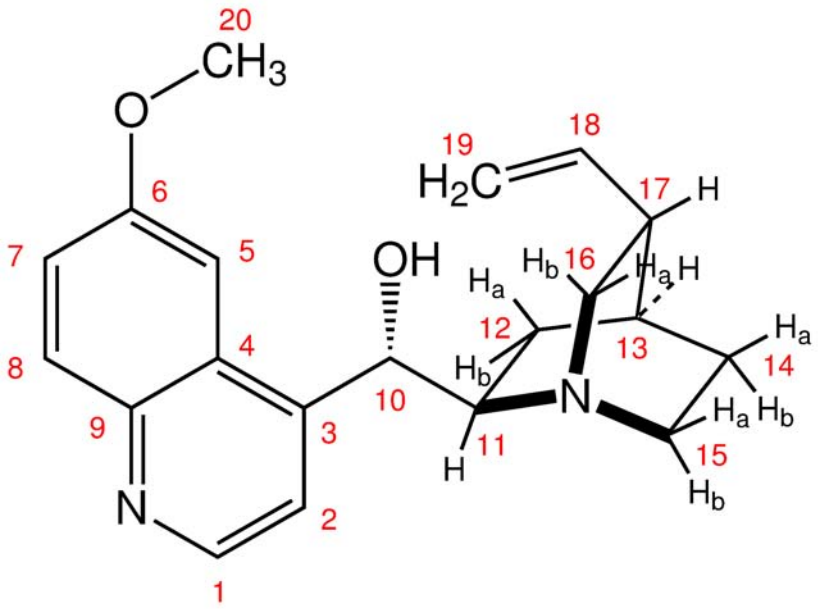
Problem 58

The ^{1}H and ^{13}C{^{1}H} NMR spectra of quinidine ($C_{20}H_{24}N_2O_2$) recorded in DMSO-d_6 solution at 298 K and 600 MHz are given below.

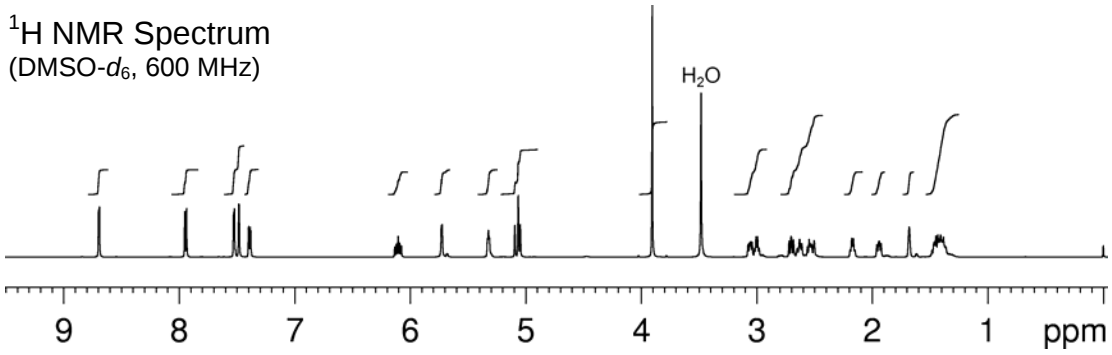
The ^{1}H NMR spectrum has signals at δ 1.38 (m, 1H), 1.43 (m, 2H), 1.68 (m, 1H), 1.94 (m, 1H), 2.17 (m, 1H), 2.53 (m, 1H), 2.63 (m, 1H), 2.70 (m, 1H), 3.00 (m, 1H), 3.06 (m, 1H), 3.90 (s, 3H), 5.05 (m, 1H), 5.08 (m, 1H), 5.32 (dd, J = 4.7, 6.2 Hz, 1H), 5.73 (d, J = 4.7 Hz, 1H), 6.10 (ddd, J = 7.5, 10.2, 17.5 Hz, 1H), 7.39 (dd, J = 2.8, 9.3 Hz, 1H), 7.48 (d, J = 2.8 Hz, 1H), 7.53 (d, J = 4.4 Hz, 1H), 7.94 (d, J = 9.3 Hz, 1H) and 8.69 (d, J = 4.4 Hz, 1H) ppm.

The ^{13}C{^{1}H} NMR spectrum has signals at δ 23.1, 26.2, 27.8, 39.8, 48.4, 49.1, 55.3, 60.5, 70.7, 102.3, 114.2, 118.9, 120.9, 126.9, 131.0, 141.2, 143.8, 147.4, 149.4 and 156.7 ppm.

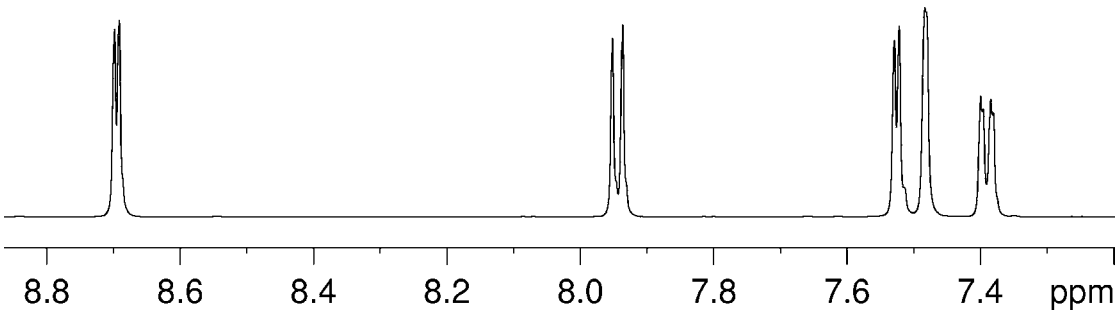
The 2D ^{1}H–^{1}H COSY, multiplicity-edited ^{1}H–^{13}C HSQC, ^{1}H–^{13}C HMBC and ^{1}H–^{1}H NOESY spectra are given on the following pages. Use these spectra to assign the ^{1}H and ^{13}C{^{1}H} resonances for this compound.



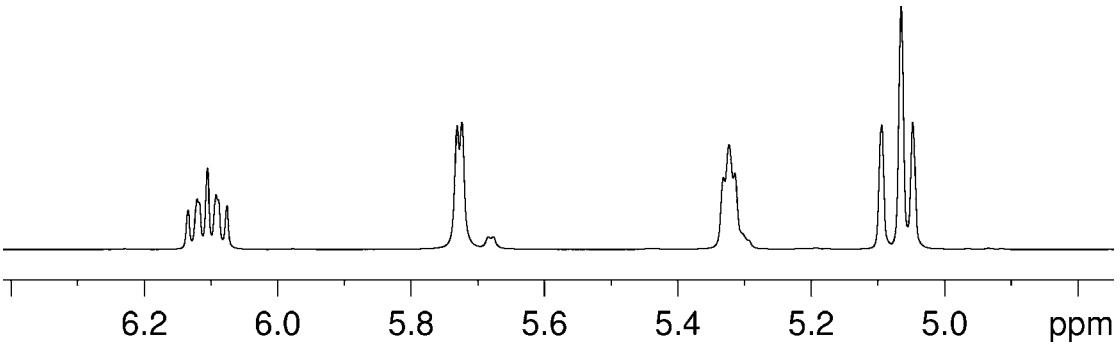
^{1}H NMR Spectrum
(DMSO-d_6, 600 MHz)



