

Supporting Information

Hypervalent iodine initiated intramolecular alkene dimerisation: a stereodivergent entry to cyclobutanes

Yuxiang Zhu,^{a,†} Ignacio Colomer^{a,†} and Timothy J. Donohoe^a

*Department of Chemistry, University of Oxford, Chemistry Research Laboratory, Mansfield Road,
Oxford, OX1 3TA (UK)*

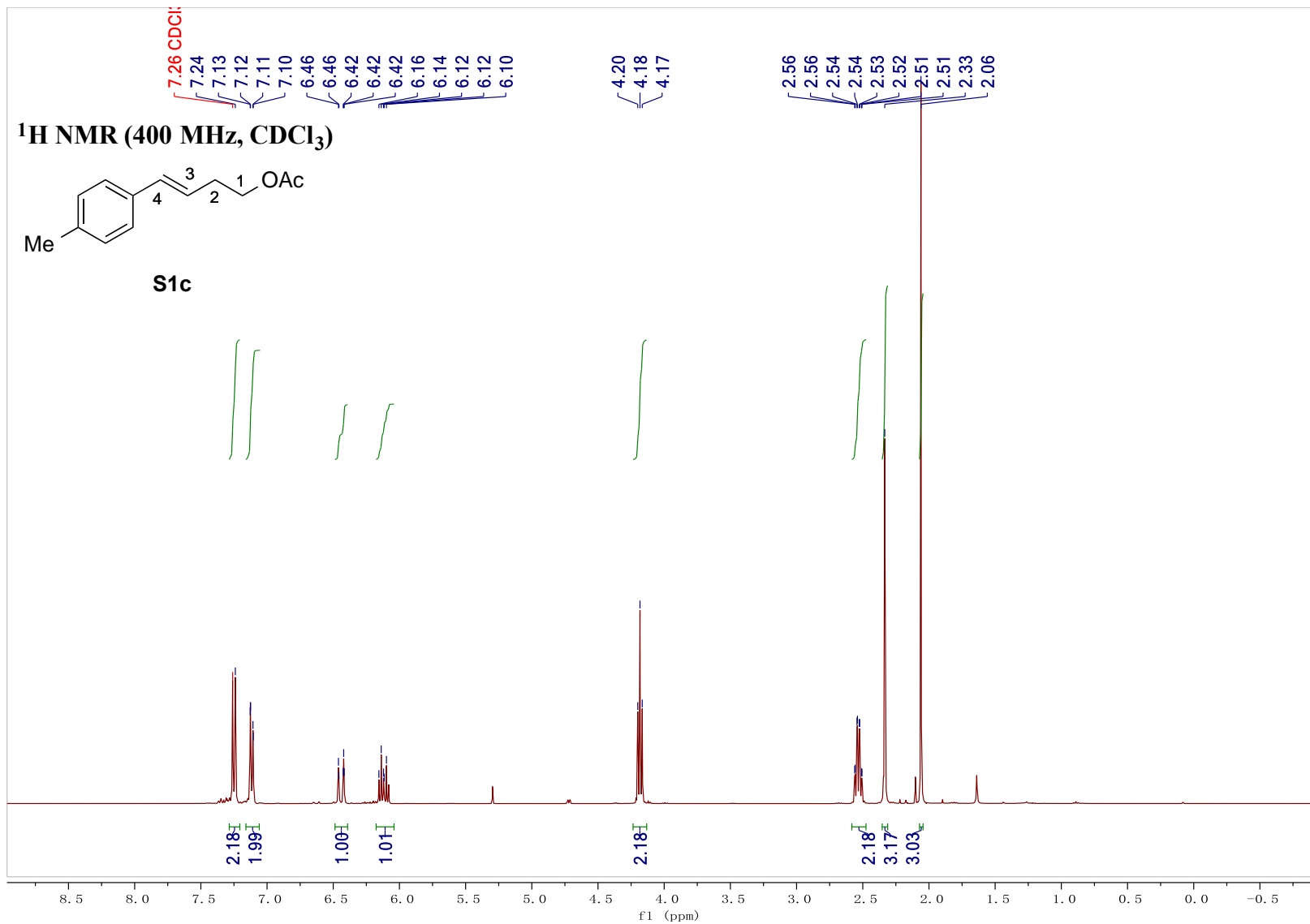
E-mail: timothy.donohoe@chem.ox.ac.uk

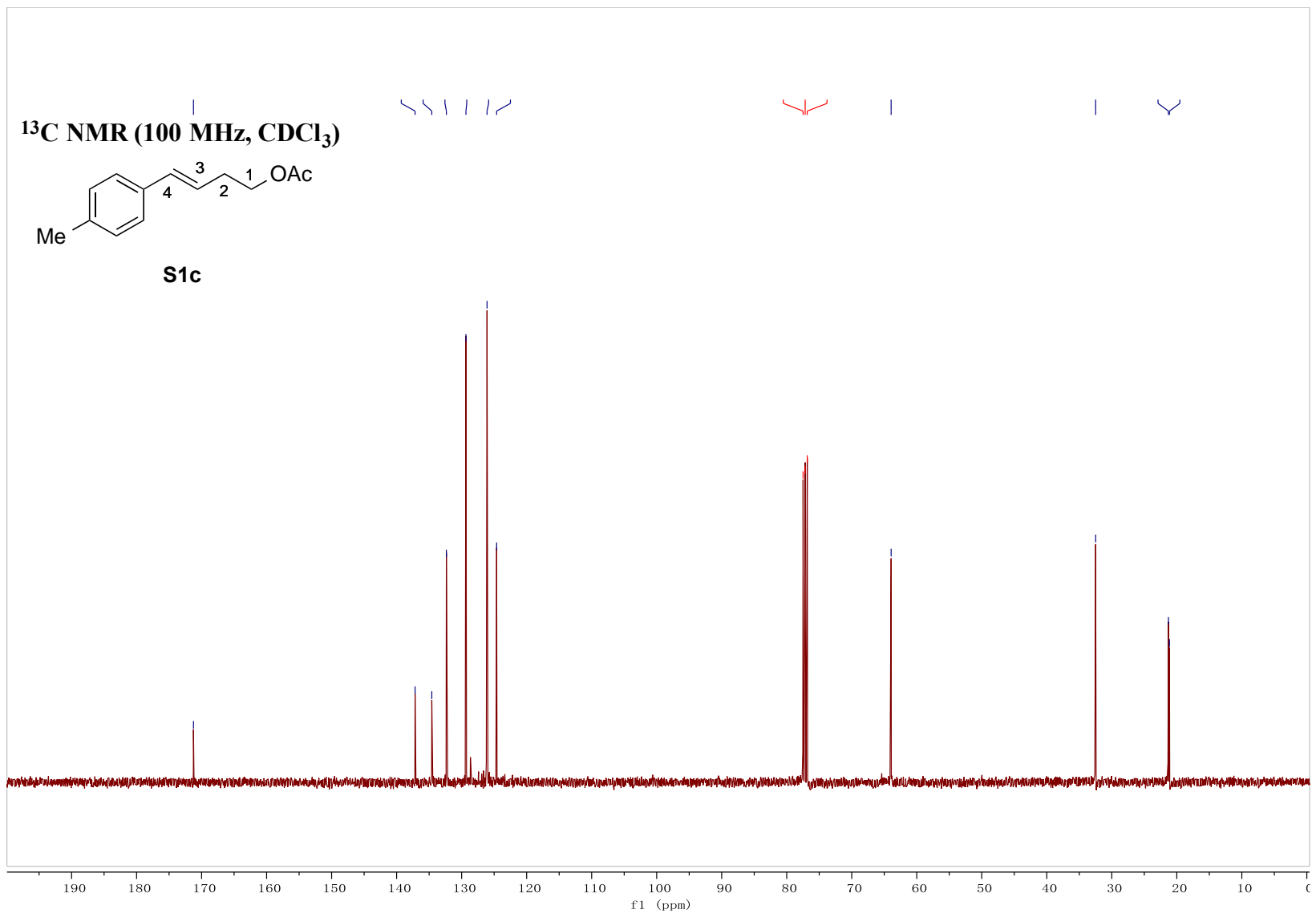
† These authors contributed equally.

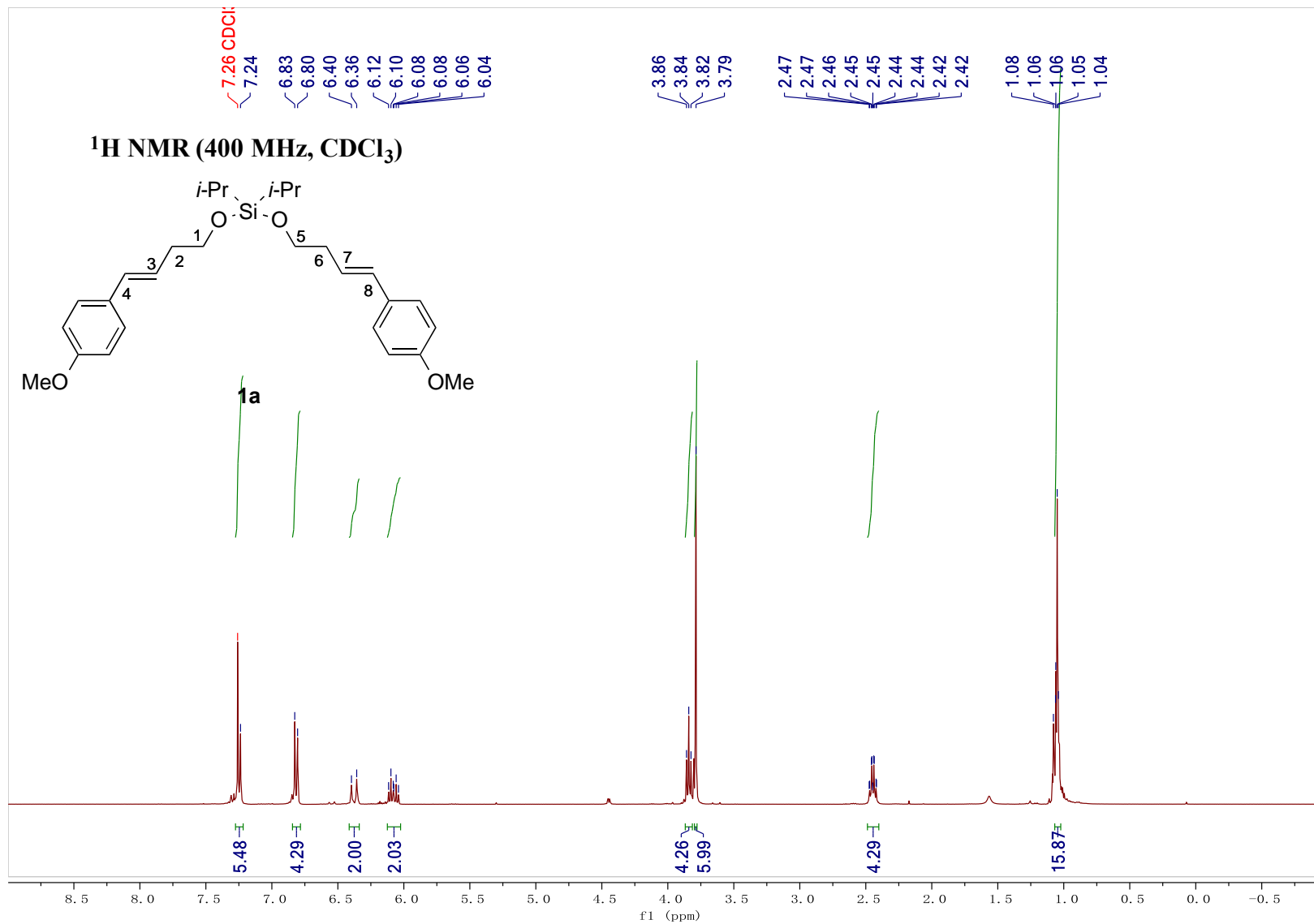
Table of Contents

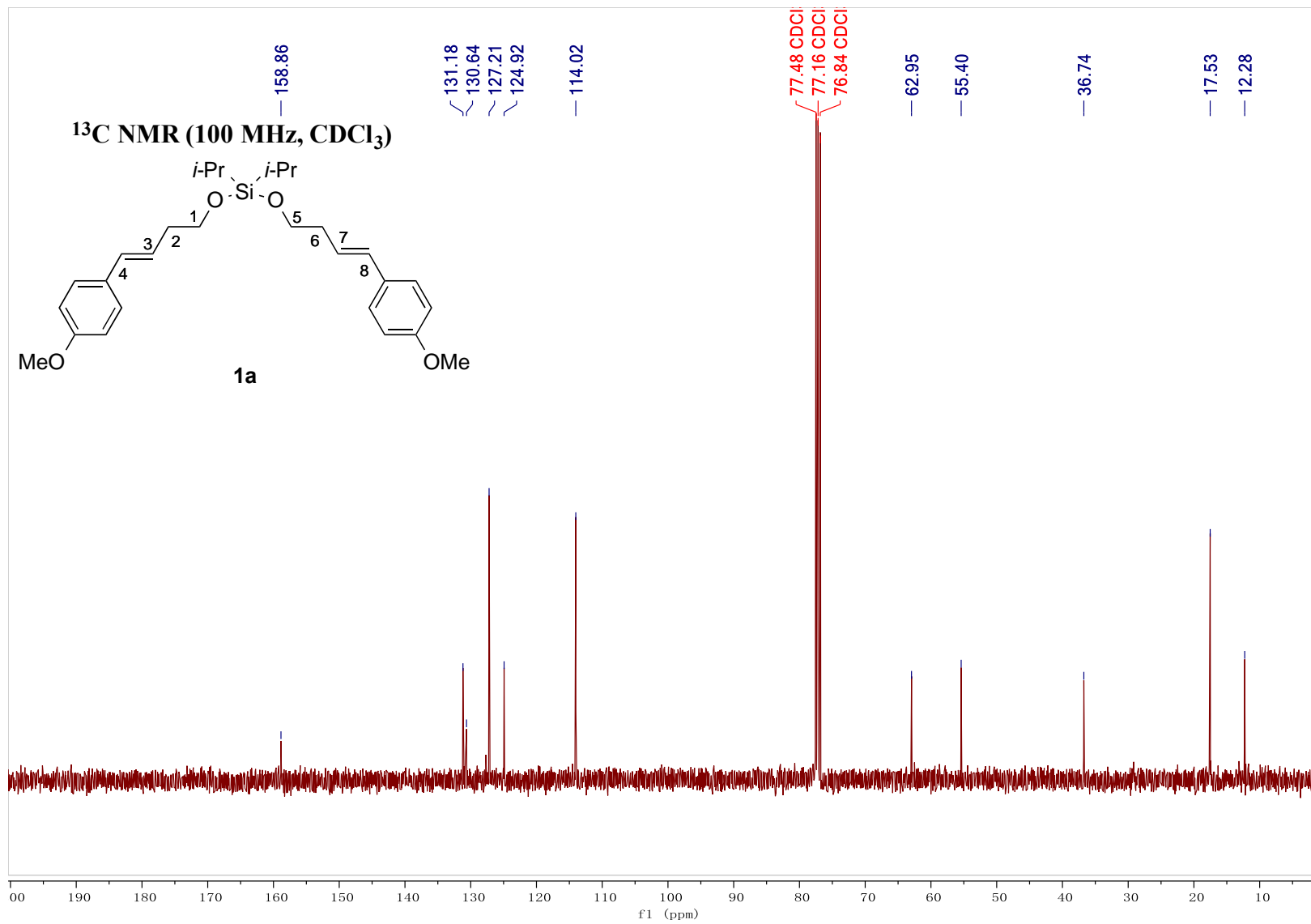
Compound (<i>E</i>)-S1c: ¹ H NMR and ¹³ C NMR	S4
Compound (<i>E</i>)-1a: ¹ H NMR and ¹³ C NMR	S6
Compound (<i>E</i>)-1b: ¹ H NMR and ¹³ C NMR	S8
Compound (<i>E</i>)-1c: ¹ H NMR and ¹³ C NMR	S10
Compound (<i>E</i>)-1e: ¹ H NMR and ¹³ C NMR	S12
Compound (<i>E</i>)-1j: ¹ H NMR and ¹³ C NMR	S14
Compound (<i>E</i>)-1k: ¹ H NMR and ¹³ C NMR	S16
Compound (<i>E</i>)-1l: ¹ H NMR and ¹³ C NMR	S18
Compound (<i>E</i>)-1m: ¹ H NMR and ¹³ C NMR	S20
Compound (<i>E</i>)-1d: ¹ H NMR and ¹³ C NMR	S22
Compound (<i>E</i>)-1f: ¹ H NMR and ¹³ C NMR	S24
Compound (<i>E</i>)-1g: ¹ H NMR and ¹³ C NMR	S26
Compound (<i>E</i>)-1h: ¹ H NMR and ¹³ C NMR	S28
Compound (<i>E</i>)-1i: ¹ H NMR and ¹³ C NMR	S30
Compound (<i>E</i>)-1n: ¹ H NMR and ¹³ C NMR	S32
Compound 4c: ¹ H NMR and ¹³ C NMR	S34
Compound 4d: ¹ H NMR and ¹³ C NMR	S36
Compound 4e: ¹ H NMR and ¹³ C NMR	S38
Compound 4g: ¹ H NMR and ¹³ C NMR	S40
Compound 2a: ¹ H NMR and ¹³ C NMR	S42
Compound 2b: ¹ H NMR and ¹³ C NMR	S44
Compound 2c: ¹ H NMR and ¹³ C NMR	S46
Compound 2d: ¹ H NMR and ¹³ C NMR	S48
Compounds 2e and 3e: ¹ H NMR and ¹³ C NMR	S50
Compound 2f: ¹ H NMR and ¹³ C NMR	S52
Compounds 2g:3g: ¹ H NMR, ¹³ C NMR	S54
Compounds 3h:3h: ¹ H NMR, ¹³ C NMR, COSY, HSQC and NOESY-2D	S56
Compounds 2i:3i: ¹ H NMR and ¹³ C NMR	S61
Compound 2j: ¹ H NMR and ¹³ C NMR	S63
Compound 3j: ¹ H NMR and ¹³ C NMR	S65
Compound 2k: ¹ H NMR and ¹³ C NMR	S67
Compound 3k: ¹ H NMR and ¹³ C NMR, COSY, HSQC and NOESY-2D	S69

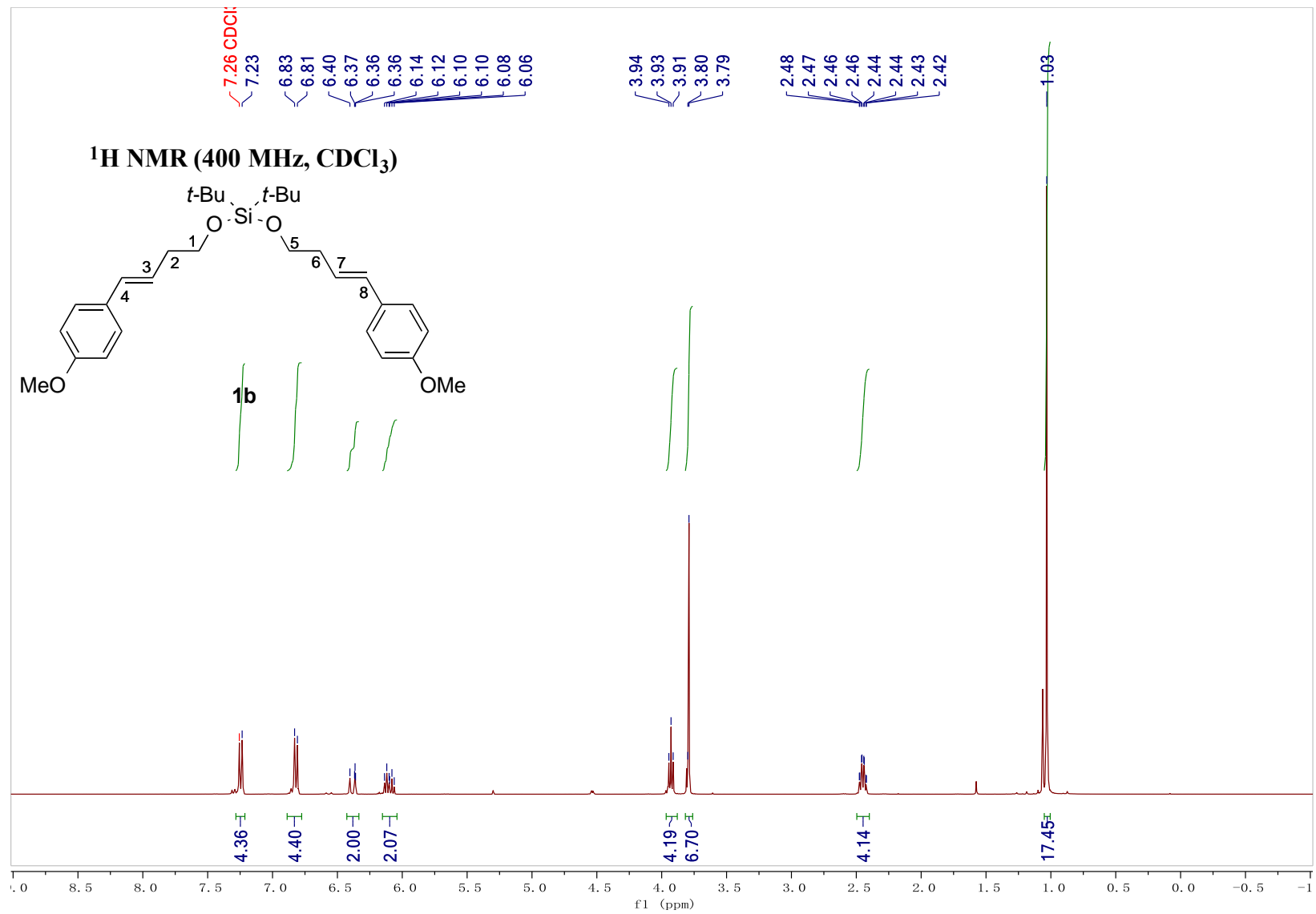
Compound 2l:3l : ^1H NMR and ^{13}C NMR	S74
Compound 2m : ^1H NMR and ^{13}C NMR	S76
Compound 3m : ^1H NMR and ^{13}C NMR	S78
Compounds 2n:3n : ^1H NMR and ^{13}C NMR	S80
Compound 5c : ^1H NMR and ^{13}C NMR	S82
Compound 5d : ^1H NMR and ^{13}C NMR	S84
Compound 5e : ^1H NMR and ^{13}C NMR	S86
Compound 5g : ^1H NMR and ^{13}C NMR, COSY, HSQC and NOESY-2D	S88
Compound 6a : ^1H NMR and ^{13}C NMR	S93
Compound 6b : ^1H NMR and ^{13}C NMR	S95
Compound 7a : ^1H NMR and ^{13}C NMR	S97
Compound 8a : ^1H NMR and ^{13}C NMR, COSY, HSQC and NOESY-2D	S99
Compound 8b : ^1H NMR and ^{13}C NMR	S104
Compound 8c : ^1H NMR and ^{13}C NMR, COSY, HSQC and NOESY-2D	S106
Compound 8d : ^1H NMR and ^{13}C NMR	S111

