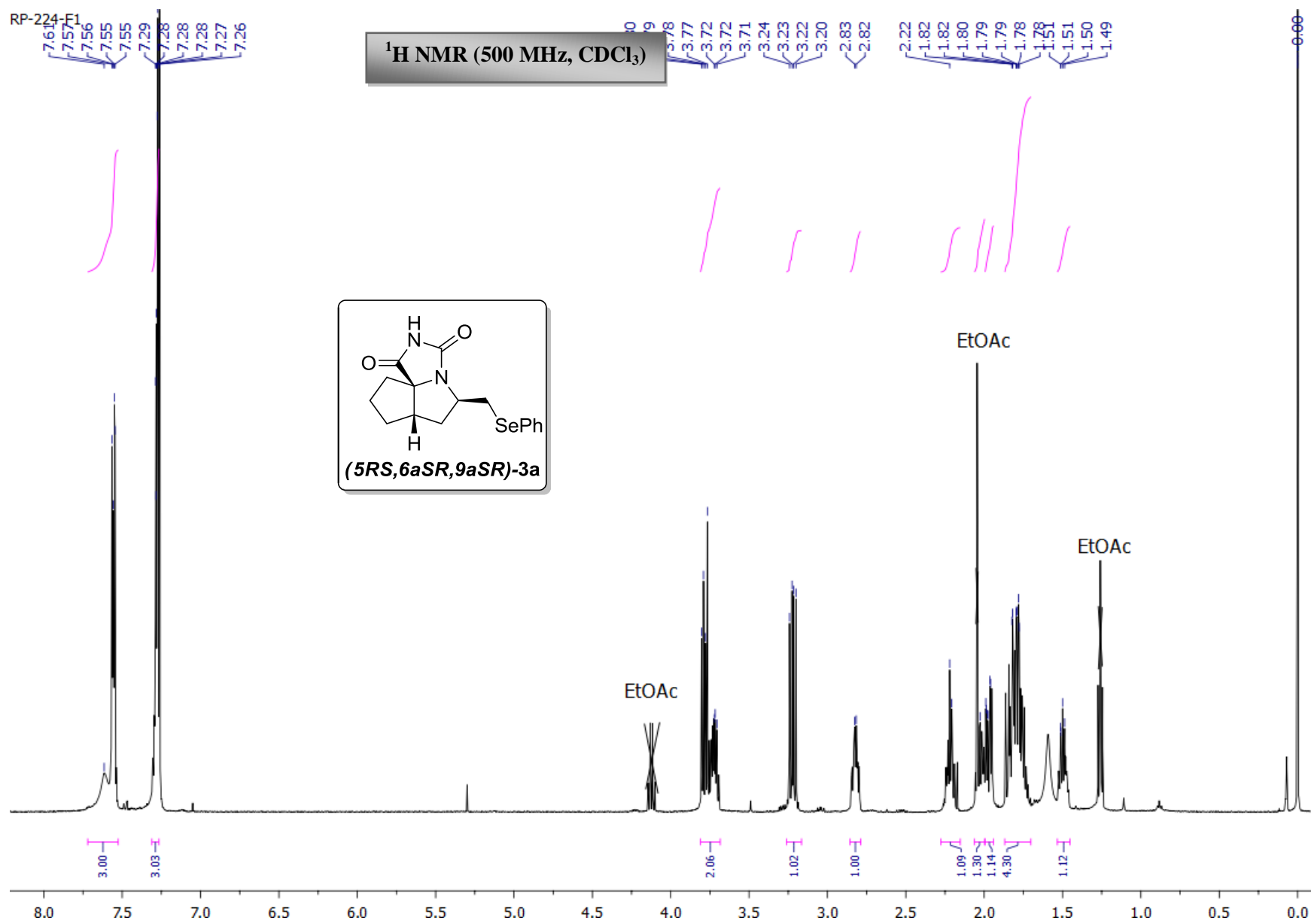
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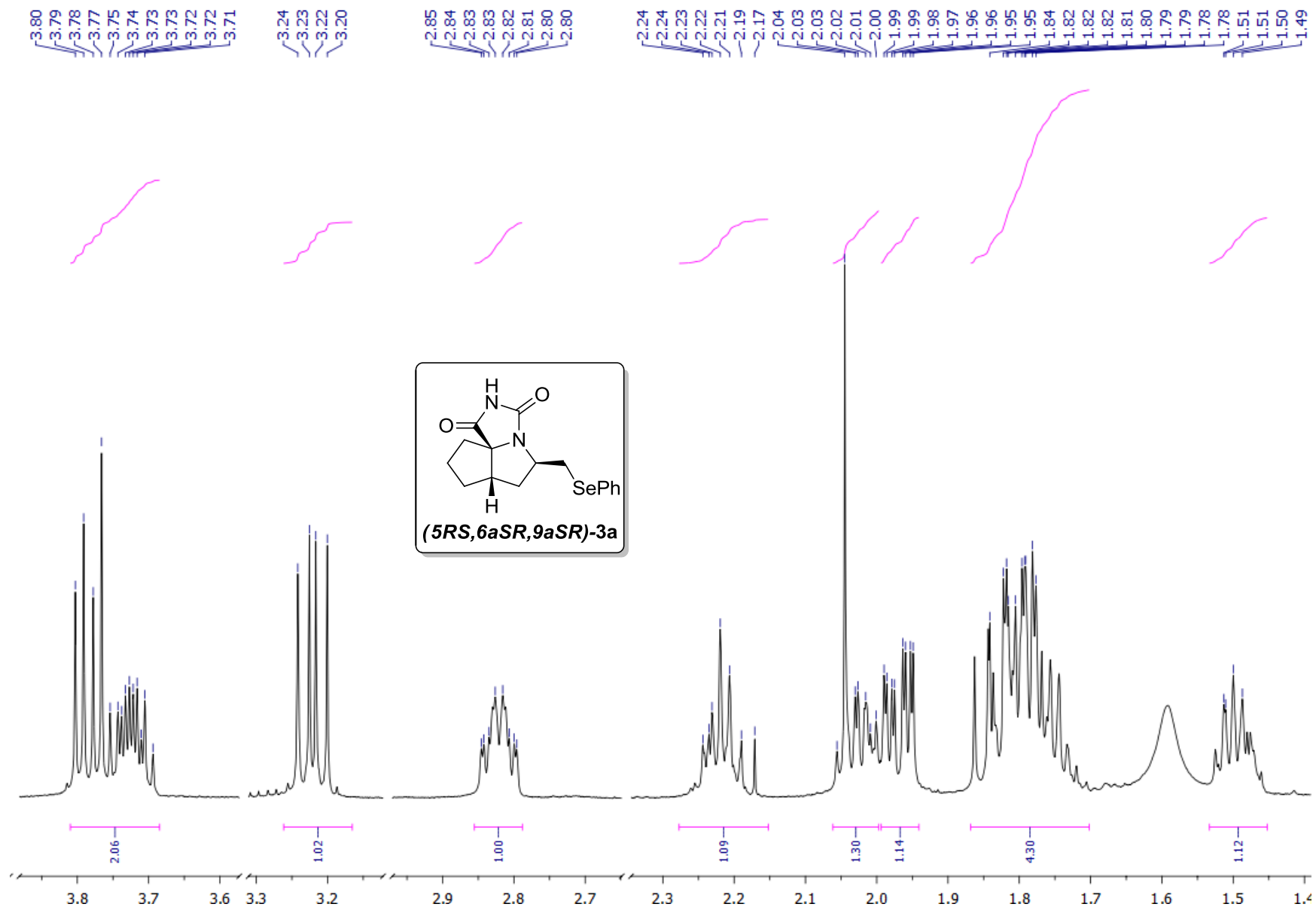
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21.76



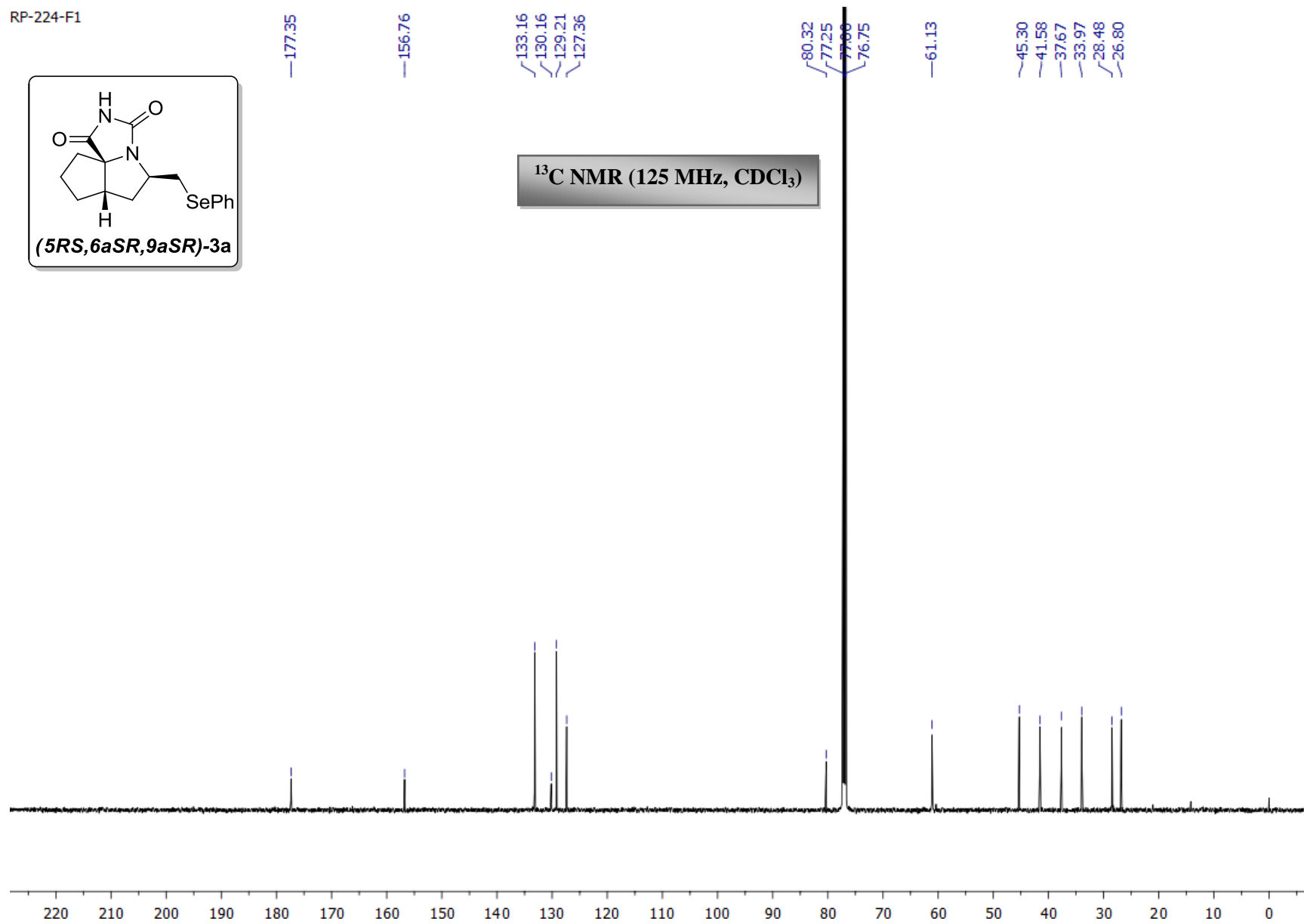
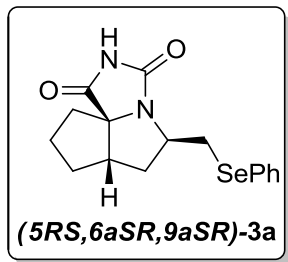
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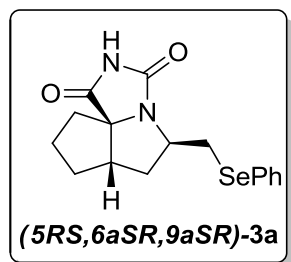




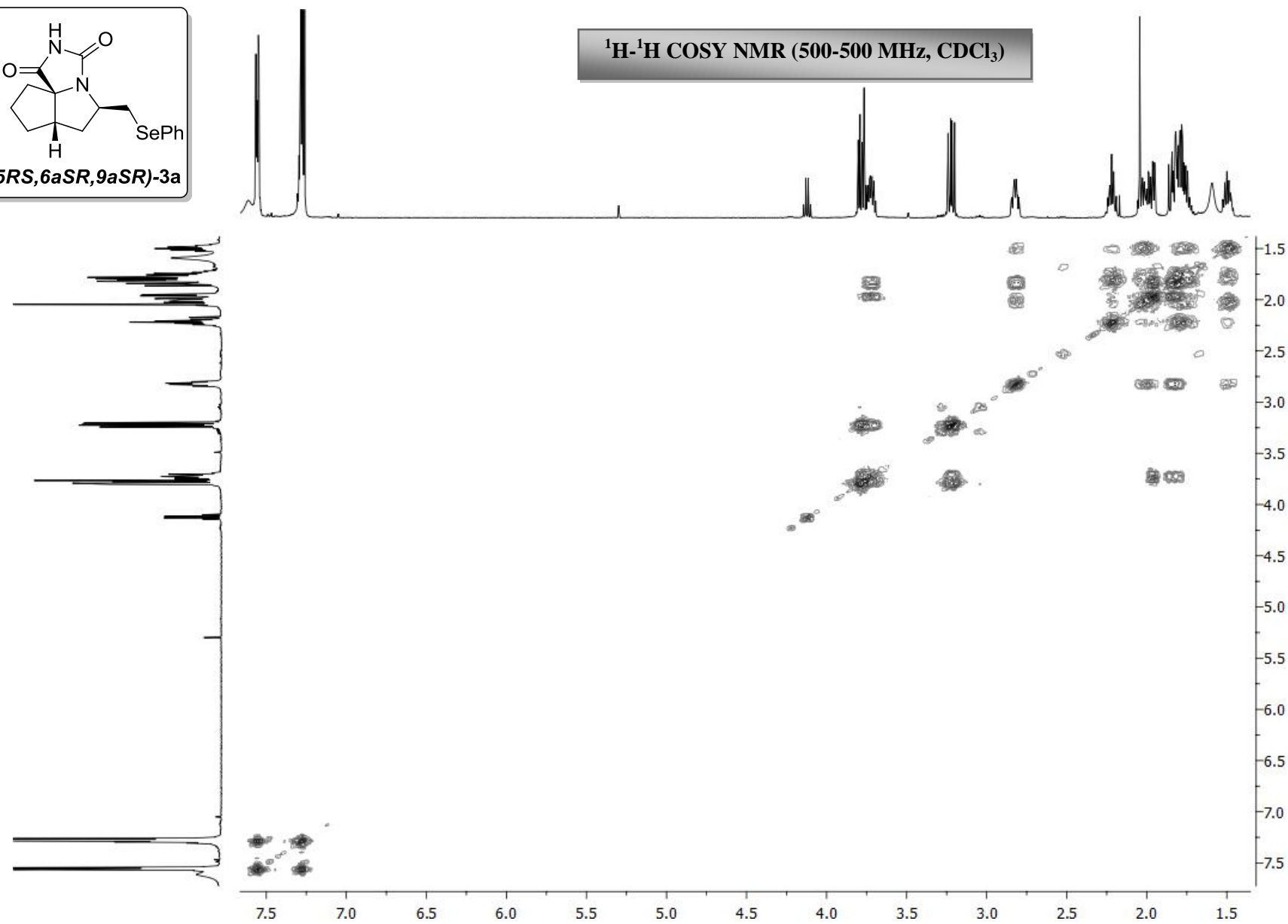


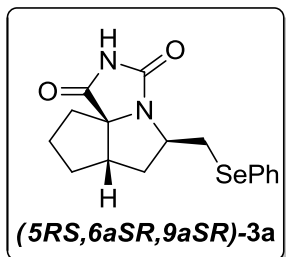
RP-224-F1



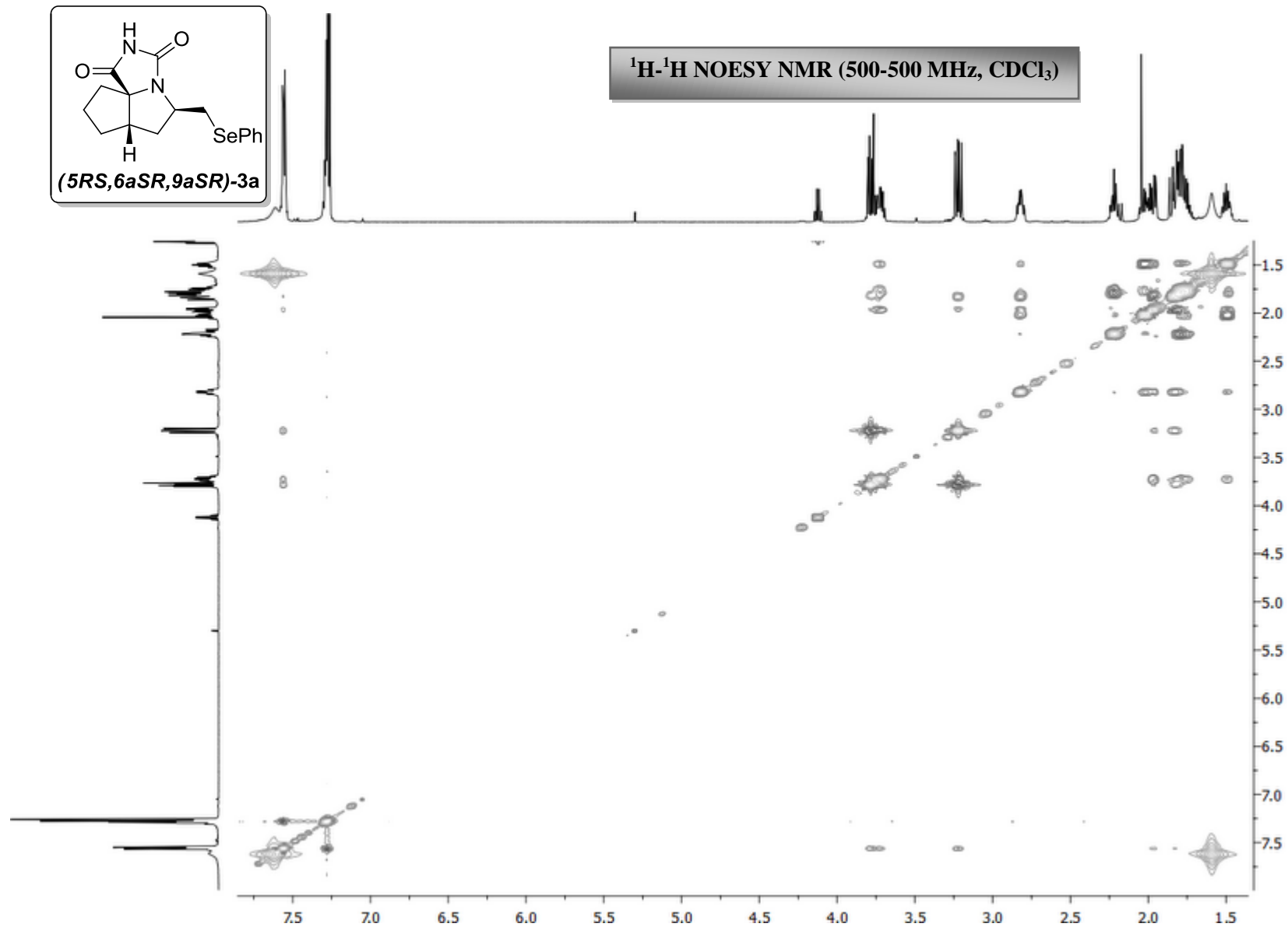


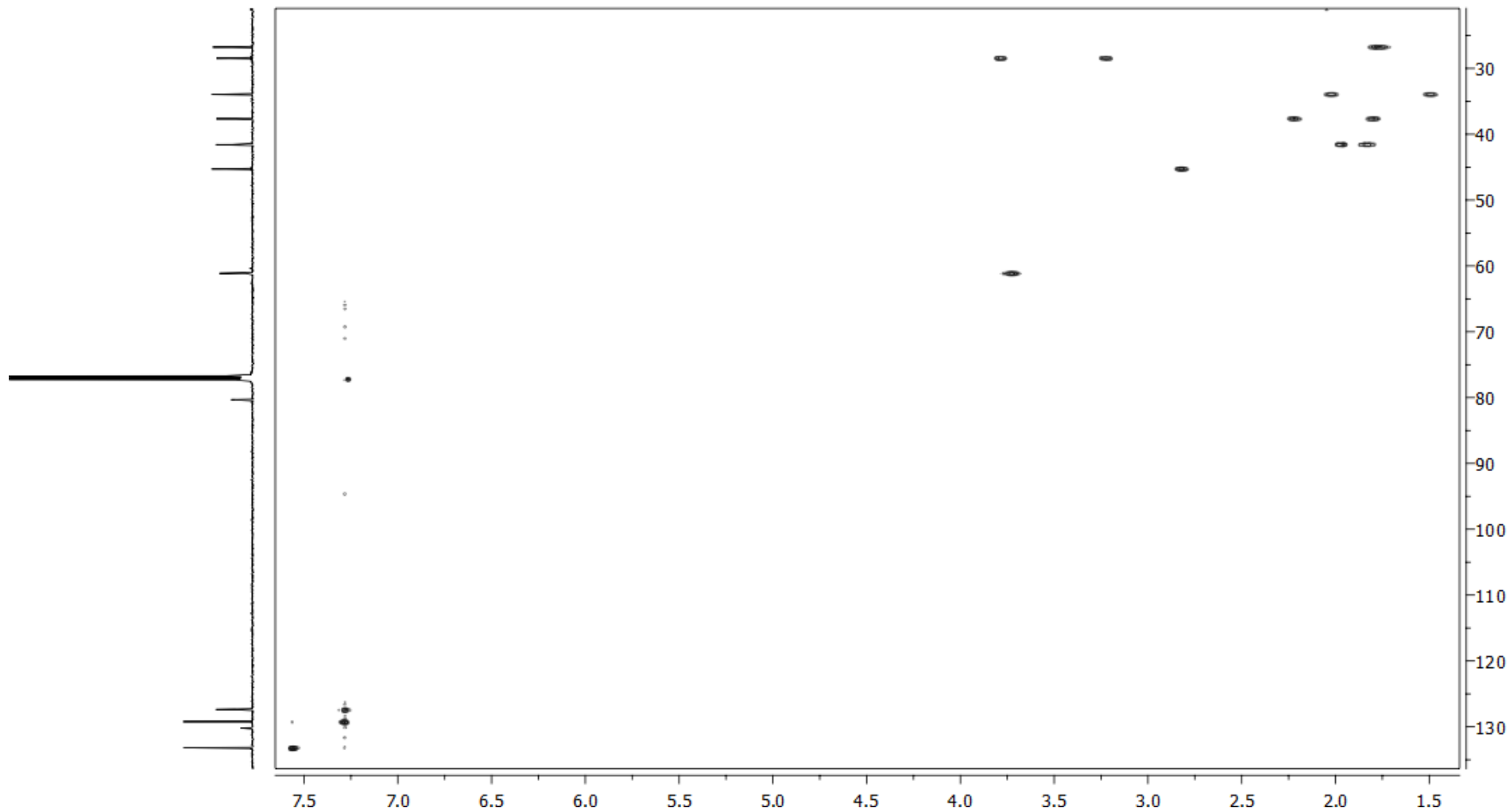
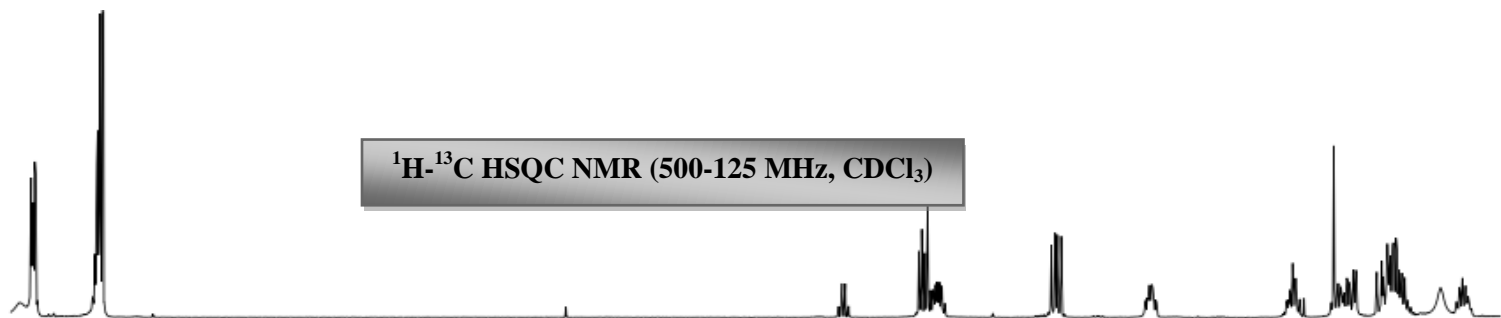
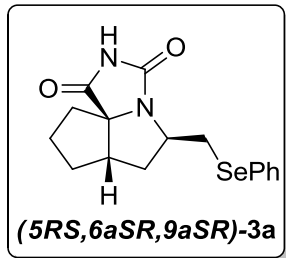
¹H-¹H COSY NMR (500-500 MHz, CDCl₃)

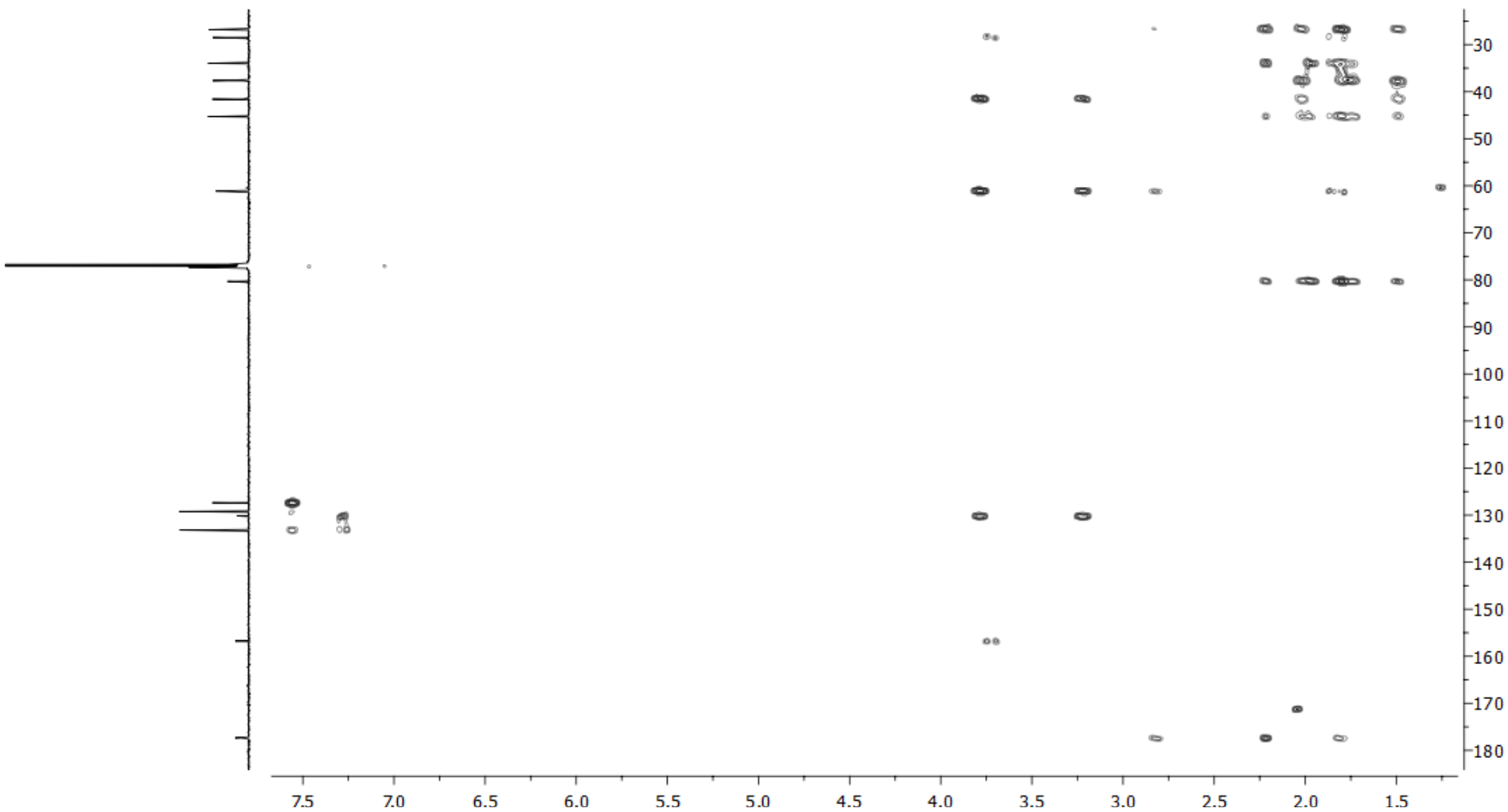
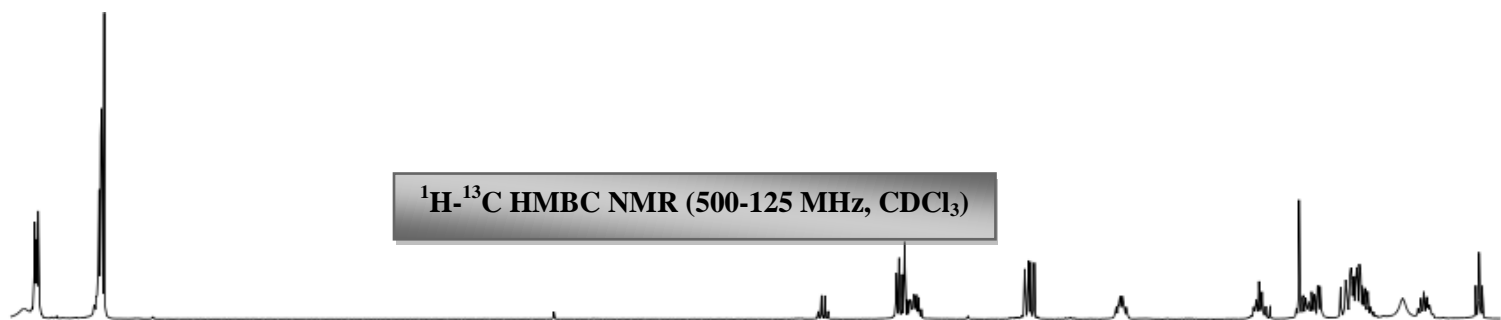
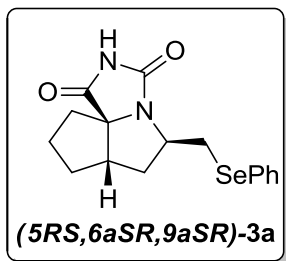




¹H-¹H NOESY NMR (500-500 MHz, CDCl₃)







RP-224

8.667

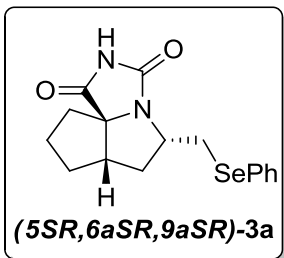
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7.27
7.26
7.25

4.23
4.22
4.21
4.20

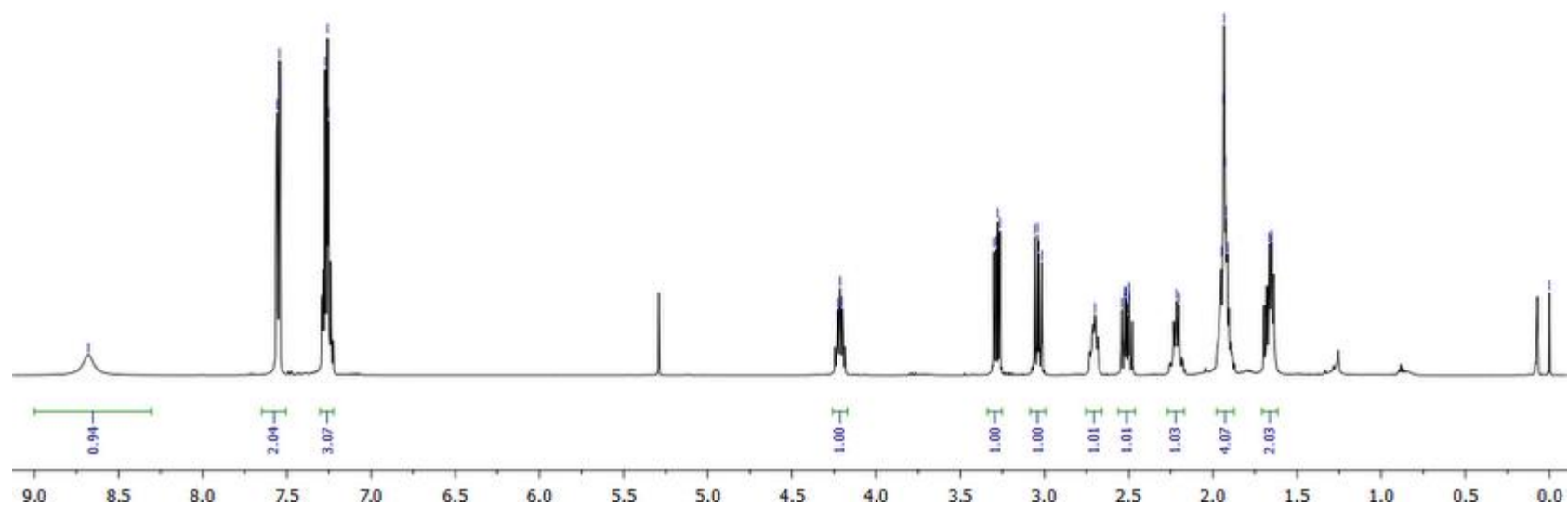
3.30
3.29
3.28
3.26
3.06
3.04
3.03

2.52
2.51
2.50
2.21
2.20
1.95
1.94
1.93
1.93
1.92
1.92
1.67
1.67
1.65
1.65

0.00



¹H NMR (500 MHz, CDCl₃)



