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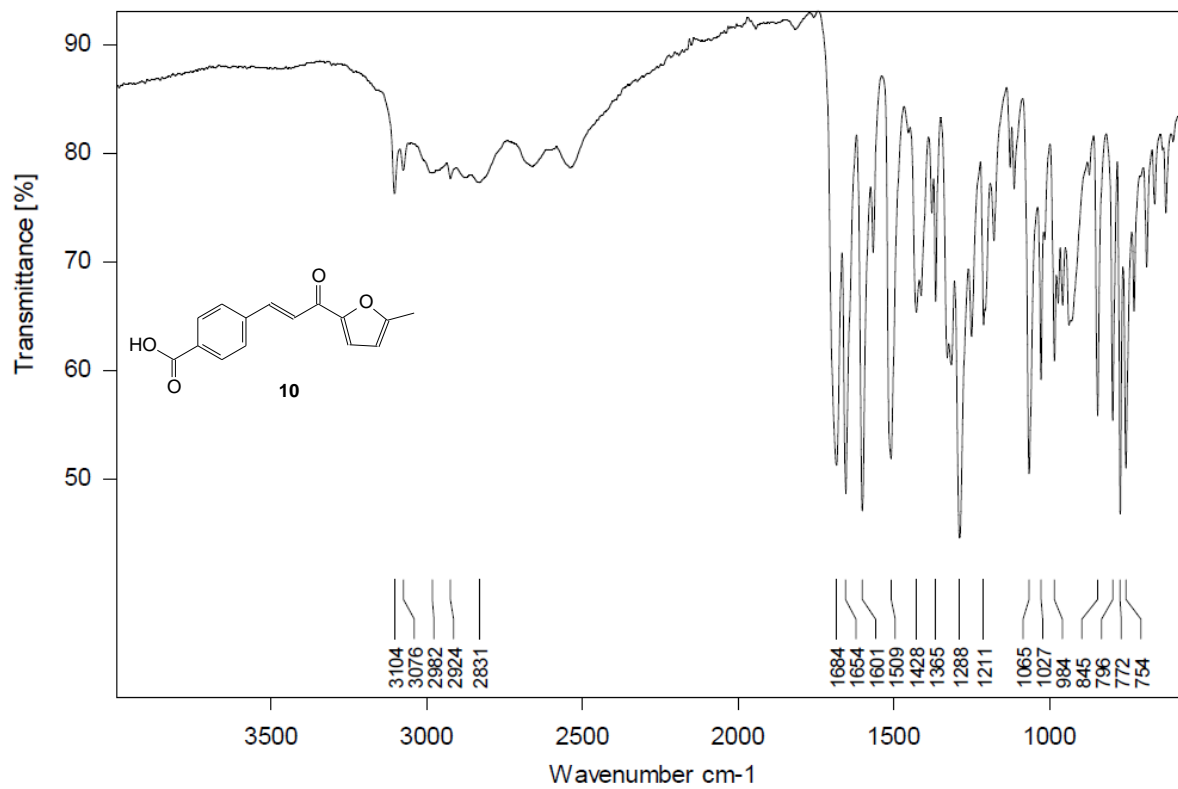
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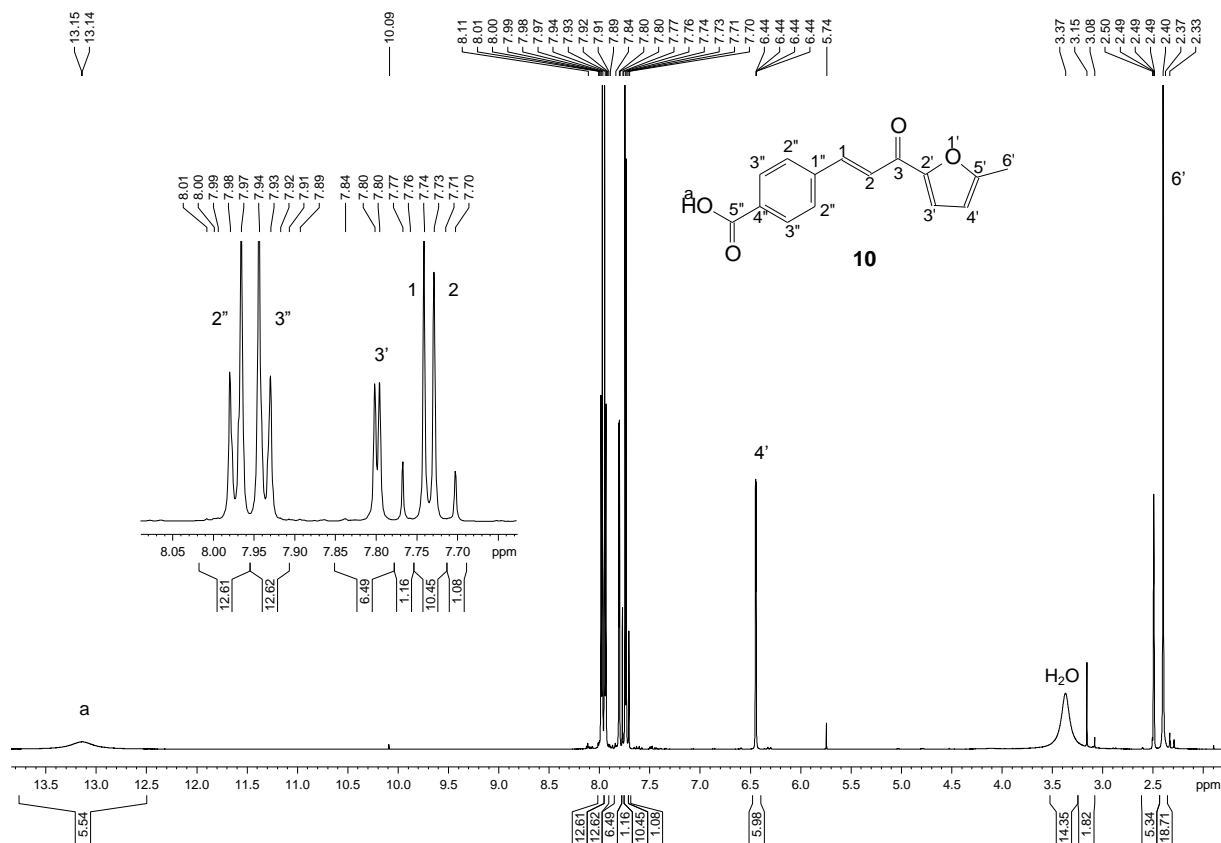
# Addendum A: Analytical data for Chapter 3

IR: 10

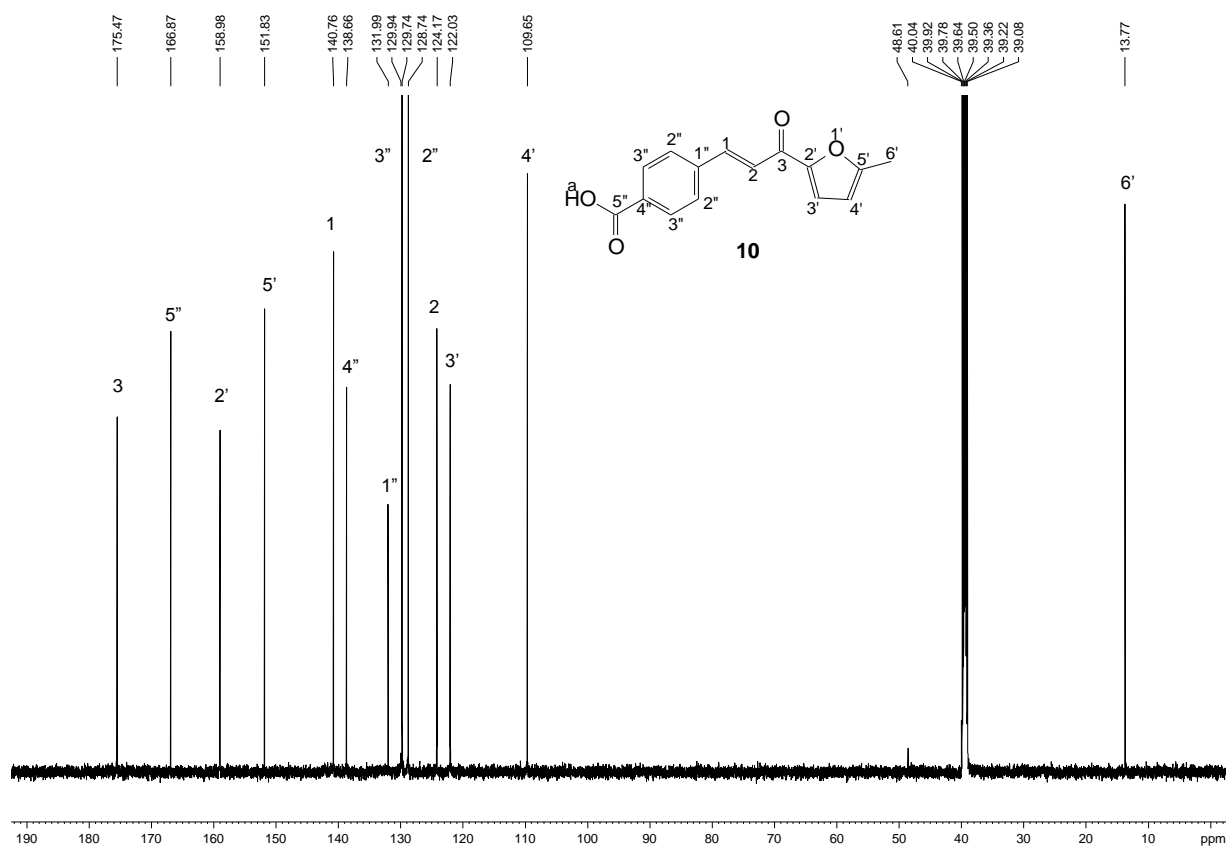


# Addendum A – Chapter 3

## <sup>1</sup>H NMR in DMSO: 10

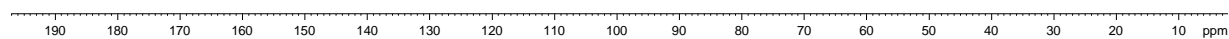
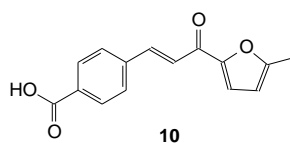
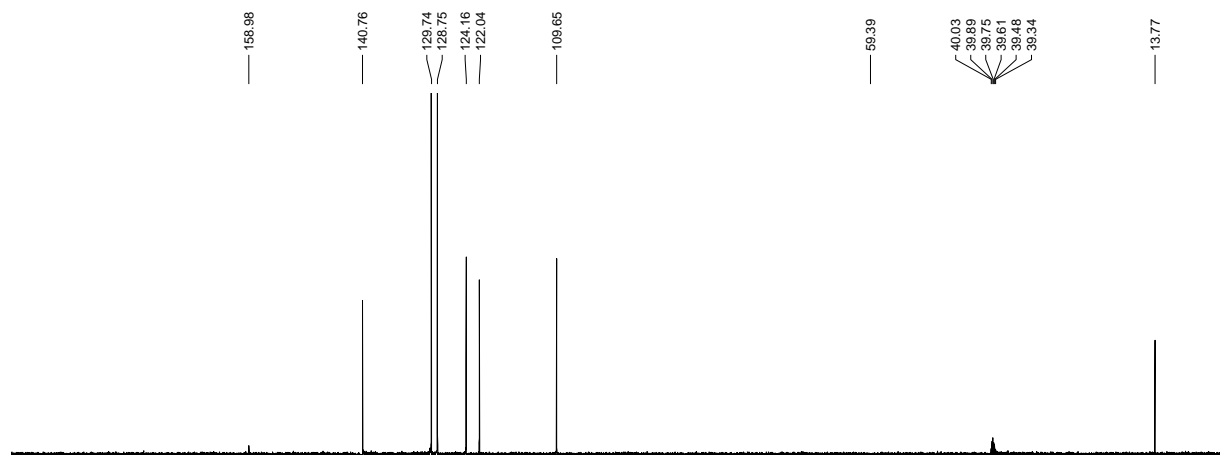


## <sup>13</sup>C NMR in DMSO: 10

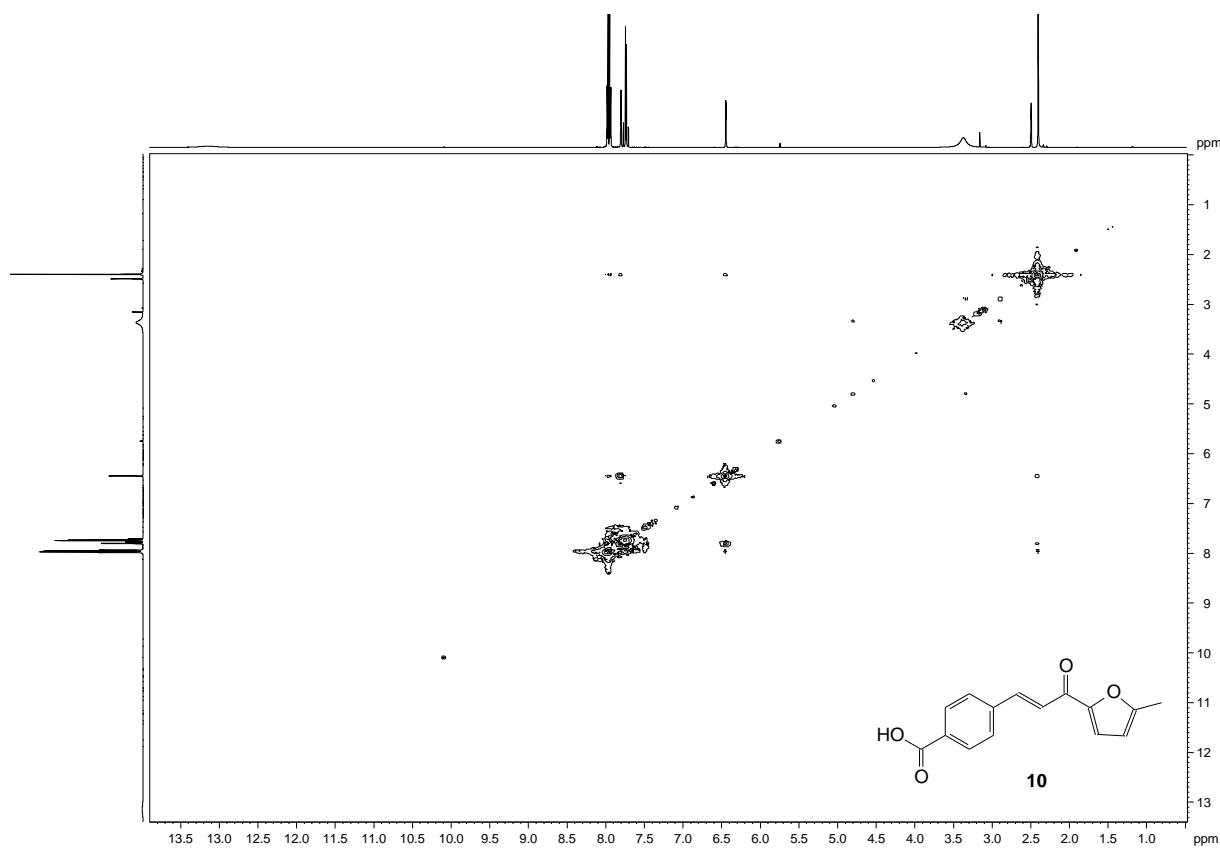


# Addendum A – Chapter 3

## DEPT135 in DMSO: 10

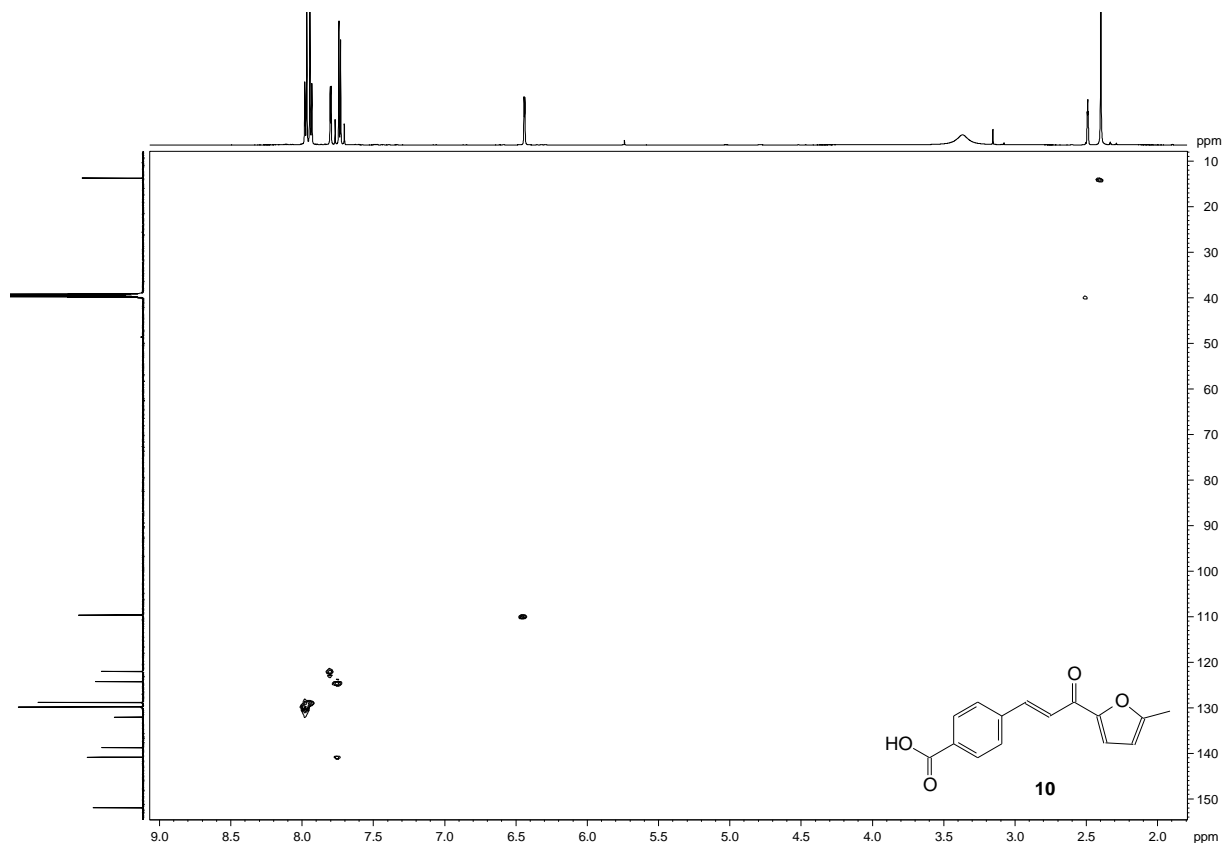


## COSY in DMSO: 10



## Addendum A – Chapter 3

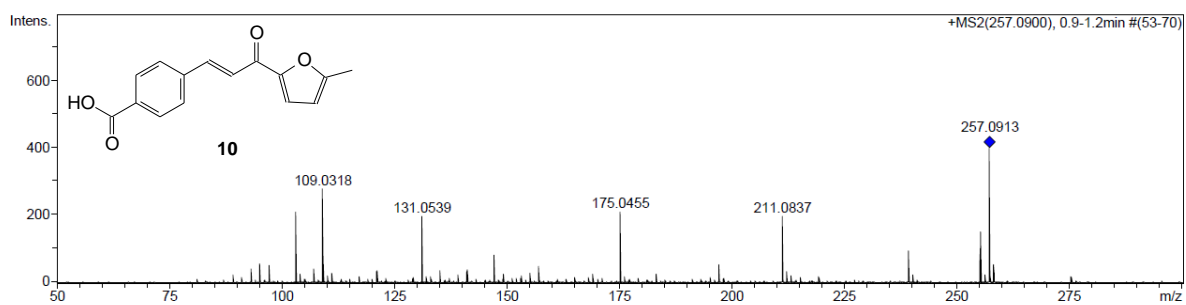
### HSQC in DMSO: **10**



### HRMS: **10**

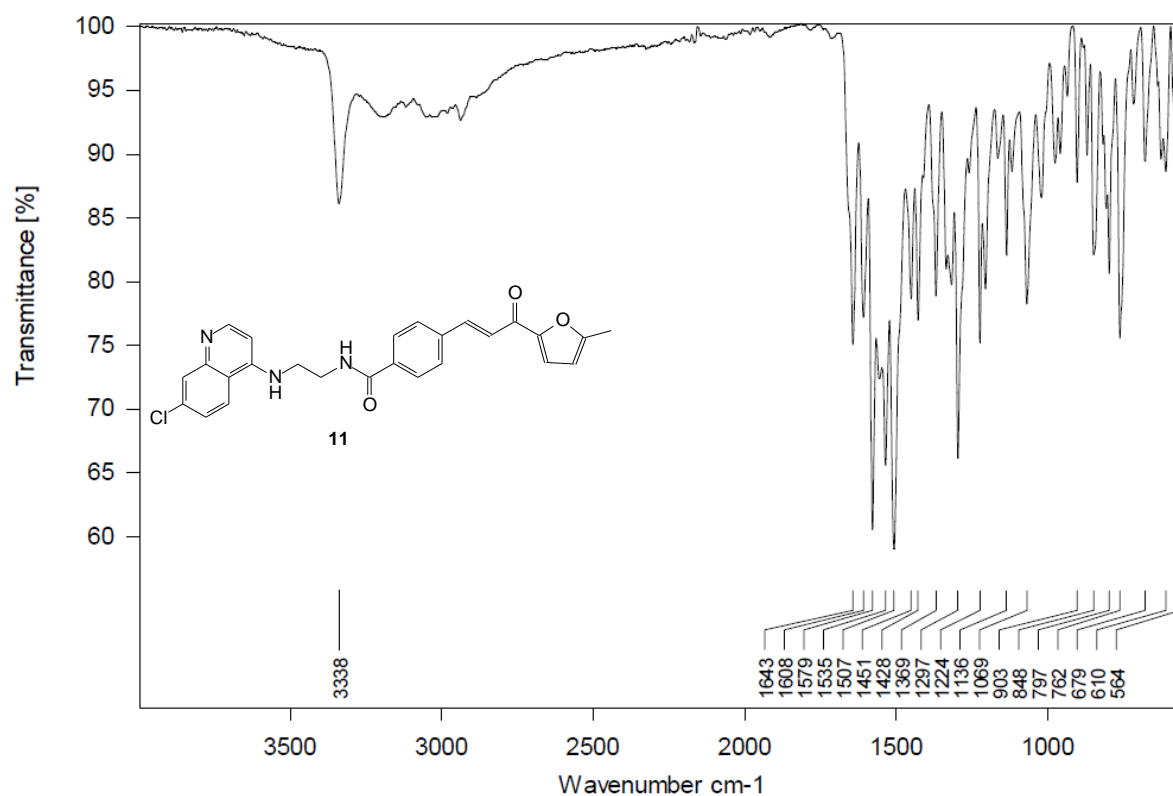
#### Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	3000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste

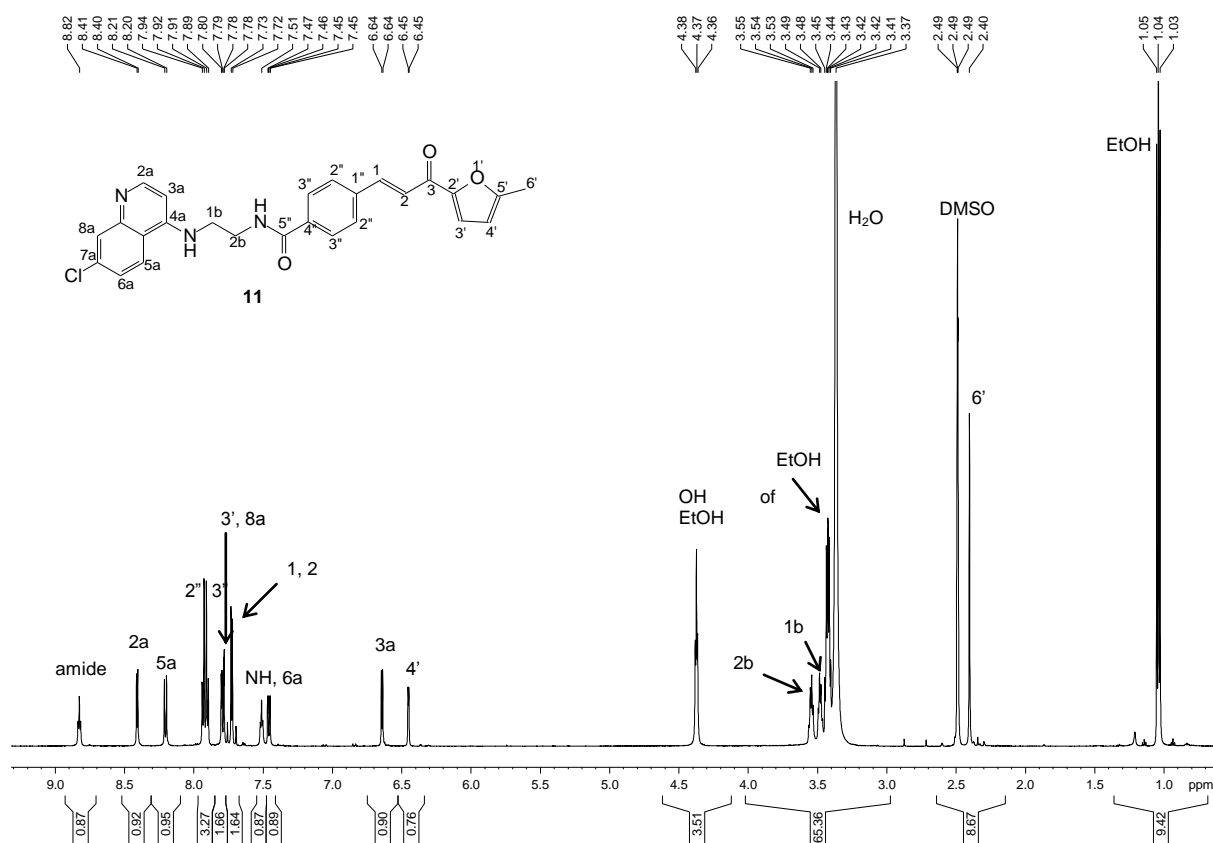


Addendum A – Chapter 3

IR: 11



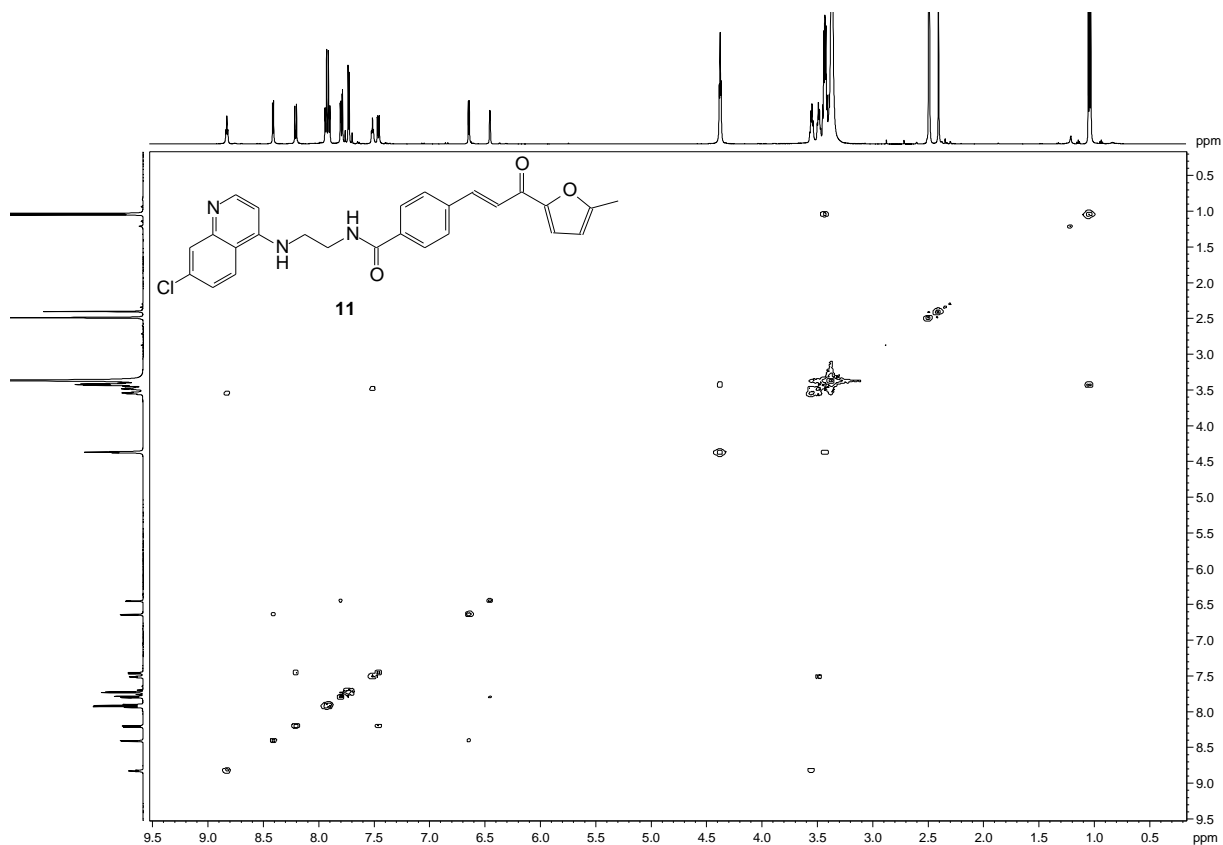
<sup>1</sup>H NMR in DMSO: 11



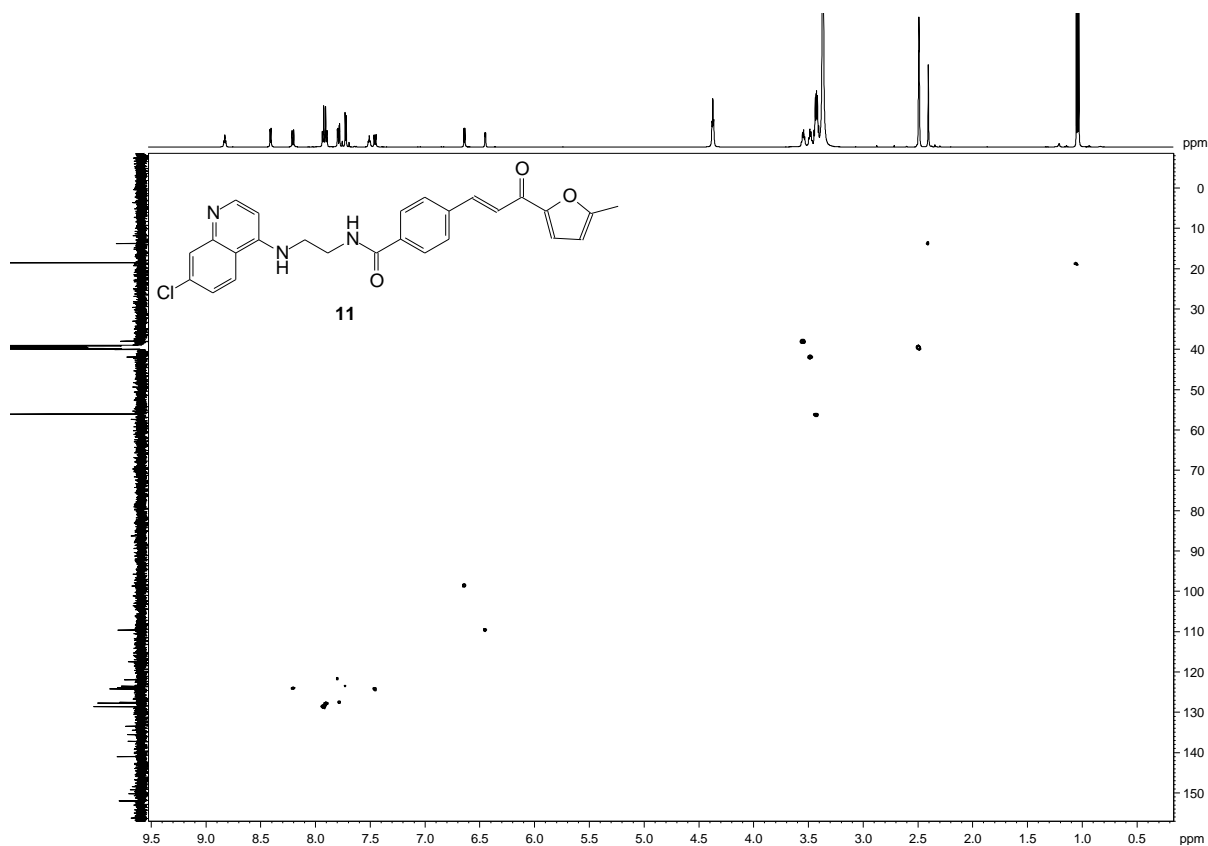


# Addendum A – Chapter 3

## COSY in DMSO: 11



## HSQC in DMSO: 12

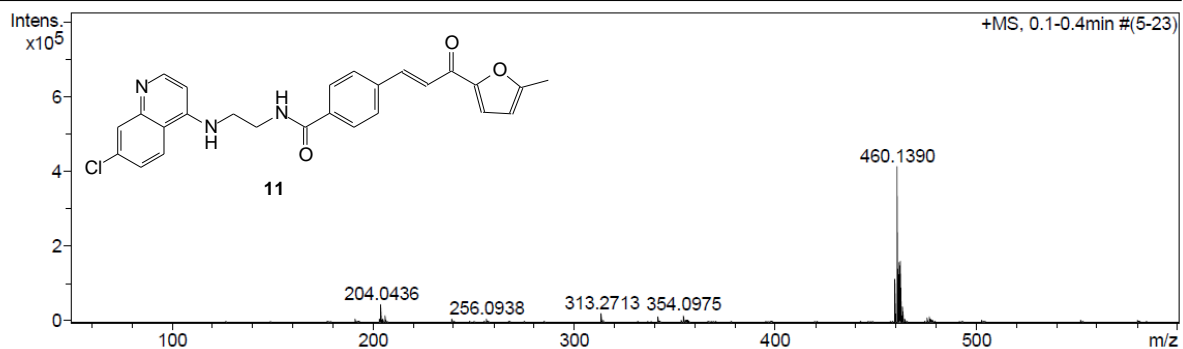


# Addendum A – Chapter 3

## HRMS: 11

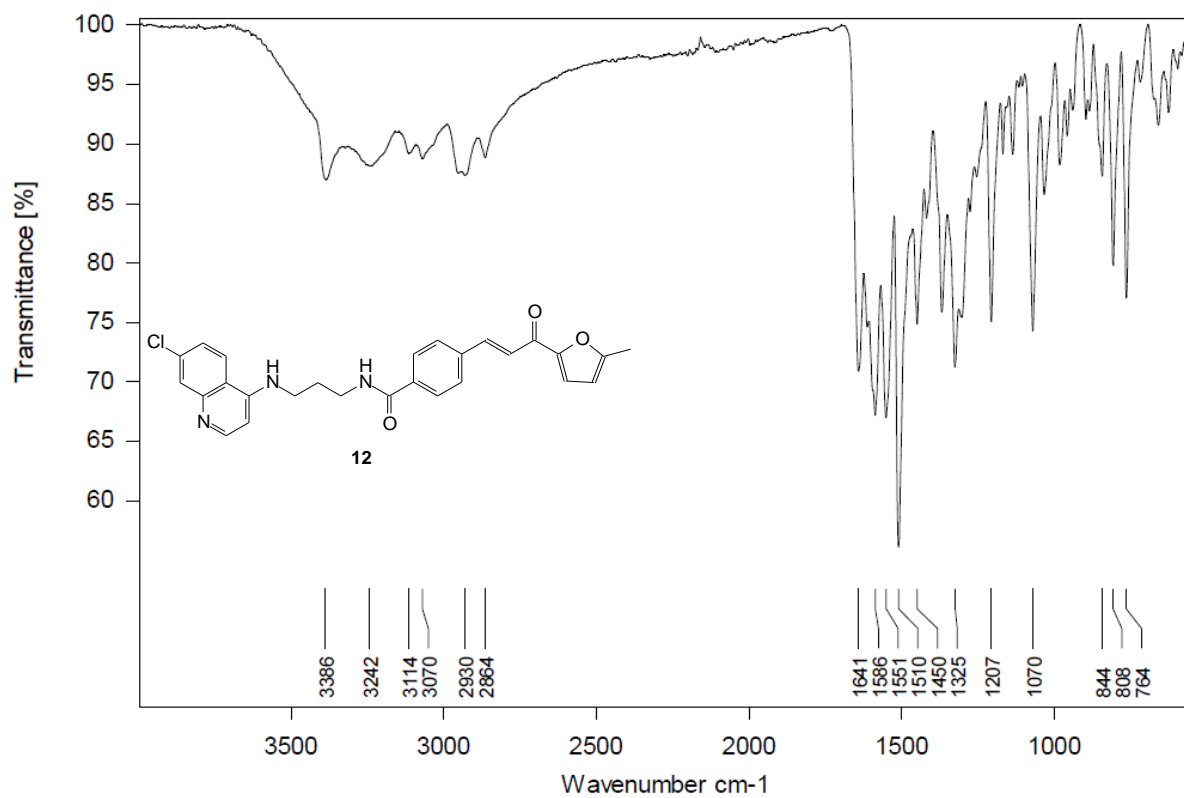
### Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	3000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste

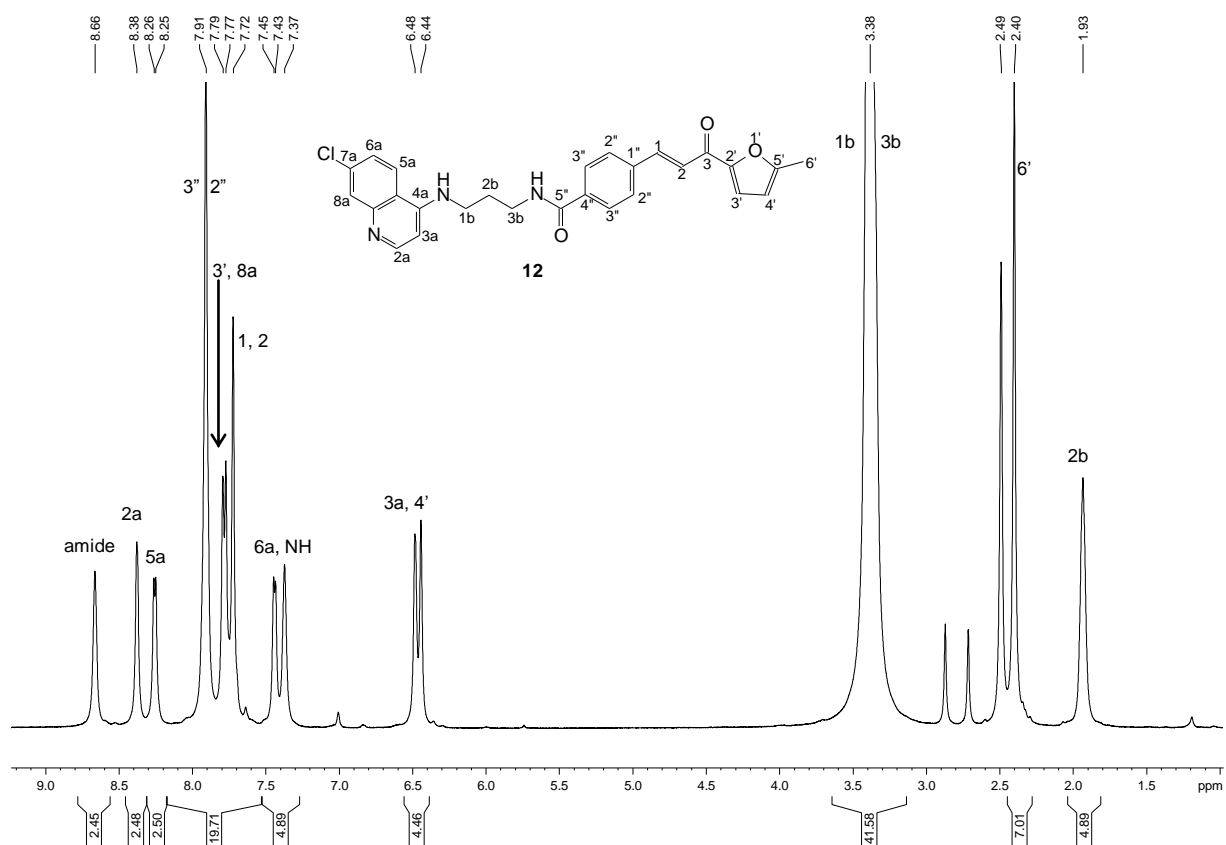


Addendum A – Chapter 3

IR: 12

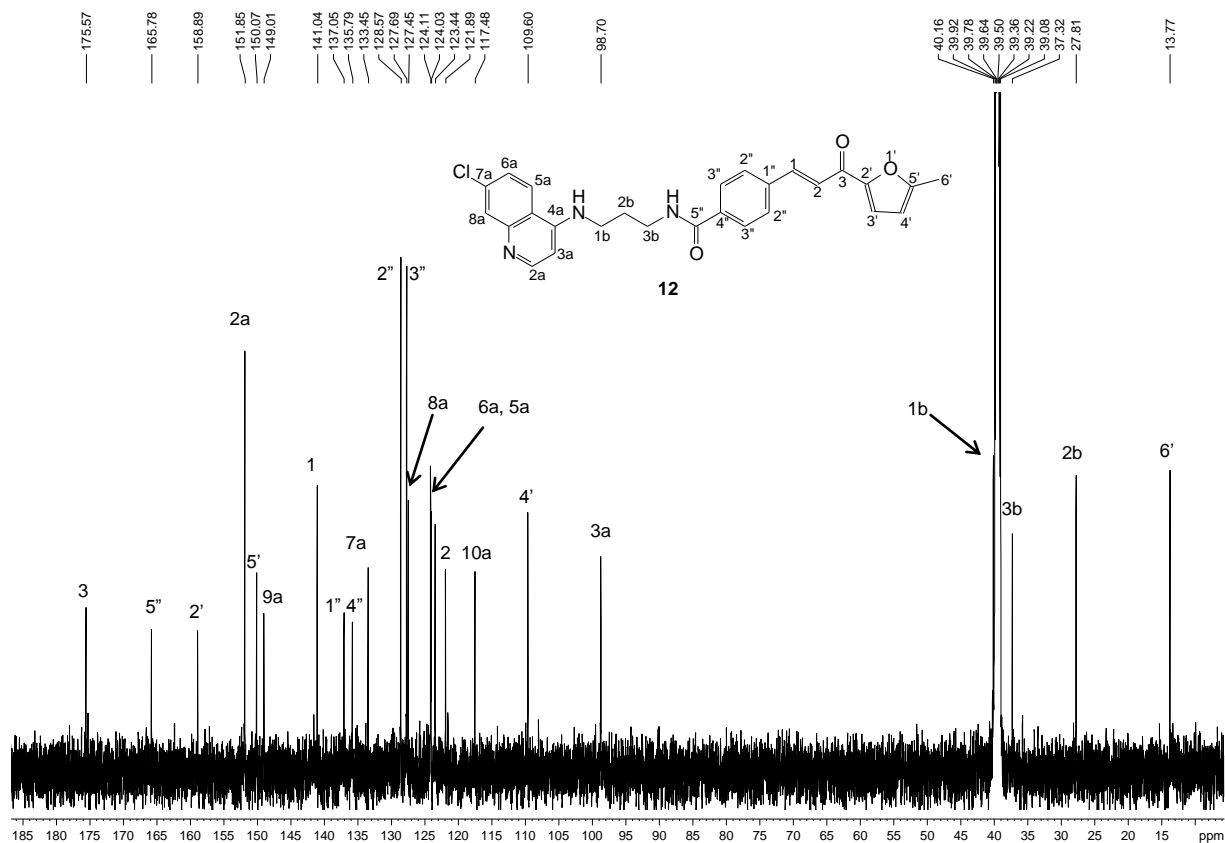


<sup>1</sup>H NMR in DMSO: 12

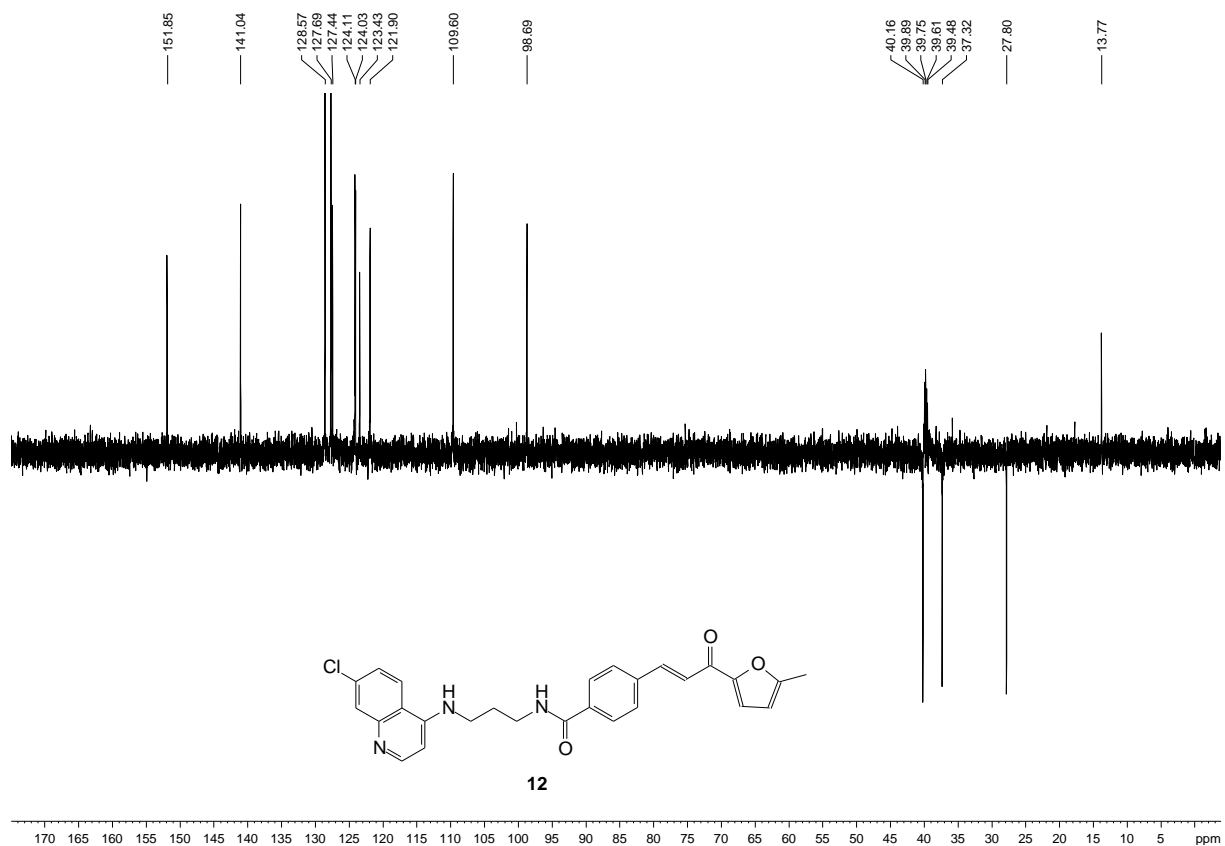


# Addendum A – Chapter 3

## <sup>13</sup>C NMR in DMSO: 12

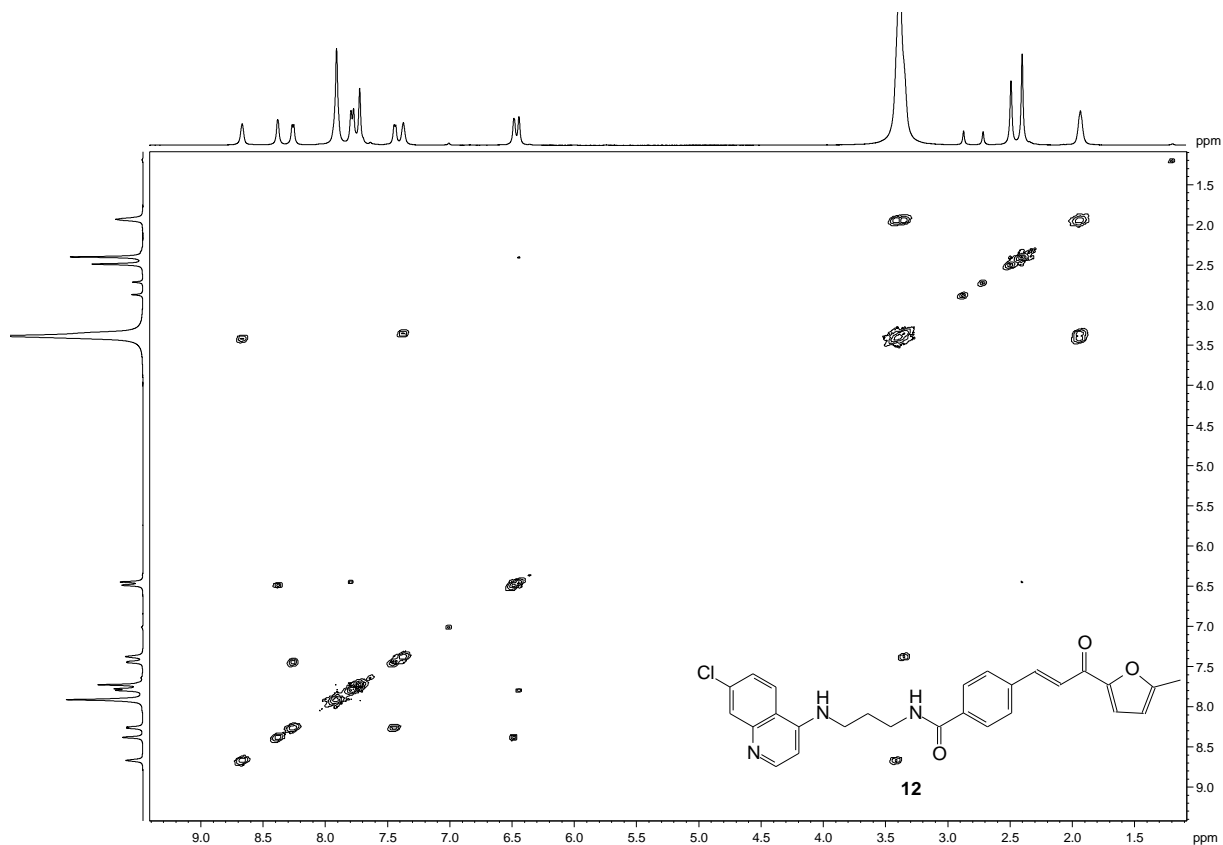


## DEPT135 in DMSO: 12

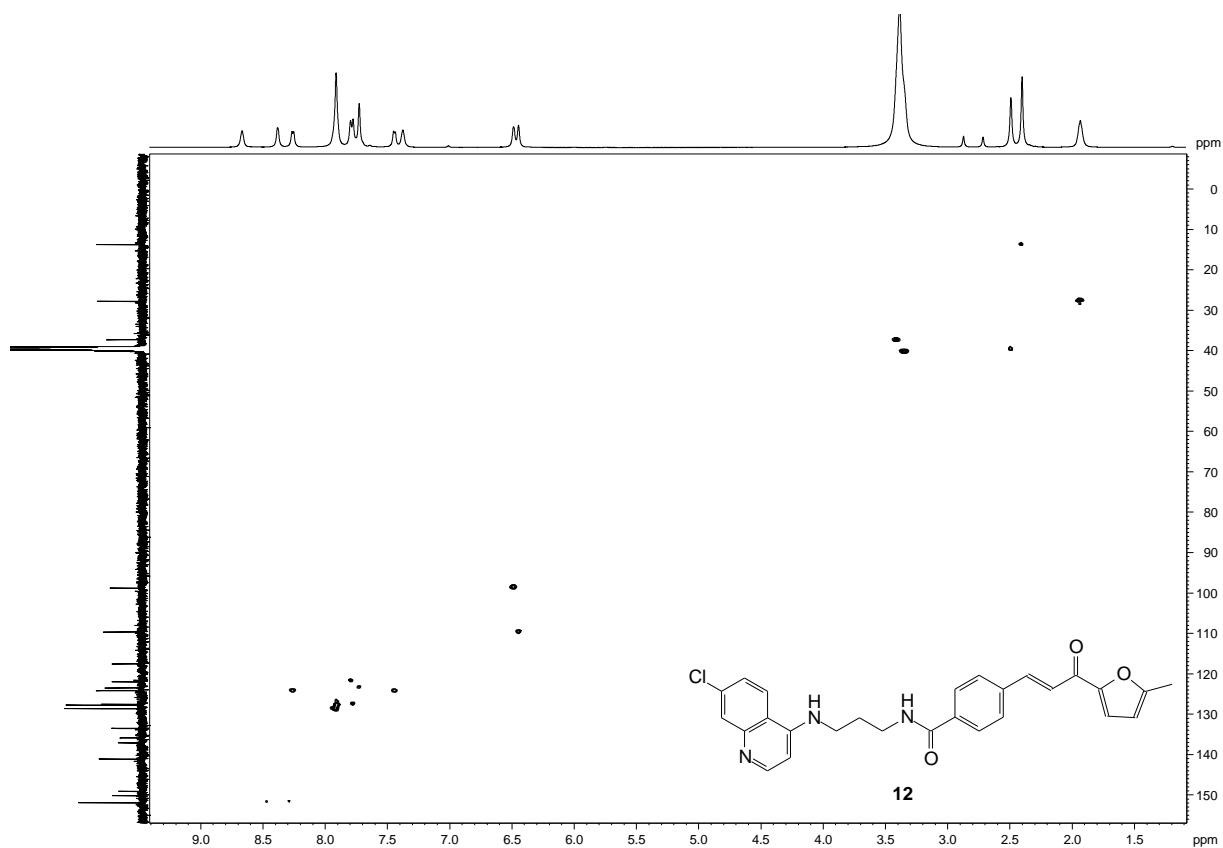


Addendum A – Chapter 3

COSY in DMSO: 12

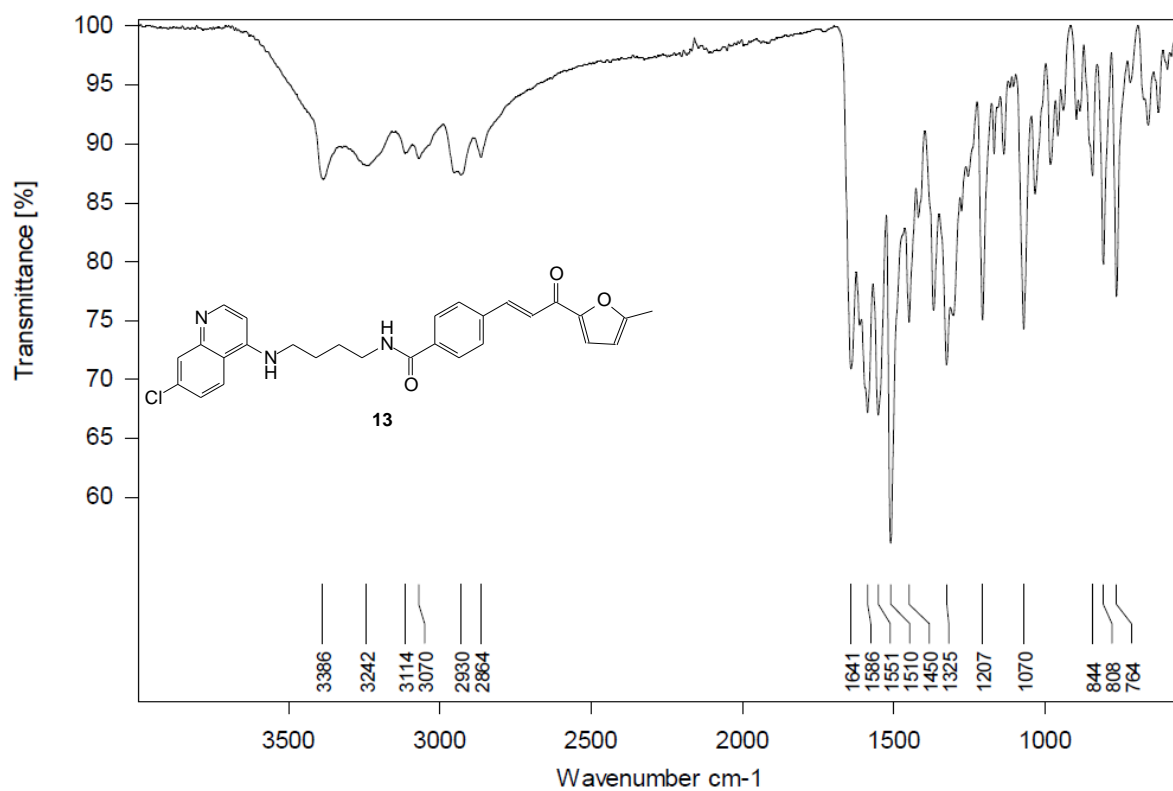


HSQC in DMSO: 12

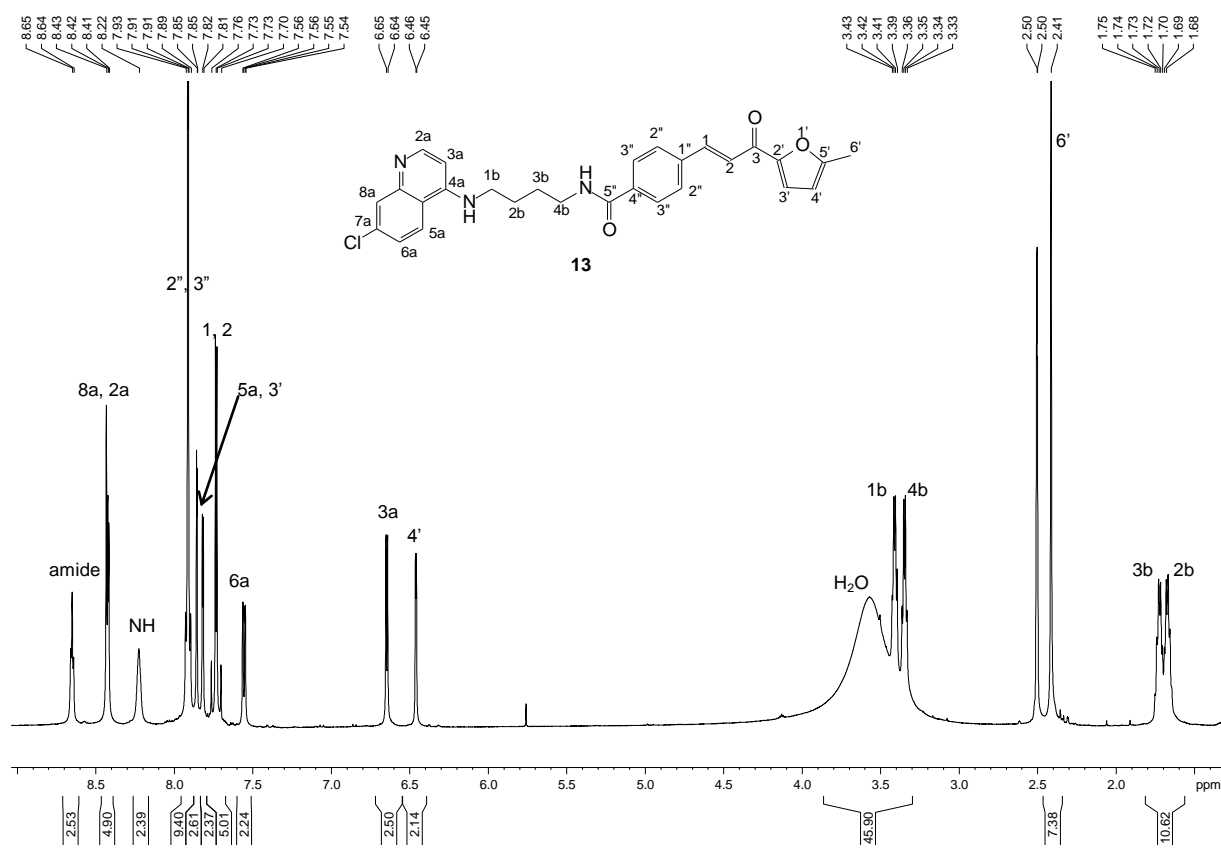




IR: 13

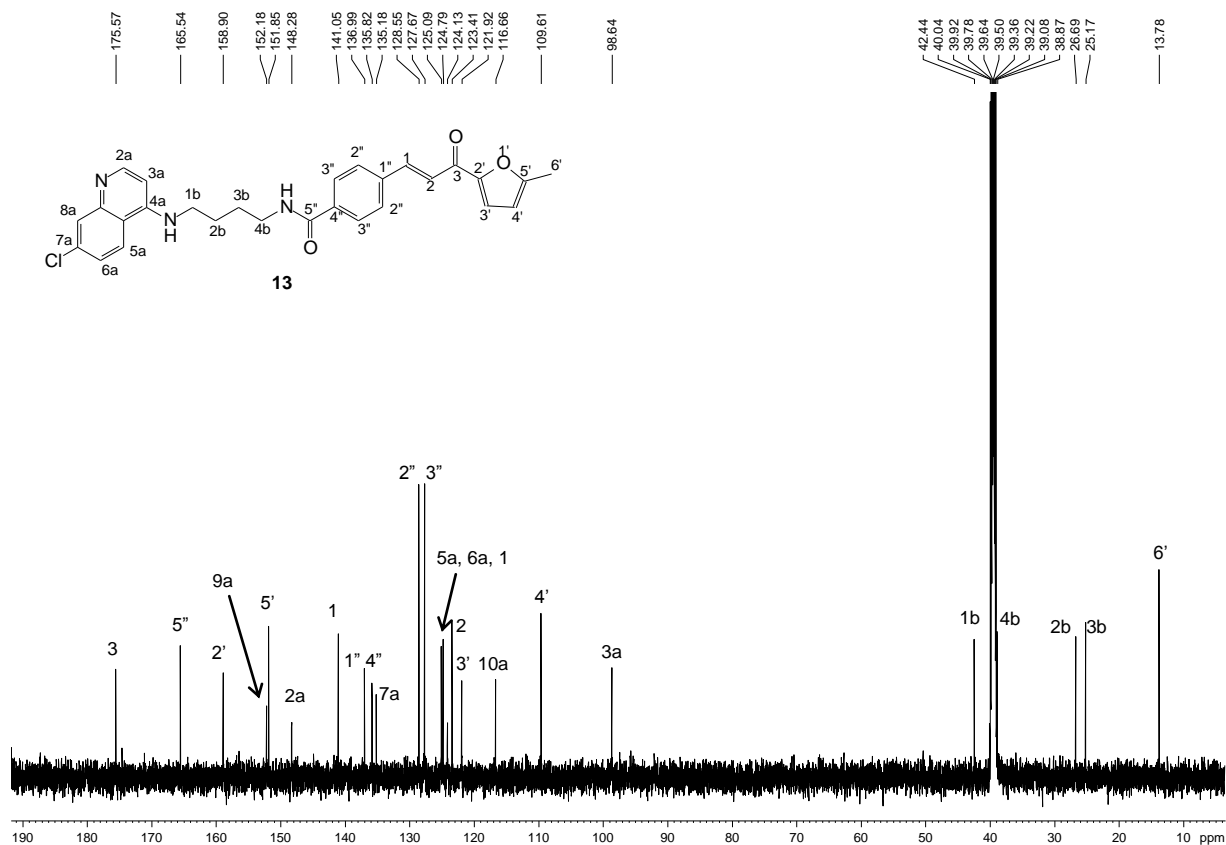


<sup>1</sup>H NMR in DMSO: 13

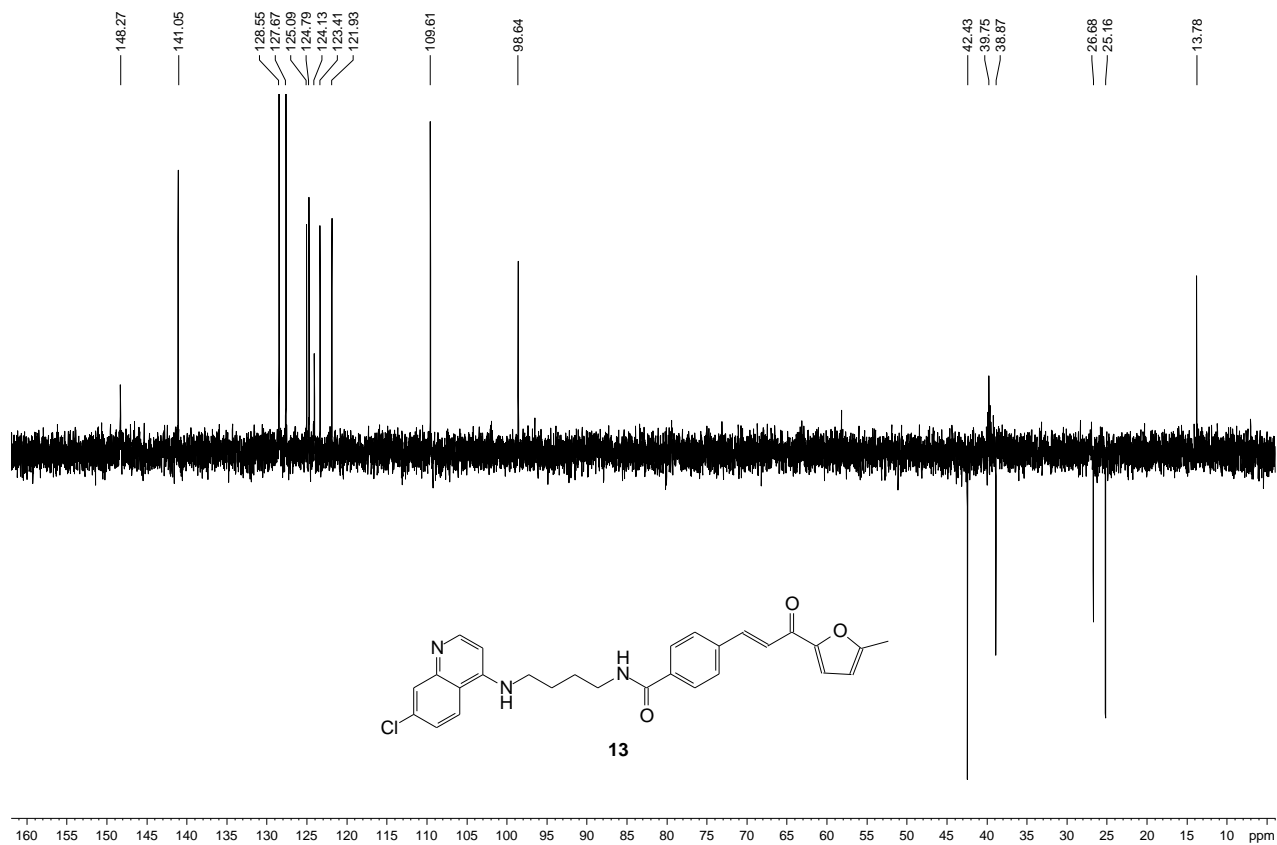


# Addendum A – Chapter 3

## <sup>13</sup>C NMR in DMSO: **13**

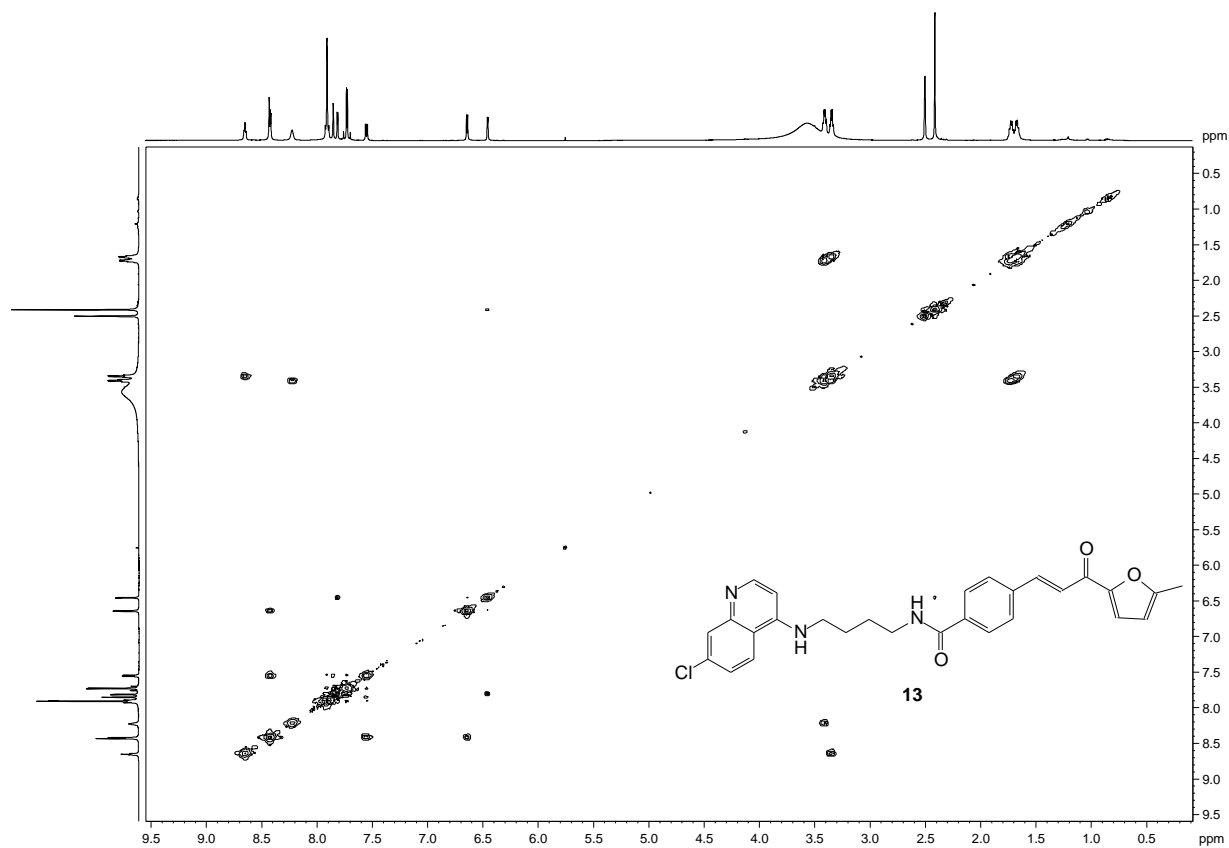


## DEPT135 in DMSO: **13**

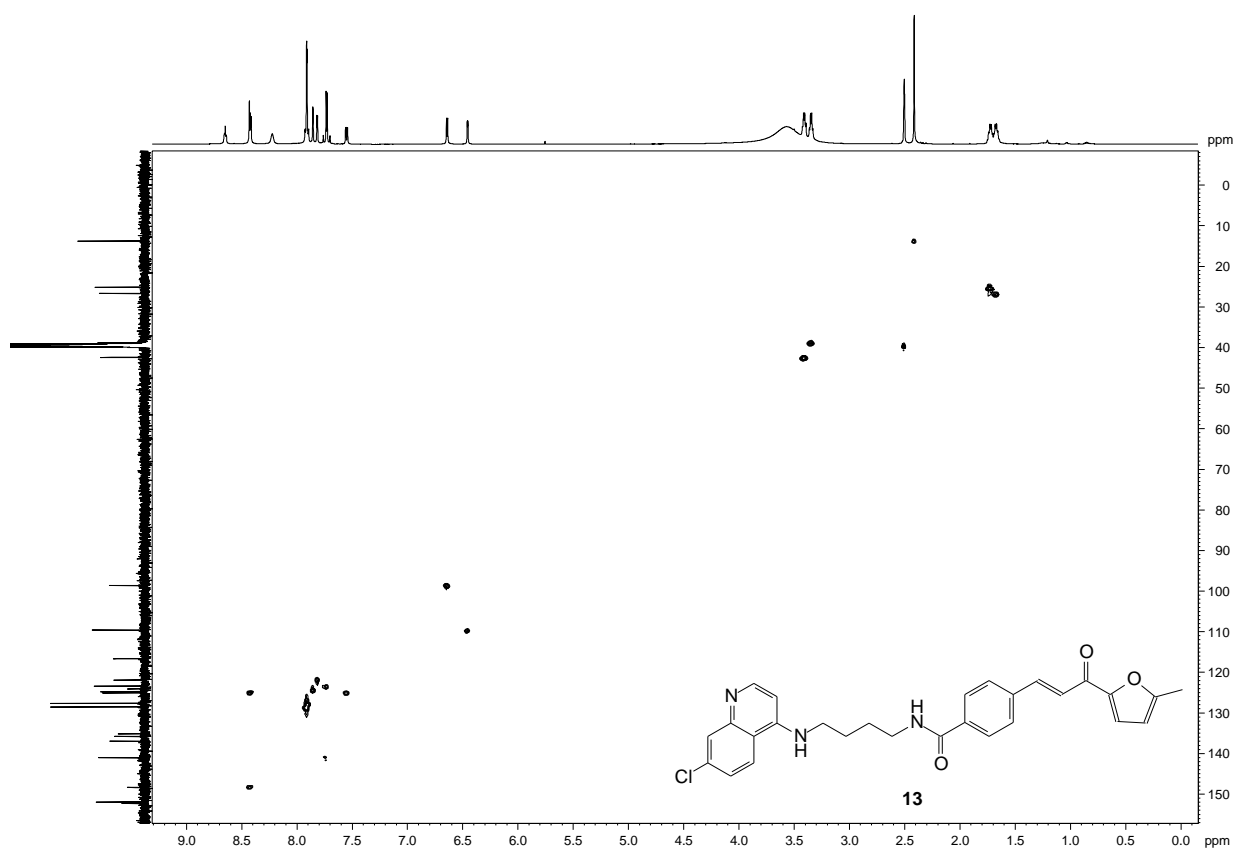


Addendum A – Chapter 3

COSY in DMSO: 13



HSQC in DMSO: 13

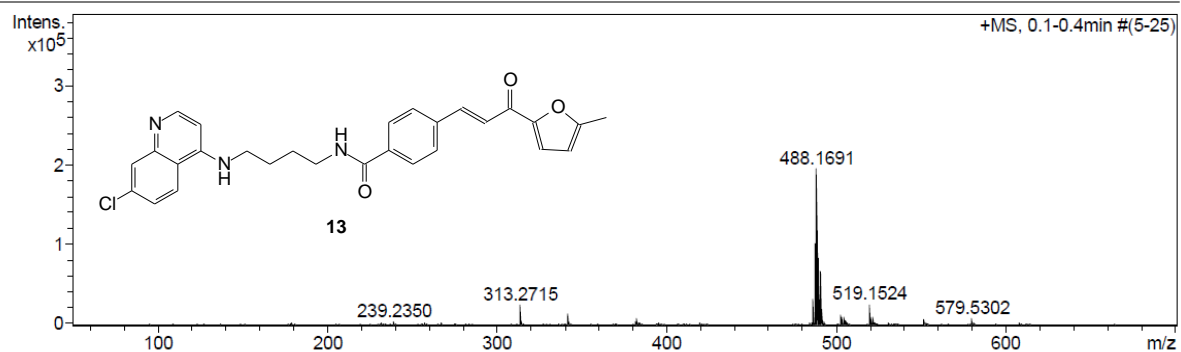


# Addendum A – Chapter 3

## HRMS: 13

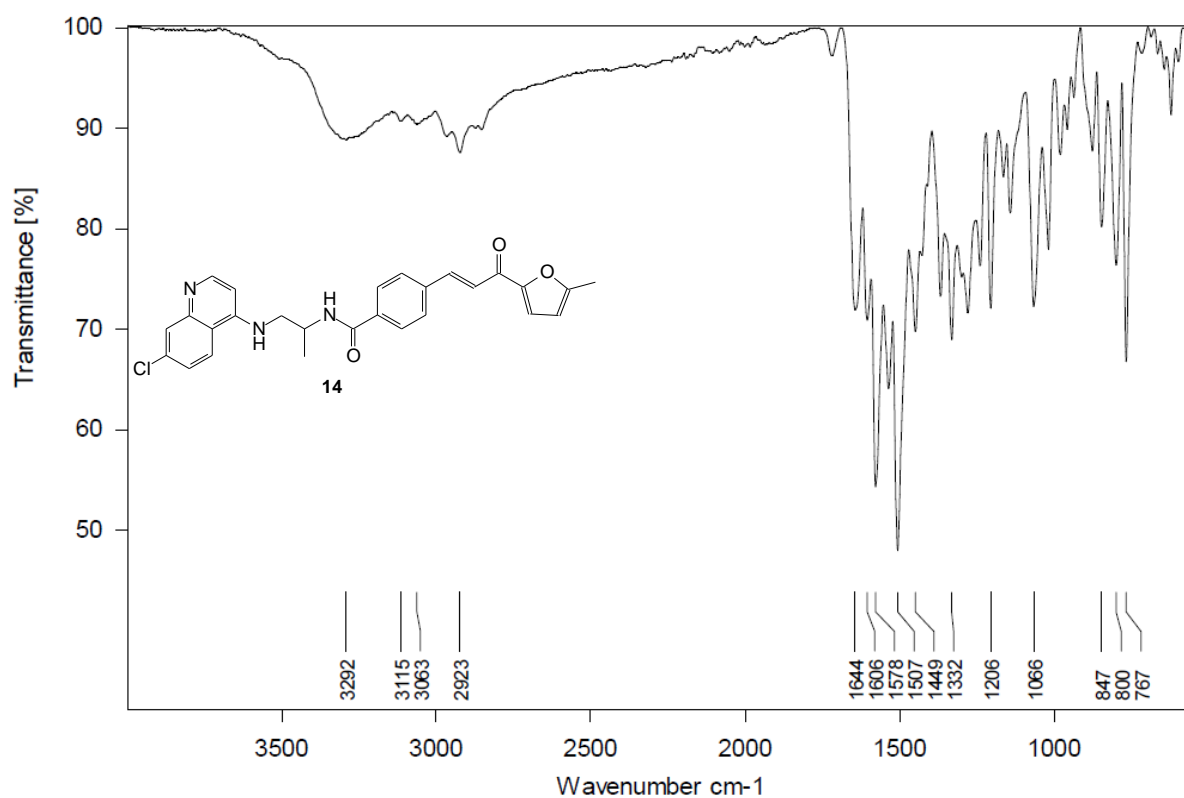
### Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	3000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste

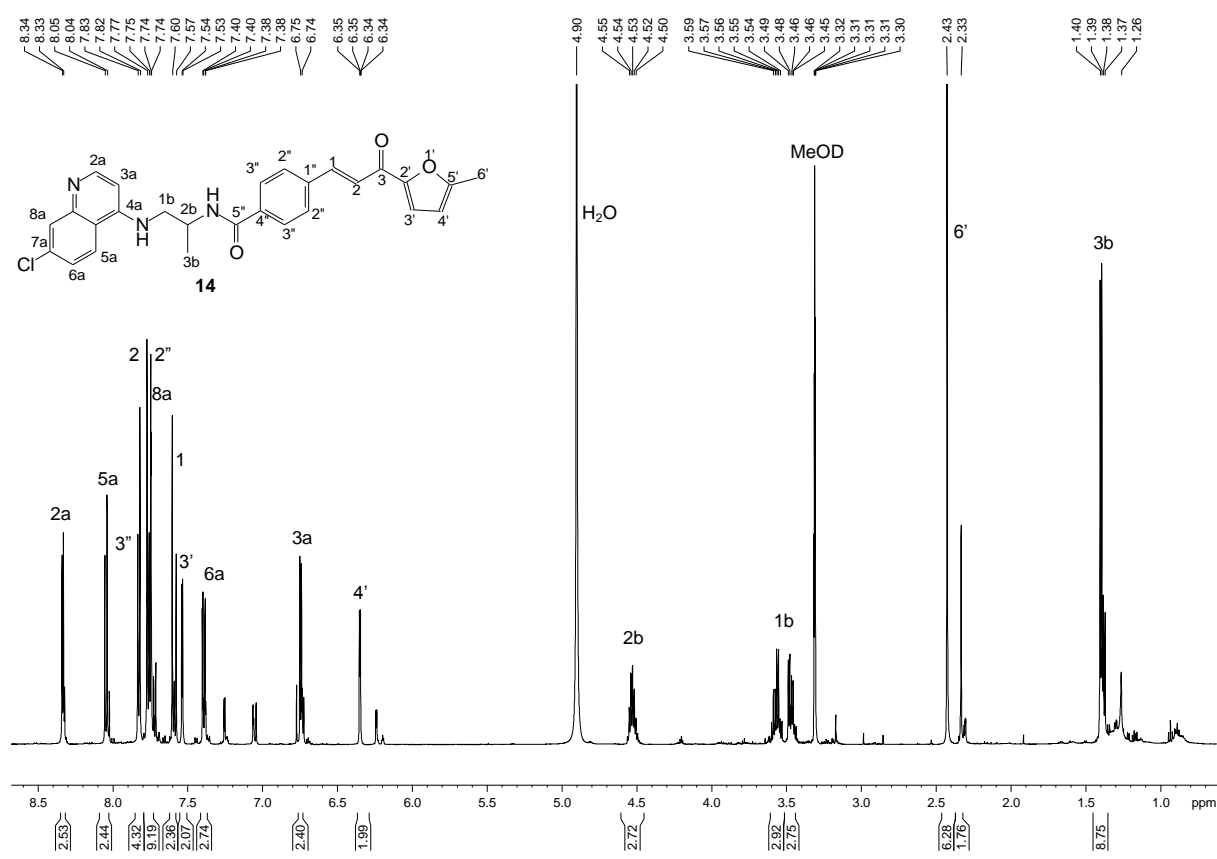


Addendum A – Chapter 3

IR: 14

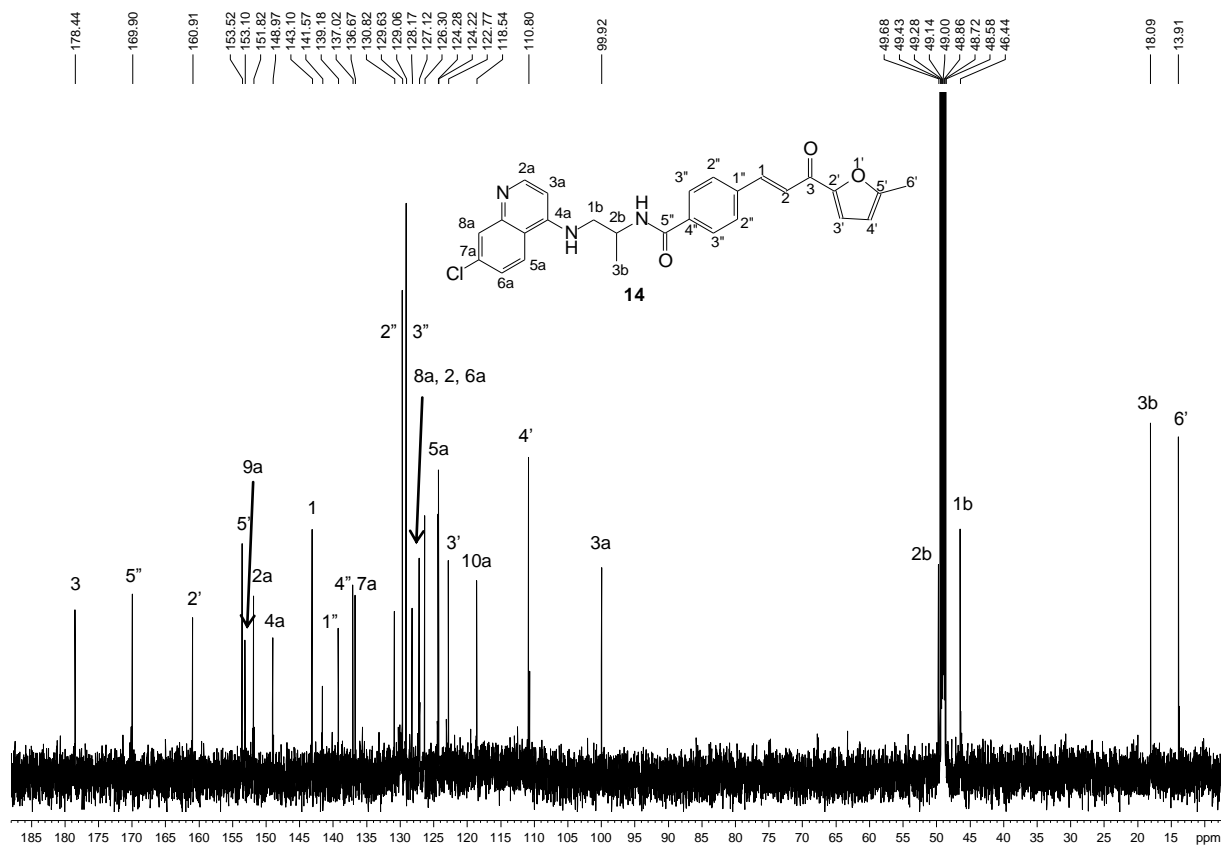


<sup>1</sup>H NMR in DMSO: 14

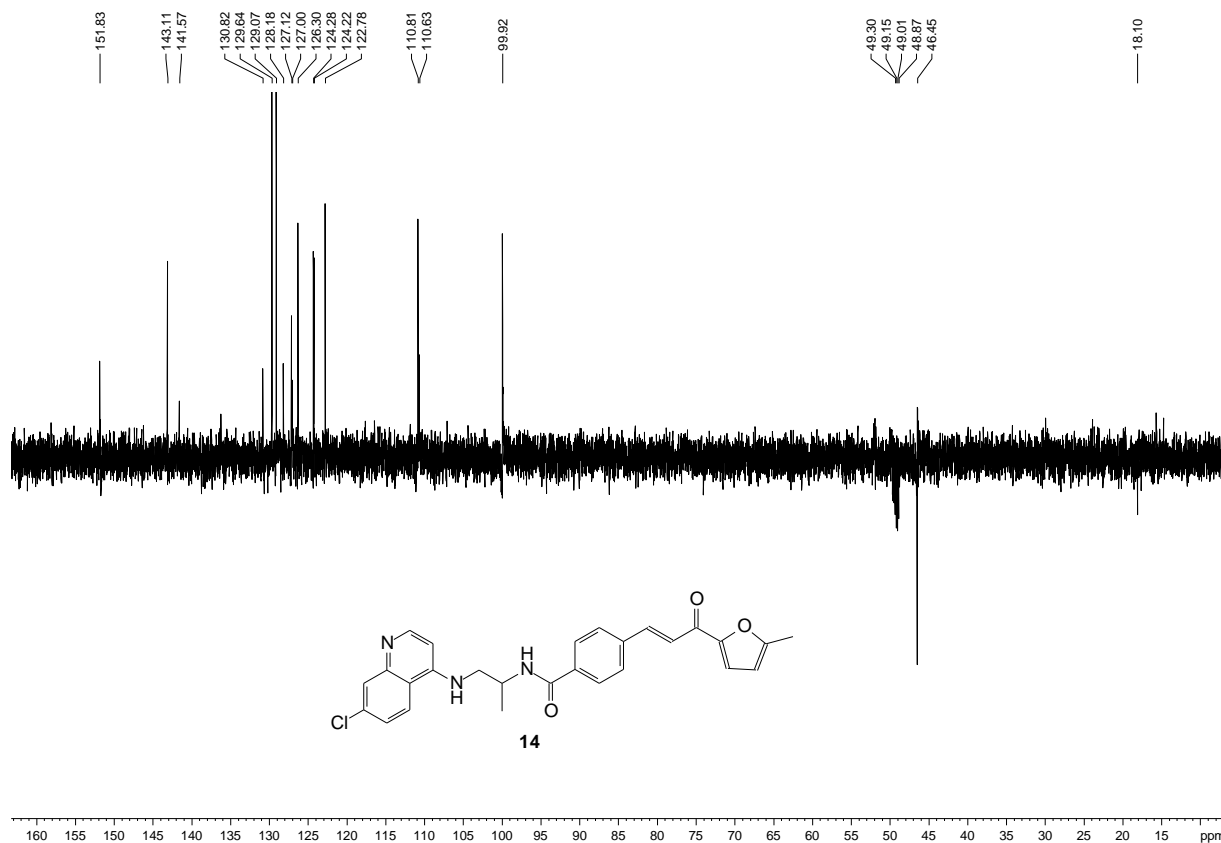


# Addendum A – Chapter 3

## <sup>13</sup>C NMR in DMSO: 14

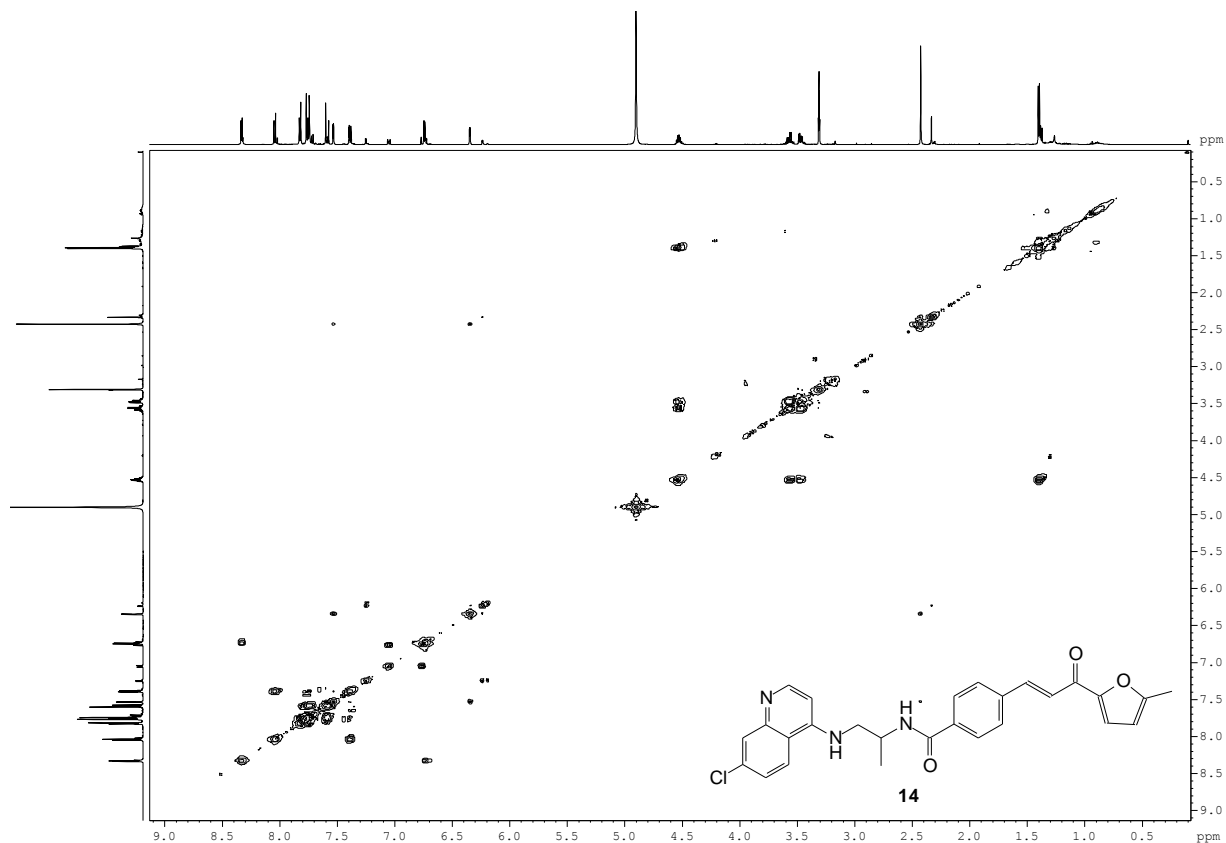


## DEPT135 in DMSO: 14

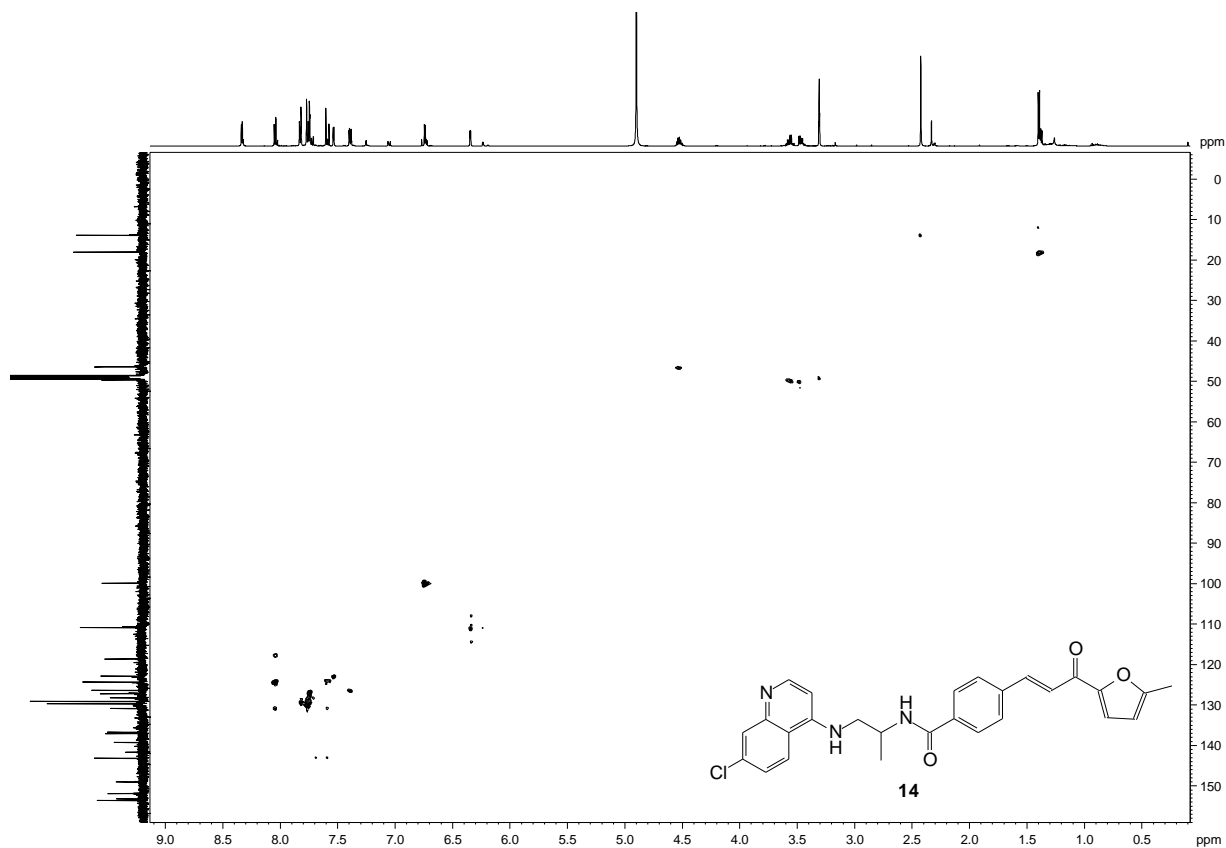


Addendum A – Chapter 3

COSY in DMSO: 14



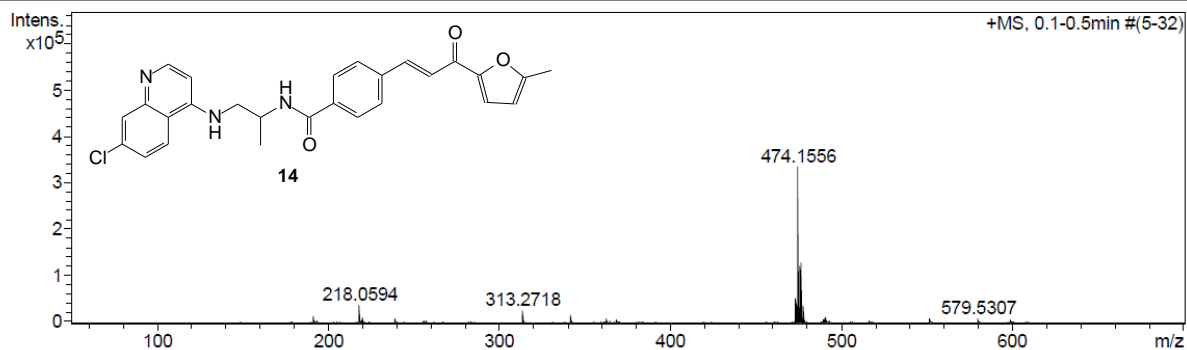
HSQC in DMSO: 14



# Addendum A – Chapter 3

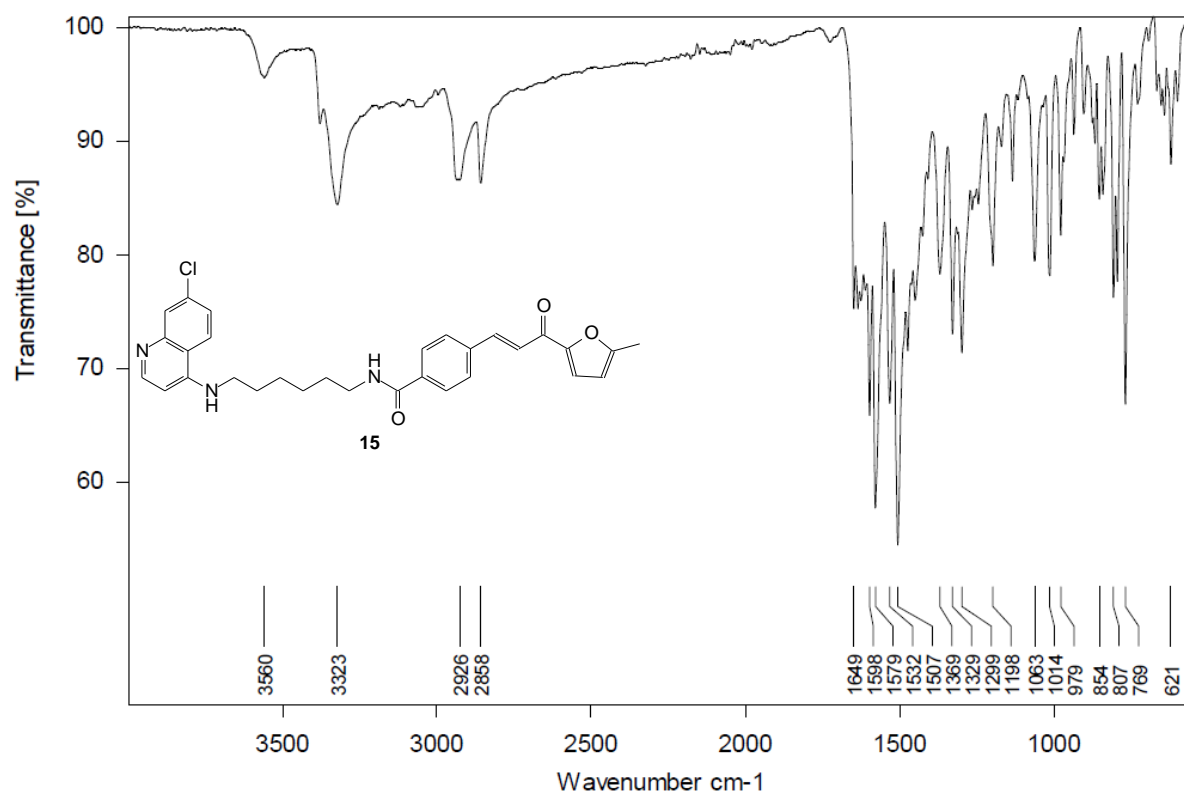
## Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	3000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste

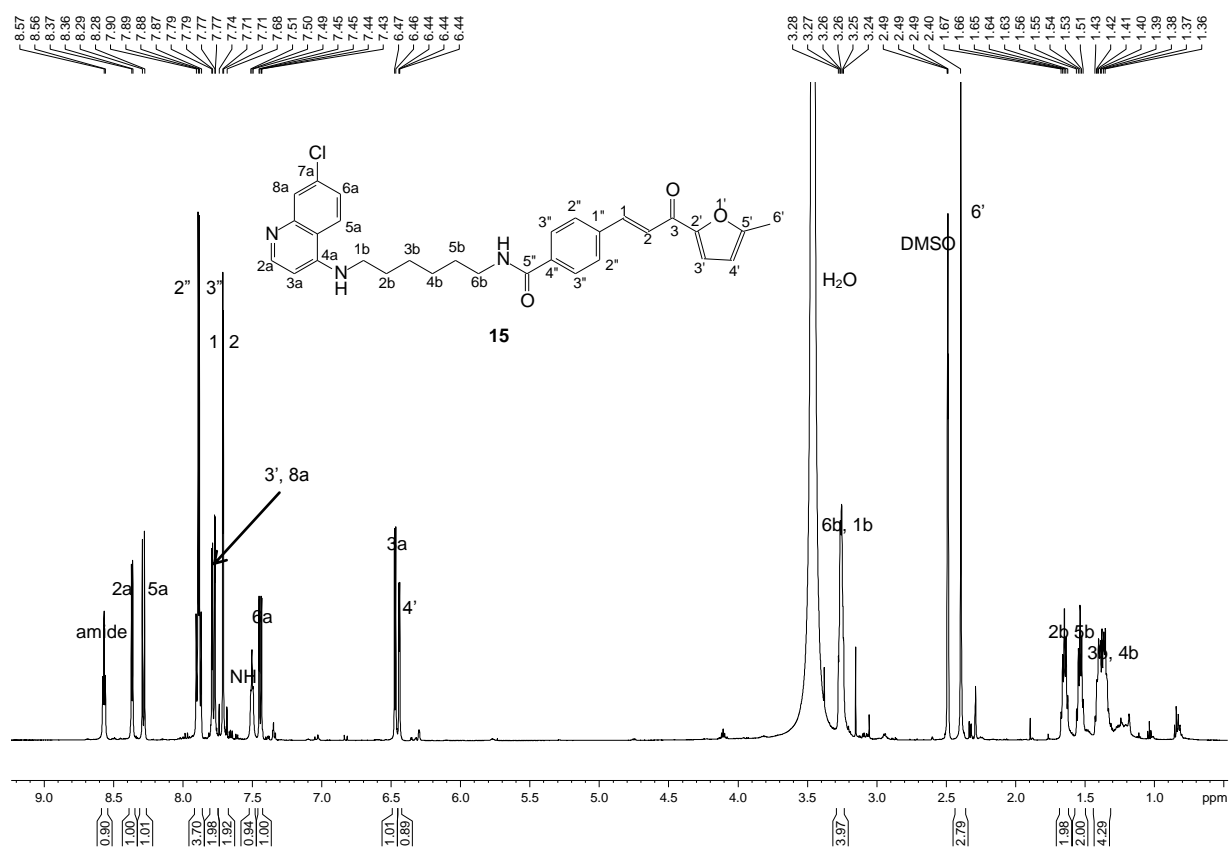


Addendum A – Chapter 3

IR: 15

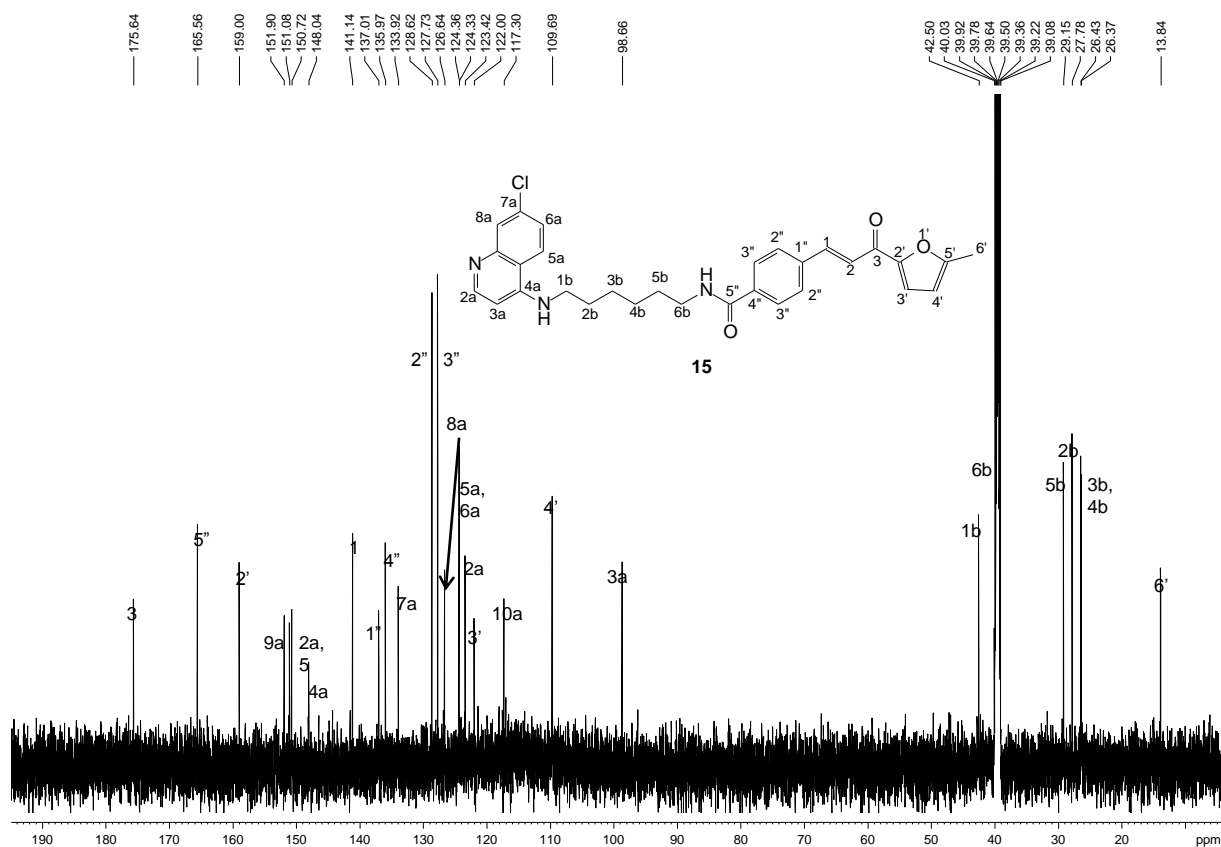


<sup>1</sup>H NMR in DMSO: 15

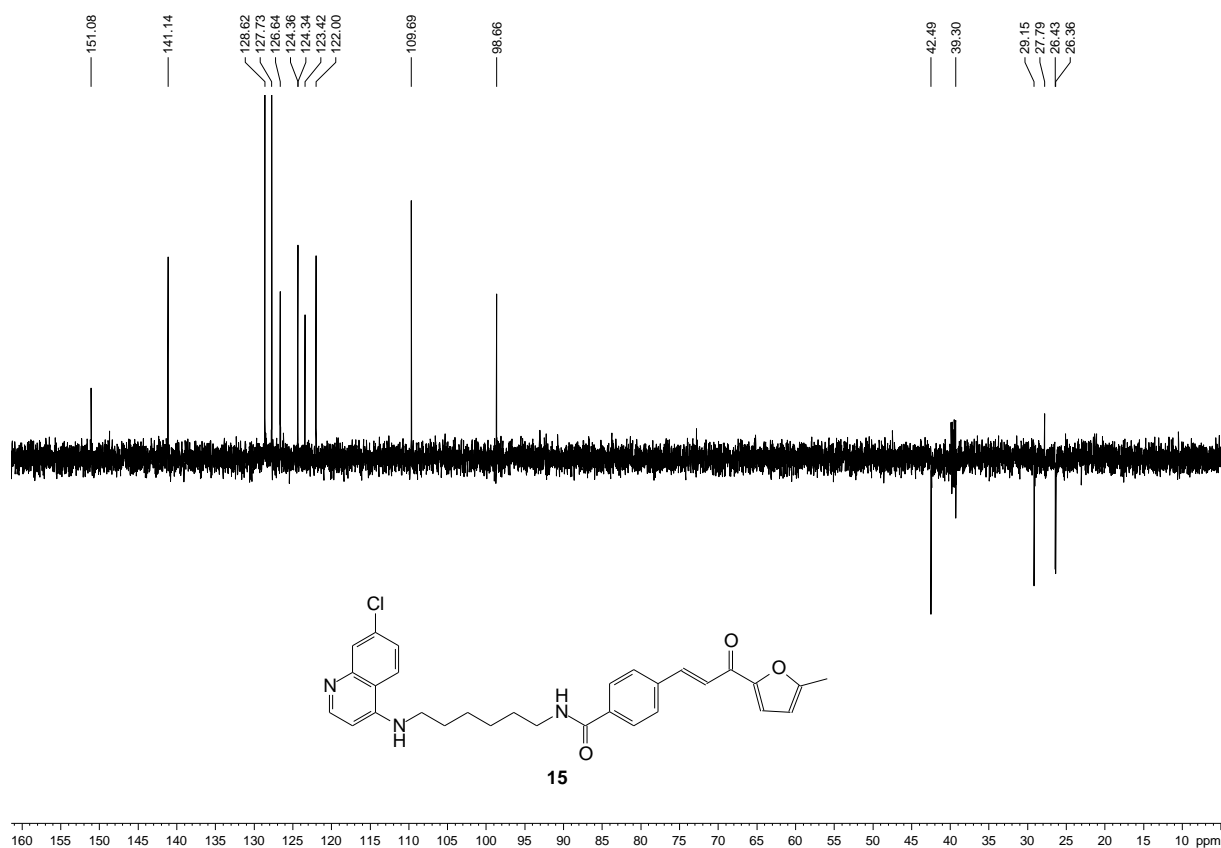


# Addendum A – Chapter 3

## <sup>13</sup>C NMR in DMSO: 15

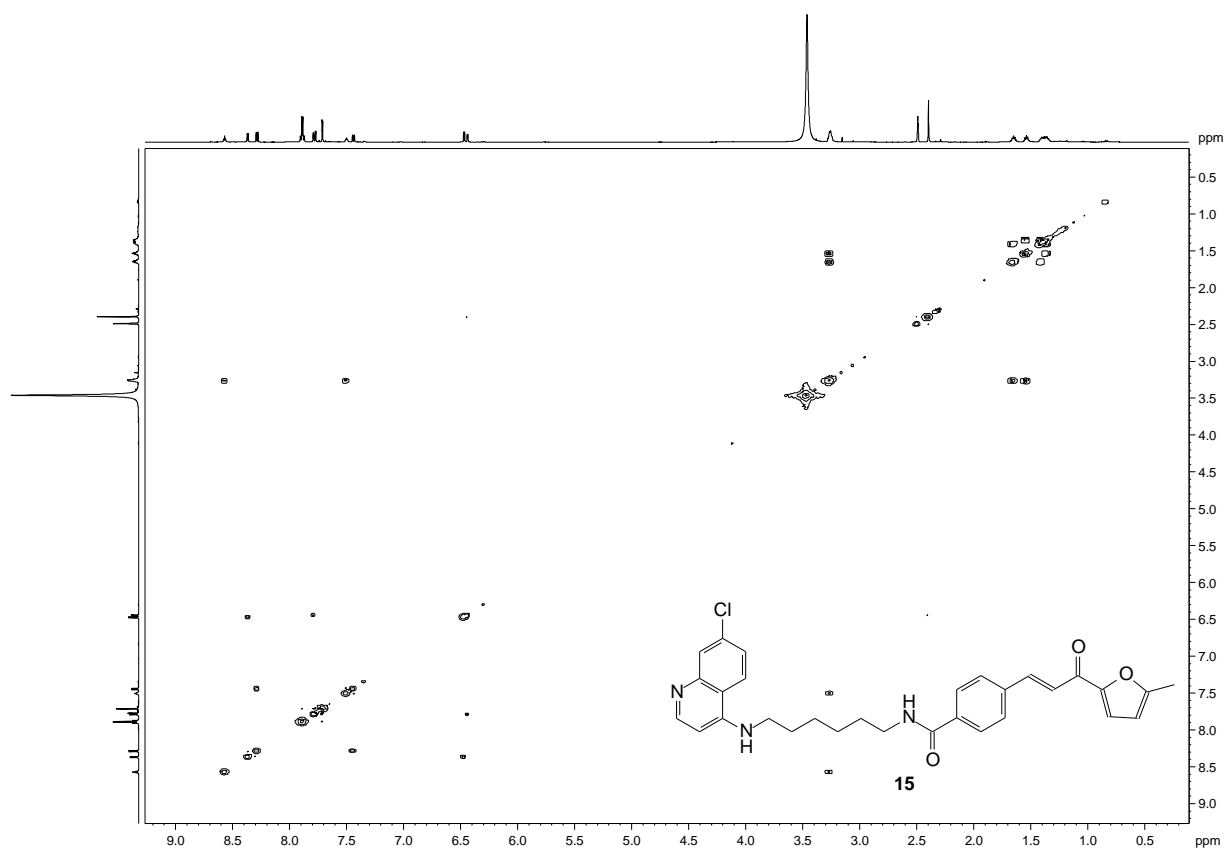


## DEPT135 in DMSO: 15

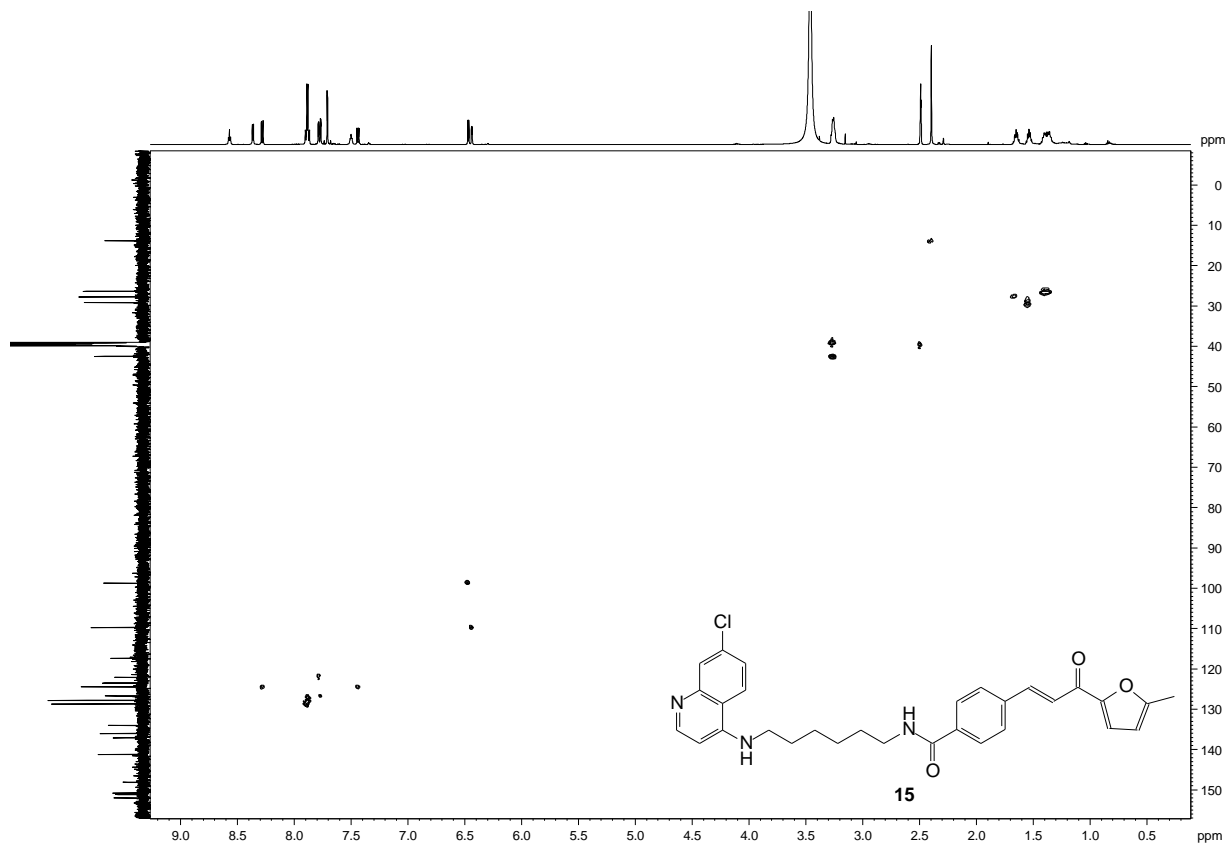


Addendum A – Chapter 3

COSY in DMSO: 15



HSQC in DMSO: 15

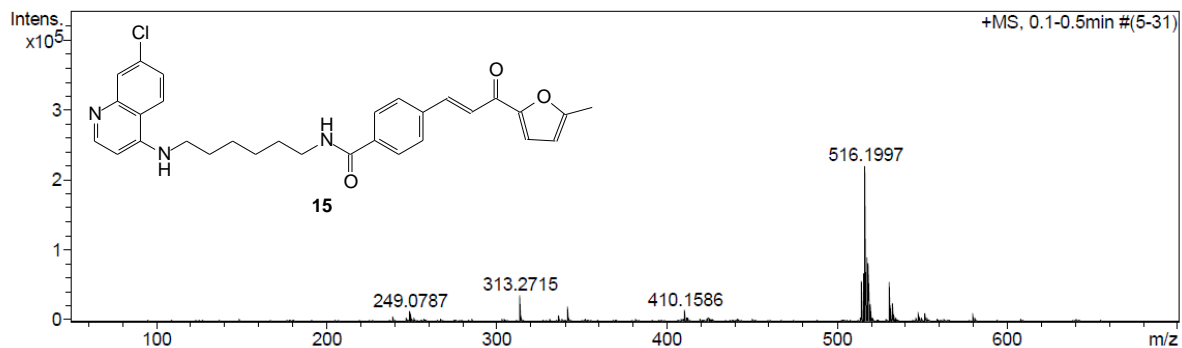


# Addendum A – Chapter 3

## HRMS: 15

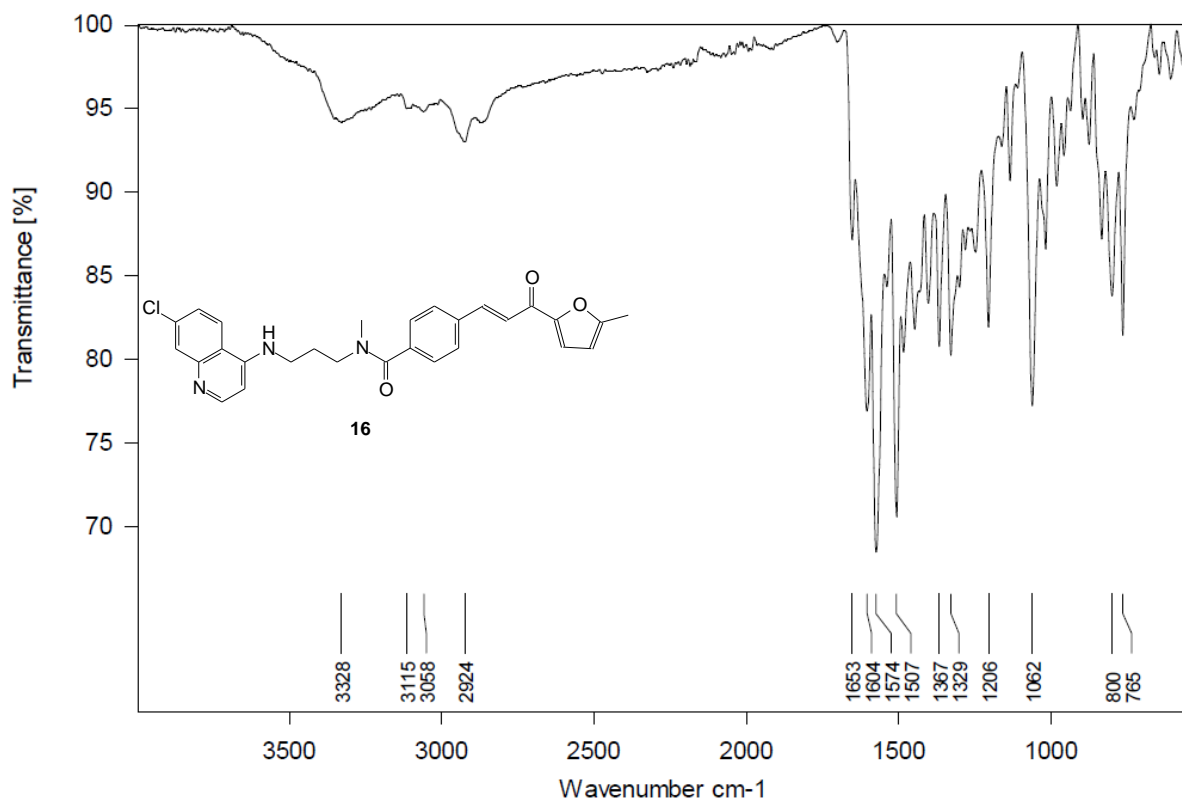
### Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	3000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste

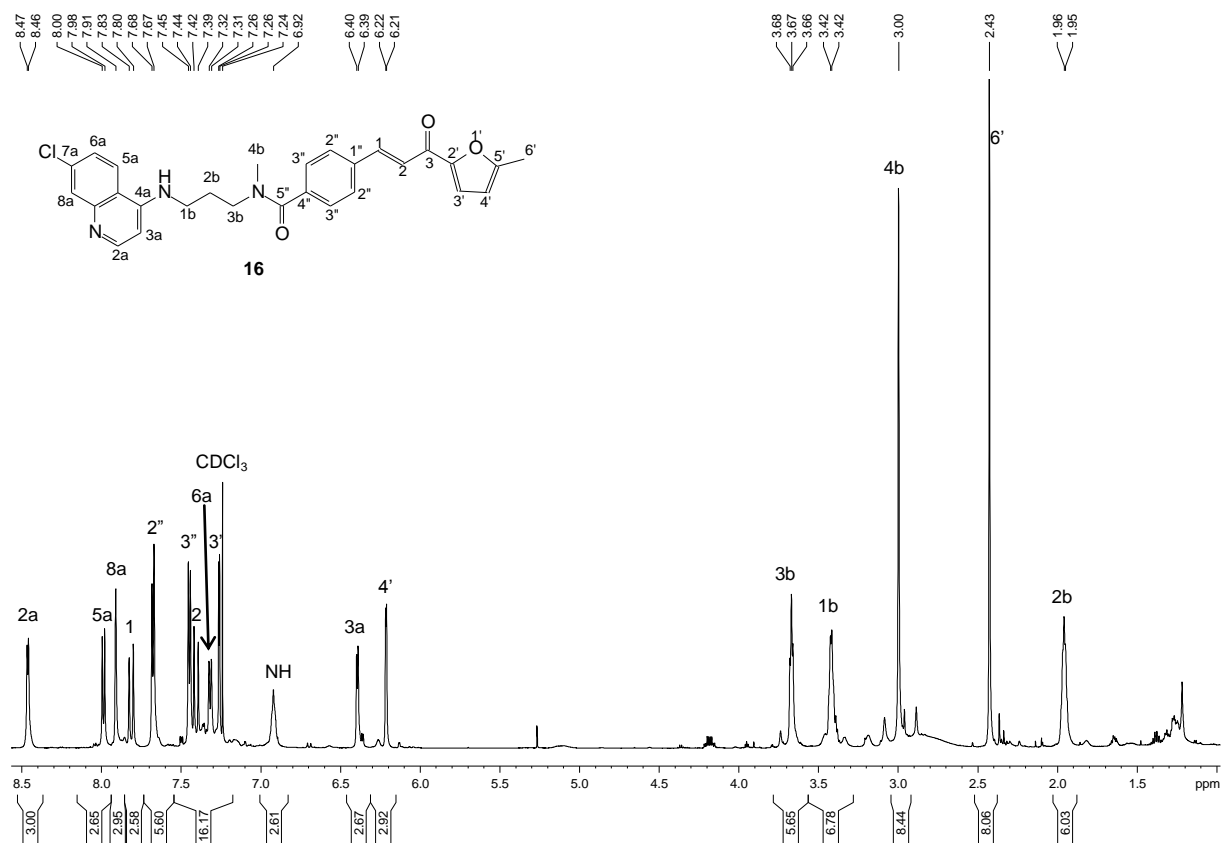


Addendum A – Chapter 3

IR: 16

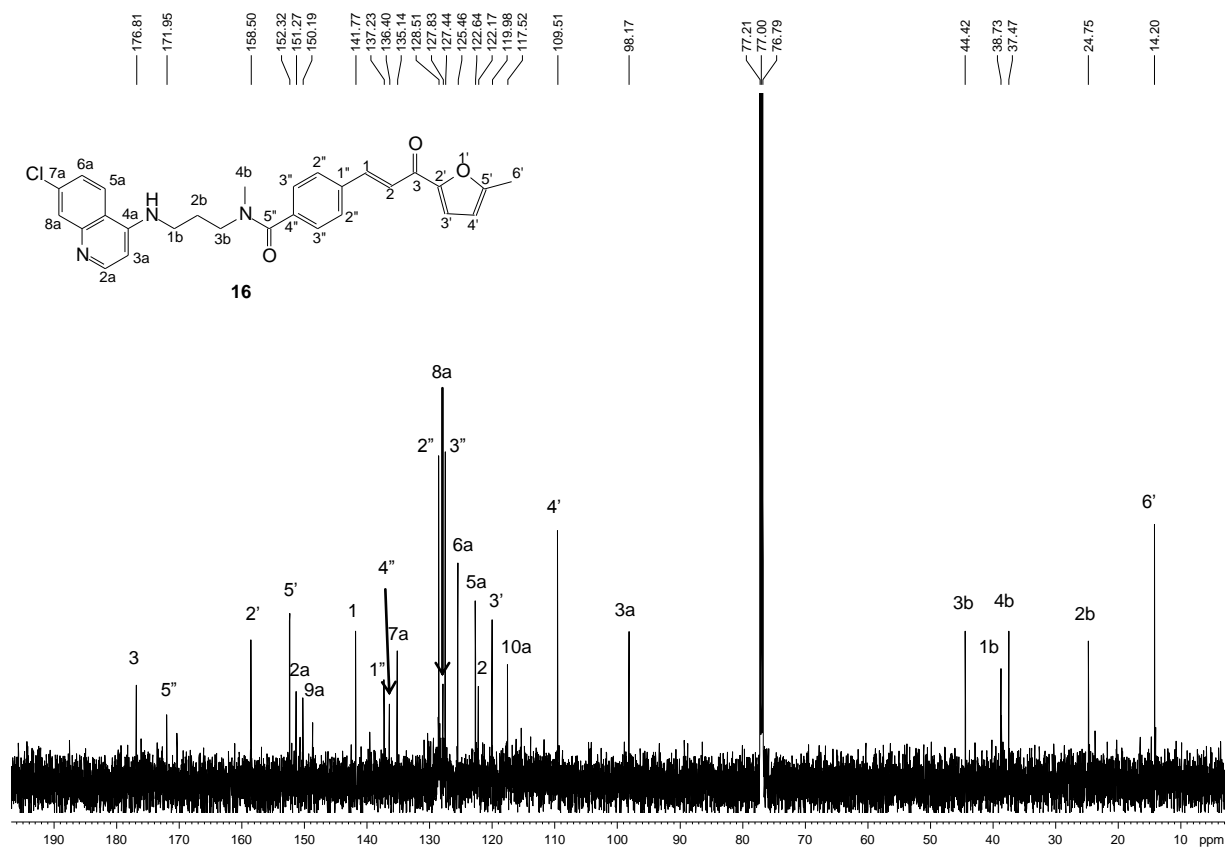


<sup>1</sup>H NMR in DMSO: 16

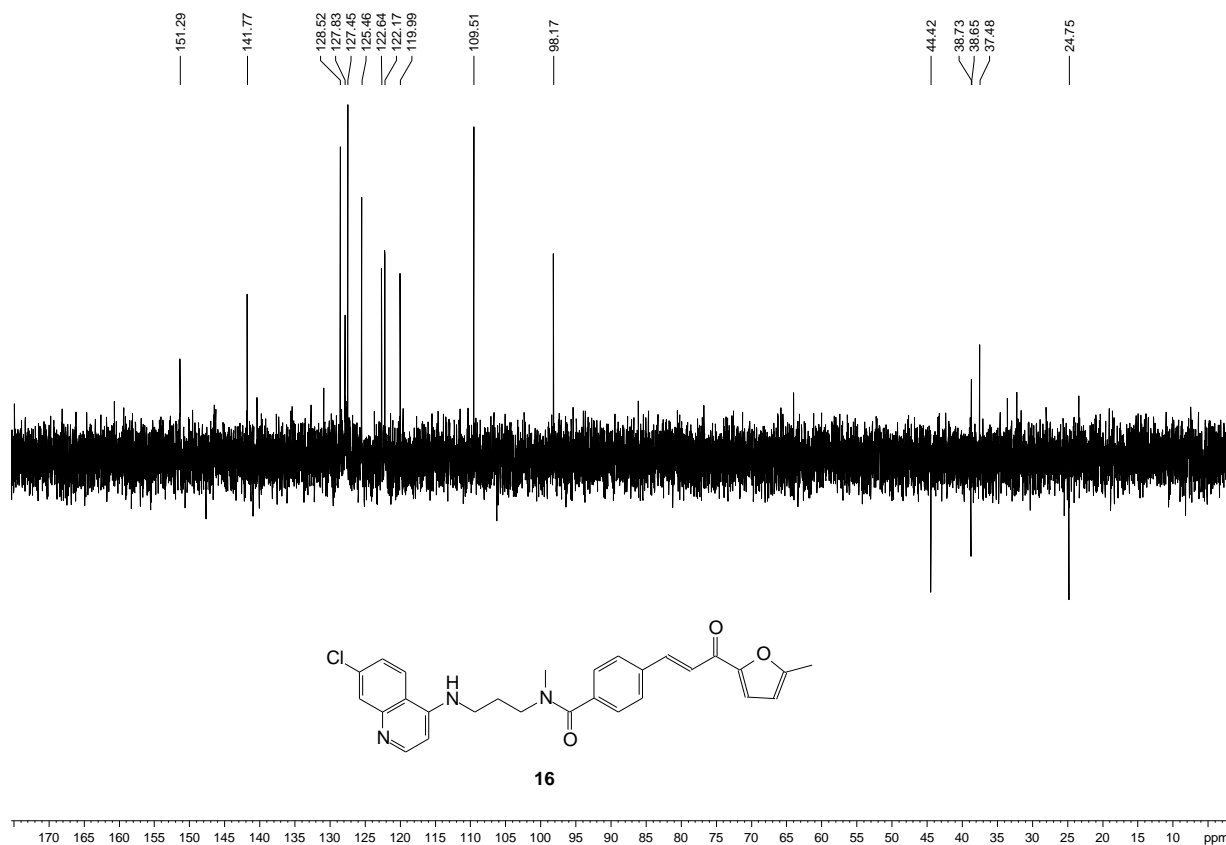


# Addendum A – Chapter 3

## <sup>13</sup>C NMR in DMSO: 16

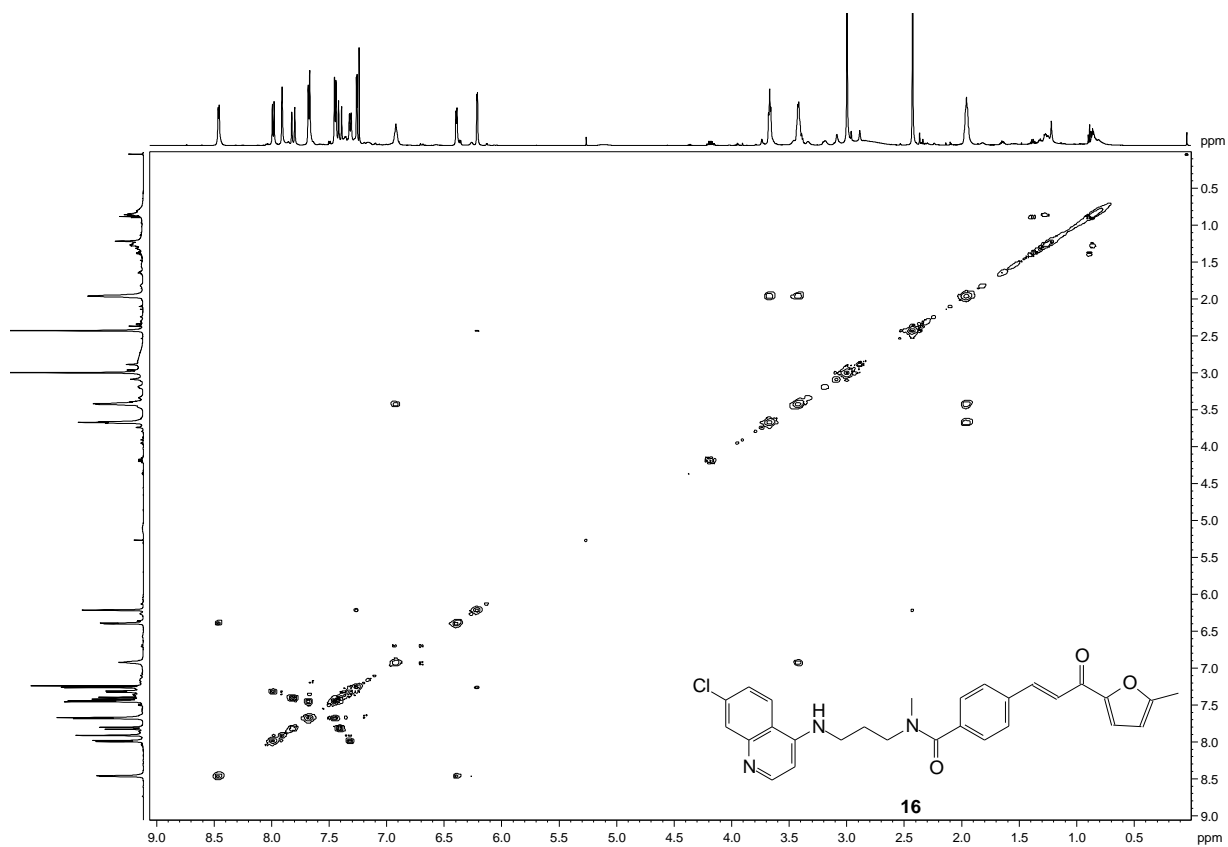


## DEPT135 in DMSO: 16

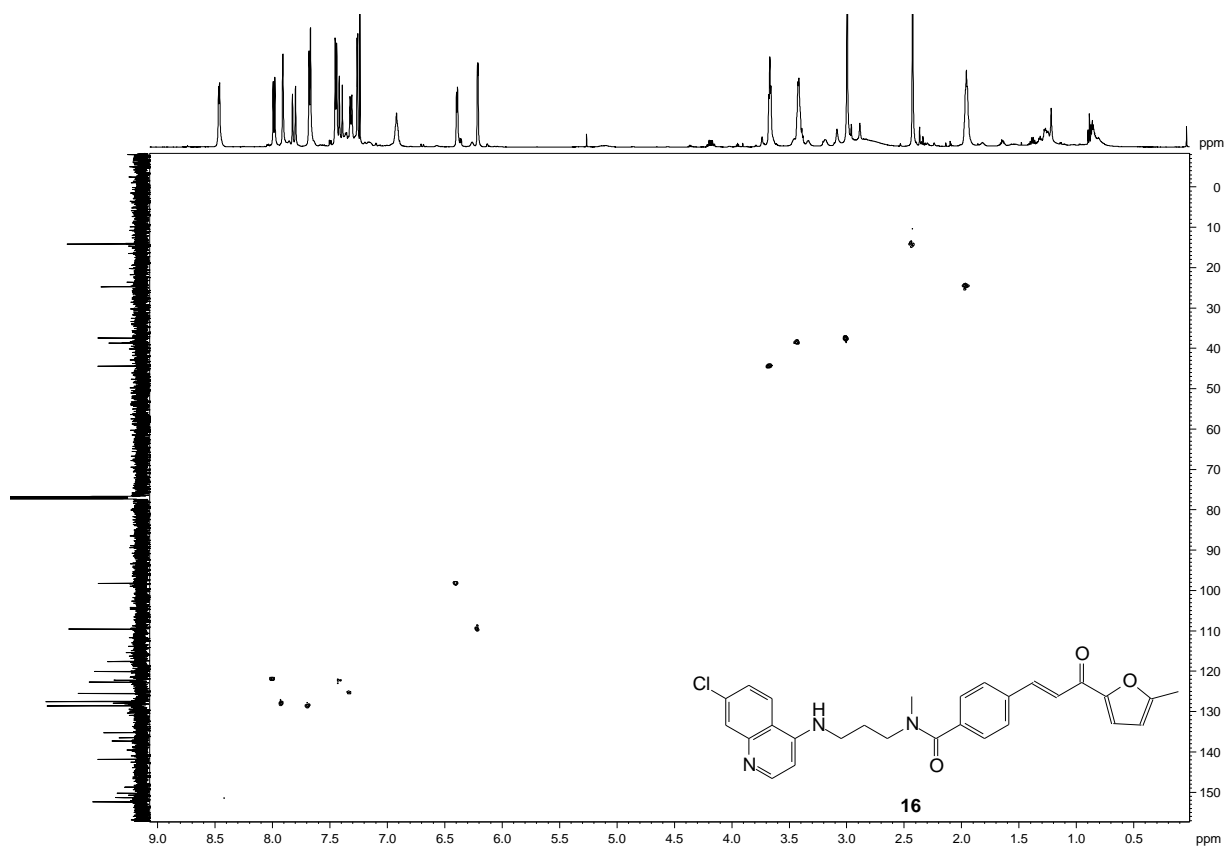


Addendum A – Chapter 3

COSY in DMSO: **16**



HSQC in DMSO: **16**

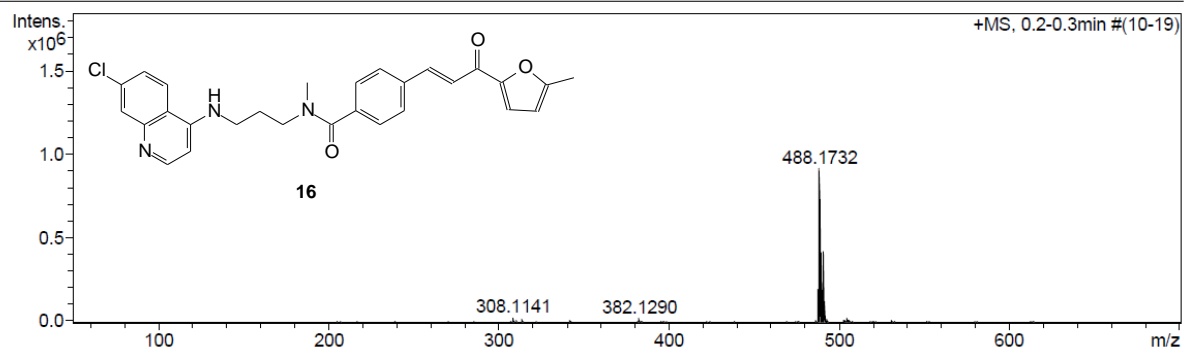


# Addendum A – Chapter 3

## HRMS: 16

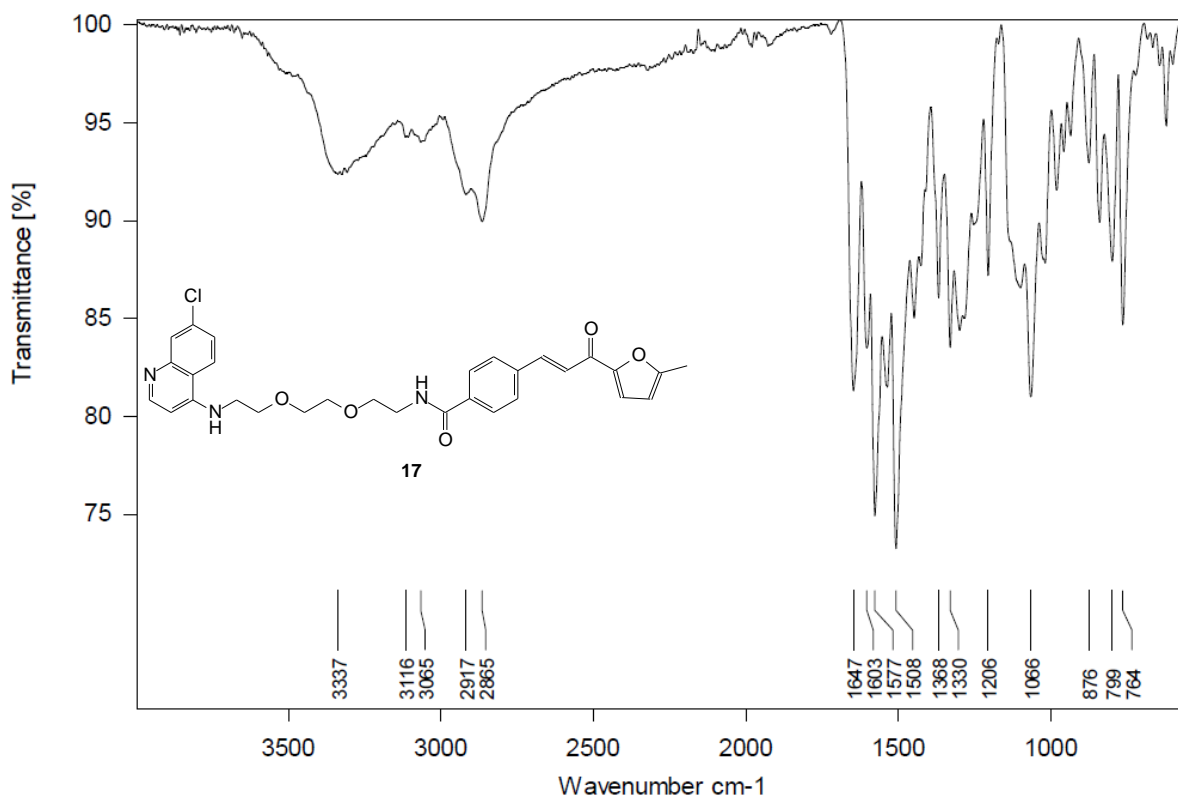
### Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	3000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste

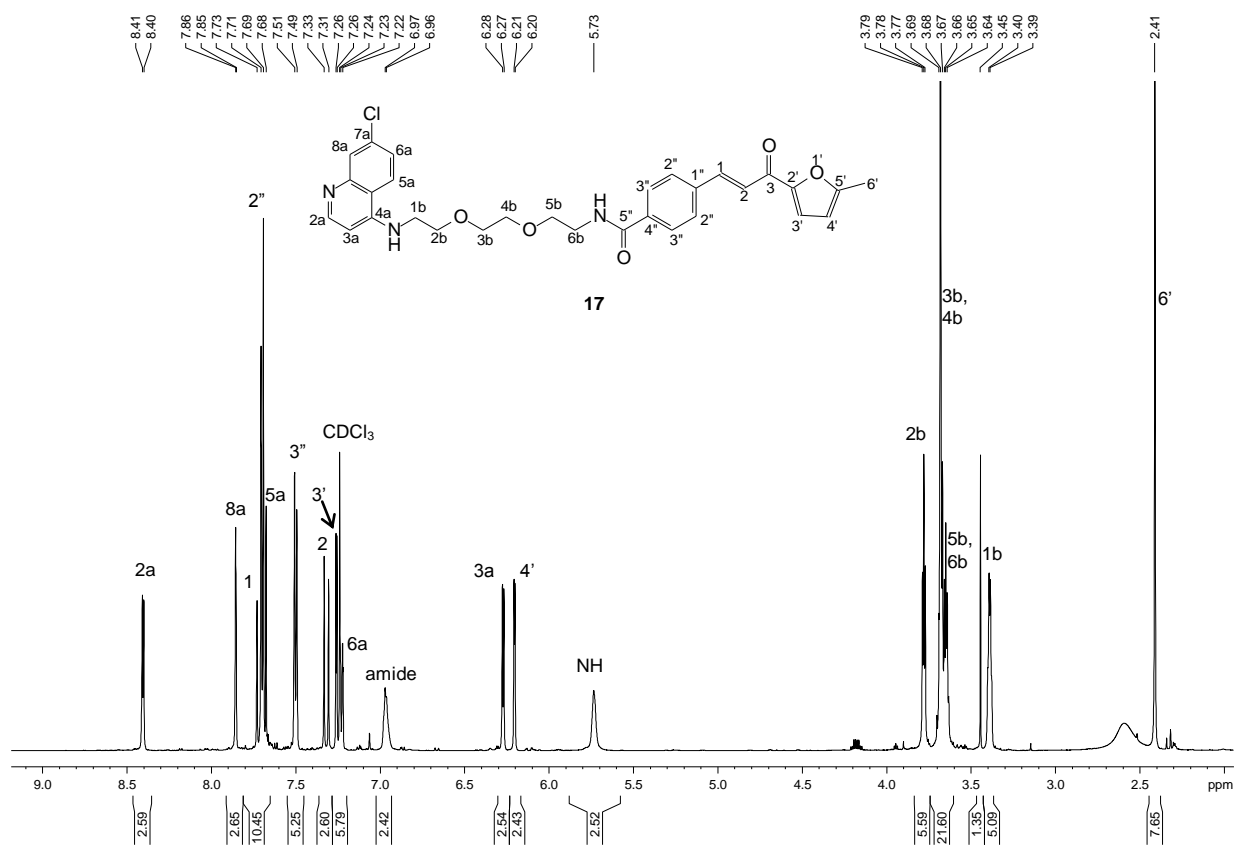


# Addendum A – Chapter 3

IR: 17

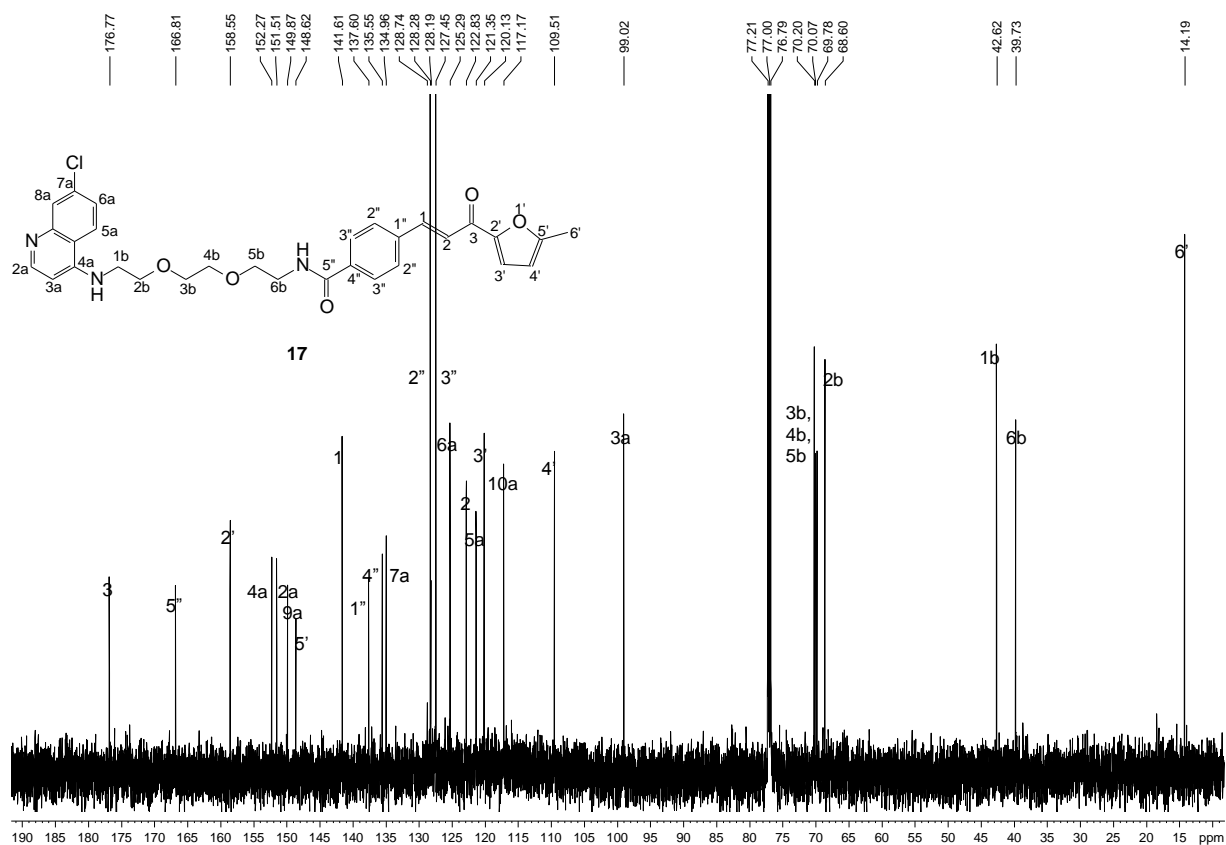


<sup>1</sup>H NMR in DMSO: 17

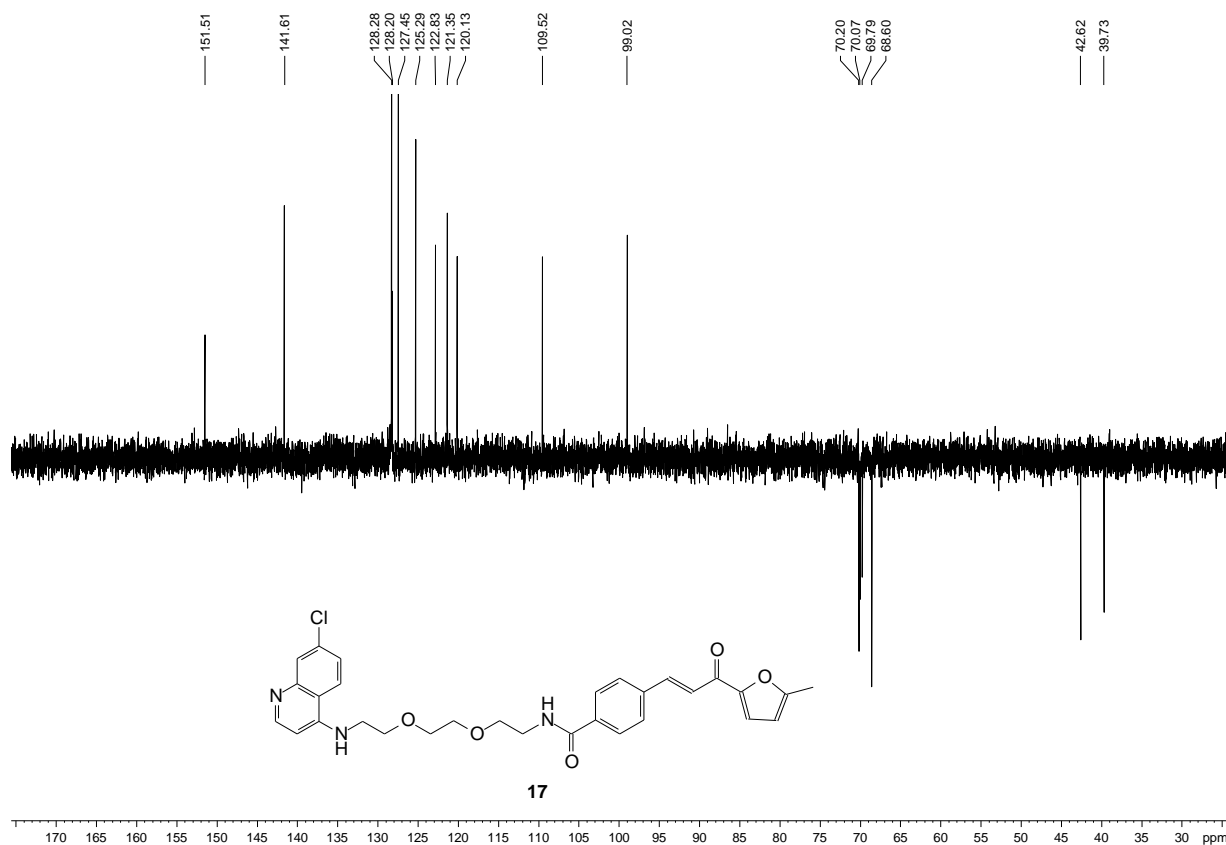


# Addendum A – Chapter 3

## <sup>13</sup>C NMR in DMSO: 17

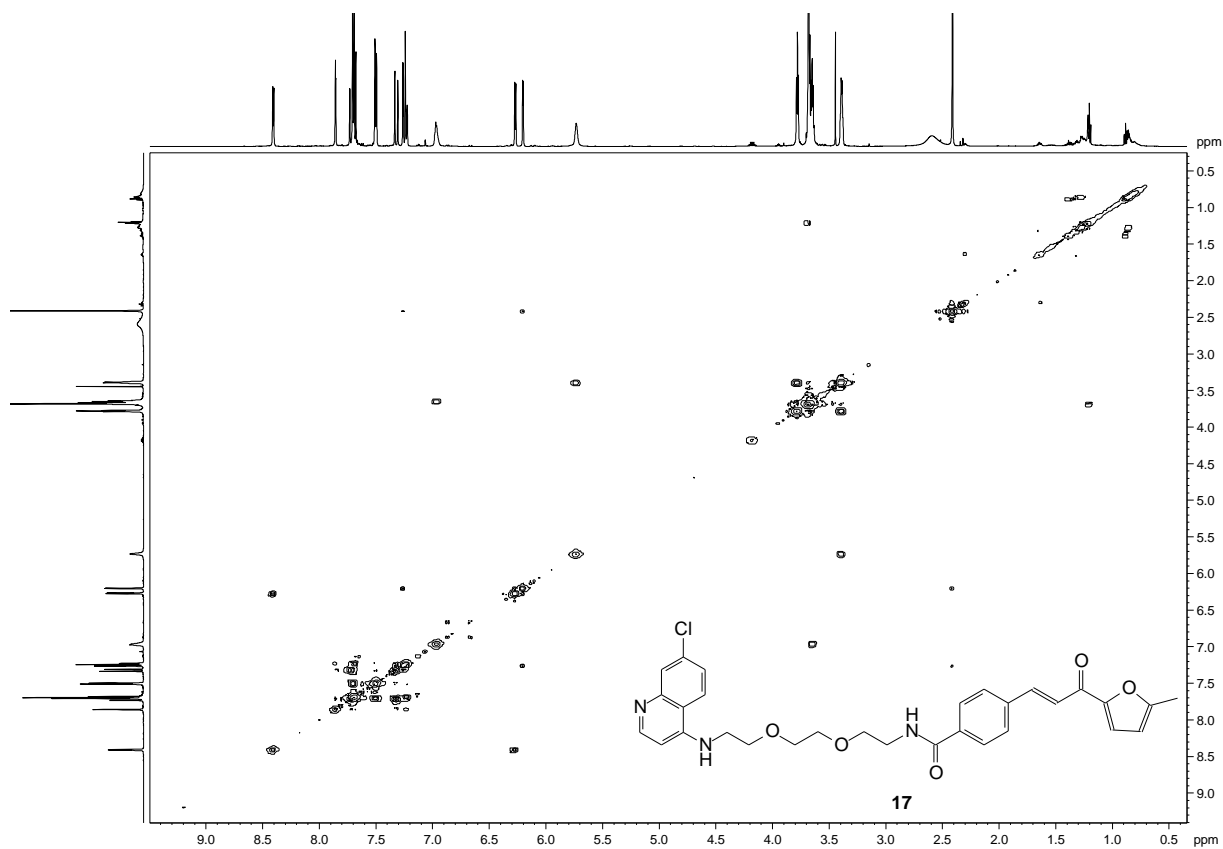


## DEPT135 in DMSO: 17

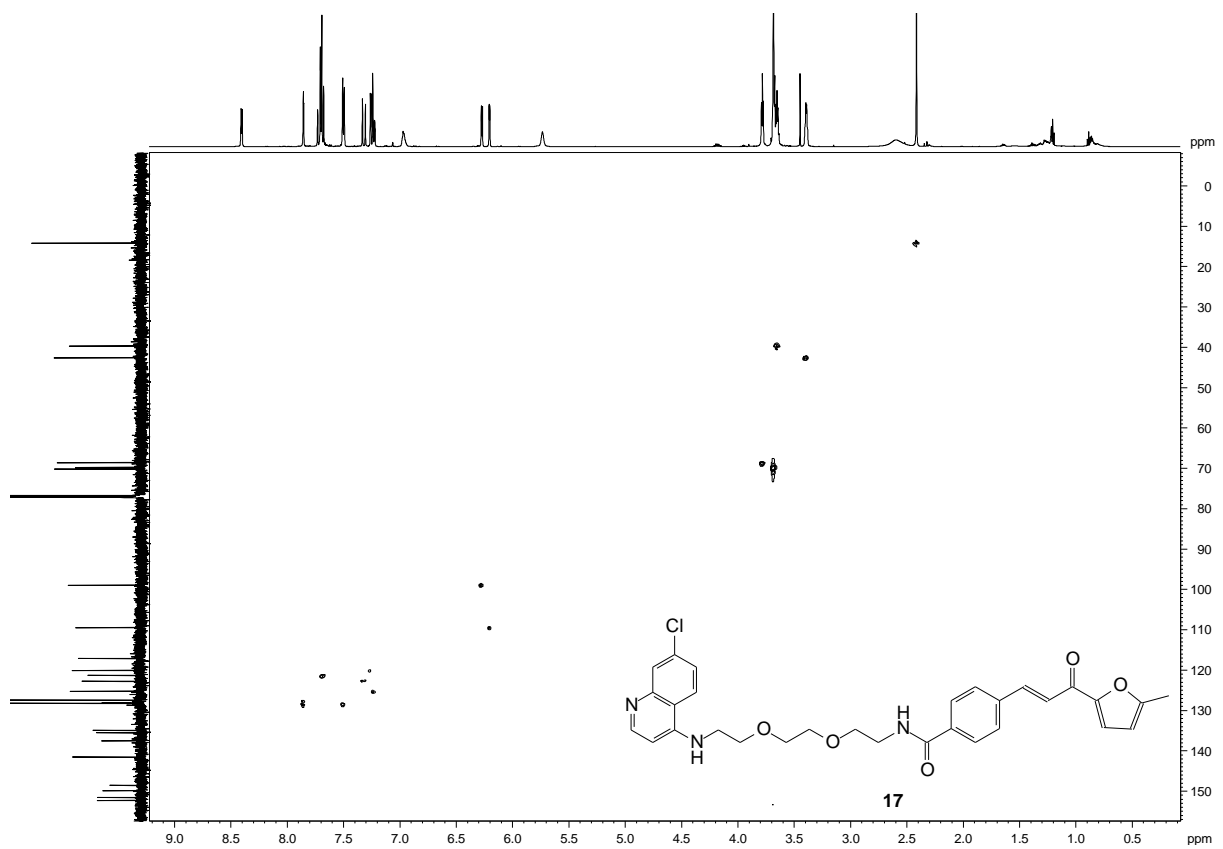


Addendum A – Chapter 3

COSY in DMSO: 17



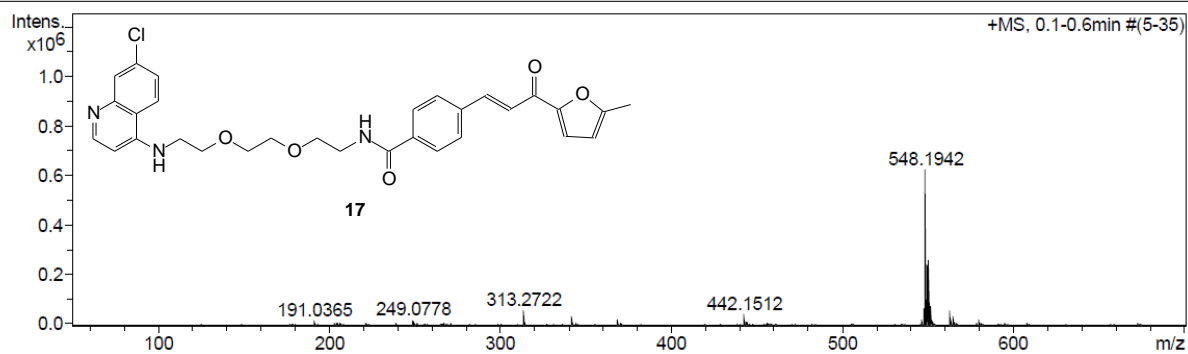
HSQC in DMSO: 17



# Addendum A – Chapter 3

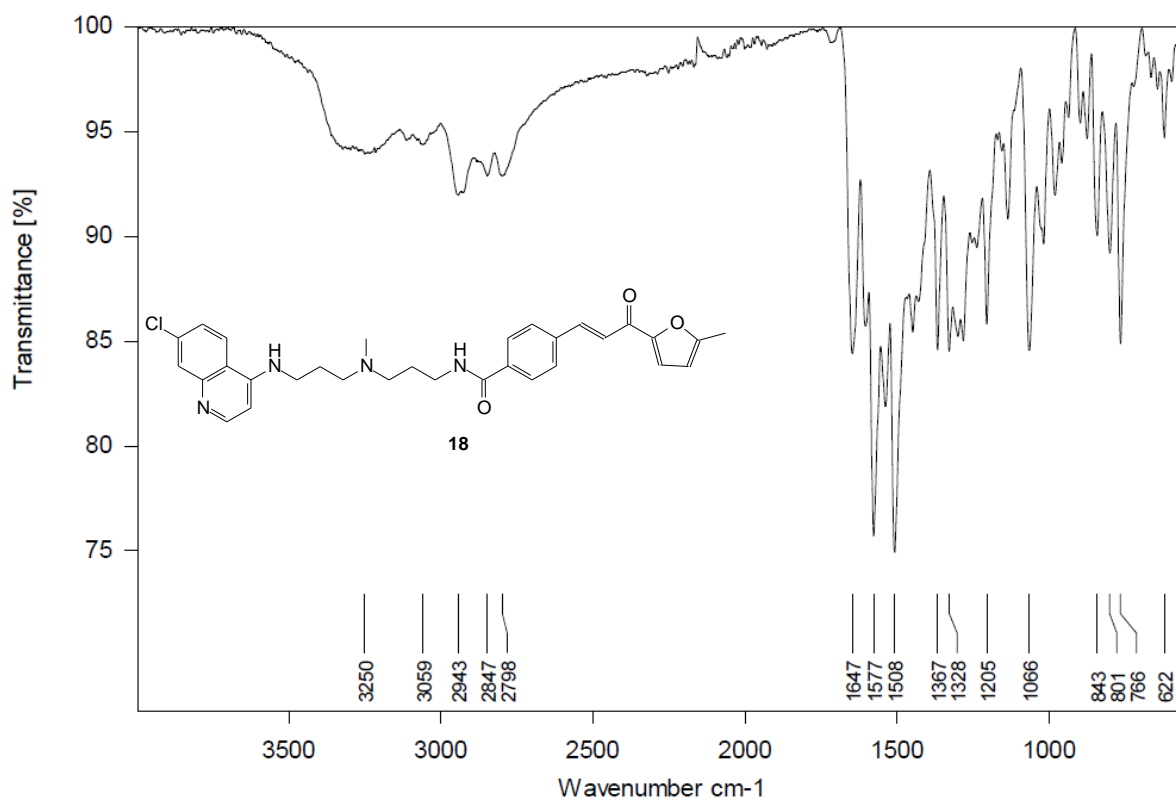
## Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	3000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste

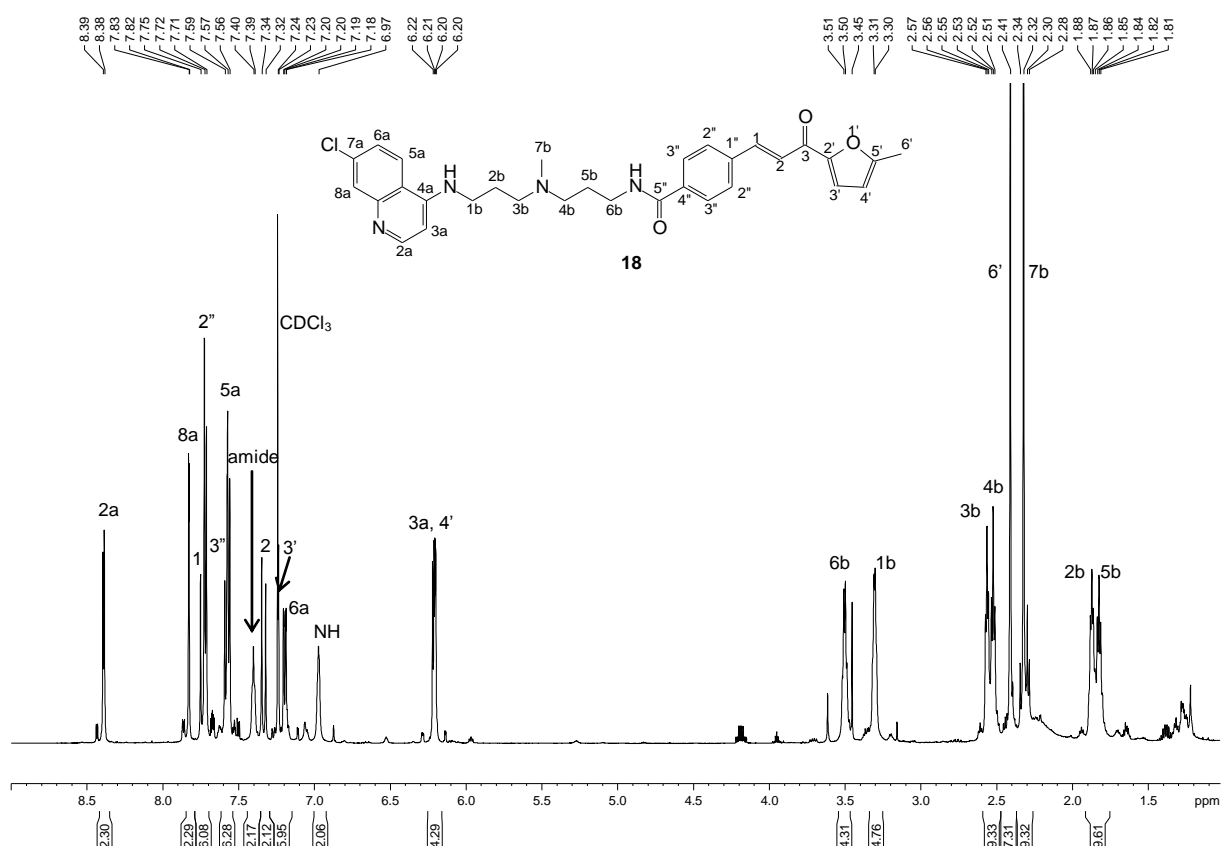


# Addendum A – Chapter 3

IR: **18**

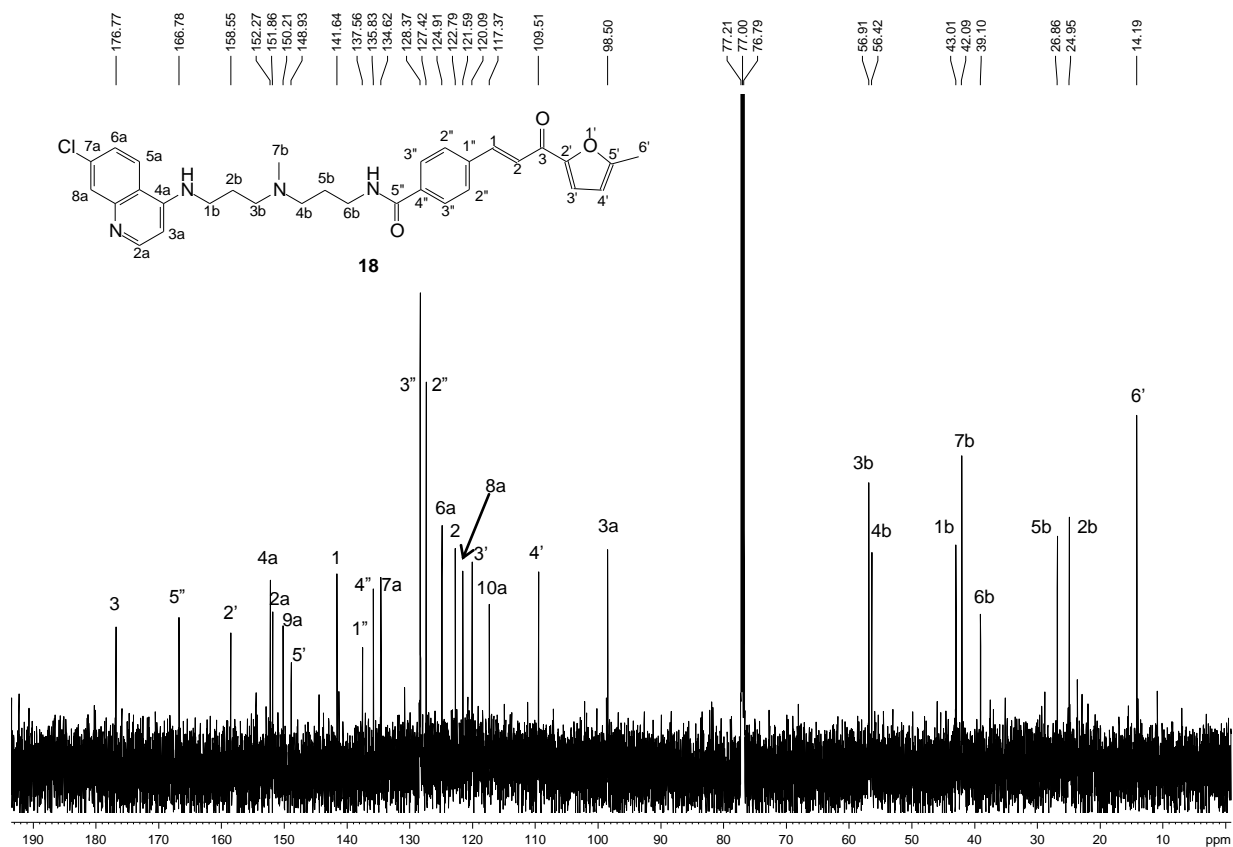


$^1\text{H}$  NMR in  $\text{CDCl}_3$ : **18**

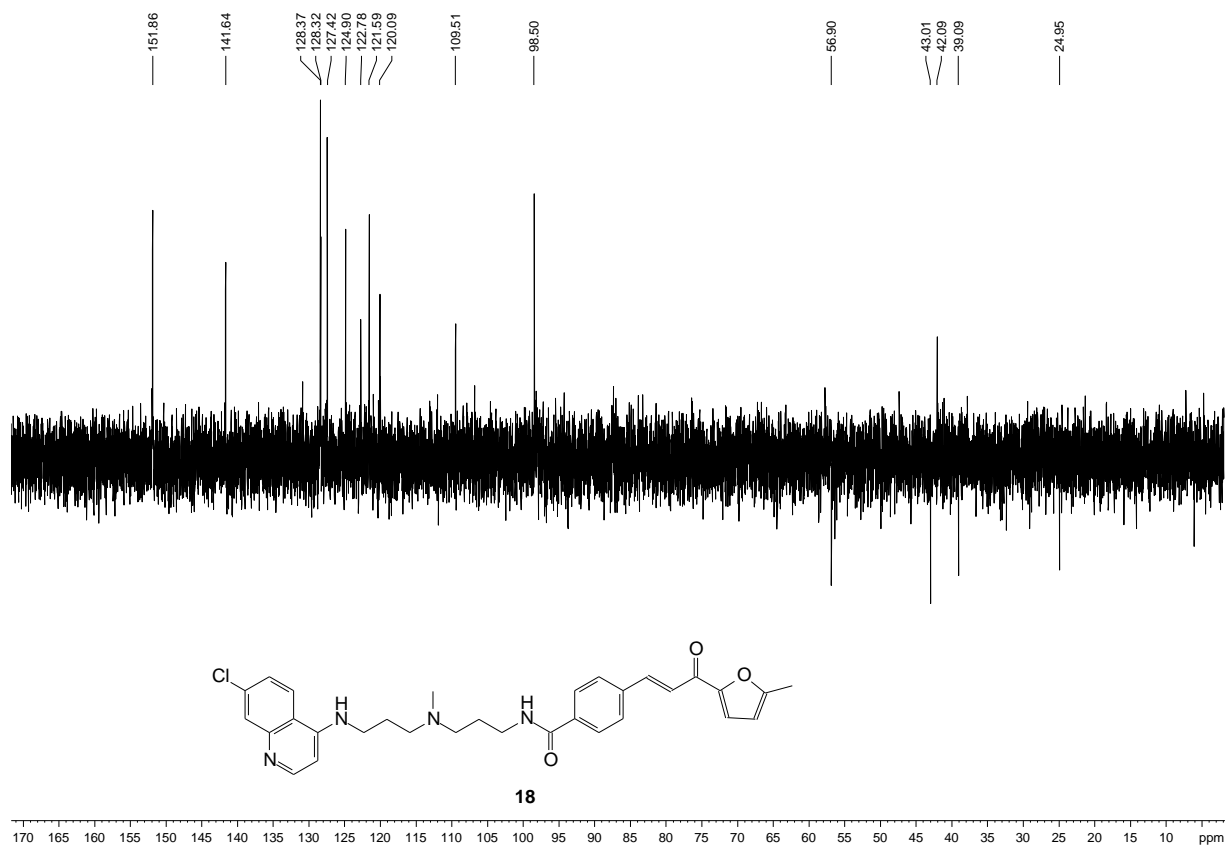


# Addendum A – Chapter 3

## <sup>13</sup>C NMR in CDCl<sub>3</sub>: 18

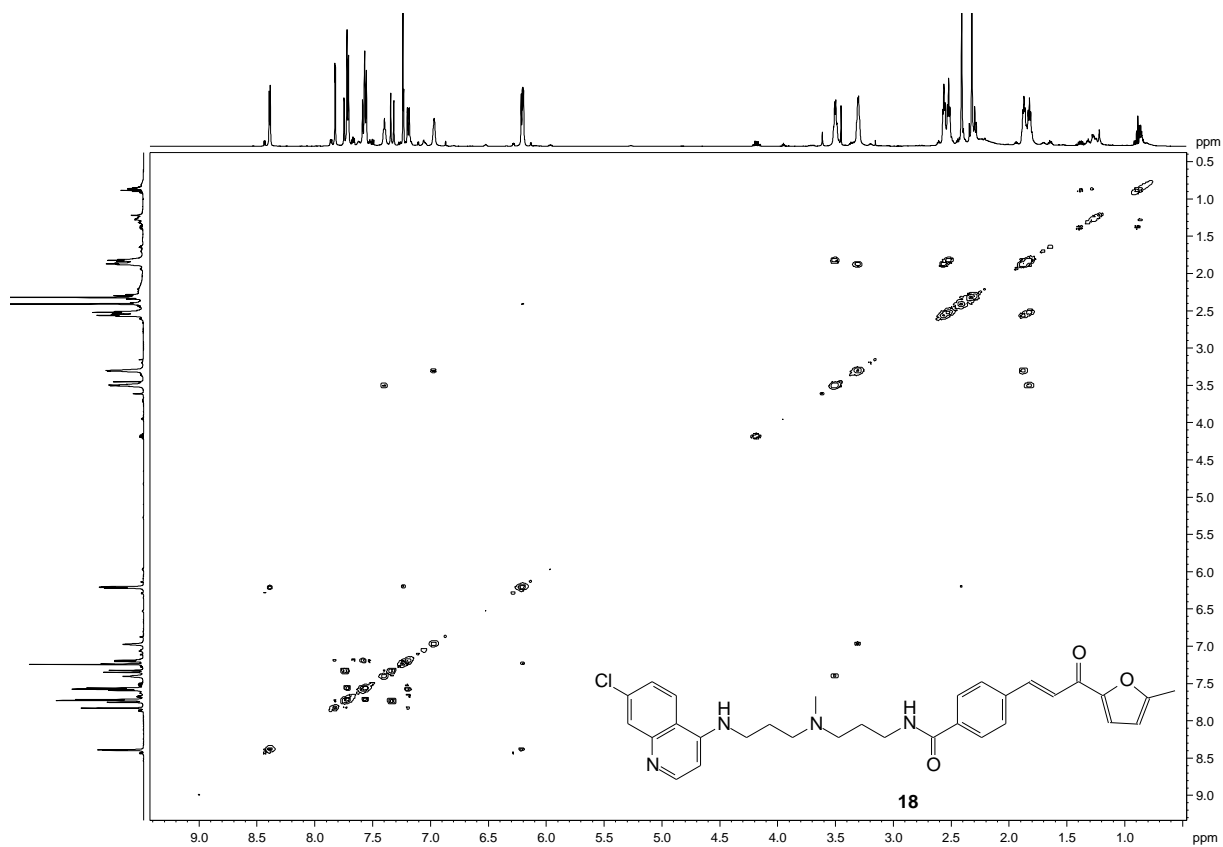


## DEPT in CDCl<sub>3</sub>: 18

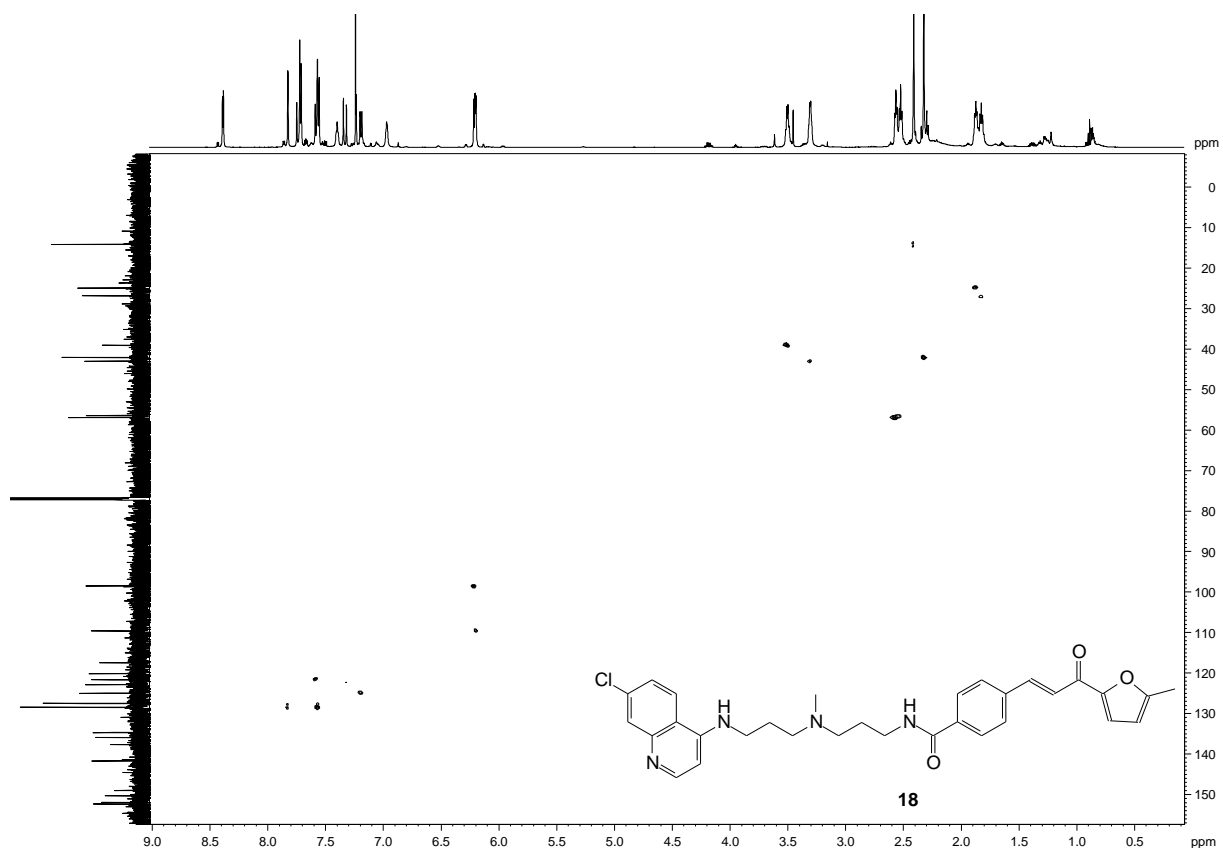


Addendum A – Chapter 3

COSY in CDCl<sub>3</sub>: **18**



HSQC in CDCl<sub>3</sub>: **18**

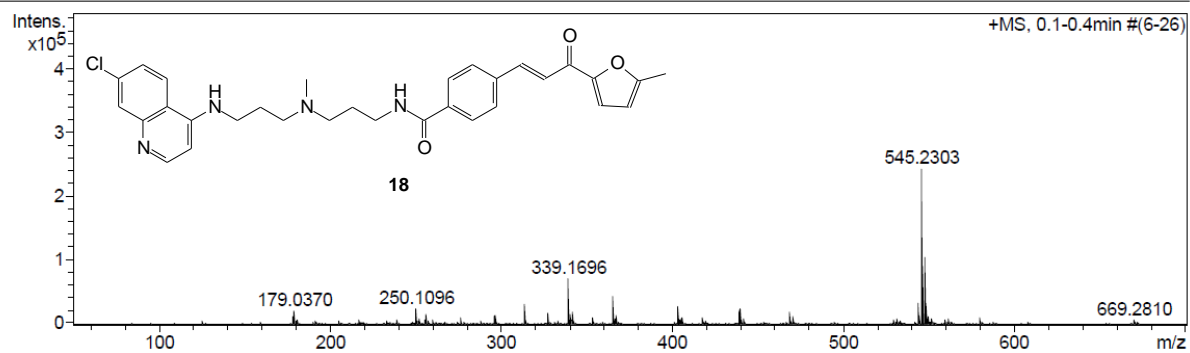


## Addendum A – Chapter 3

HRMS: 18

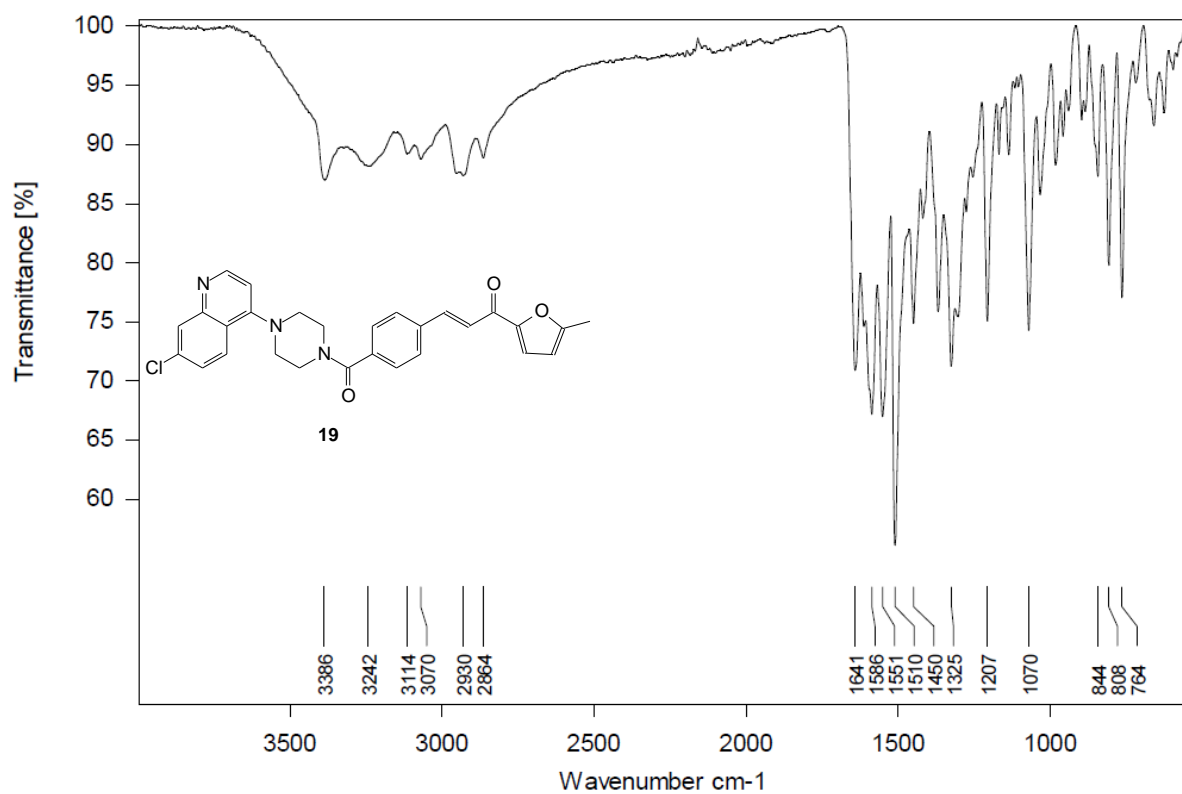
### Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	3000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste

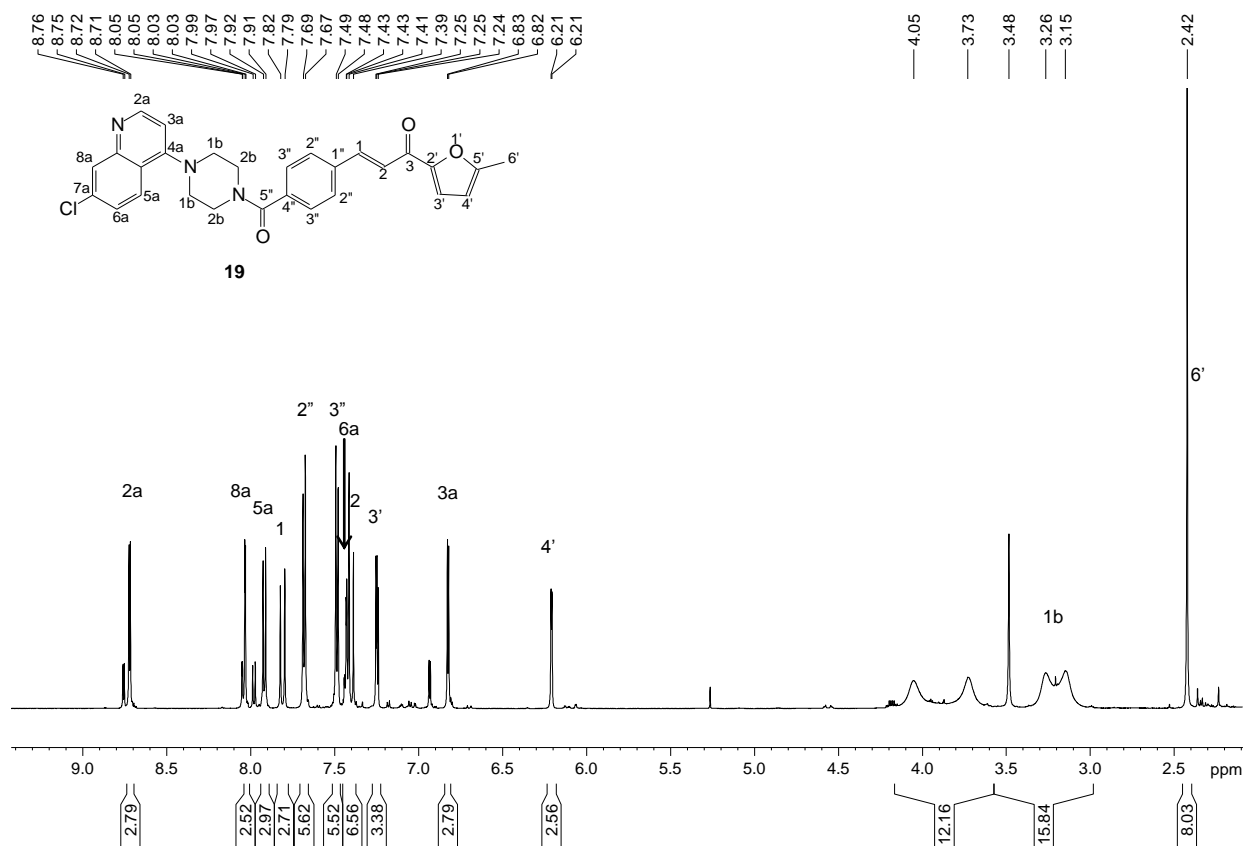


Addendum A – Chapter 3

IR: 19

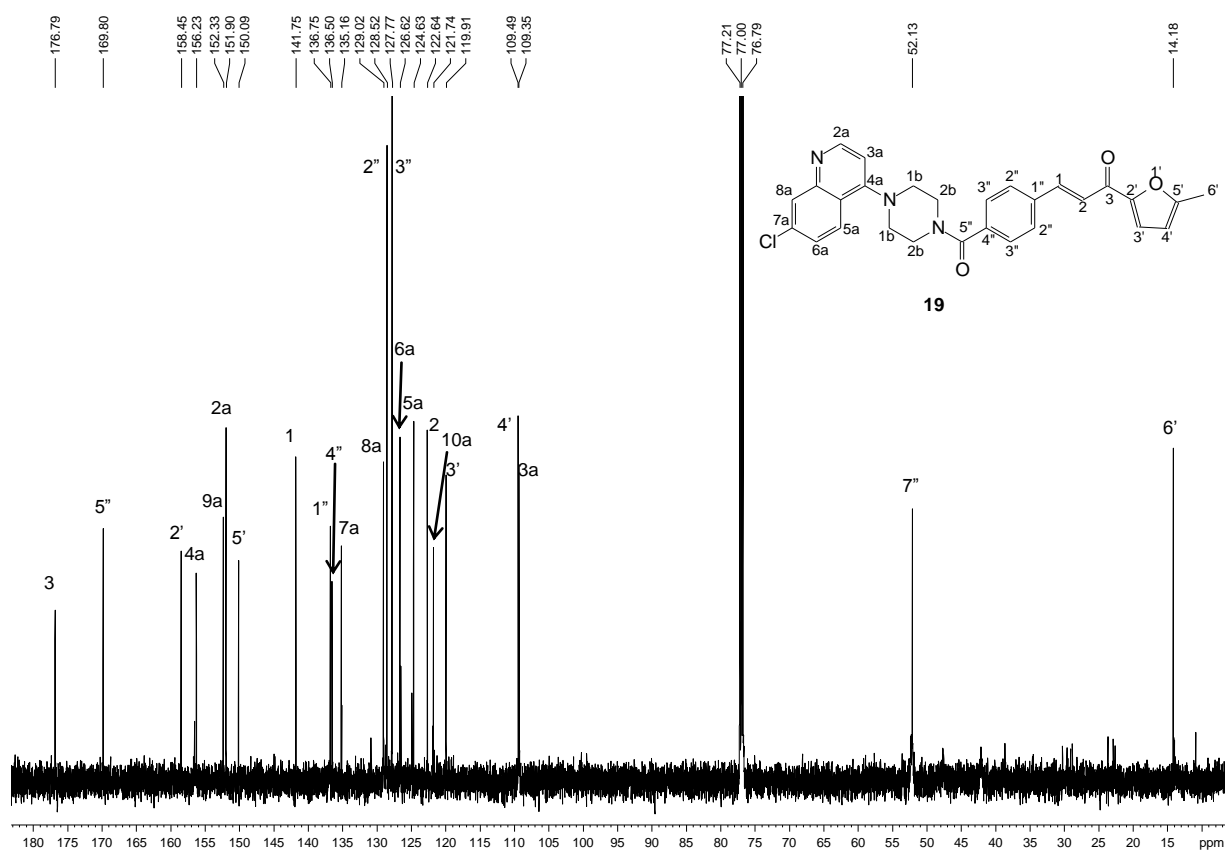


<sup>1</sup>H NMR in CDCl<sub>3</sub>: 19



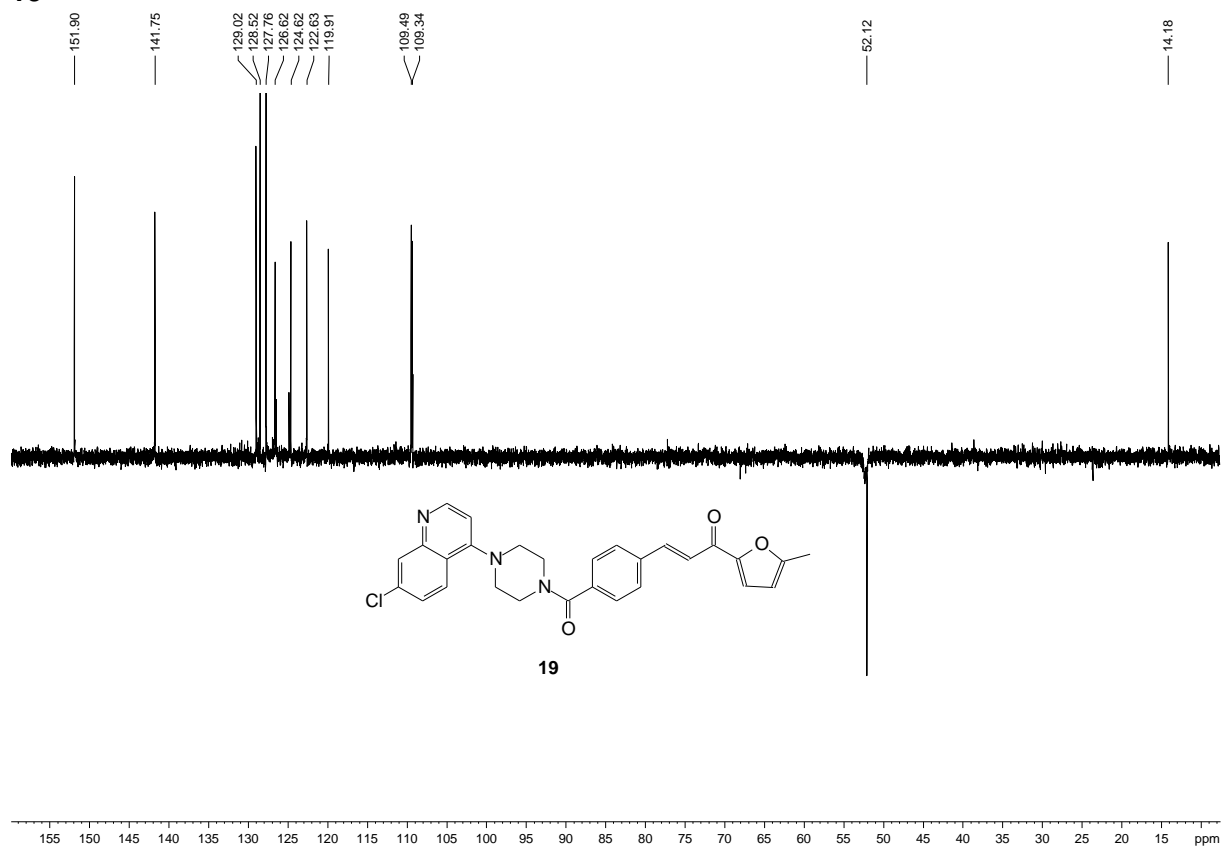
# Addendum A – Chapter 3

## <sup>13</sup>C NMR in CDCl<sub>3</sub>: 19



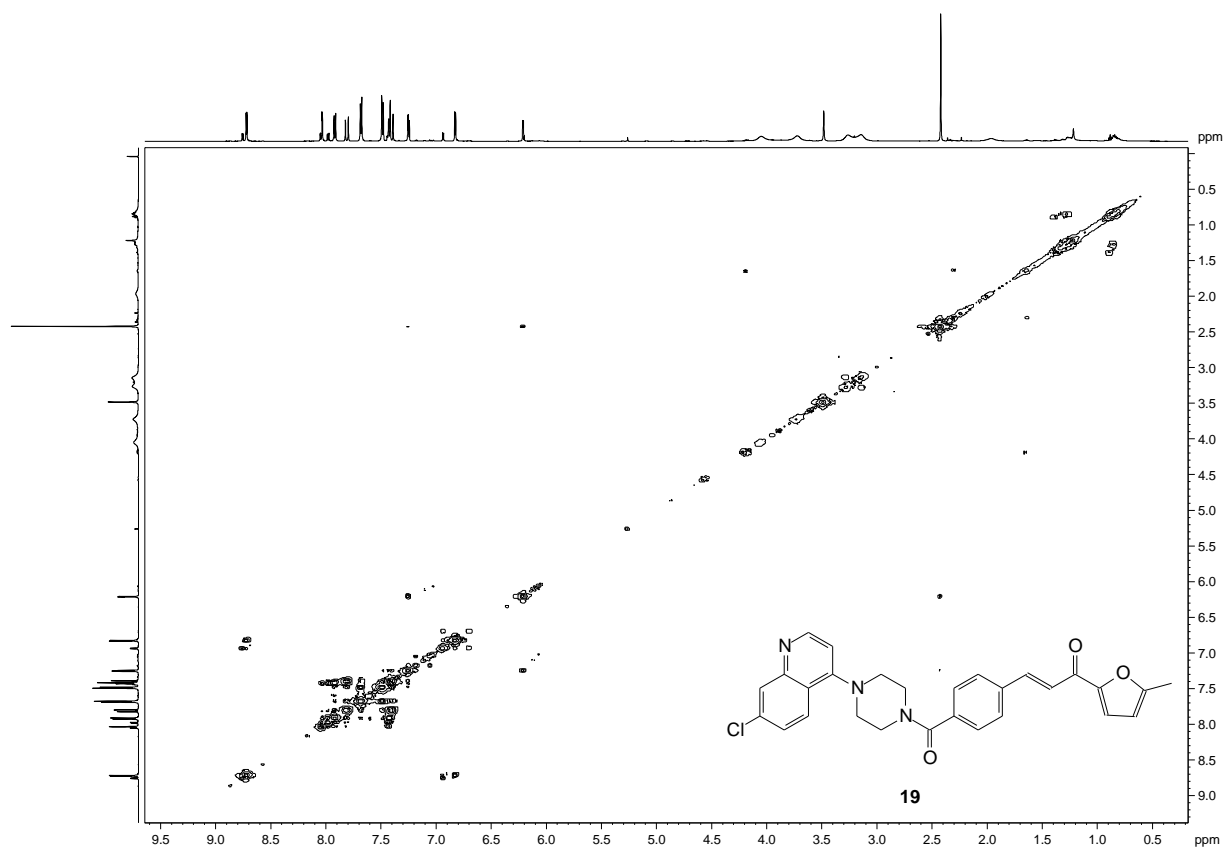
## DEPT135 in CDCl<sub>3</sub>:

### 19

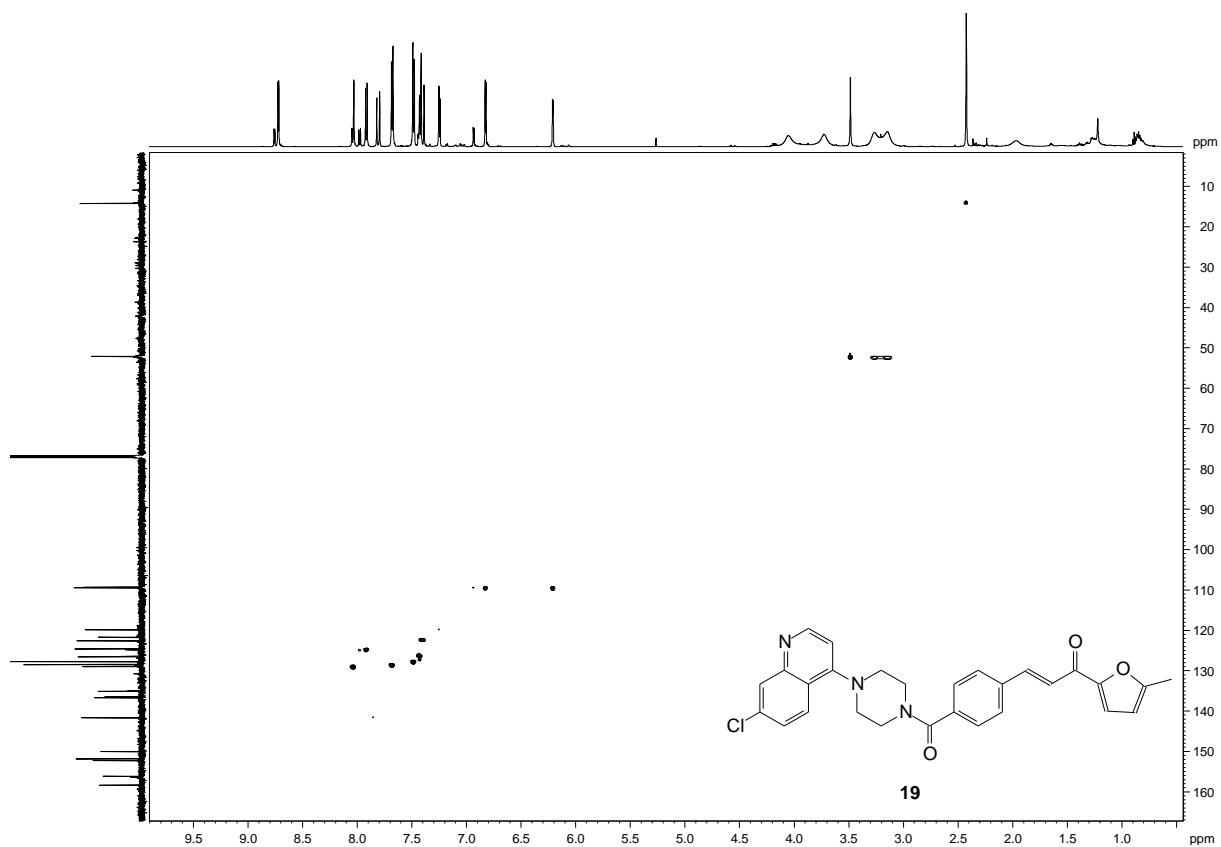


Addendum A – Chapter 3

COSY in CDCl<sub>3</sub>: **19**



HSQC in CDCl<sub>3</sub>: **19**

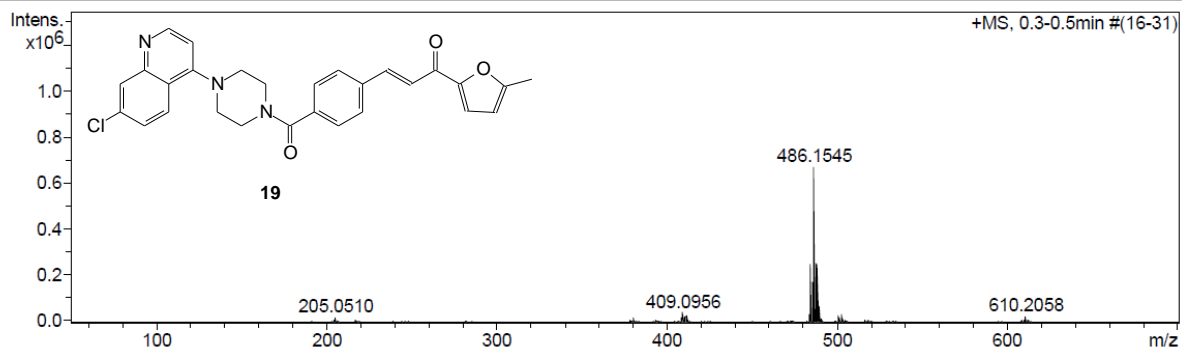


# Addendum A – Chapter 3

## HRMS: 19

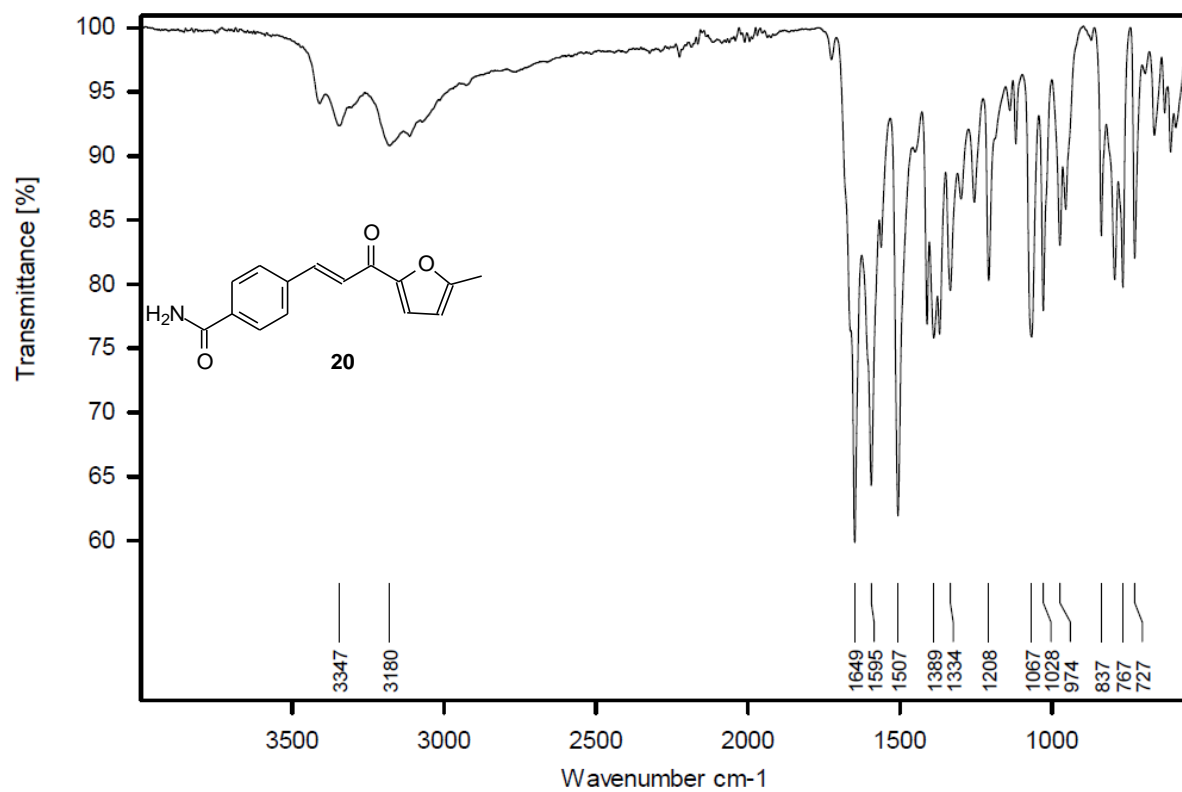
### Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	3000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste

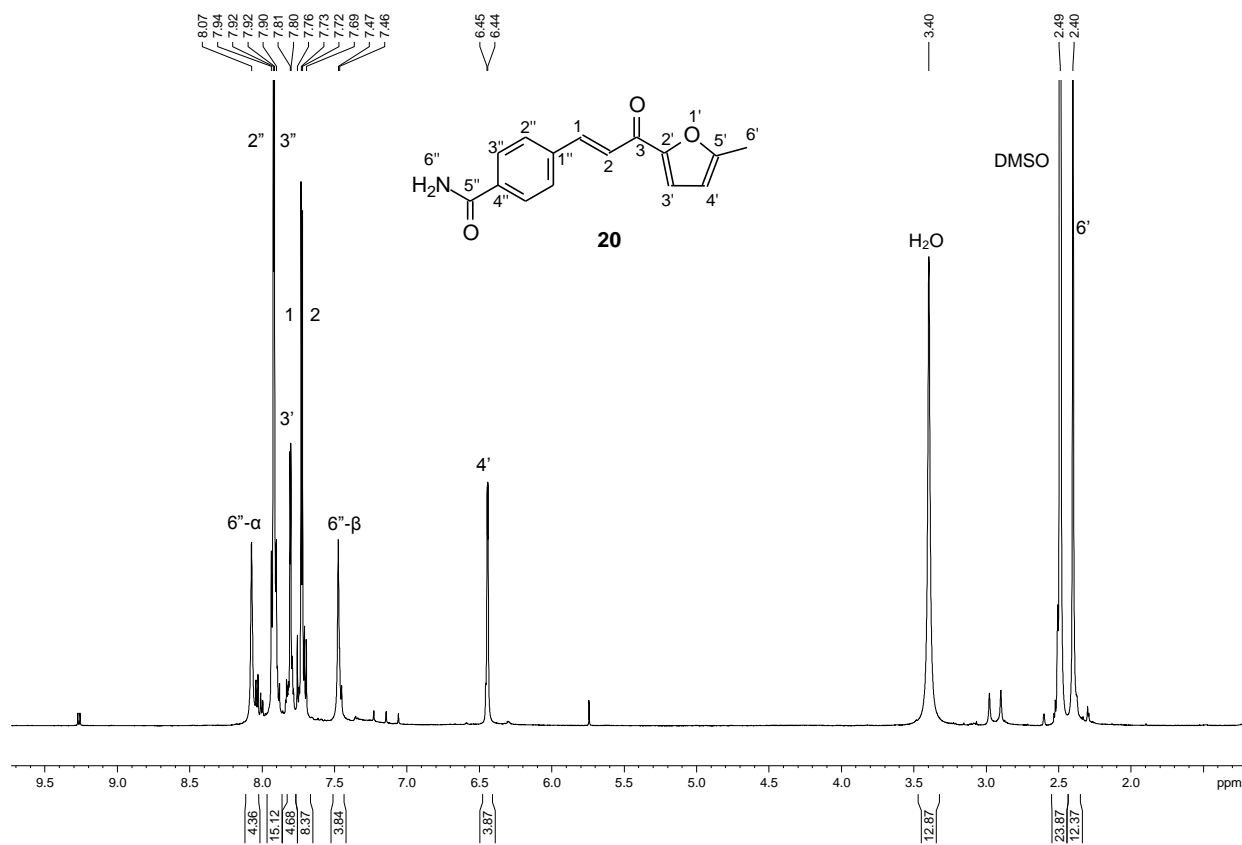


Addendum A – Chapter 3

IR: **20**

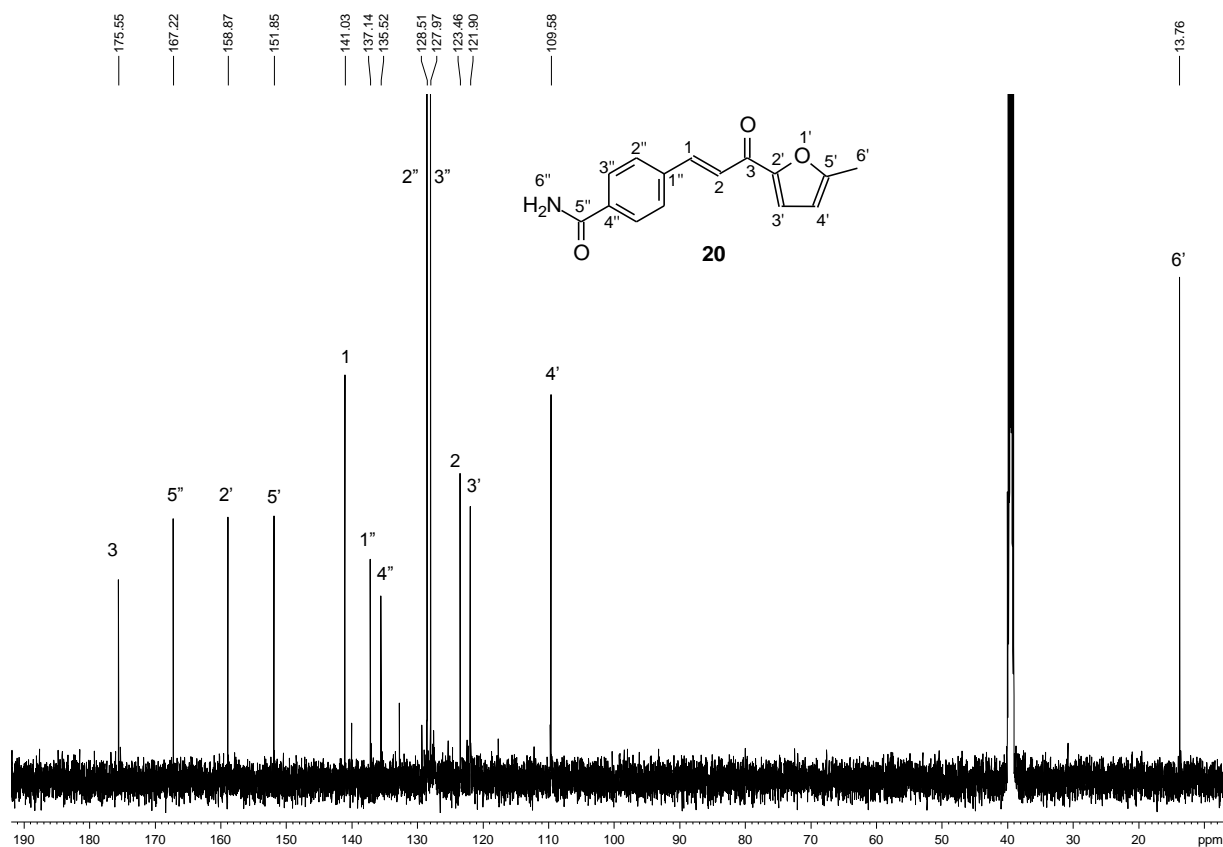


<sup>1</sup>H NMR in DMSO: **20**

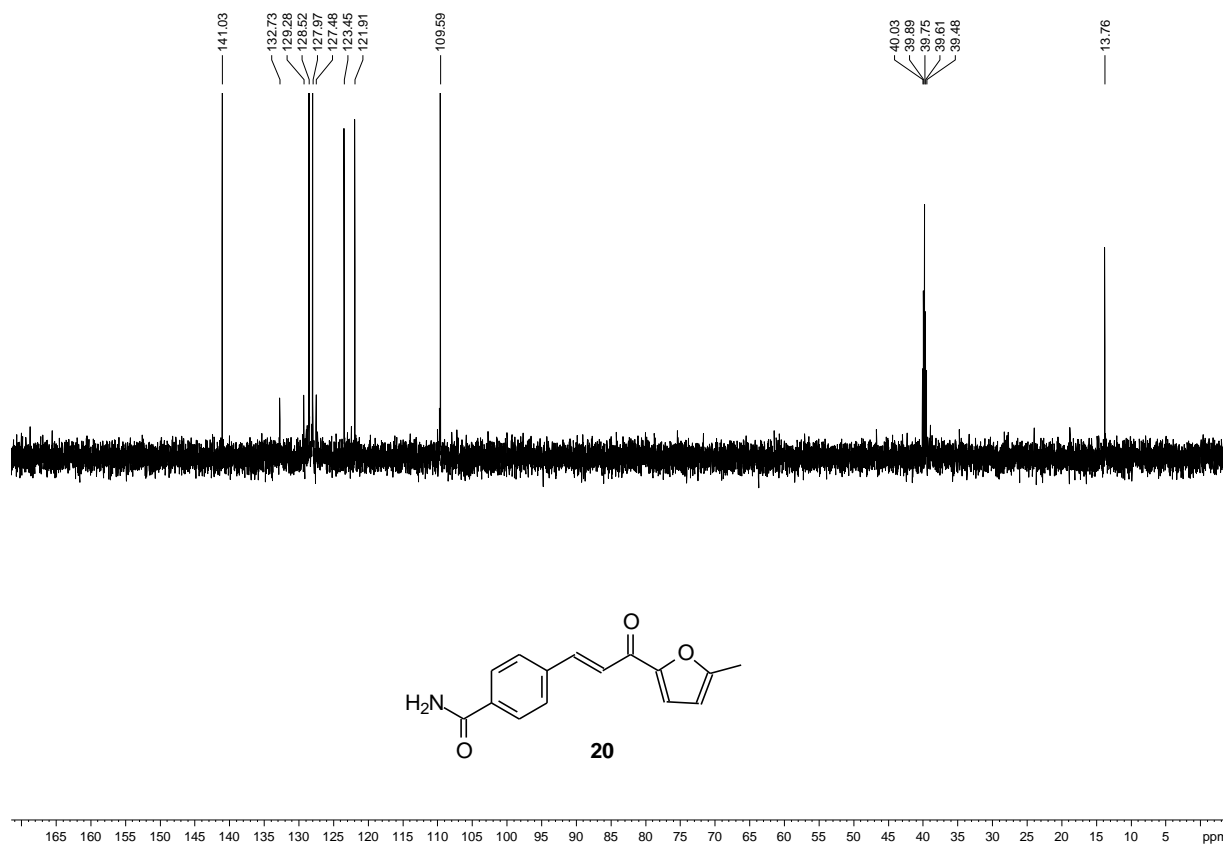


# Addendum A – Chapter 3

## <sup>13</sup>C NMR in DMSO: **20**

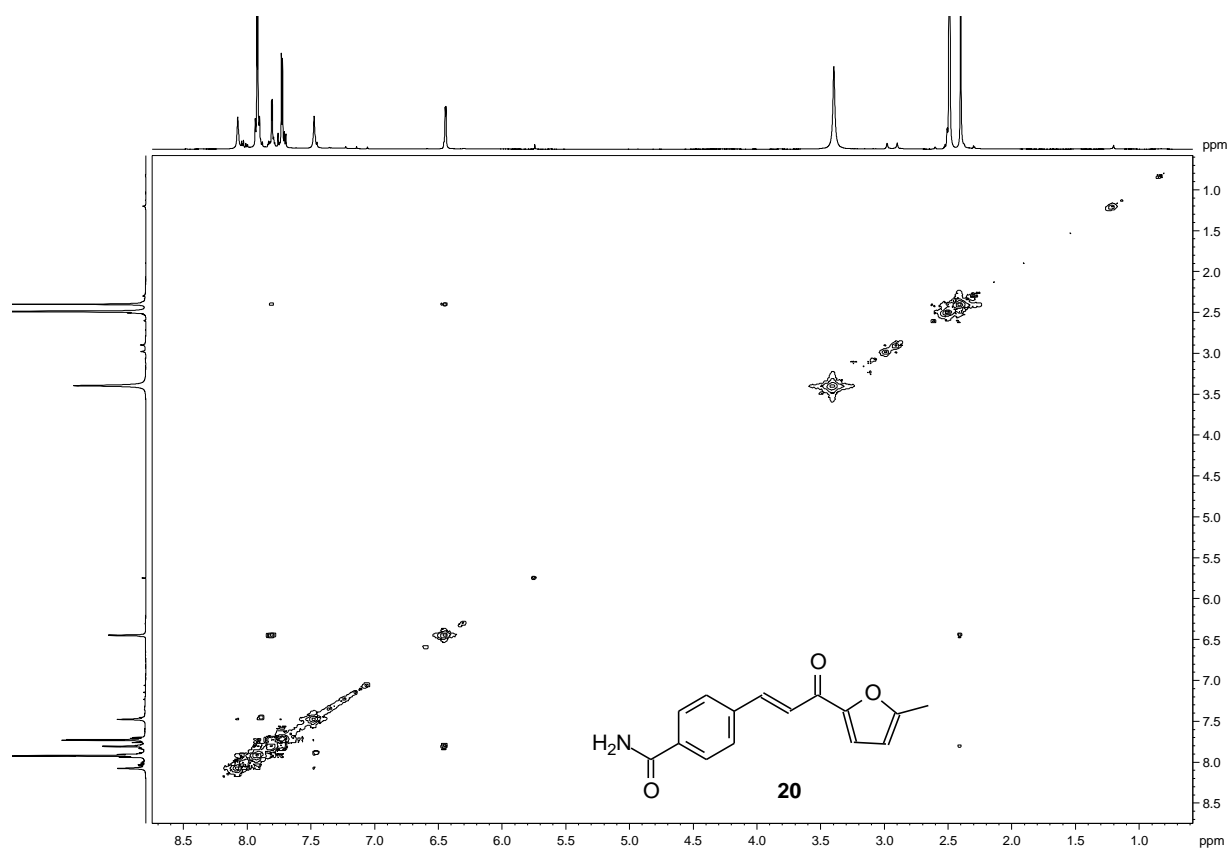


## DEPT135 in DMSO: **20**

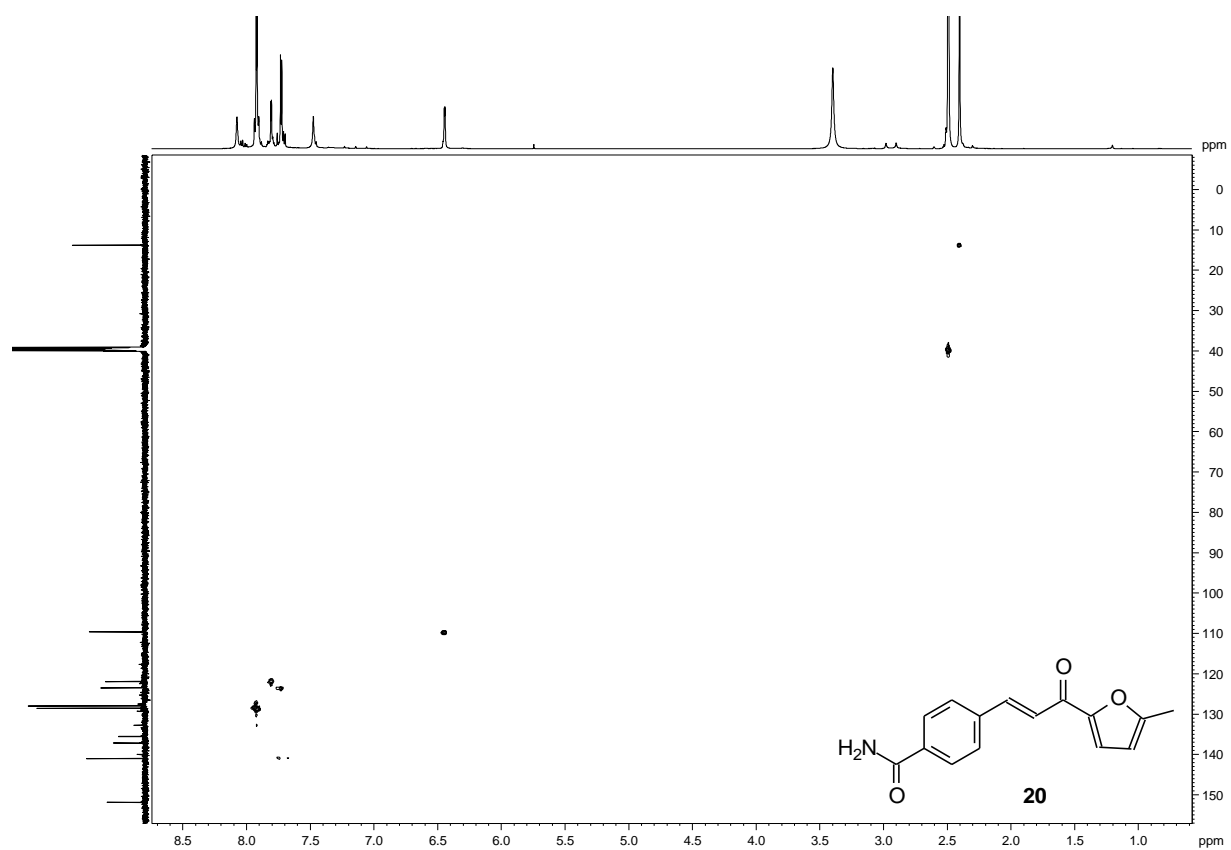


# Addendum A – Chapter 3

COSY in DMSO: **20**



HSQC in DMSO: **20**

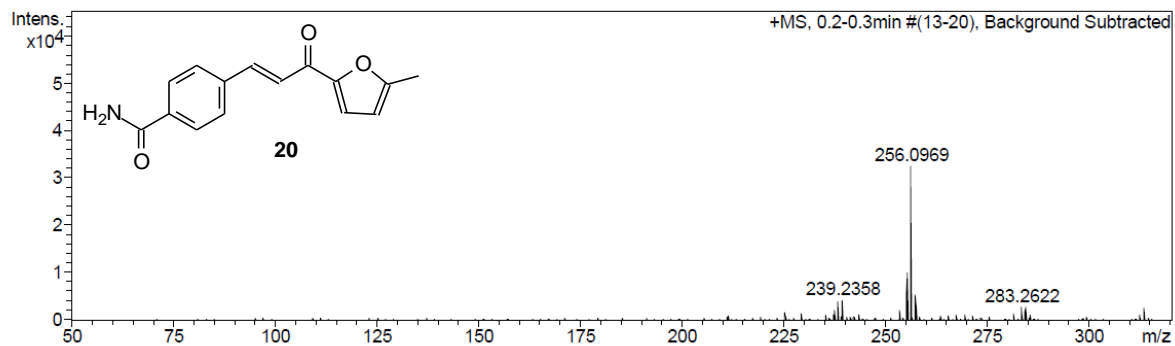


# Addendum A – Chapter 3

## HRMS: 20

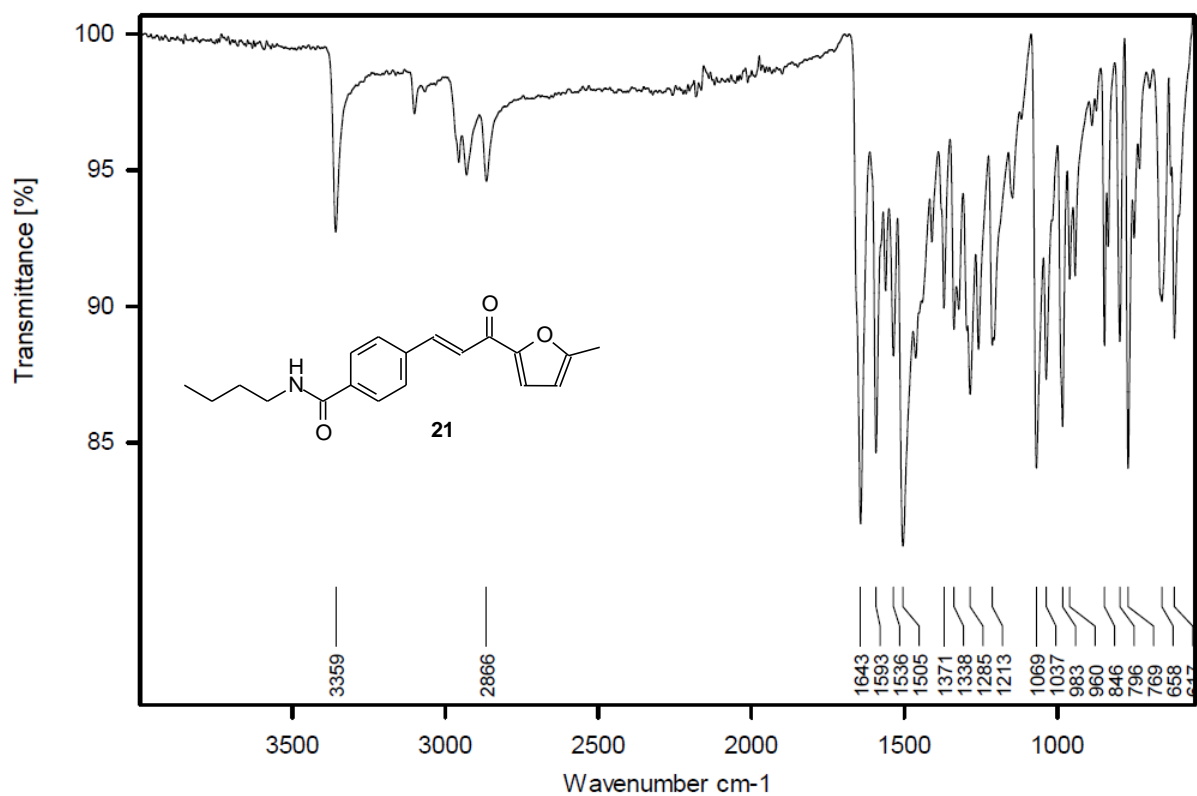
### Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

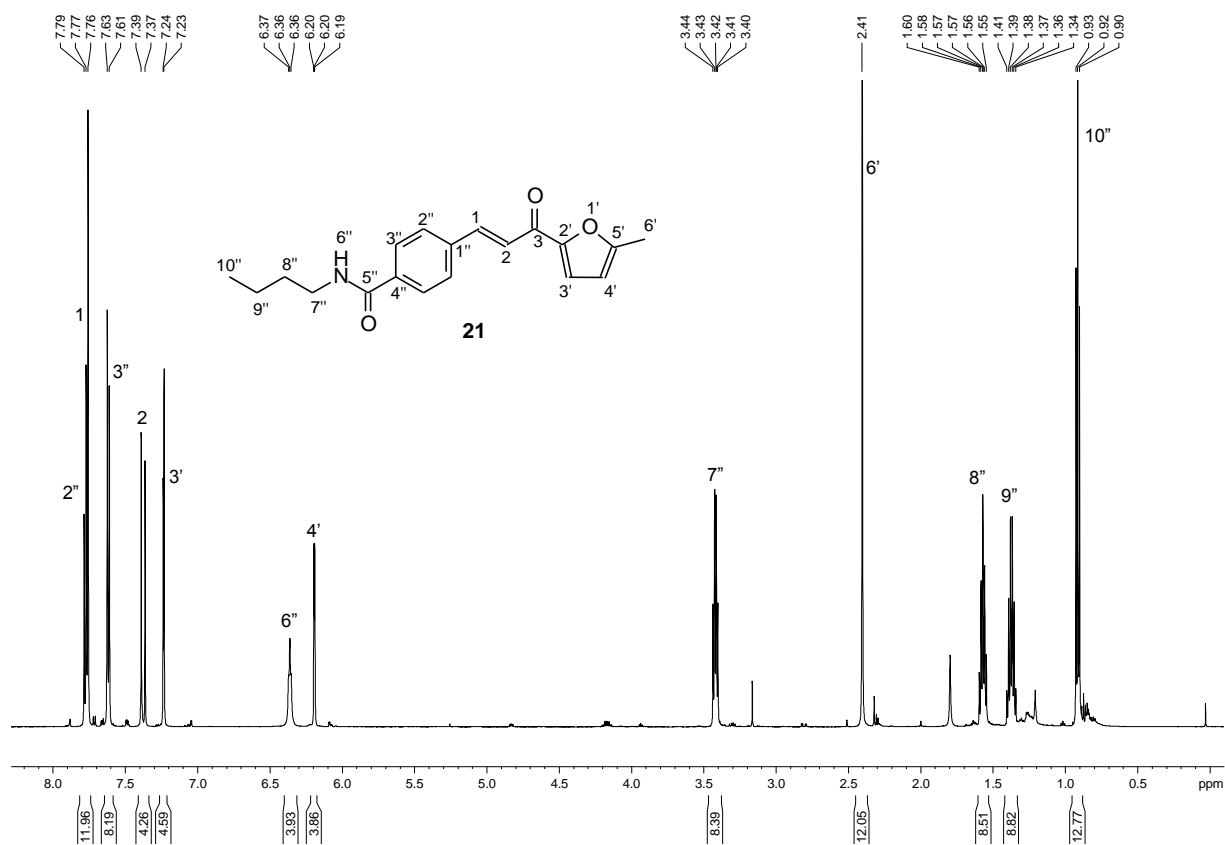


Addendum A – Chapter 3

IR: 21

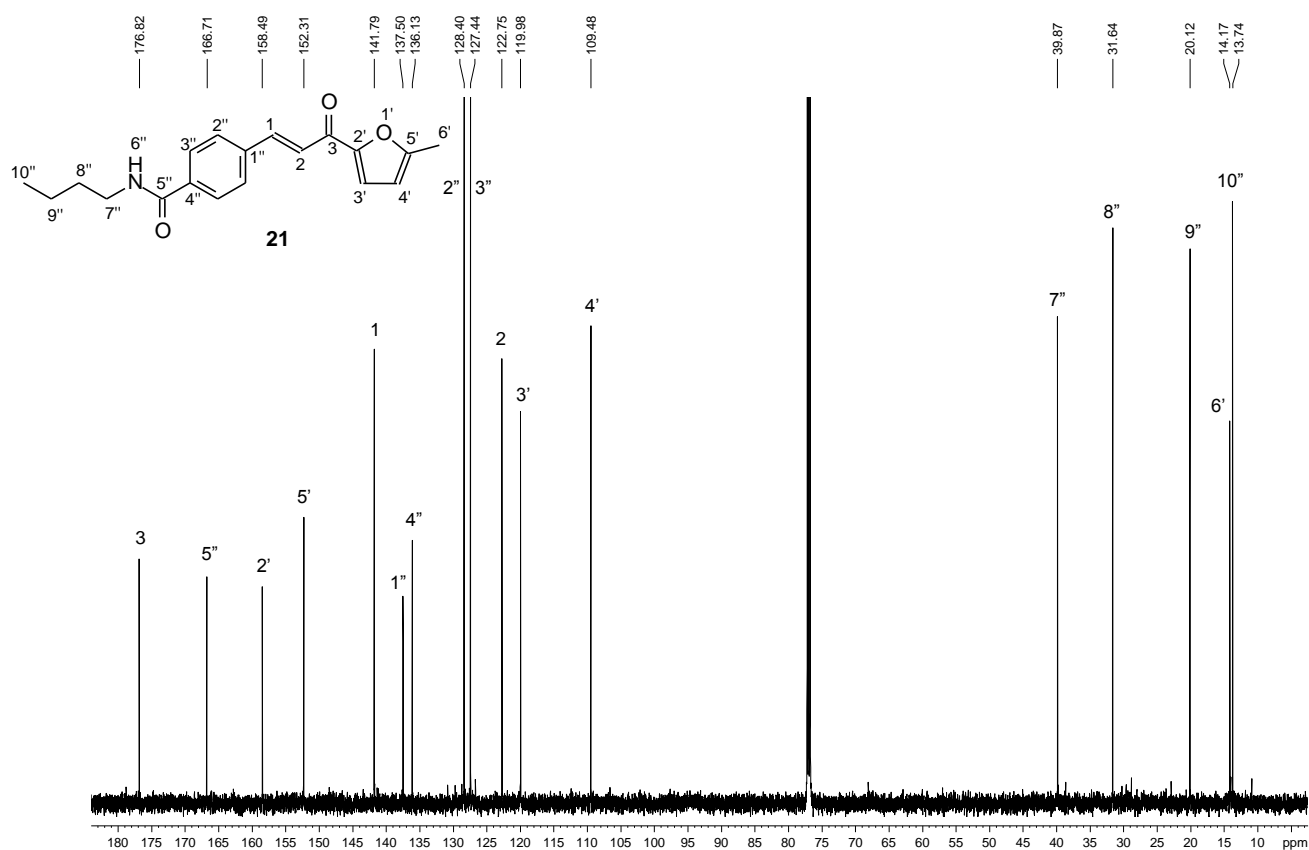


<sup>1</sup>H NMR in CDCl<sub>3</sub>: 21

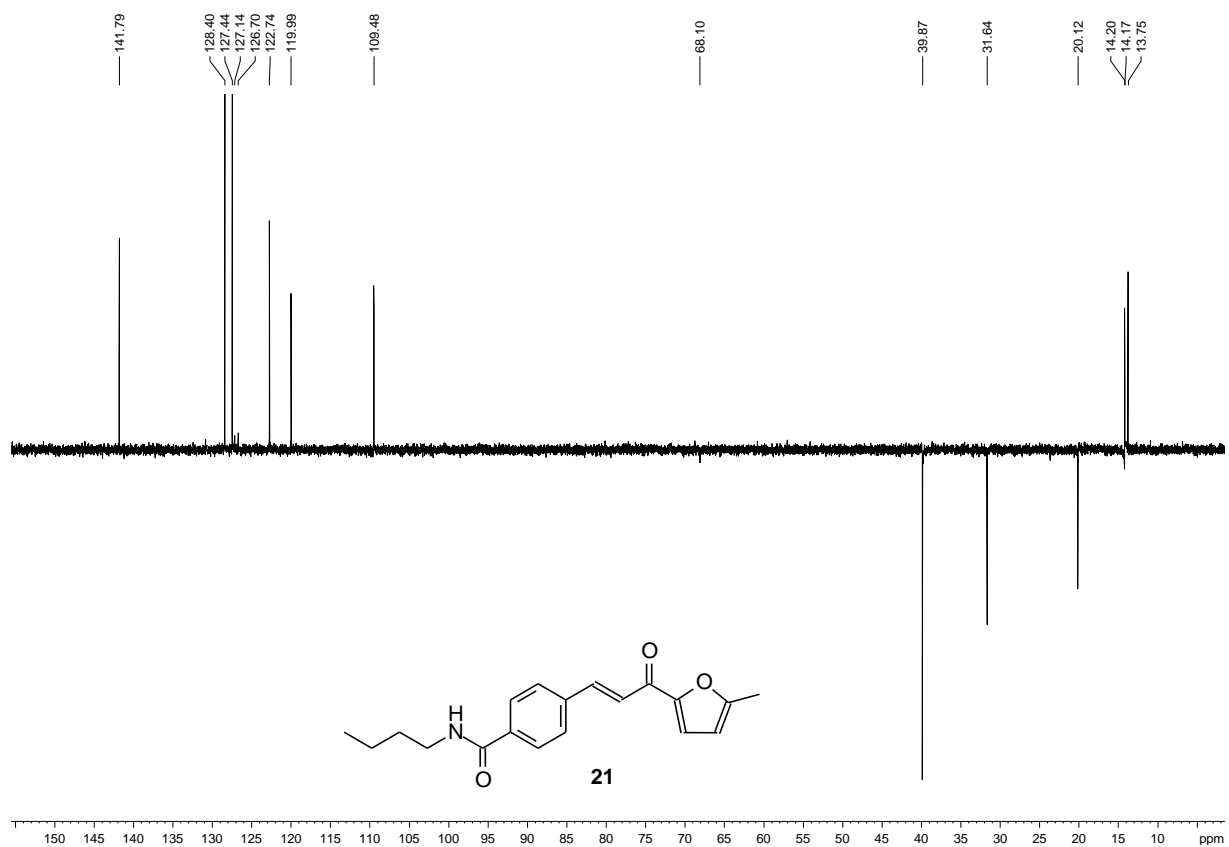


# Addendum A – Chapter 3

## <sup>13</sup>C NMR in CDCl<sub>3</sub>: 21

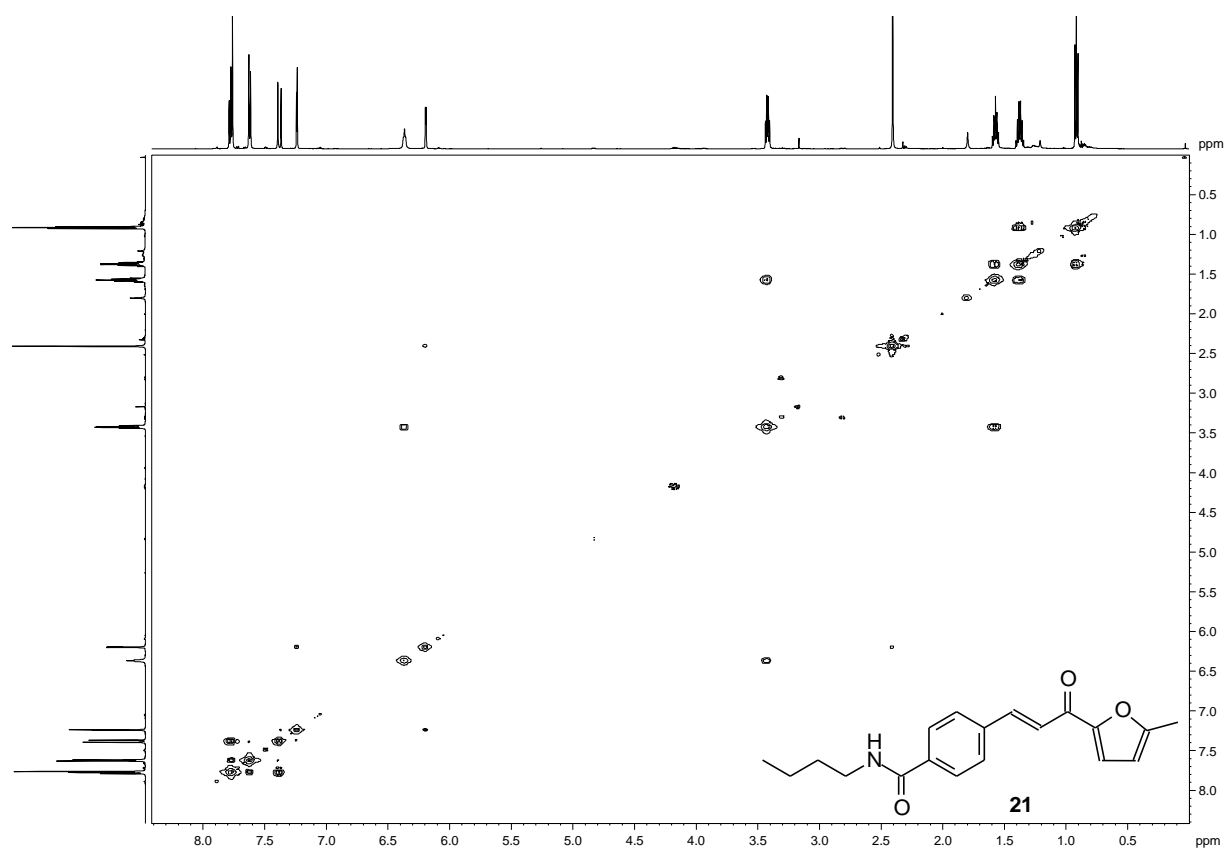


## DEPT135 in CDCl<sub>3</sub>: 21

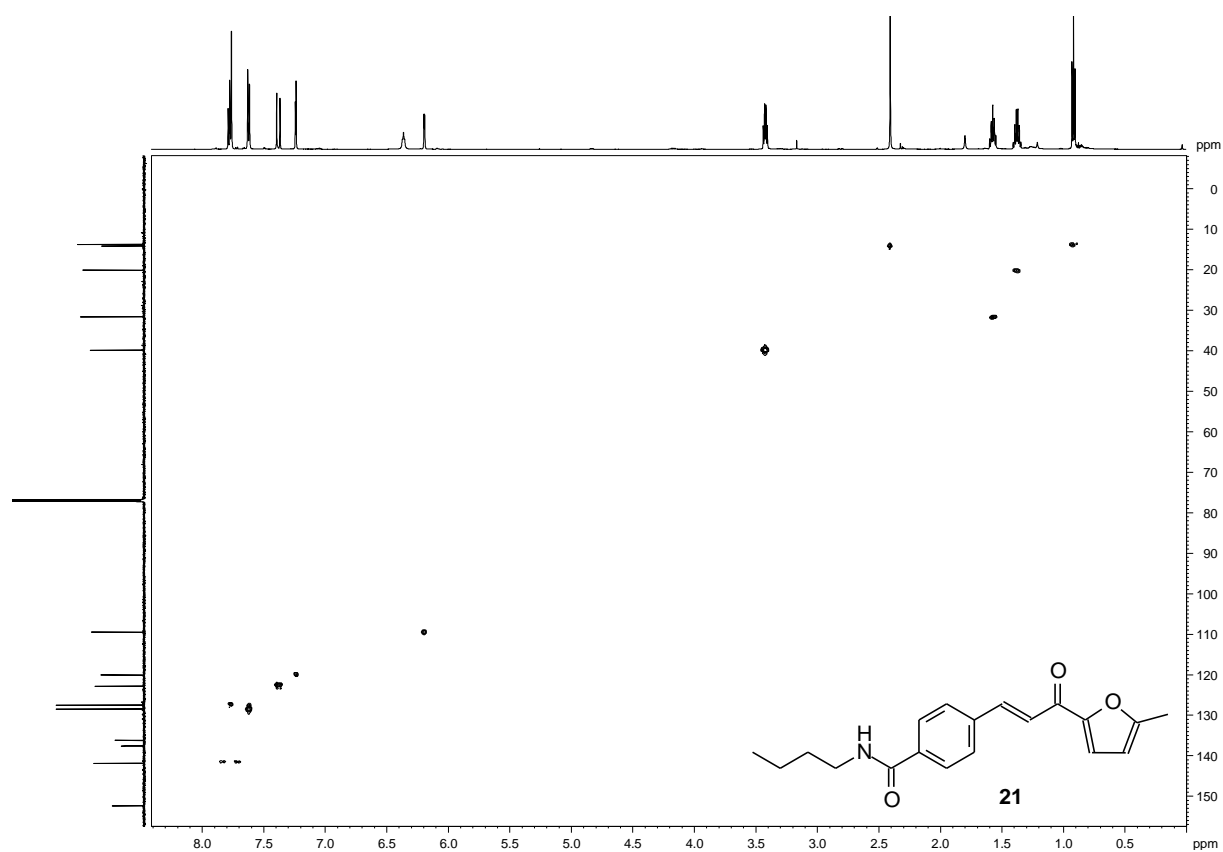


Addendum A – Chapter 3

COSY in CDCl<sub>3</sub>: 21



HSQC in CDCl<sub>3</sub>: 21

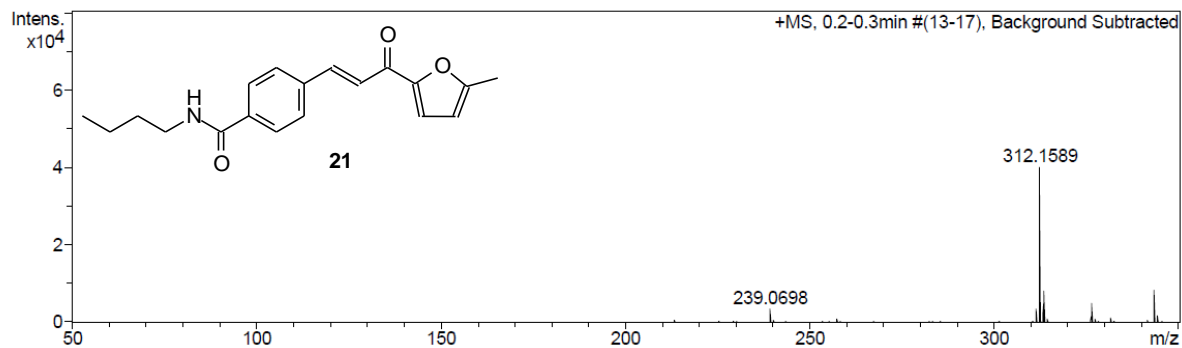


# Addendum A – Chapter 3

## HRMS: 21

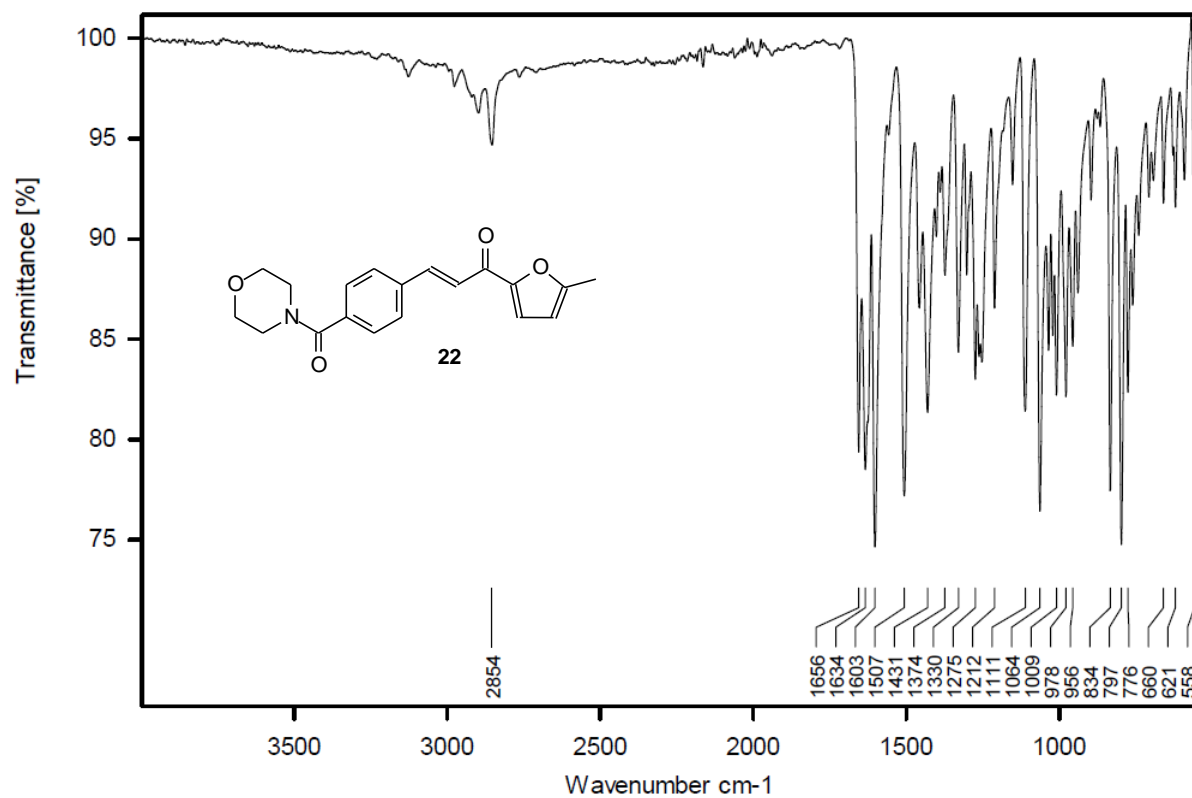
### Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

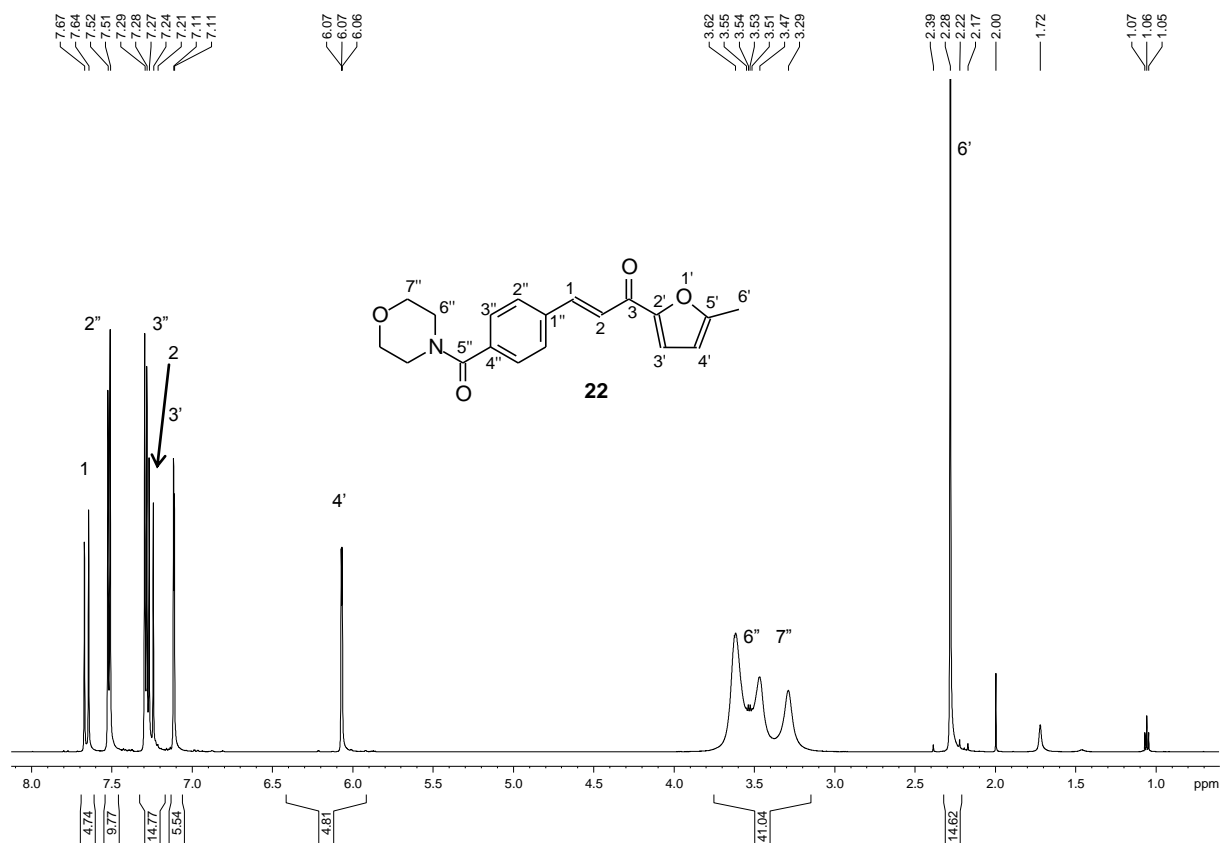


Addendum A – Chapter 3

IR: 22

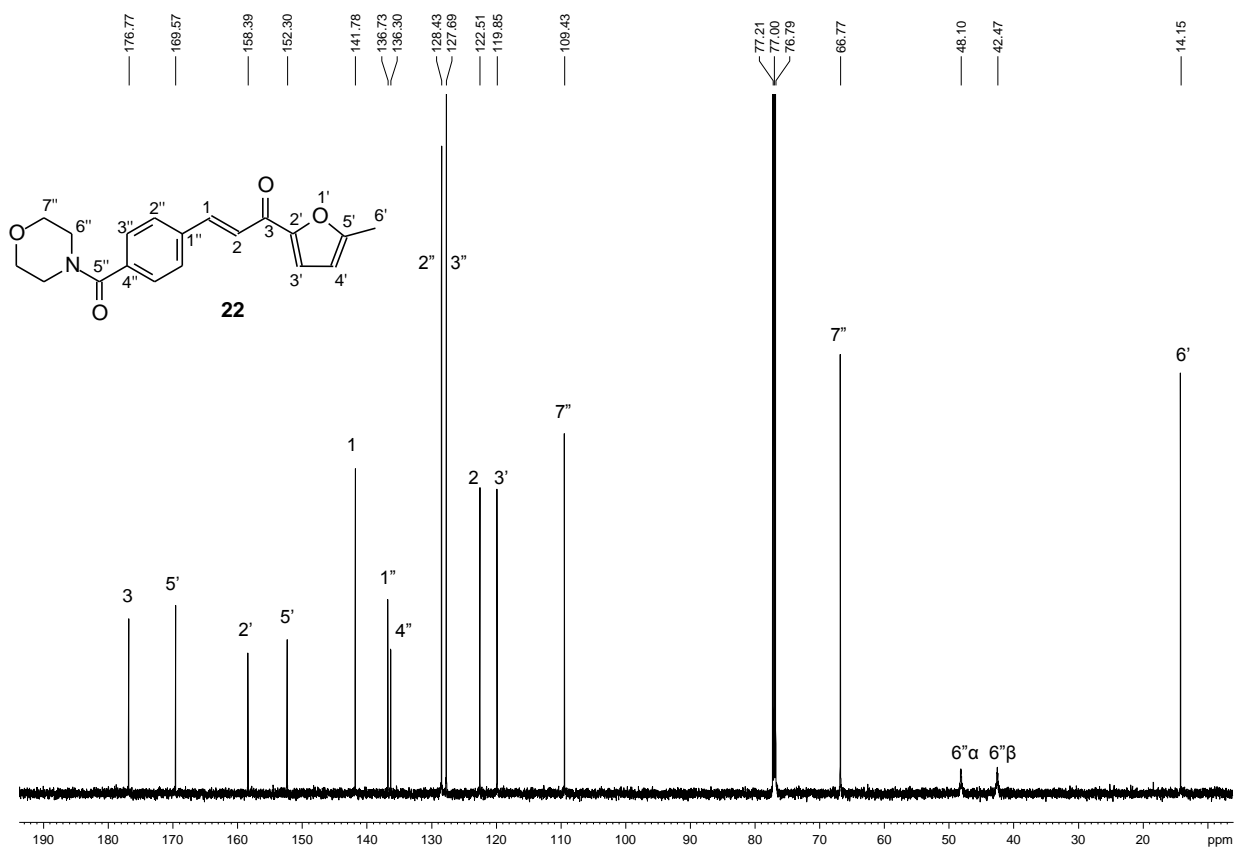


<sup>1</sup>H NMR in CDCl<sub>3</sub>: 22



## Addendum A – Chapter 3

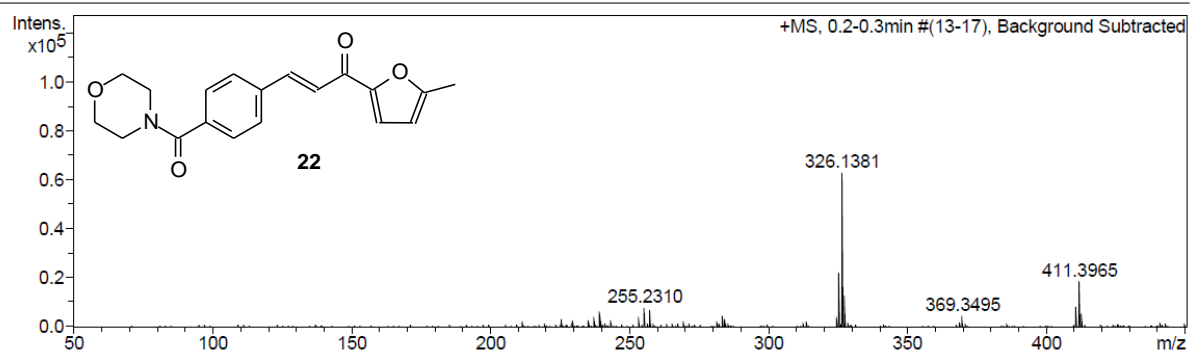
### $^{13}\text{C}$ NMR in $\text{CDCl}_3$ : **22**



### HRMS of **22**

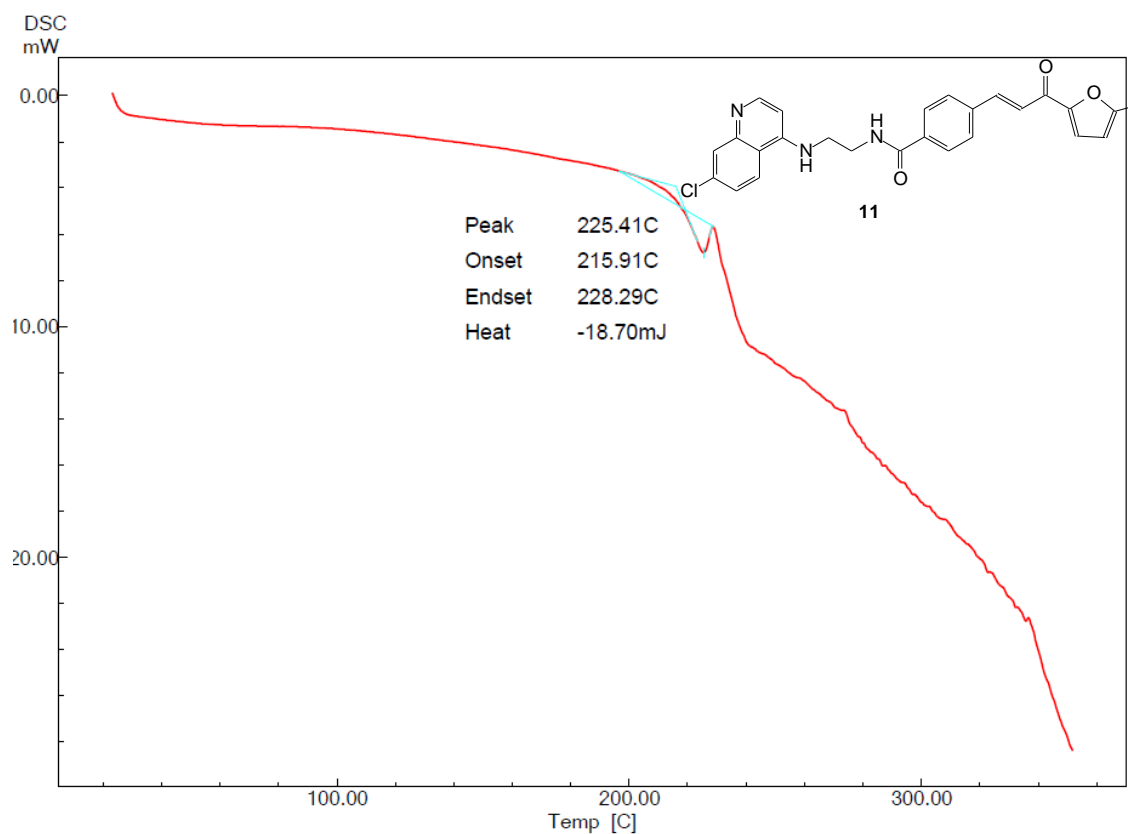
#### Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

