

SUPPORTING INFORMATION

Diastereoselective C-Alkylation of Aldimines, Derived from Chiral α -Carbon Heteroatom-Substituted Aldehydes, with Triethylborane. Application to the Synthesis of Benzylisoquinolines

David Fuentes-Ríos,^a Carmen Muñoz,^a Amelia Díaz,^{*a} Francisco Sarabia,^a and J. Manuel López-Romero^{*a}

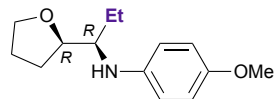
Department of Organic Chemistry, Faculty of Sciences, University of Malaga, Campus de Teatinos s/n, 29071-Málaga, SPAIN.

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6 major

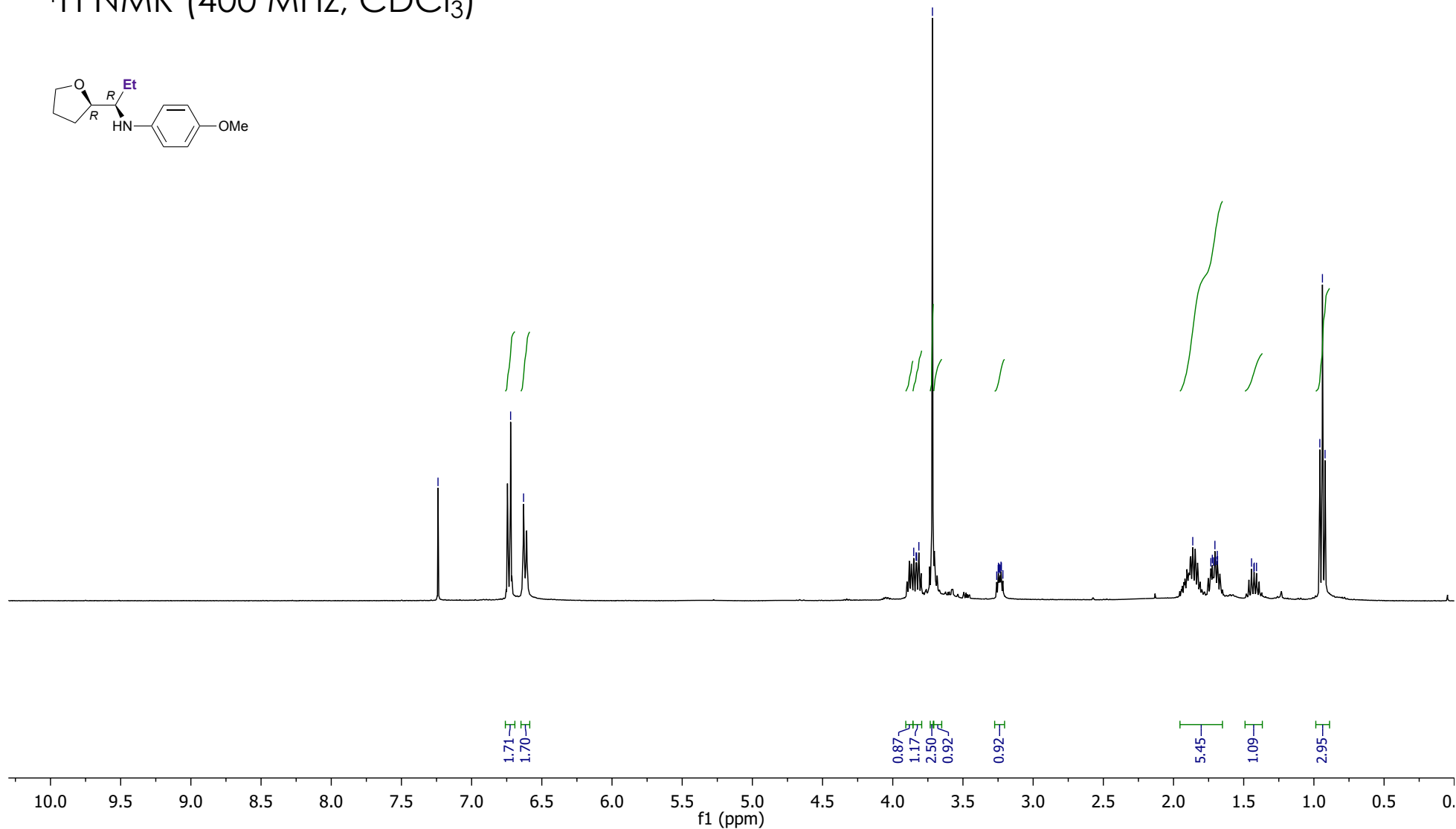
^1H NMR (400 MHz, CDCl_3)



7.24

6.72
6.63

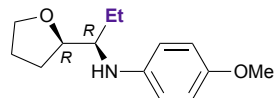
3.85
3.83
3.83
3.81
3.72
3.26
3.25
3.25
3.25
3.24
3.23
3.23
3.22
1.86
1.73
1.72
1.72
1.71
1.70
1.69
1.69
1.44
1.43
1.42
1.41
0.96
0.94



^1H NMR (400 MHz, CDCl_3) of compound **6** major diastereomer

6 major

^{13}C NMR (100 MHz, CDCl_3)



— 152.08

— 141.97

— 114.78

— 81.08

— 68.23

— 59.59

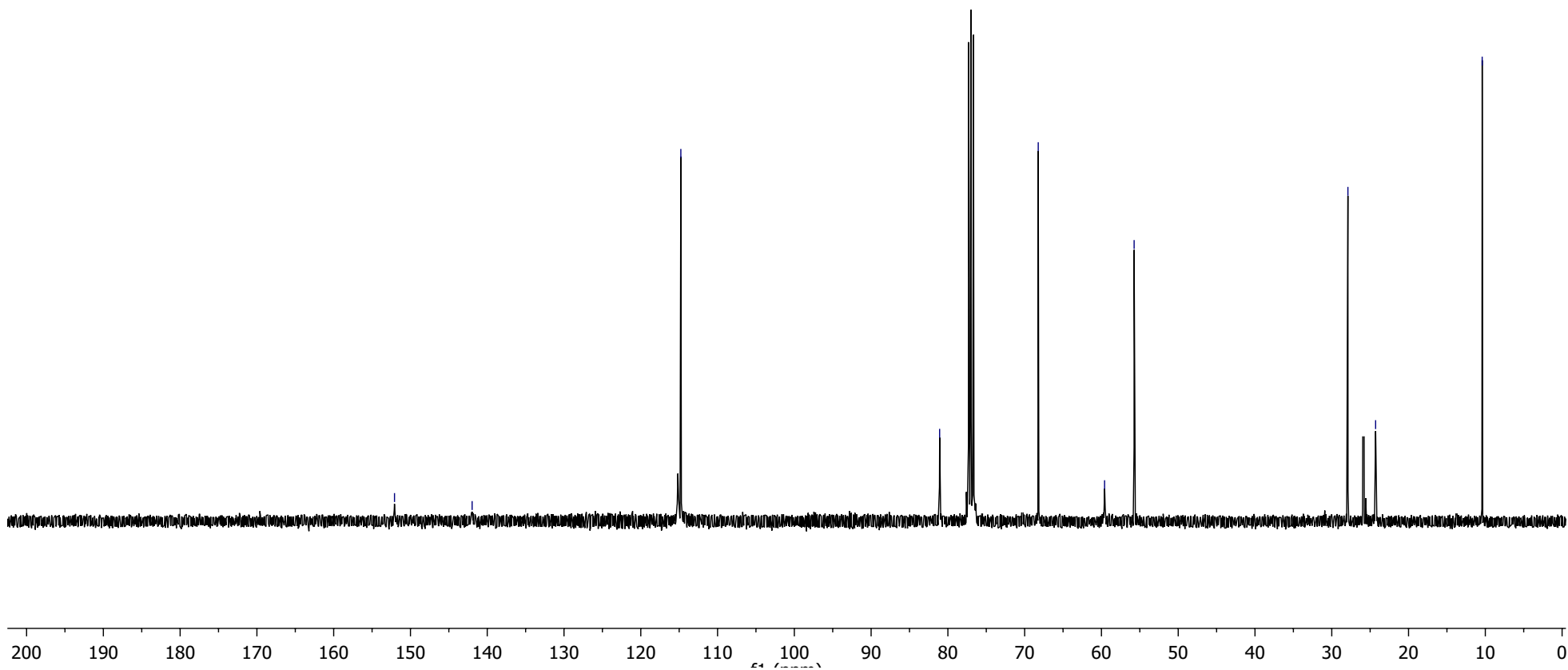
— 55.74

— 27.90

— 25.85

— 24.29

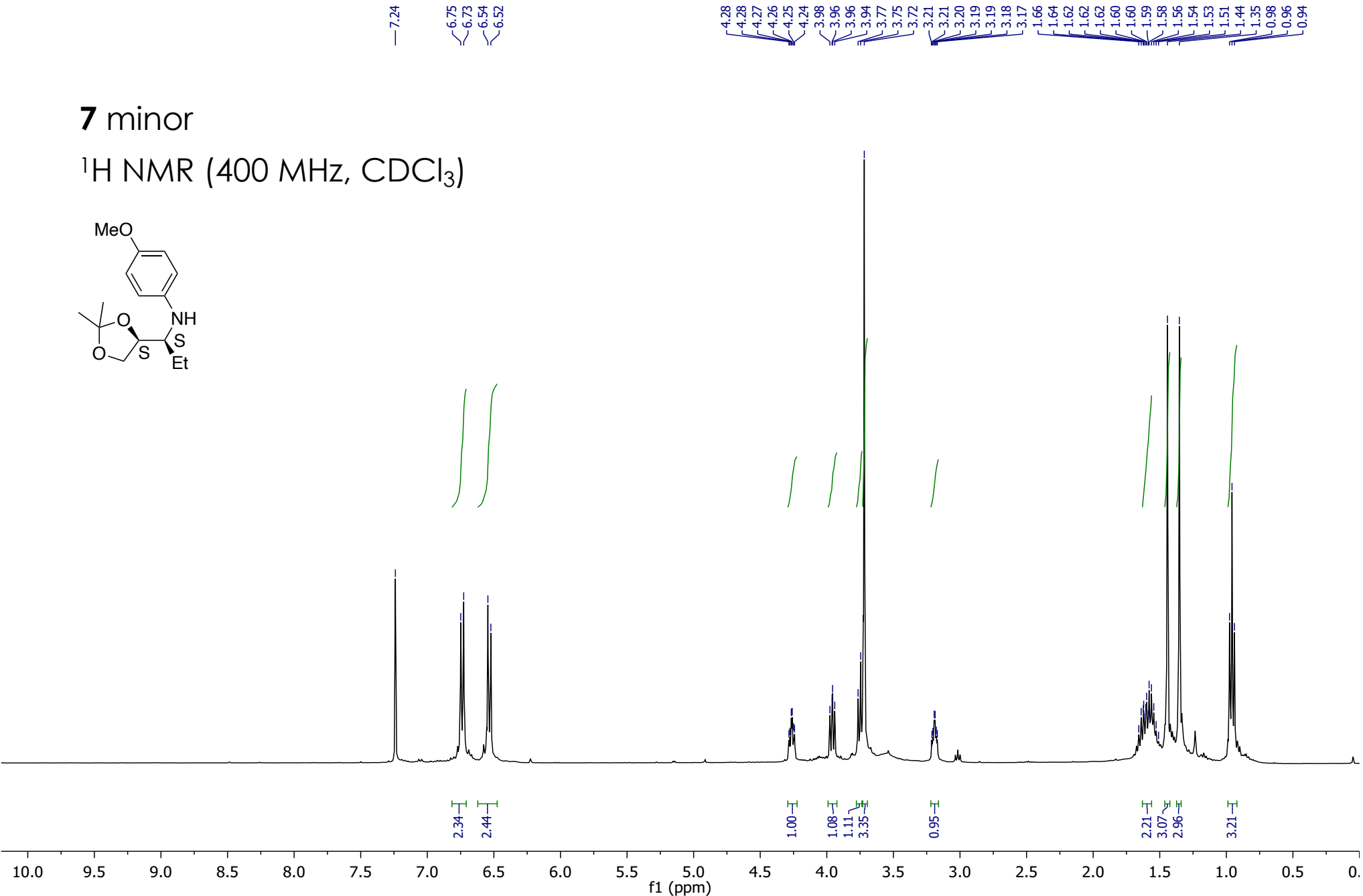
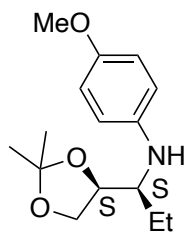
— 10.41



^{13}C NMR (100 MHz, CDCl_3) of compound **6** major diastereomer

7 minor

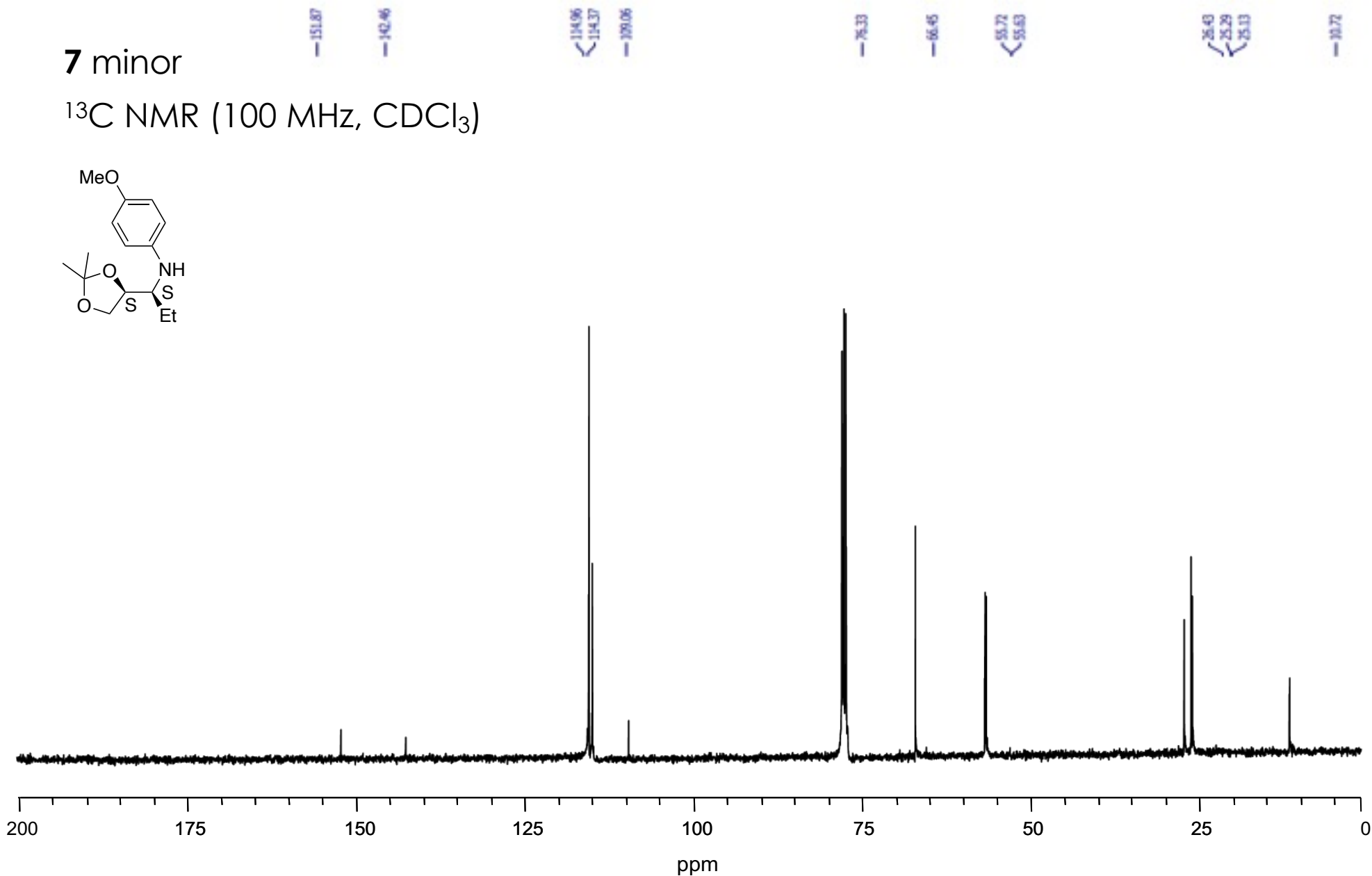
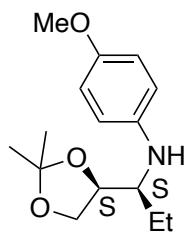
^1H NMR (400 MHz, CDCl_3)