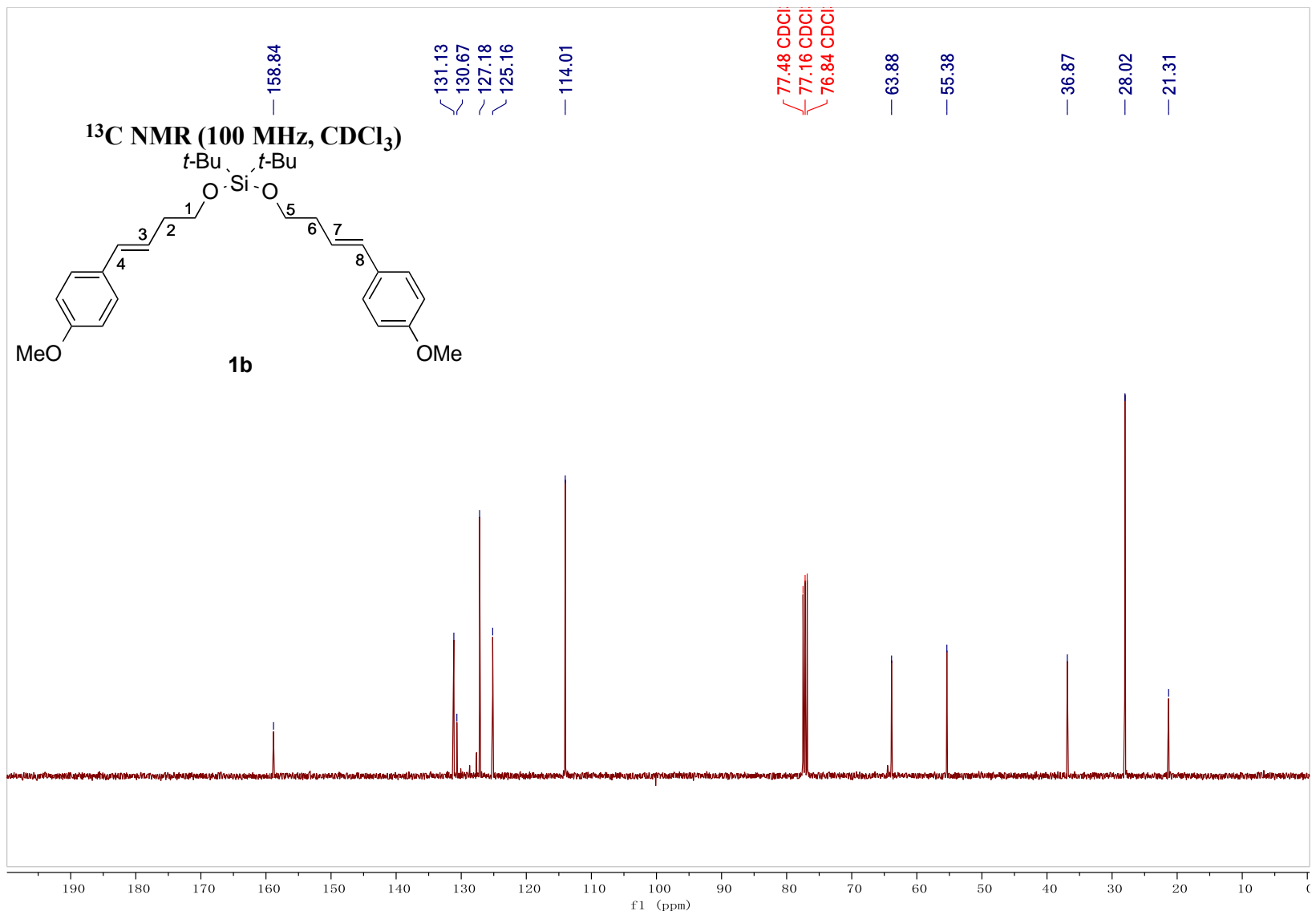


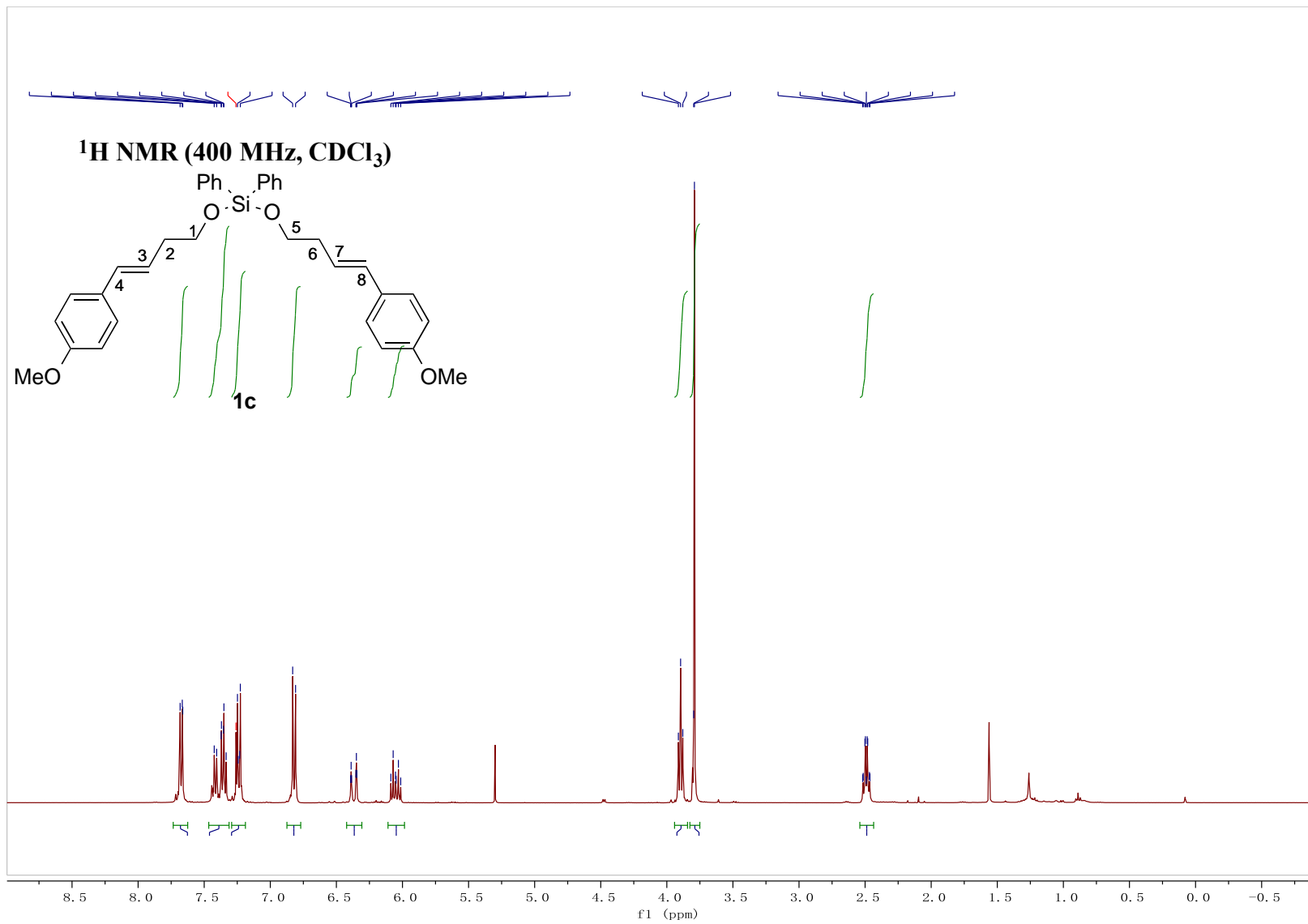


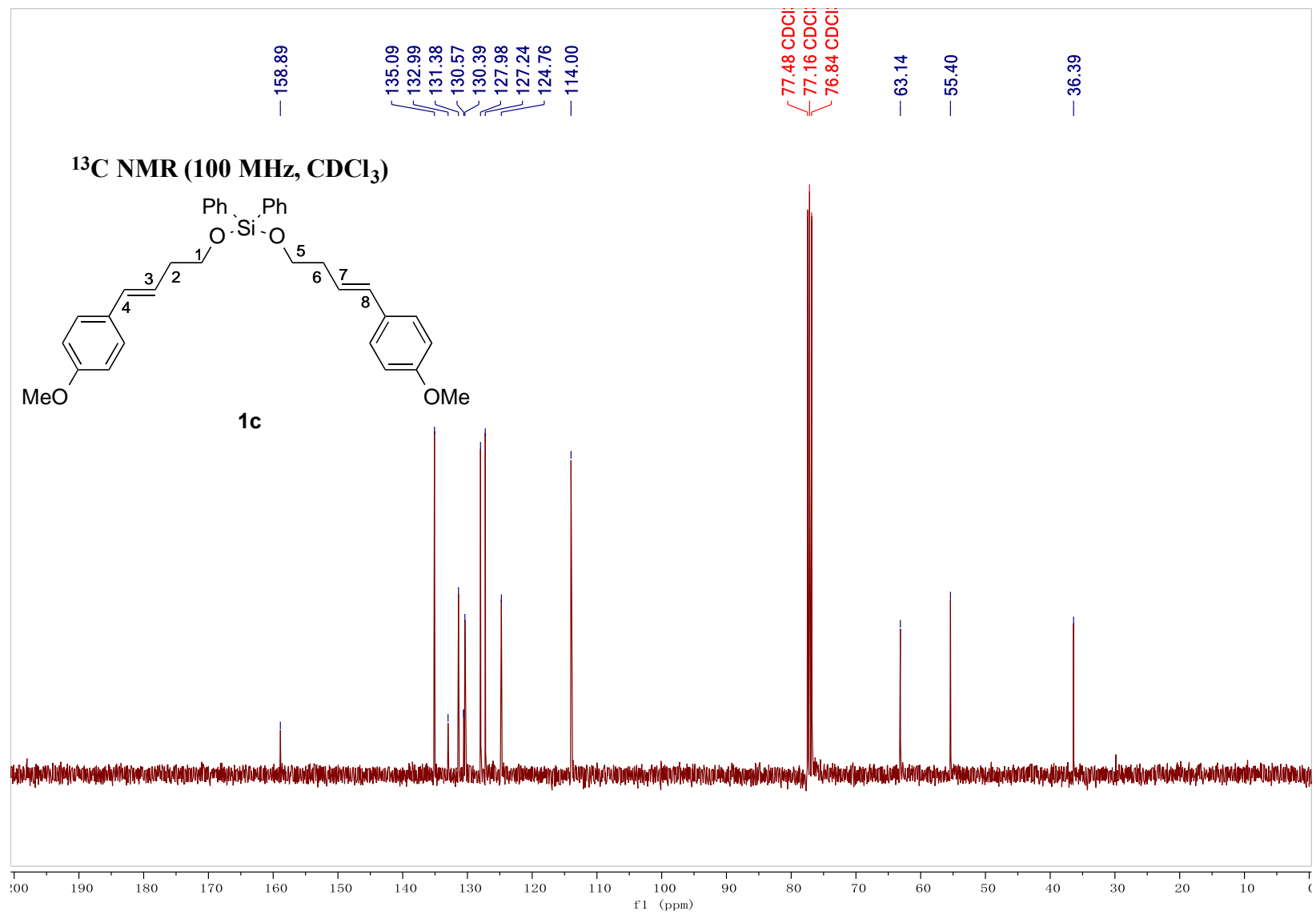


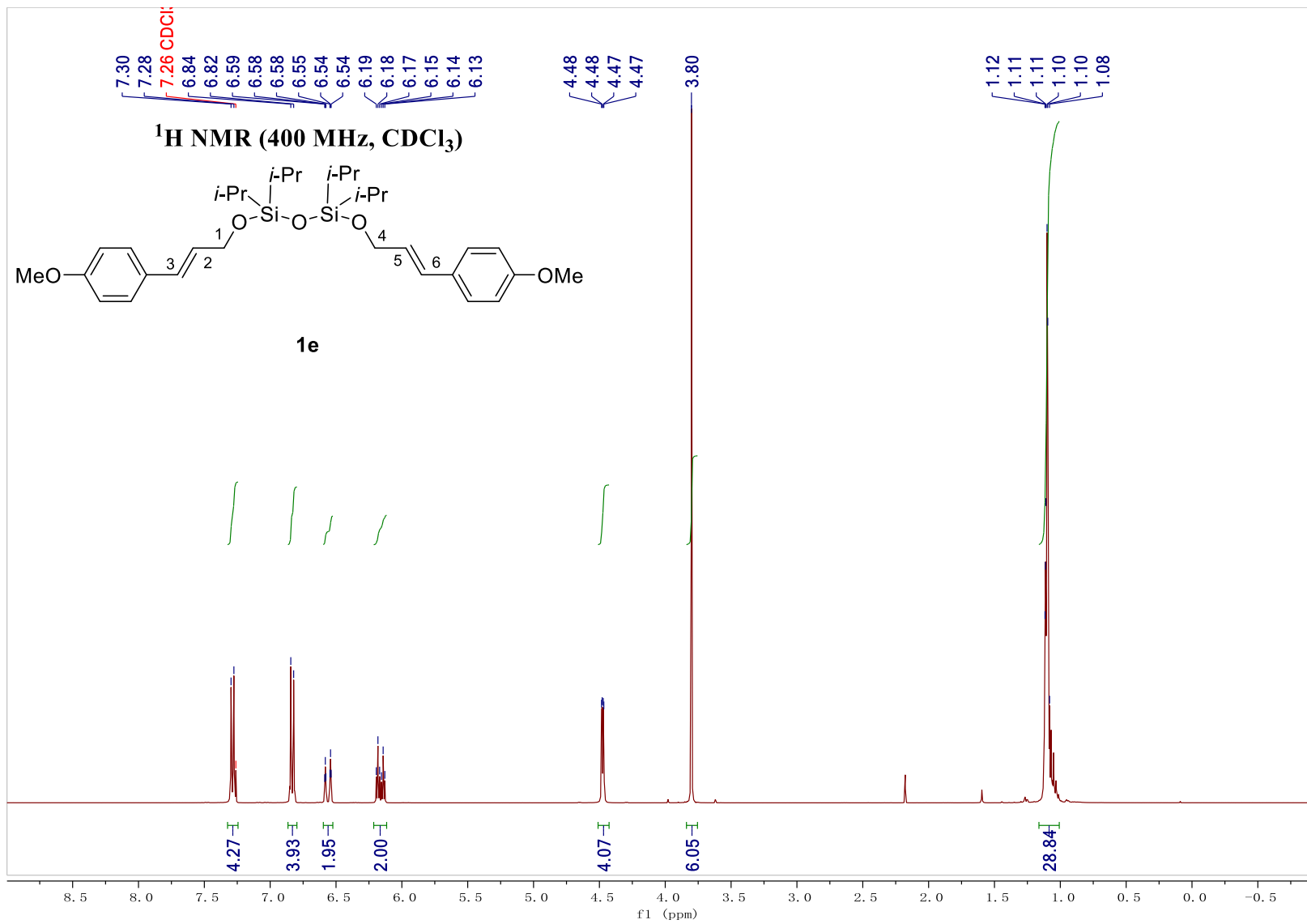


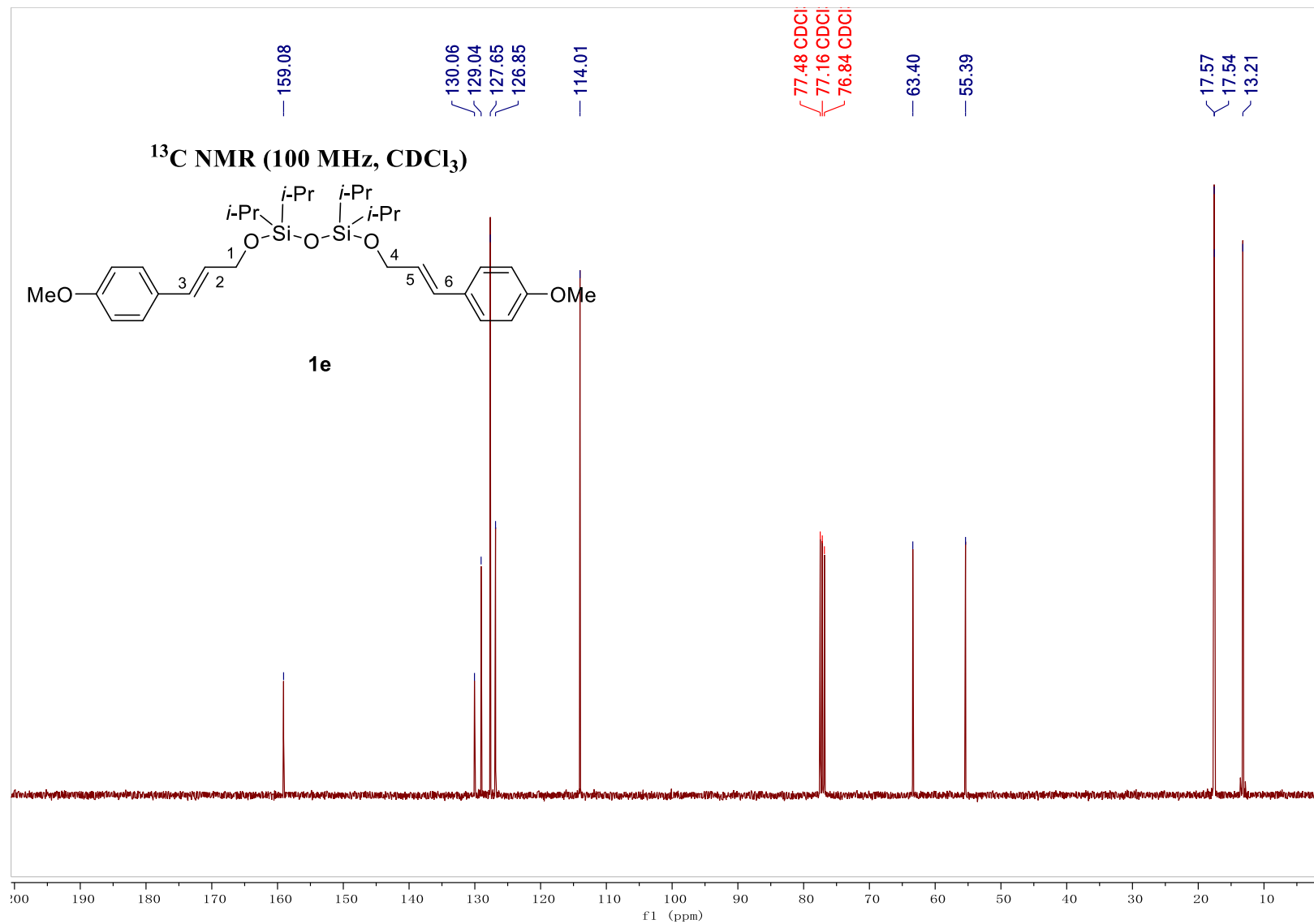


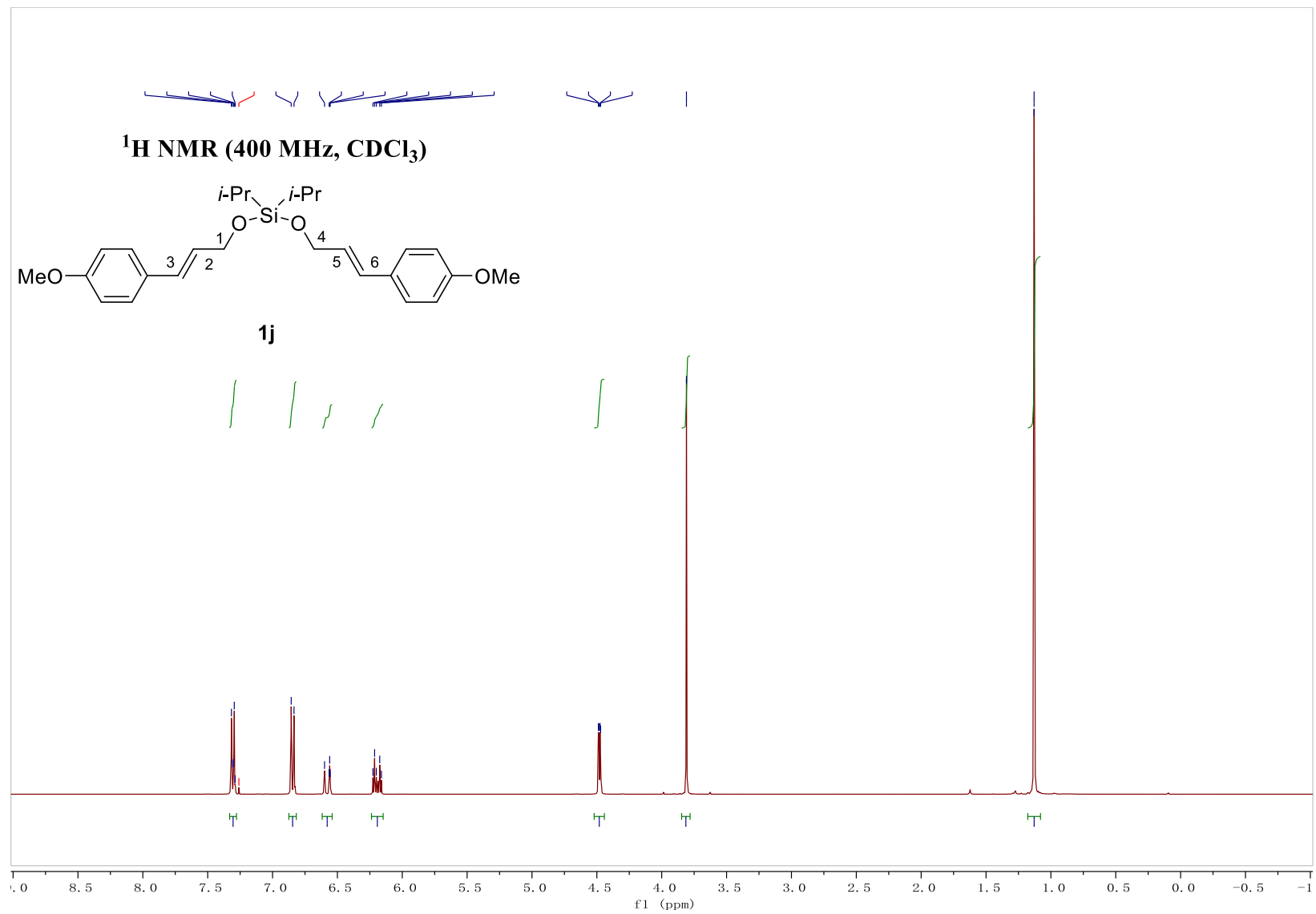


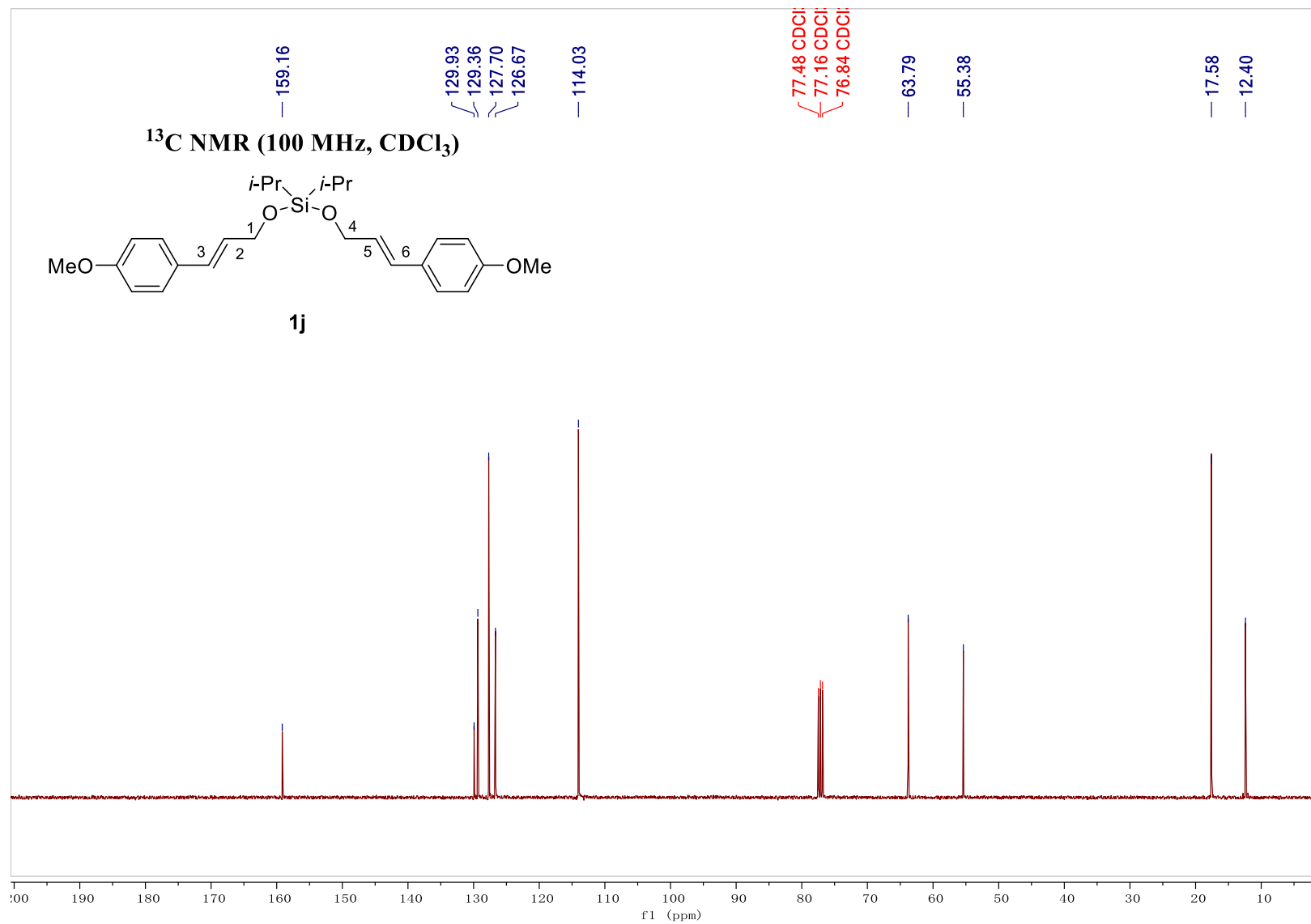


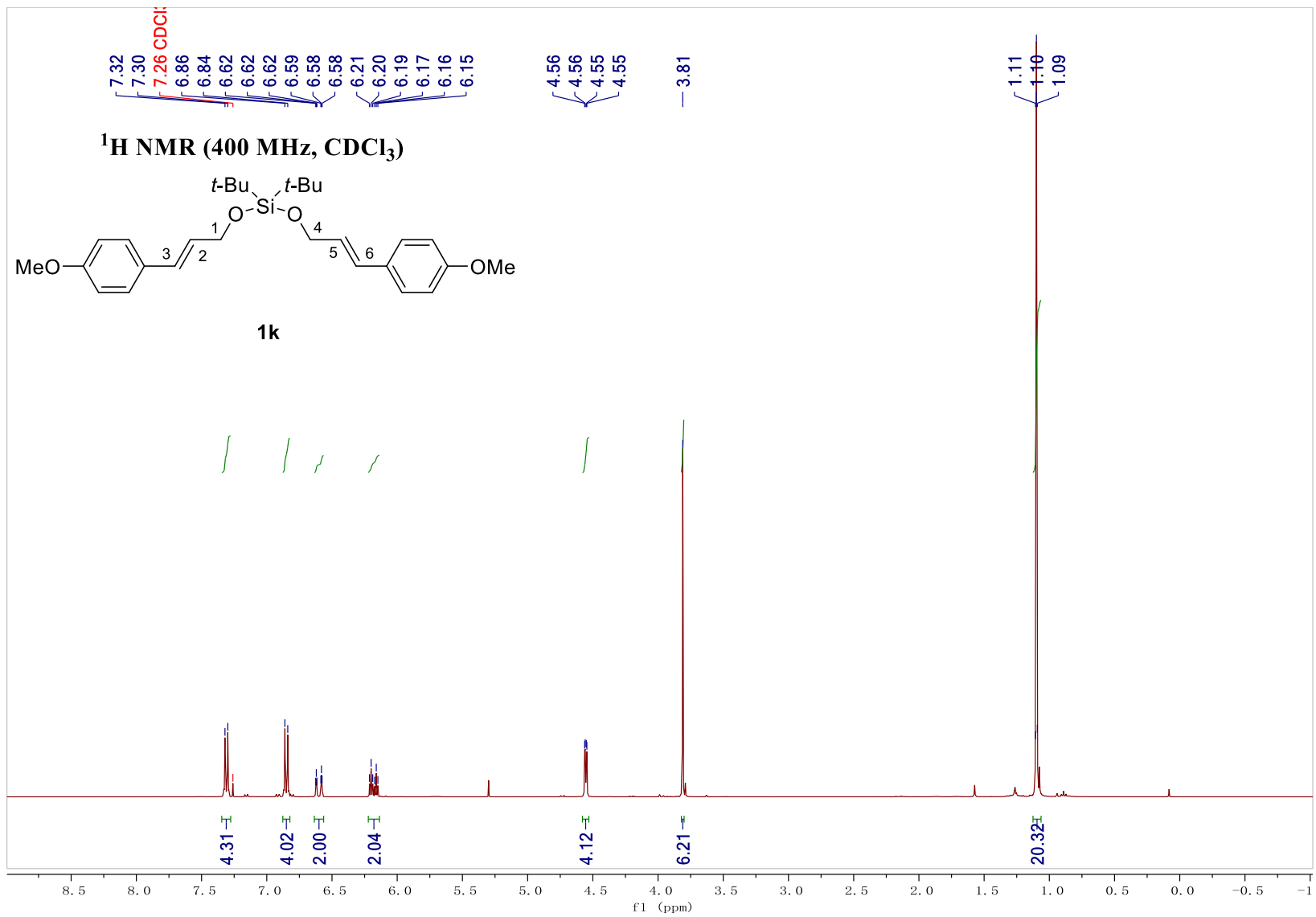


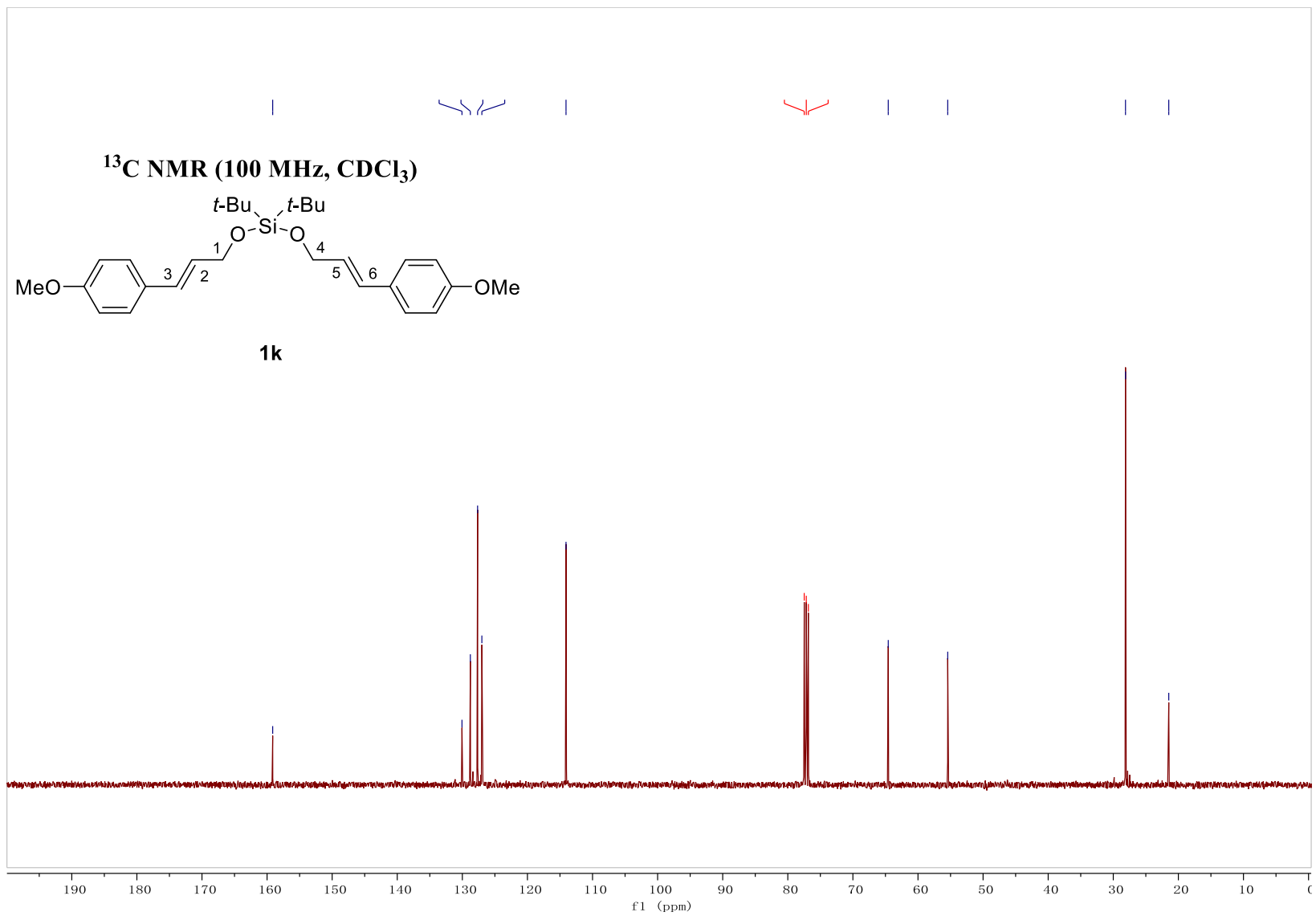


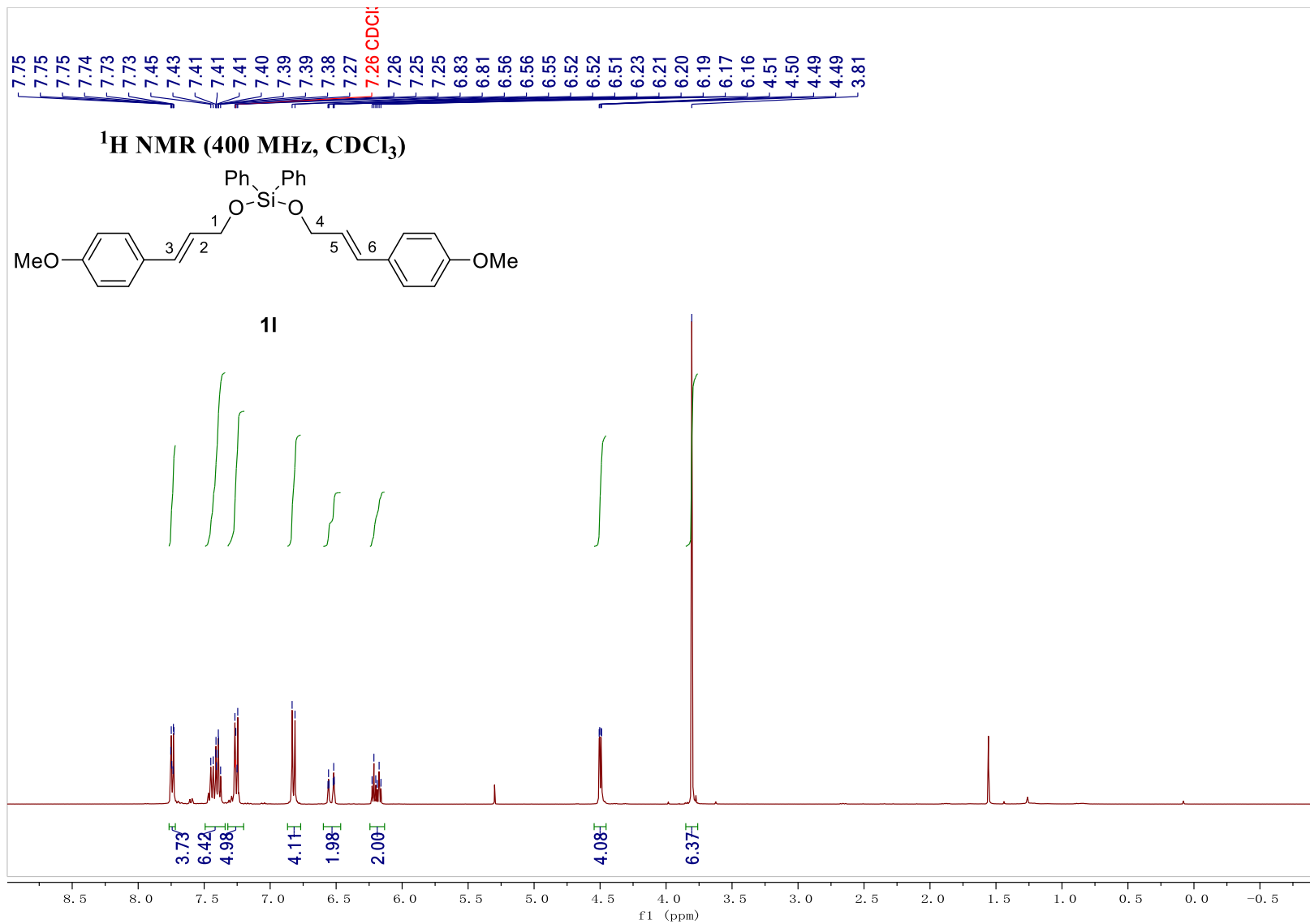


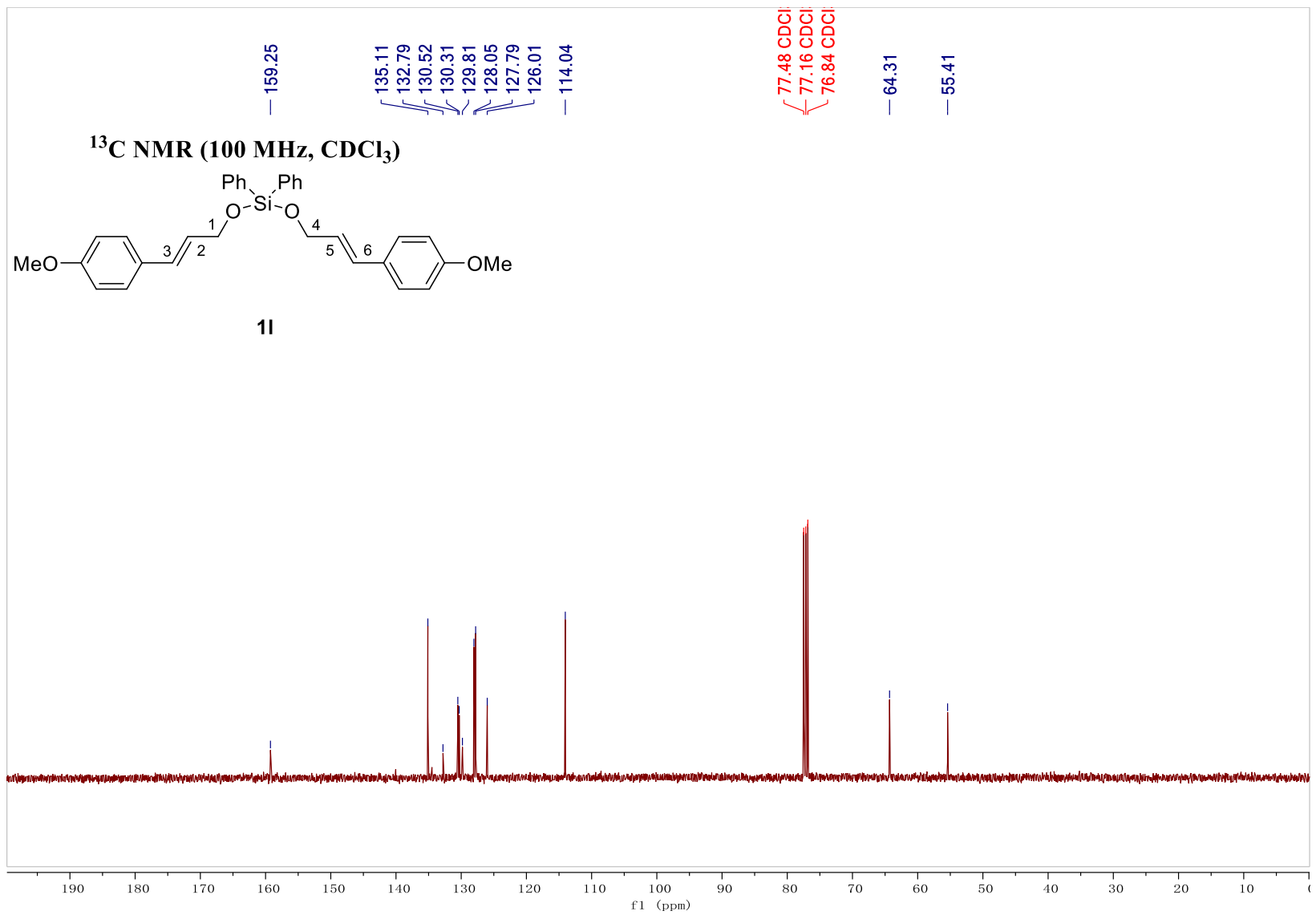


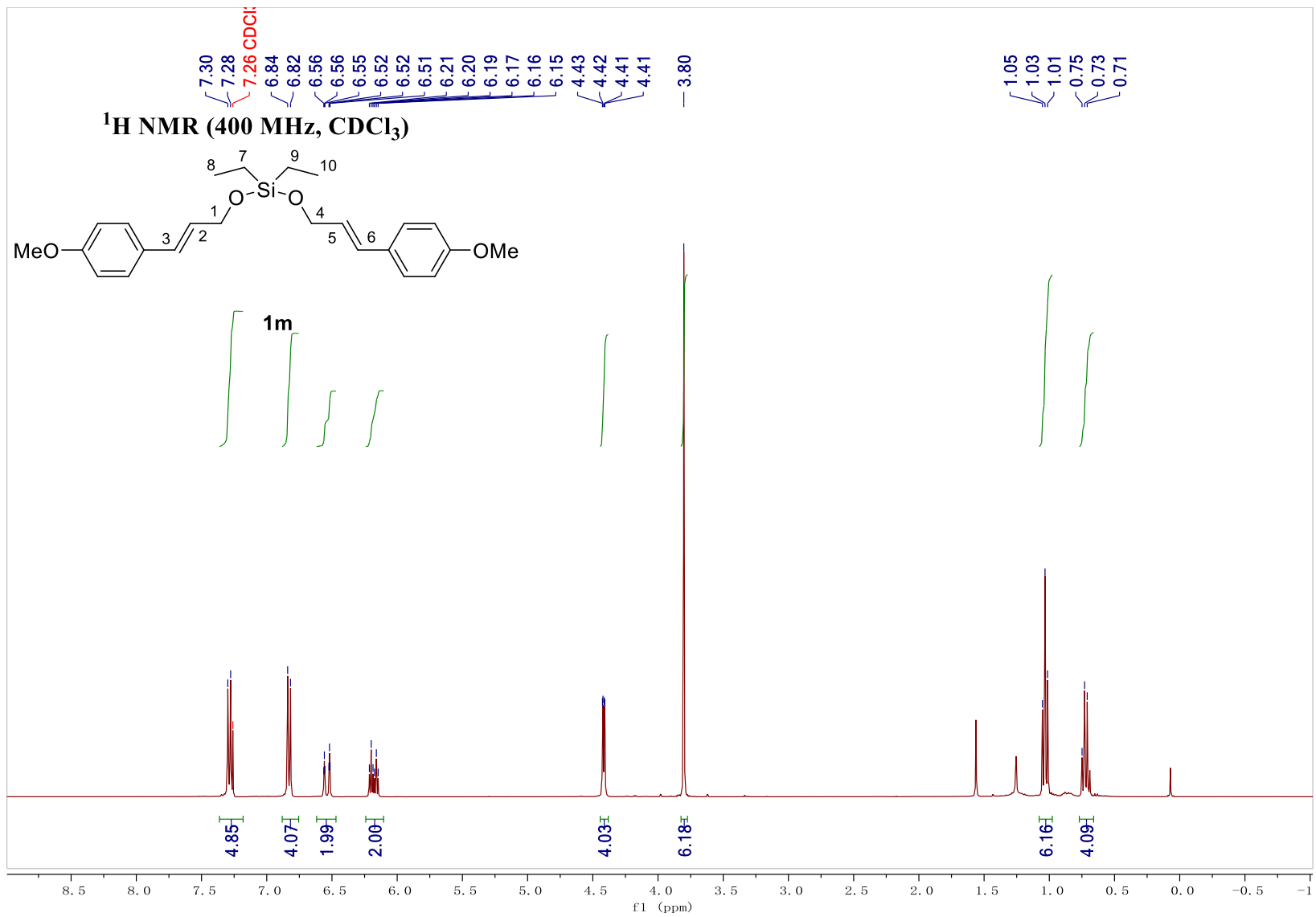


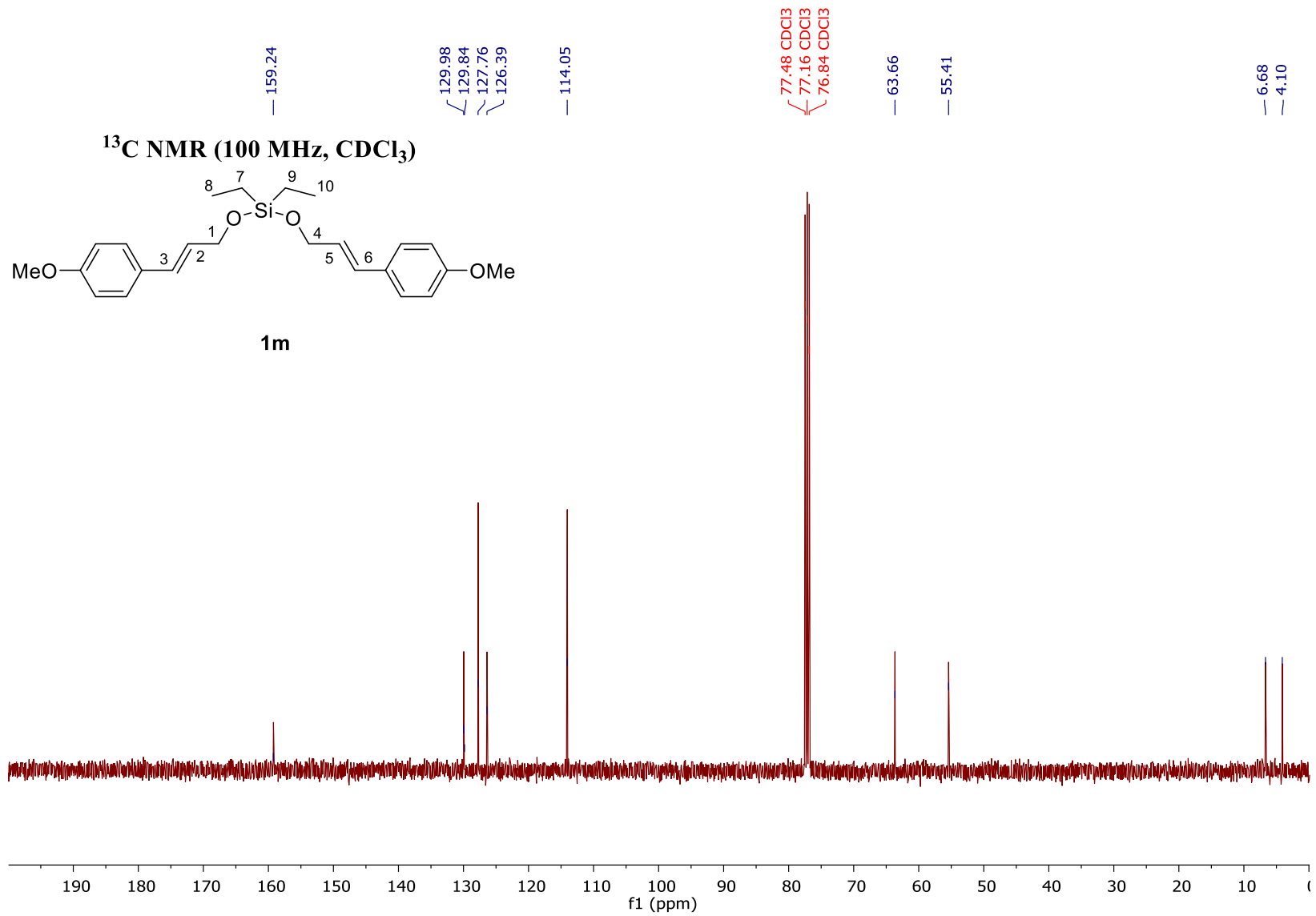


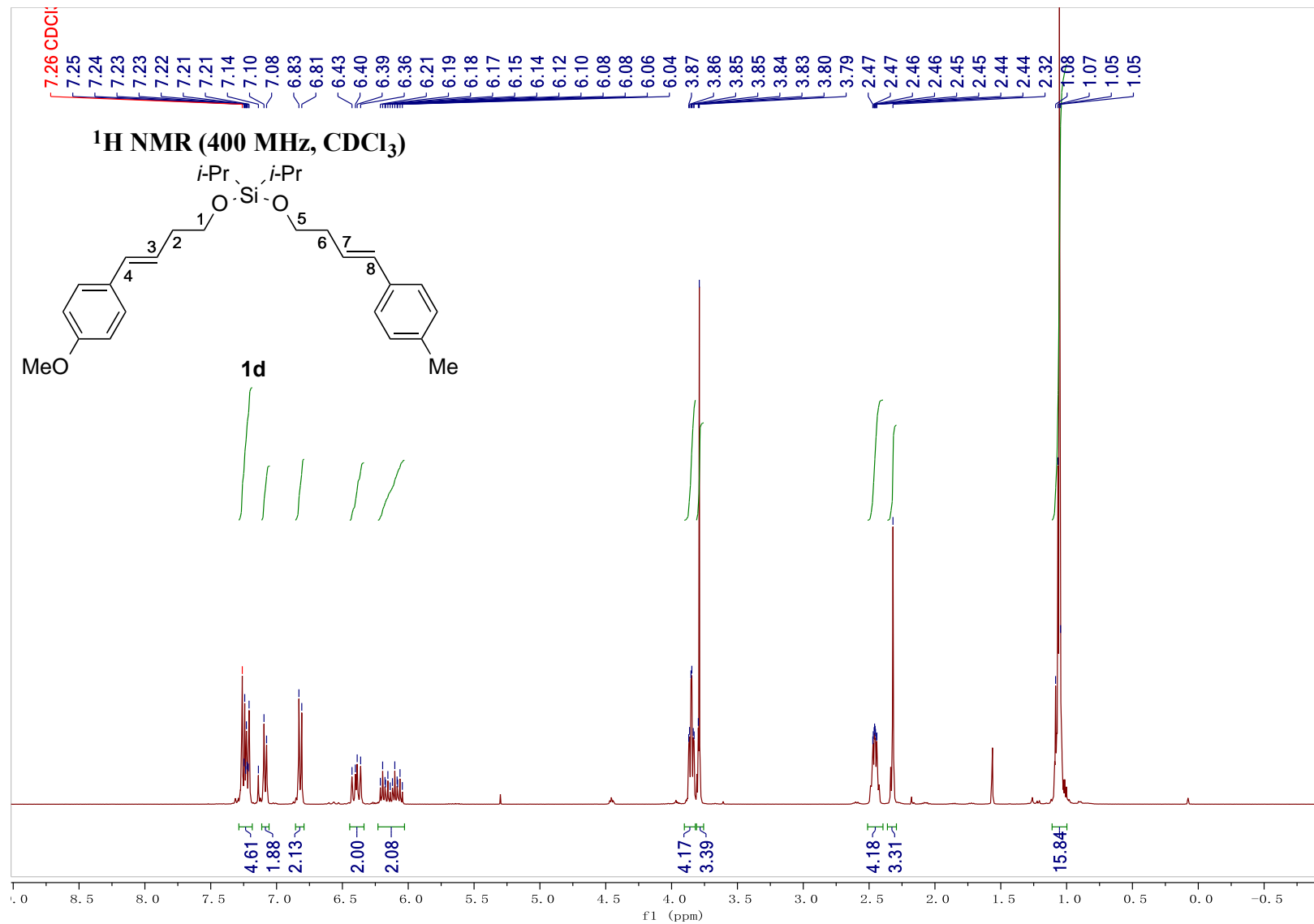


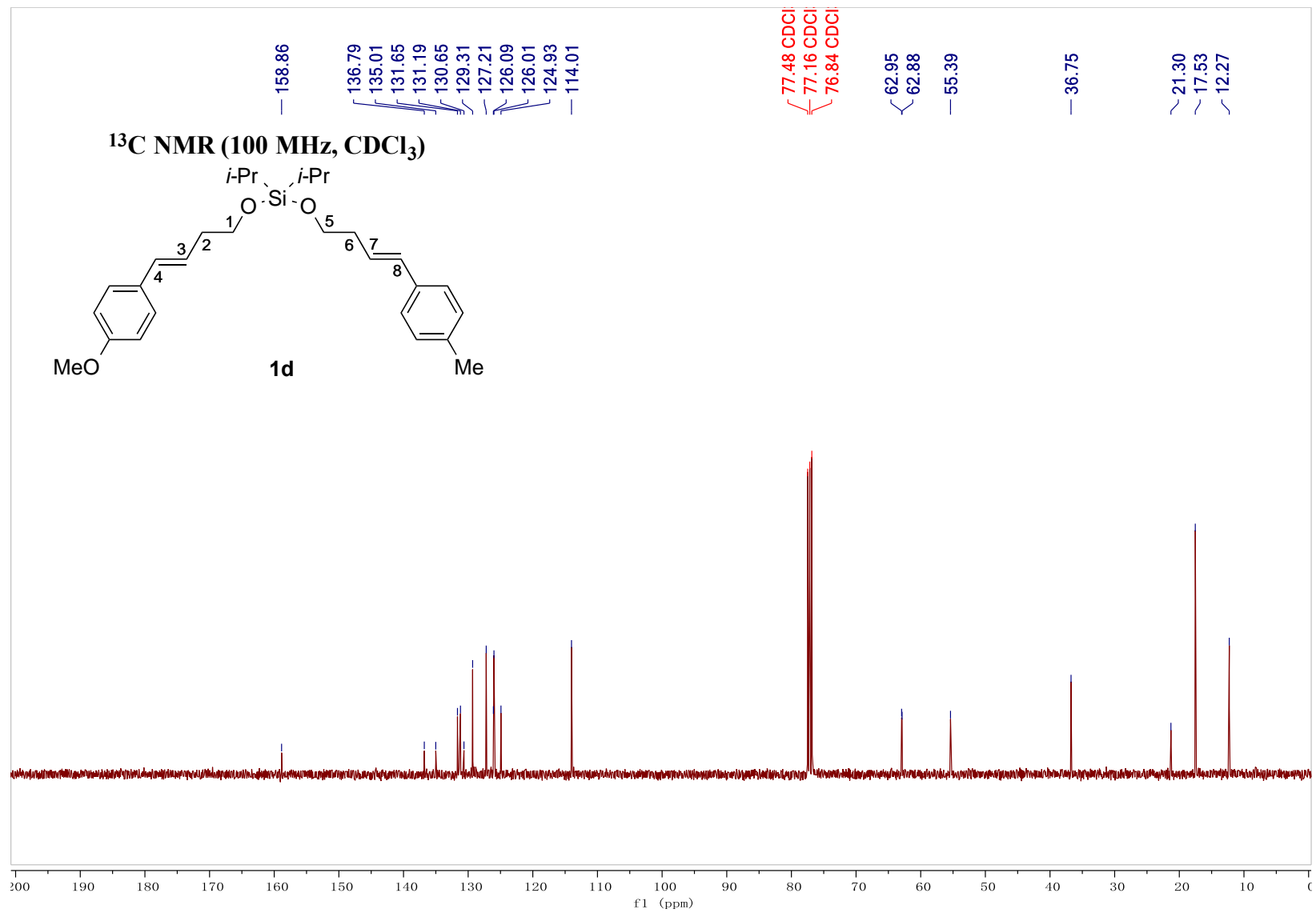


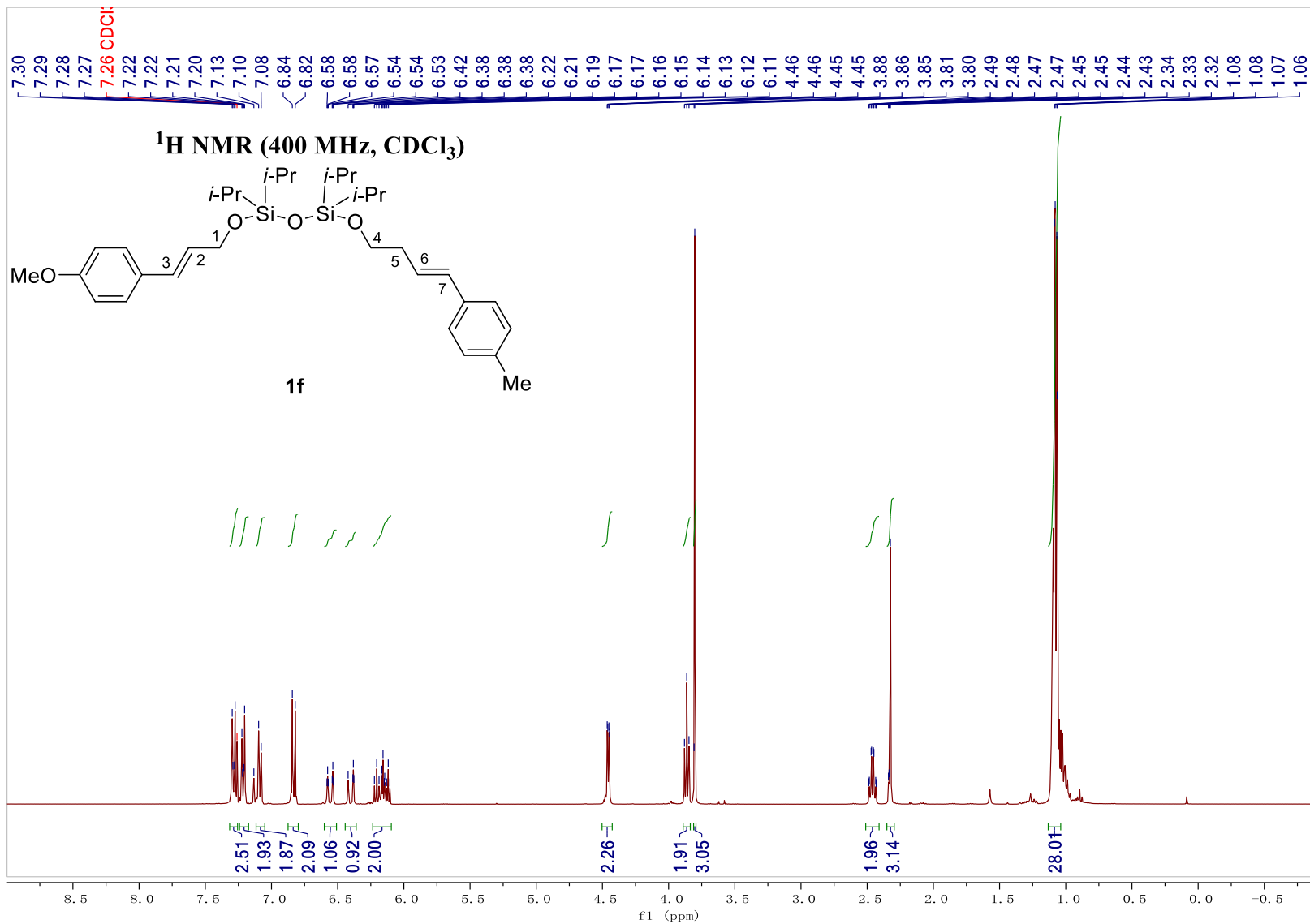


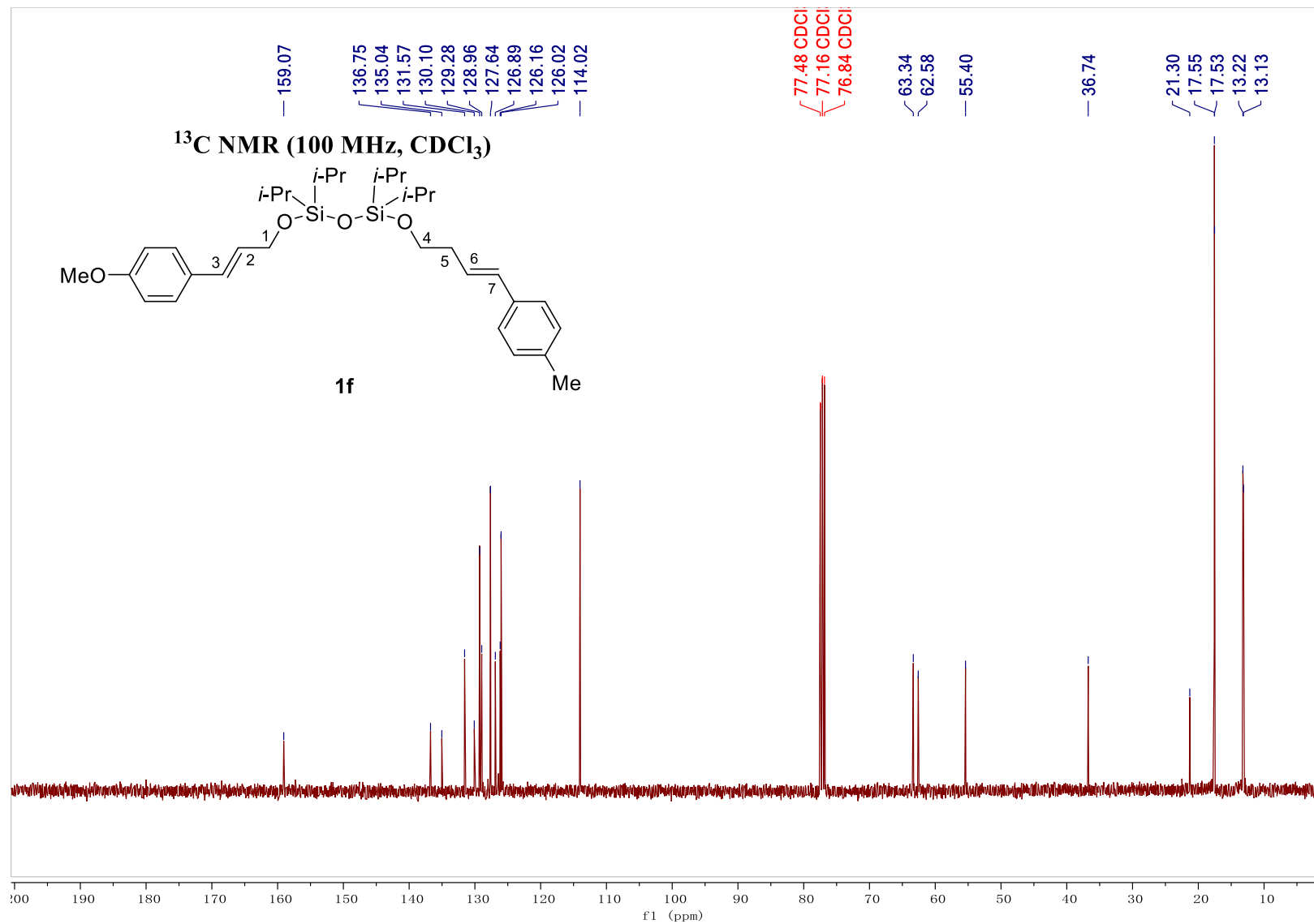


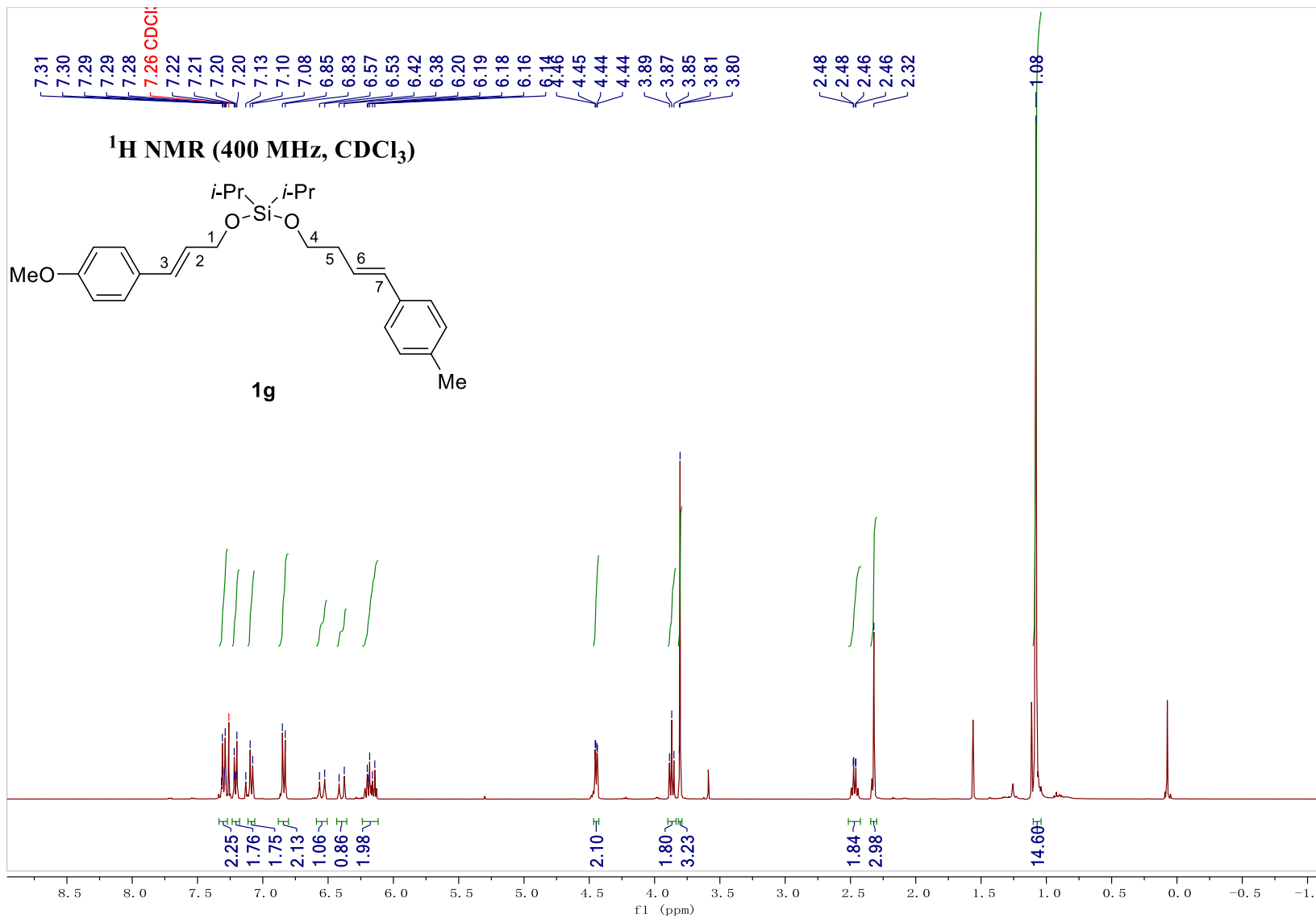