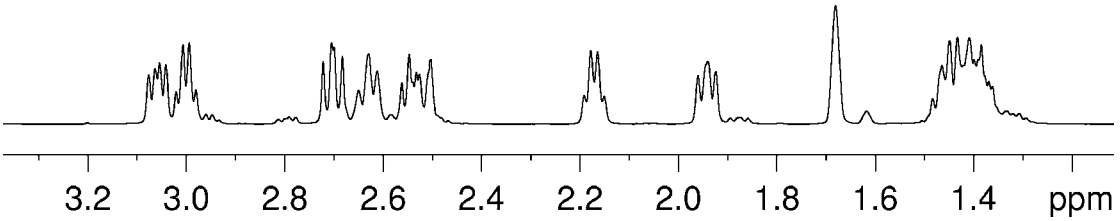
^{1}H NMR Expansion Spectrum
(DMSO-d_6, 600 MHz)



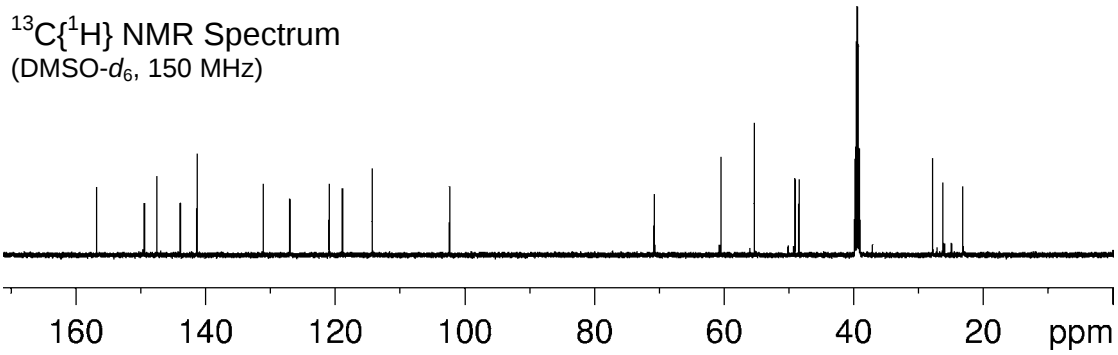
^{1}H NMR Expansion Spectrum
(DMSO-d_6, 600 MHz)



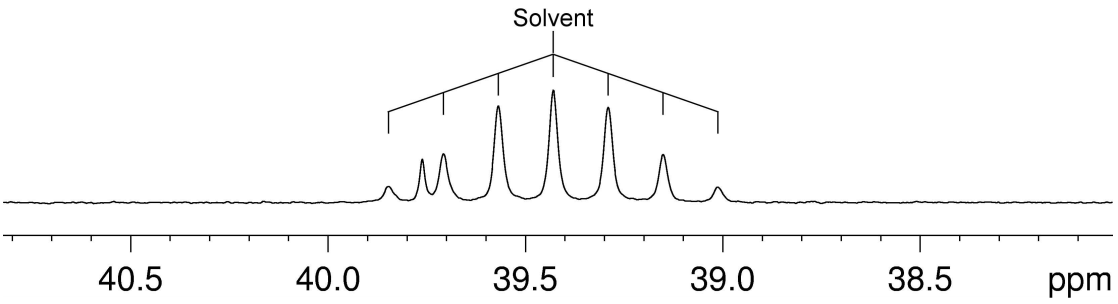
^{1}H NMR Expansion Spectrum
(DMSO-d_6, 600 MHz)