^1H NMR (400 MHz, CDCl_3) of compound 7 minor diastereomer

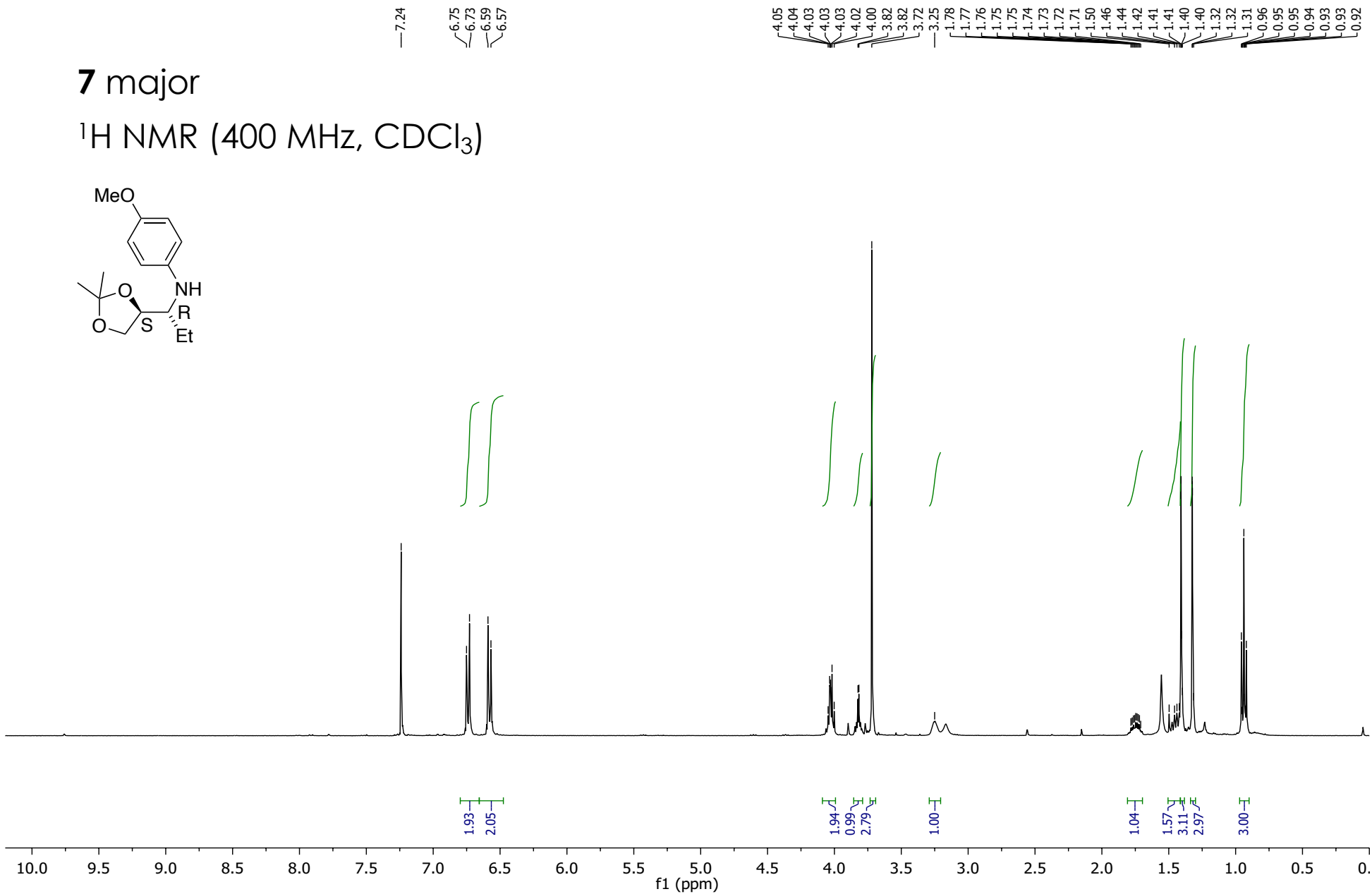
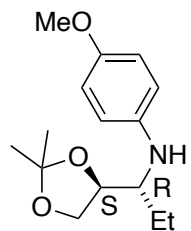
7 minor

^{13}C NMR (100 MHz, CDCl_3)



7 major

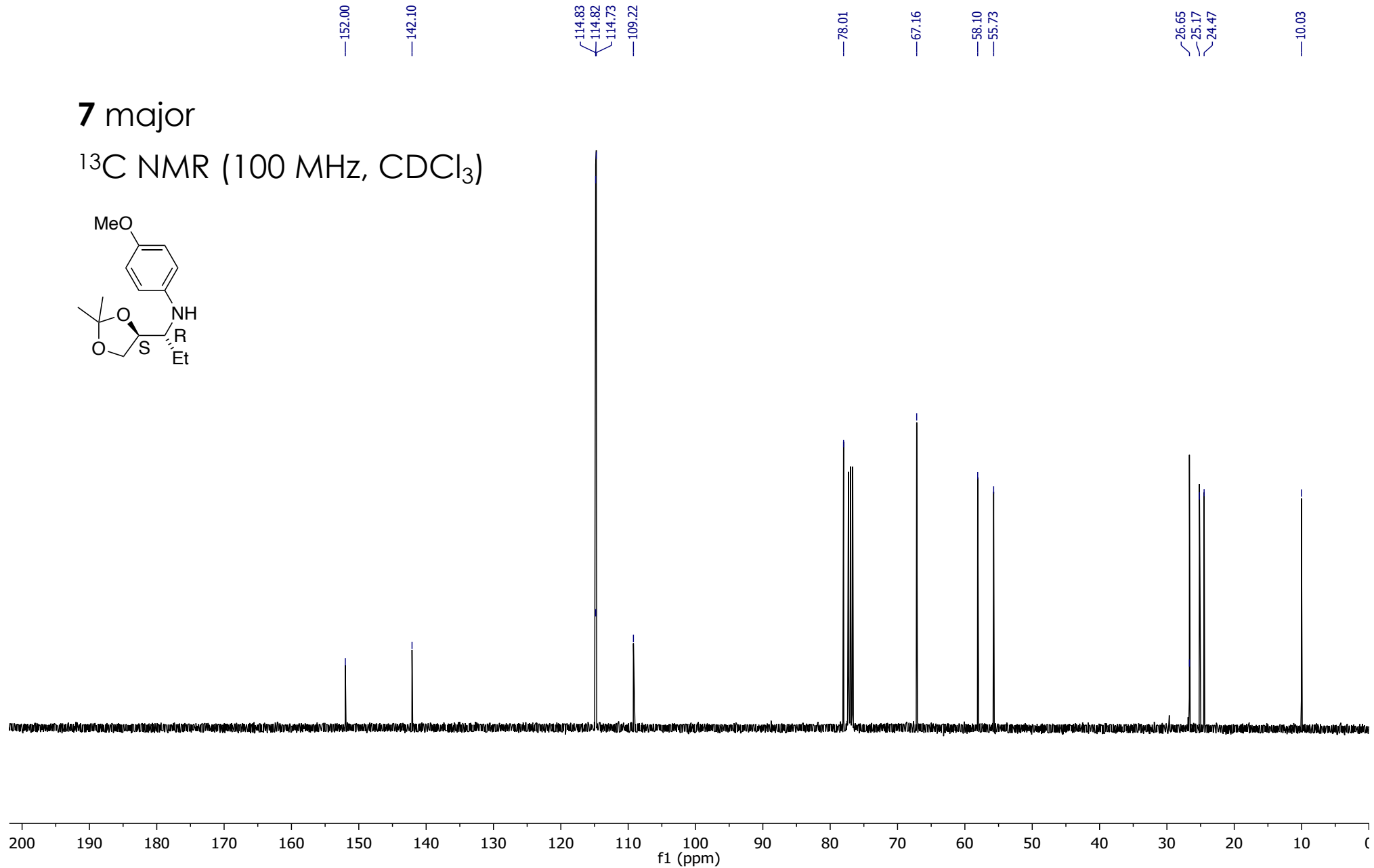
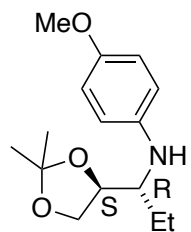
^1H NMR (400 MHz, CDCl_3)



^1H NMR (400 MHz, CDCl_3) of compound 7 major diastereomer

7 major

^{13}C NMR (100 MHz, CDCl_3)



^{13}C NMR (100 MHz, CDCl_3) of compound **7** major diastereomer

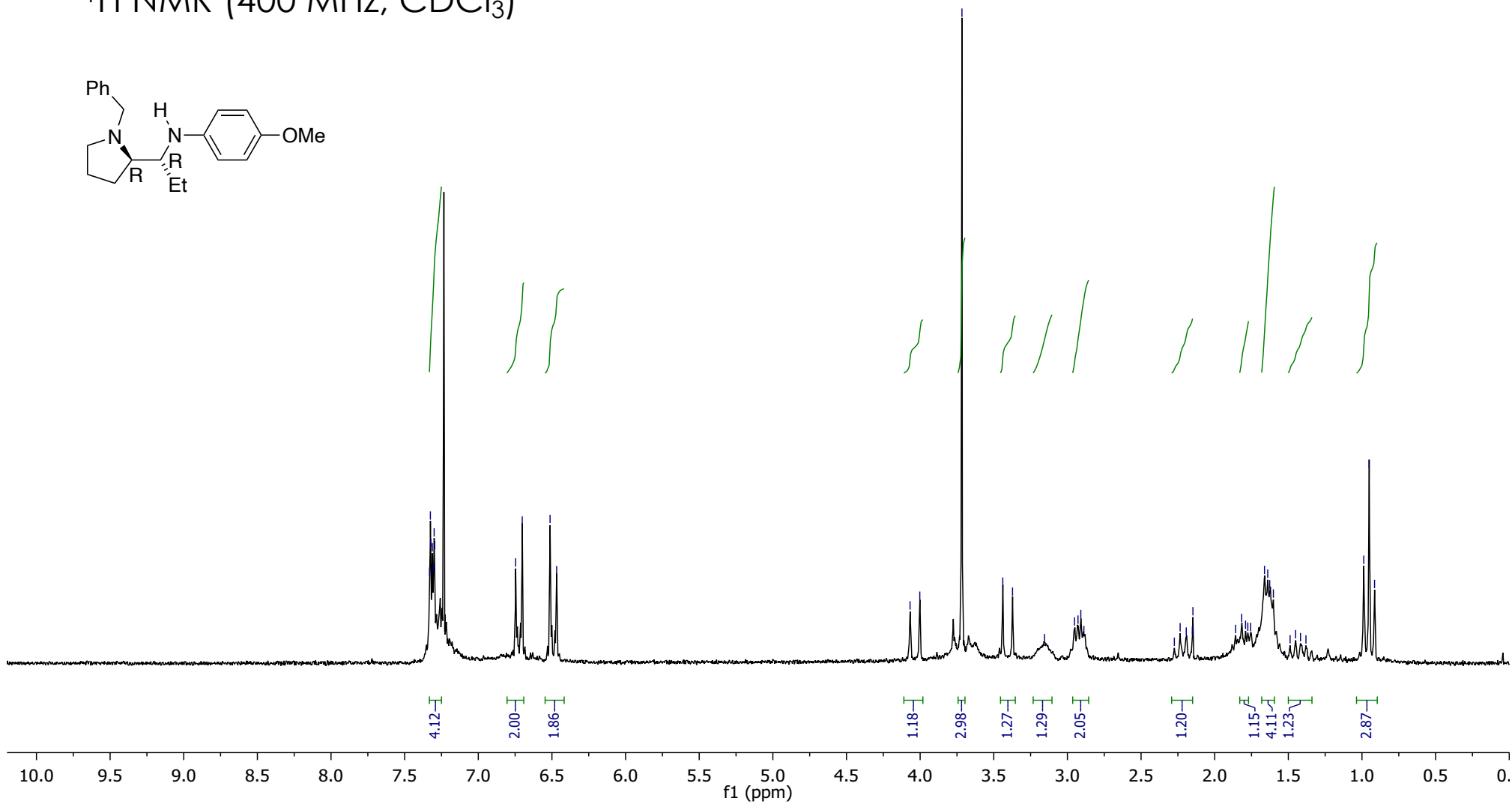
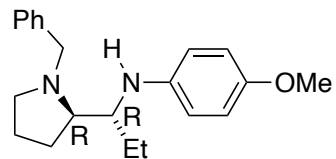
7.33
7.33
7.32
7.31
7.30
7.30
6.75
6.70
6.51
6.47

4.07
4.00
3.72
3.44
3.37
3.16
2.95
2.93
2.91
2.89

2.27
2.23
2.19
2.15
2.15
1.86
1.82
1.79
1.78
1.76
1.66
1.64
1.63
1.60
1.49
1.45
1.42
1.38
0.99
0.91

8 major

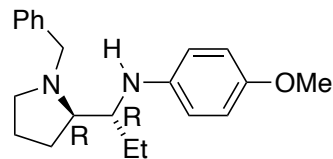
^1H NMR (400 MHz, CDCl_3)



^1H NMR (400 MHz, CDCl_3) of compound **8** major diastereomer

8 major

^{13}C NMR (100 MHz, CDCl_3)



—151.26

—143.01

—140.32

—128.49

—128.19

—126.80

—114.92

—113.91

—65.21

—60.78

—58.66

—55.84

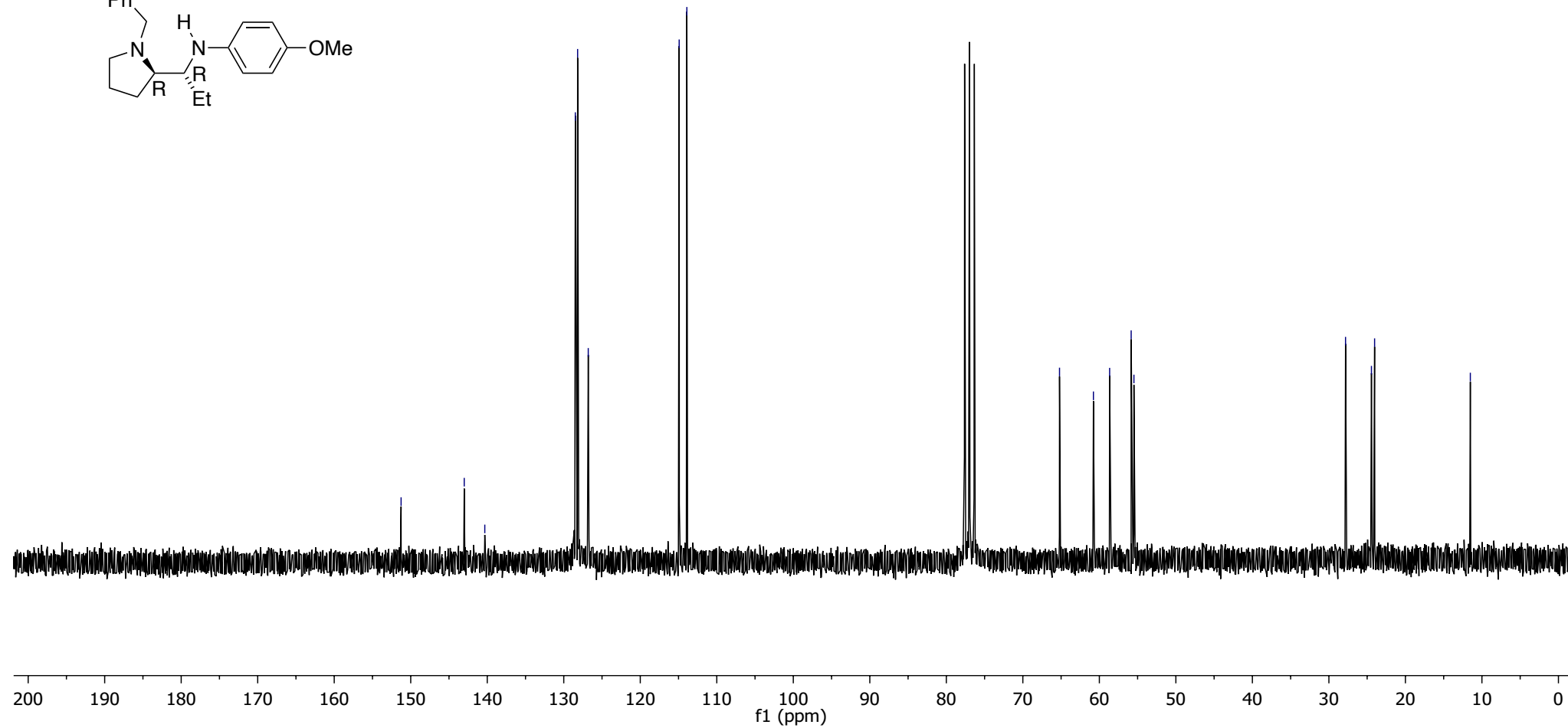
—55.48

—27.82

—24.44

—24.03

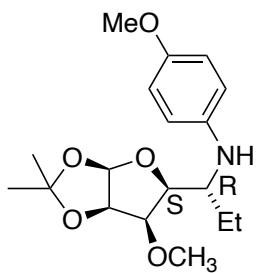
—11.51



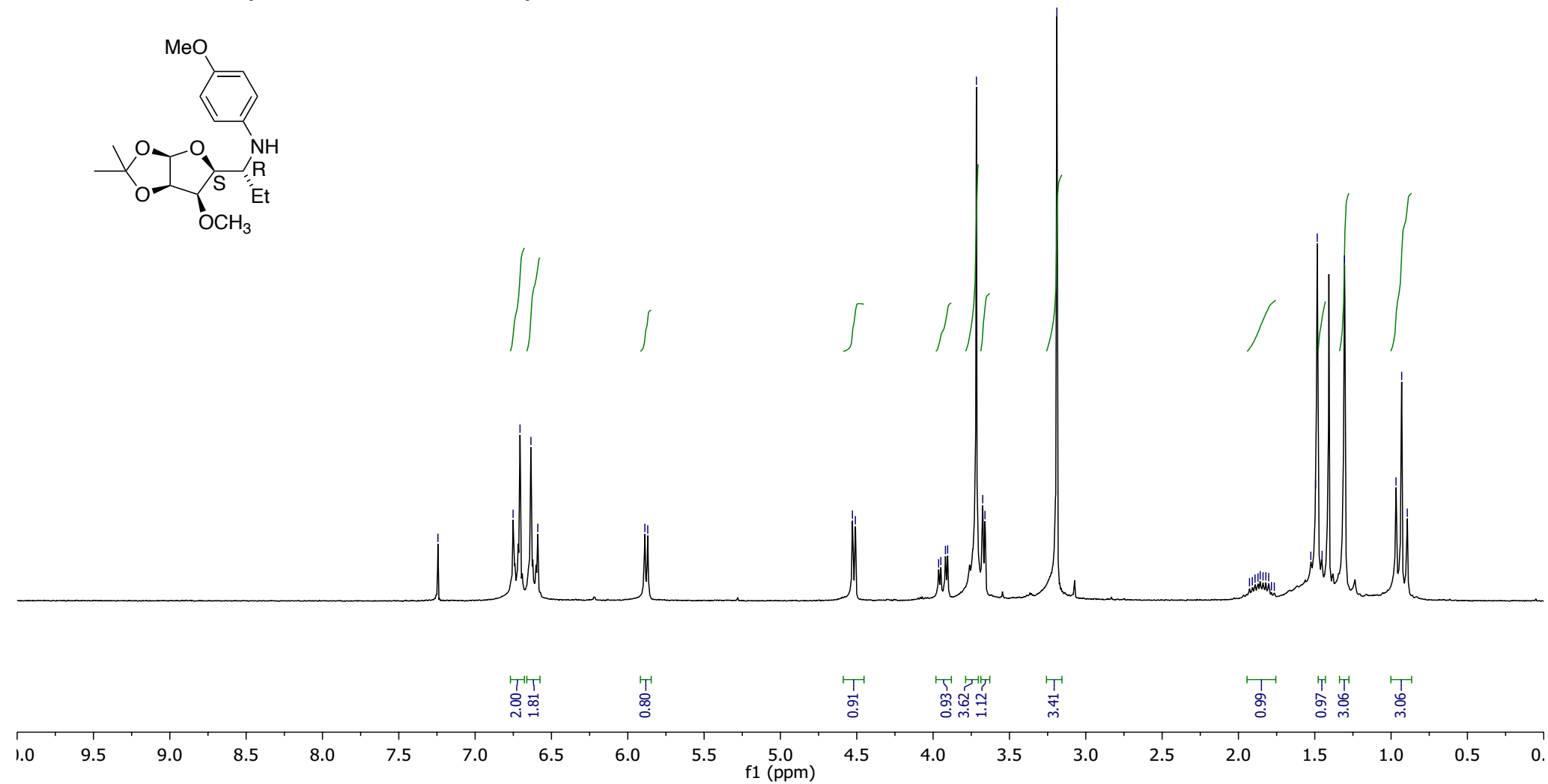
^{13}C NMR (100 MHz, CDCl_3) of compound **8** major diastereomer

