

Supplementary Material

On the role of "mental leaps" in small-molecule structure elucidation by NMR spectroscopy

Márton Weber,^{a,b} Áron Szigetvári,^a Mónika Halmi,^b Péter Keglevich,^b and Csaba Szántay Jr^{*a}

^a*Spectroscopic Research Department, Gedeon Richter Plc., Gyömrői út 19-21, Budapest H-1103, Hungary*

^b*Department of Organic Chemistry and Technology, Budapest University of Technology and Economics, Szt. Gellért tér 4, Budapest, H-1111, Hungary*

Email: cs.szantay@richter.hu

Table of Contents

NMR spectra of Compound **6**

¹ H NMR spectrum.....	S2
¹³ C NMR spectrum.....	S6
HSQC spectrum	S7
HMBC spectrum	S11
COSY spectrum.....	S16
ROESY spectrum.....	S20

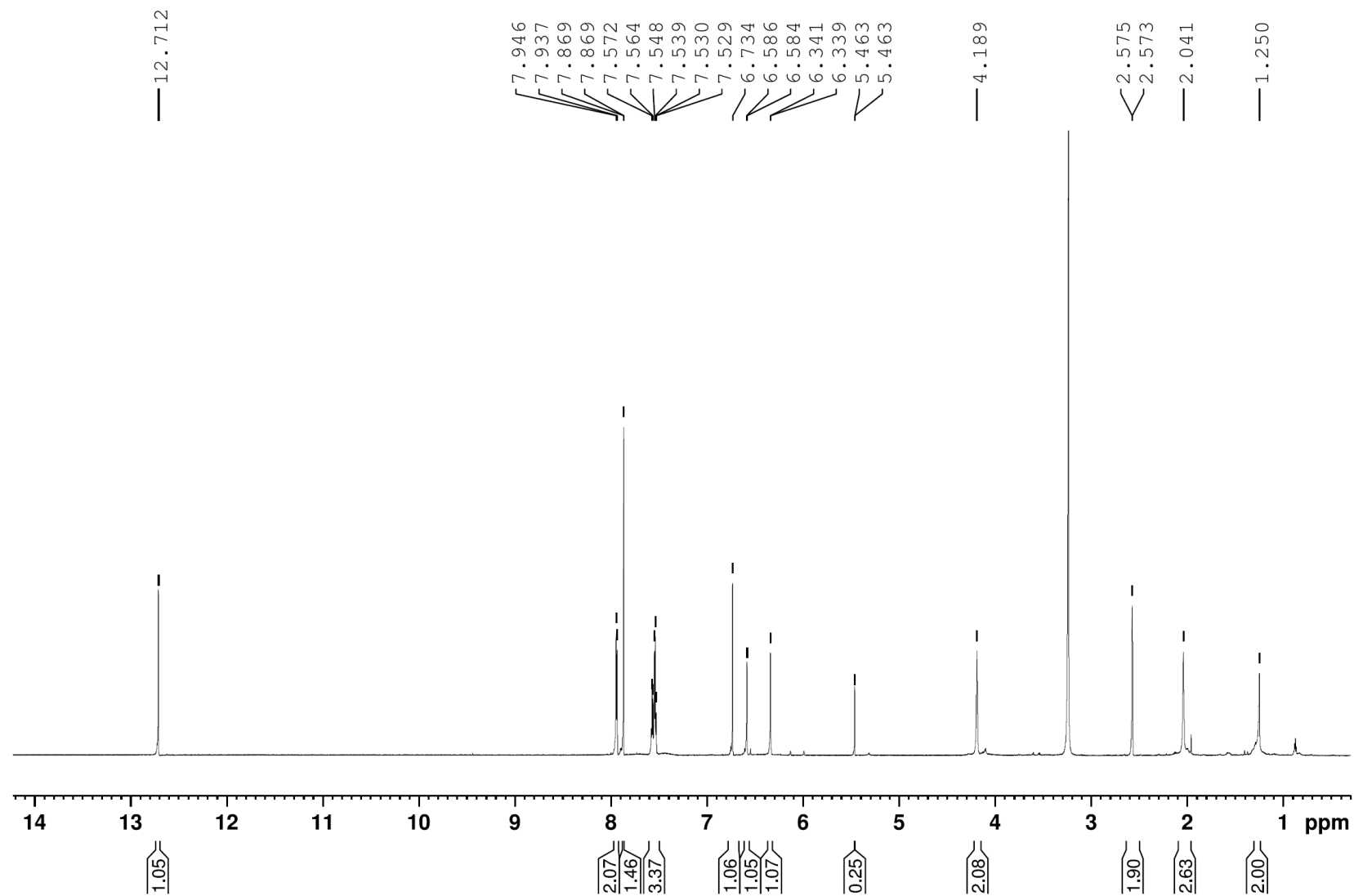
NMR spectra of Compound **10**

¹ H NMR spectrum.....	S24
¹³ C NMR spectrum.....	S30
HSQC spectrum	S31
HMBC spectrum optimized to ⁿ J _{C,H} = 8 Hz.....	S36
COSY spectrum.....	S43
ROESY spectrum.....	S48
HMBC spectrum optimized to ⁿ J _{C,H} = 2 Hz.....	S52
1,1-ADEQUATE spectrum	S60

NMR spectra of the mixture of Compounds **7**, **14** and **15**

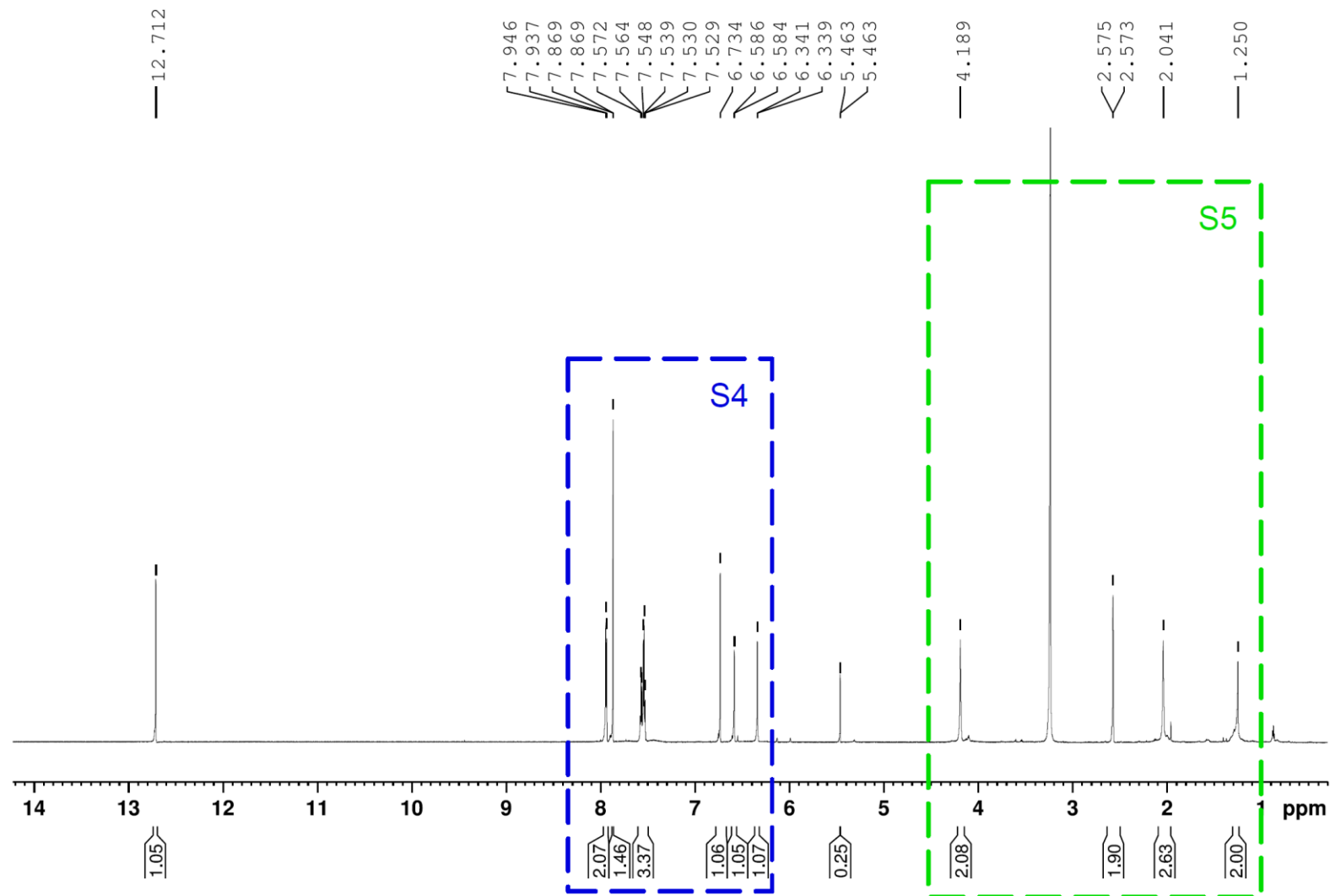
¹ H NMR spectrum.....	S64
¹³ C NMR spectrum.....	S68
HSQC spectrum	S69
HMBC spectrum	S72