4.23
4.23
4.22
4.21
4.21
4.20
4.20
4.19

3.30
3.29
3.28
3.26

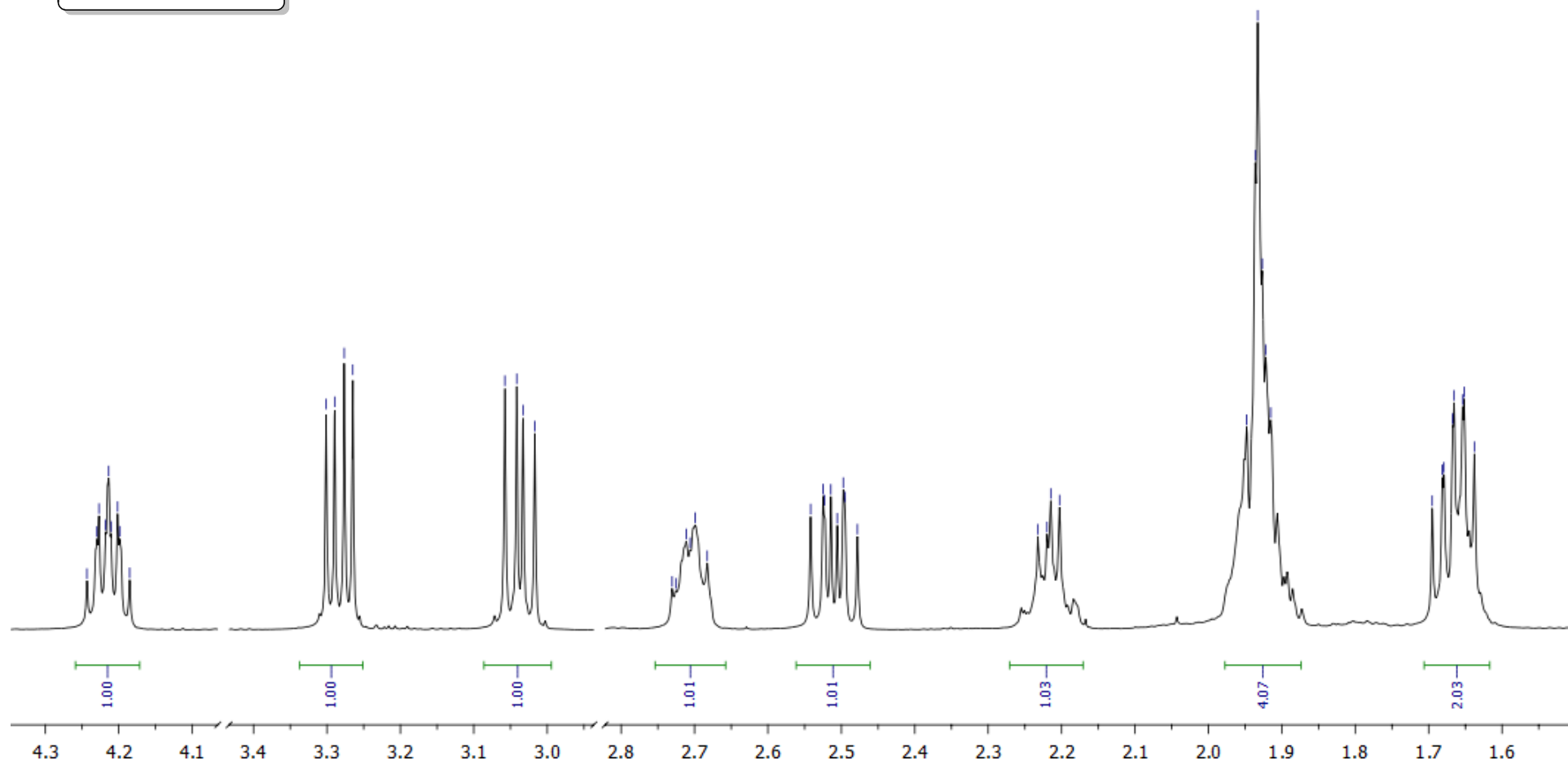
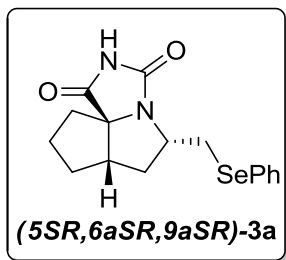
3.06
3.04
3.03
3.02

2.73
2.73
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2.71
2.70
2.68
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2.51
2.51
2.50
2.50
2.48

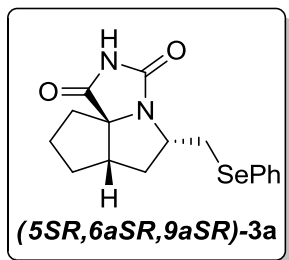
2.23
2.22
2.21
2.20

1.95
1.94
1.93
1.93
1.92
1.92

1.70
1.68
1.68
1.67
1.67
1.65
1.65
1.64



RP-224-F2



—178.45

—160.18

132.58
129.49
129.15
127.09

80.22
77.25
77.00
76.75

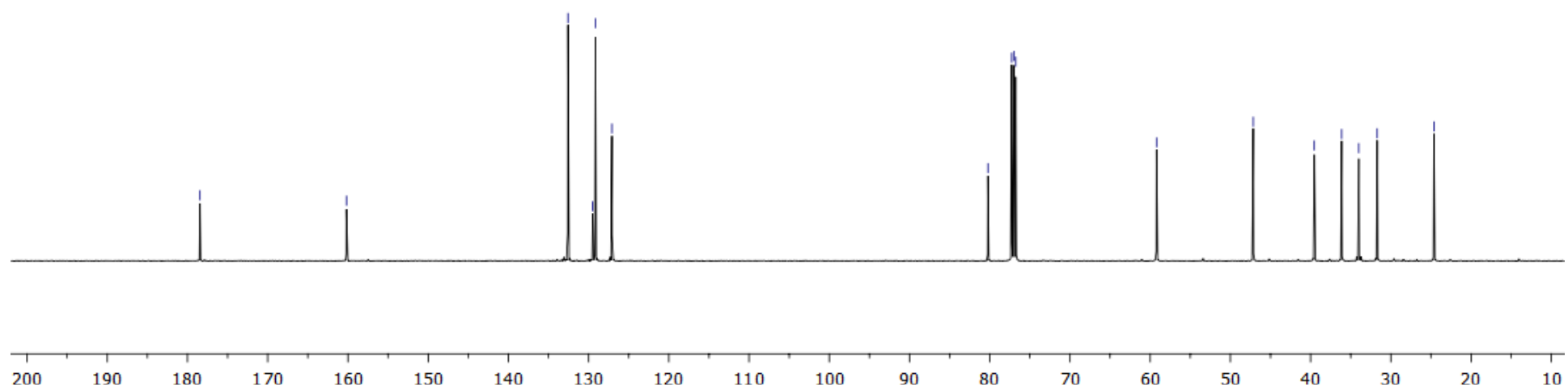
—59.19

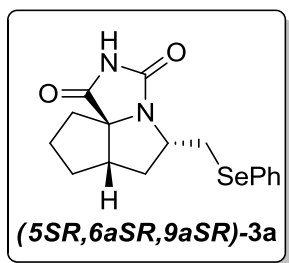
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39.54
36.13
33.99
31.69

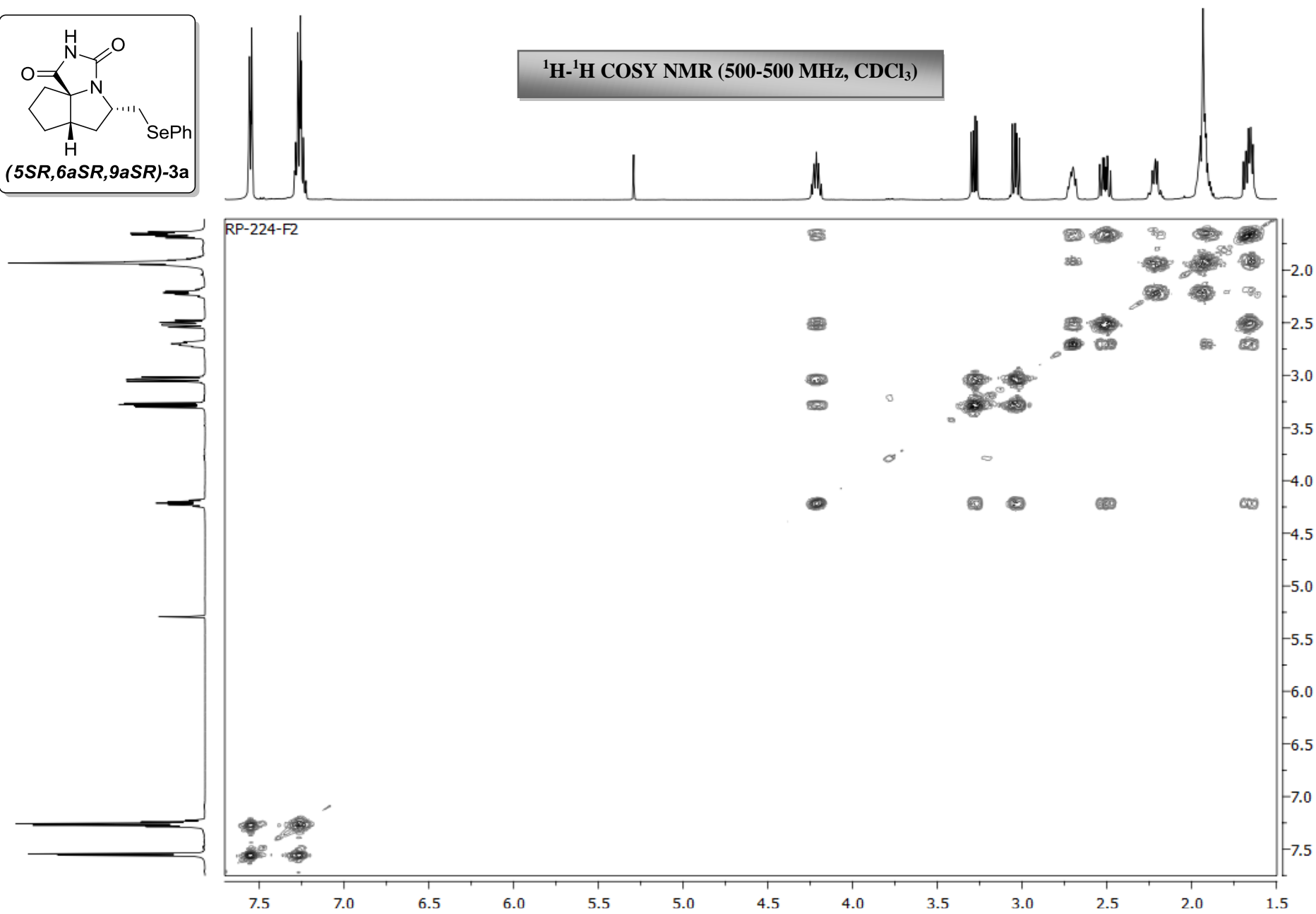
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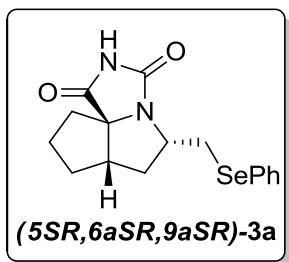
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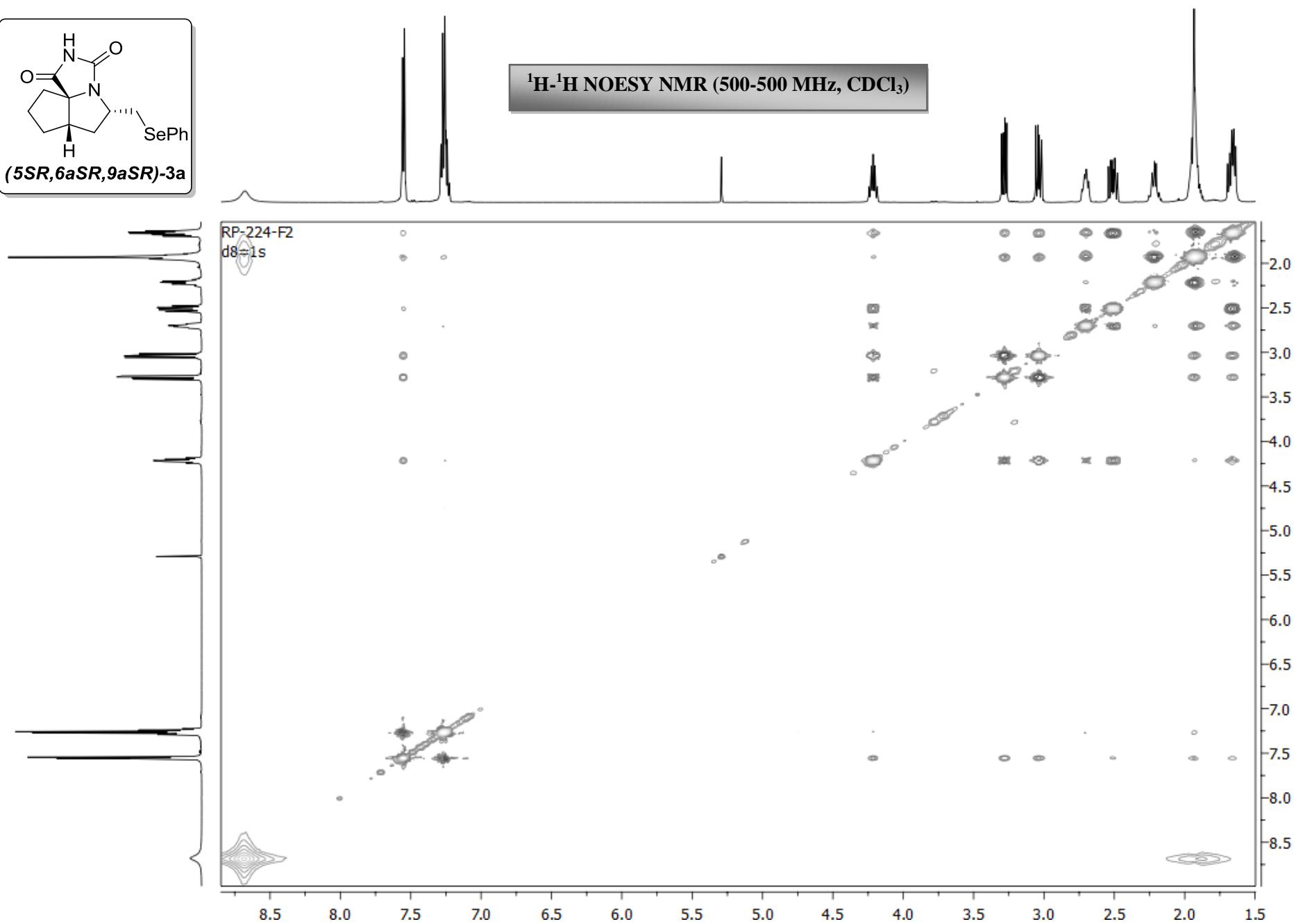


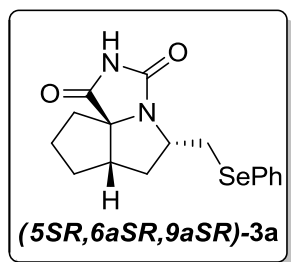
^1H - ^1H COSY NMR (500-500 MHz, CDCl_3)



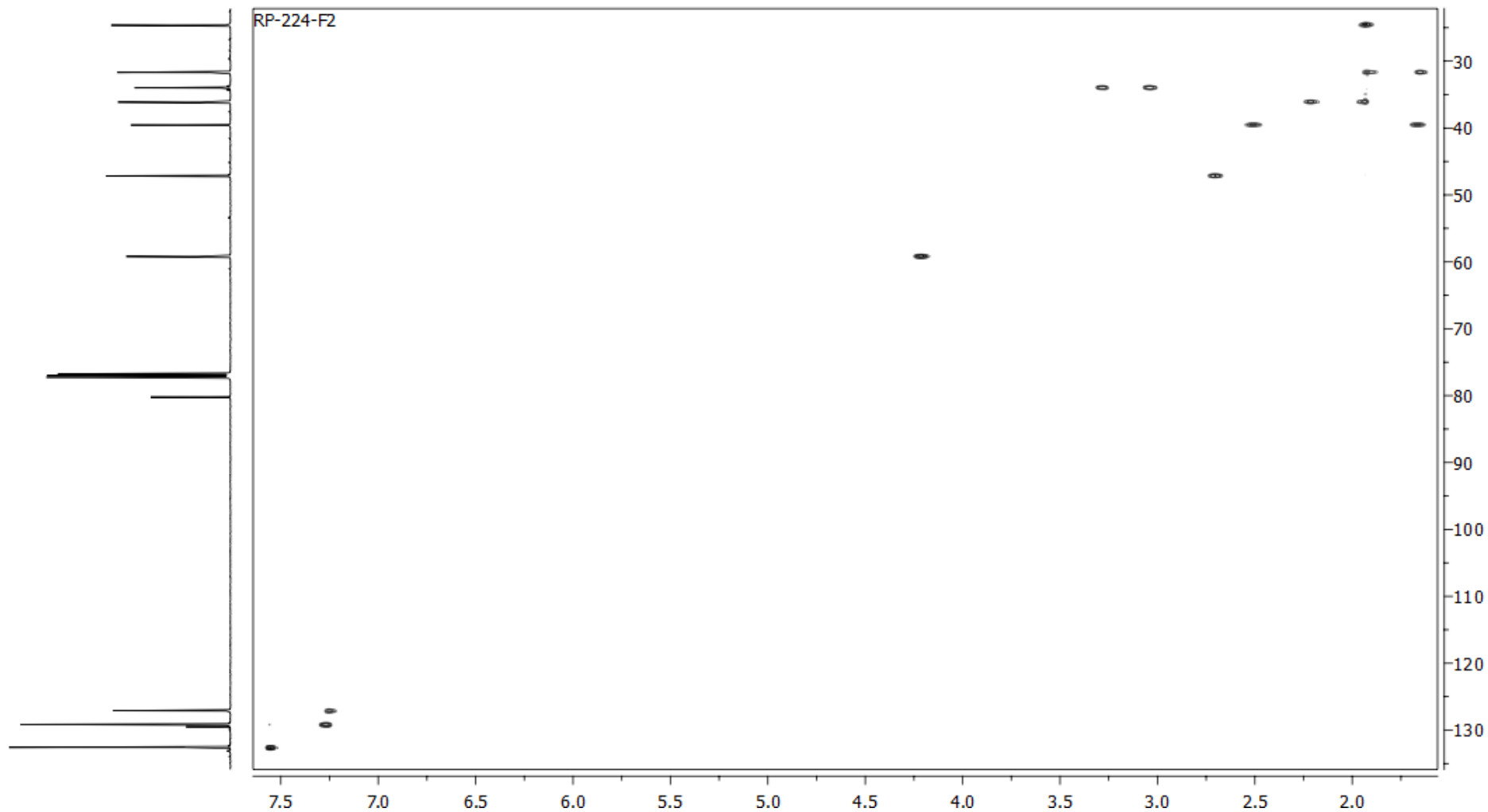
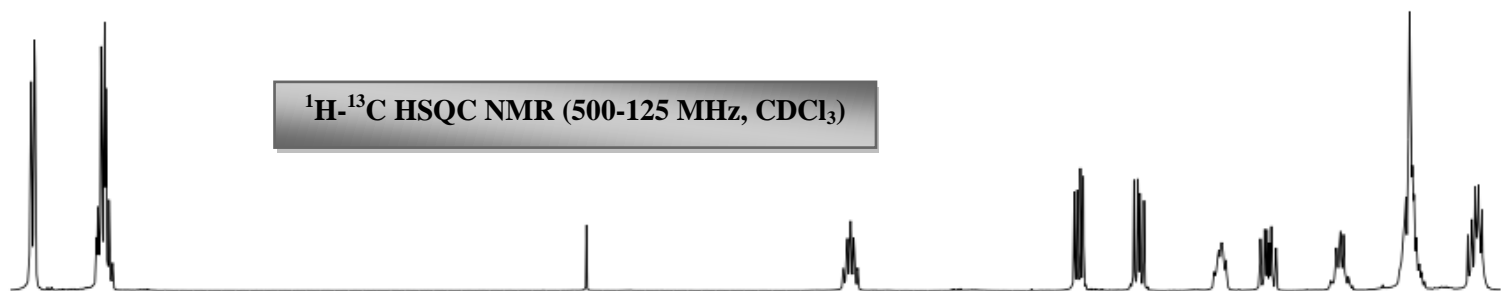


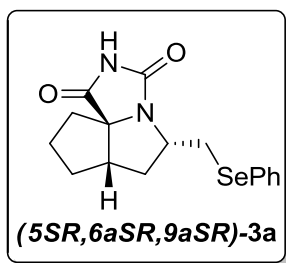
^1H - ^1H NOESY NMR (500-500 MHz, CDCl_3)



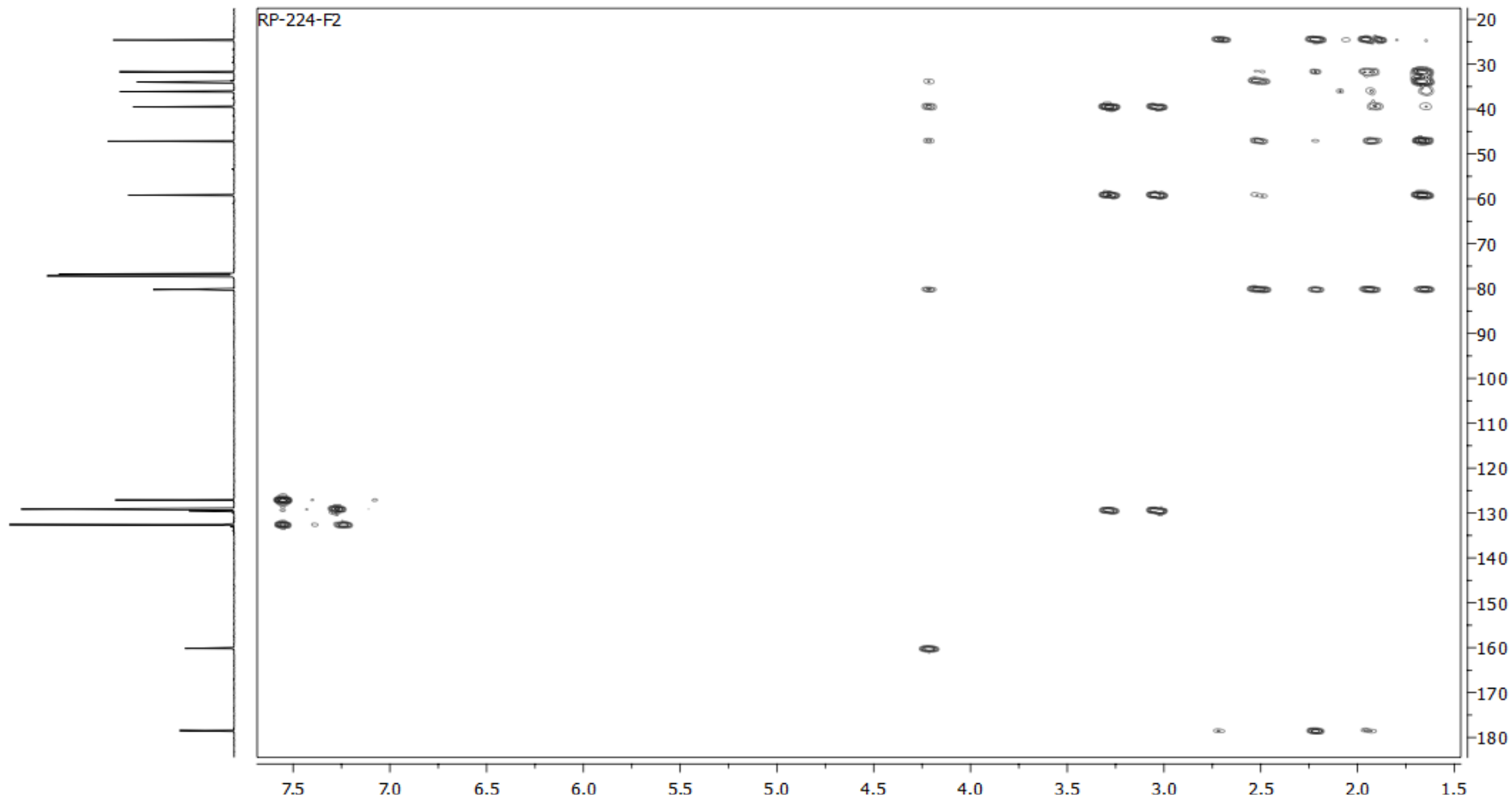
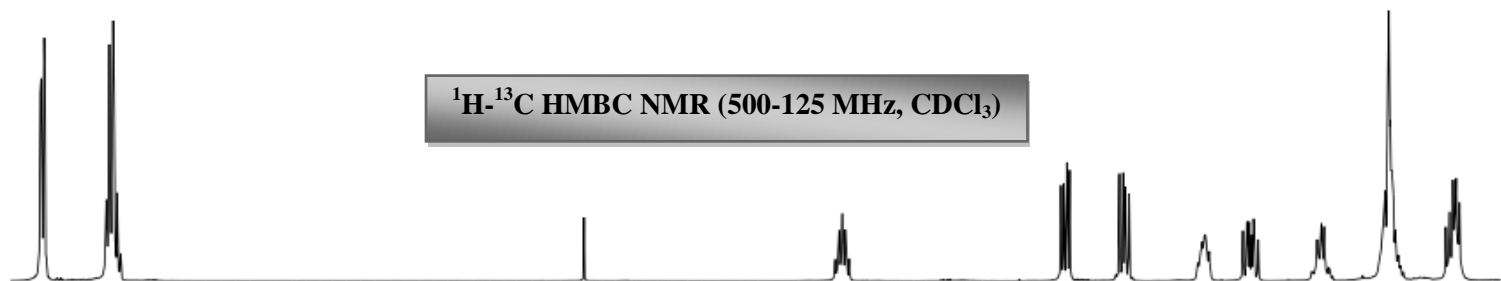


^1H - ^{13}C HSQC NMR (500-125 MHz, CDCl_3)



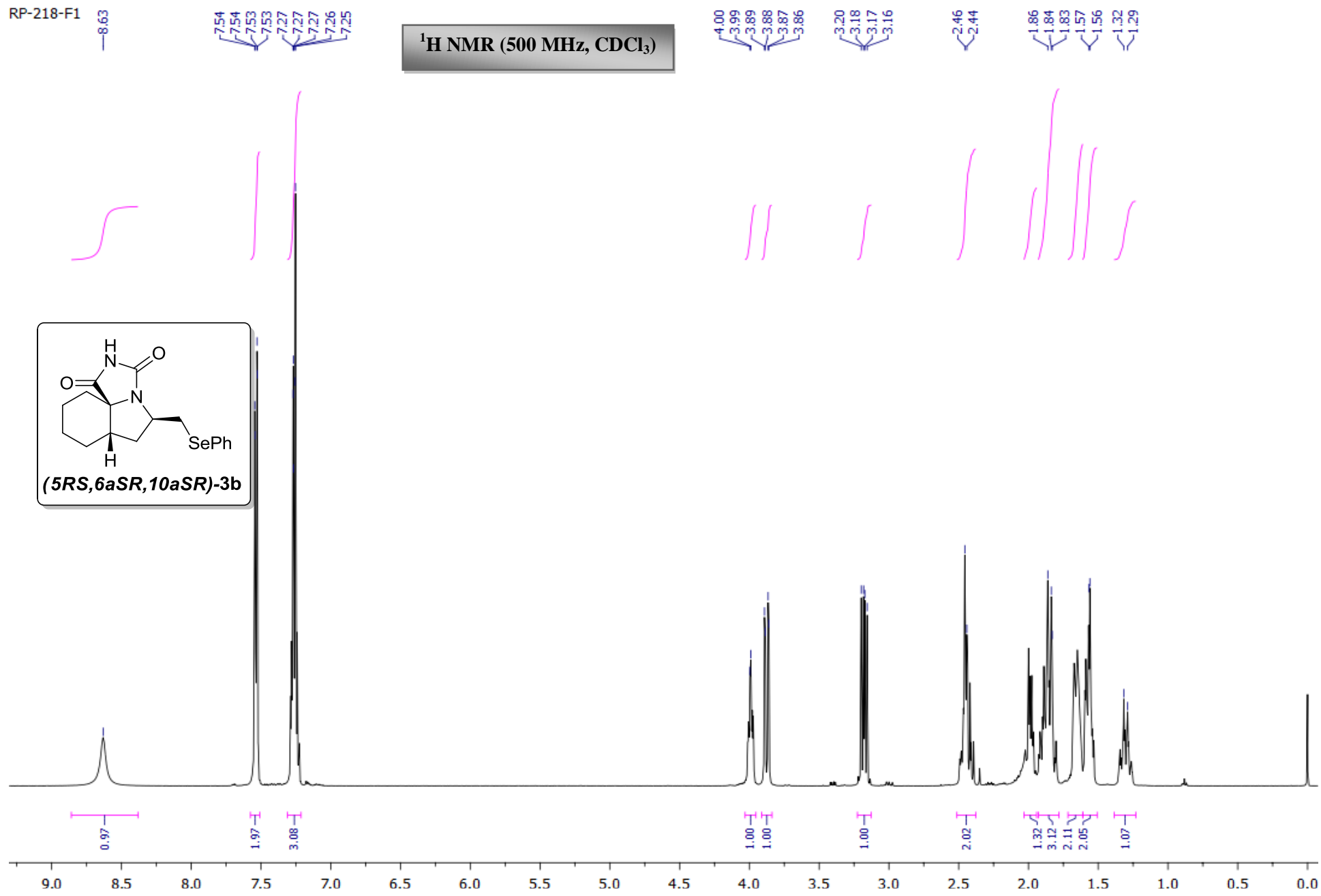
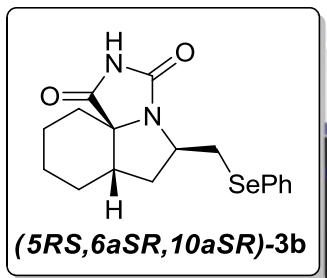