9 major

^1H NMR (400 MHz, CDCl_3)



7.24
6.75
6.71
6.63
6.59
5.89
5.87
4.53
4.51
3.96
3.95
3.92
3.90
3.72
3.67
3.66
3.19
1.93
1.91
1.89
1.87
1.86
1.84
1.82
1.80
1.78
1.77
1.53
1.49
1.48
1.45
1.31
0.97
0.93
0.89



^1H NMR (400 MHz, CDCl_3) of compound 9 major diastereomer

—151.73

—142.26

—114.81

—114.60

—111.30

—104.81

—83.55

—82.33

—81.07

—57.36

—55.65

—53.36

—26.64

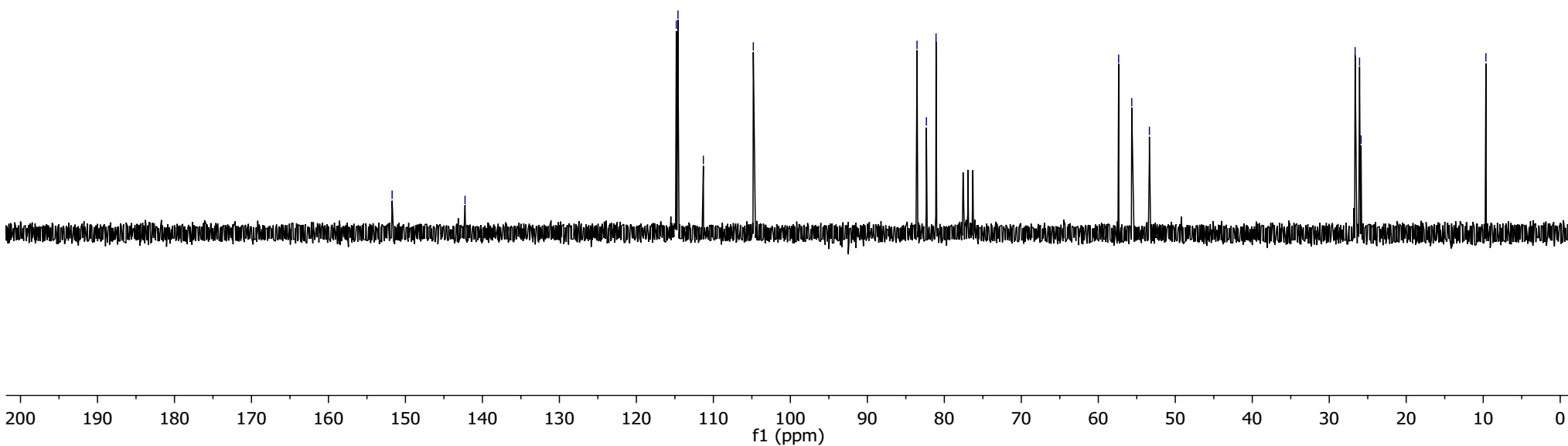
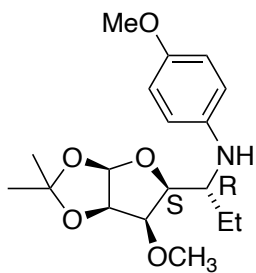
—26.06

—25.87

—9.65

9 major

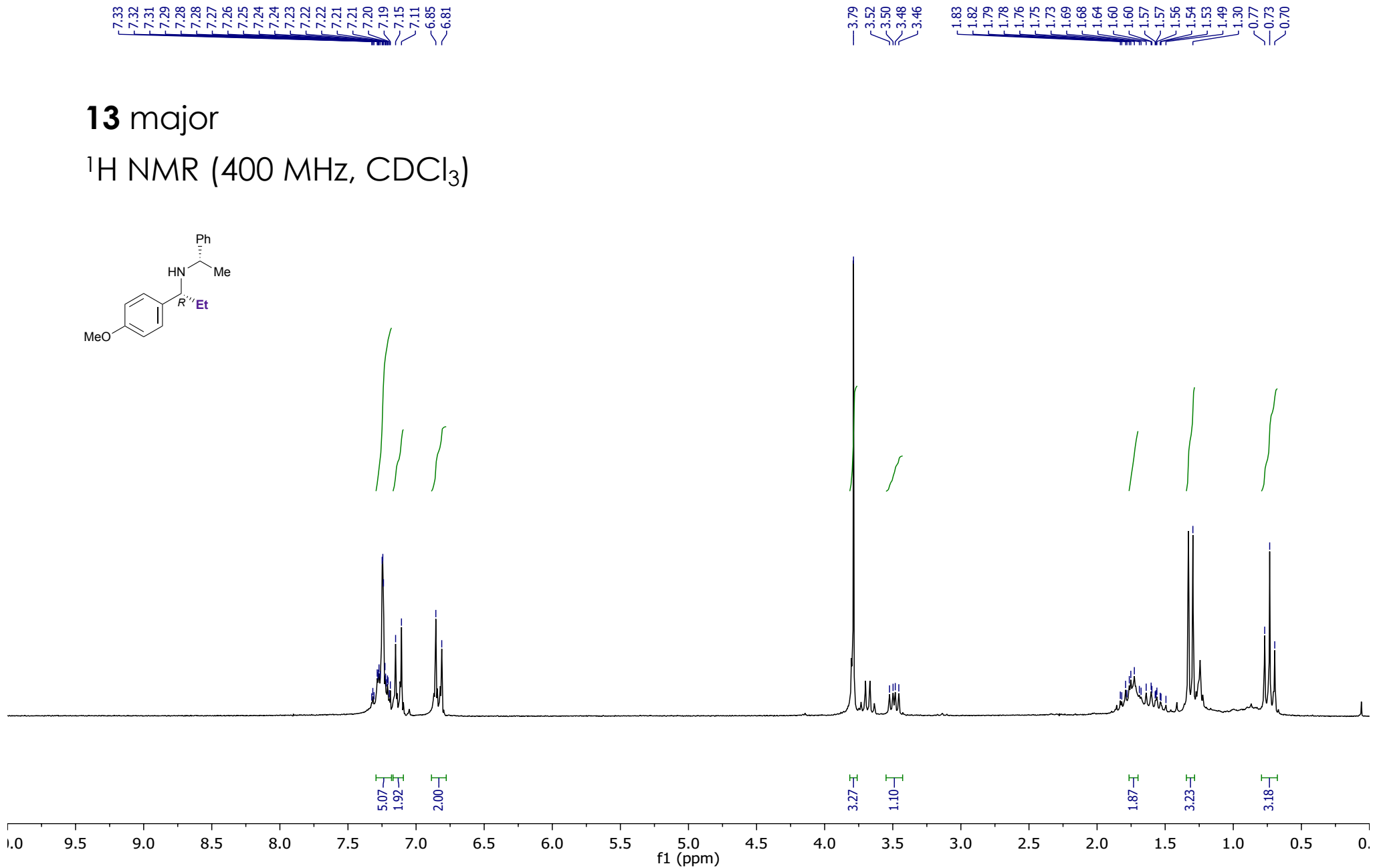
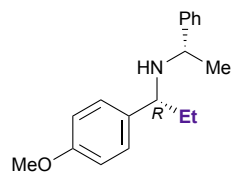
^{13}C NMR (100 MHz, CDCl_3)



^{13}C NMR (100 MHz, CDCl_3) of compound **9** major diastereomer

13 major

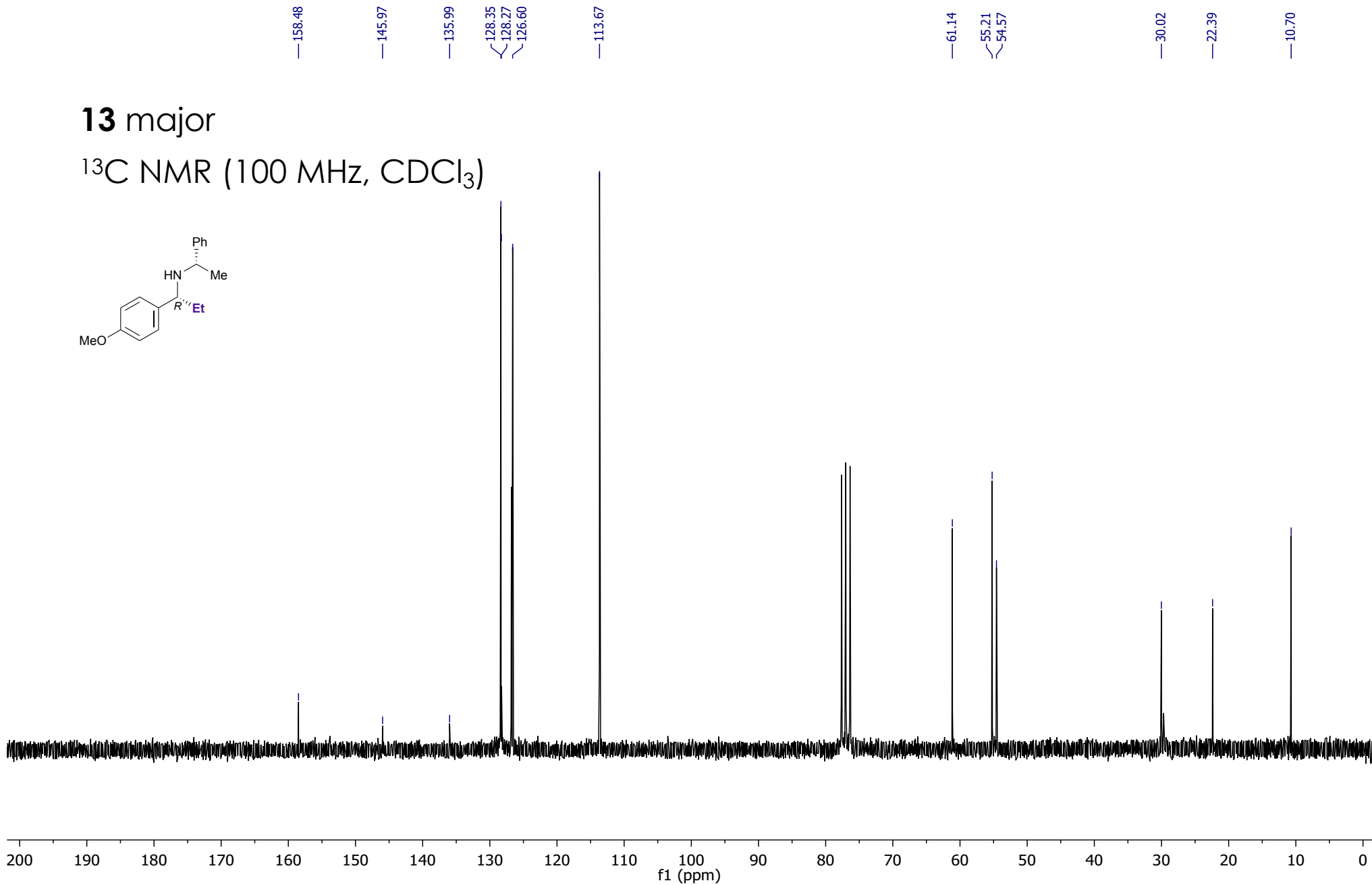
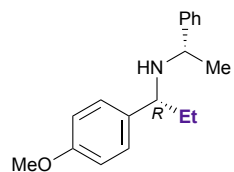
^1H NMR (400 MHz, CDCl_3)



^1H NMR (400 MHz, CDCl_3) of compound **13** minor diastereomer

13 major

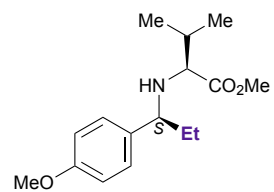
^{13}C NMR (100 MHz, CDCl_3)



^{13}C NMR (100 MHz, CDCl_3) of compound **13** minor diastereomer

14 major

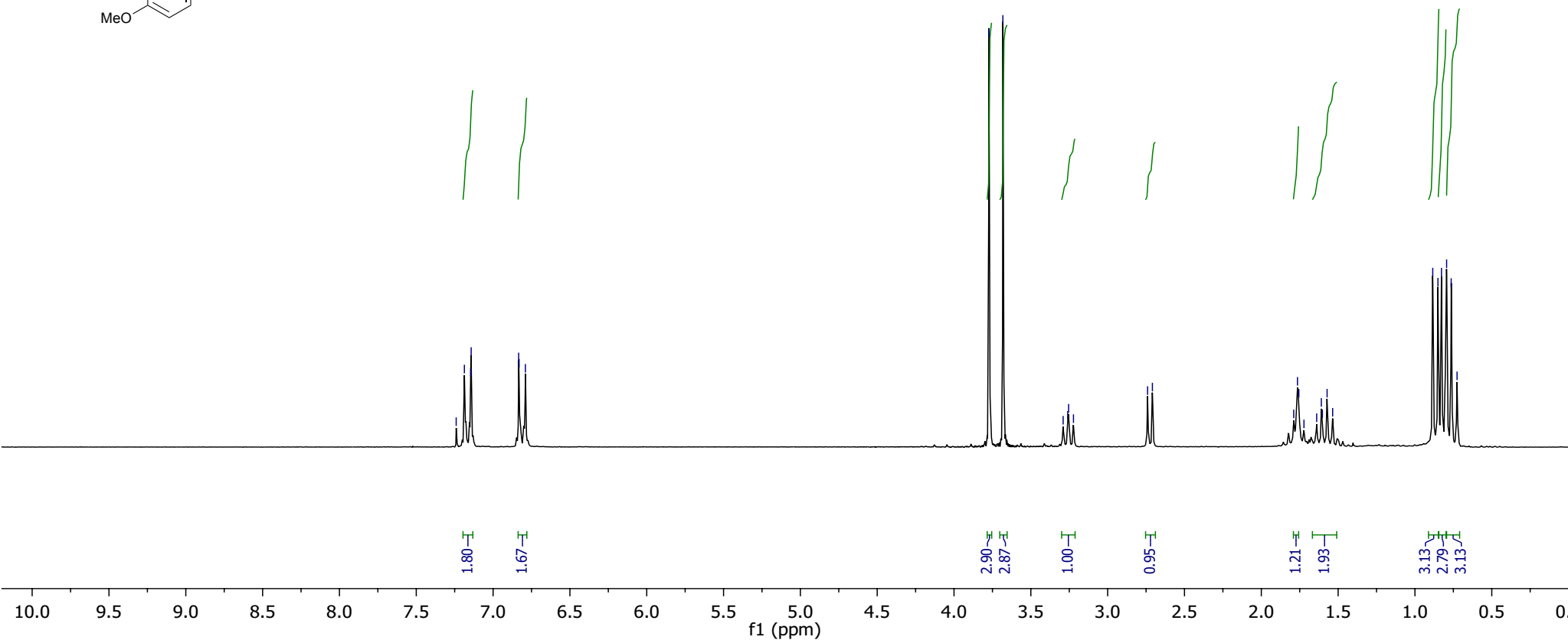
^1H NMR (400 MHz, CDCl_3)



7.24
7.19
7.15
7.14
6.83
6.83
6.79

3.77
3.68
3.29
3.26
3.25
3.22
2.74
2.71

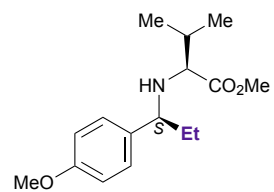
1.79
1.76
1.76
1.72
1.64
1.61
1.60
1.57
1.54
0.88
0.85
0.83
0.79
0.76
0.73



^1H NMR (400 MHz, CDCl_3) of compound **14** major diastereomer

14 major

^{13}C NMR (100 MHz, CDCl_3)