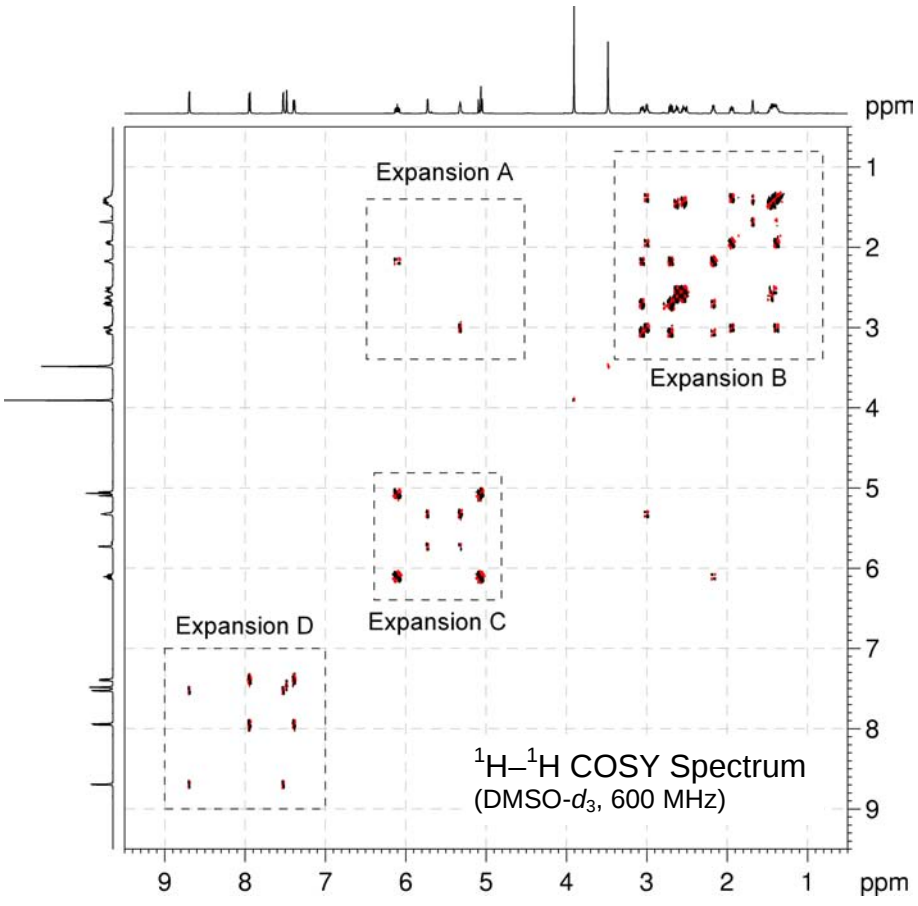


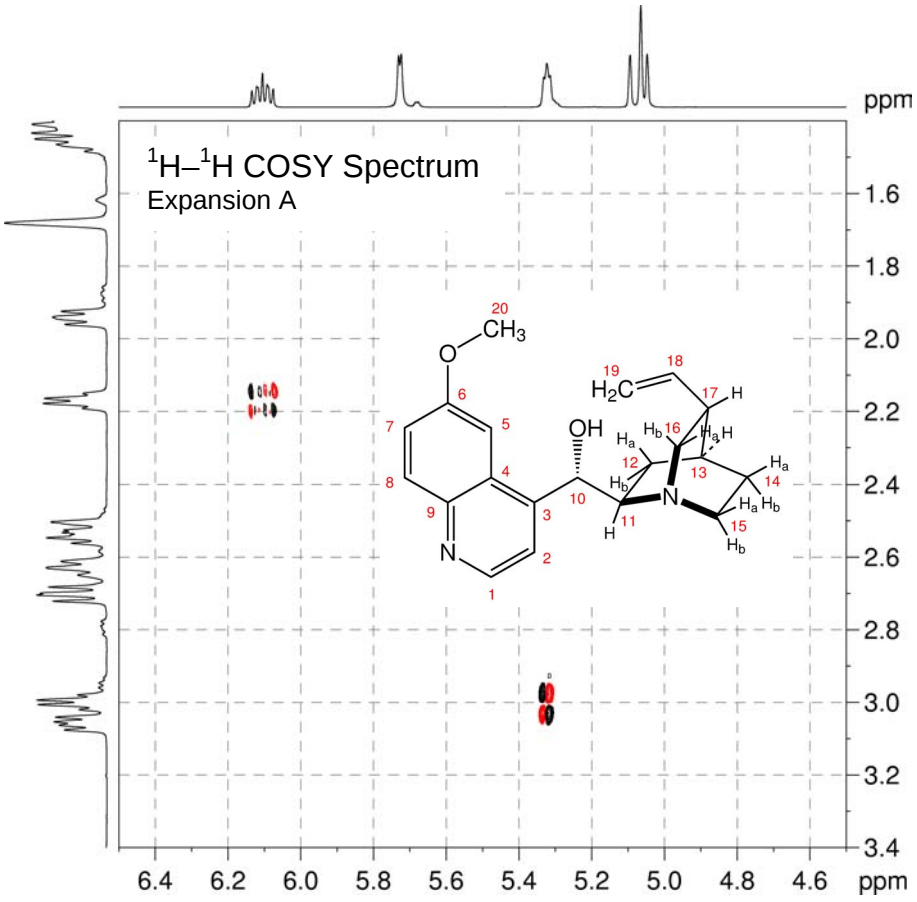
$^{13}C\{^{1}H\}$ NMR Spectrum
(DMSO-d_6, 150 MHz)

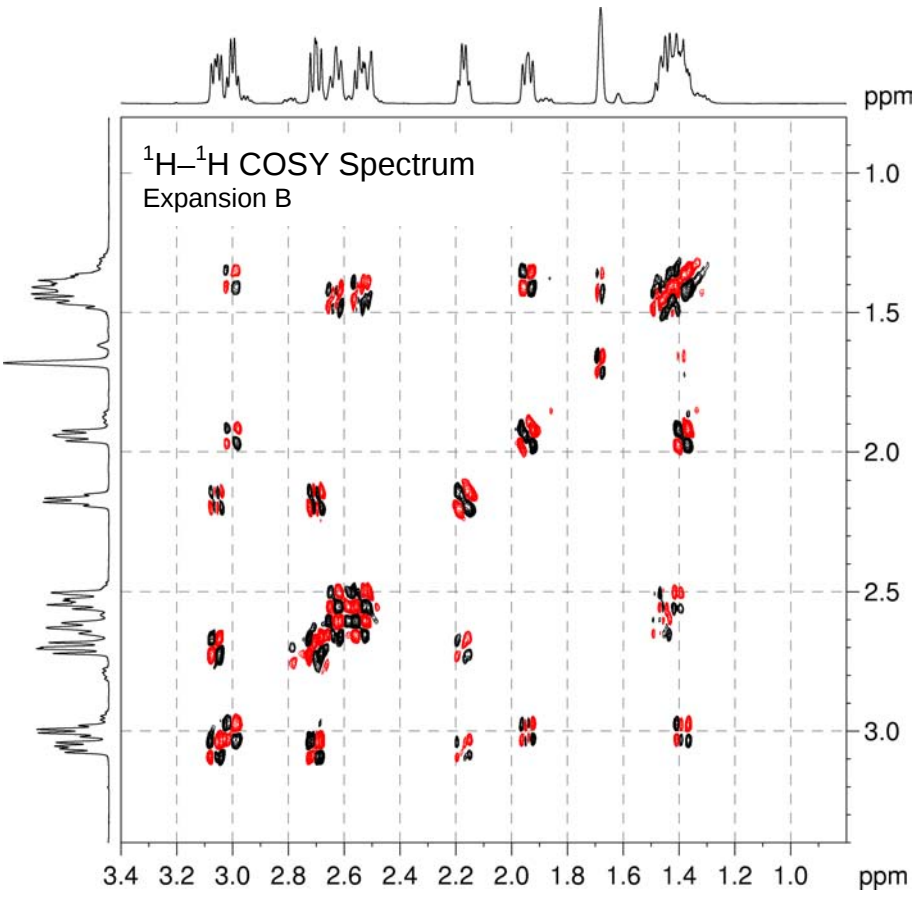


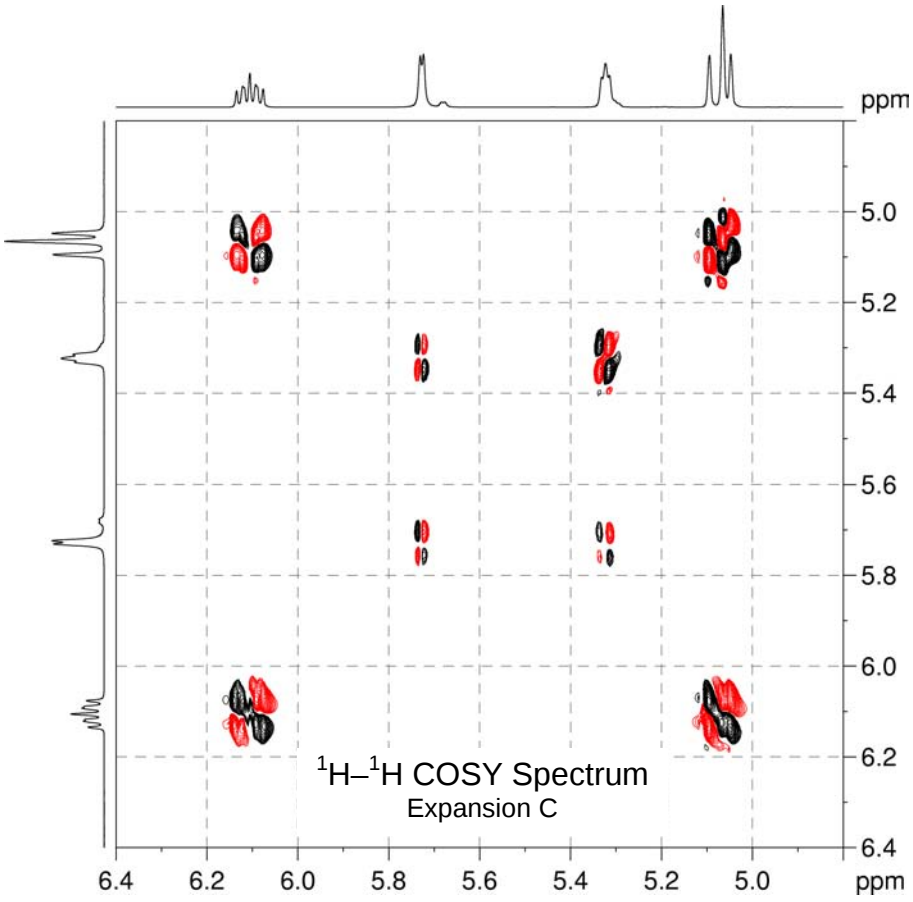
$^{13}C\{^{1}H\}$ NMR Expansion Spectrum
(DMSO-d_6, 150 MHz)



