



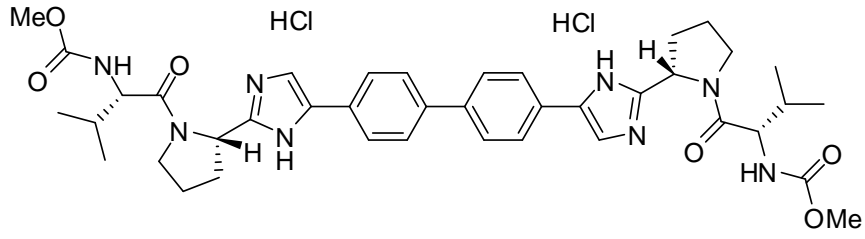
**Australian Government**  
**National Measurement  
Institute**

## 1H AND 13C NMR OF DACLATASVIR.



ORGANISATION: NATIONAL MEASUREMENT INSTITUTE

# DACLASTVIR



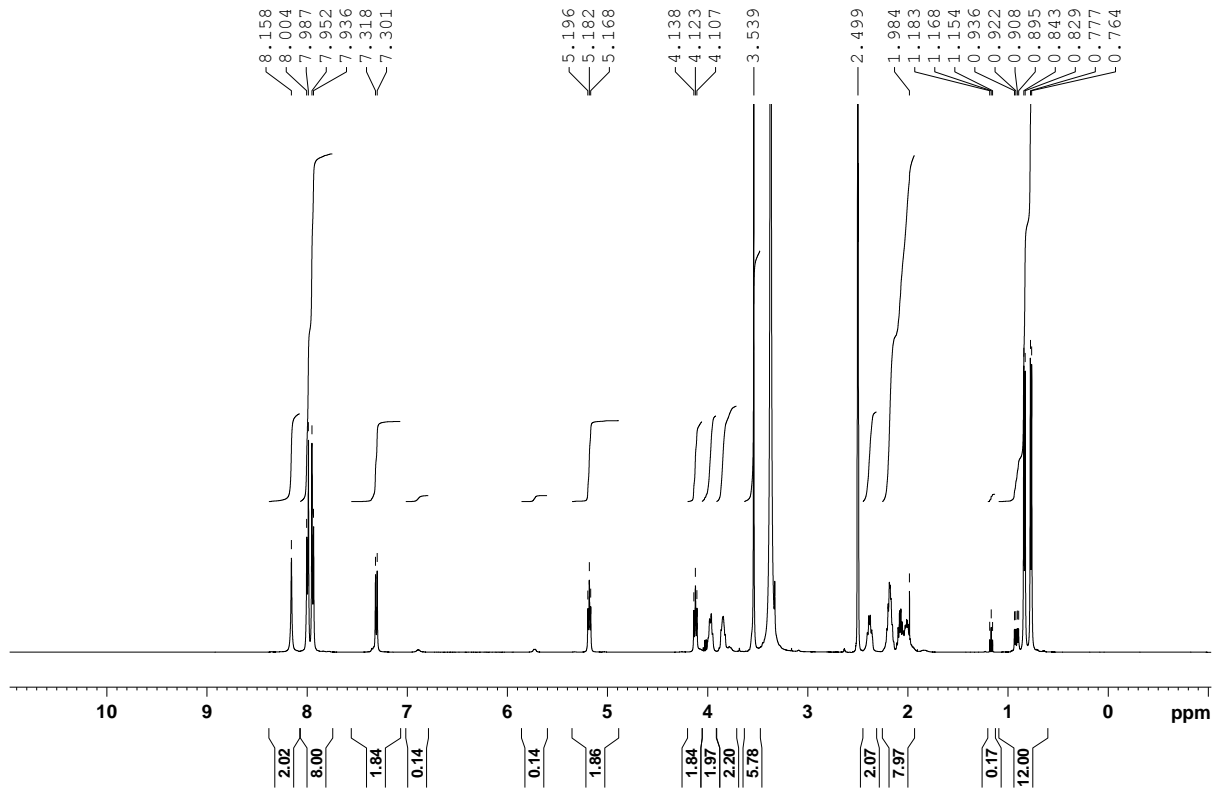
## <sup>1</sup>H NMR in DMSO-d<sub>6</sub>

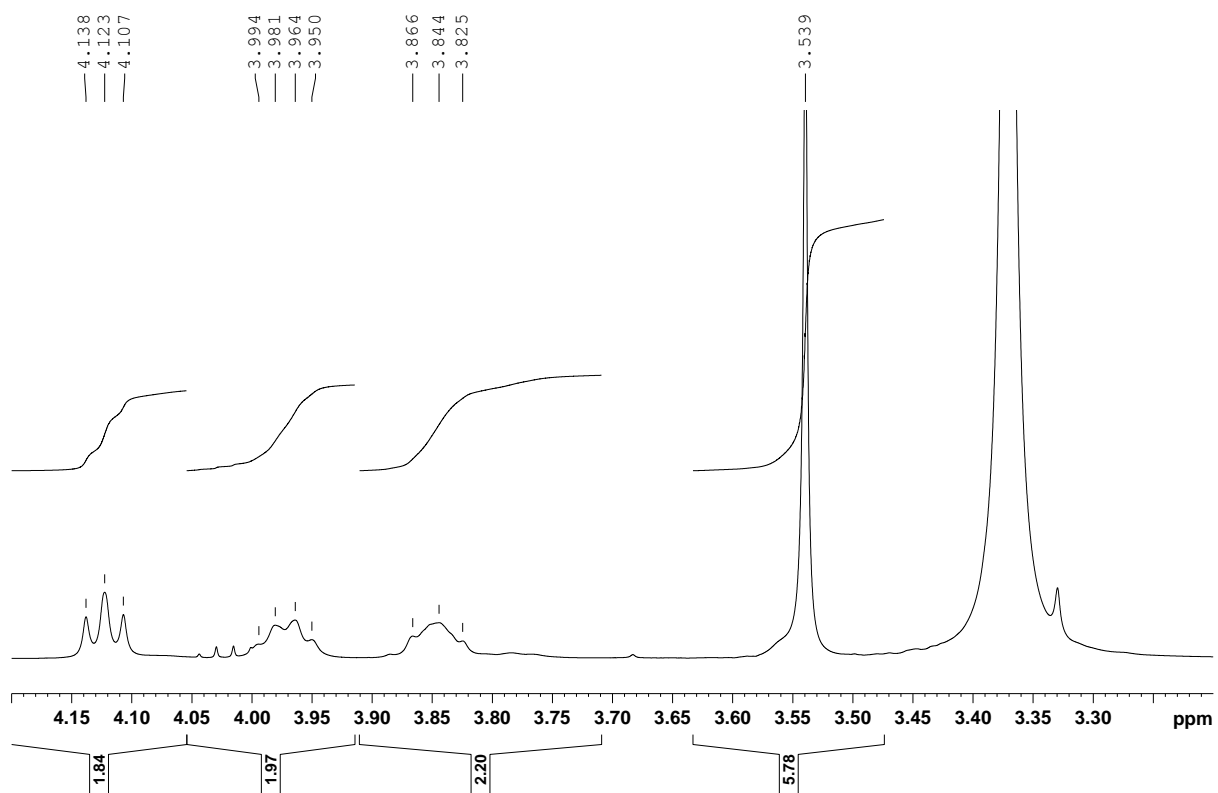
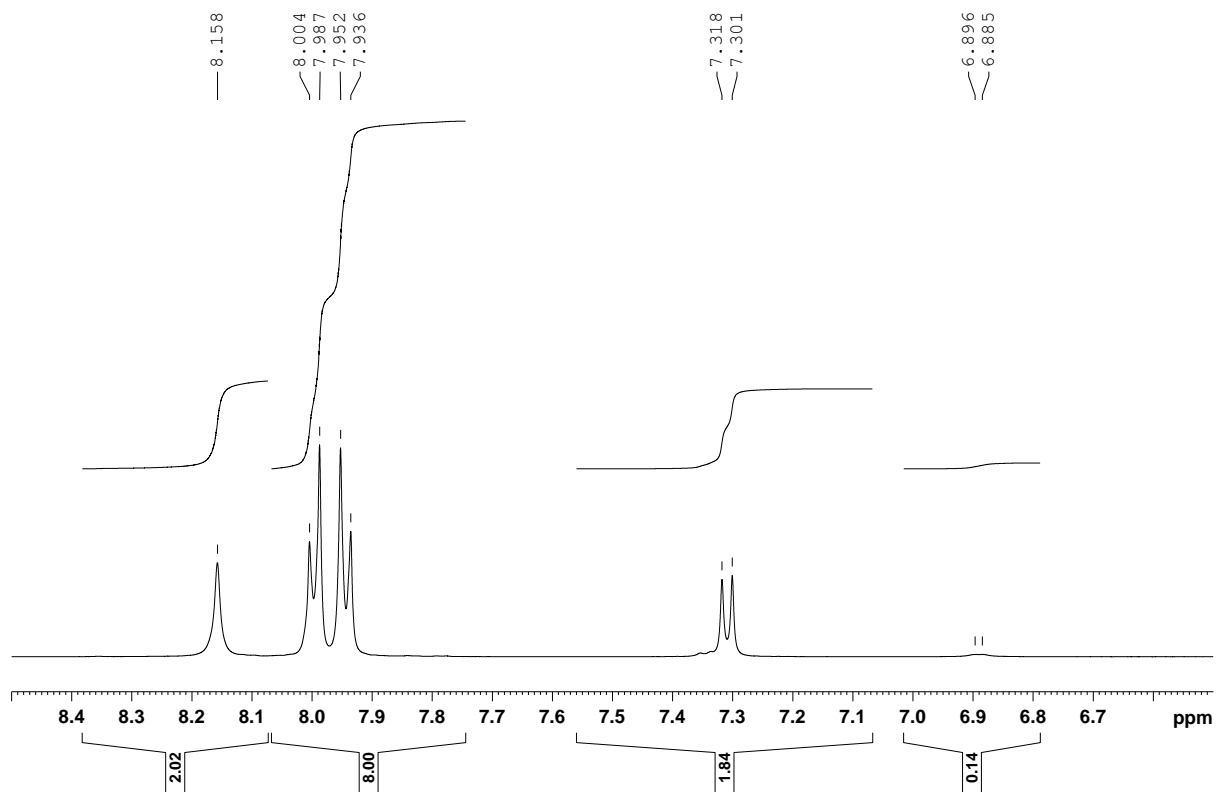
SF01 = 500.13 MHz