— 176.41

— 158.60

— 135.66

— 128.74

— 113.45

— 64.38

— 62.88

— 55.16

— 51.24

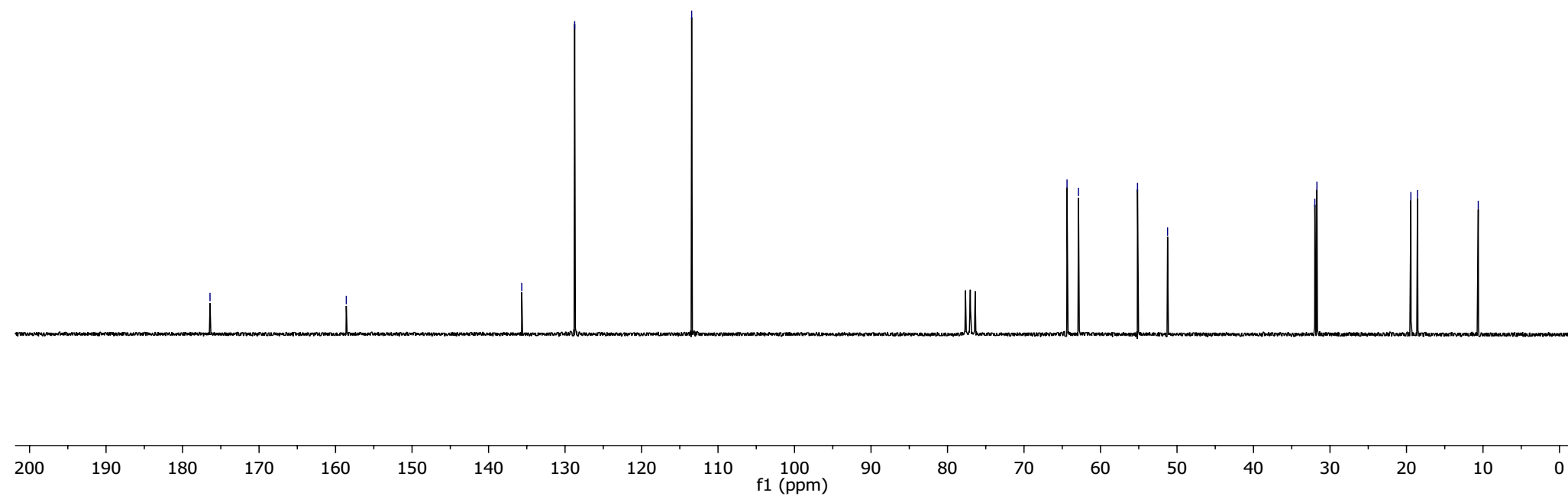
— 31.98

— 31.71

— 19.43

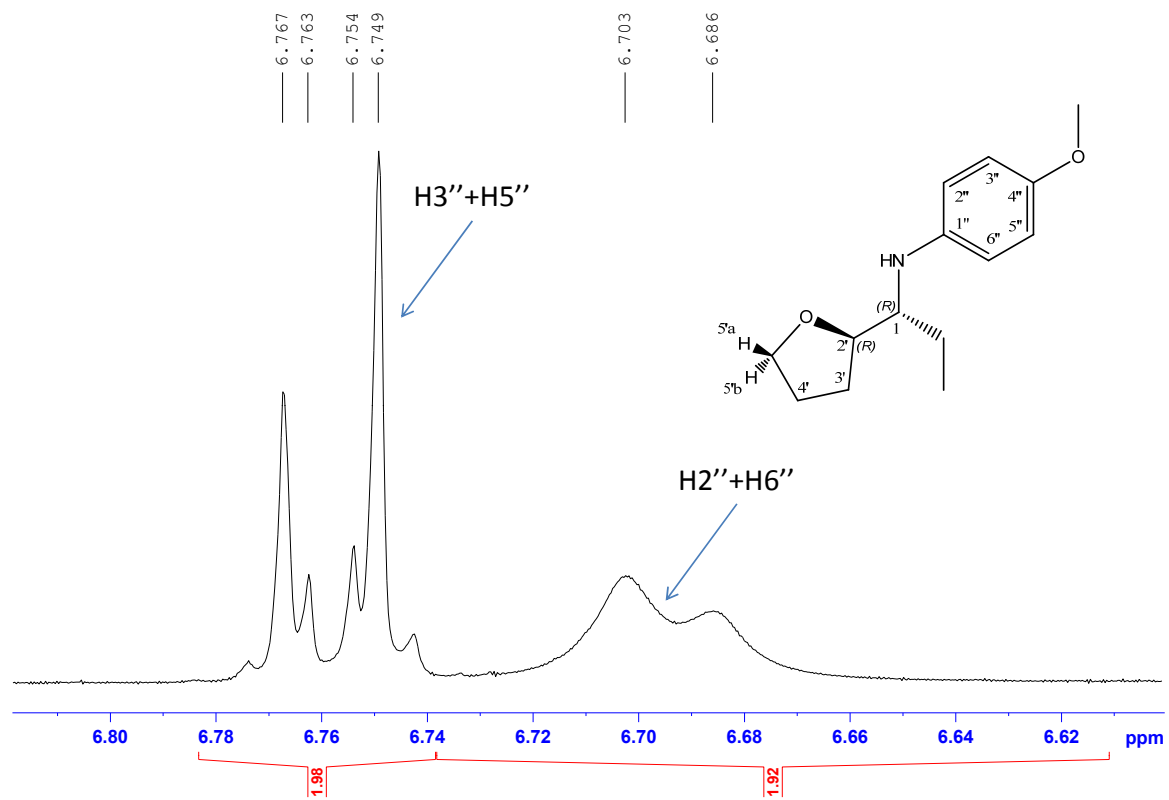
— 18.57

— 10.62



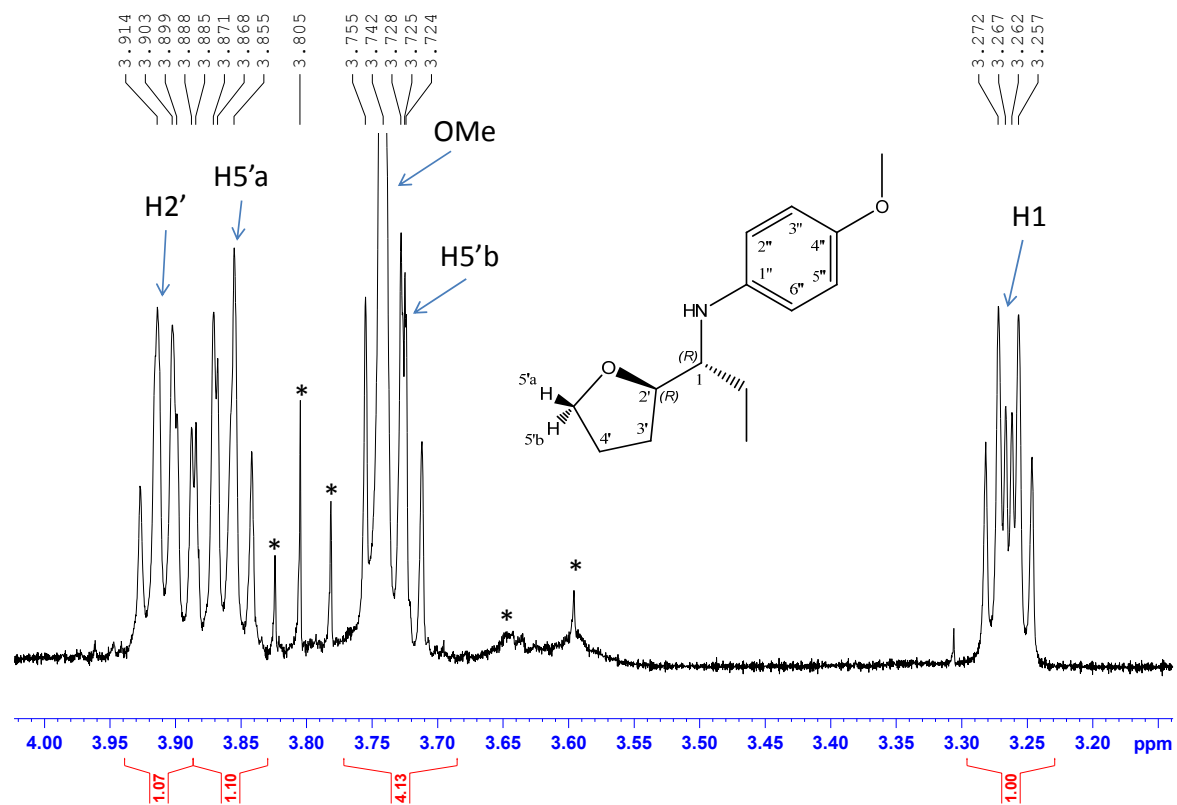
^{13}C NMR (100 MHz, CDCl_3) of compound **14** major diastereomer

6 major
nOe



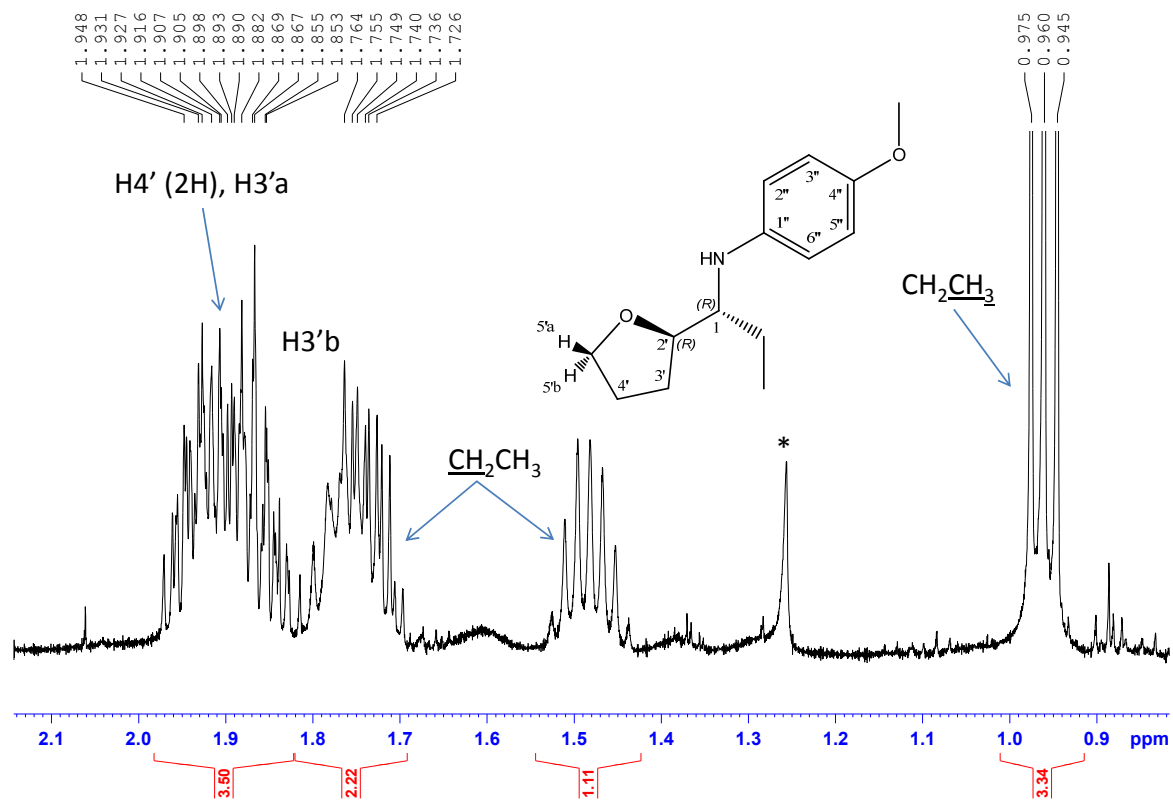
¹H NMR (400 MHz, CDCl₃) NOE for compound **6** major diastereomer

6 major
nOe



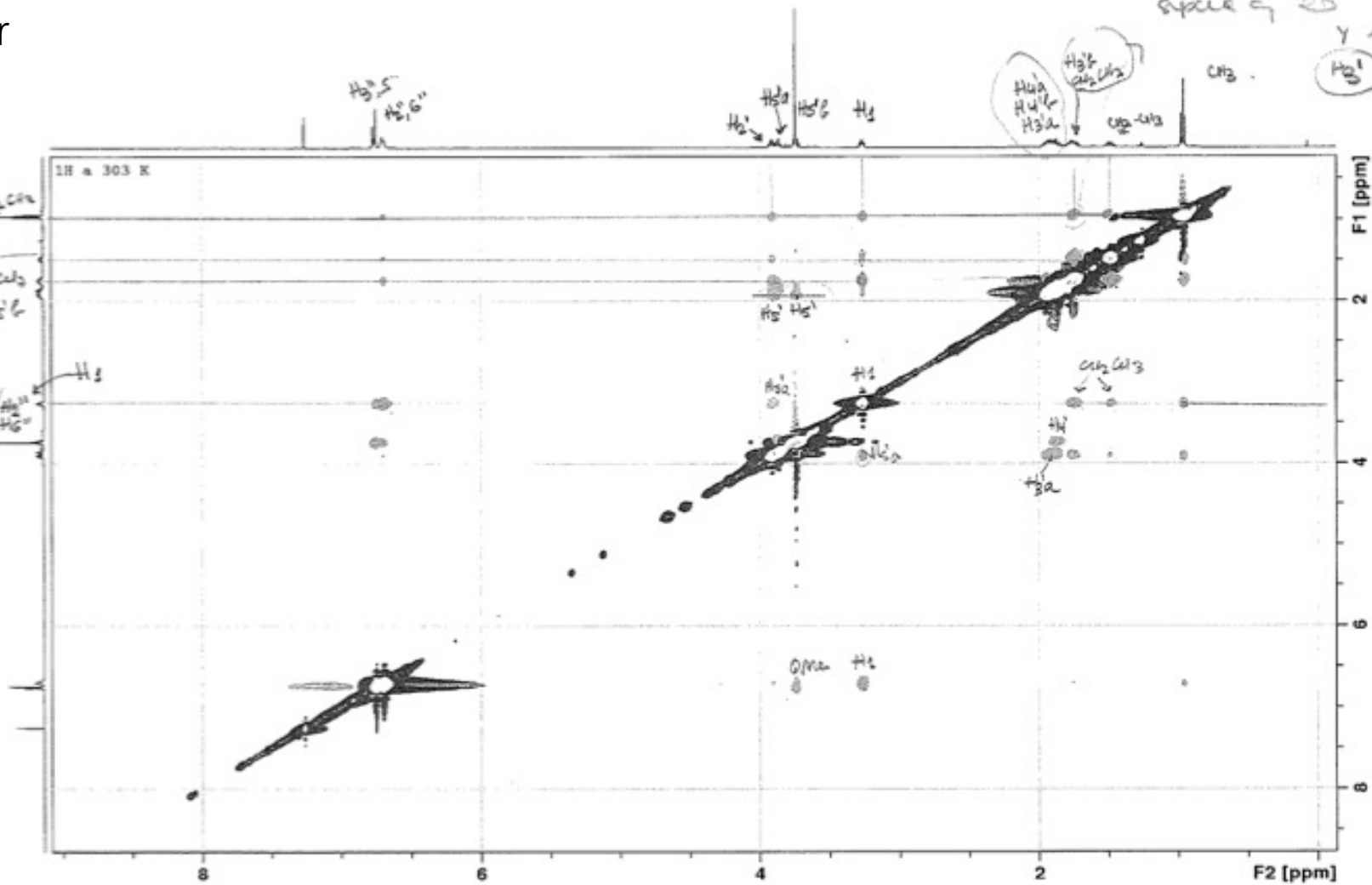
^1H NMR (400 MHz, CDCl_3) NOE for compound **6** major diastereomer

6 major
nOe



¹H NMR (400 MHz, CDCl₃) NOE for compound **6** major diastereomer

6 major NOESY

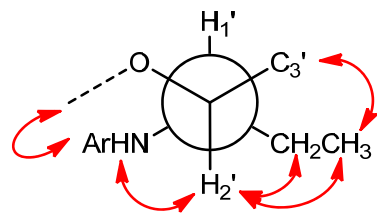
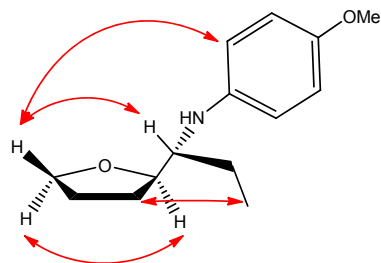


¹H NMR (400 MHz, CDCl₃) NOESY for compound **6** major diastereomer

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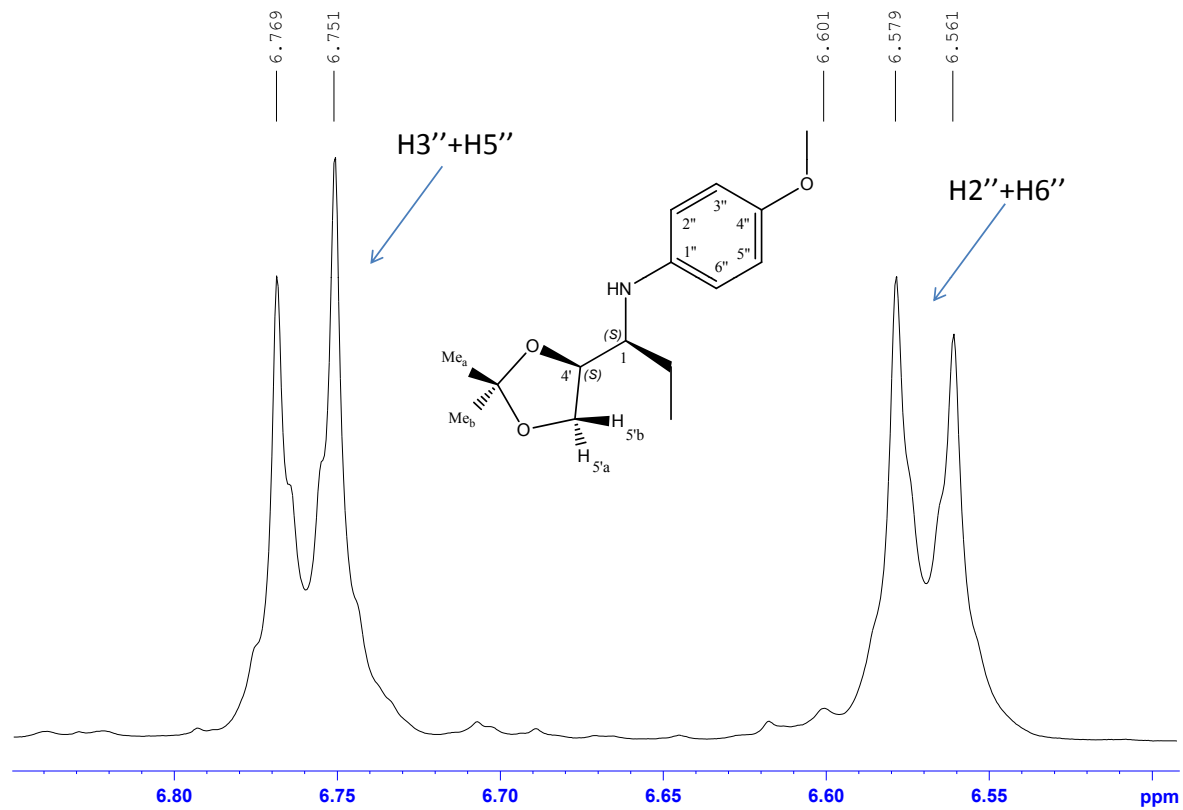
6 major