Detailed NMR assignments of Compounds 6 , 7 , 10 , 14 and 15	S76
---	-----

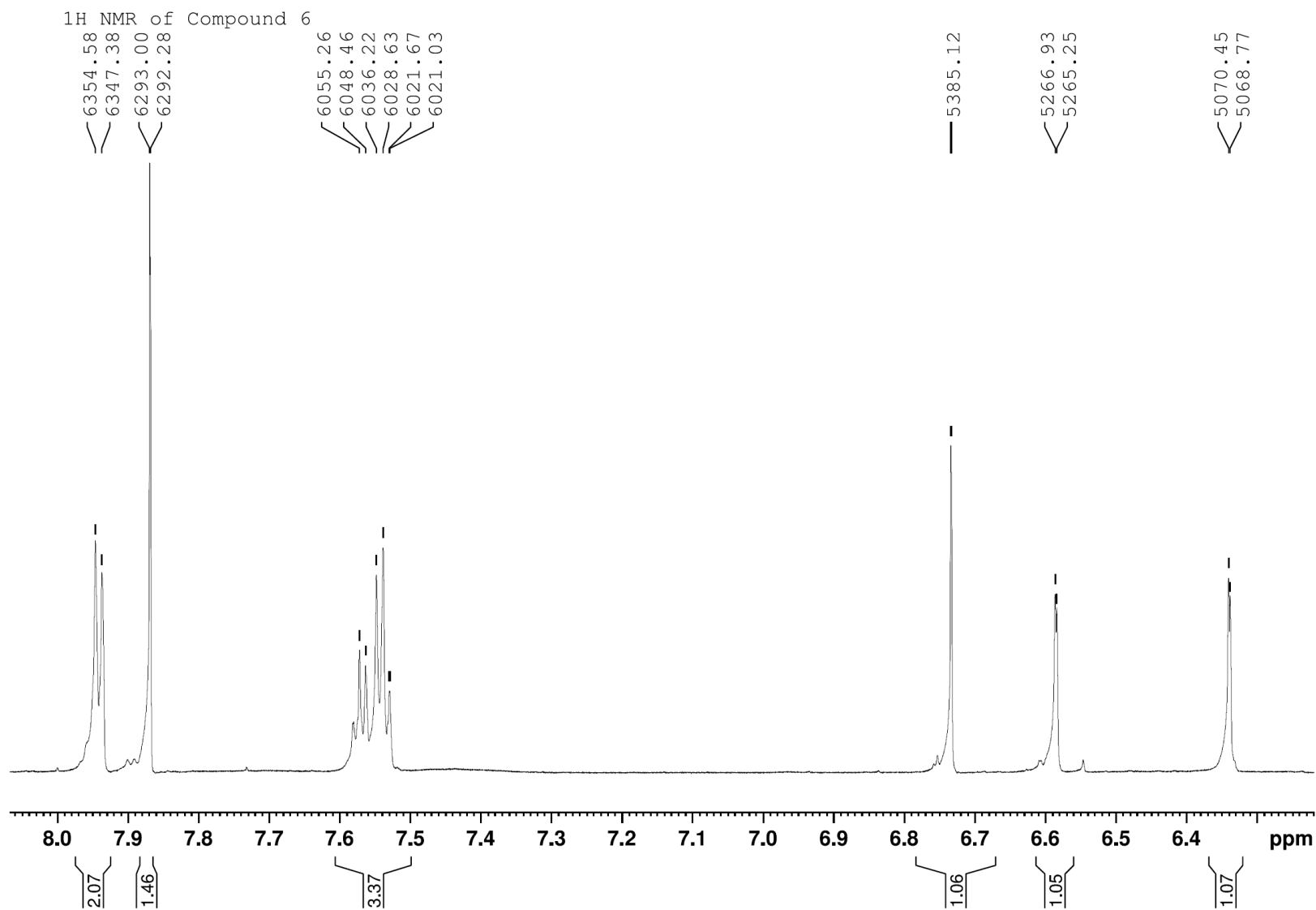
¹H NMR of Compound 6

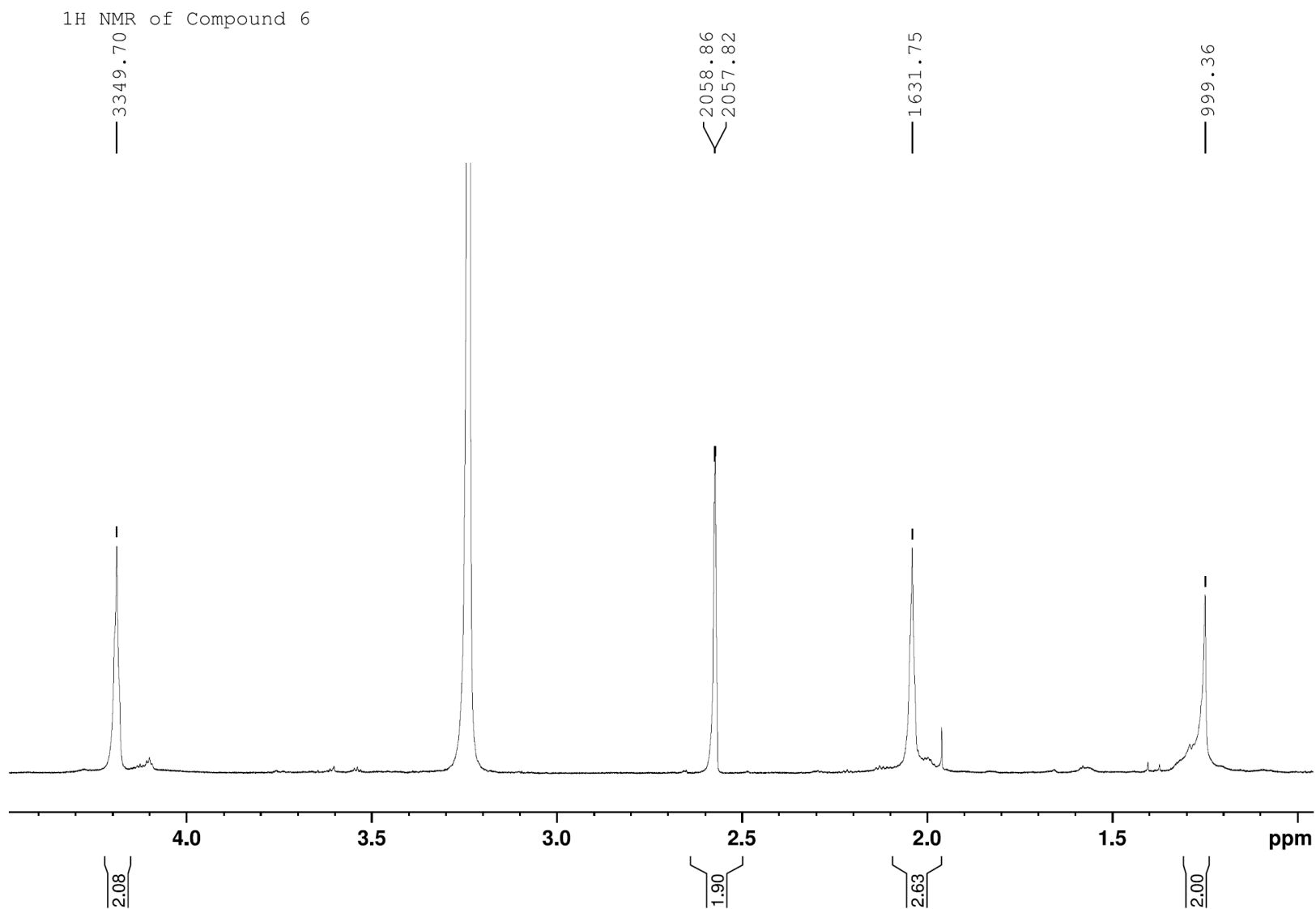
S2

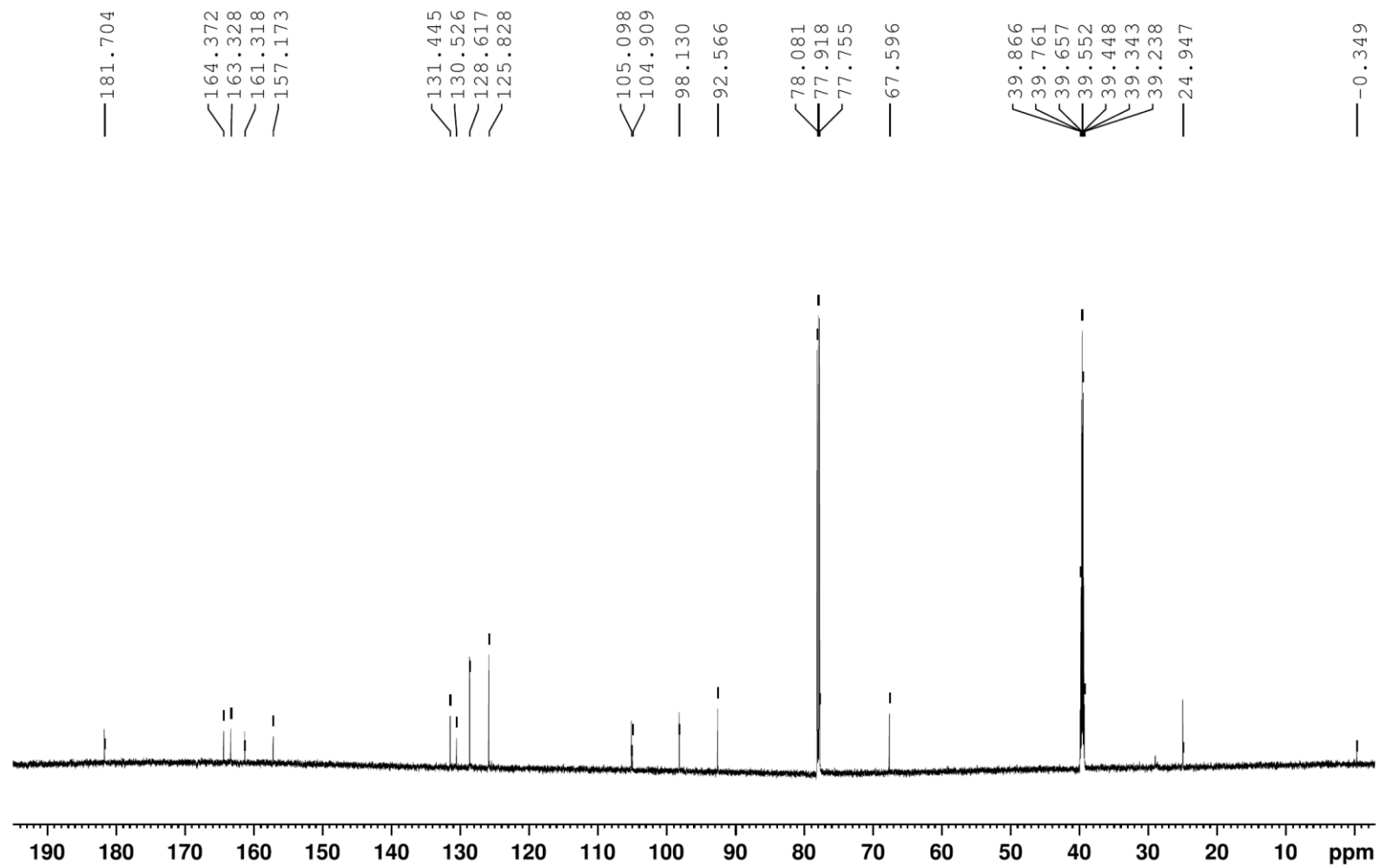
¹H NMR of Compound 6



S3

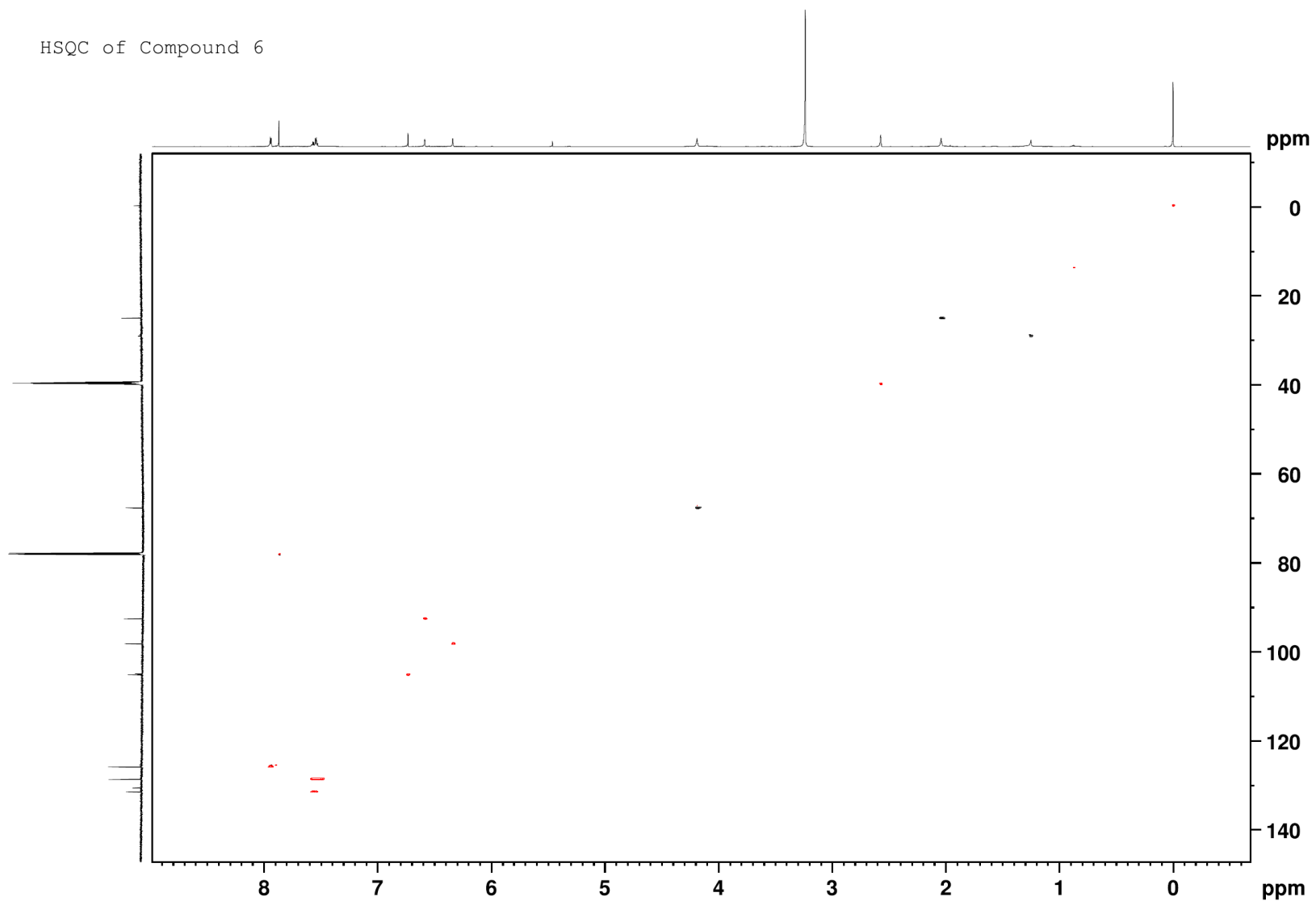




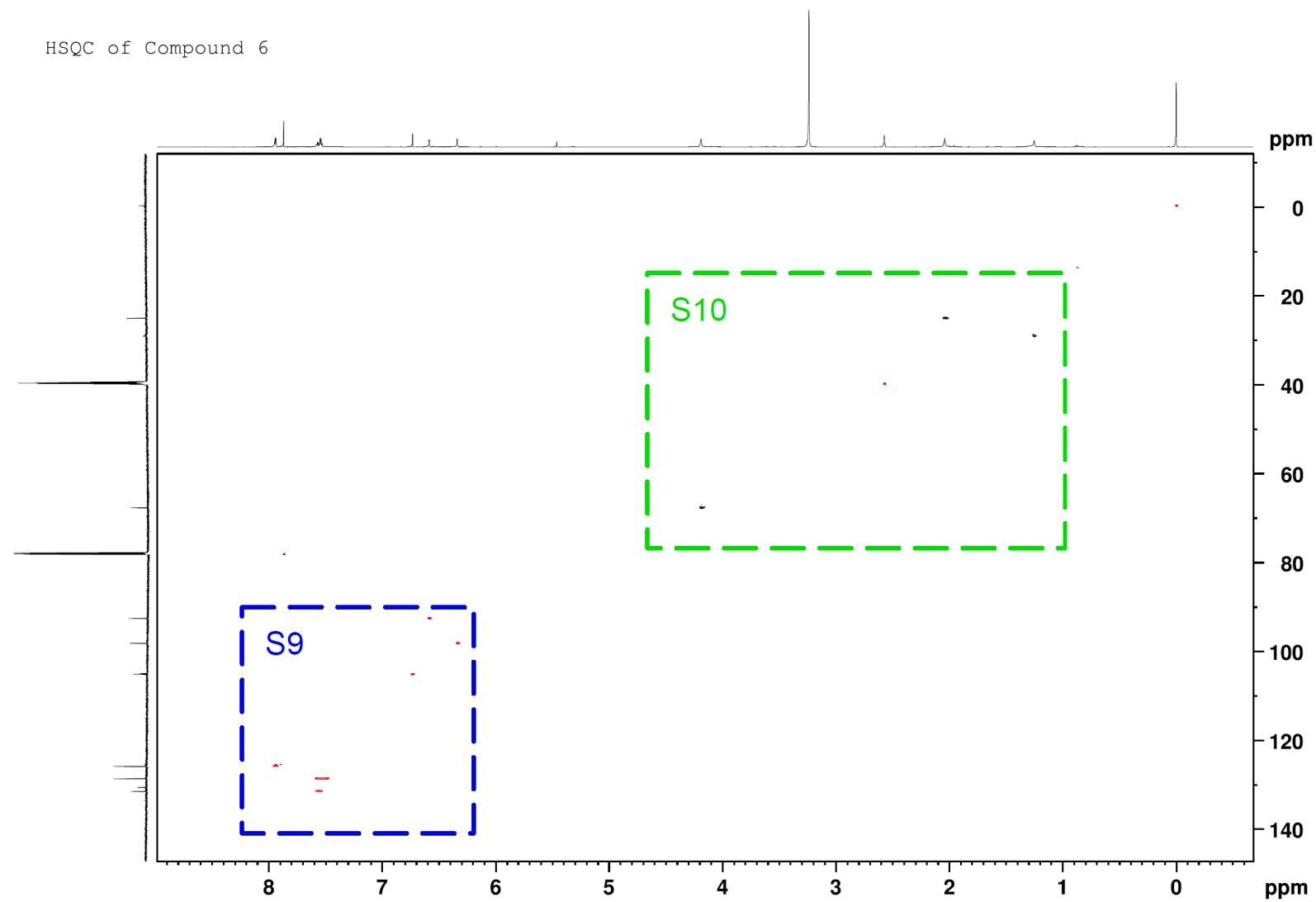
¹³C NMR of Compound 6

S6

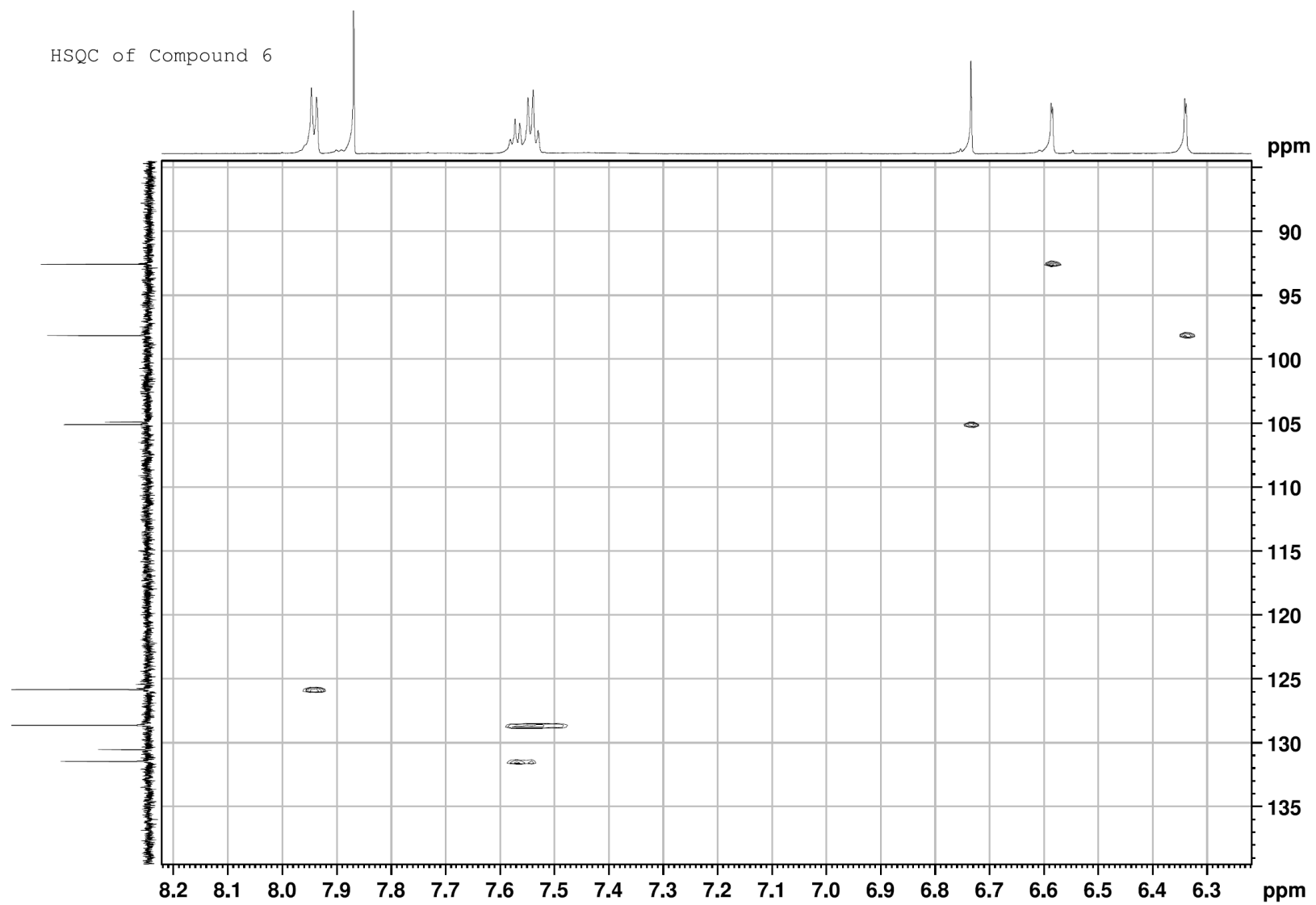
HSQC of Compound 6

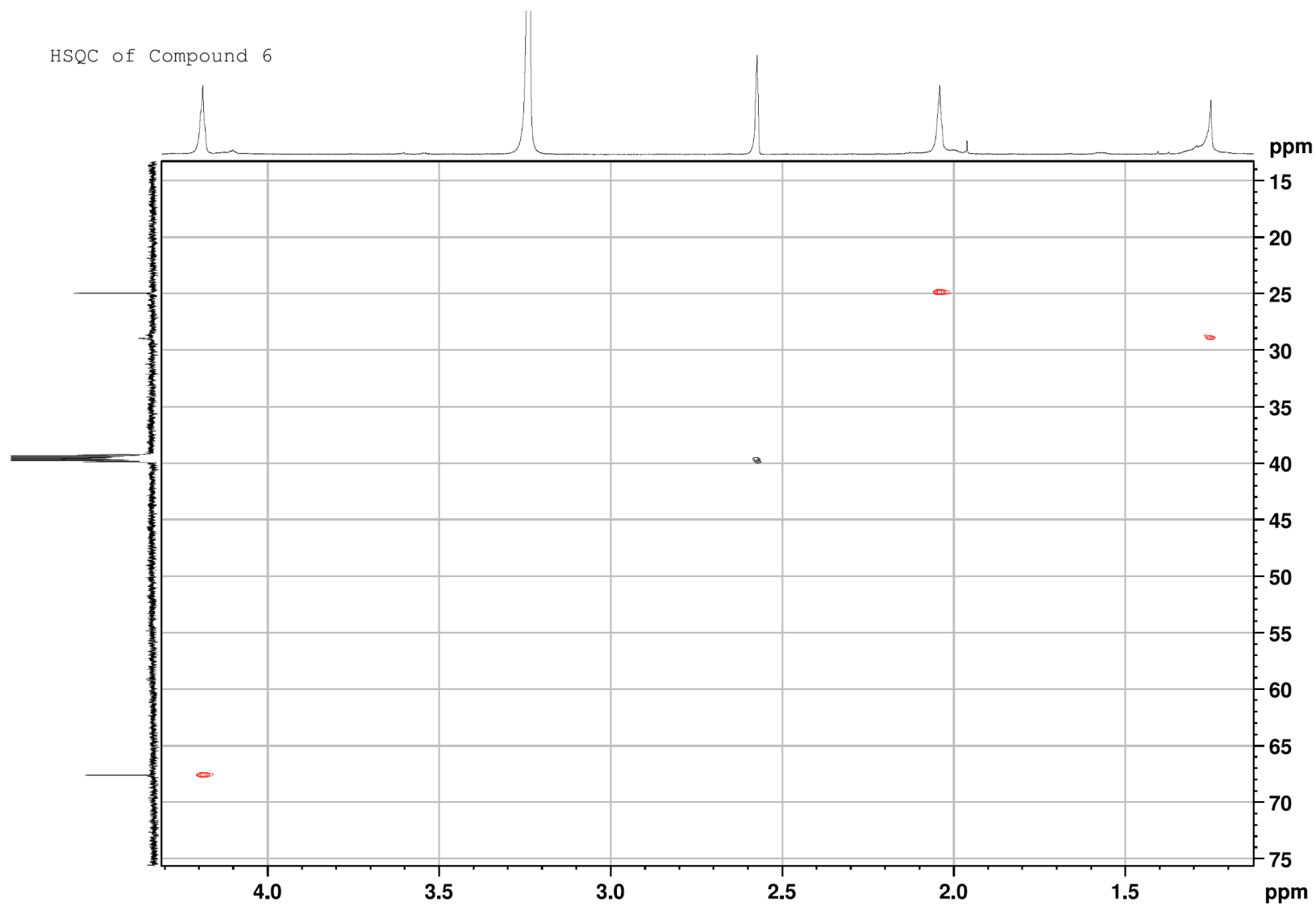


HSQC of Compound 6

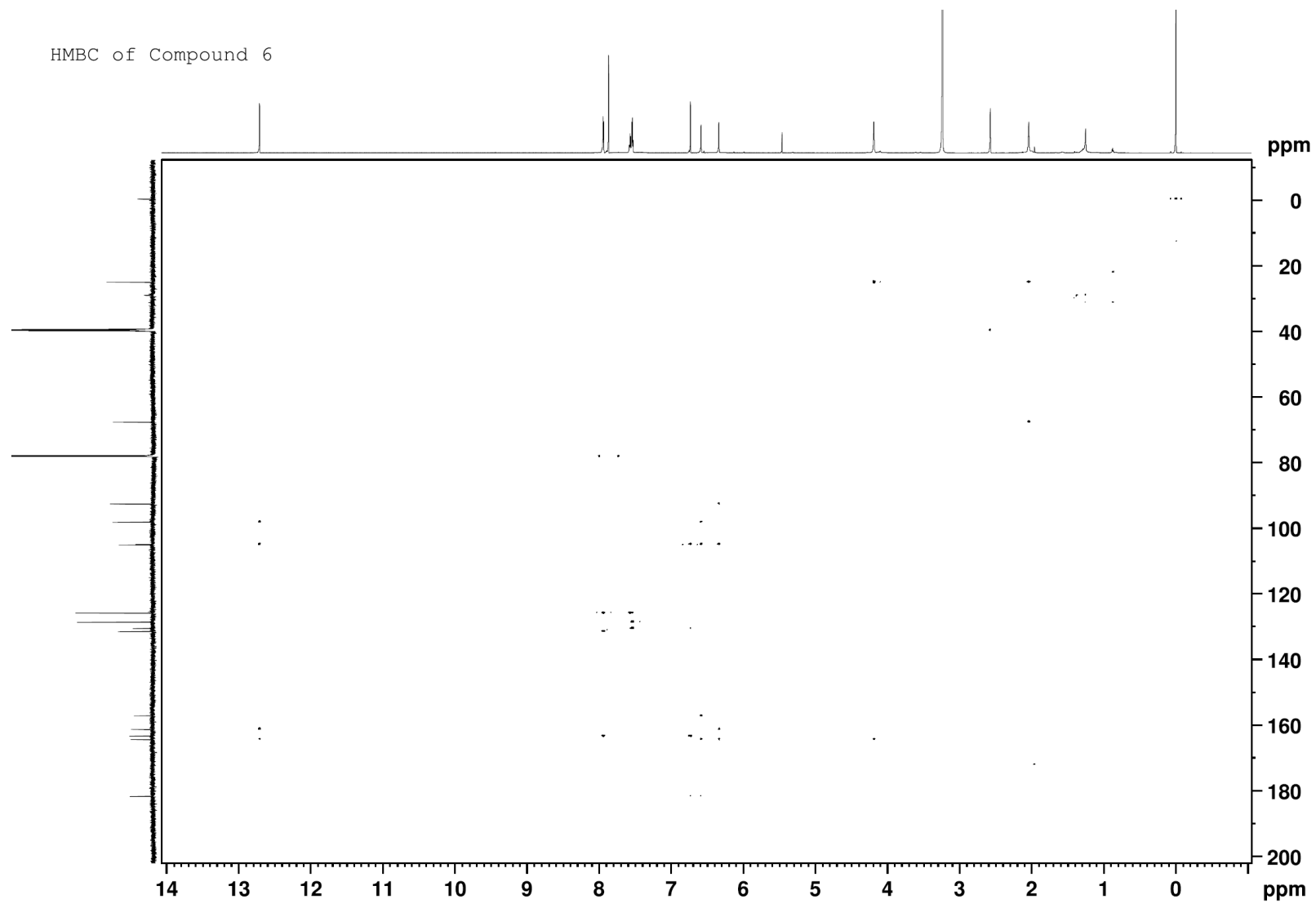


S8



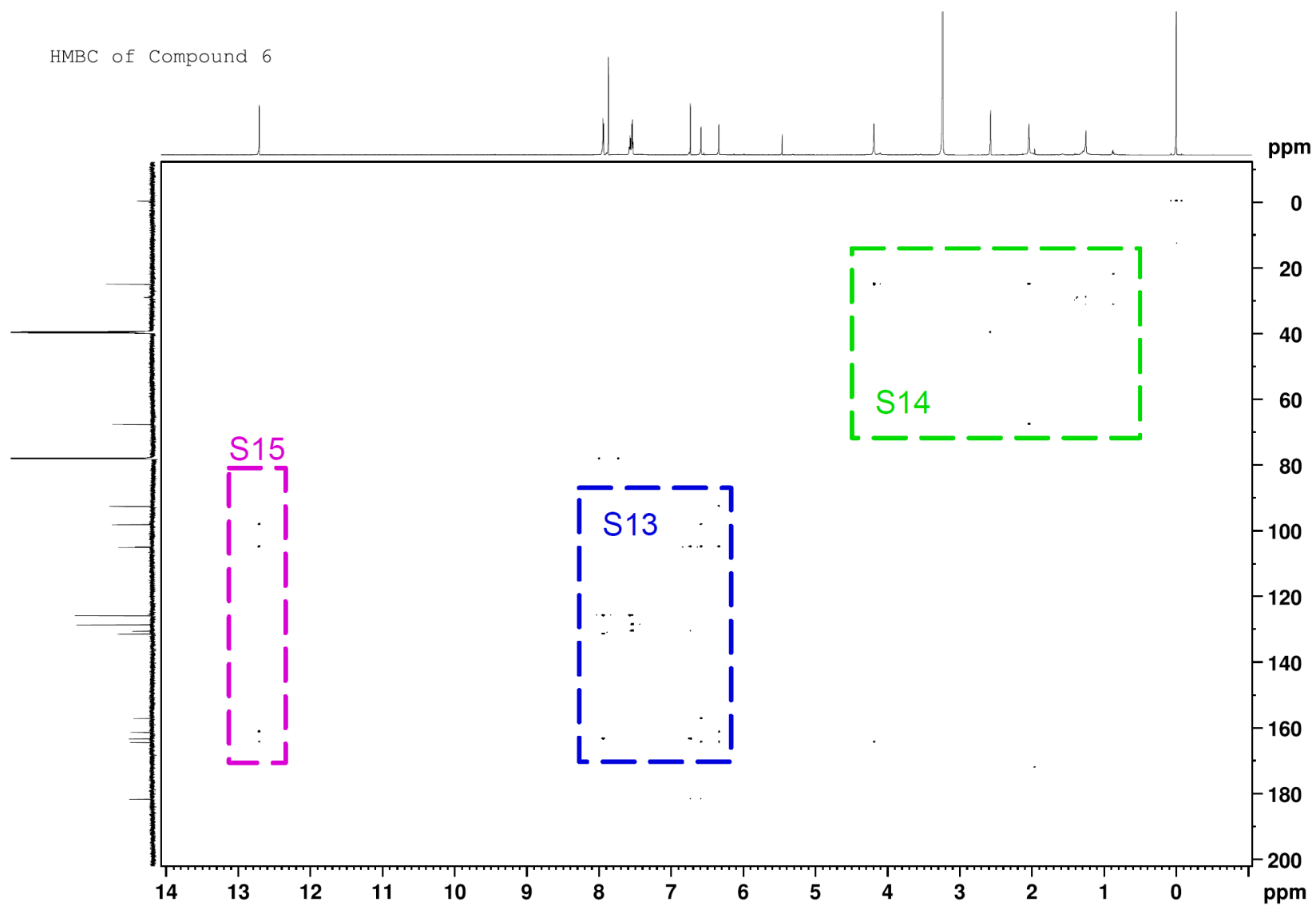


S10

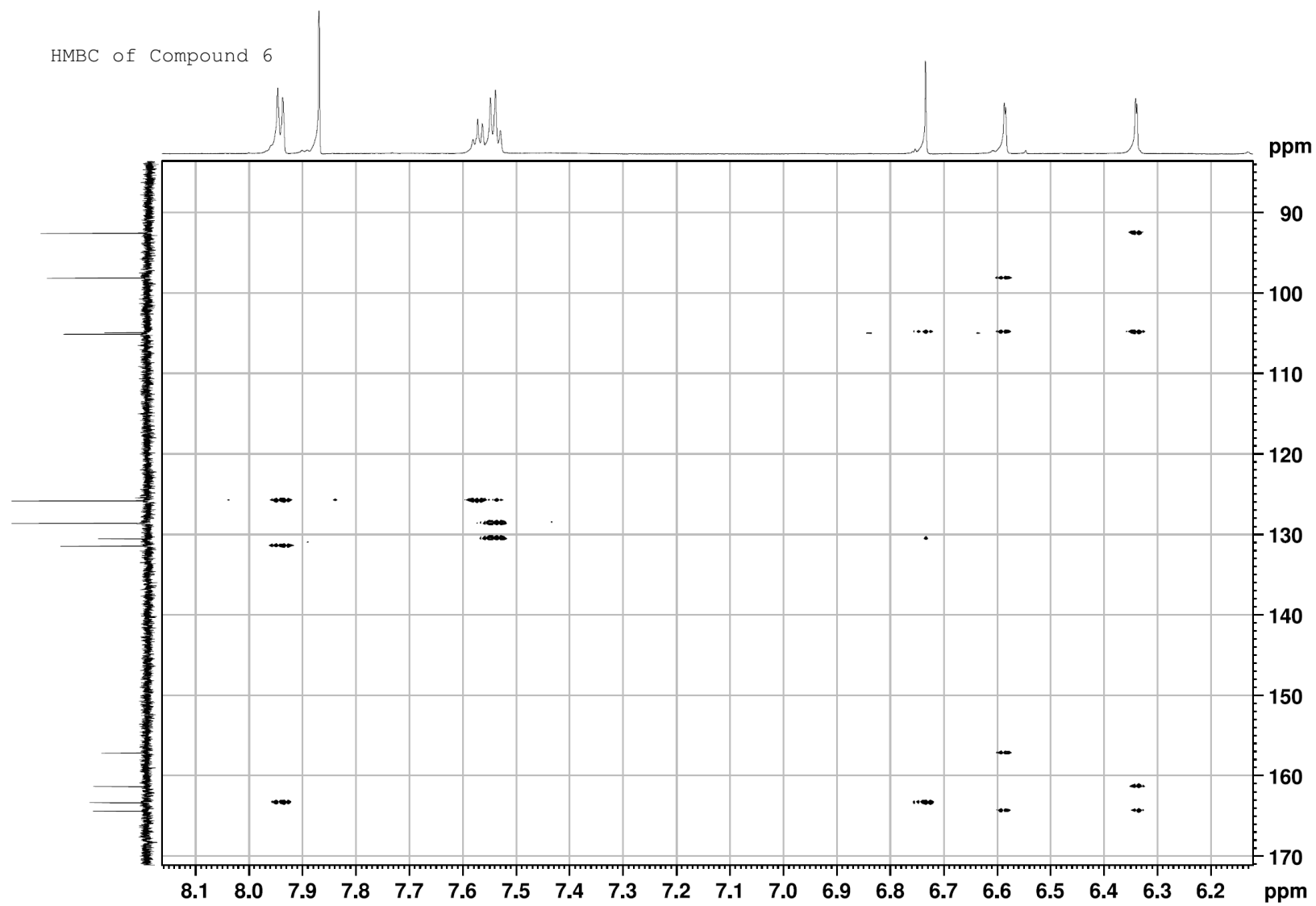


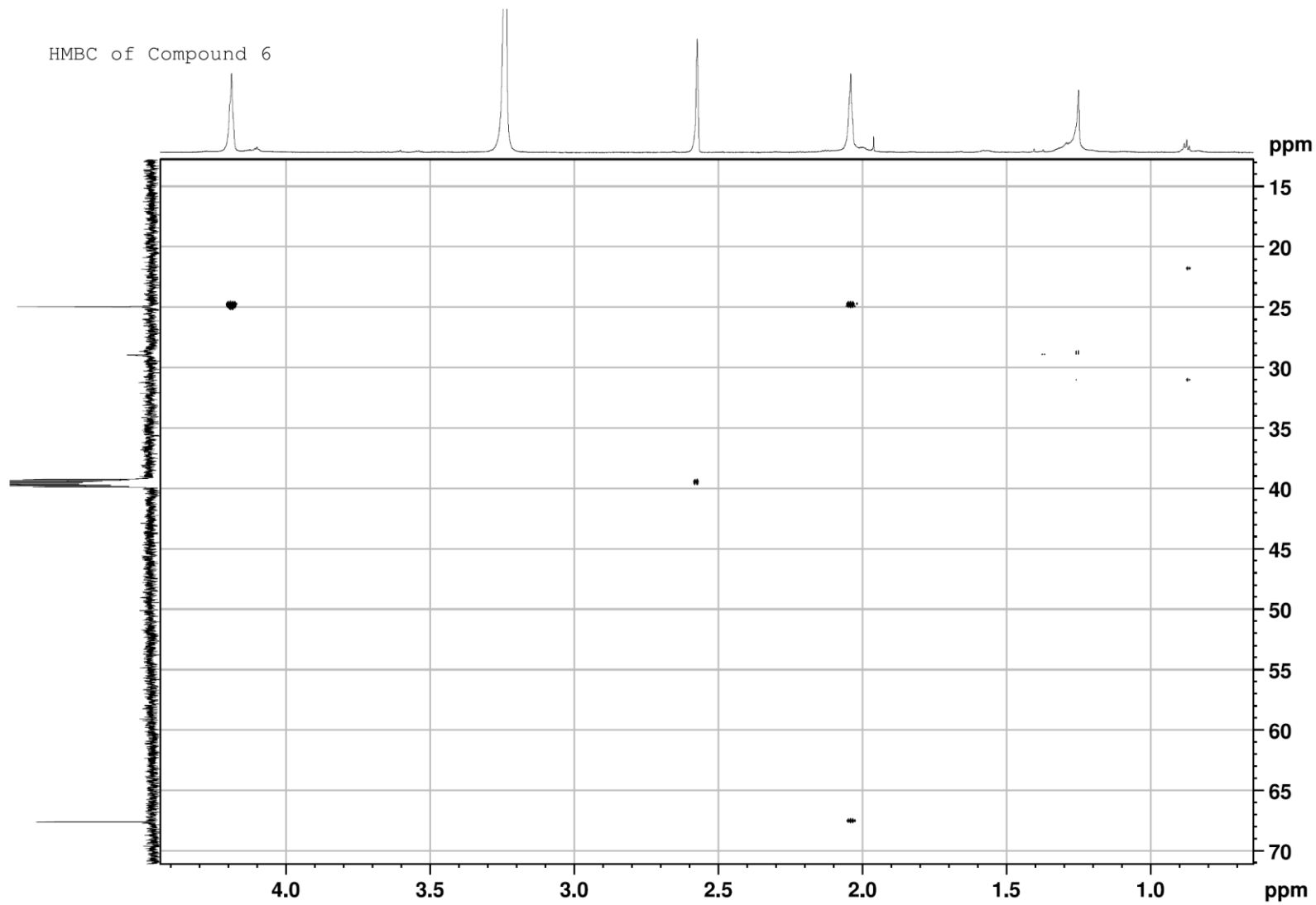
S11

HMBC of Compound 6