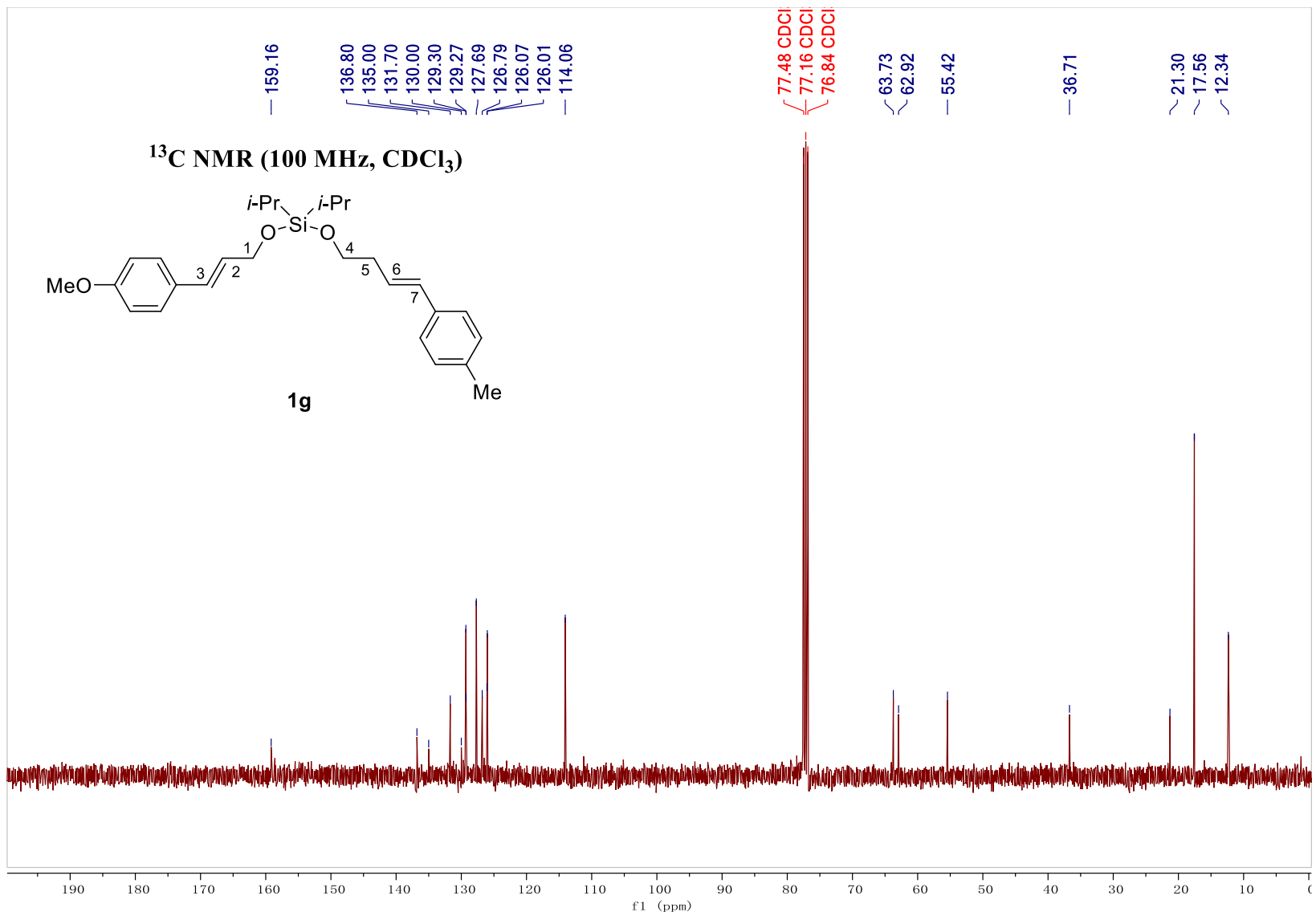


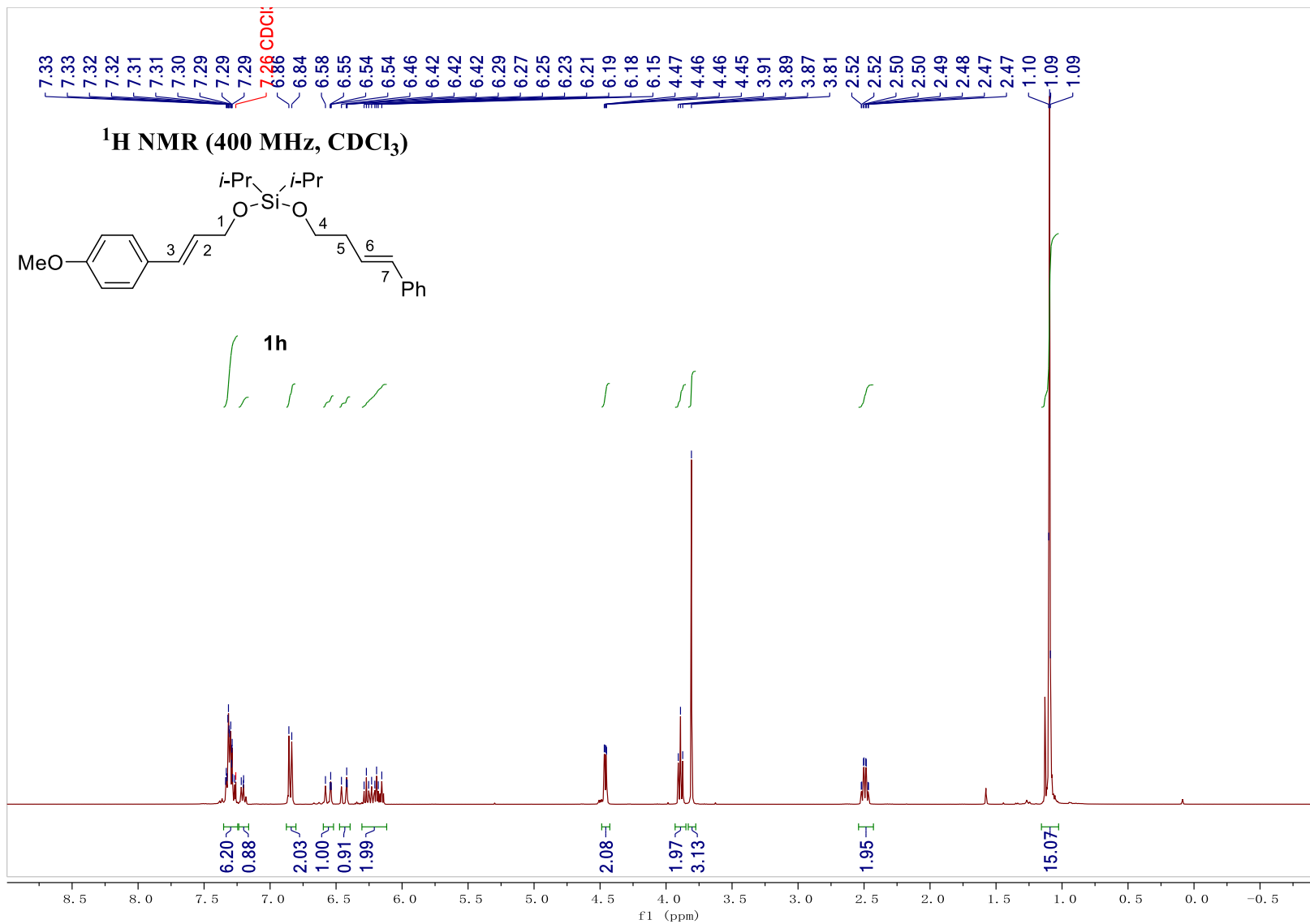


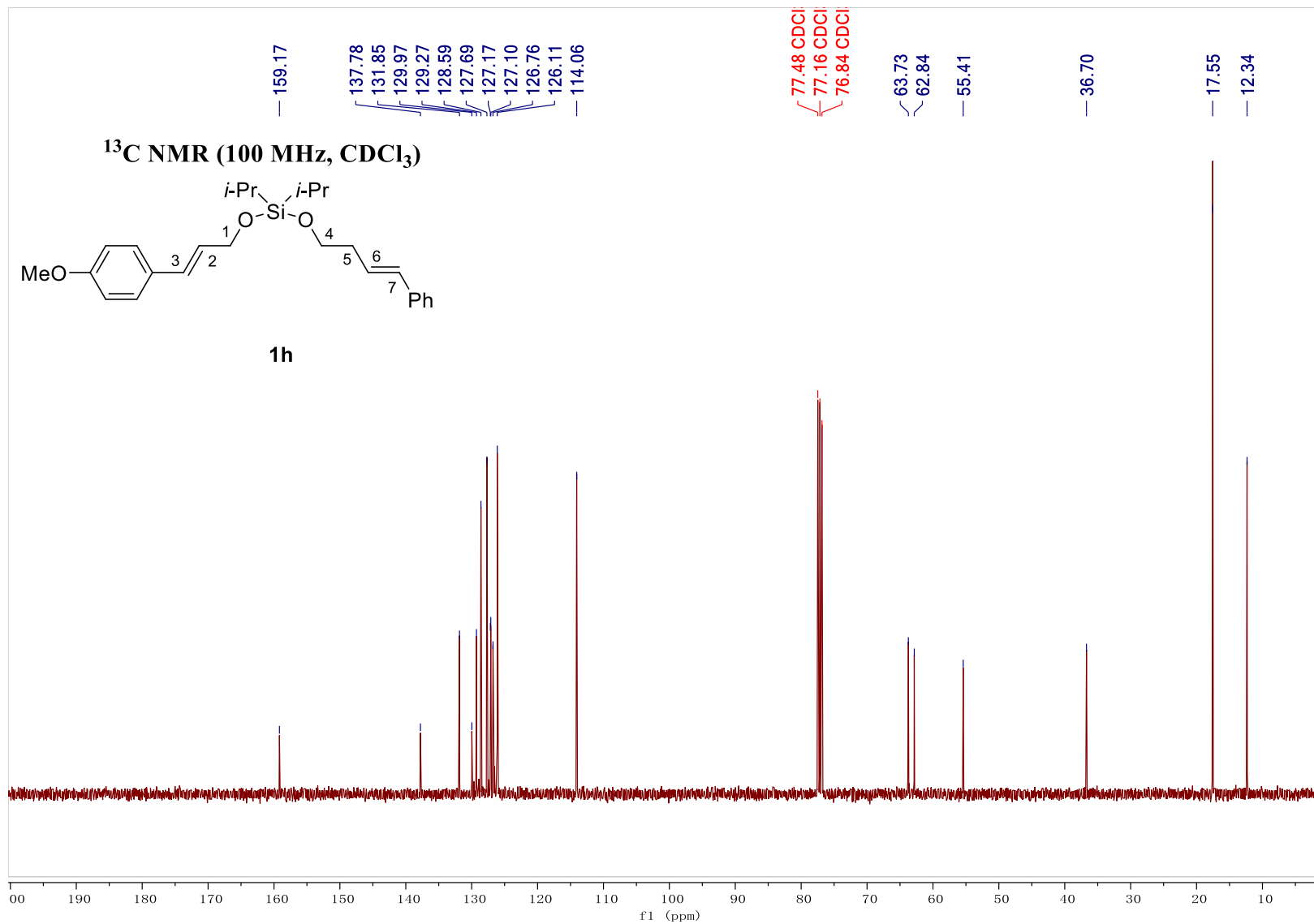


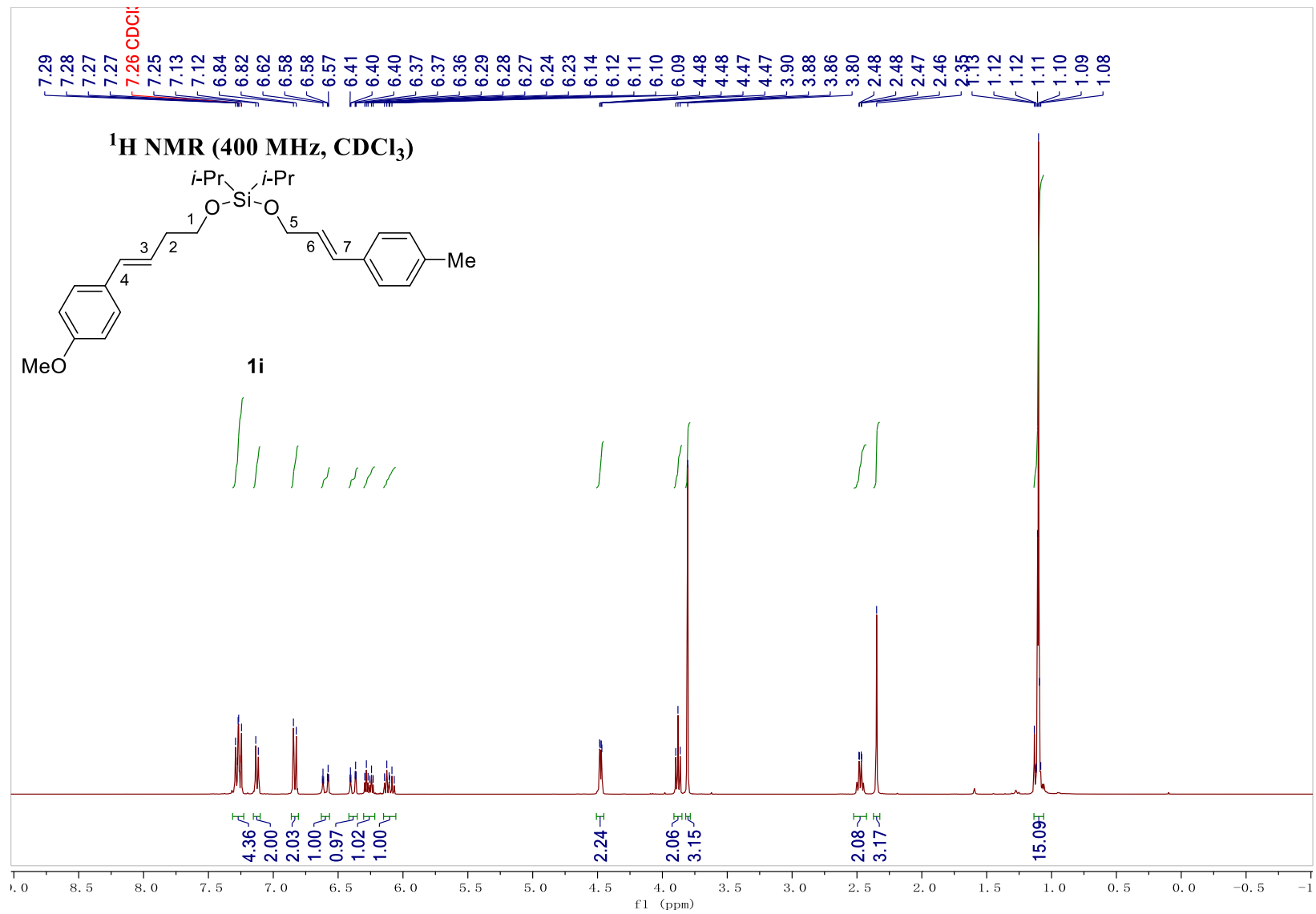


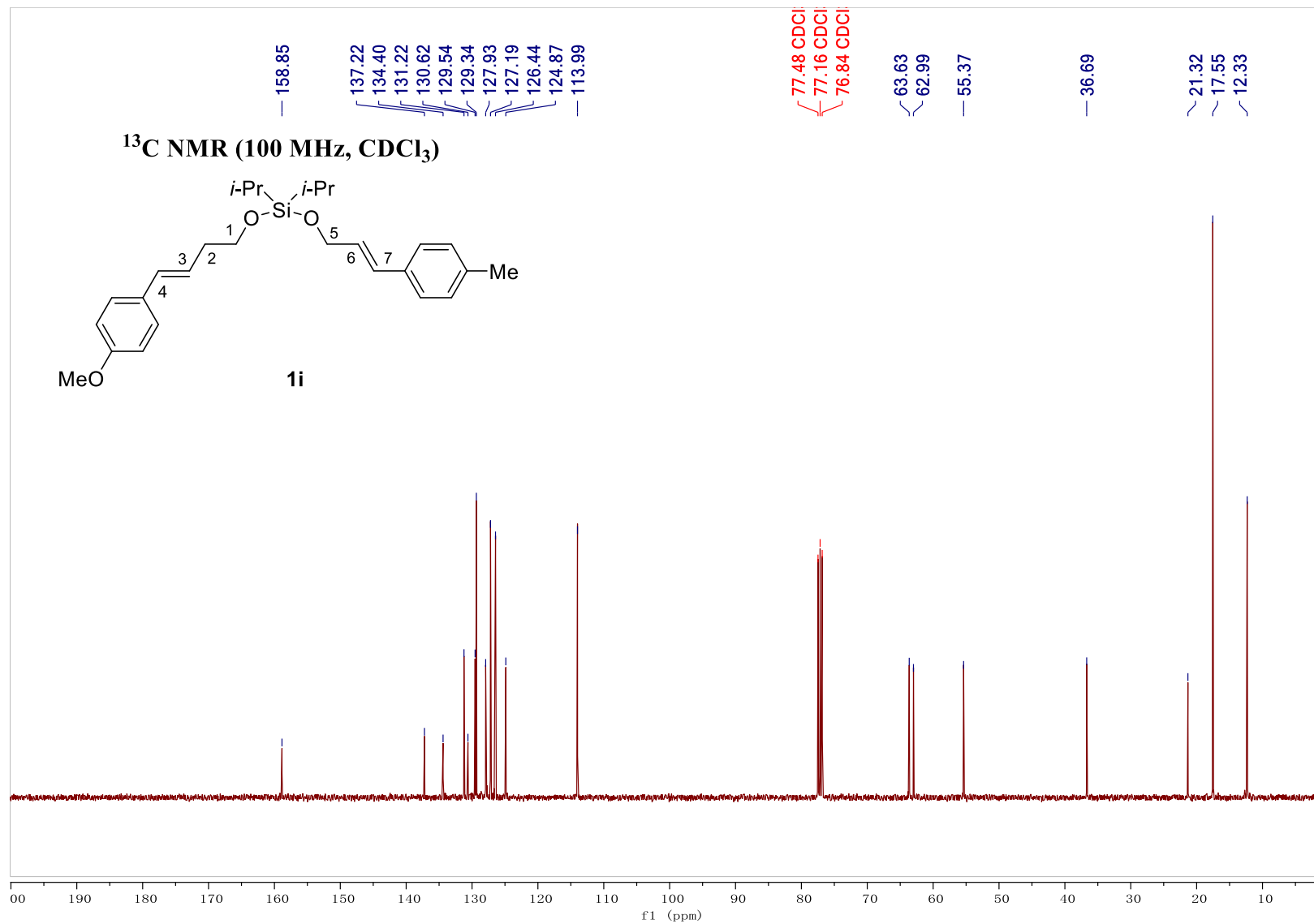


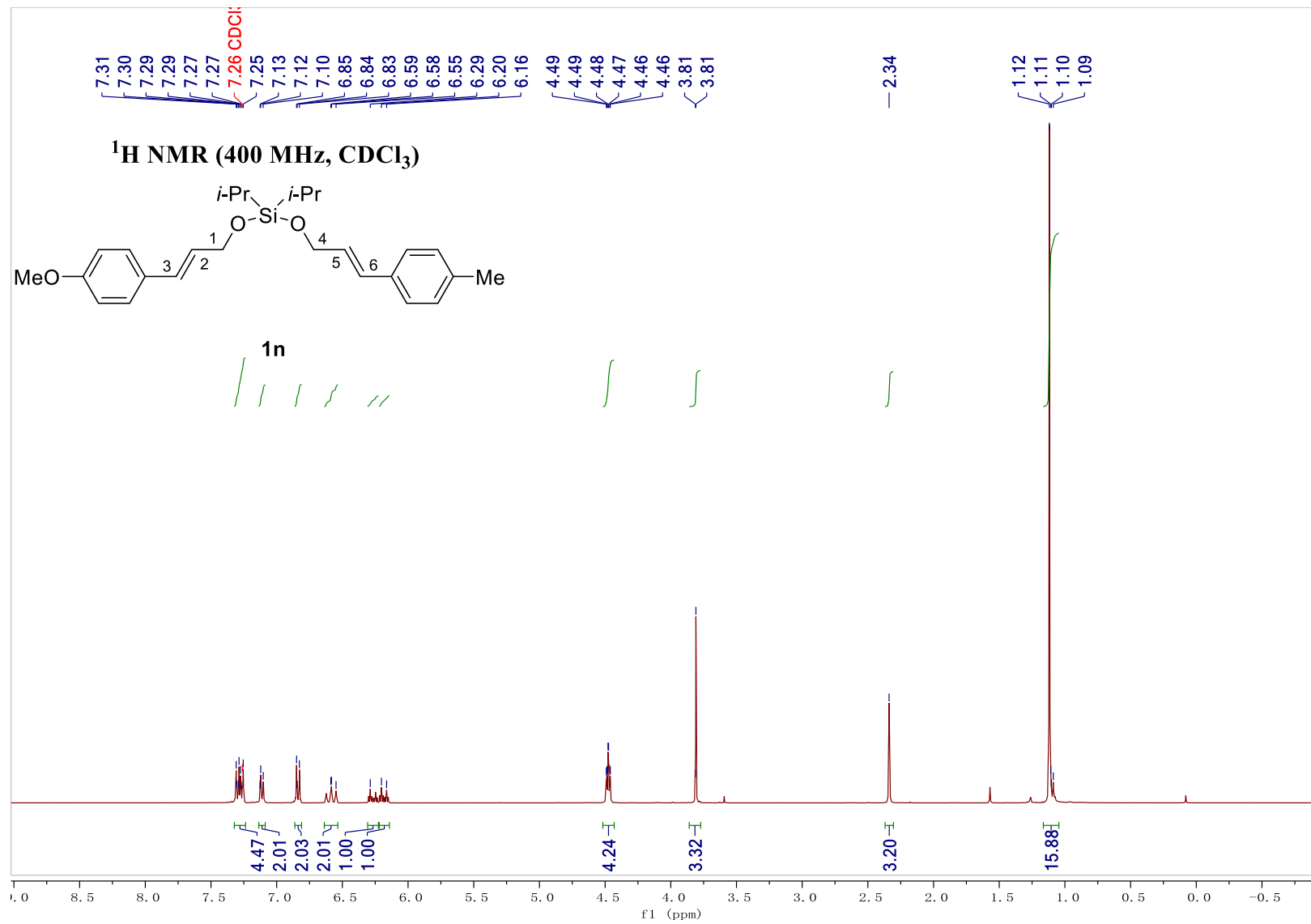


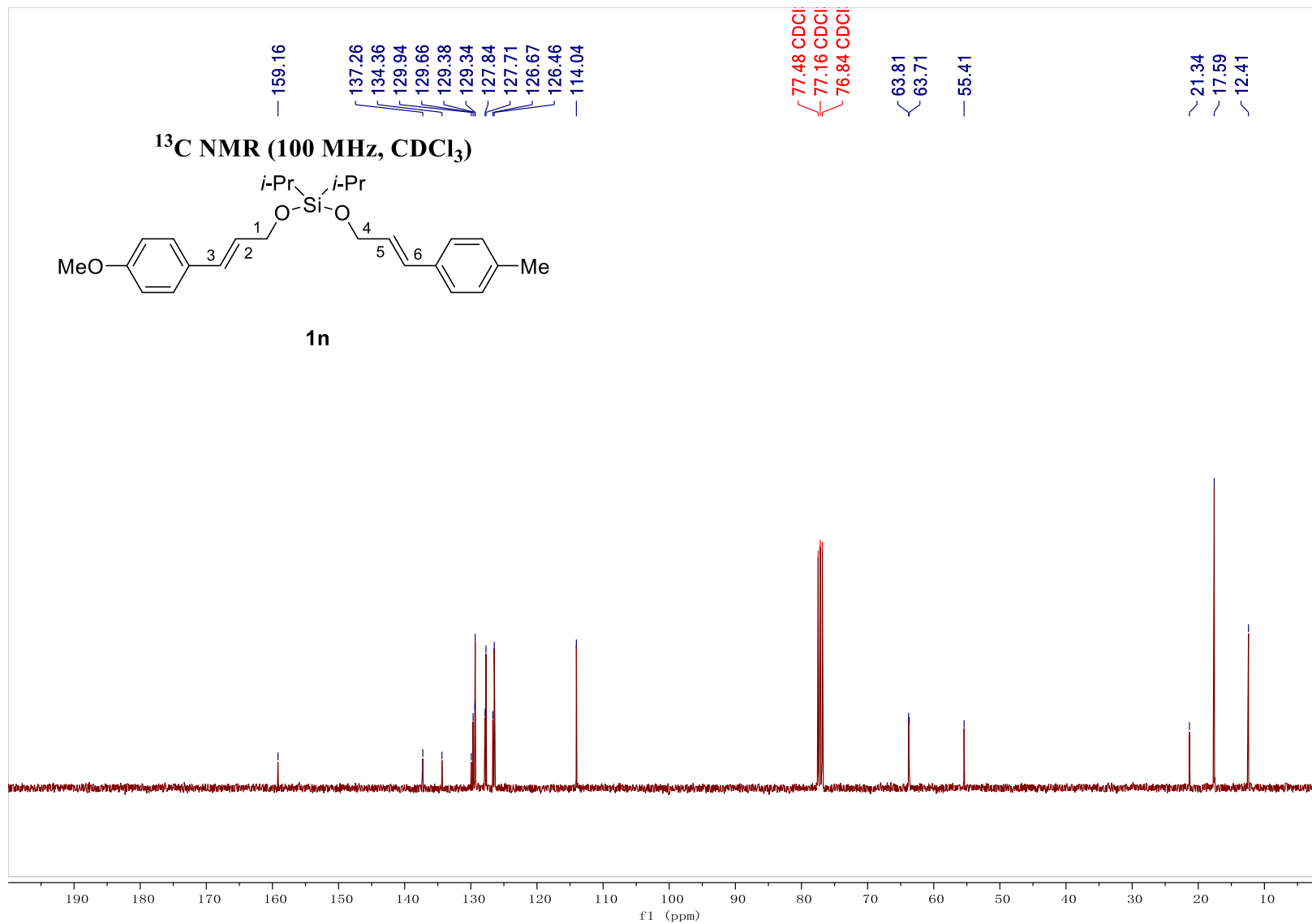


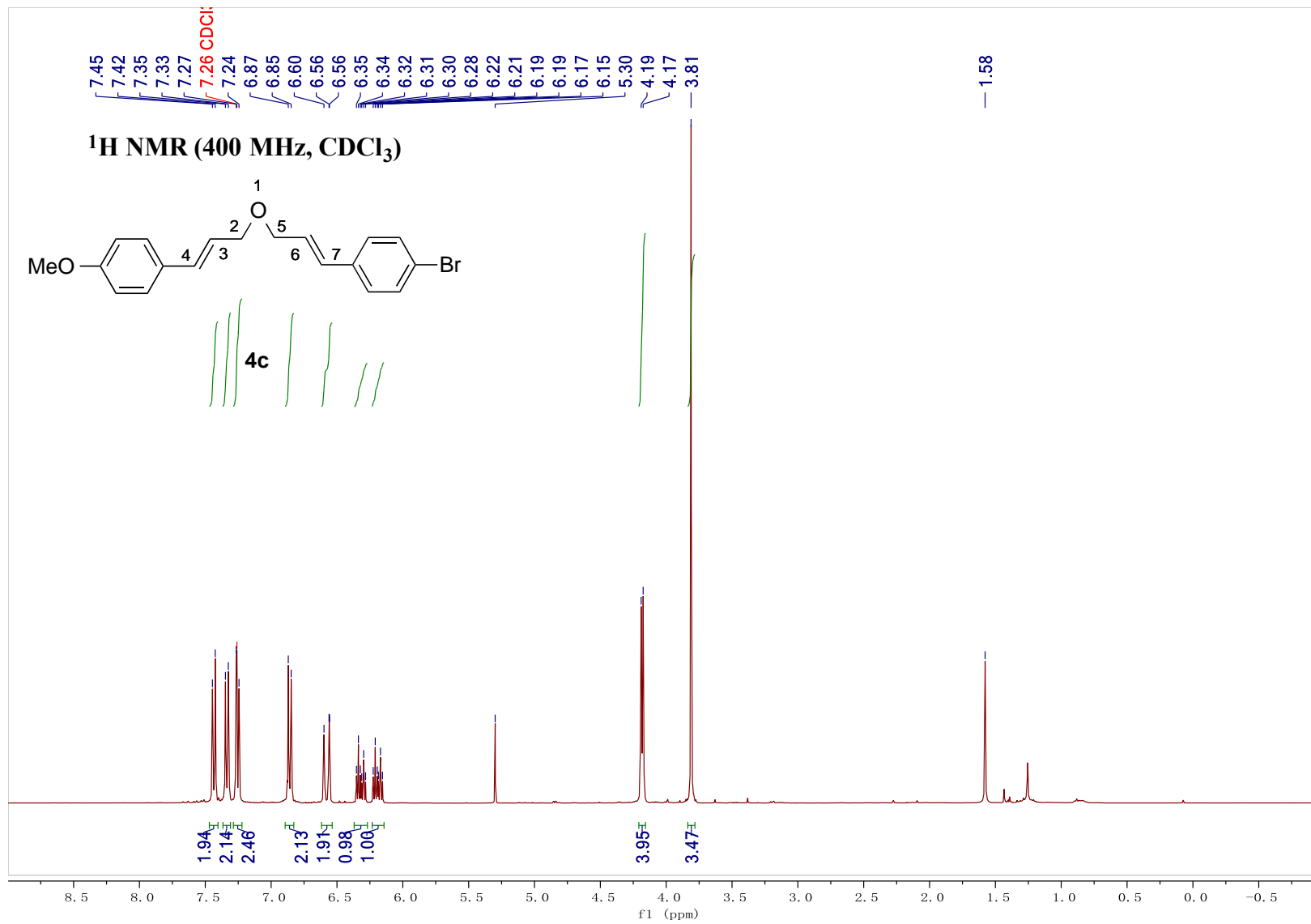


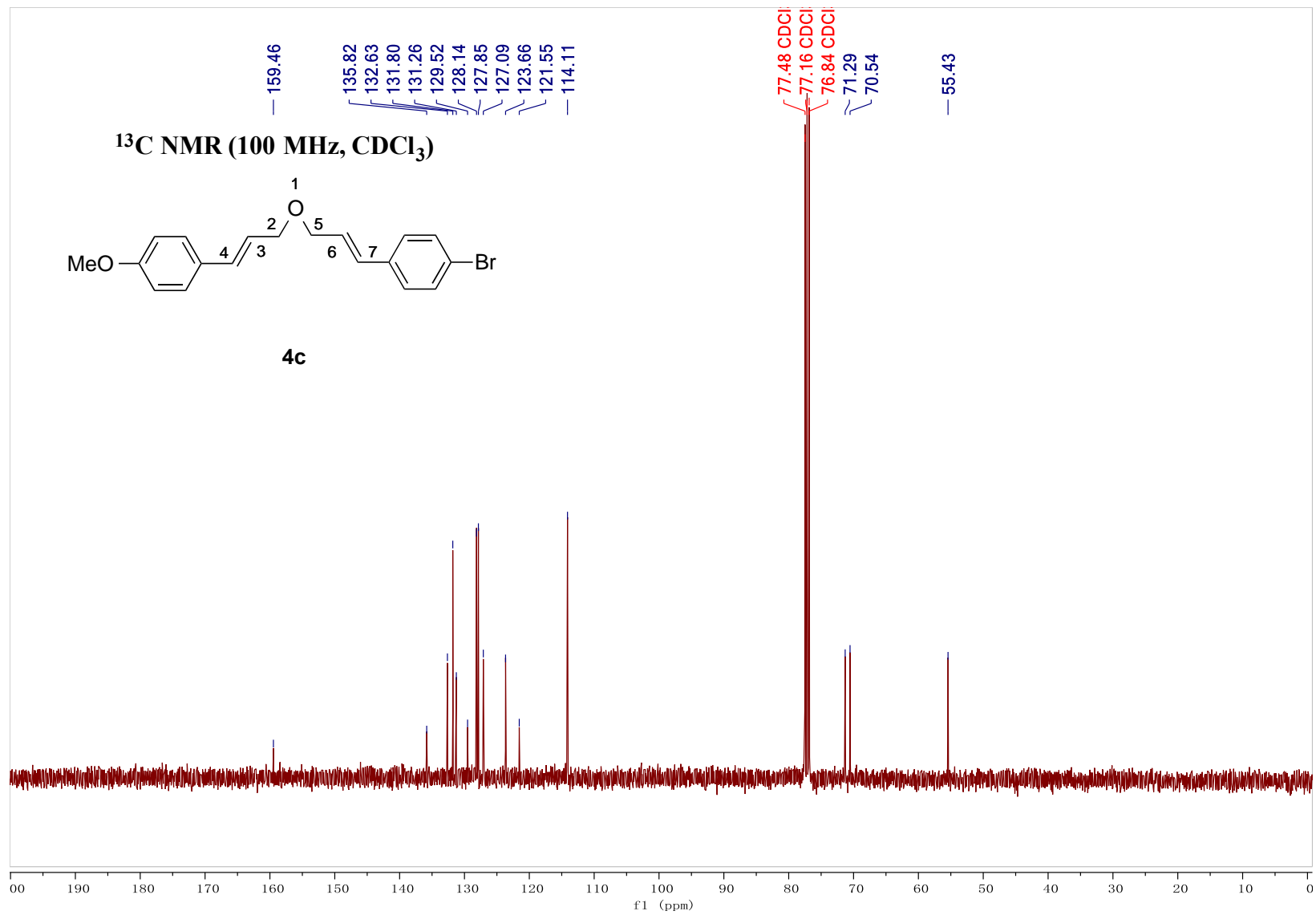


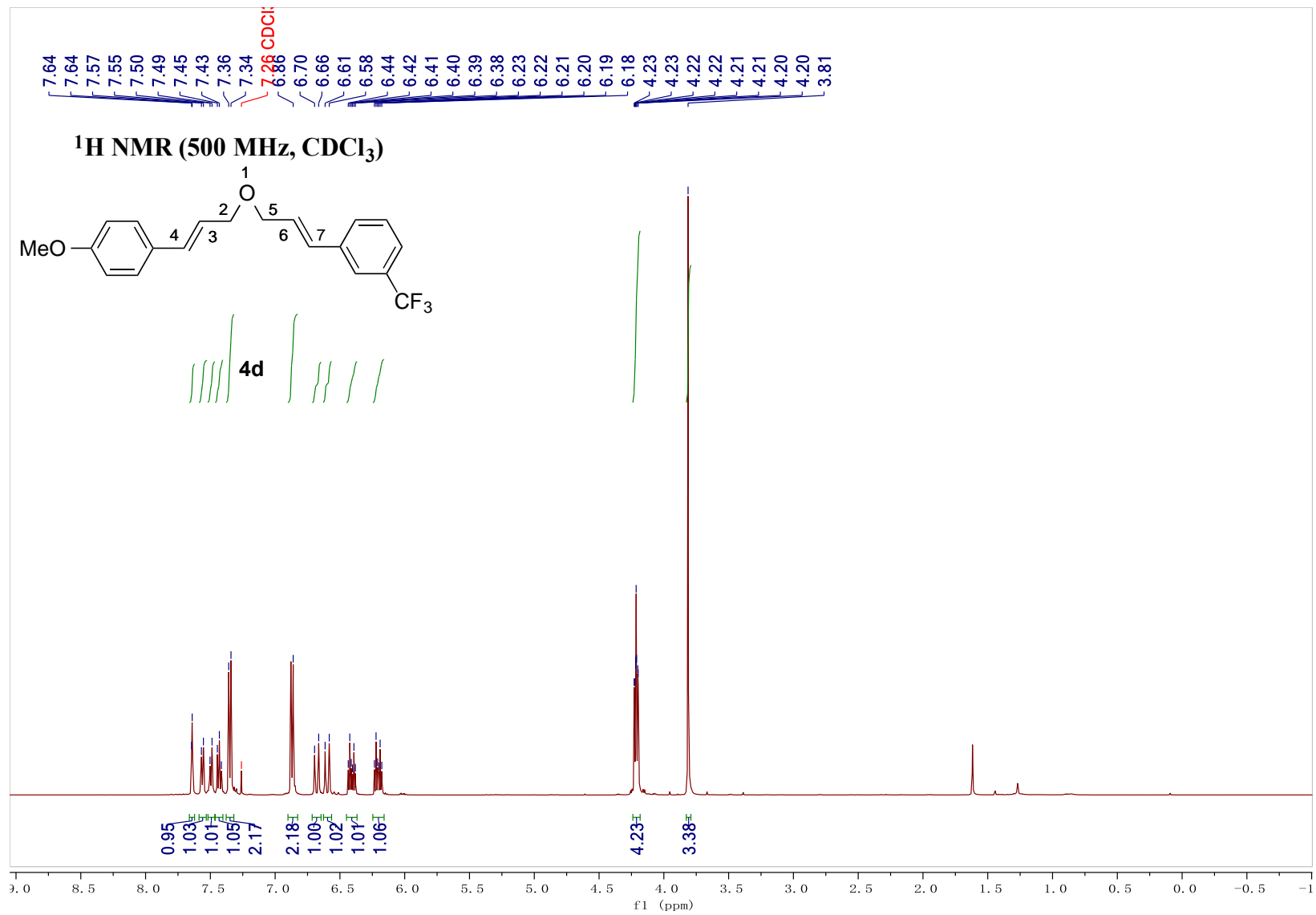


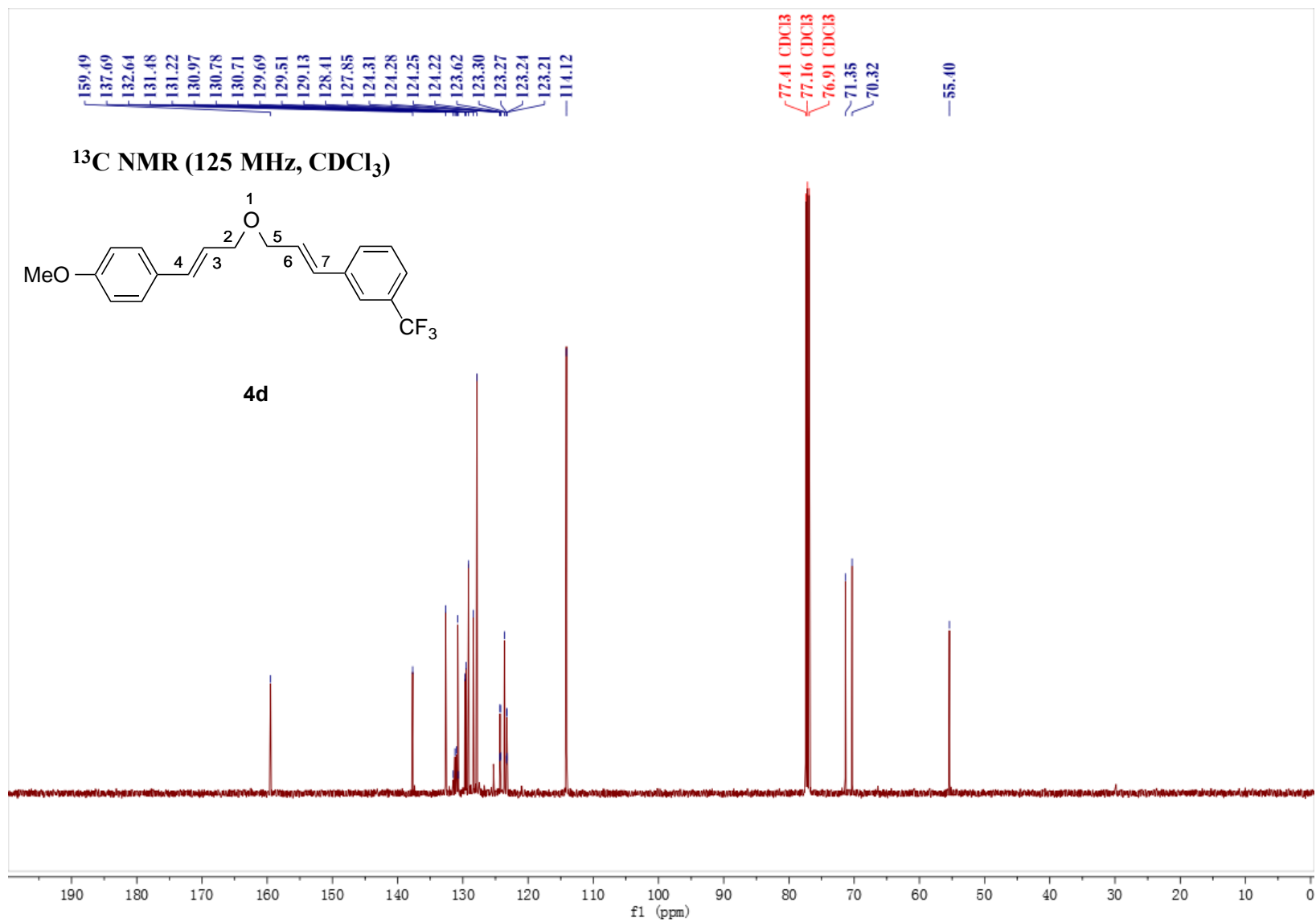


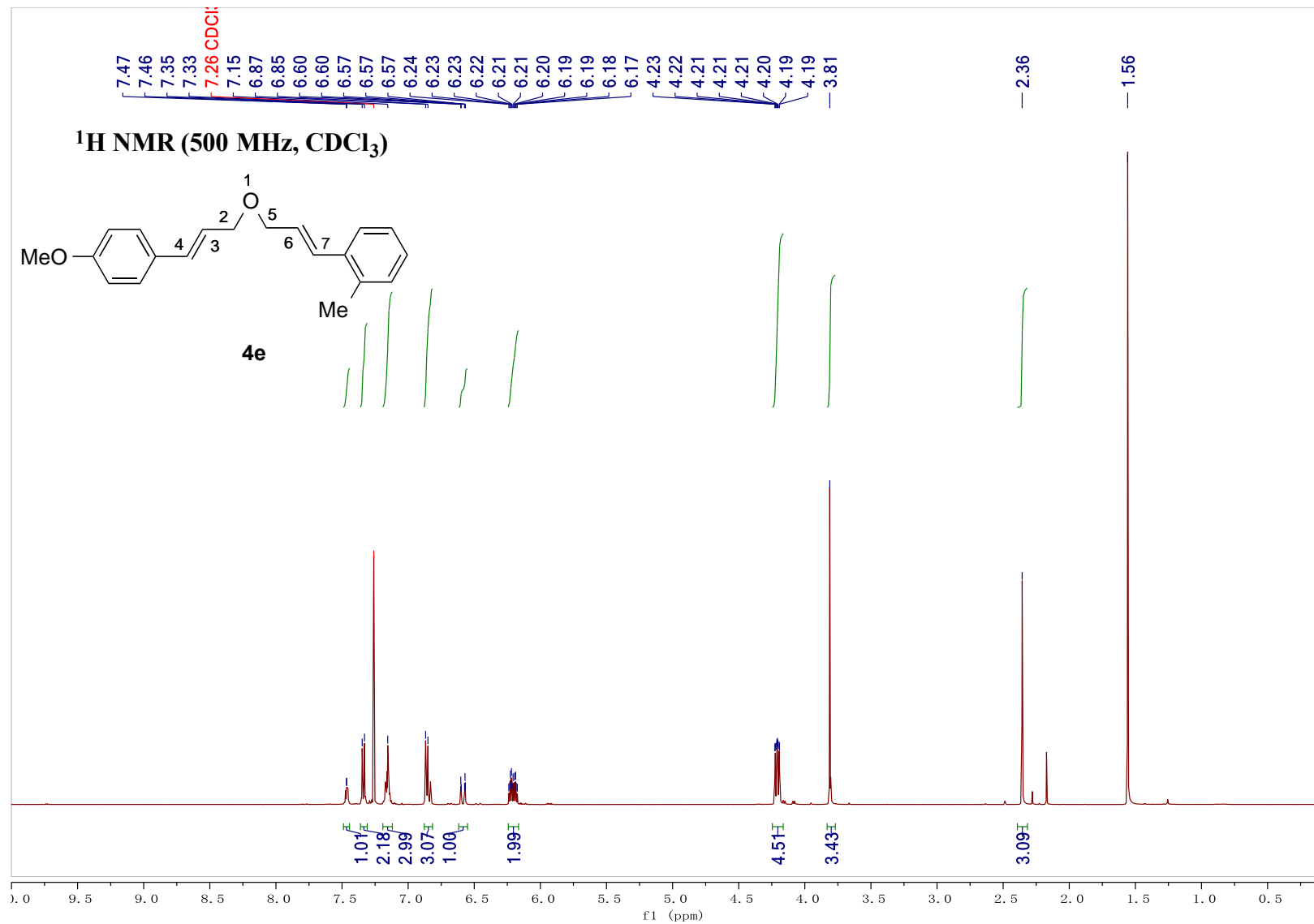


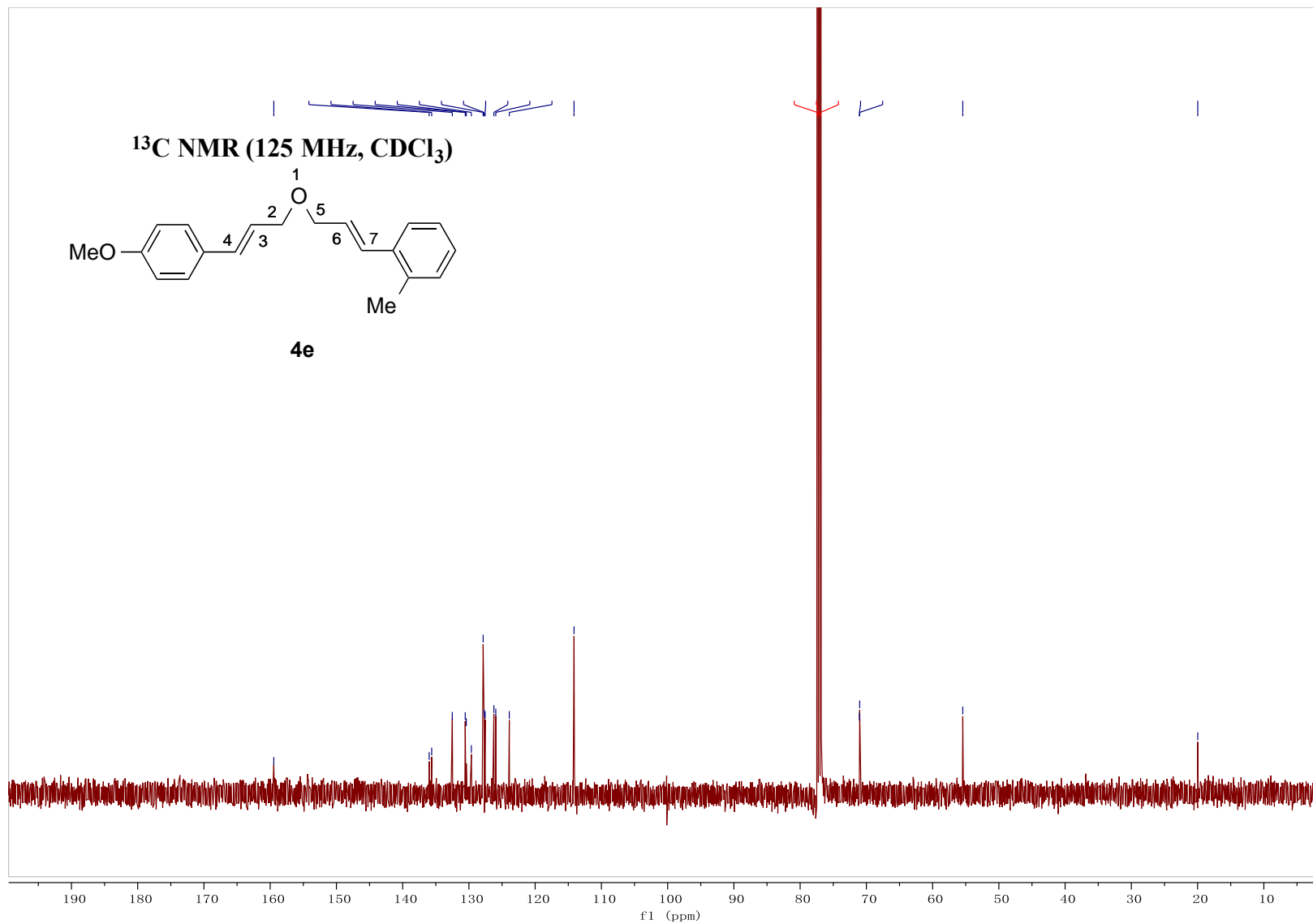


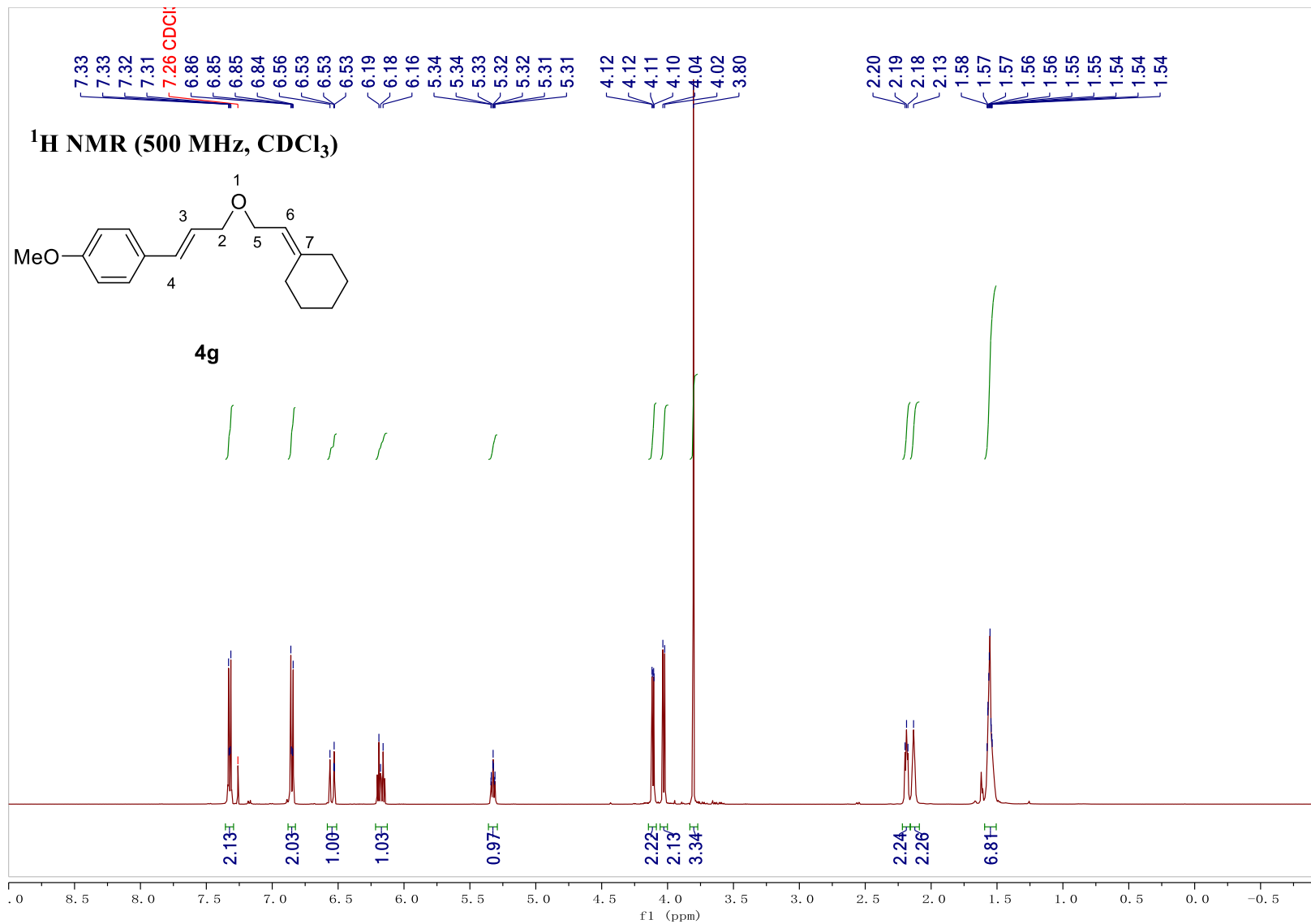


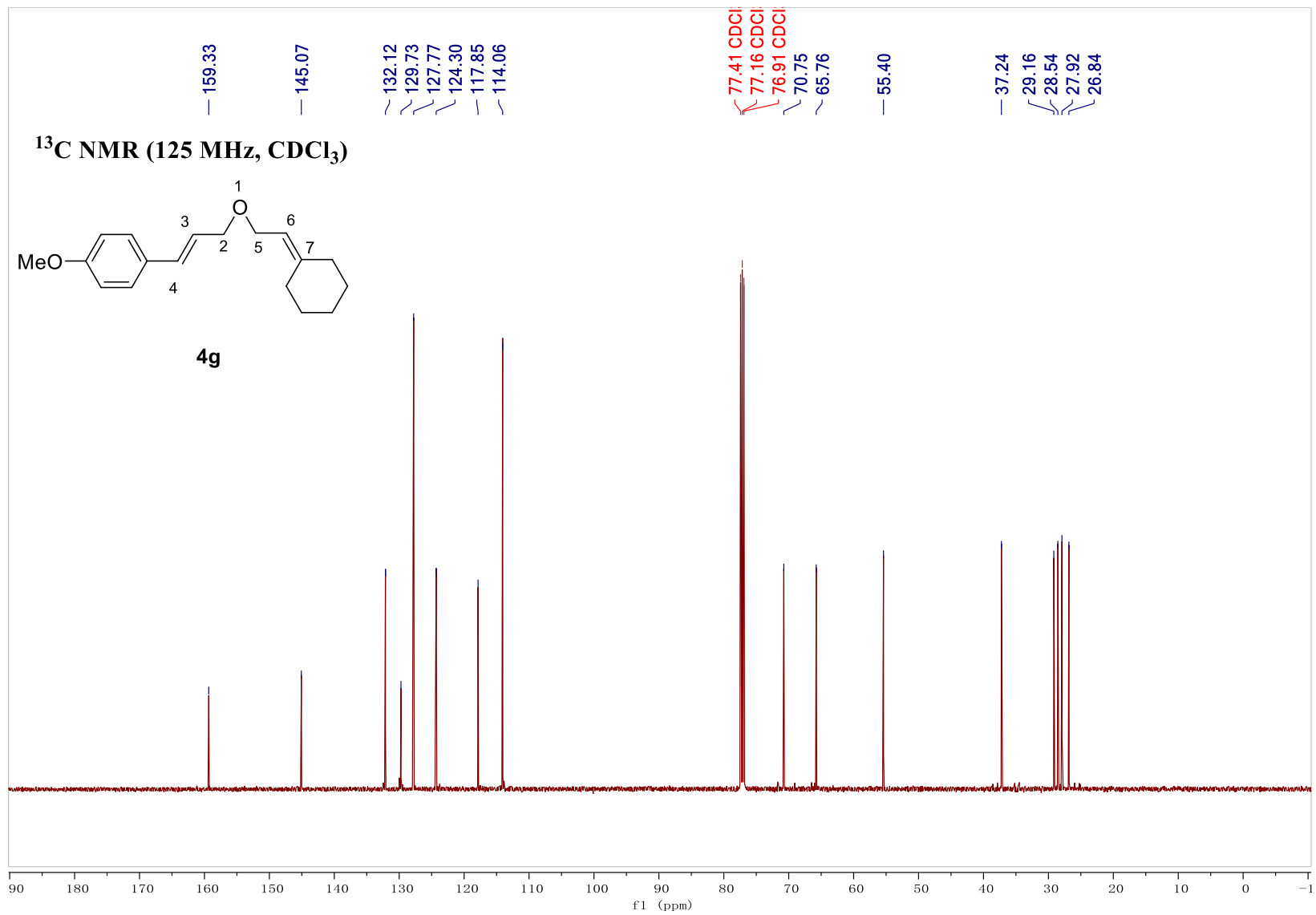


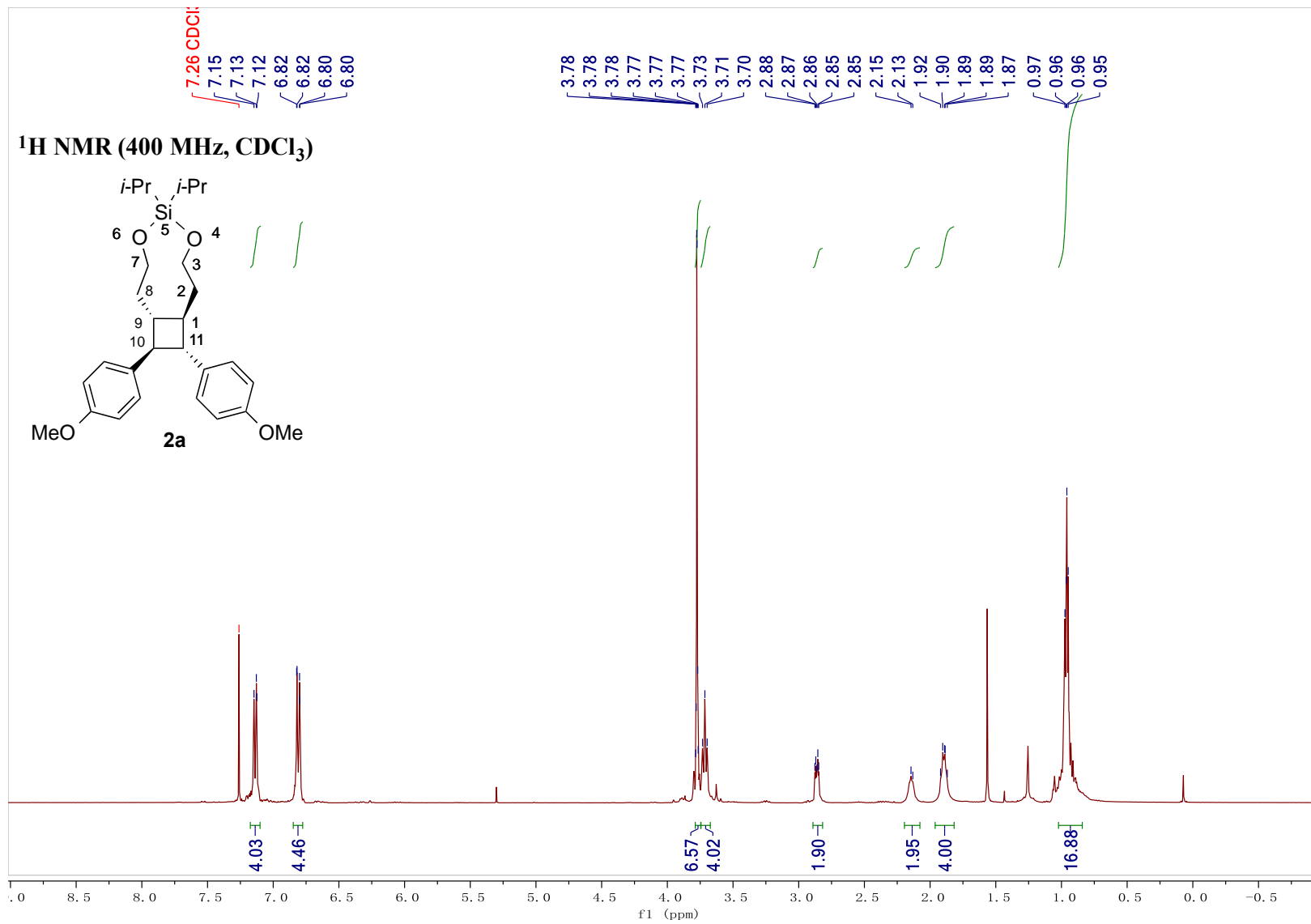




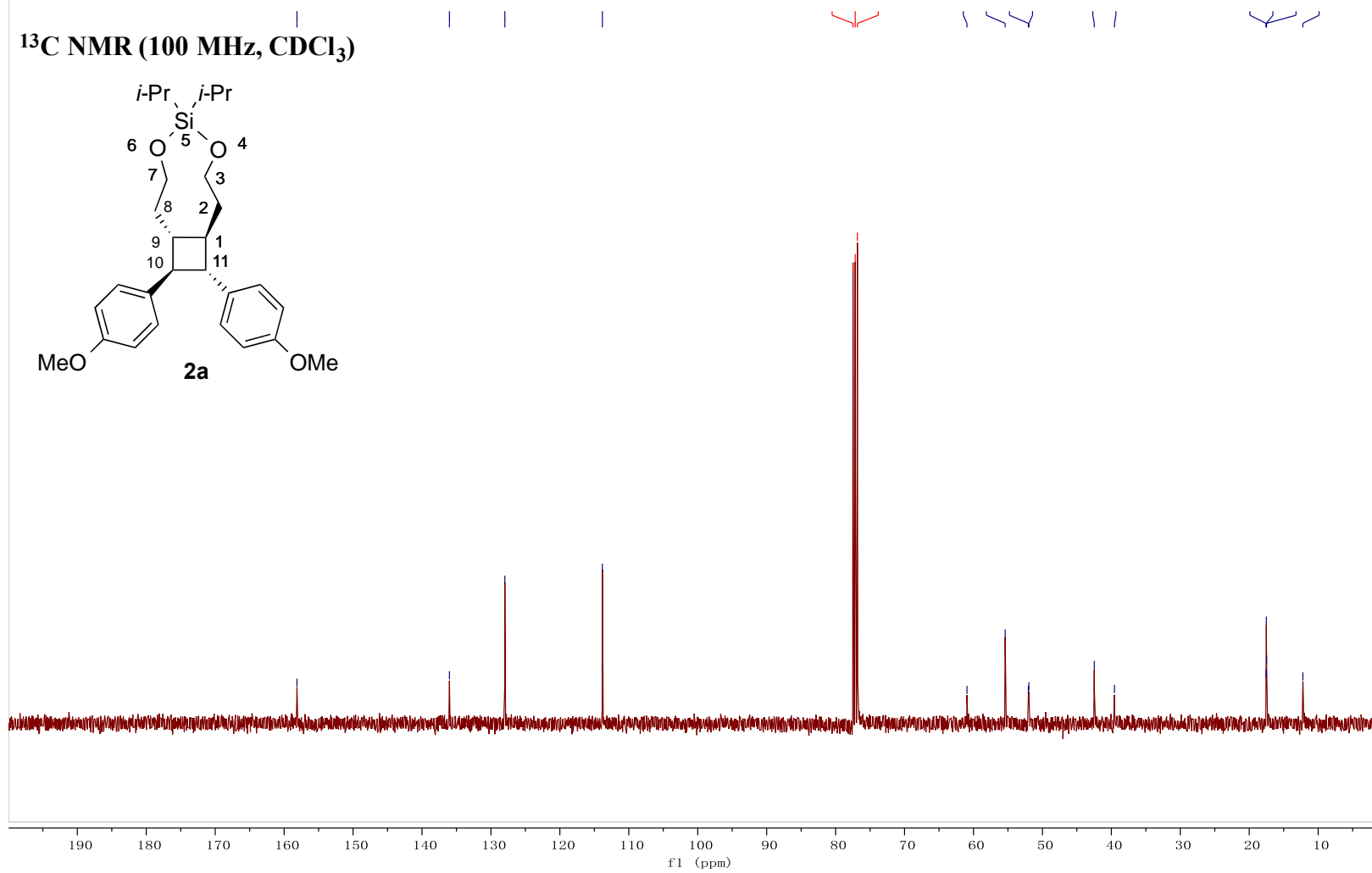
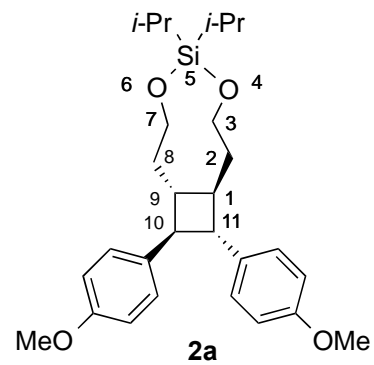