STEREOCHEMISTRY and observed nOe



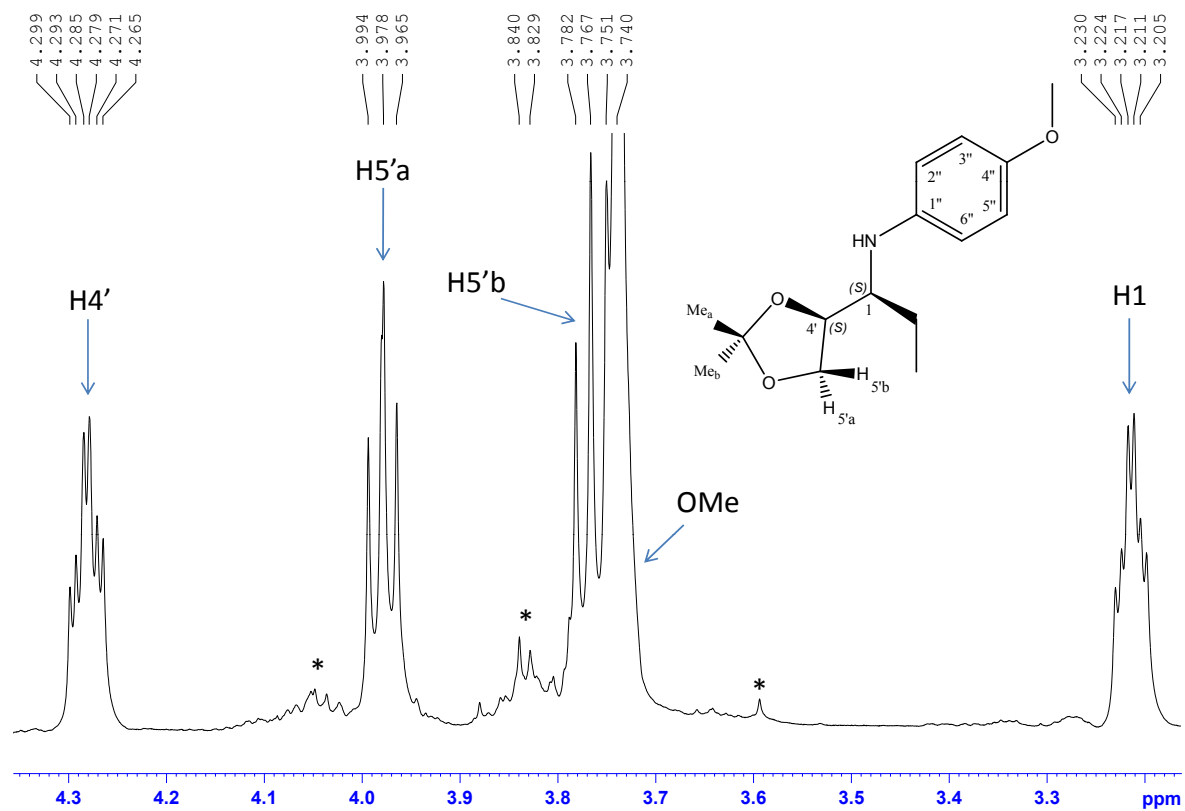
Stereochemistry and observed NOE for compound **6** major diastereomer

7 minor
nOe



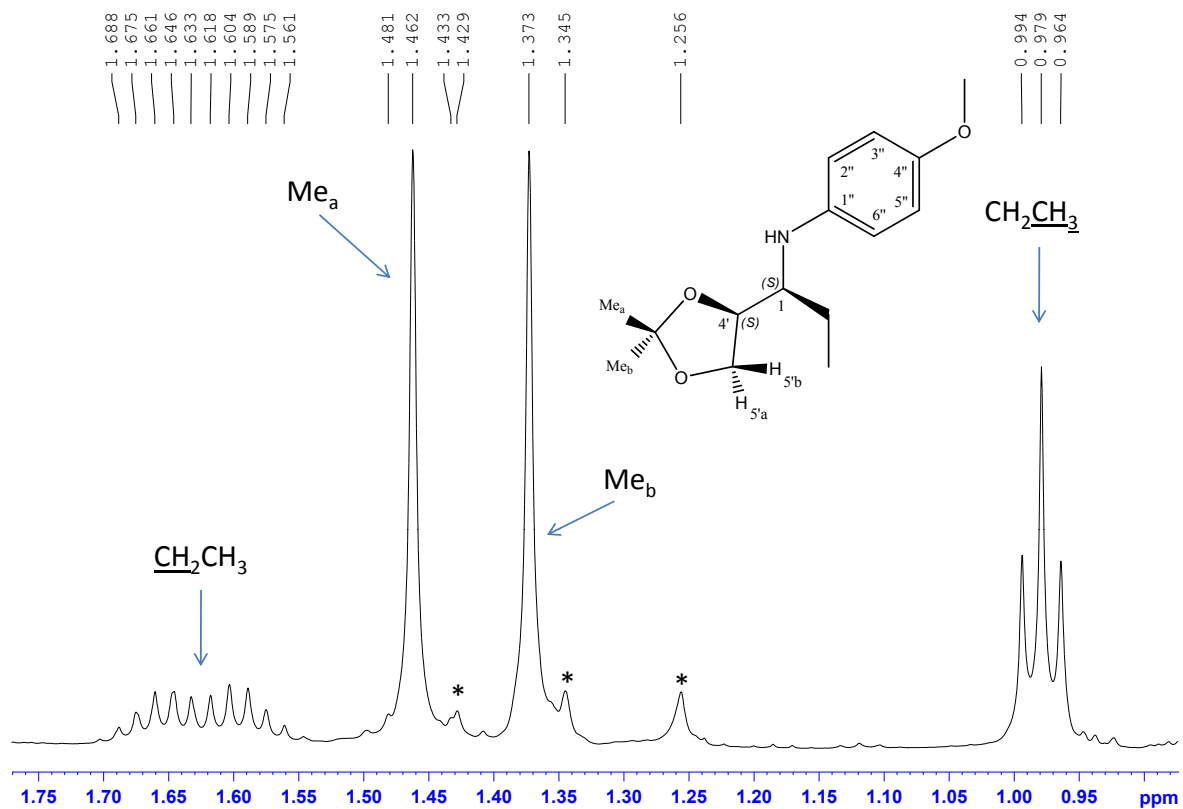
^1H NMR (400 MHz, CDCl_3) NOE for compound **7** minor diastereomer

7 minor
nOe



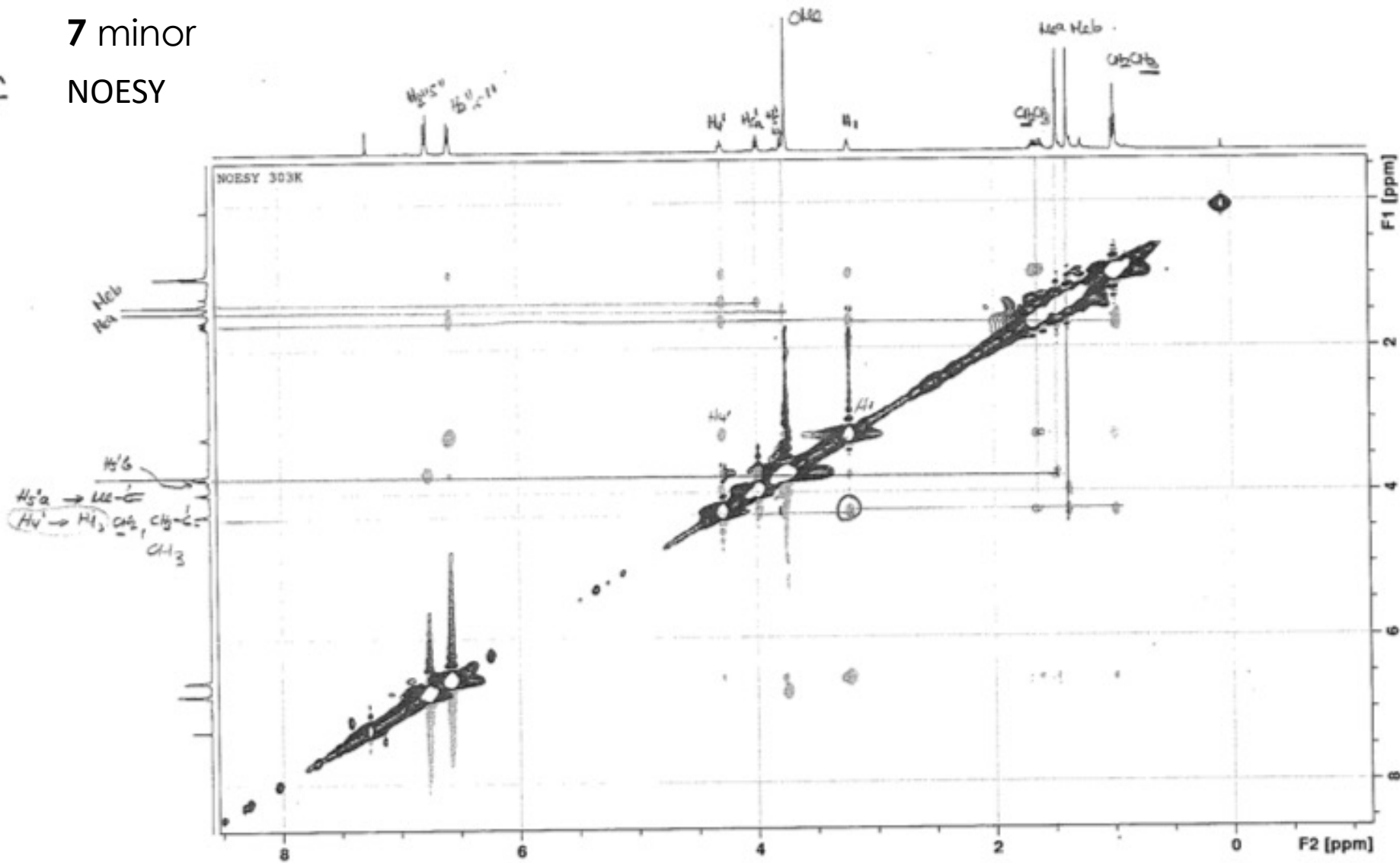
^1H NMR (400 MHz, CDCl_3) NOE for compound **7** minor diastereomer

7 minor
nOe



¹H NMR (400 MHz, CDCl₃) NOE for compound **7** minor diastereomer

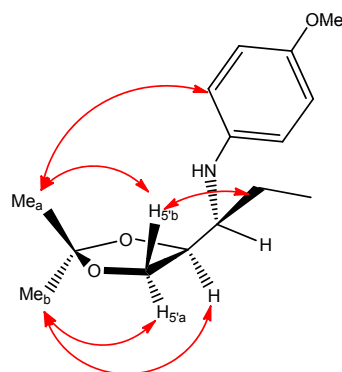
7 minor
NOESY



¹H NMR (400 MHz, CDCl₃) NOESY for compound **7** minor diastereomer

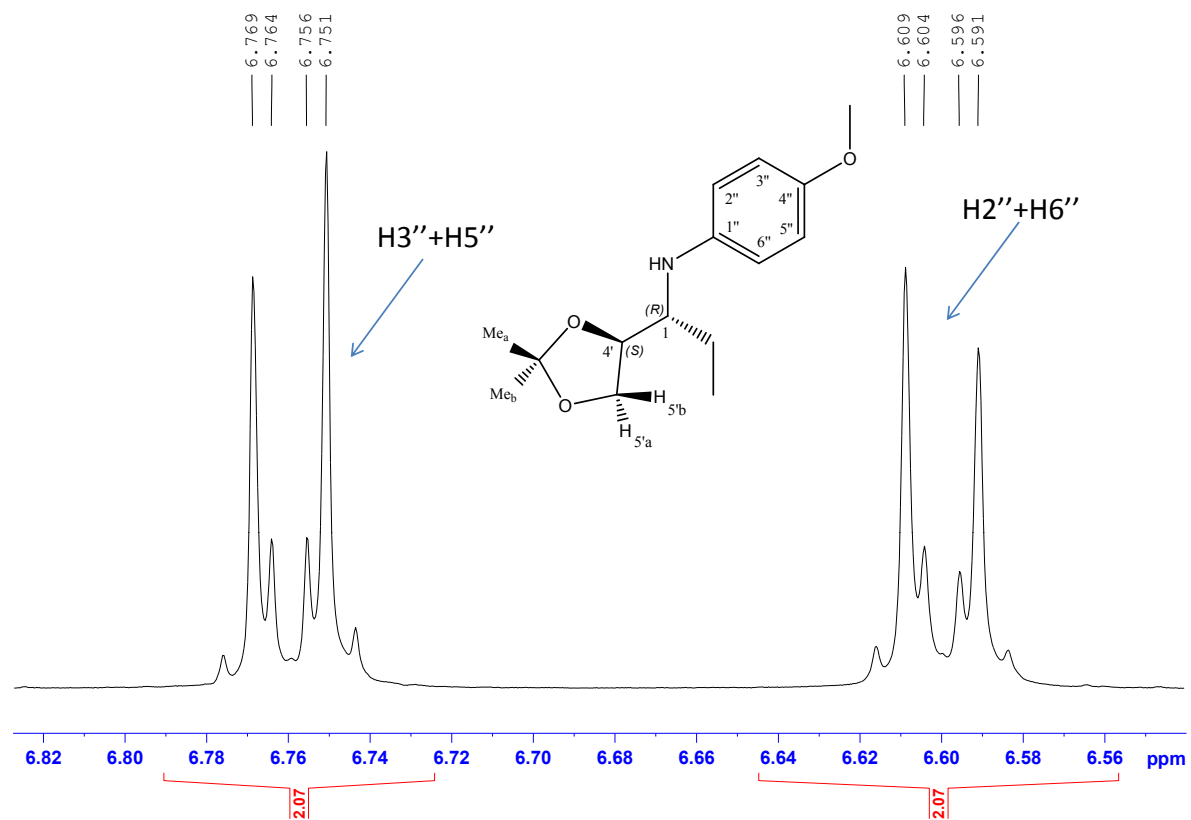
7 minor

STEREOCHEMISTRY and observed nOe



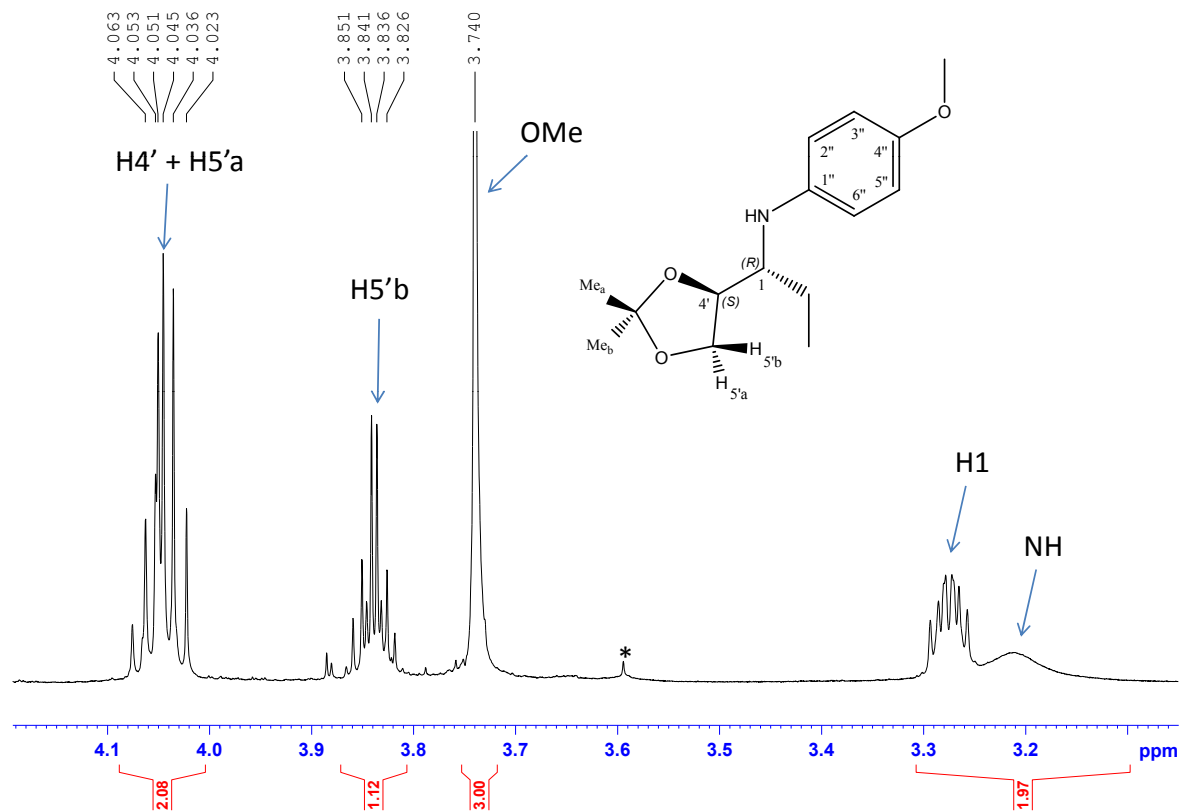
Stereochemistry and observed NOE for compound **7** minor diastereomer