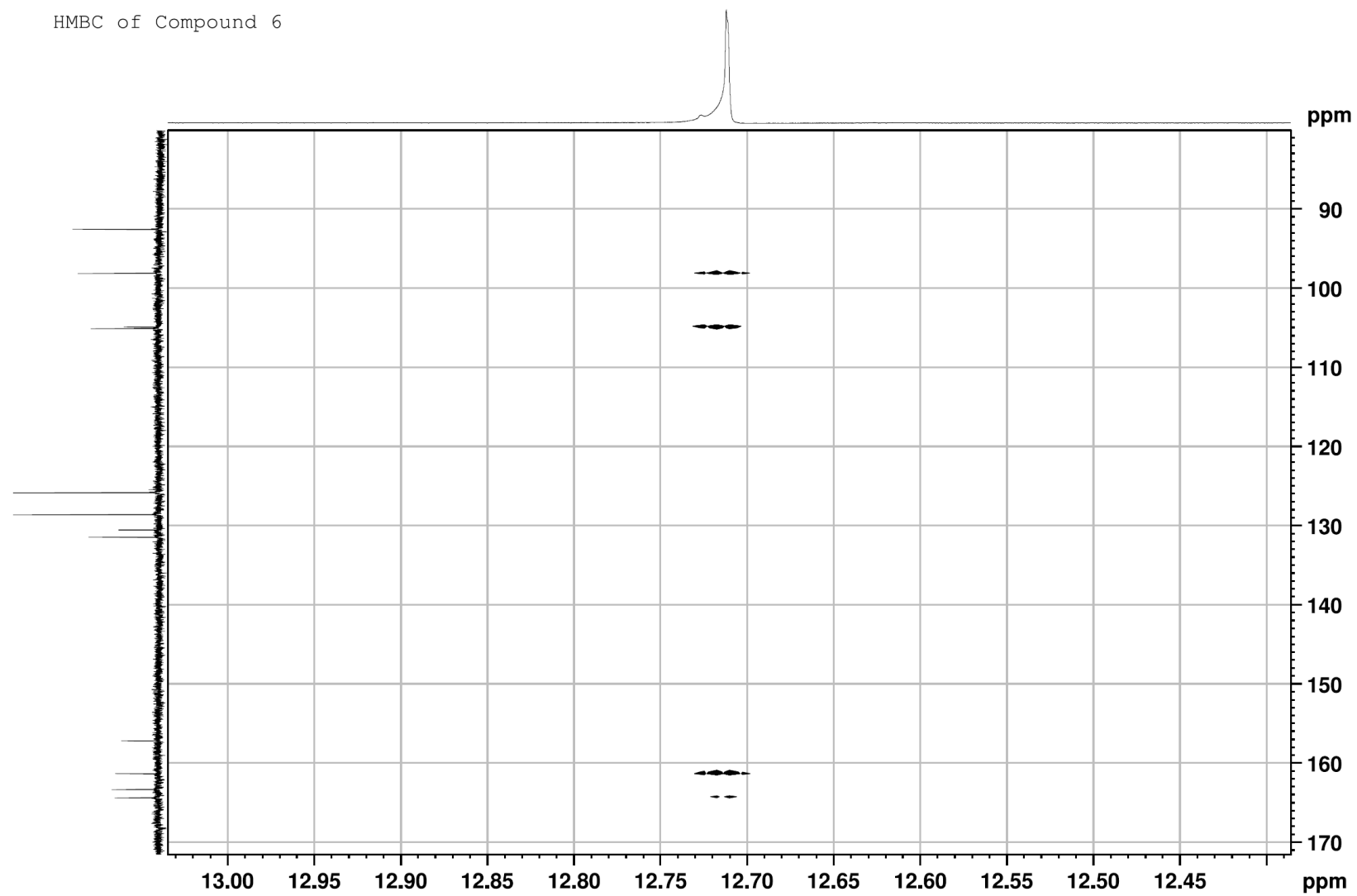
S12



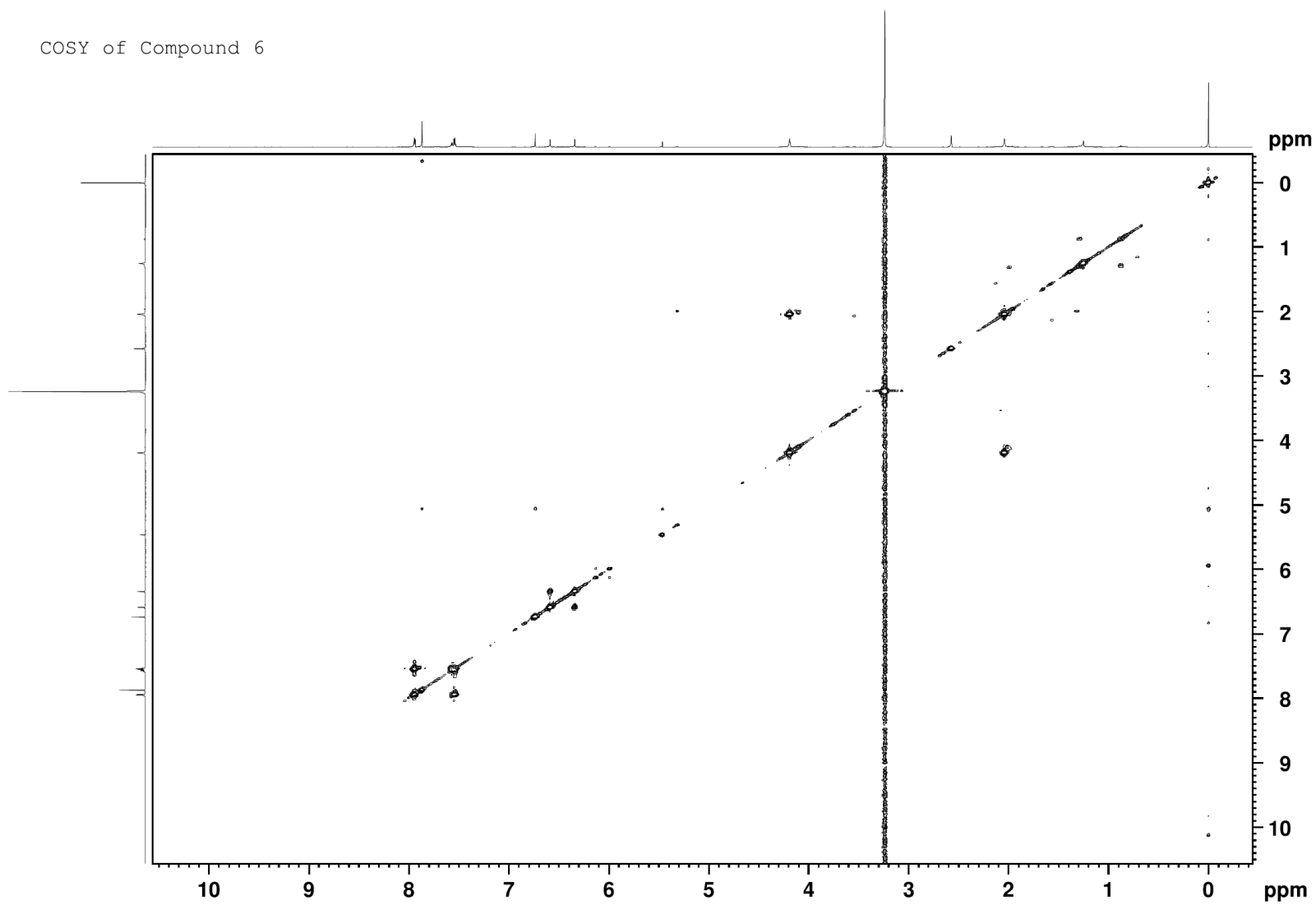


S14

HMBC of Compound 6

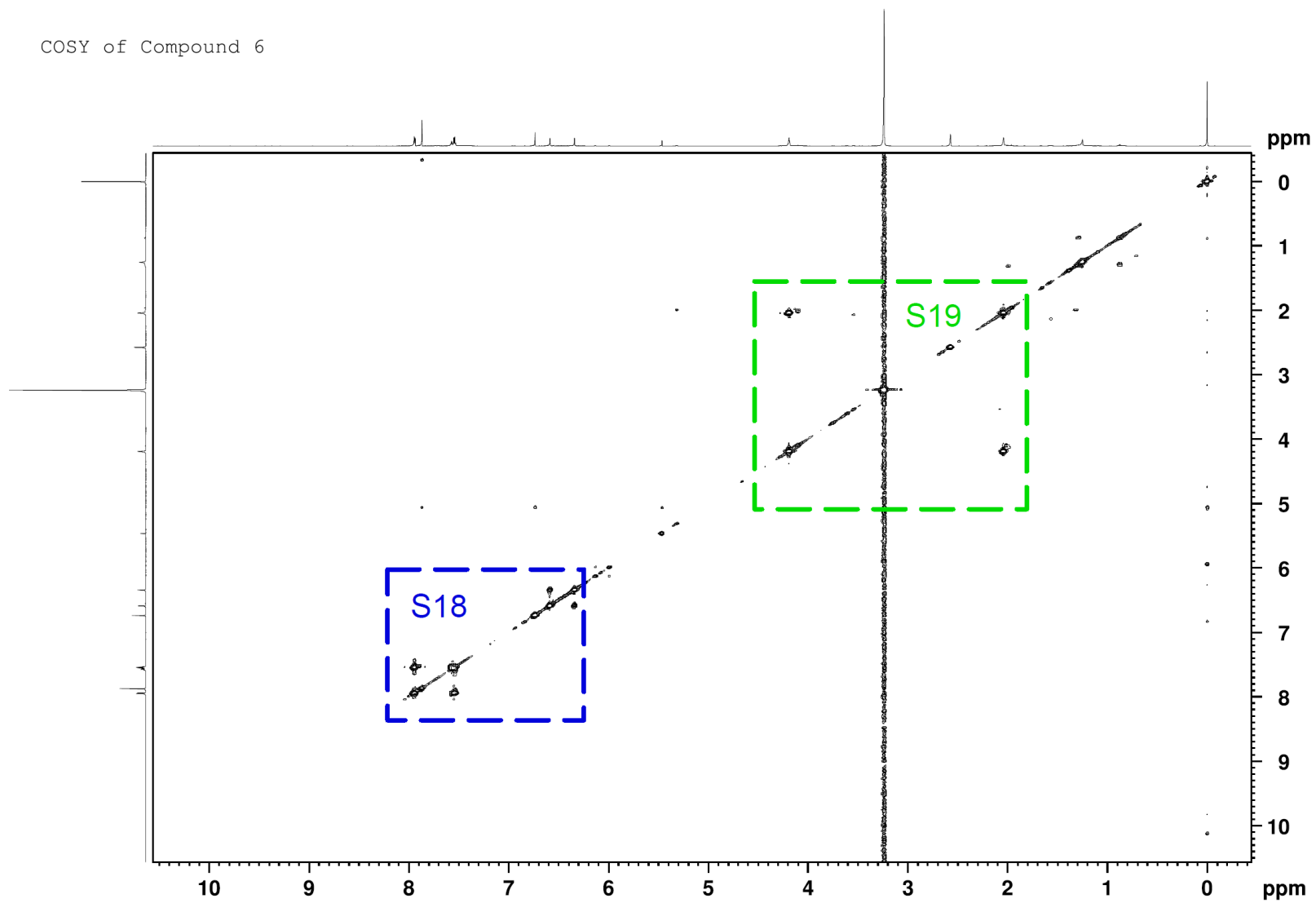


COSY of Compound 6



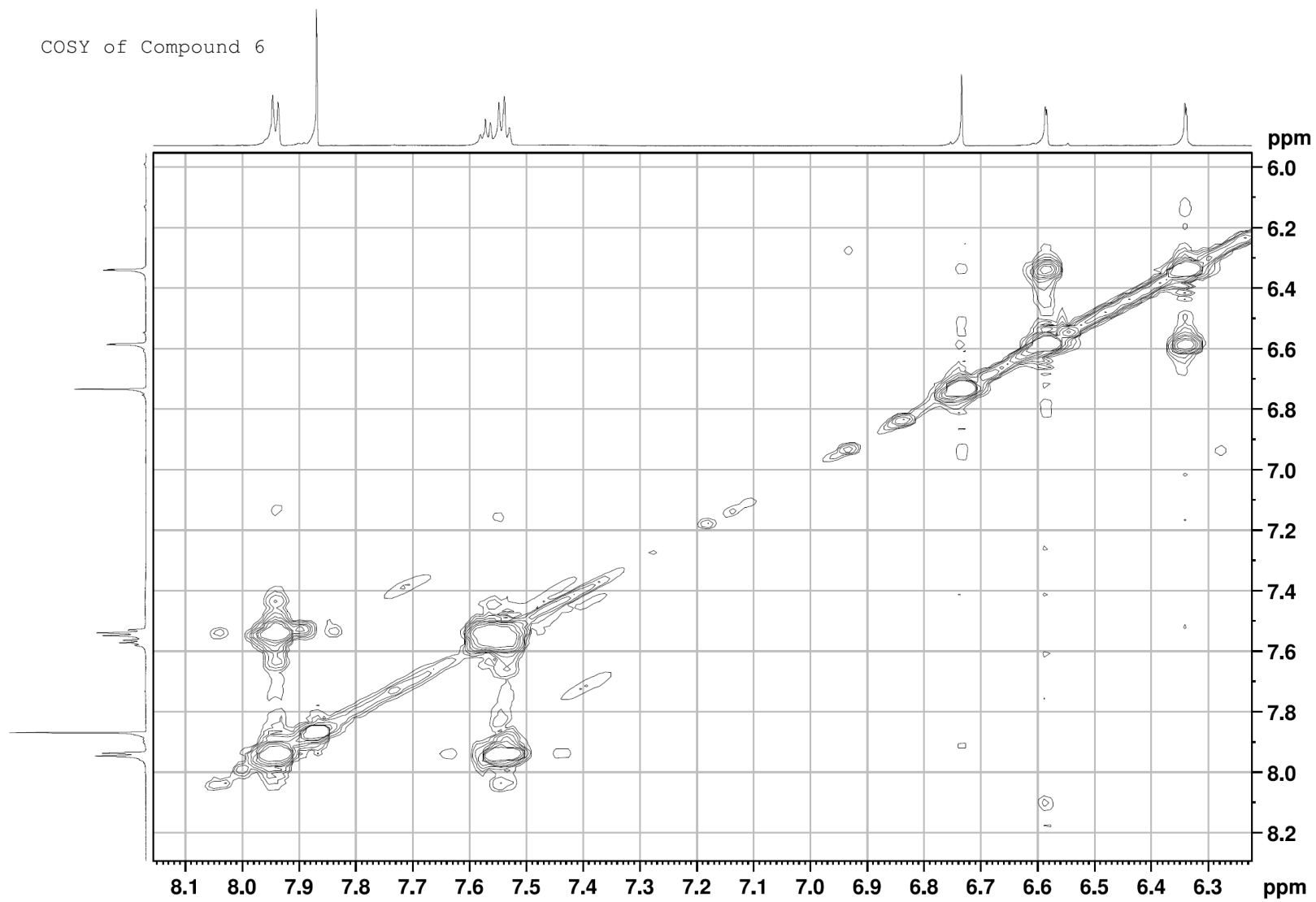
S16

COSY of Compound 6

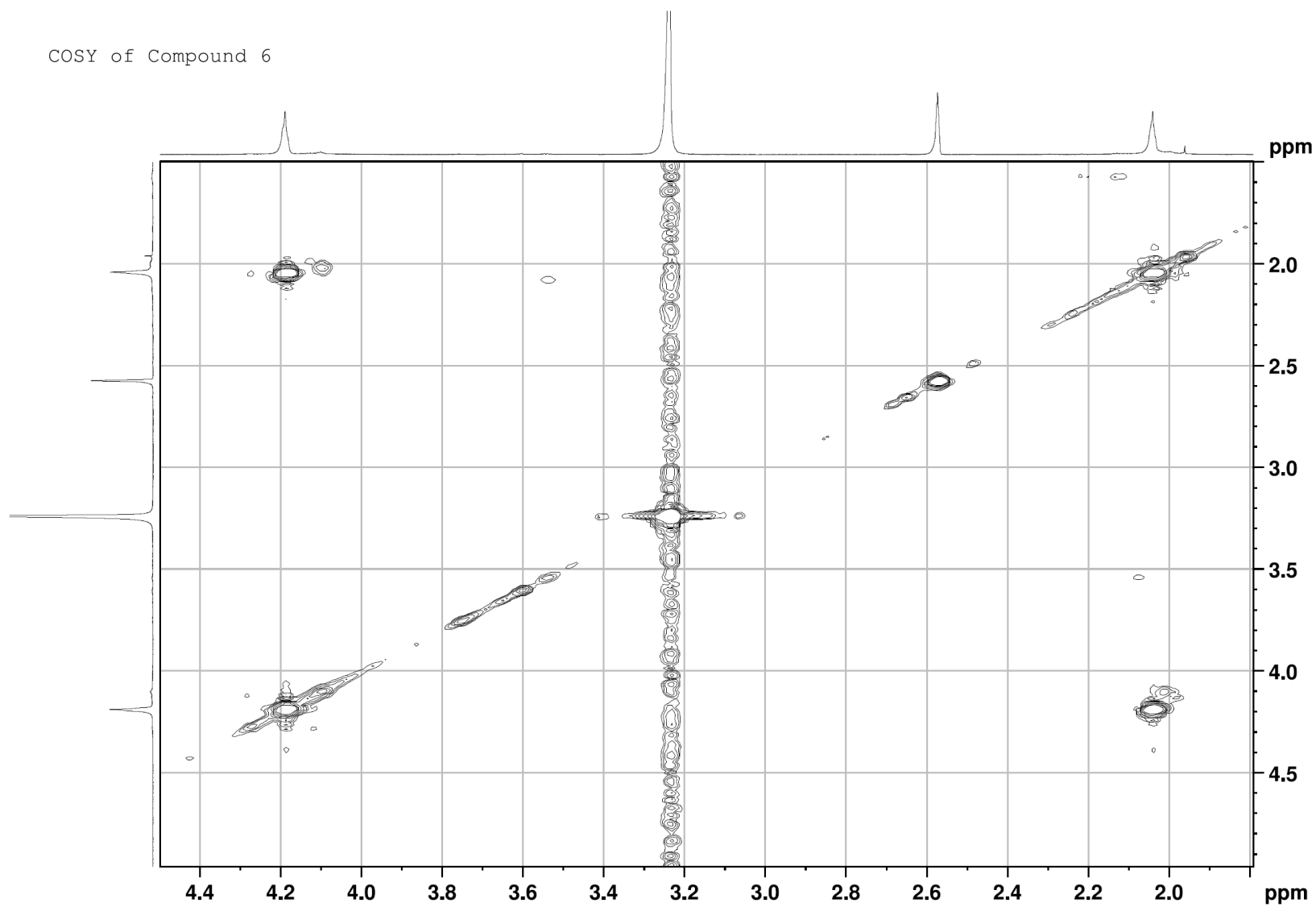


S17

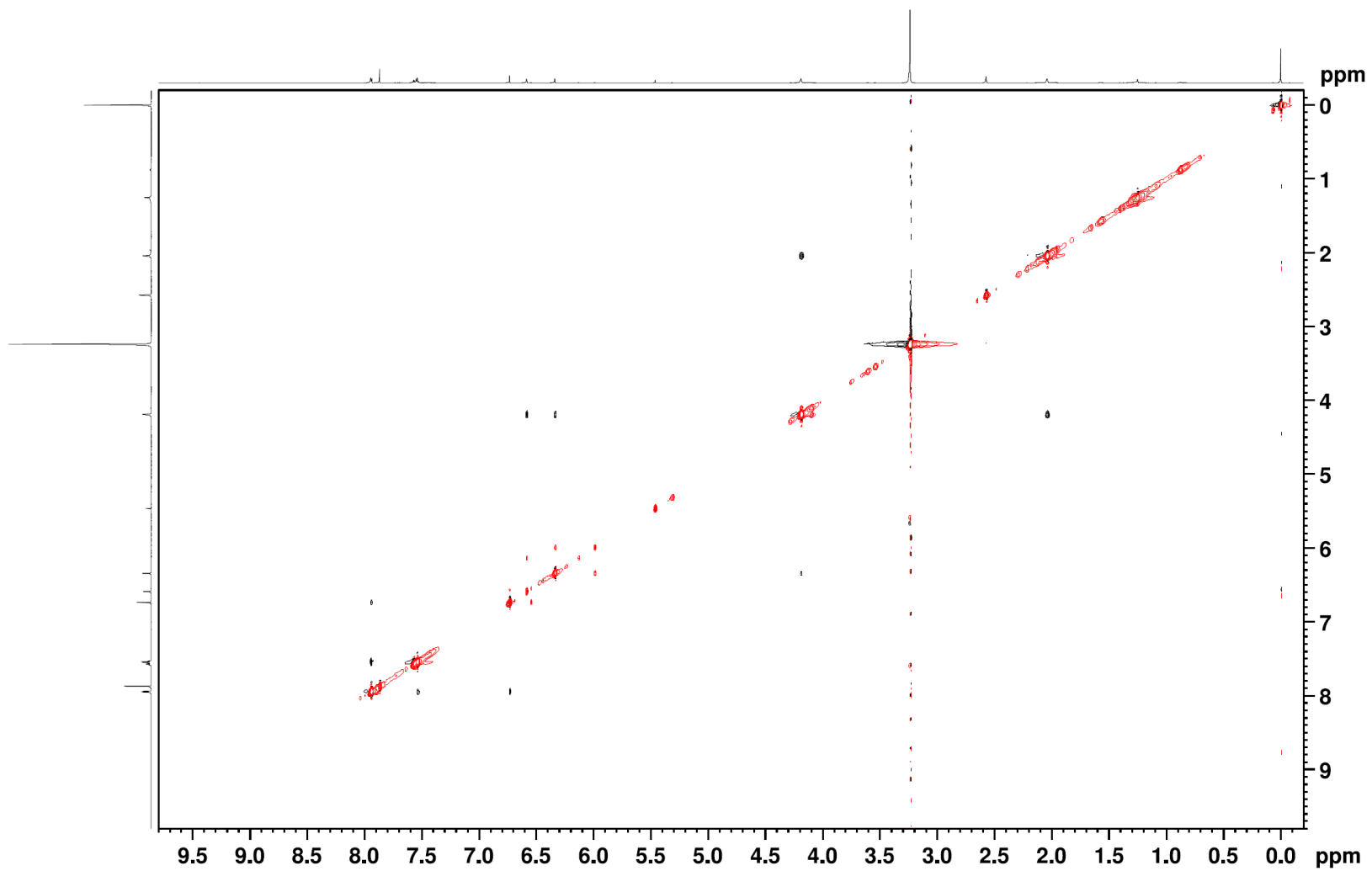
COSY of Compound 6



COSY of Compound 6

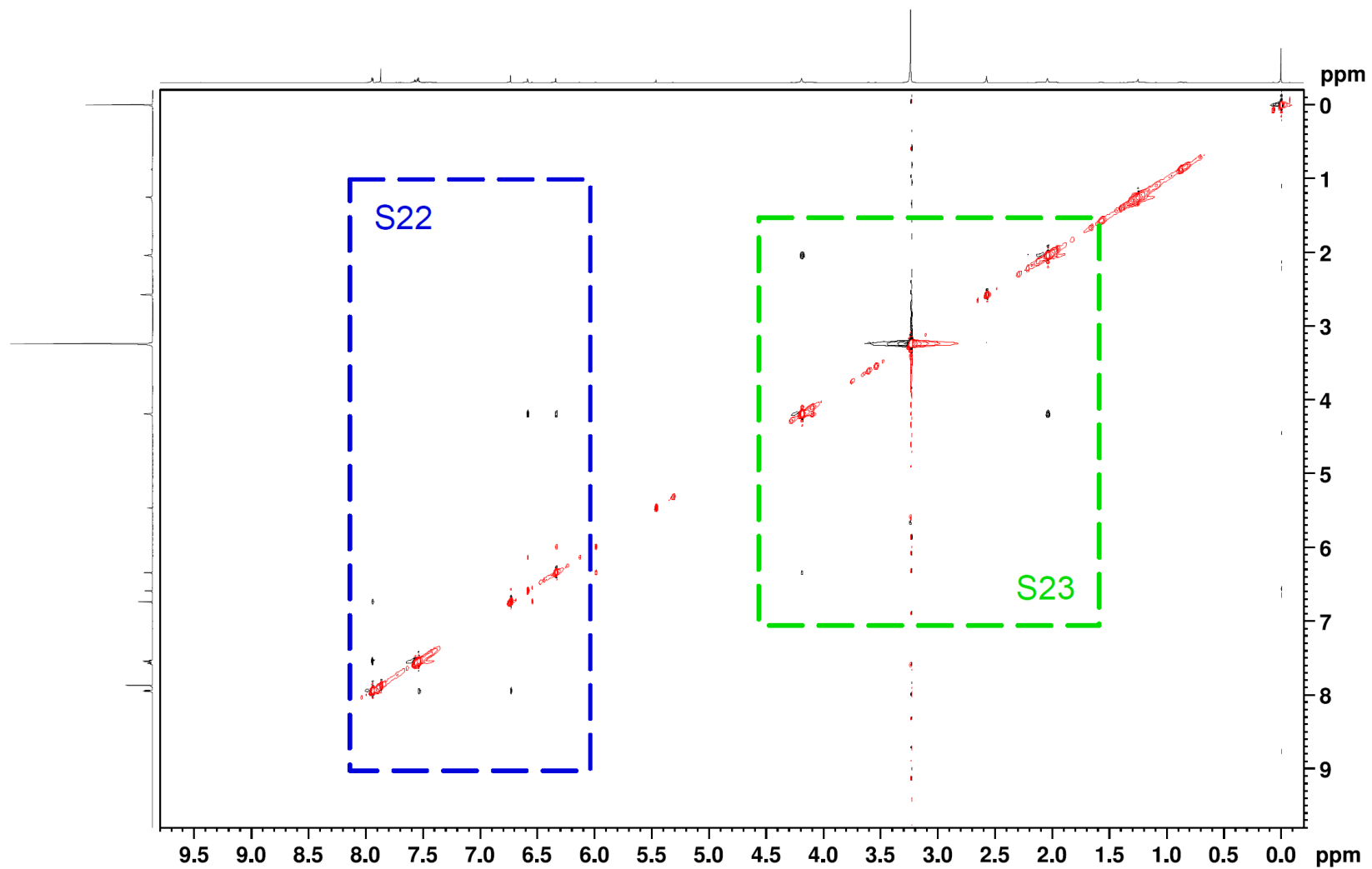


ROESY of Compound 6

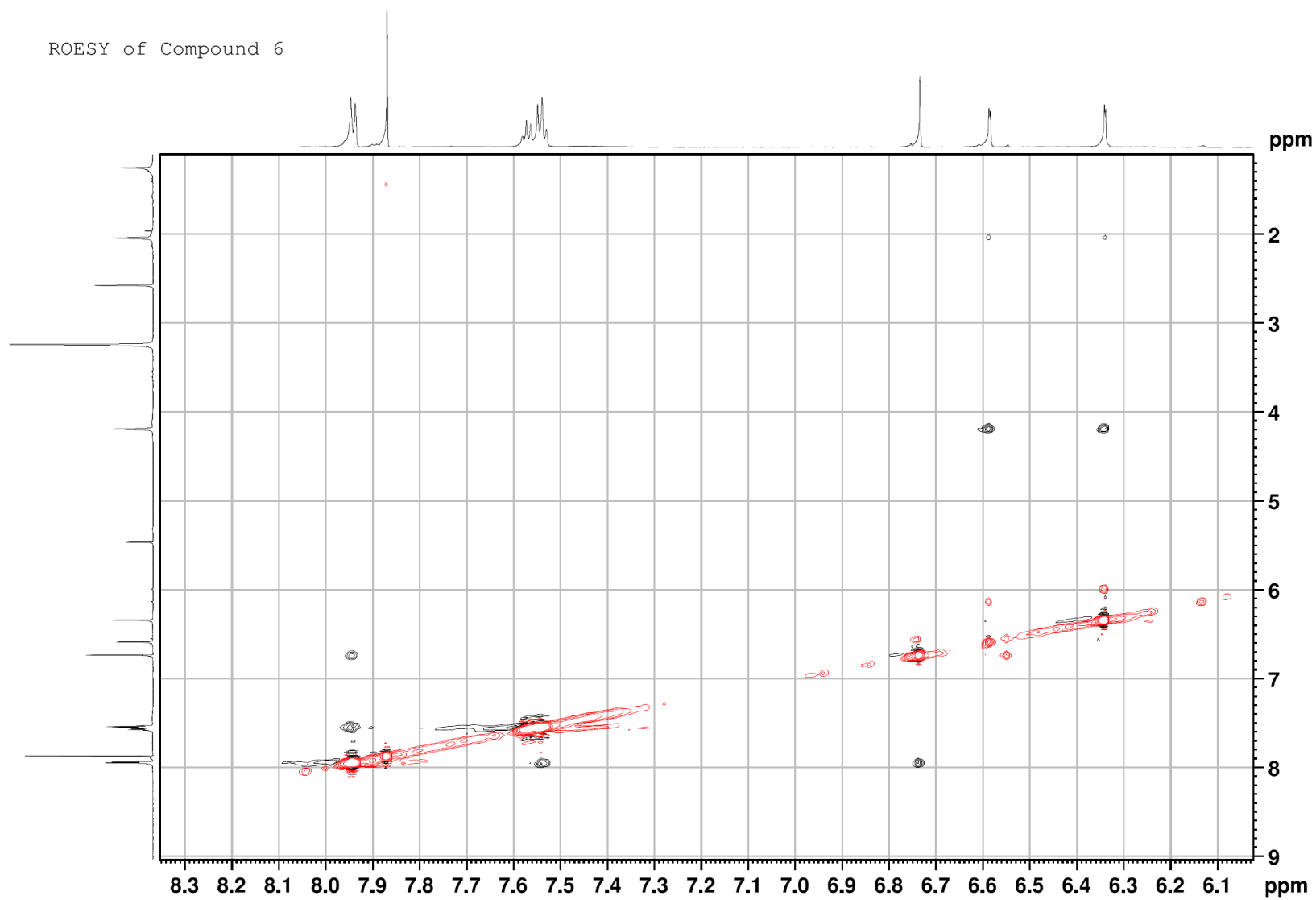


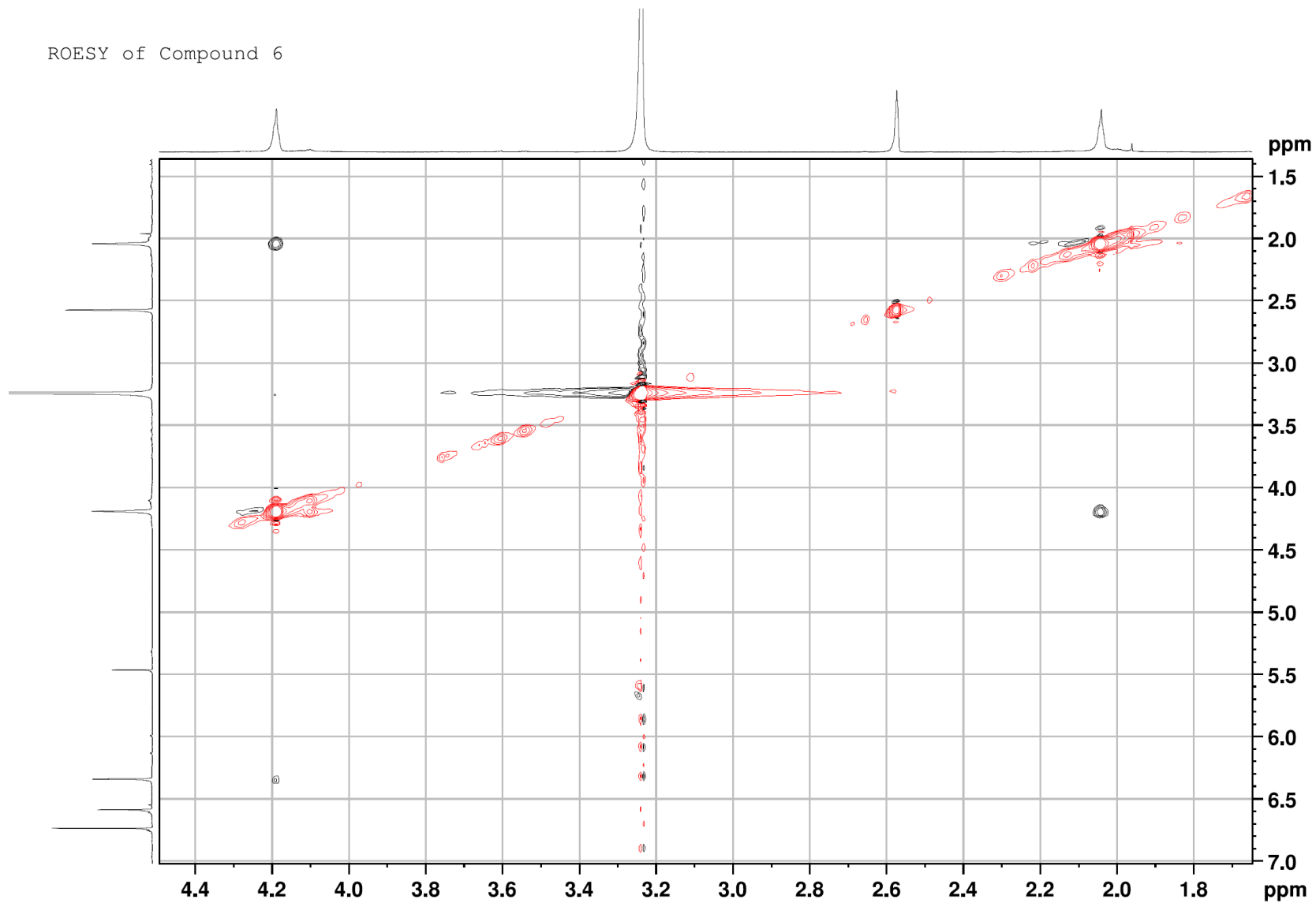
S20

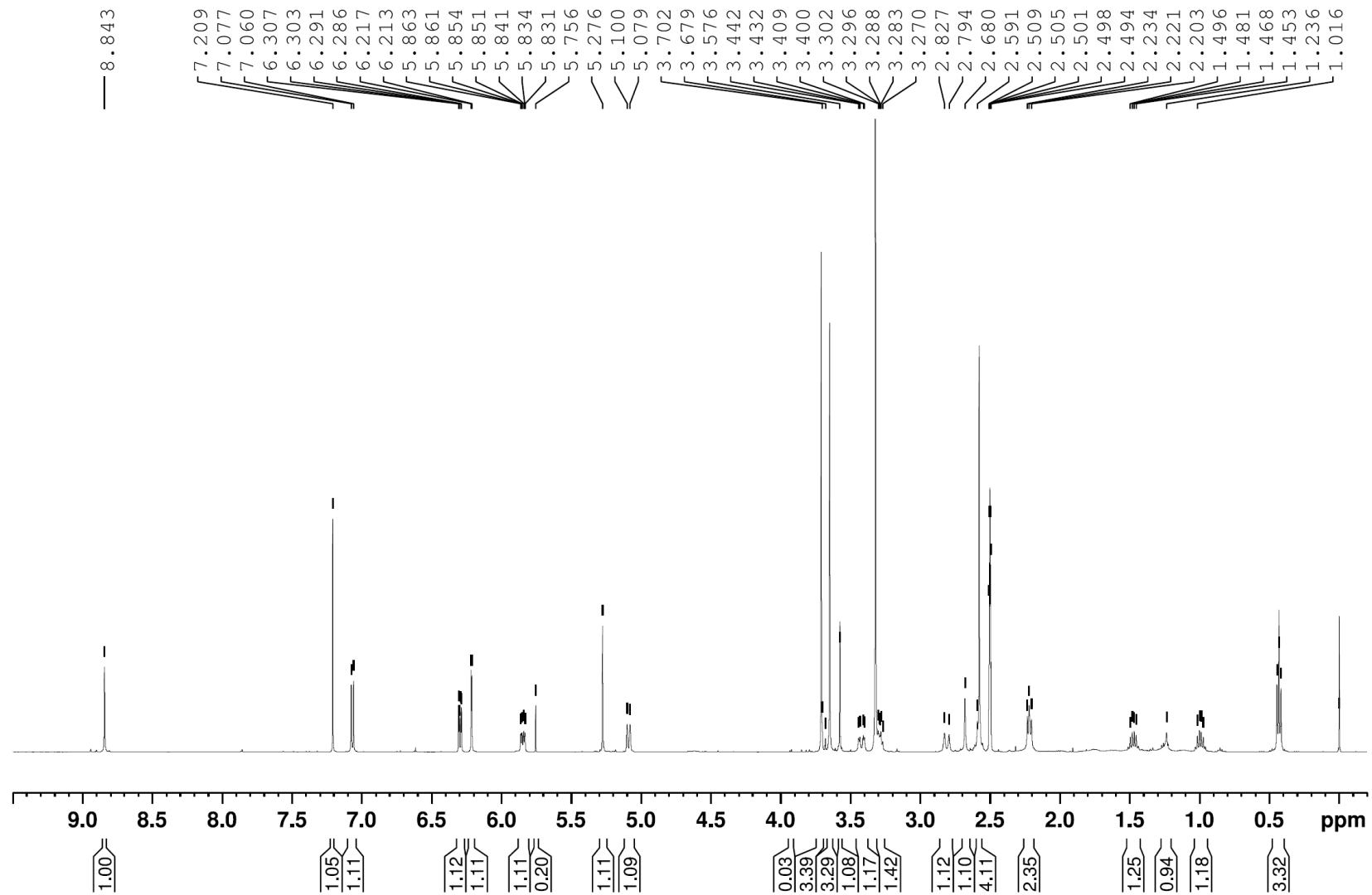
ROESY of Compound 6



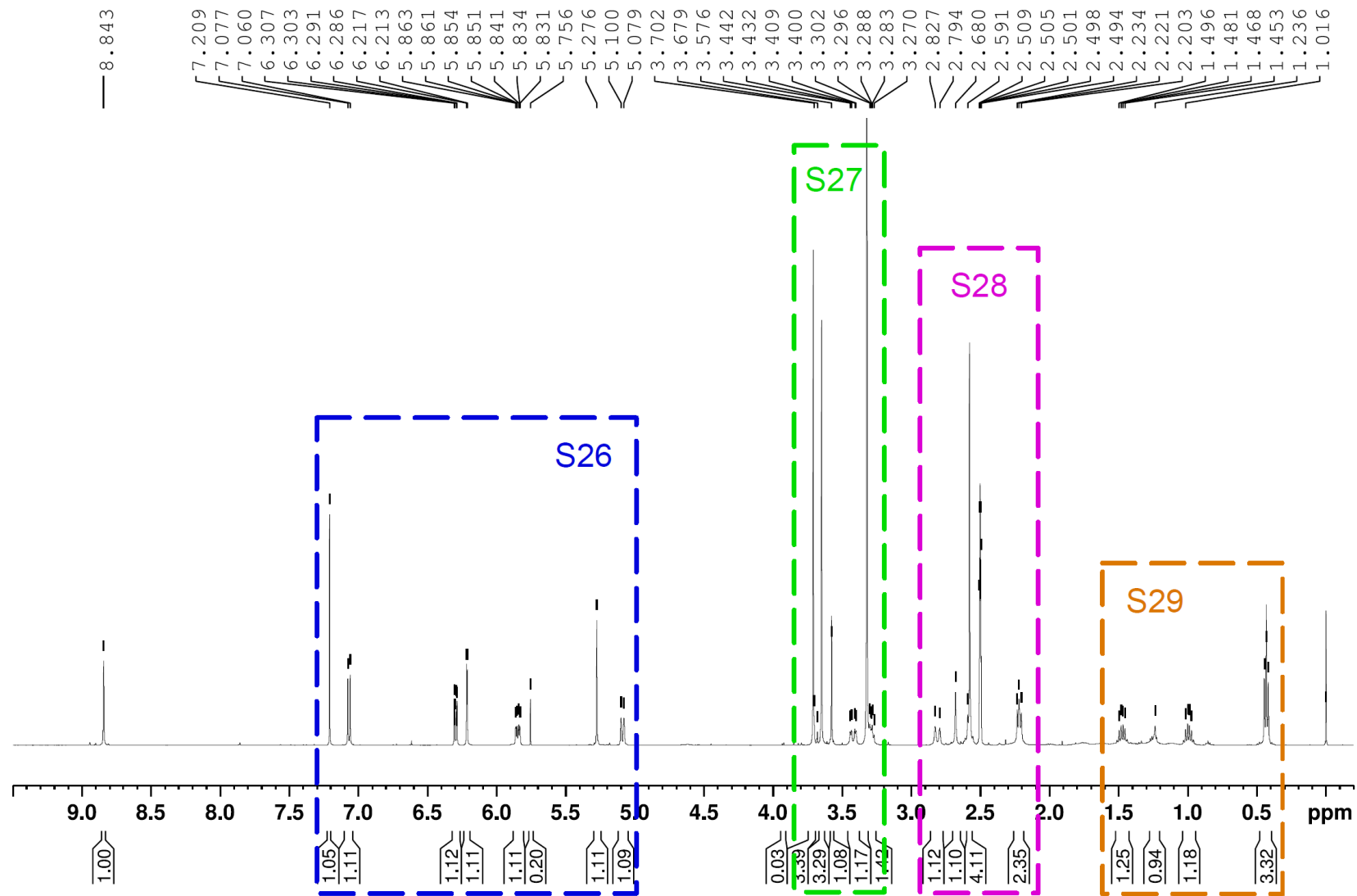
S21



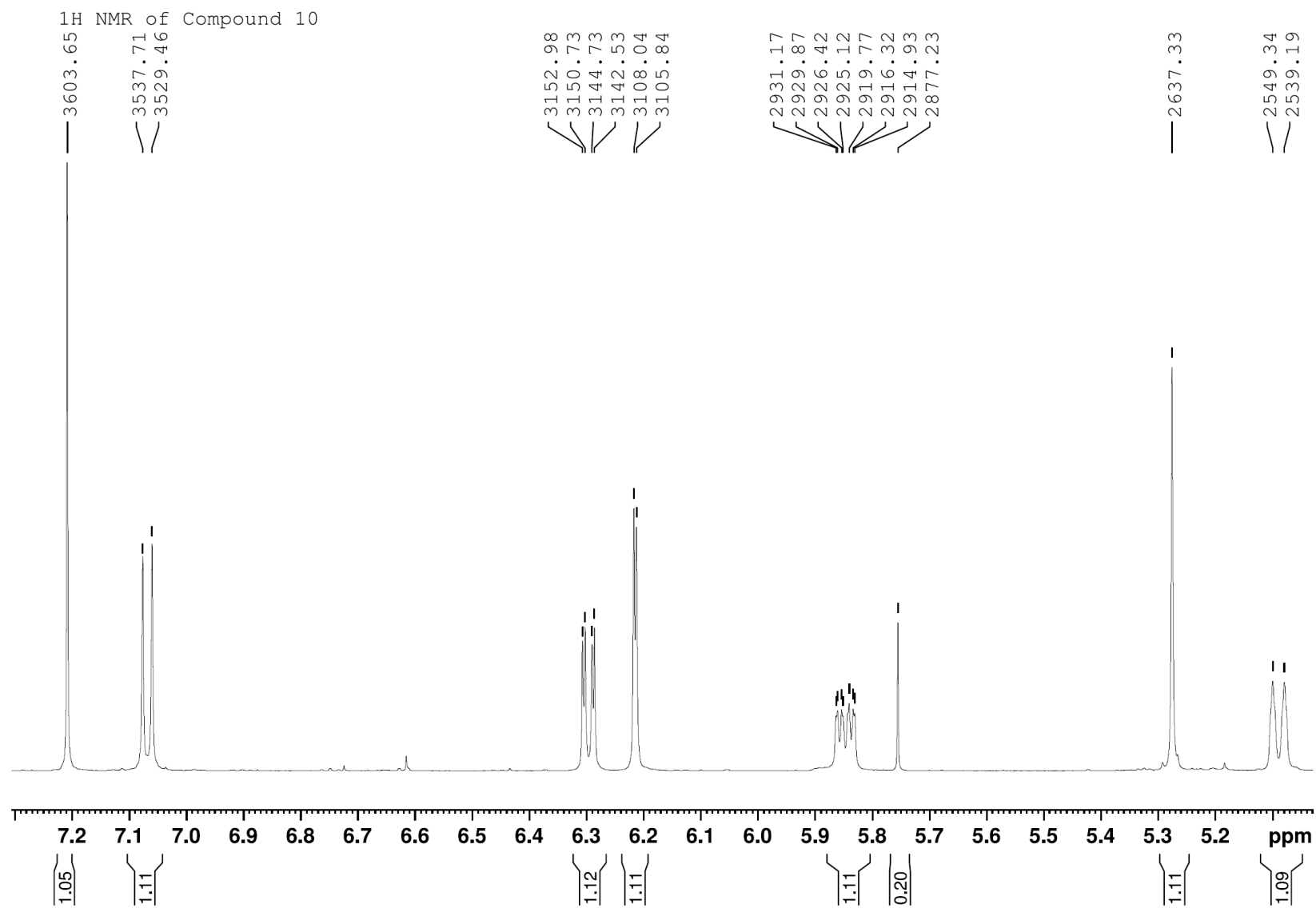


¹H NMR of Compound 10

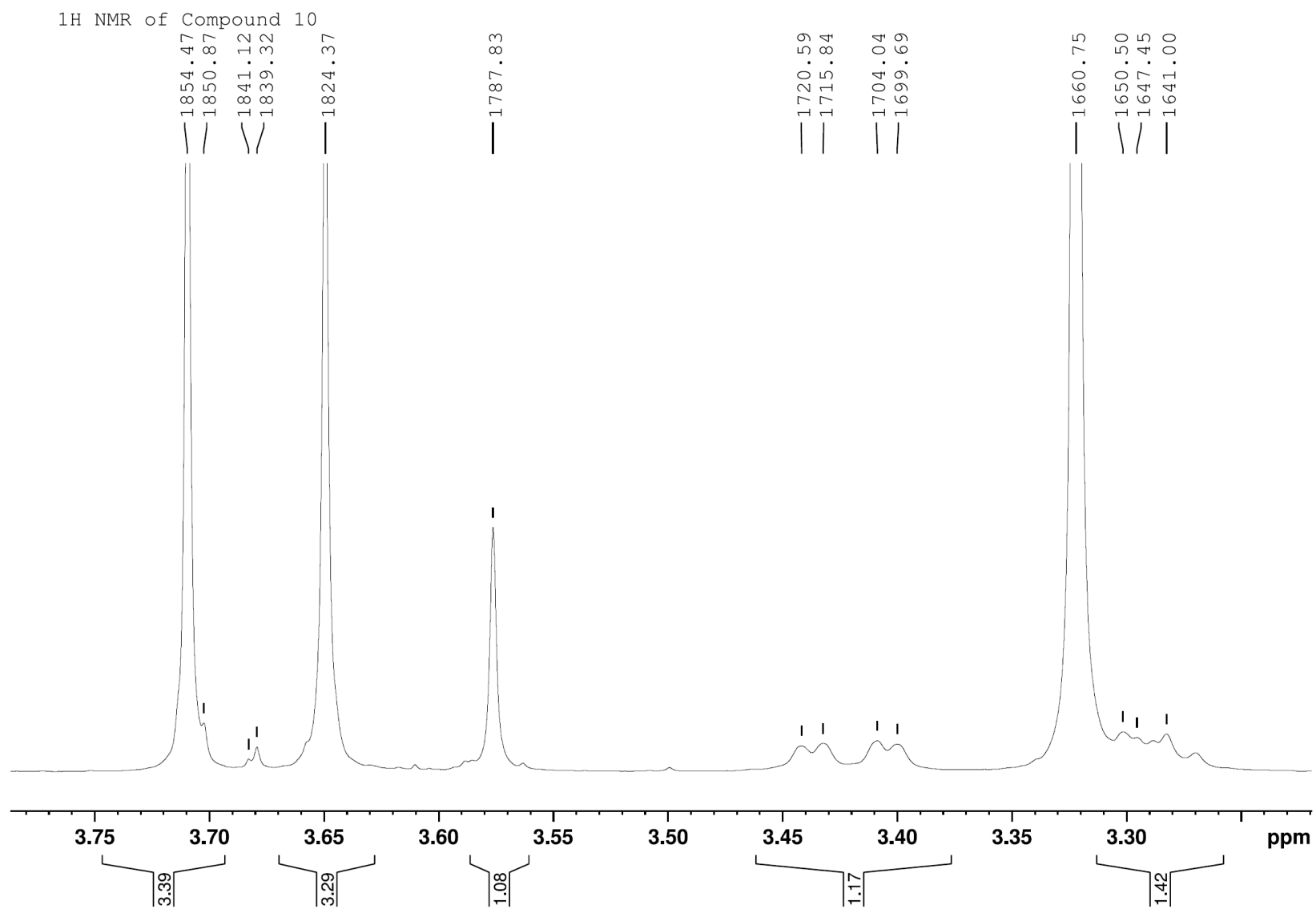