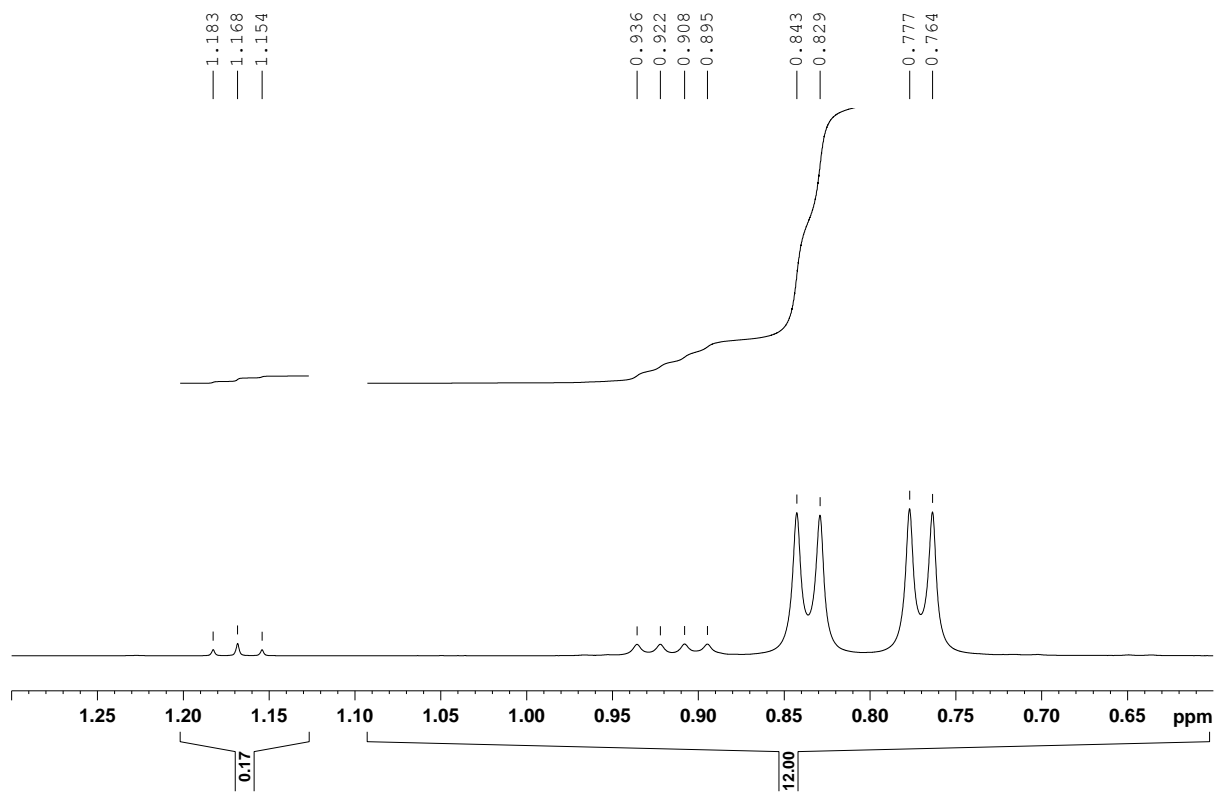
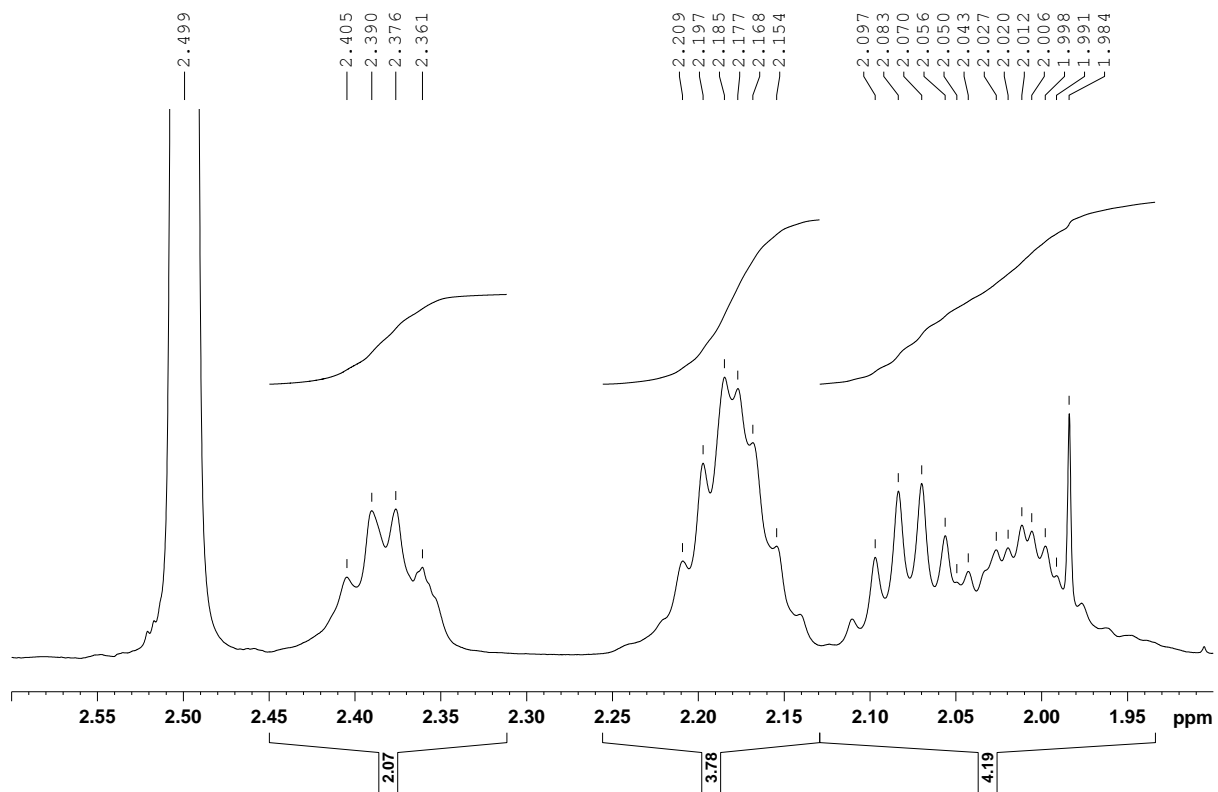
SW = 12.0016 Hz

D1 = 40 seconds

NS = 64 scans







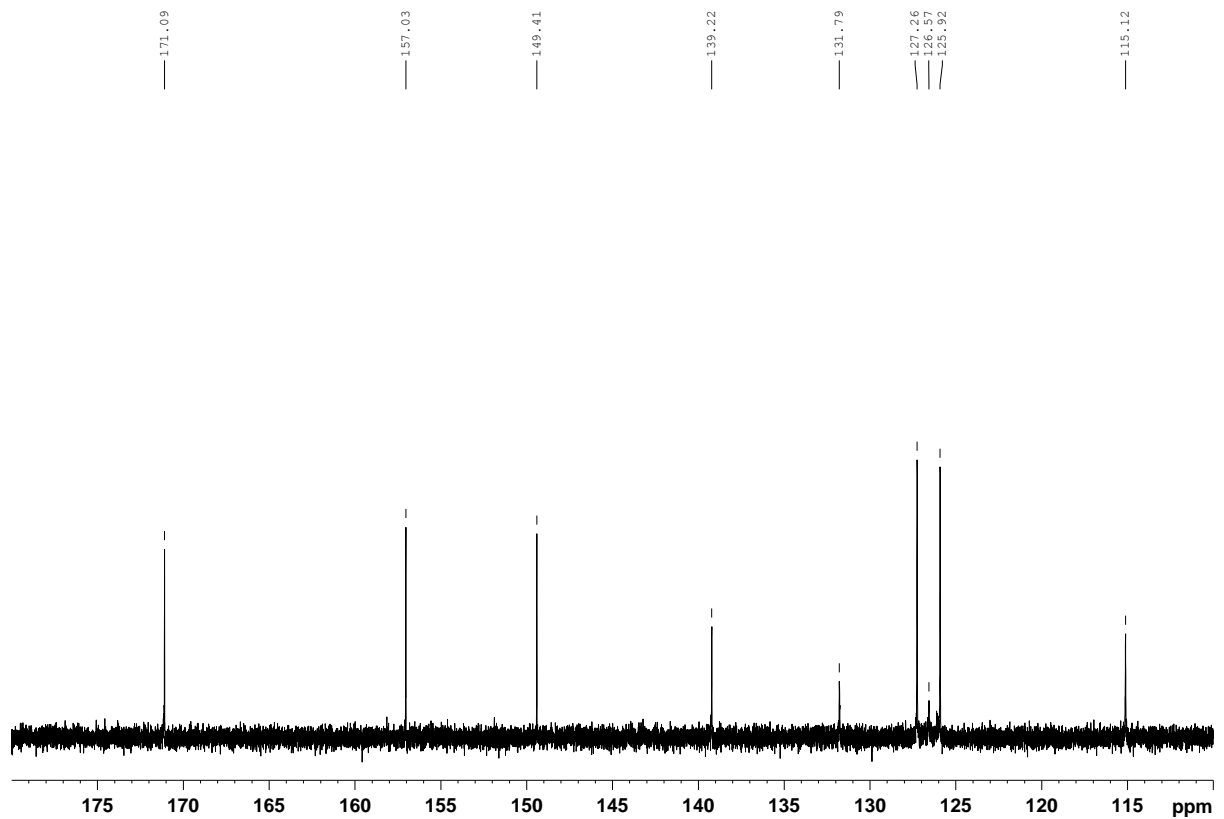
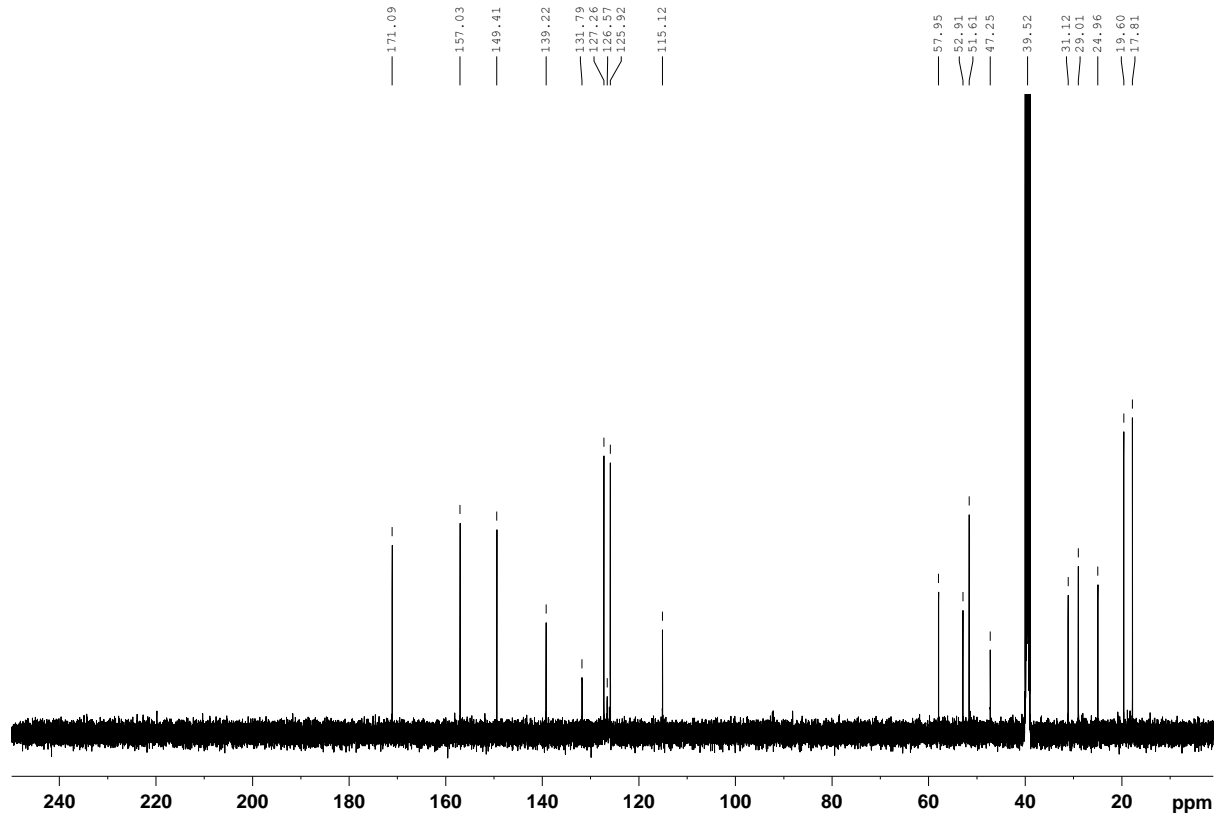
**<sup>13</sup>C NMR in DMSO-d6**