7 major
nOe



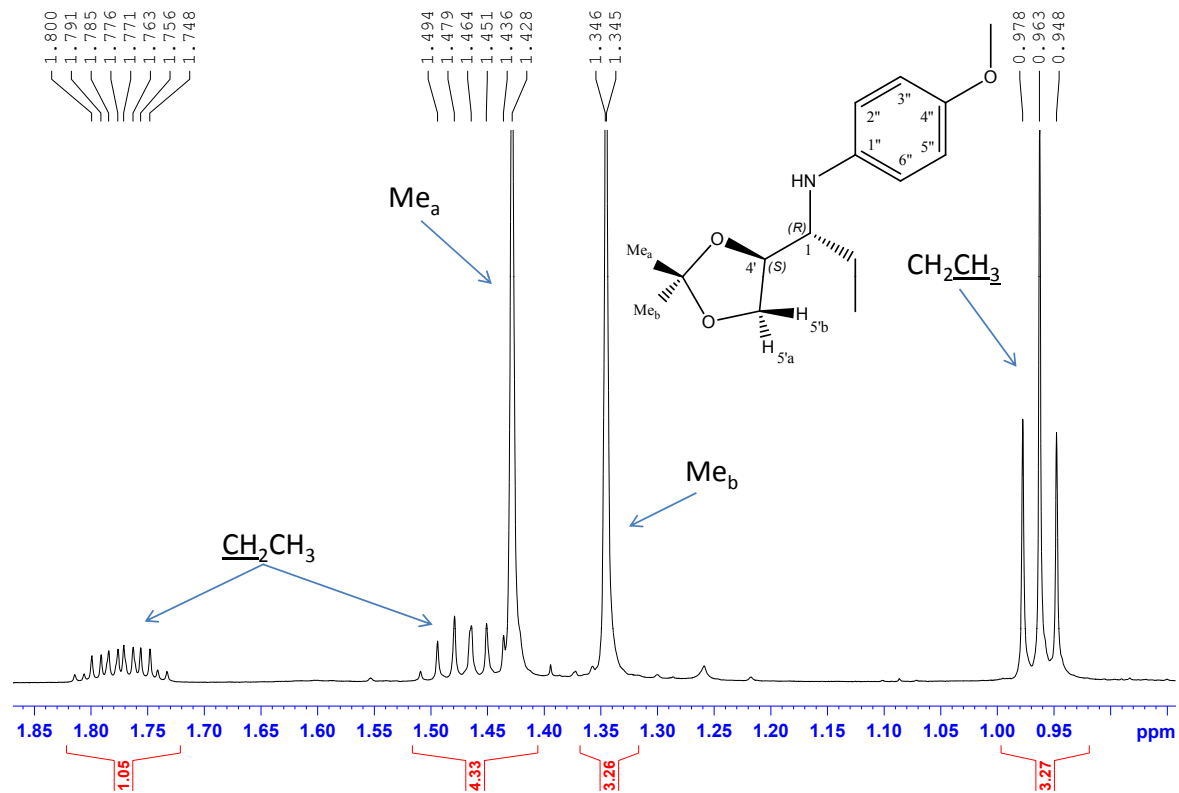
^1H NMR (400 MHz, CDCl_3) NOE for compound **7** major diastereomer

7 major
nOe



^1H NMR (400 MHz, CDCl_3) NOE for compound **7** major diastereomer

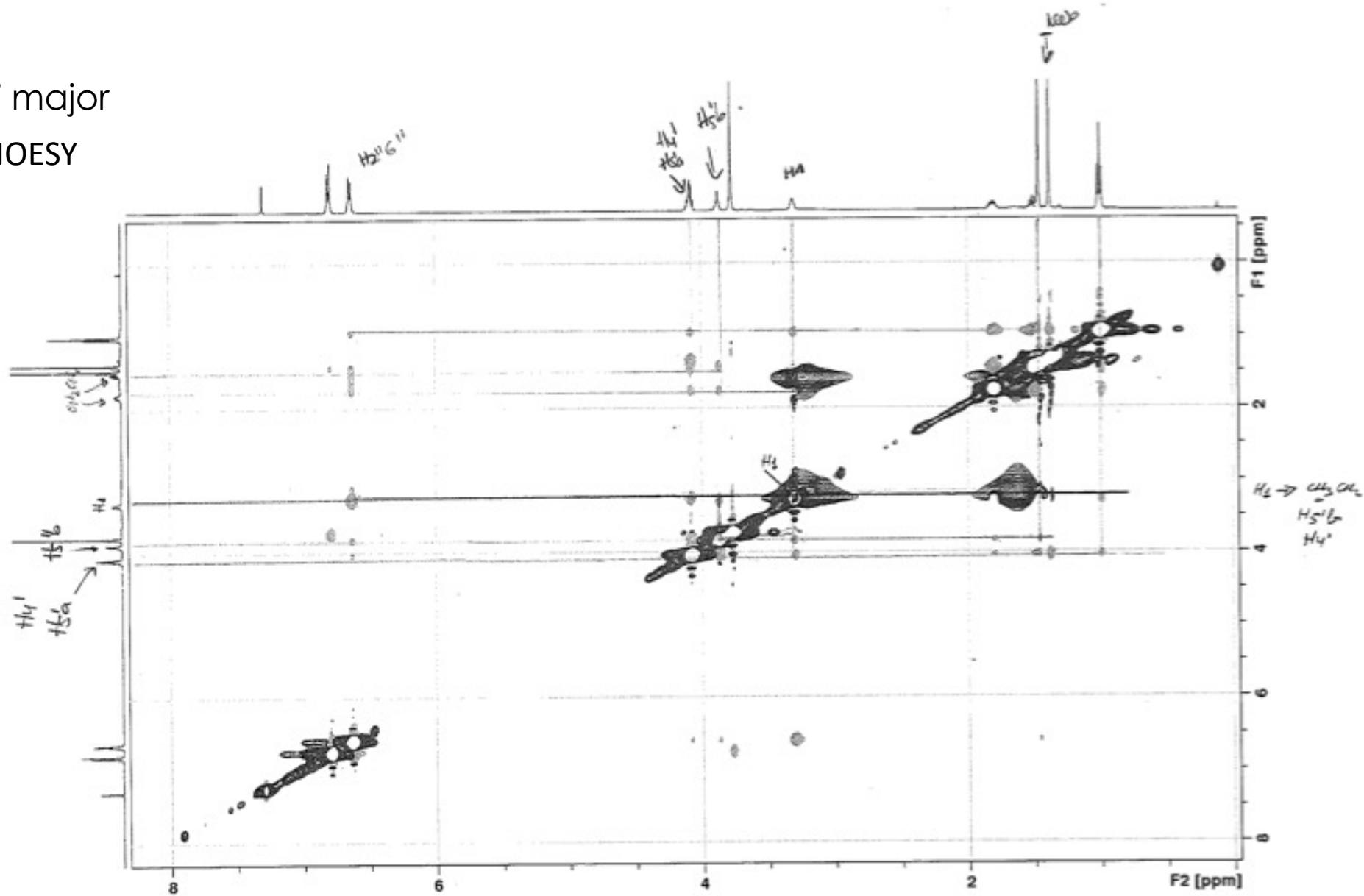
7 major
nOe



¹H NMR (400 MHz, CDCl₃) NOE for compound 7 major diastereomer

TR

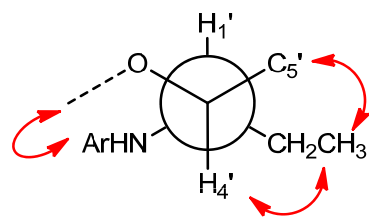
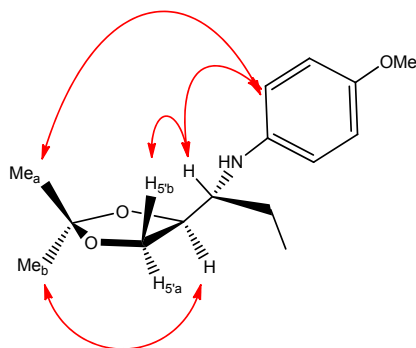
7 major NOESY



¹H NMR (400 MHz, CDCl₃) NOESY for compound **7** major diastereomer

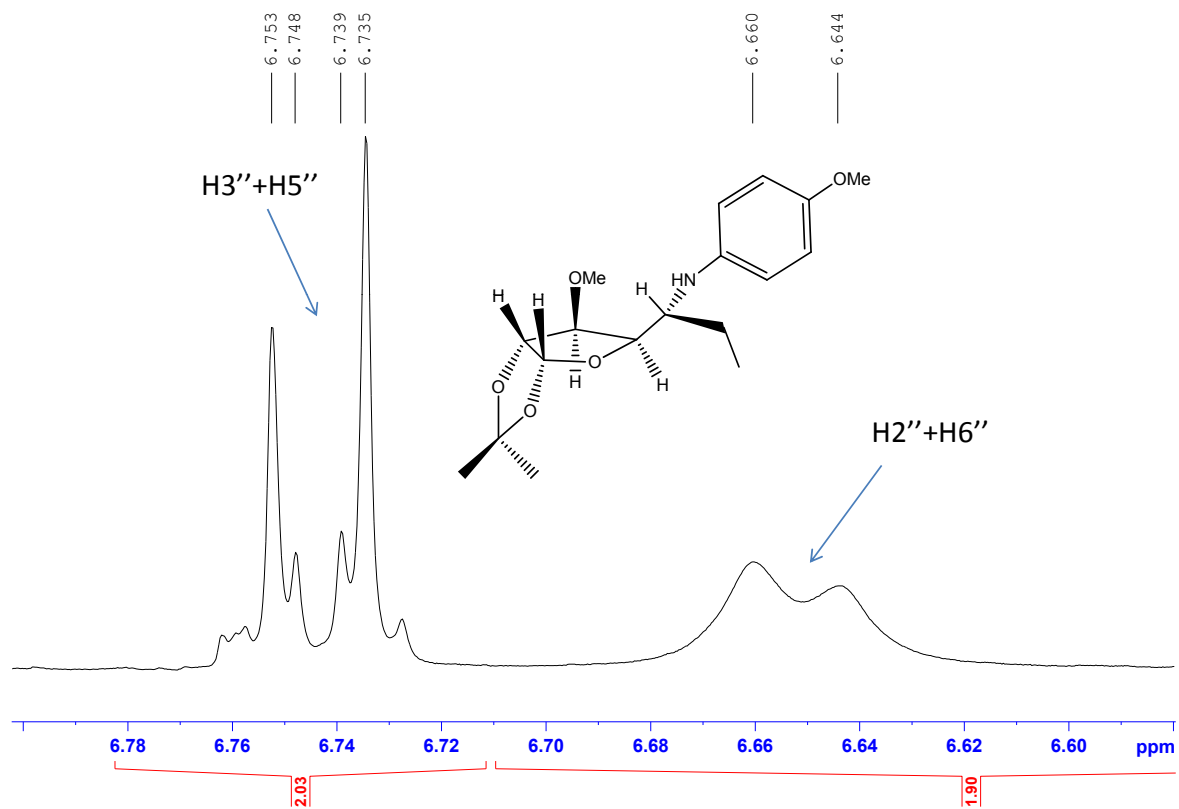
7 major
nOe

STEREOCHEMISTRY and observed nOe



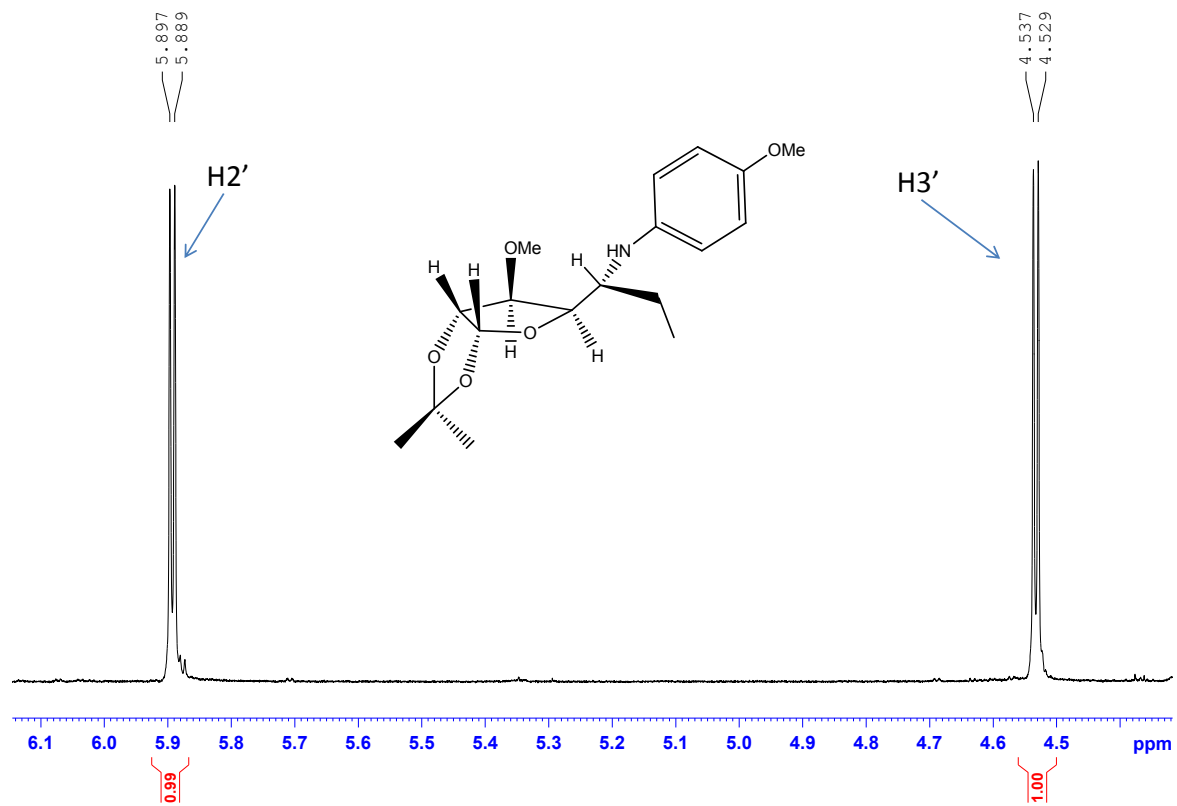
Stereochemistry and observed NOE for compound **7** major diastereomer

9 major
nOe



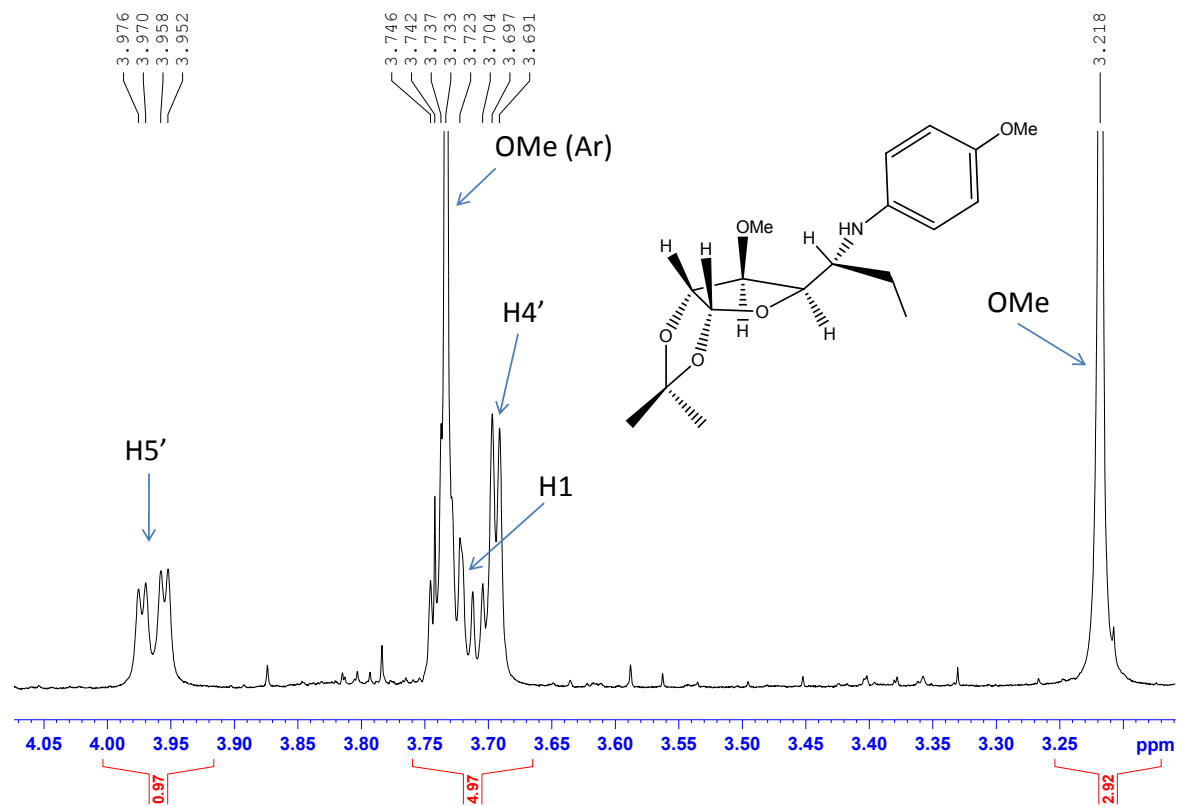
¹H NMR (400 MHz, CDCl₃) NOE for compound 9 major diastereomer