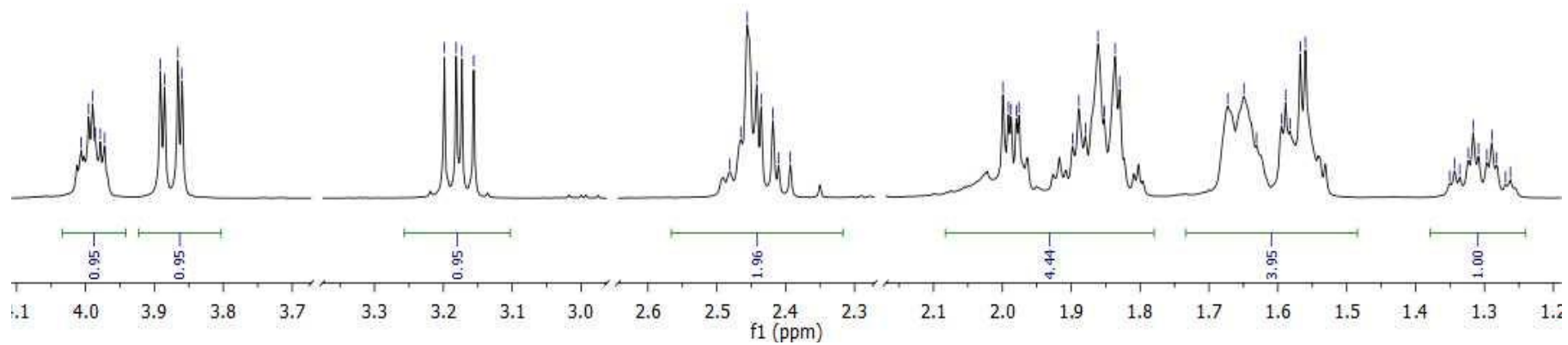
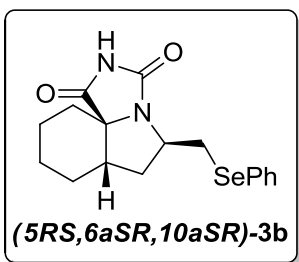
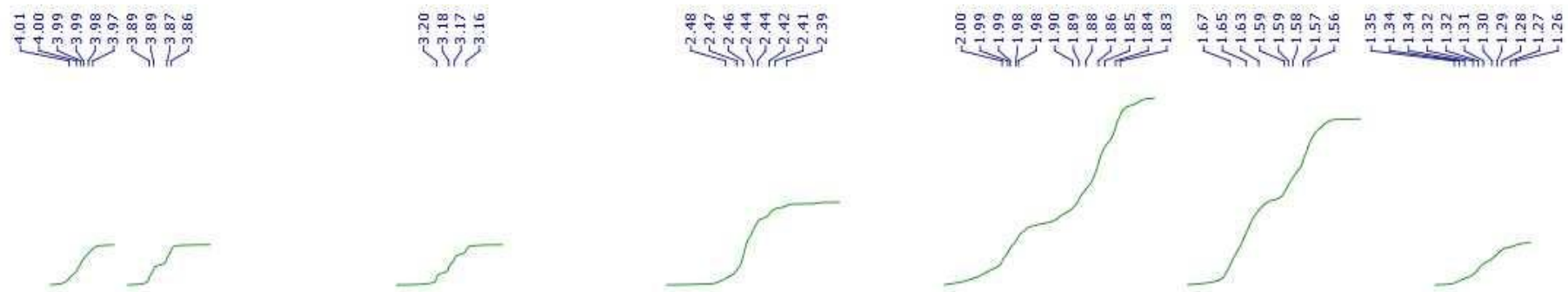
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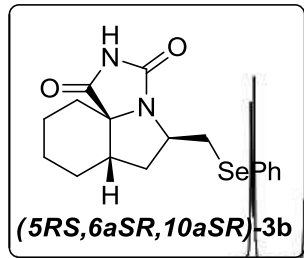


RP-218-F1

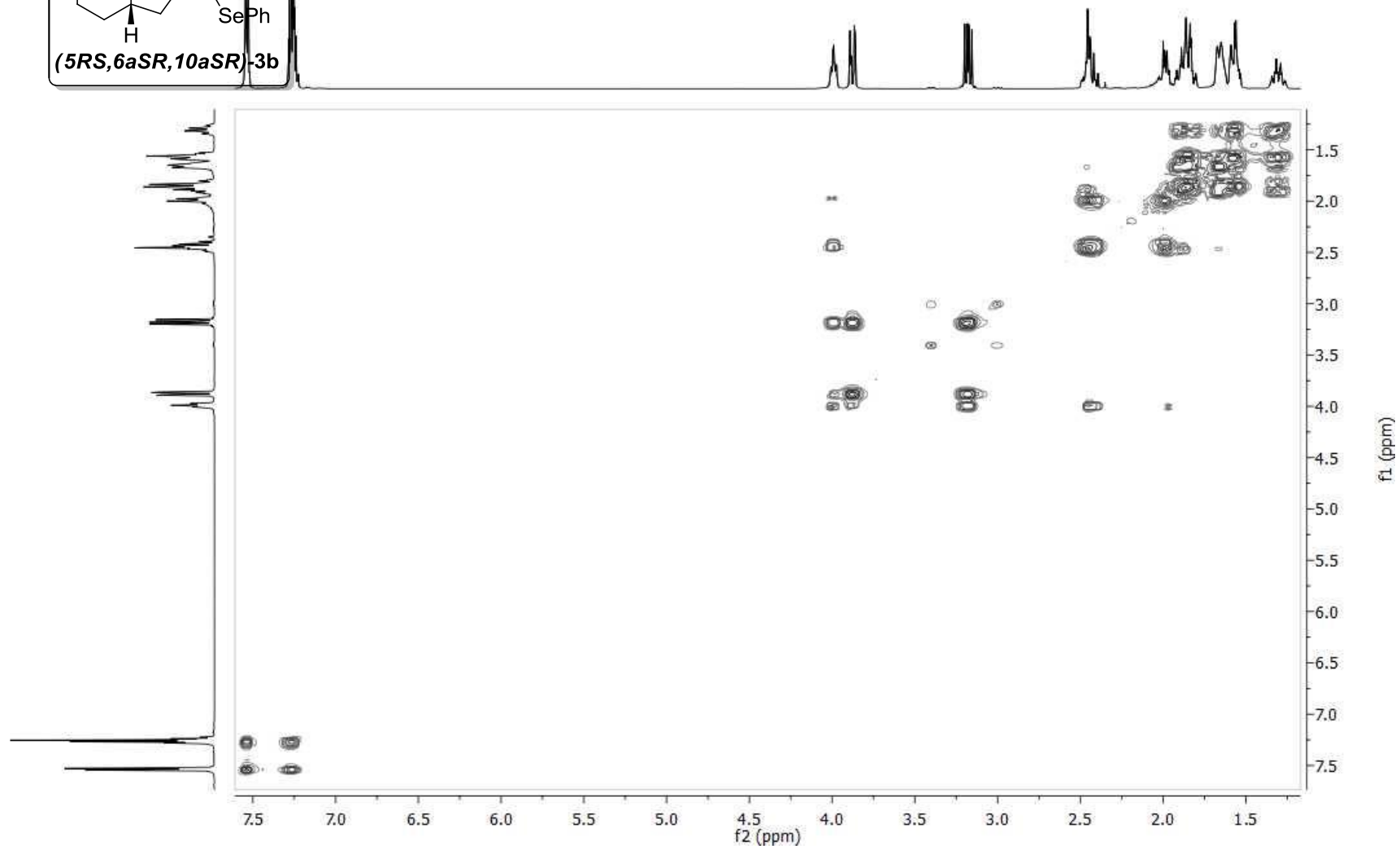
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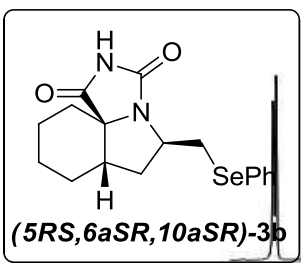




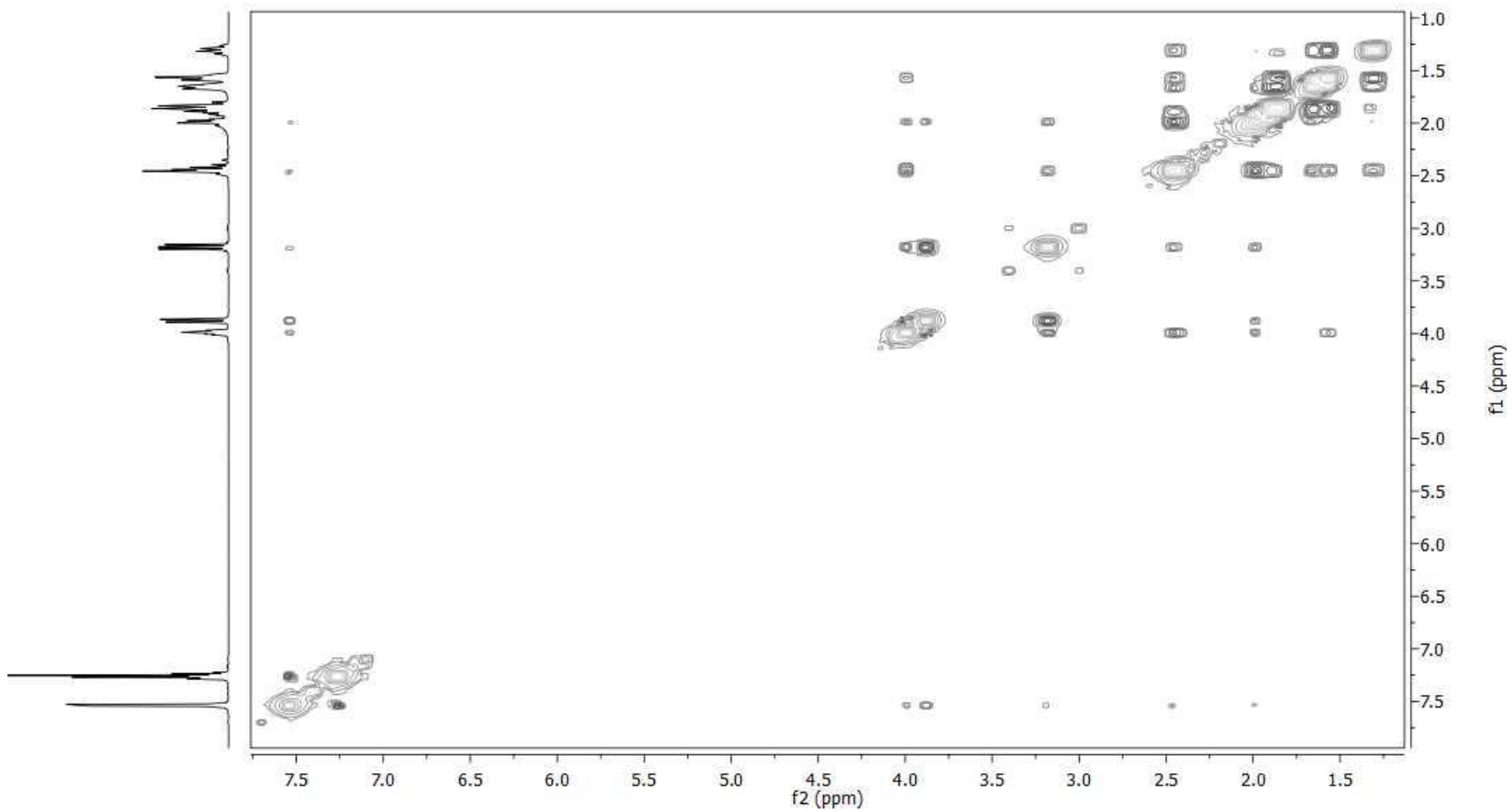


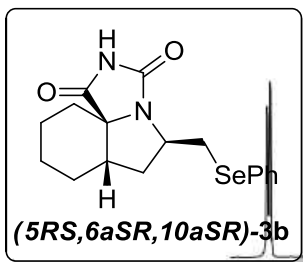
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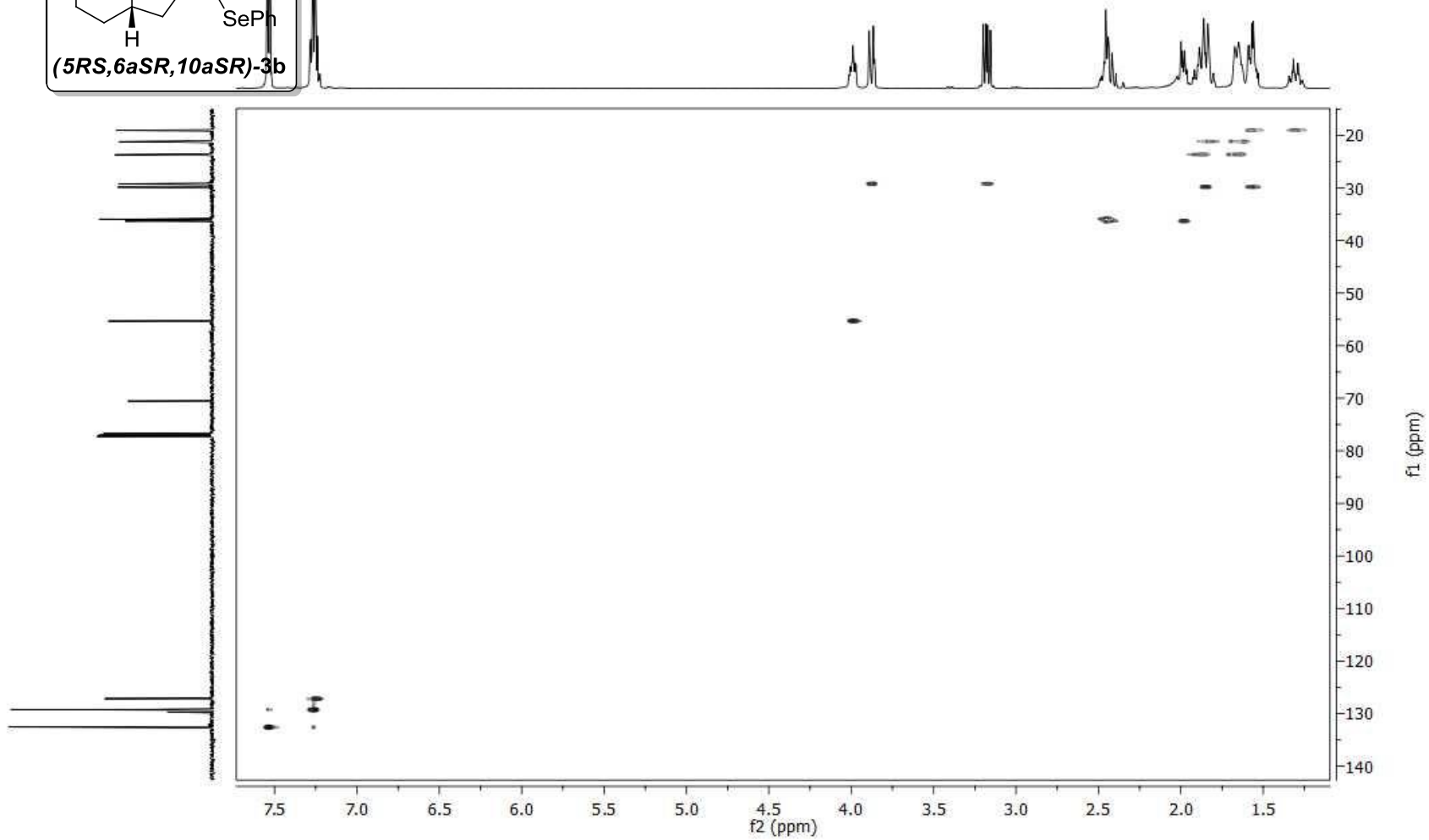


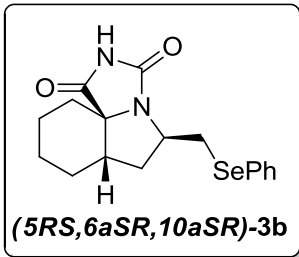
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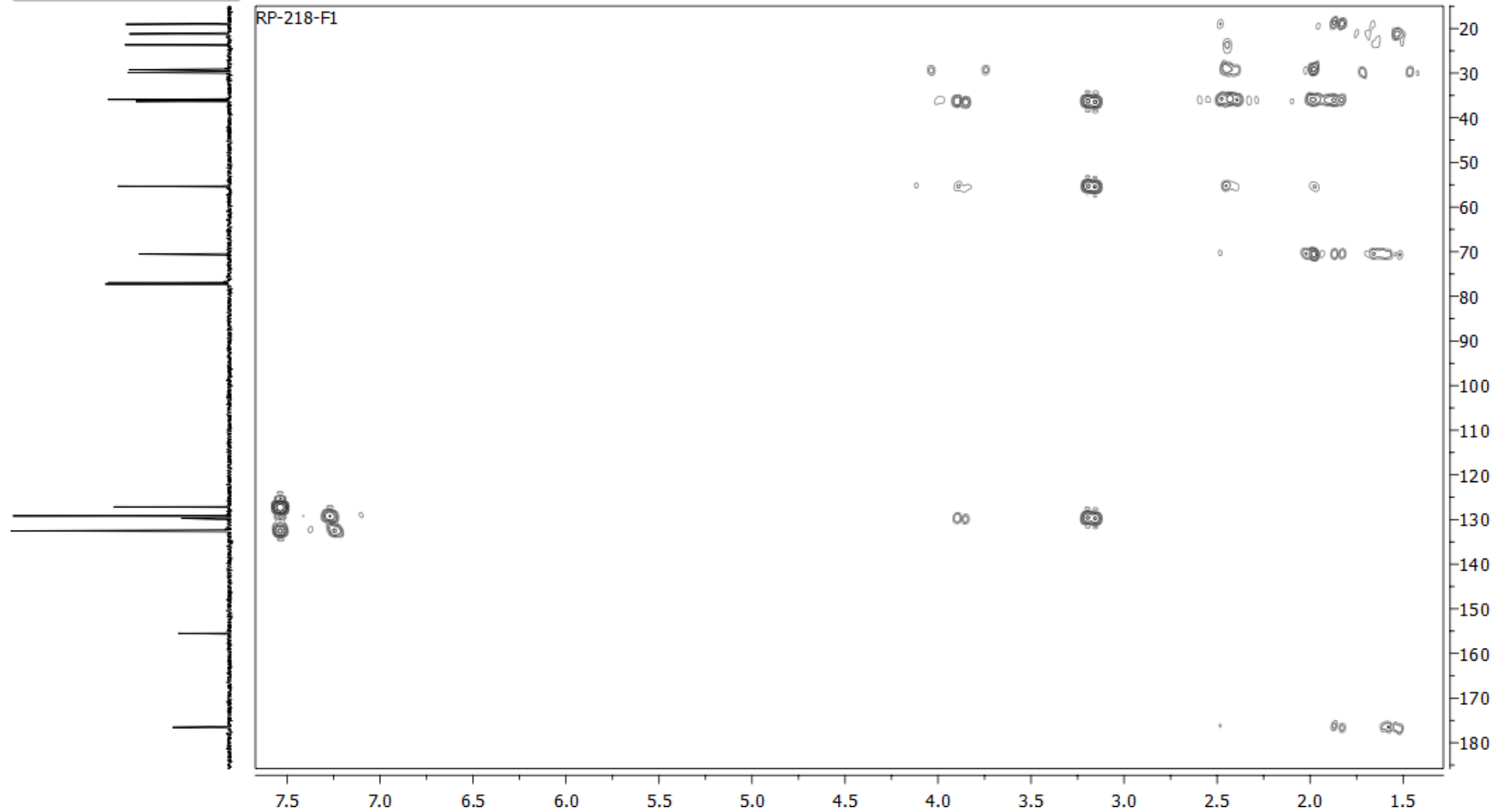
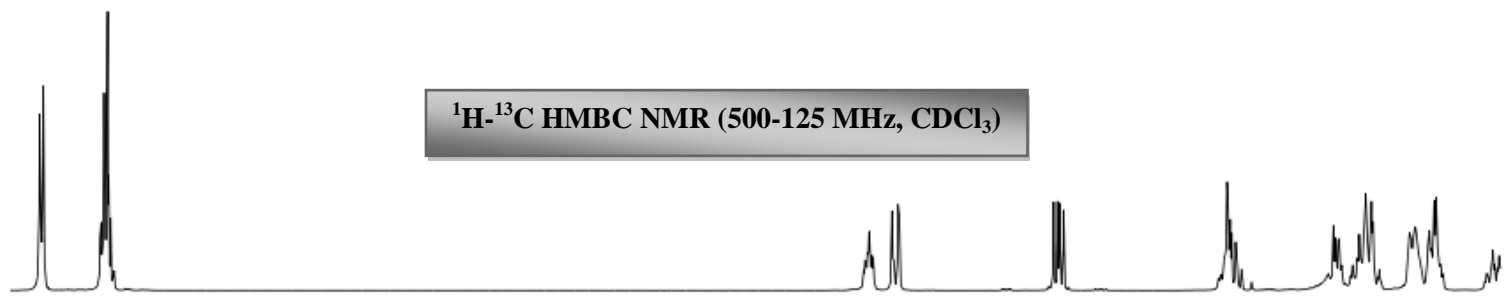


^1H - ^{13}C HSQC NMR (500-125 MHz, CDCl_3)

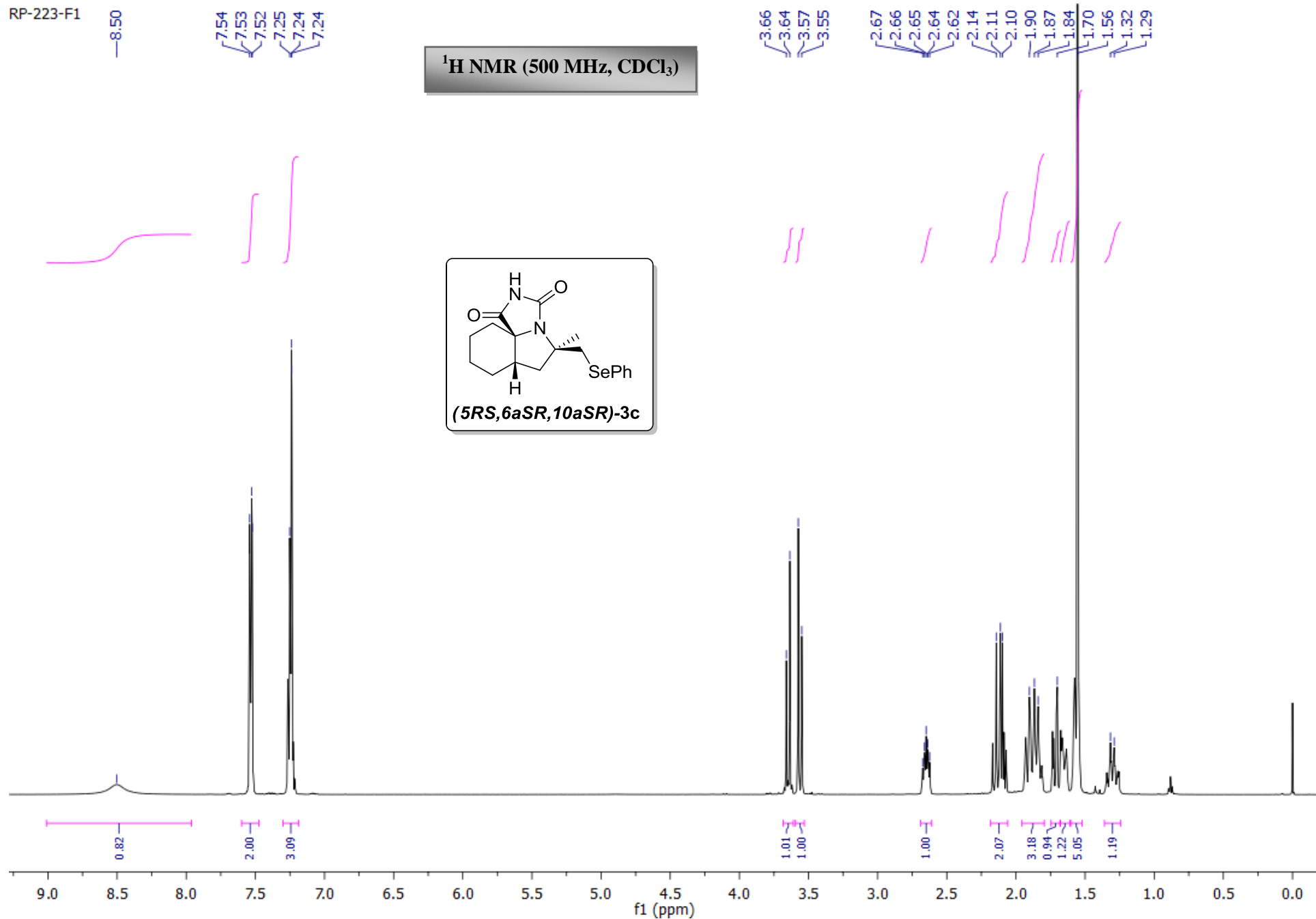


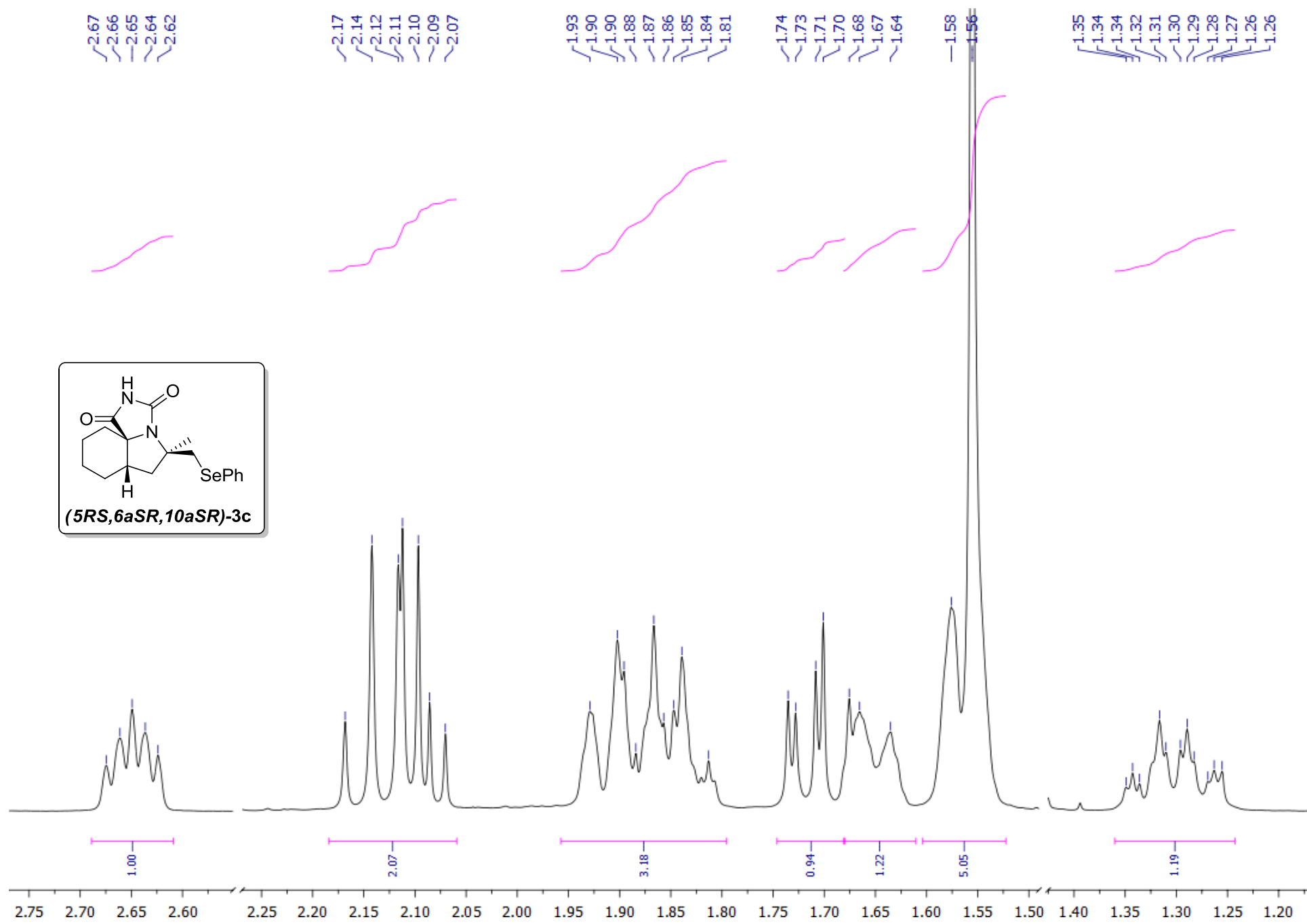


^1H - ^{13}C HMBC NMR (500-125 MHz, CDCl_3)



RP-223-F1





RP-223-F1

—176.62

—155.69

—132.87

—130.47

—129.16

—127.22

—77.25

—77.00

—76.75

—70.55

—63.48

—43.34

—36.67

—36.55

—31.44

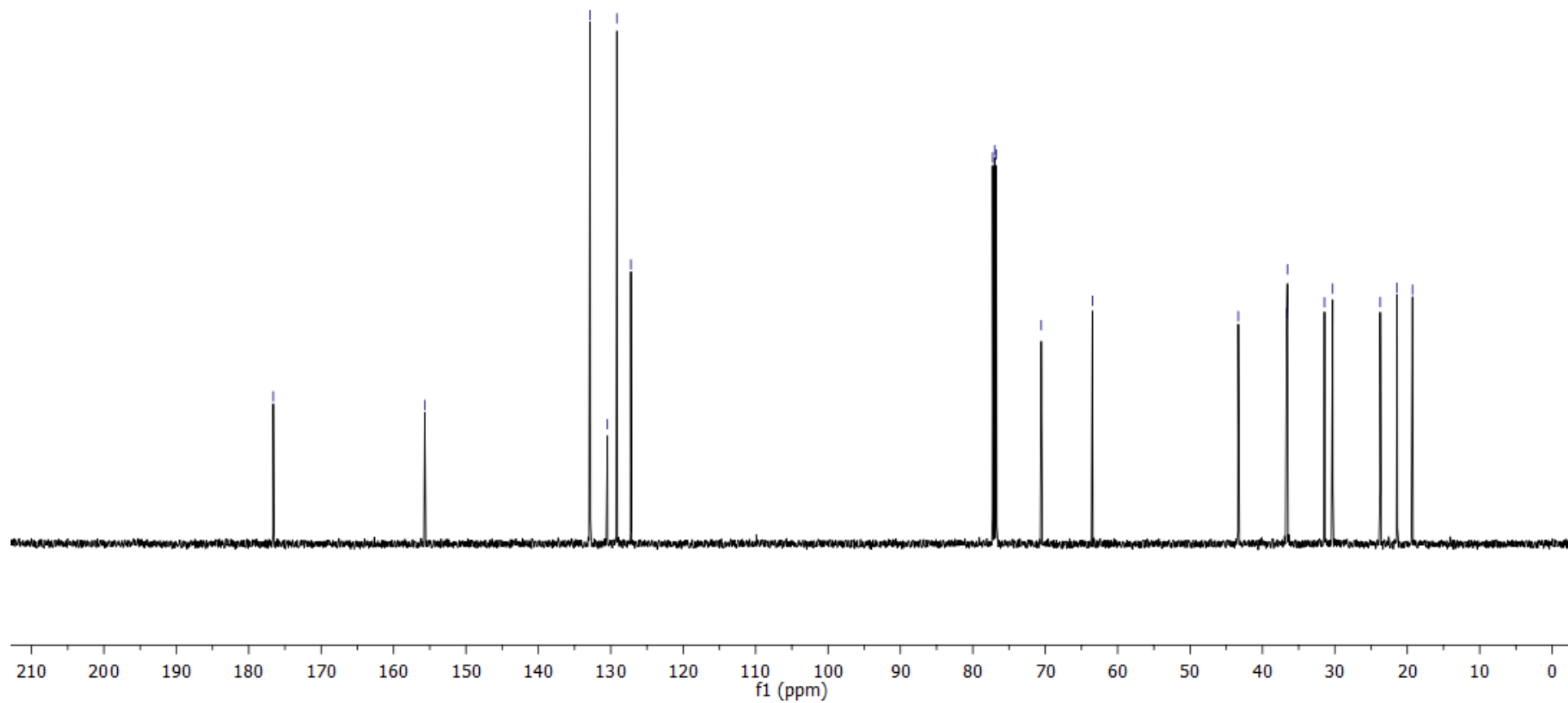
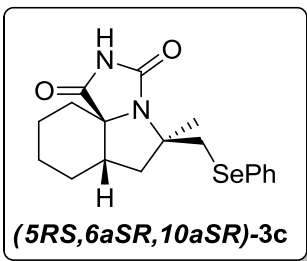
—30.31