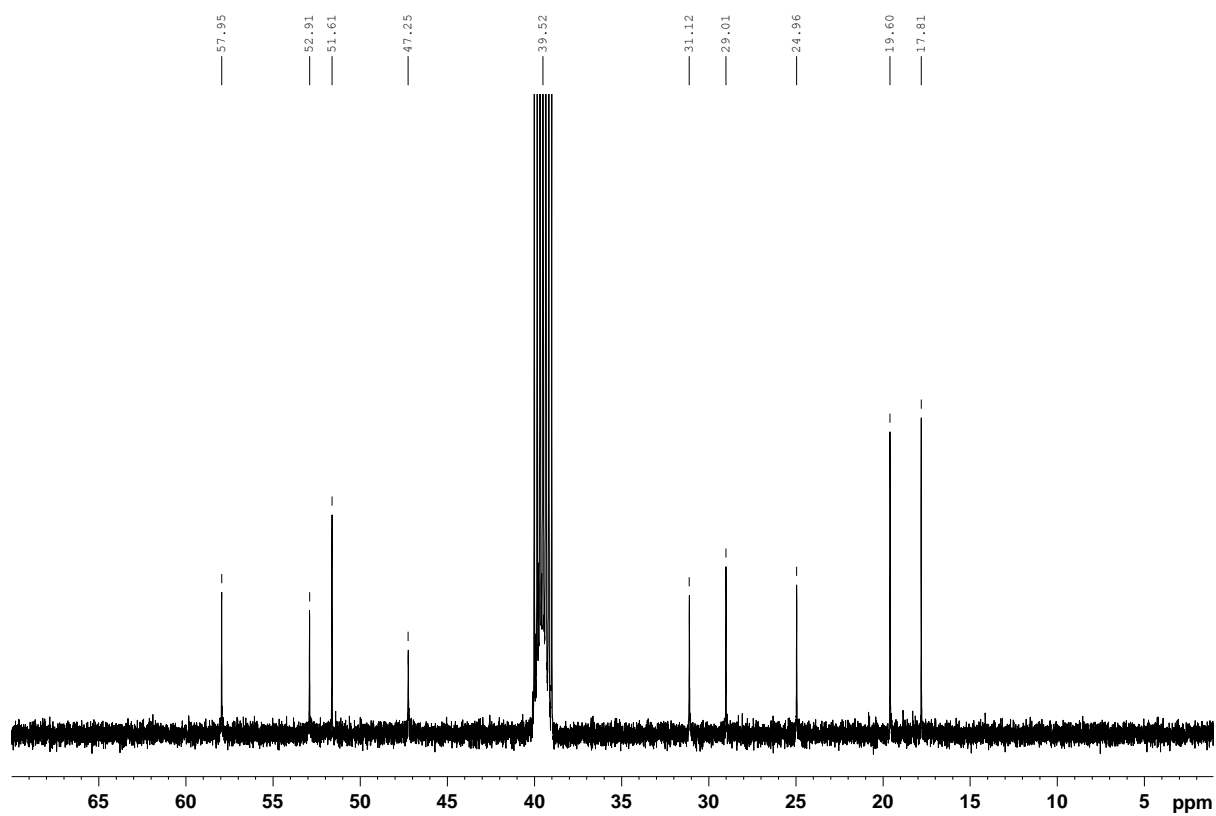
SF01 = 125.77 MHz

SW = 250.55 ppm

D1 = 2 seconds

NS = 1024 scans



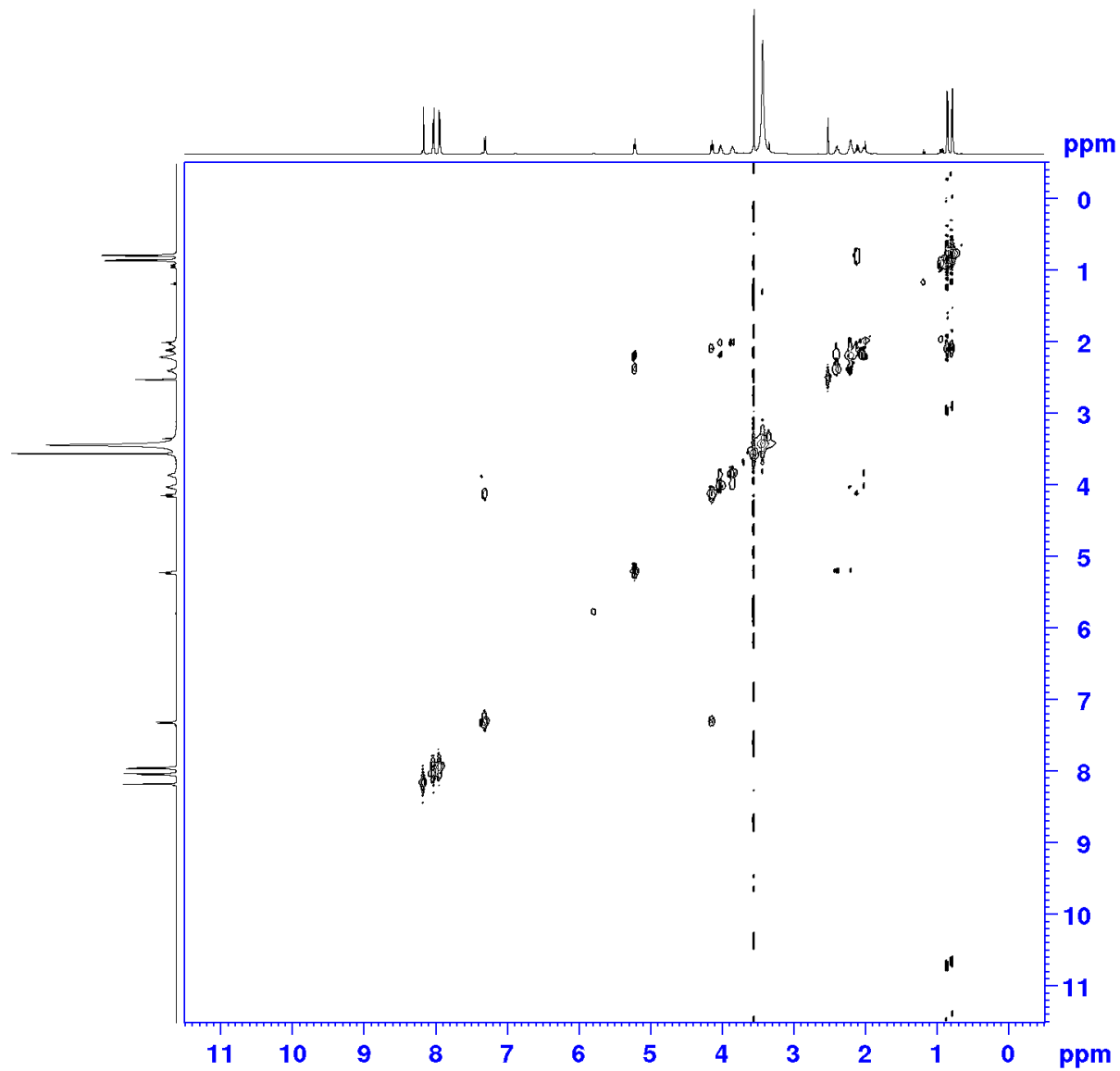


**COSY in DMSO-d6**

SF01 = 500.133 MHz

SW = 12.016 ppm

NS = 4 scans

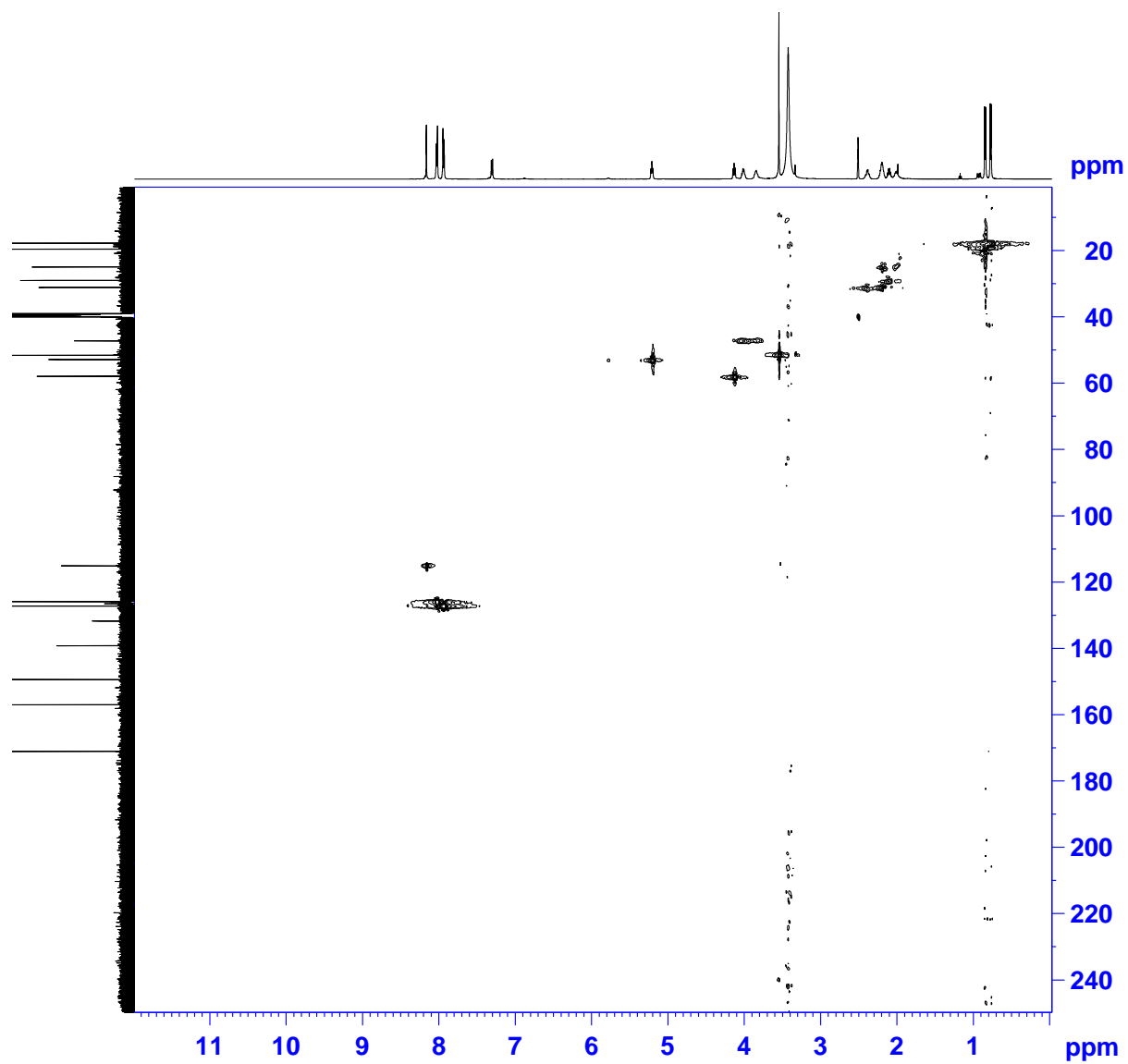


# HSQC in DMSO-d6

<sup>13</sup>C  