9 major
nOe



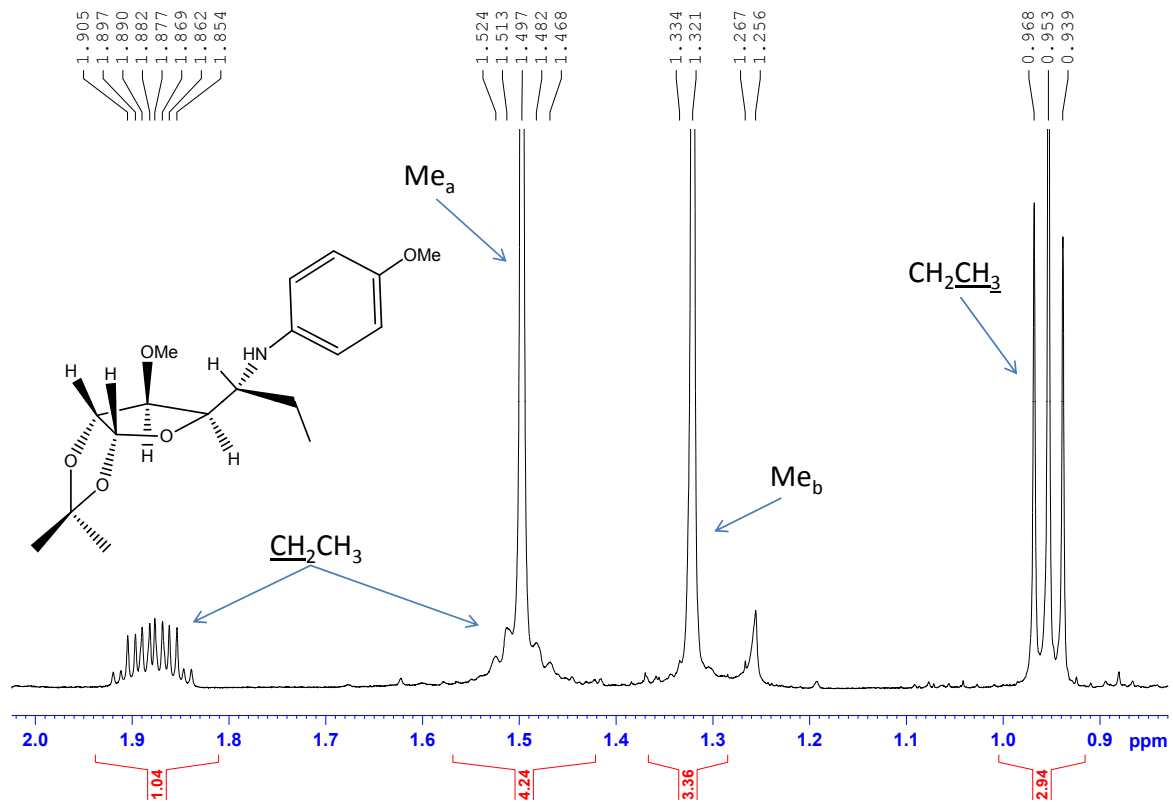
¹H NMR (400 MHz, CDCl₃) NOE for compound **9** major diastereomer

9 major
nOe



^1H NMR (400 MHz, CDCl_3) NOE for compound **9** major diastereomer

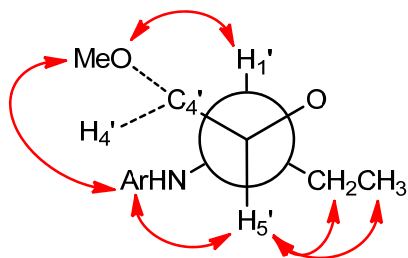
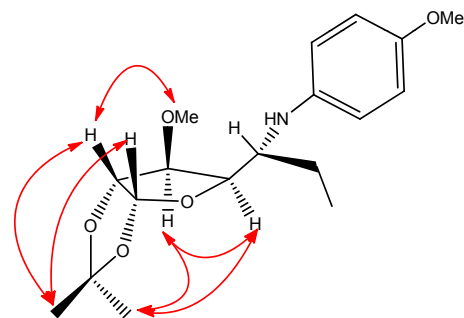
9 major
nOe



^1H NMR (400 MHz, CDCl_3) NOE for compound **9** major diastereomer

9 major

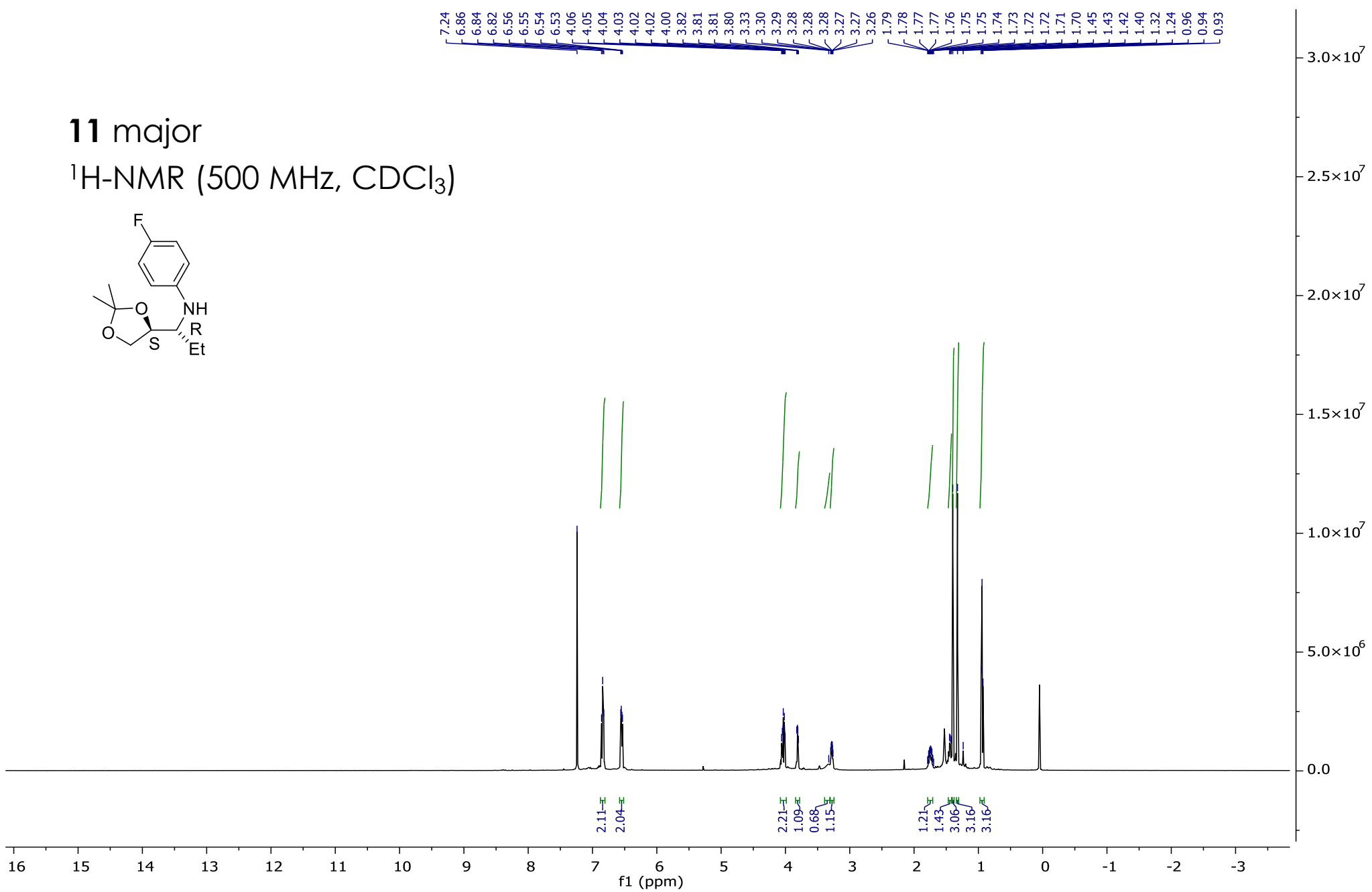
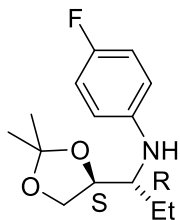
STEREOCHEMISTRY and observed nOe



Stereochemistry and observed NOE for compound 9 major diastereomer

11 major

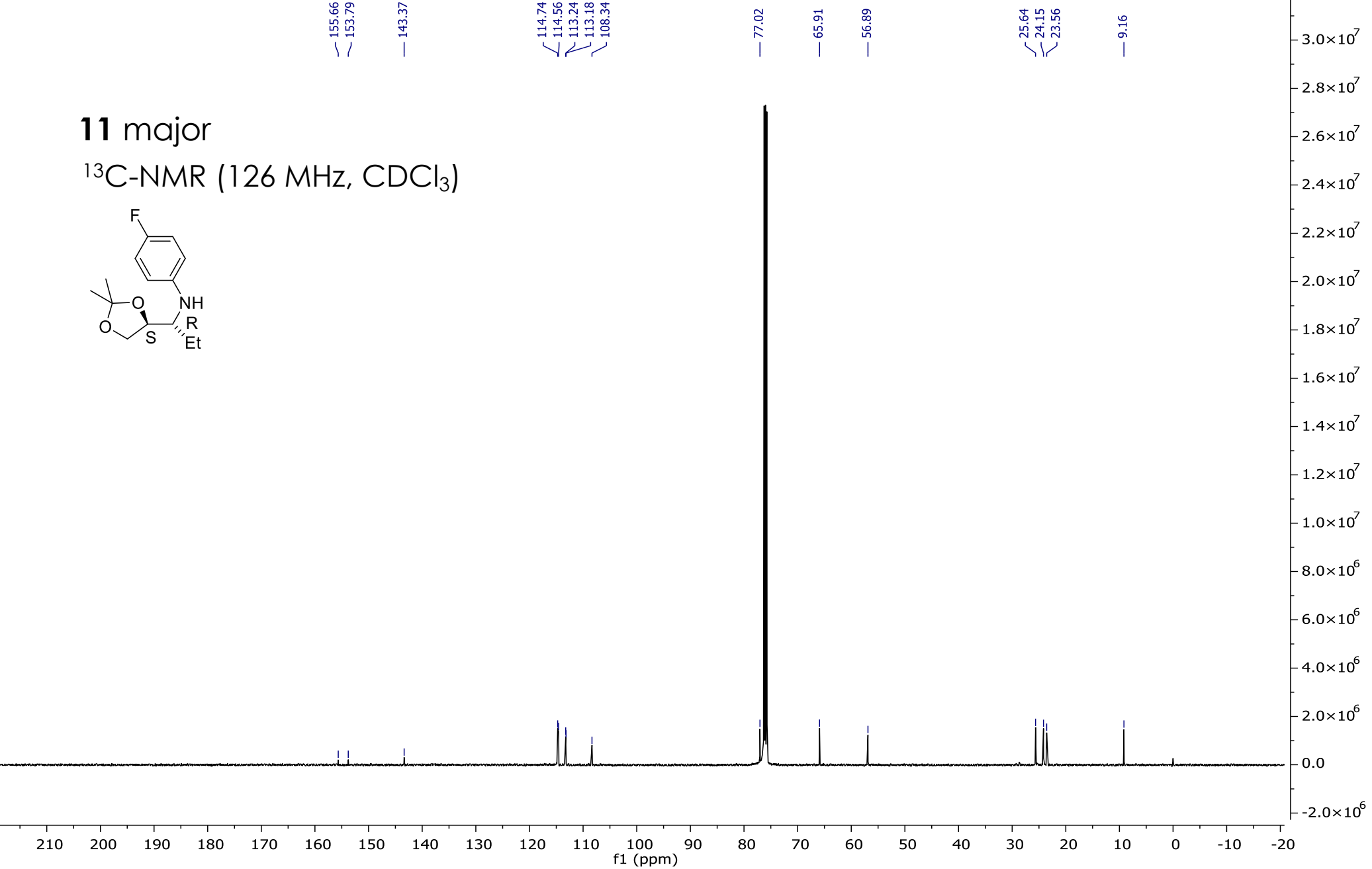
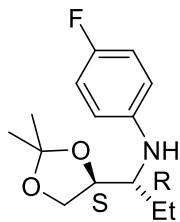
¹H-NMR (500 MHz, CDCl₃)



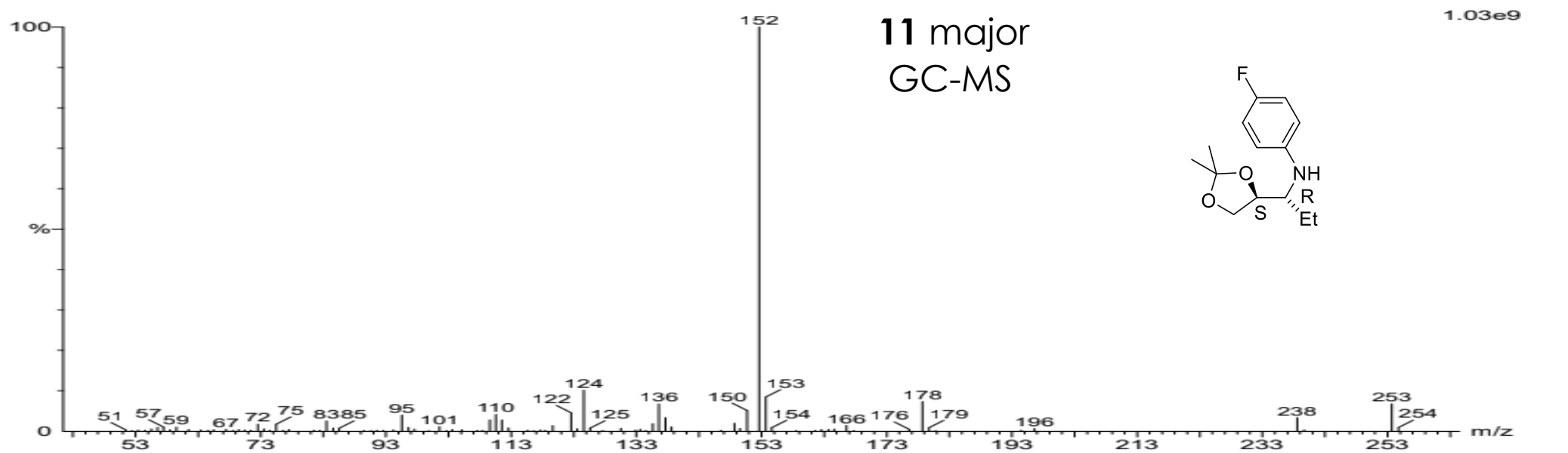
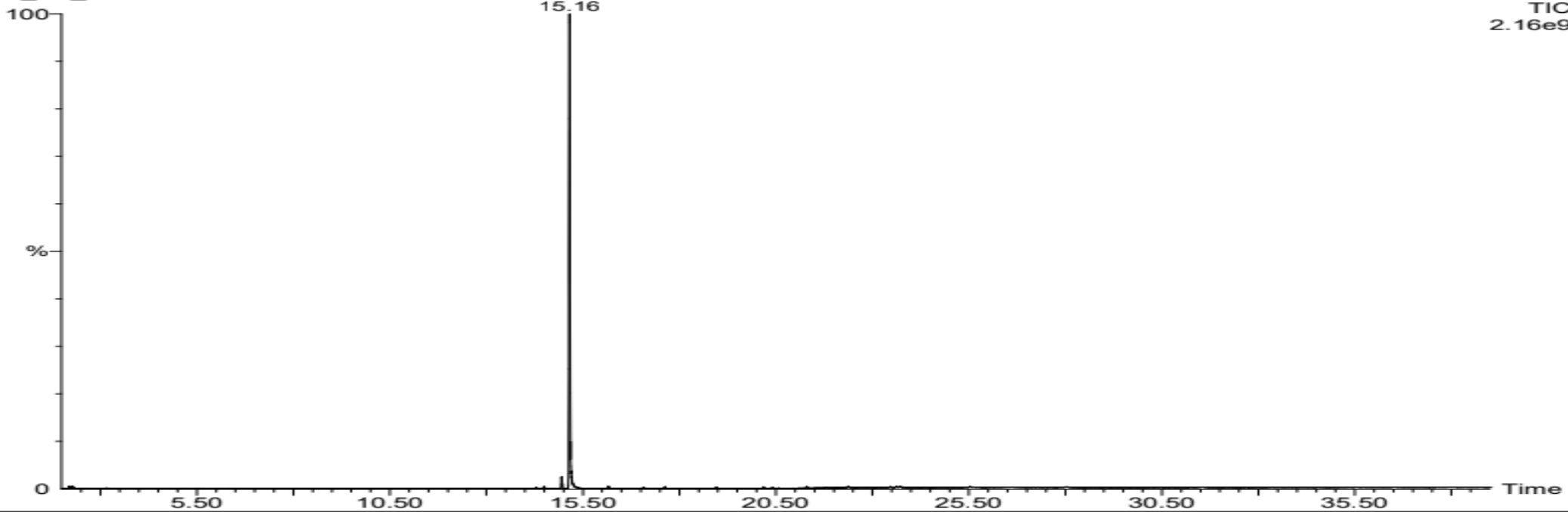
¹H NMR (500 MHz, CDCl₃) of compound **11** major diastereomer

11 major

^{13}C -NMR (126 MHz, CDCl_3)