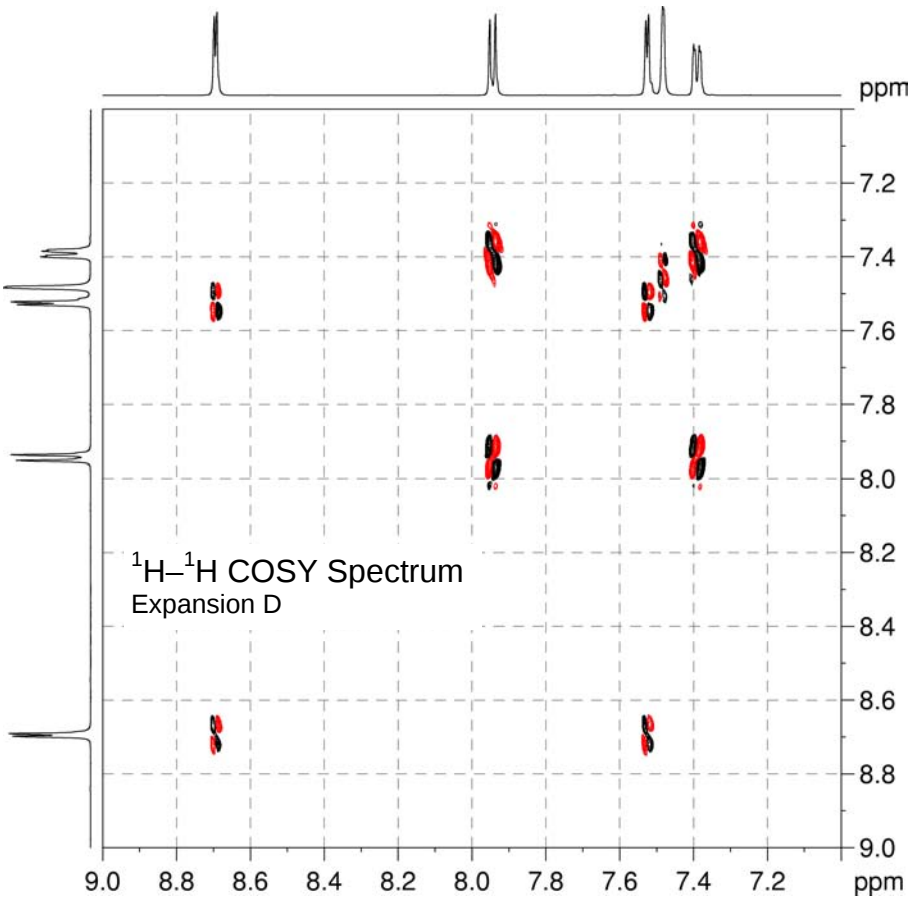



^{1}H–^{1}H COSY Spectrum
Expansion A
ppm
1.6
1.8
2.0
2.2
2.4
2.6
2.8
3.0
3.2
3.4
6.4
6.2
6.0
5.8
5.6
5.4
5.2
5.0
4.8
4.6
ppm

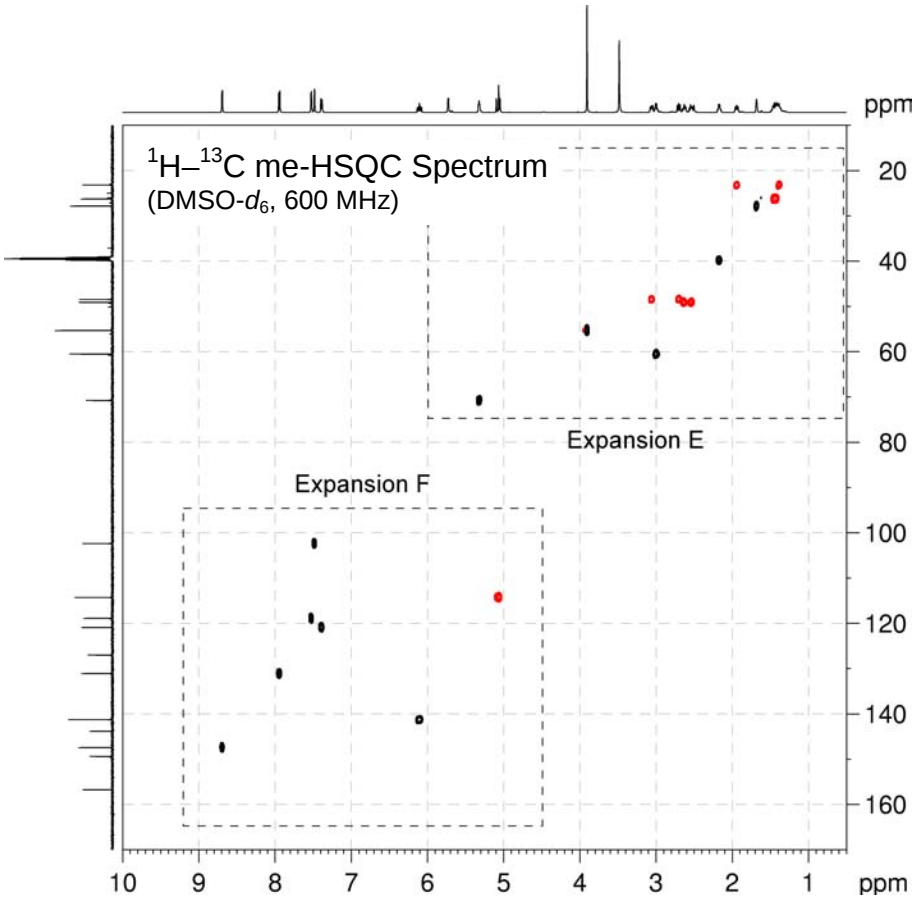

^{1}H–^{1}H COSY Spectrum
Expansion B
ppm
1.0
1.5
2.0
2.5
3.0
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
ppm