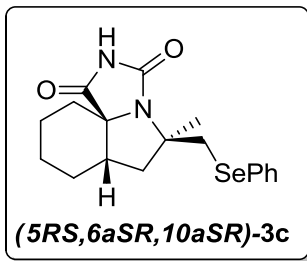
—23.73

—21.40

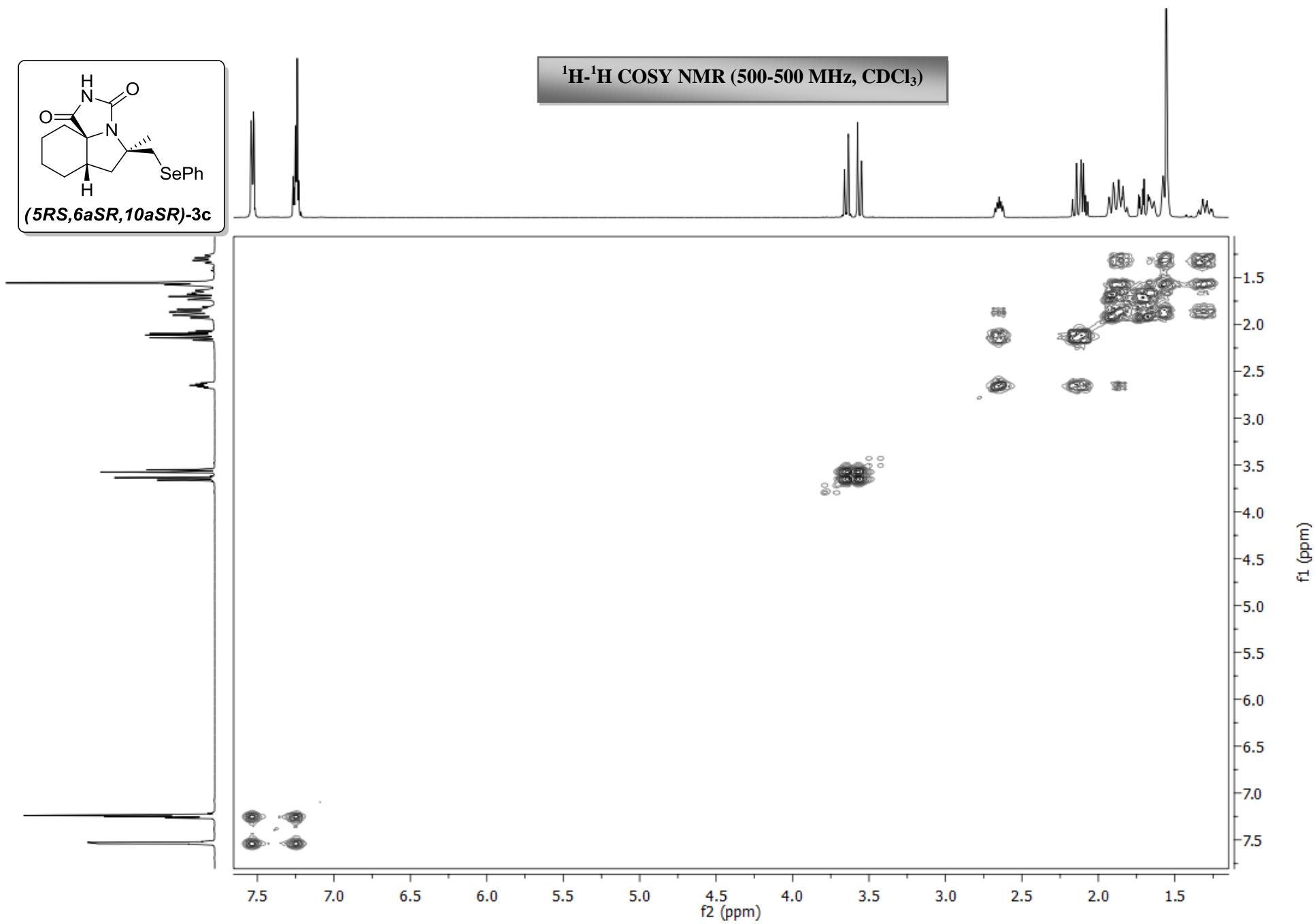
—19.29

¹³C NMR (125 MHz, CDCl₃)

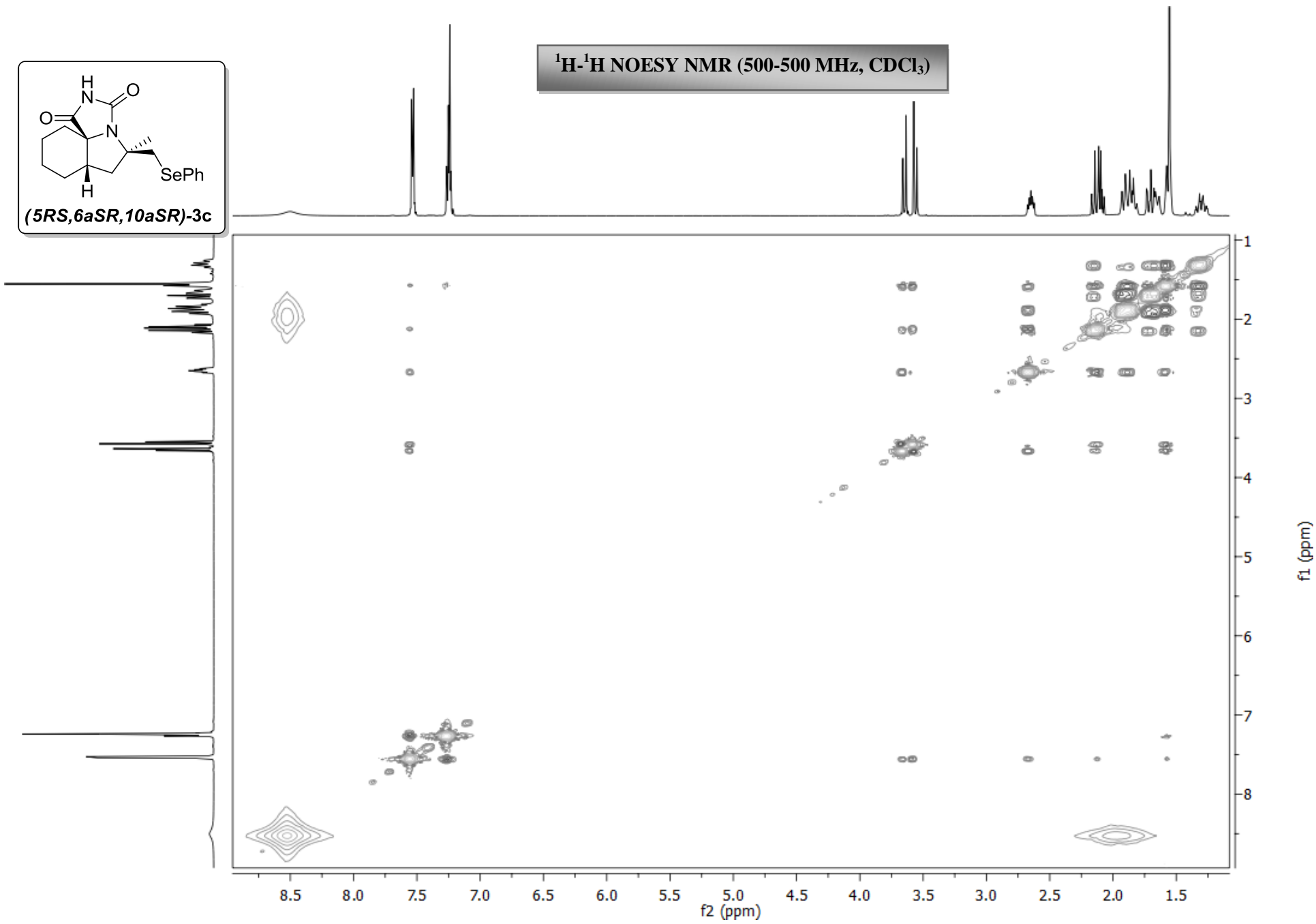
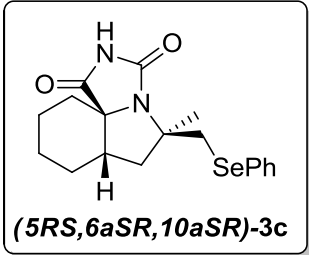


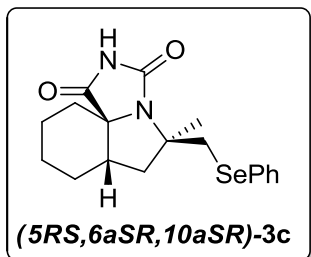


¹H-¹H COSY NMR (500-500 MHz, CDCl₃)

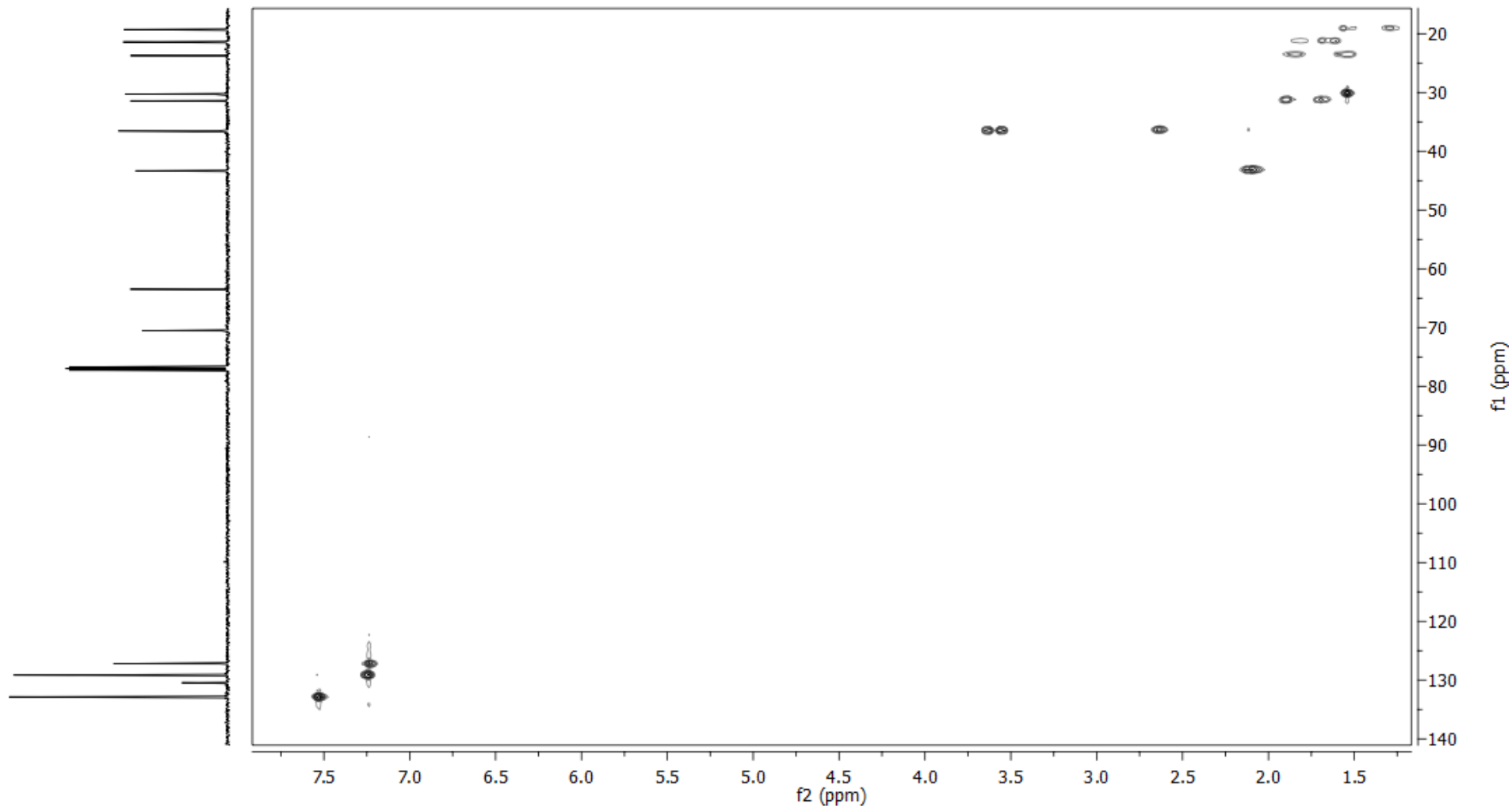


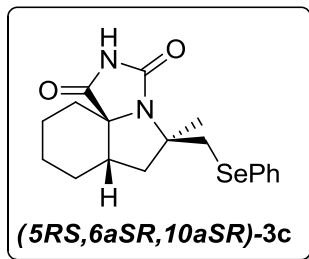
¹H-¹H NOESY NMR (500-500 MHz, CDCl₃)



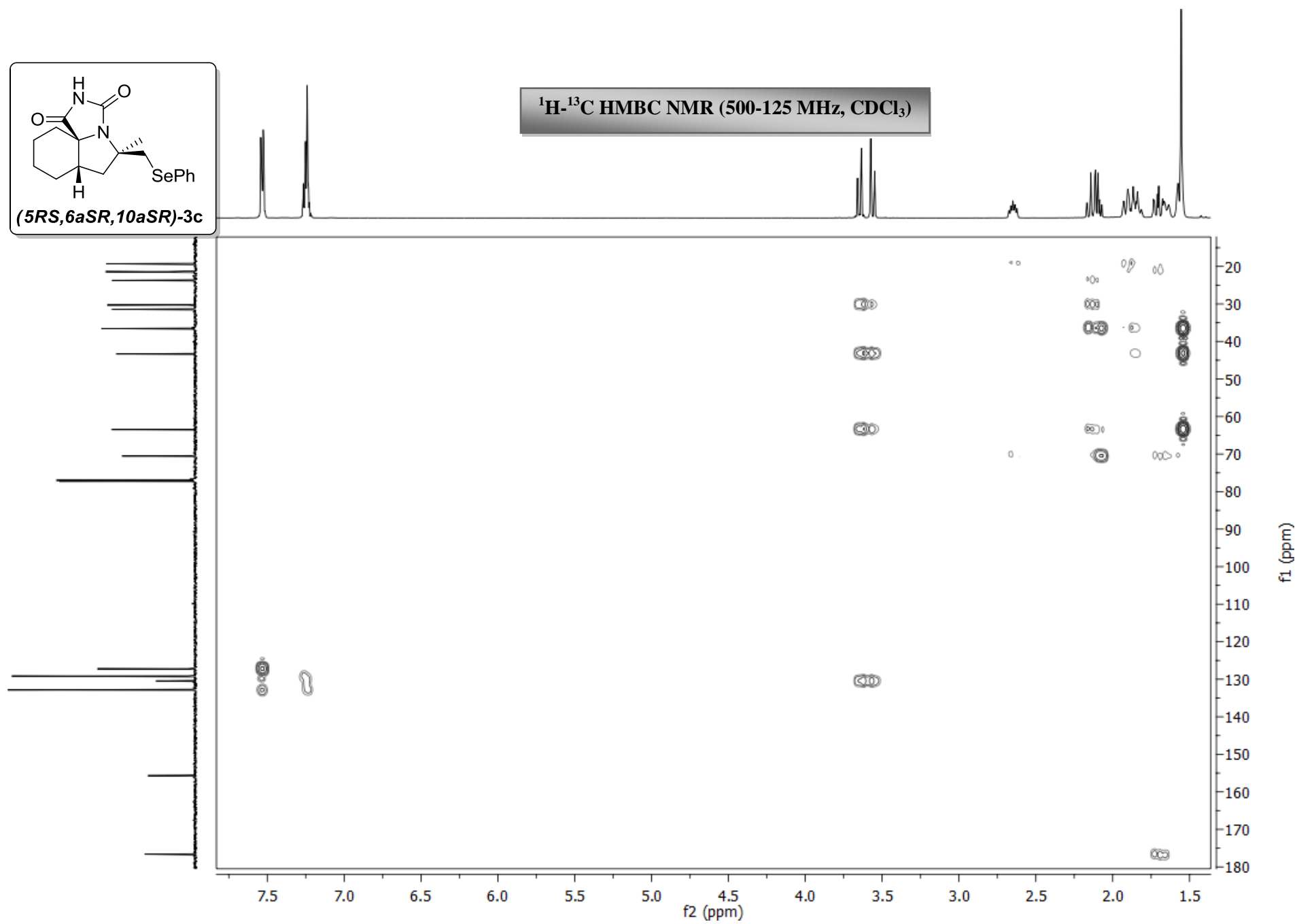


^1H - ^{13}C HSQC NMR (500-125 MHz, CDCl_3)

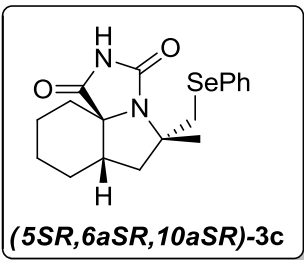




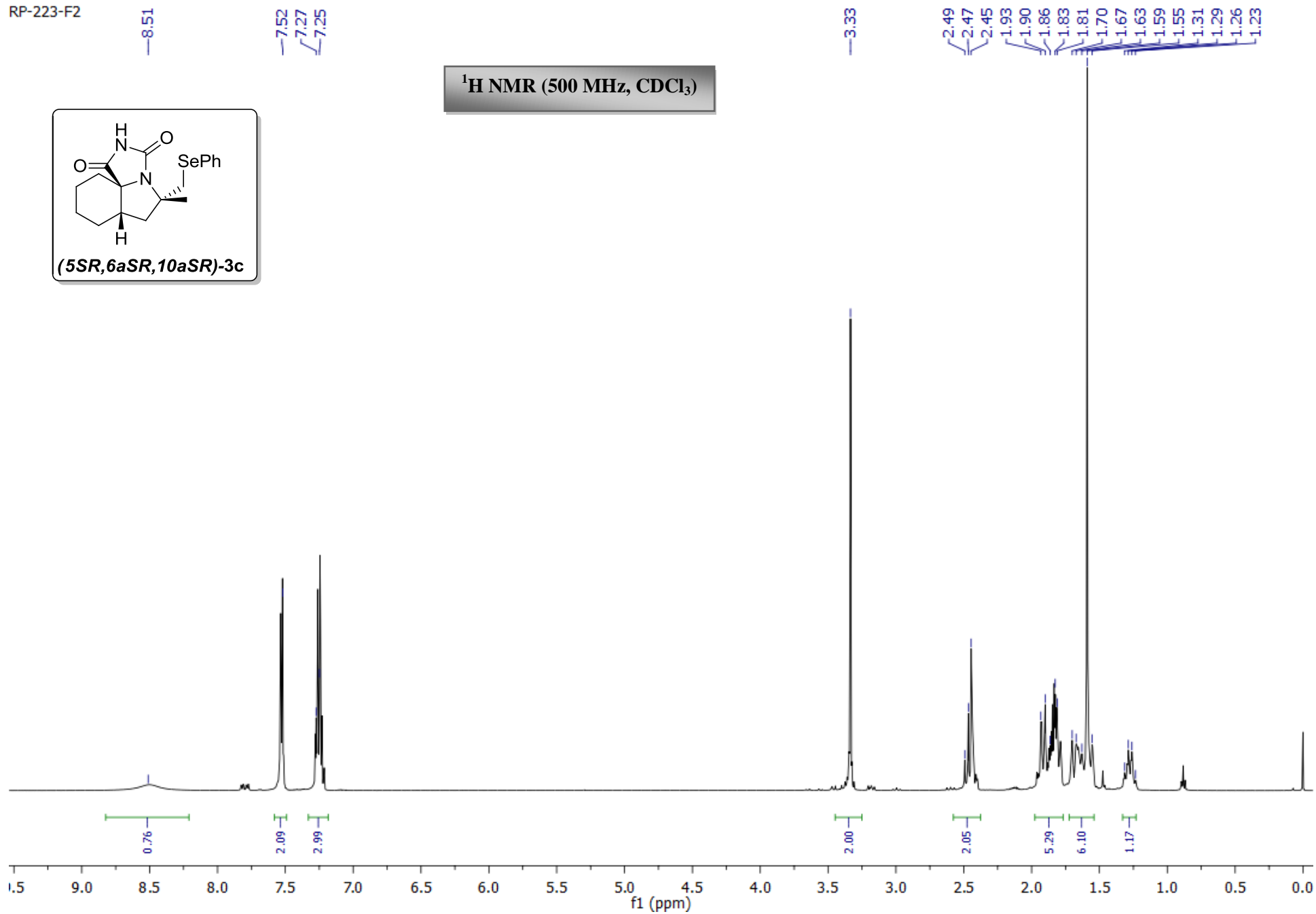
^1H - ^{13}C HMBC NMR (500-125 MHz, CDCl_3)



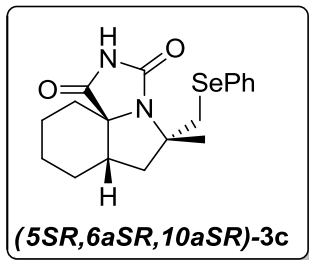
RP-223-F2



¹H NMR (500 MHz, CDCl₃)



RP-223-F2



—176.93

—156.46

132.32

130.70

129.10

126.92

77.25

77.00

76.74

70.57

—63.97

43.73

40.94

36.17

31.30

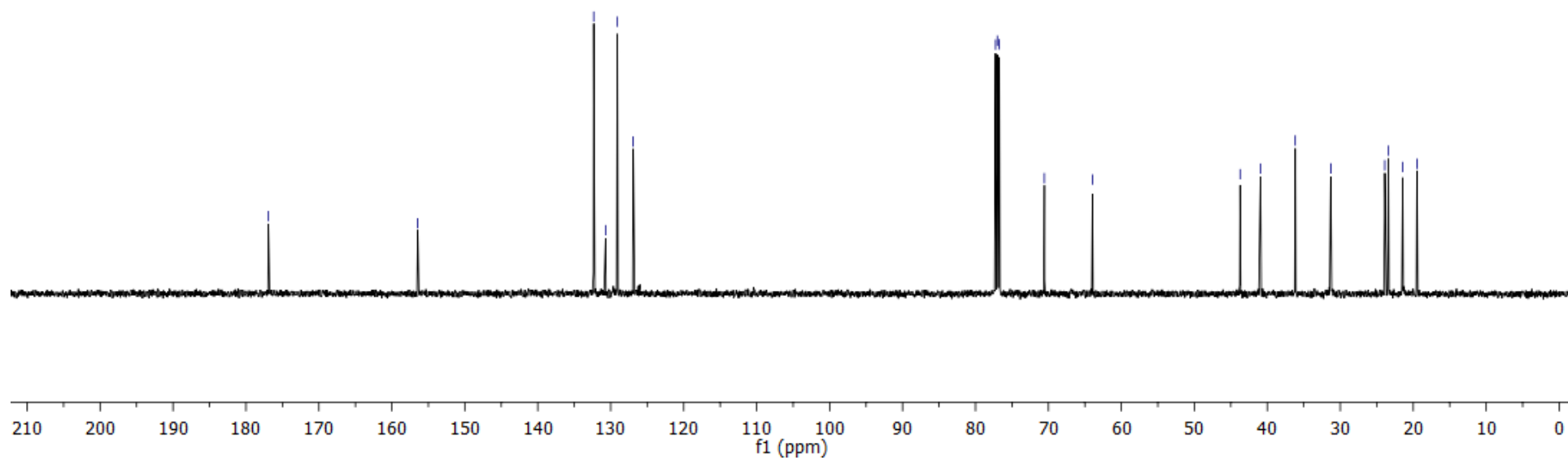
23.90

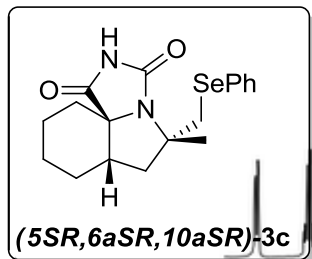
23.41

21.44

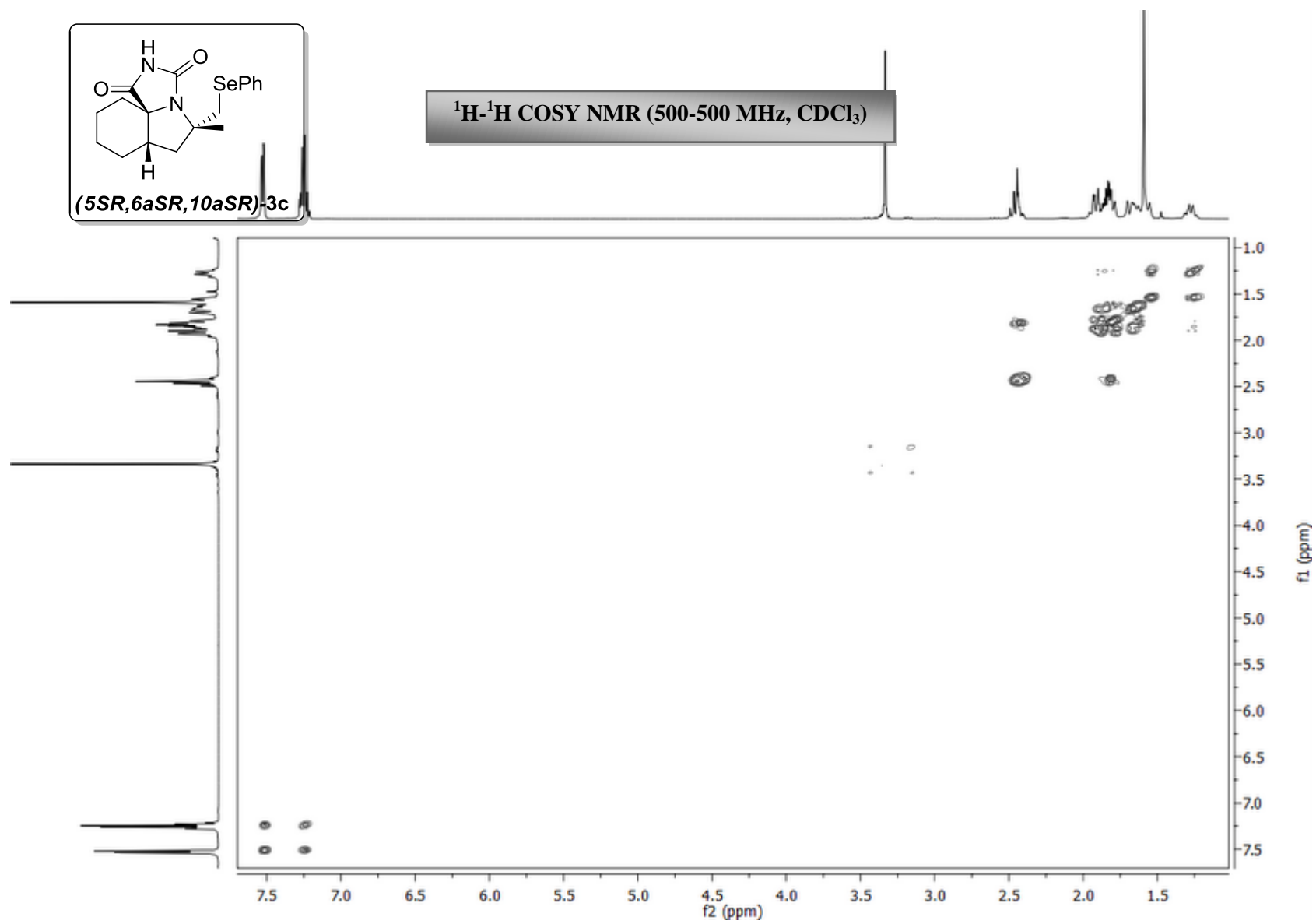
19.49

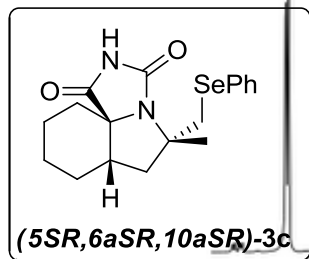
¹³C NMR (125 MHz, CDCl₃)



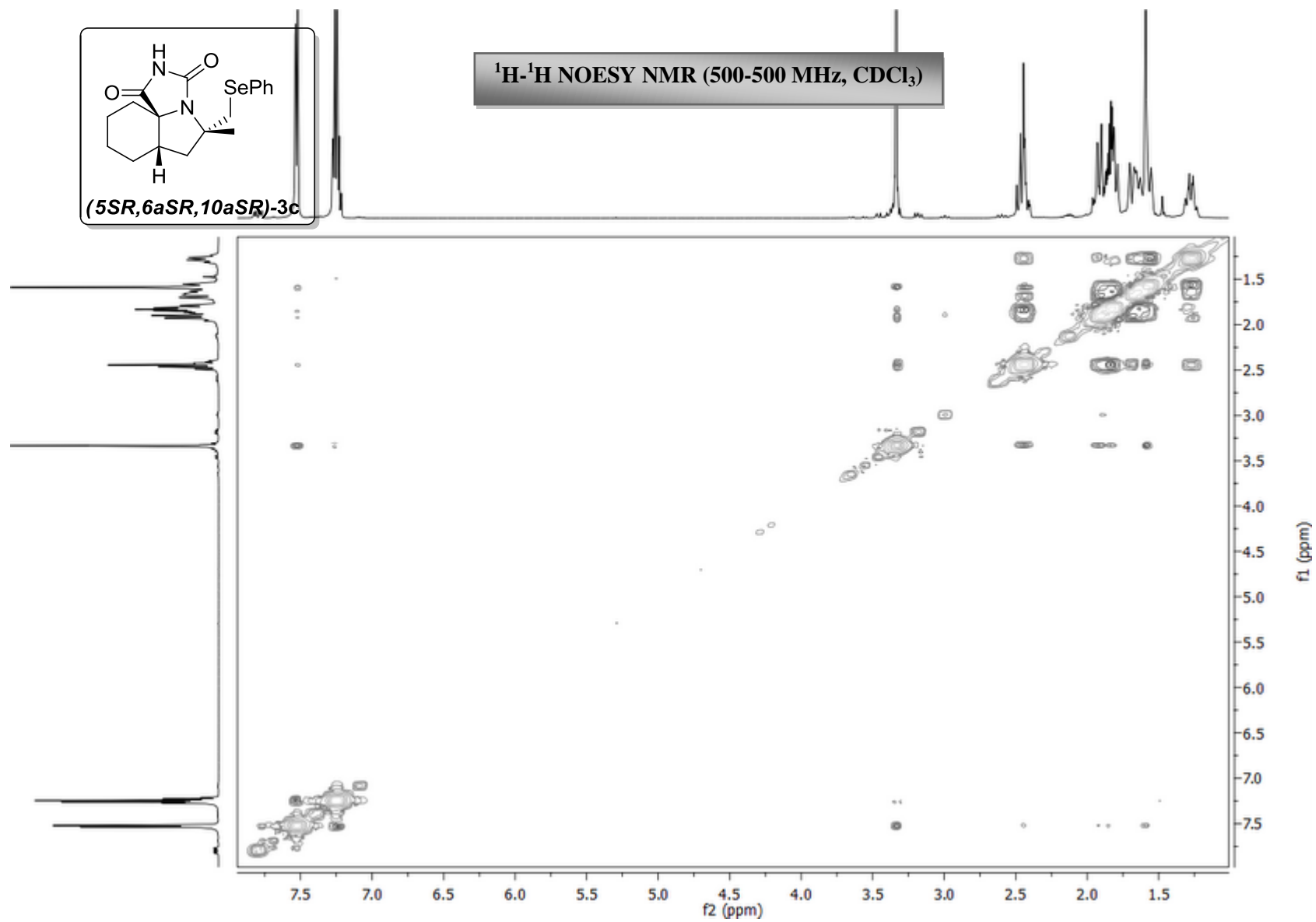


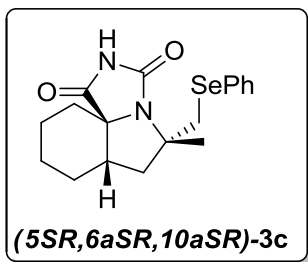
^1H - ^1H COSY NMR (500-500 MHz, CDCl_3)