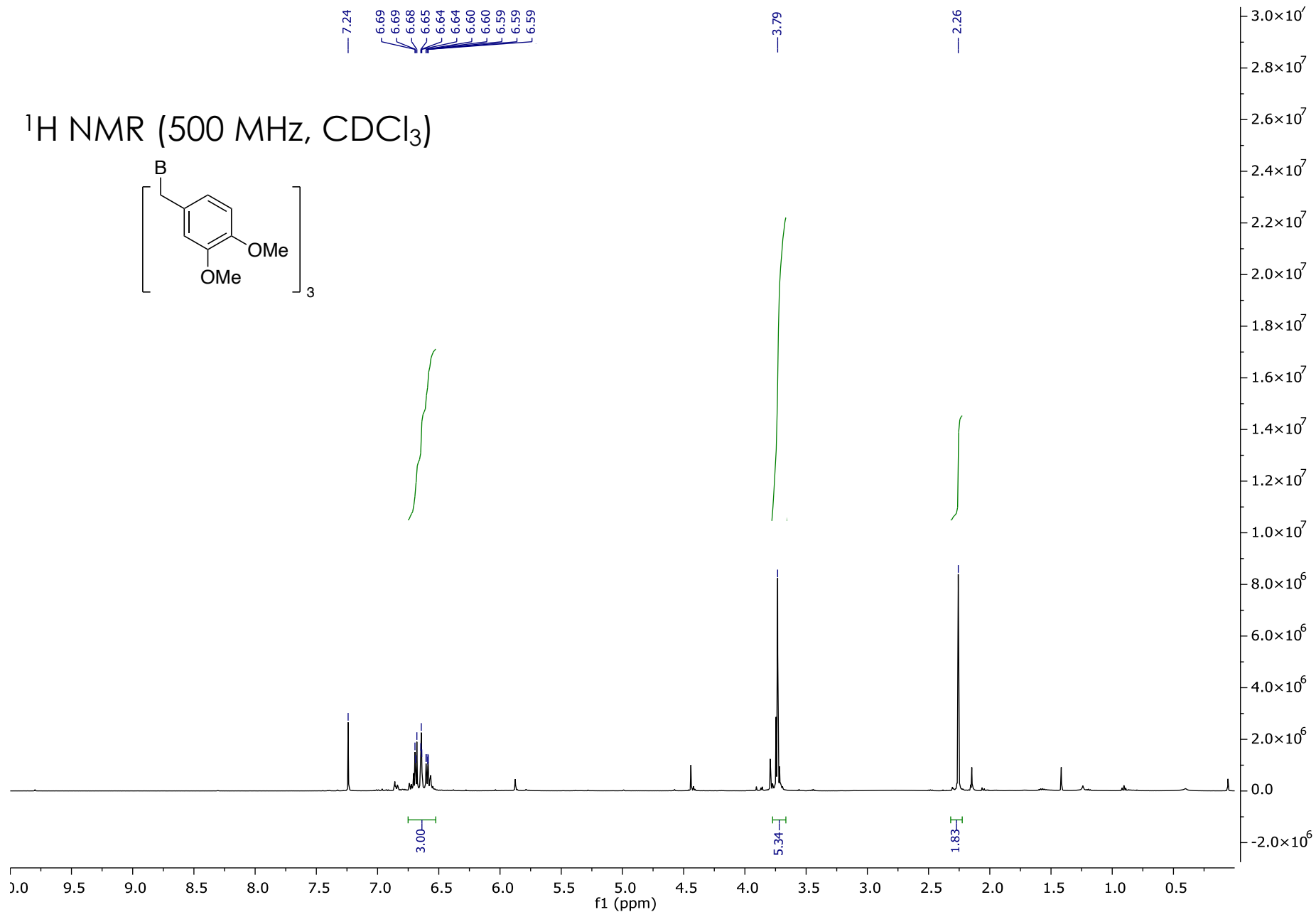
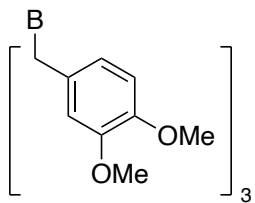


^{13}C NMR (126 MHz, CDCl_3) of compound **11** major diastereomer



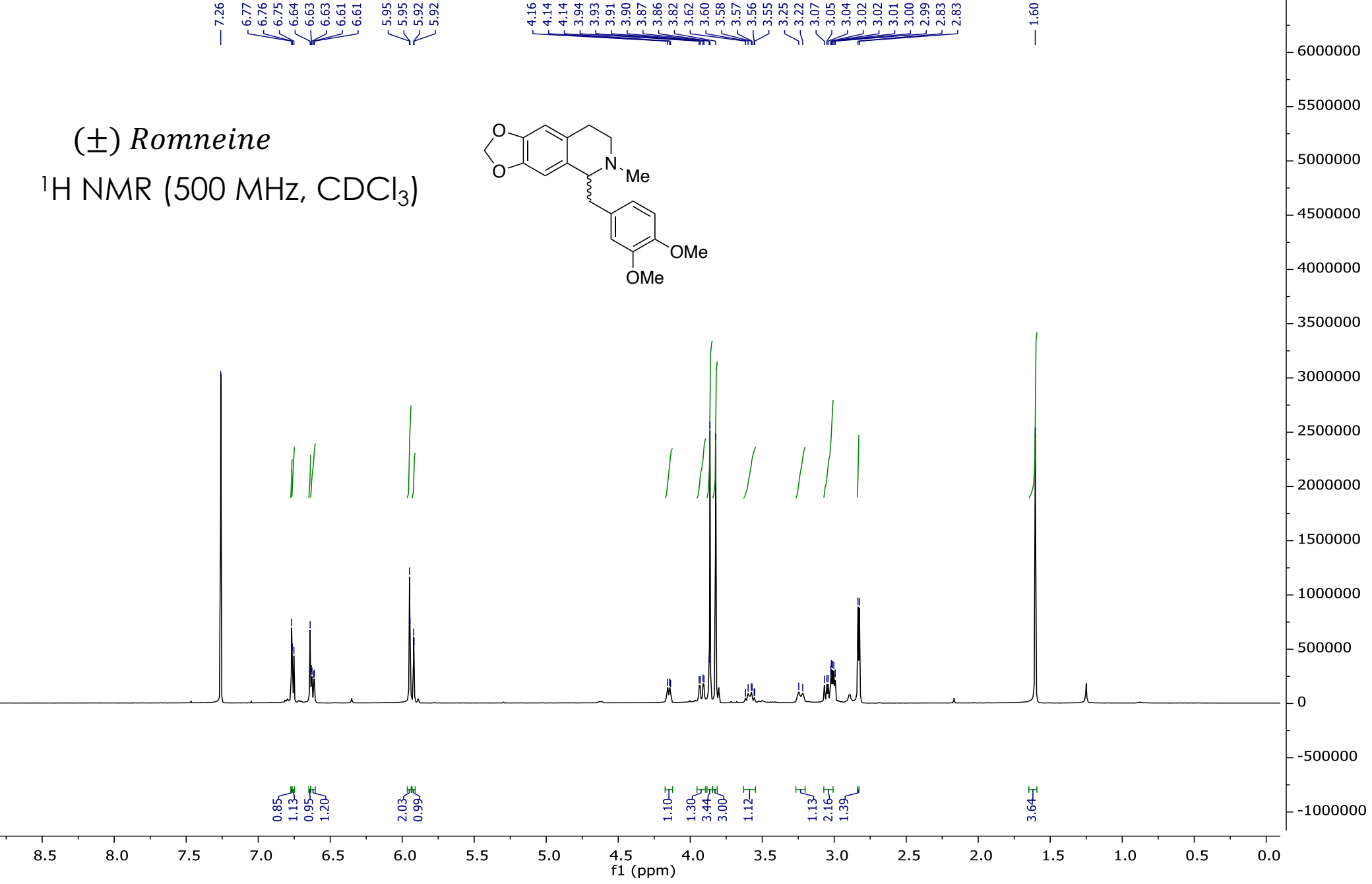
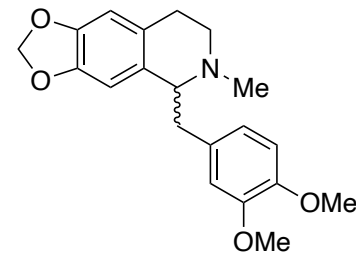
GC-MS of compound **11** major diastereomer

^1H NMR (500 MHz, CDCl_3)



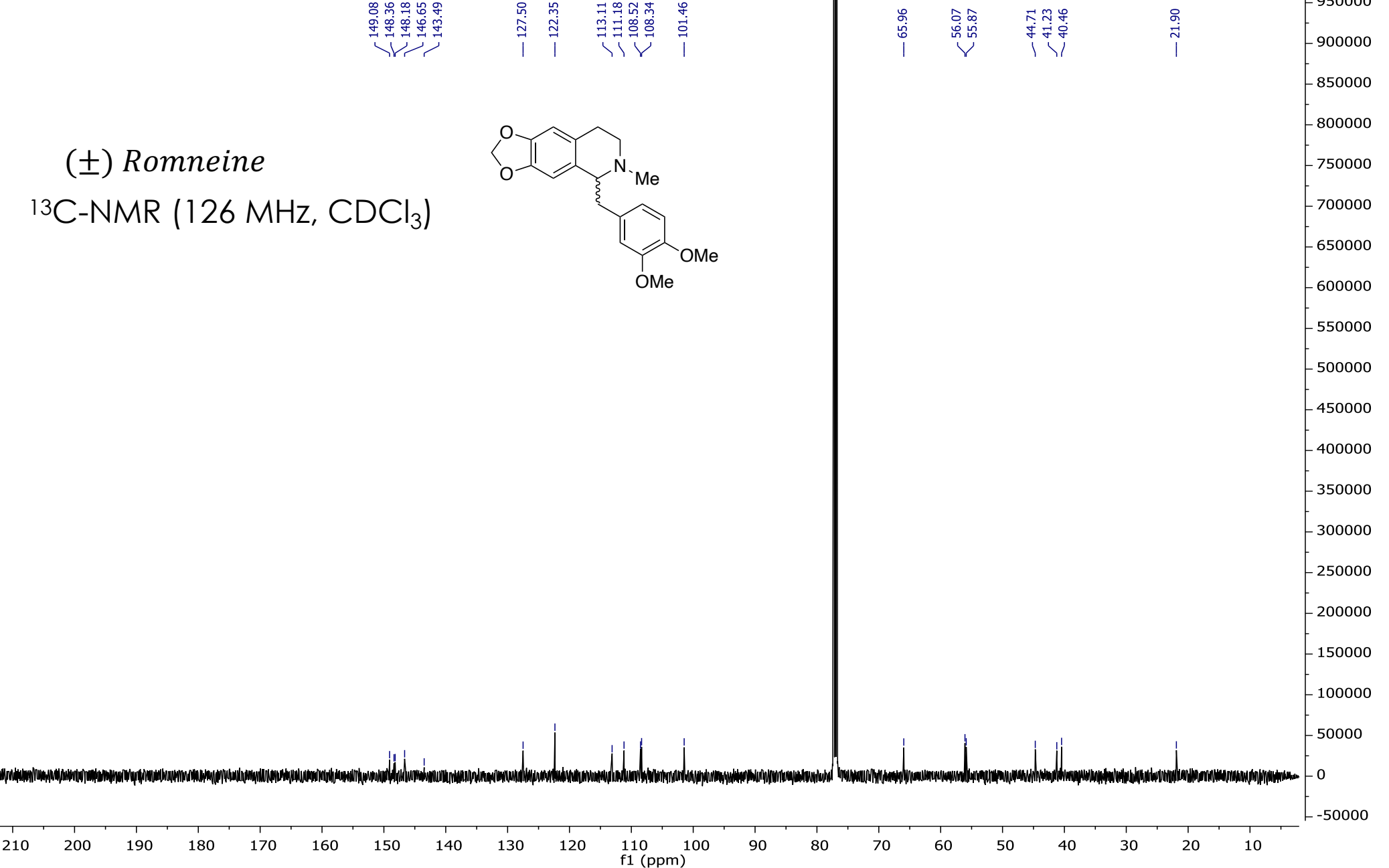
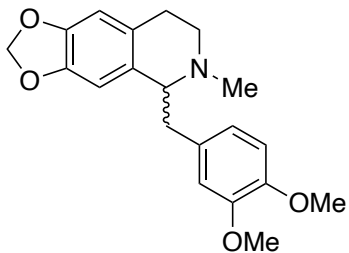
^1H NMR (500 MHz, CDCl_3) of borane **20**

(±) Romneine
¹H NMR (500 MHz, CDCl₃)



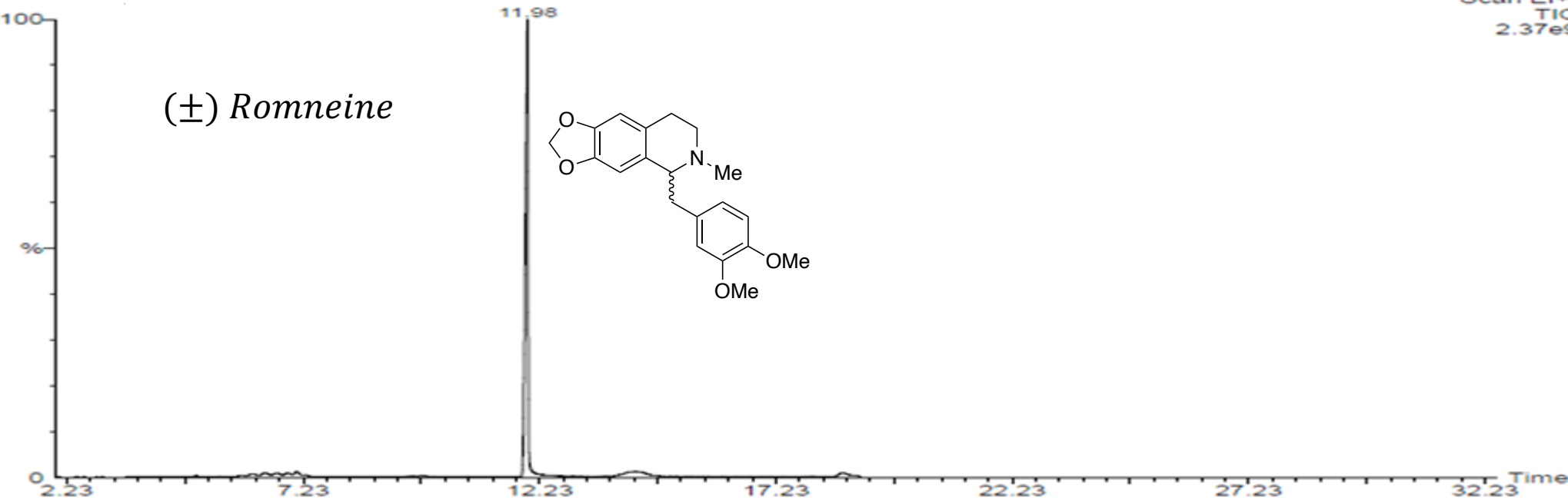
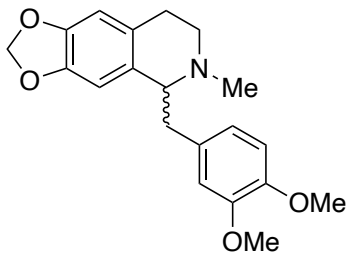
¹H NMR (500 MHz, CDCl₃) of (±)-Romneine

(±) *Romneine*
¹³C-NMR (126 MHz, CDCl₃)



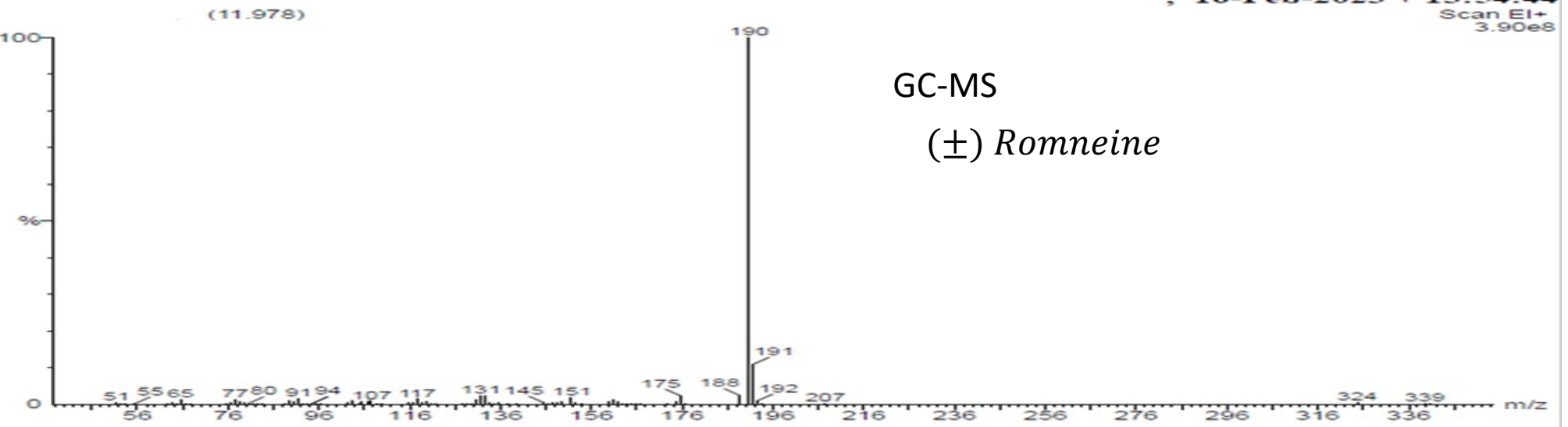
¹³C NMR (126 MHz, CDCl₃) of (±)-Romneine

(±) Romneine



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GC-MS
(±) Romneine



GC-MS of (±)-Romneine