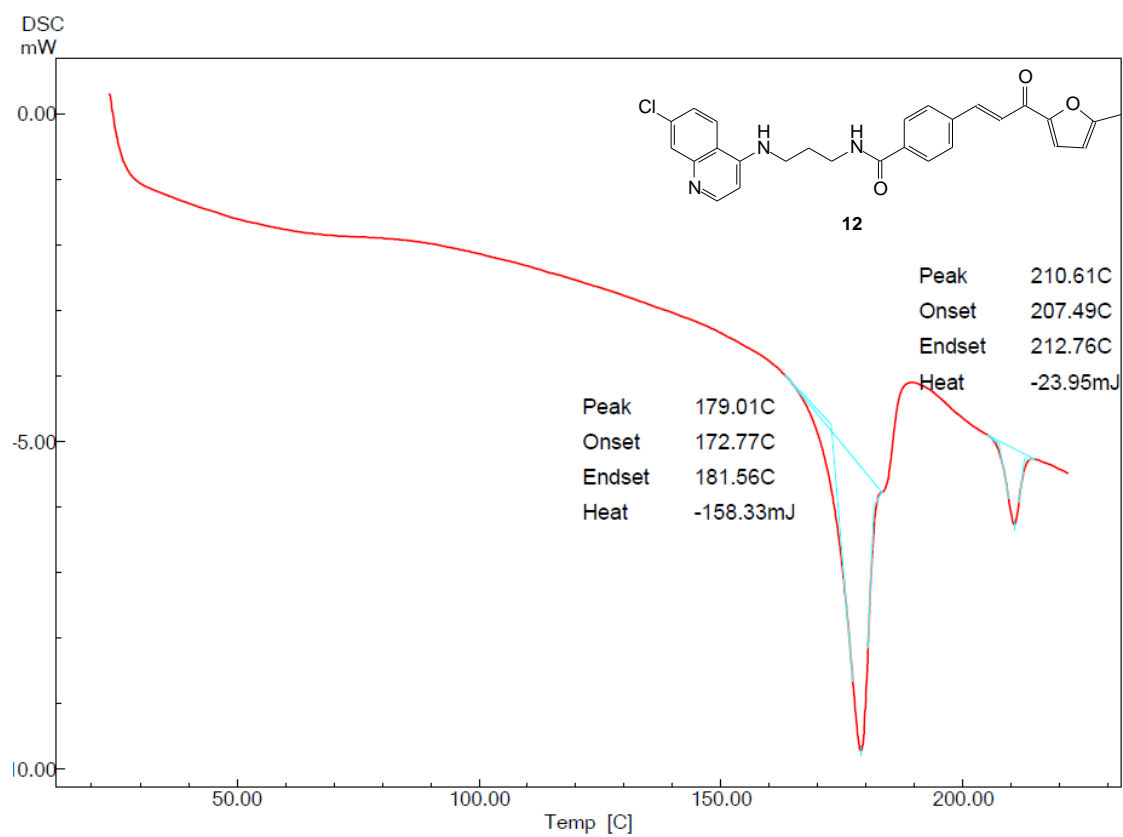


### Addendum A – Chapter 3

#### DSC Thermgraph: 11

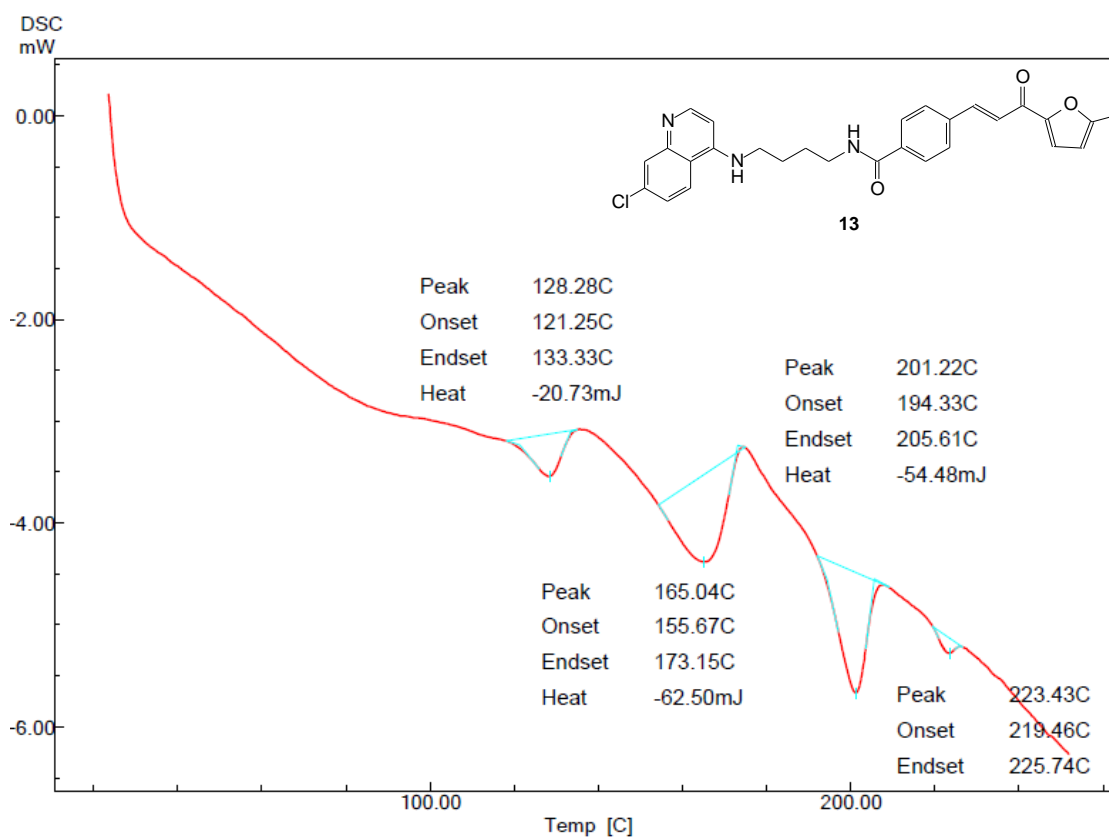


#### DSC Thermgraph: 12

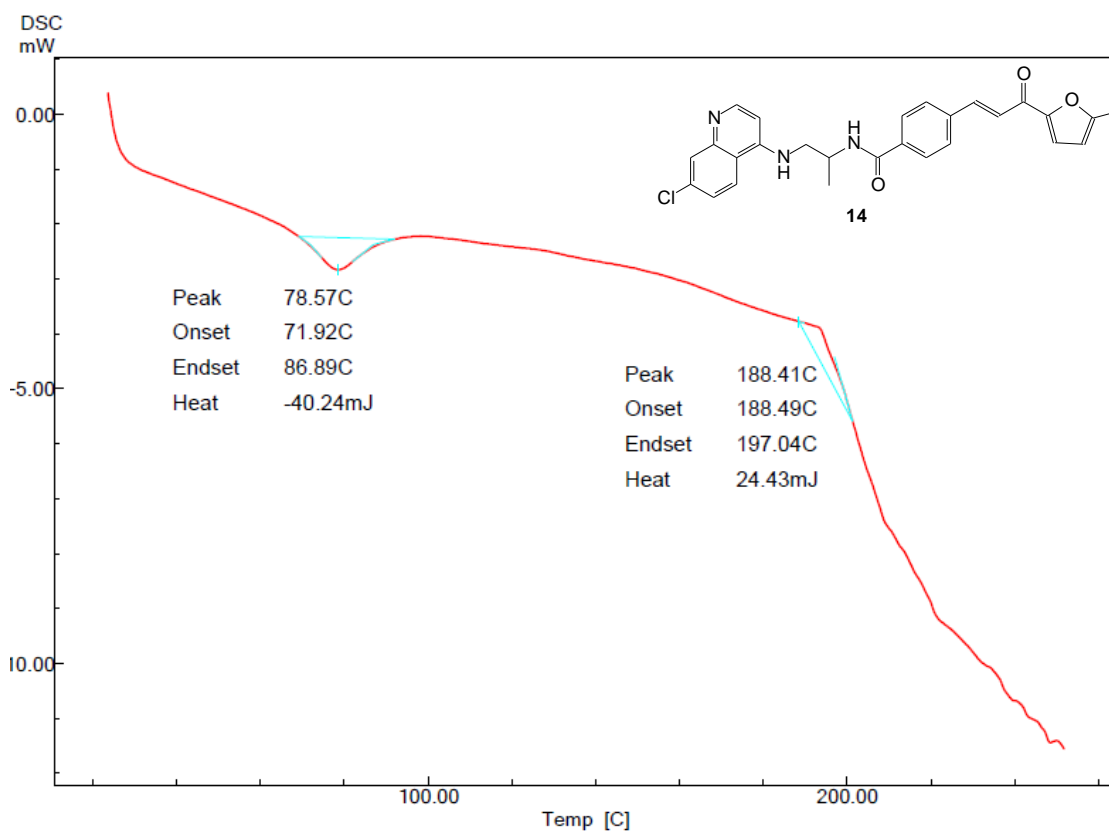


Addendum A – Chapter 3

DSC Thermgraph: 13

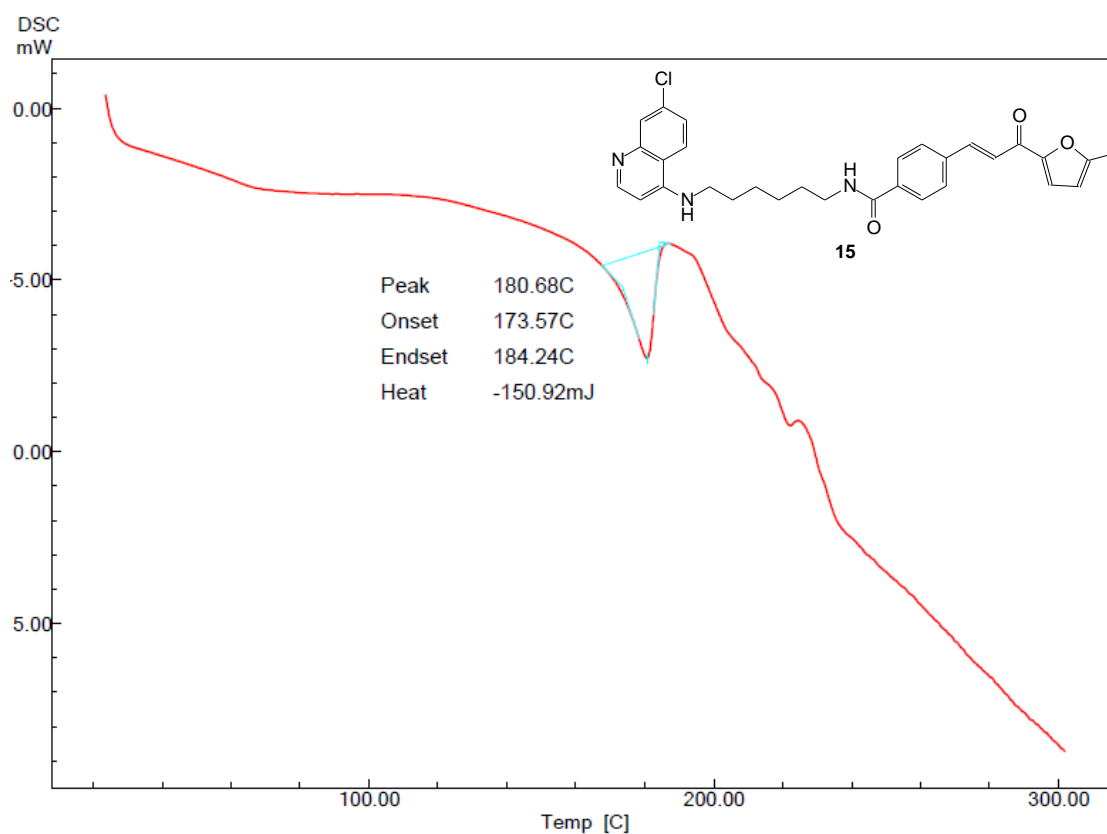


DSC Thermgraph: 14

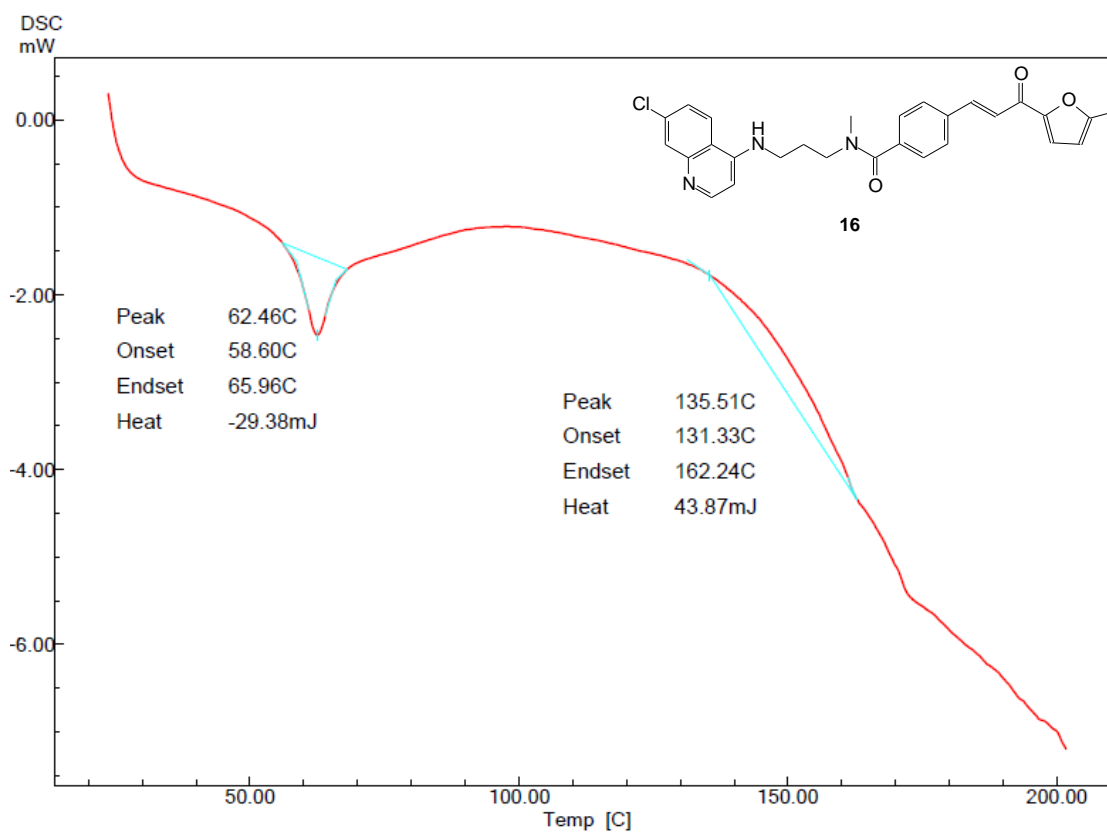


### Addendum A – Chapter 3

#### DSC Thermgraph: 15

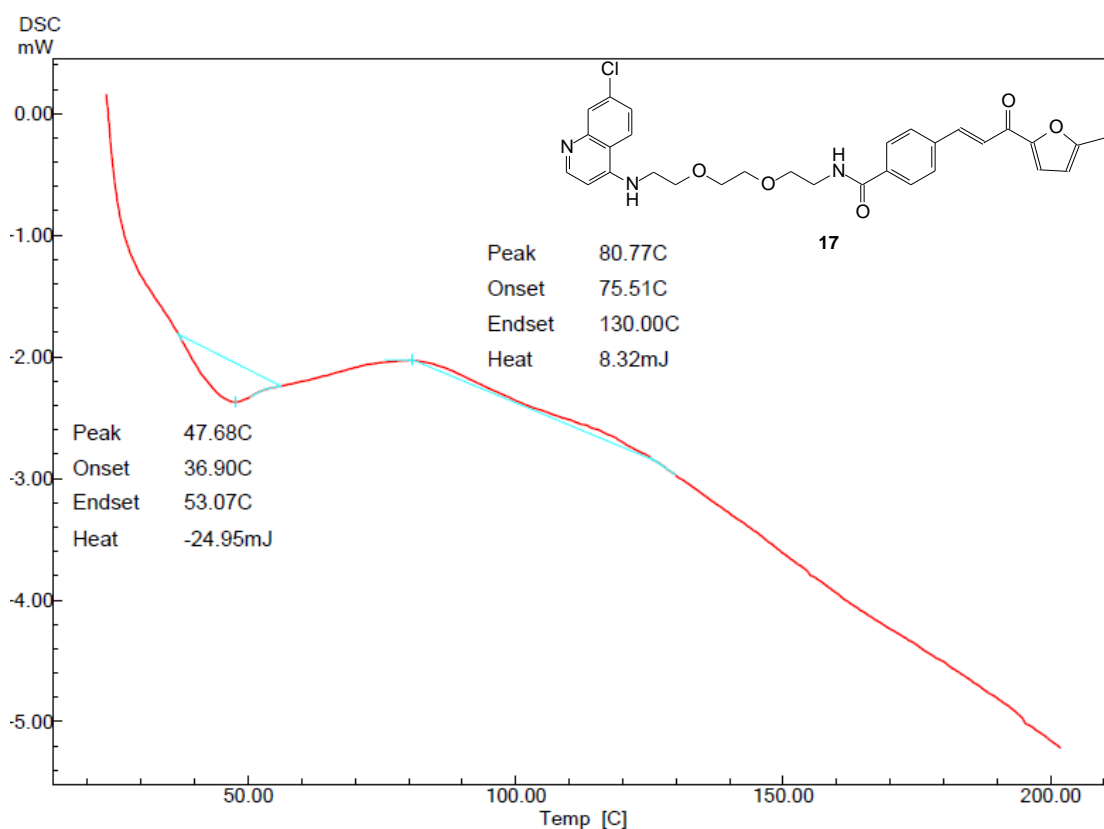


#### DSC Thermgraph: 16

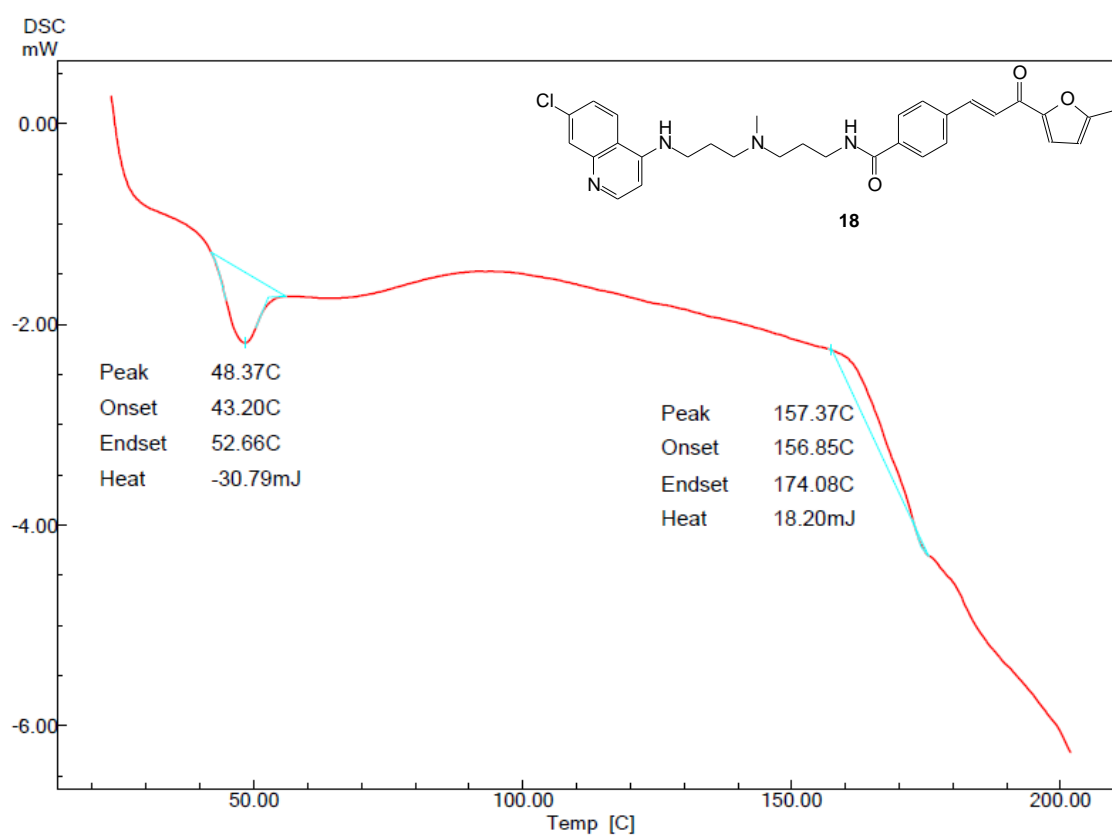


### Addendum A – Chapter 3

#### DSC Thermgraph: 17

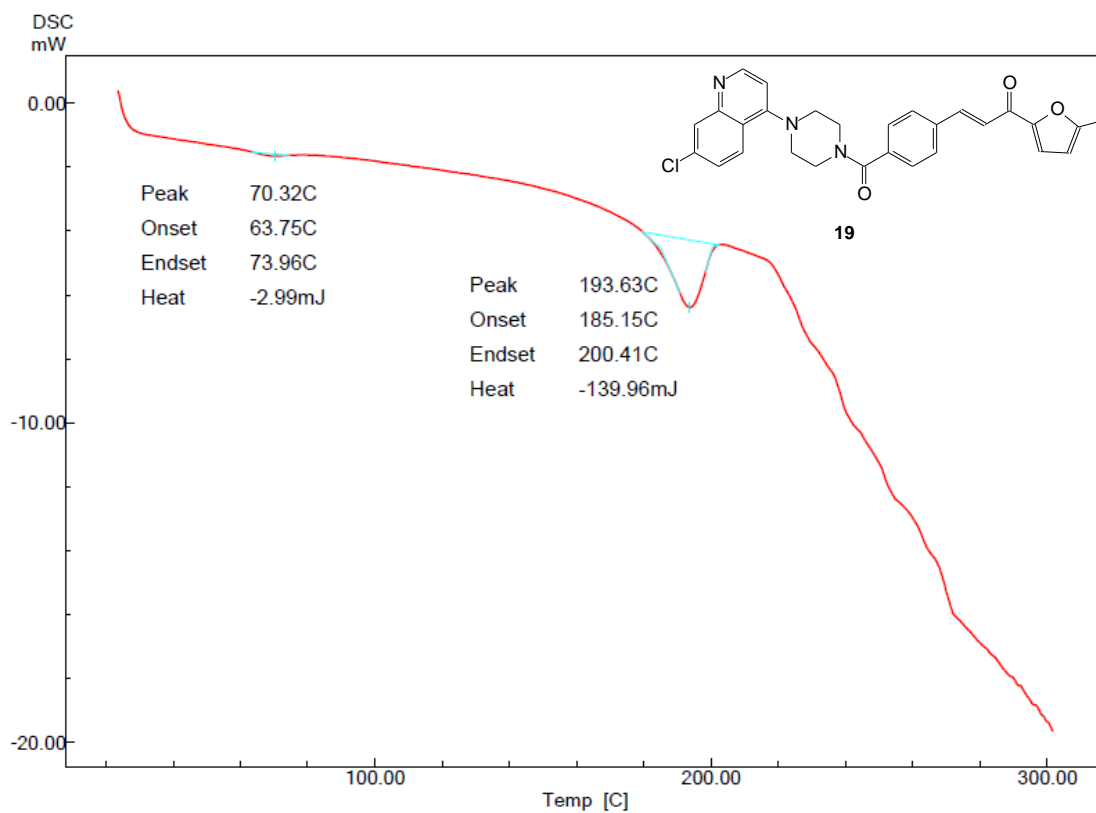


#### DSC Thermgraph: 18

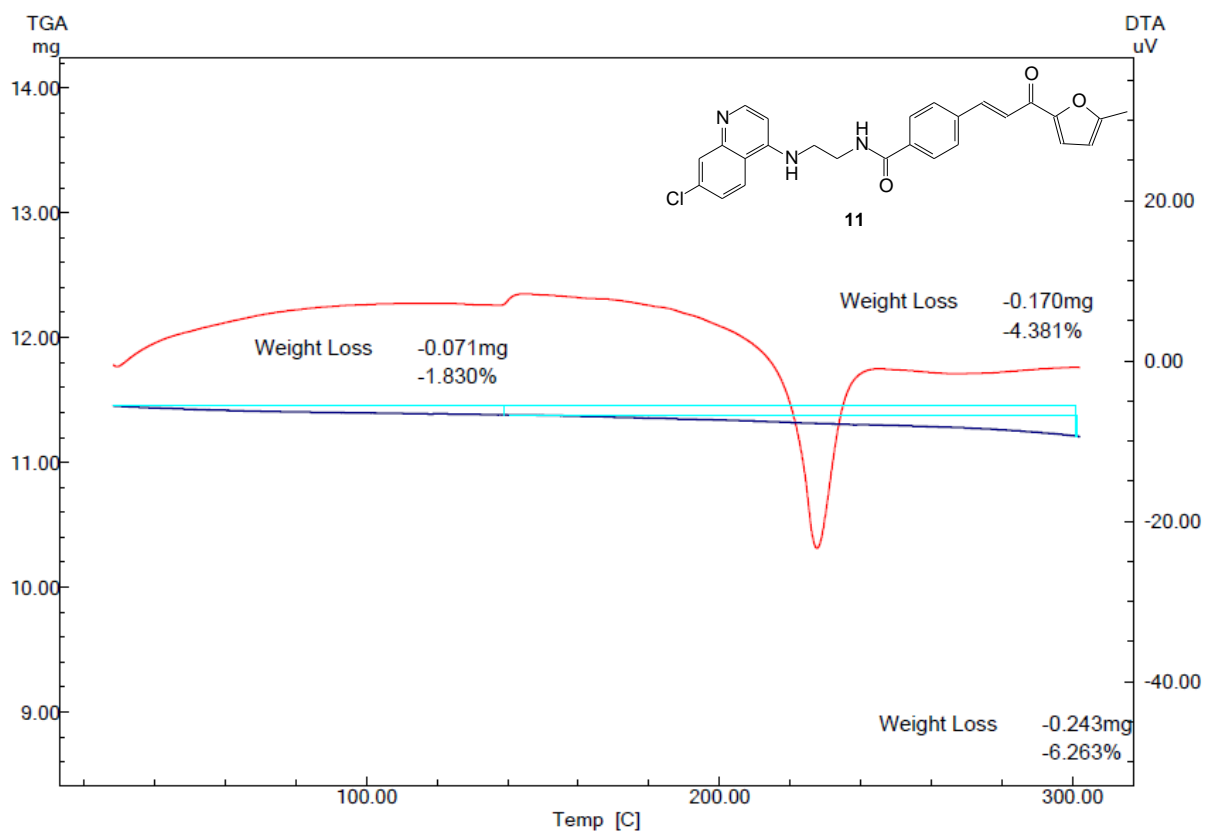


# Addendum A – Chapter 3

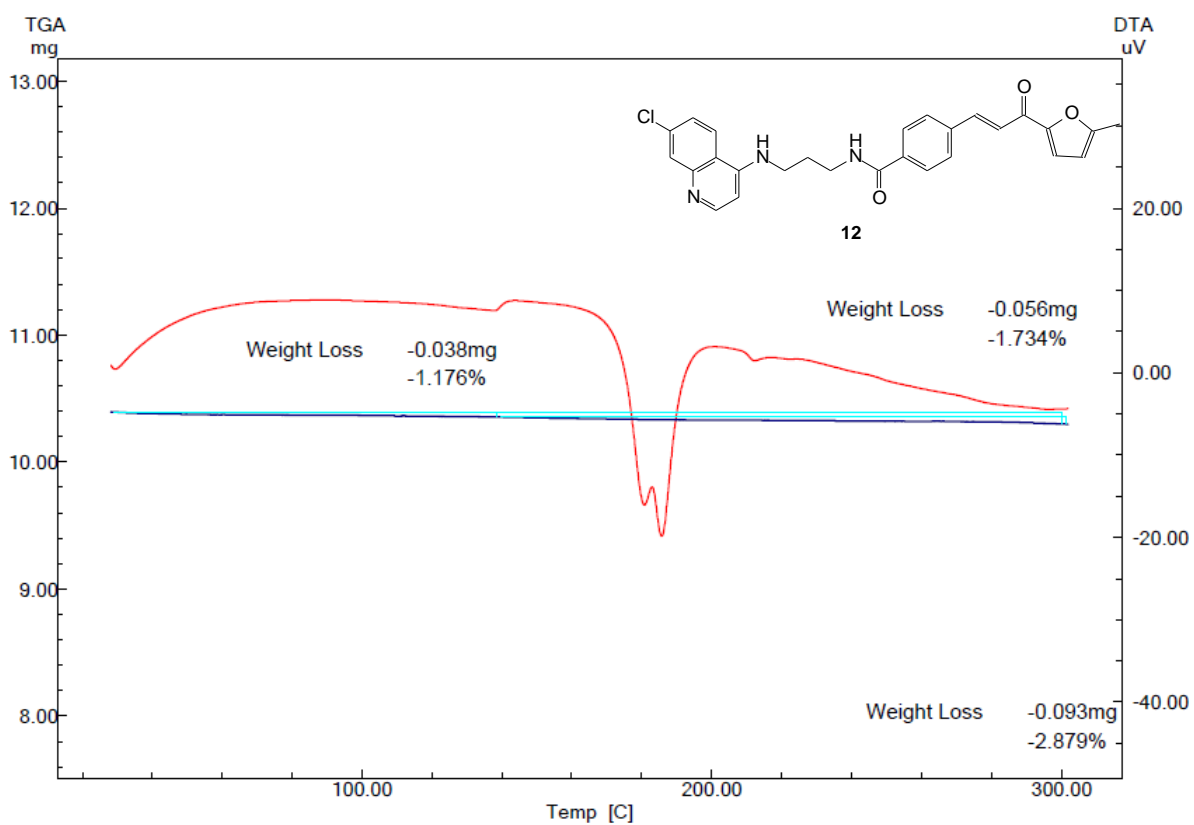
## DSC Thermgraph: 19



TGA Thermgraph: 11

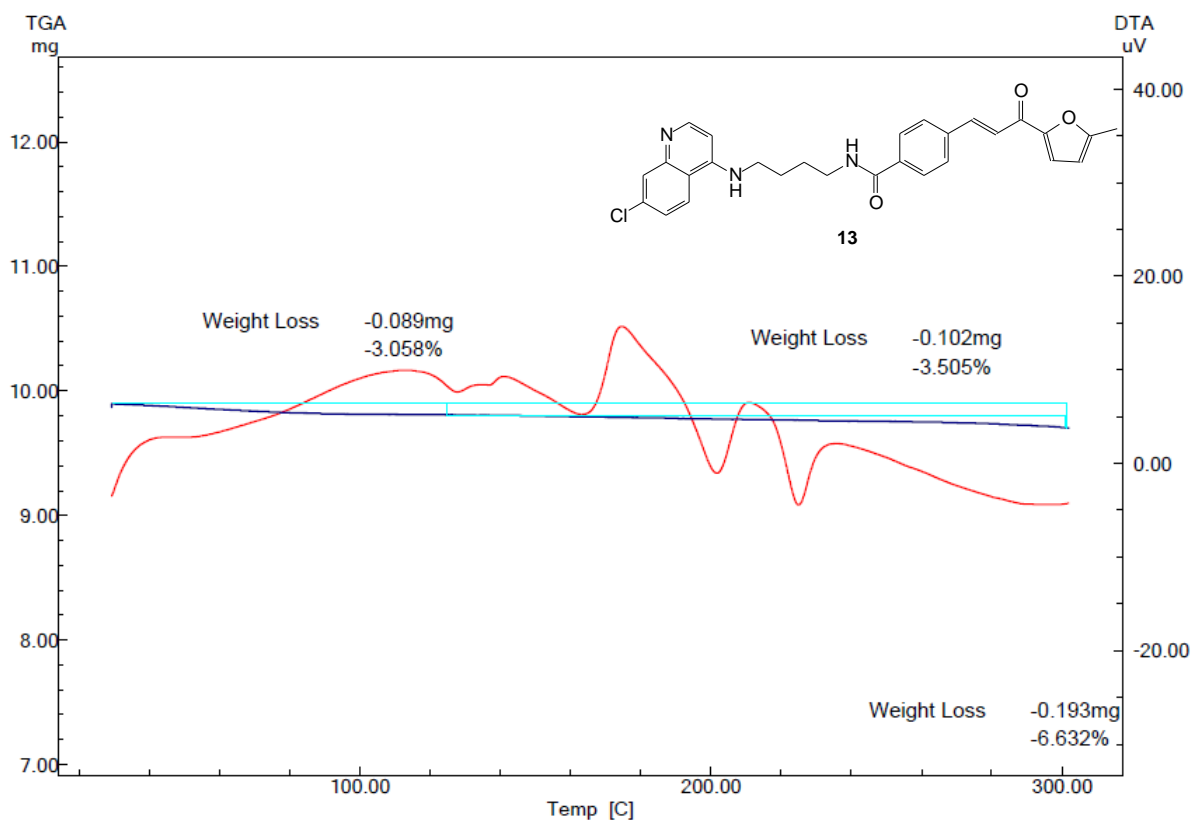


TGA Thermgraph: 12

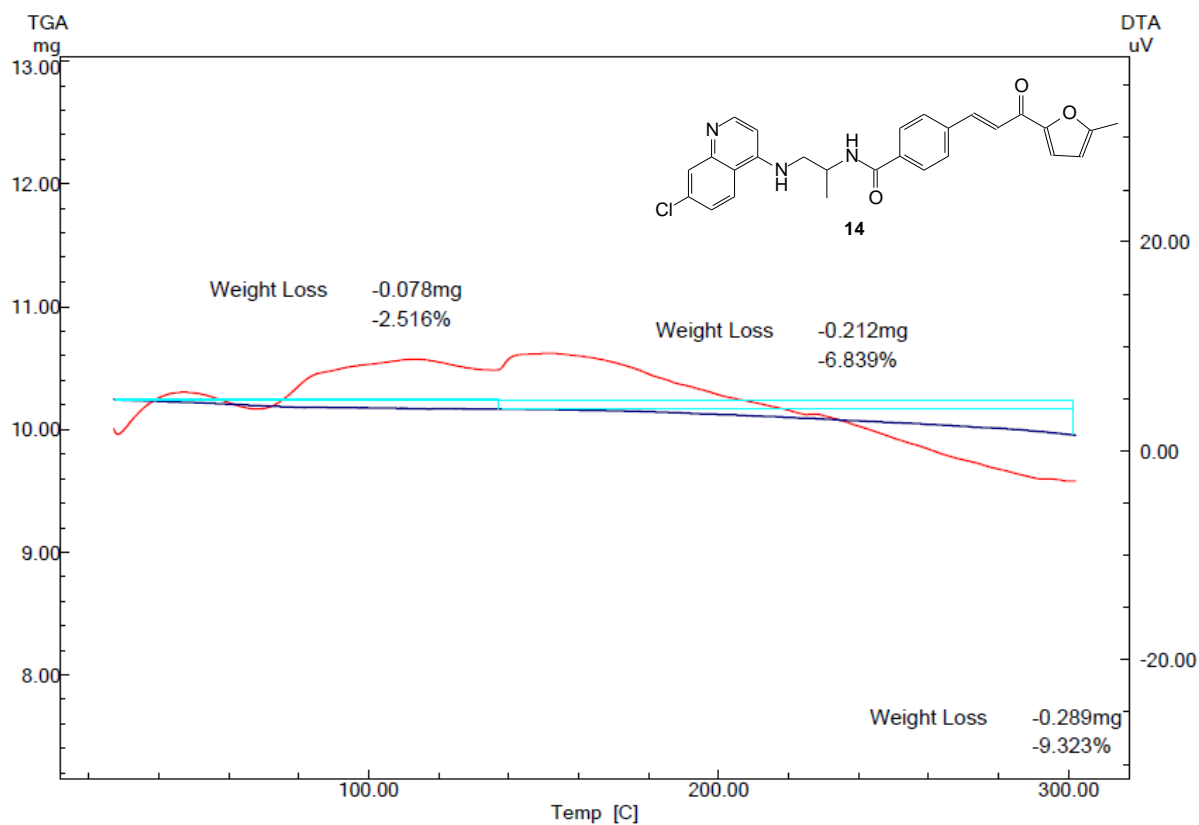


### Addendum A – Chapter 3

#### TGA Thermgraph: 13

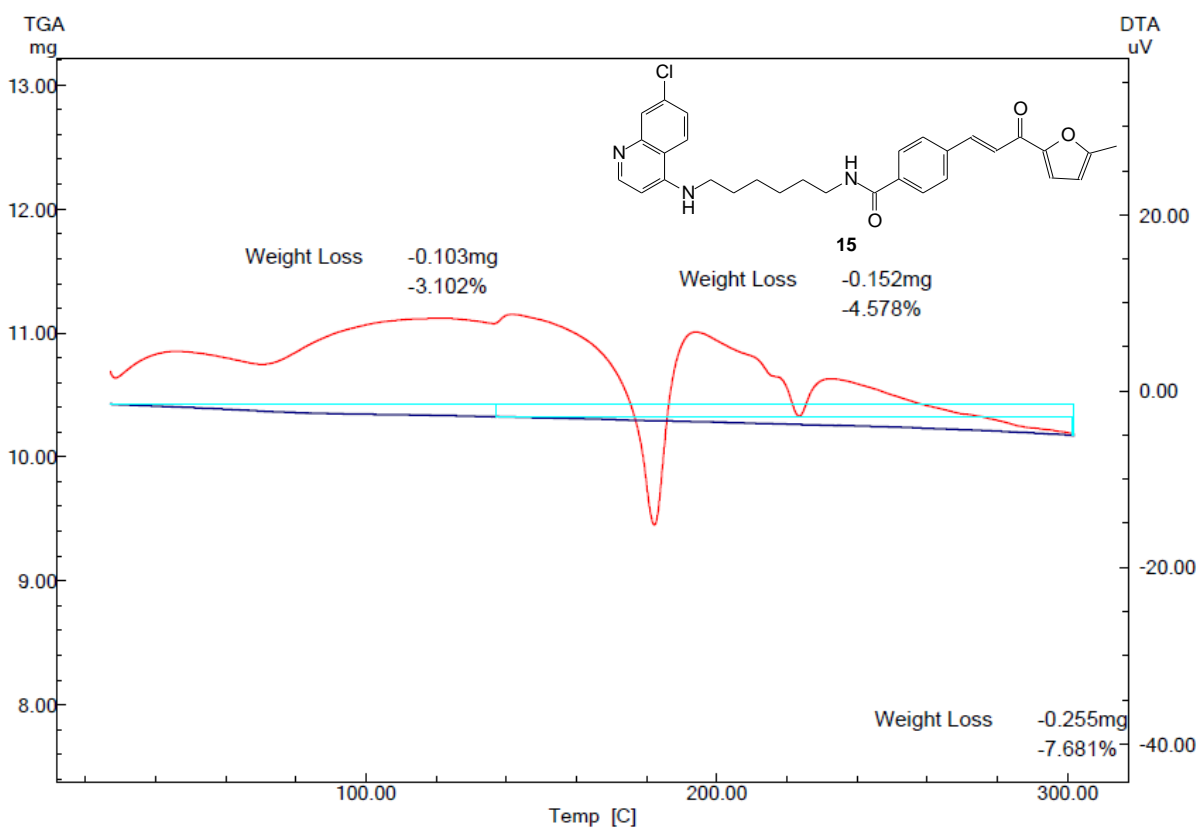


#### TGA Thermgraph: 14

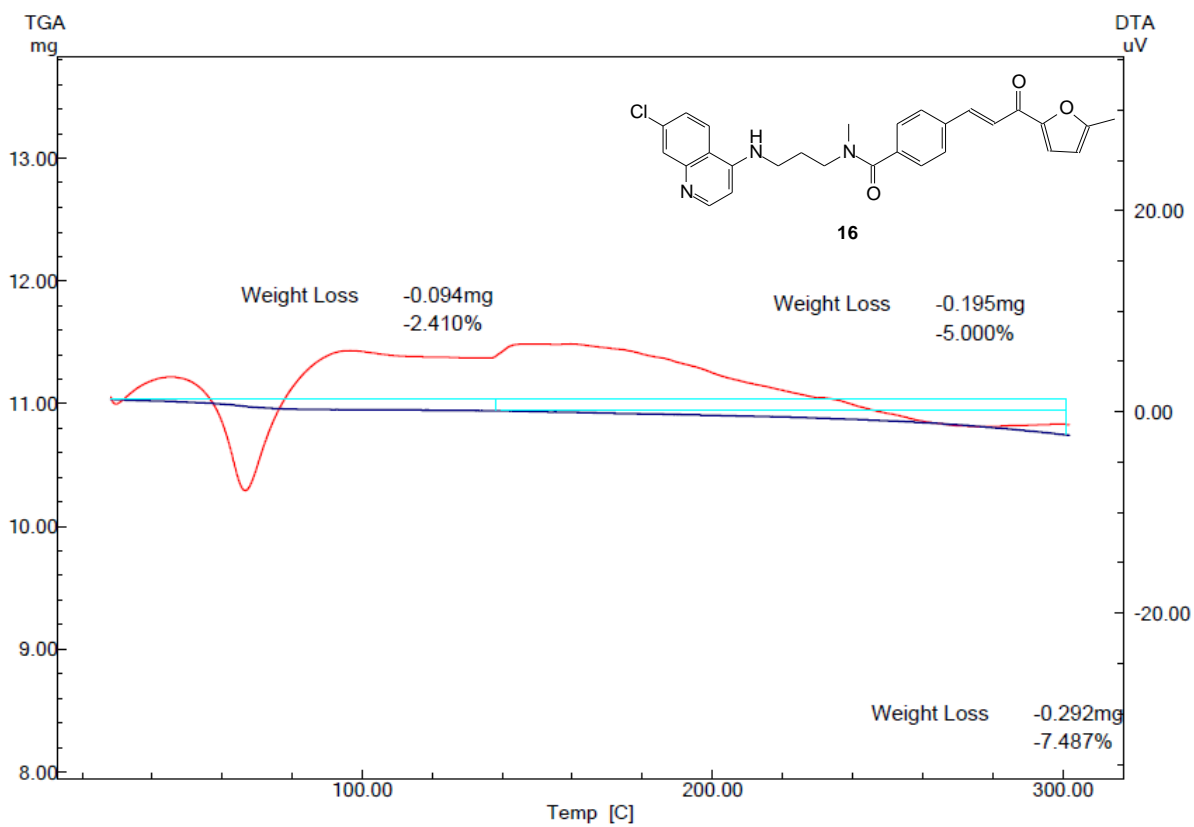


### Addendum A – Chapter 3

#### TGA Thermgraph: 15

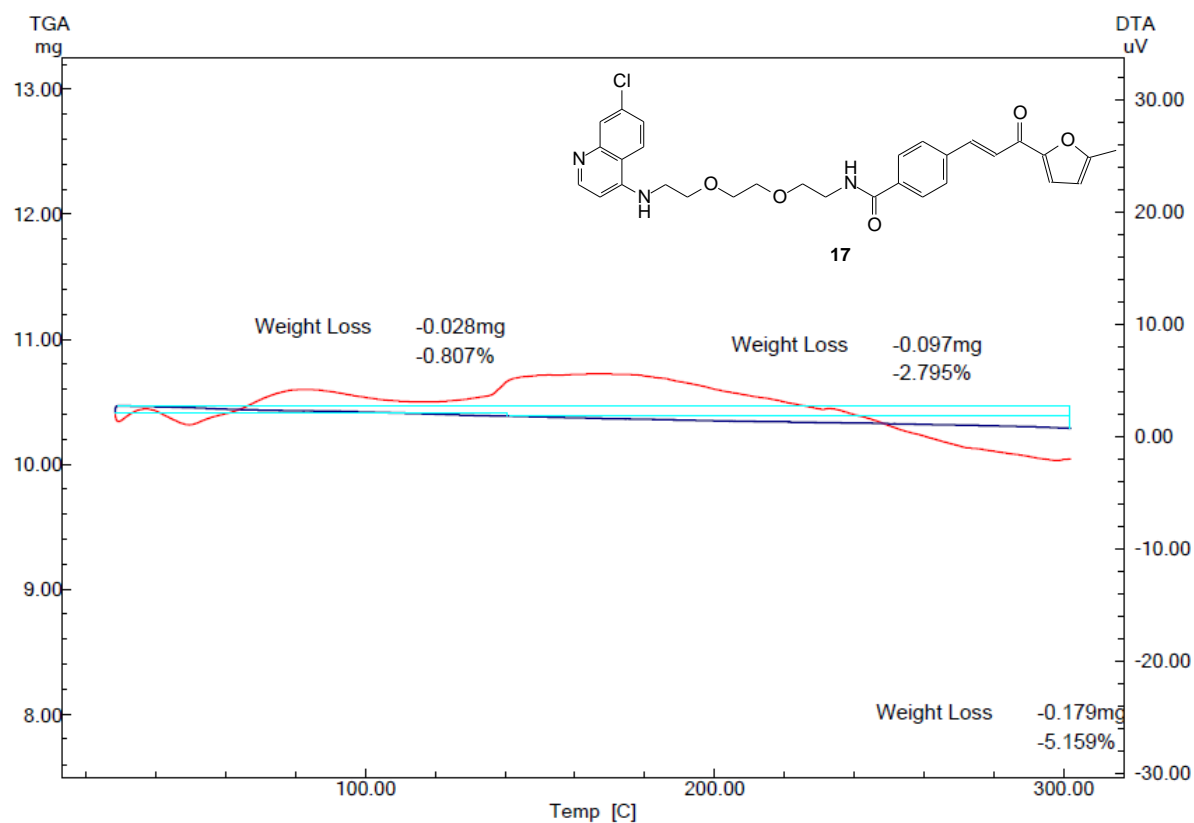


#### TGA Thermgraph: 16

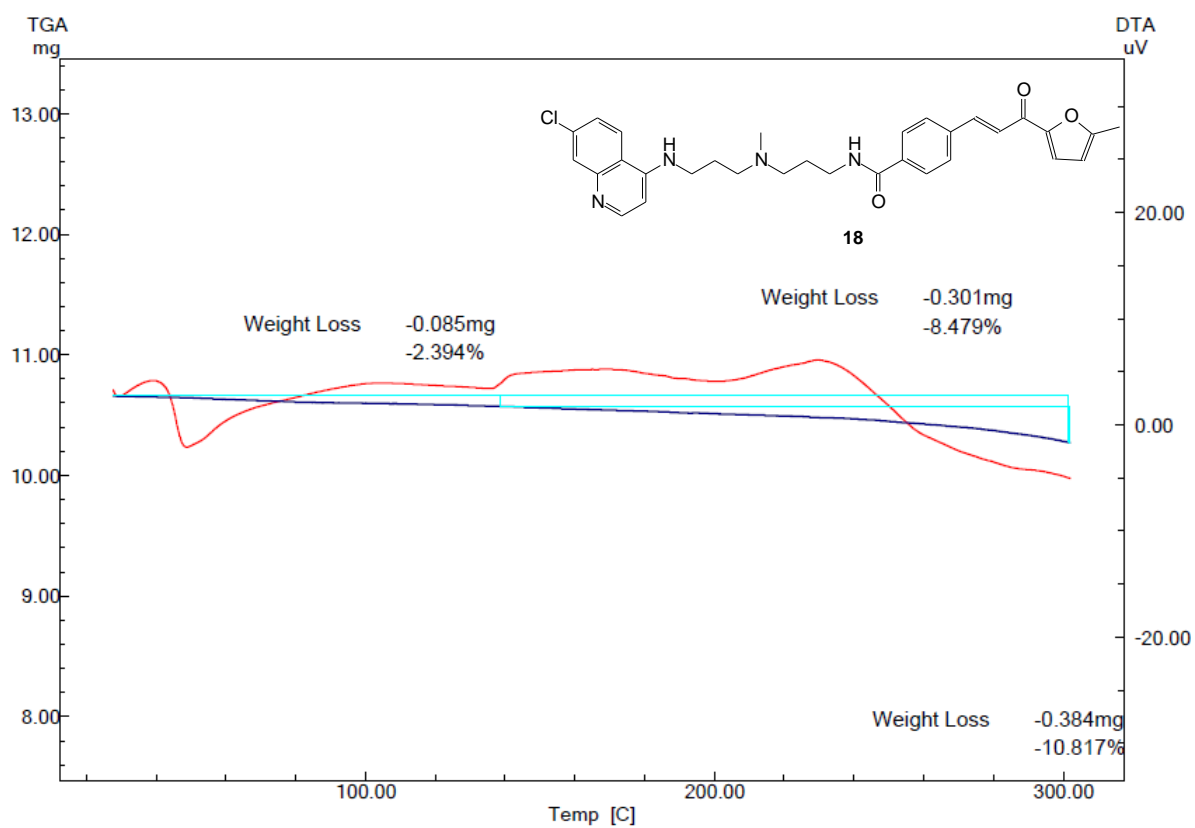


### Addendum A – Chapter 3

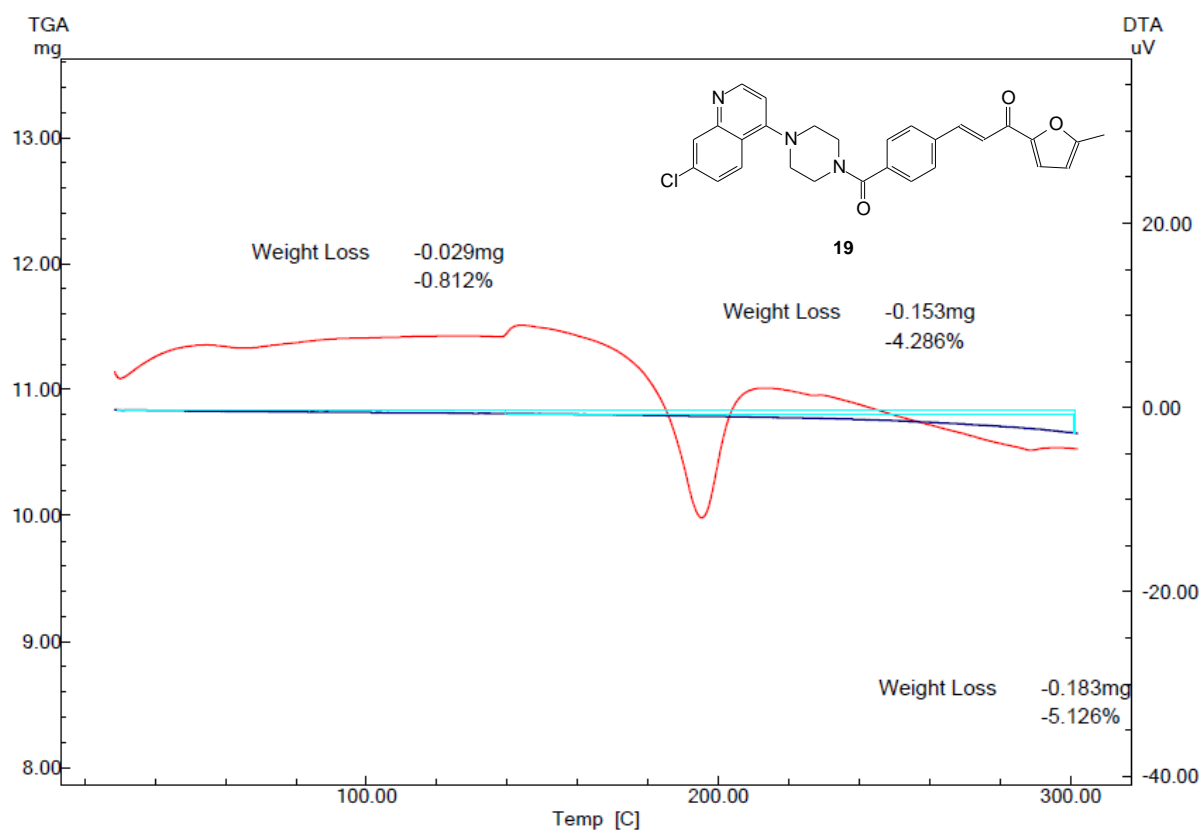
#### TGA Thermgraph: 17



#### TGA Thermgraph: 18

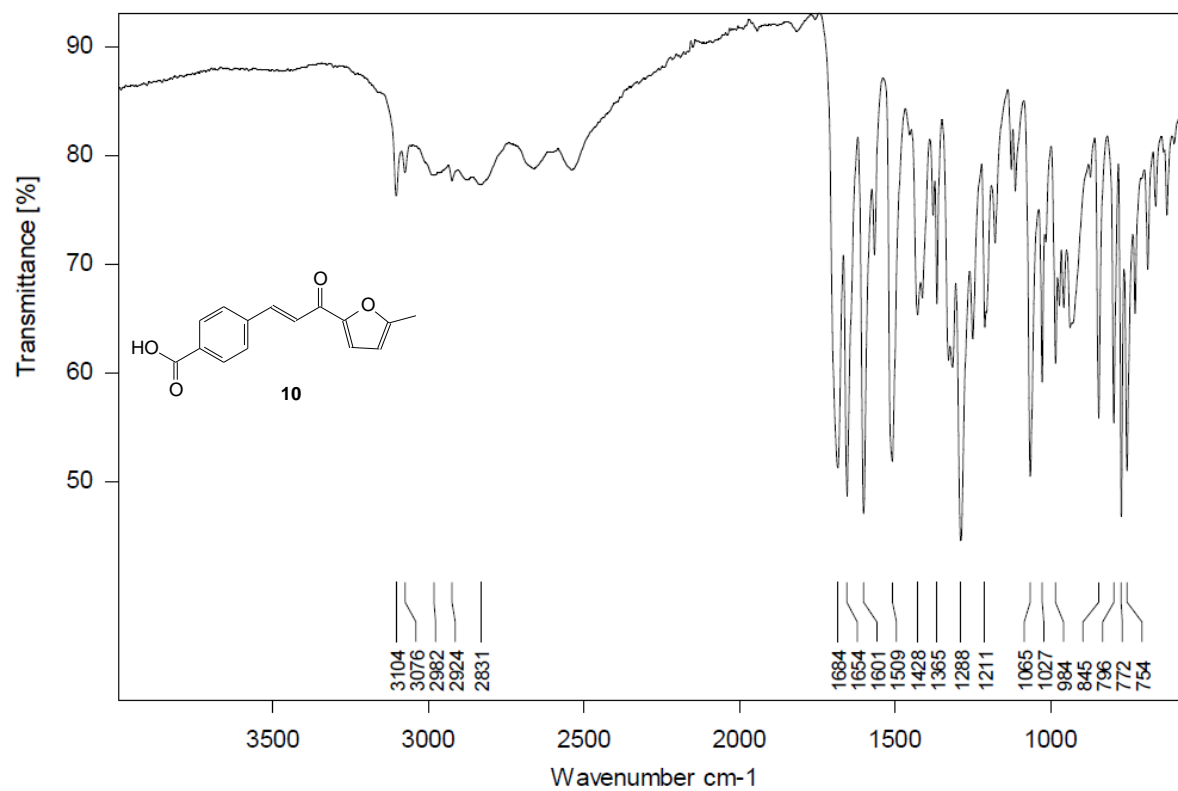


TGA Thermgraph: 19



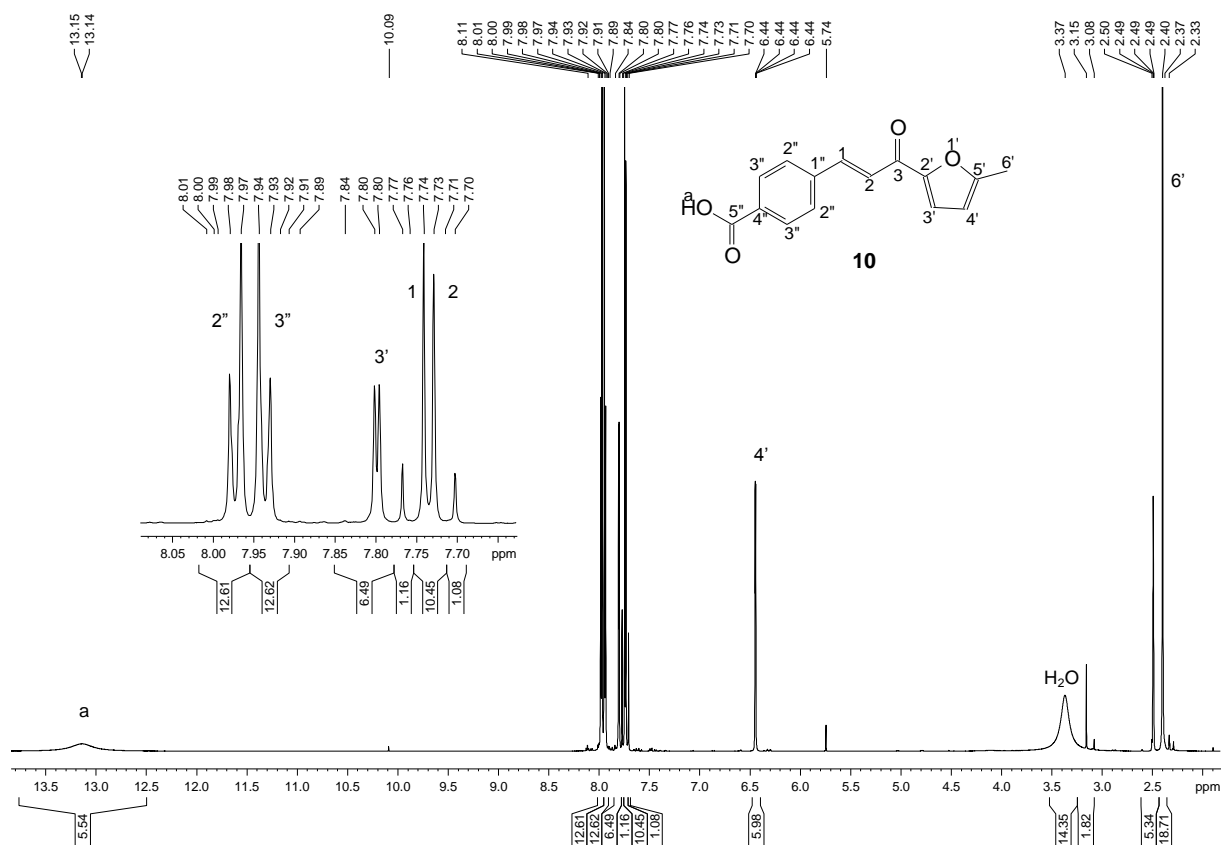
# Addendum B: Analytical data for Chapter 4

IR: 10

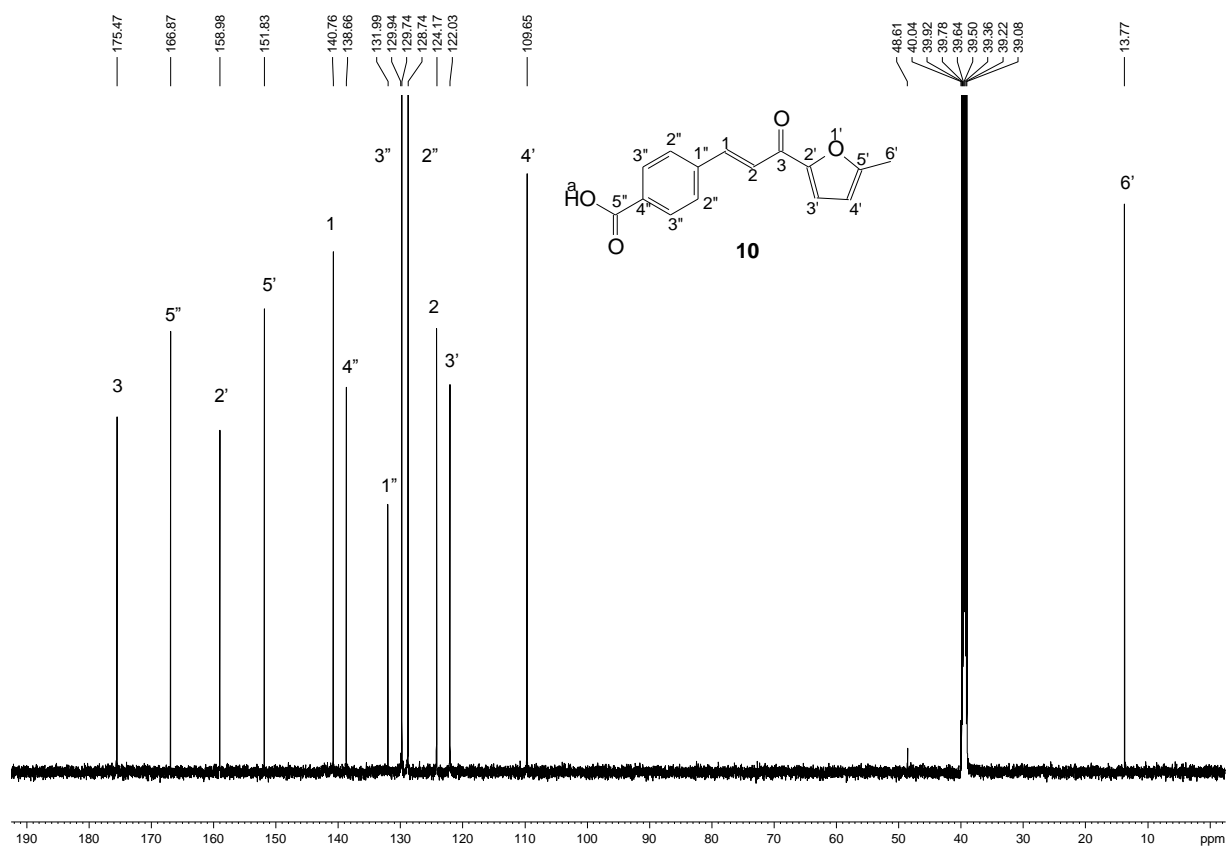


# Addendum B – Chapter 4

## <sup>1</sup>H NMR in DMSO: 10

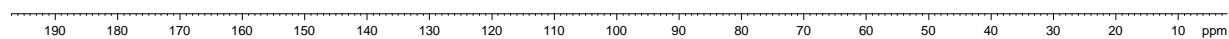
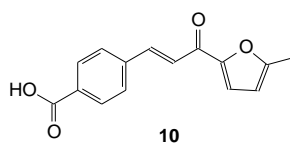
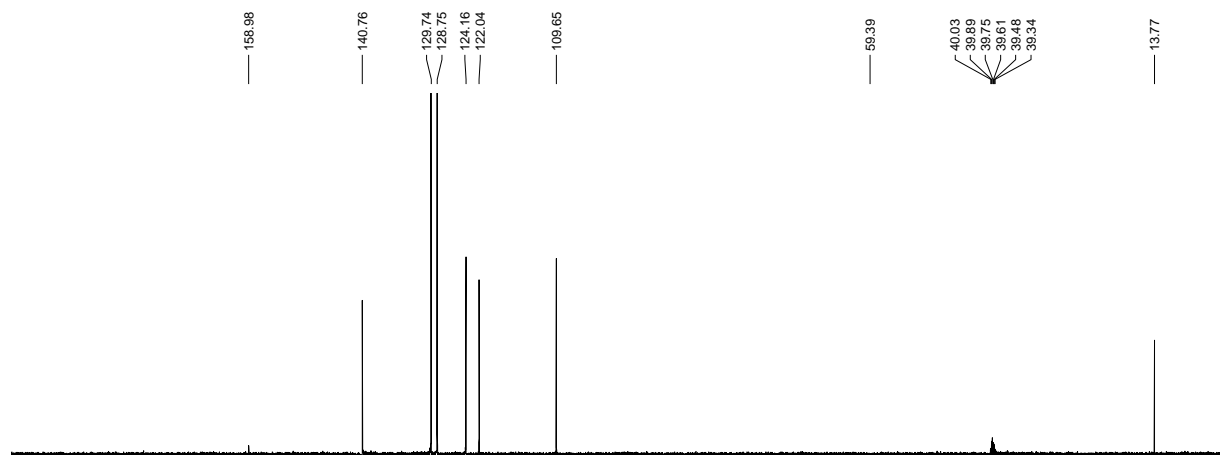


## <sup>13</sup>C NMR in DMSO: 10

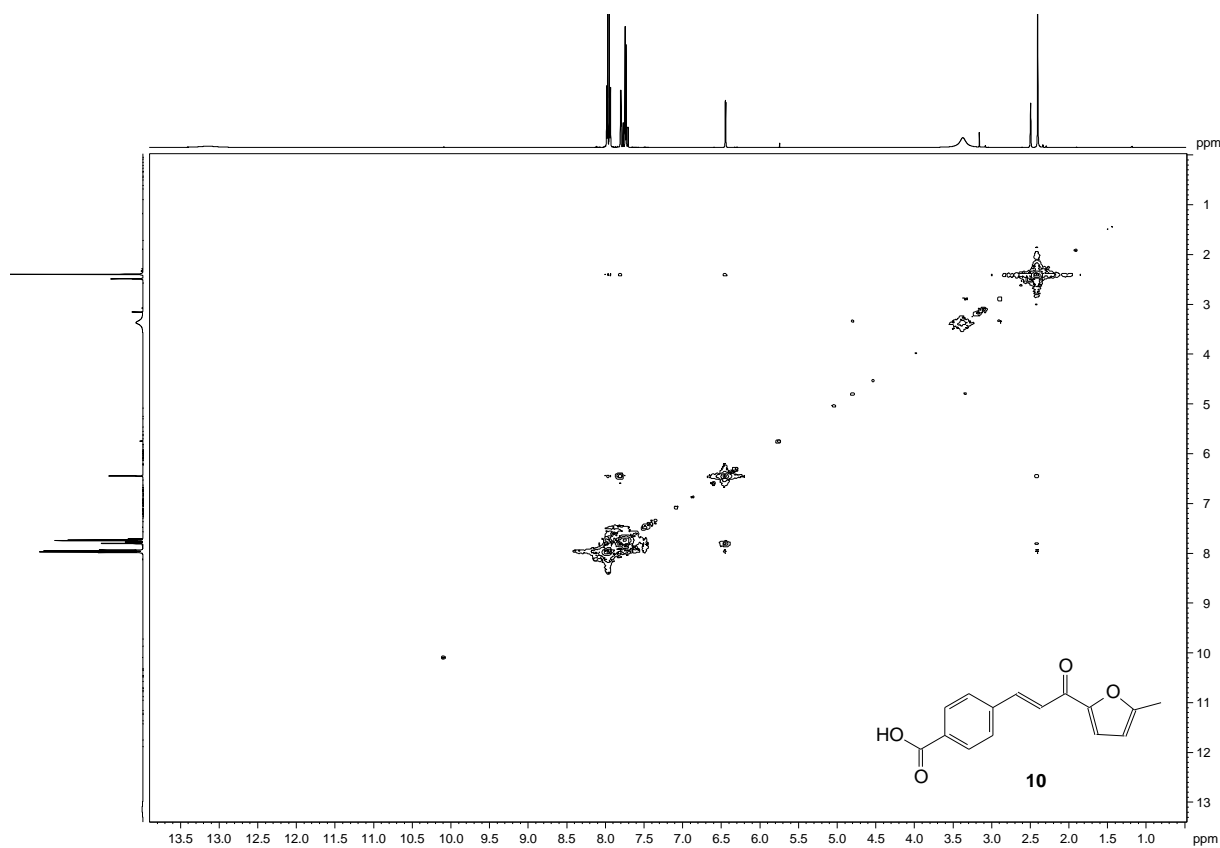


# Addendum B – Chapter 4

## DEPT135 in DMSO: 10

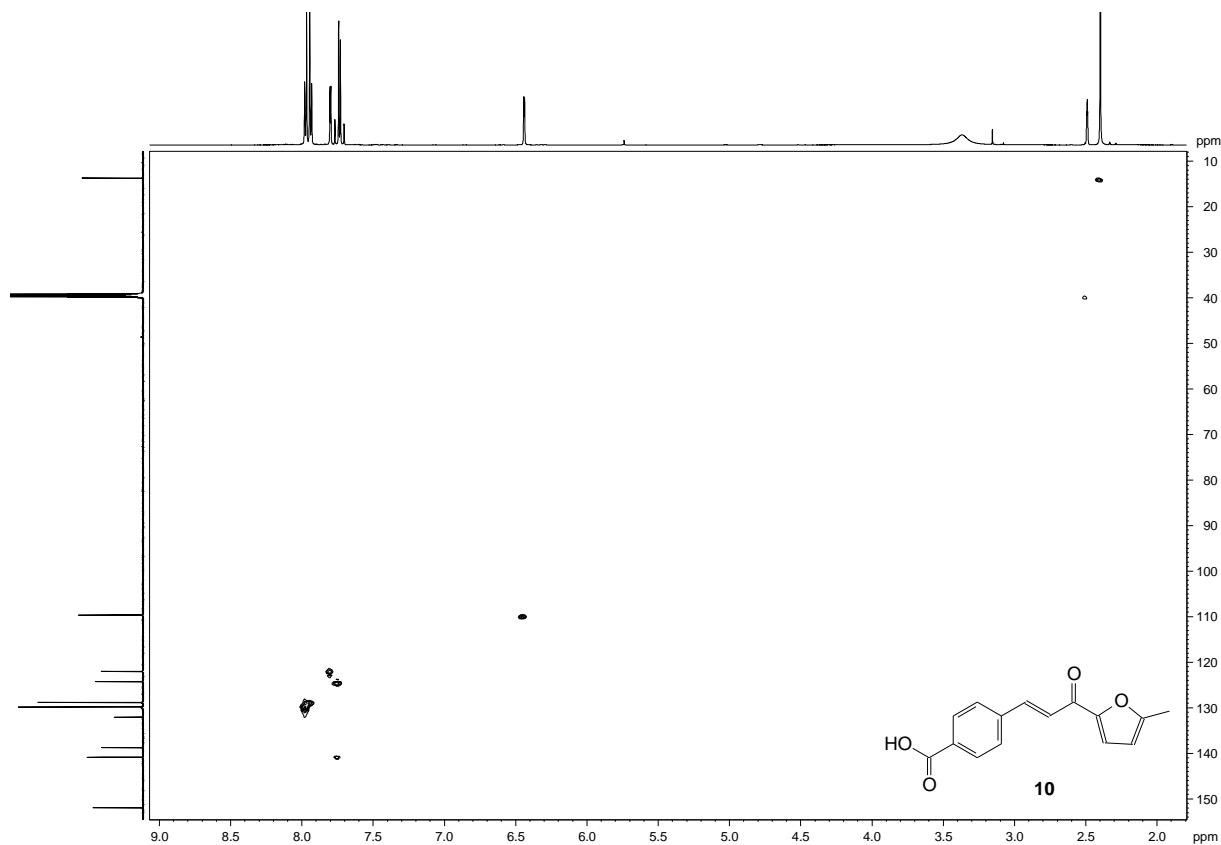


## COSY in DMSO: 10



## Addendum B – Chapter 4

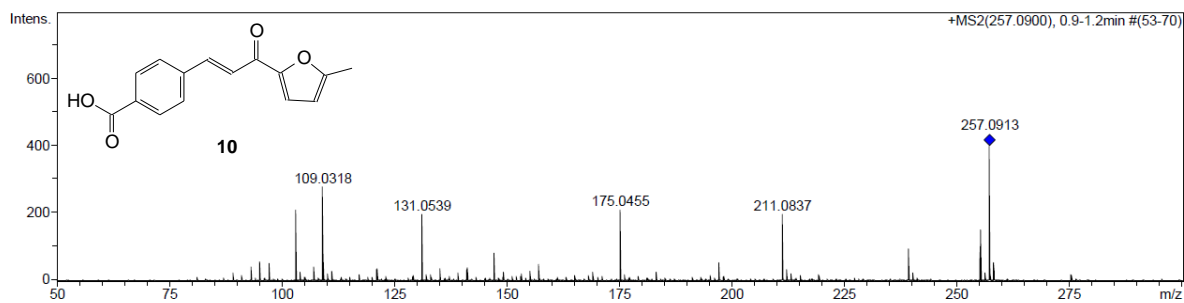
### HSQC in DMSO: **10**



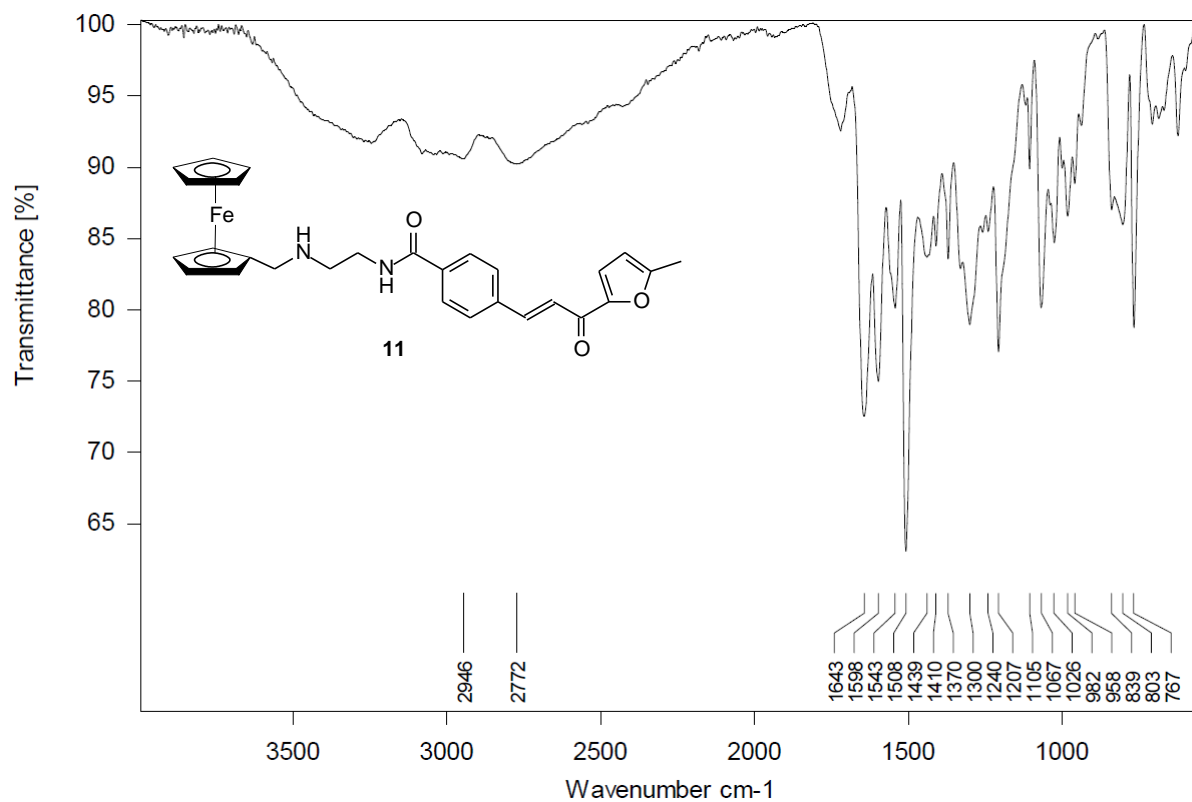
### HRMS: **10**

#### Acquisition Parameter

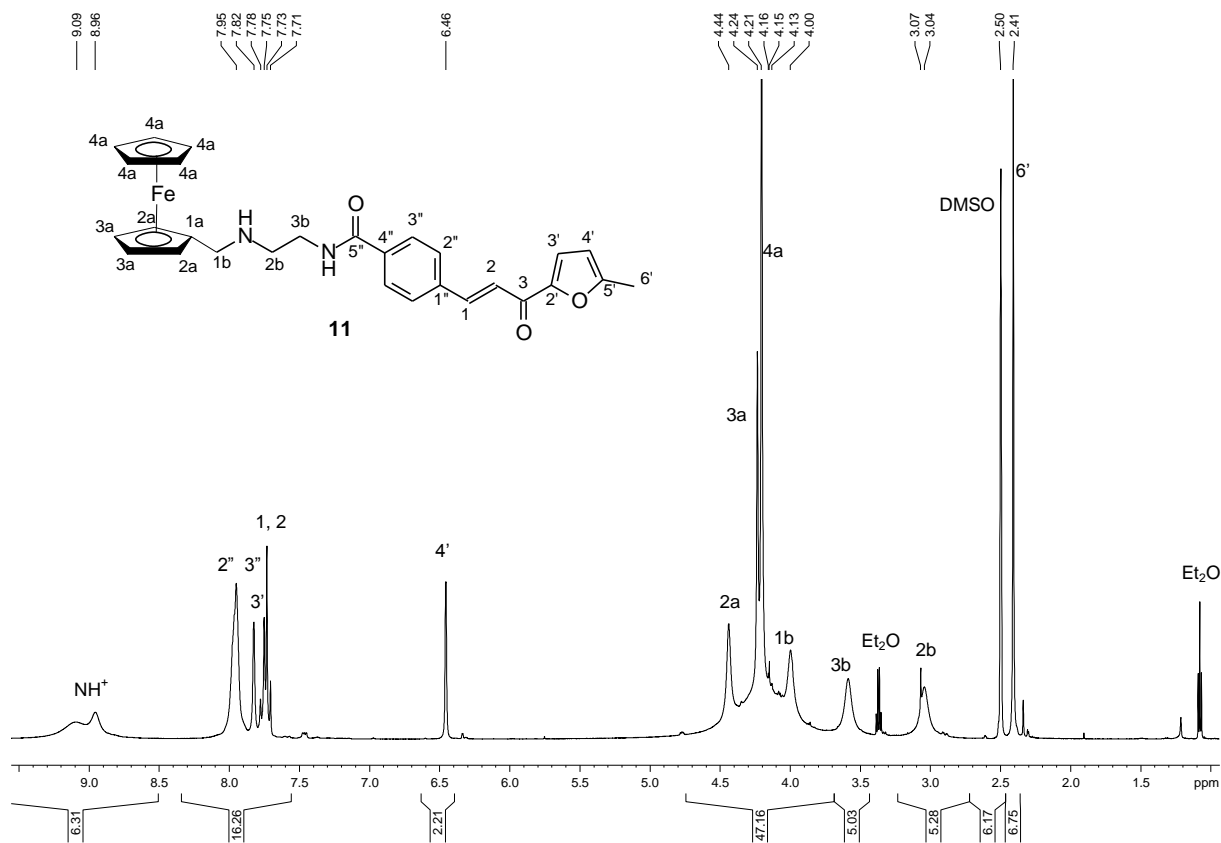
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	3000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste



IR: 11

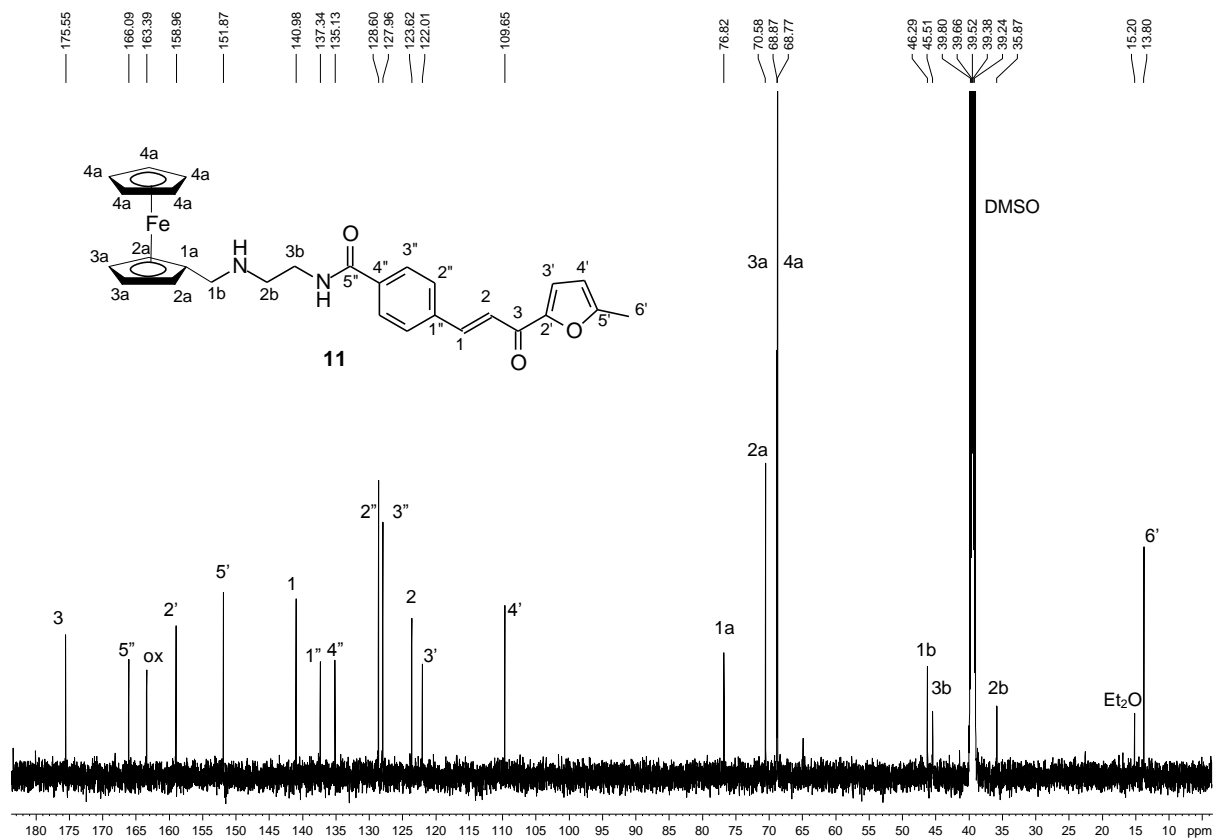


<sup>1</sup>H NMR in DMSO: 11

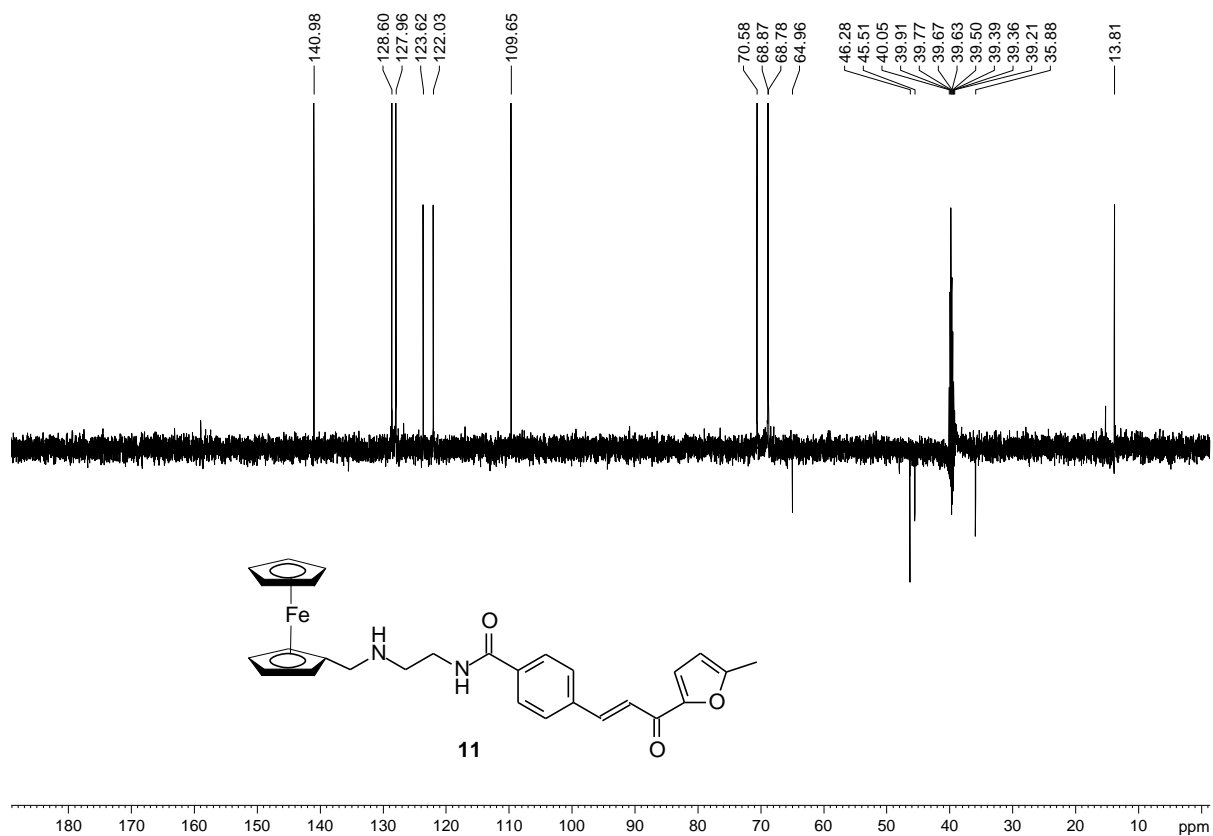


# Addendum B – Chapter 4

## <sup>13</sup>C NMR in DMSO: 11

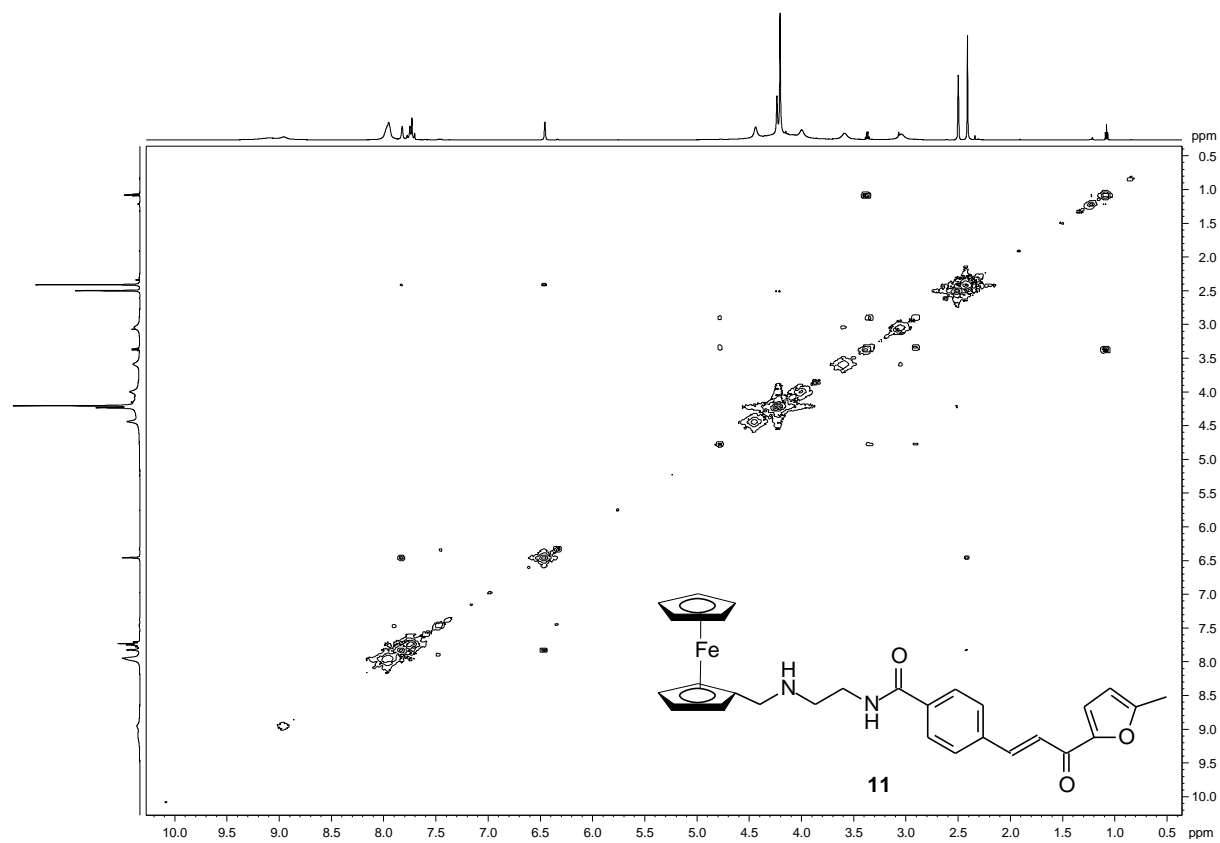


## DEPT135 in DMSO: 11

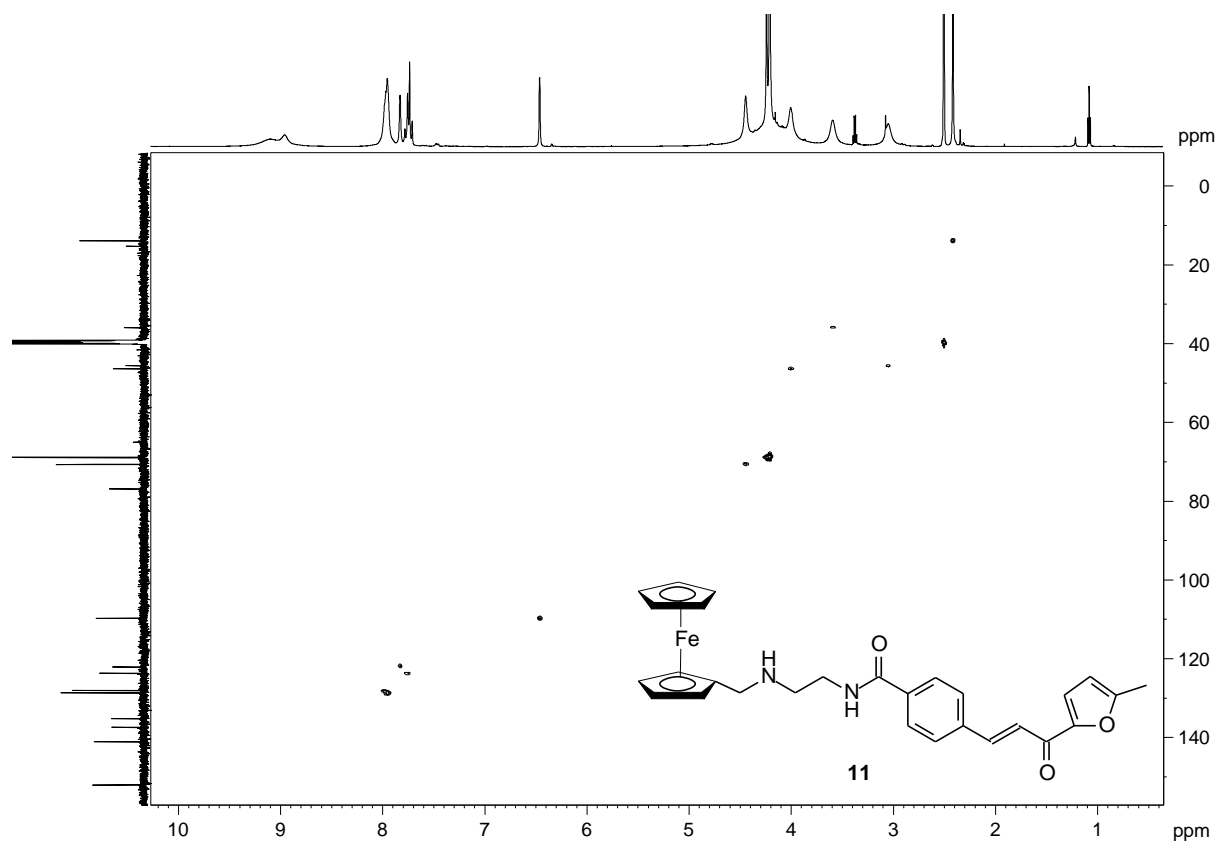


Addendum B – Chapter 4

COSY in DMSO: 11



HSQC in DMSO: 11

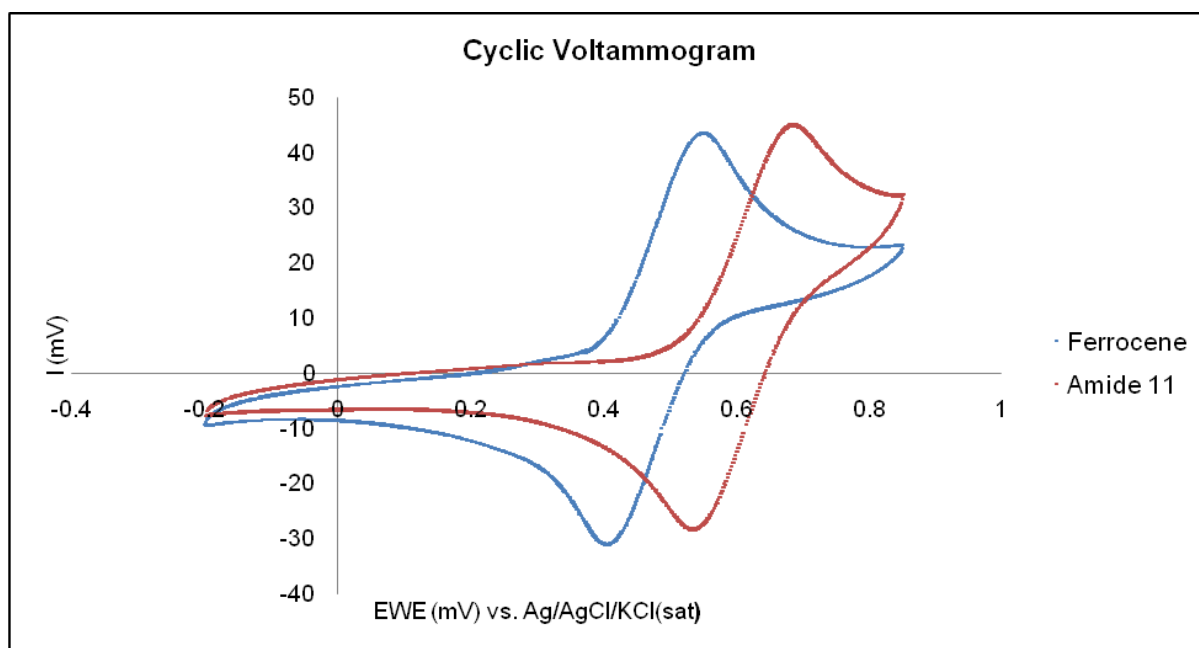
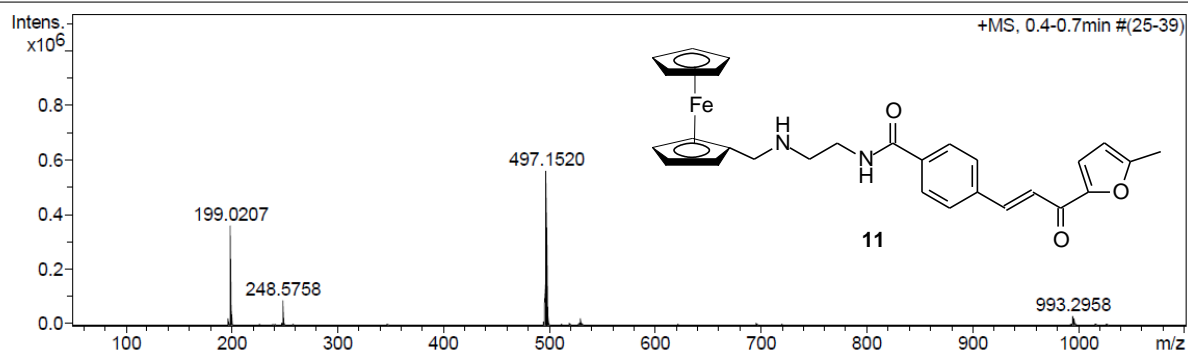


## Addendum B – Chapter 4

### HRMS: 11

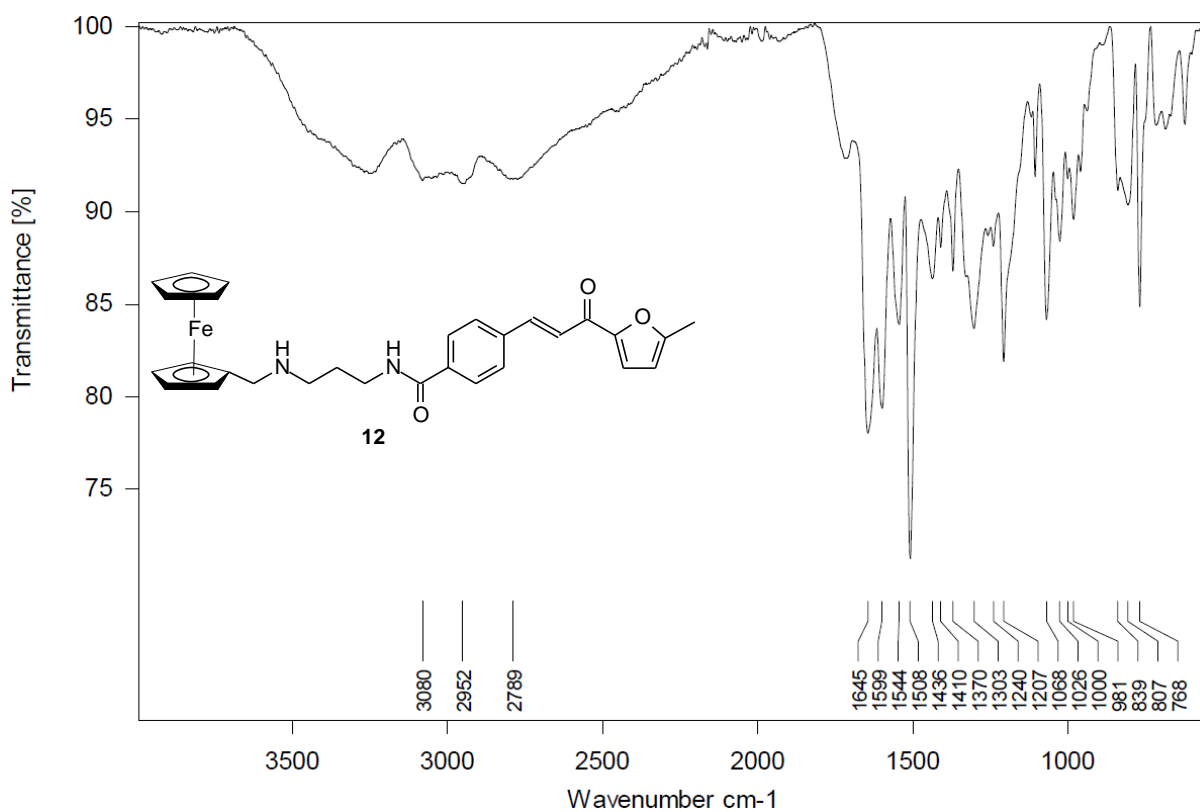
#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

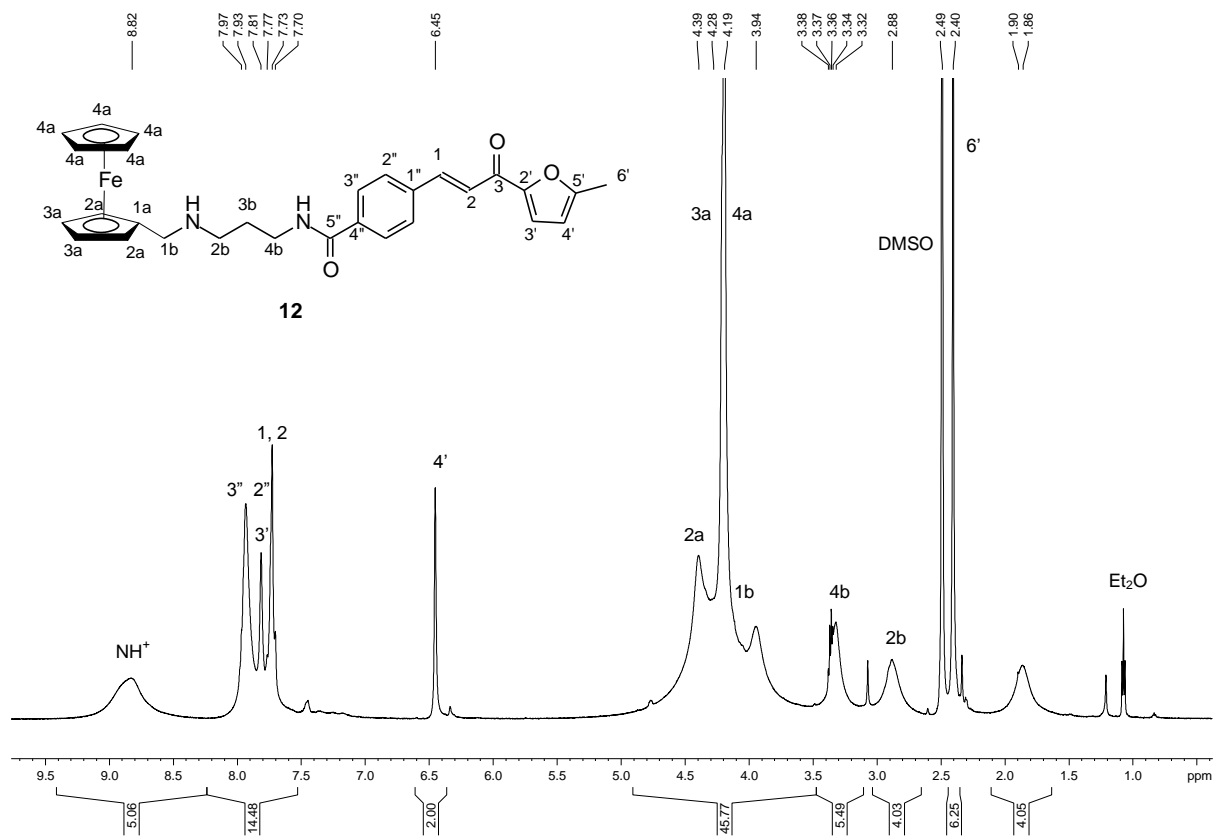


# Addendum B – Chapter 4

IR: 12

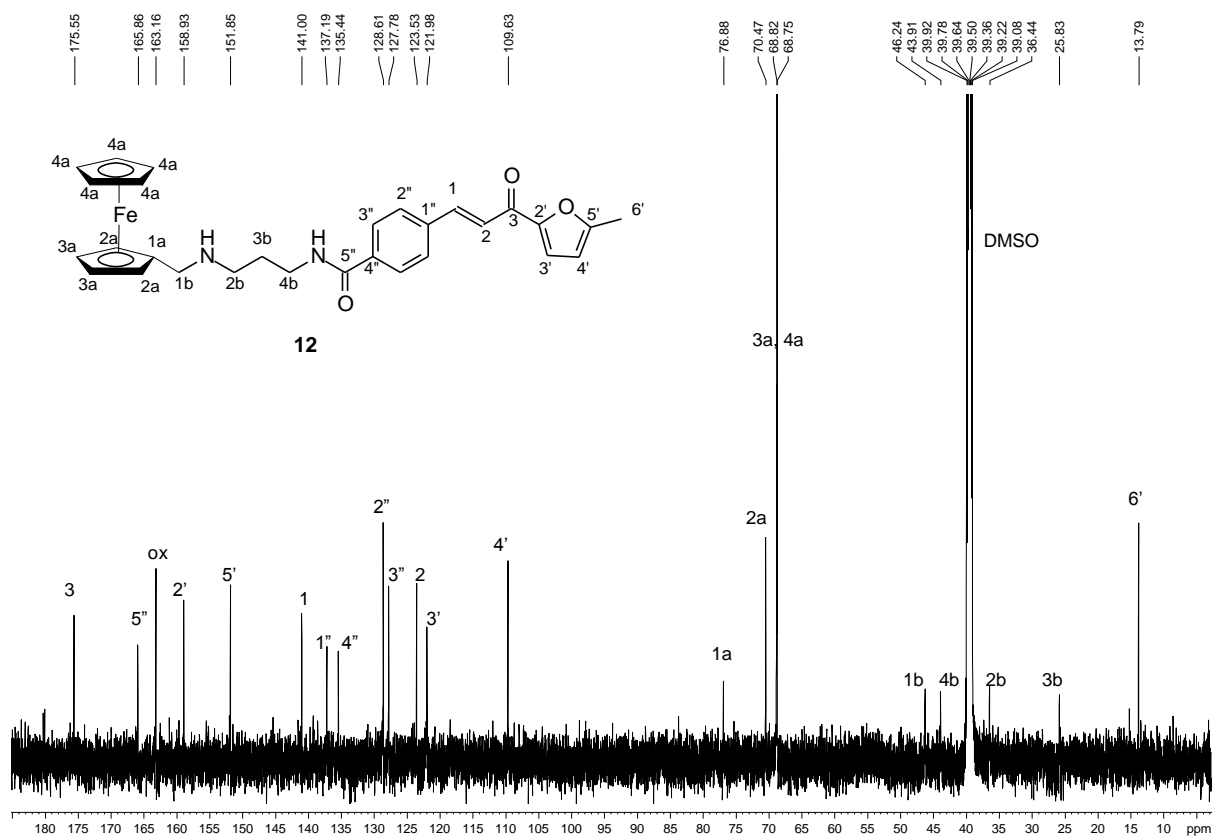


<sup>1</sup>H NMR in DMSO: 12

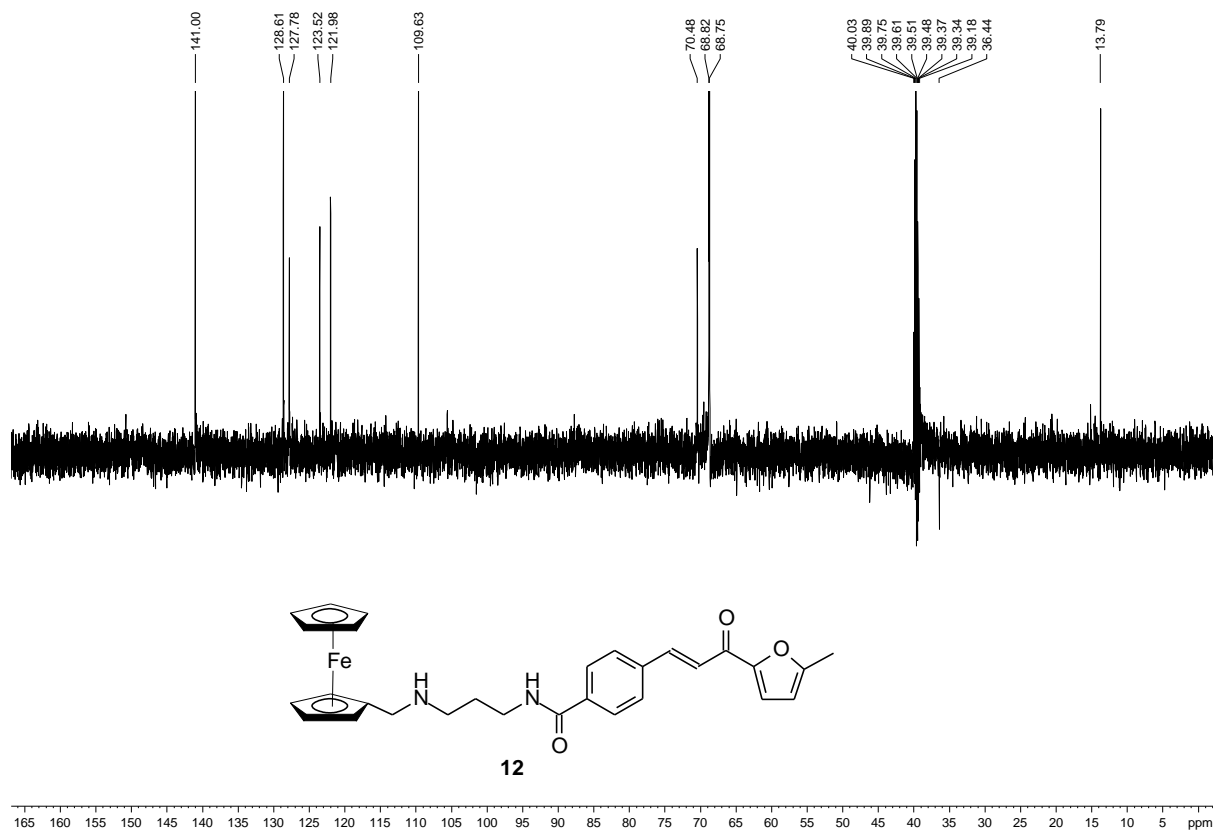


## Addendum B – Chapter 4

### <sup>13</sup>C NMR in DMSO: **12**

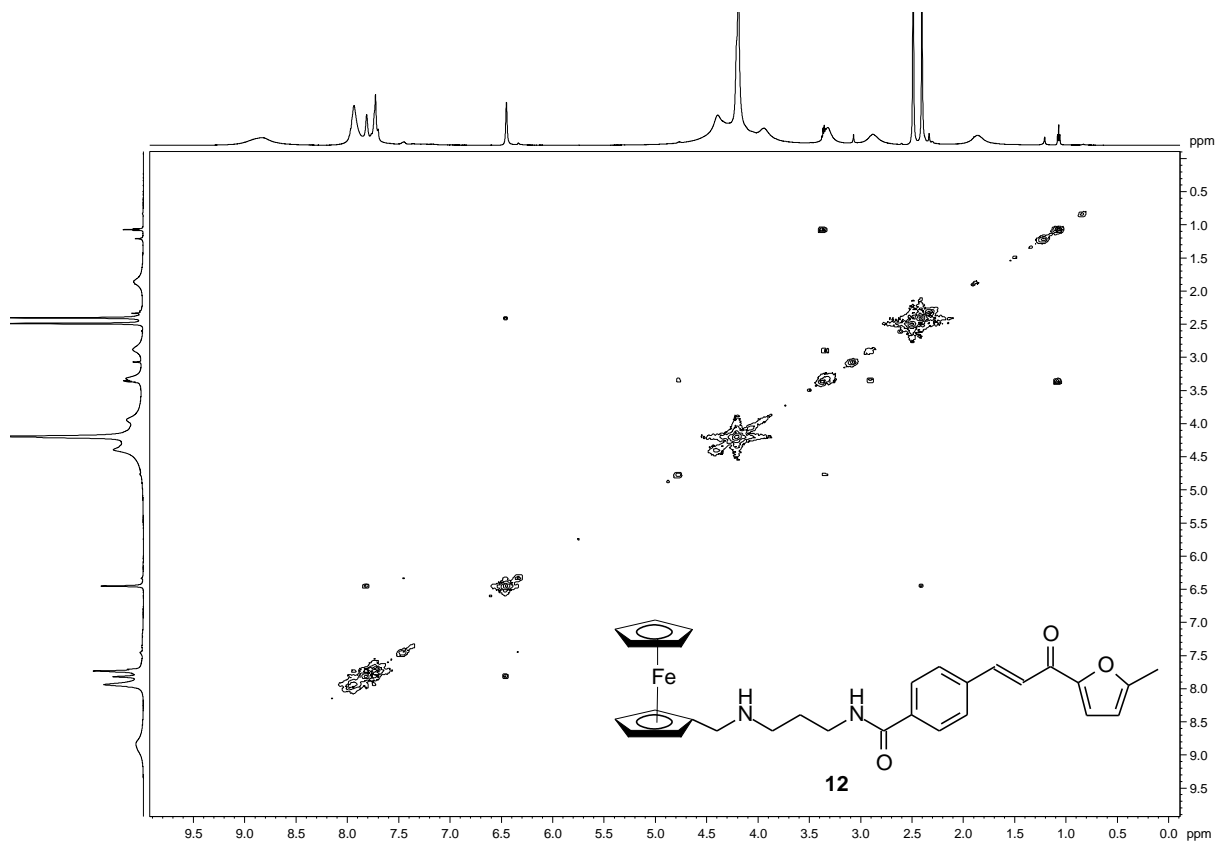


### DEPT135 in DMSO: **12**

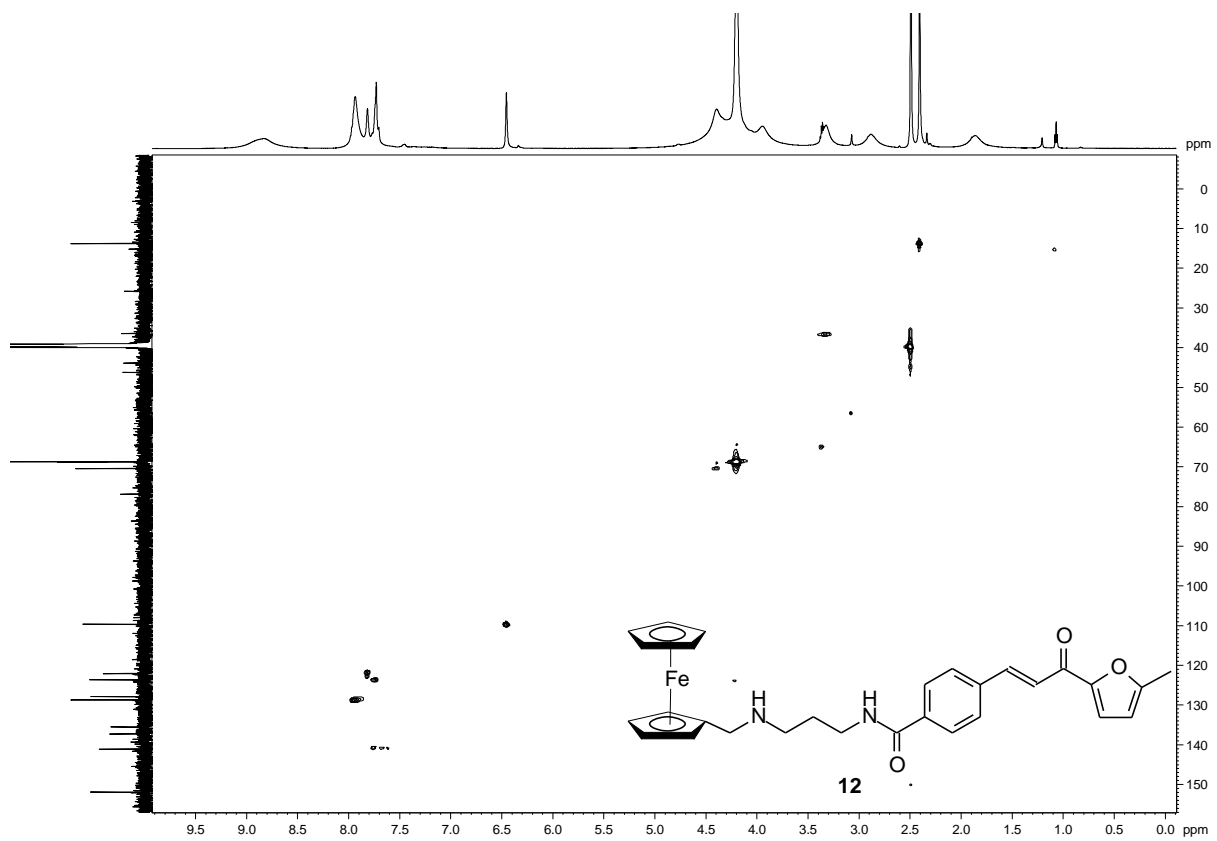


Addendum B – Chapter 4

COSY in DMSO: 12



HSQC in DMSO: 12

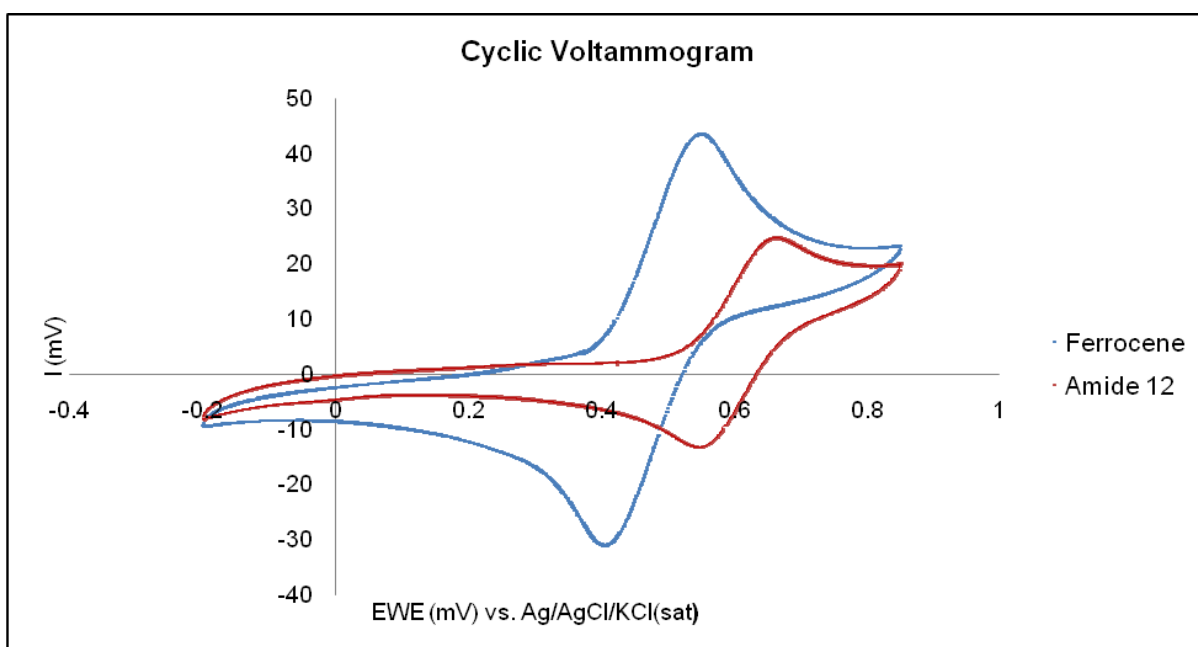
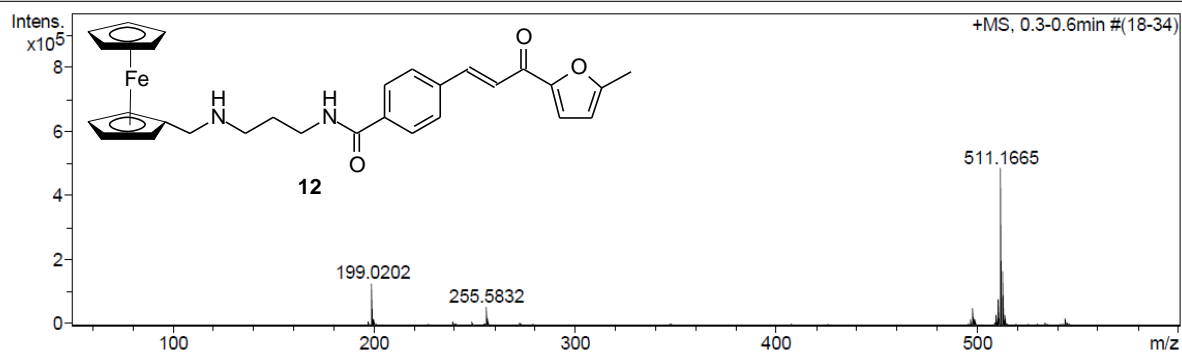


## Addendum B – Chapter 4

### HRMS: 12

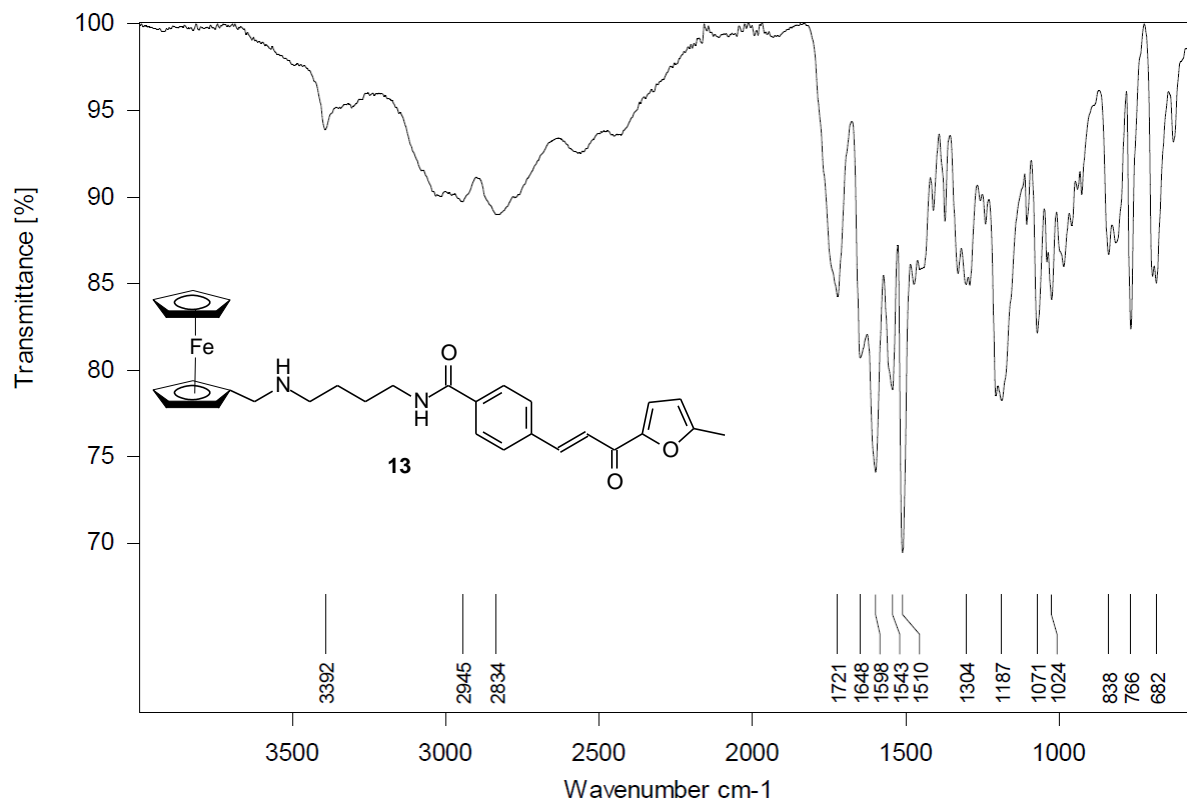
#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

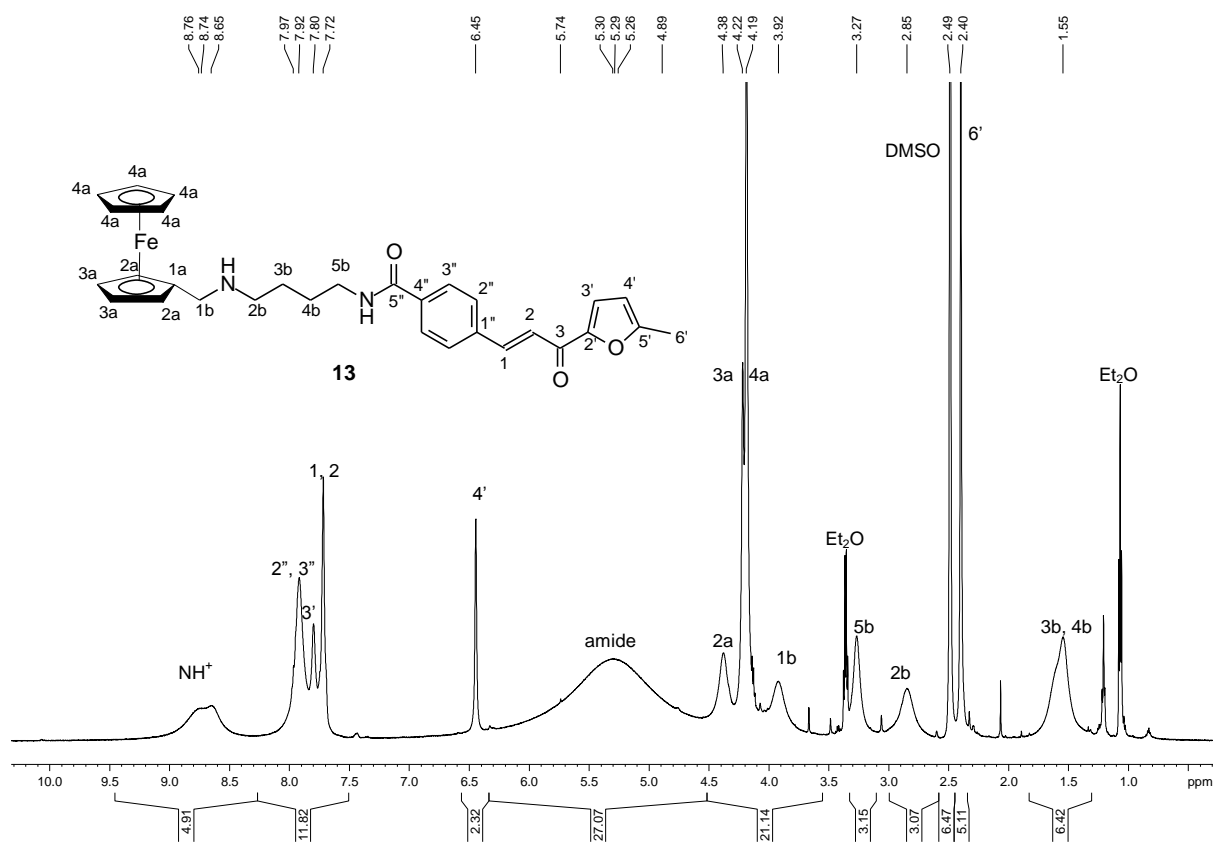


Addendum B – Chapter 4

IR: 13

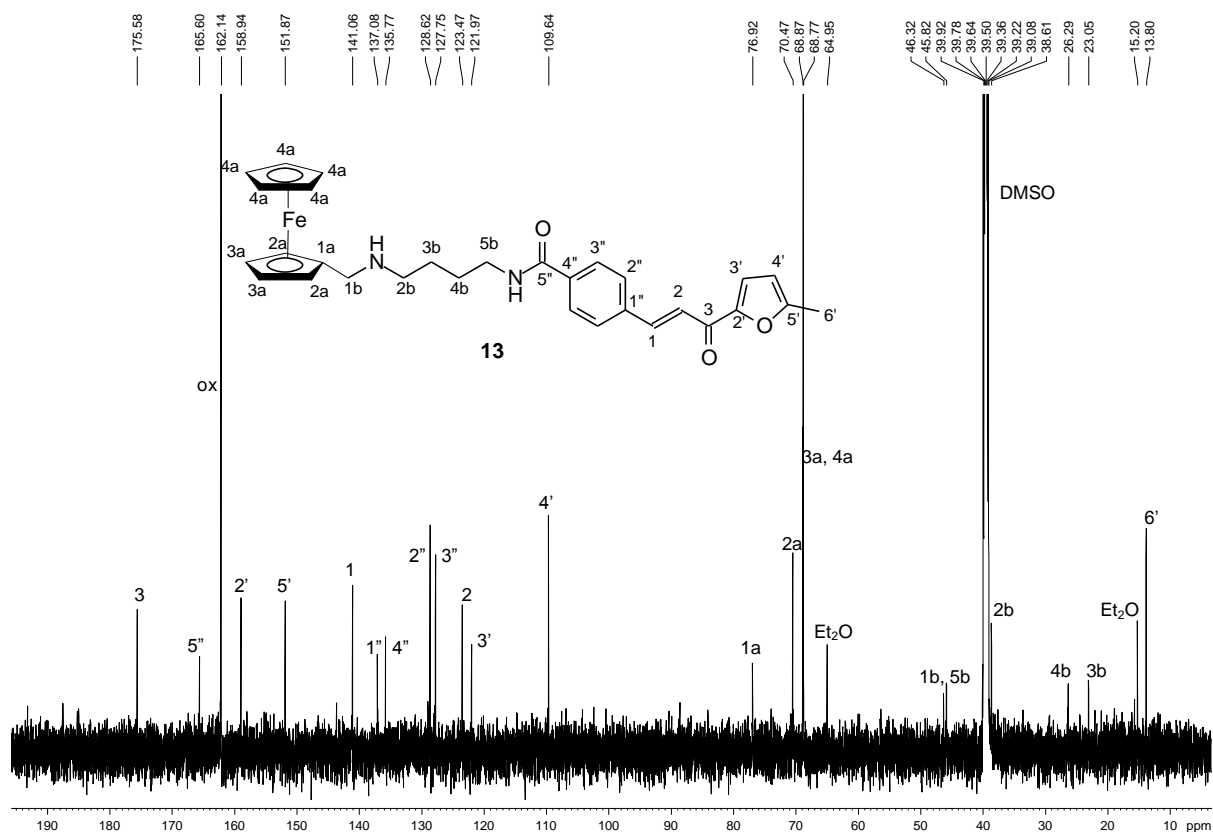


<sup>1</sup>H NMR in DMSO: 13

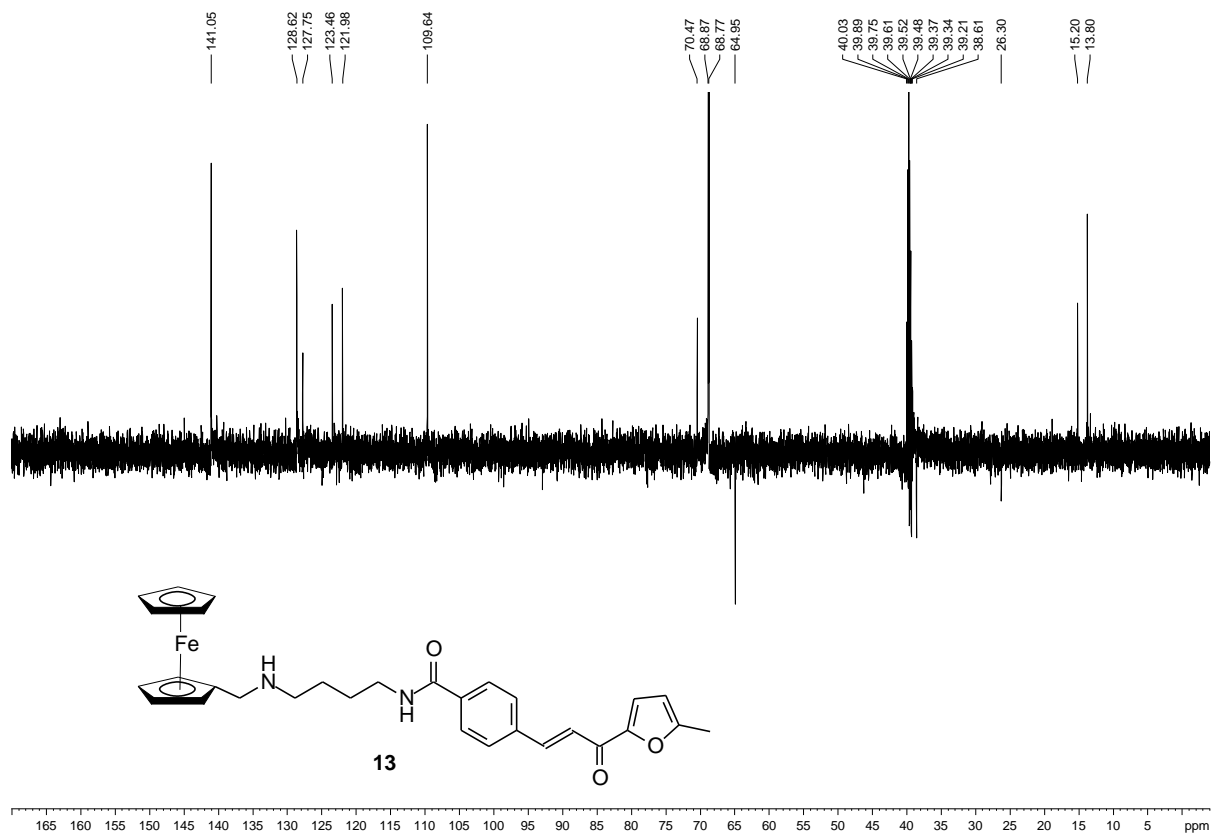


# Addendum B – Chapter 4

## <sup>13</sup>C NMR in DMSO: 13

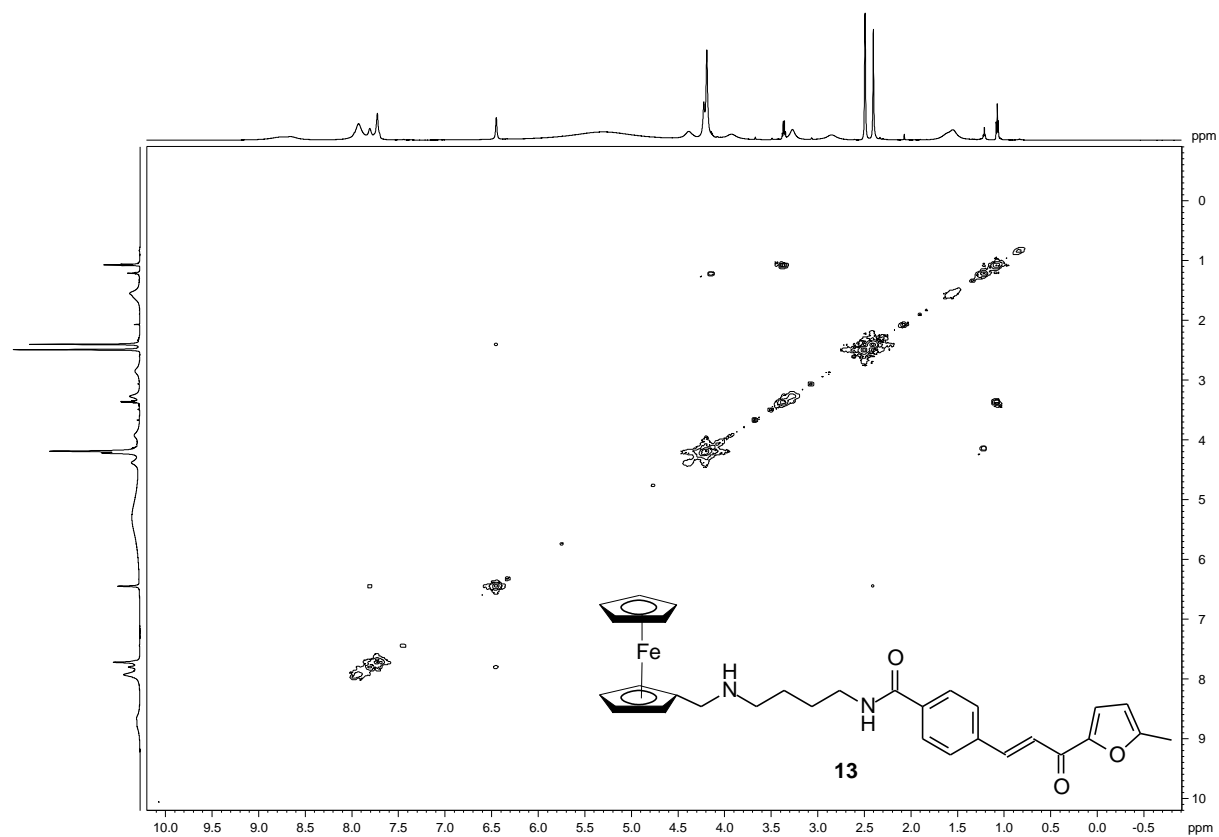


## DEPT135 in DMSO: 13

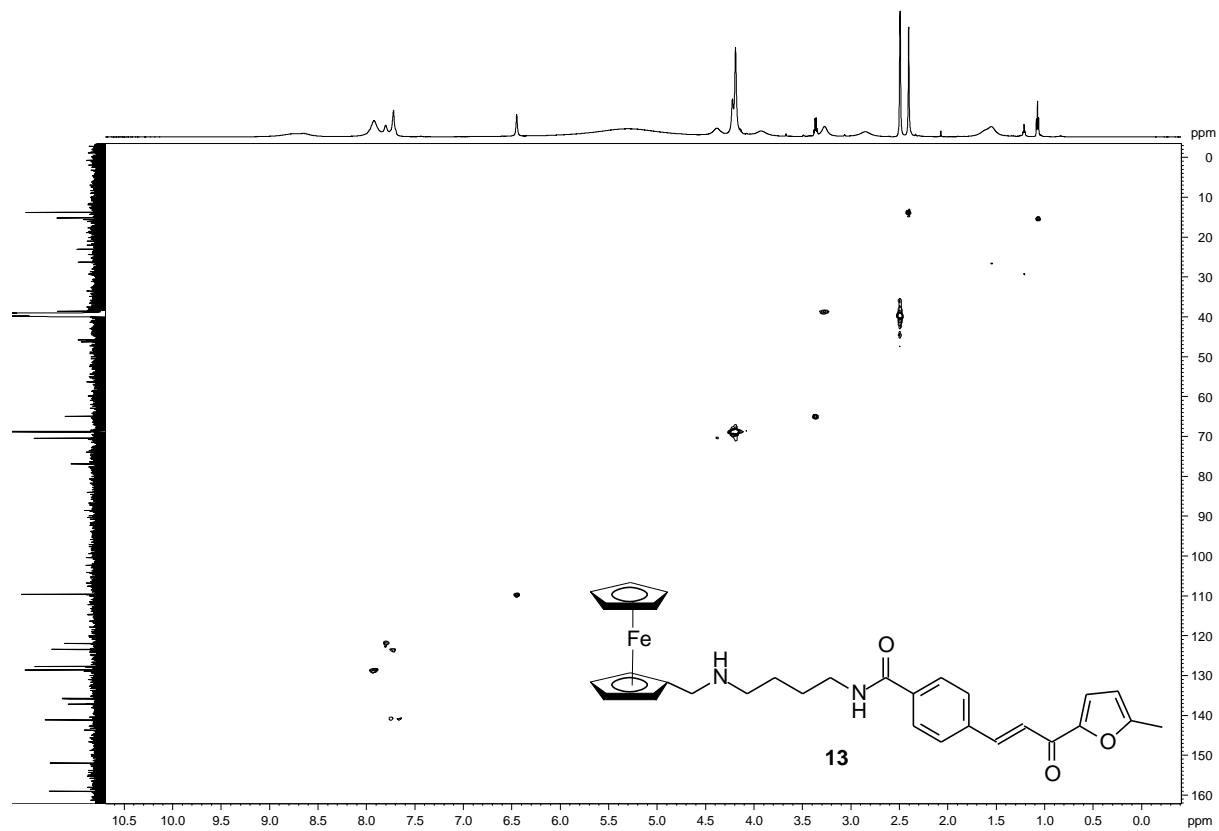


Addendum B – Chapter 4

COSY in DMSO: 13



HSQC in DMSO: 13

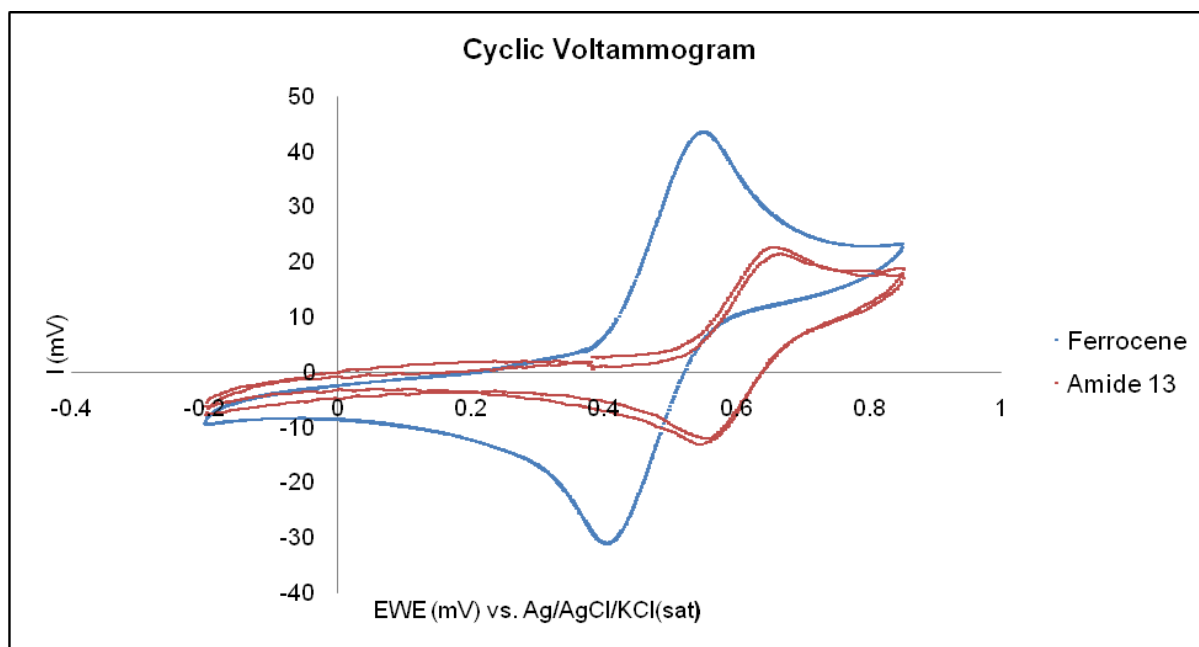
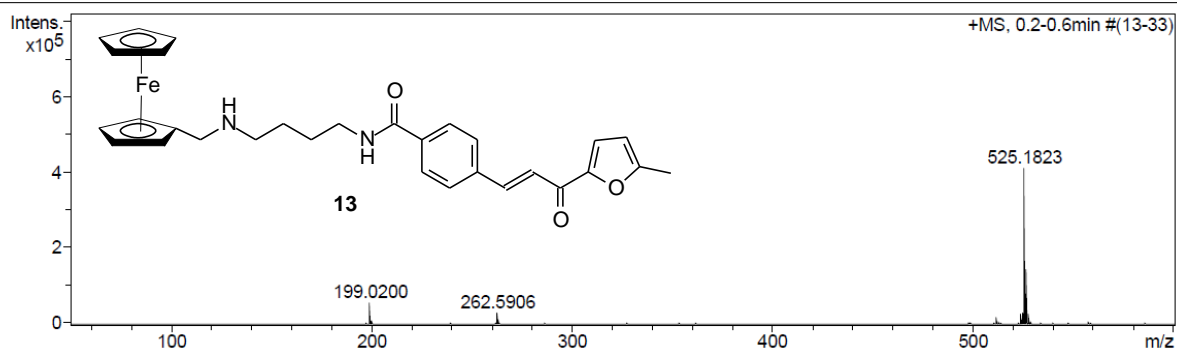