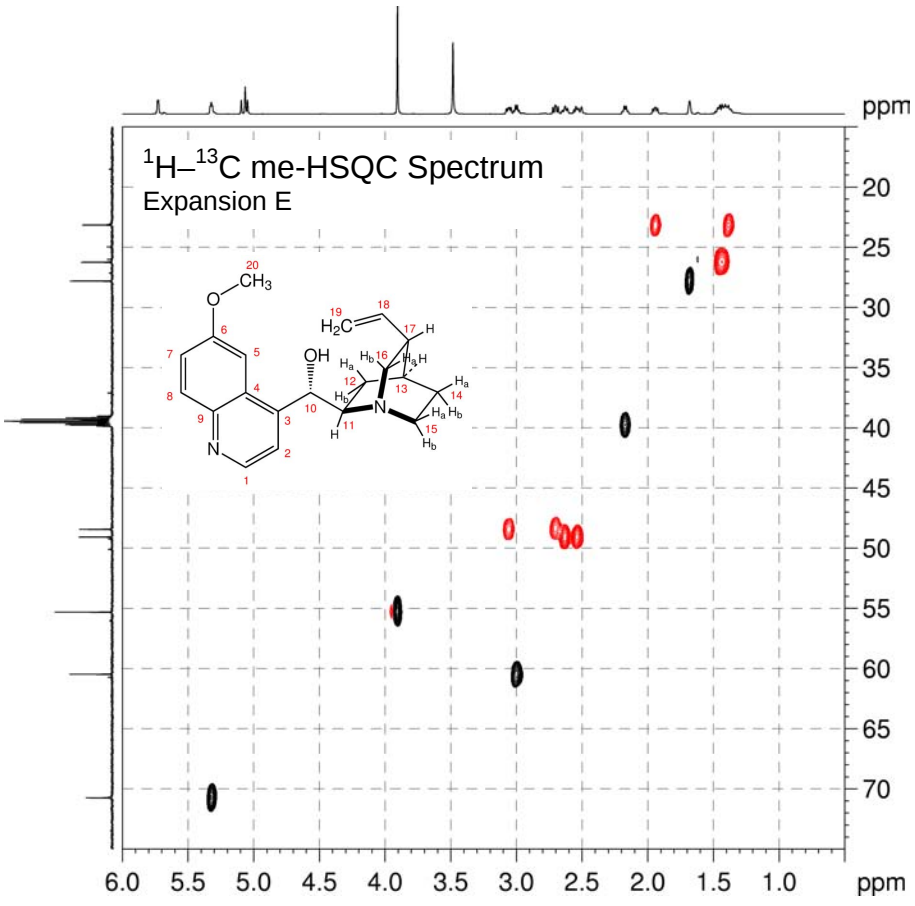


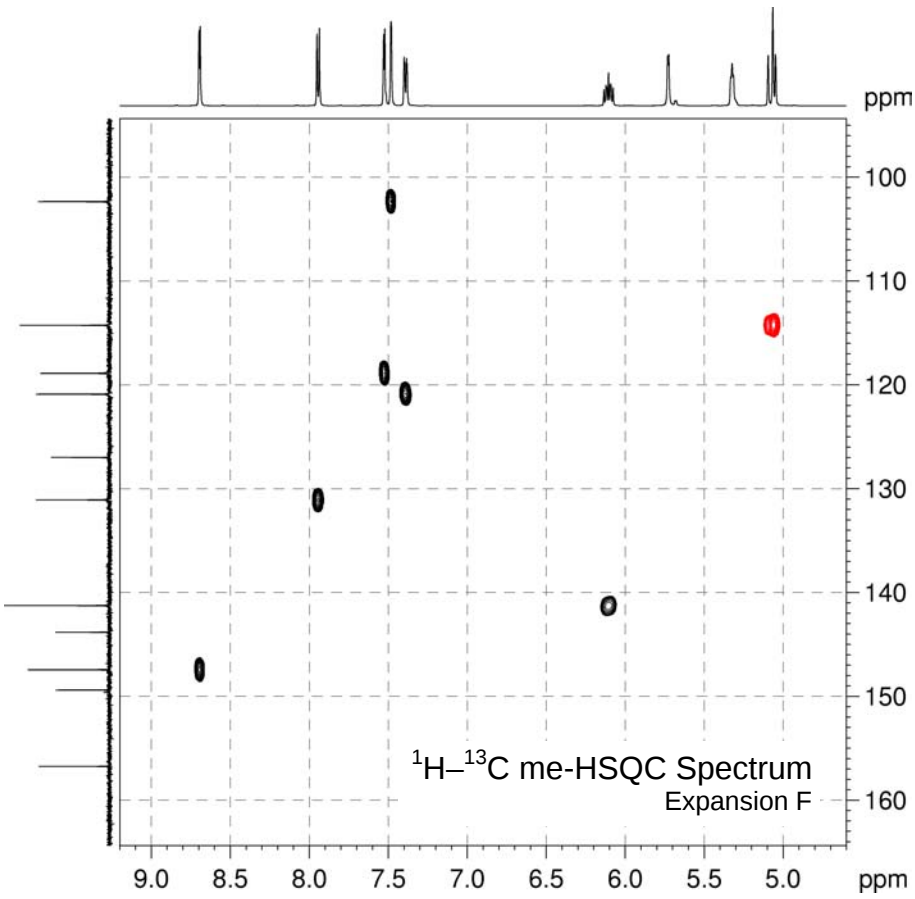
$^{1}H–^{1}H$ COSY Spectrum
Expansion C

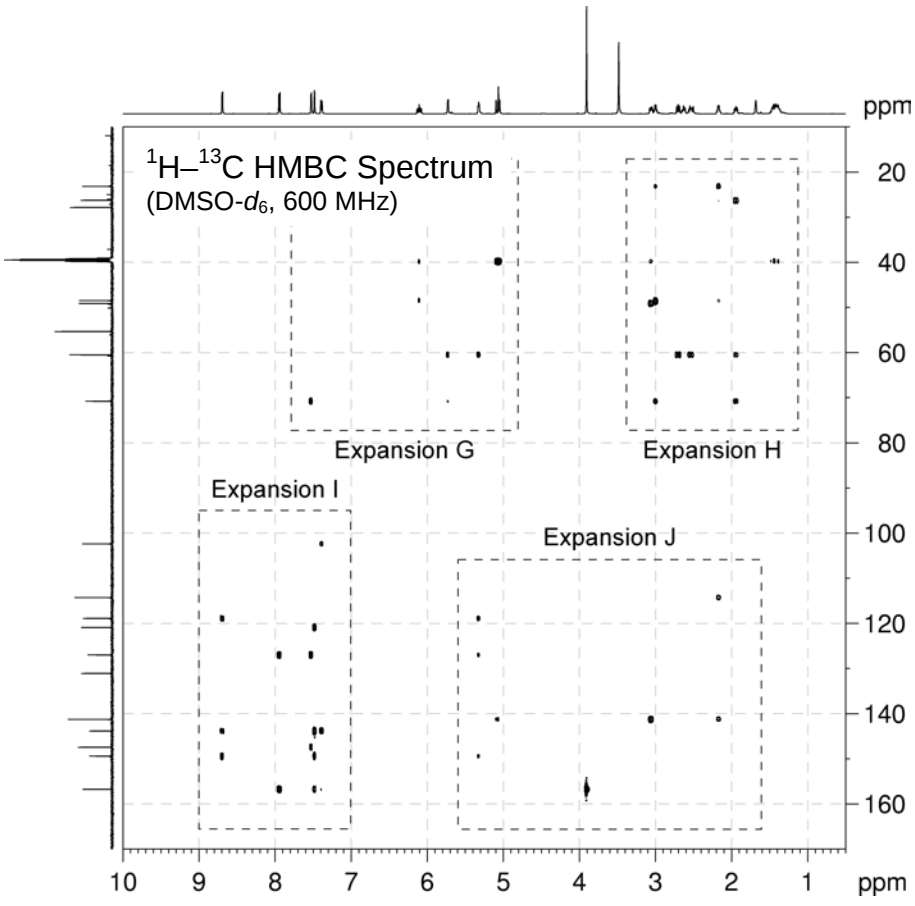


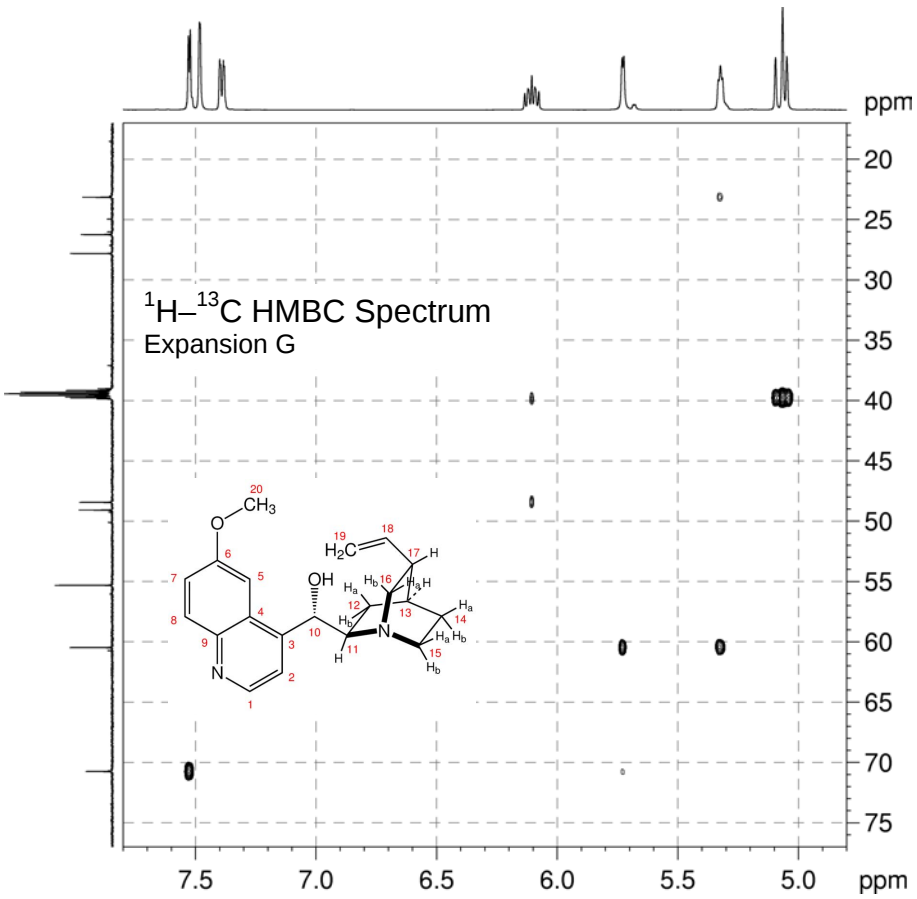
$^{1}H–^{1}H$ COSY Spectrum
Expansion D


^{1}H–^{13}C me-HSQC Spectrum
(DMSO-d_6, 600 MHz)
Expansion E
Expansion F
ppm
20
40
60
80
100
120
140
160
10
9
8
7
6
5
4
3
2
1
ppm

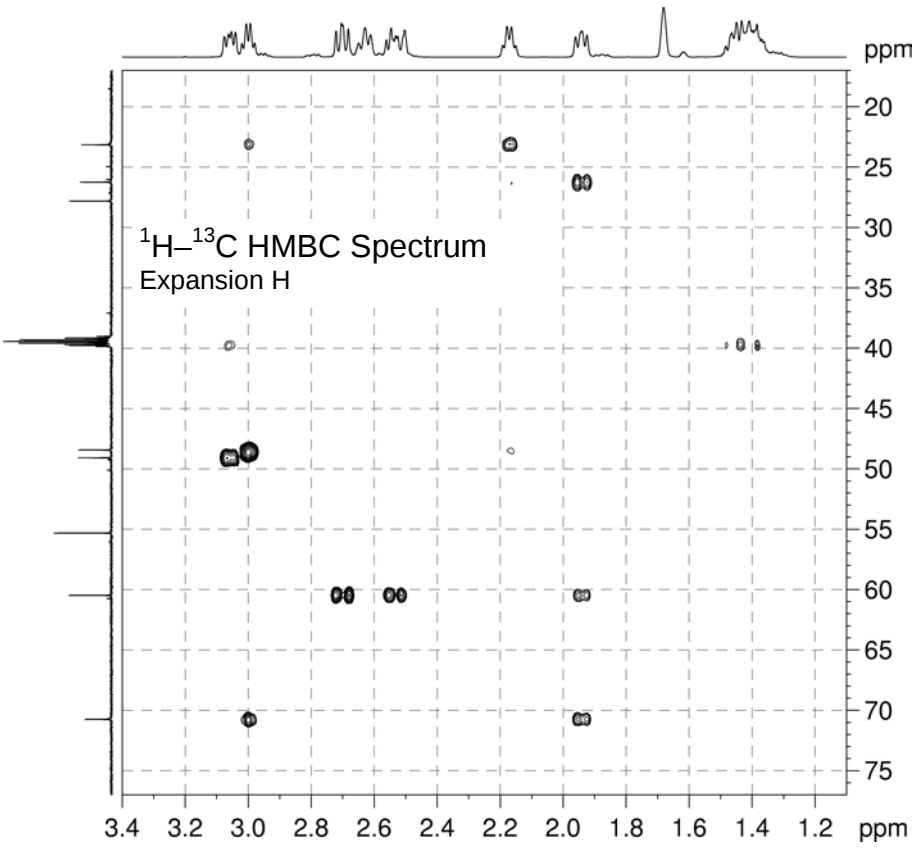

^{1}H–^{13}C me-HSQC Spectrum