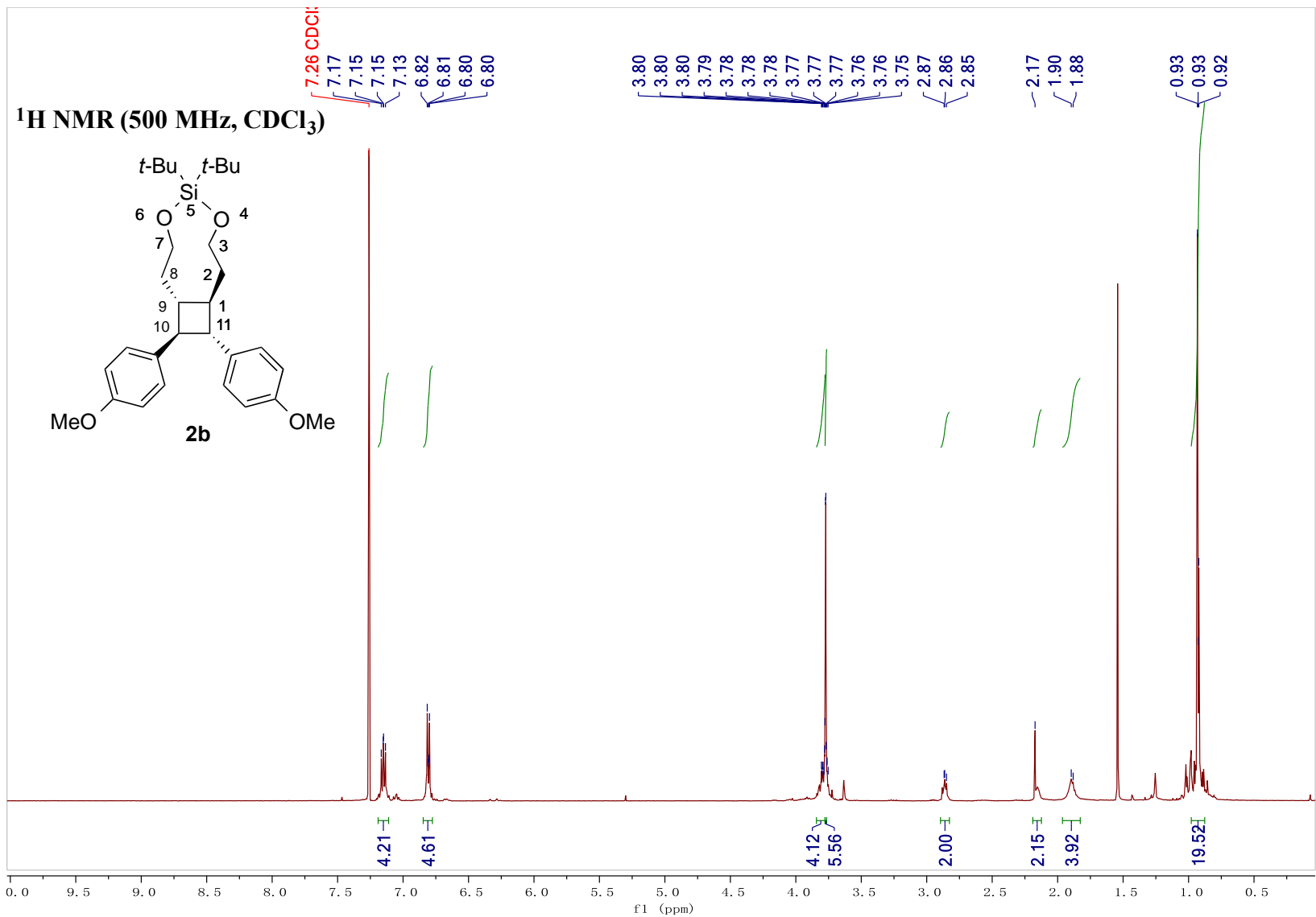


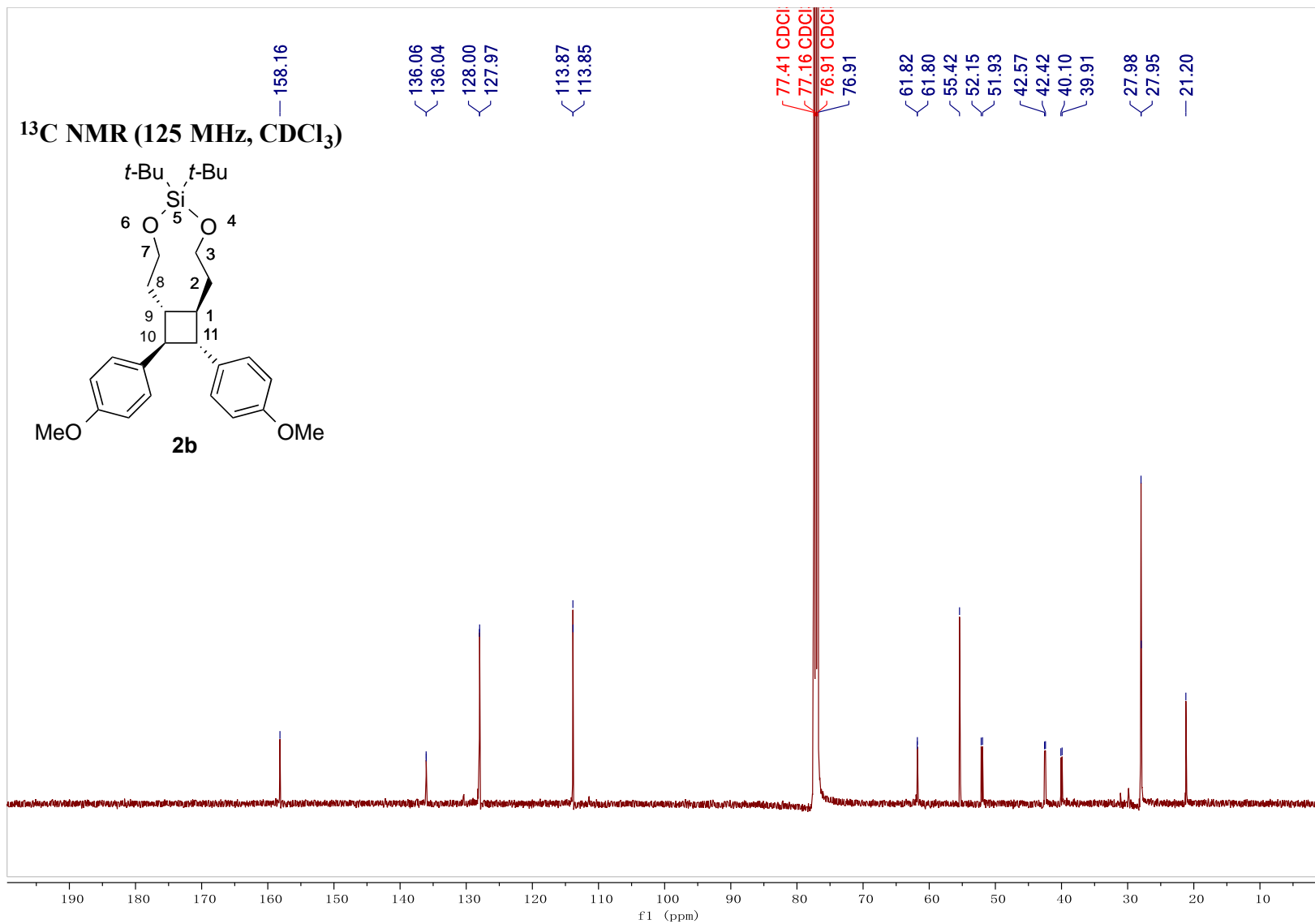


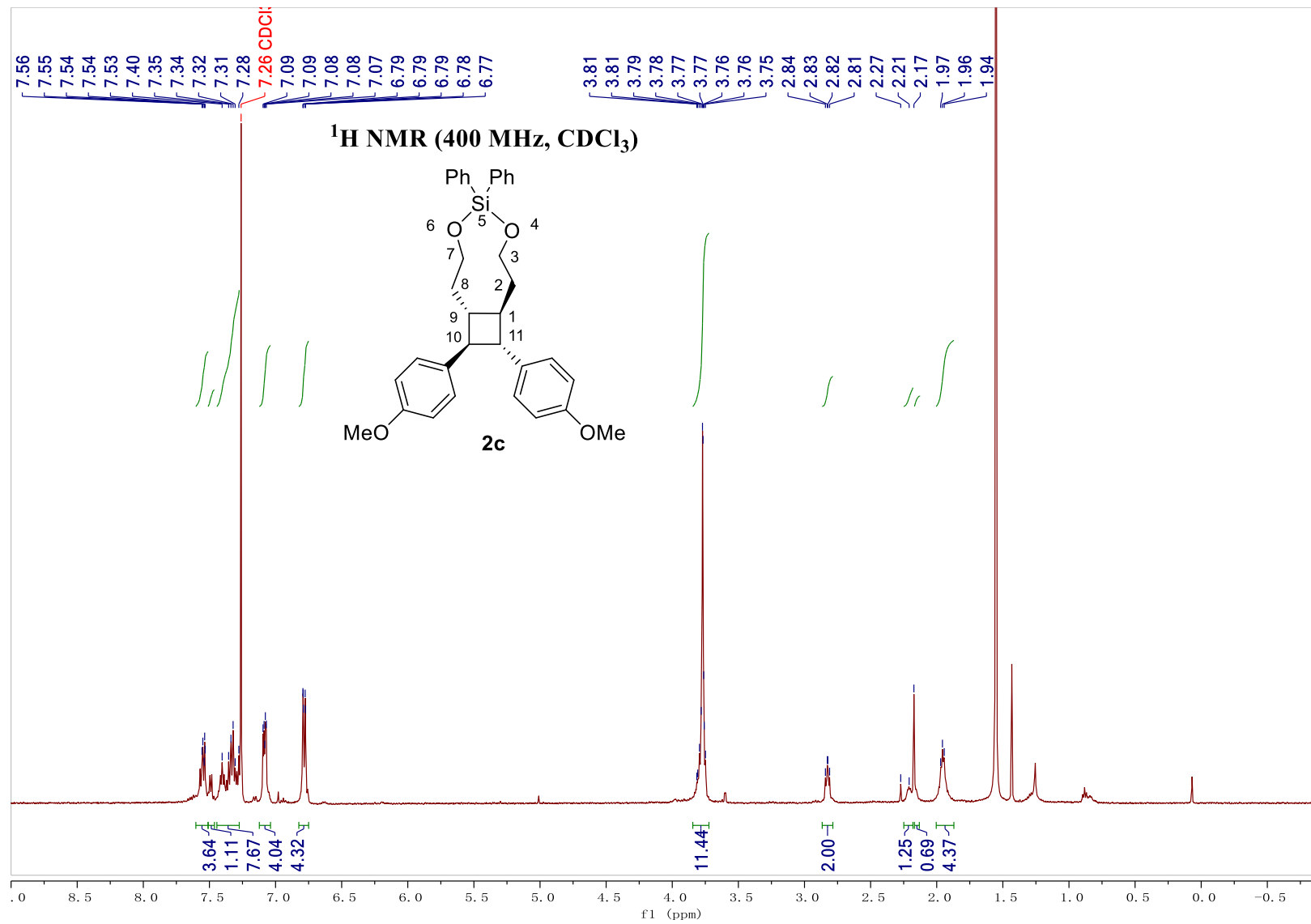


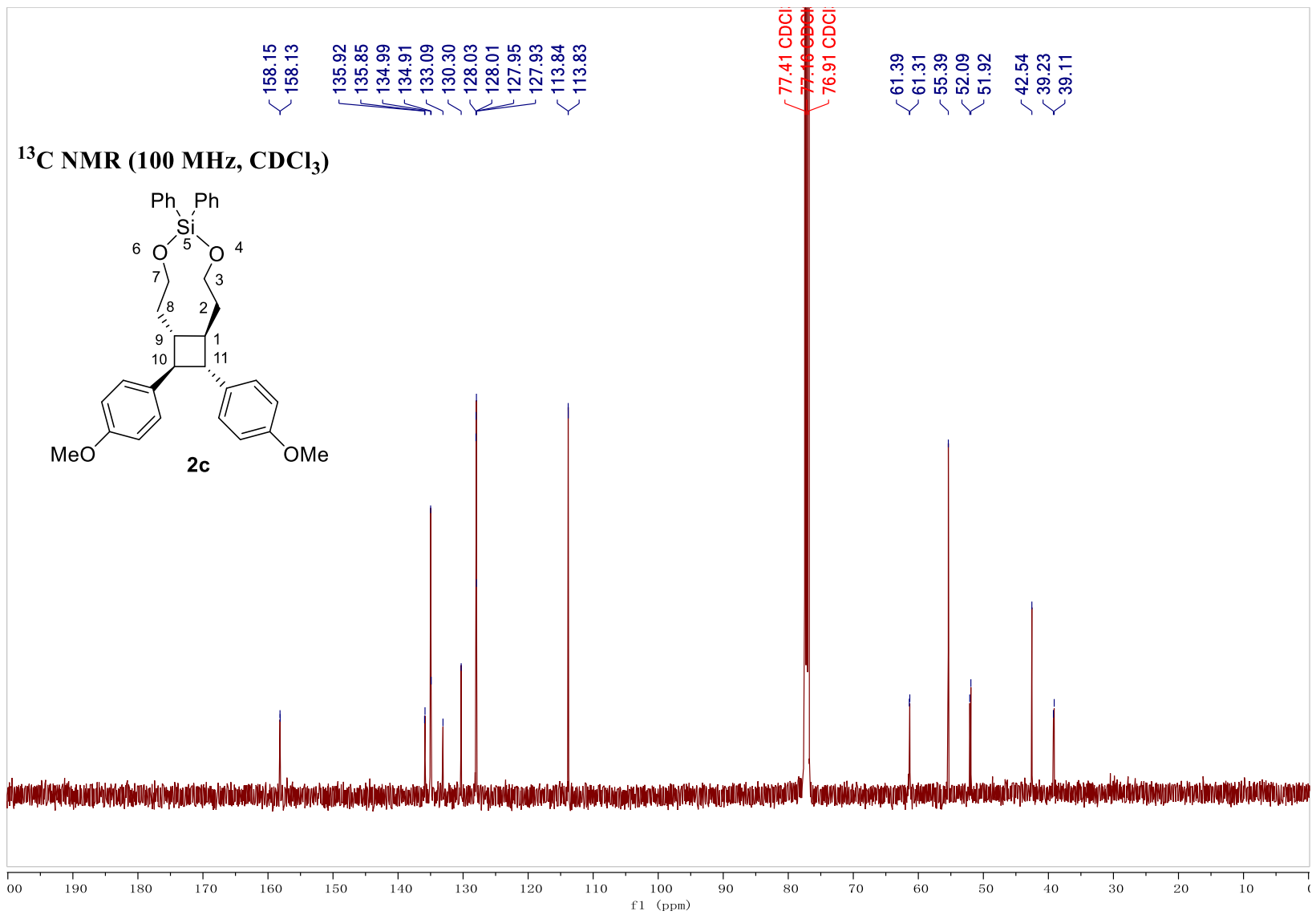
¹³C NMR (100 MHz, CDCl₃)