SF01 = 125.77 MHz  
SW = 250 ppm

<sup>1</sup>H  
SF01 = 500.13 MHz  
SW = 6685 ppm

NS = 4 scans





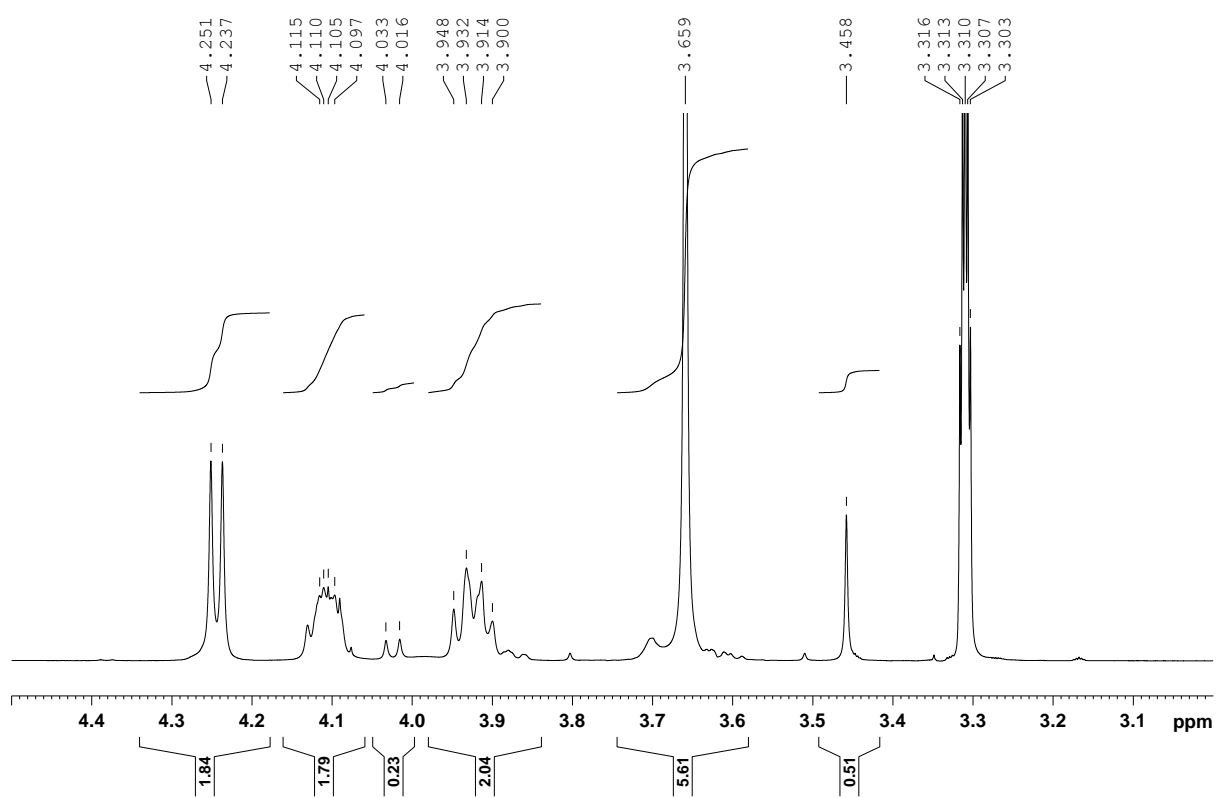
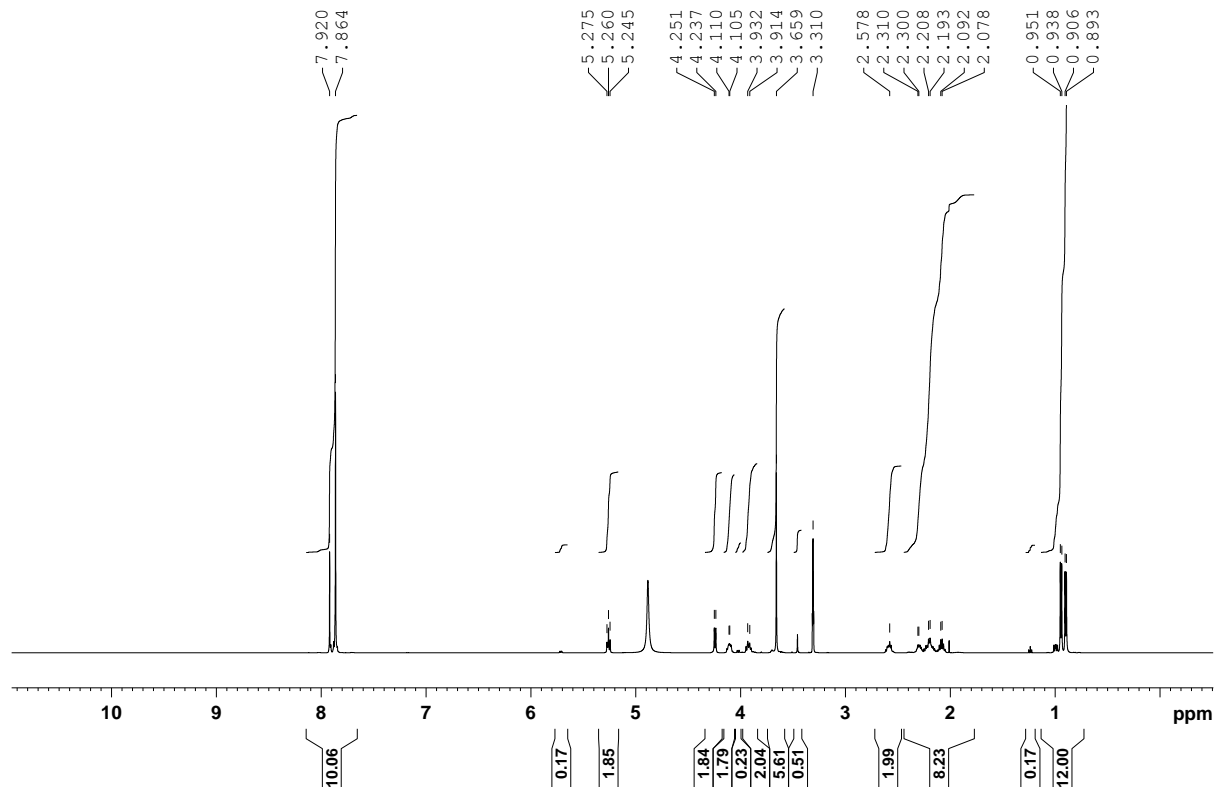
**<sup>1</sup>H NMR in methanol-d4**

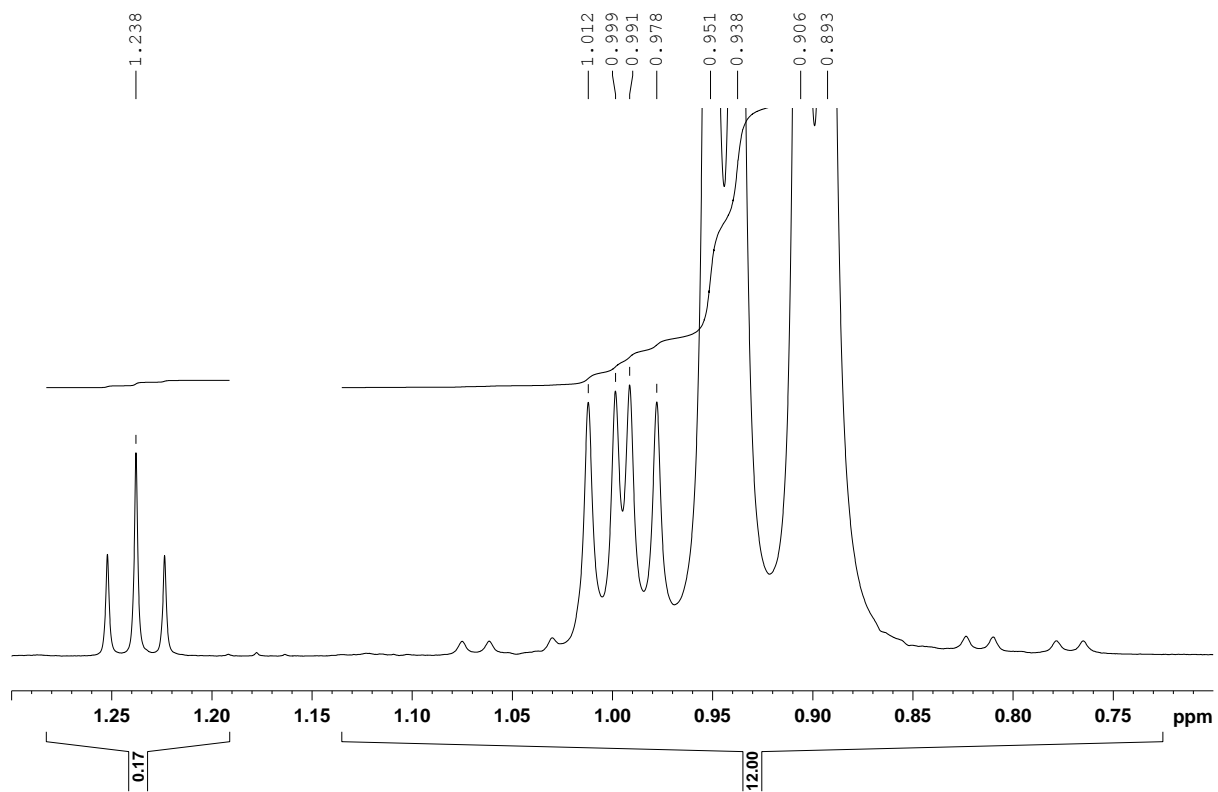
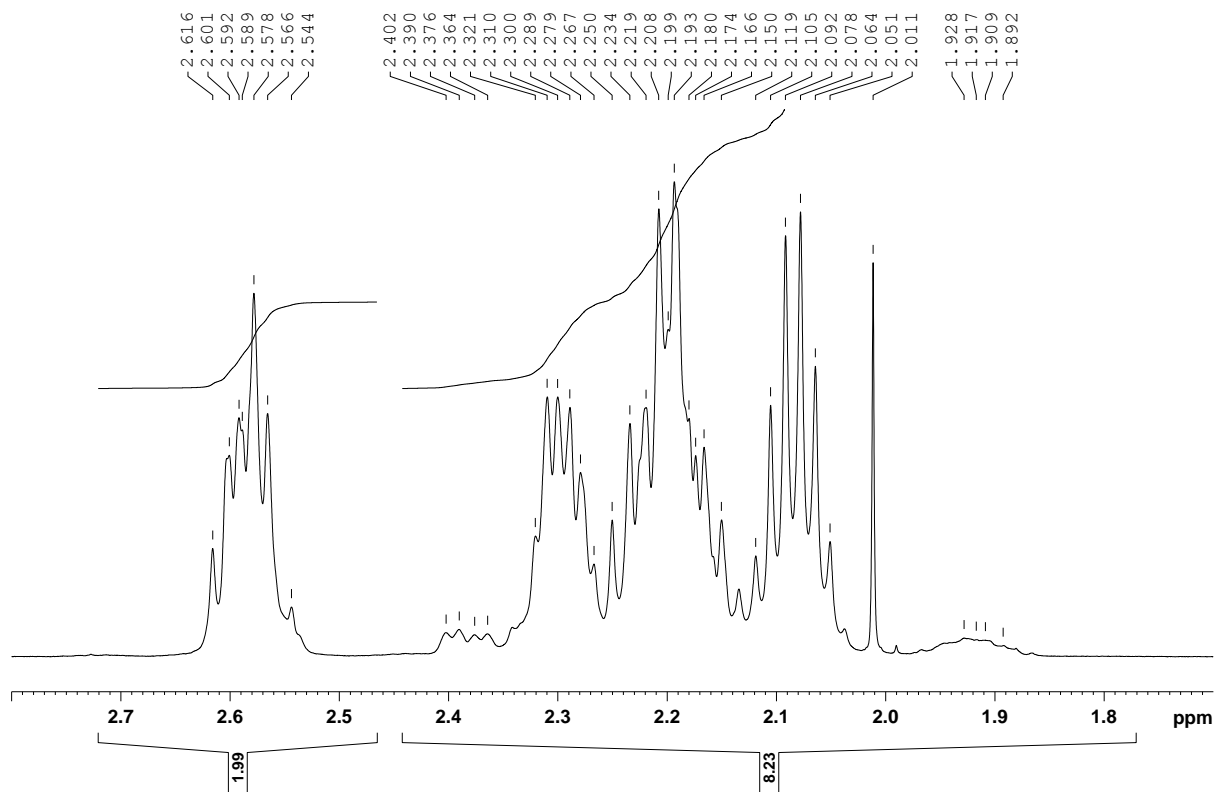
SF01 = 500.13 MHz