Expansion E
ppm
20
25
30
35
40
45
50
55
60
65
70
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm


ppm
100
110
120
130
140
150
160
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
ppm
^{1}H–^{13}C me-HSQC Spectrum
Expansion F

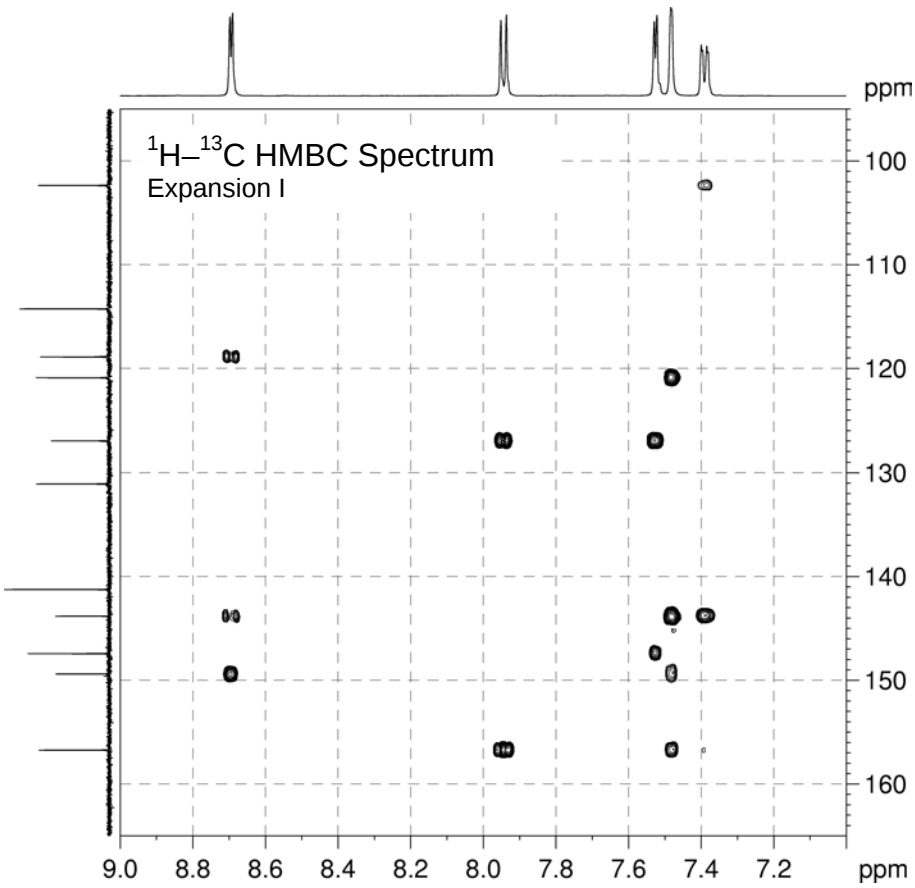

ppm
^{1}H–^{13}C HMBC Spectrum
(DMSO-d_6, 600 MHz)
20
40
60
80
100
120
140
160
Expansion G
Expansion H
Expansion I
Expansion J
10
9
8
7
6
5
4
3
2
1
ppm