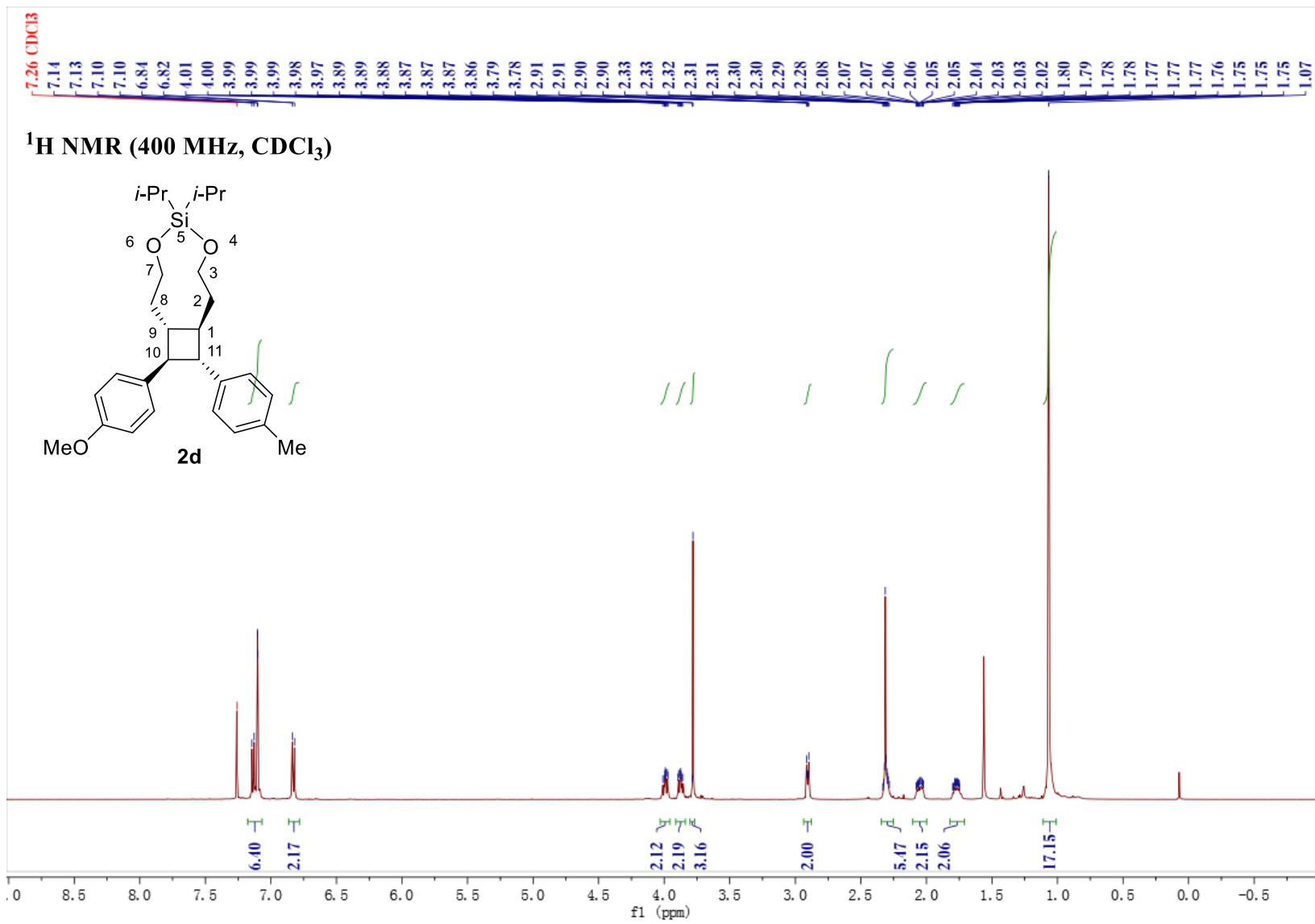


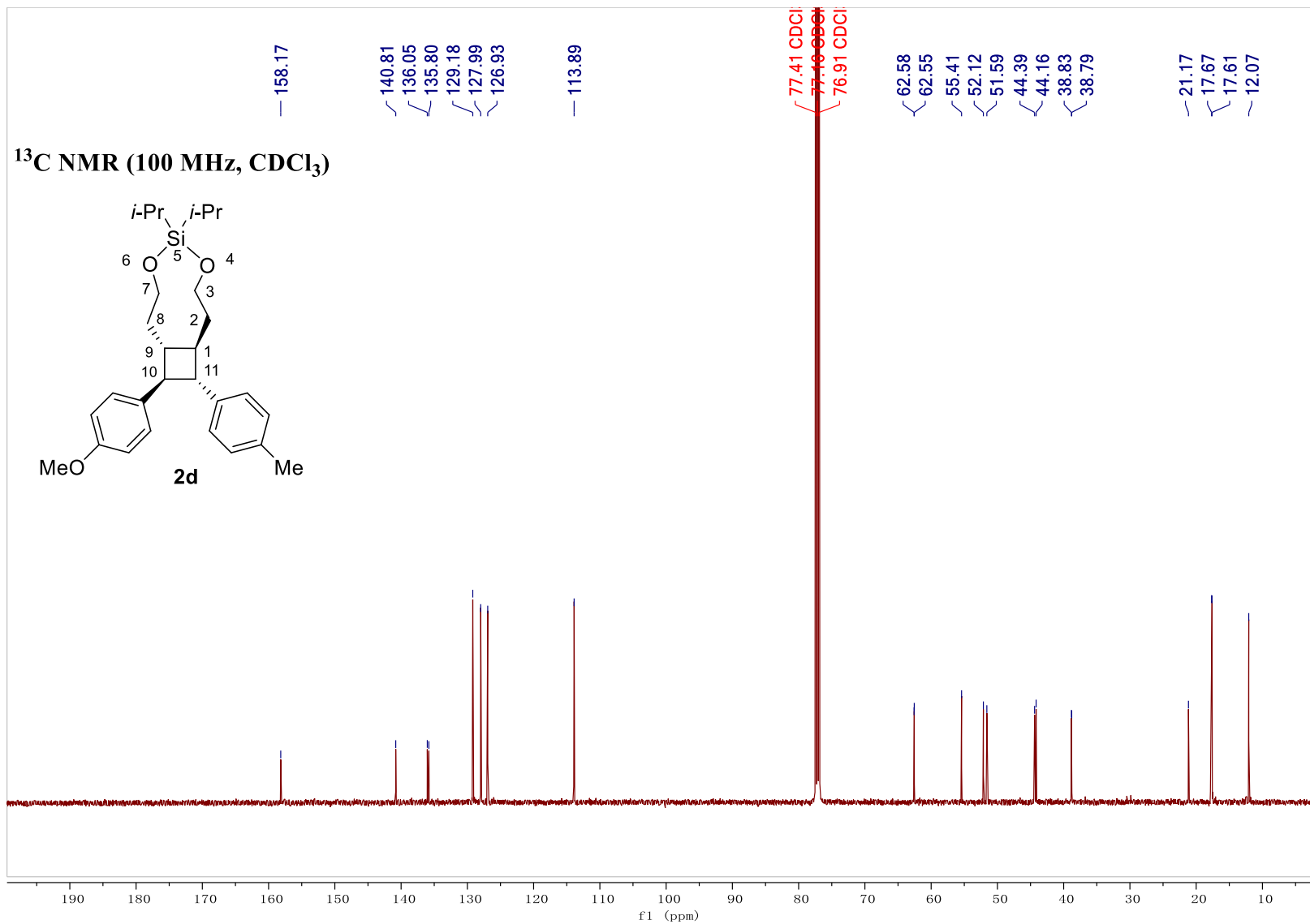


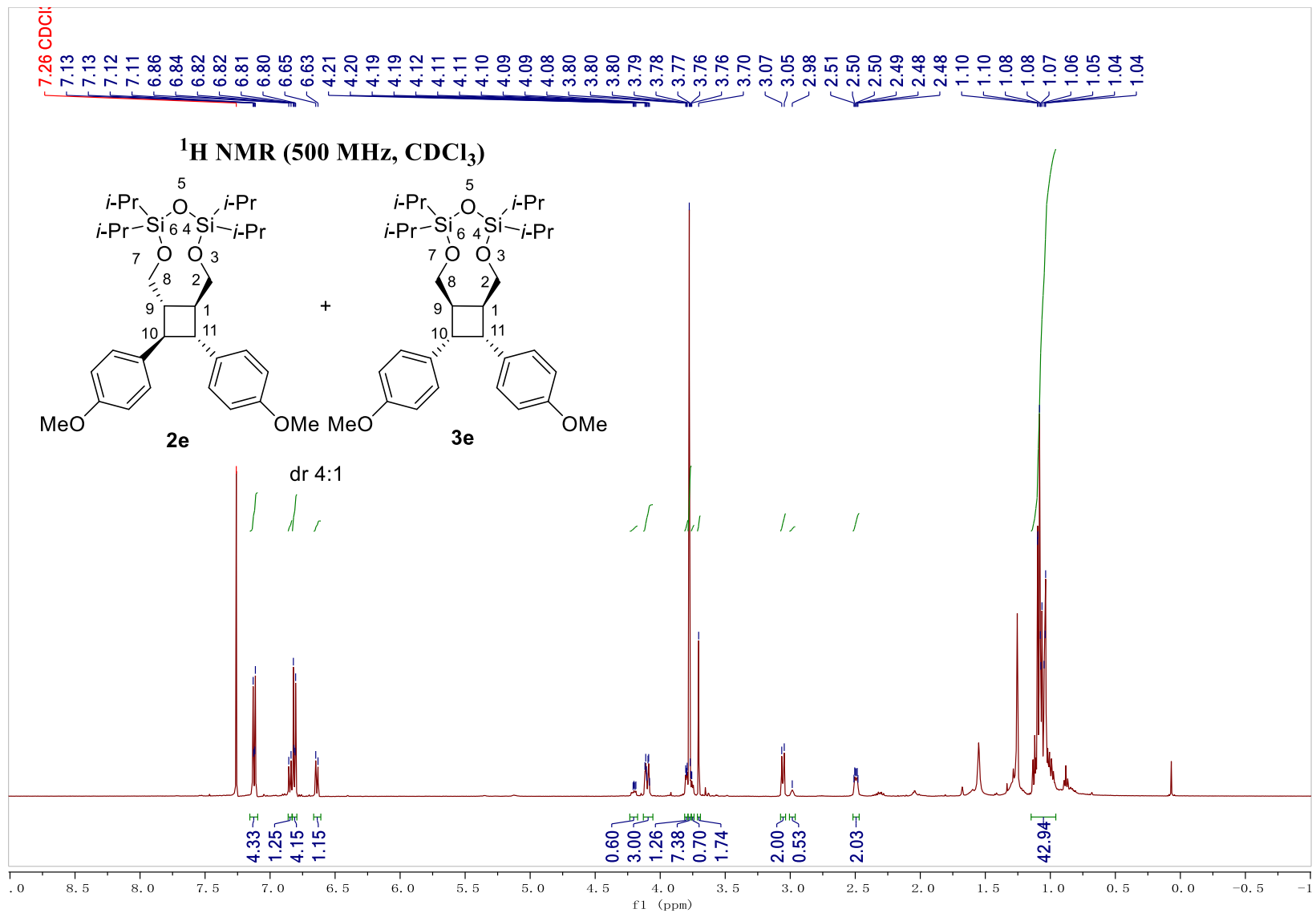


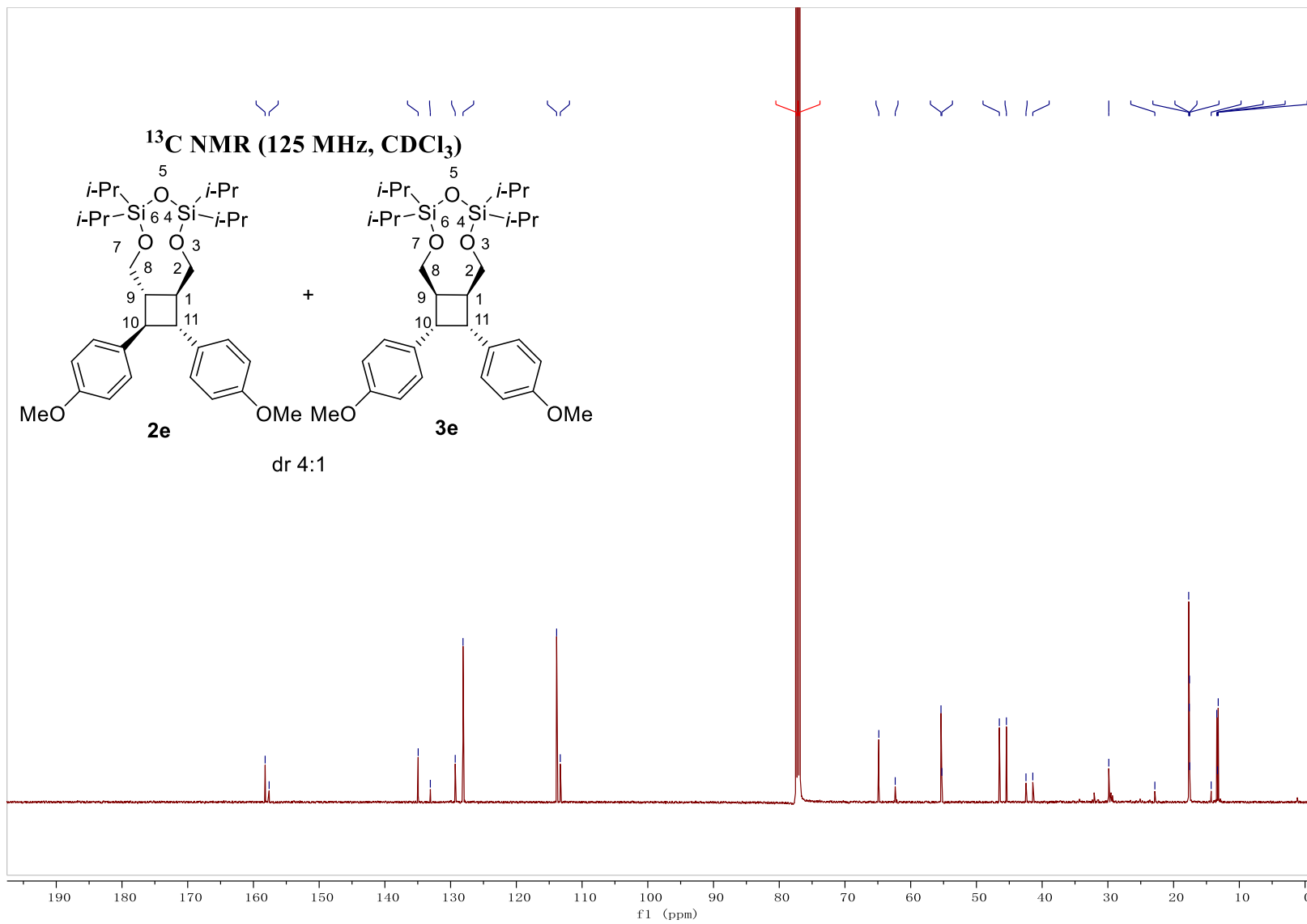


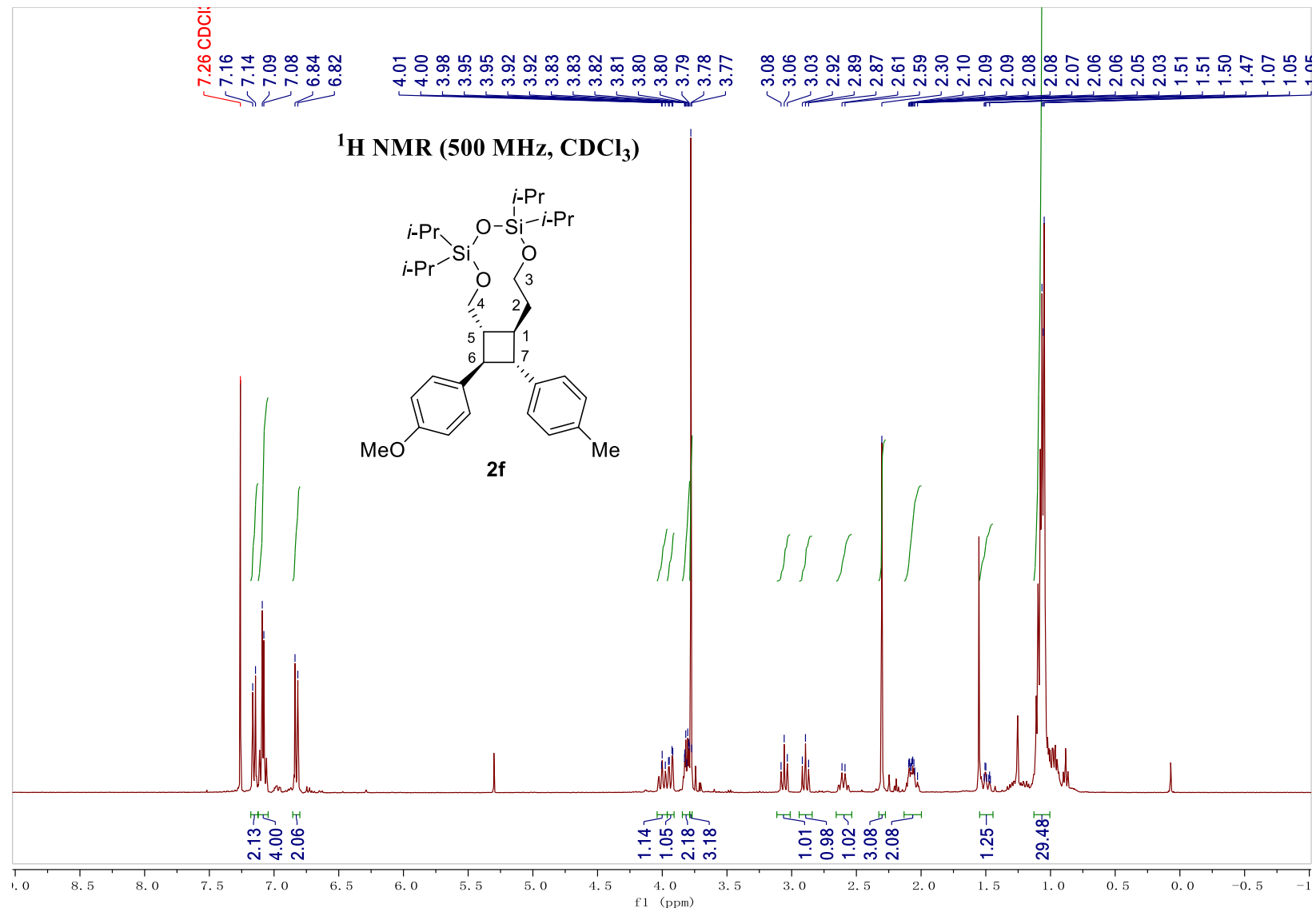


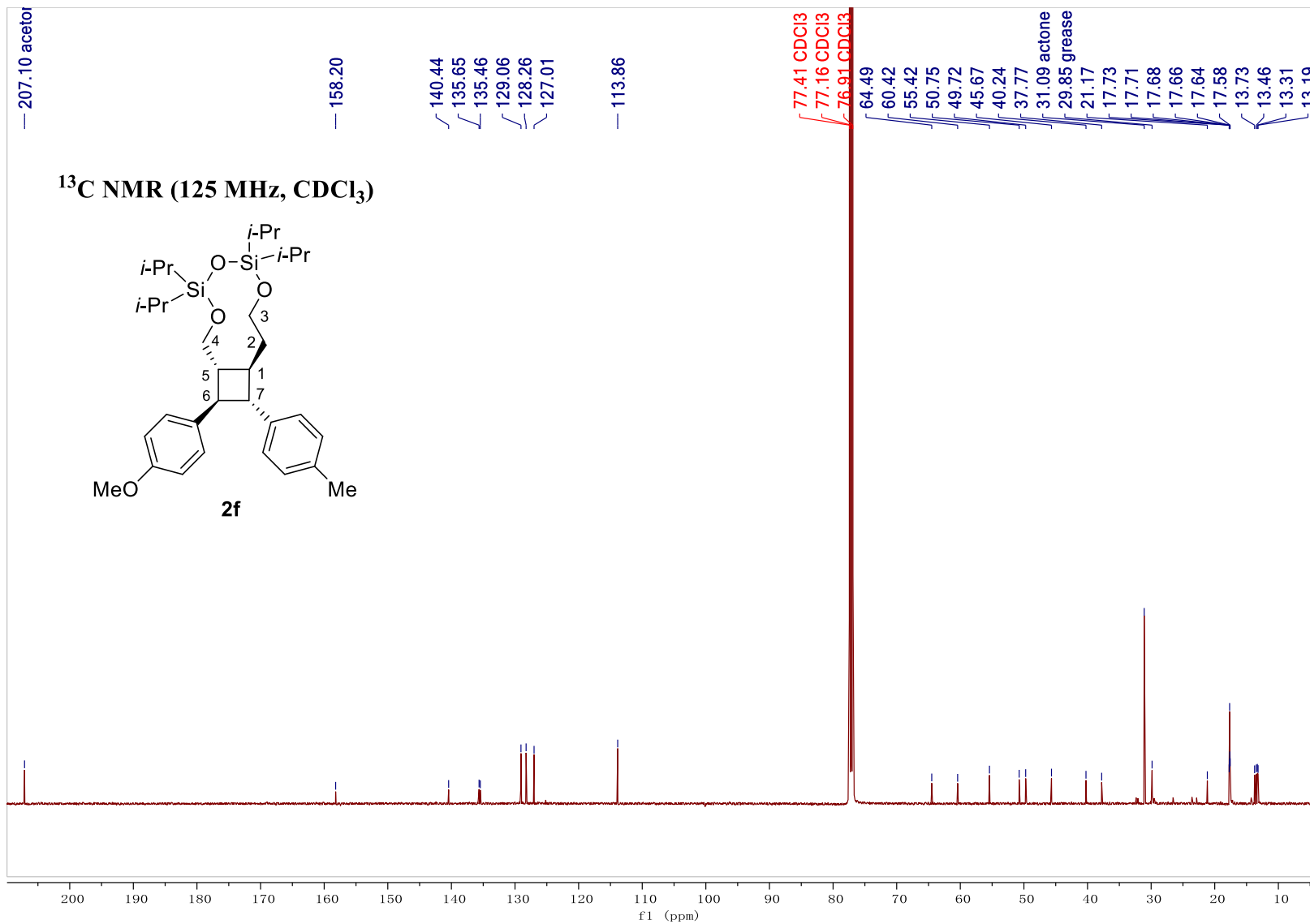


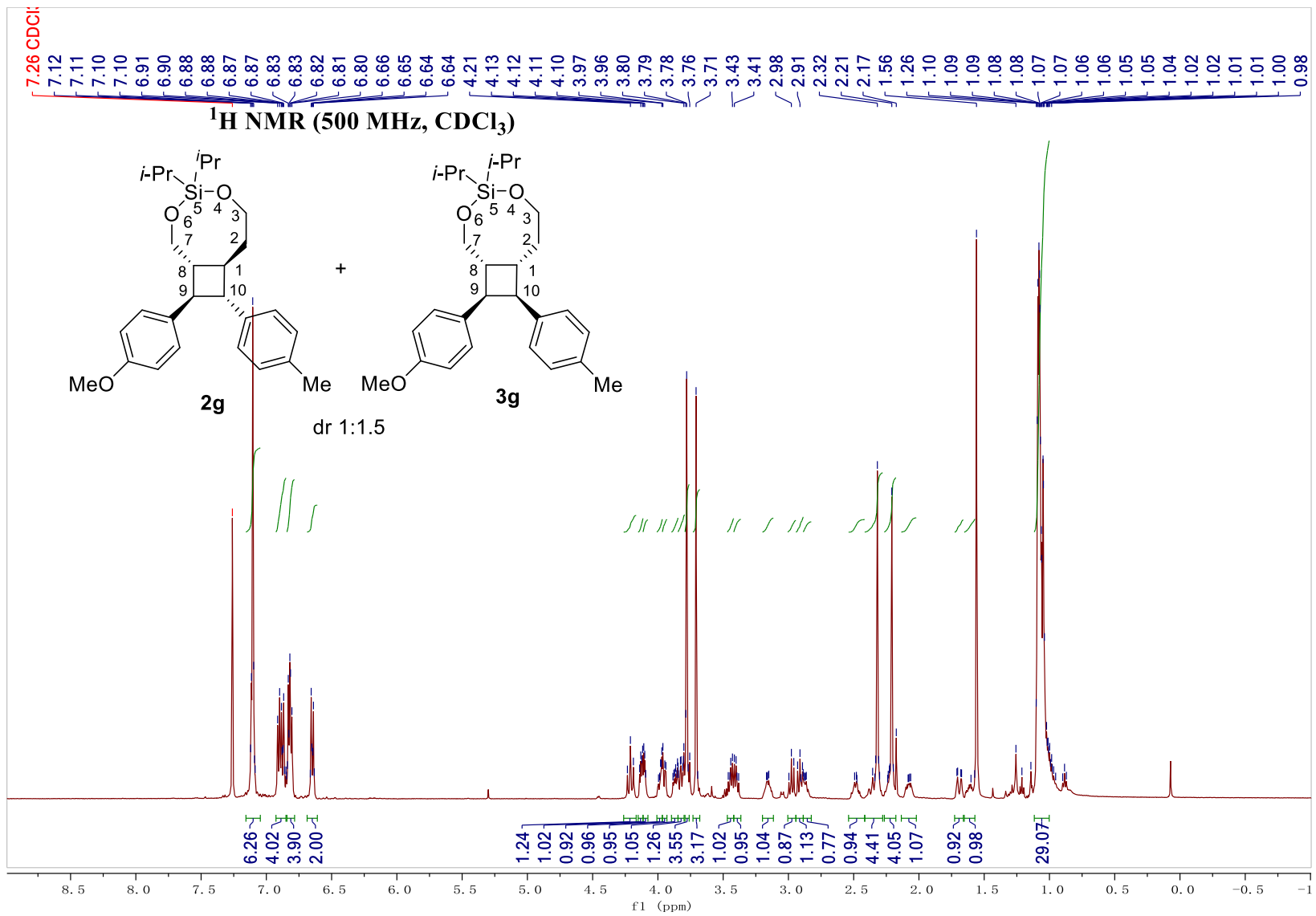


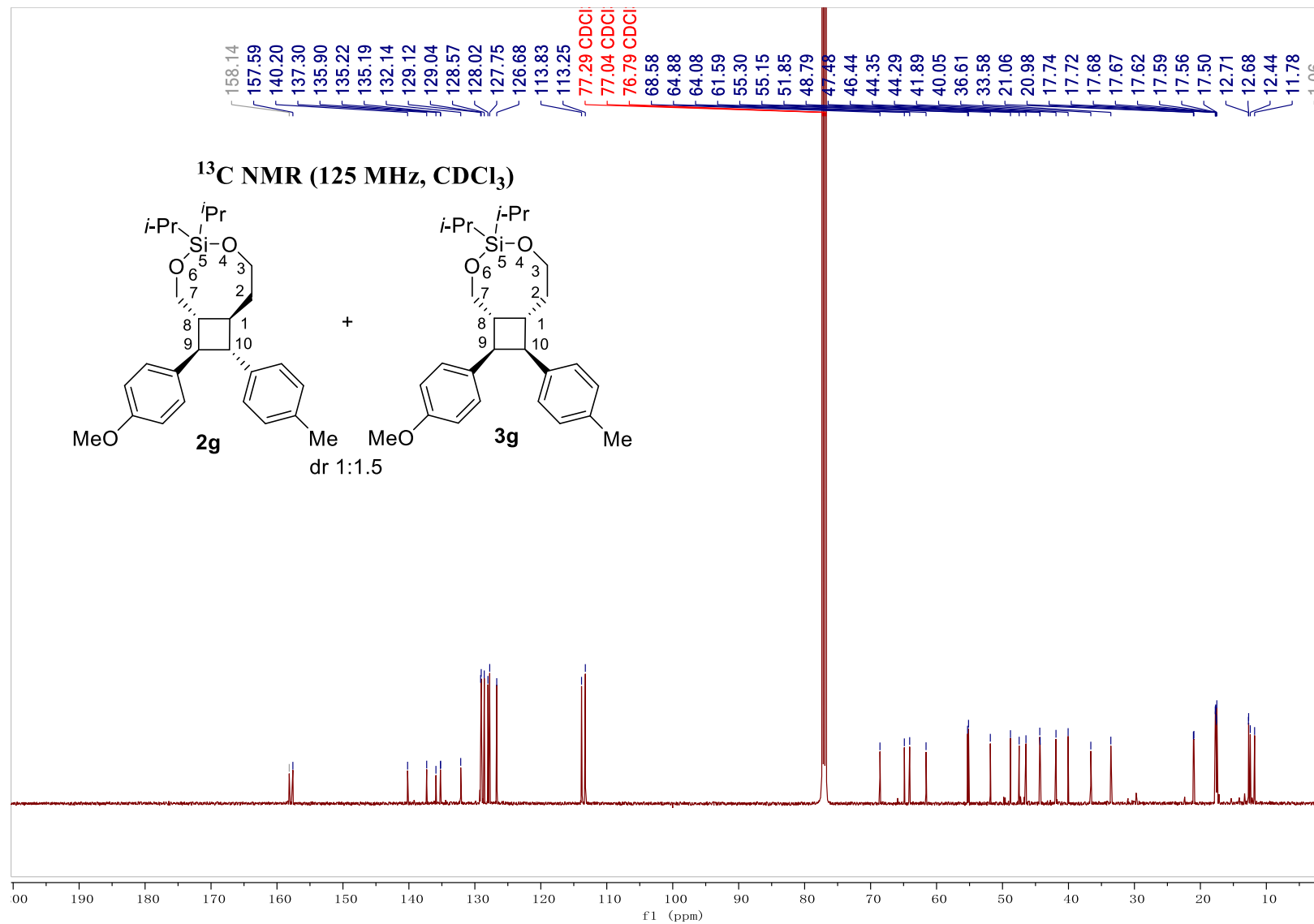


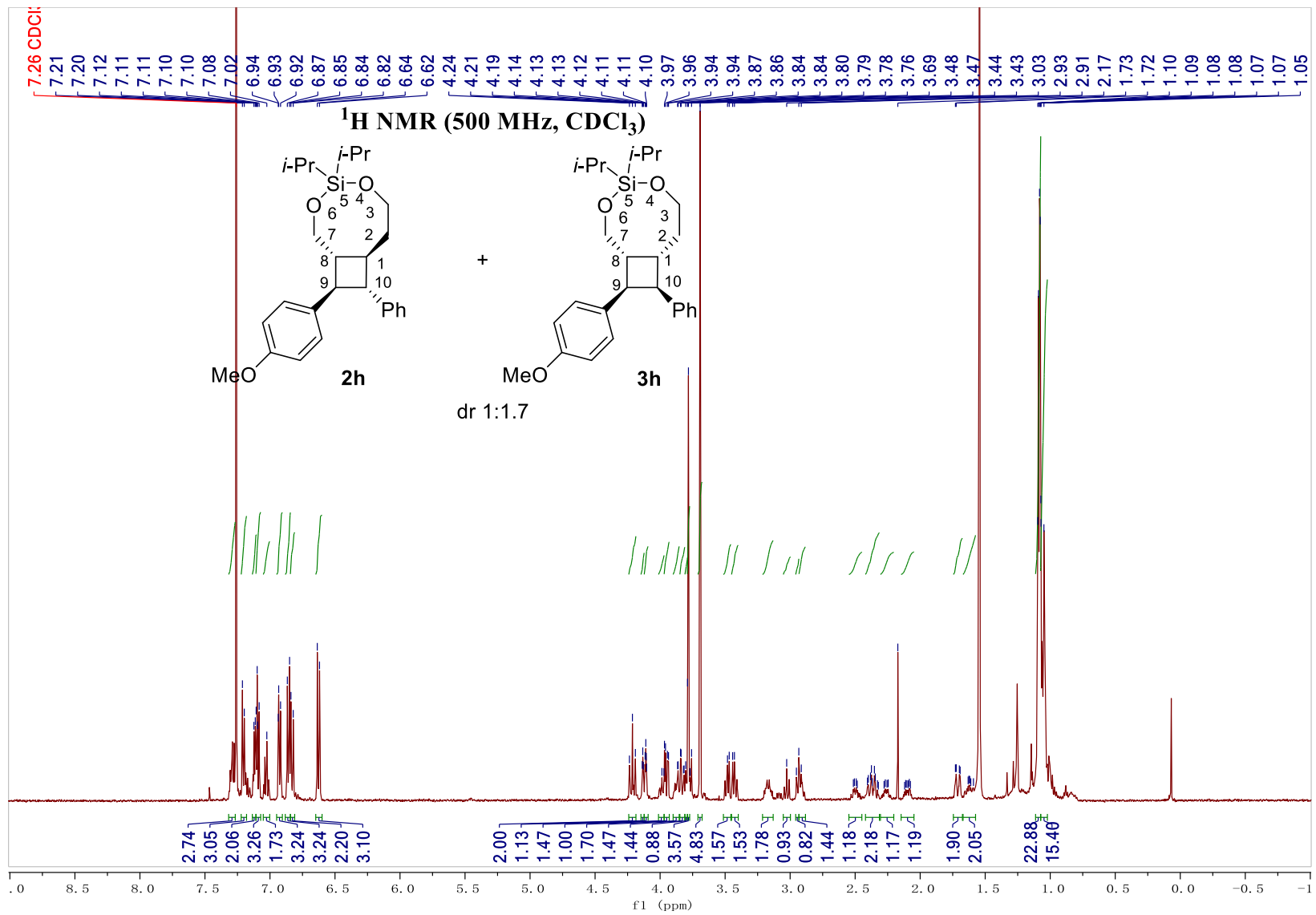


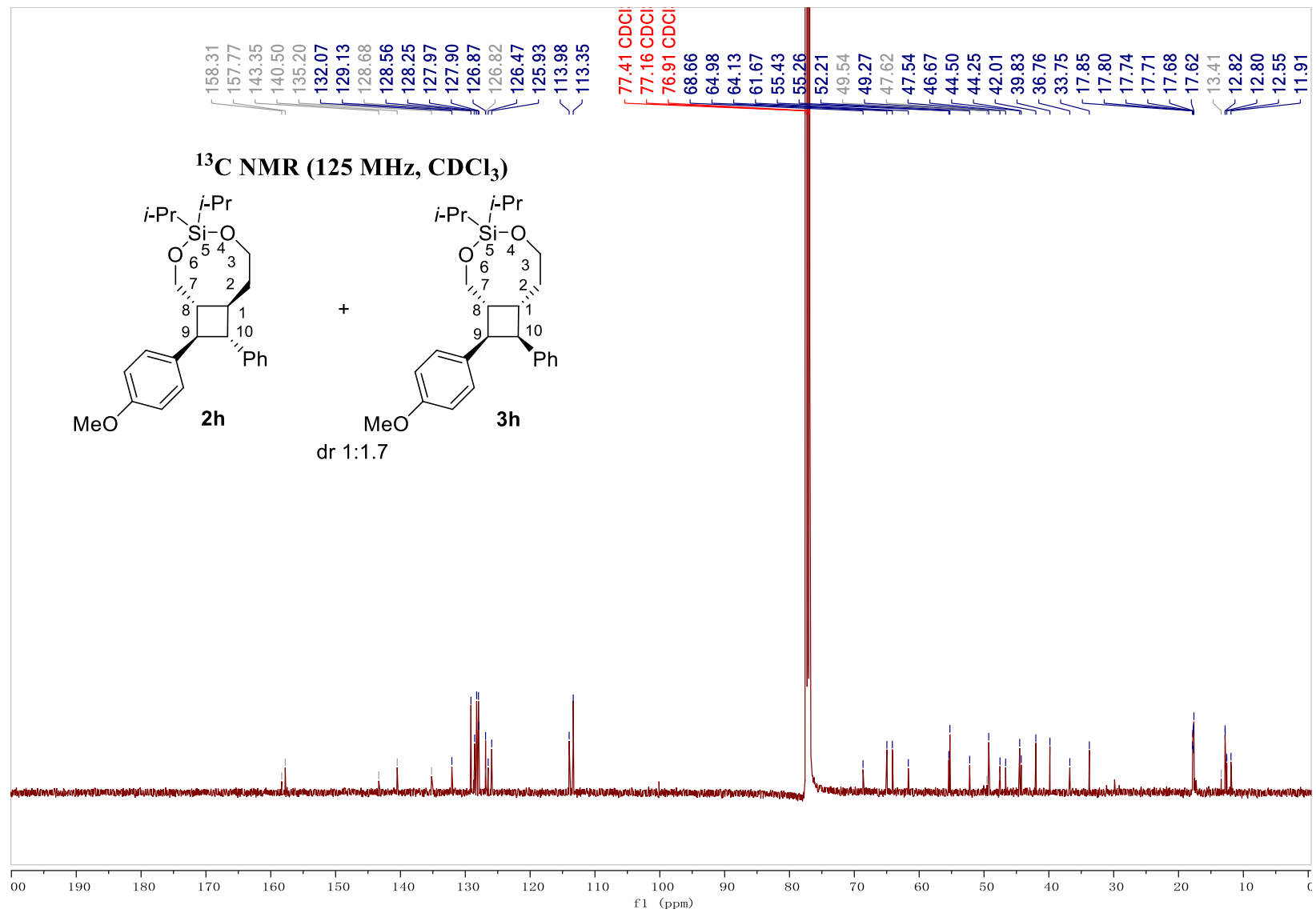


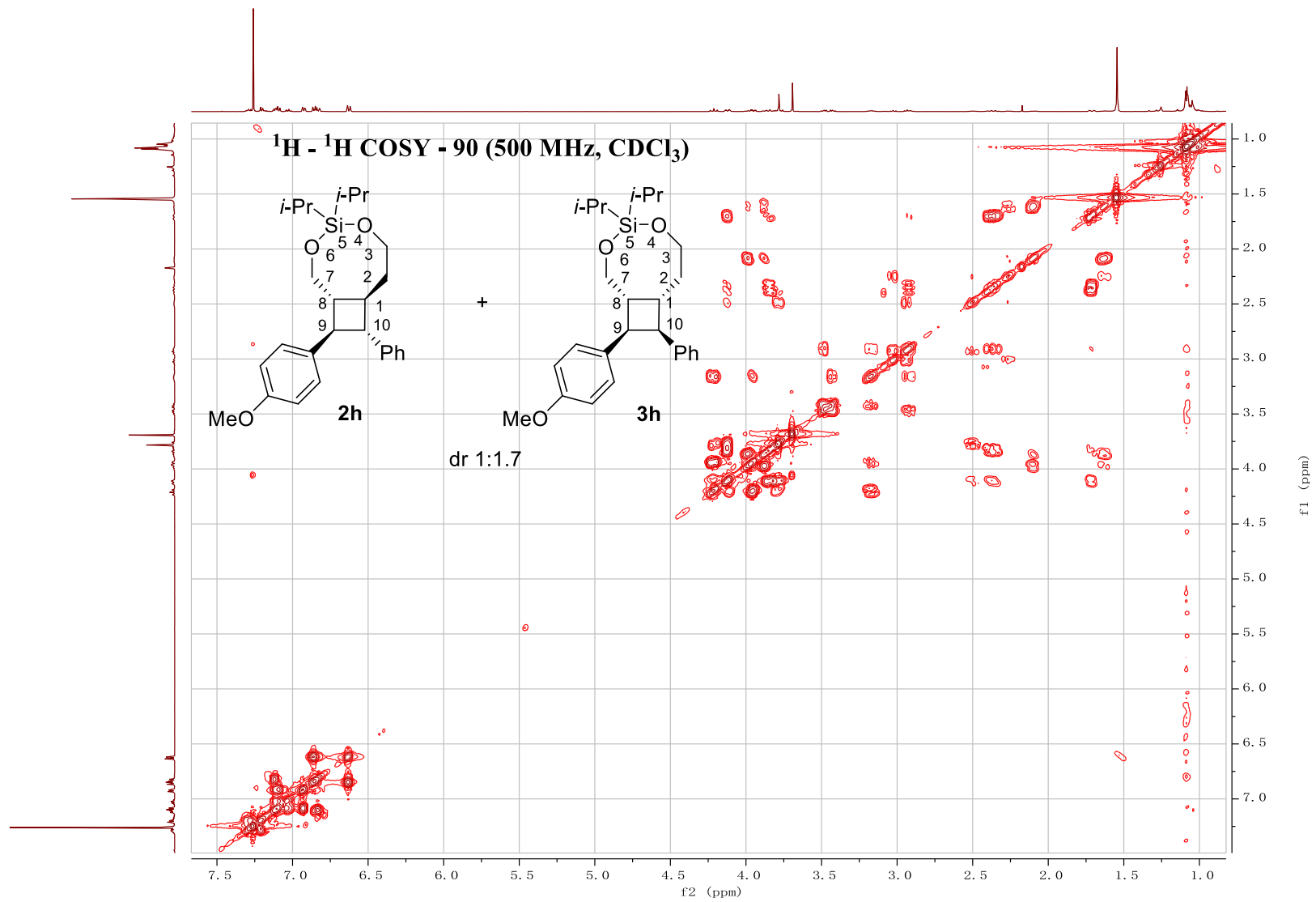


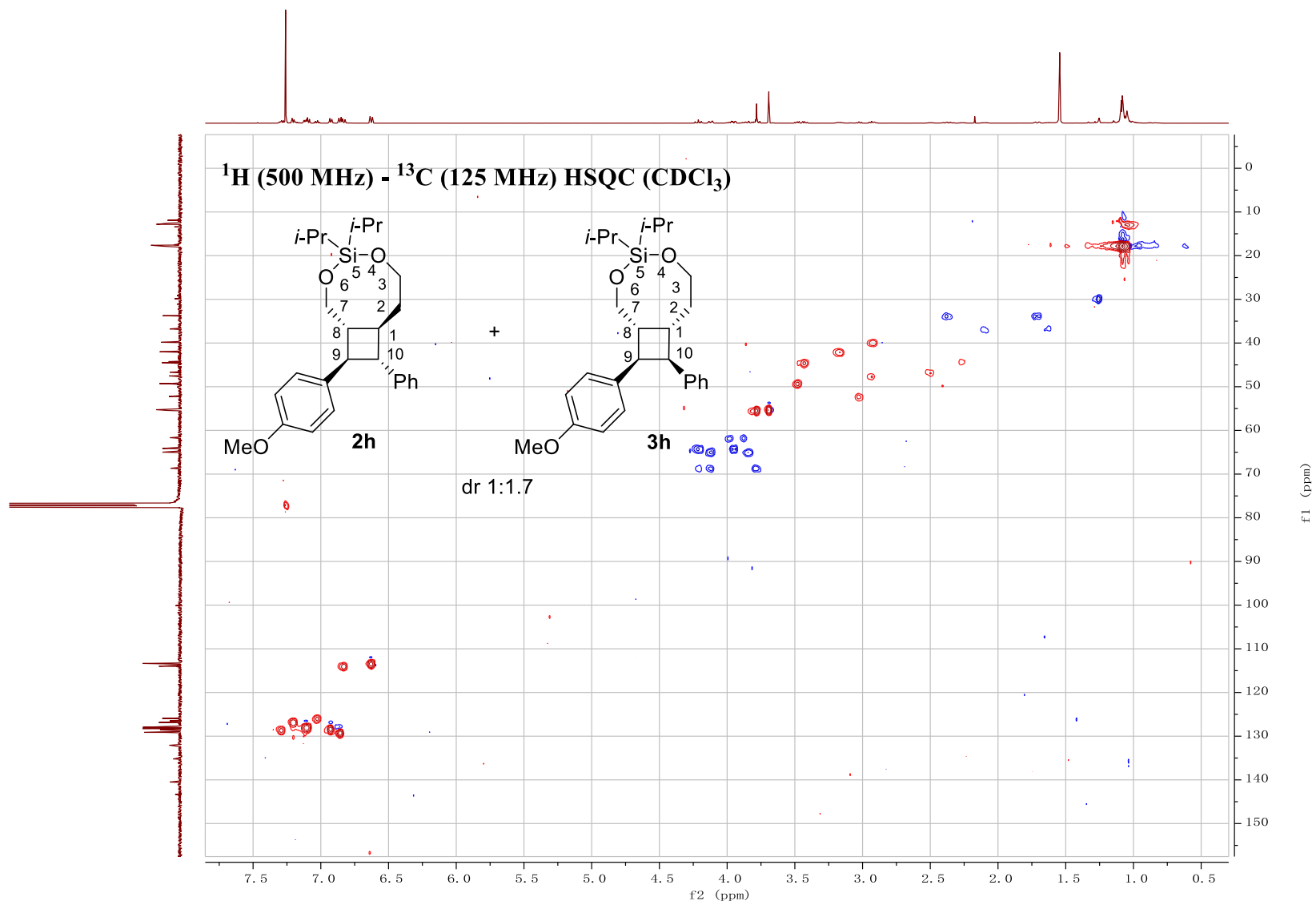




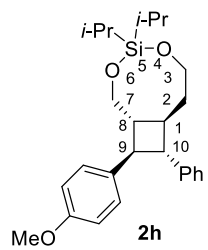




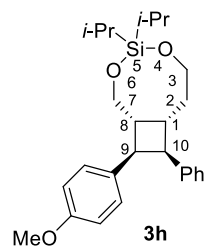




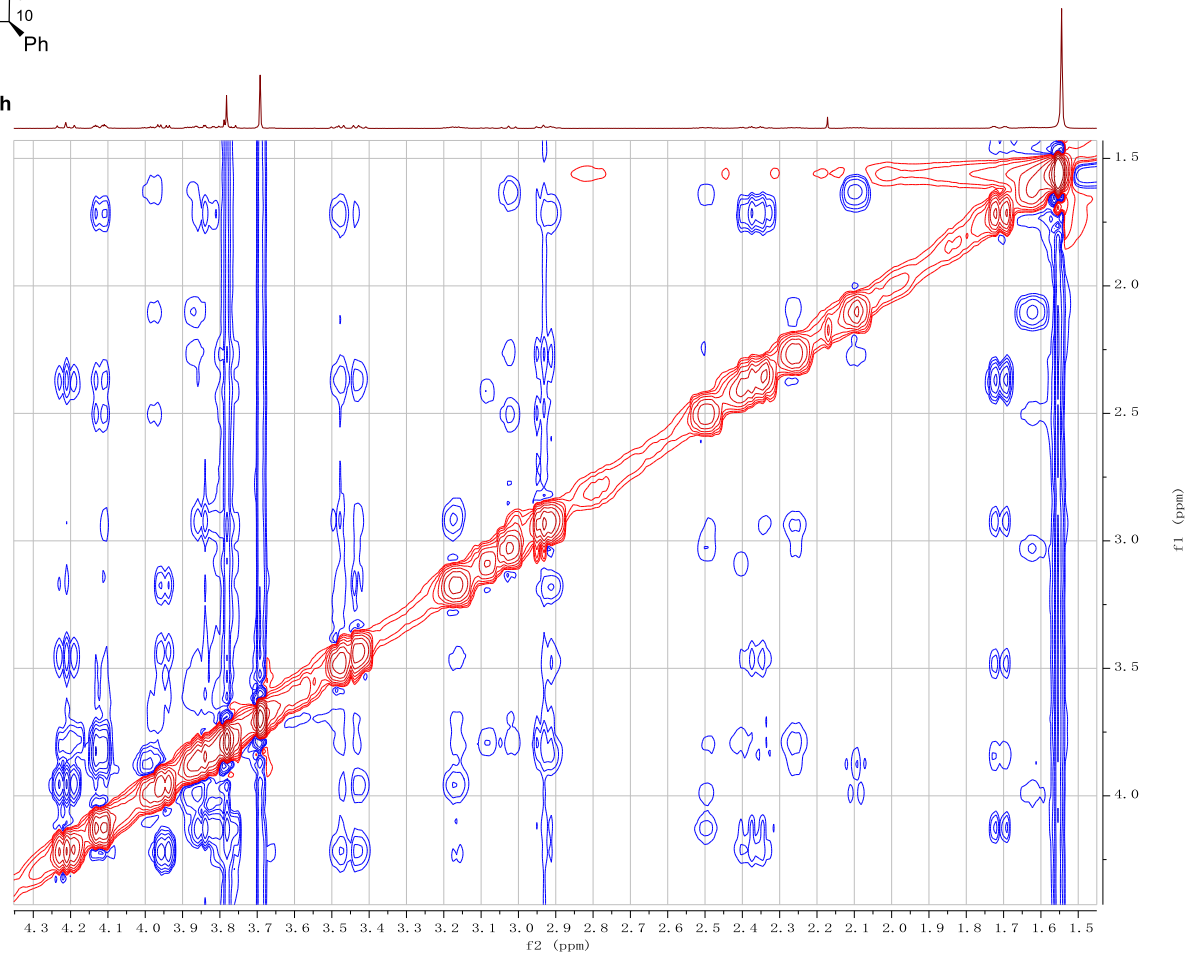
NOESY-2D (500 MHz, CDCl₃)

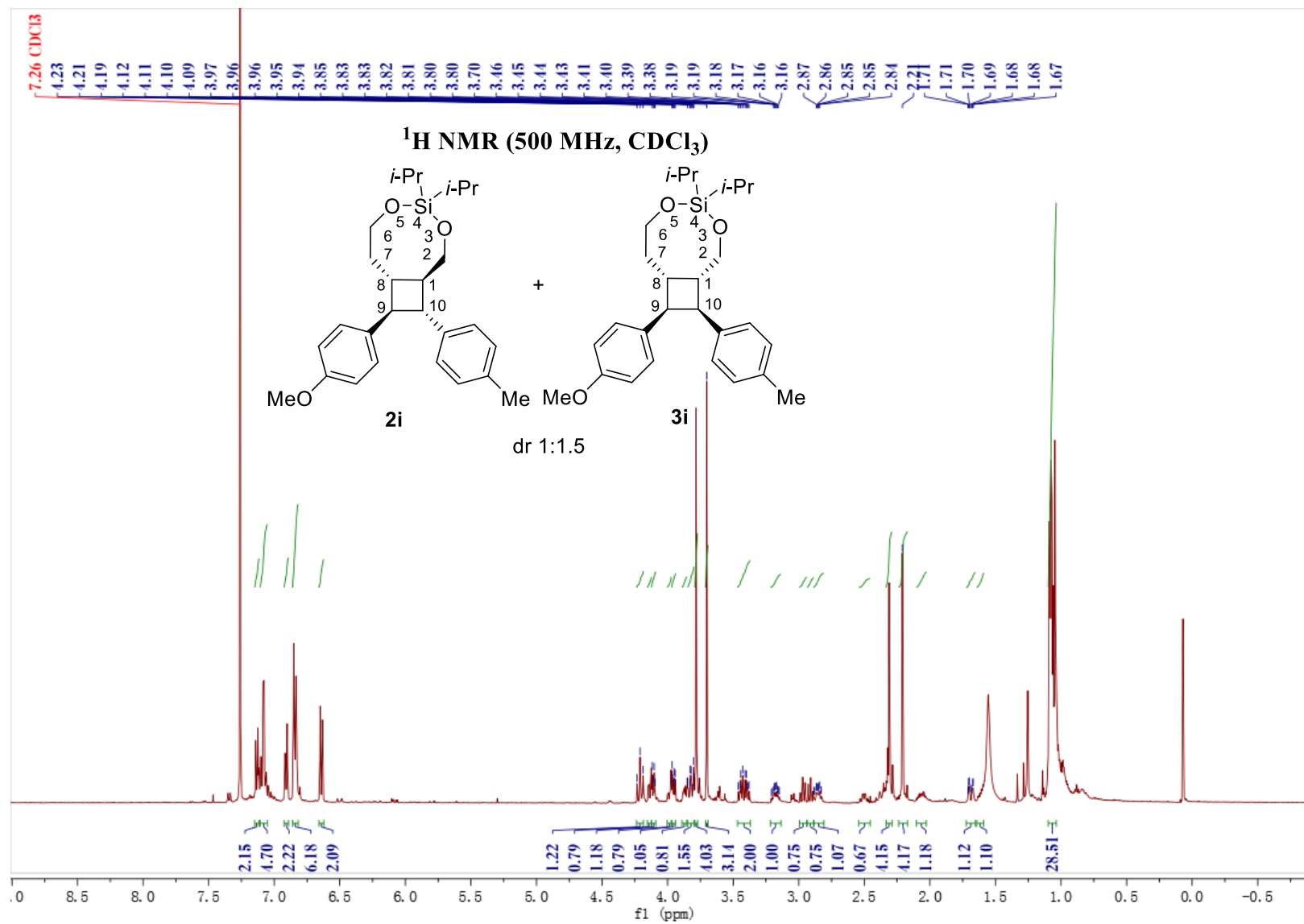


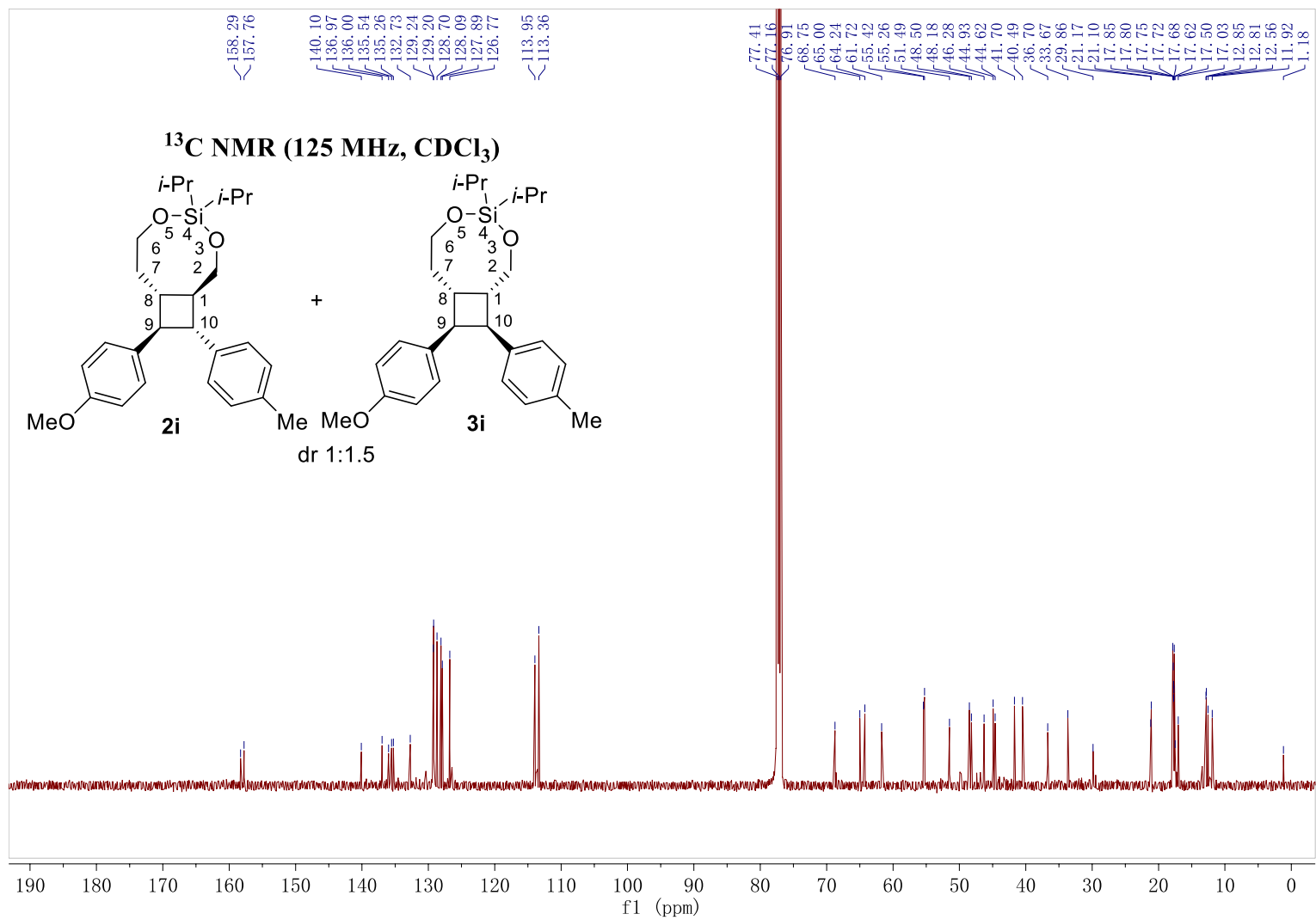
+

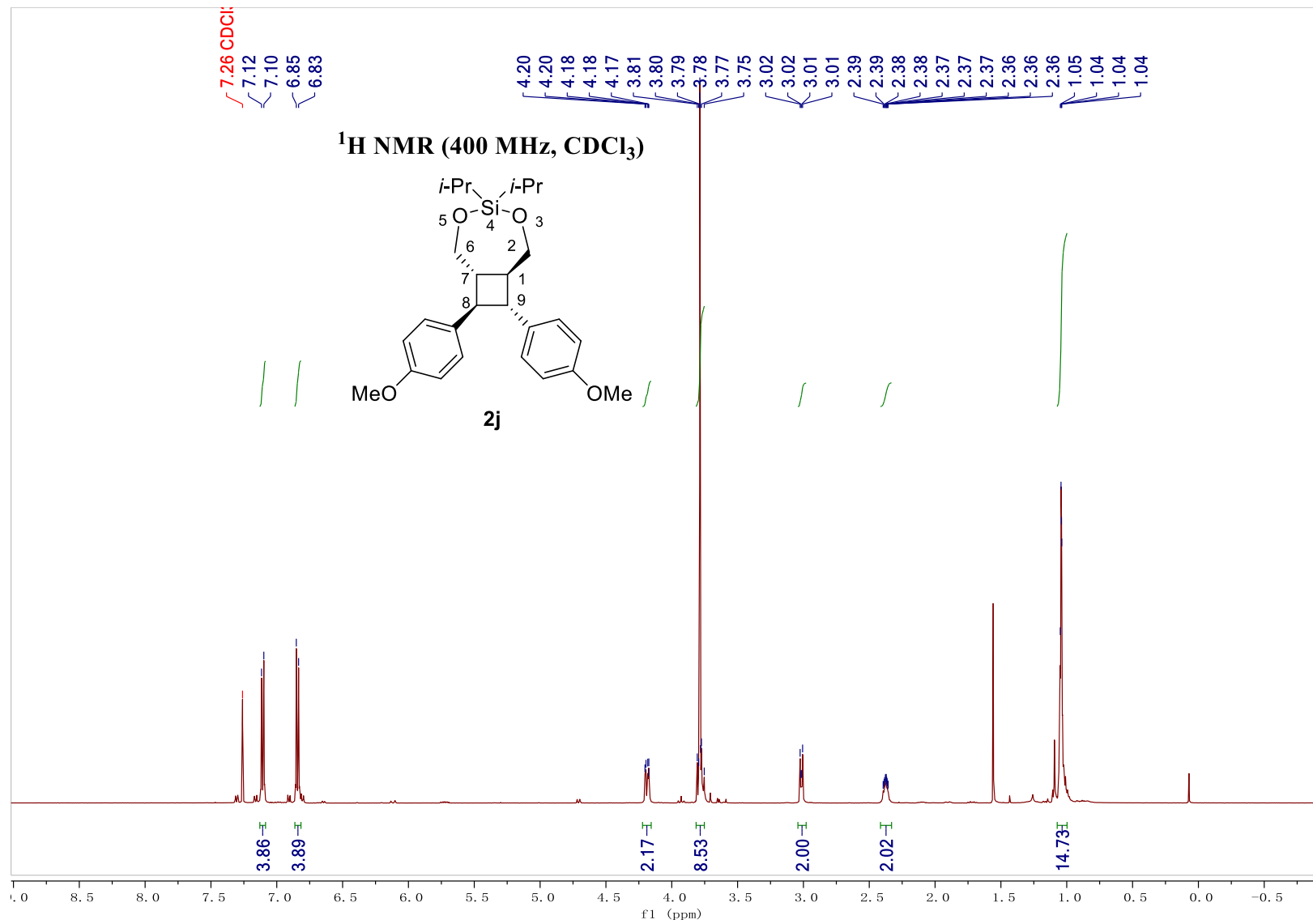


dr 1:1.7

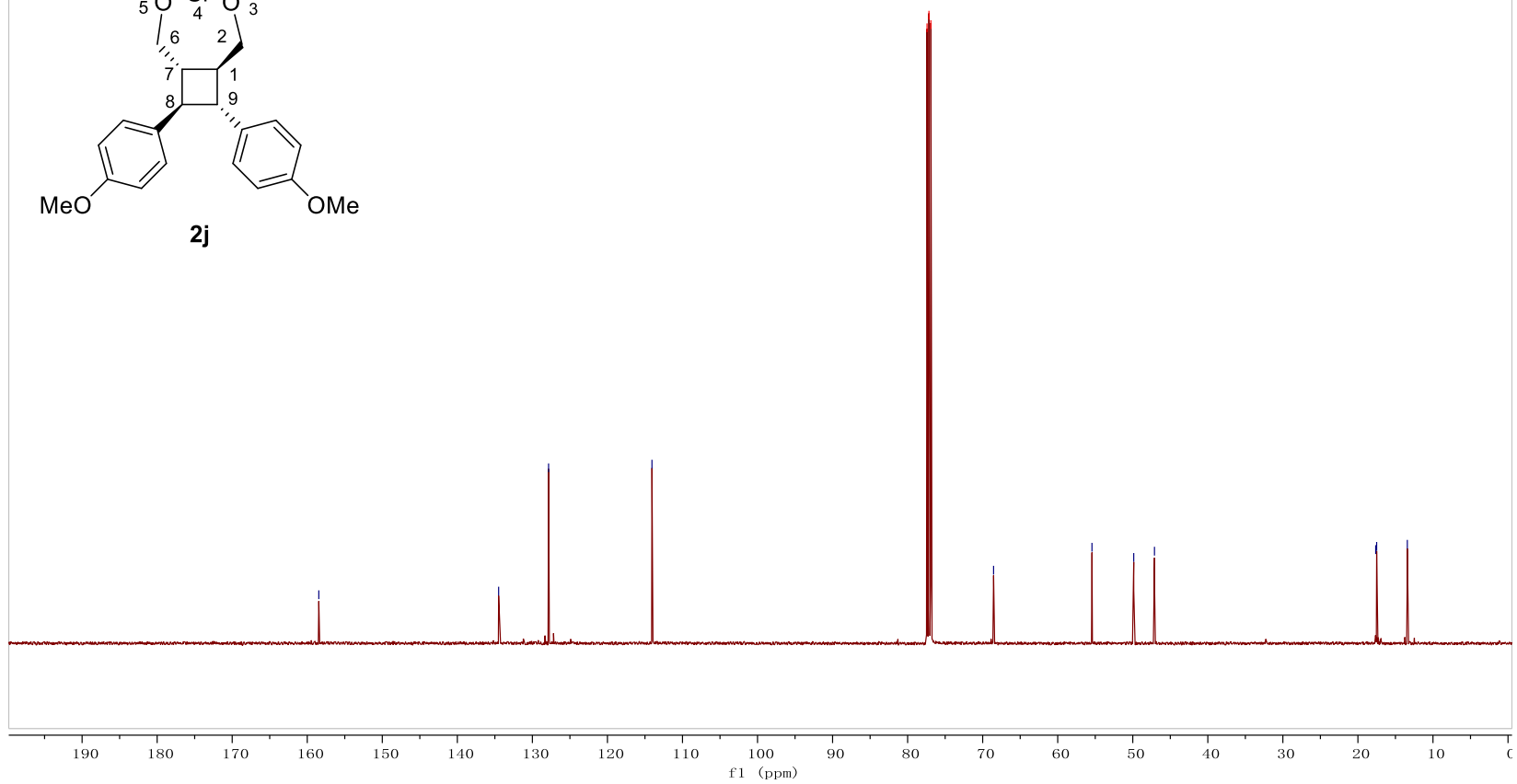
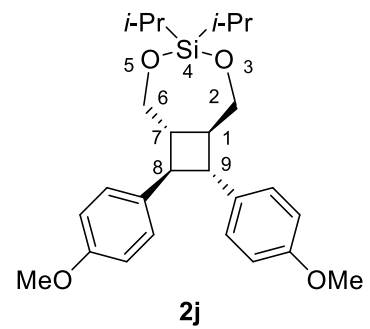


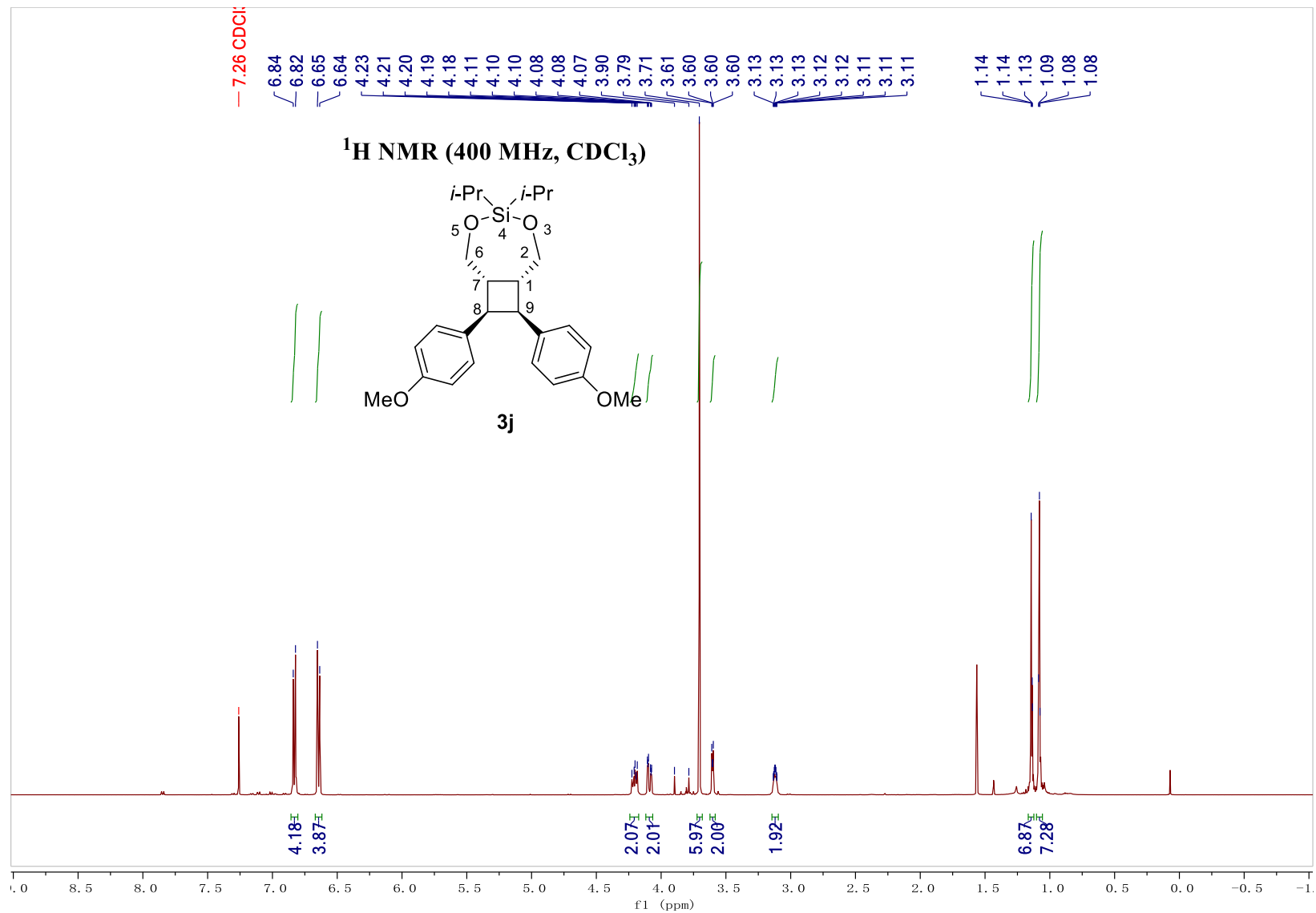


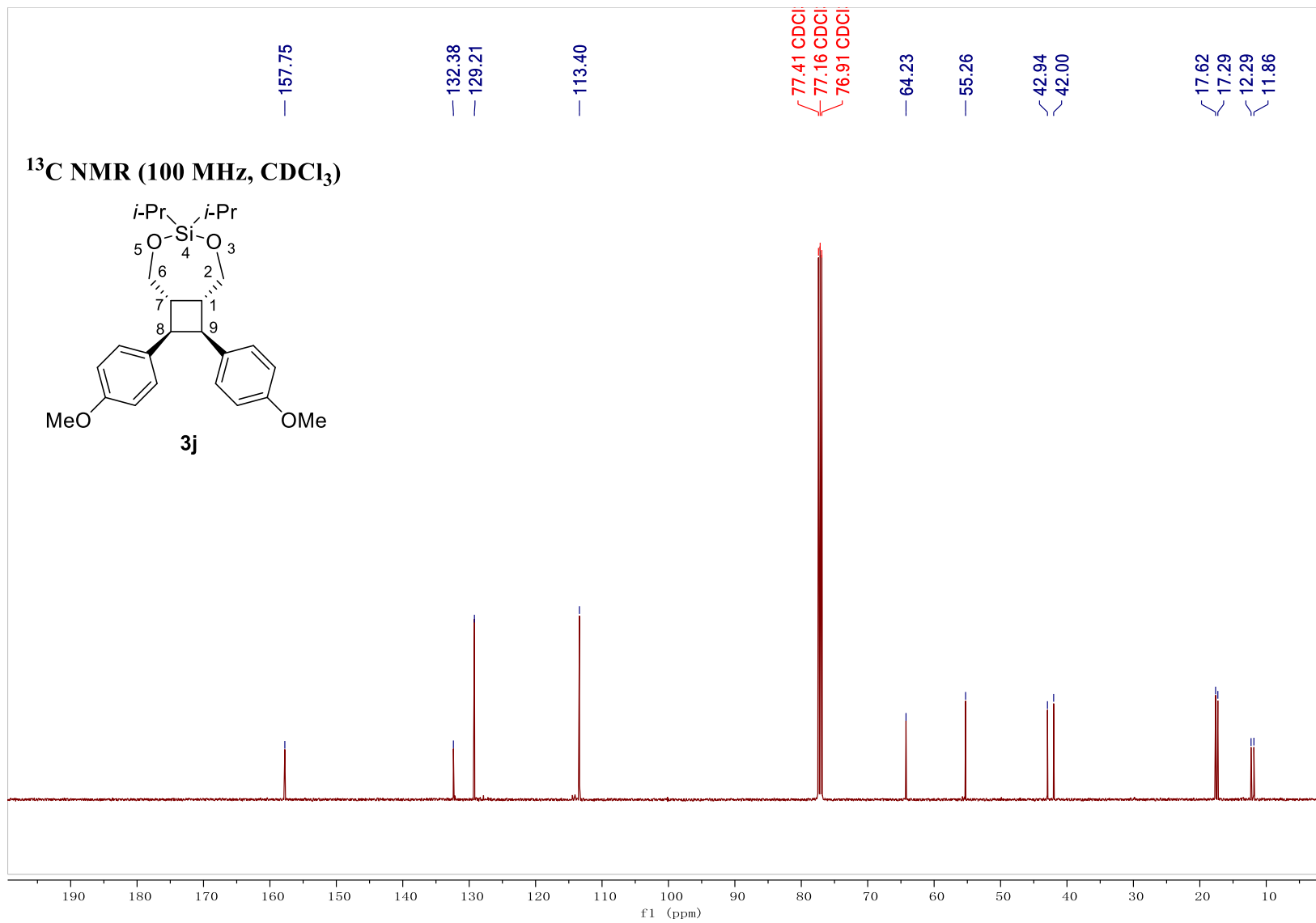


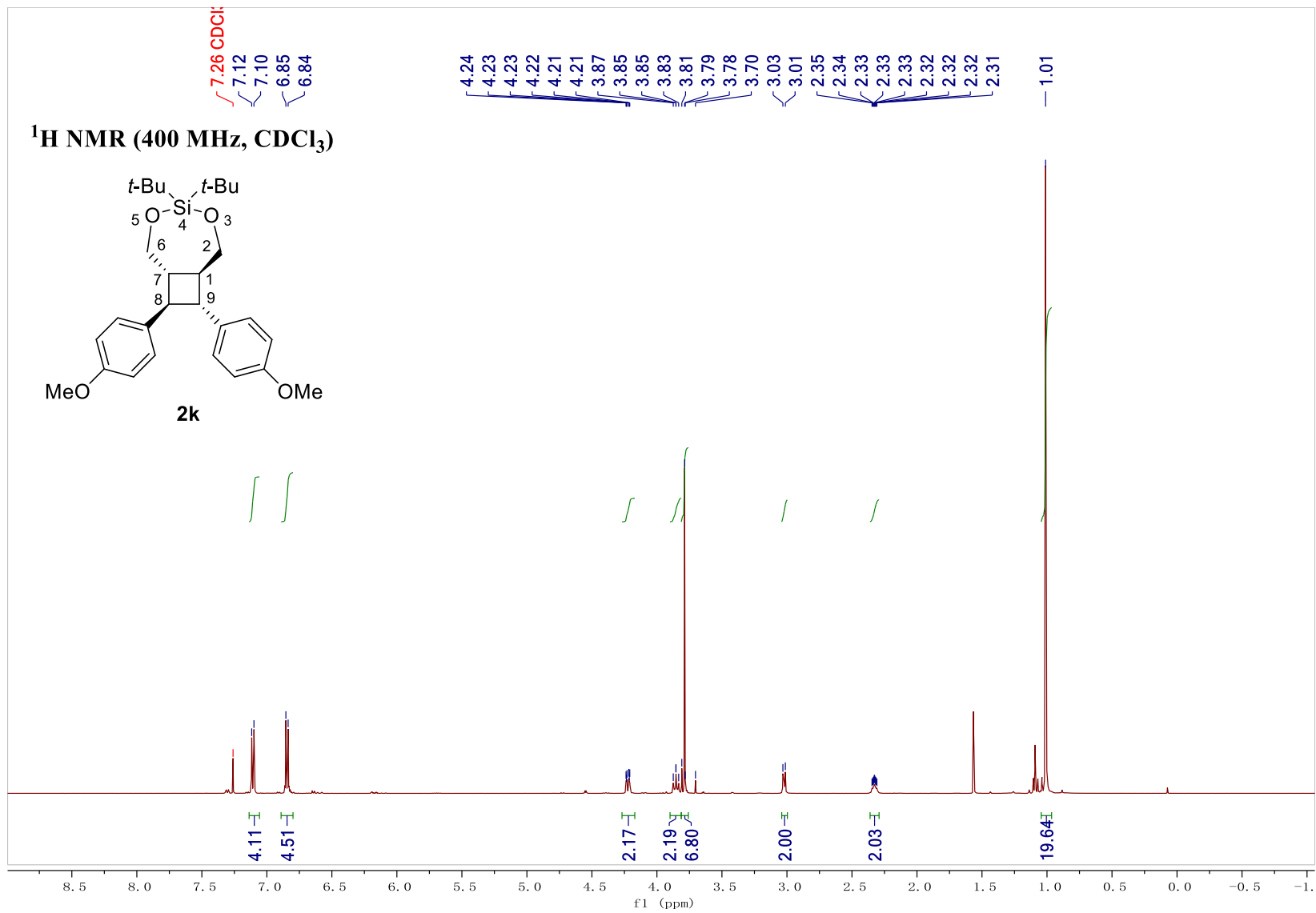


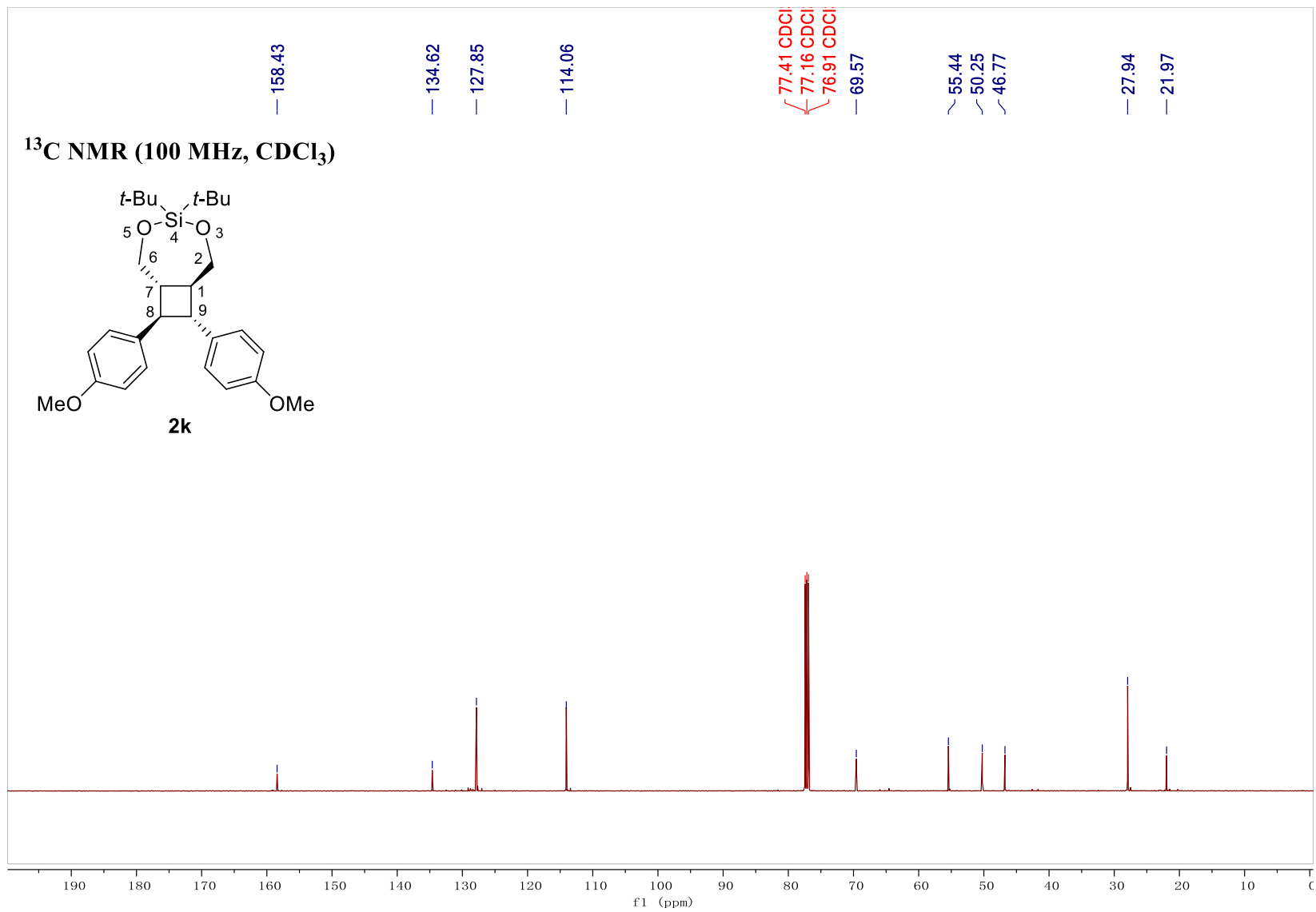
¹³C NMR (100 MHz, CDCl₃)