## Addendum B – Chapter 4

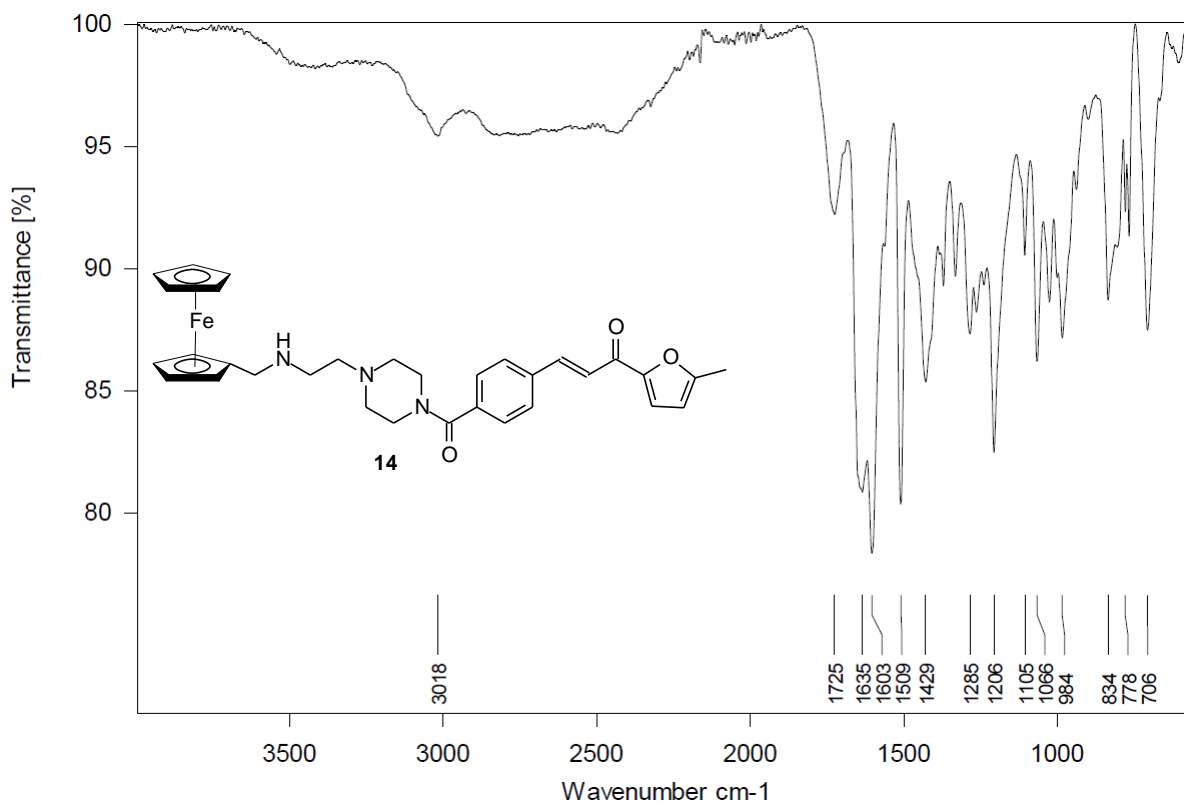
### HRMS: 13

#### Acquisition Parameter

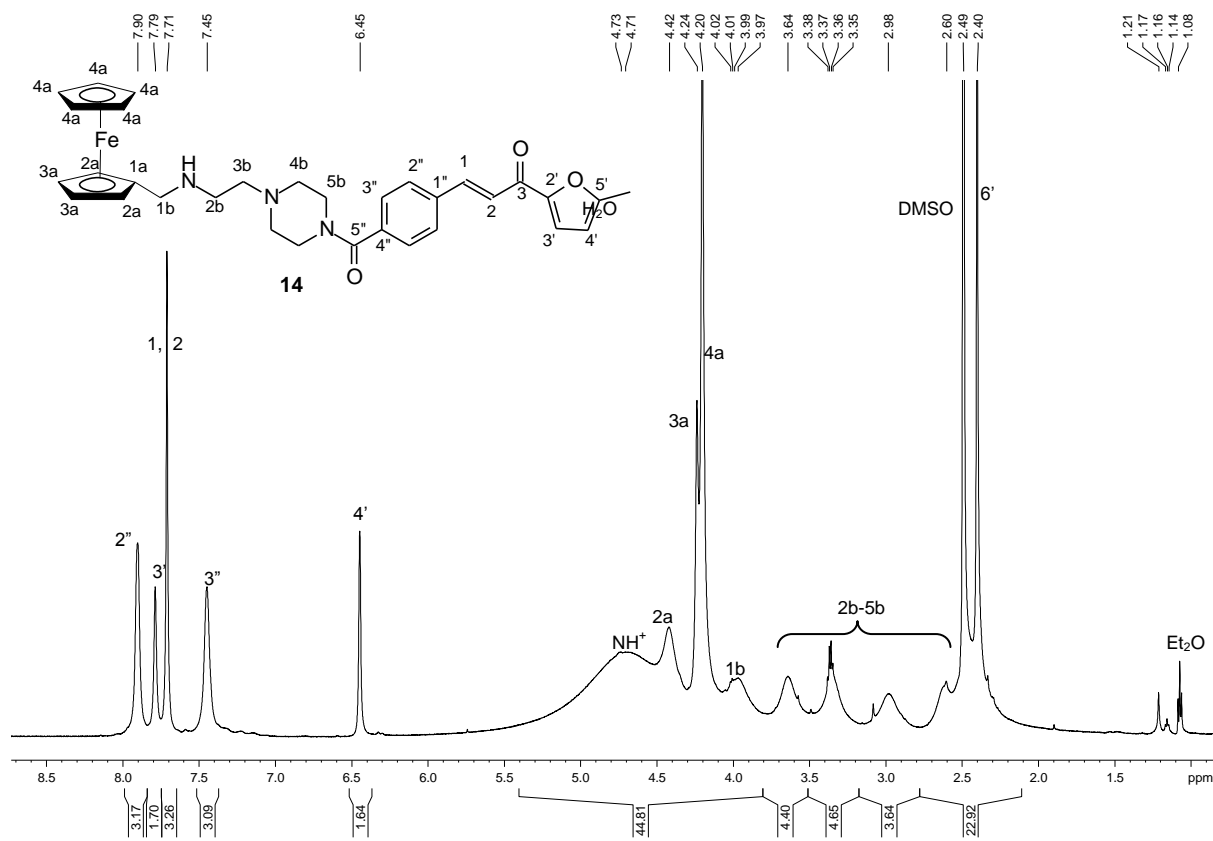
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste



IR: 14

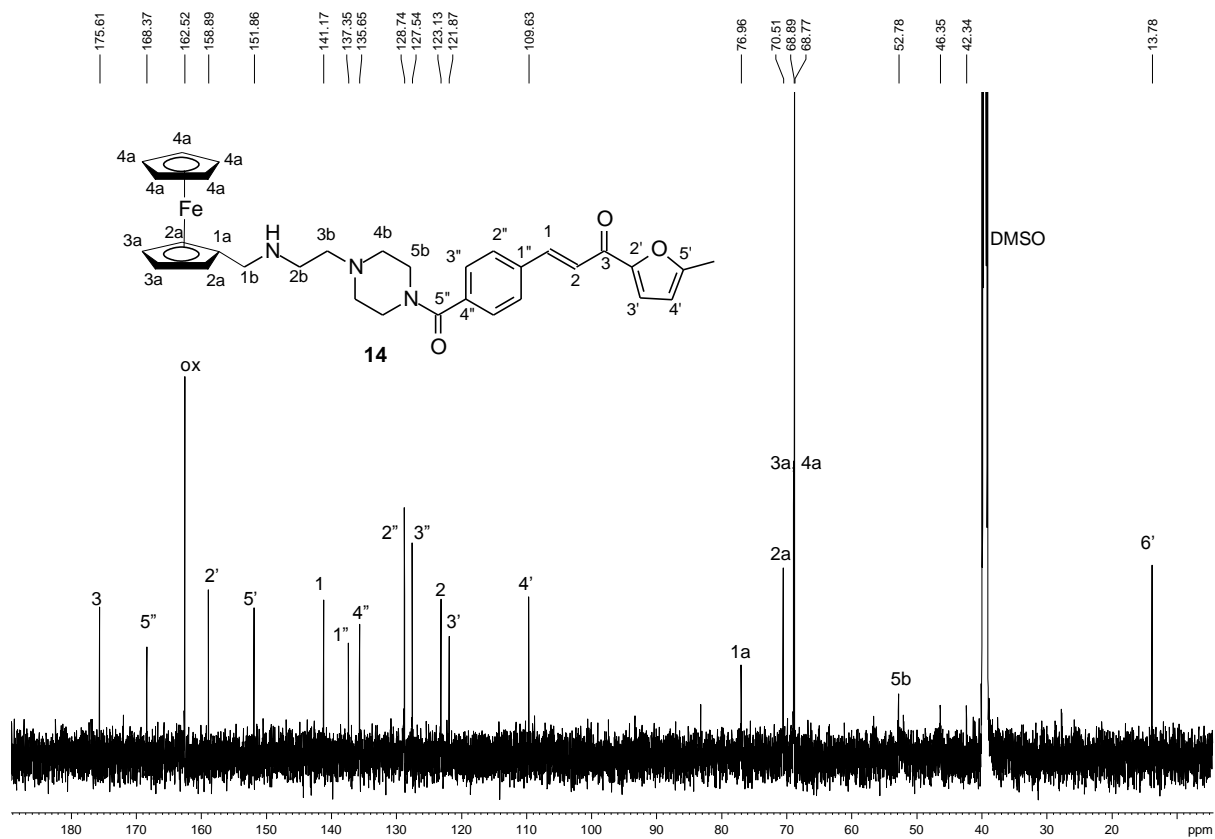


<sup>1</sup>H NMR in DMSO: 14

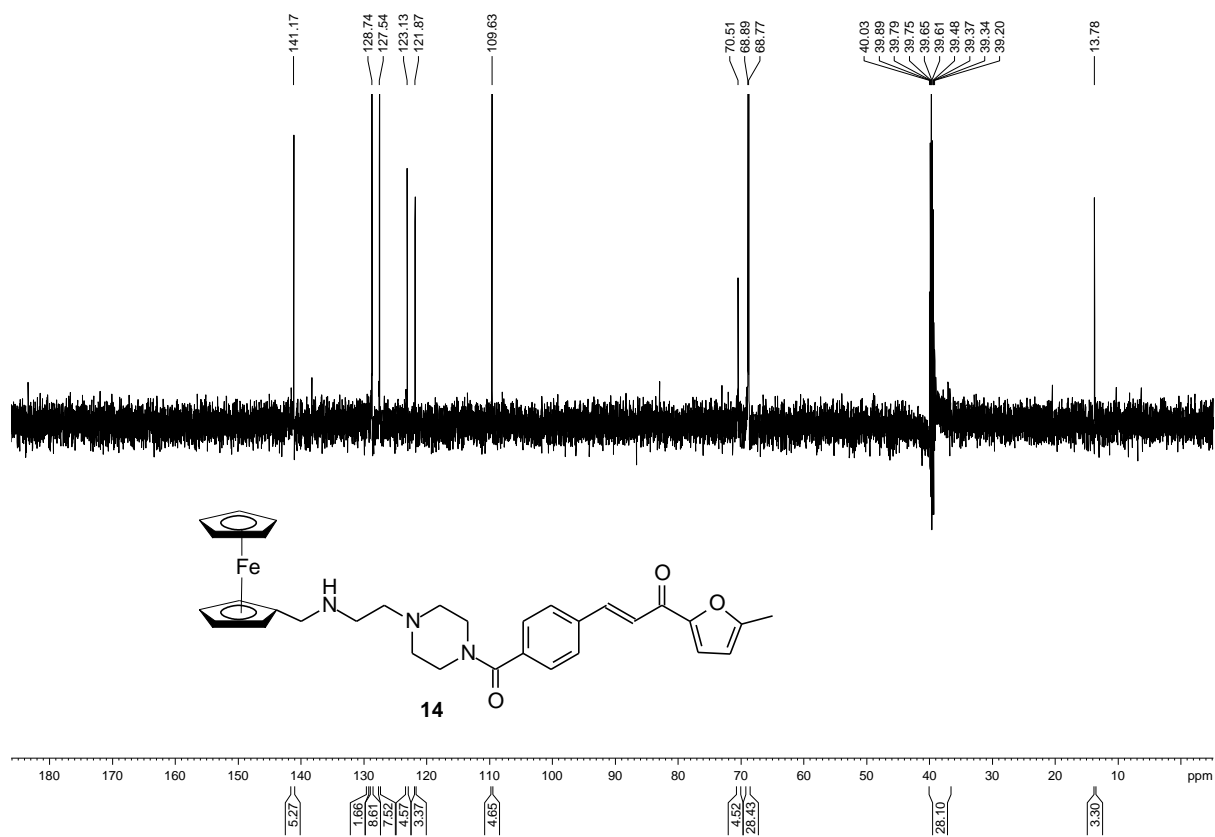


# Addendum B – Chapter 4

## <sup>13</sup>C NMR in DMSO: 14

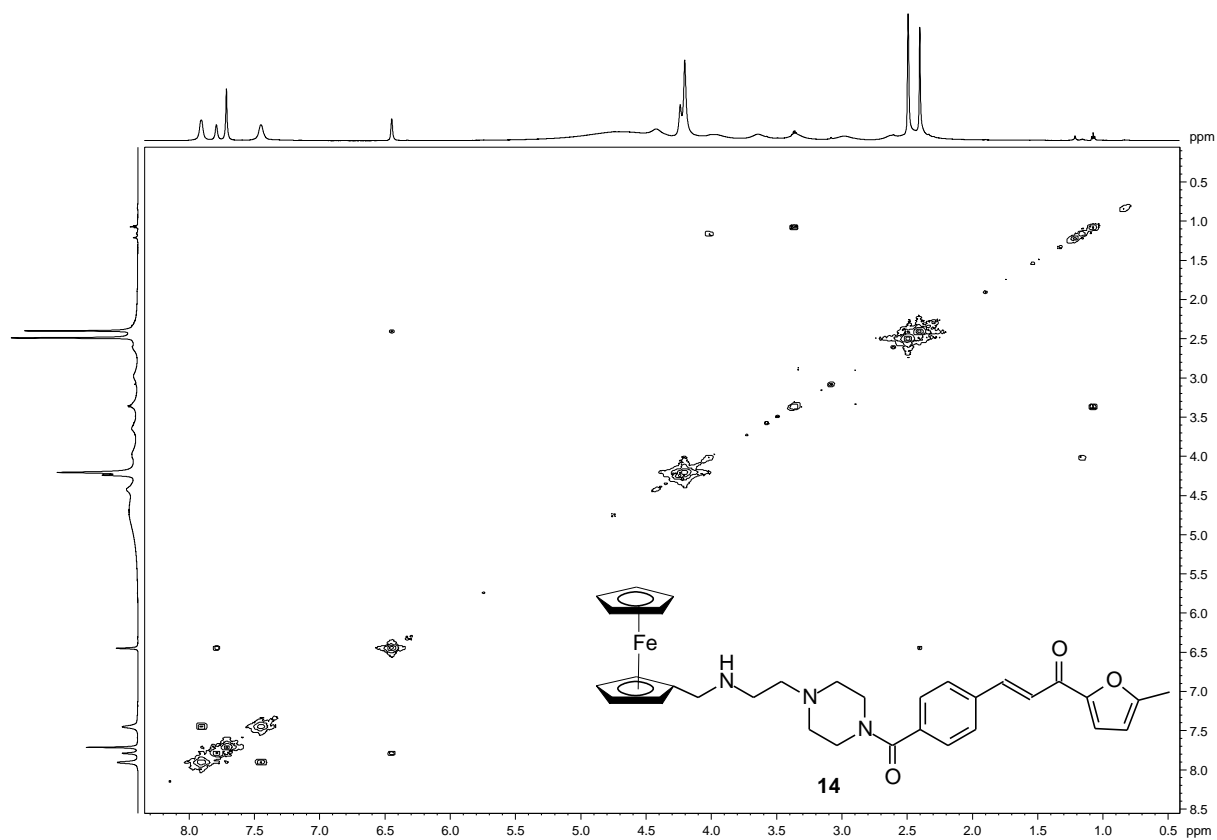


## DEPT135 in DMSO: 14

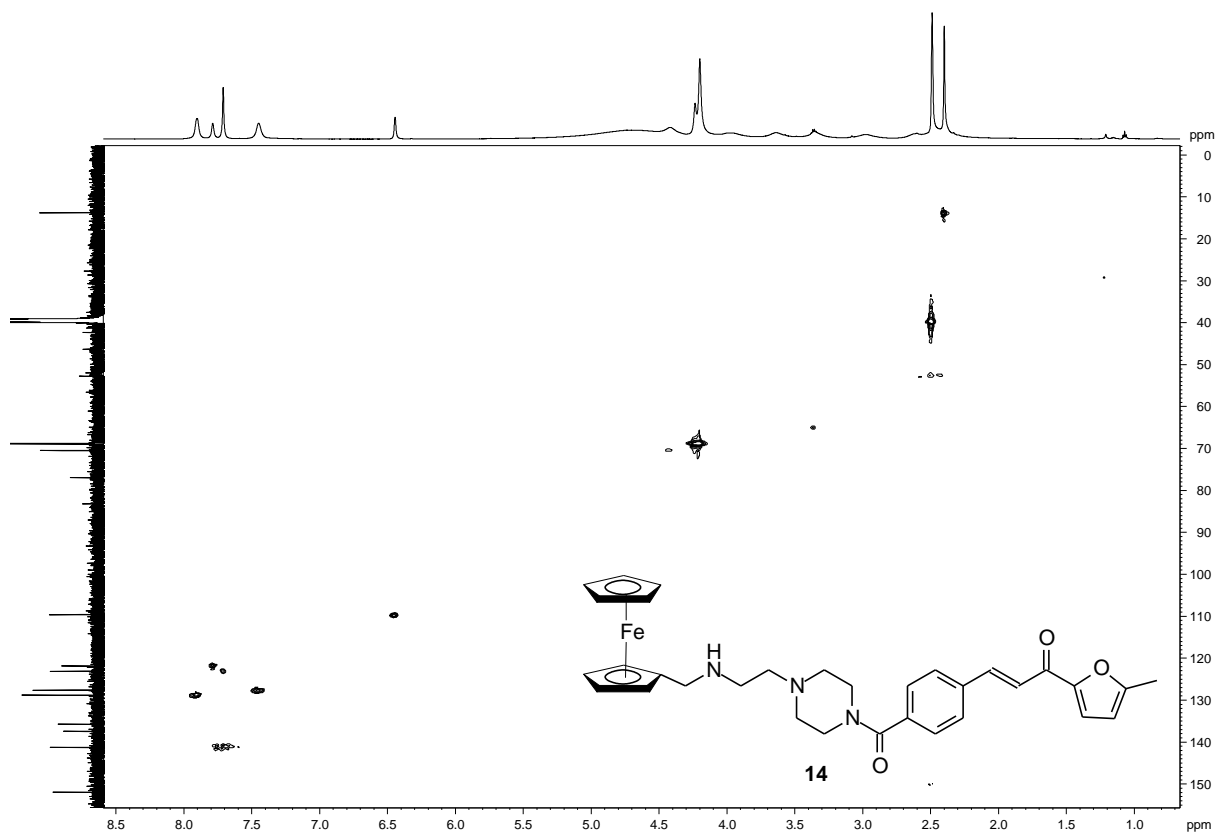


Addendum B – Chapter 4

COSY in DMSO: 14



HSQC in DMSO: 14

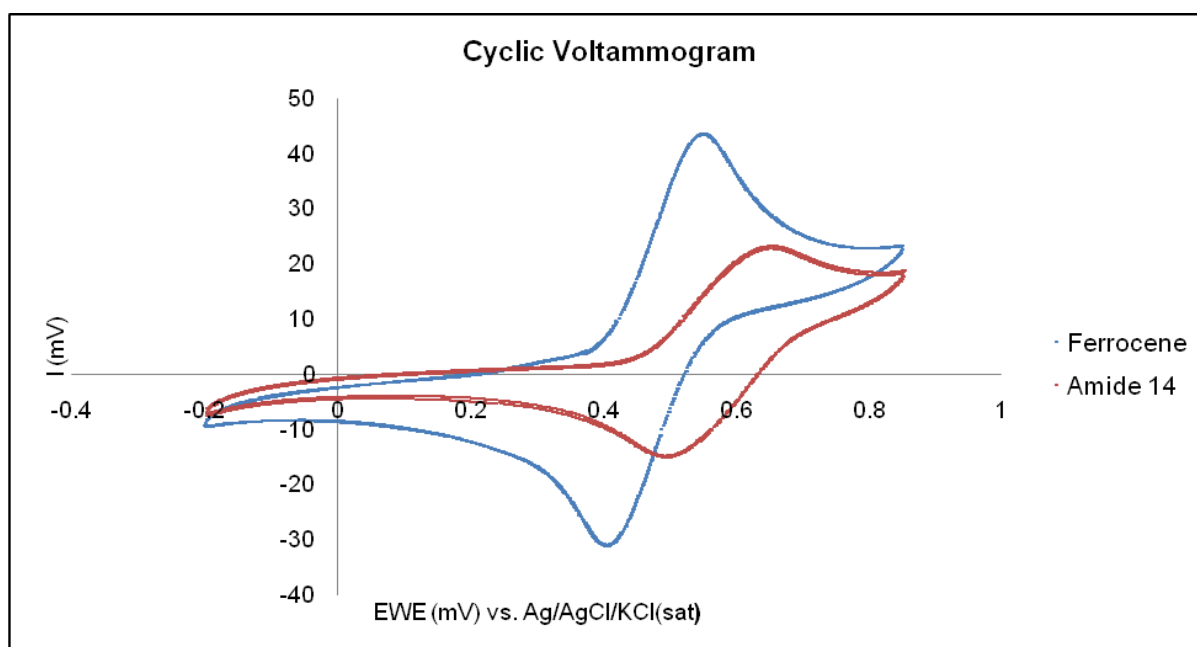
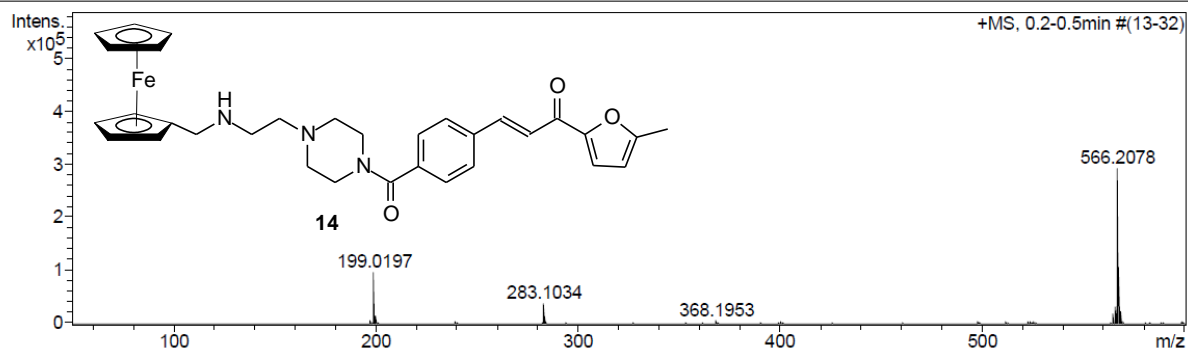


## Addendum B – Chapter 4

### HRMS: 14

#### Acquisition Parameter

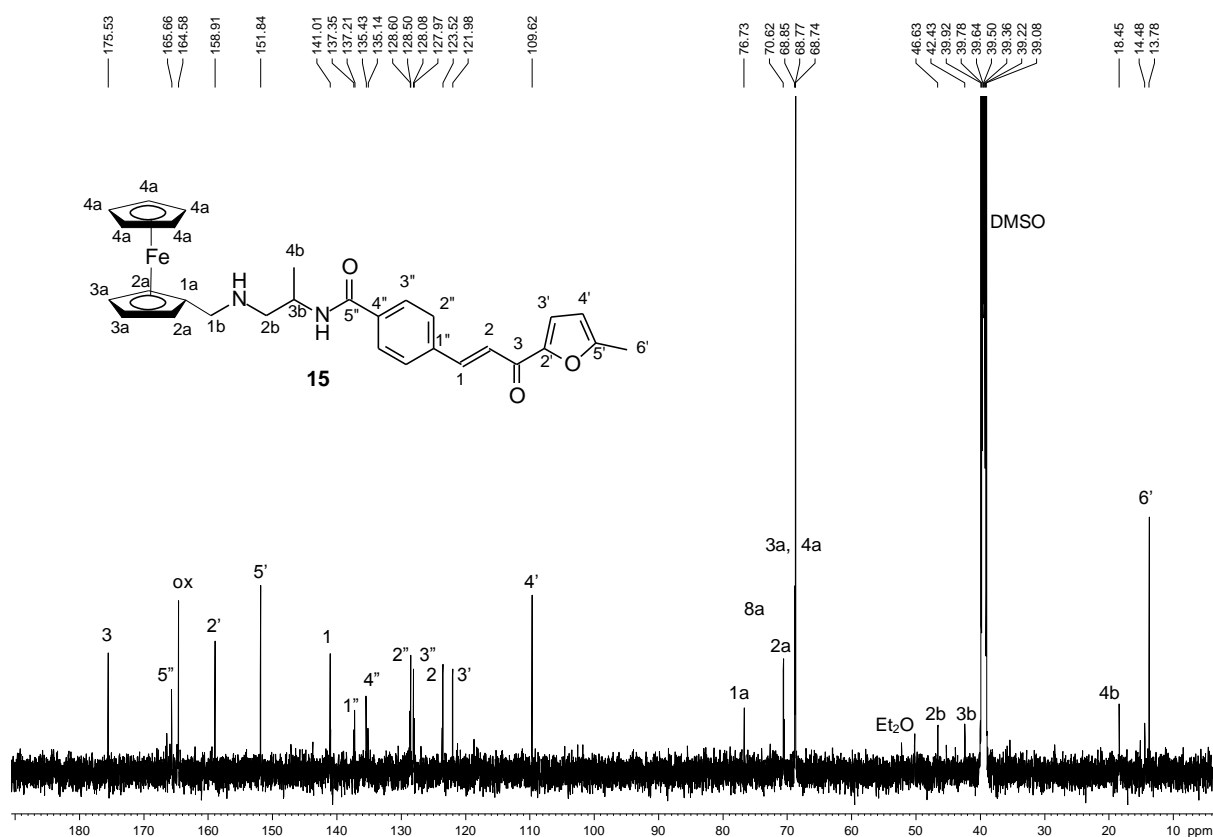
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste



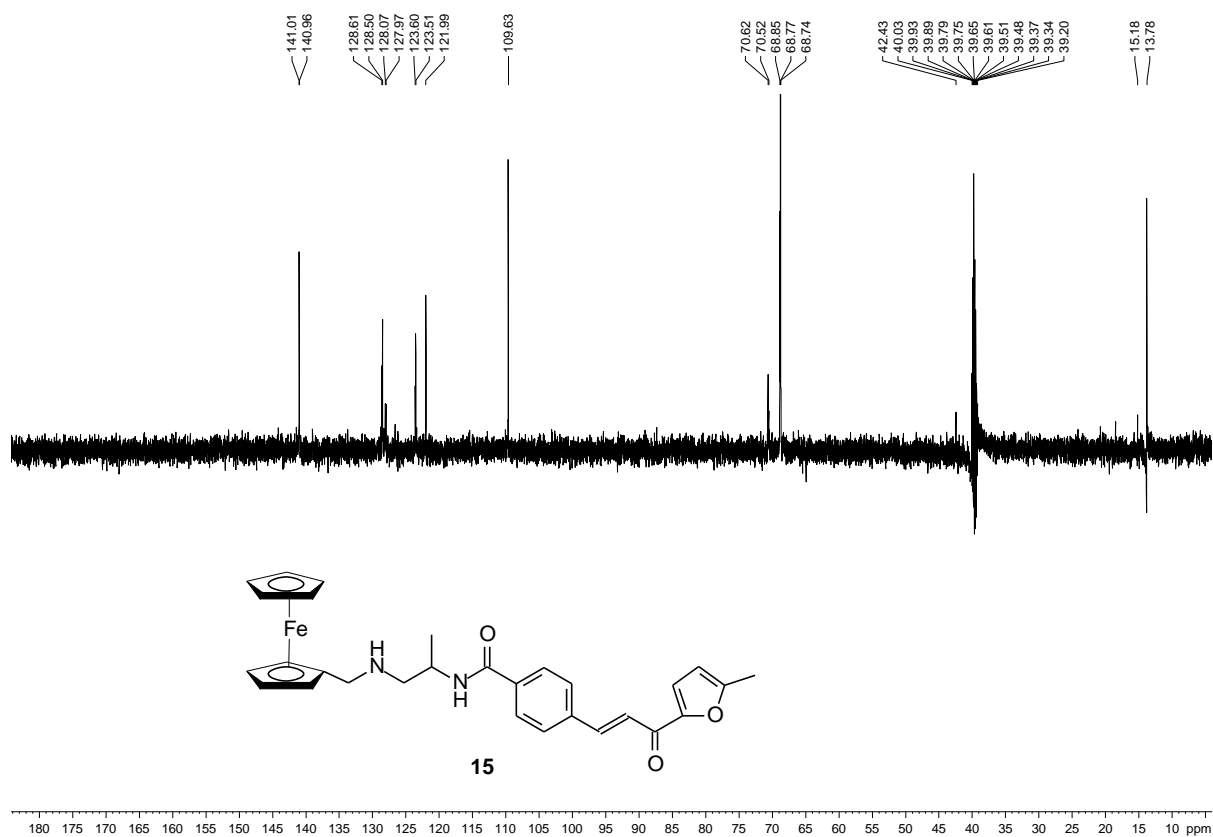


# Addendum B – Chapter 4

## <sup>13</sup>C NMR in DMSO: 15

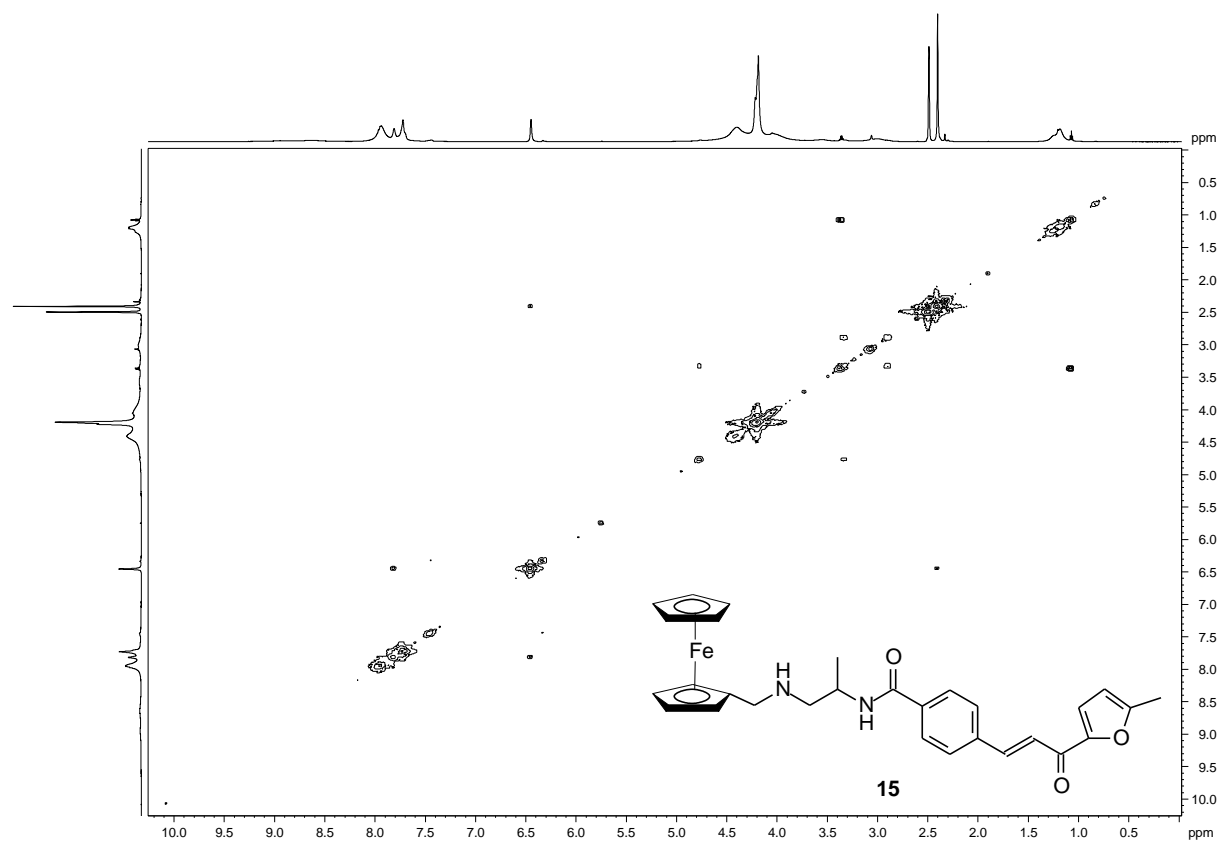


## DEPT135 in DMSO: 15

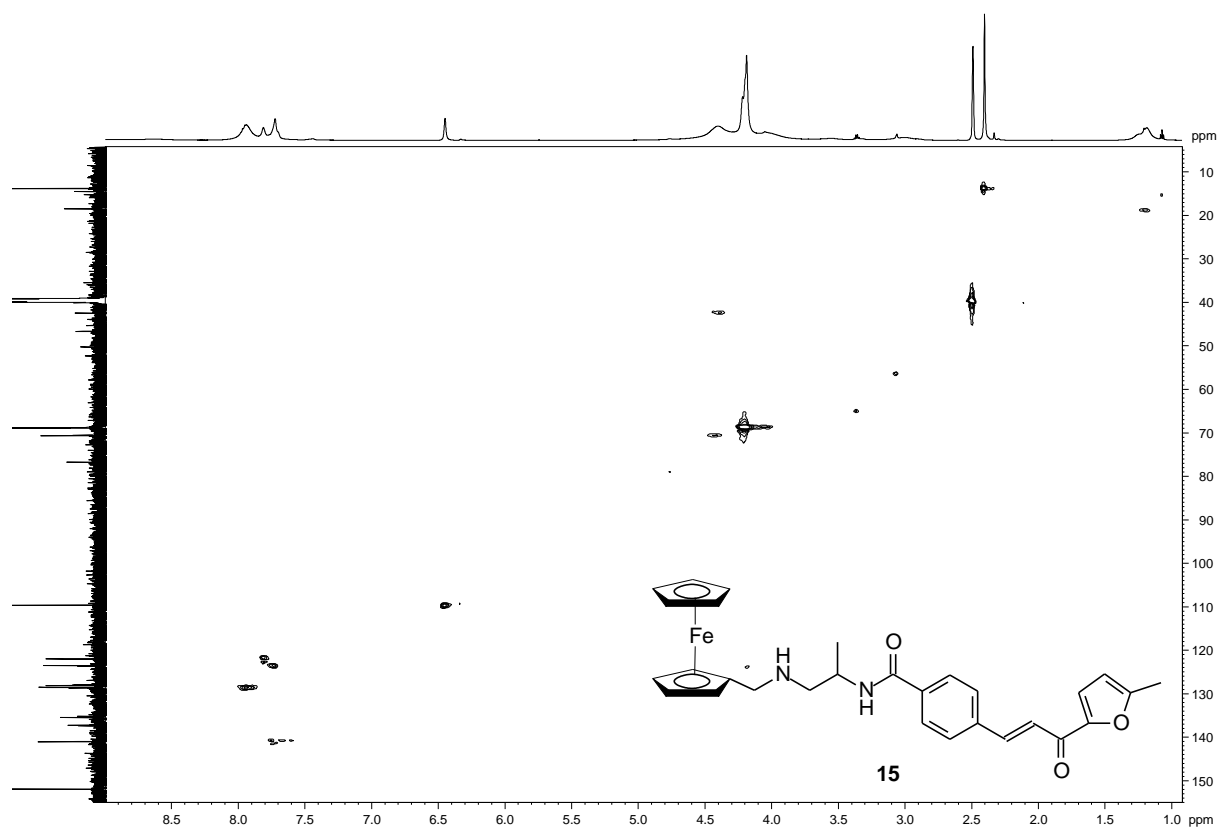


# Addendum B – Chapter 4

## COSY in DMSO: 15



## HSQC in DMSO: 15

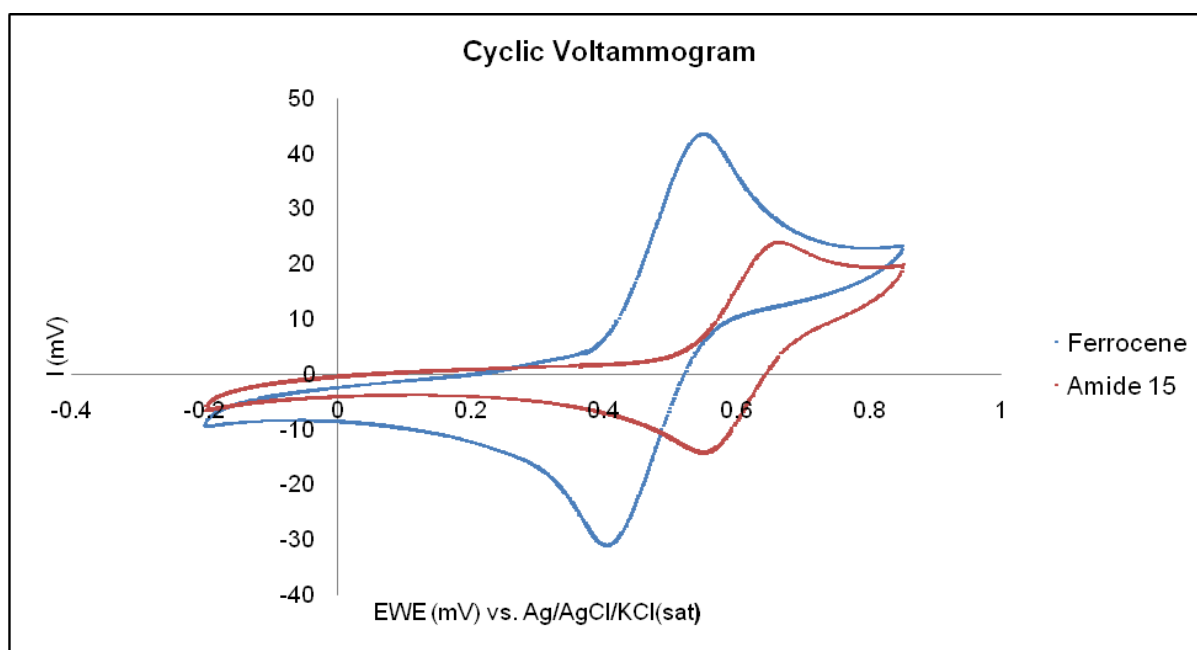
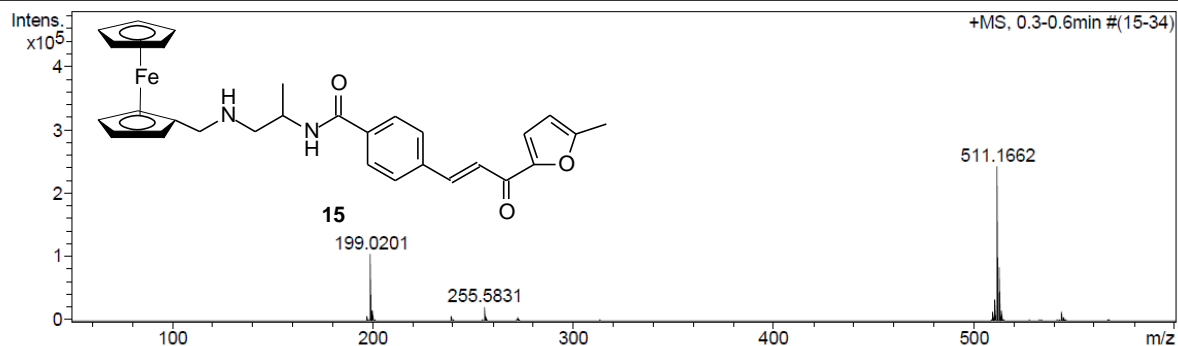


## Addendum B – Chapter 4

### HRMS: 15

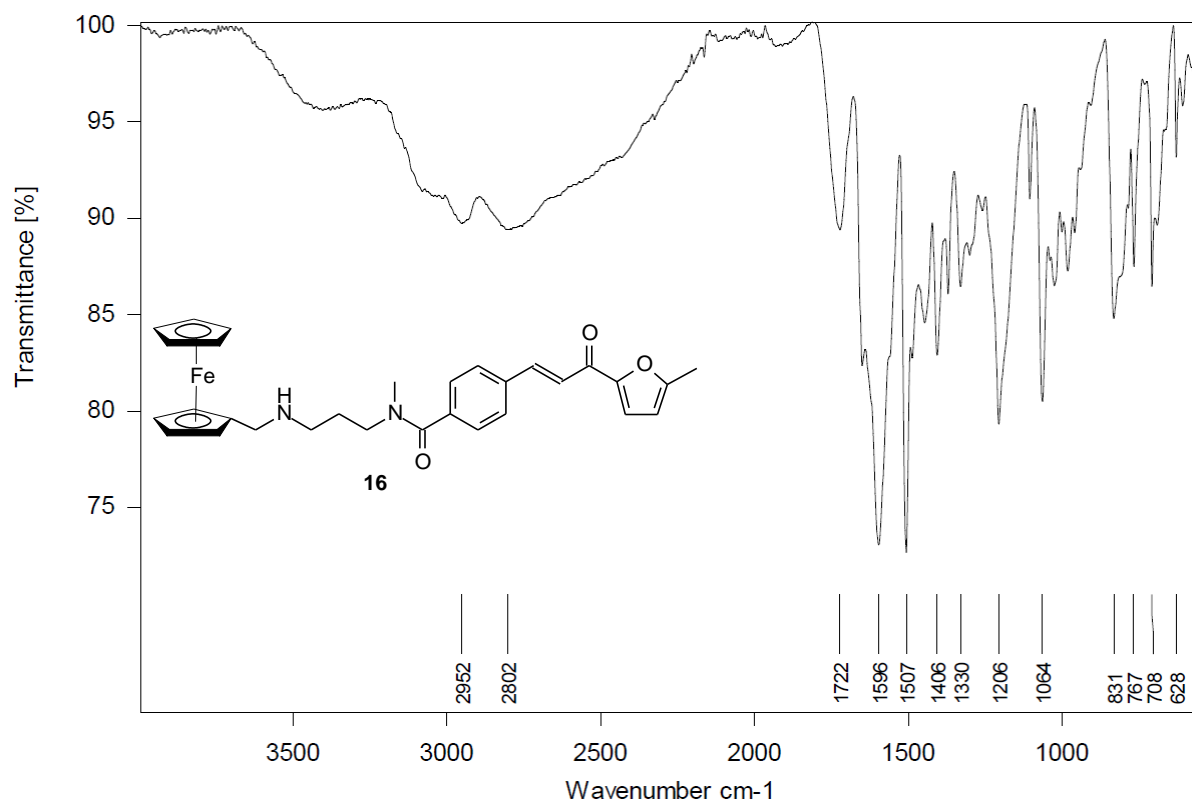
#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

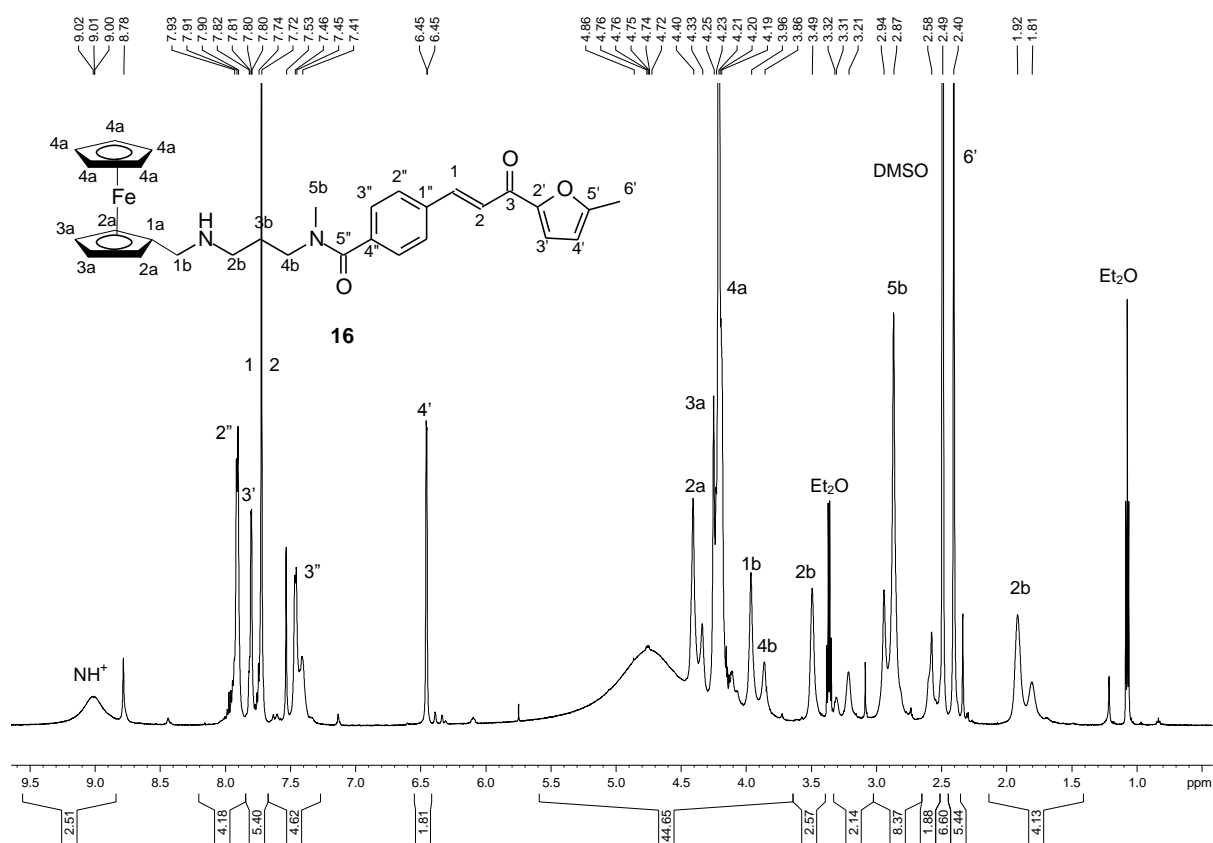


Addendum B – Chapter 4

IR: 16



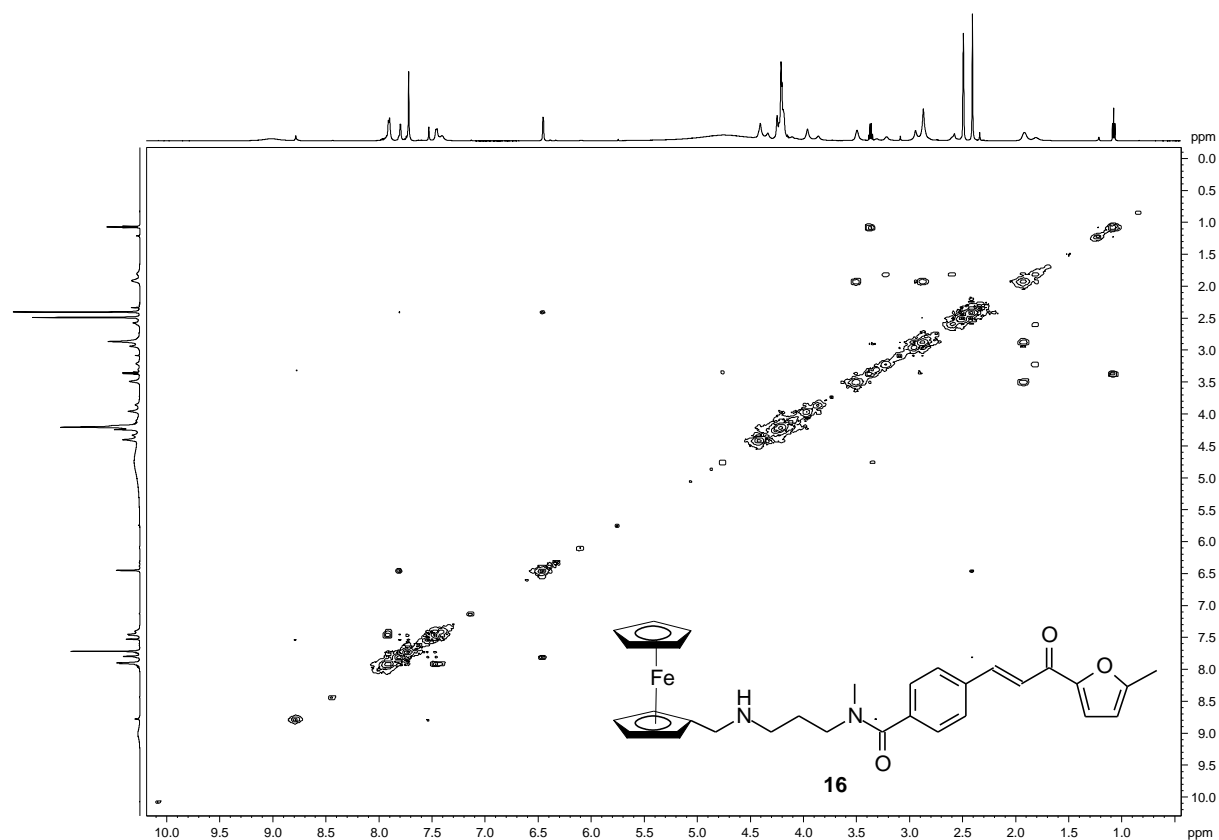
<sup>1</sup>H NMR in DMSO: 16



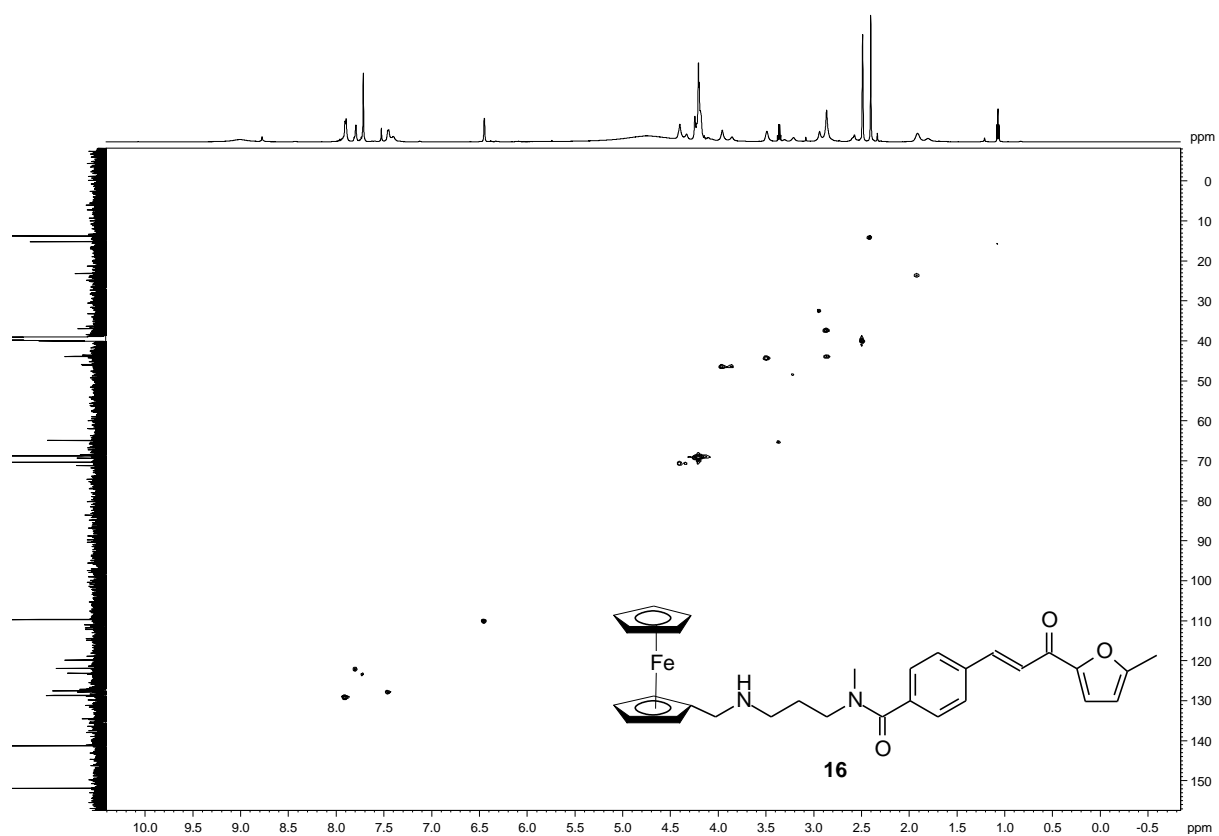


# Addendum B – Chapter 4

## COSY in DMSO: 16



## HSQC in DMSO: 16

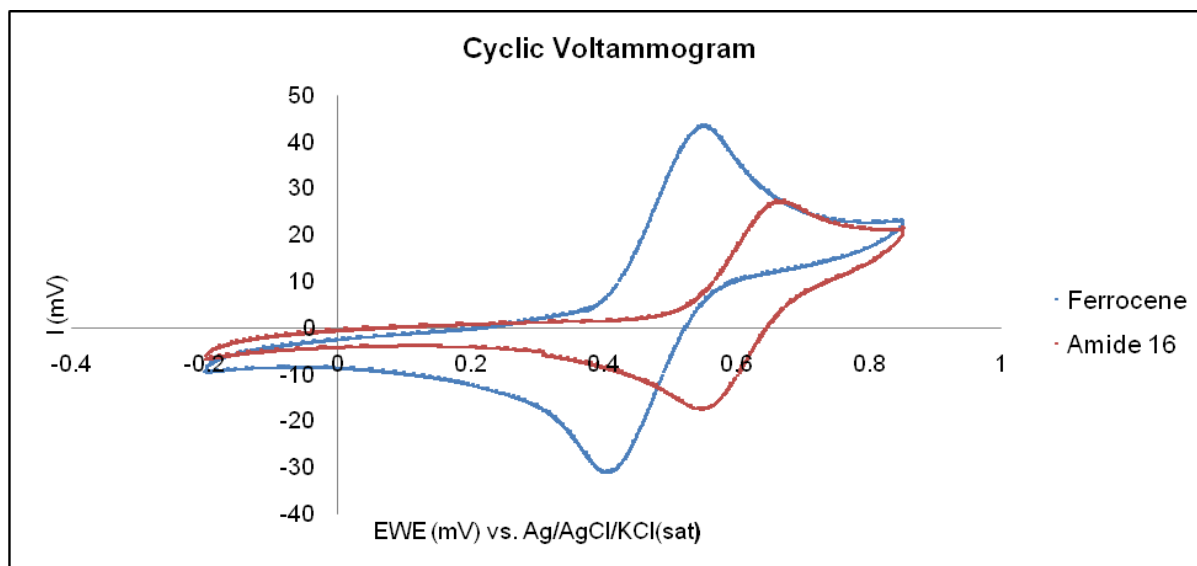
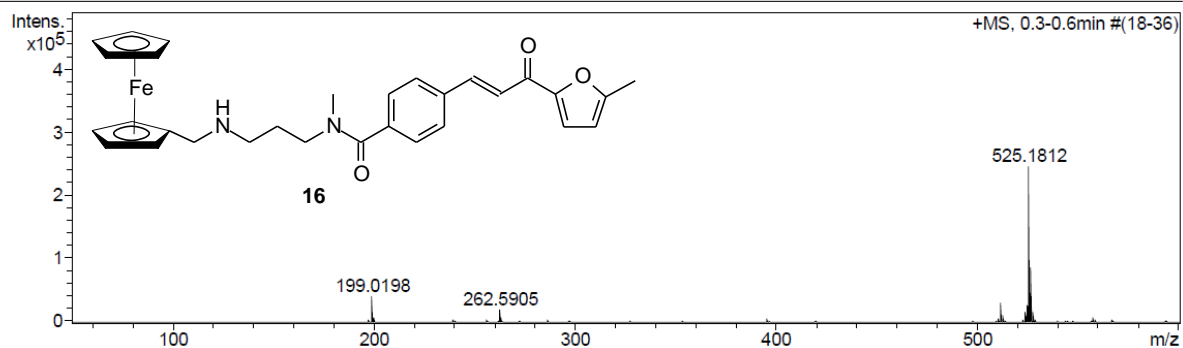


## Addendum B – Chapter 4

### HRMS: 16

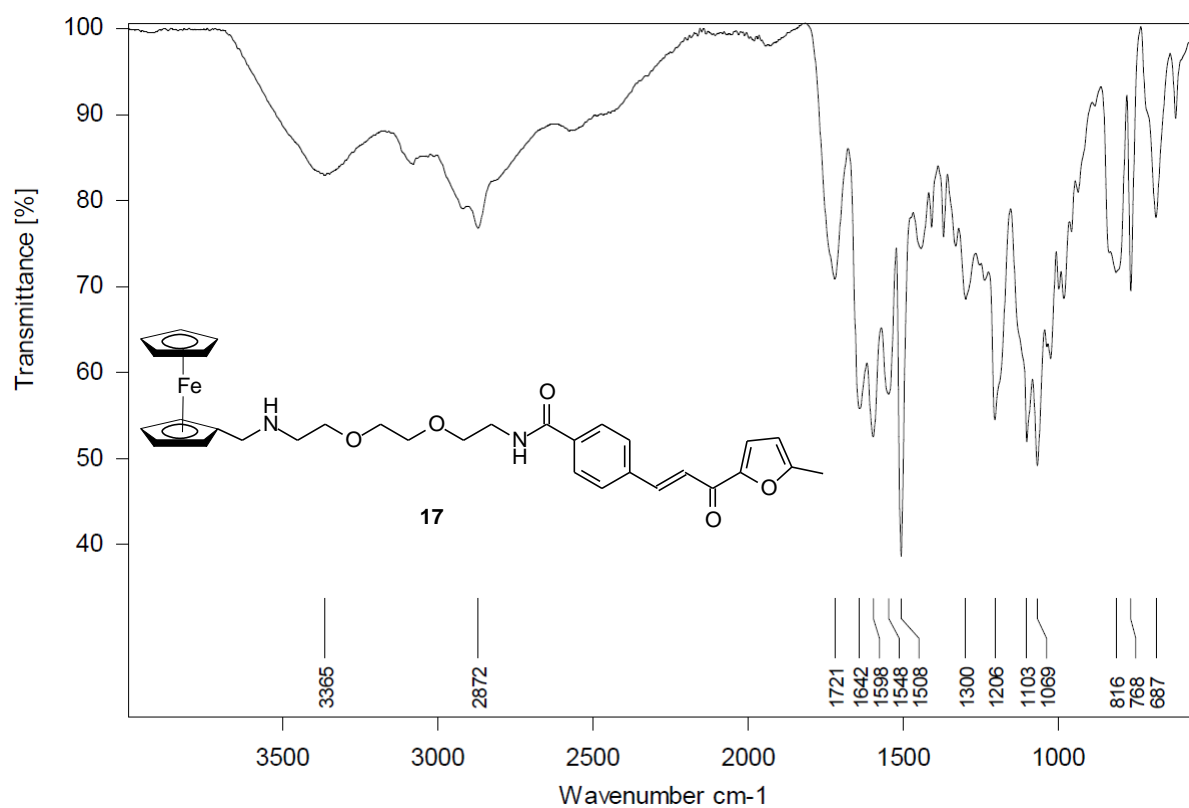
#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