SW = 6000 Hz

D1 = 40 seconds

NS = 64 scans





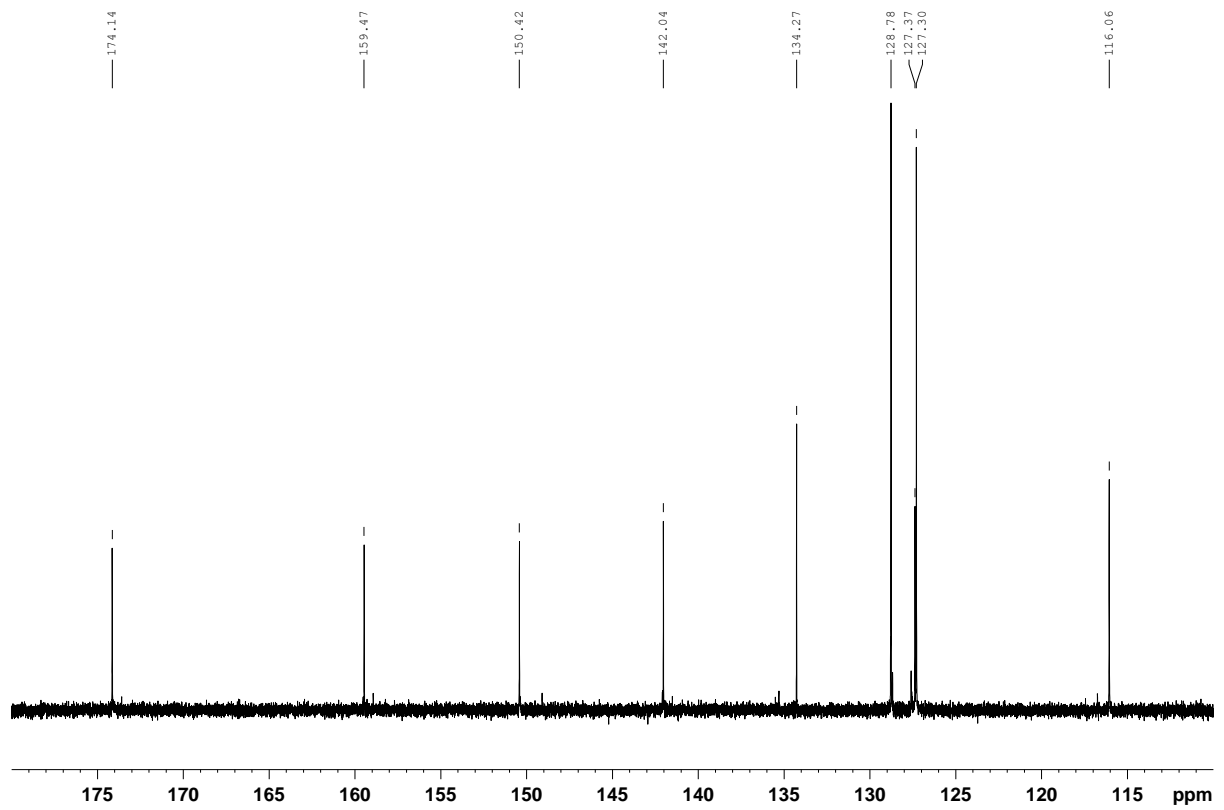
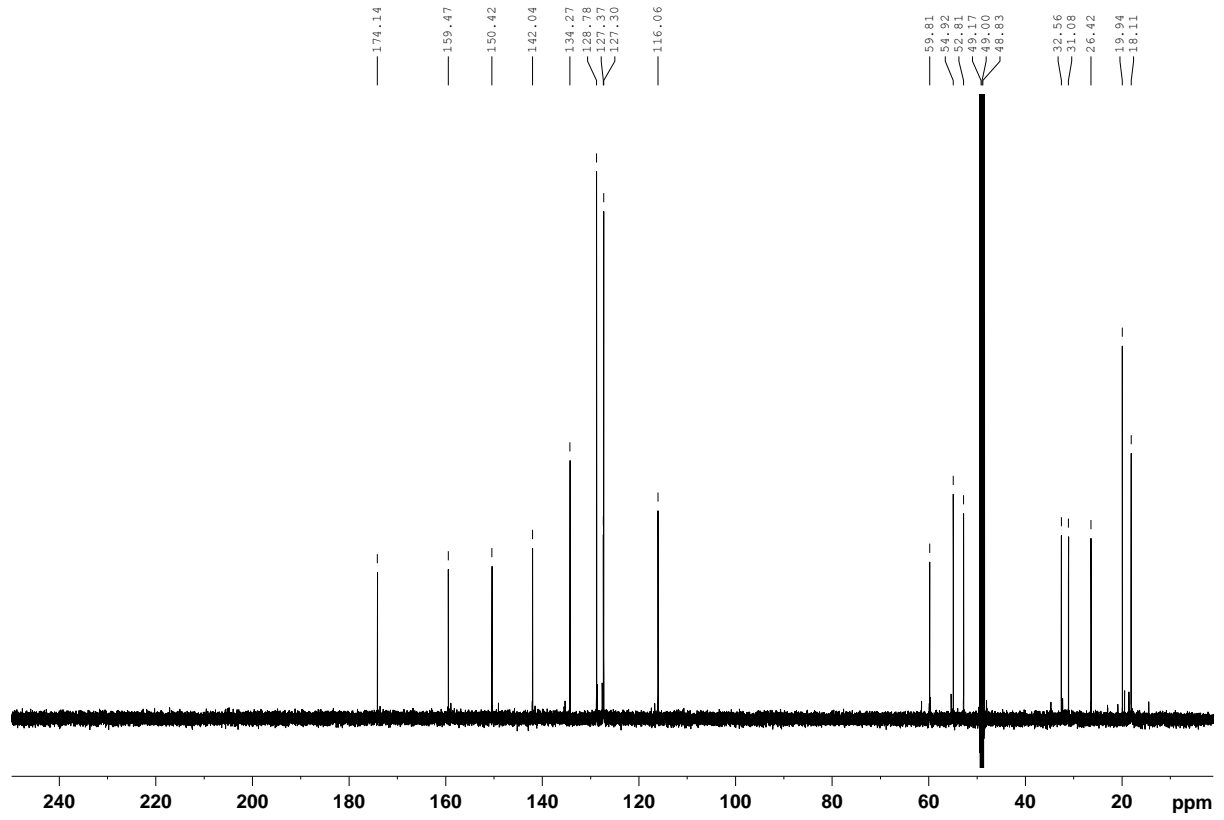
**<sup>13</sup>C NMR in MeOH-d4**