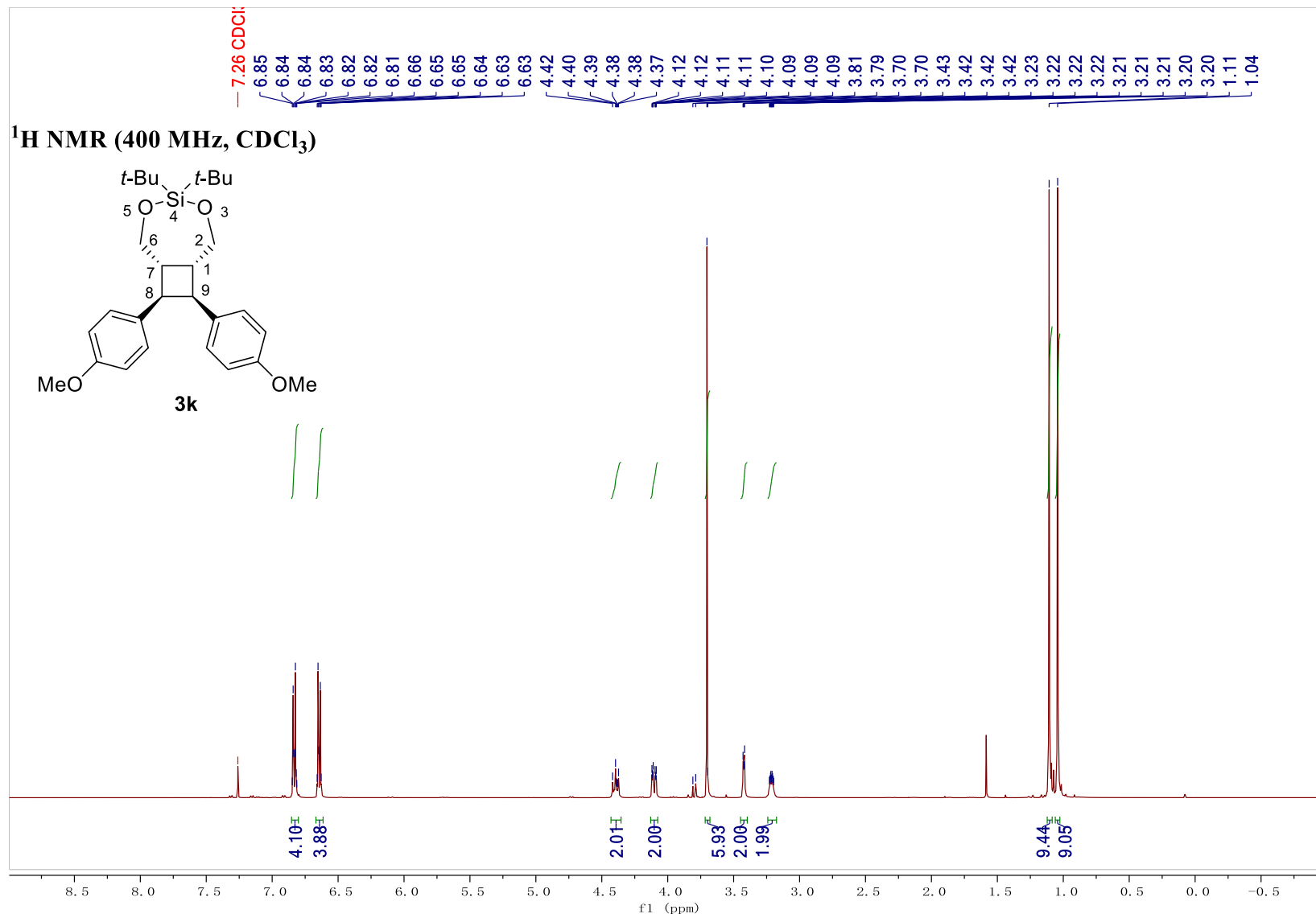


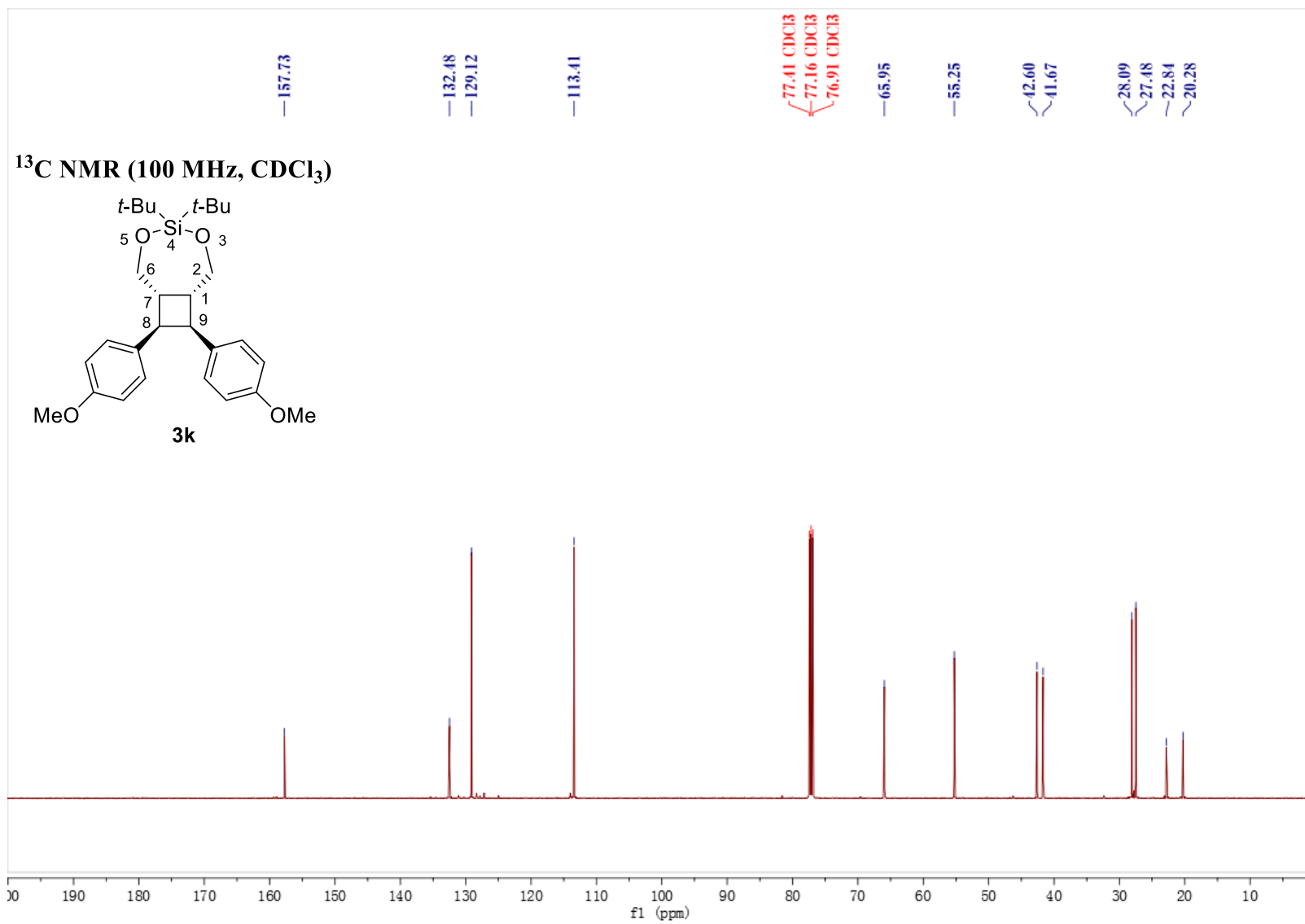




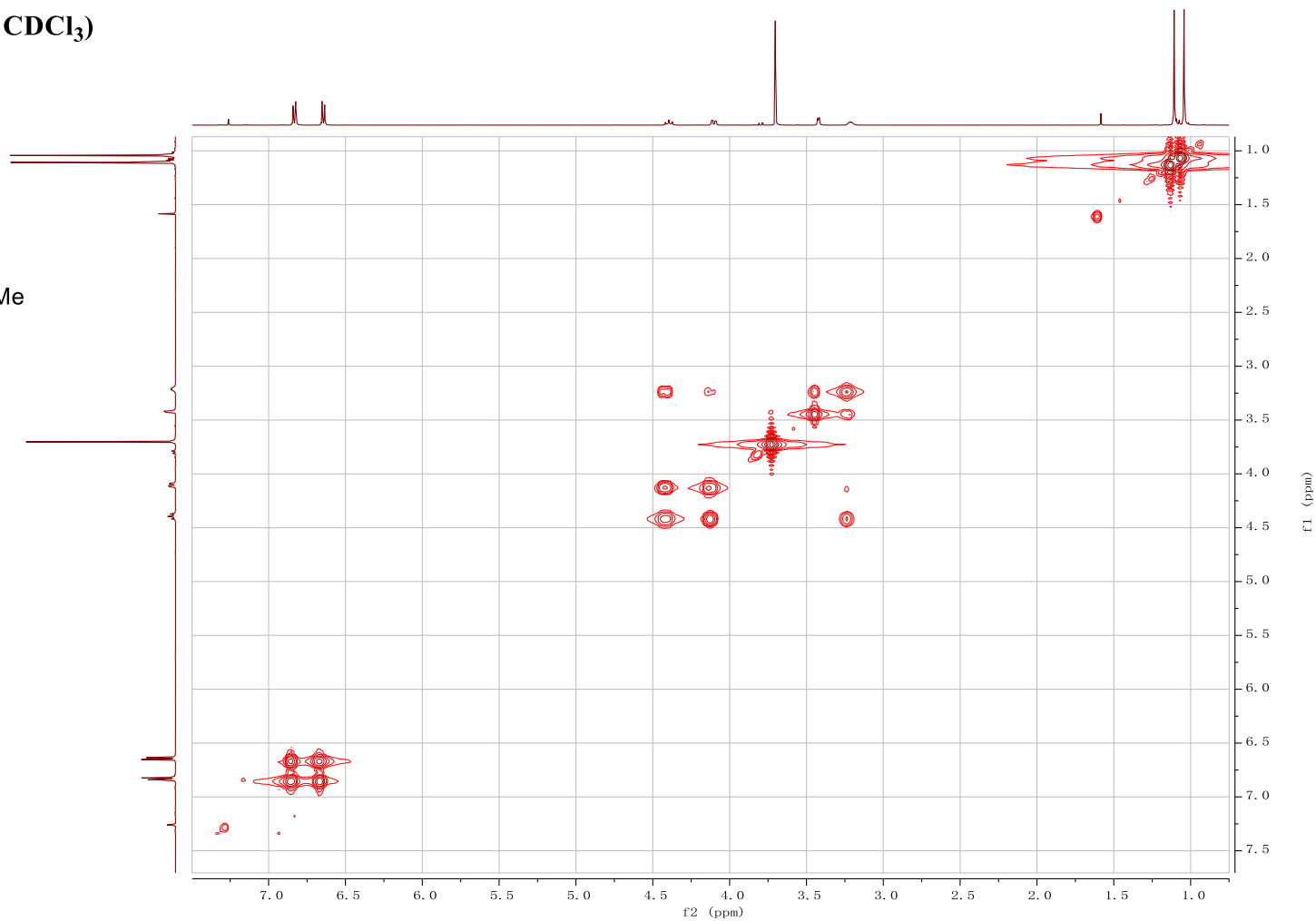
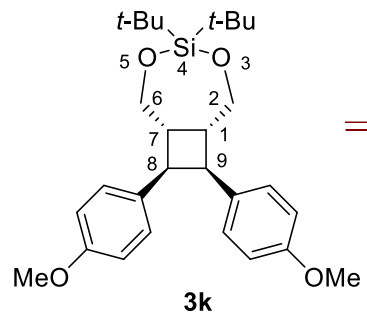




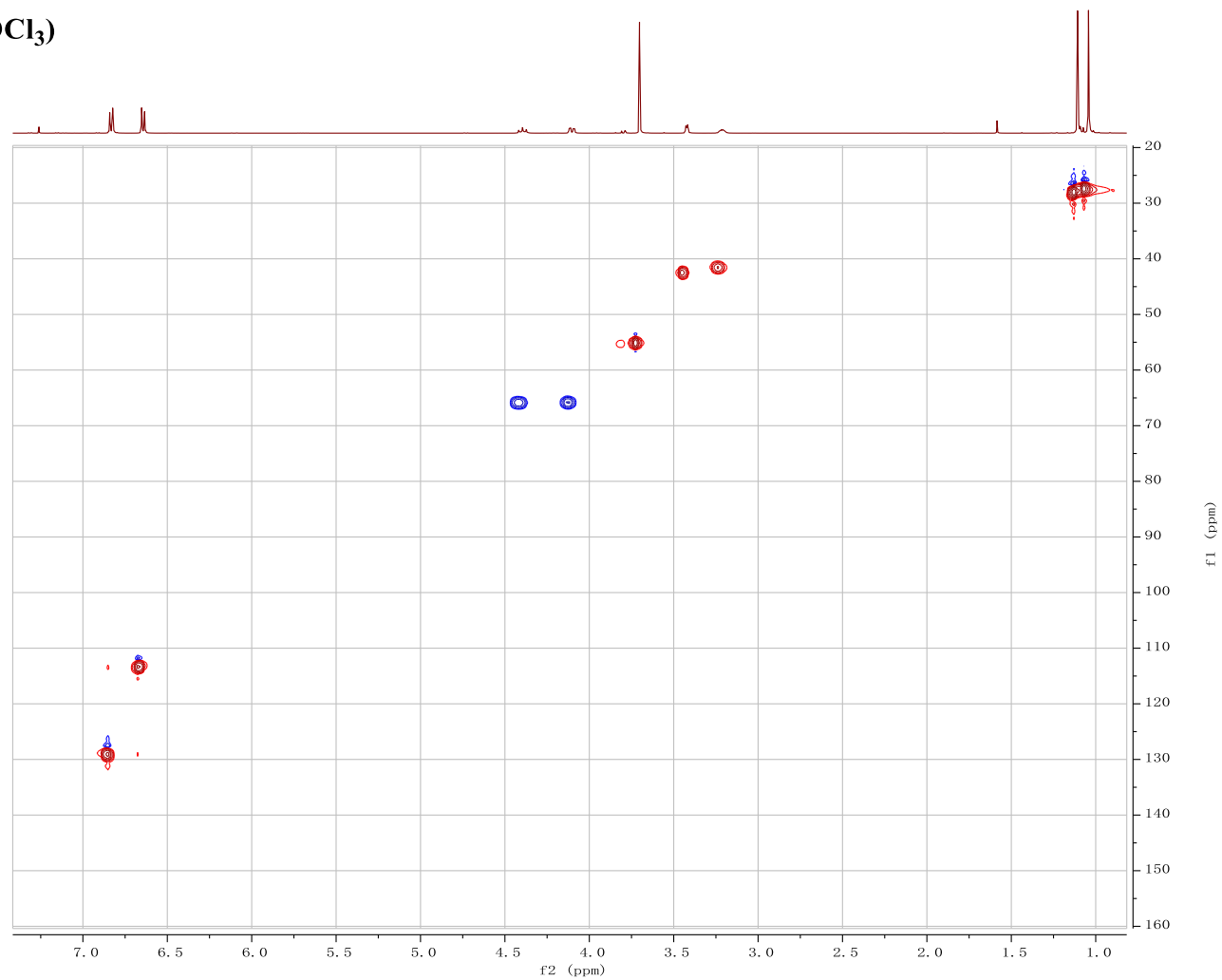
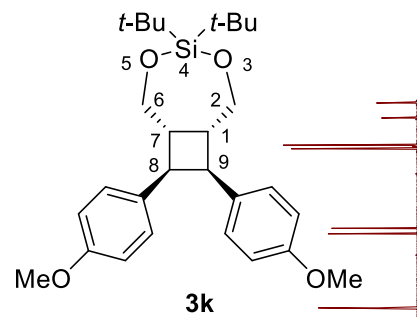




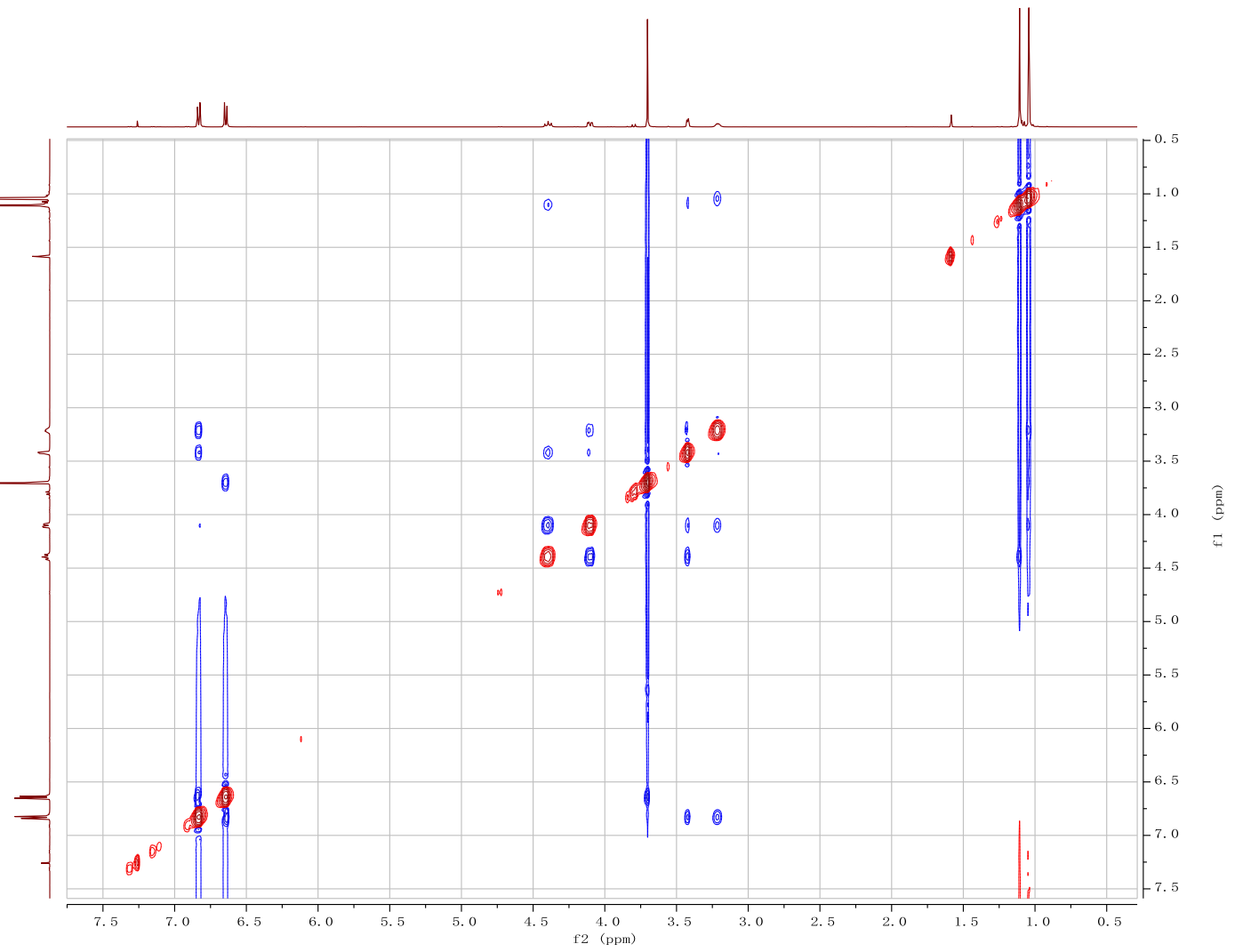
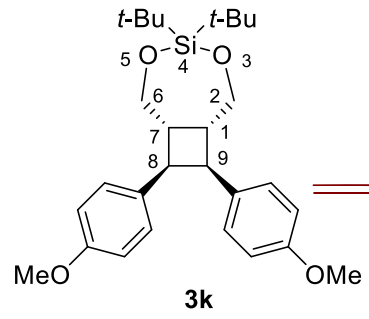
$^1\text{H} - ^1\text{H}$ COSY - 90 (400 MHz, CDCl_3)

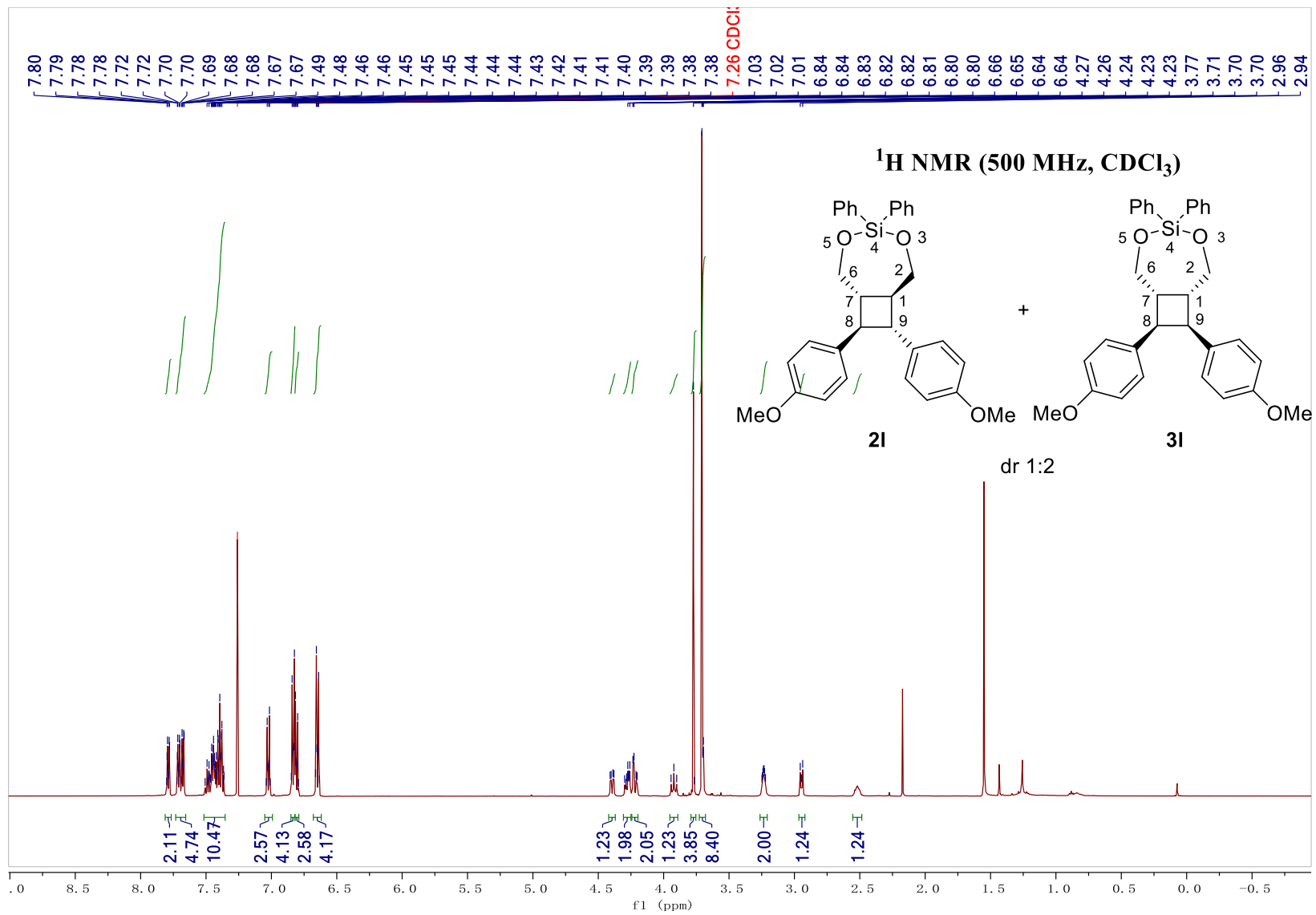


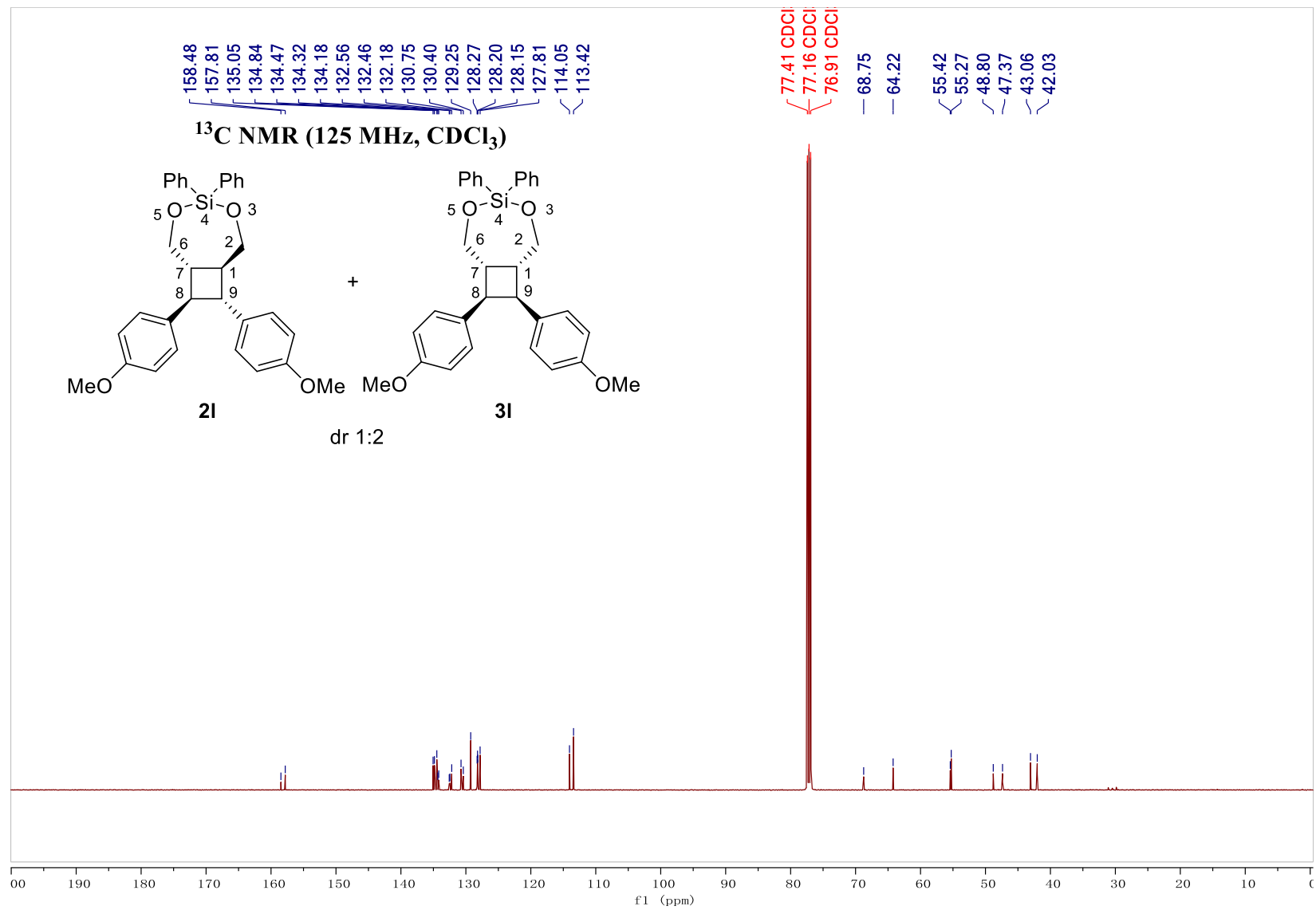
^1H (400 MHz) - ^{13}C (100 MHz) HSQC (CDCl_3)

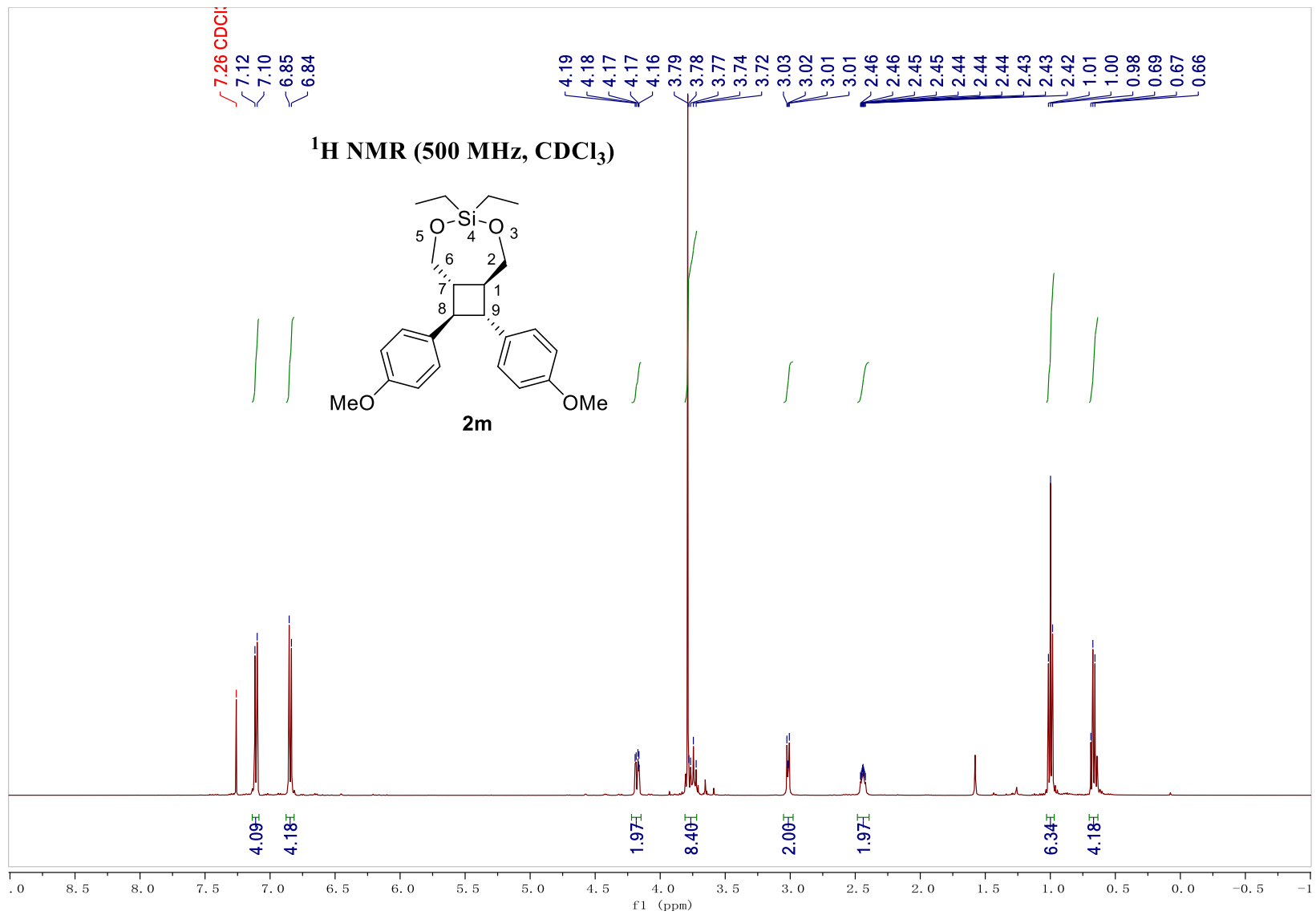


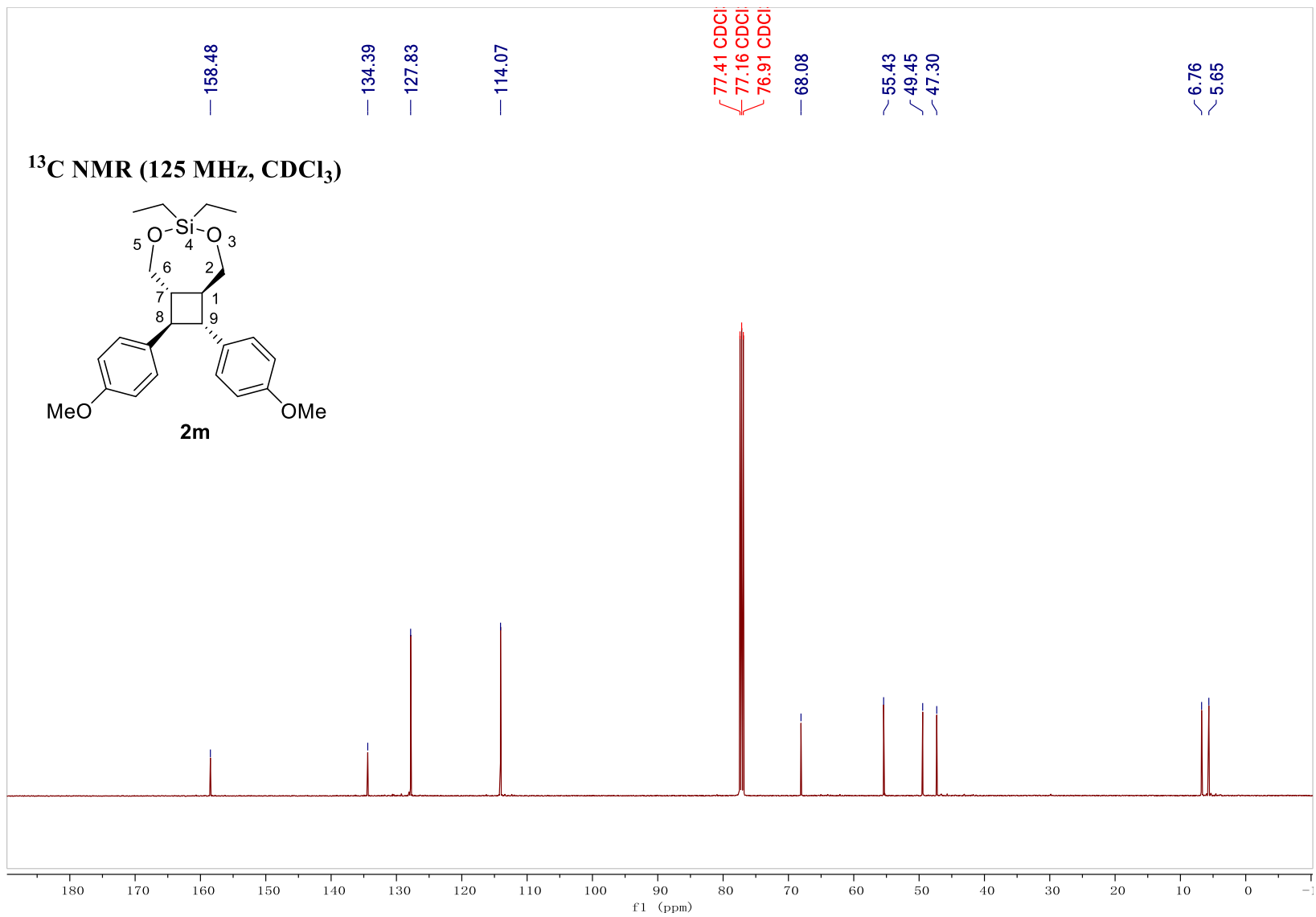
NOESY-2D (400 MHz, CDCl₃)