¹H NMR of Compound 10



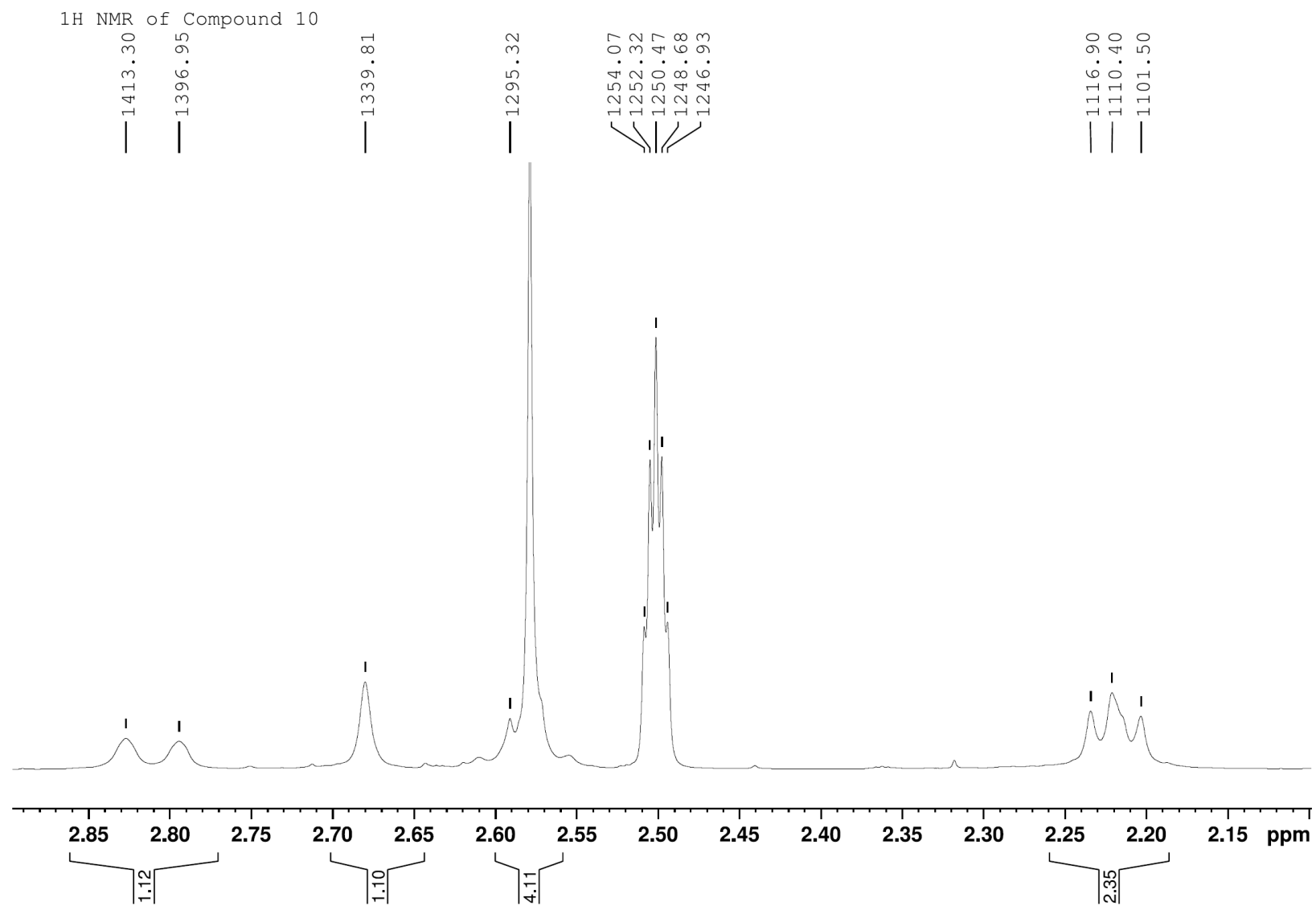
S25

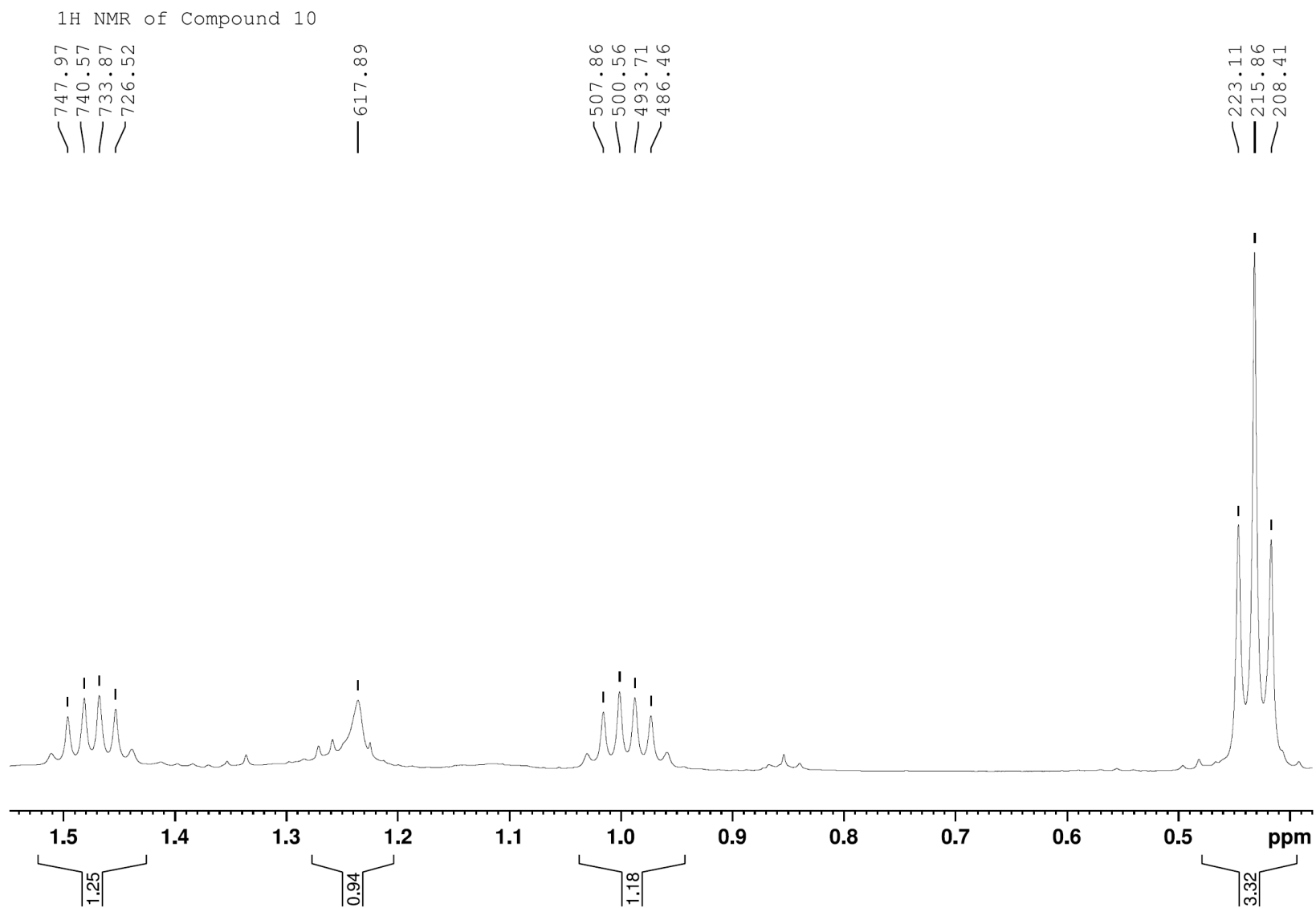


S26

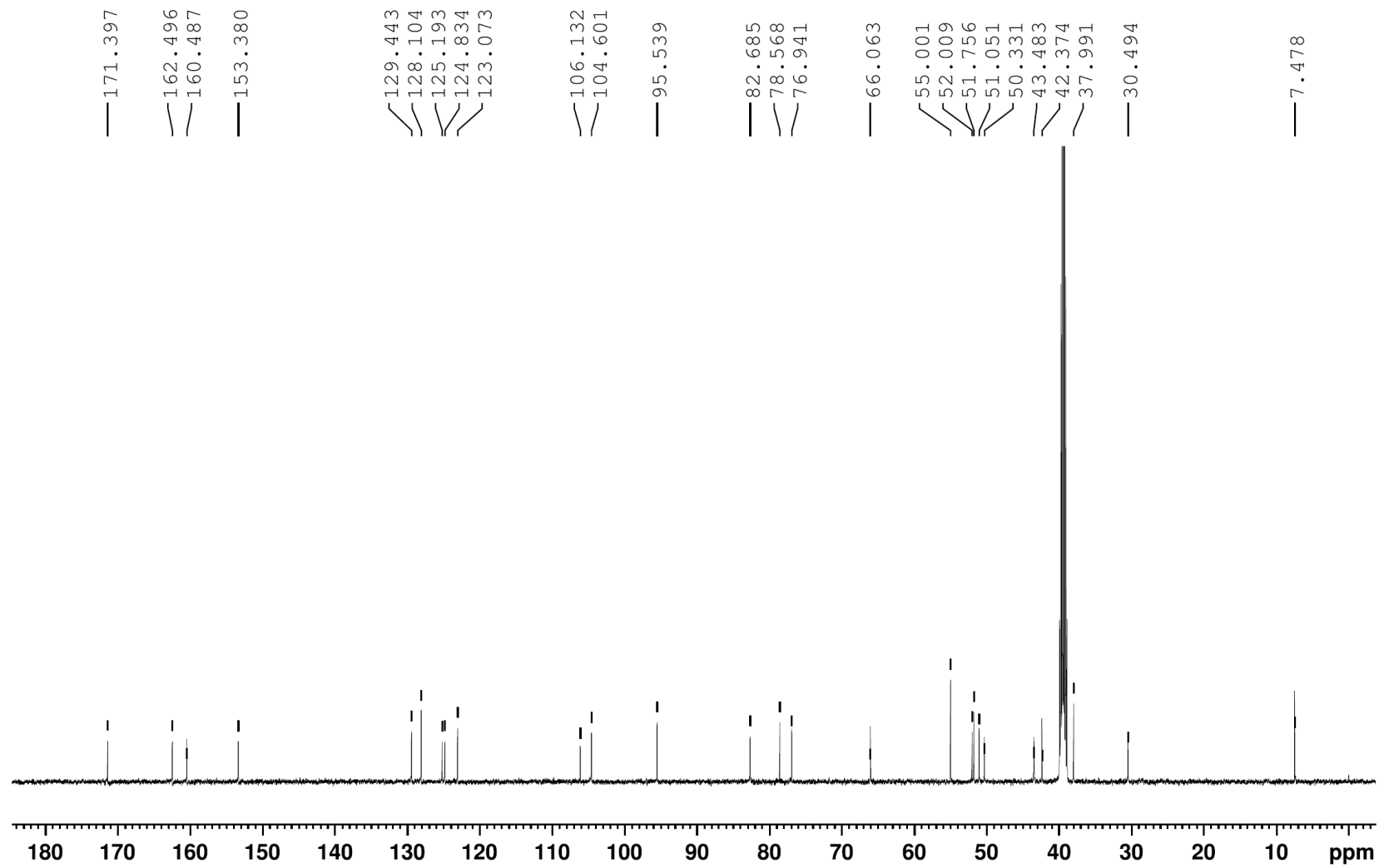


S27

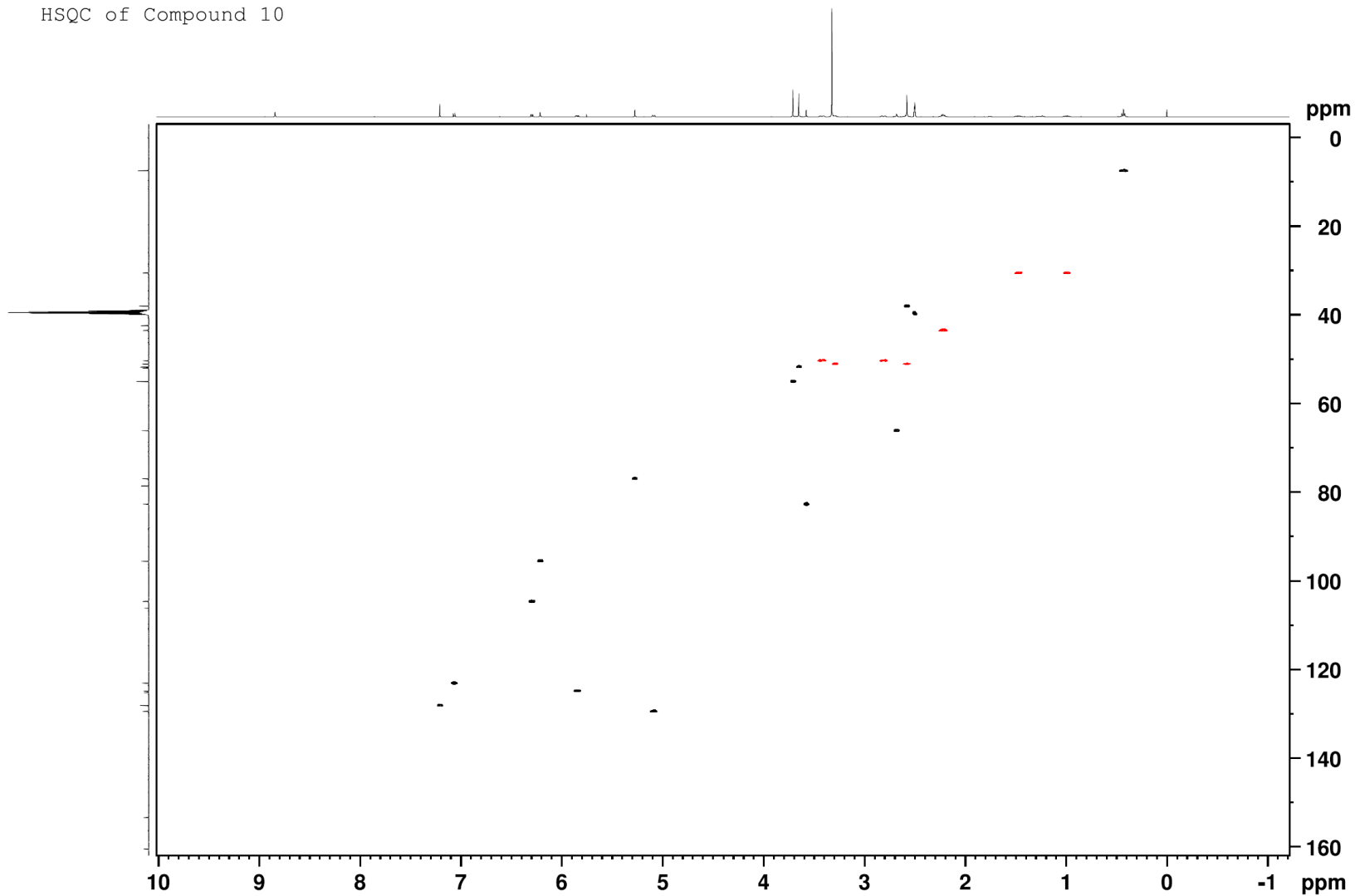




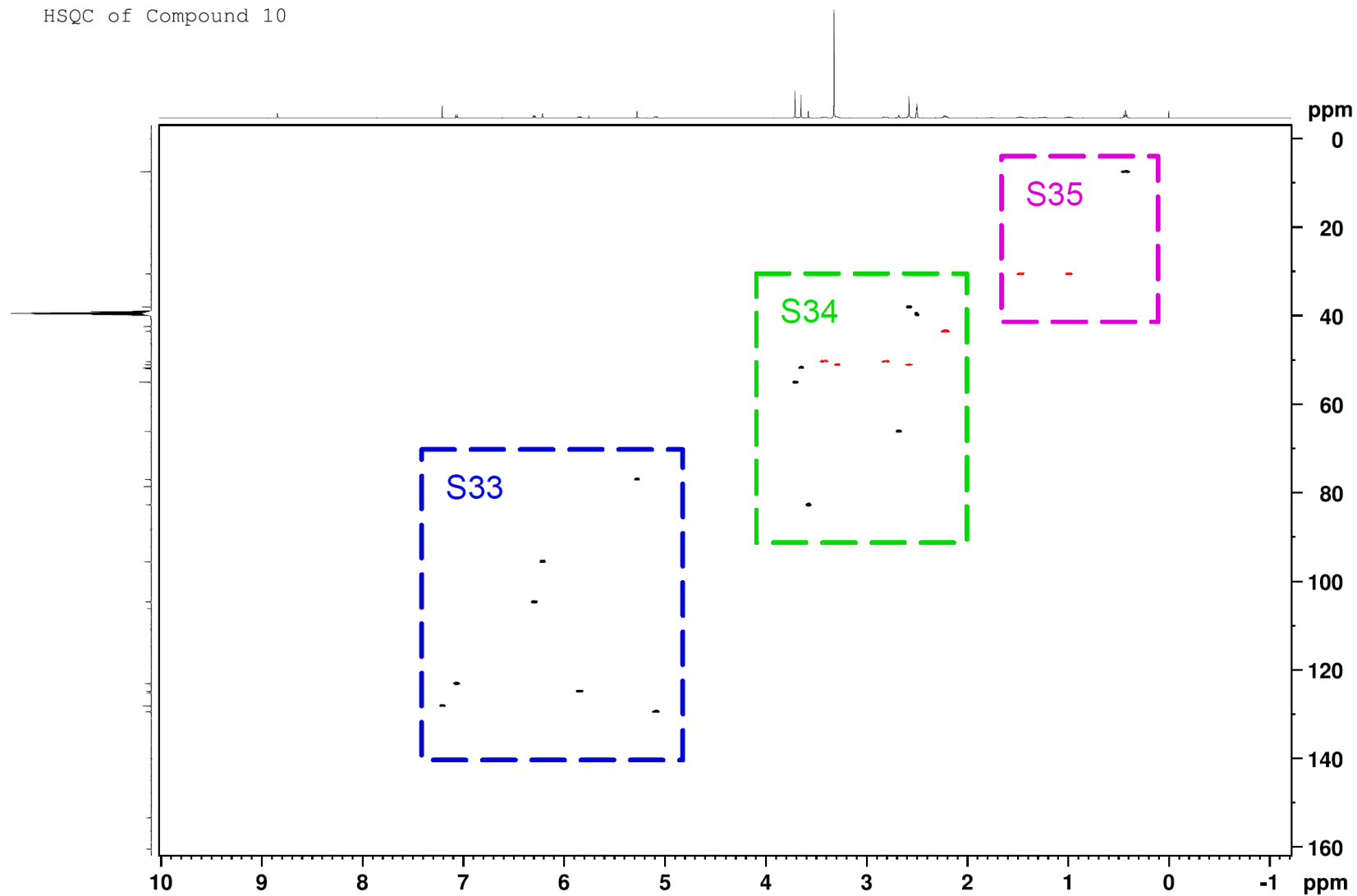
S29

^{13}C NMR of Compound 10

HSQC of Compound 10

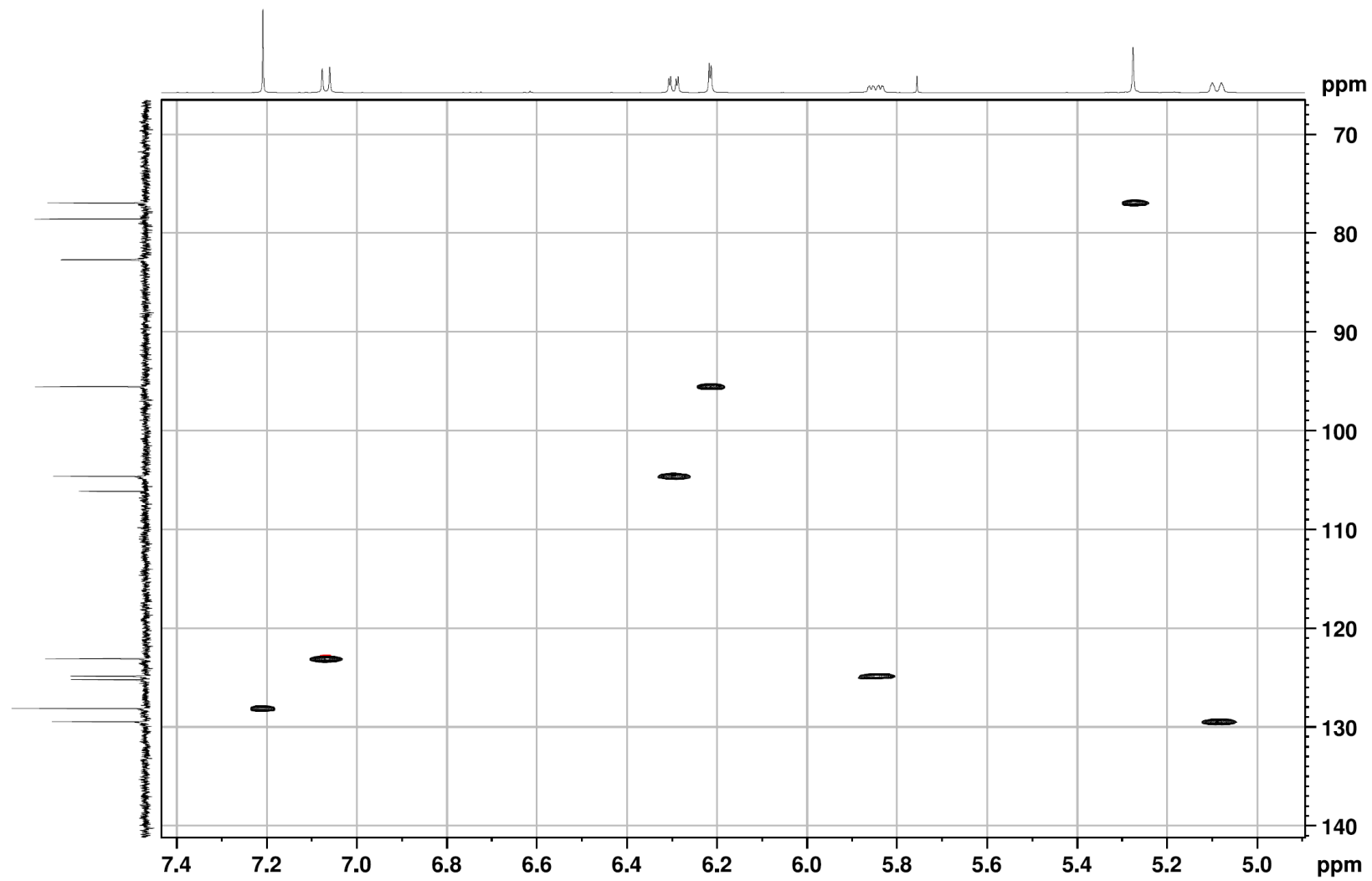


HSQC of Compound 10



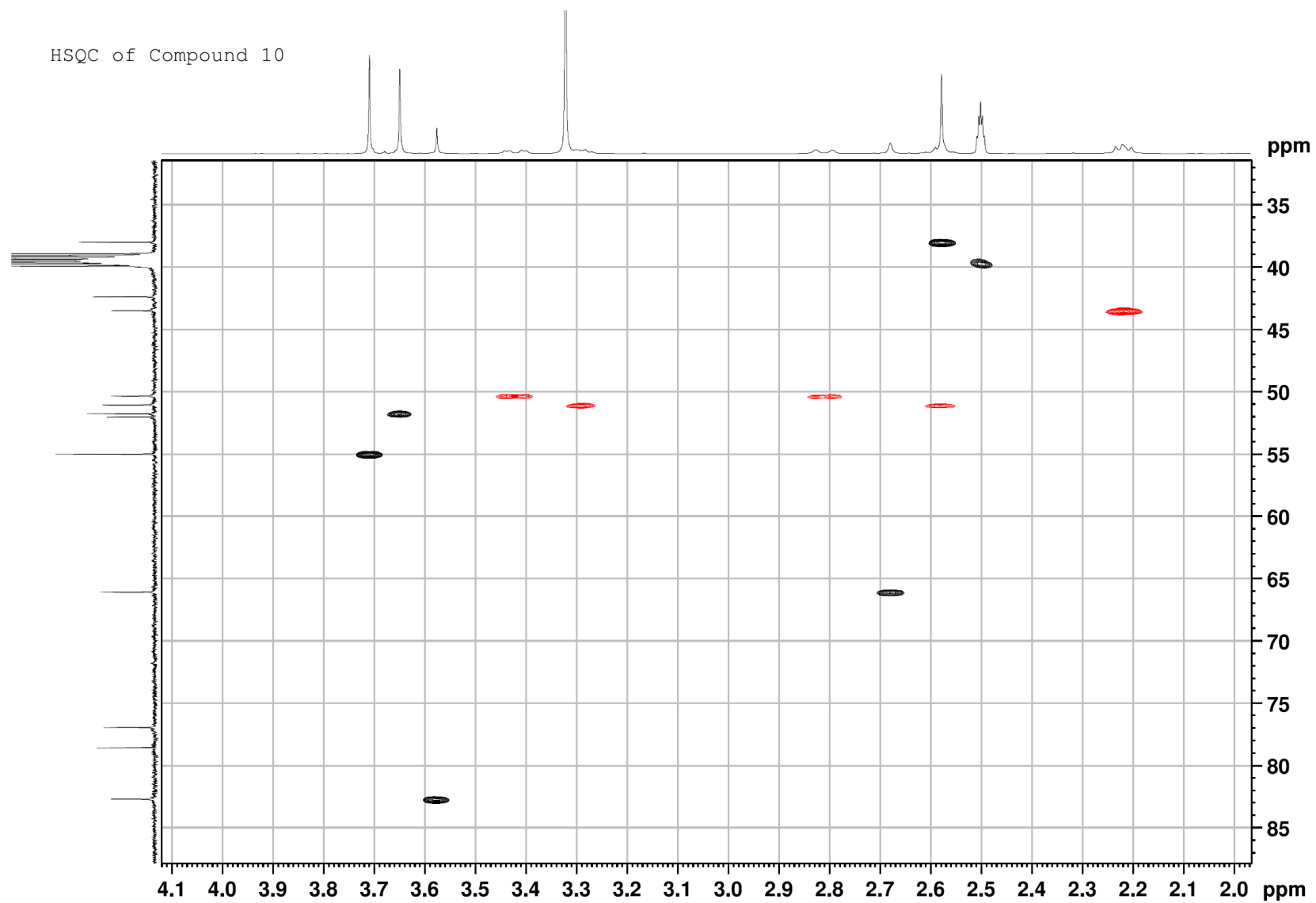
S32

HSQC of Compound 10

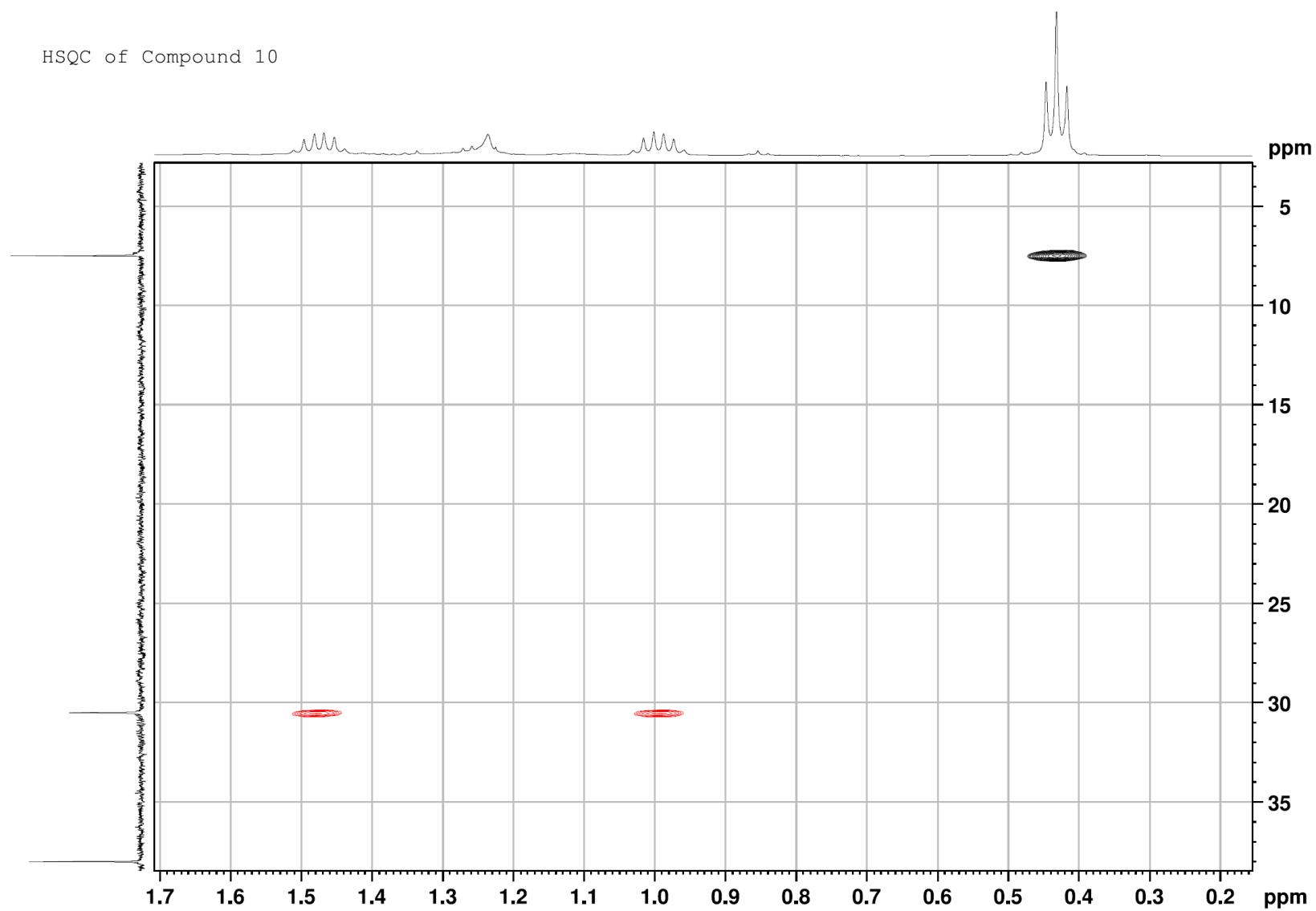


S33

HSQC of Compound 10

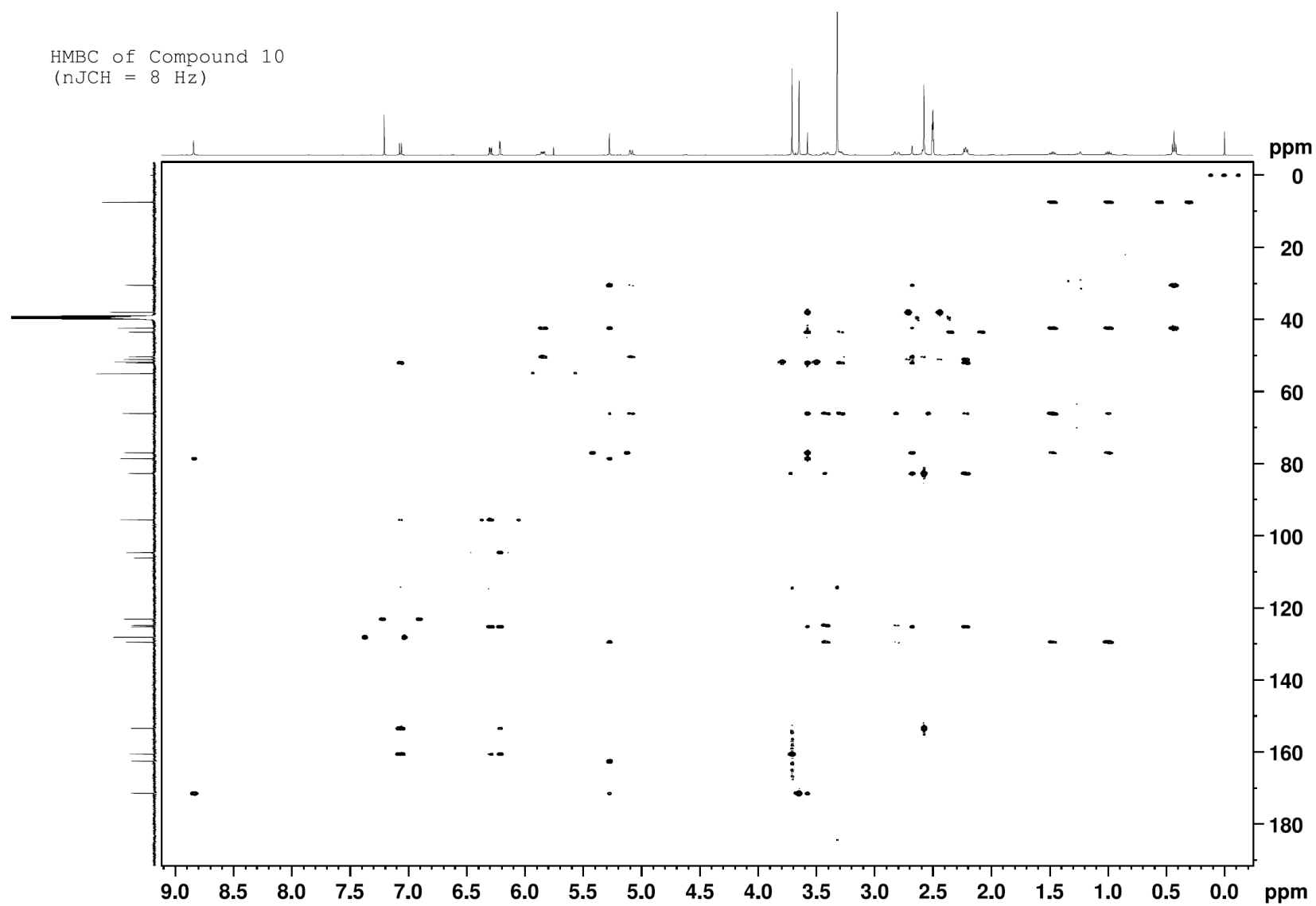


HSQC of Compound 10

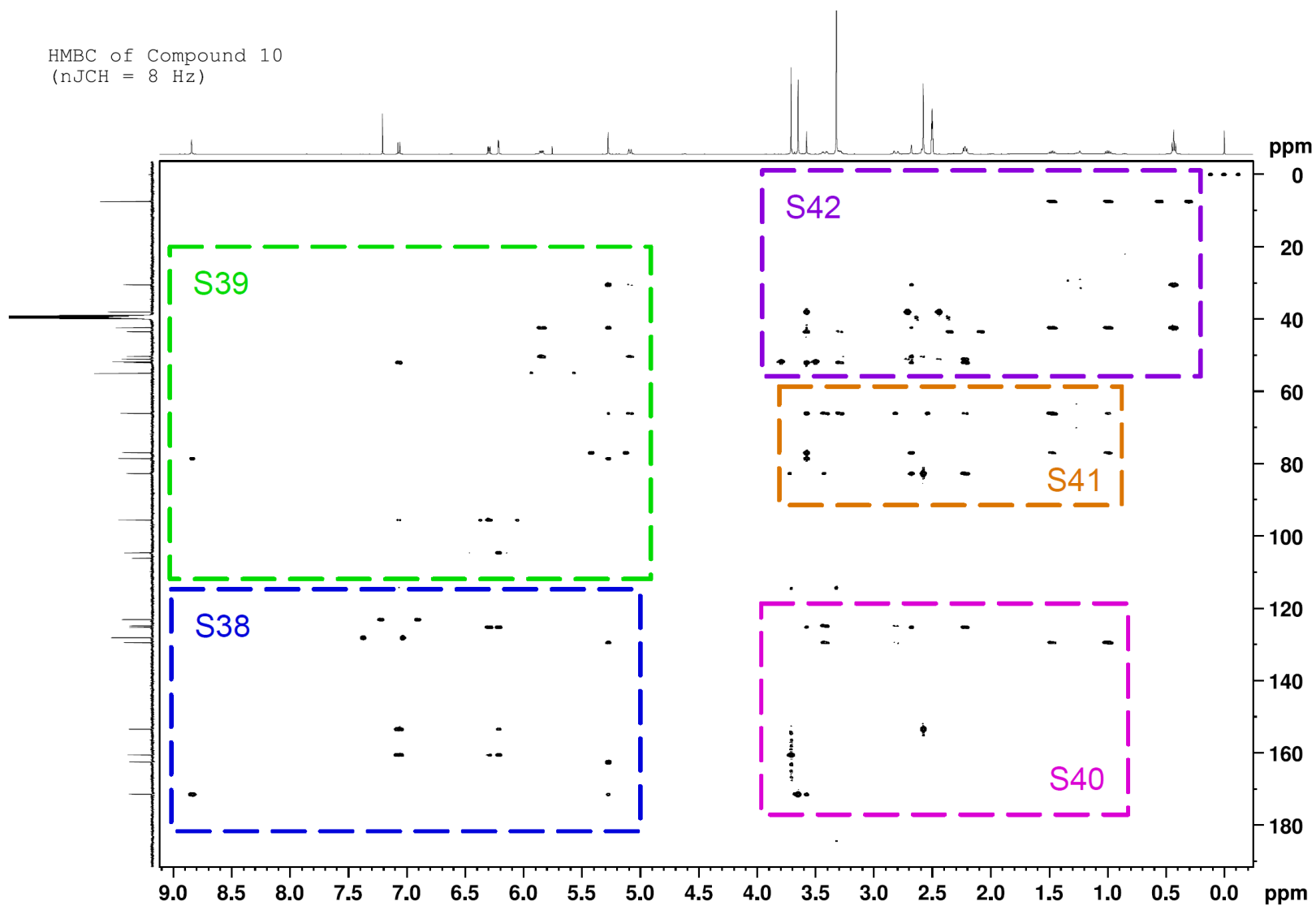


S35

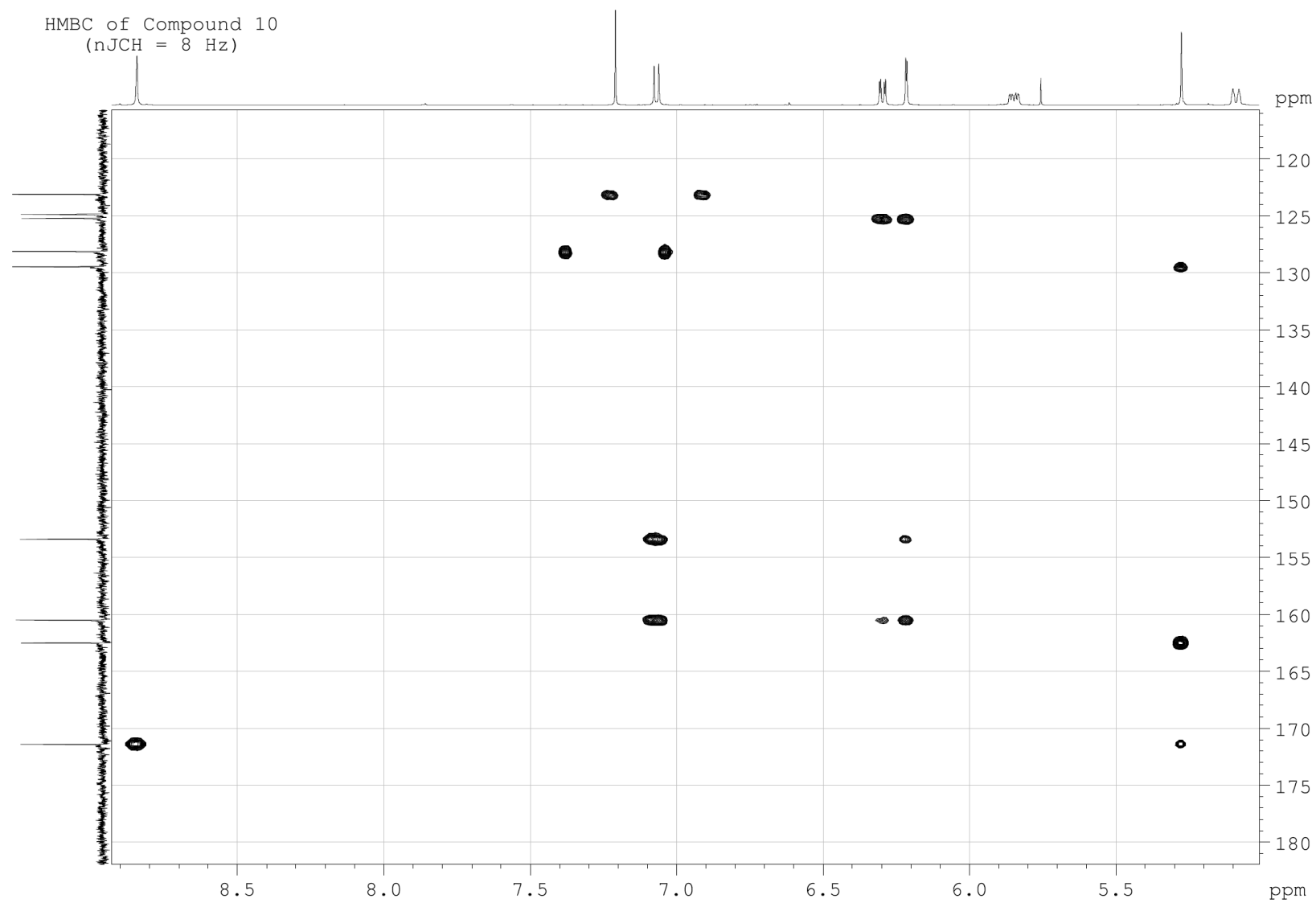
HMBC of Compound 10
($nJ_{CH} = 8$ Hz)