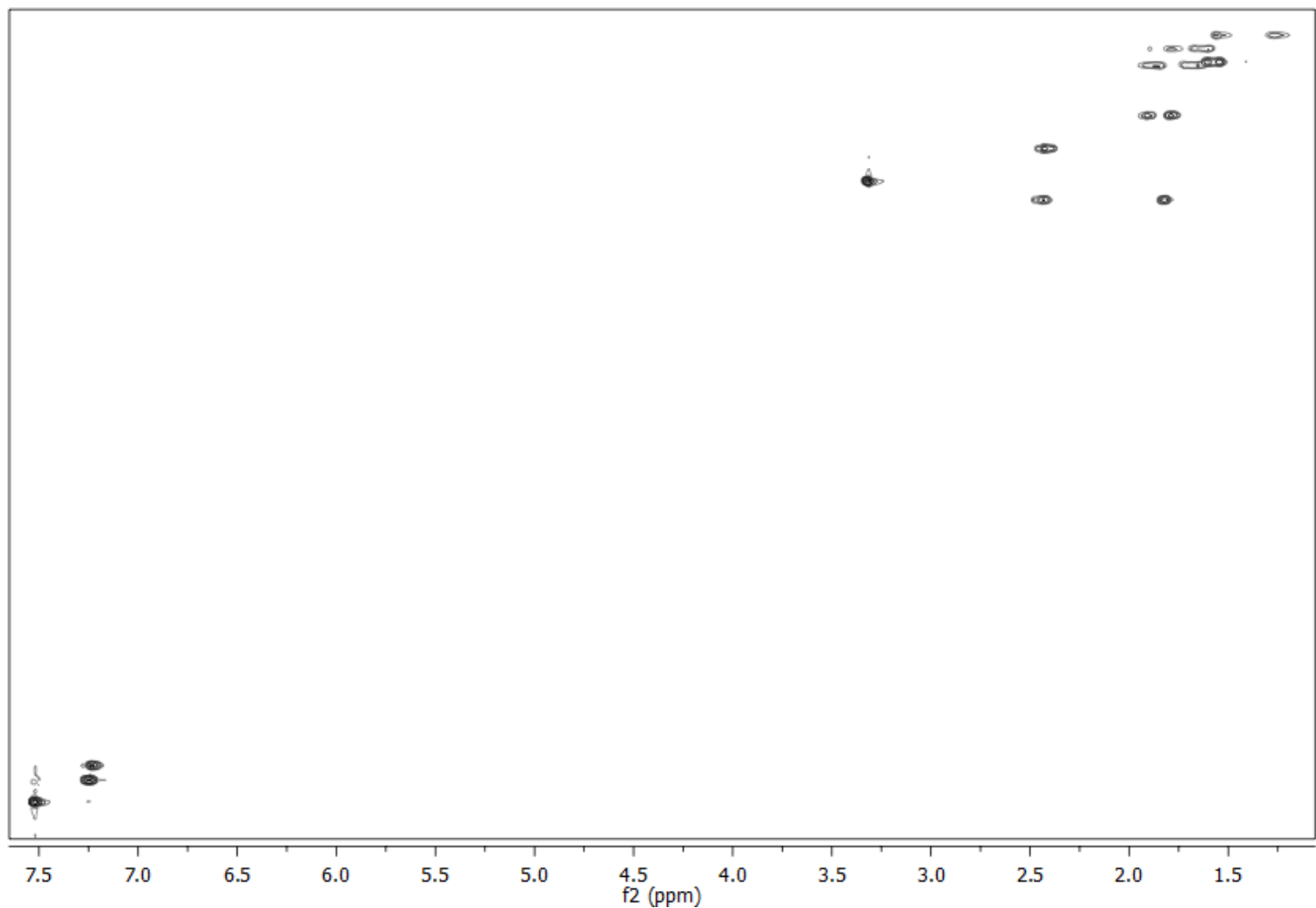
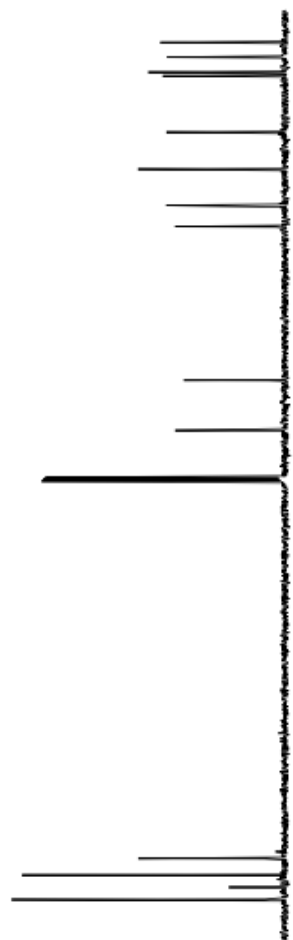
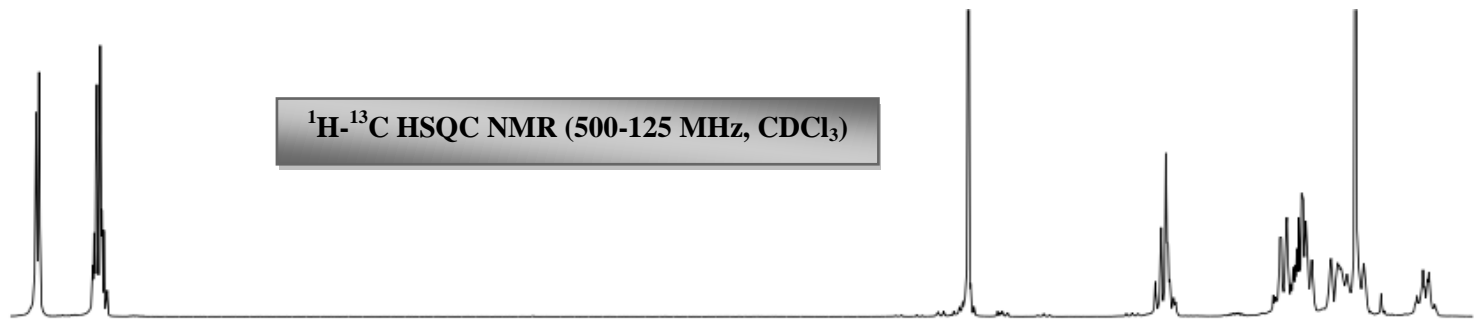


^1H - ^1H NOESY NMR (500-500 MHz, CDCl_3)



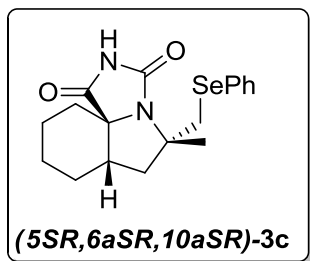


^1H - ^{13}C HSQC NMR (500-125 MHz, CDCl_3)

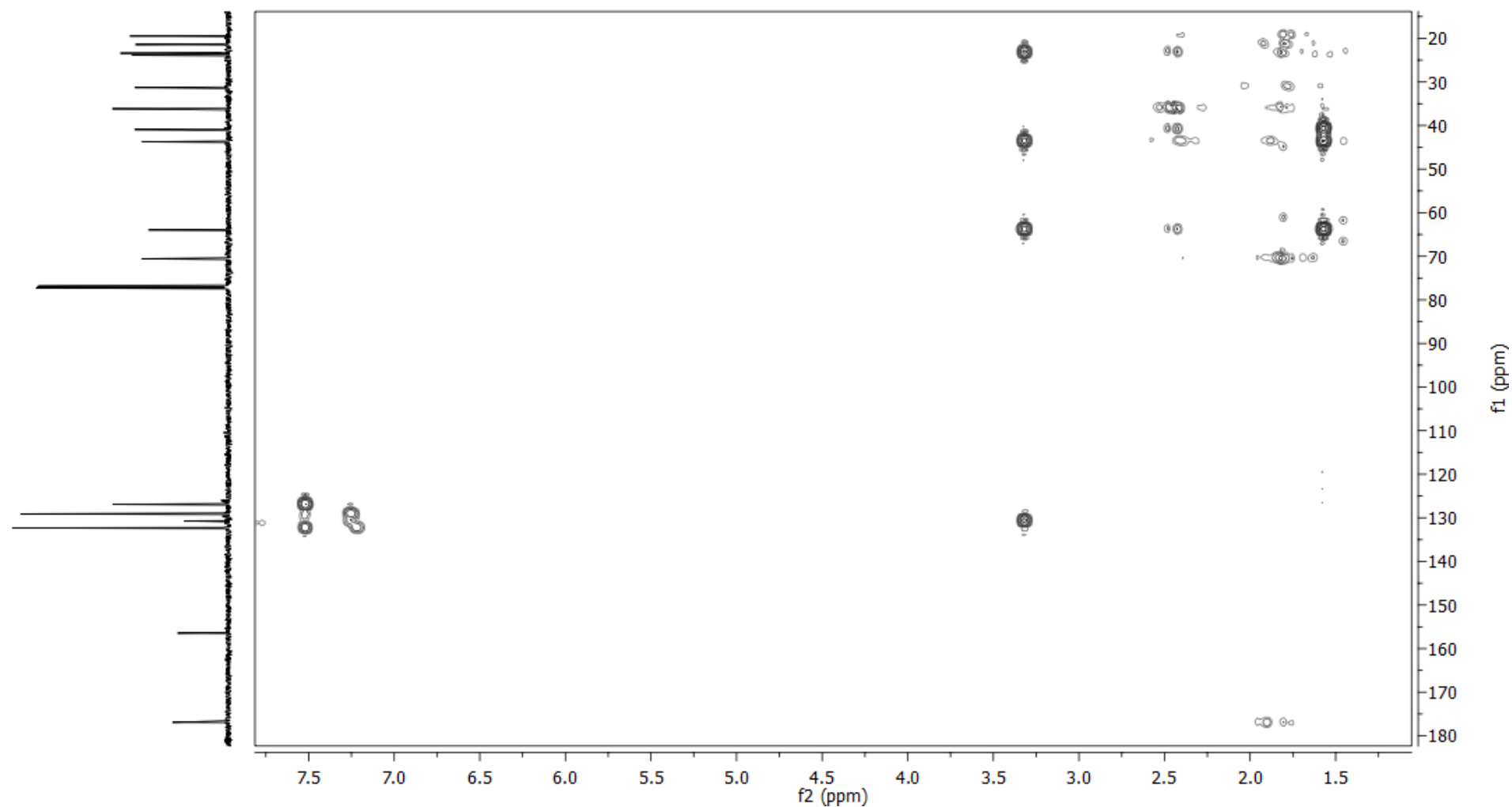
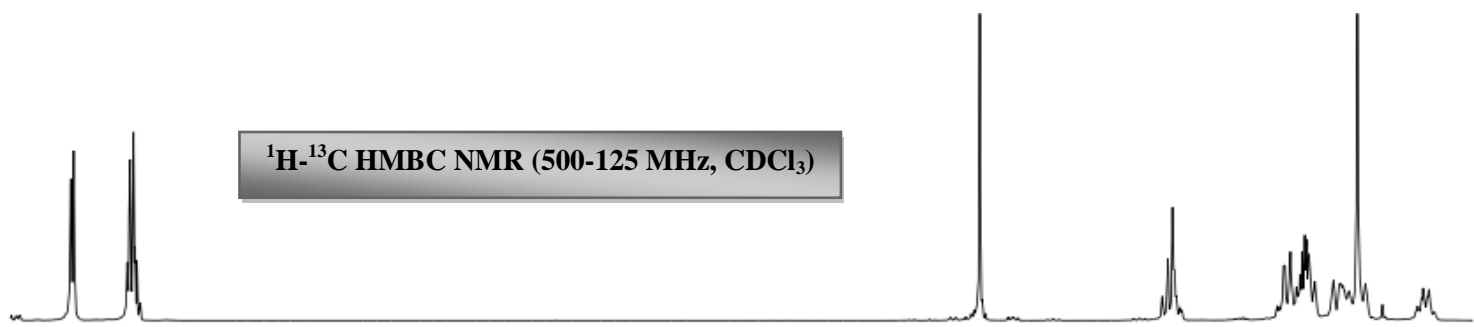


f1 (ppm)

f2 (ppm)



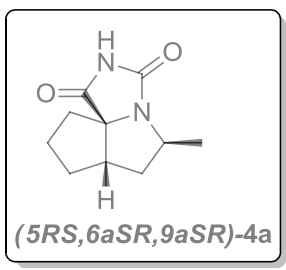
^1H - ^{13}C HMBC NMR (500-125 MHz, CDCl_3)



RP-231

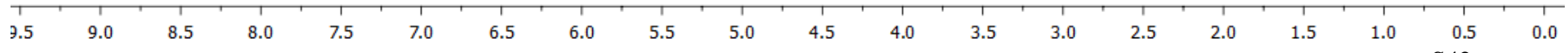


8.76



¹H NMR (500 MHz, CDCl₃)

3.63
3.63
3.61
2.81
2.81
2.80
2.80
2.22
2.21
2.05
2.04
2.03
2.03
1.82
1.82
1.81
1.81
1.79
1.79
1.59
1.58
1.54
1.53
0.00



1.00

1.00

1.00

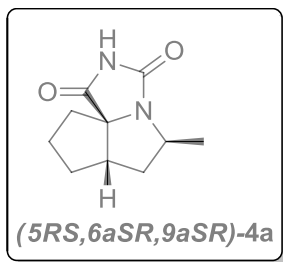
1.04

1.17

5.13

4.06

RP-231



—178.35

—157.42

80.21
77.25
77.00
76.75

—56.04

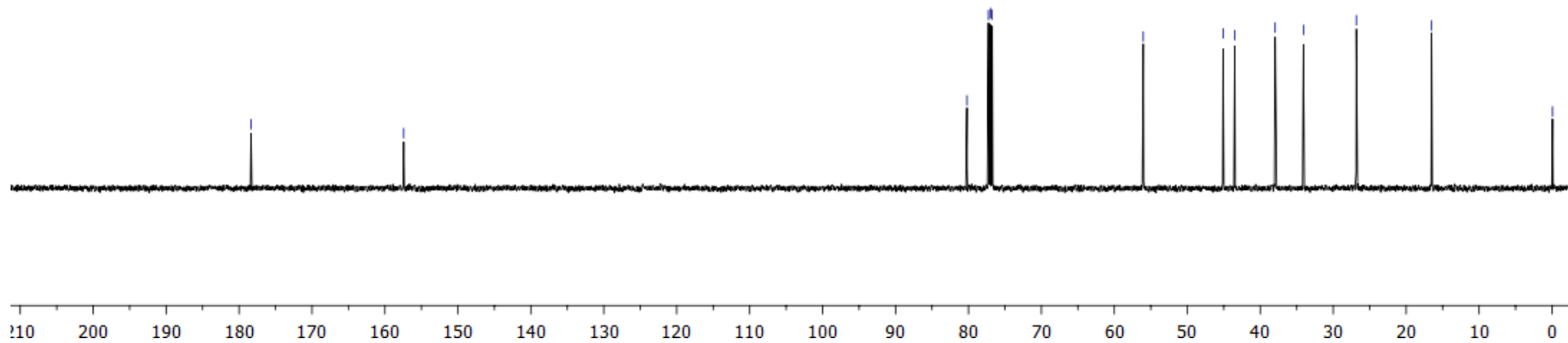
45.10
43.50
37.95
34.07

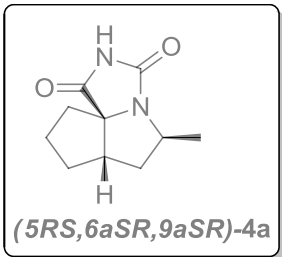
—26.83

—16.51

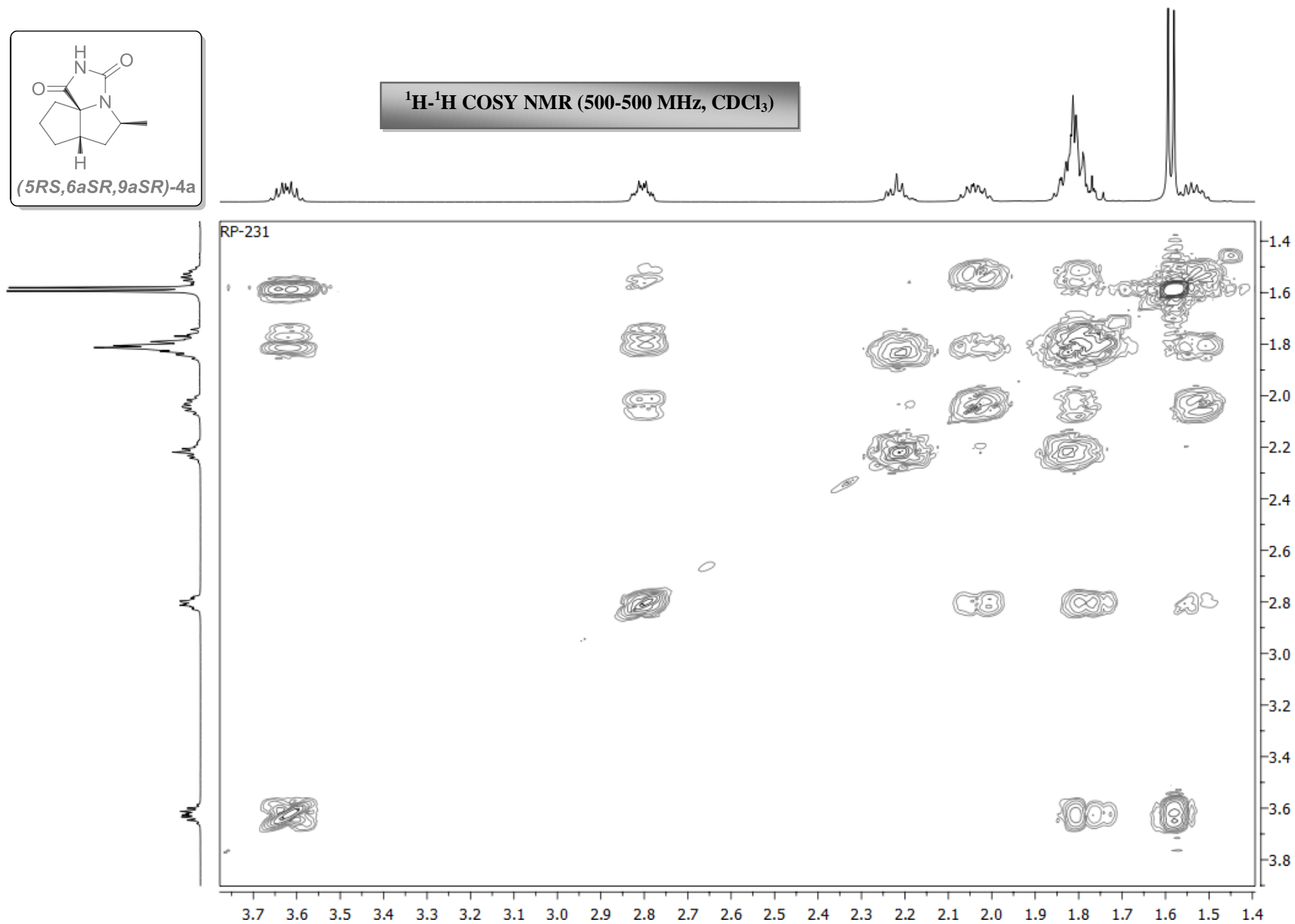
—0.08

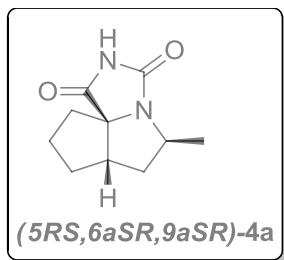
¹³C NMR (125 MHz, CDCl₃)



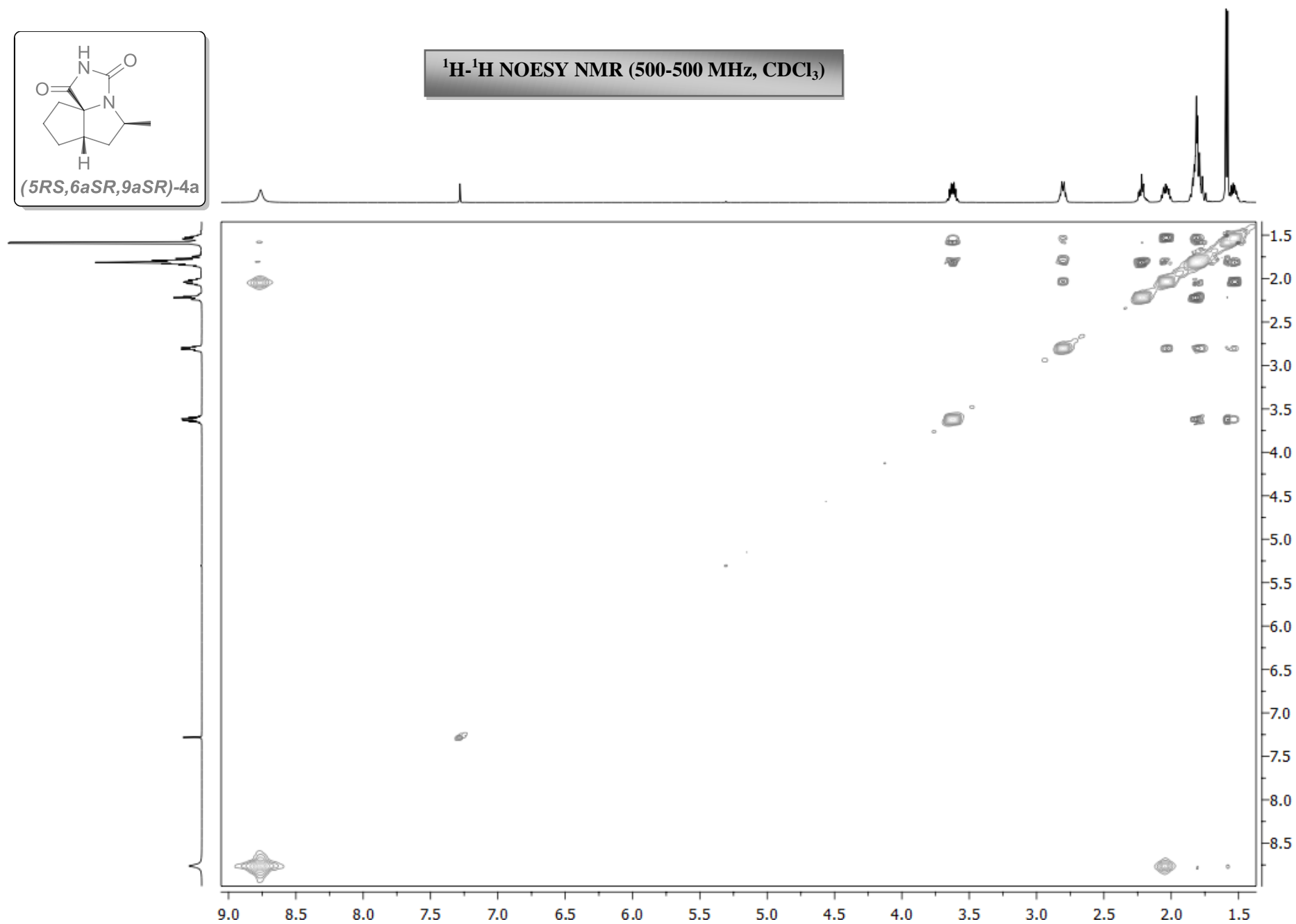


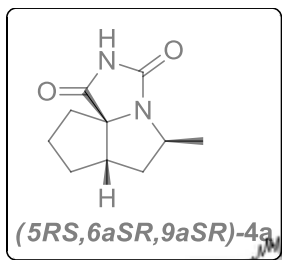
¹H-¹H COSY NMR (500-500 MHz, CDCl₃)



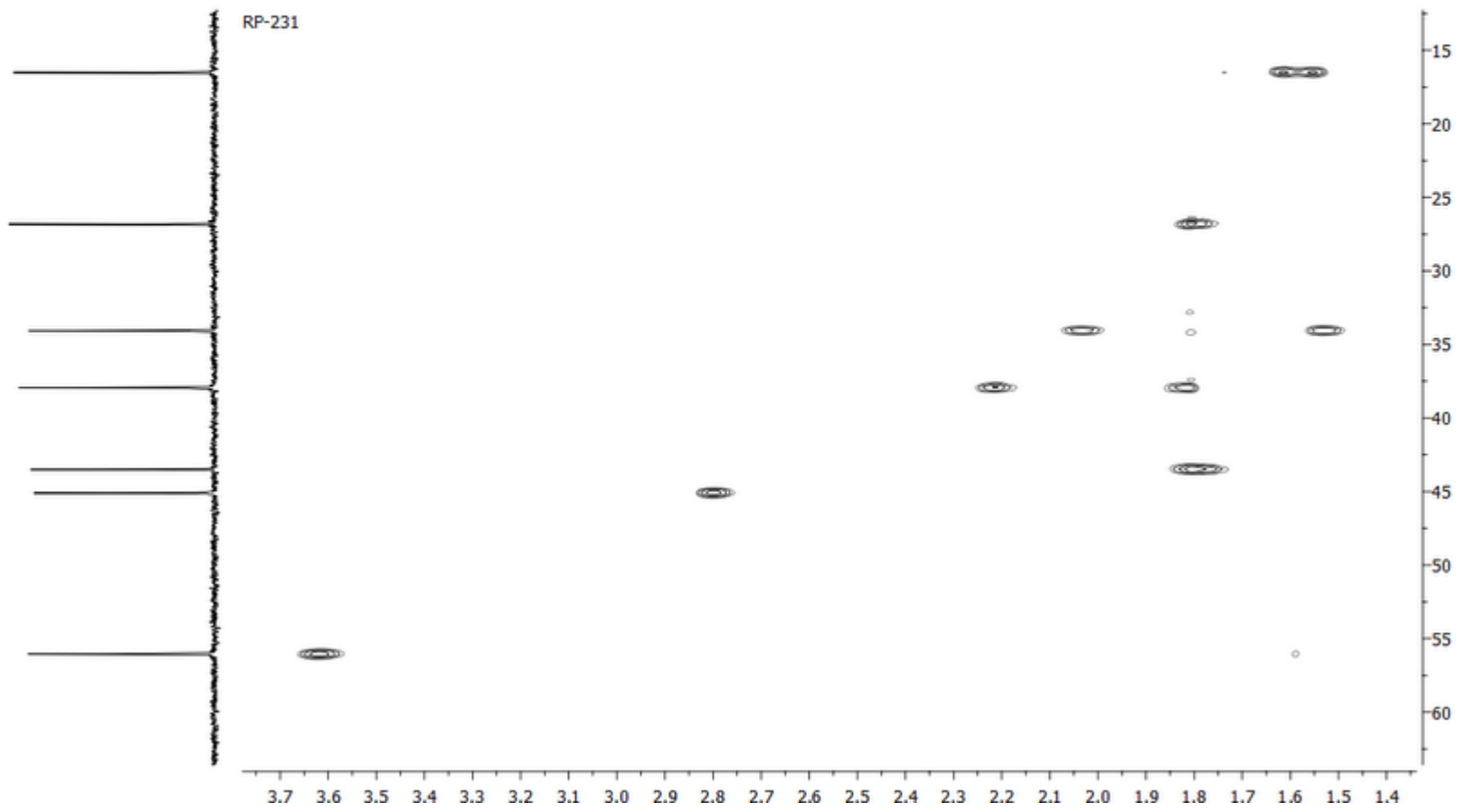


¹H-¹H NOESY NMR (500-500 MHz, CDCl₃)





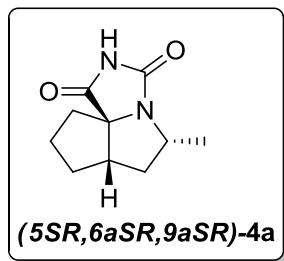
^1H - ^{13}C HSQC NMR (500-125 MHz, CDCl_3)



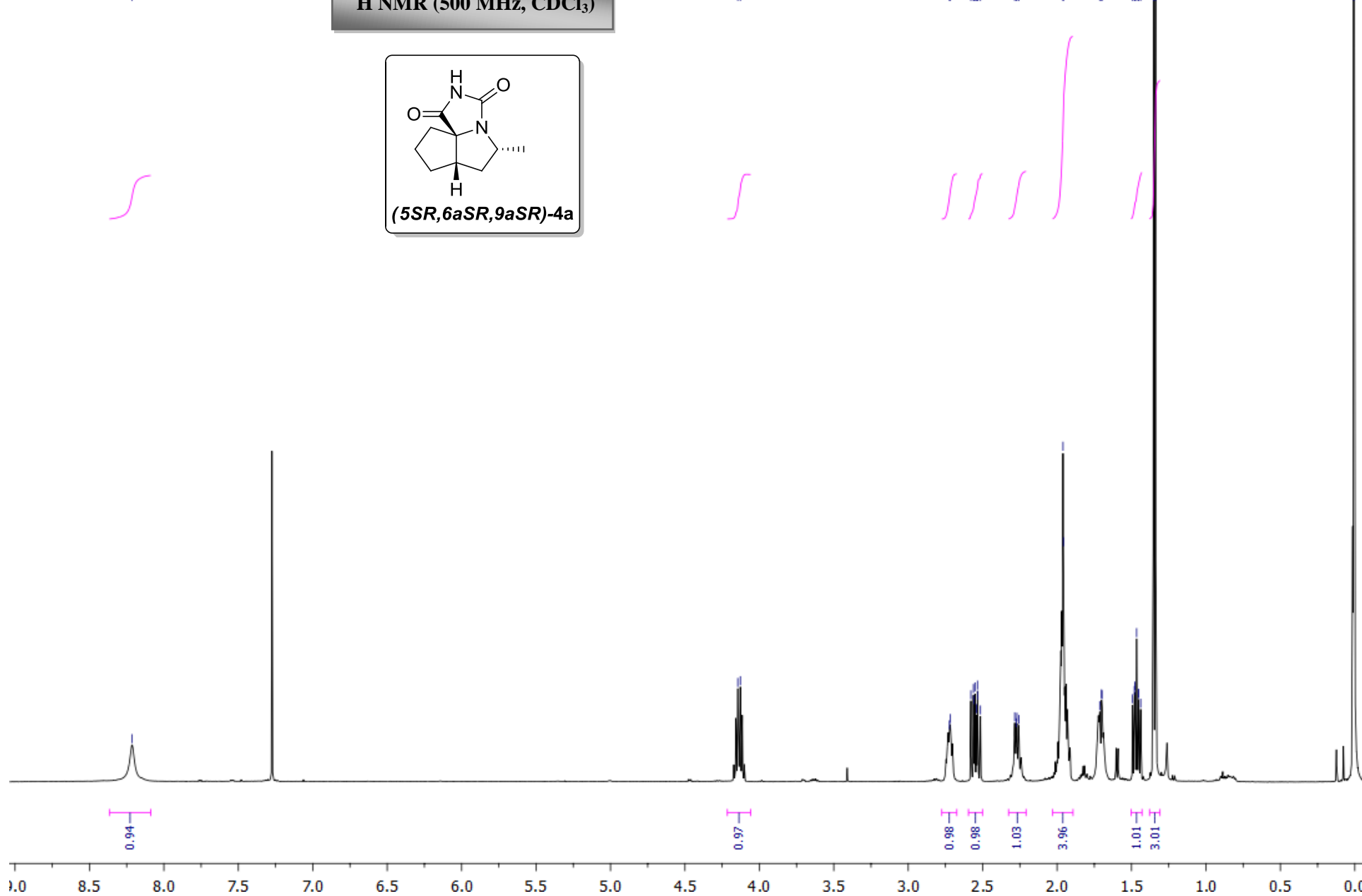
RP-233

—8.21

¹H NMR (500 MHz, CDCl₃)



4.14
4.13
2.72
2.72
2.58
2.56
2.56
2.55
2.54
2.53
2.53
2.51
2.28
2.27
2.27
2.26
1.96
1.96
1.71
1.70
1.70
1.49
1.48
1.48
1.47
1.45
1.45
1.44
1.35
1.34
0.01



4.17
4.16
4.15
4.14
4.14
4.13
4.13
4.12
4.11
4.10

2.74
2.73
2.72
2.72
2.70

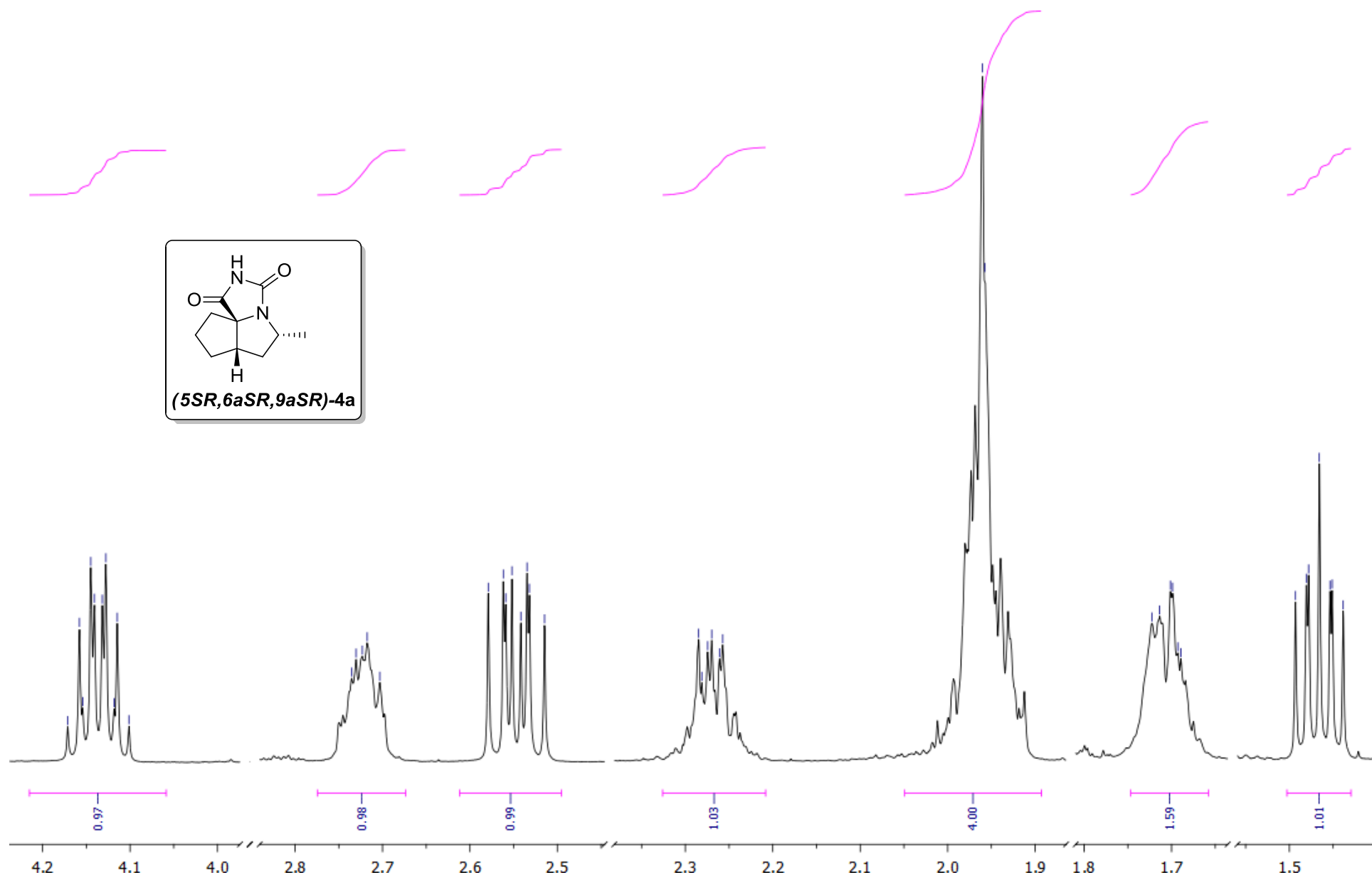
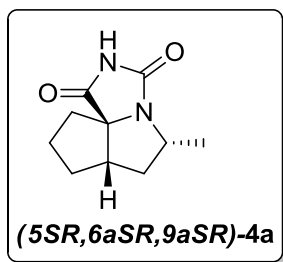
2.58
2.56
2.56
2.55
2.54
2.53
2.53
2.51