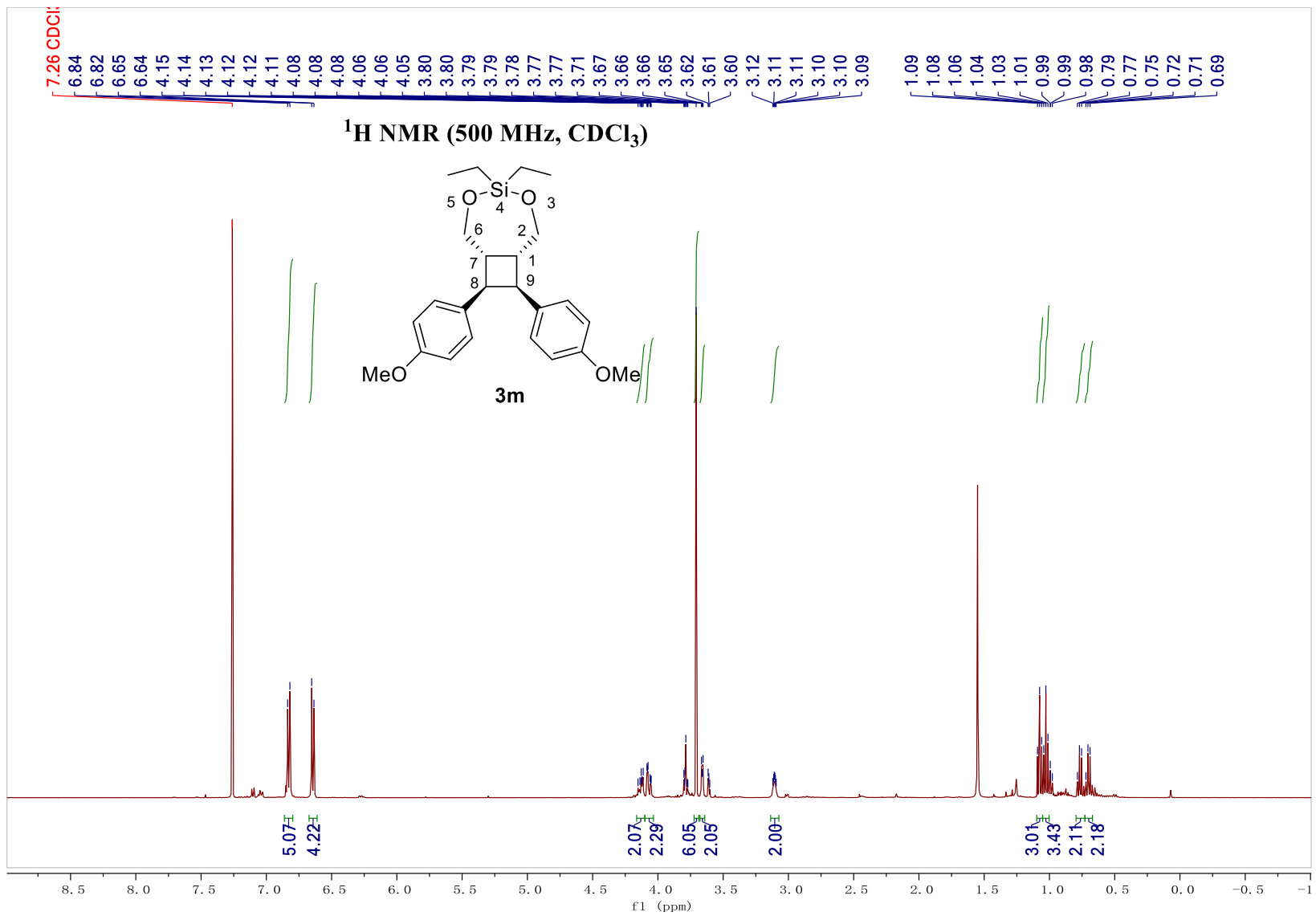


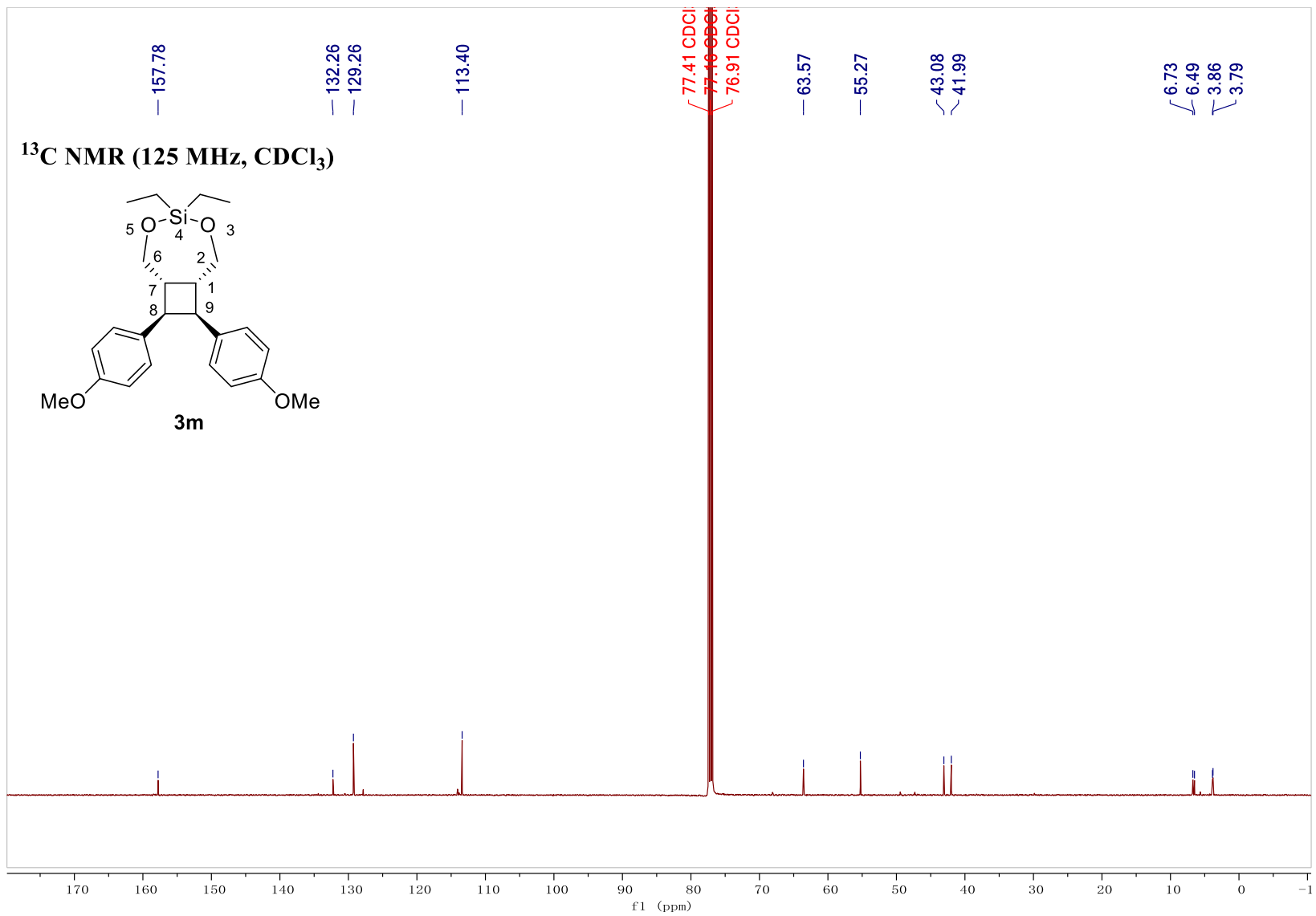


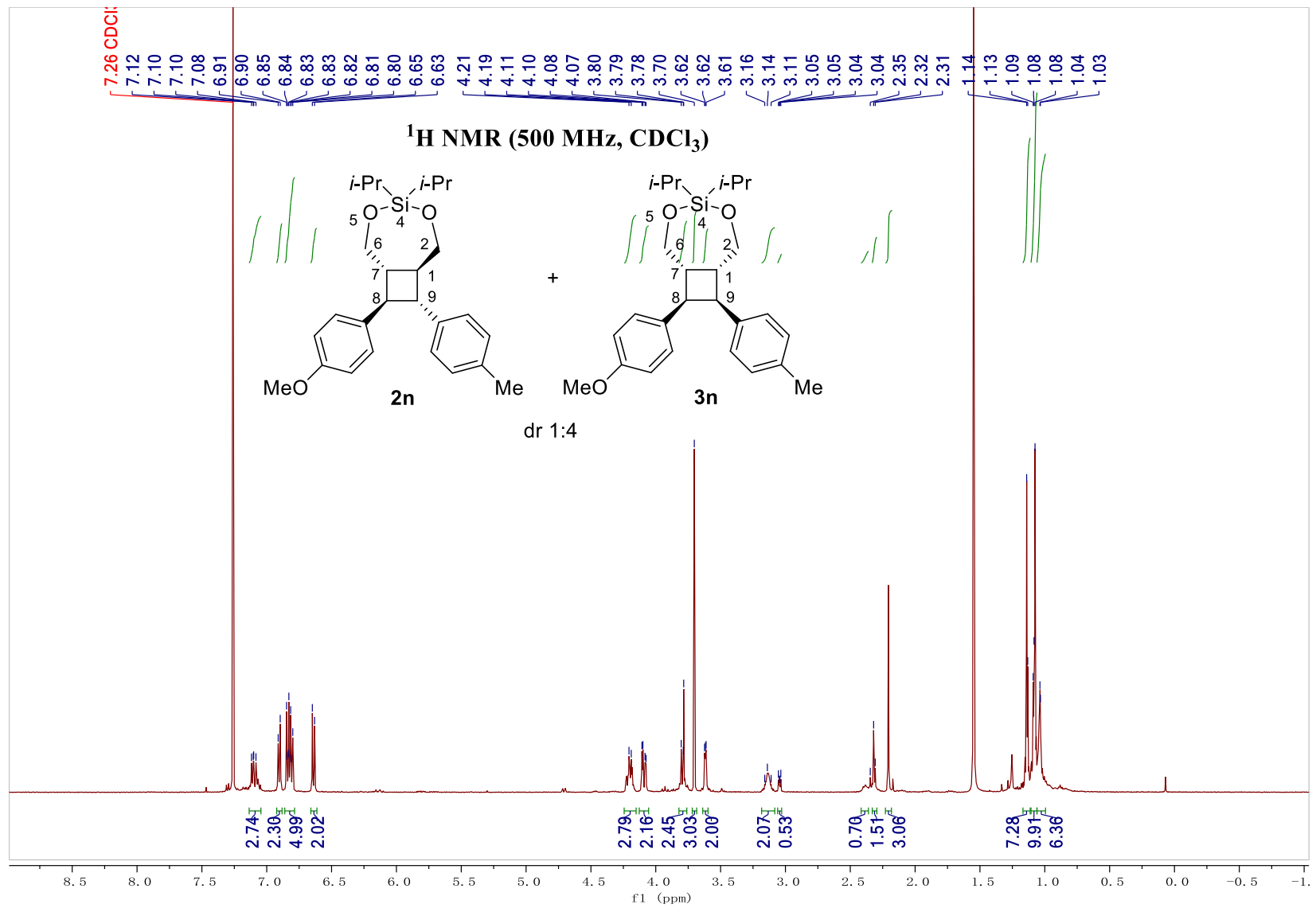


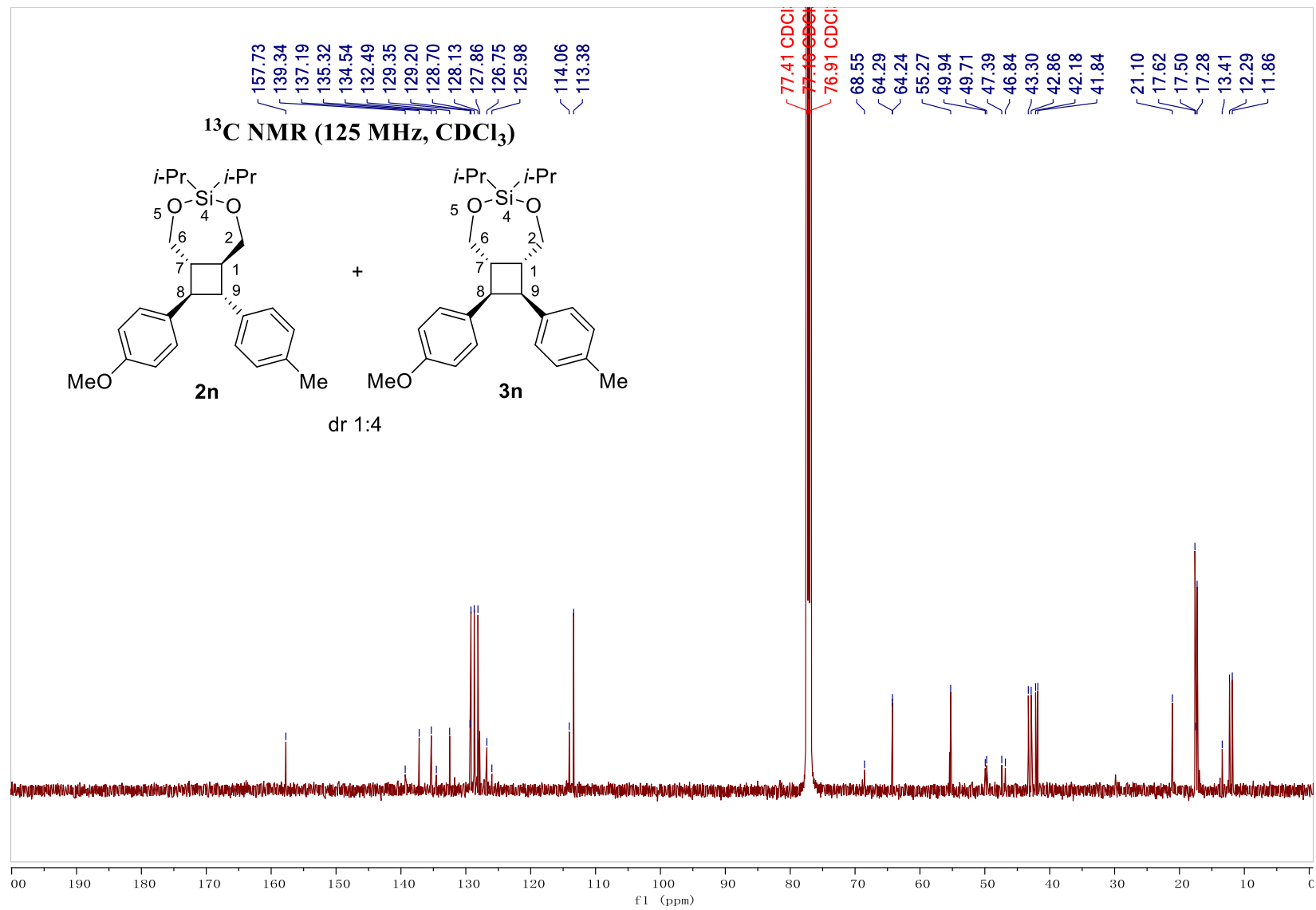


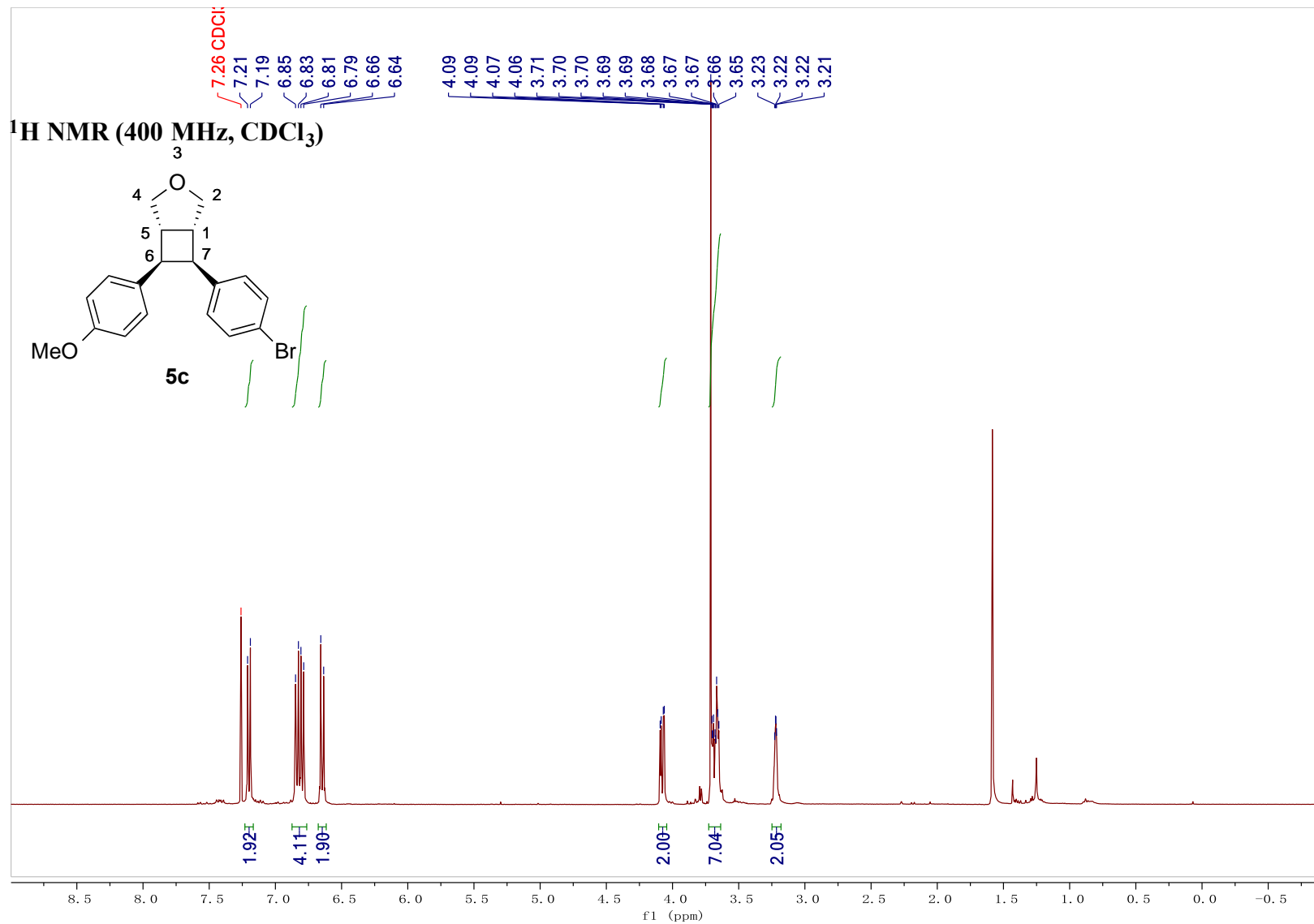


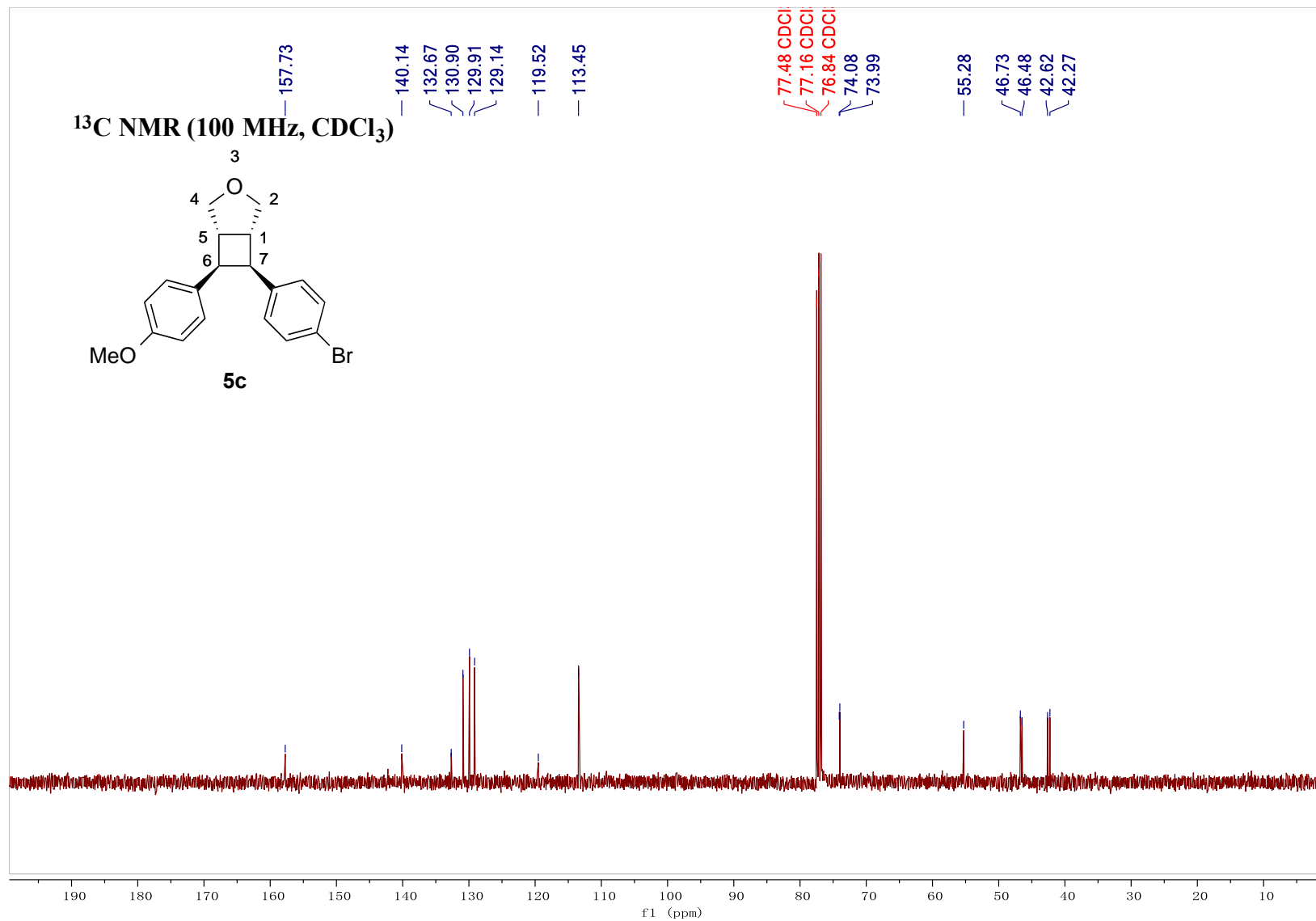


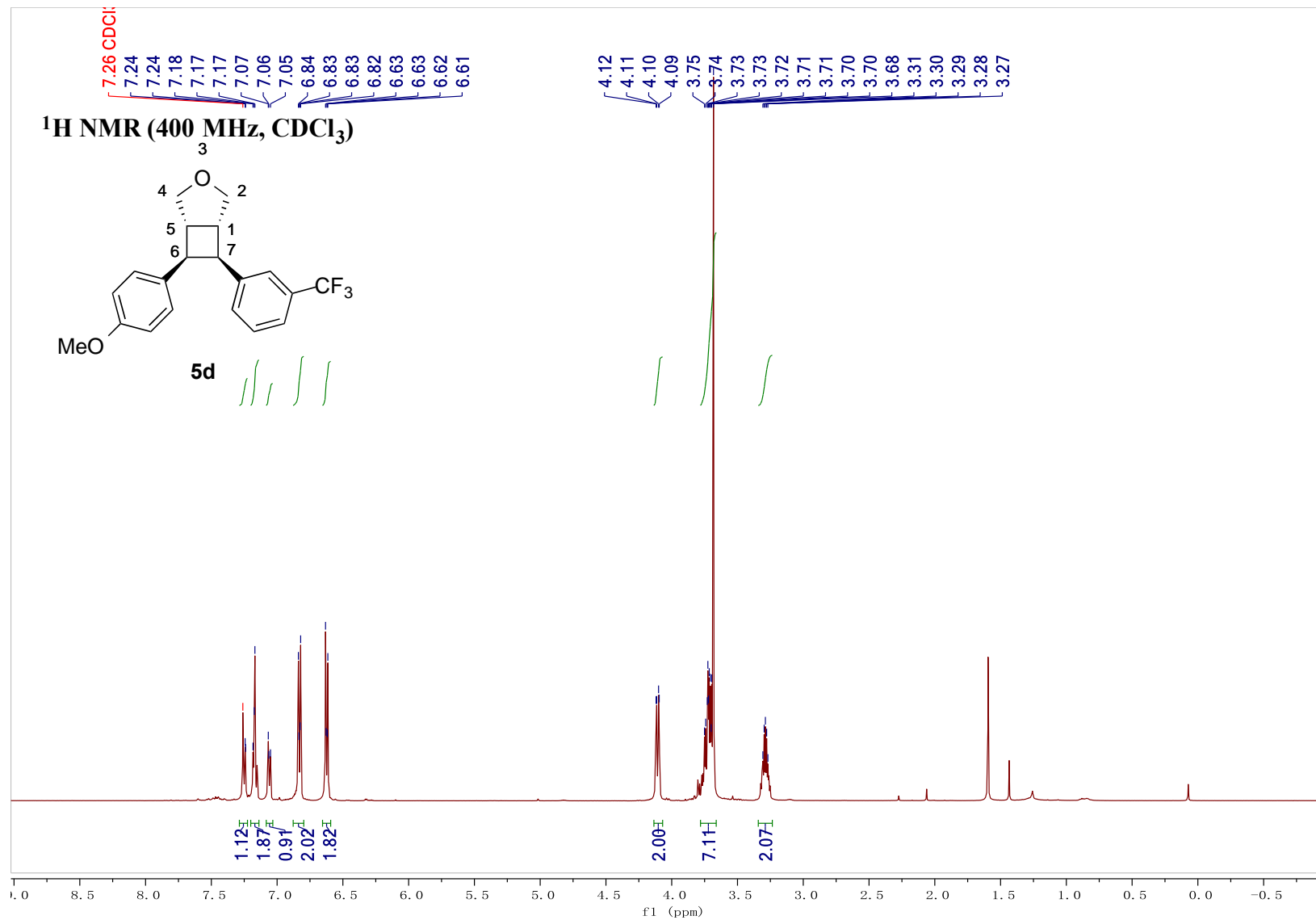


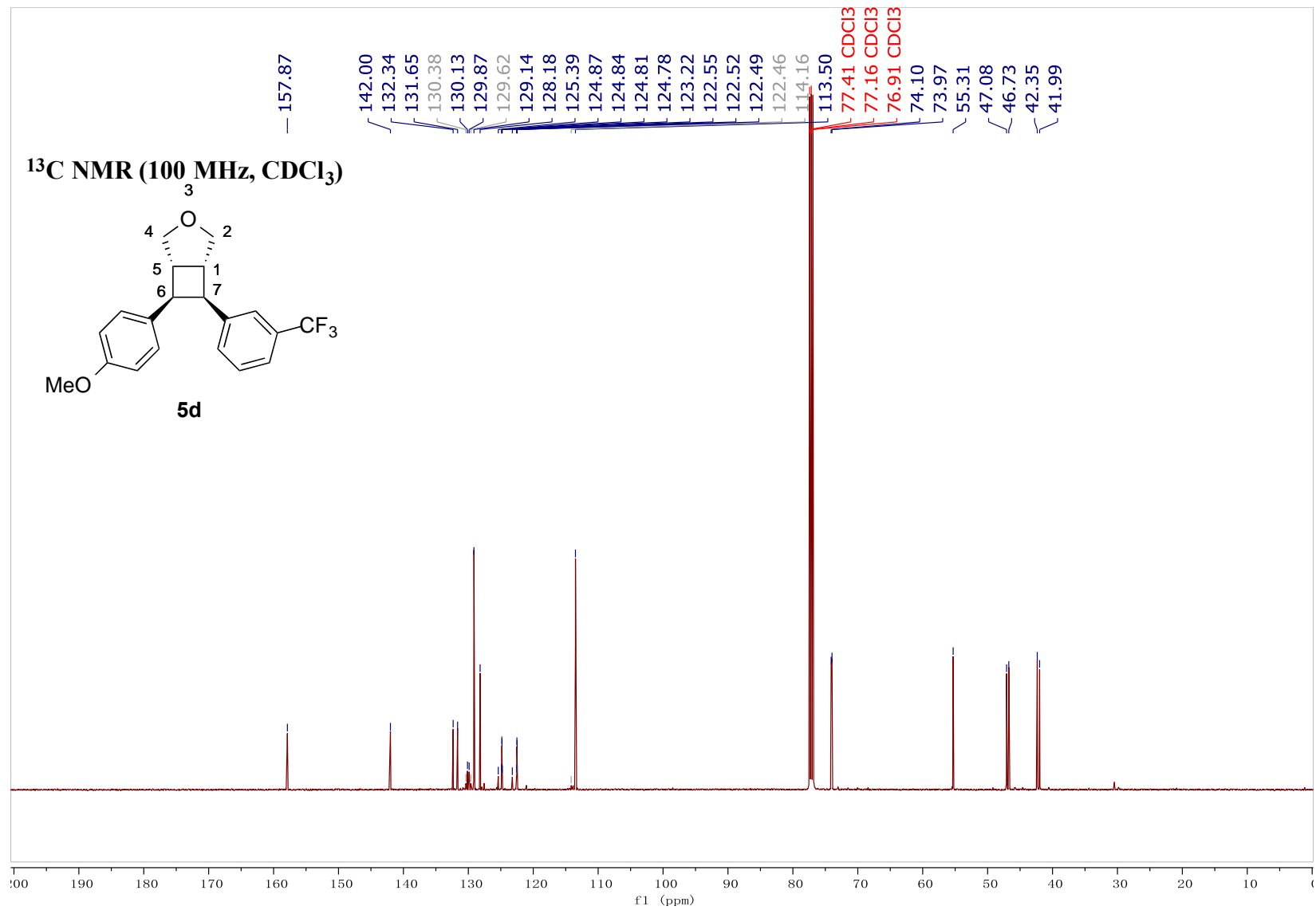


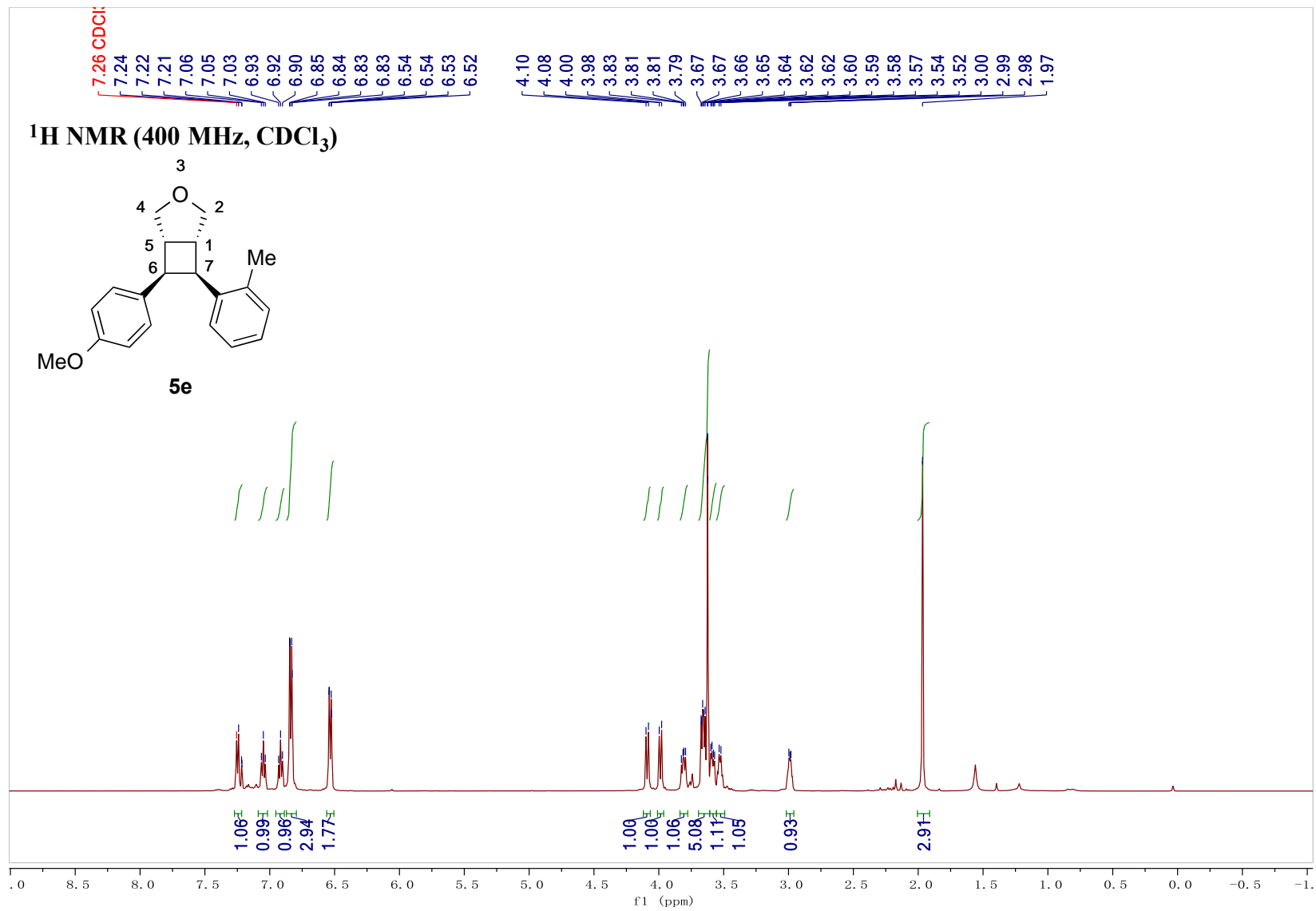


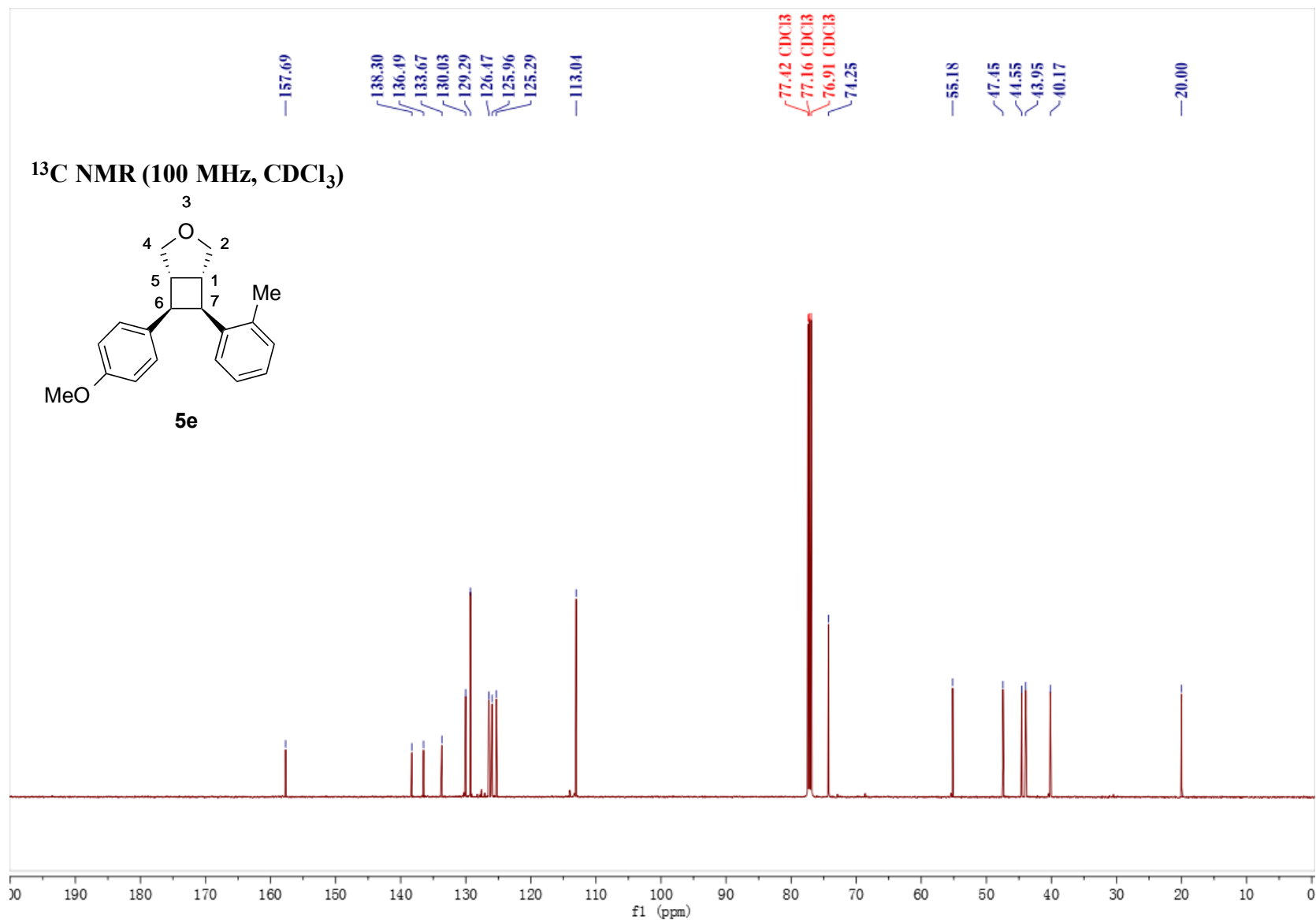


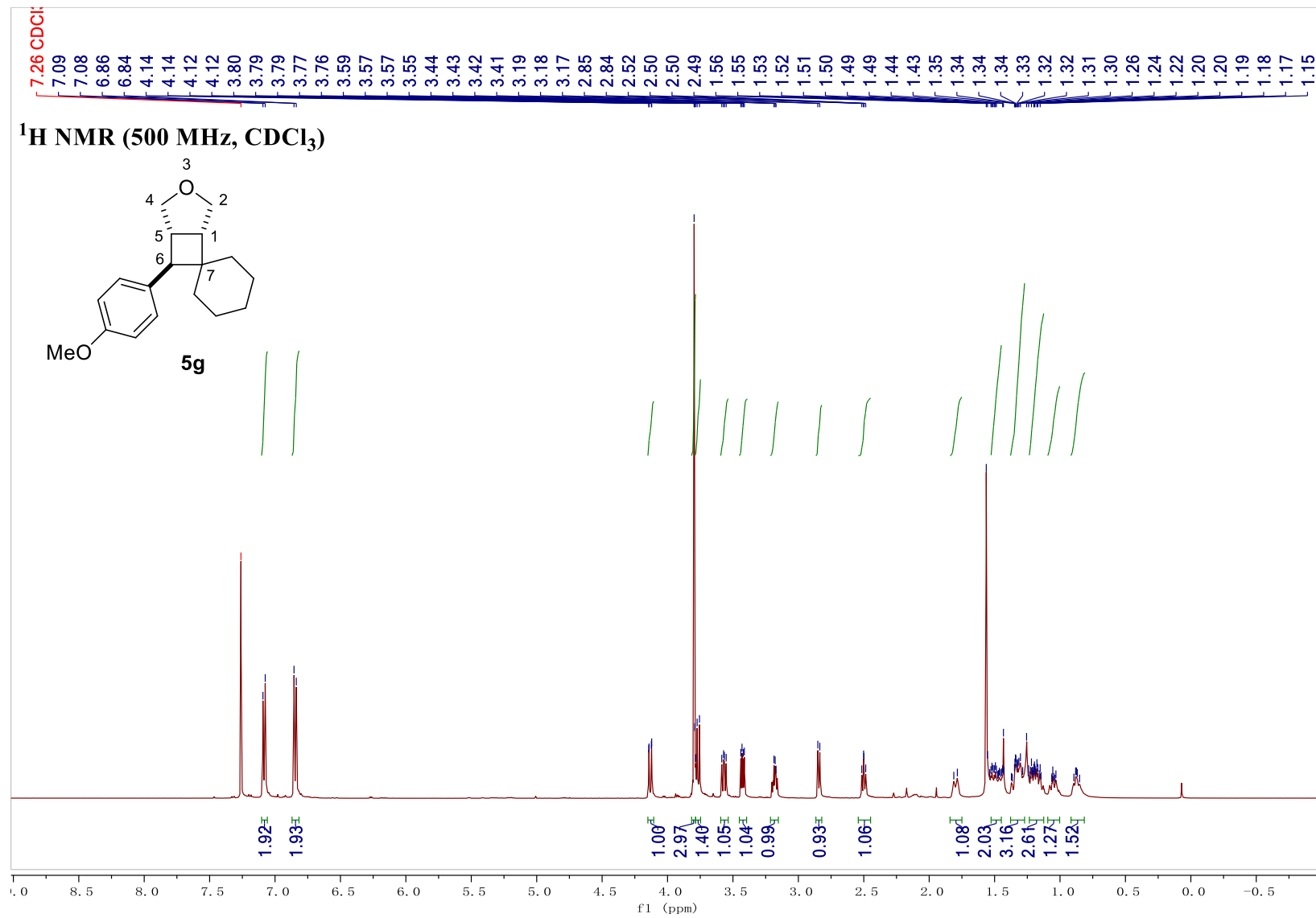


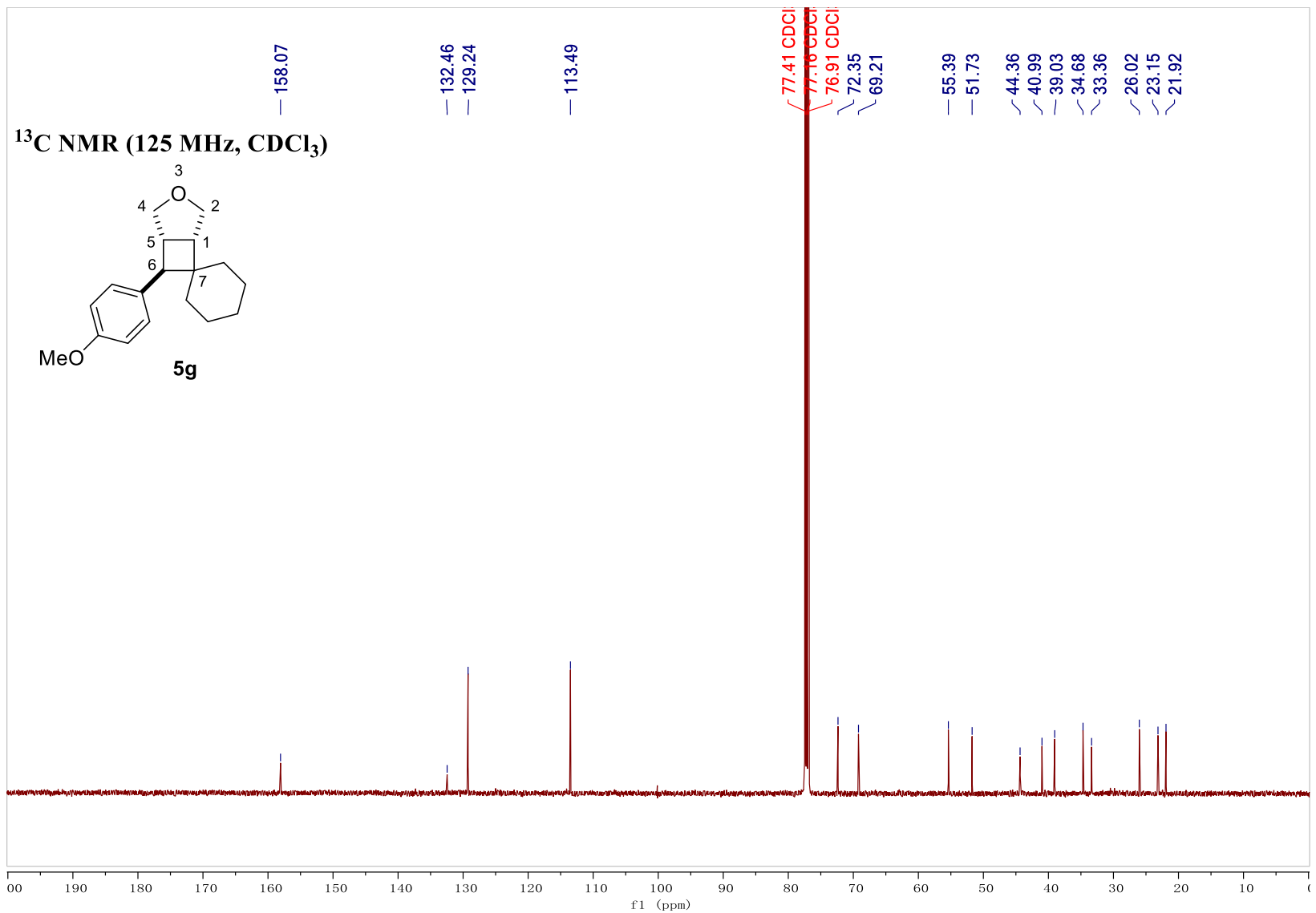




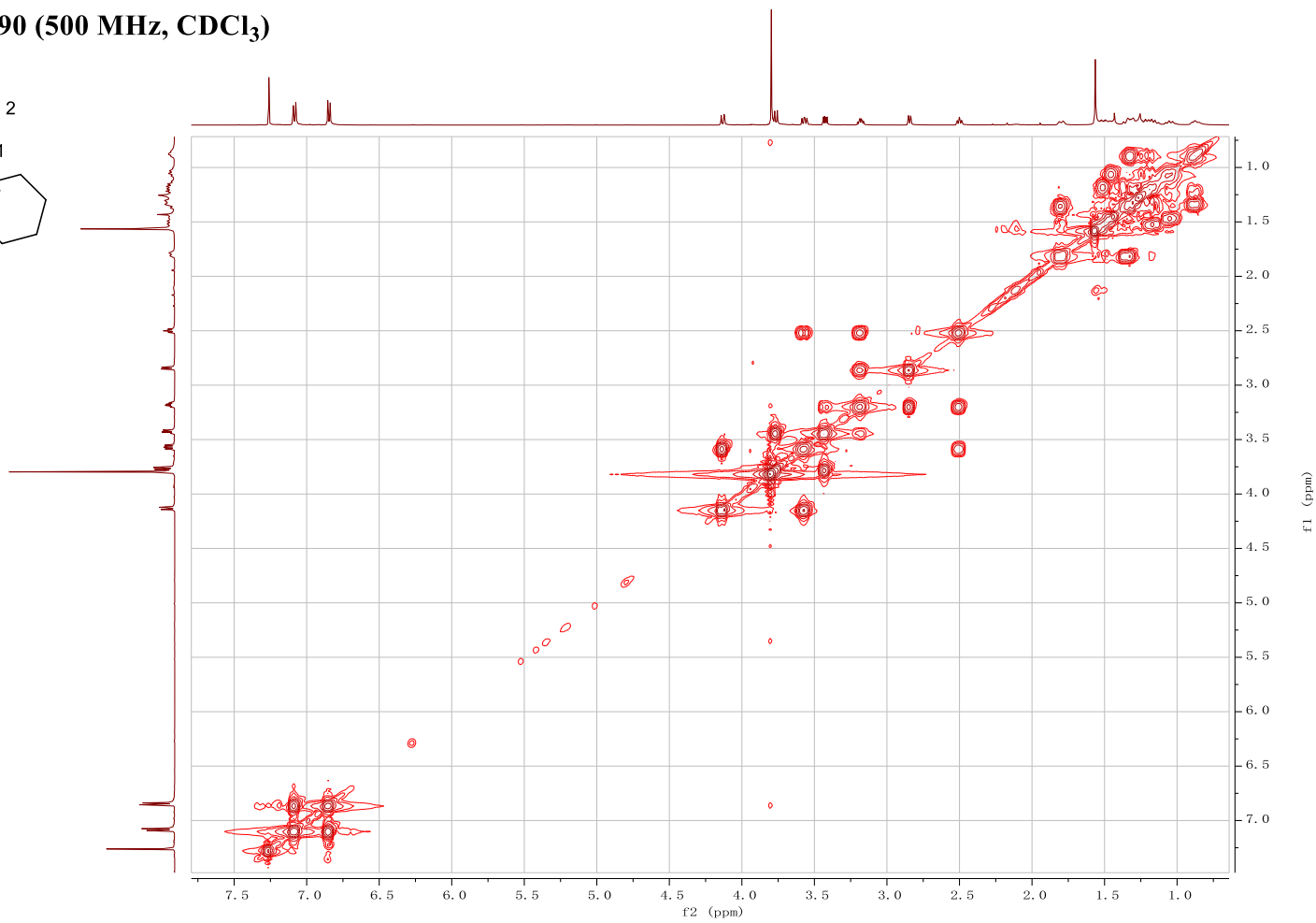
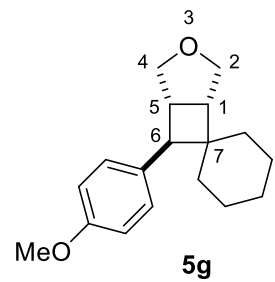




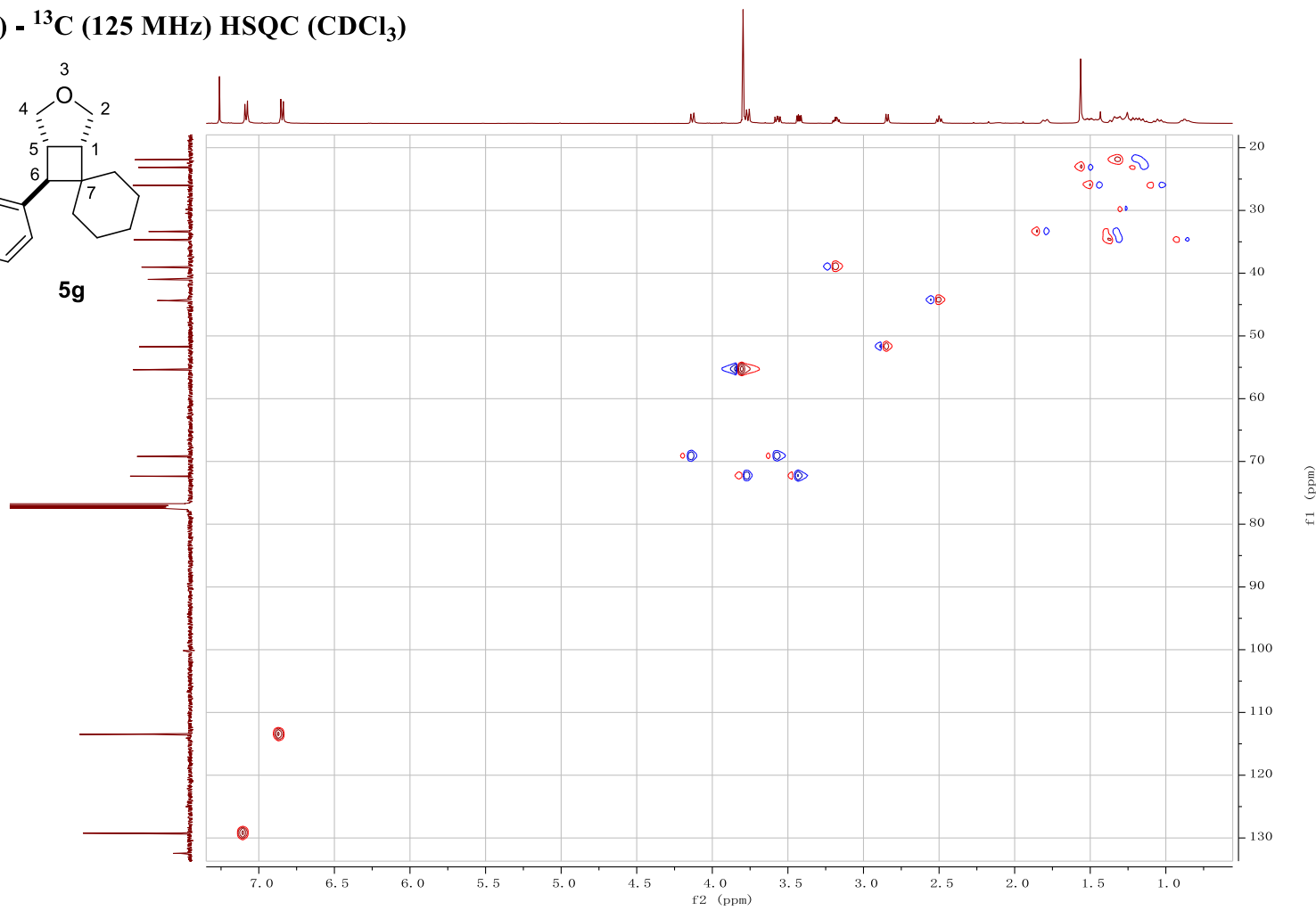
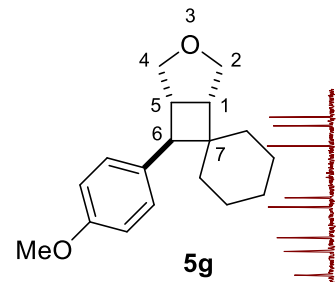




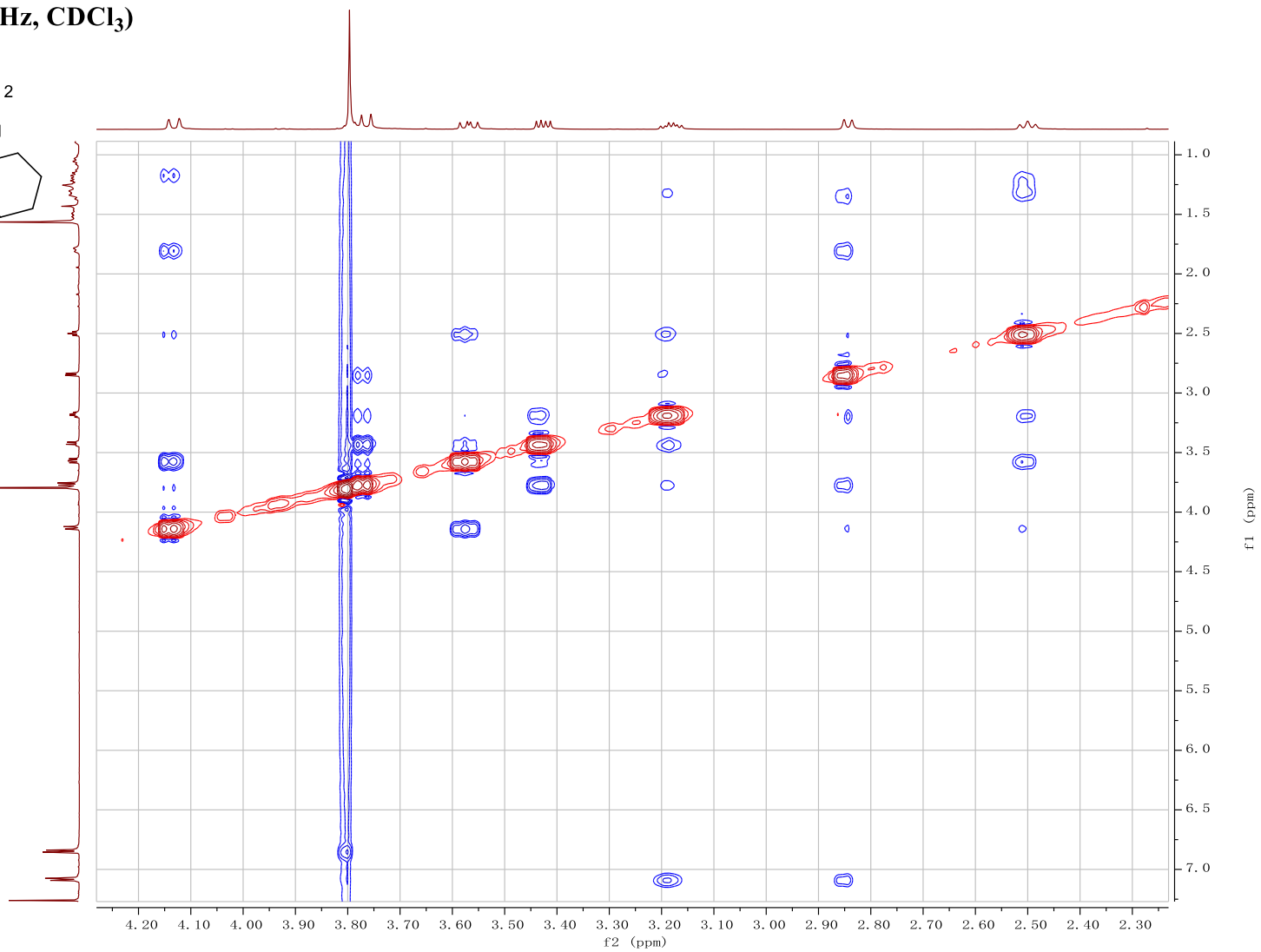
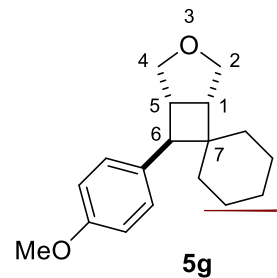
$^1\text{H} - ^1\text{H}$ COSY - 90 (500 MHz, CDCl_3)

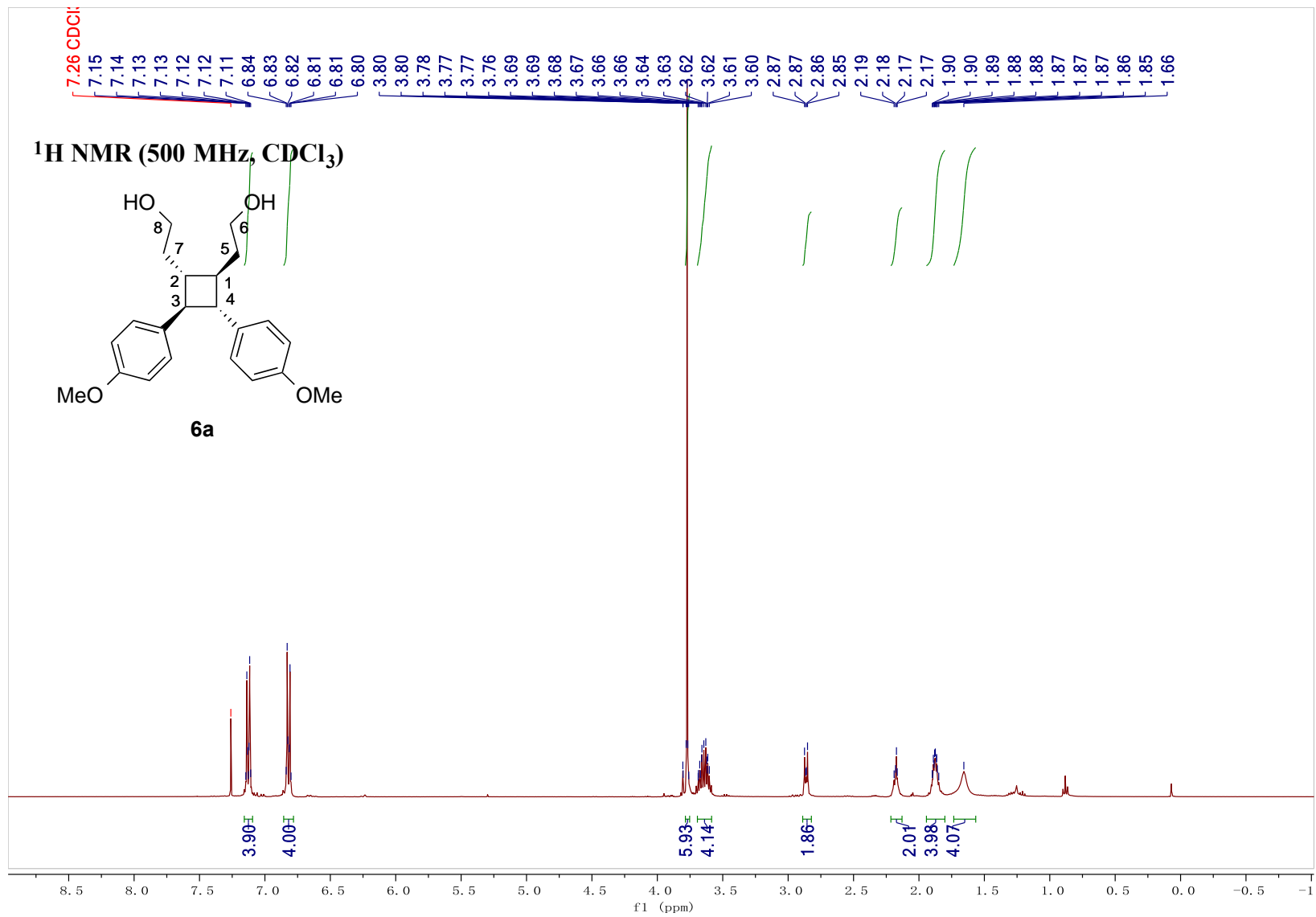


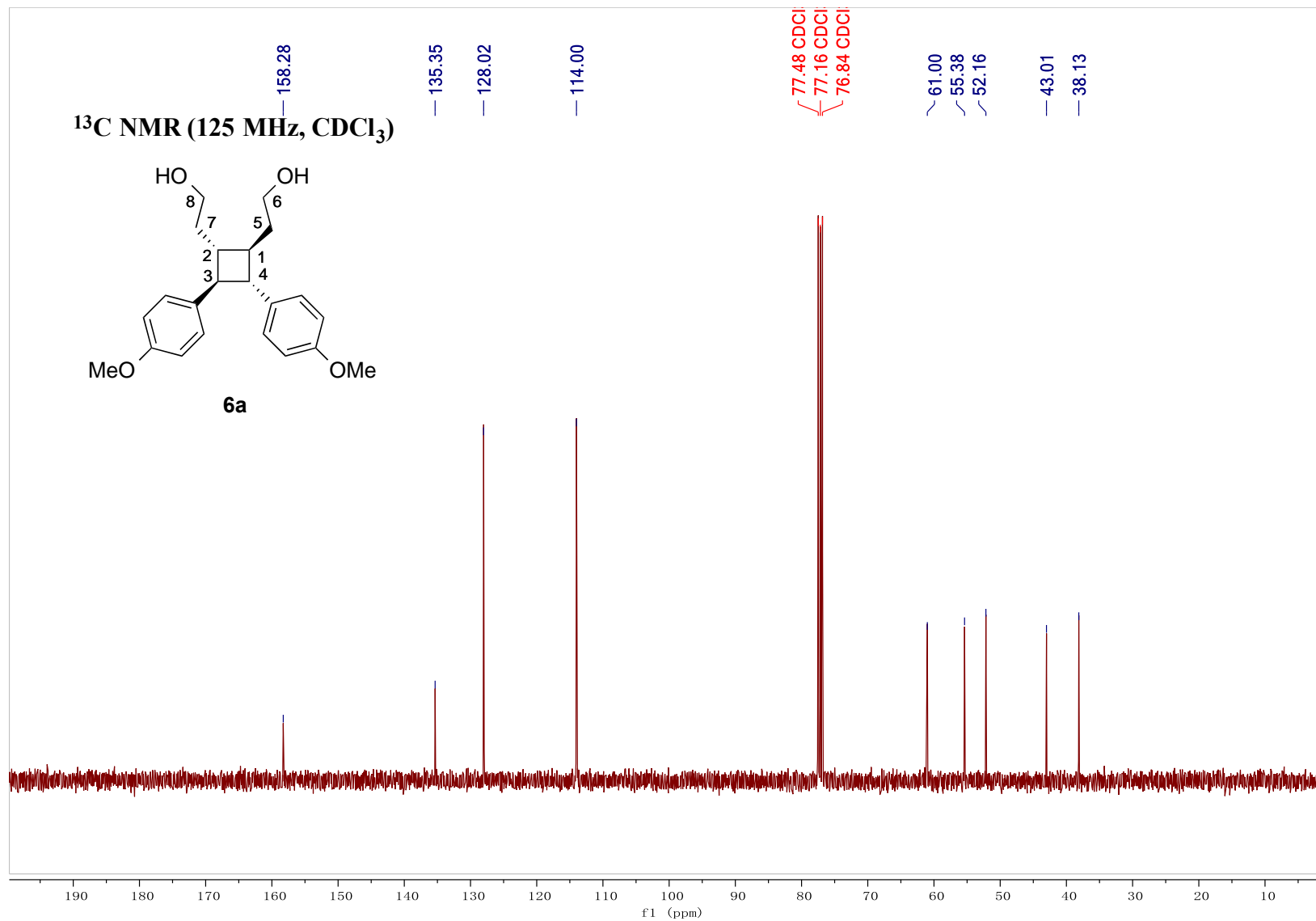
^1H (500 MHz) - ^{13}C (125 MHz) HSQC (CDCl_3)

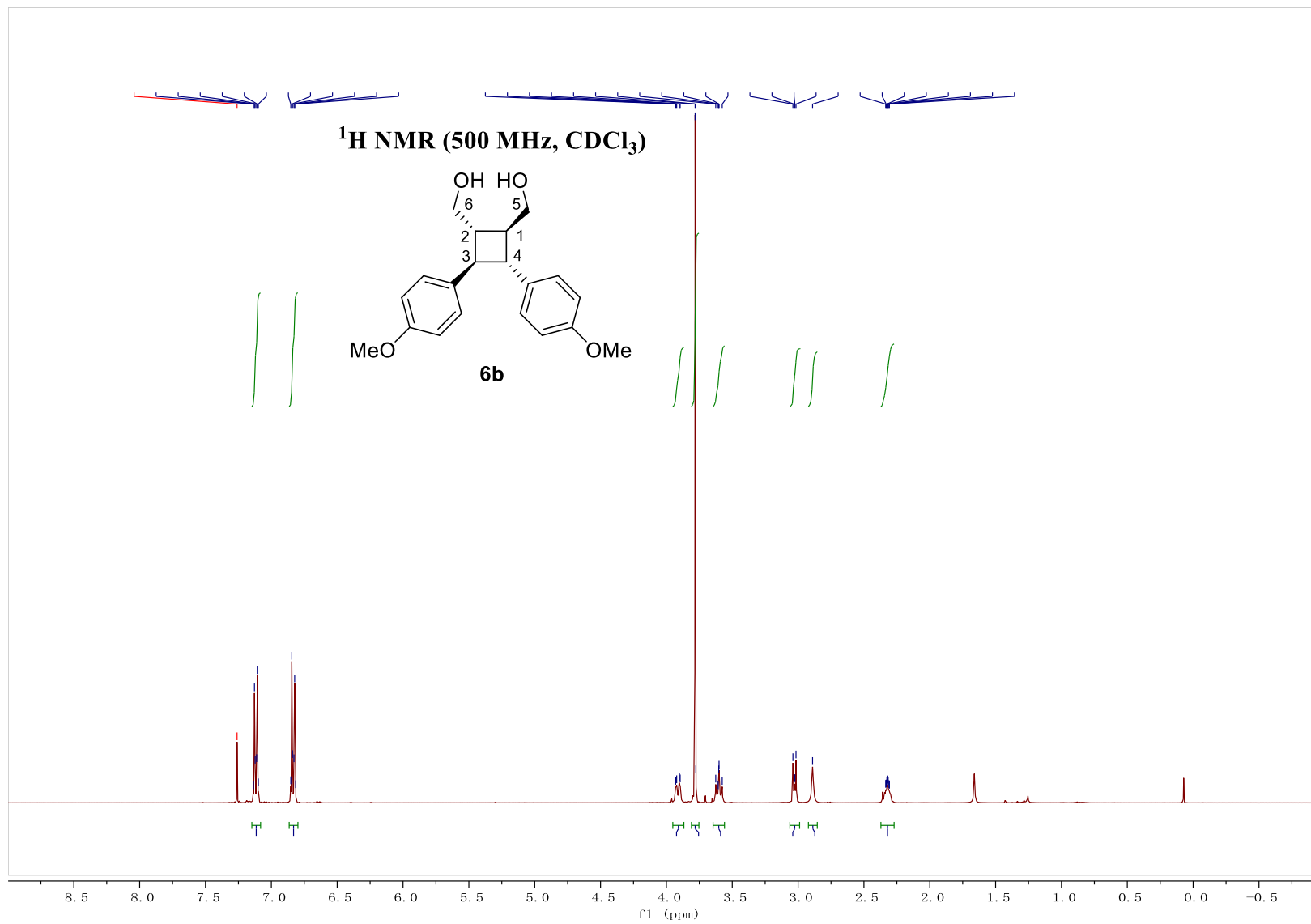


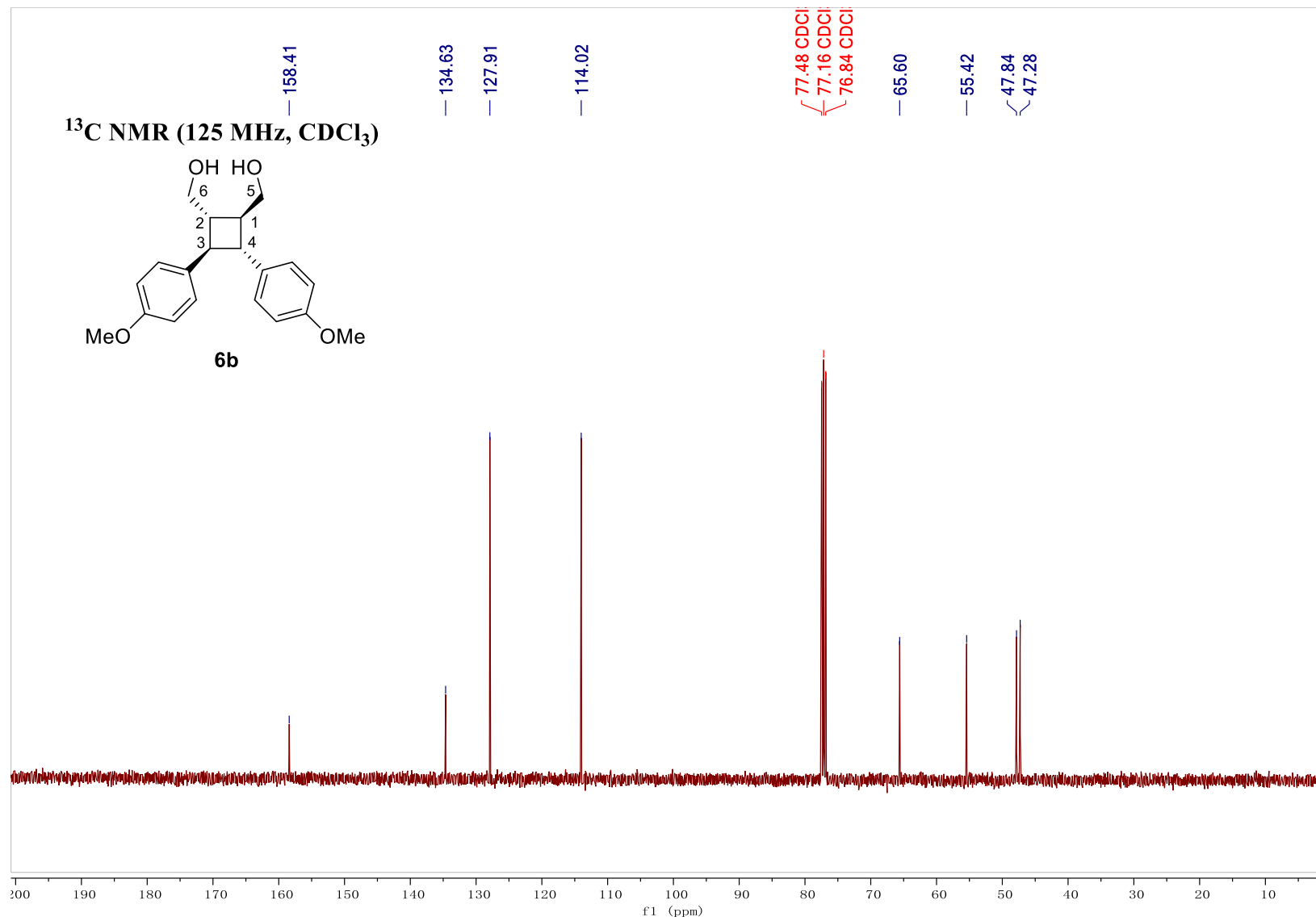
NOESY-2D (500 MHz, CDCl₃)