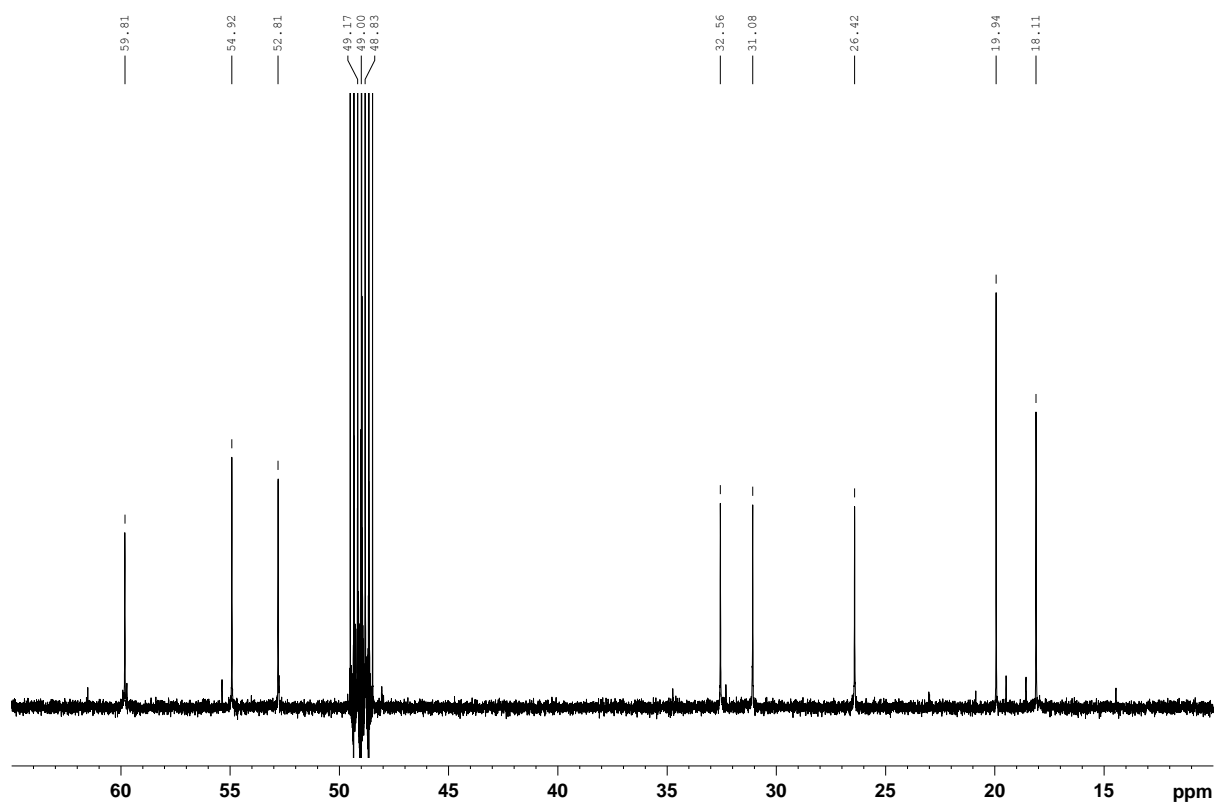
SF01 = 125.77 MHz

SW = 250.55 ppm

D1 = 2 seconds

NS = 1024 scans

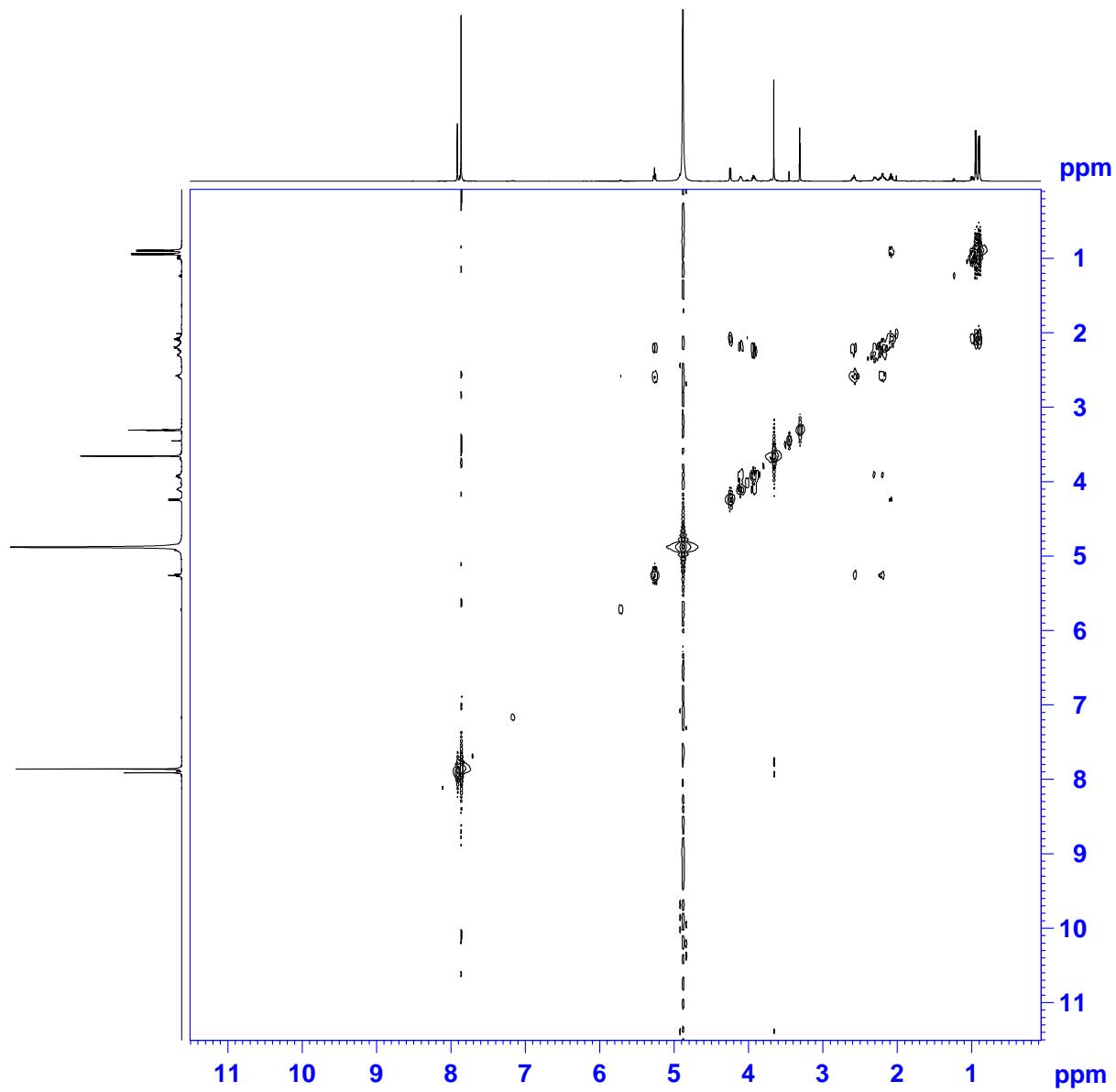




**COSY in MeOH-d4**

SF01 = 500.133 MHz  
SW = 12.016 ppm

NS = 4 scans

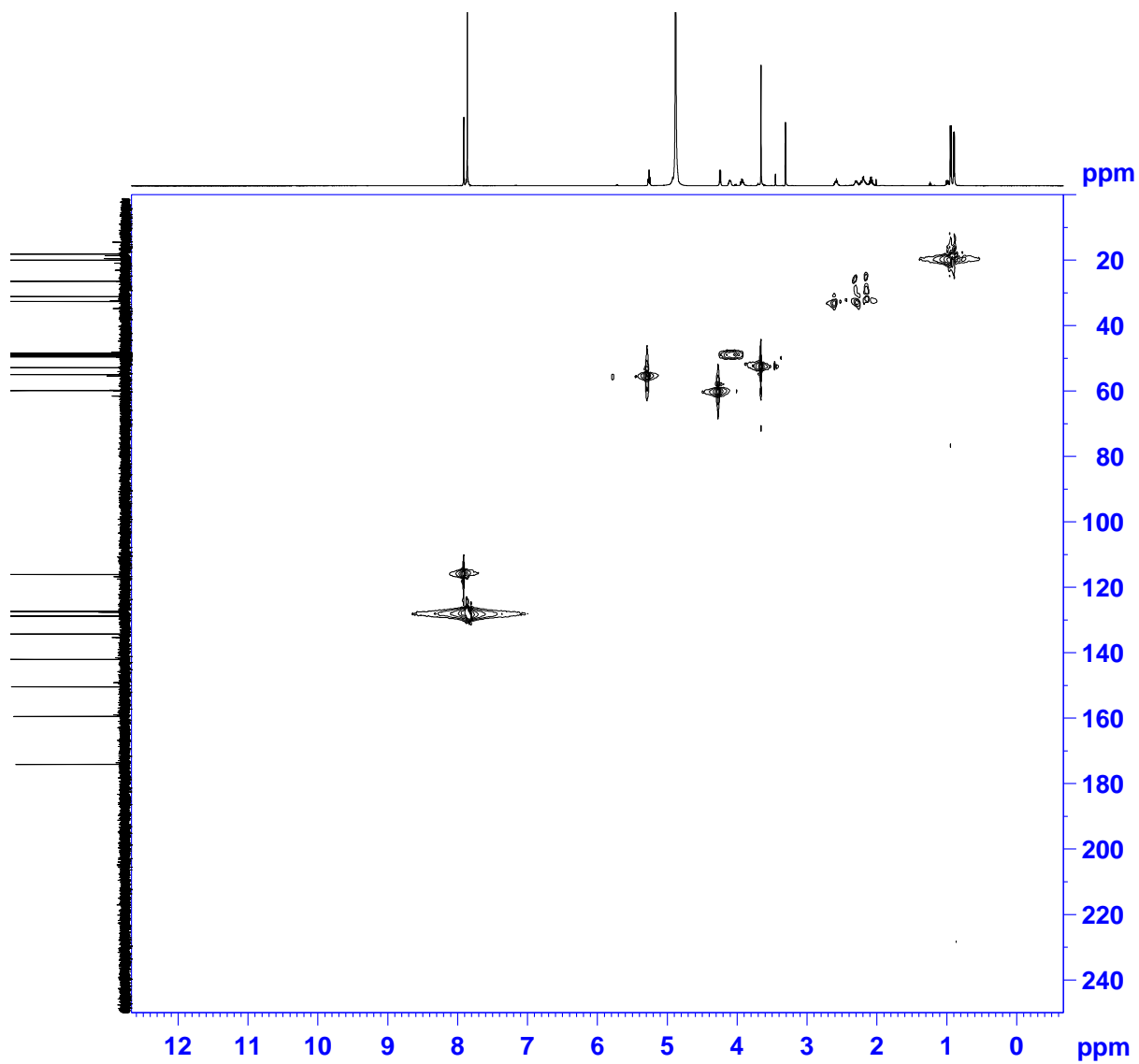


# HSQC in MeOH-d4

<sup>13</sup>C  
SF01 = 125.77 MHz  
SW = 250 ppm

<sup>1</sup>H  
SF01 = 500.13 MHz  
SW = 13.3654 ppm