2.28
2.28
2.27
2.27
2.26
2.26

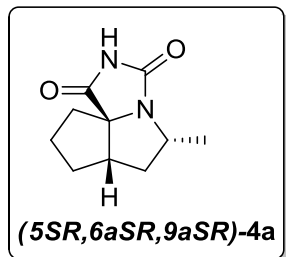
1.96
1.96

1.72
1.71
1.70
1.70
1.69
1.69

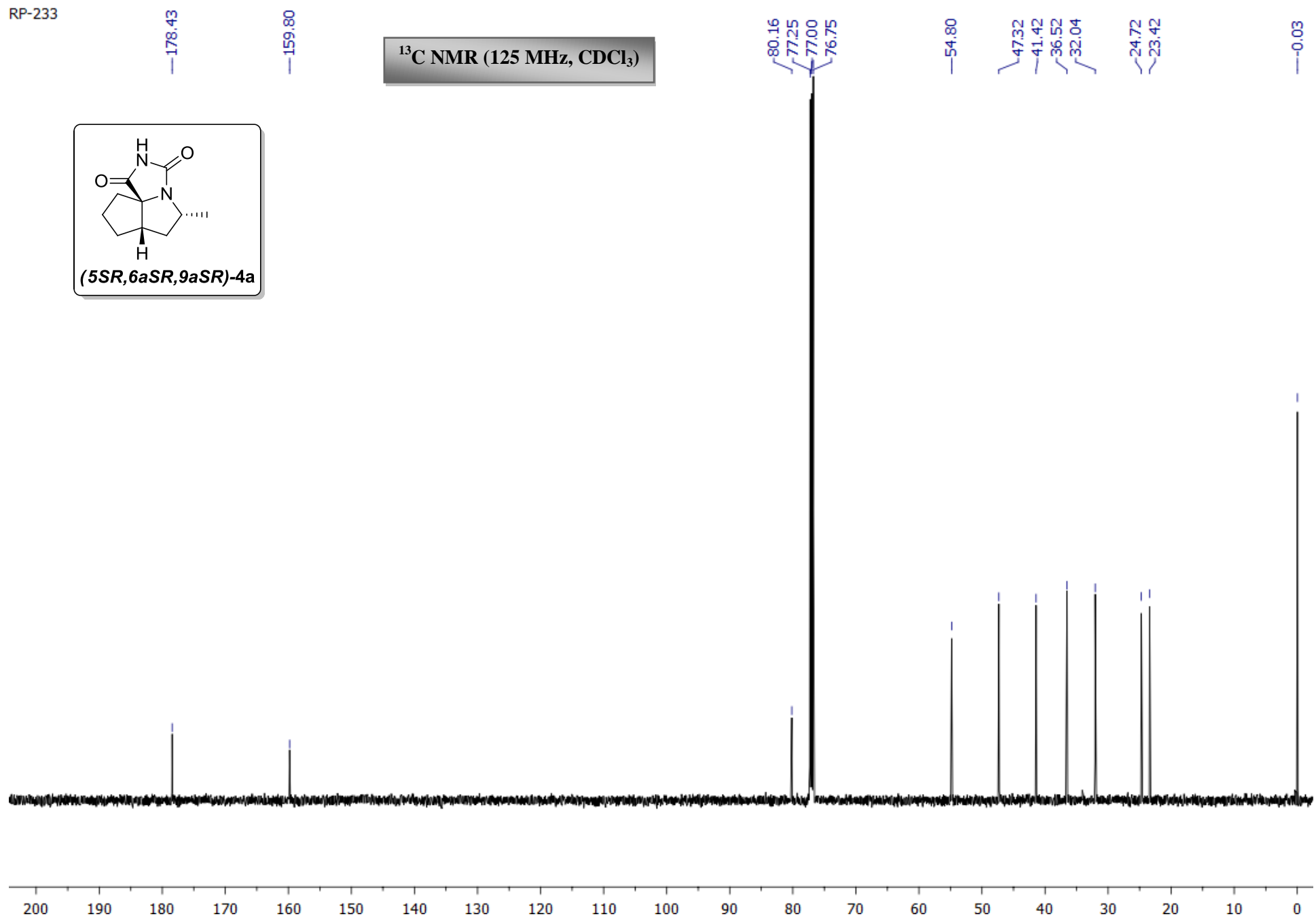
1.49
1.48
1.48
1.47
1.45
1.45

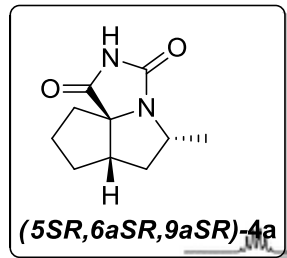


RP-233

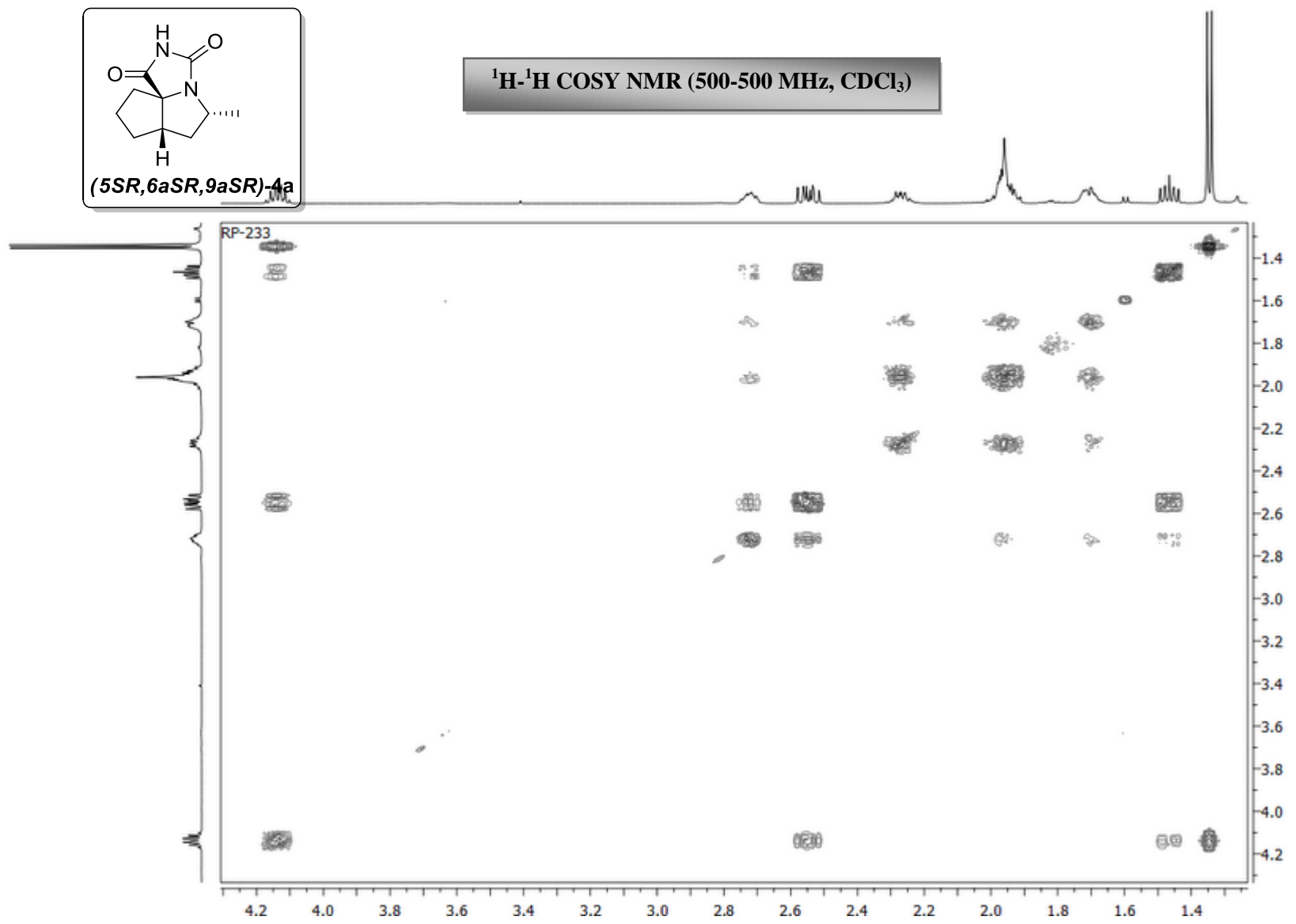


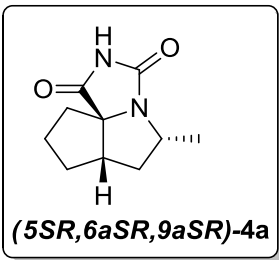
¹³C NMR (125 MHz, CDCl₃)



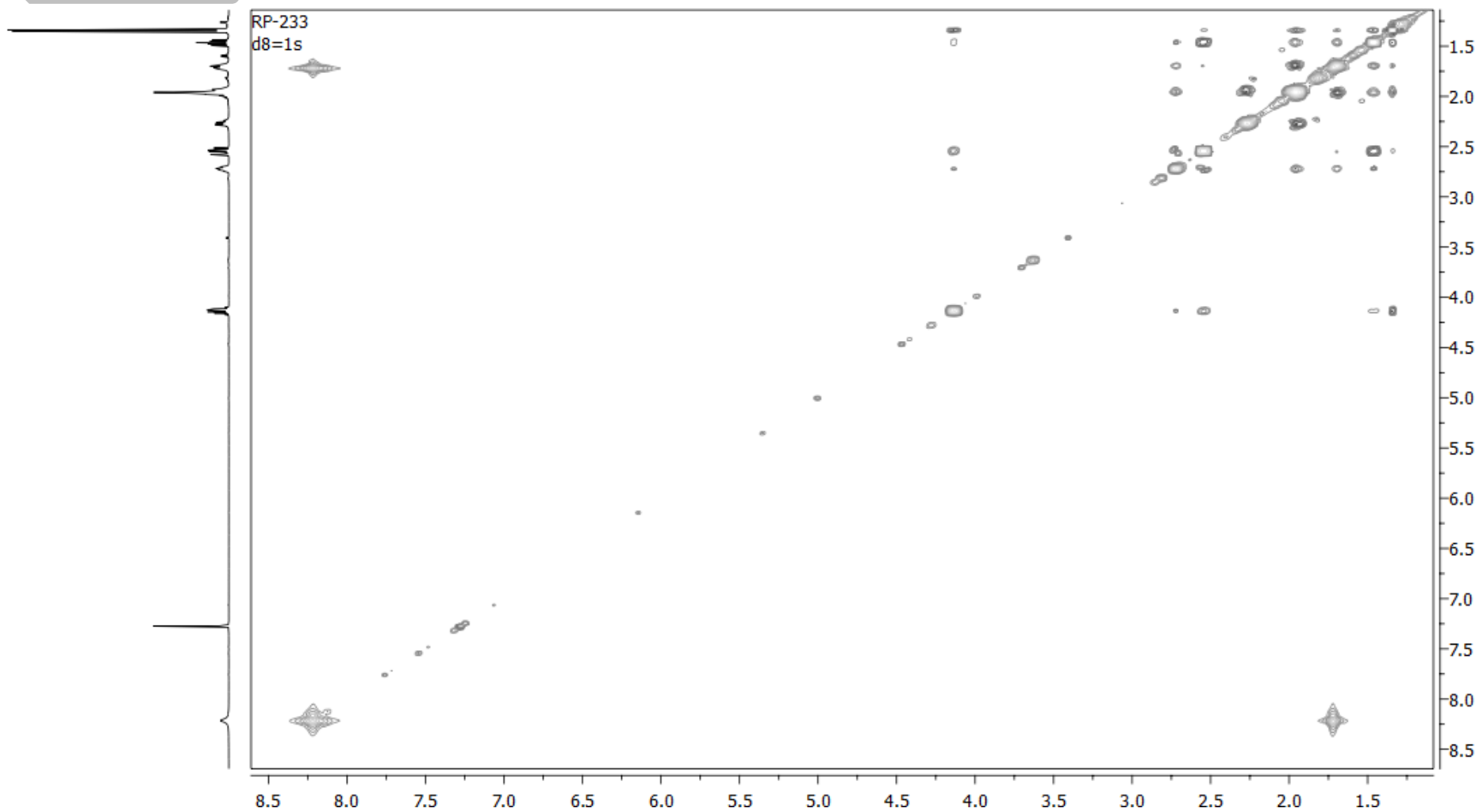


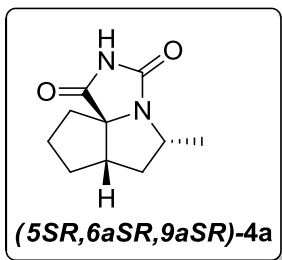
^1H - ^1H COSY NMR (500-500 MHz, CDCl_3)



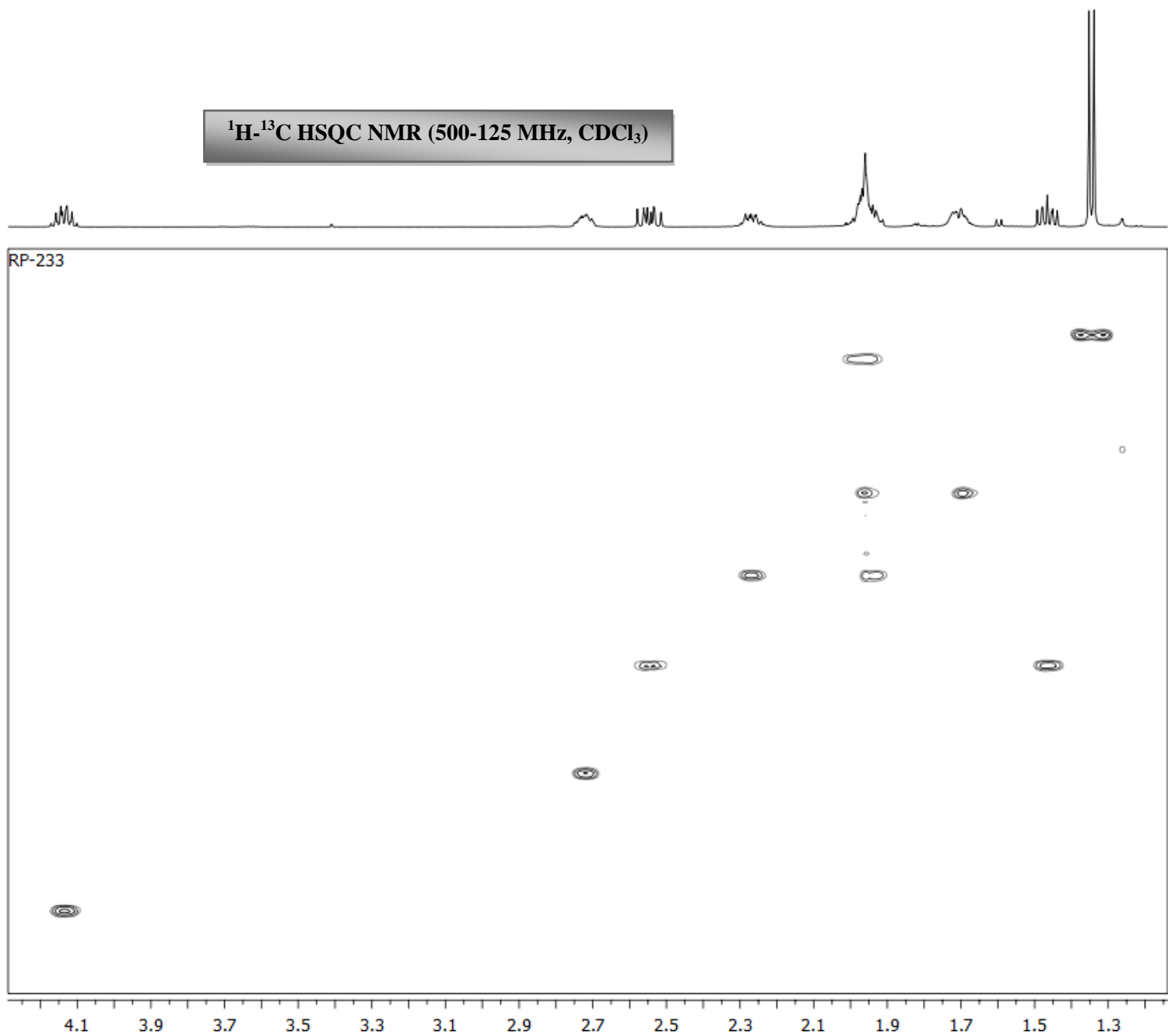


¹H-¹H NOESY NMR (500-500 MHz, CDCl₃)





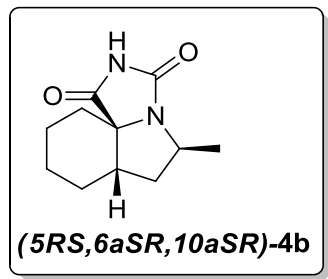
^1H - ^{13}C HSQC NMR (500-125 MHz, CDCl_3)



RP-227

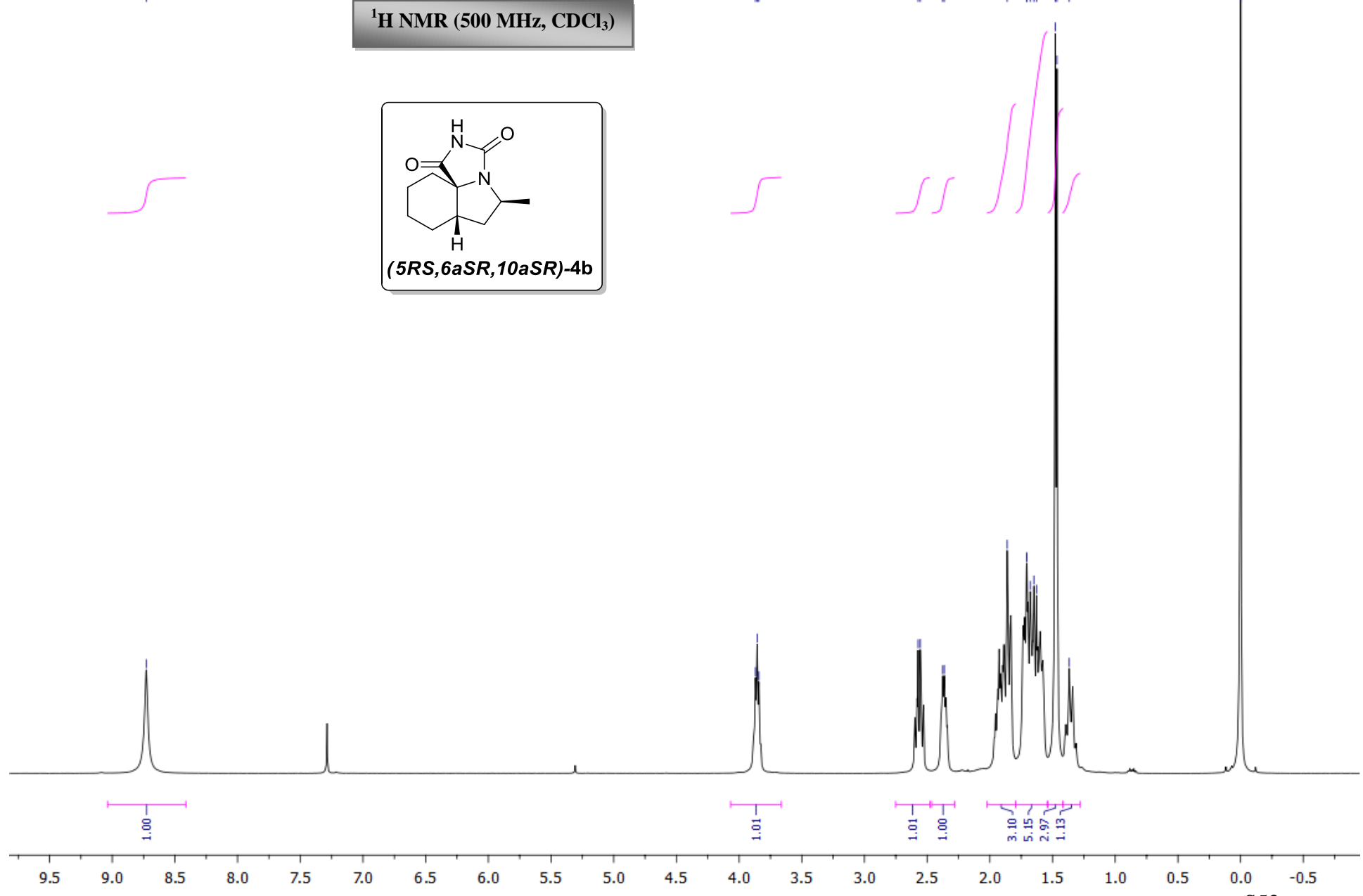
8.73

¹H NMR (500 MHz, CDCl₃)



3.87
3.86
3.84
2.57
2.55
2.38
2.36
1.86
1.71
1.70
1.68
1.65
1.63
1.48
1.46
1.37

0.00



RP-227

3.88
3.87
3.86
3.84
3.83

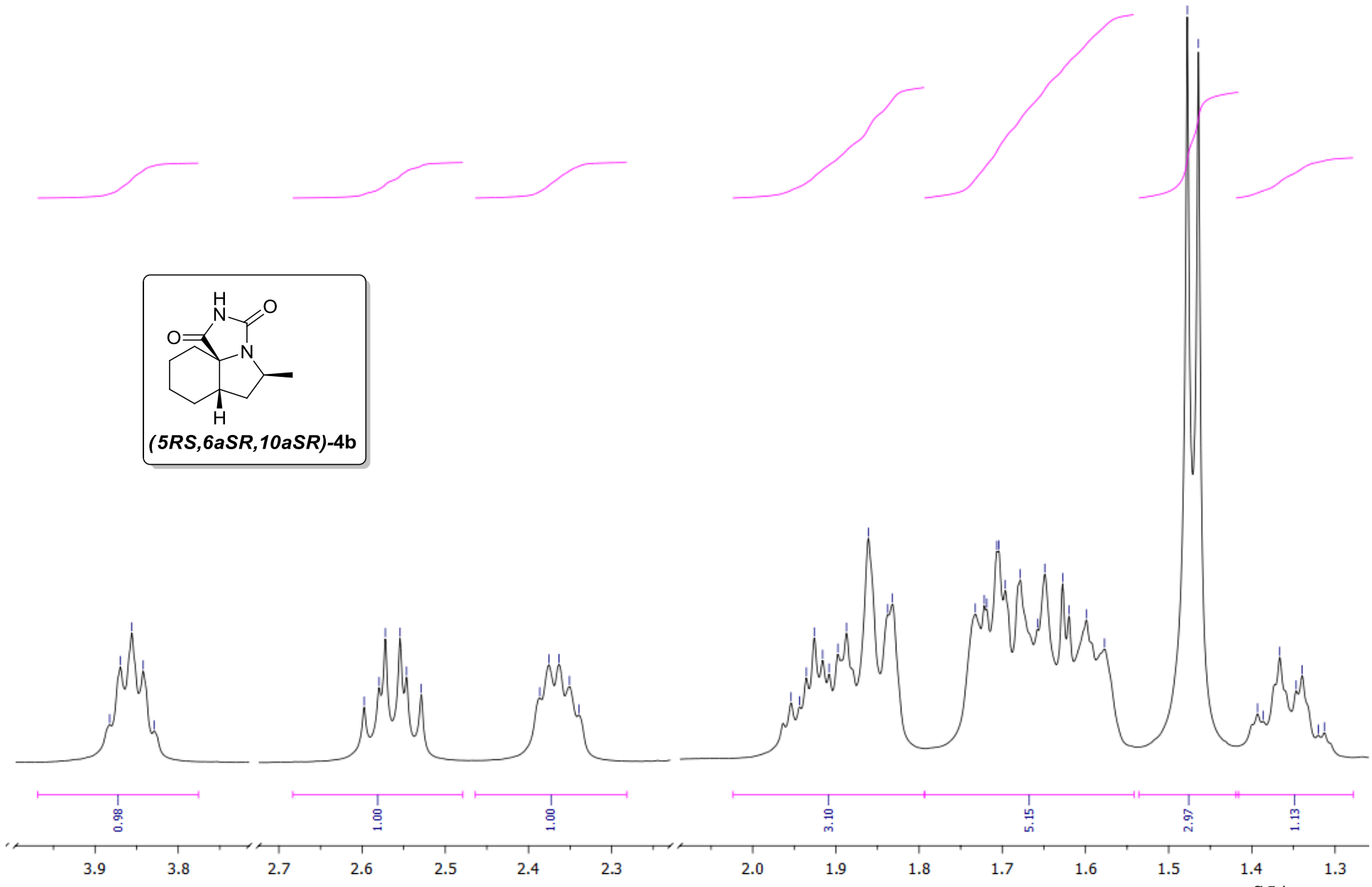
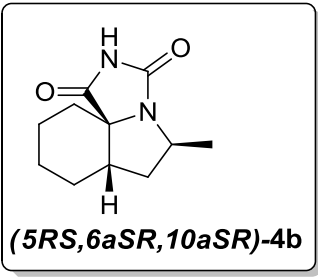
2.60
2.58
2.57
2.55
2.55
2.53

2.39
2.38
2.36
2.35
2.34

1.95
1.94
1.94
1.93
1.92
1.91
1.90
1.89
1.86
1.84
1.83

1.73
1.72
1.72
1.71
1.70
1.70
1.68
1.65
1.63
1.62
1.60
1.48
1.46

1.39
1.39
1.37
1.35
1.34
1.32
1.31

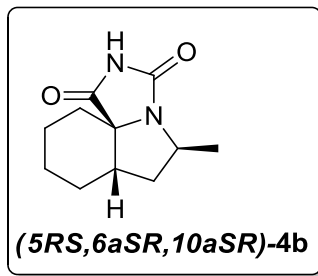


RP-227

—176.99

—155.85

¹³C NMR (125 MHz, CDCl₃)

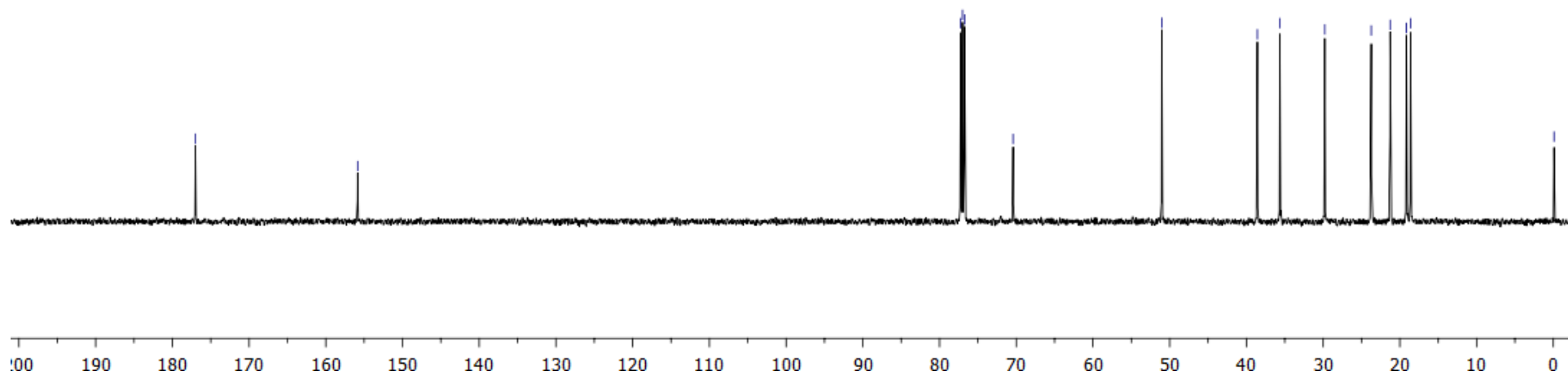


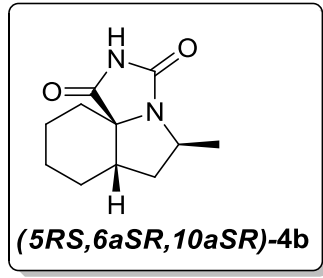
77.25
77.00
76.75
70.42

—51.04

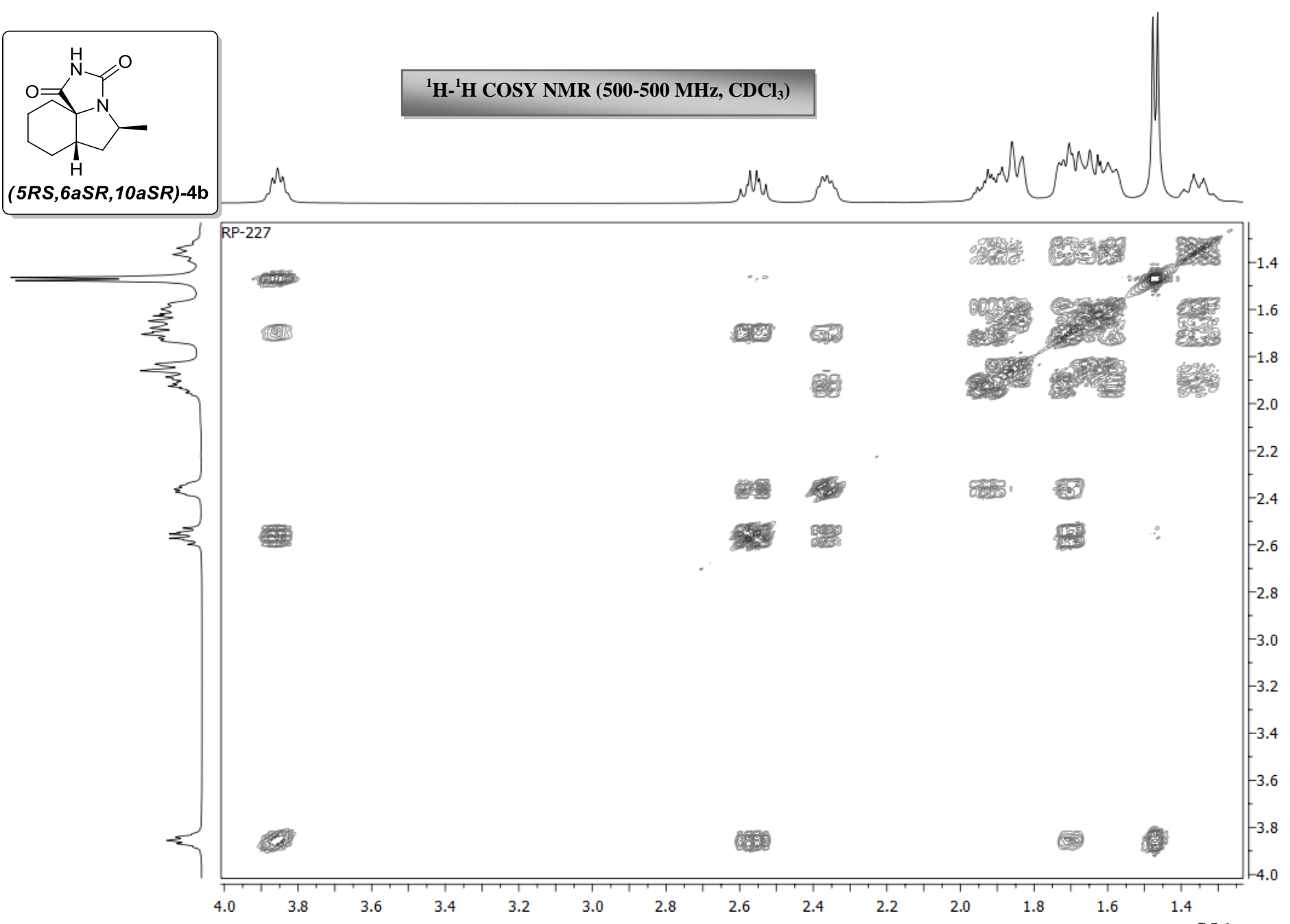
38.57
35.65
29.78
23.74
21.26
19.15
18.61