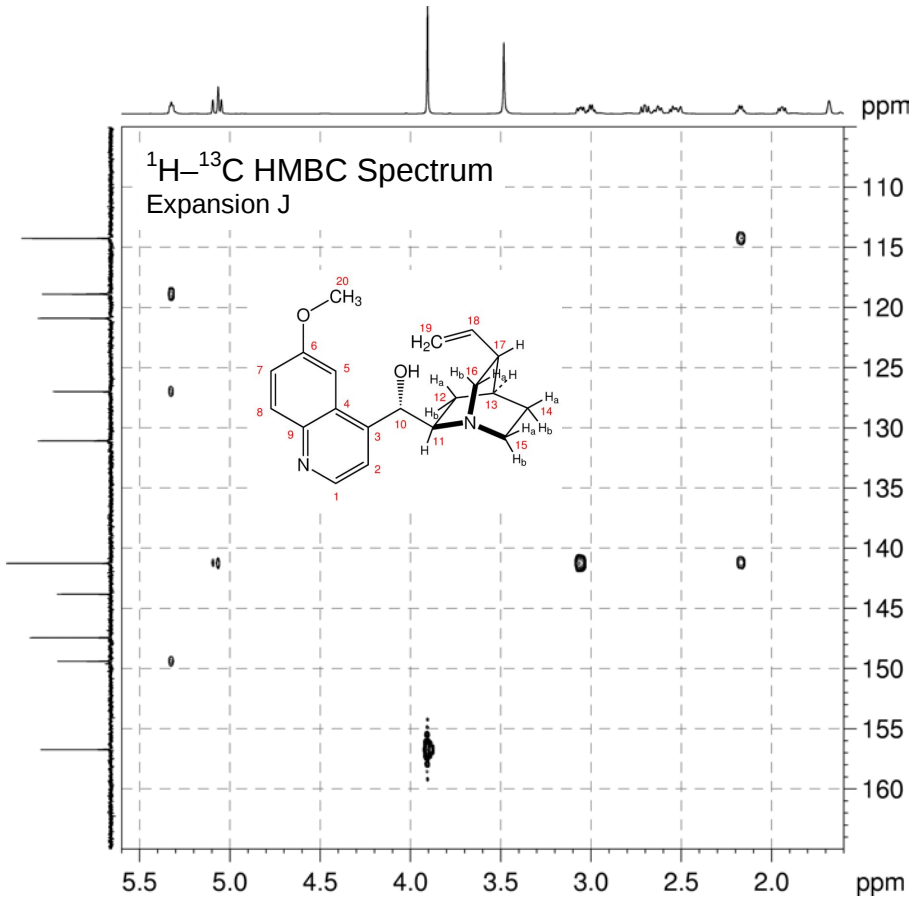


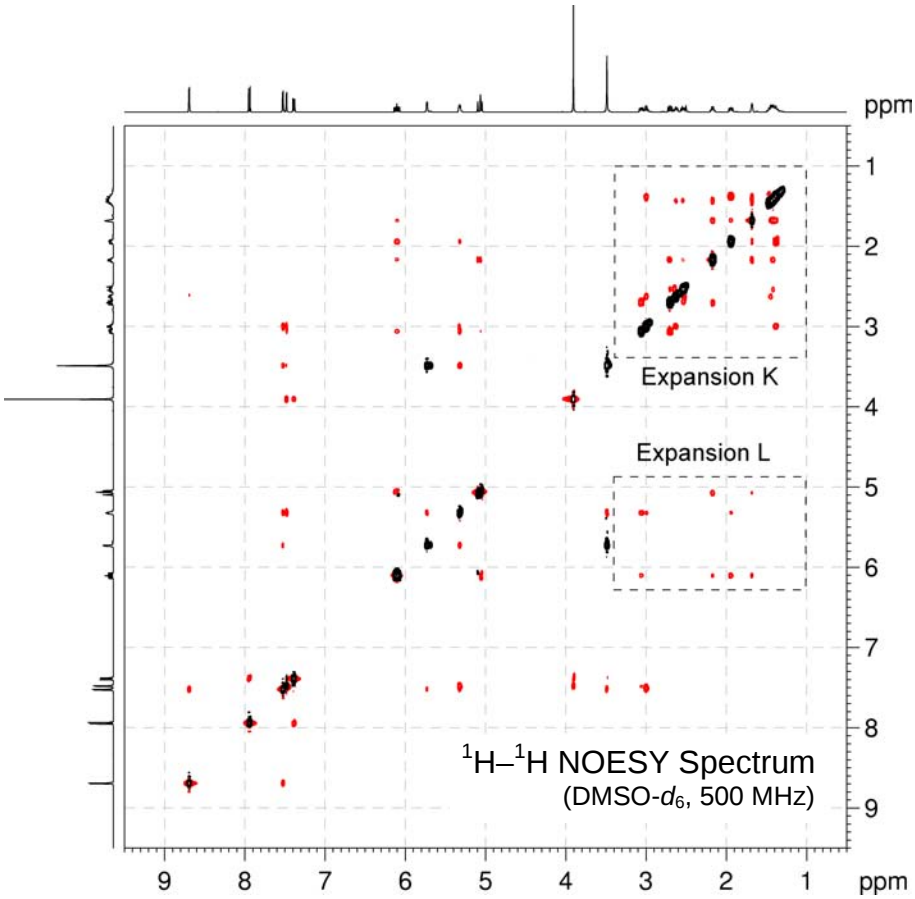
^{1}H–^{13}C HMBC Spectrum
Expansion G

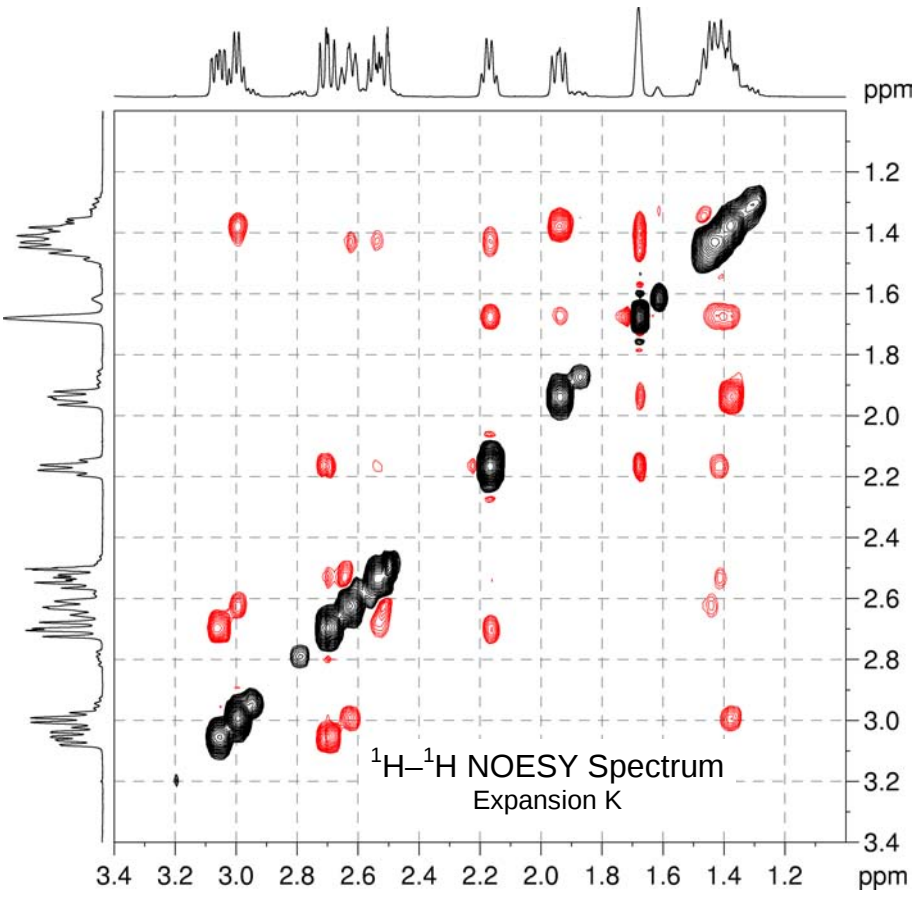


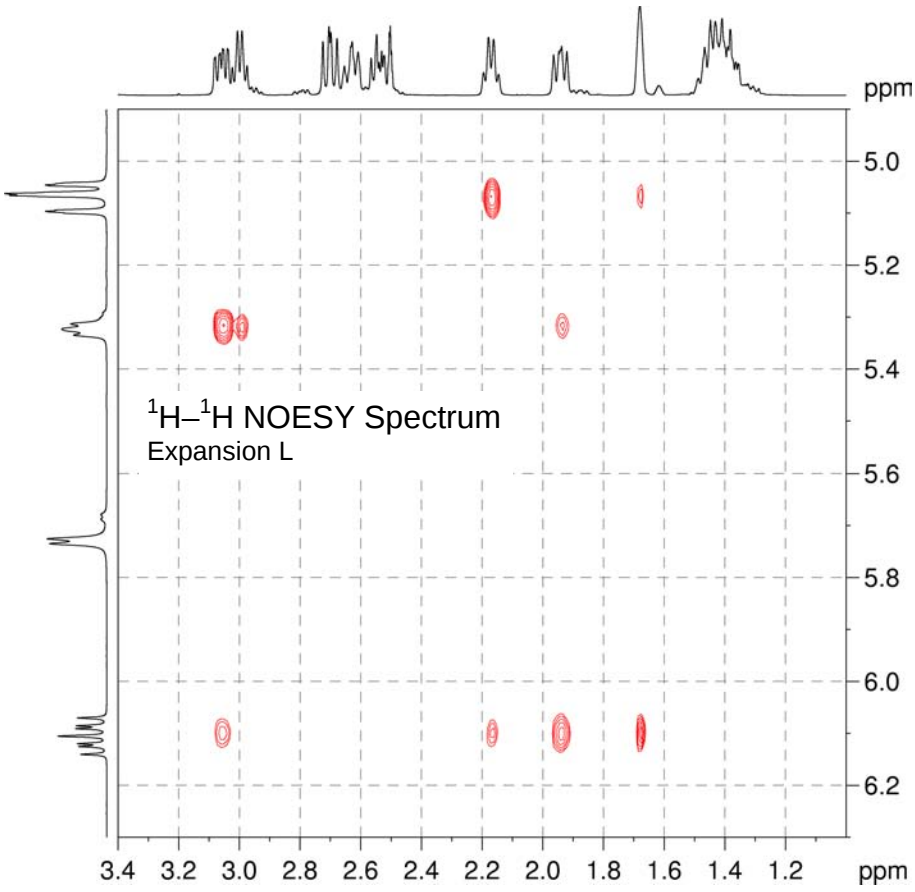
^{1}H–^{13}C HMBC Spectrum
Expansion H


ppm
^{1}H–^{13}C HMBC Spectrum
Expansion I
100
110
120
130
140
150
160
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
ppm

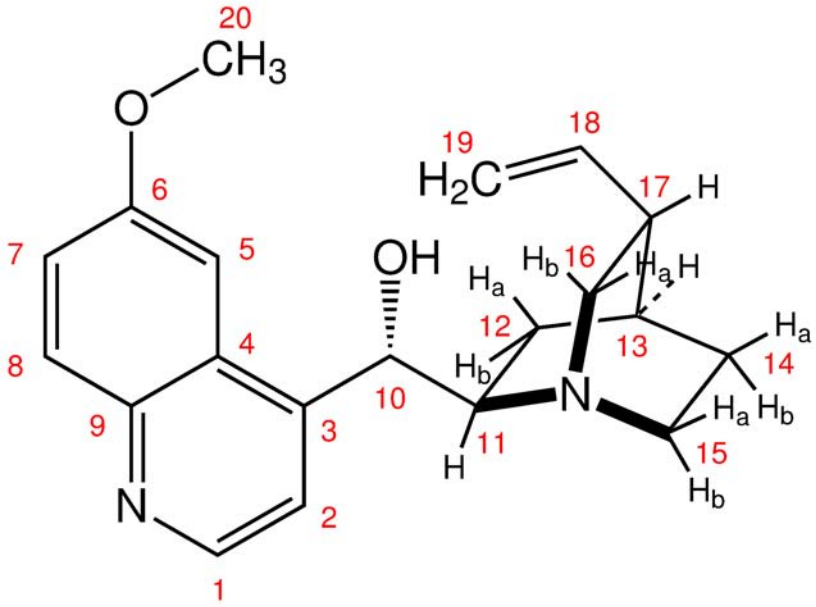

ppm
^{1}H–^{13}C HMBC Spectrum
Expansion J
110
115
120
125
130
135
140
145
150
155
160
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm


ppm
Expansion K
Expansion L
^{1}H–^{1}H NOESY Spectrum
(DMSO-d_6, 500 MHz)
ppm


ppm
^{1}H–^{1}H NOESY Spectrum
Expansion K
ppm



$^{1}H–^{1}H$ NOESY Spectrum
Expansion L



Proton	Chemical Shift (ppm)	Carbon	Chemical Shift (ppm)
H_1		C_1	
H_2		C_2	
		C_3	
		C_4	
H_5		C_5	
		C_6	
H_7		C_7	
H_8		C_8	
		C_9	
H_{10}		C_{10}	
H_{11}		C_{11}	
H_{12a}		C_{12}	
H_{12b}			
H_{13}		C_{13}	
H_{14a}		C_{14}	
H_{14b}			
H_{15a}		C_{15}	
H_{15b}			
H_{16a}		C_{16}	
H_{16b}			
H_{17}		C_{17}	
H_{18}		C_{18}	
H_{19a} H_{19b}		C_{19}	
H_{20}		C_{20}	
OH			