NS = 4 scans

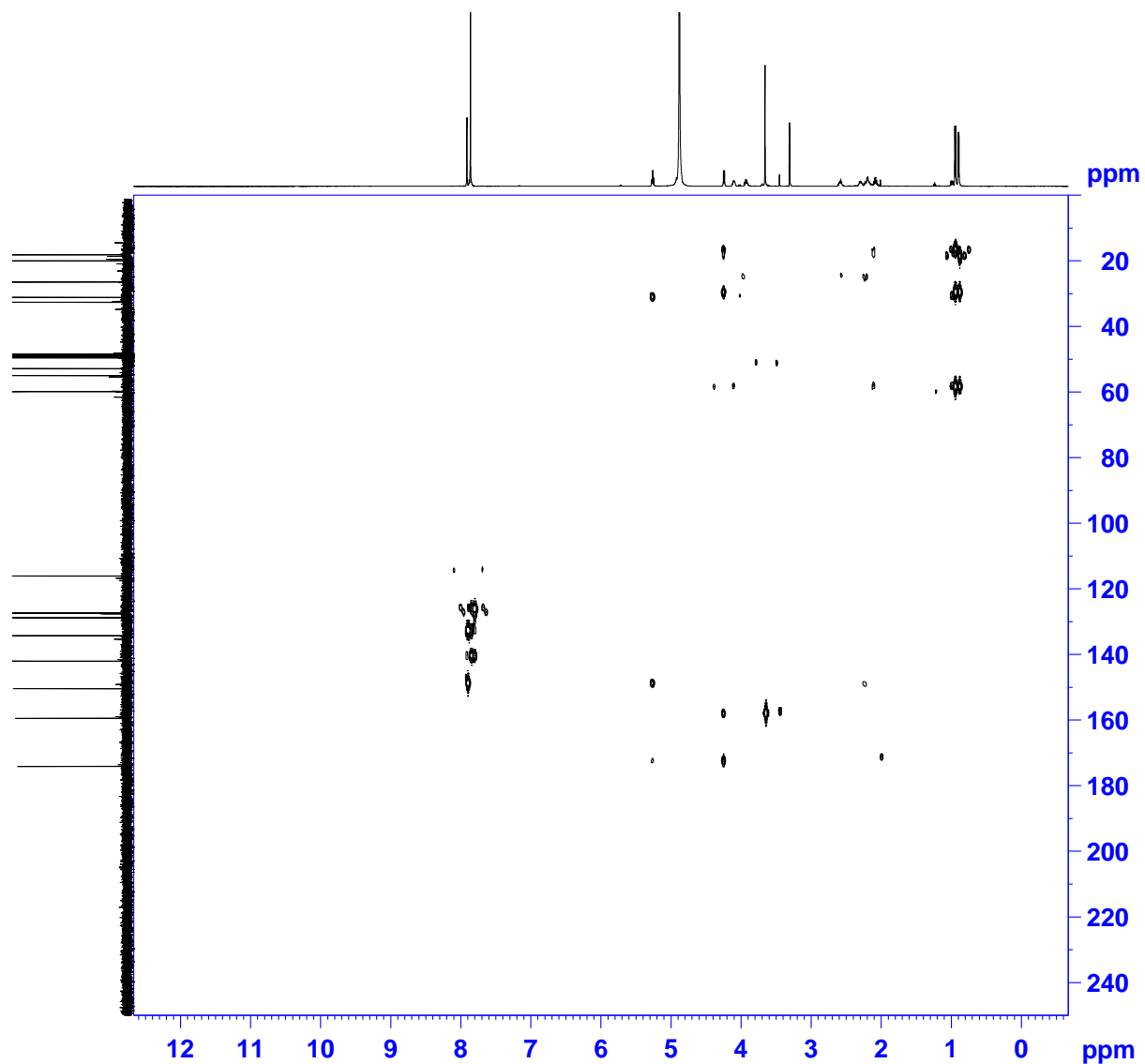


# HMBC in MeOH-d4

<sup>13</sup>C  
SF01 = 125.77 MHz  
SW = 250 ppm

<sup>1</sup>H  
SF01 = 500.13 MHz  
SW = 12.0160 ppm

NS = 8 scans



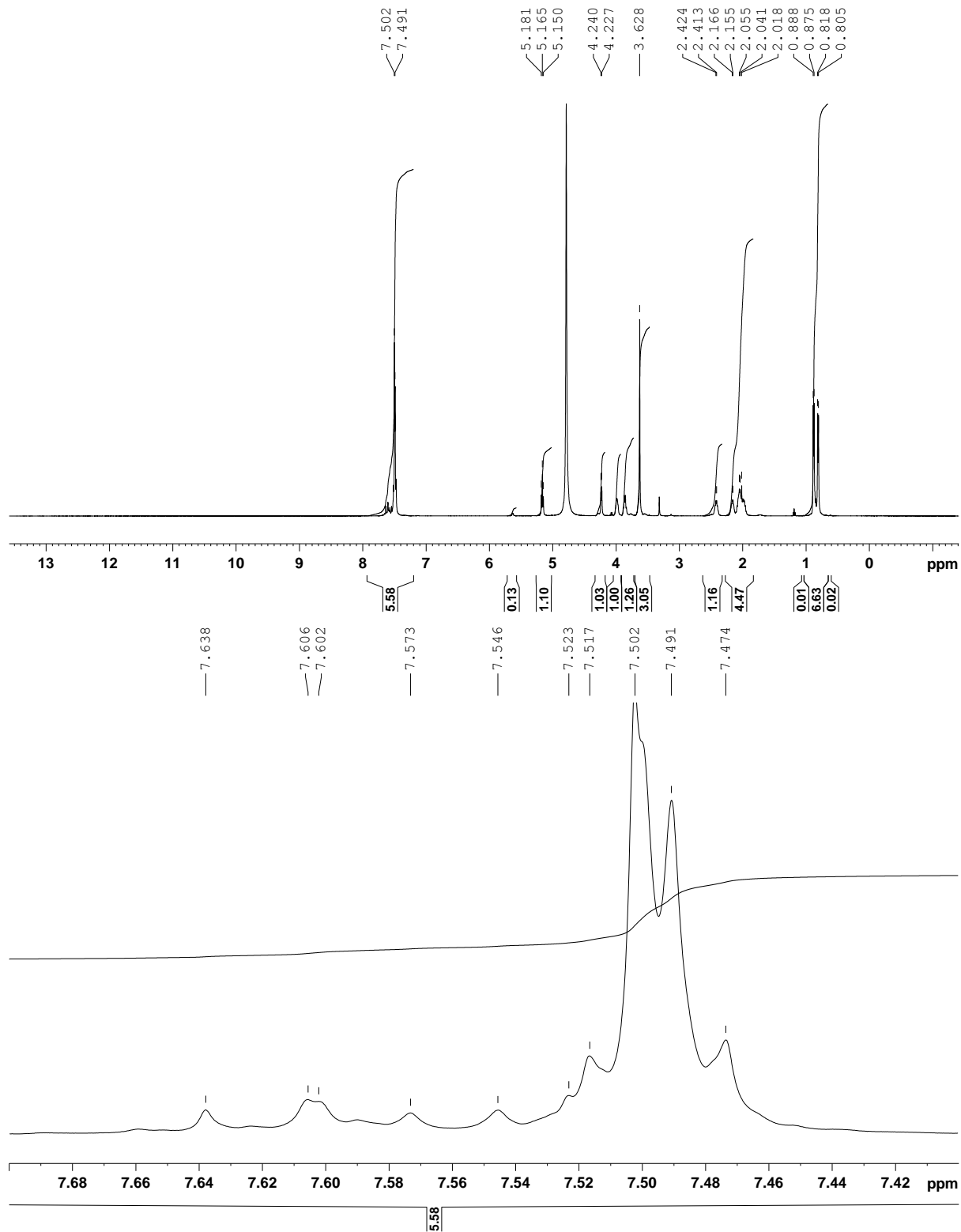
# <sup>1</sup>H NMR in D<sub>2</sub>O

SF01 = 500.13 MHz

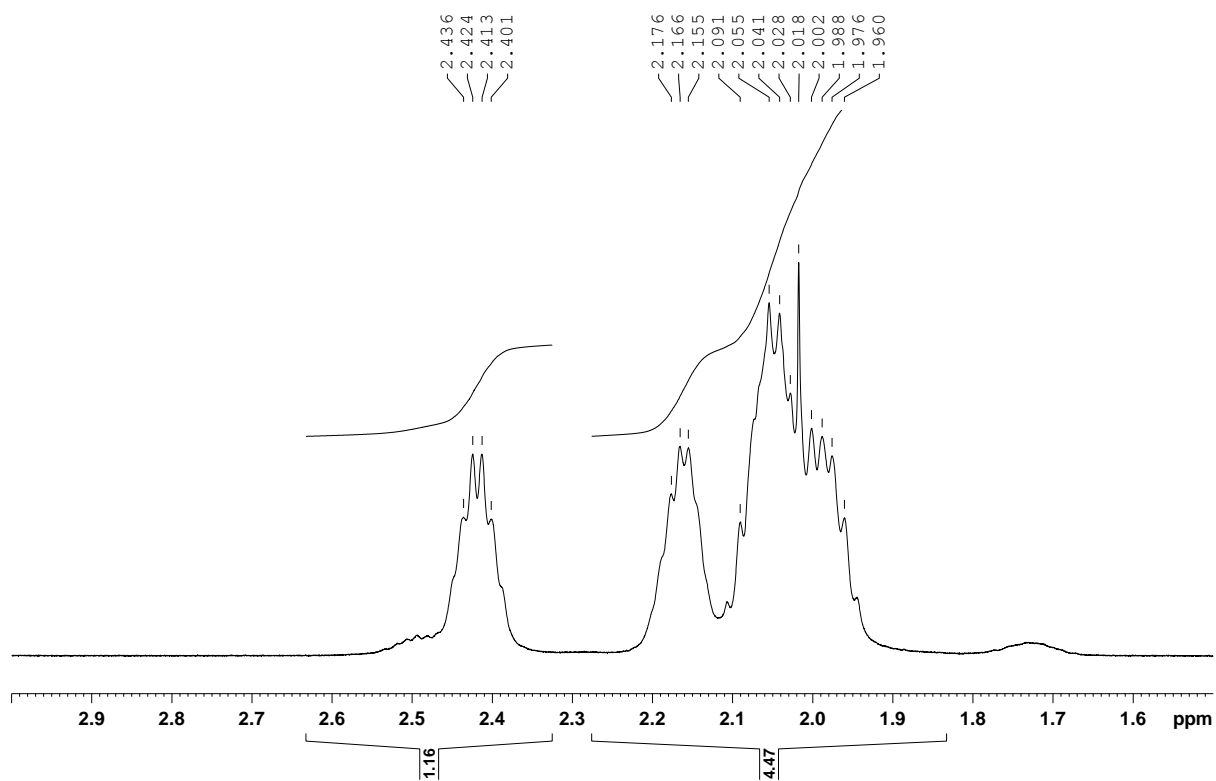
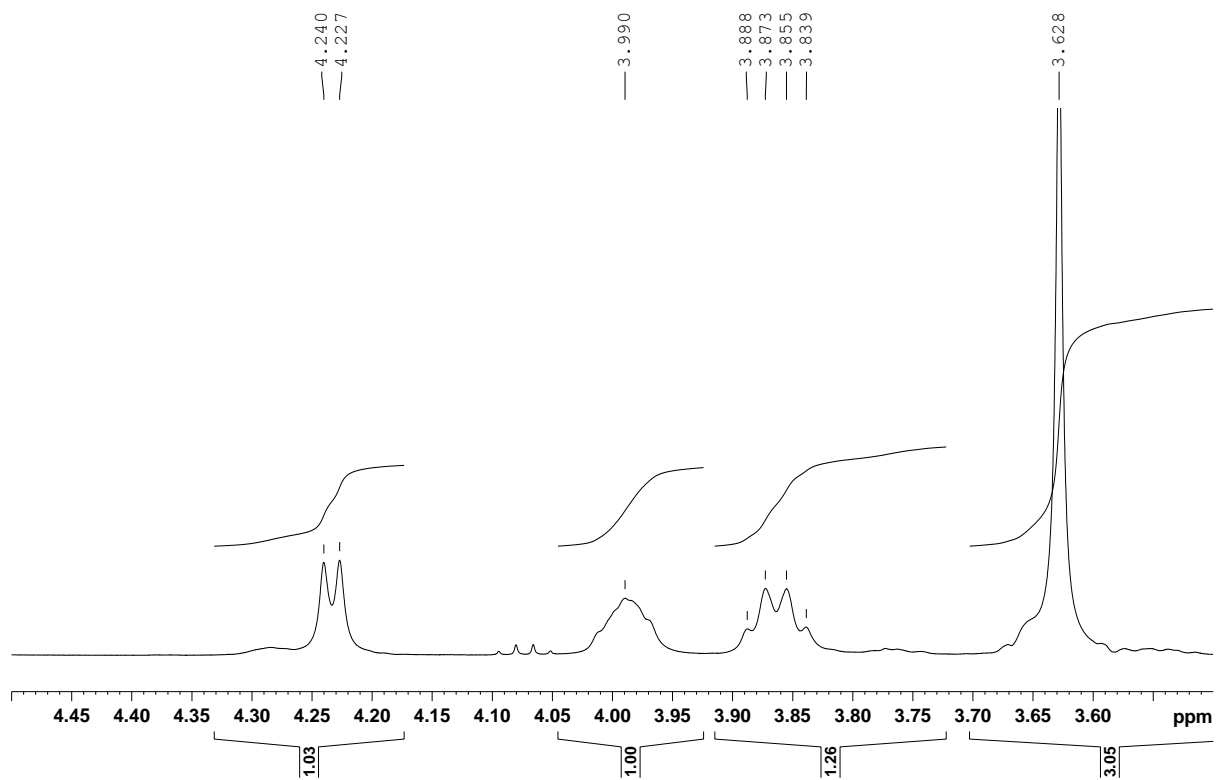
SW = 14.9960 ppm