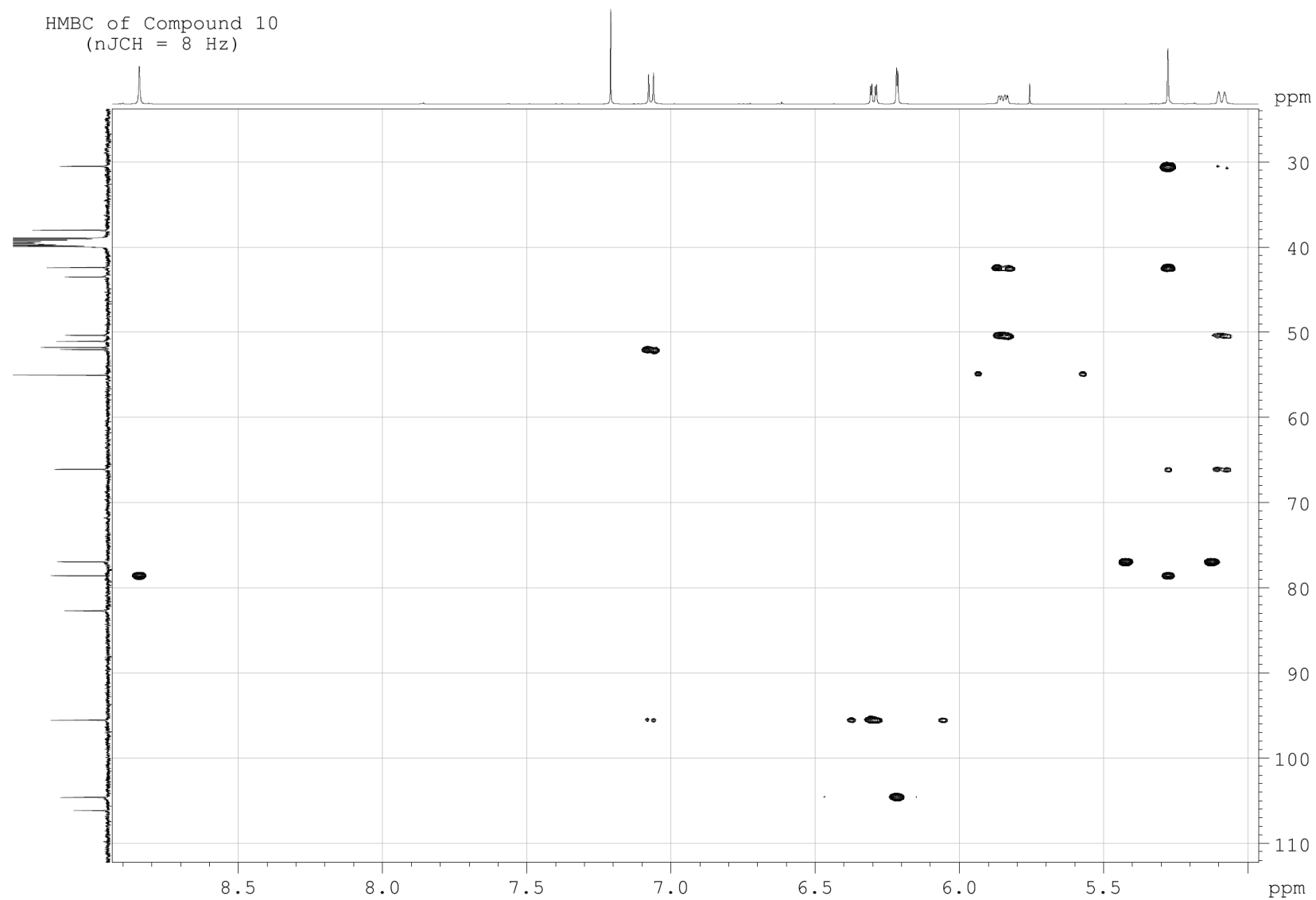


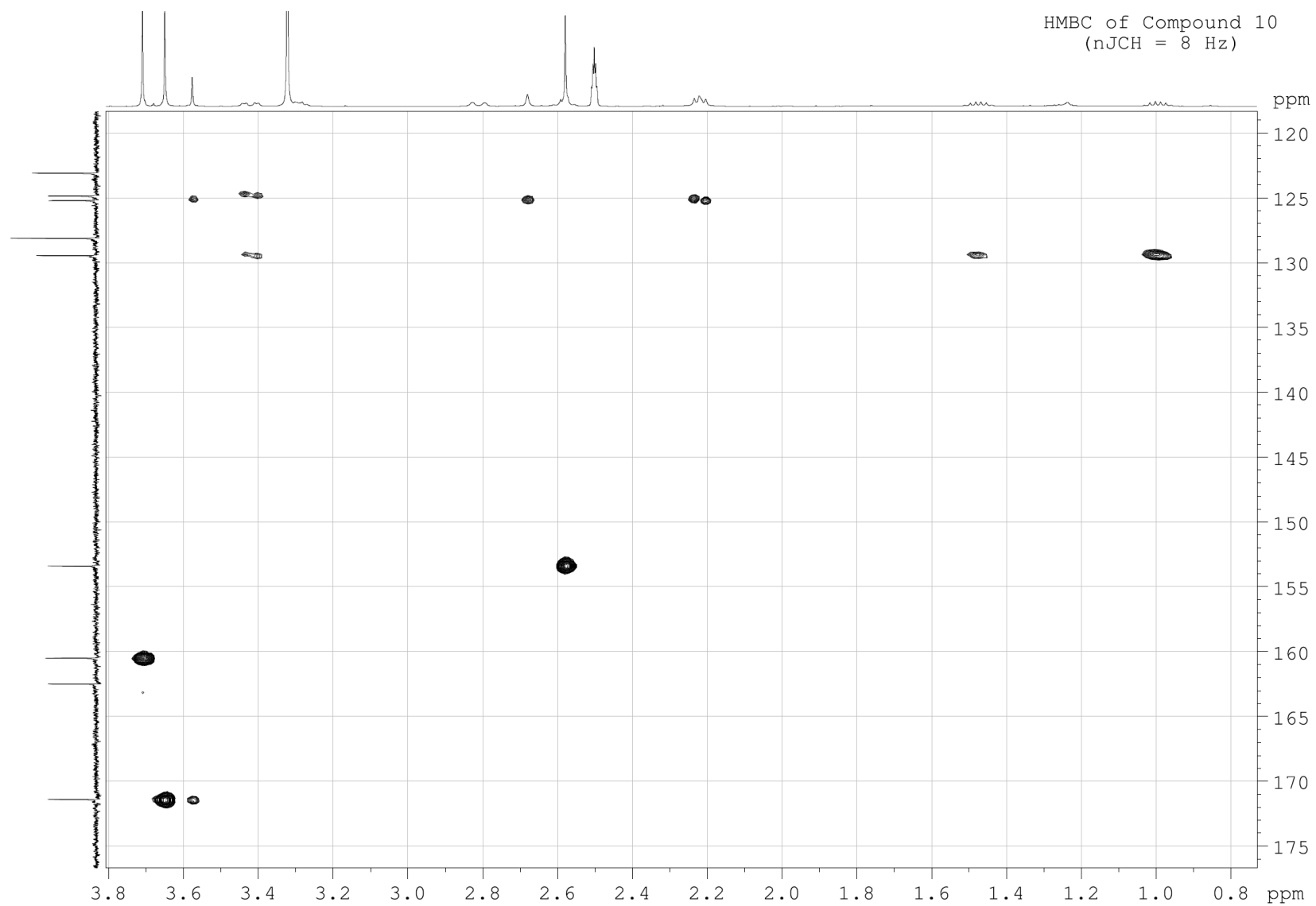
S36



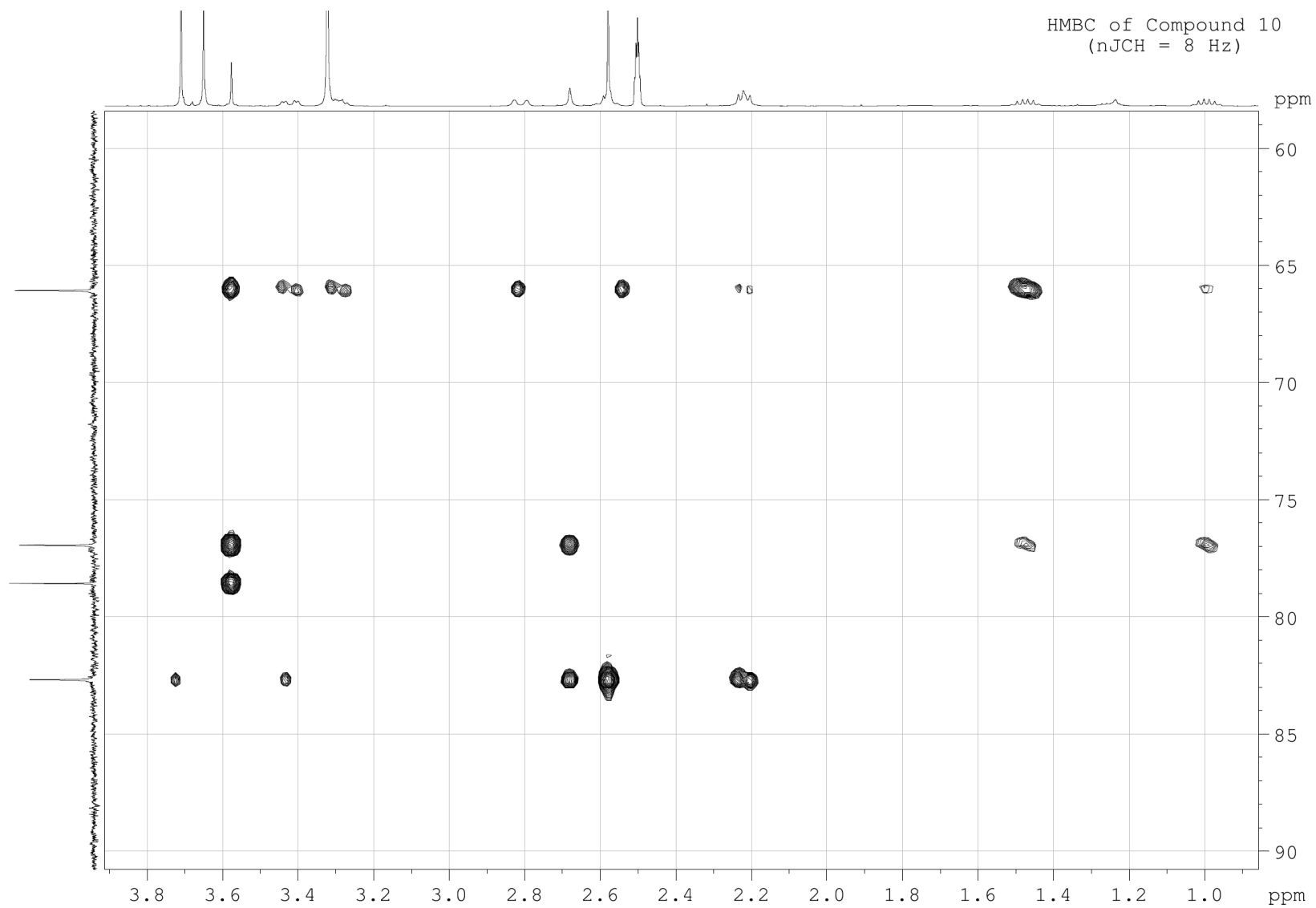
S37

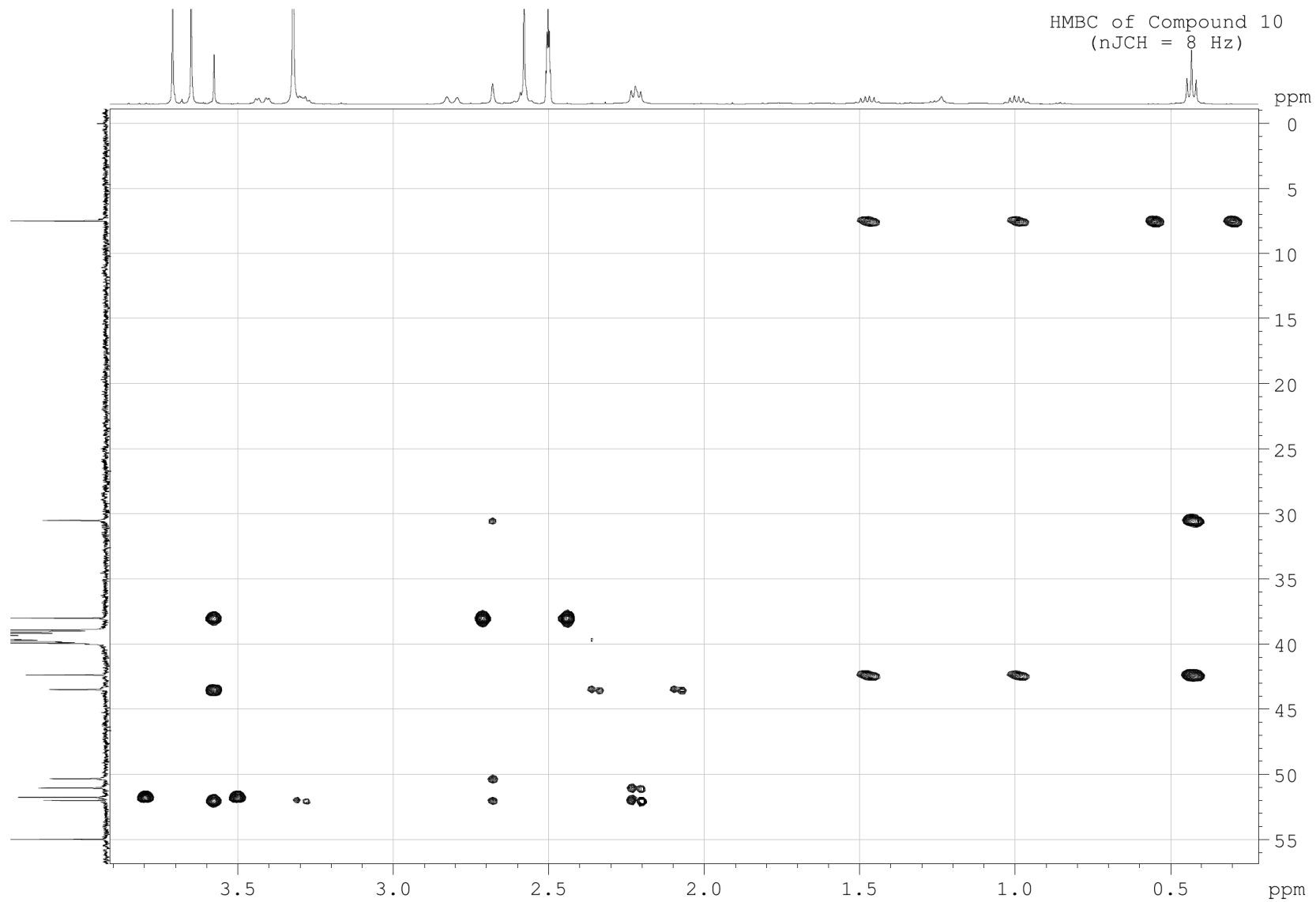




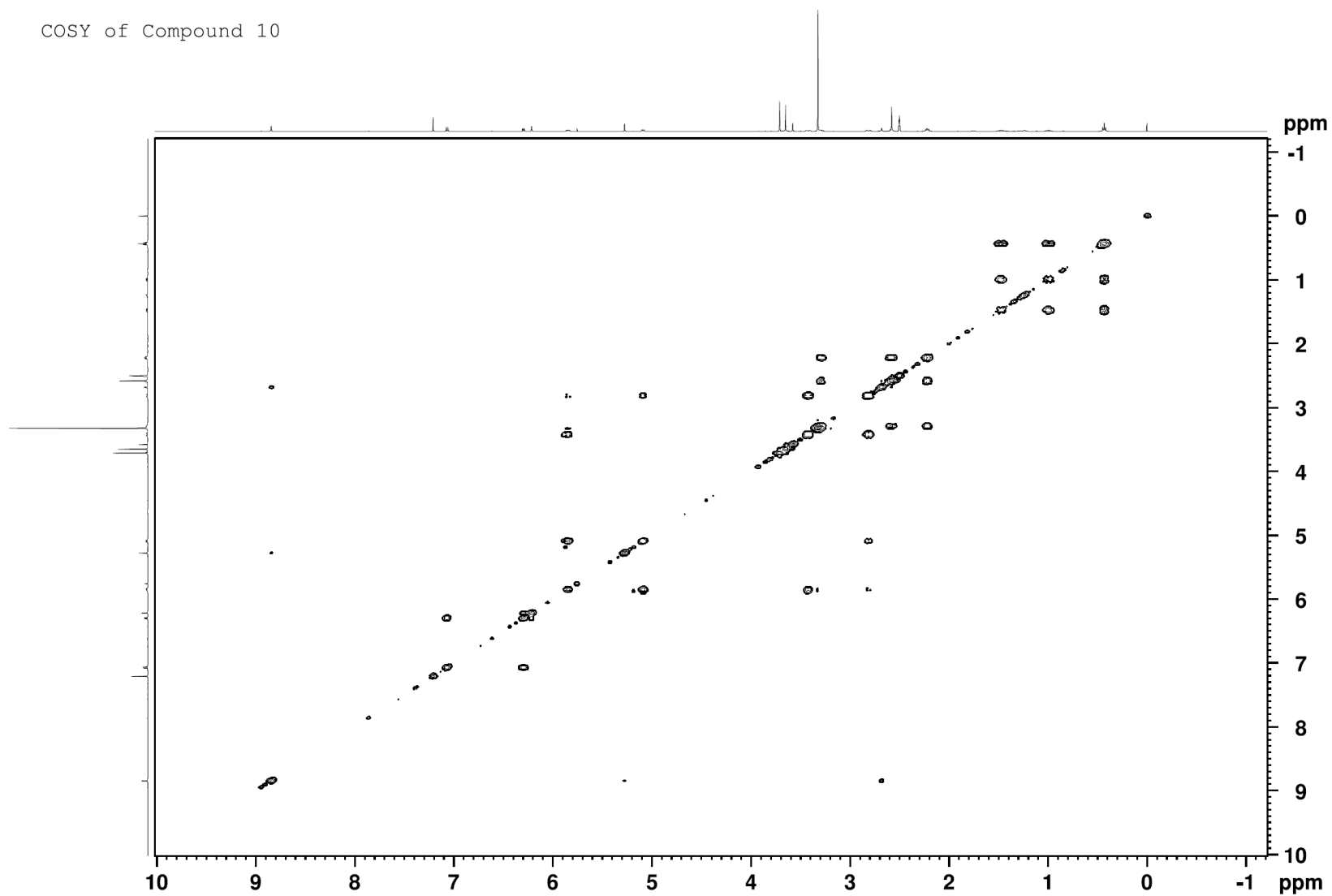


S40

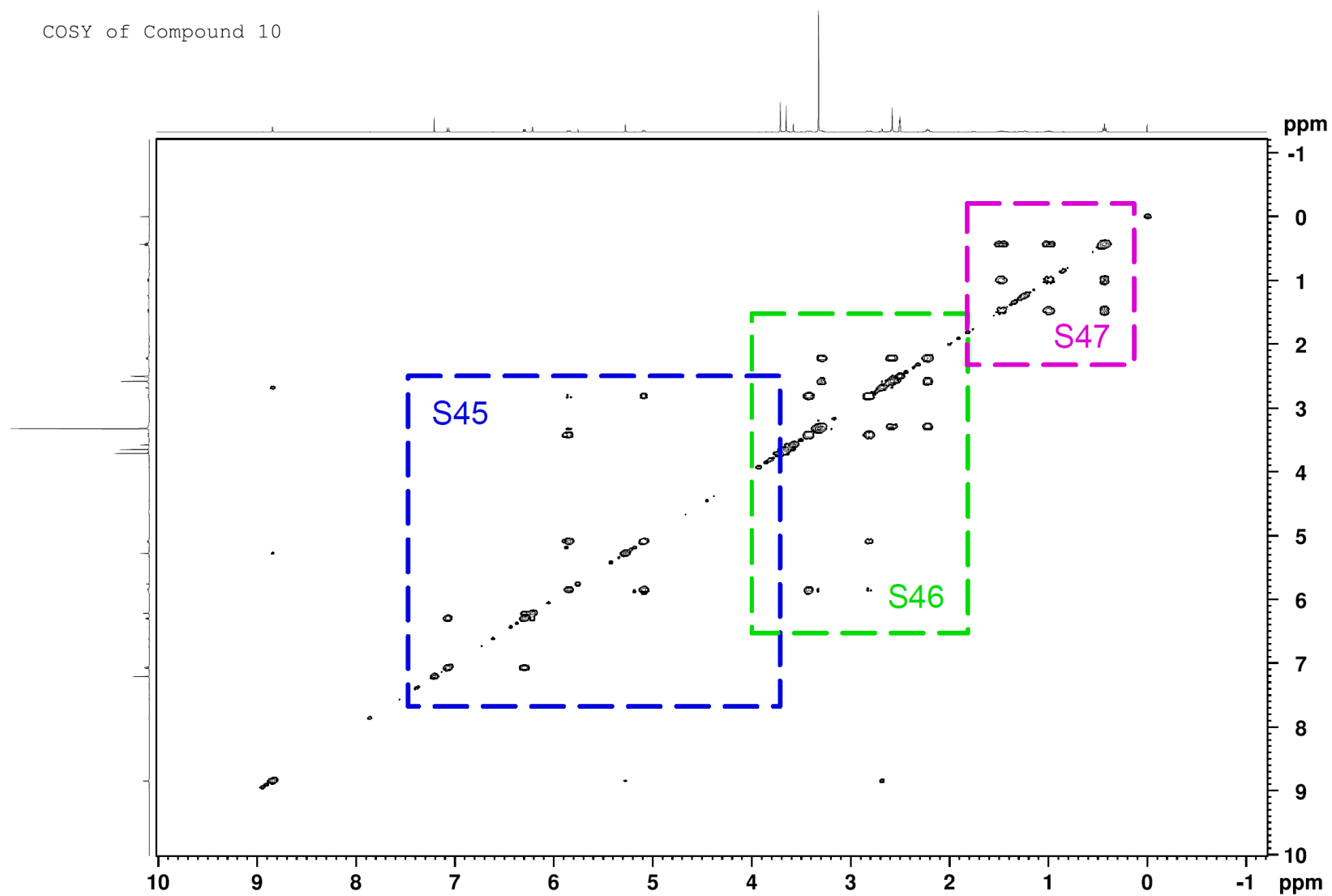




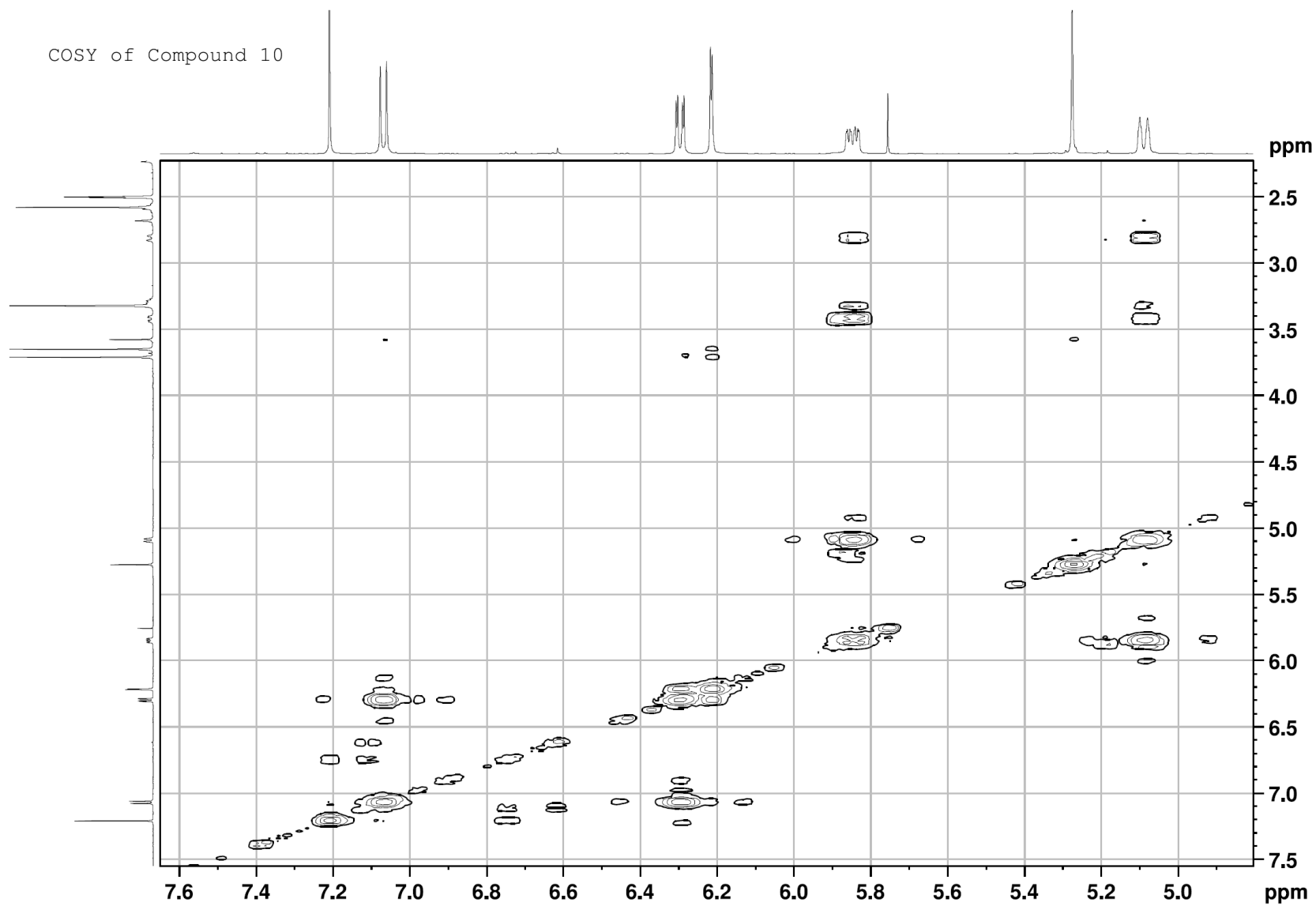
COSY of Compound 10

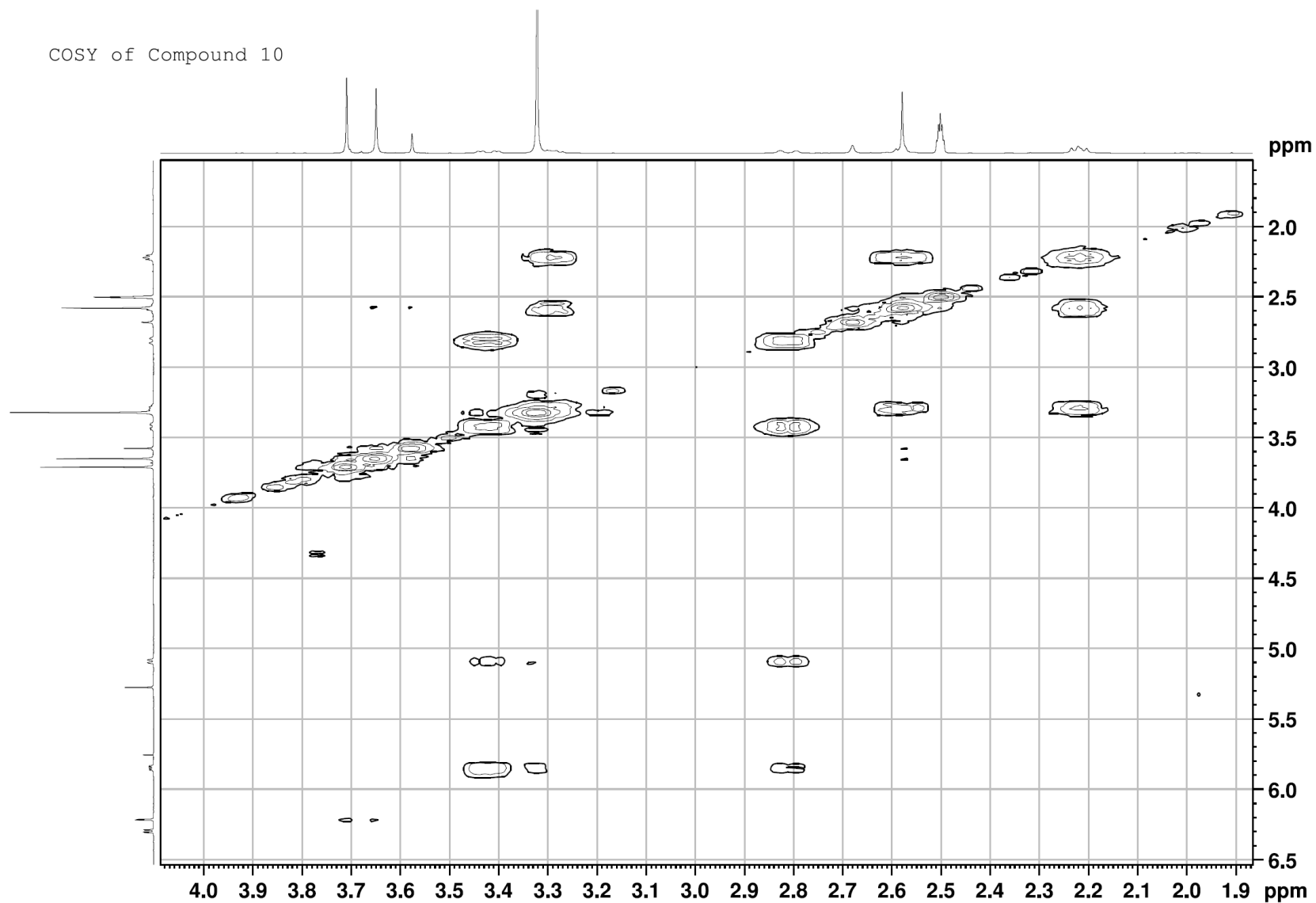


COSY of Compound 10

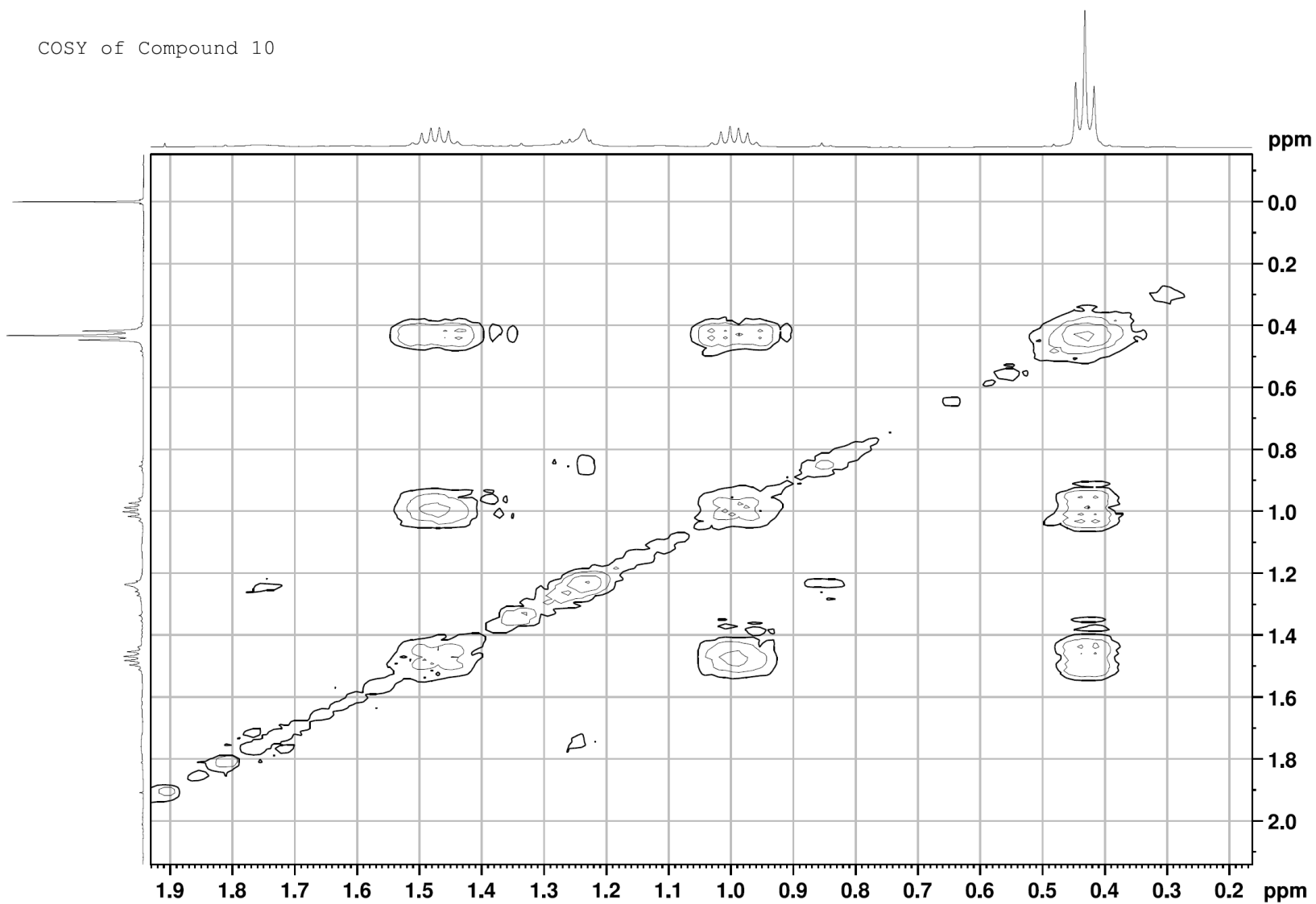


S44

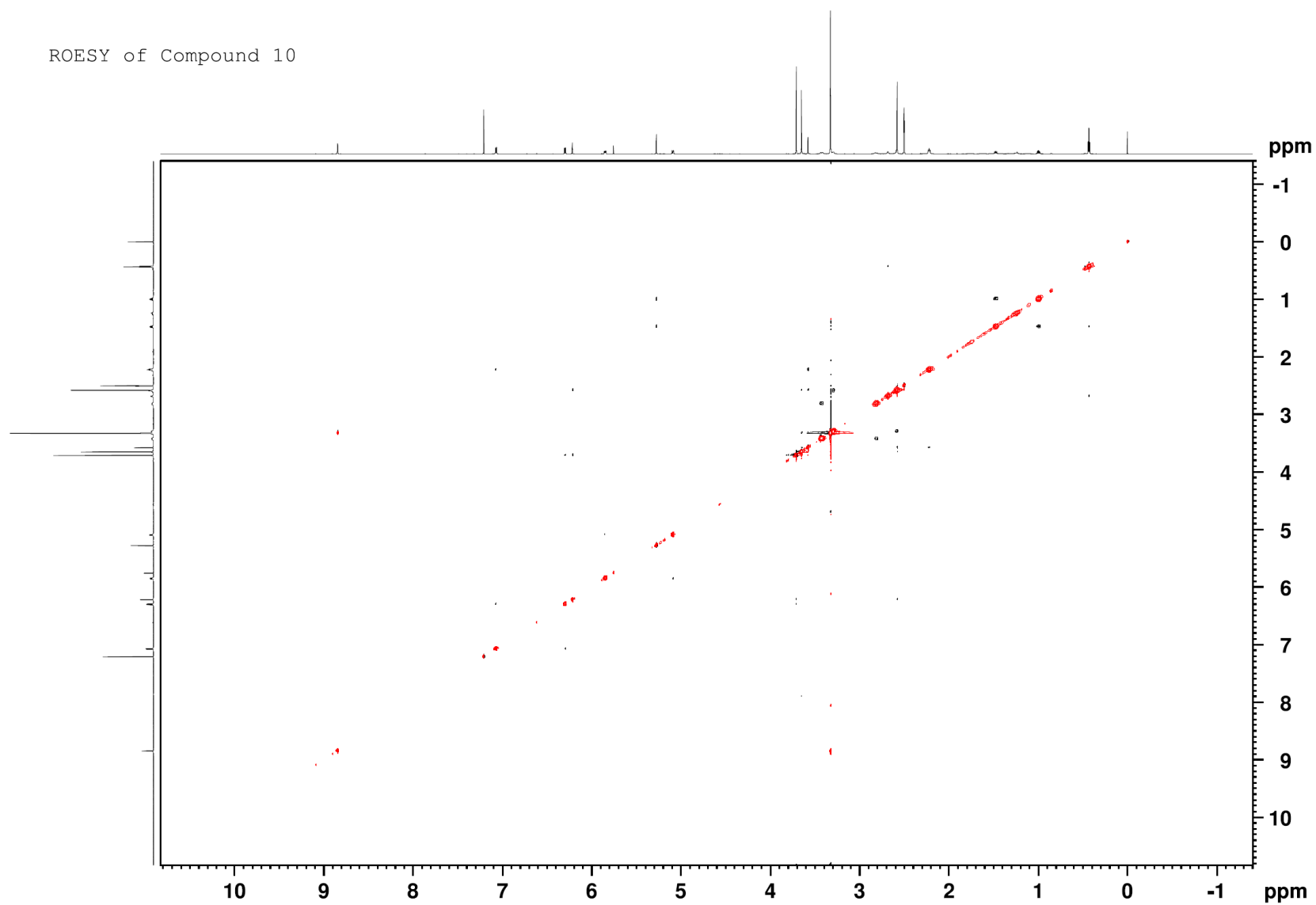