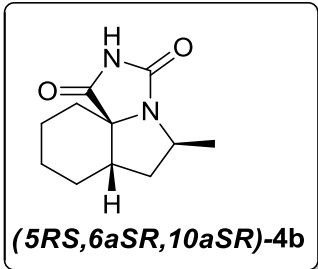
—0.09



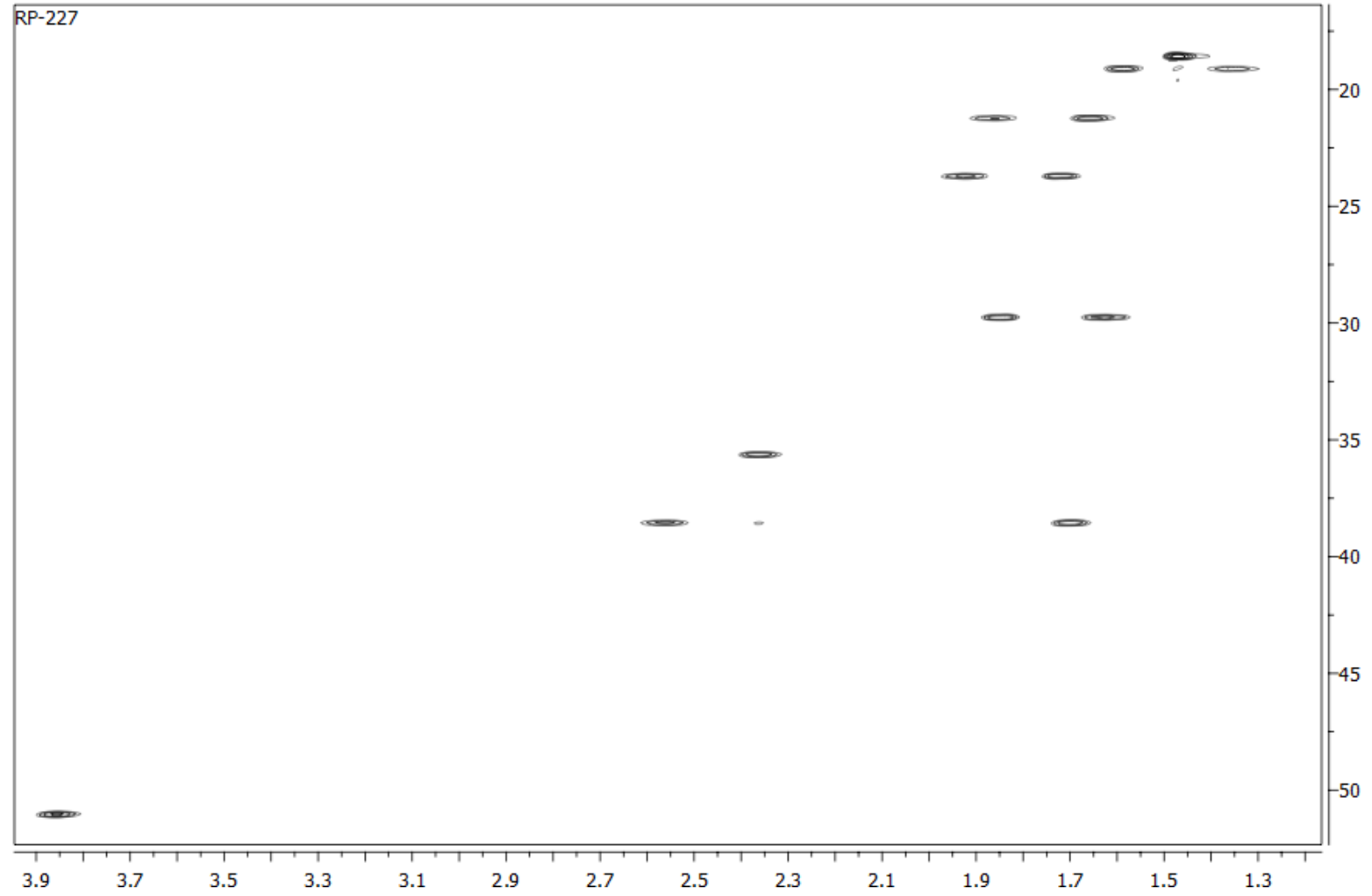
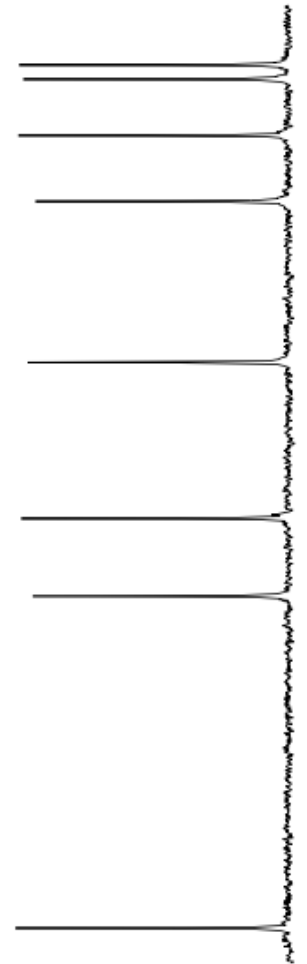
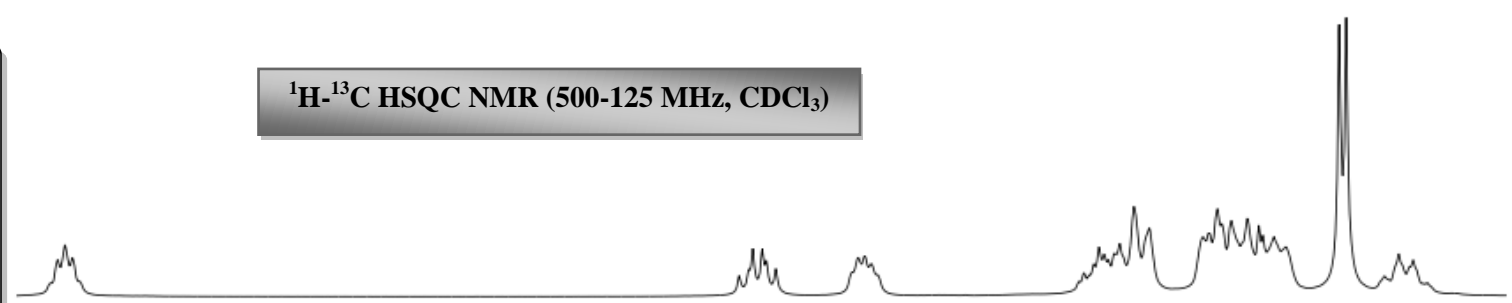


¹H-¹H COSY NMR (500-500 MHz, CDCl₃)





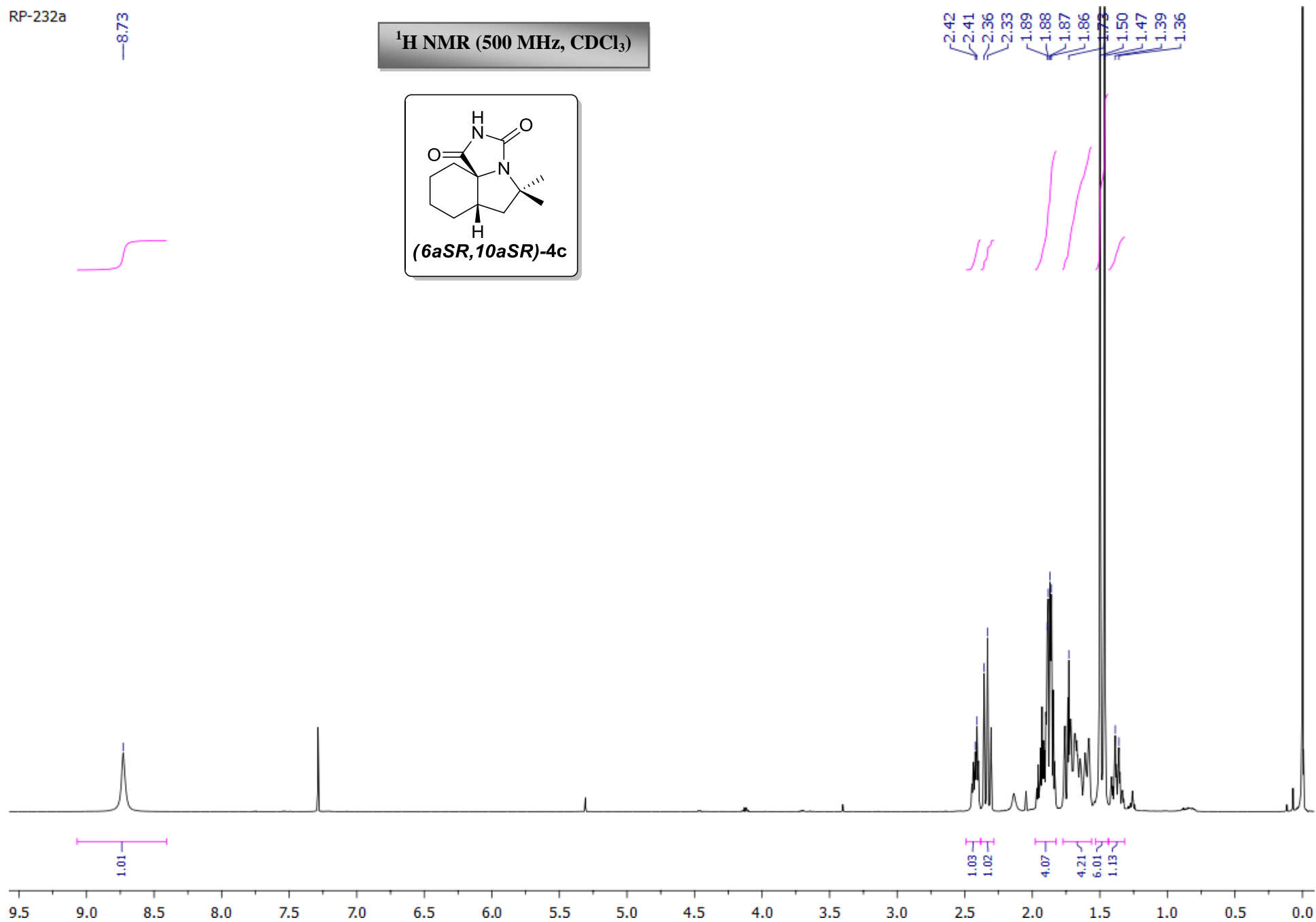
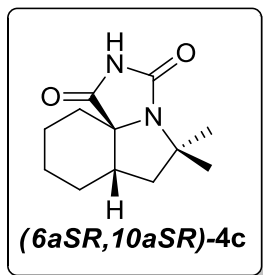
¹H-¹³C HSQC NMR (500-125 MHz, CDCl₃)



RP-232a

—8.73

¹H NMR (500 MHz, CDCl₃)



RP-232a

~2.42

~2.41

~2.36

~2.33

~1.89

~1.88

~1.87

~1.86

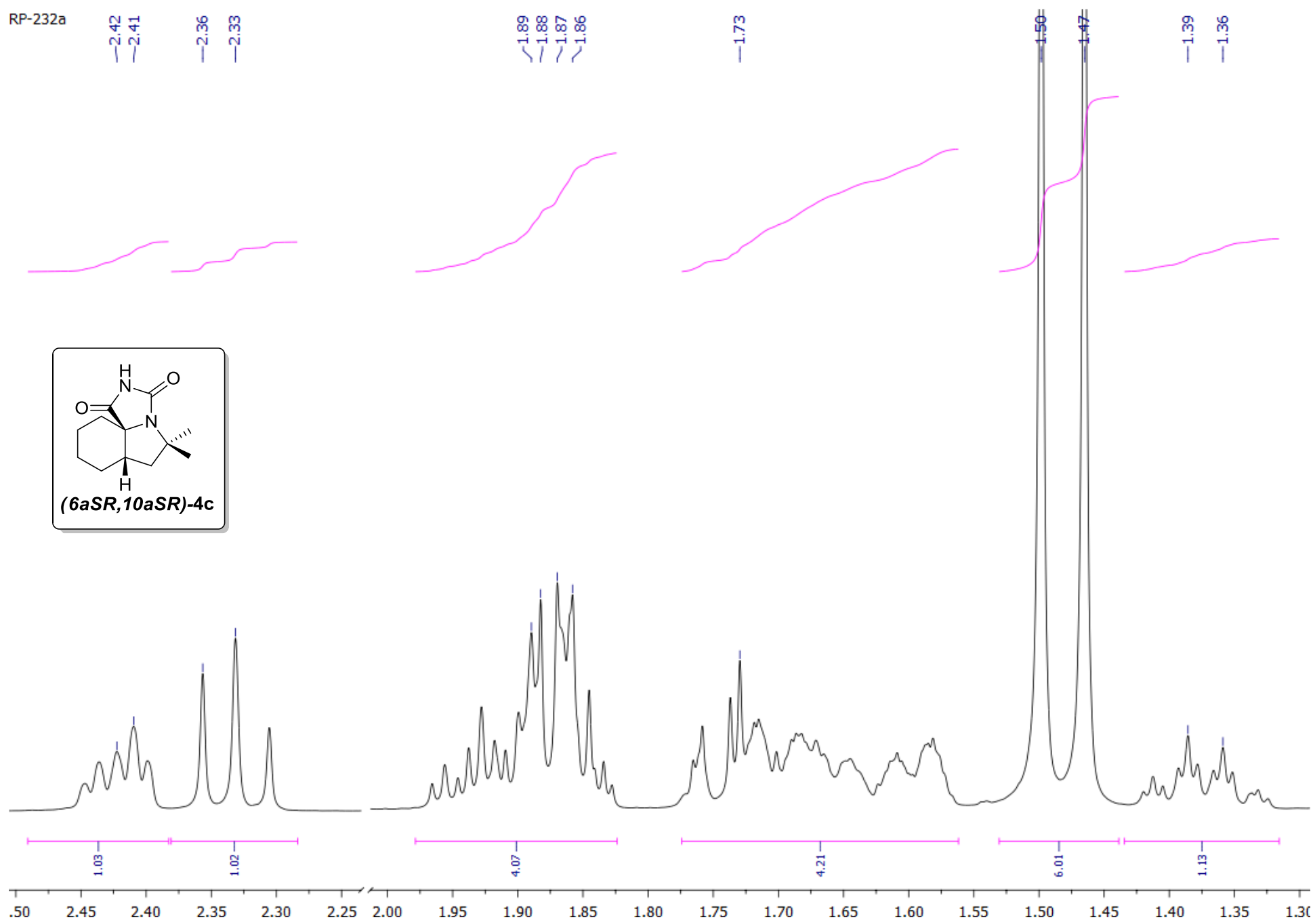
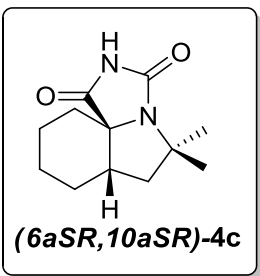
~1.73

1.50

1.47

~1.39

~1.36



RP-232a

—177.14

—156.29

77.25
77.00
76.75
—70.49

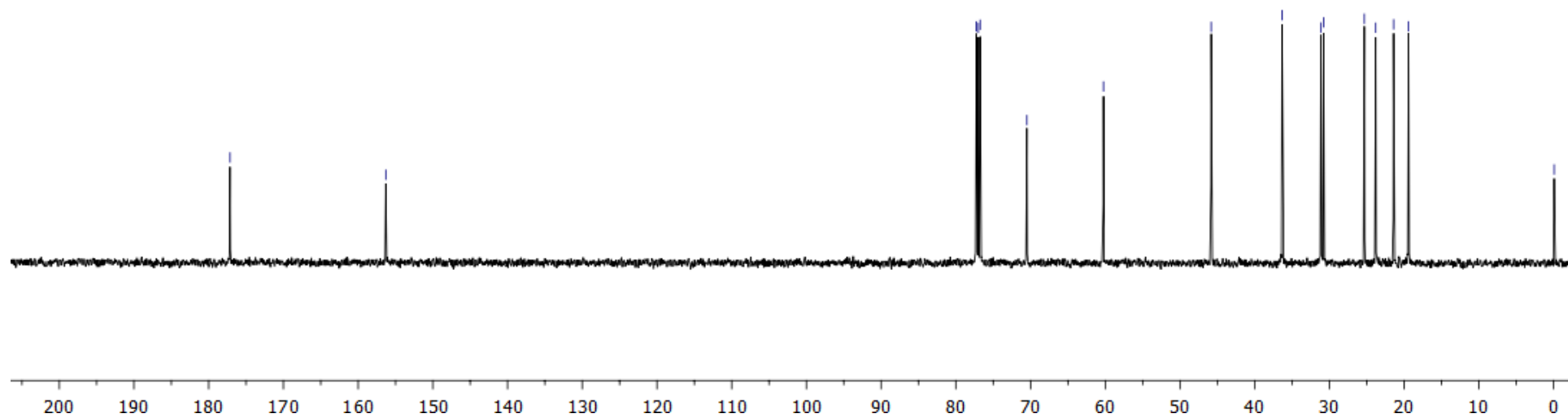
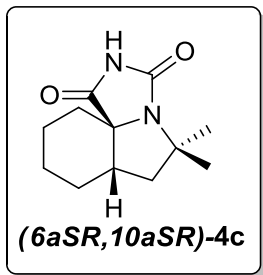
—60.24

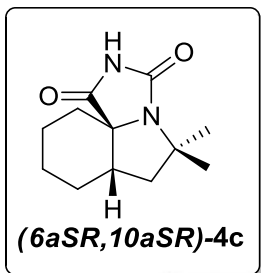
—45.82

36.33
31.14
30.77
25.32
23.81
21.41
19.40

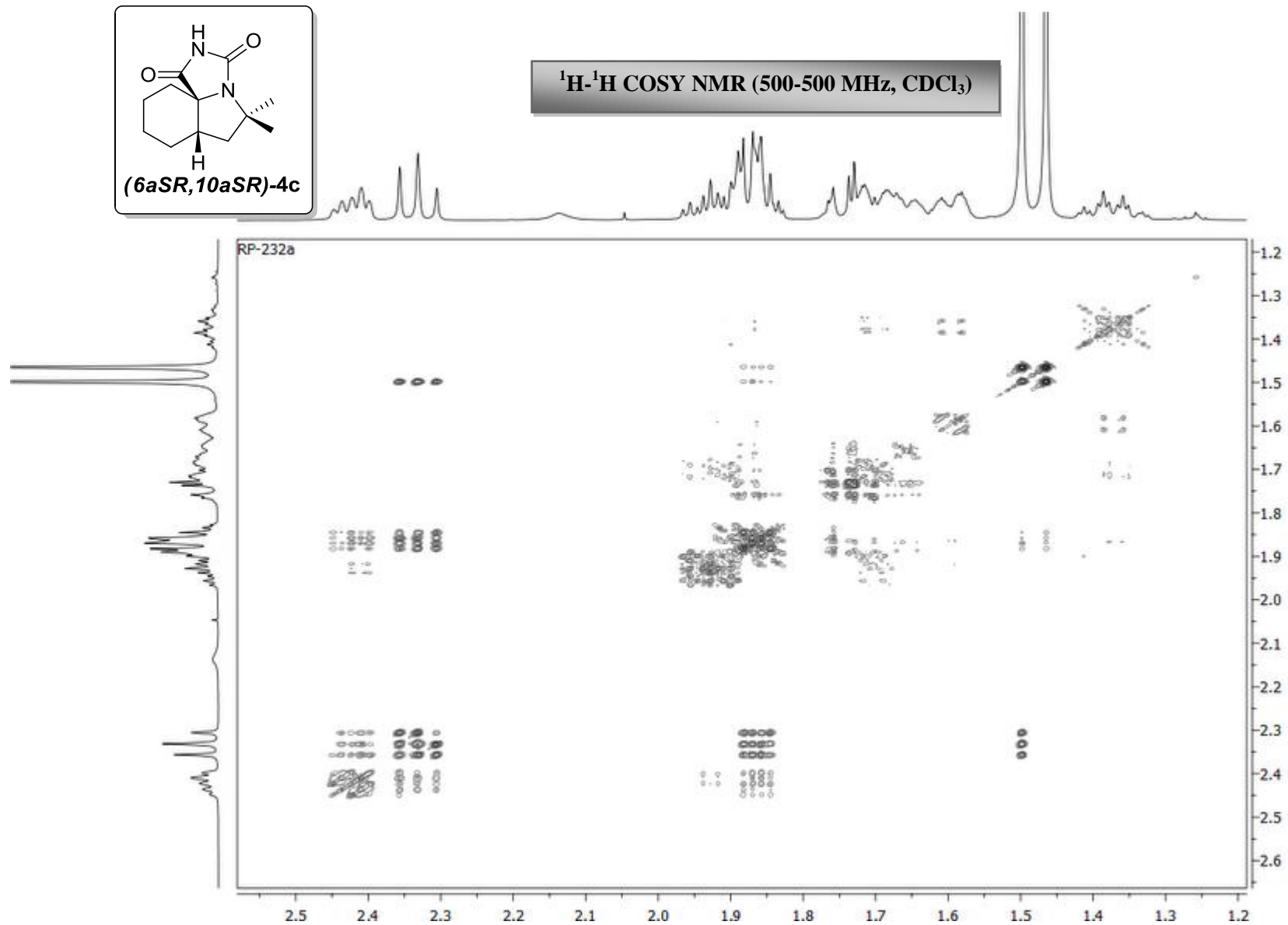
—0.09

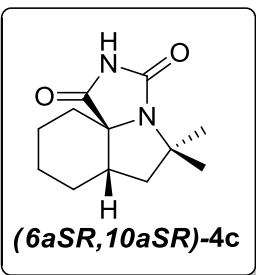
¹³C NMR (125 MHz, CDCl₃)



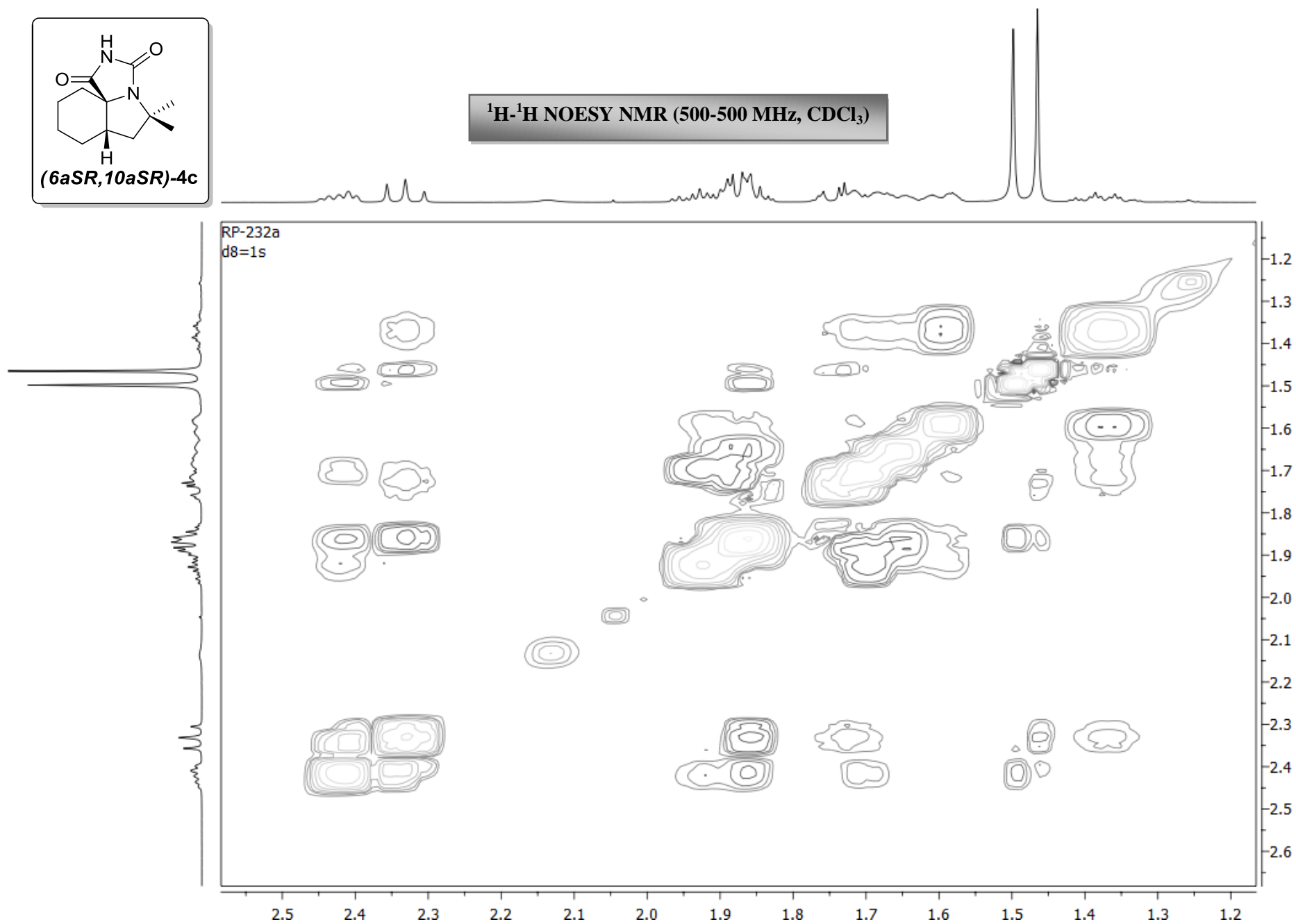


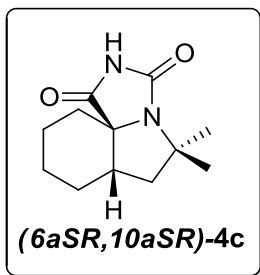
^1H - ^1H COSY NMR (500-500 MHz, CDCl_3)



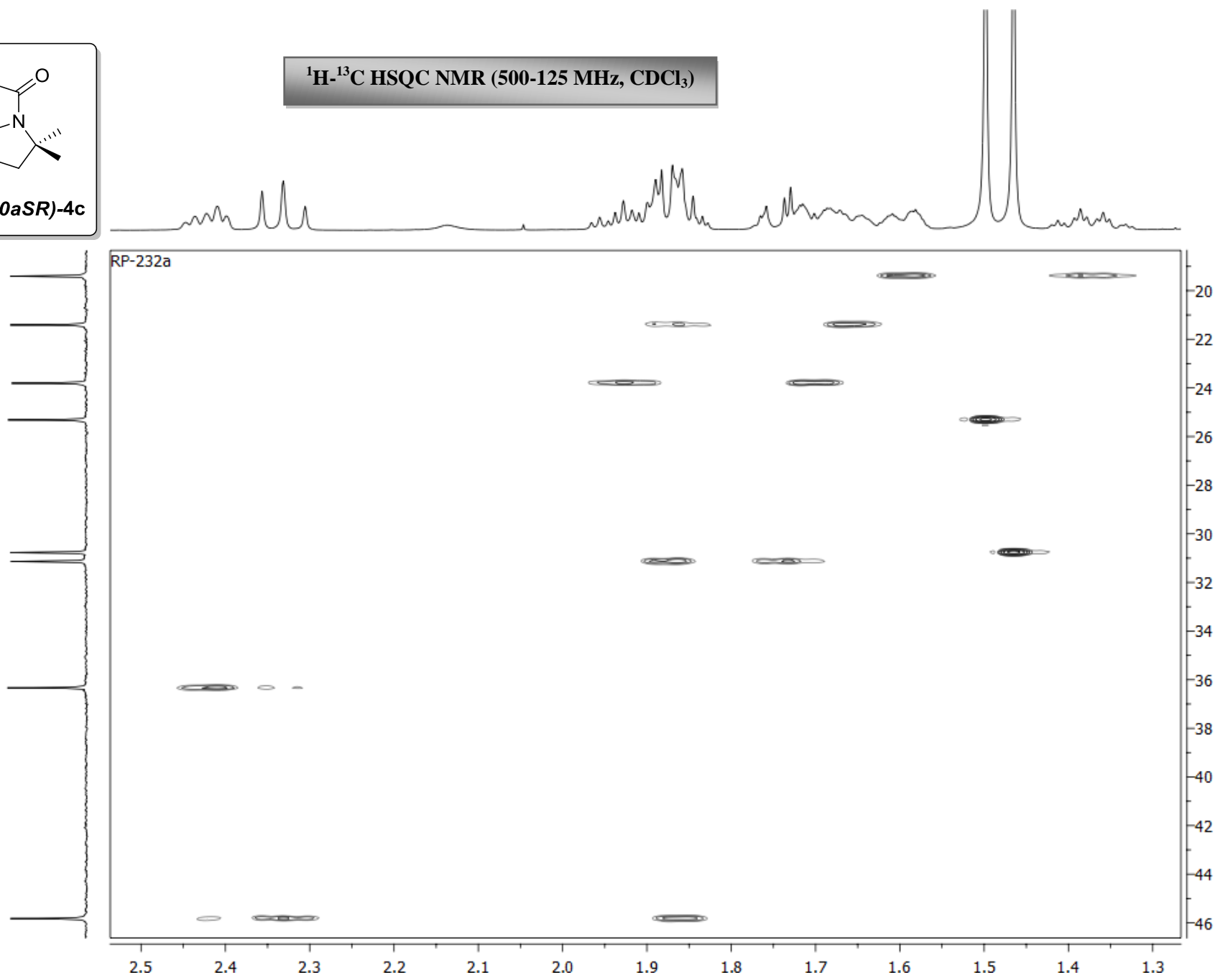


^1H - ^1H NOESY NMR (500-500 MHz, CDCl_3)



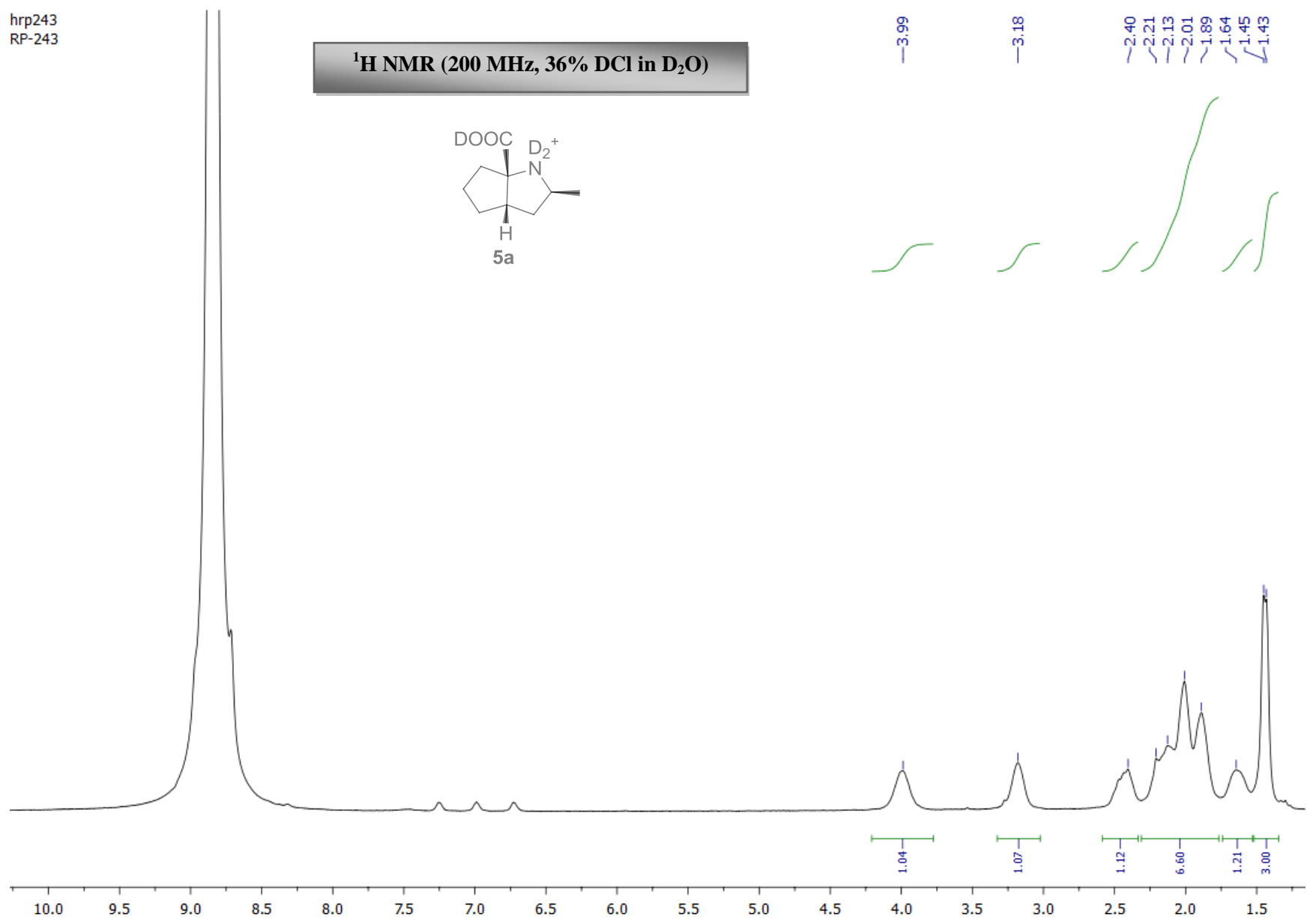
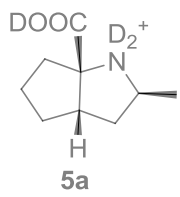


^1H - ^{13}C HSQC NMR (500-125 MHz, CDCl_3)



hrp243
RP-243

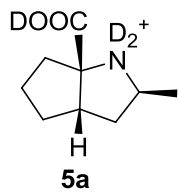
¹H NMR (200 MHz, 36% DCl in D₂O)



crp243
RP-243

—173.40

^{13}C NMR (50 MHz, 36% DCl in D_2O)