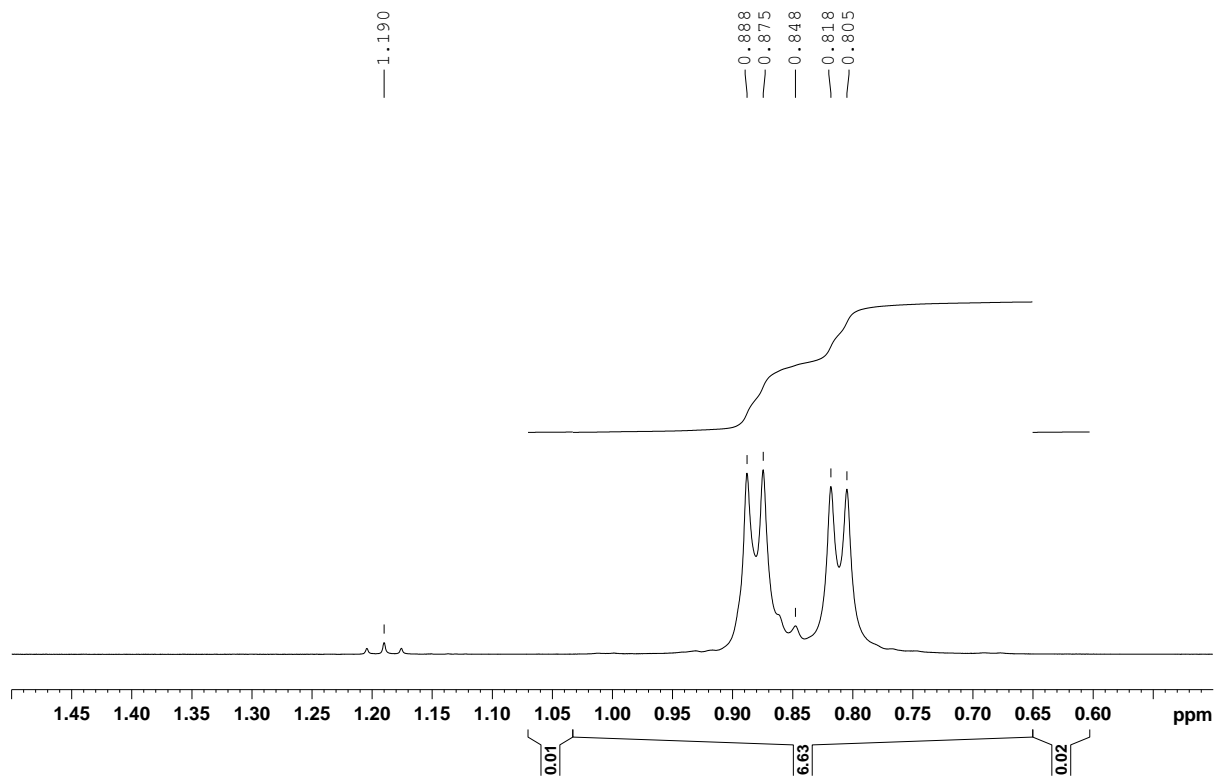
D1 = 5 seconds

NS = 8 scans

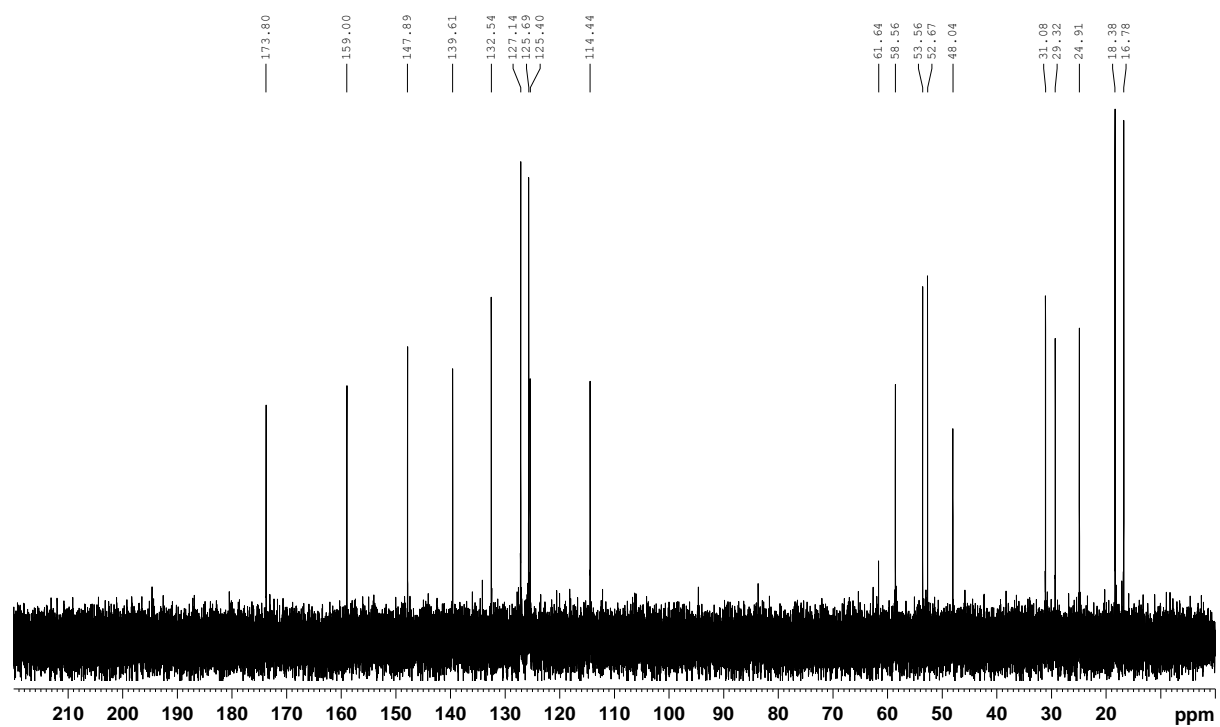


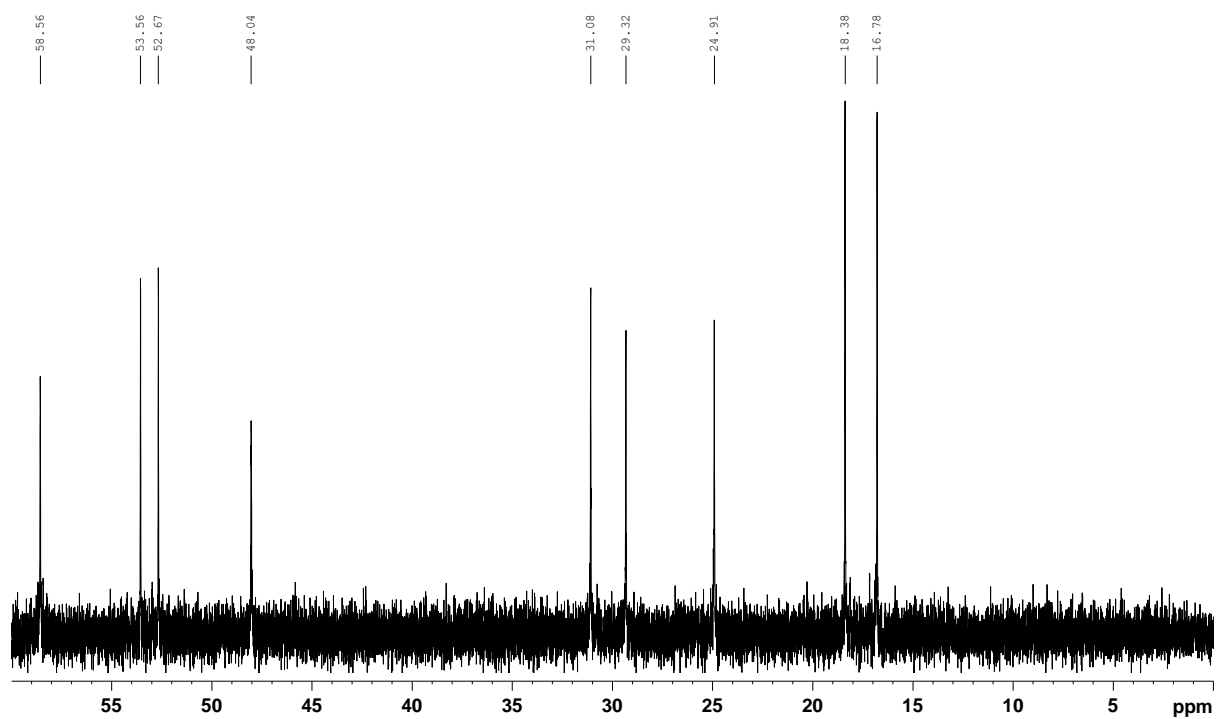
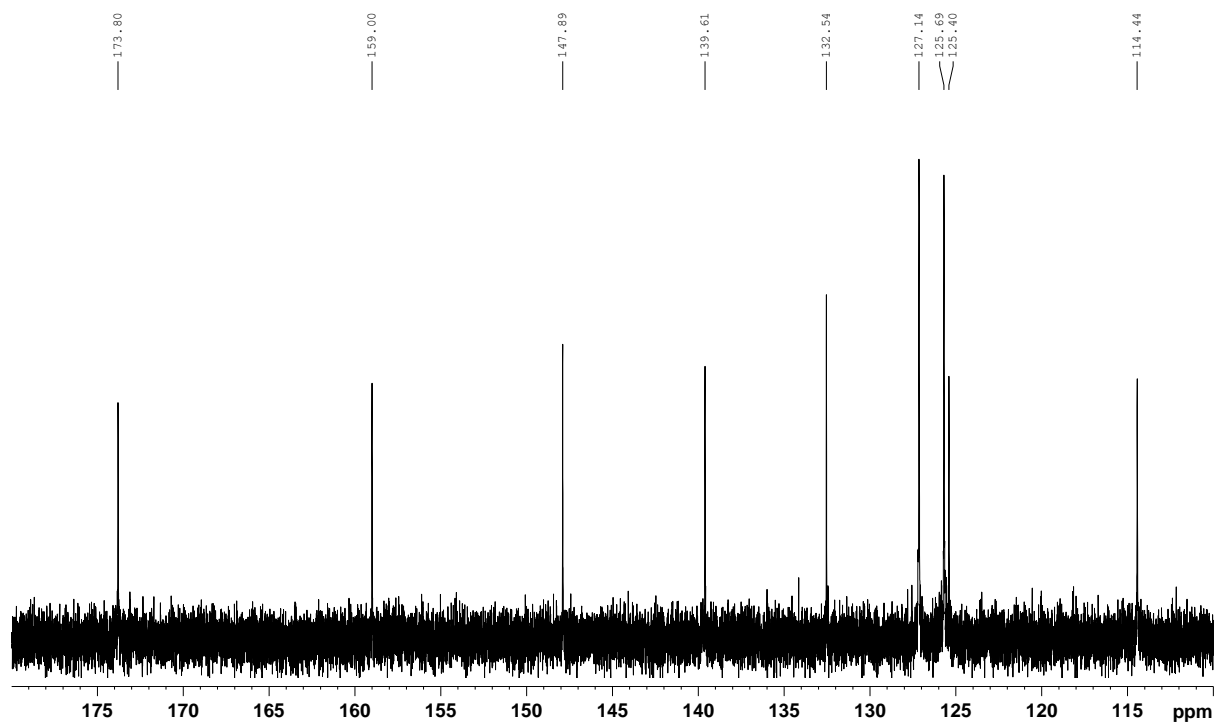






**<sup>13</sup>C NMR in D<sub>2</sub>O**  
SF01 = 125.77 MHz  
SW = 250.55 ppm  
D1 = 2 seconds  
NS = 1024 scans



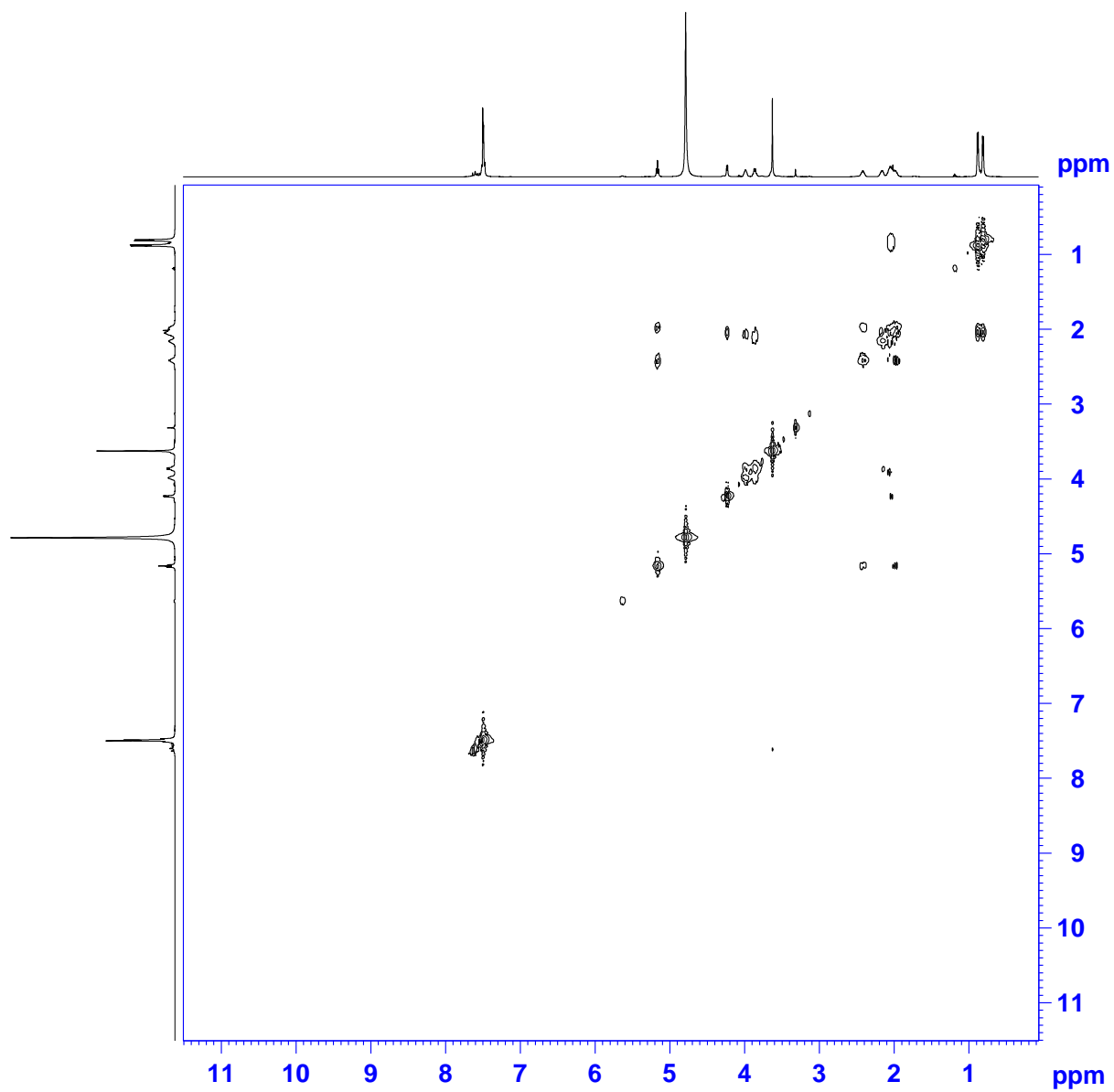


### COSY in D<sub>2</sub>O

SF01 = 500.133 MHz

SW = 12.016 ppm

NS = 4 scans



# HSQC in D<sub>2</sub>O

<sup>13</sup>C  
SF01 = 125.77 MHz  
SW = 250 ppm

<sup>1</sup>H  
SF01 = 500.13 MHz  
SW = 13.3654 ppm

NS = 4 scans