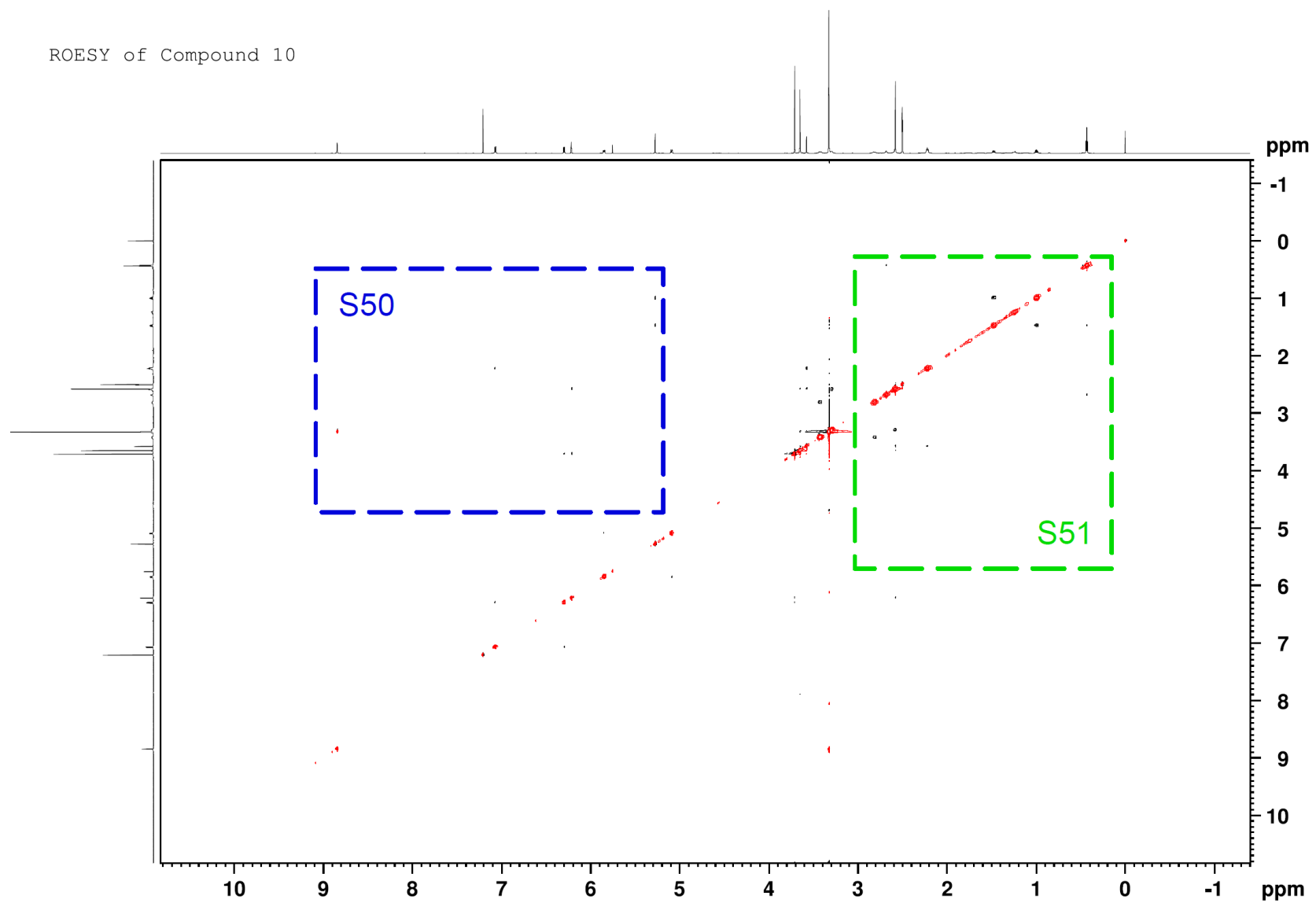
COSY of Compound 10



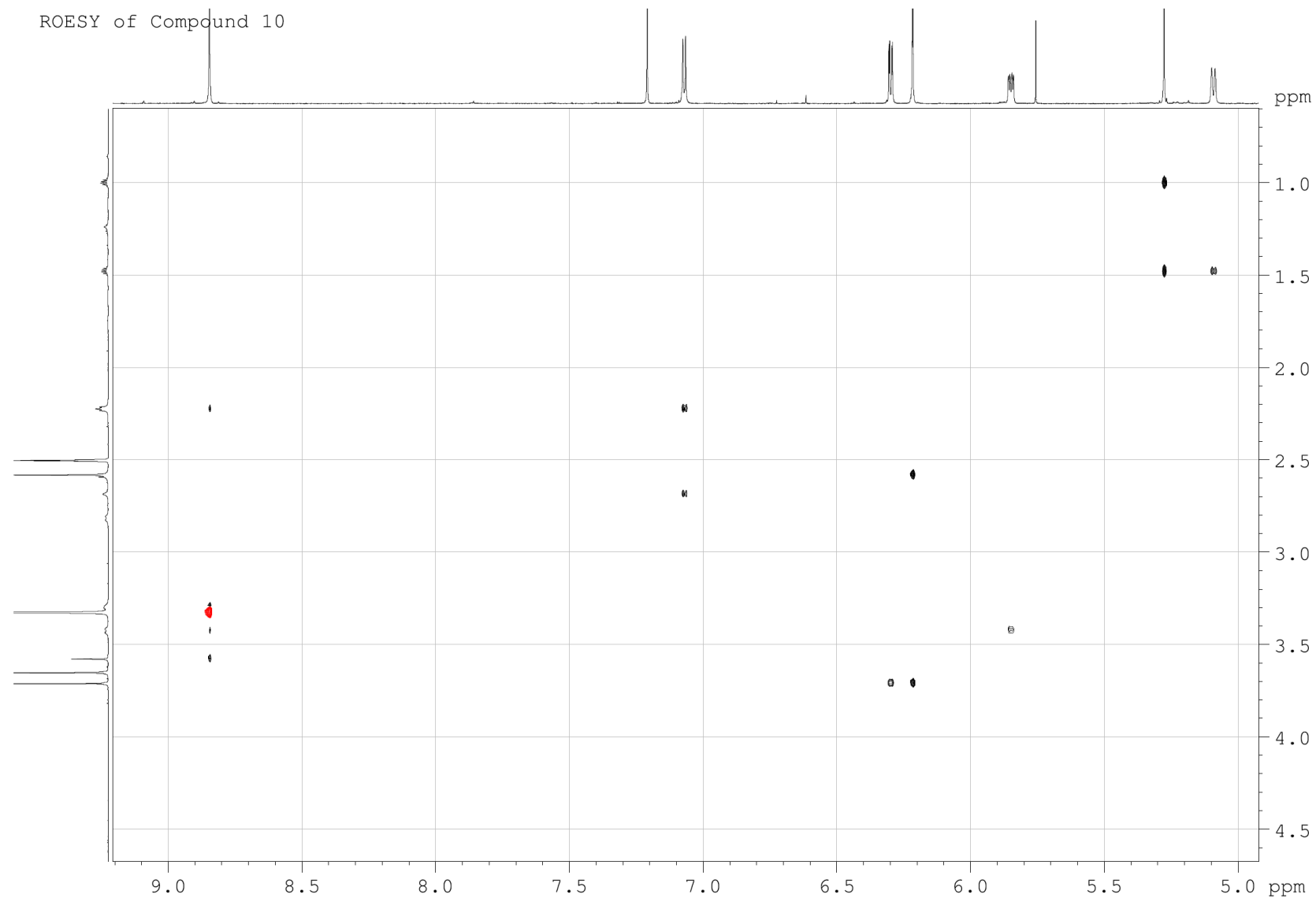
ROESY of Compound 10

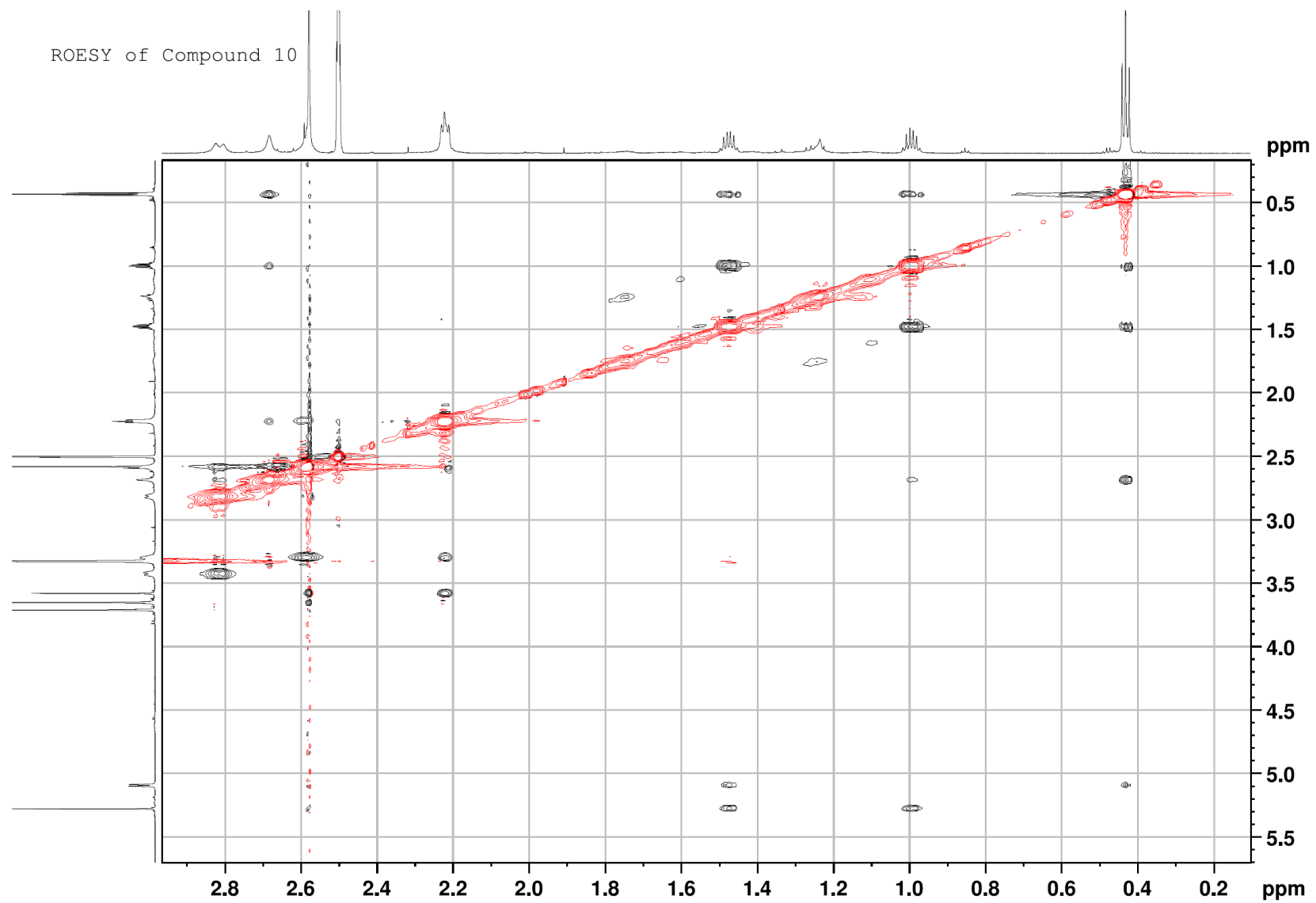


ROESY of Compound 10

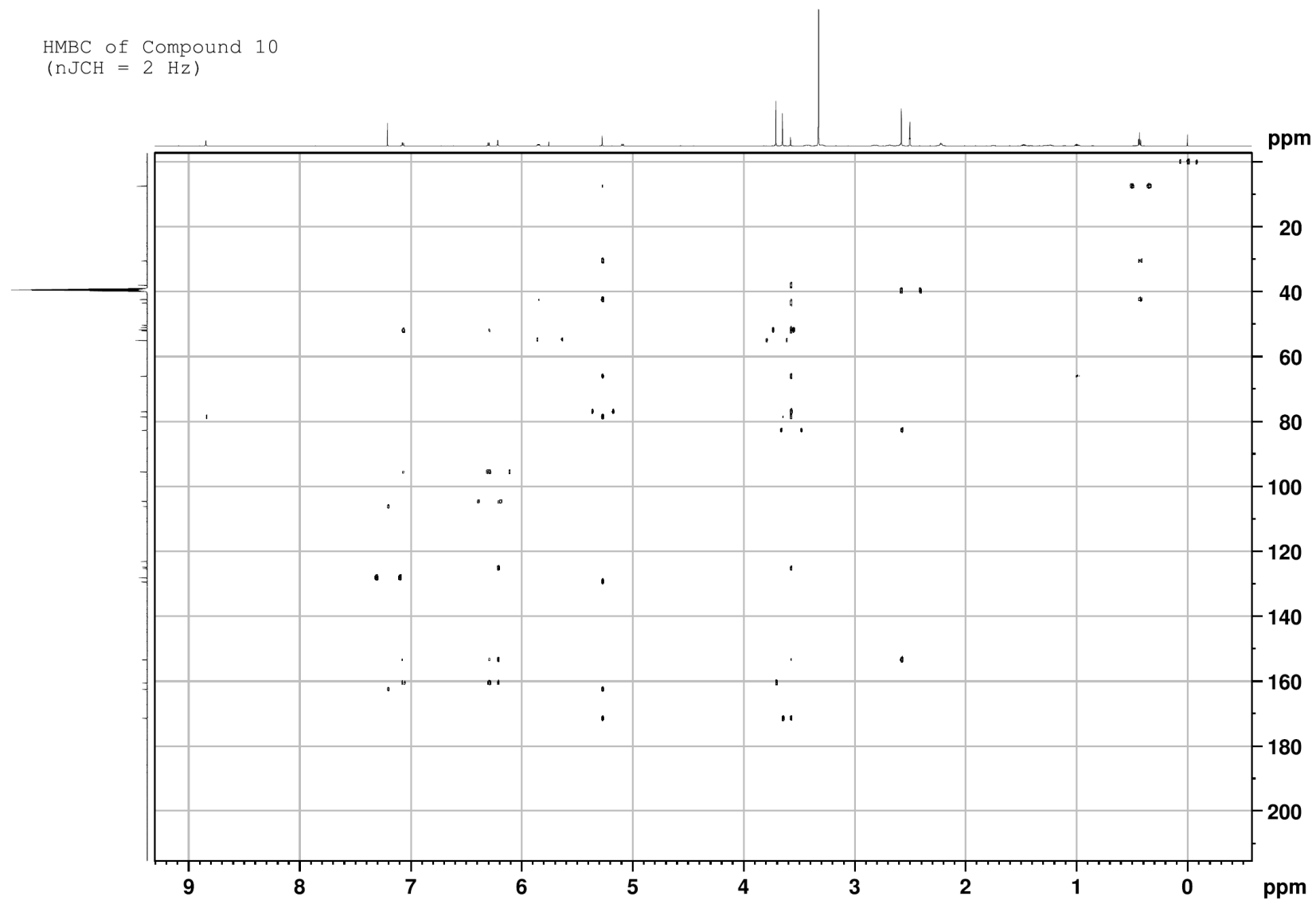


S49

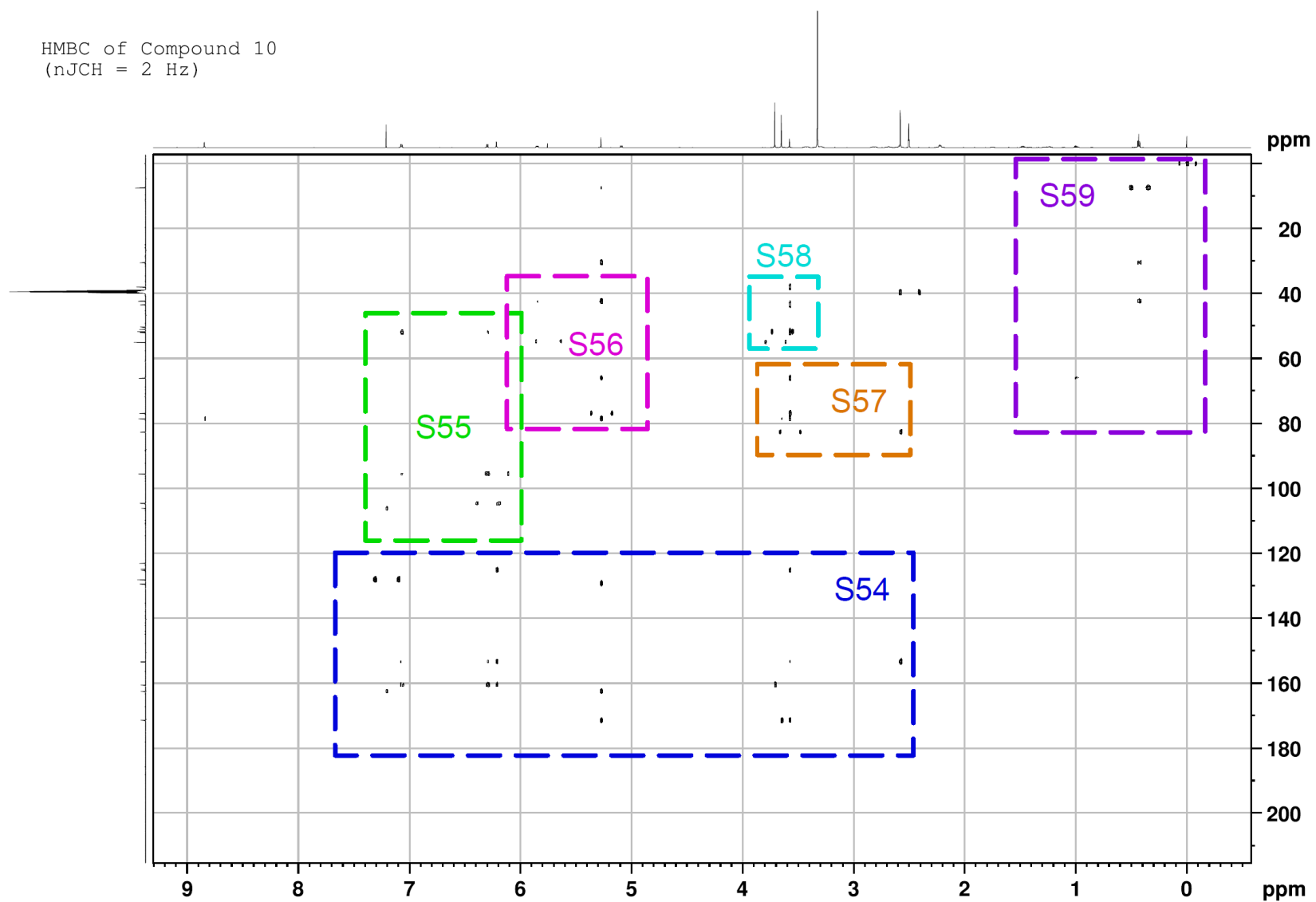




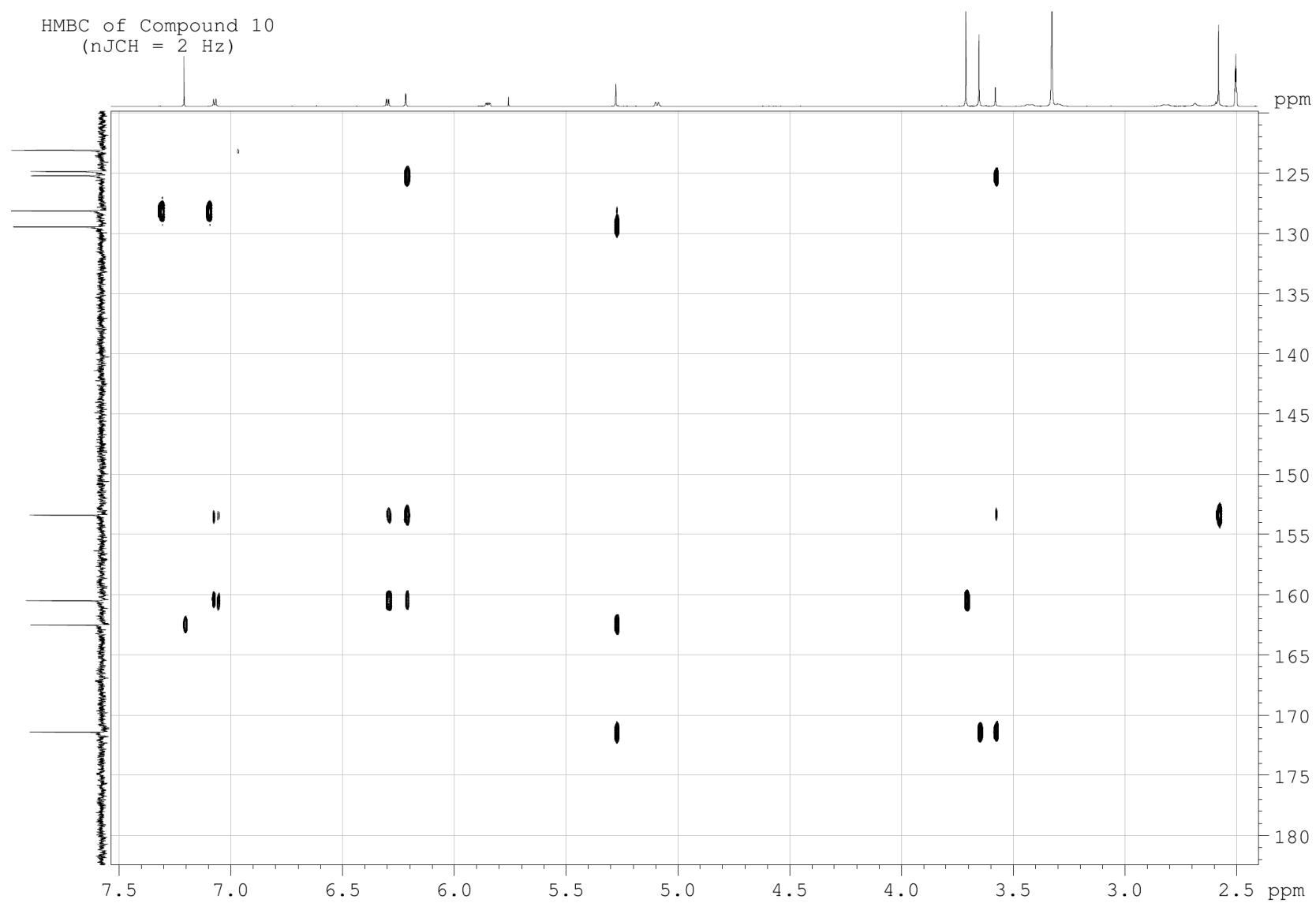
HMBC of Compound 10
($nJ_{CH} = 2$ Hz)

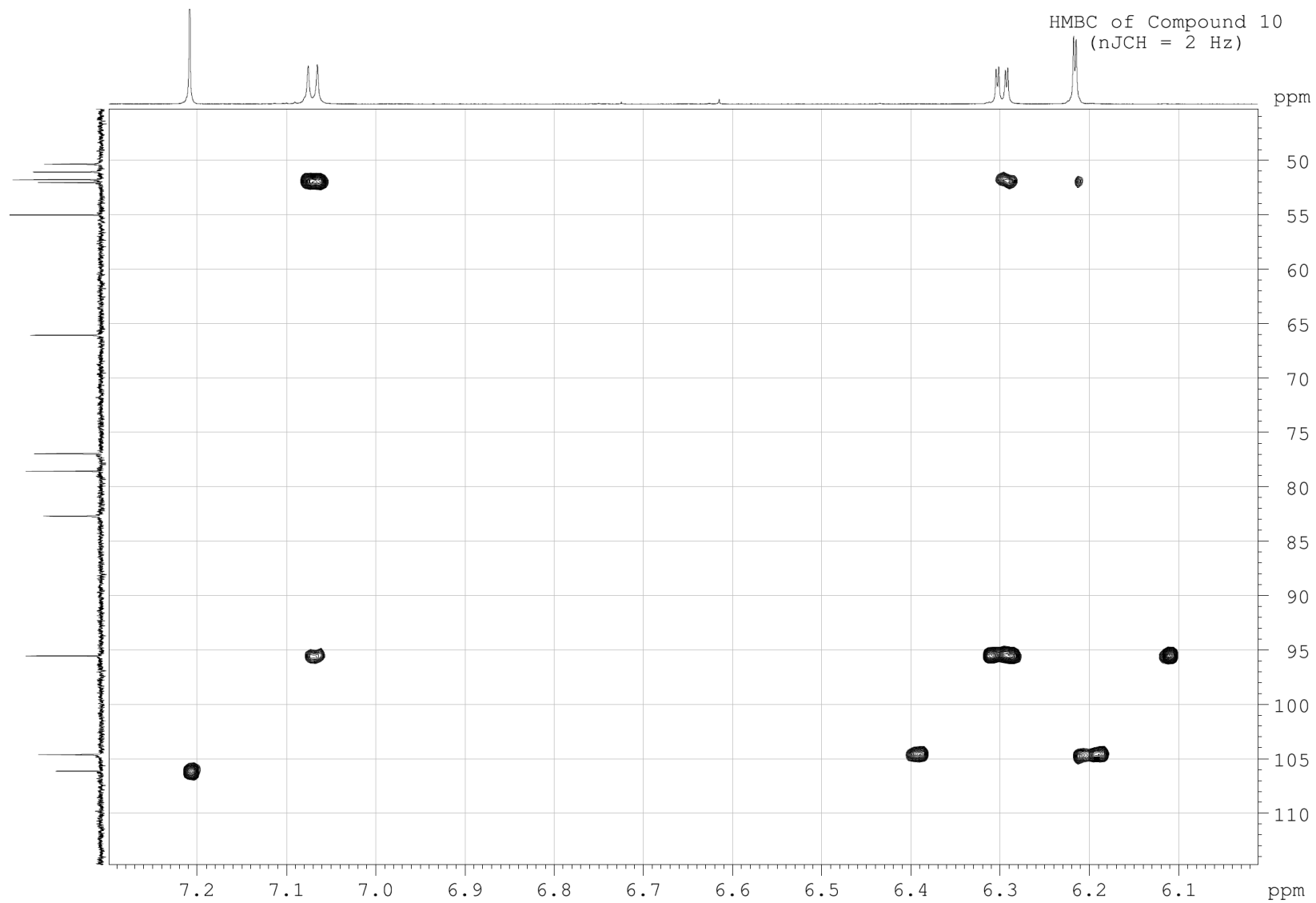


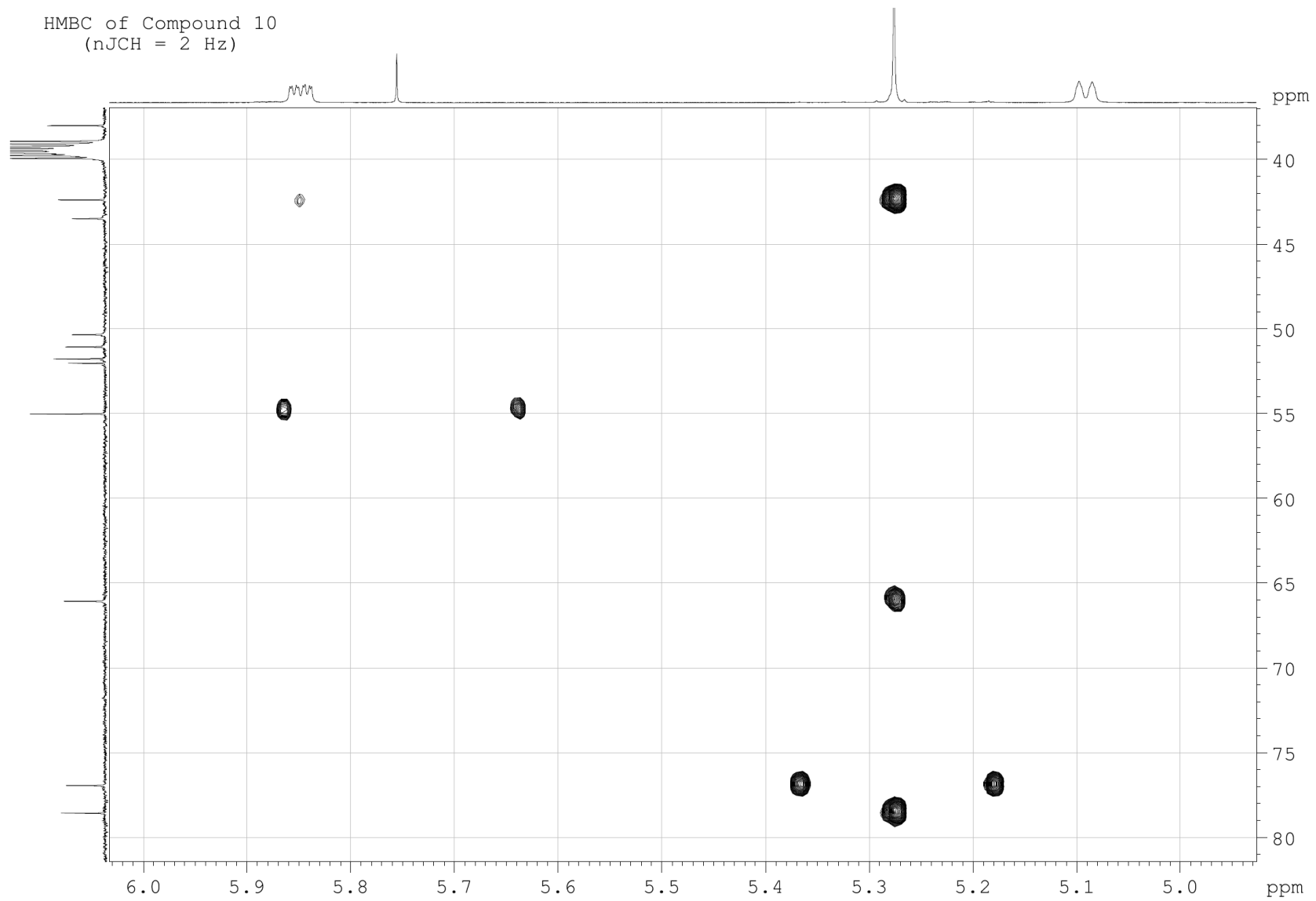
HMBC of Compound 10
($nJ_{CH} = 2$ Hz)