—76.42

—56.35

—47.73

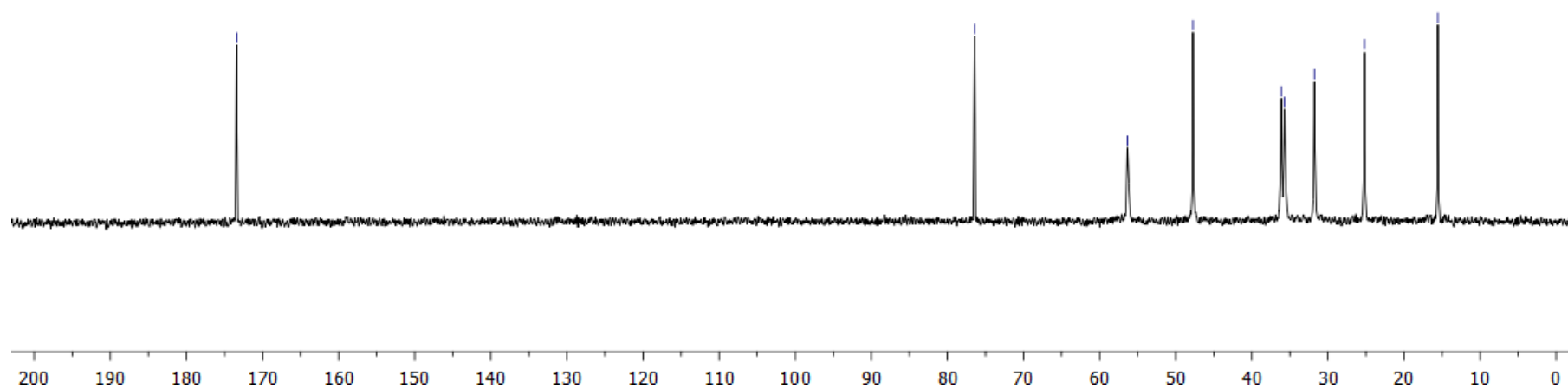
—36.15

—35.69

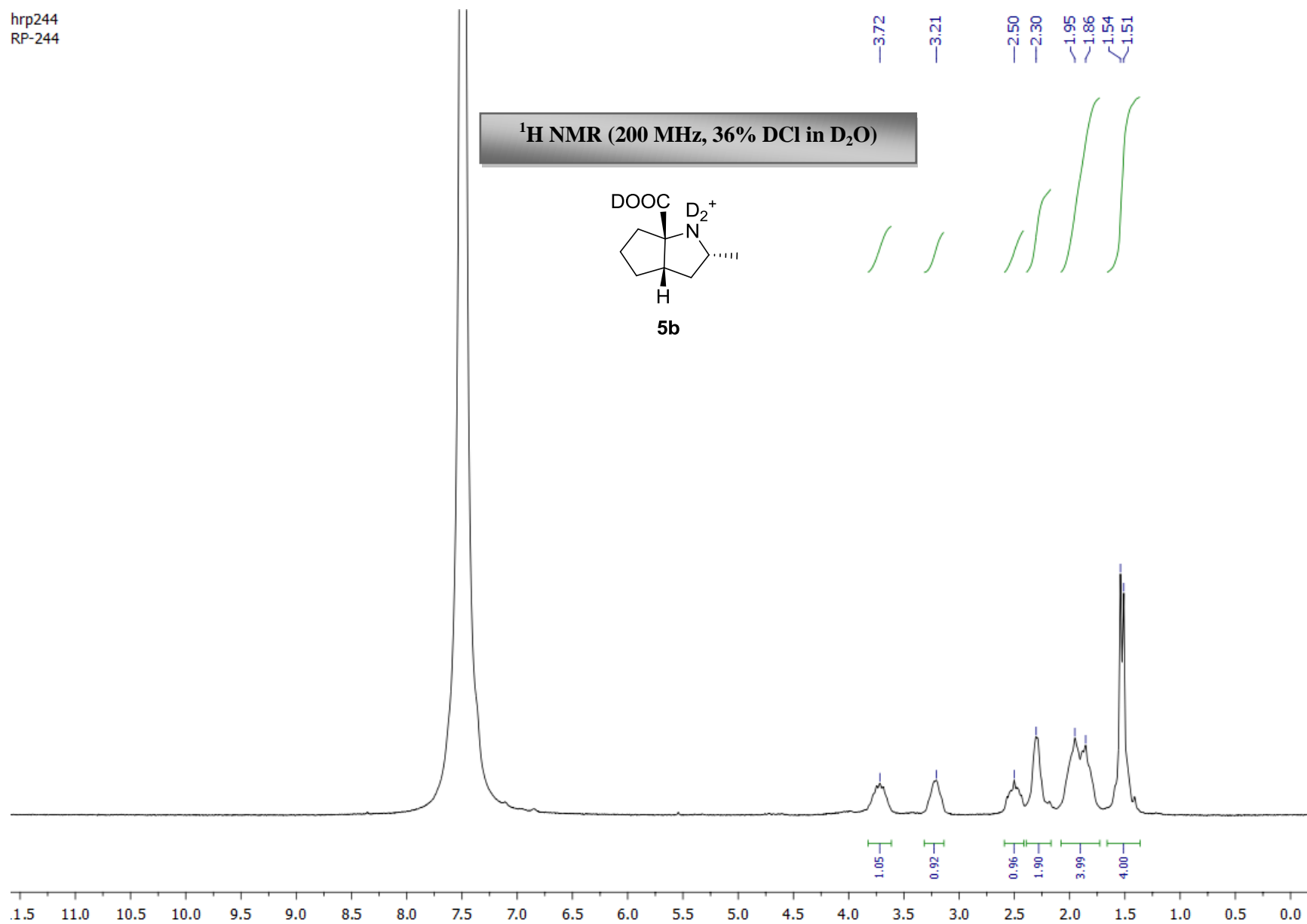
—31.77

—25.20

—15.55



hrp244
RP-244



RP-244

—174.53

^{13}C NMR (50 MHz, 36% DCl in D_2O)

—78.02

—59.07

—49.84

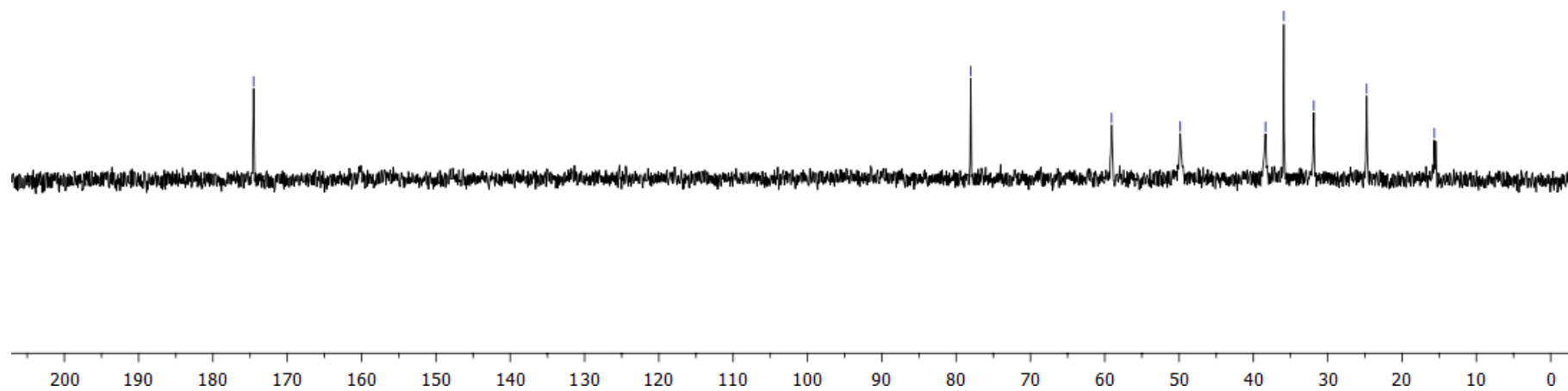
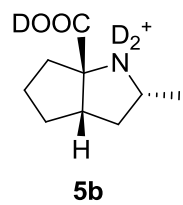
—38.38

—35.91

—31.87

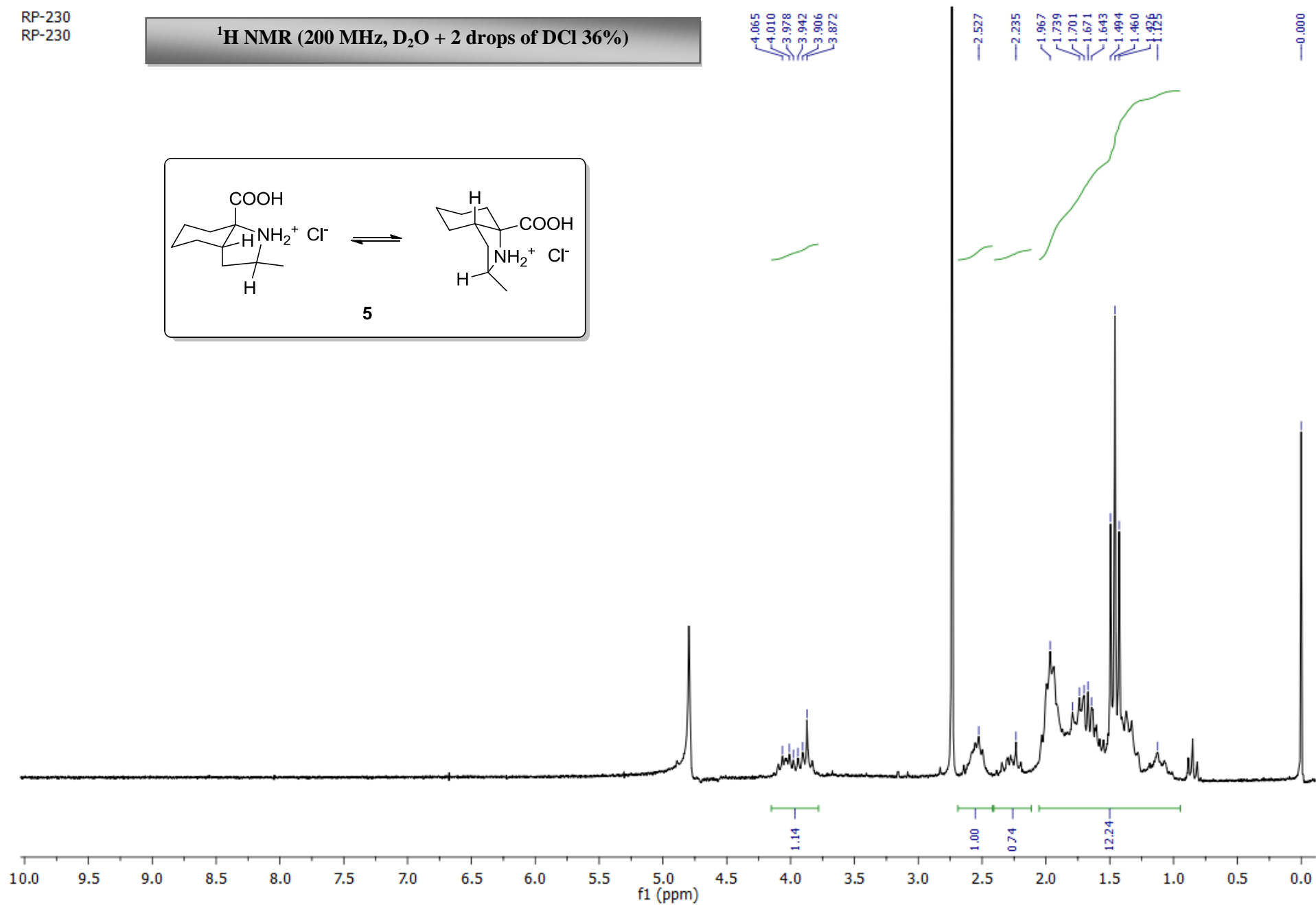
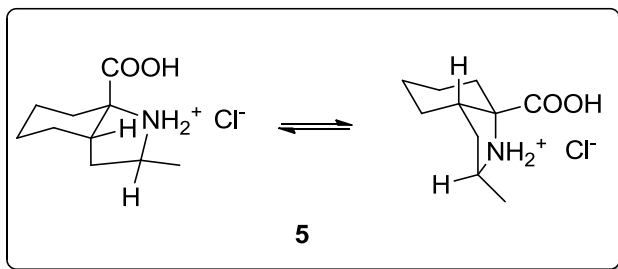
—24.76

—15.66



RP-230
RP-230

^1H NMR (200 MHz, D_2O + 2 drops of DCI 36%)



RP-230C
RP-230 + DCl

177.07
176.47

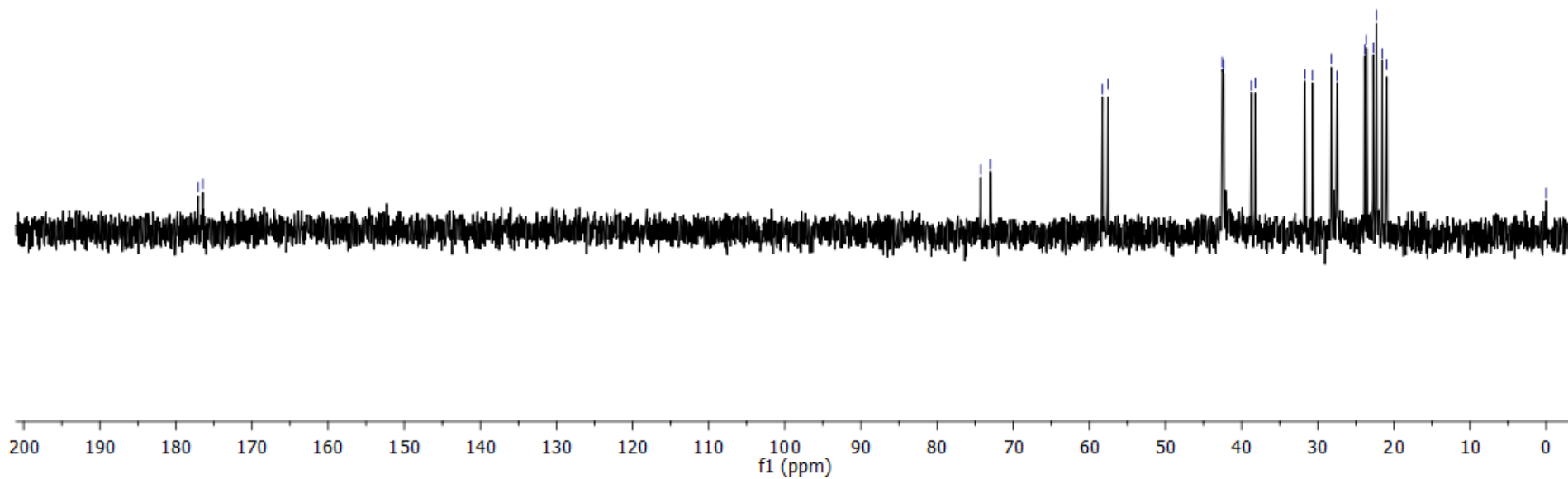
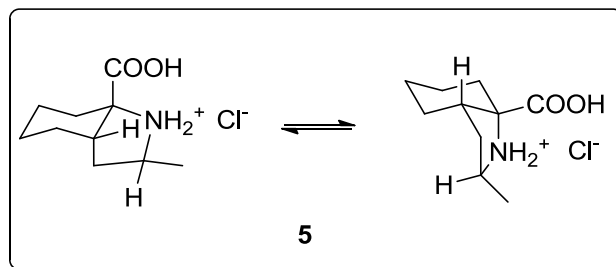
¹³C NMR (50 MHz, D₂O + 2 drops of DCl 36%)

74.28
73.01

58.29
57.58

42.53
42.38
38.72
38.22
31.70
30.68
28.21
27.47
23.86
23.62
22.72
22.31
21.55
20.94

0.00



RP-217-rs
RP-217-rs

8.440

7.542
7.530
7.293
7.287
7.283
7.274
7.263
7.260
7.250

4.251
4.218
4.188
3.798
3.750

3.221
3.086
3.045

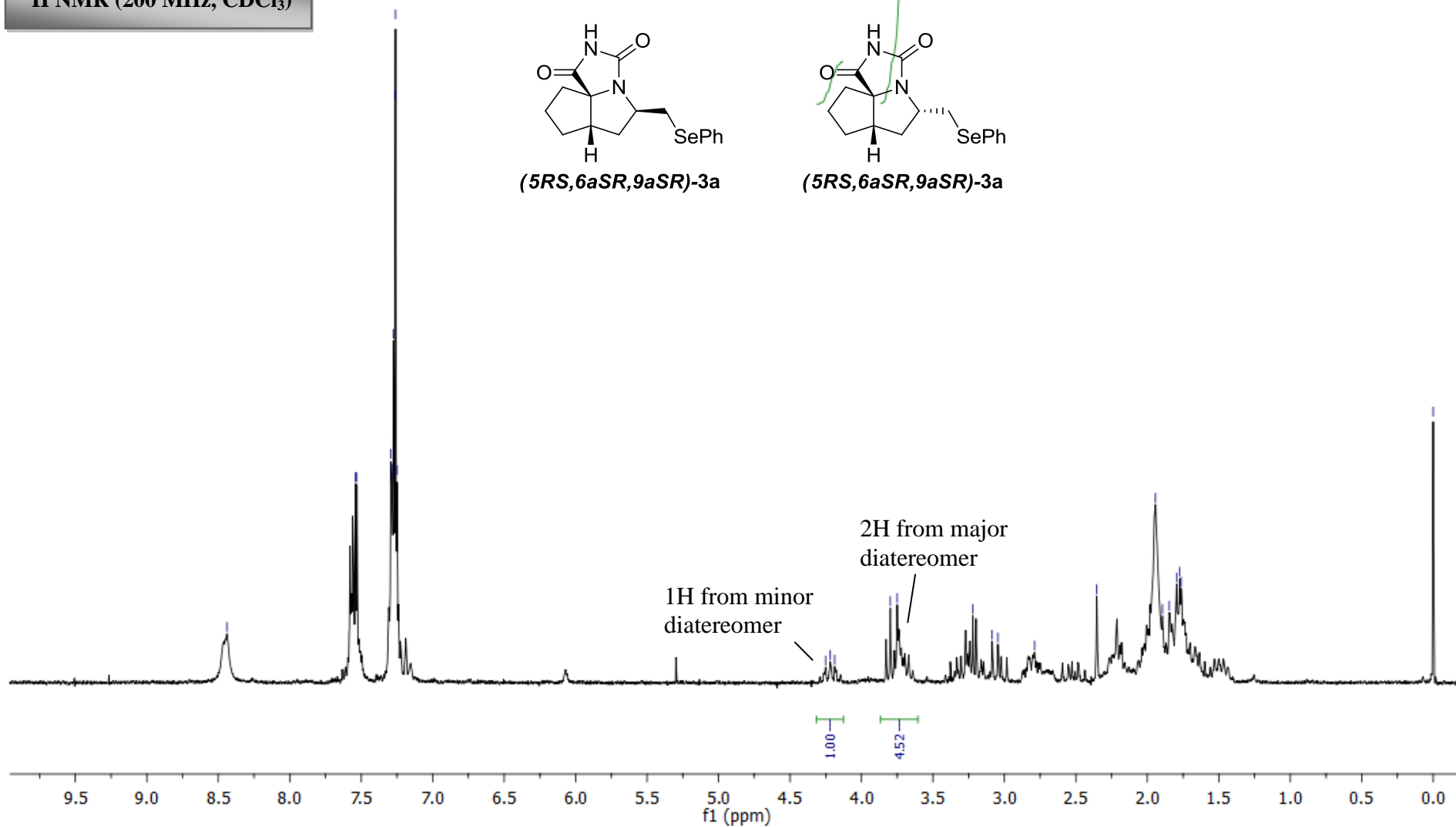
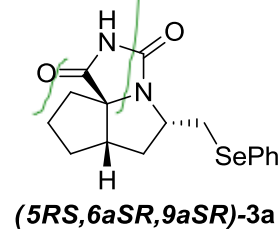
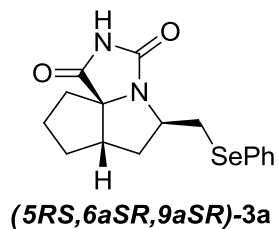
2.789

2.354
1.943
1.894
1.847
1.795
1.774
1.762

0.000

¹H NMR (200 MHz, CDCl₃)

Reaction mixture



RP-218-rs
RP-218-rs

8.57

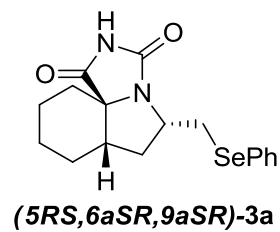
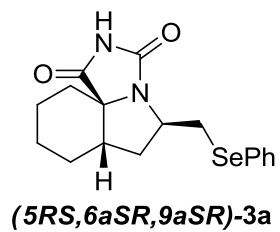
8.18

4.02
4.00
3.96
3.91
3.89
3.84
3.83
3.24
3.20
3.18
3.14

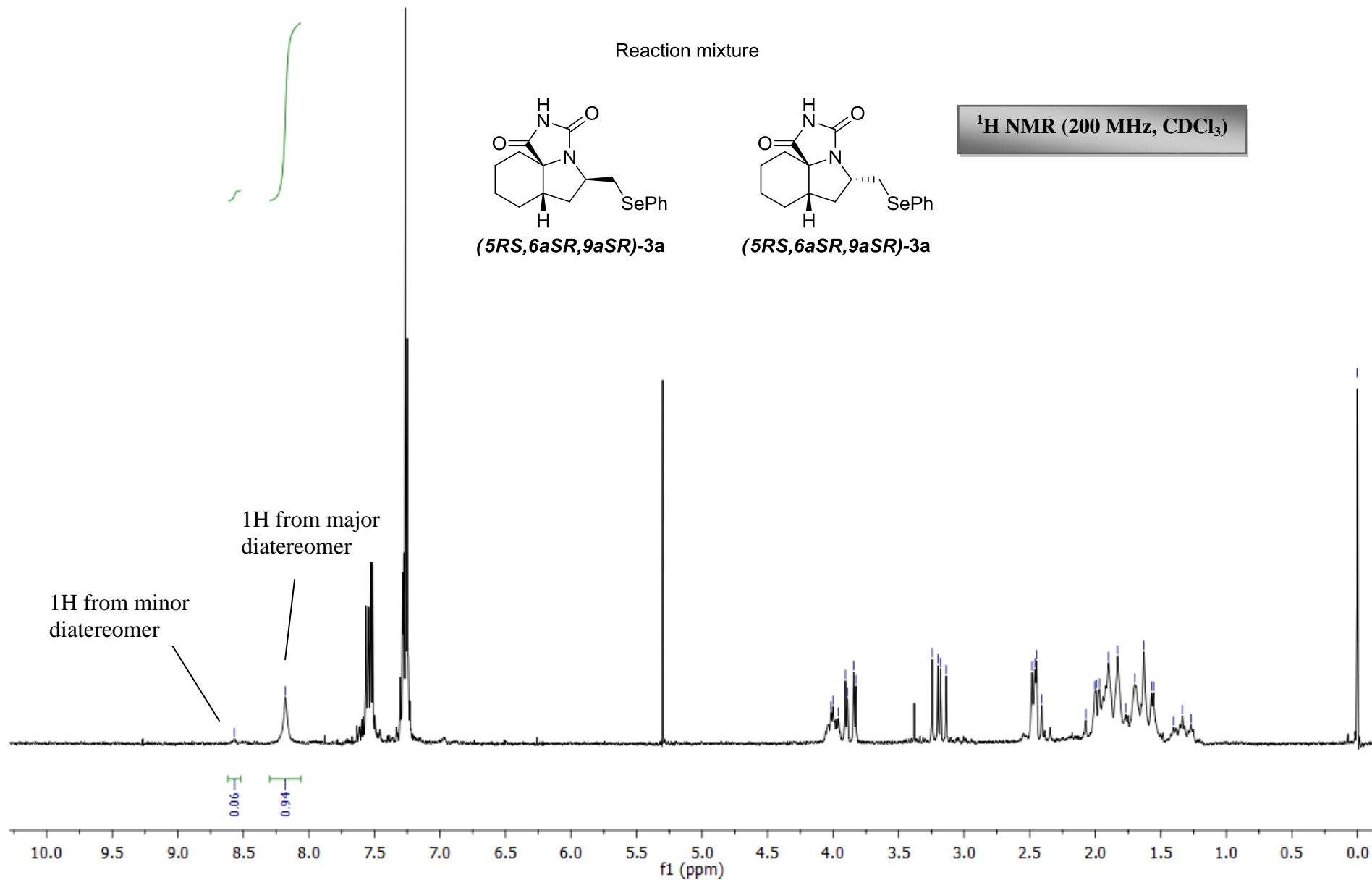
2.48
2.46
2.45
2.41
2.07
2.00
1.99
1.97
1.90
1.83
1.77
1.70
1.63
1.57
1.56
1.40
1.34
1.27

0.00

Reaction mixture



¹H NMR (200 MHz, CDCl₃)



RP-223-rs
RP-223-rs

¹H NMR (200 MHz, CDCl₃)

Reaction mixture

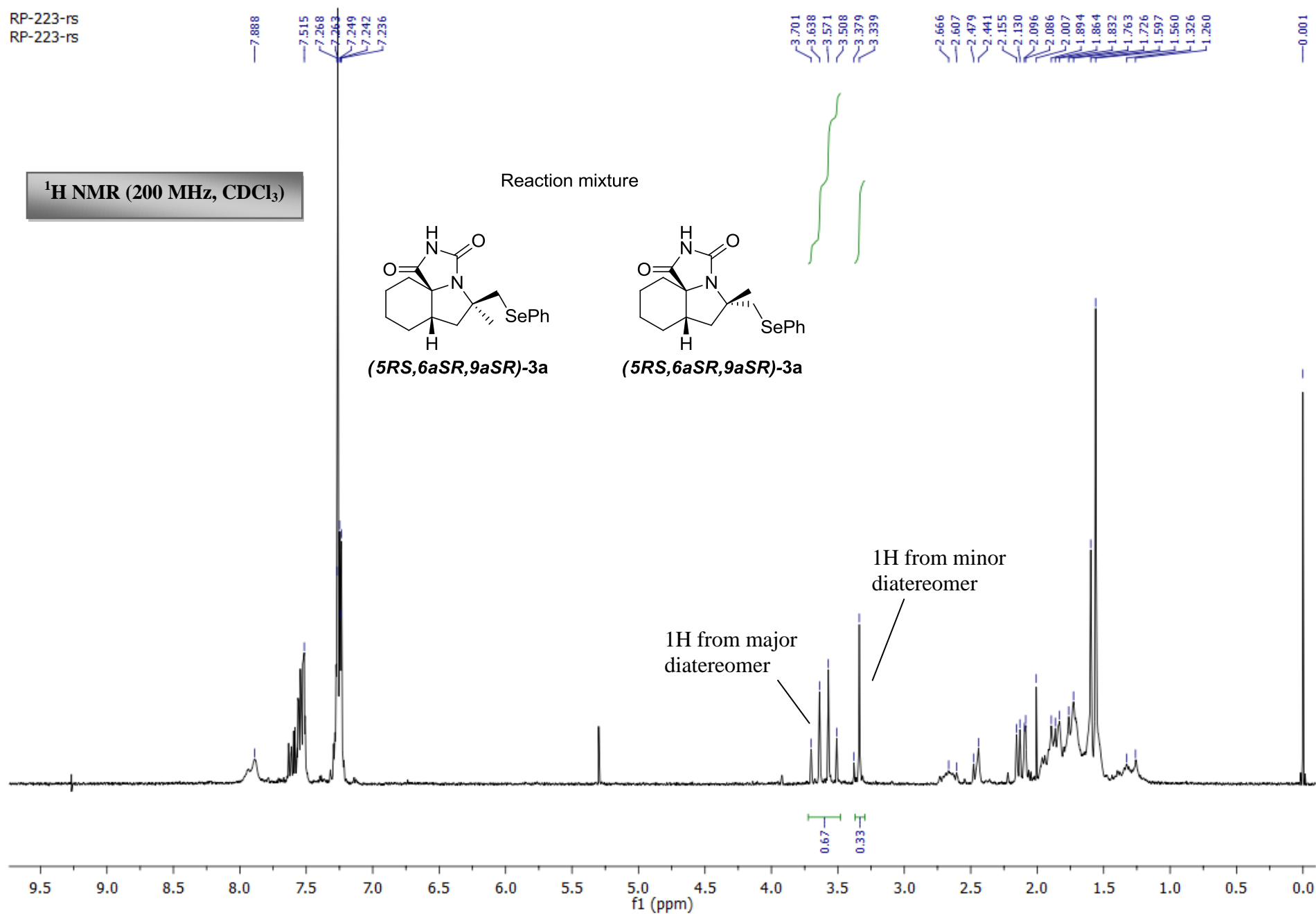
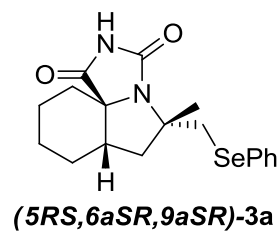
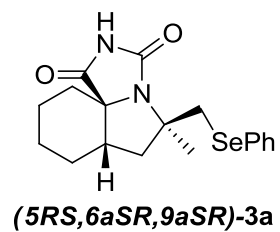


Table S2 Crystallographic data, experimental and refinement details for **2c** and **3b**

	(2c)	(3b)
Crystal data		
Chemical formula	C ₁₂ H ₁₈ N ₂ O ₂ ·H ₂ O	C ₁₇ H ₂₀ N ₂ O ₂ Se
<i>M</i> _r	480.6	363.31
Crystal system, space group	Monoclinic, <i>I</i> 2/ <i>a</i>	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>
Temperature (K)	294	294
<i>a</i> , <i>b</i> , <i>c</i> (Å)	12.7811 (4), 6.2674 (2), 33.3511 (9)	6.7697 (4), 18.4108 (9), 13.0431 (10)
β (°)	93.650 (3)	99.042 (7)
<i>V</i> (Å ³)	2666.15 (14)	1605.43 (18)
<i>Z</i>	4	4
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α
μ (mm ⁻¹)	0.09	2.35
Crystal size (mm)	0.49 × 0.44 × 0.04	0.59 × 0.15 × 0.06
Data collection		
Diffractometer	Gemini S (Oxford Diffraction)	Gemini S (Oxford Diffraction)
Absorption correction	Multi-scan	Multi-scan
<i>T</i> _{min} , <i>T</i> _{max}	0.852, 1	0.650, 1
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	11300, 3164, 2773	7207, 3665, 2432
<i>R</i> _{int}	0.018	0.039
(sin θ/λ) _{max} (Å ⁻¹)	0.685	0.683
Refinement		
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.067, 0.172, 1.14	0.066, 0.227, 1.07
No. of reflections	3164	3665
No. of parameters	167	203
No. of restraints	4	1
H-atom treatment	Mixture of independent and constrained refinement	Mixture of independent and constrained refinement
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.35, -0.18	1.29, -0.93

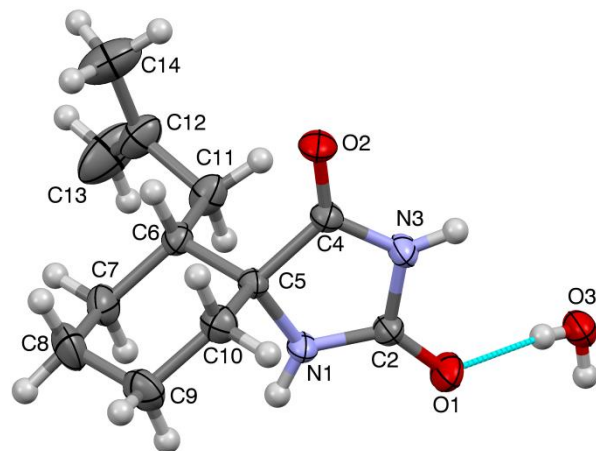


Figure S1. Molecular structure of **2c**. Ellipsoids are drawn at 40% probability level, whereas hydrogen atoms are depicted as spheres of arbitrary radii

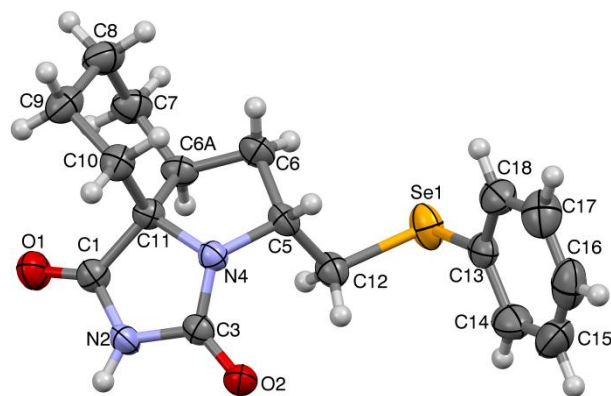


Figure S2. Molecular structure of **3b**. Ellipsoids are drawn at 40% probability level, whereas hydrogen atoms are depicted as spheres of arbitrary radii