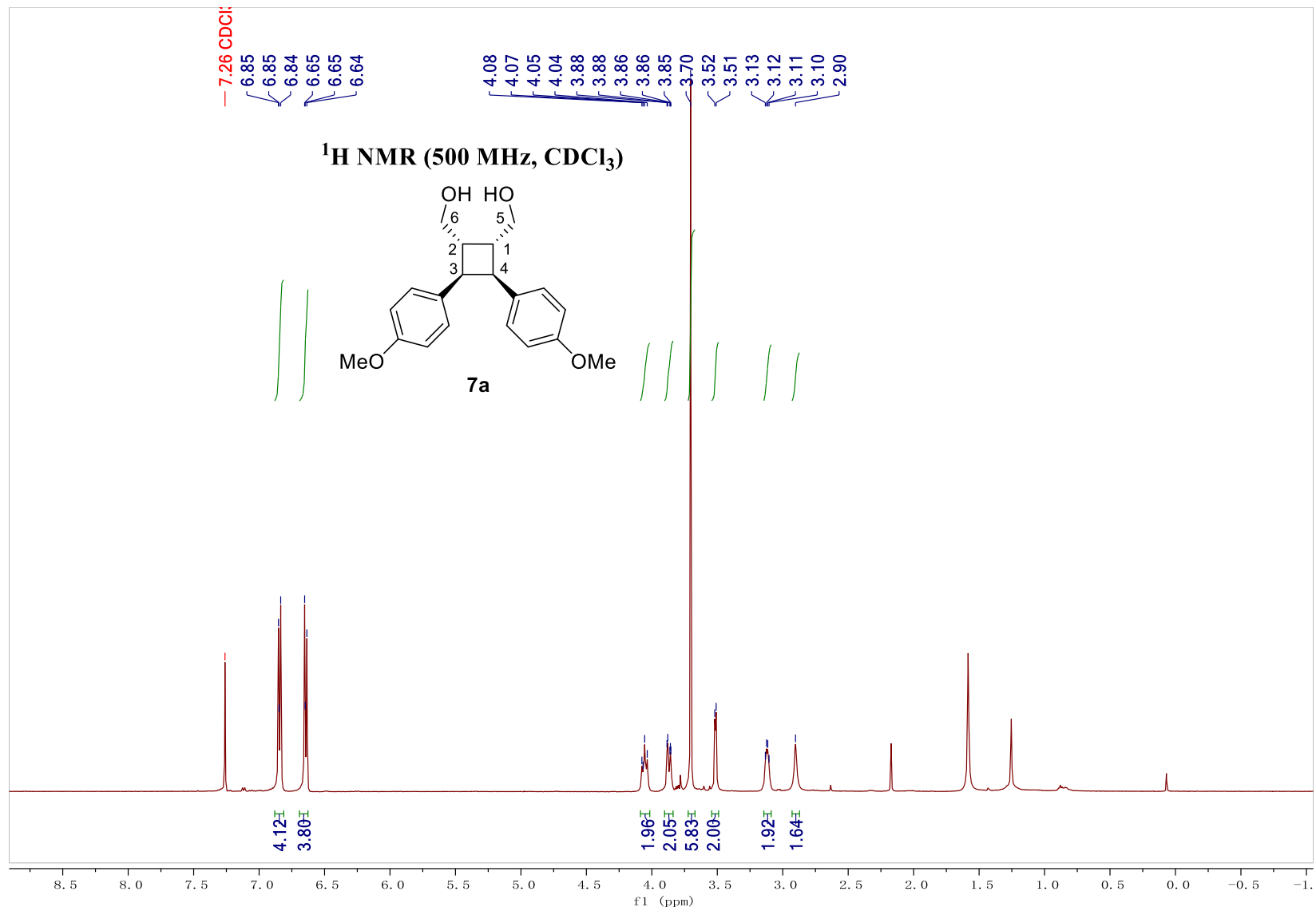


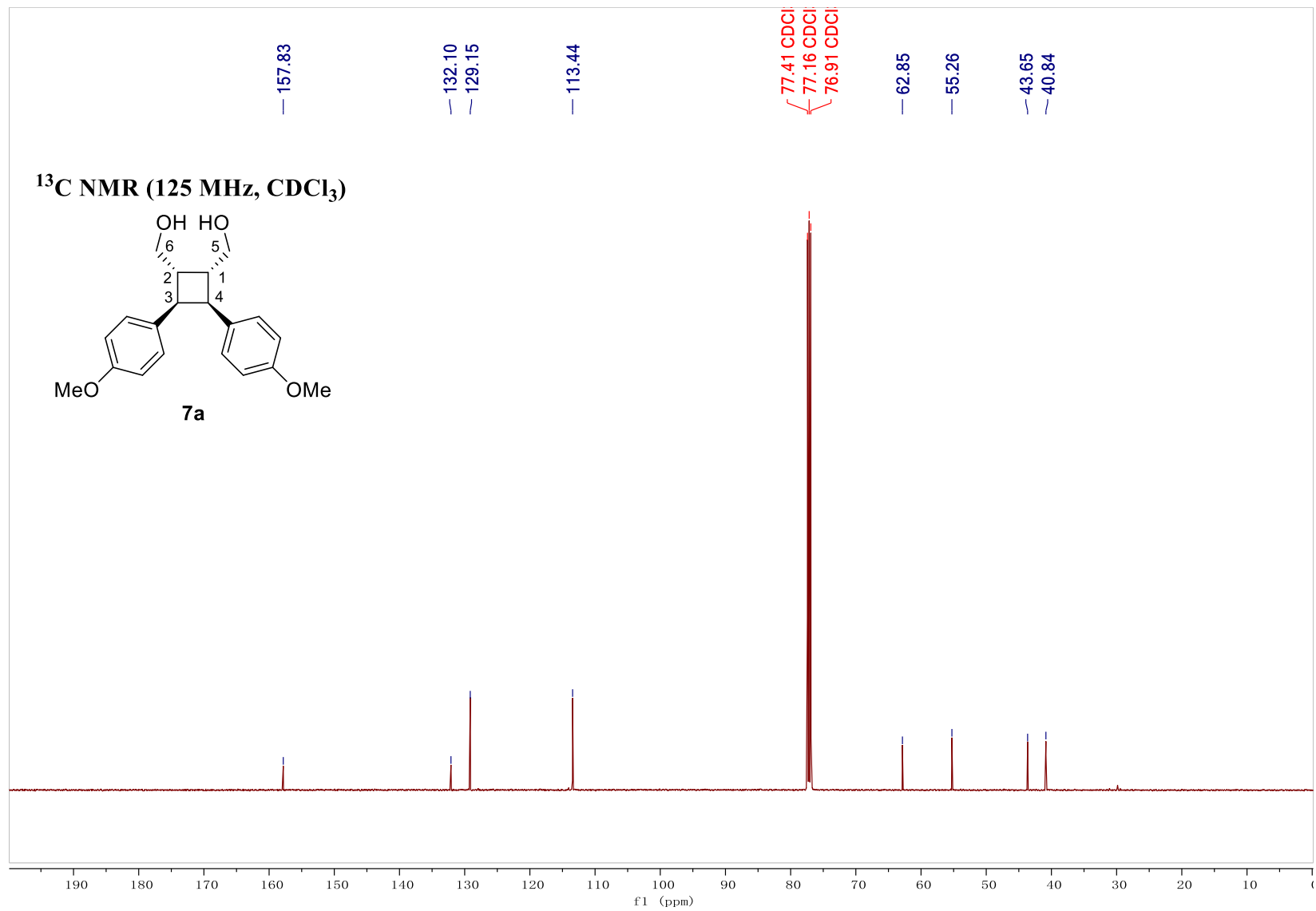


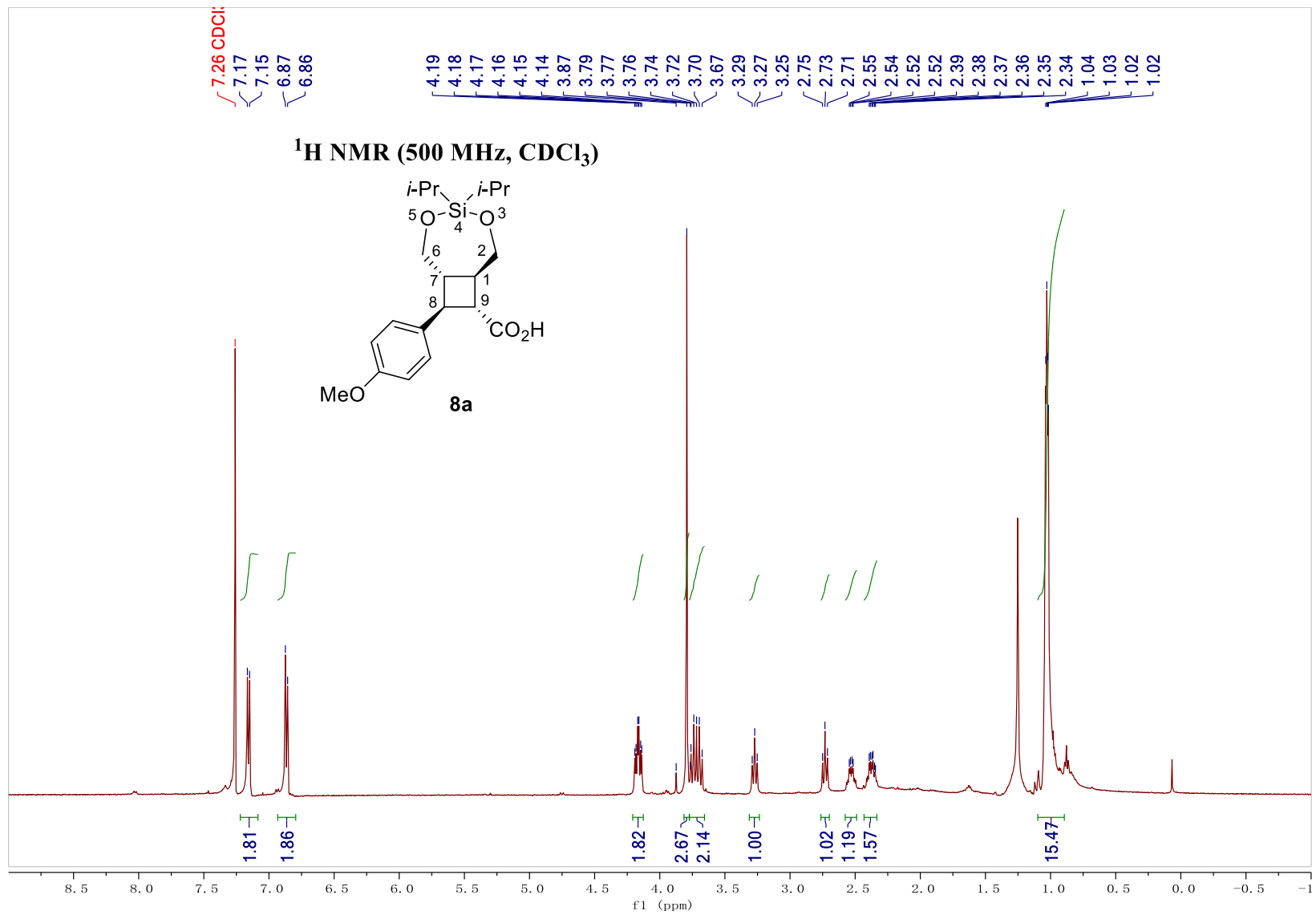




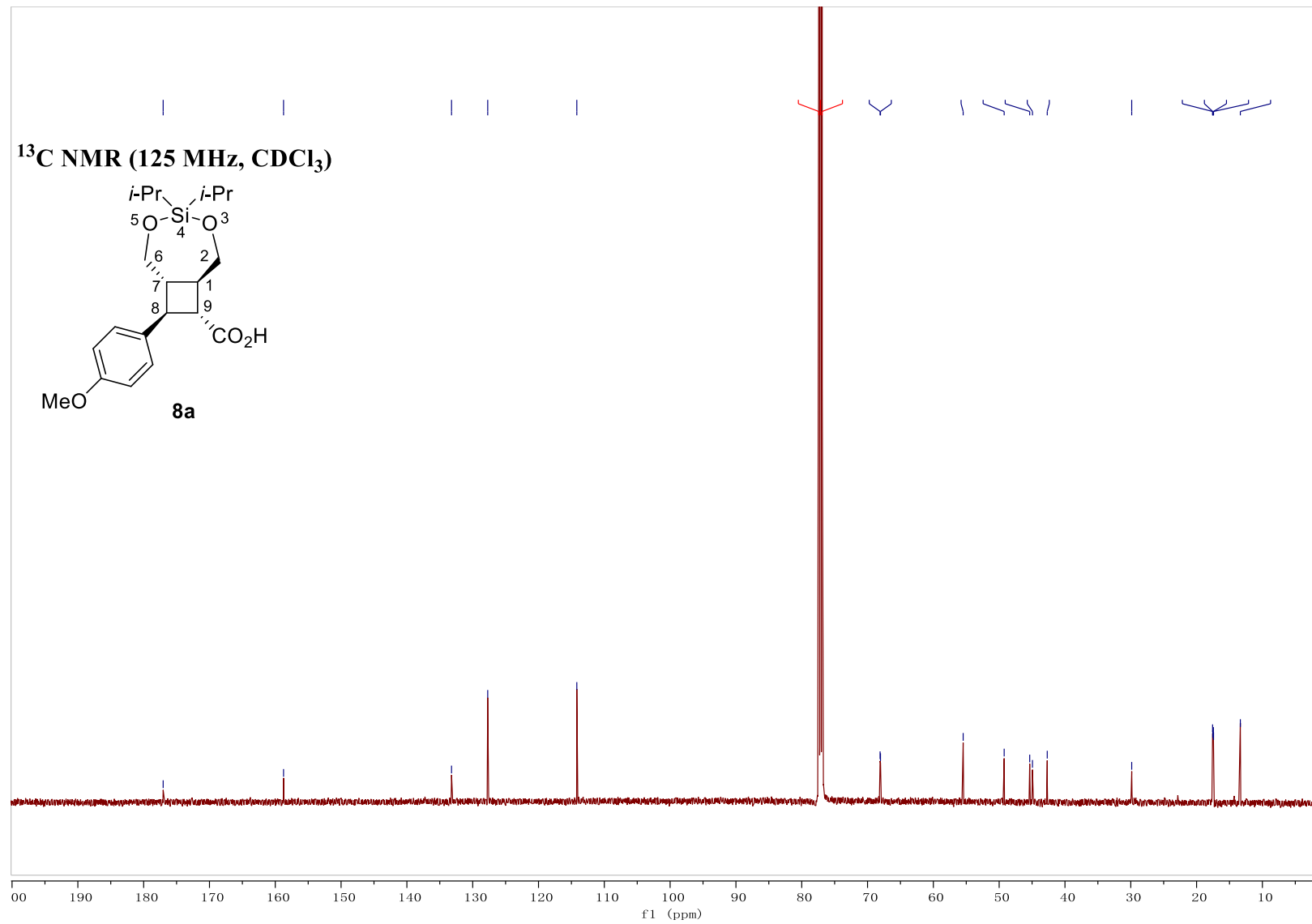
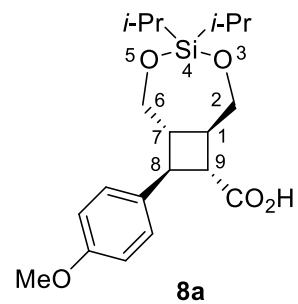




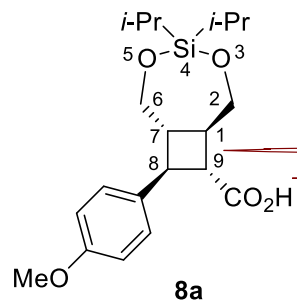




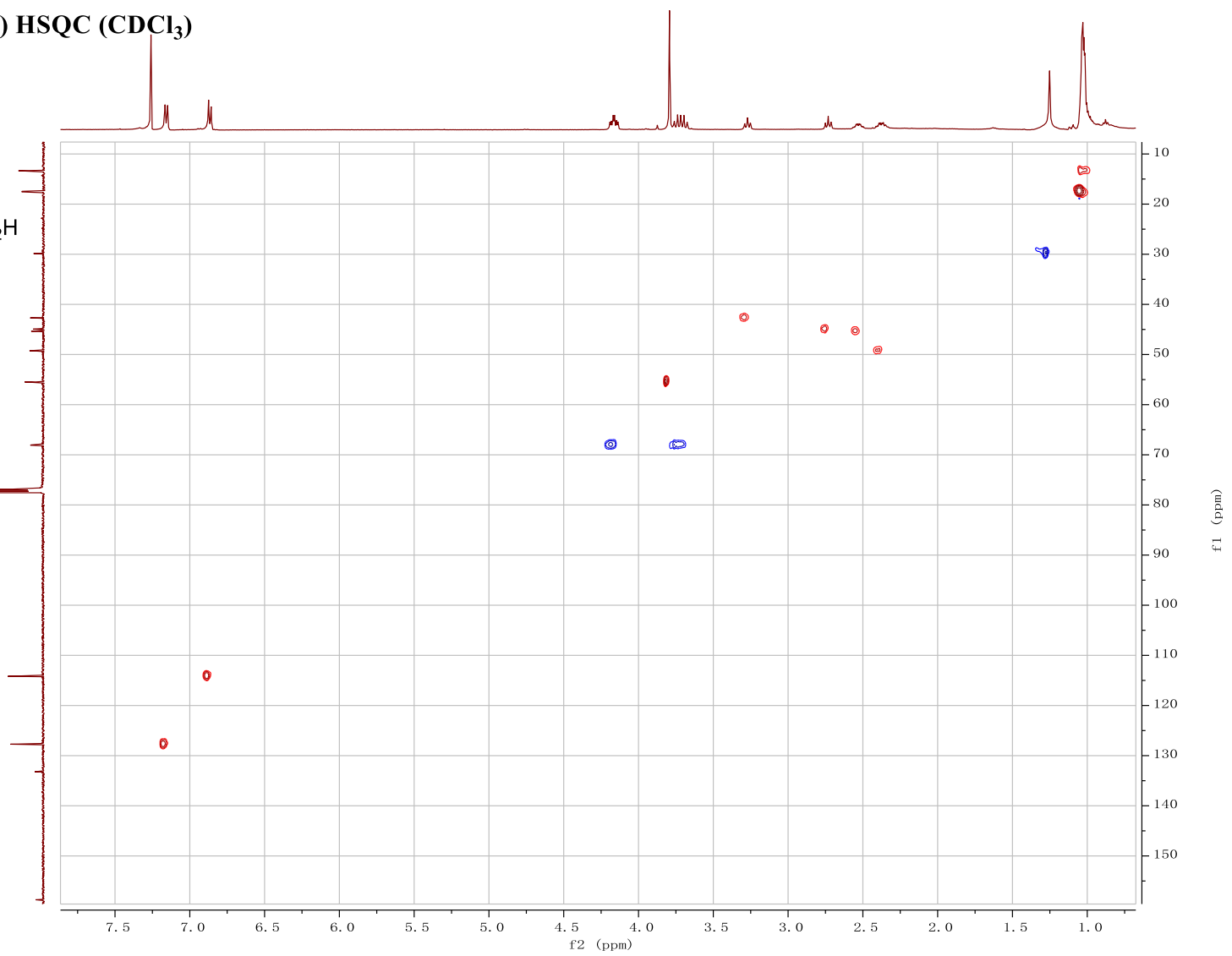
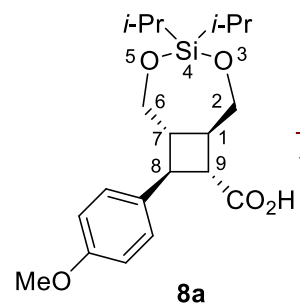
^{13}C NMR (125 MHz, CDCl_3)



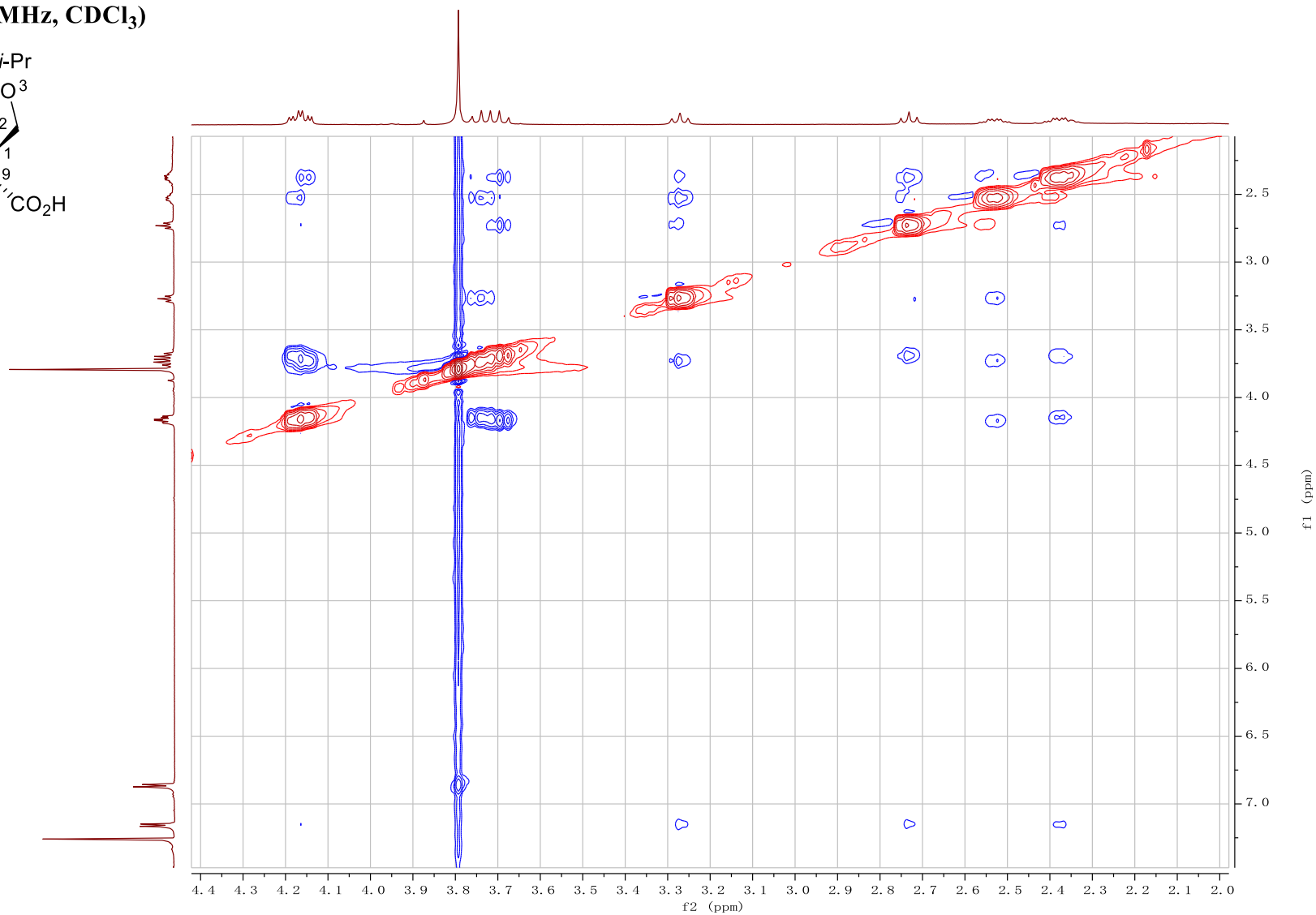
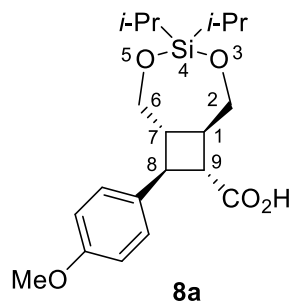
$^1\text{H} - ^1\text{H}$ COSY - 90 (500 MHz, CDCl_3)

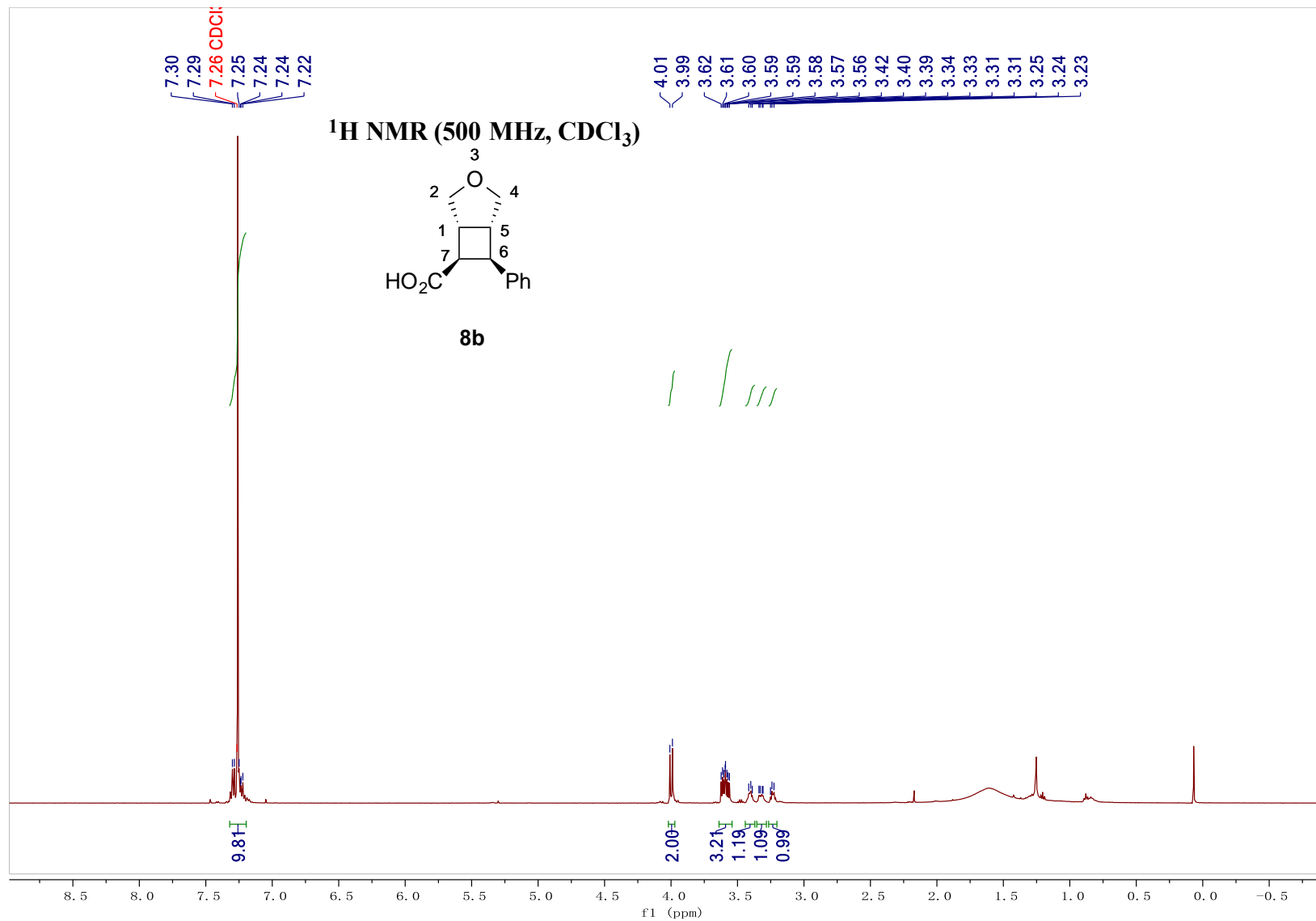


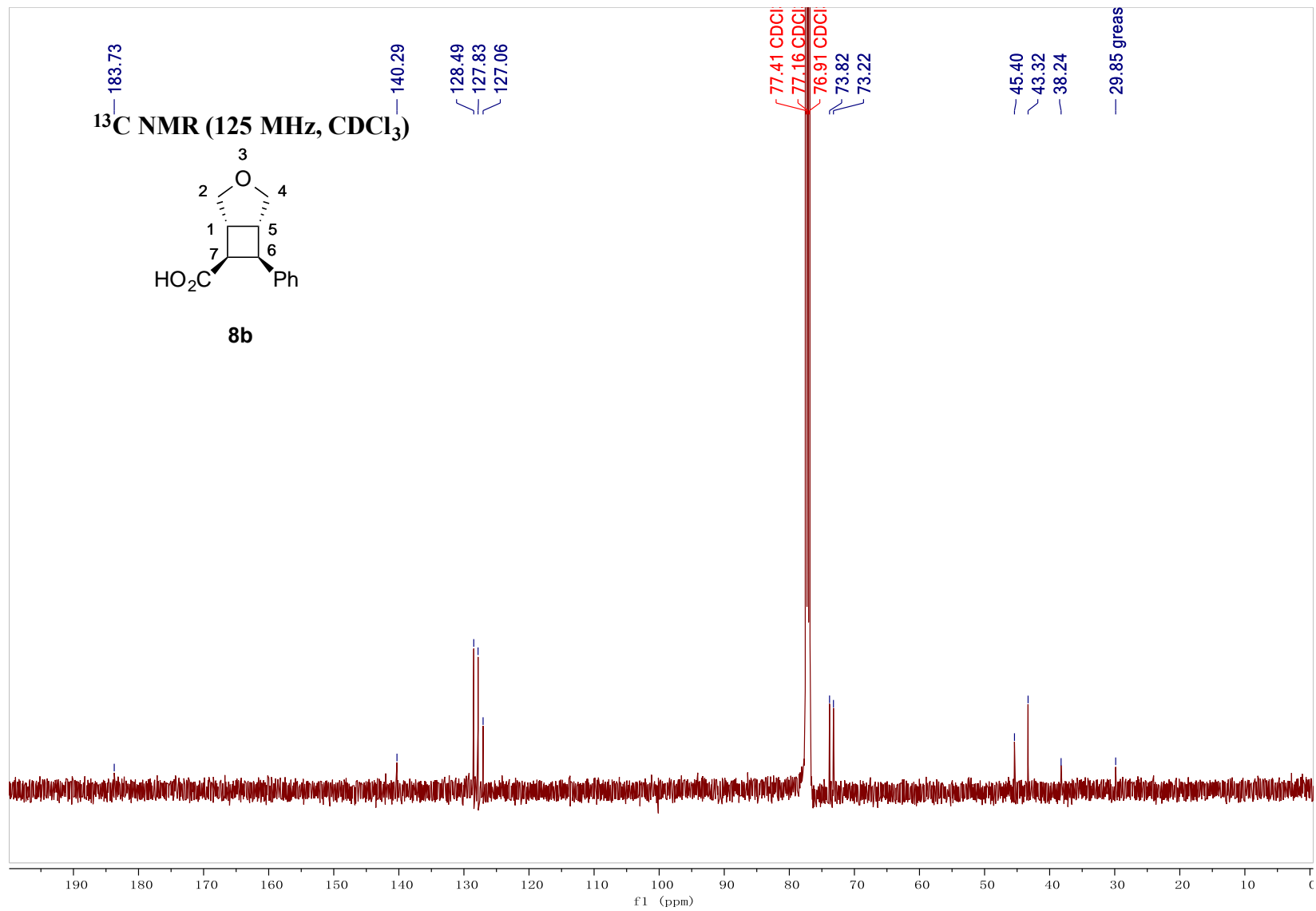
^1H (500 MHz) - ^{13}C (125 MHz) HSQC (CDCl_3)

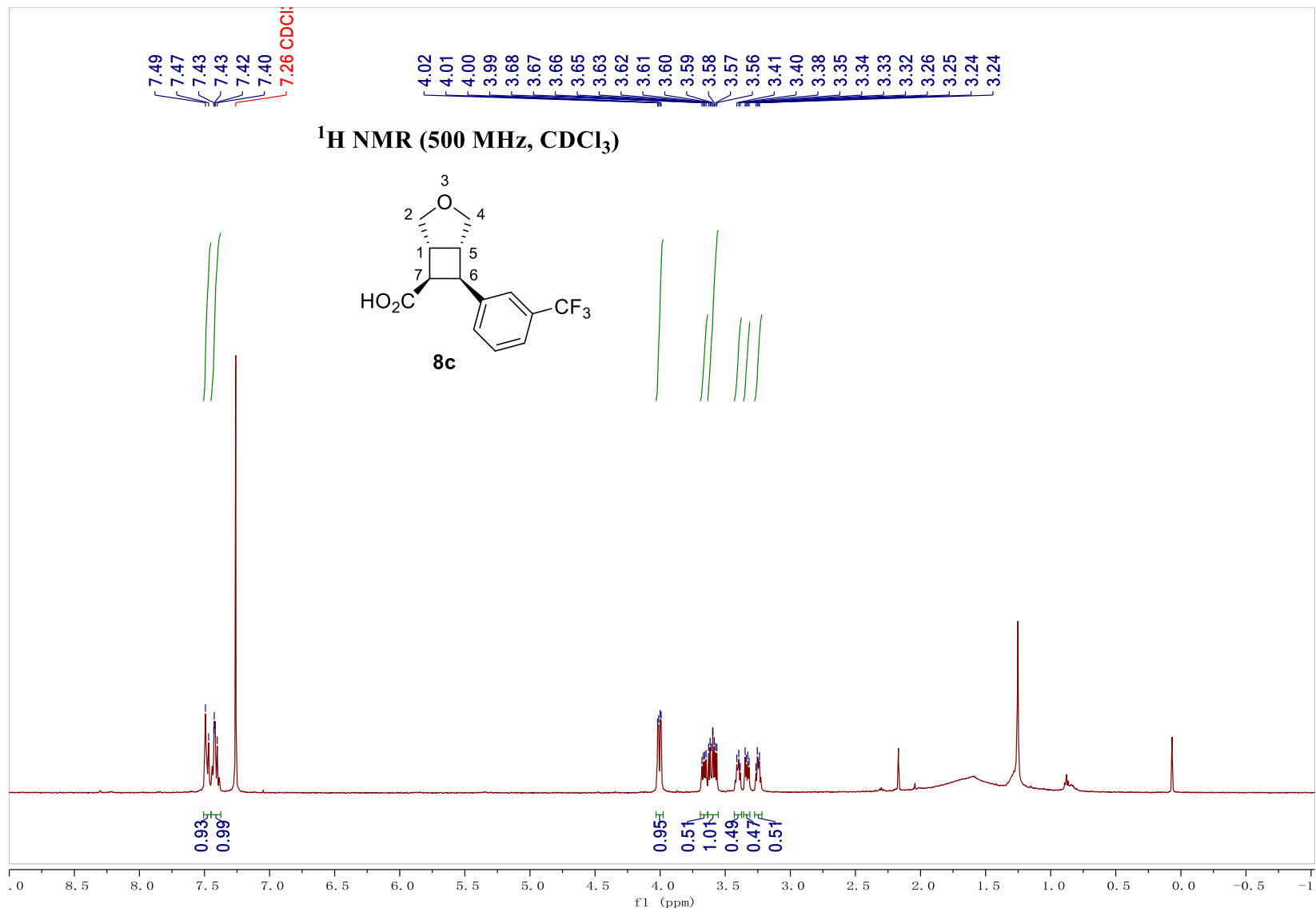


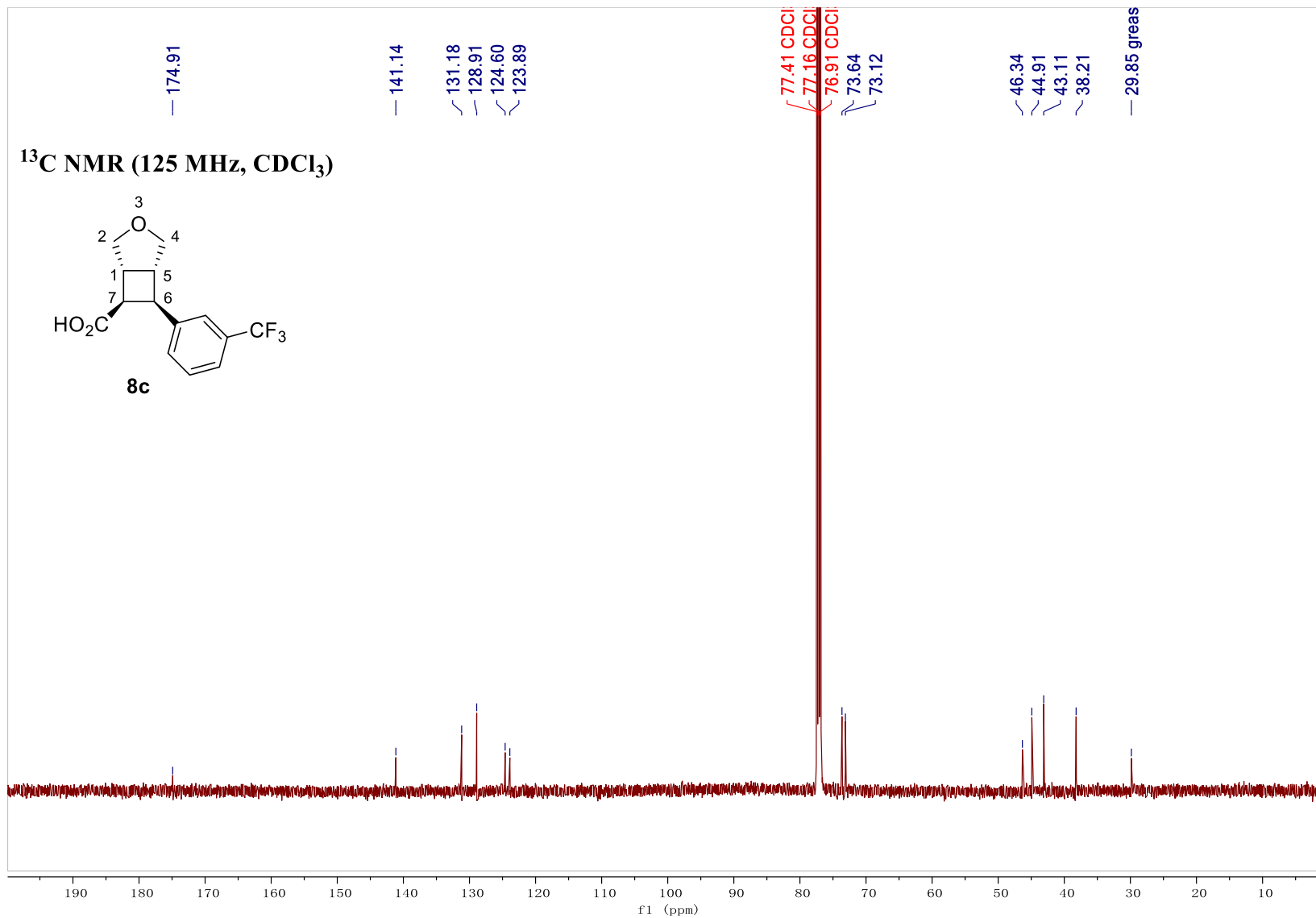
NOESY-2D (500 MHz, CDCl₃)



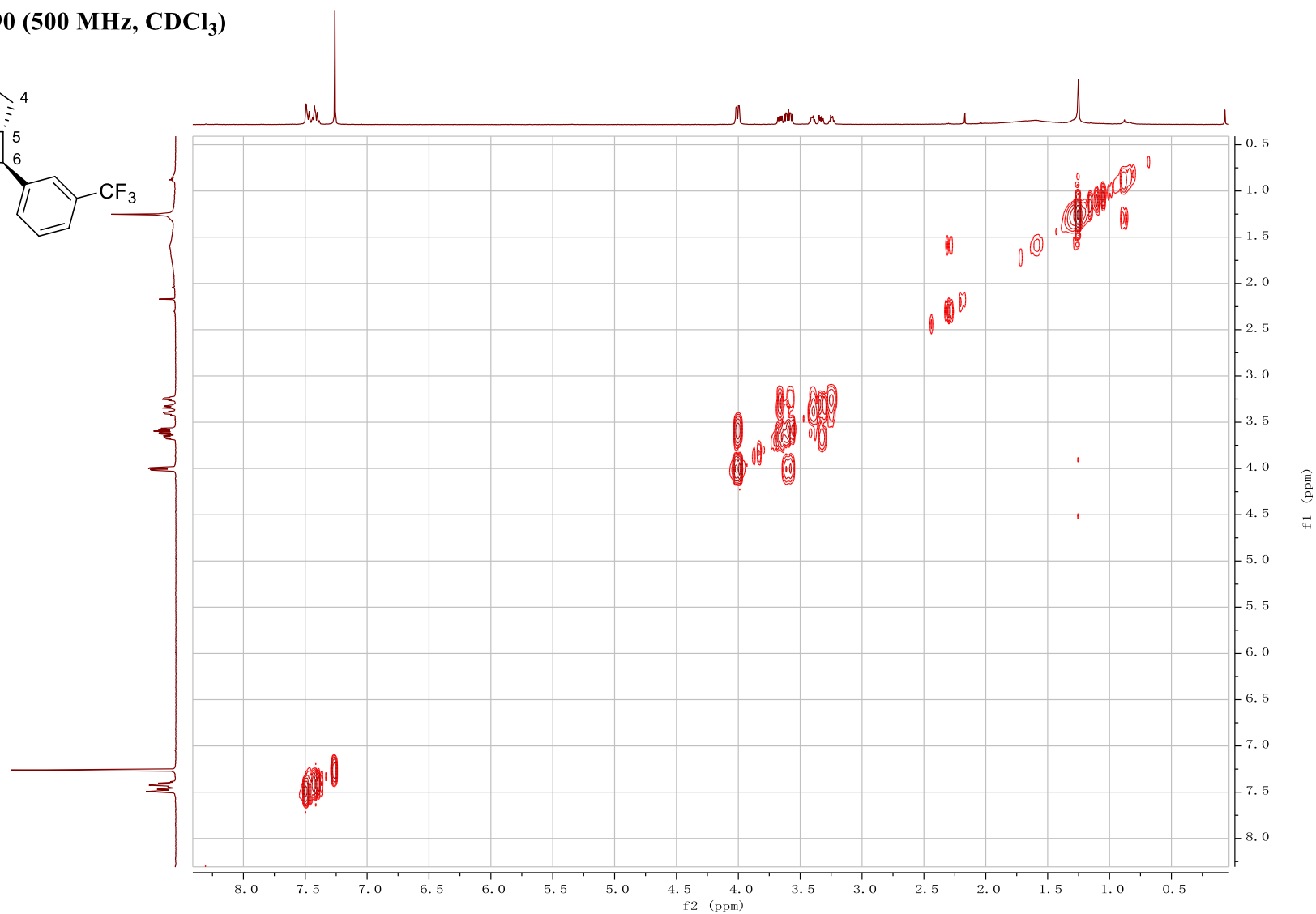
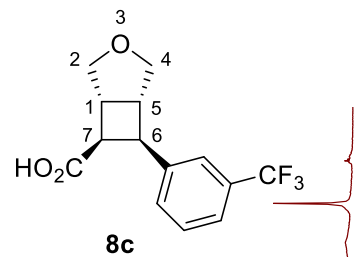




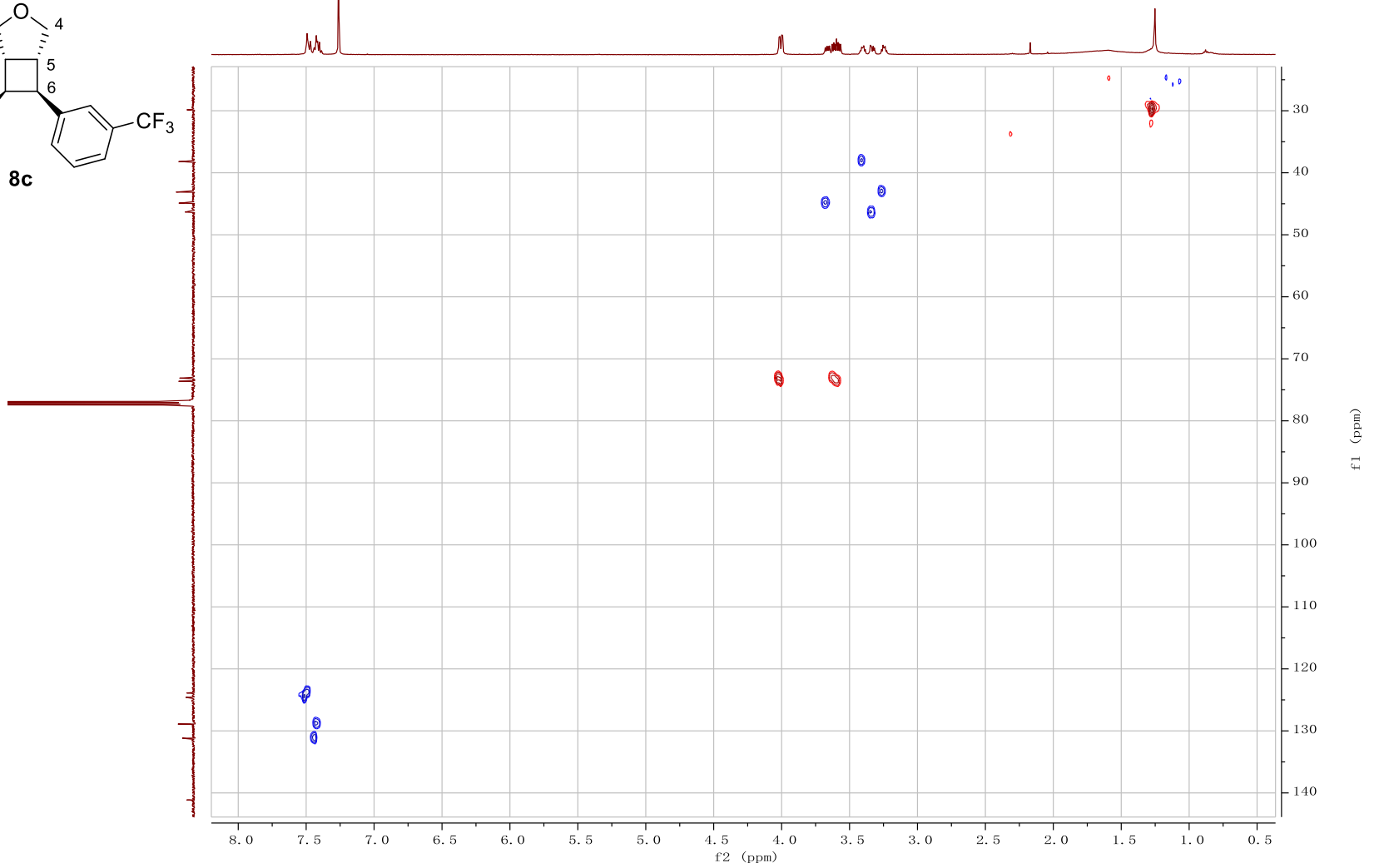
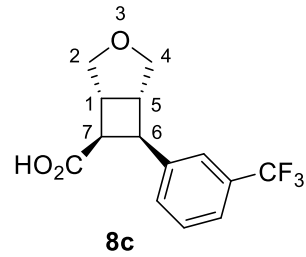




$^1\text{H} - ^1\text{H}$ COSY - 90 (500 MHz, CDCl_3)



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



NOESY-2D (500 MHz, CDCl₃)