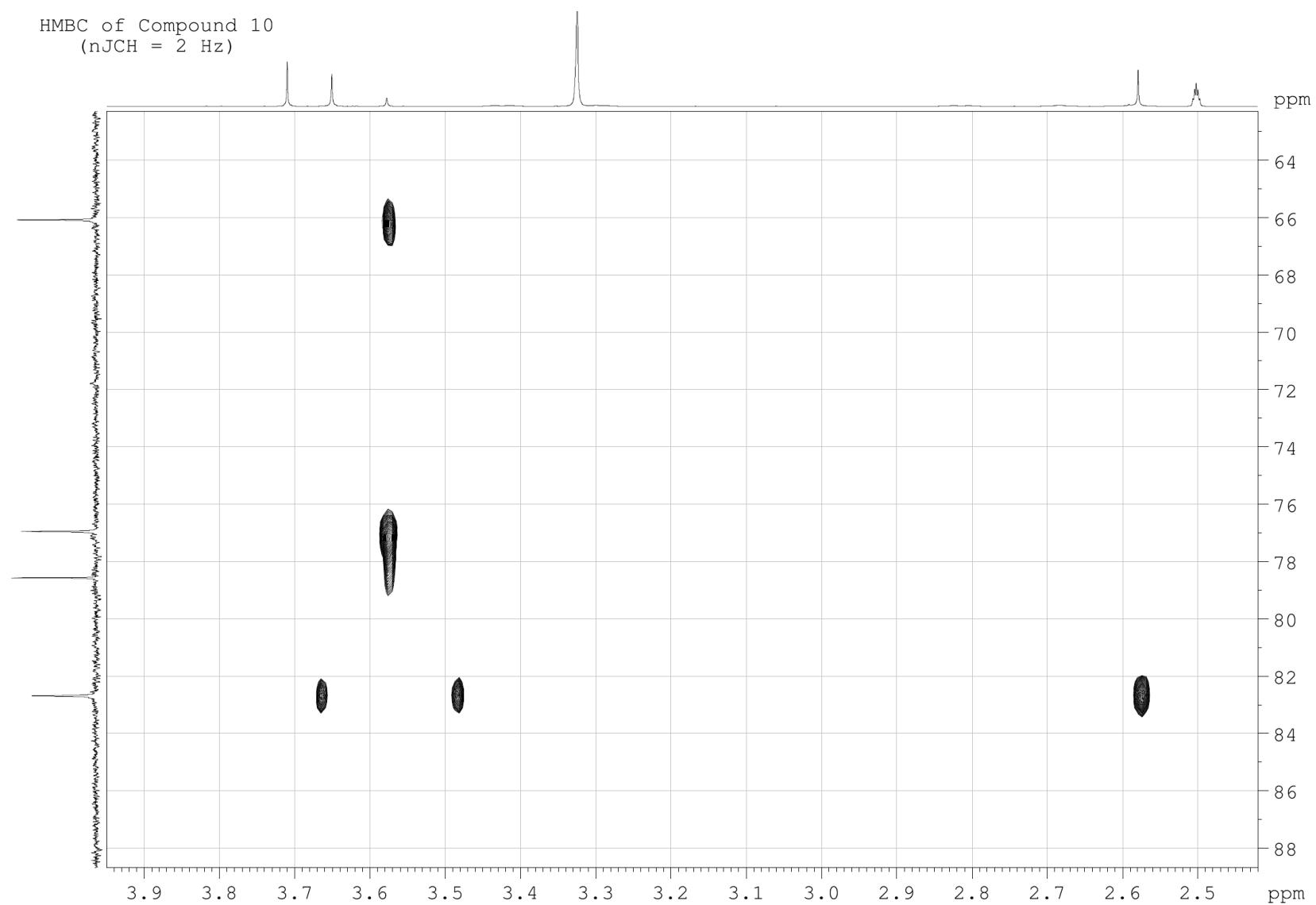


S53

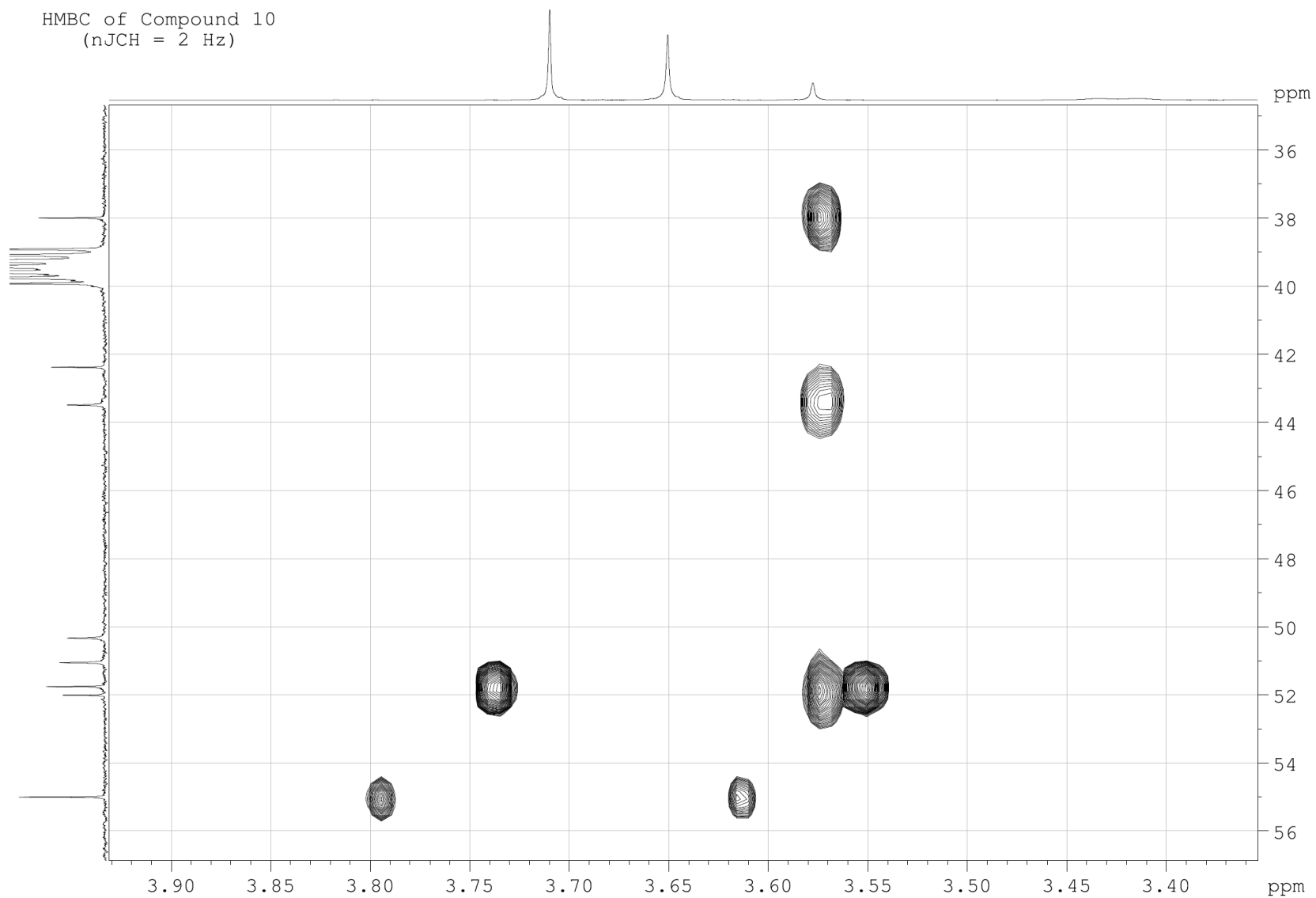


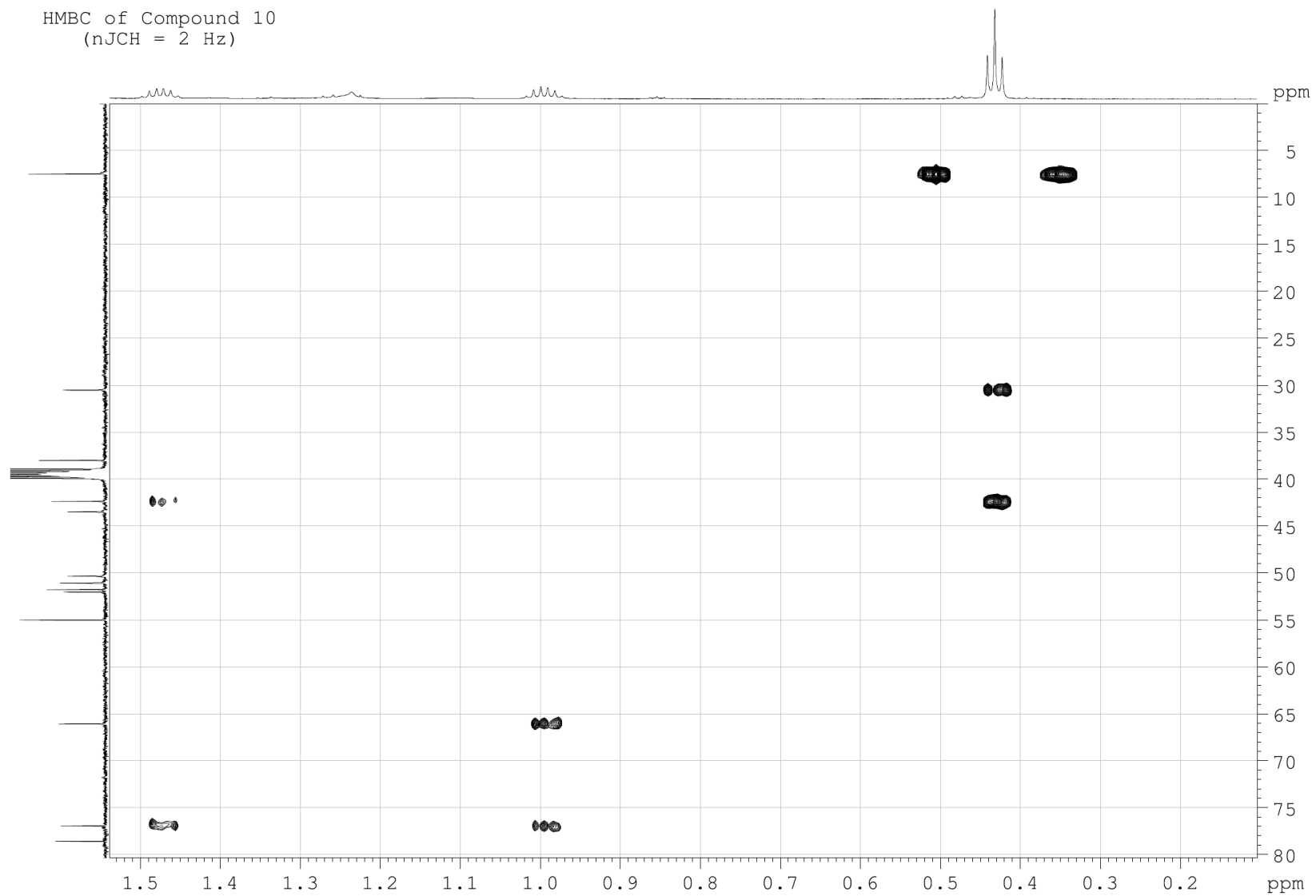




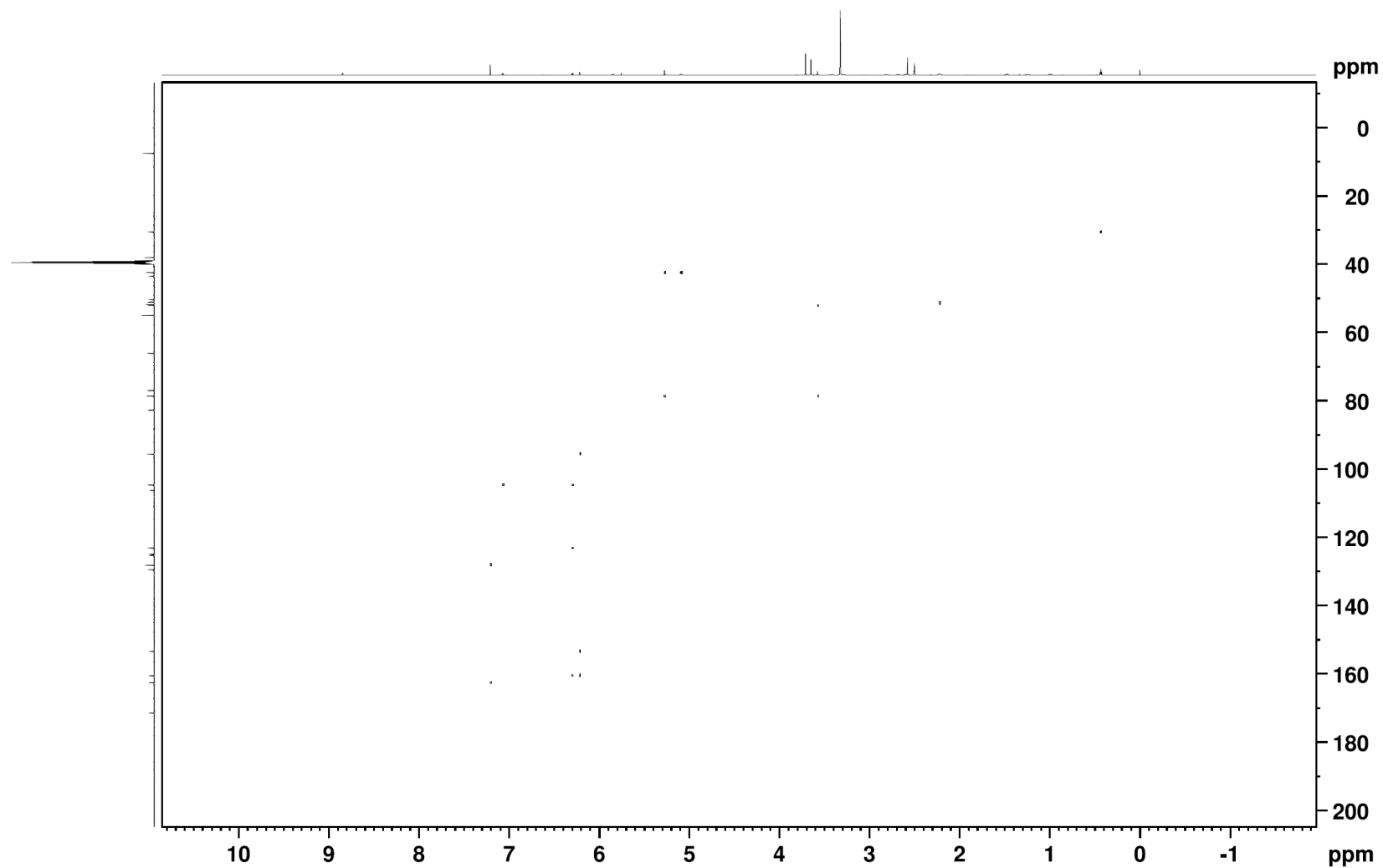


S57



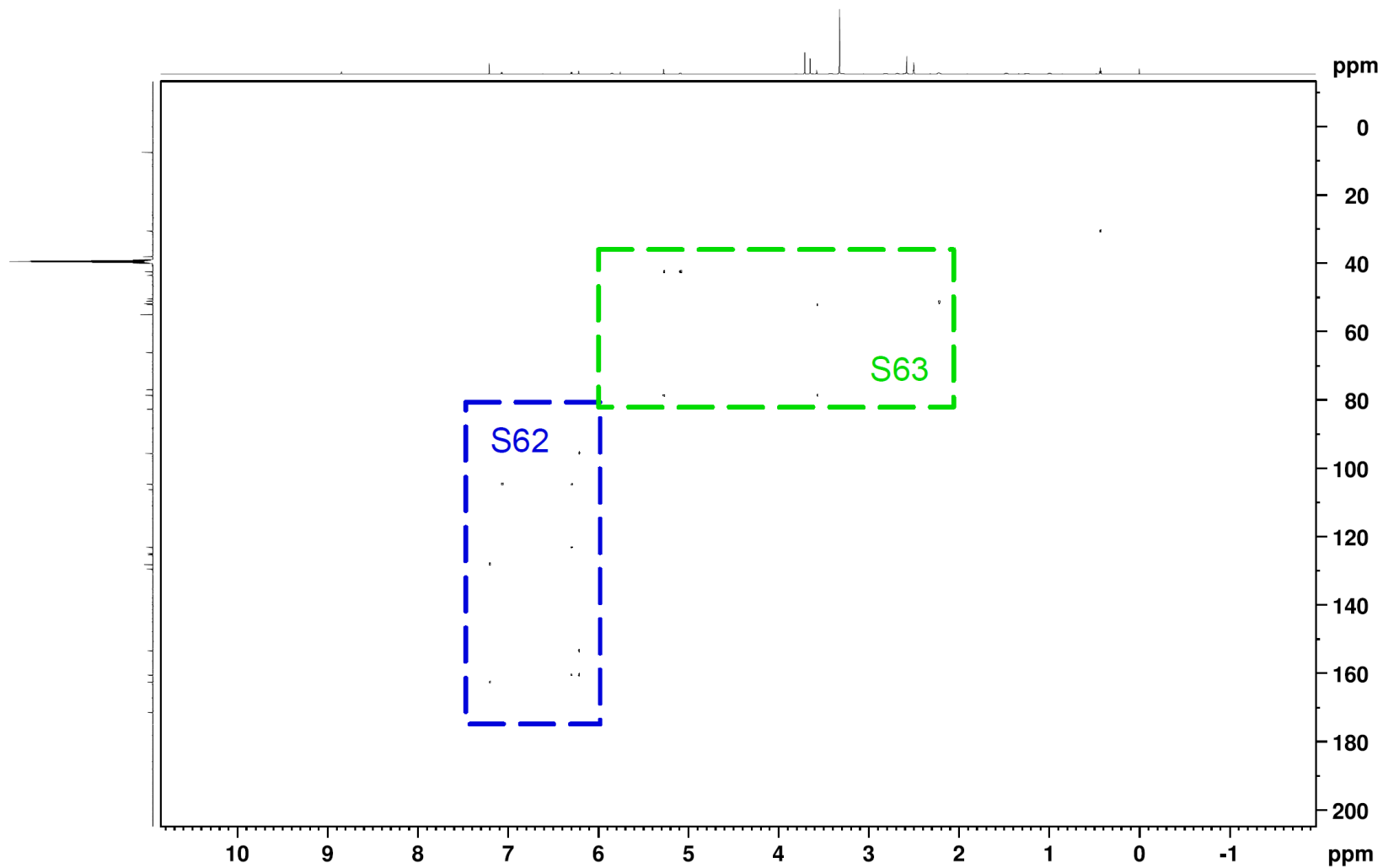


1,1-ADEQUATE of Compound 10

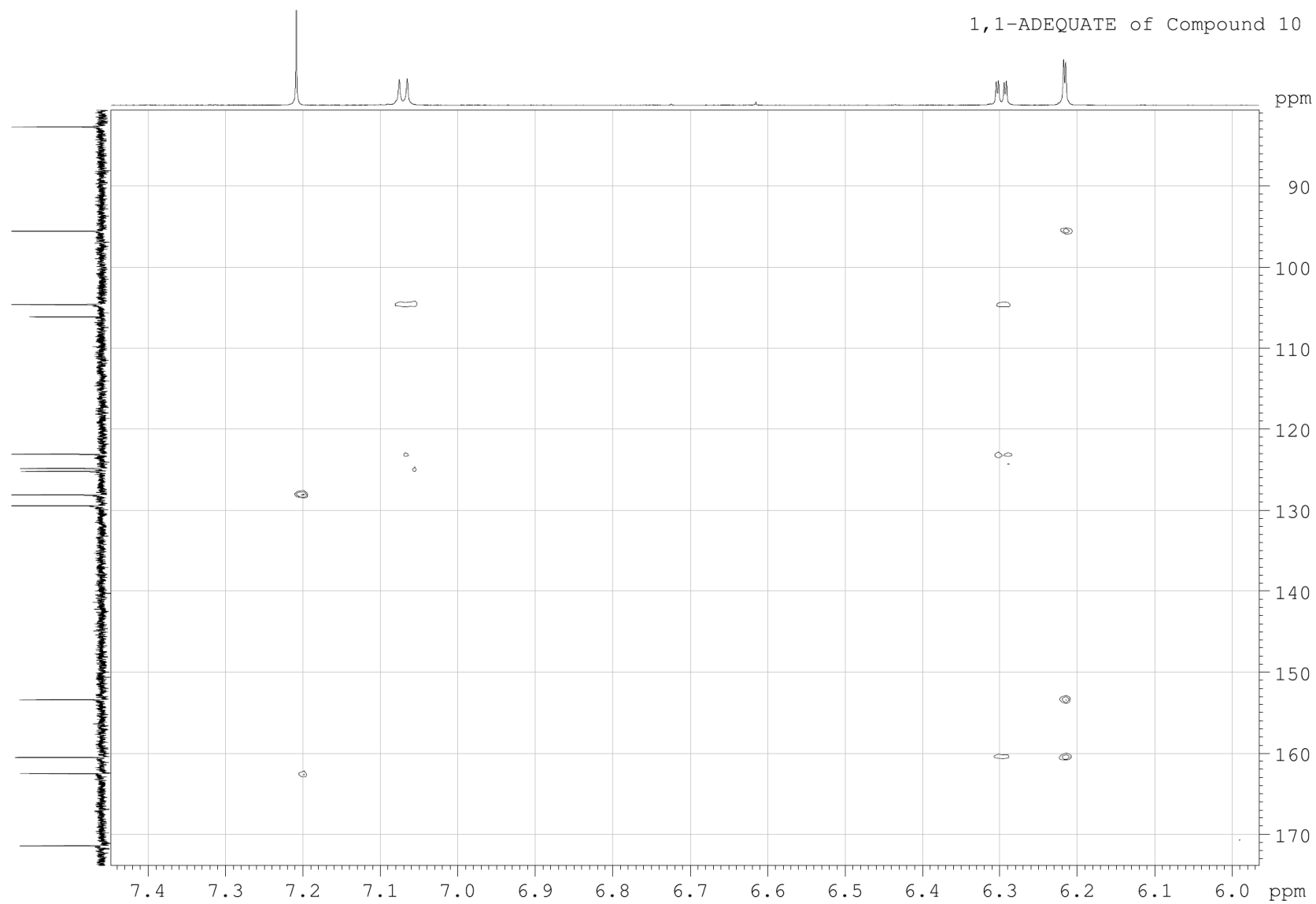


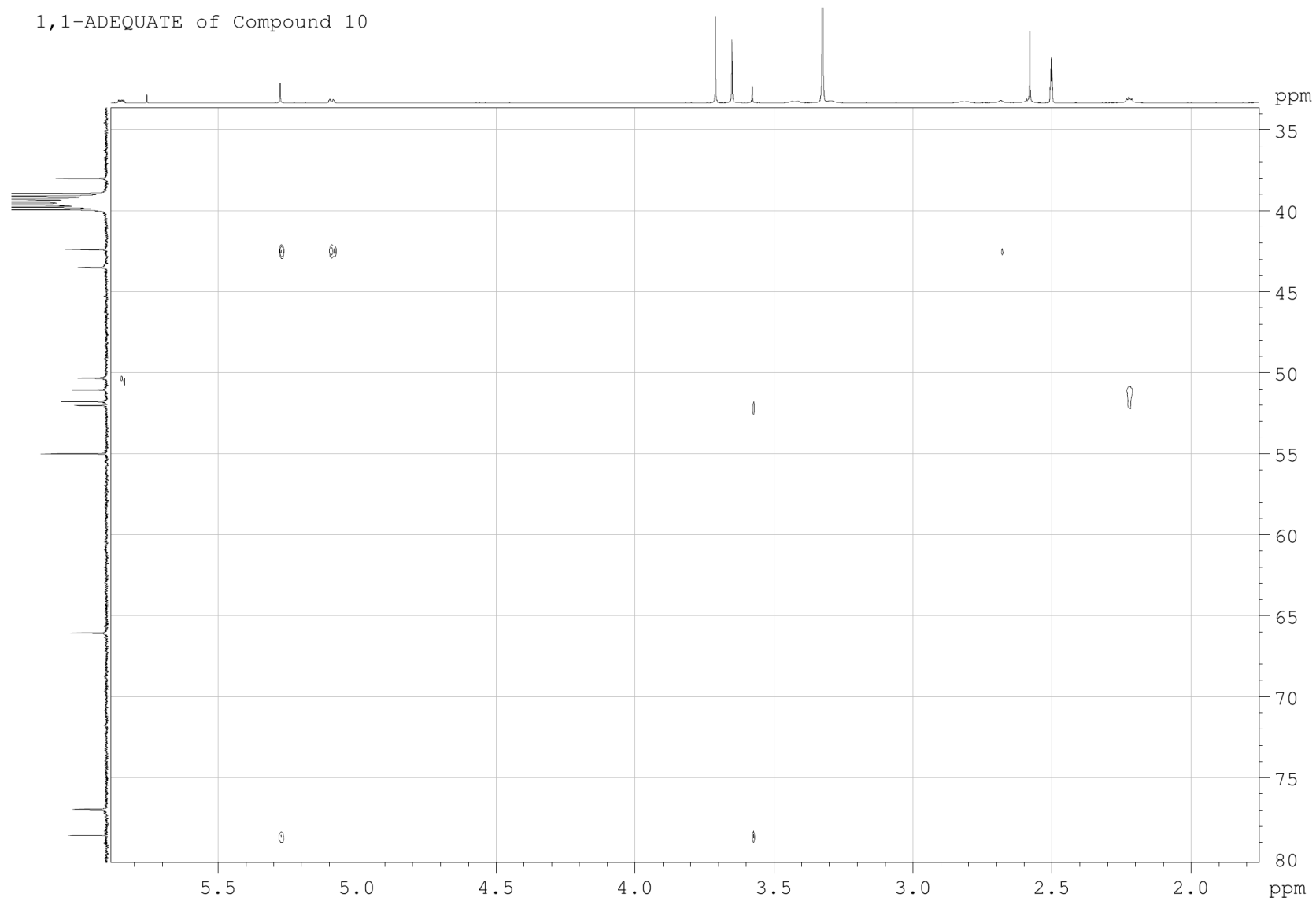
S60

1,1-ADEQUATE of Compound 10

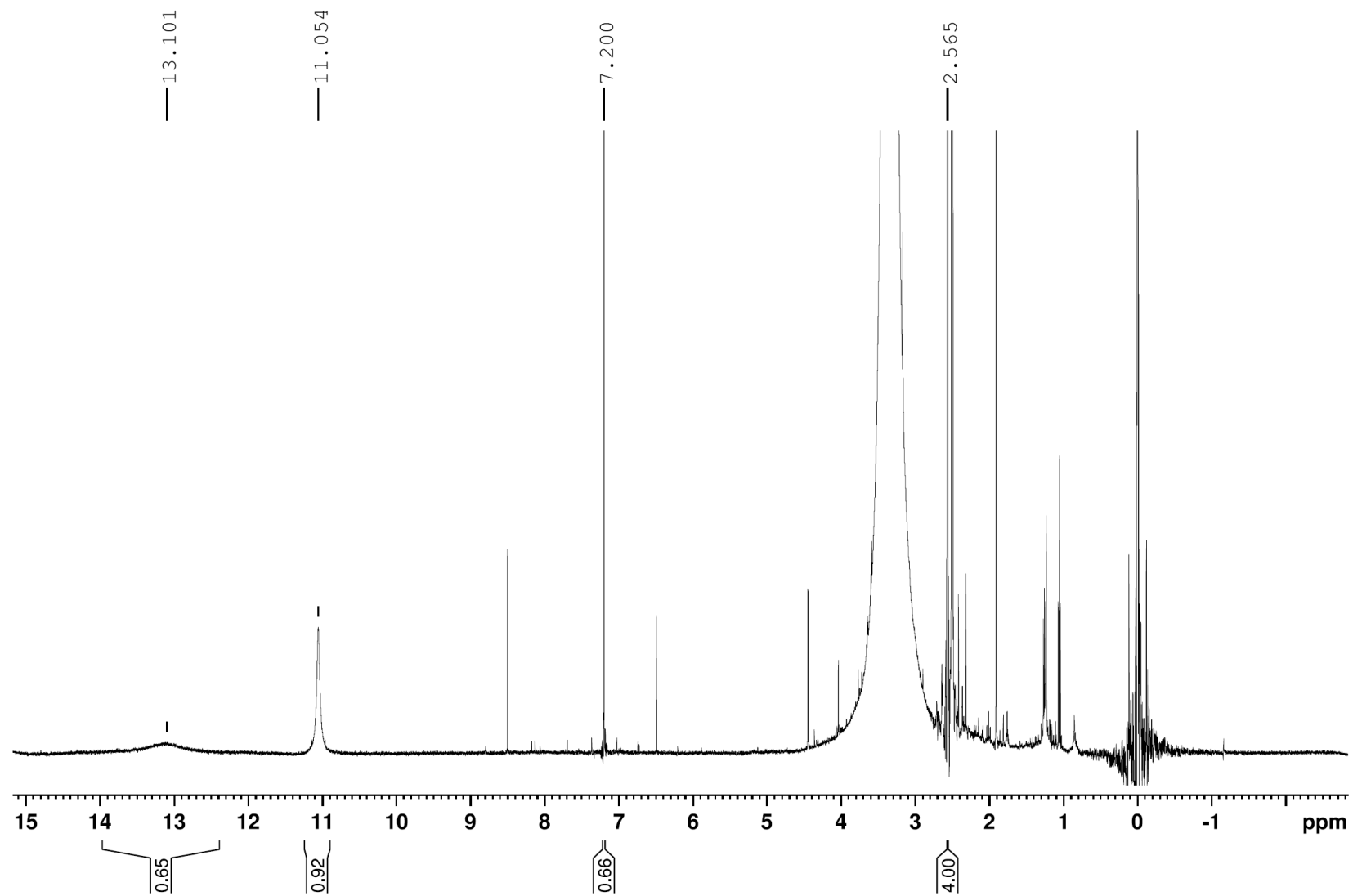


S61



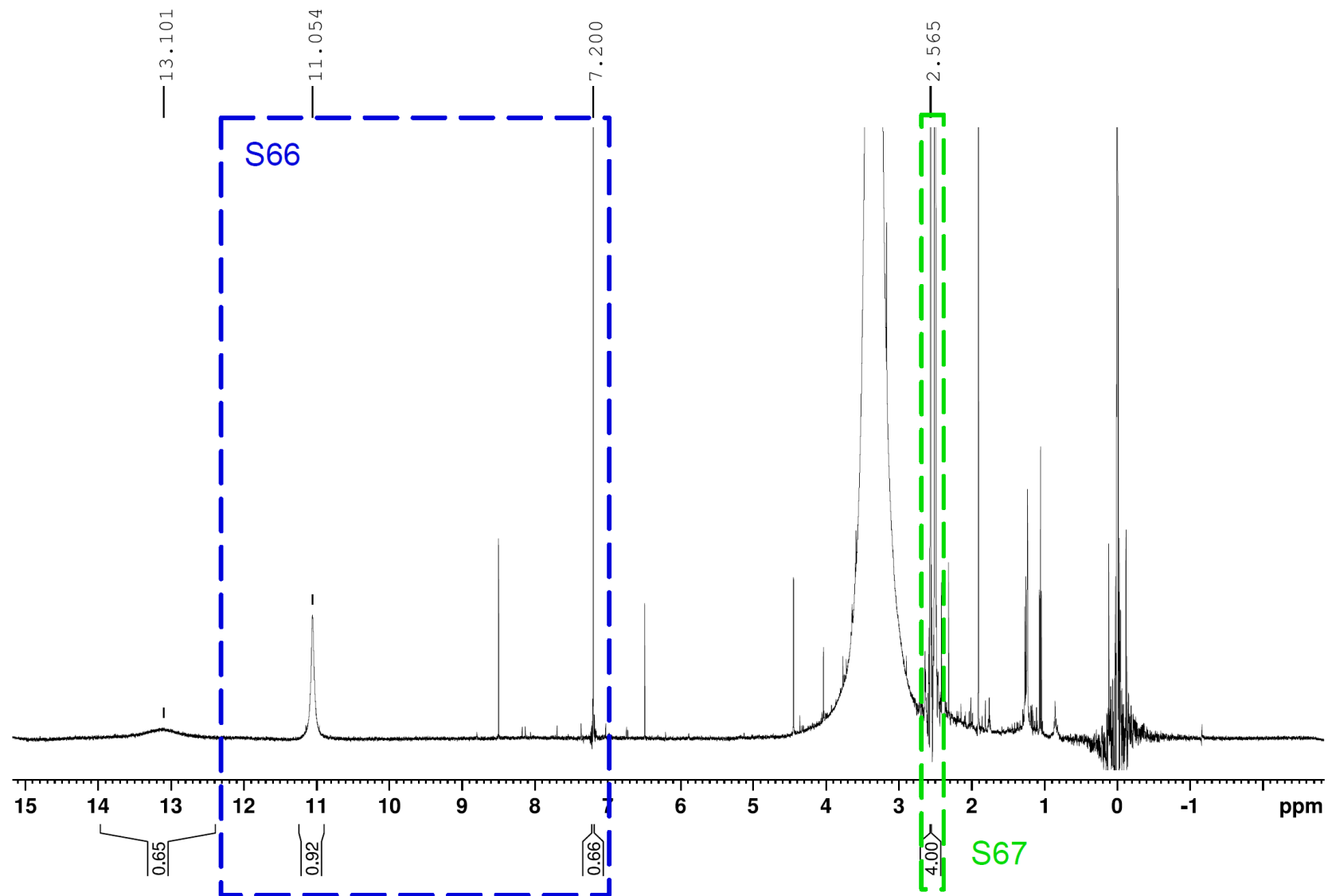


¹H NMR of Compounds 7, 14 and 15

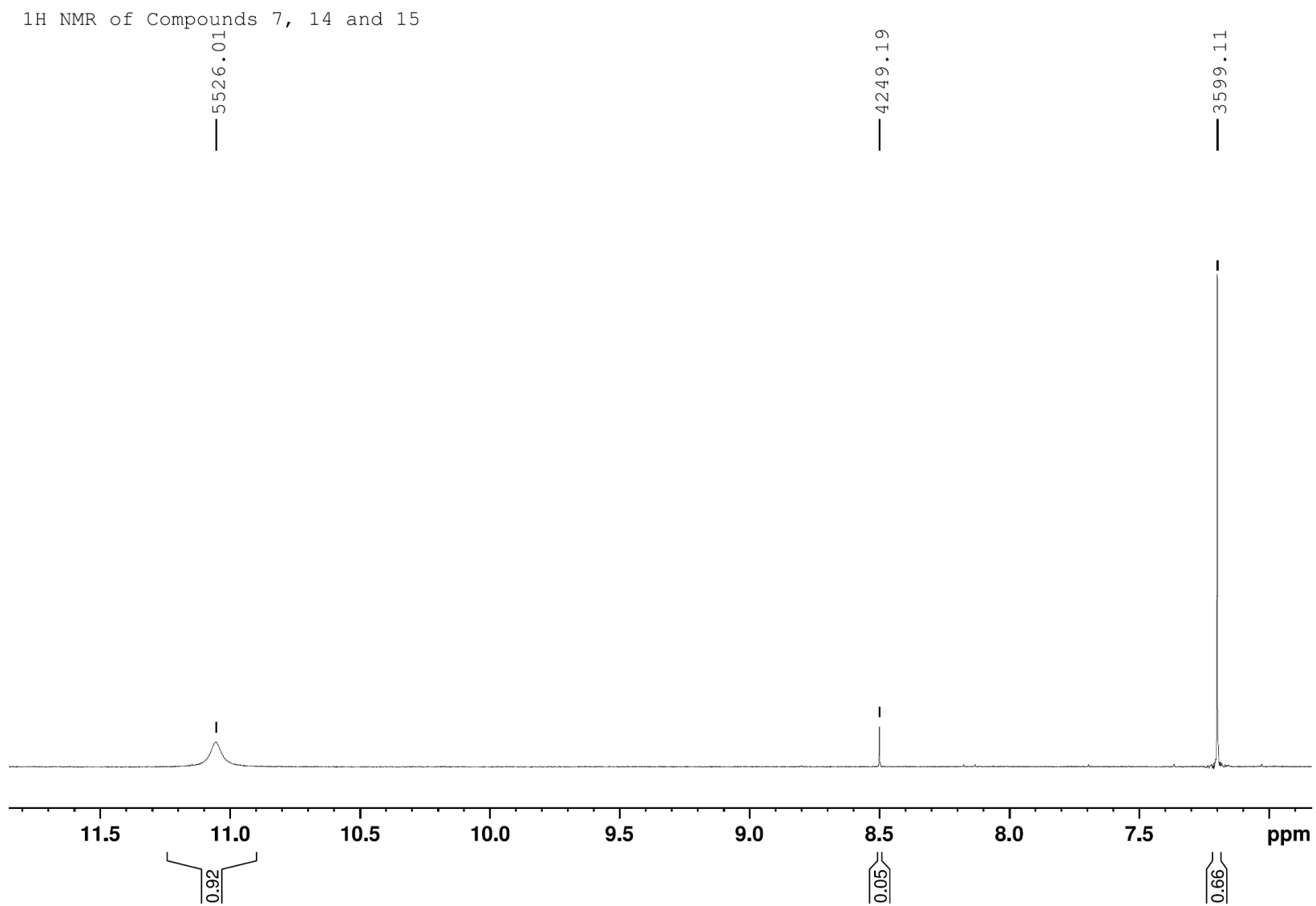


S64

^1H NMR of Compounds 7, 14 and 15

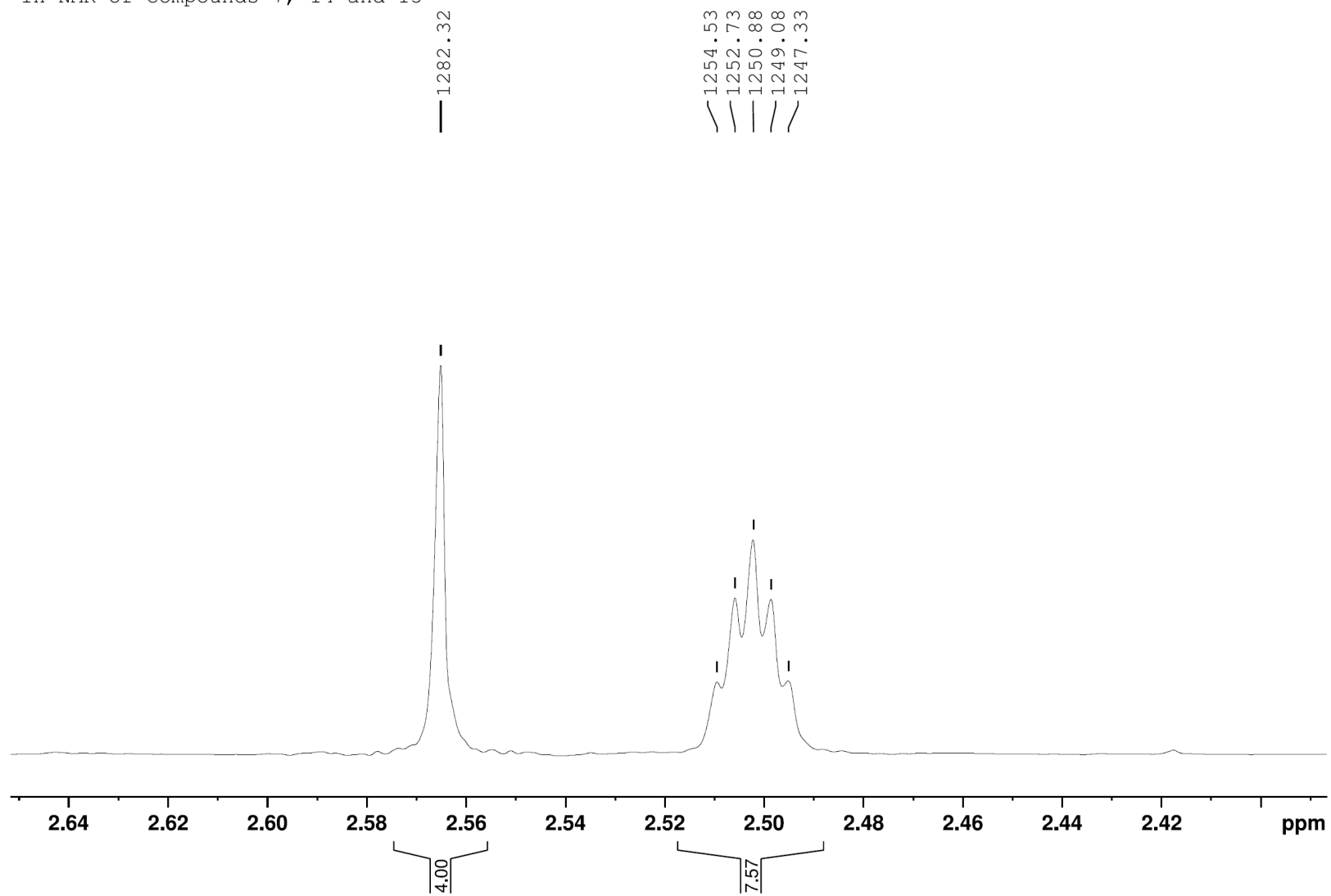


S65



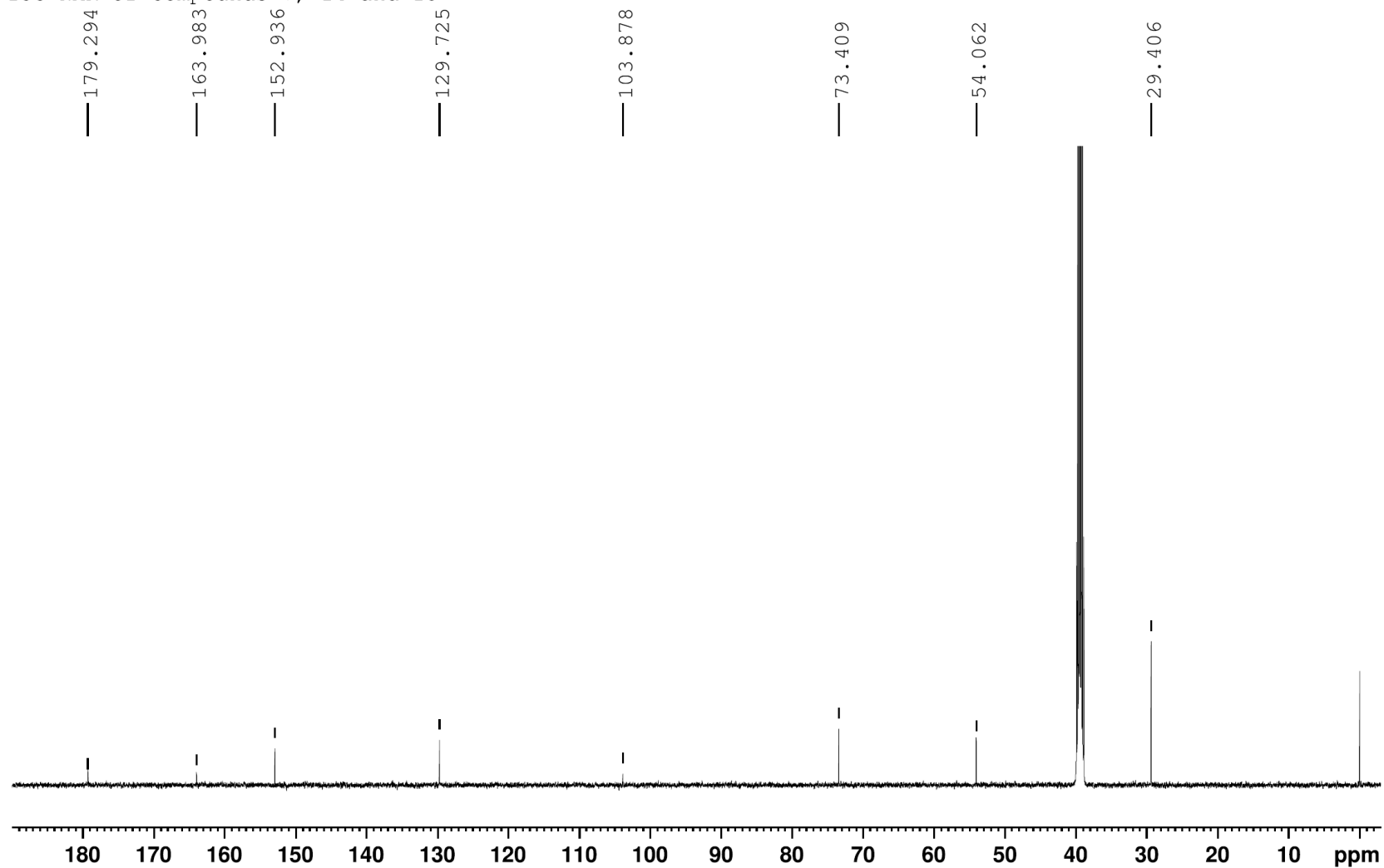
S66

¹H NMR of Compounds 7, 14 and 15

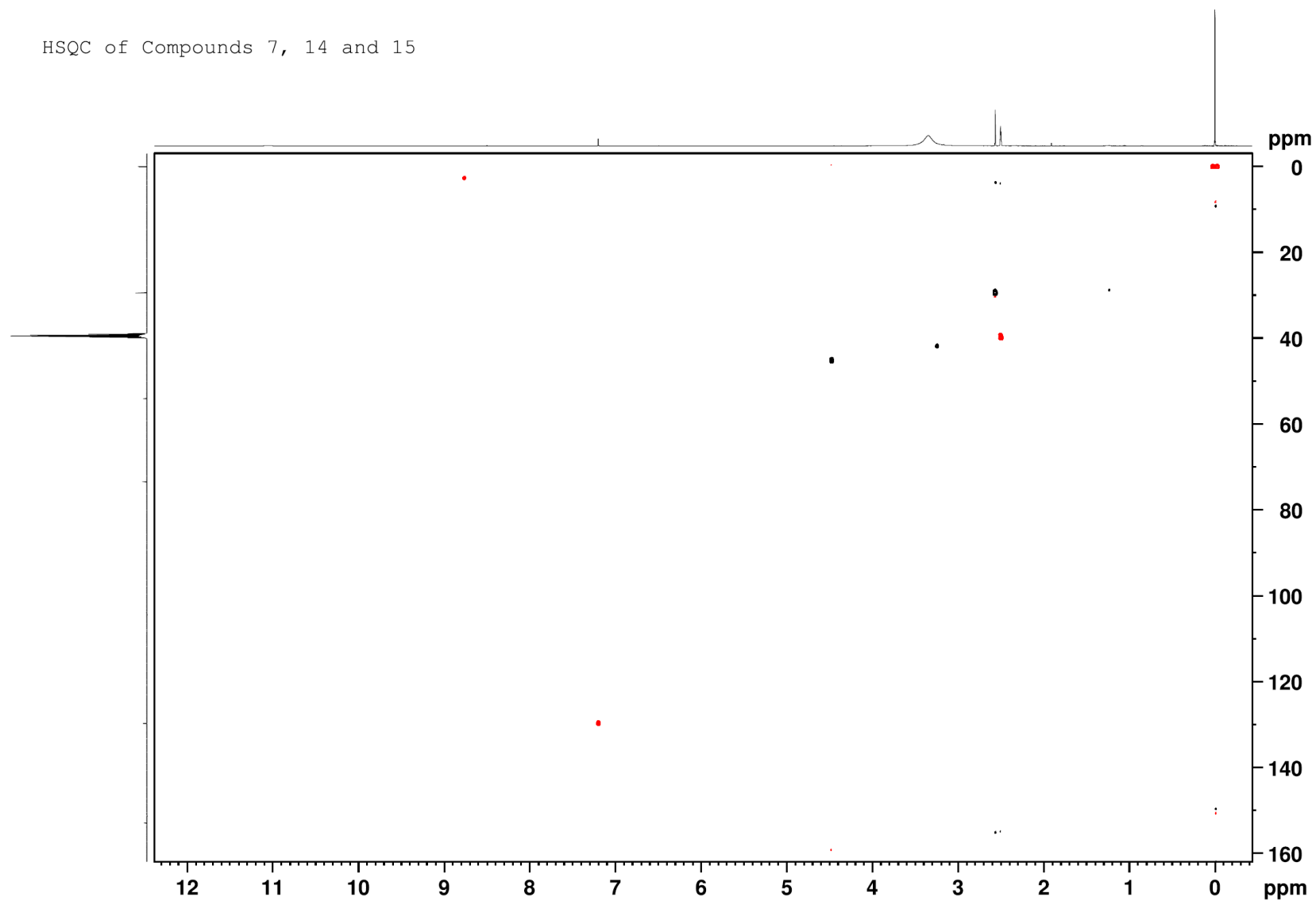


S67

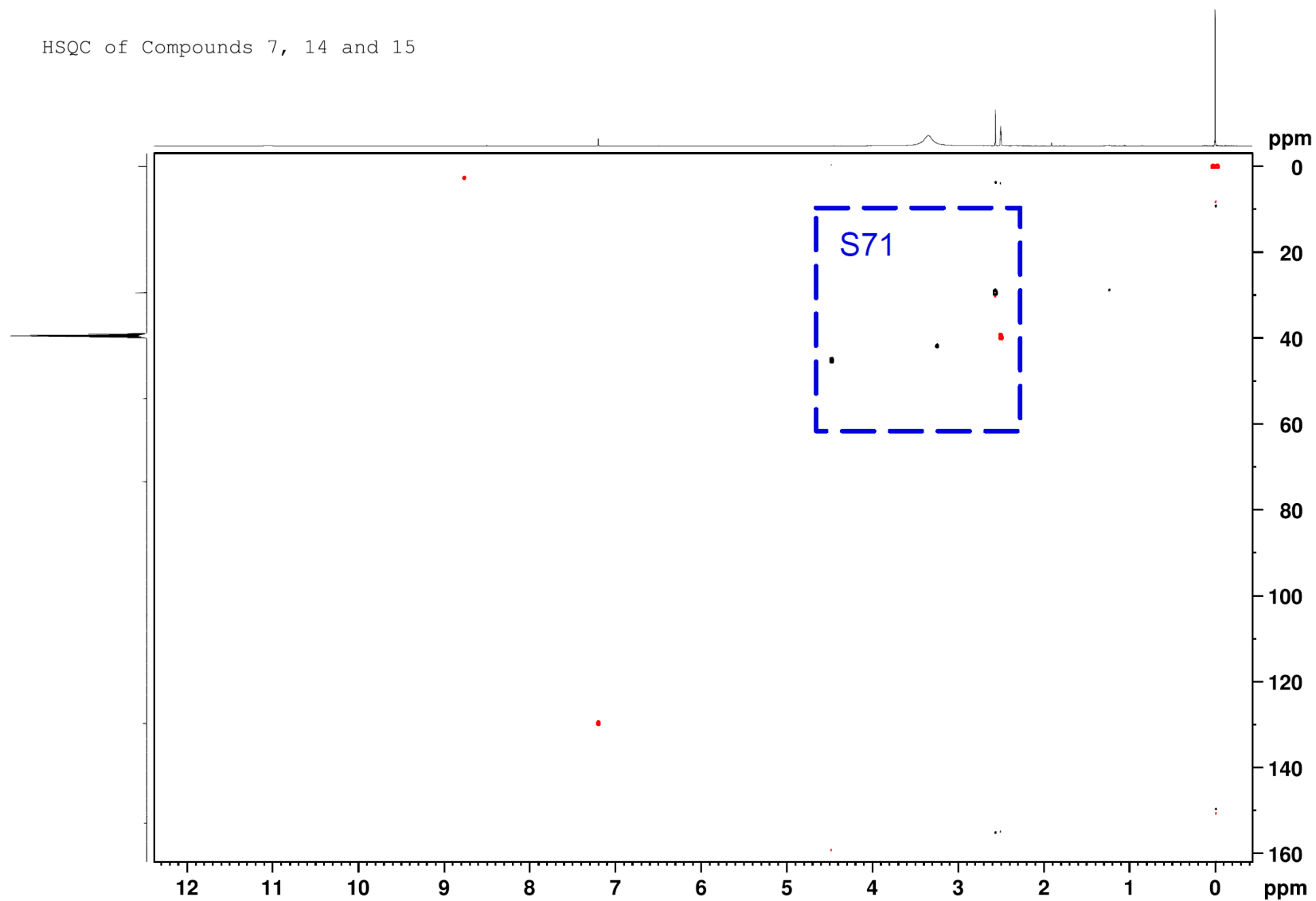
¹³C NMR of Compounds 7, 14 and 15



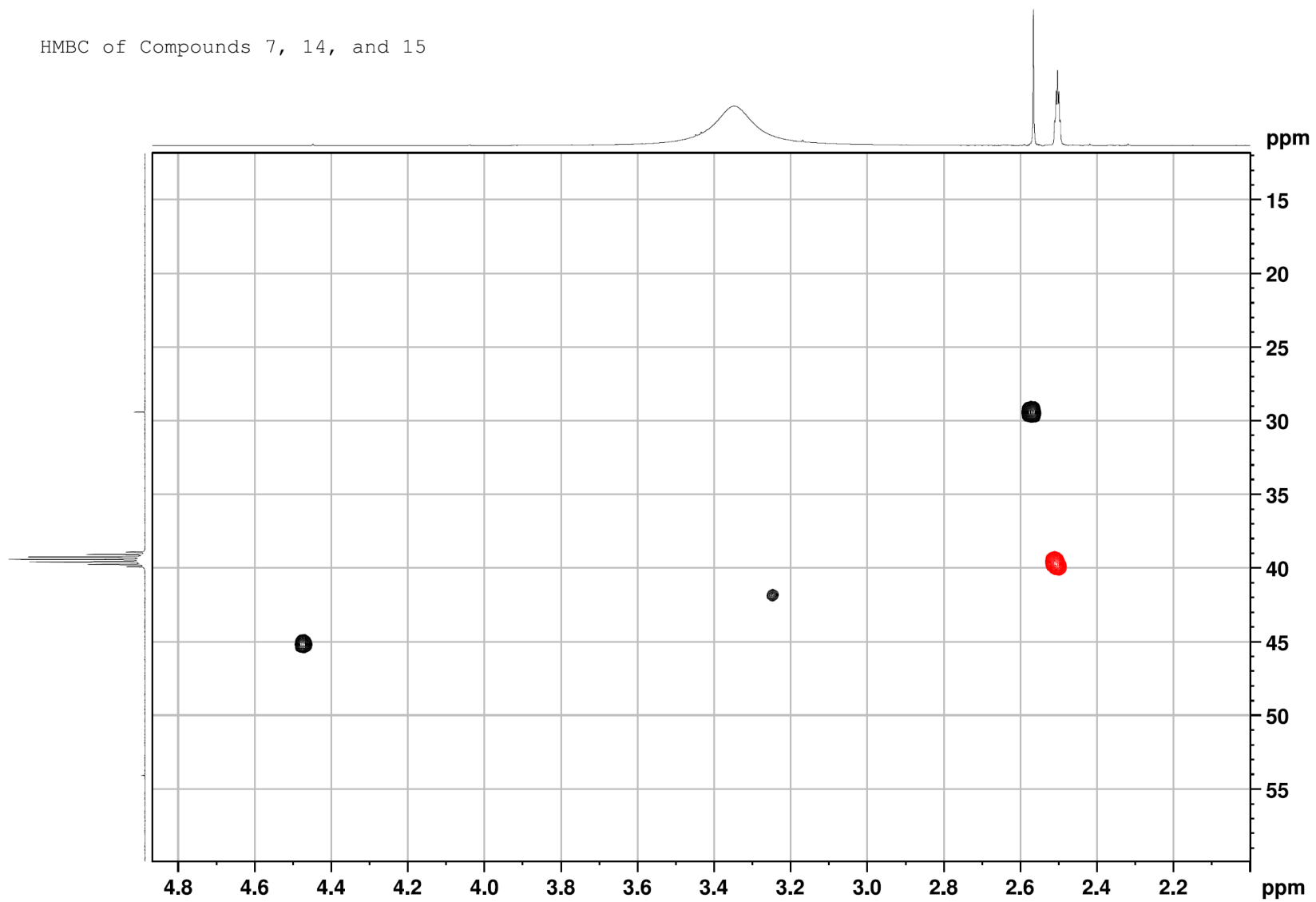
HSQC of Compounds 7, 14 and 15



HSQC of Compounds 7, 14 and 15

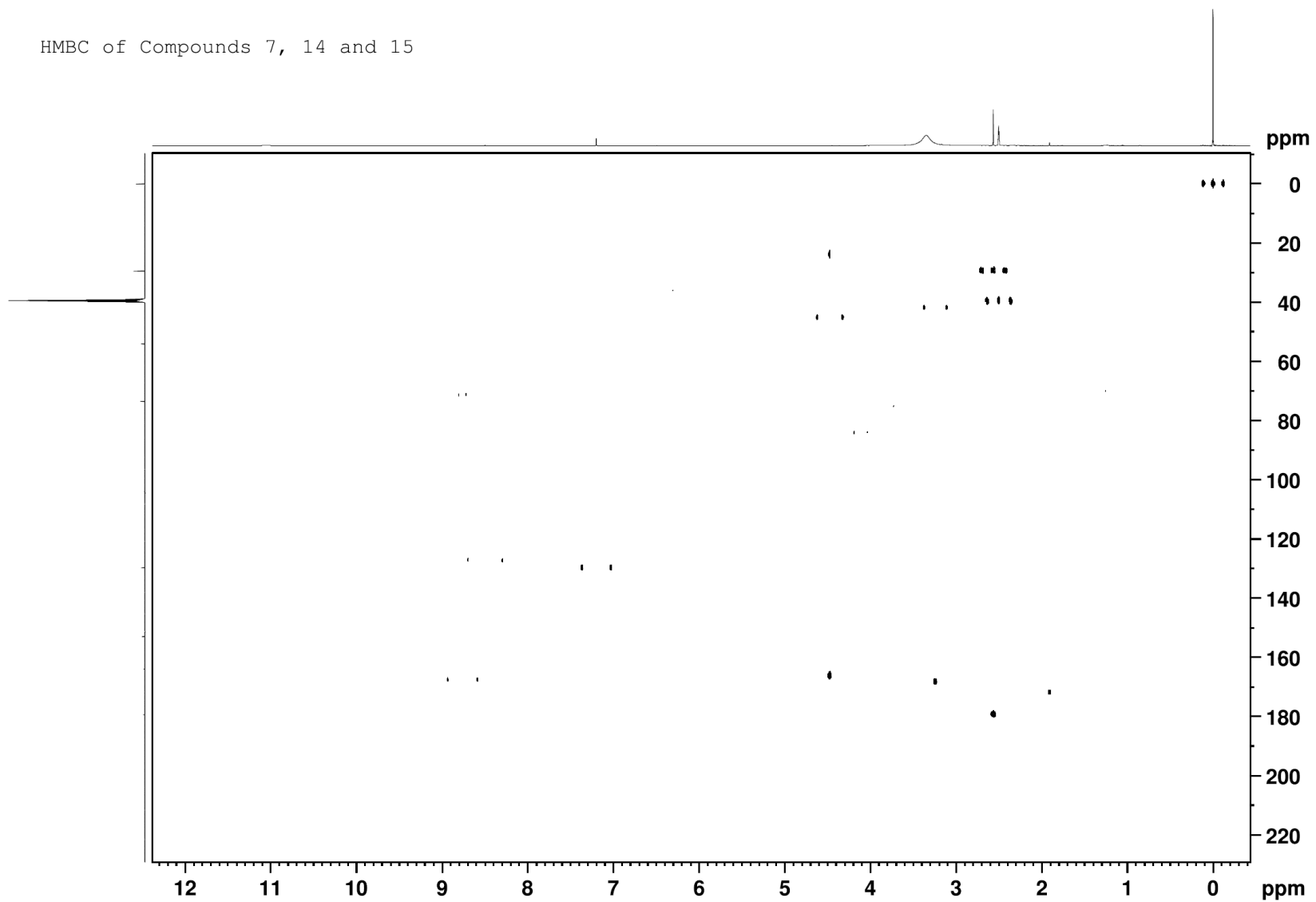


HMBC of Compounds 7, 14, and 15

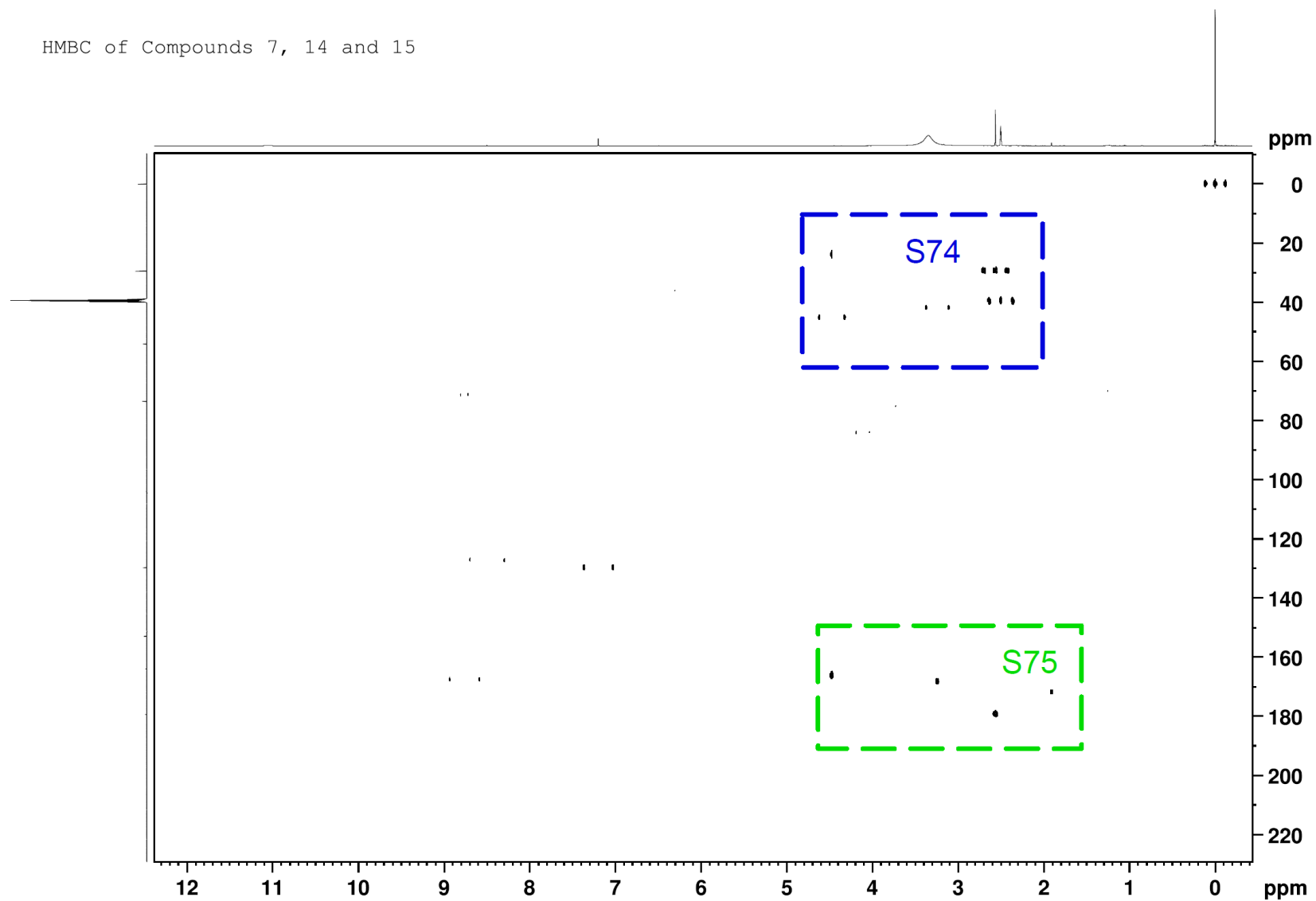


S71

HMBC of Compounds 7, 14 and 15

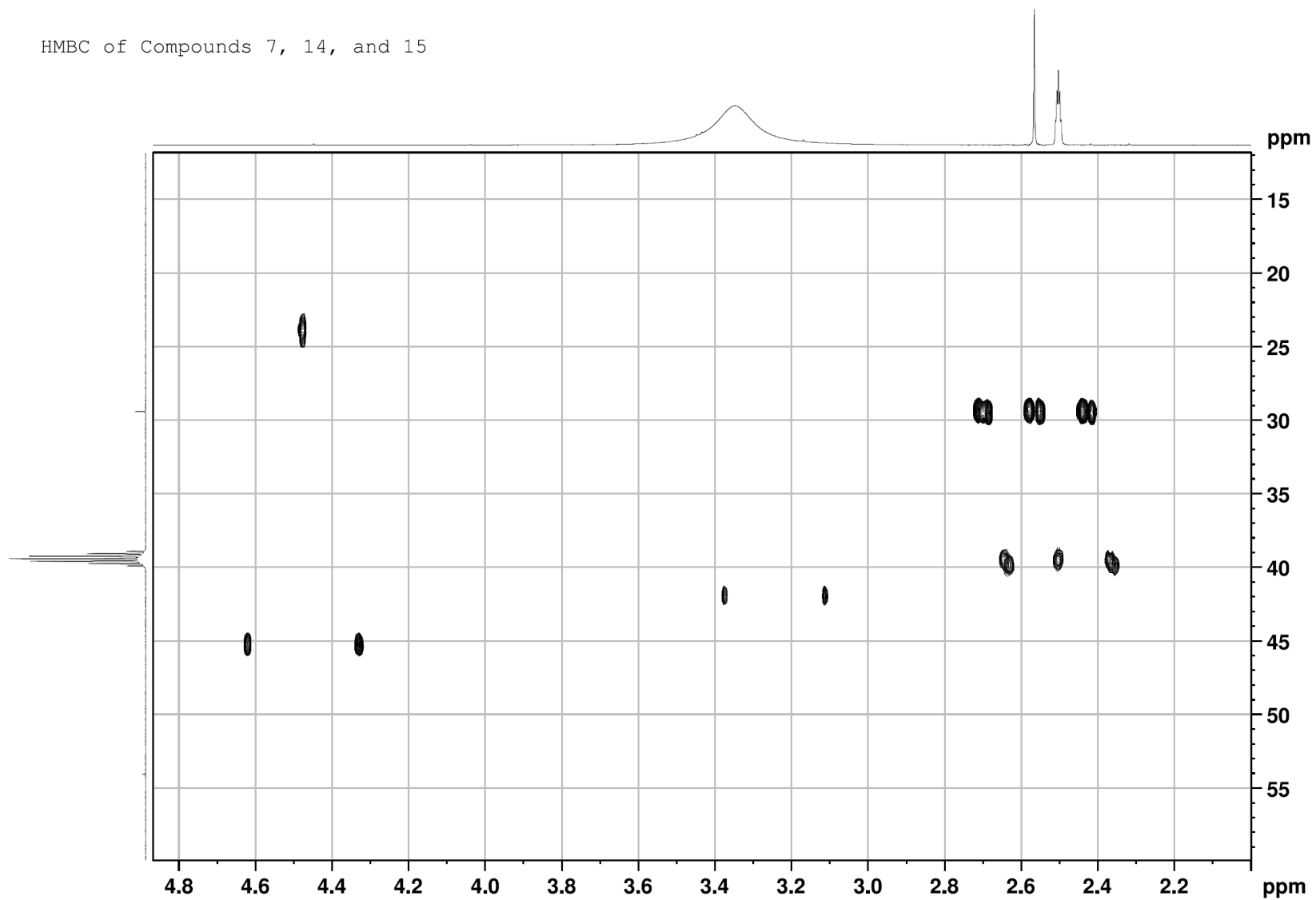


HMBC of Compounds 7, 14 and 15

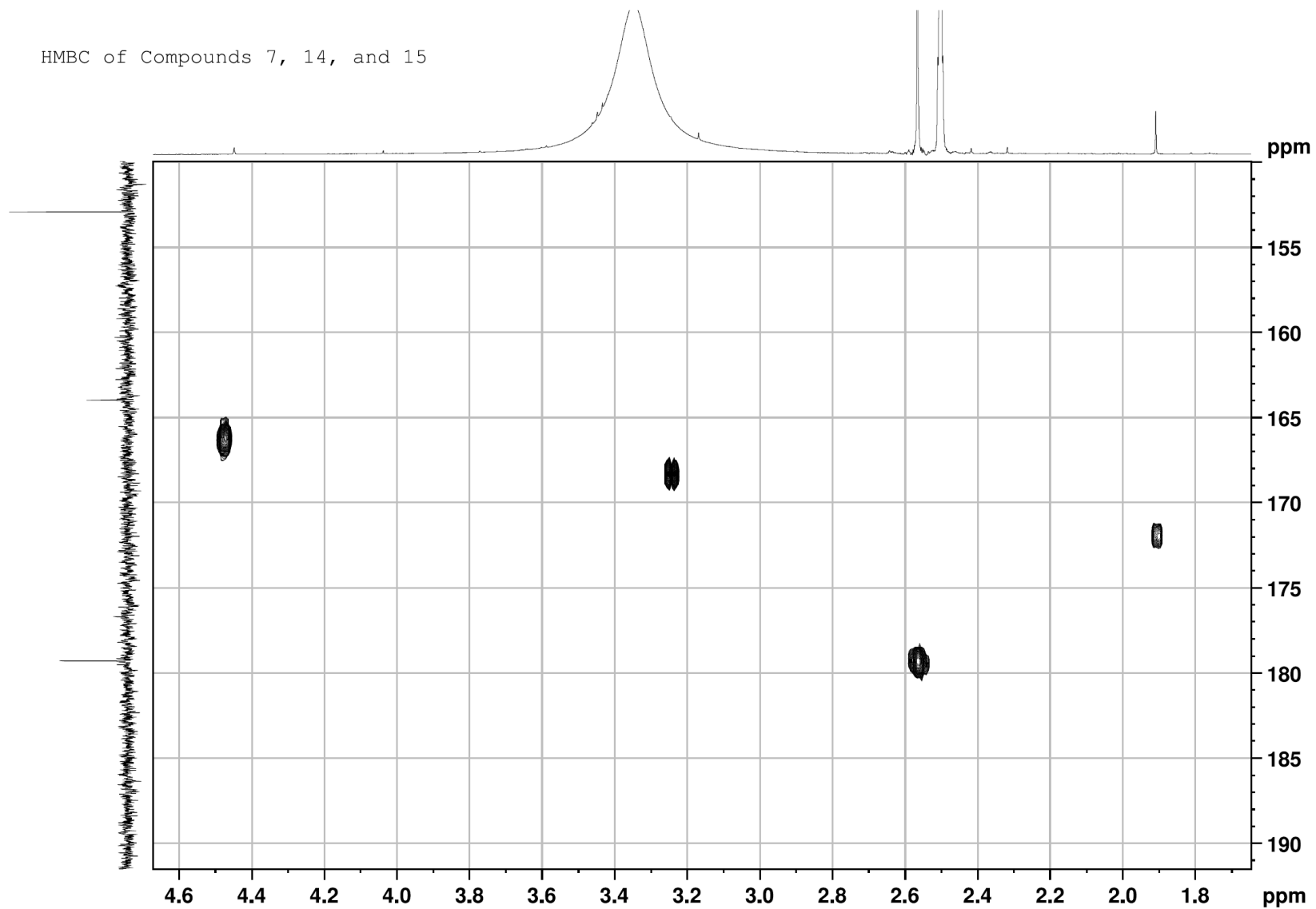


S73

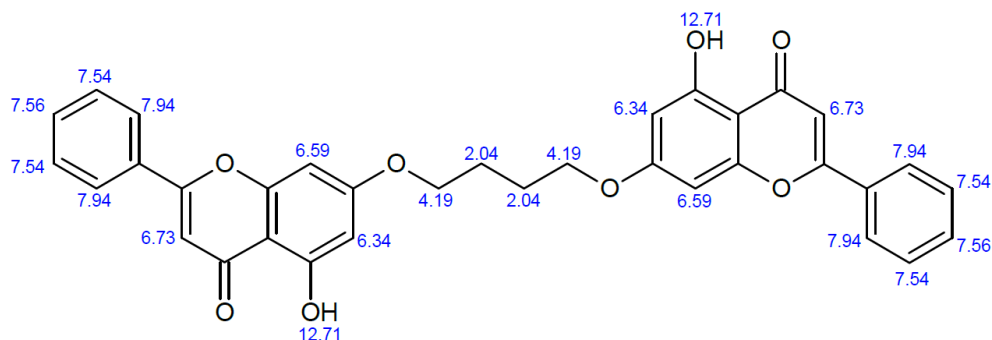
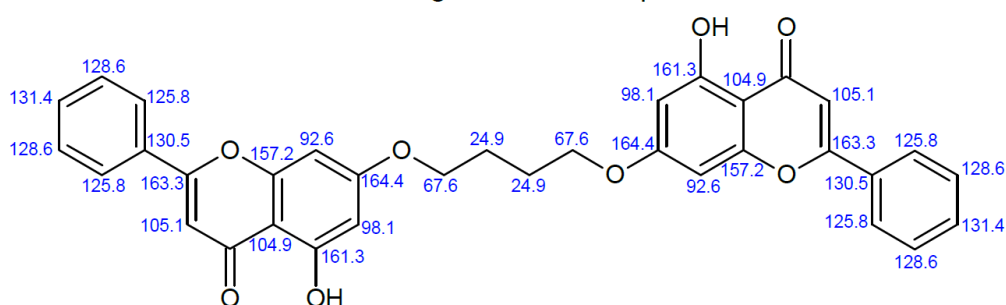
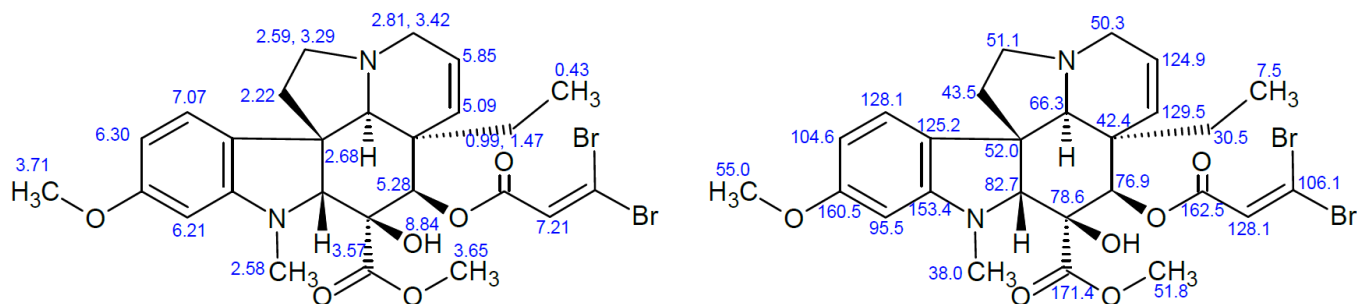
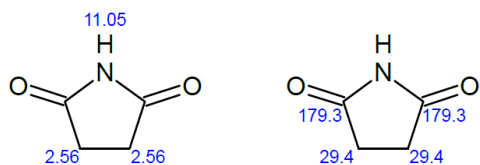
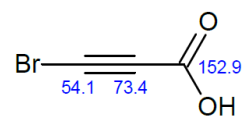
HMBC of Compounds 7, 14, and 15



HMBC of Compounds 7, 14, and 15



Detailed NMR assignments of Compounds 6, 7, 10, 14 and 15

 ^1H NMR assignments of Compound 6 ^{13}C NMR assignments of Compound 6 ^1H NMR and ^{13}C NMR assignments of Compound 10 ^1H NMR and ^{13}C NMR assignments of Compound 14 ^{13}C NMR assignments of Compound 7 ^1H NMR and ^{13}C NMR assignments of Compound 15