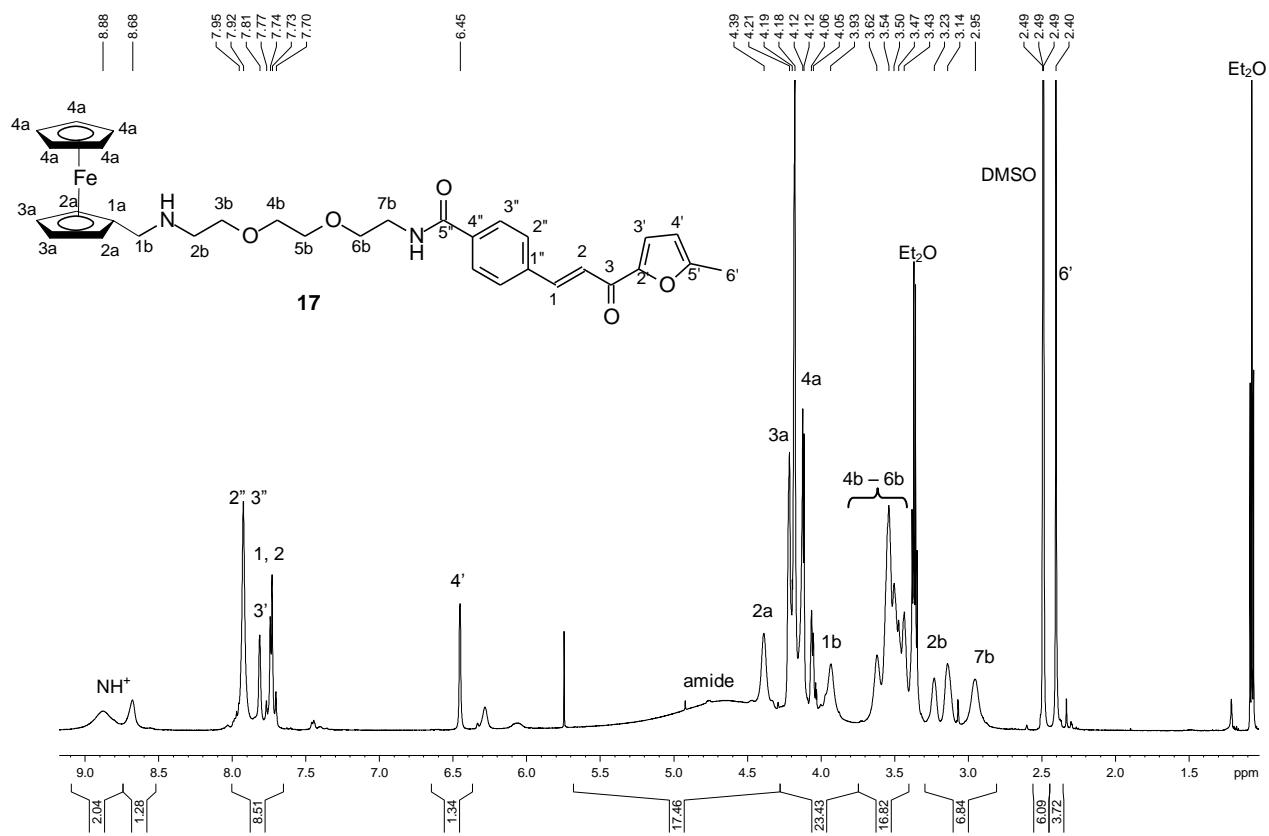


# Addendum B – Chapter 4

IR: 17

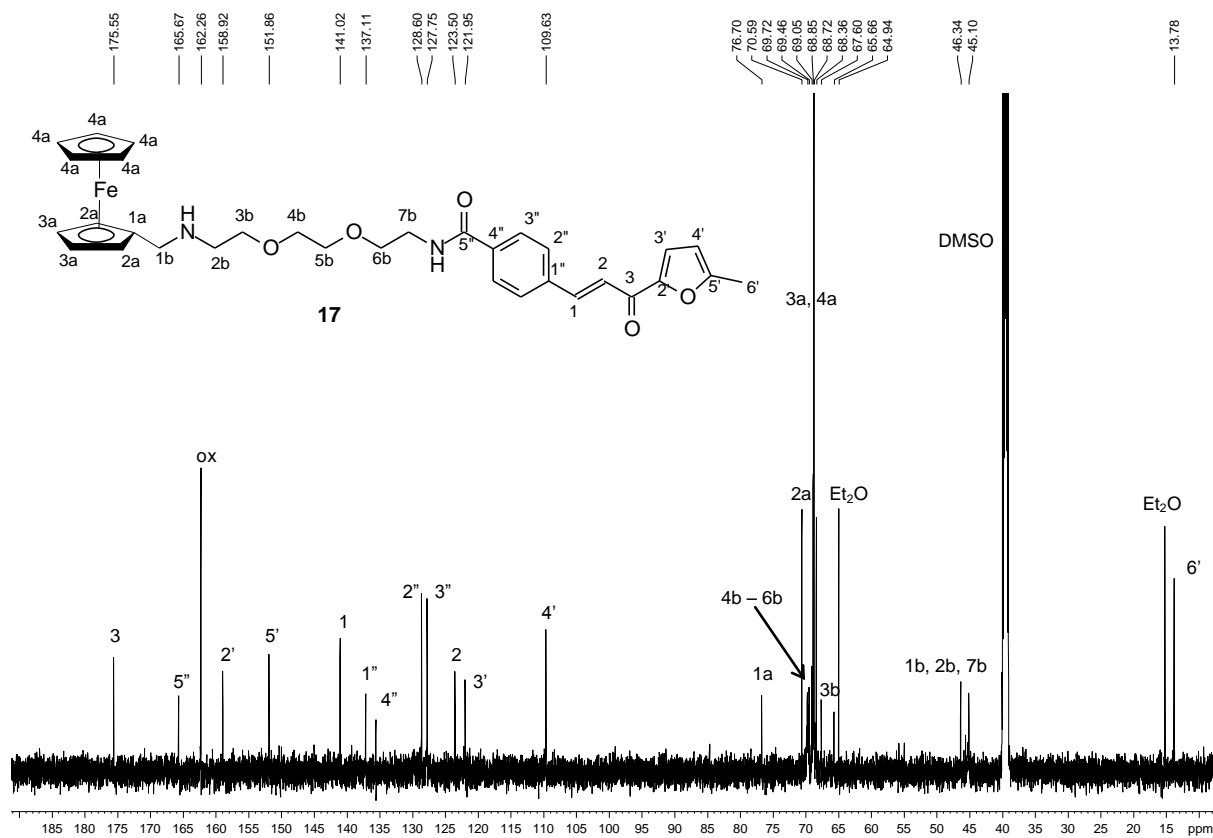


<sup>1</sup>H NMR in DMSO: 17



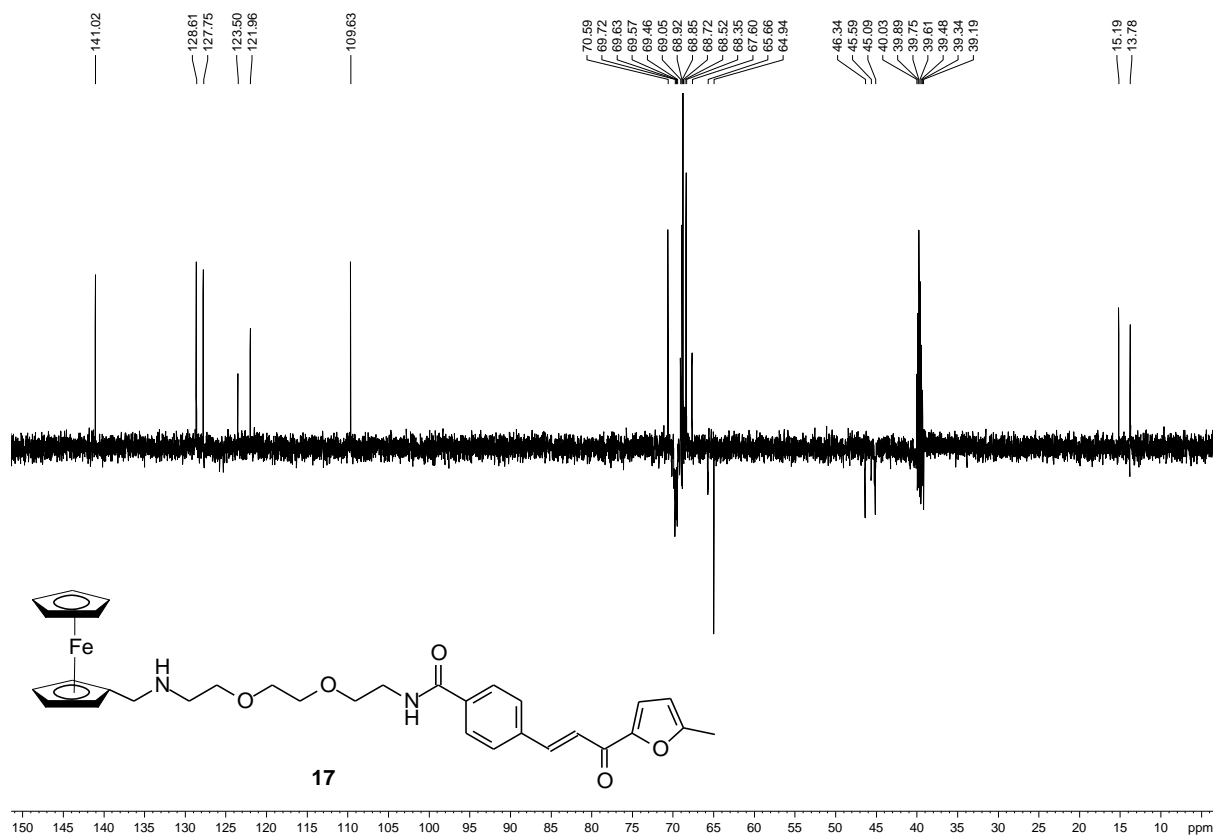
# Addendum B – Chapter 4

## <sup>13</sup>C NMR in DMSO: 17

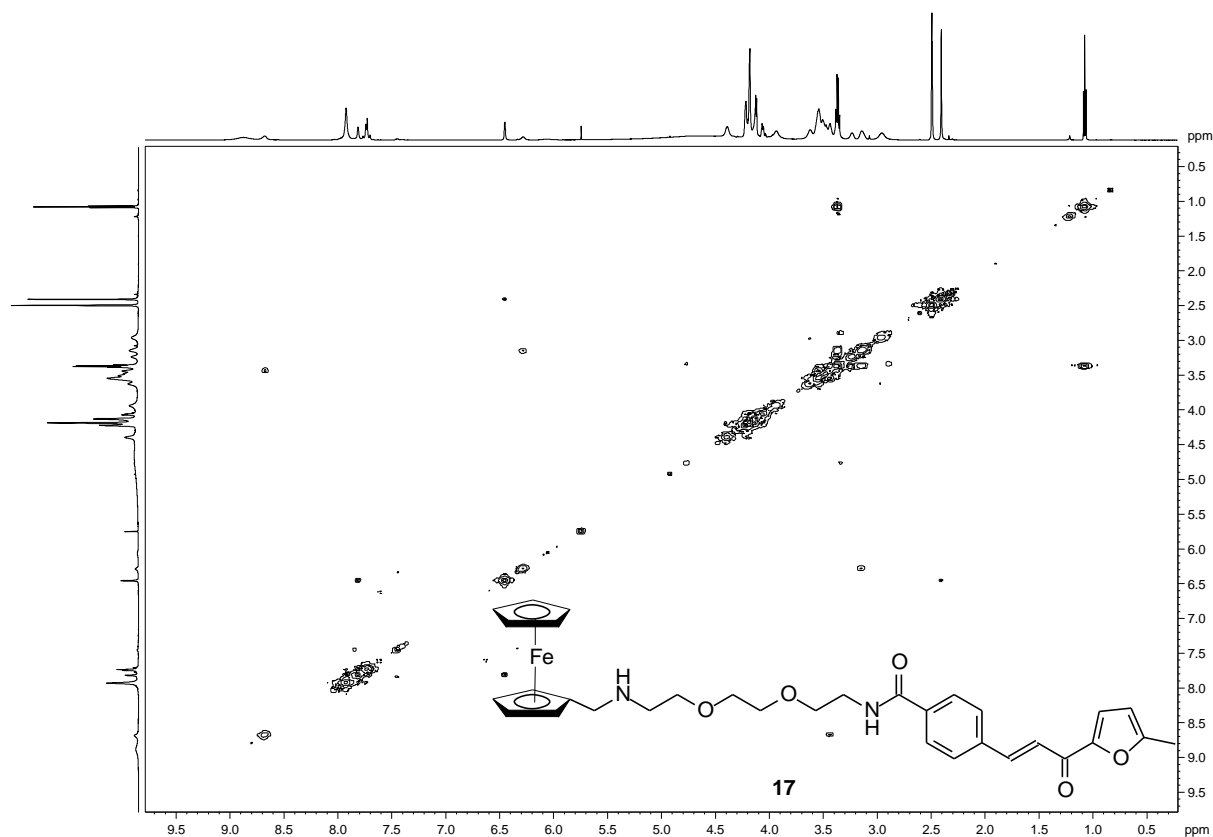


## DEPT135 in DMSO: 17

# Addendum B – Chapter 4

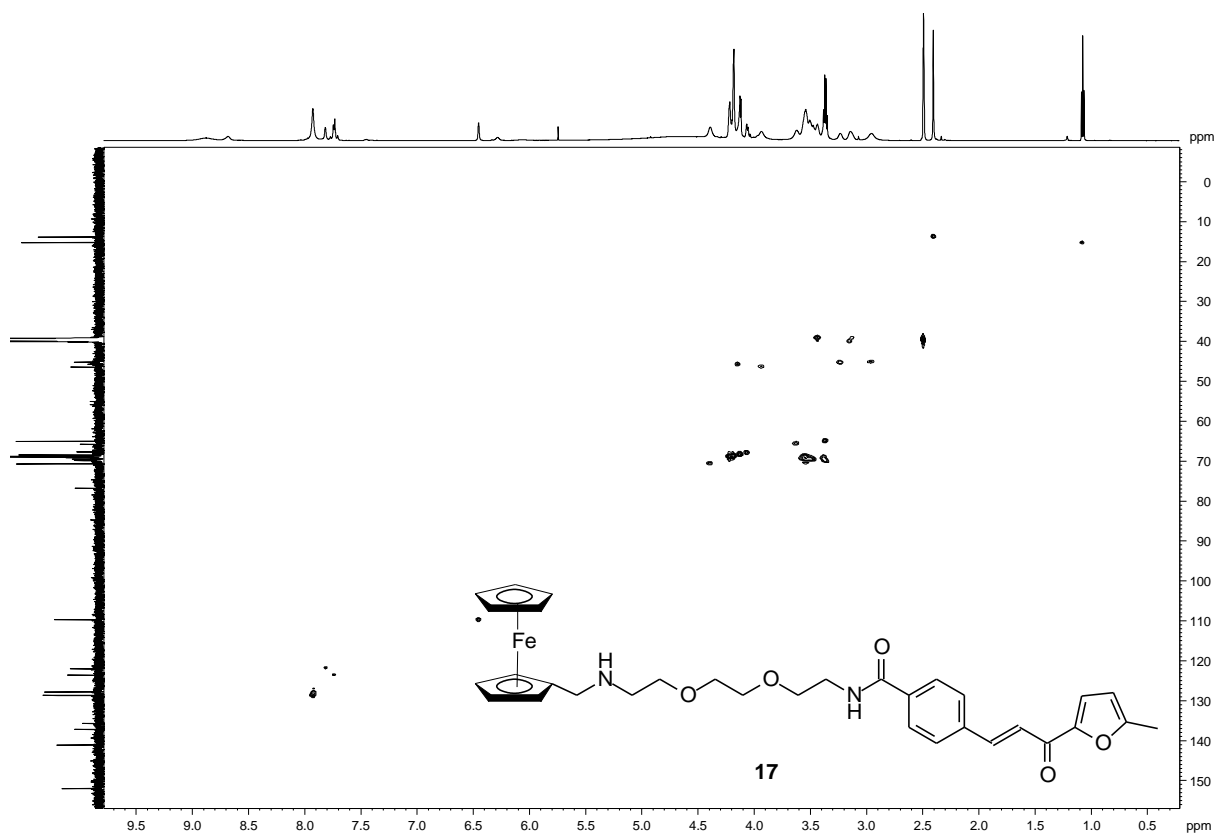


## COSY in DMSO: 17



## HSQC in DMSO: 17

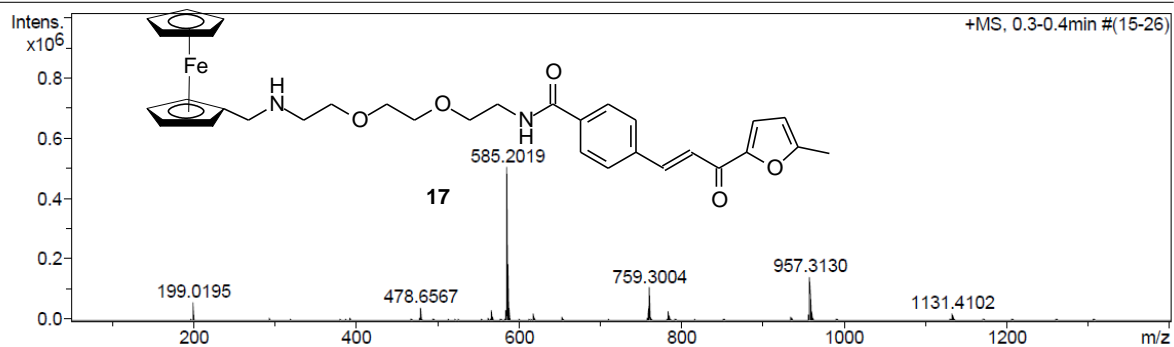
# Addendum B – Chapter 4

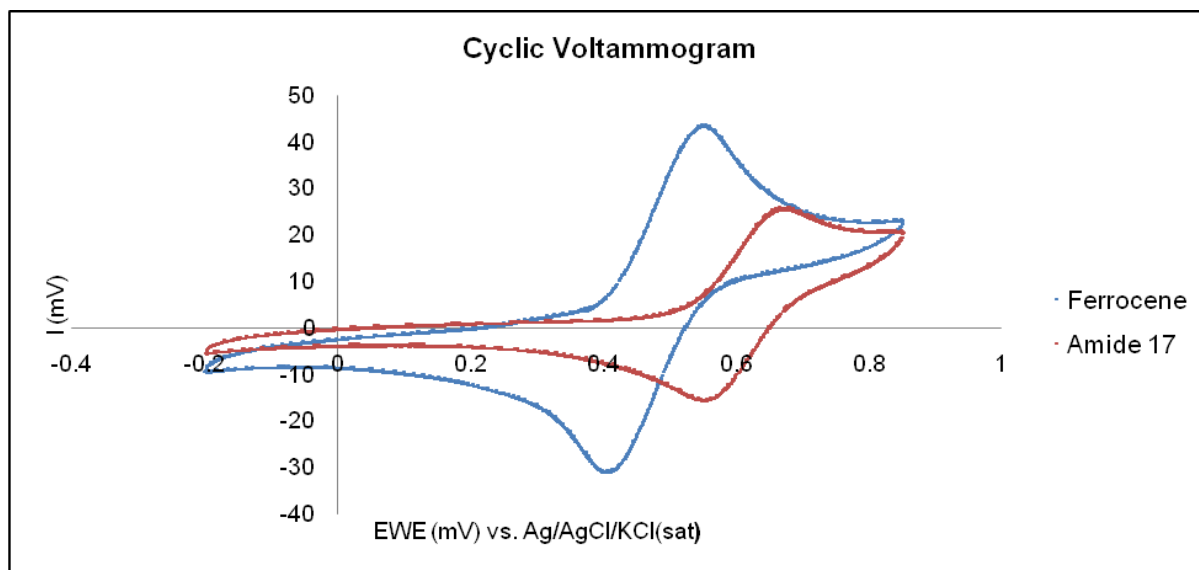


HRMS: 17

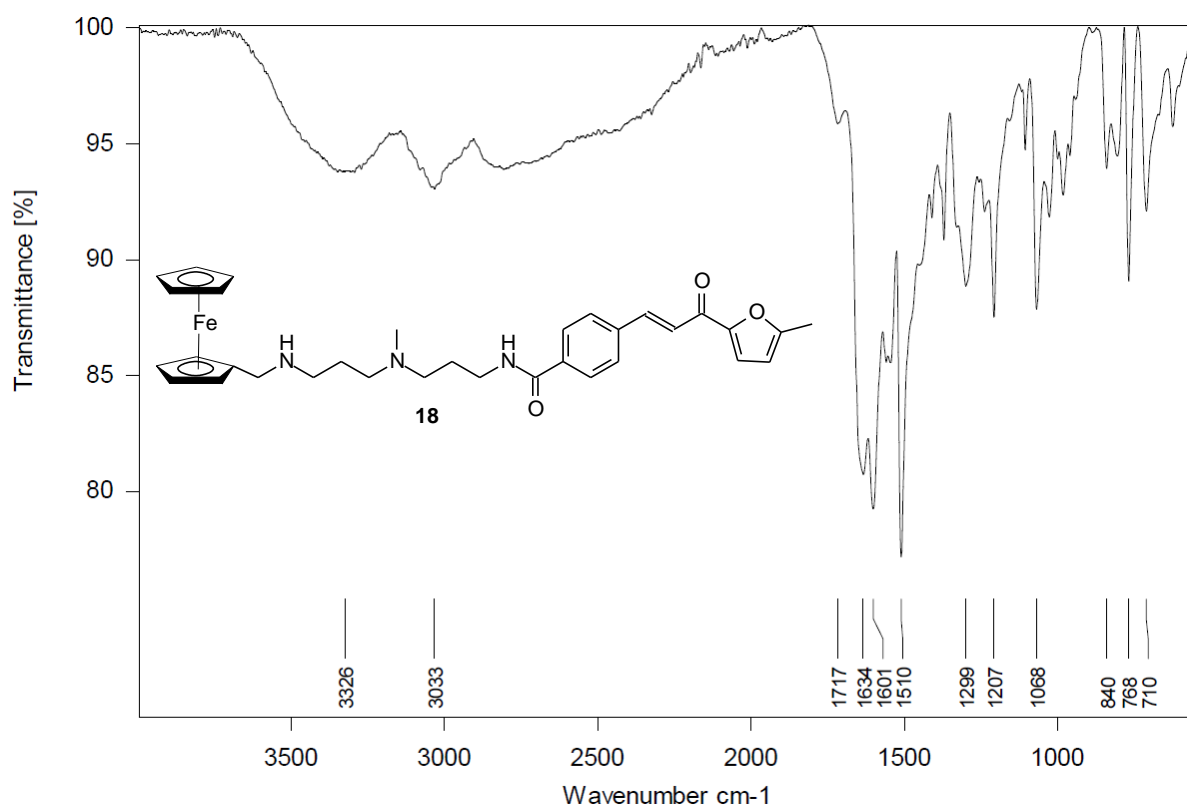
### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

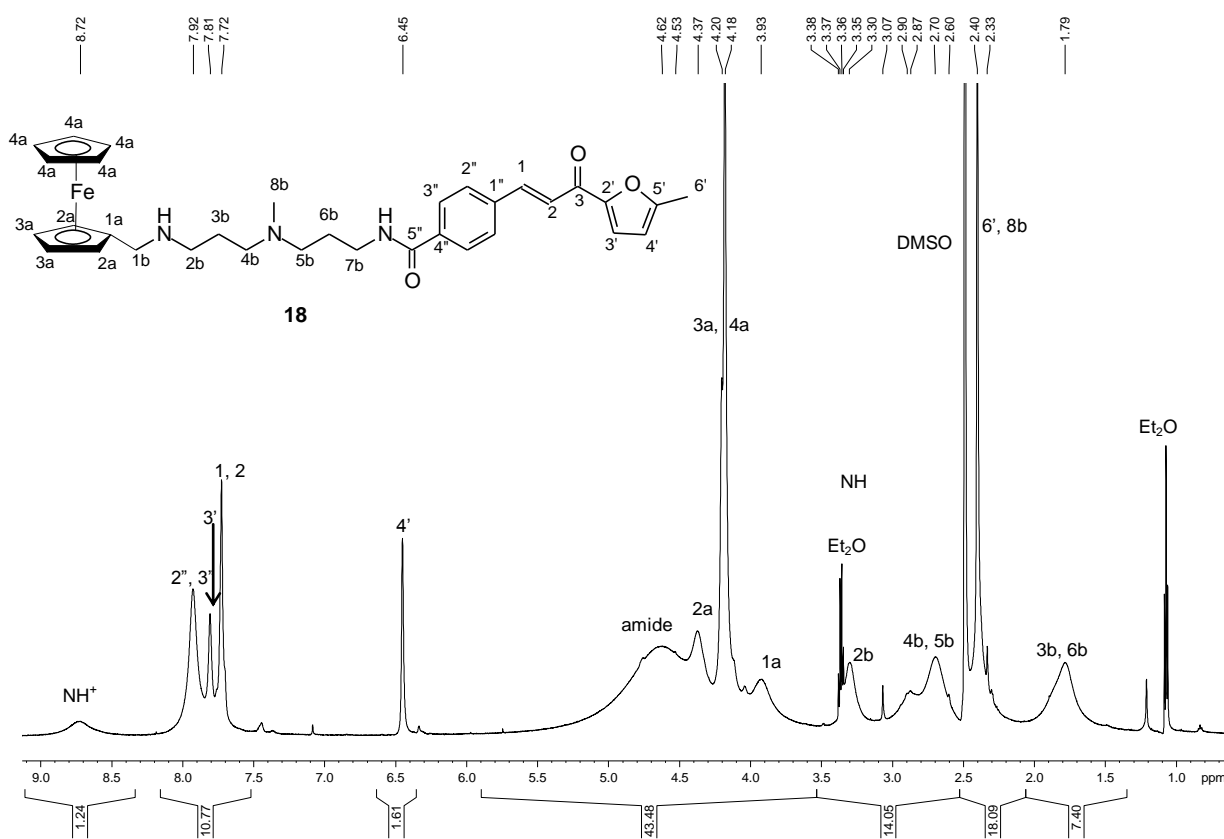




IR: **18**

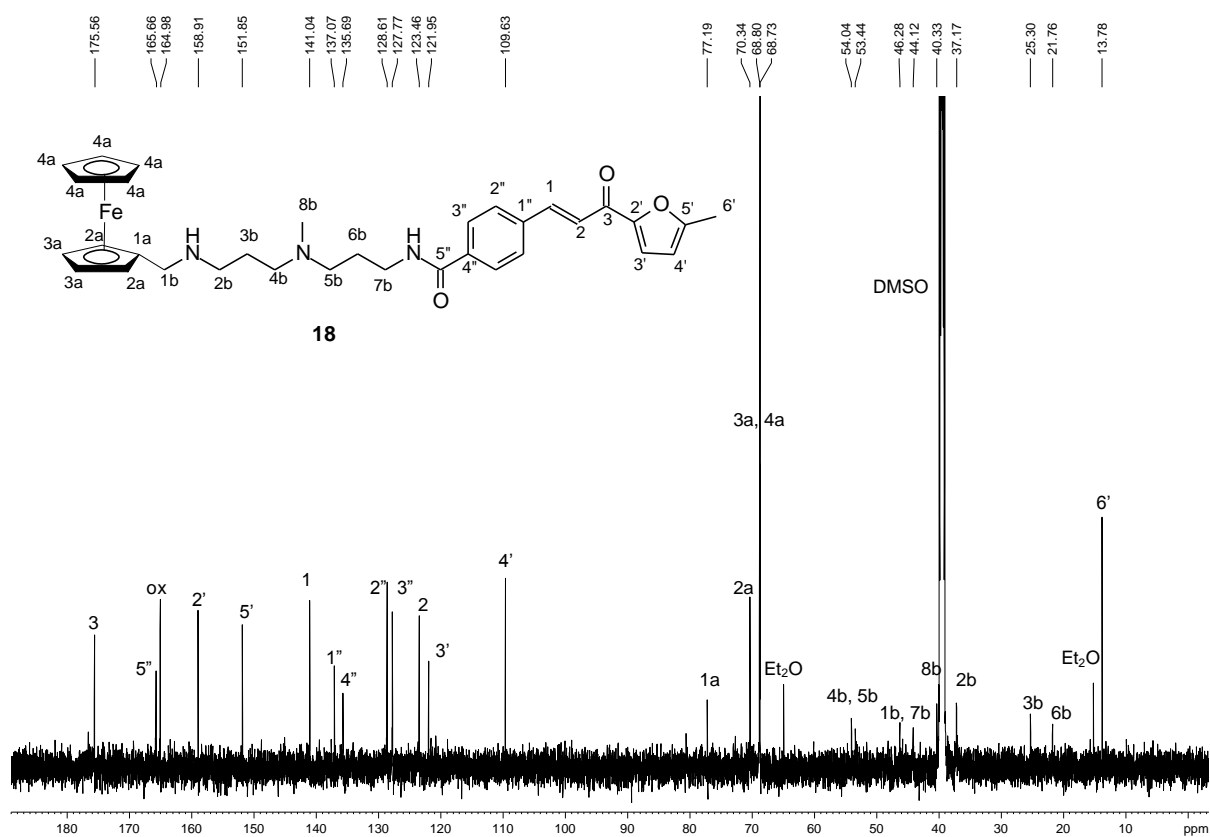


<sup>1</sup>H NMR in DMSO: **18**

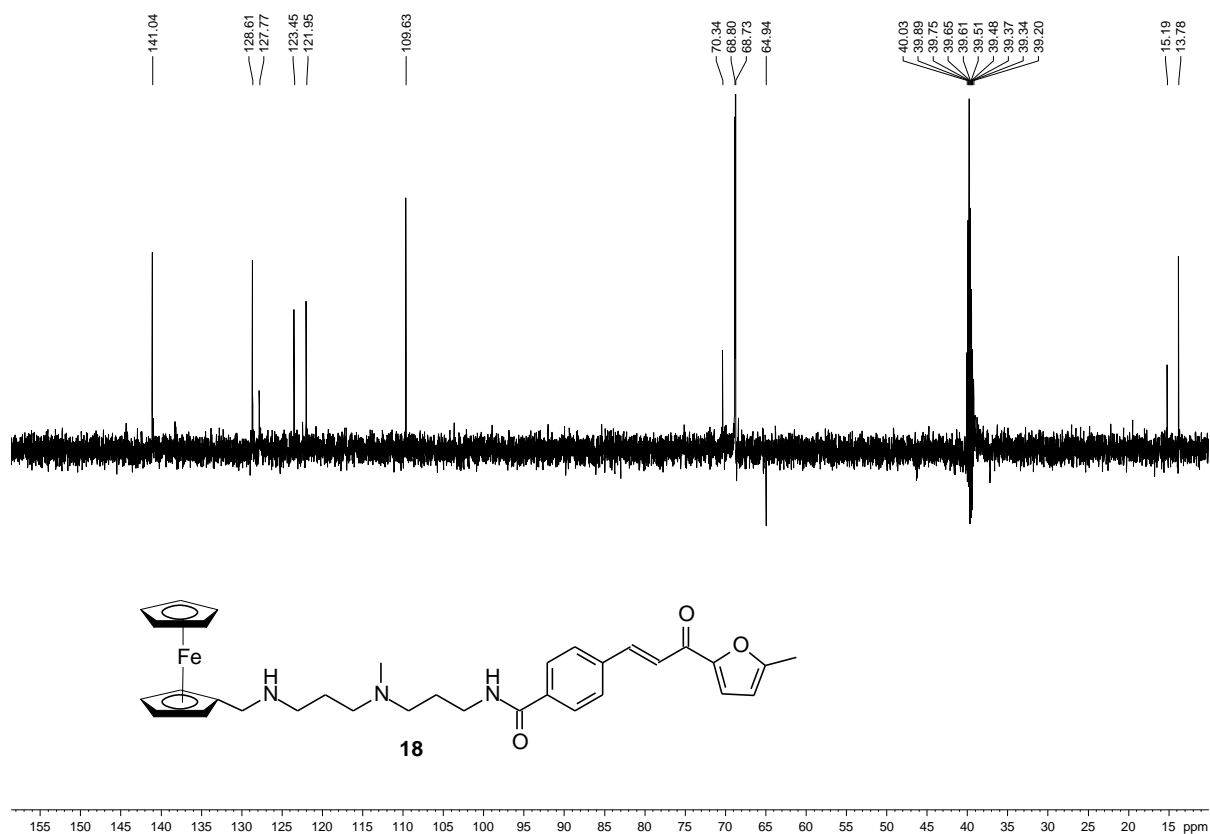


# Addendum B – Chapter 4

## <sup>13</sup>C NMR in DMSO: **18**

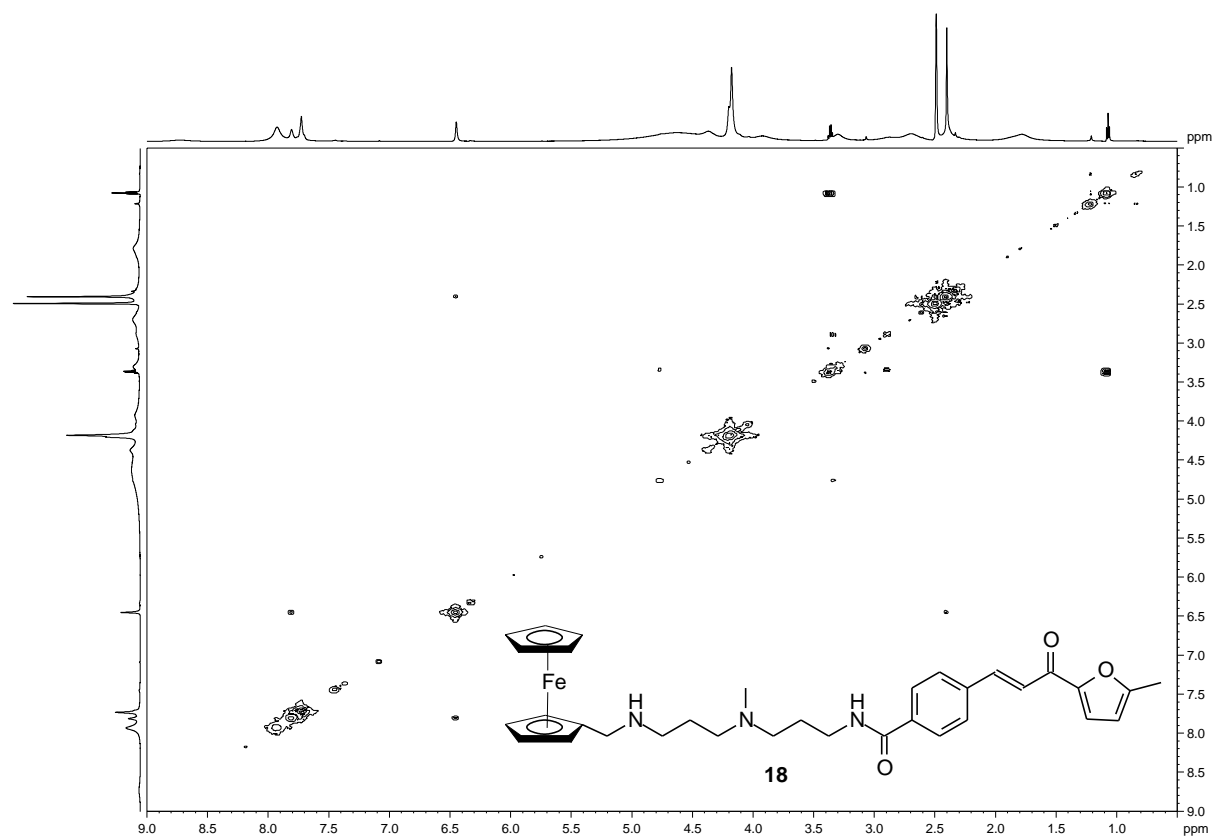


## DEPT135 in DMSO: **18**

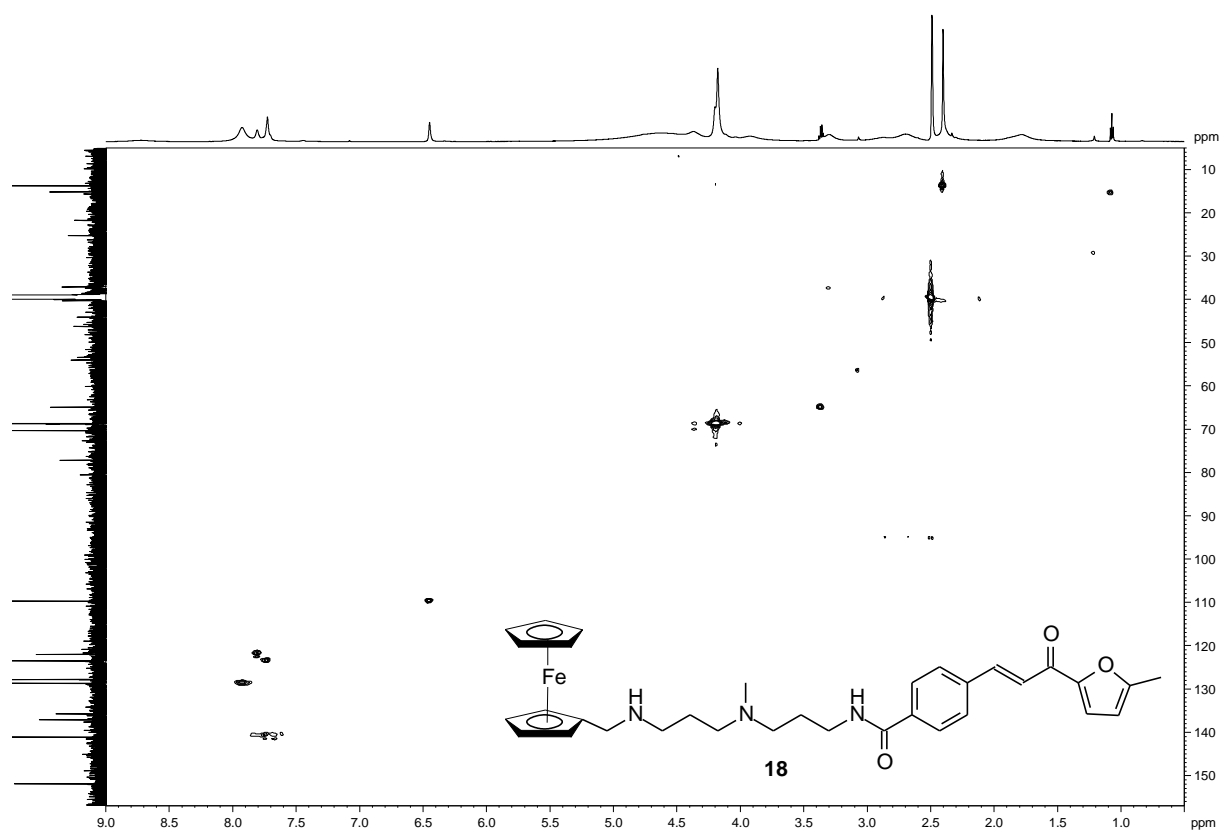


Addendum B – Chapter 4

COSY in DMSO: **18**



HSQC in DMSO: **18**

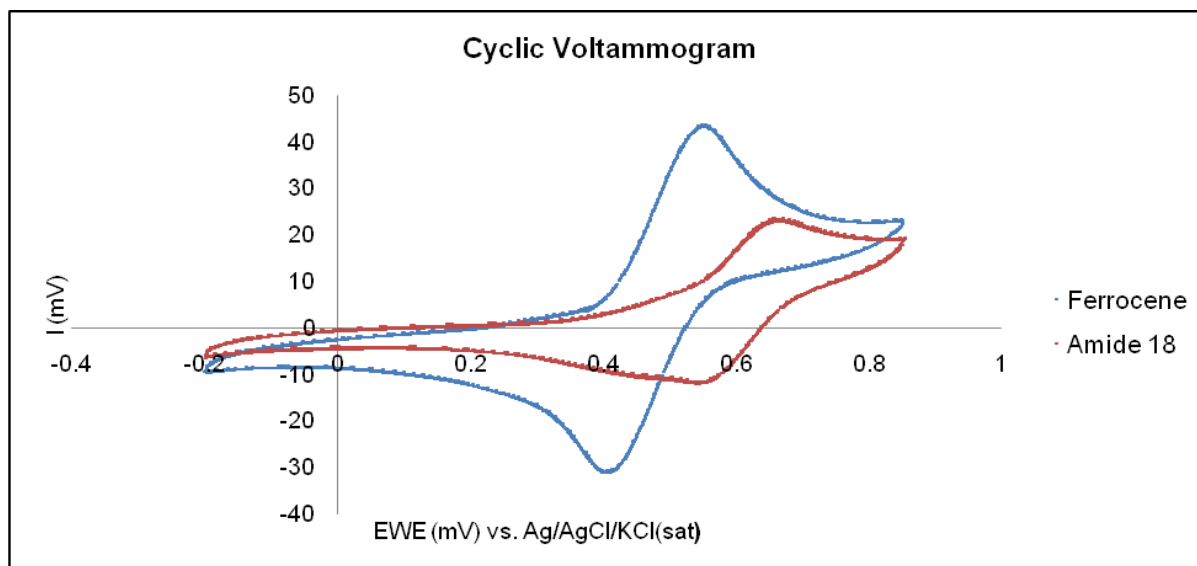
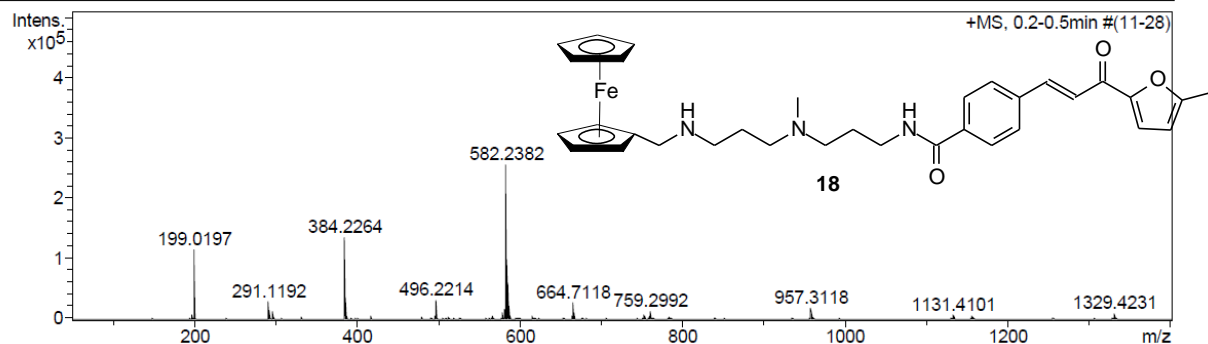


## Addendum B – Chapter 4

### HRMS: 18

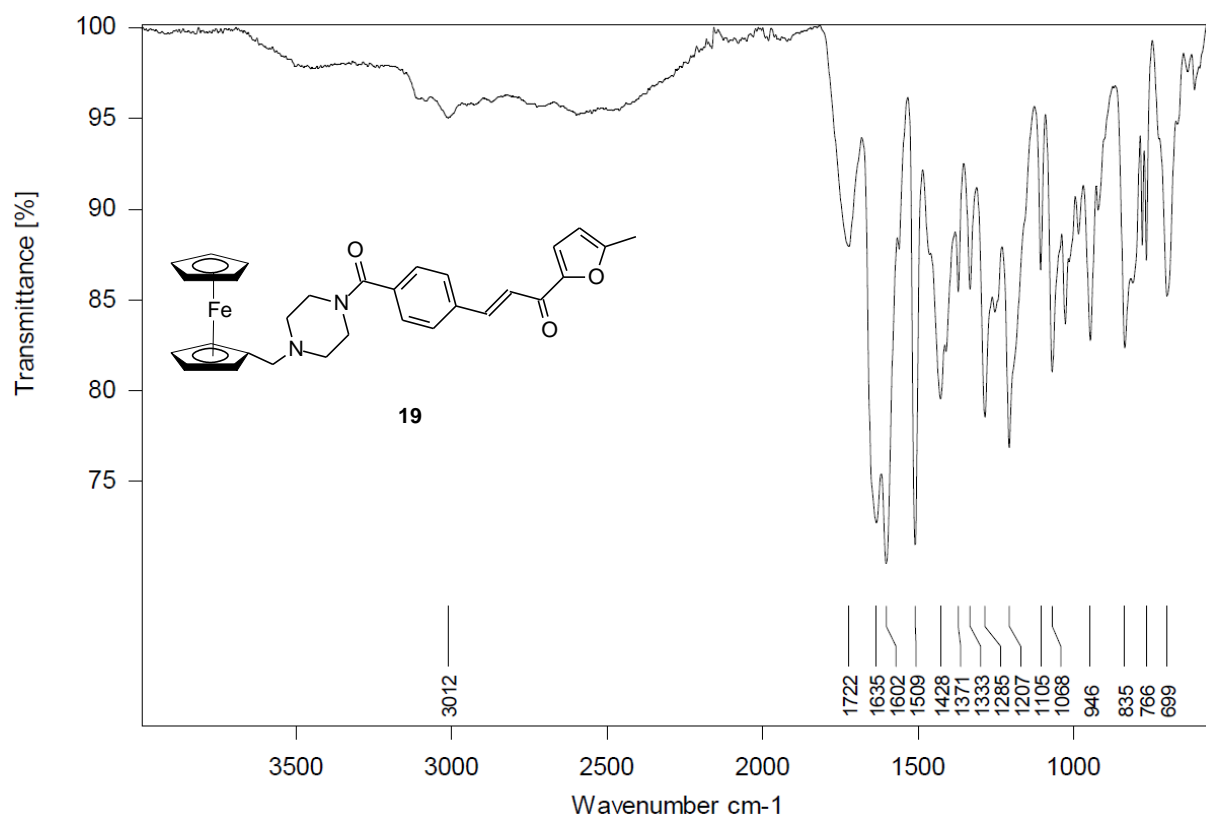
#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

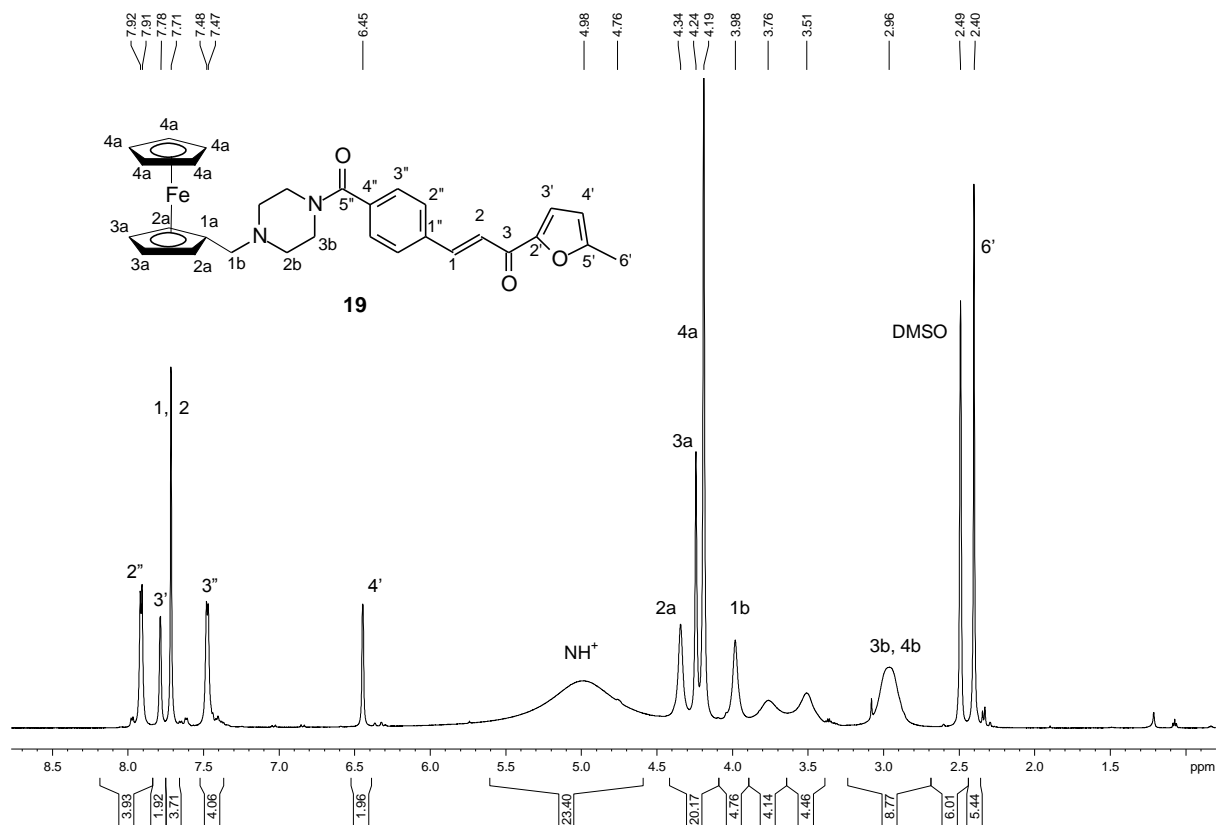


Addendum B – Chapter 4

IR: 19

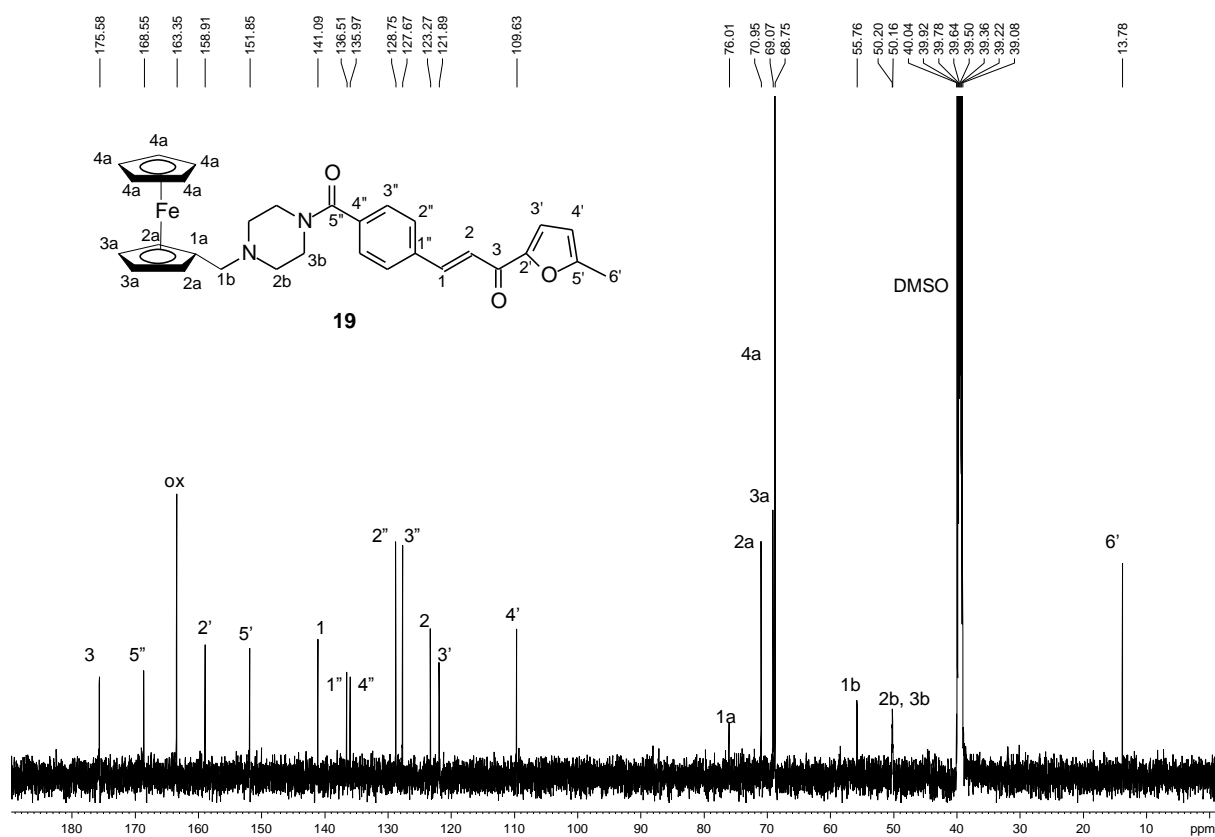


<sup>1</sup>H NMR in DMSO: 19

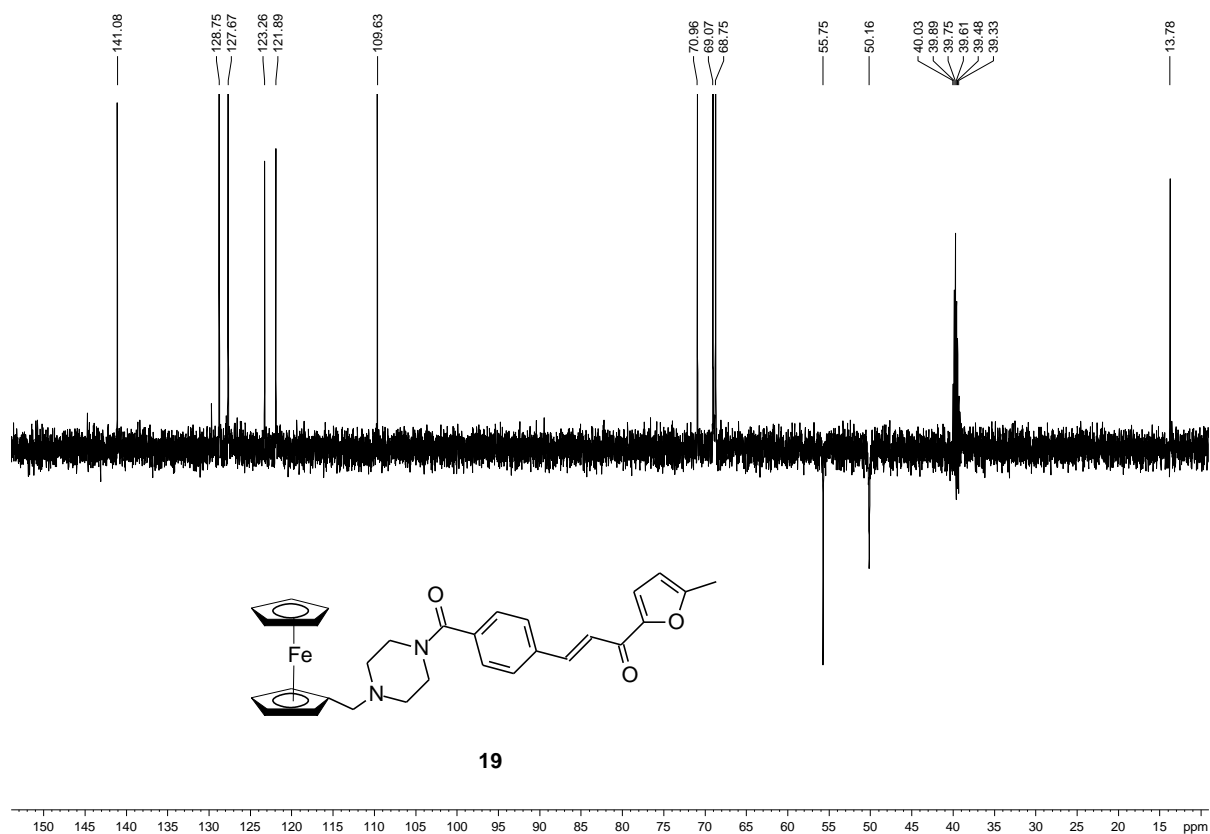


# Addendum B – Chapter 4

## <sup>13</sup>C NMR in DMSO: 19

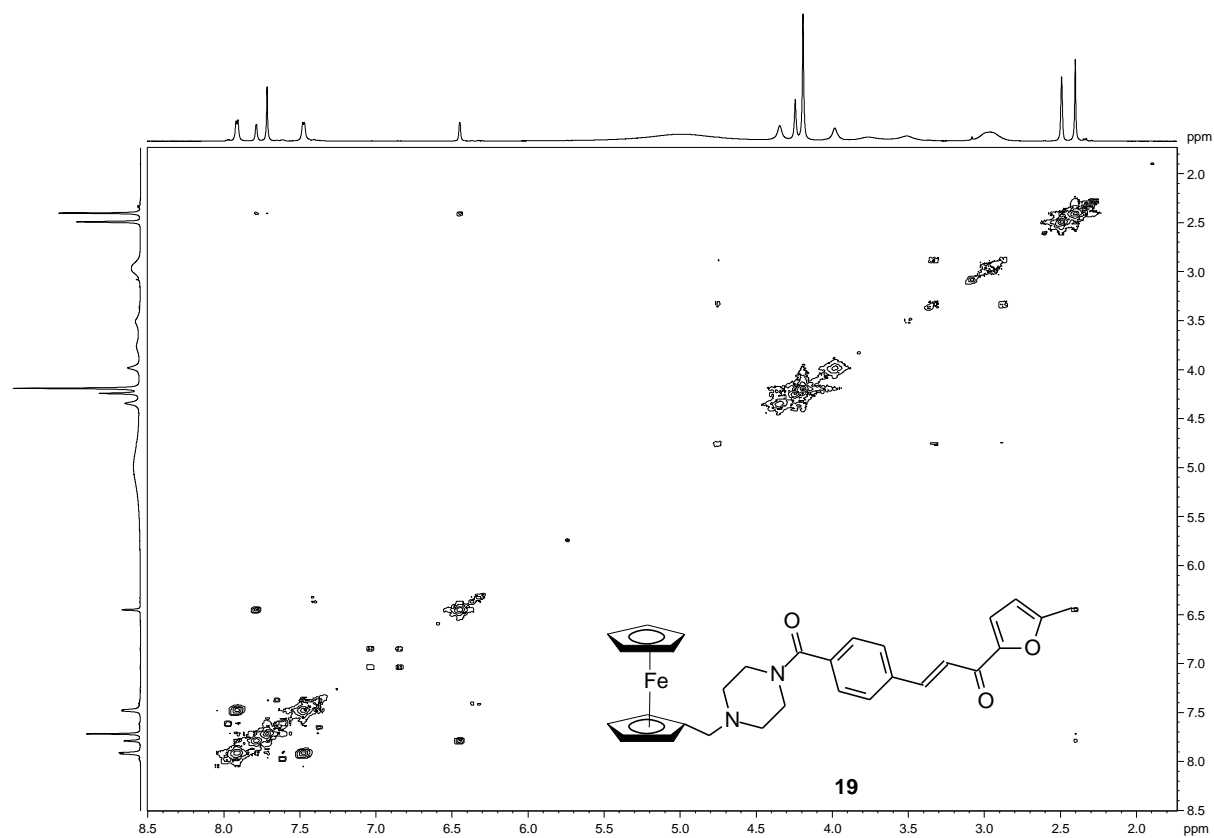


## DEPT135 in DMSO: 19

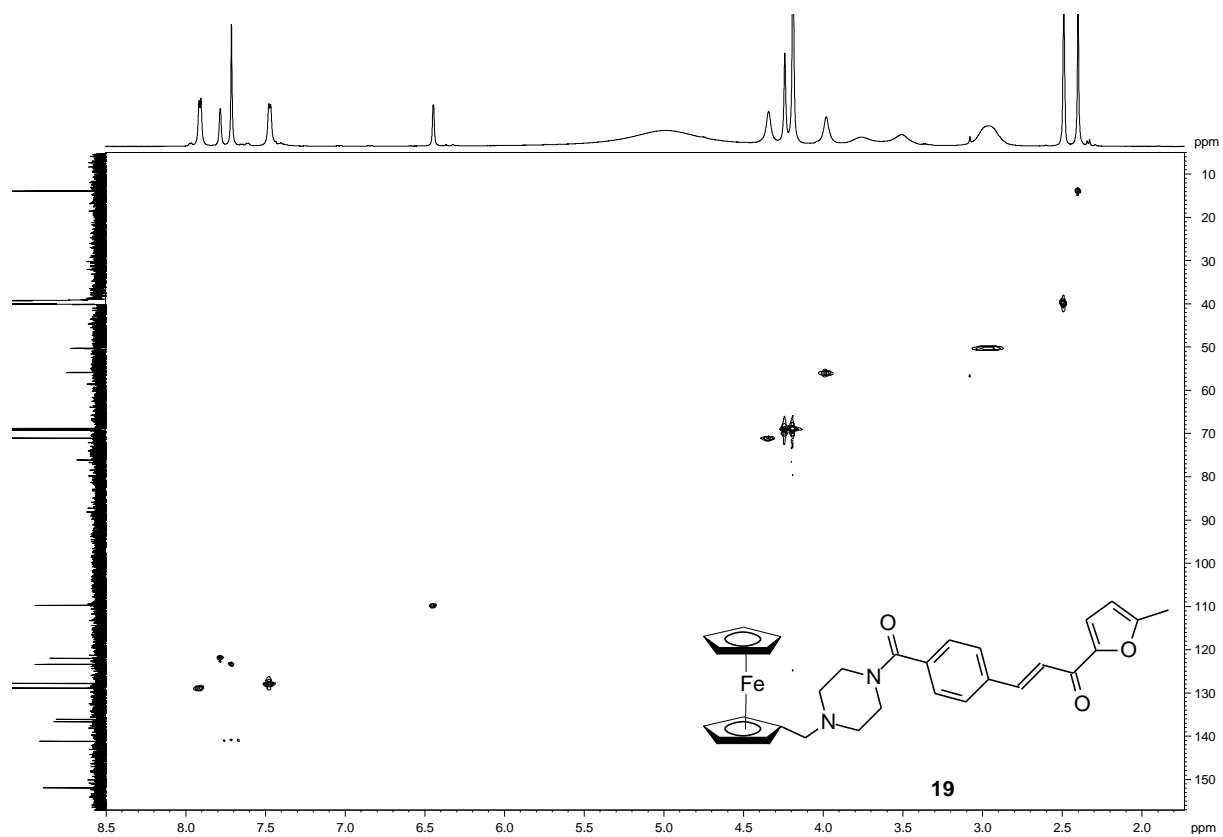


## Addendum B – Chapter 4

COSY in DMSO: **19**



HSQC in DMSO: **19**

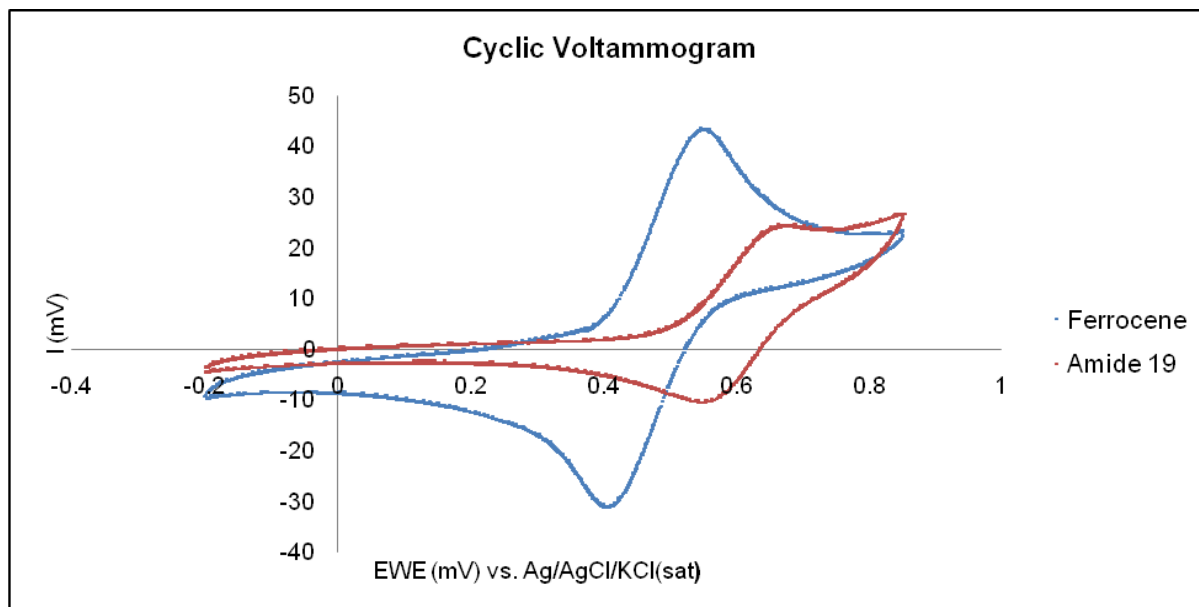
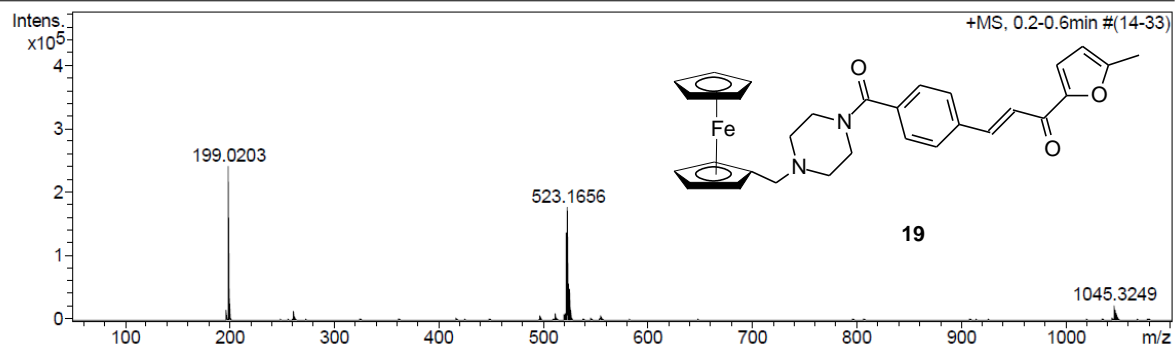


## Addendum B – Chapter 4

### HRMS: 19

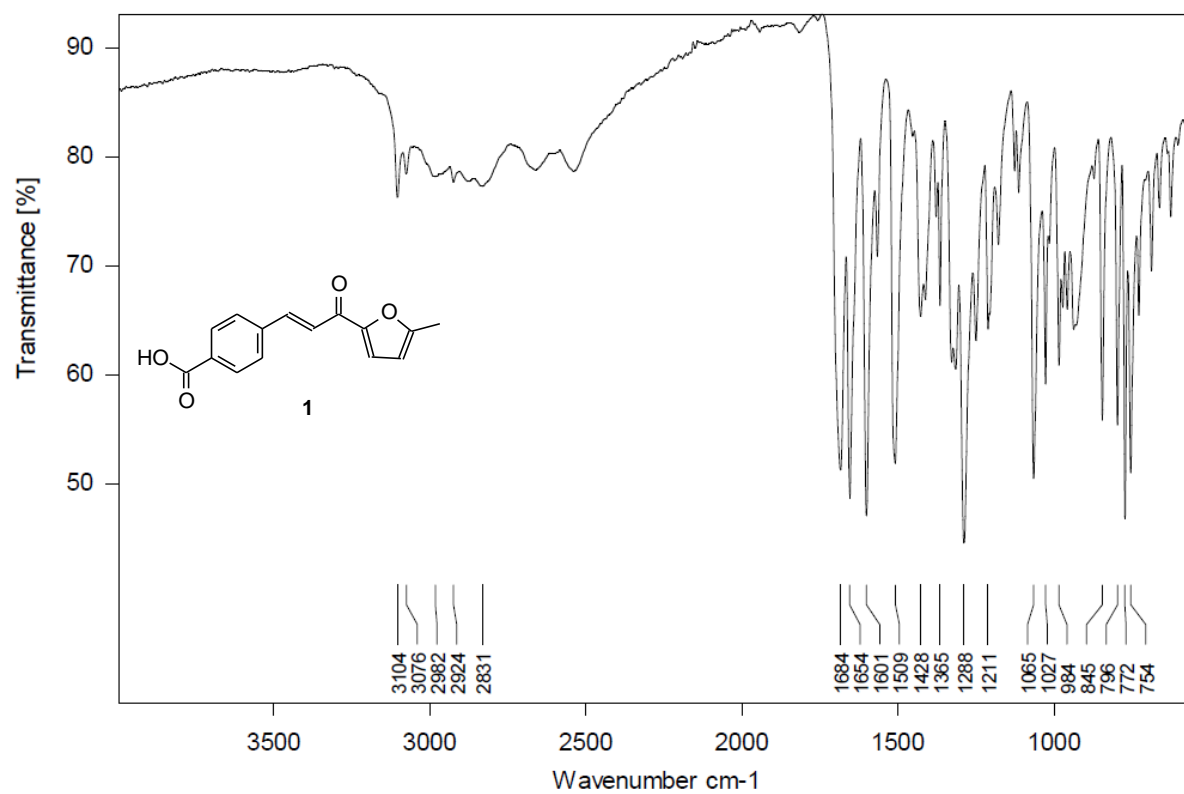
#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste



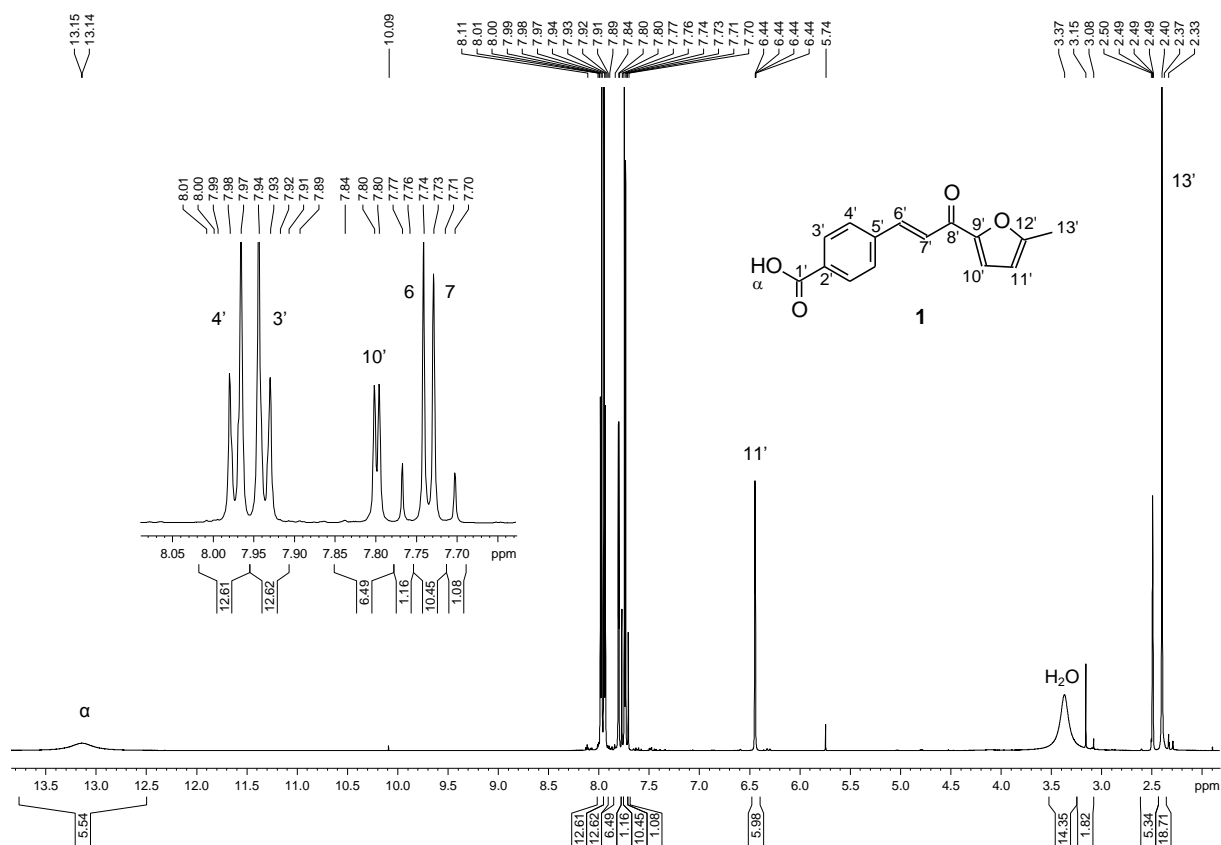
# Addendum C: Analytical data for Chapter 3

IR: 1

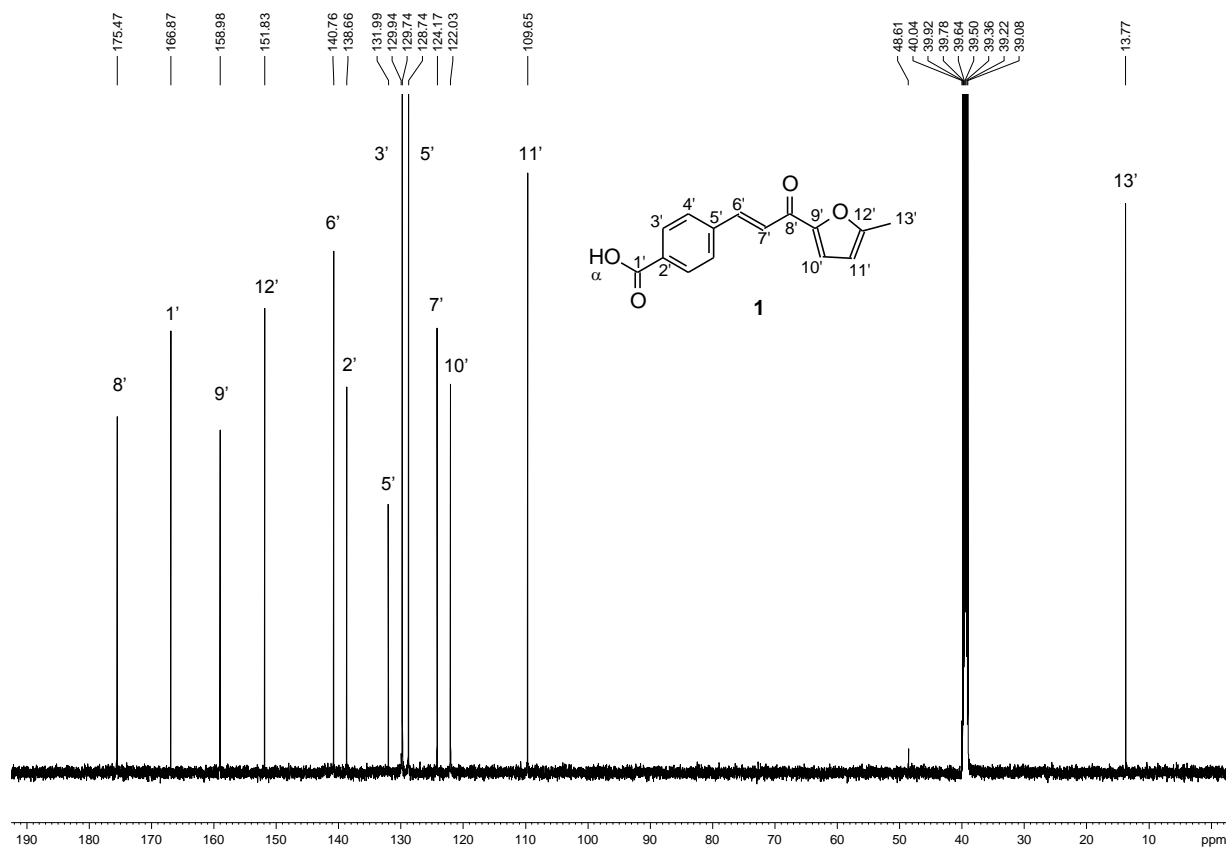


# Addendum C – Chapter 5:

## <sup>1</sup>H NMR in DMSO: 1

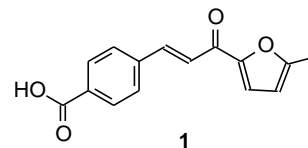
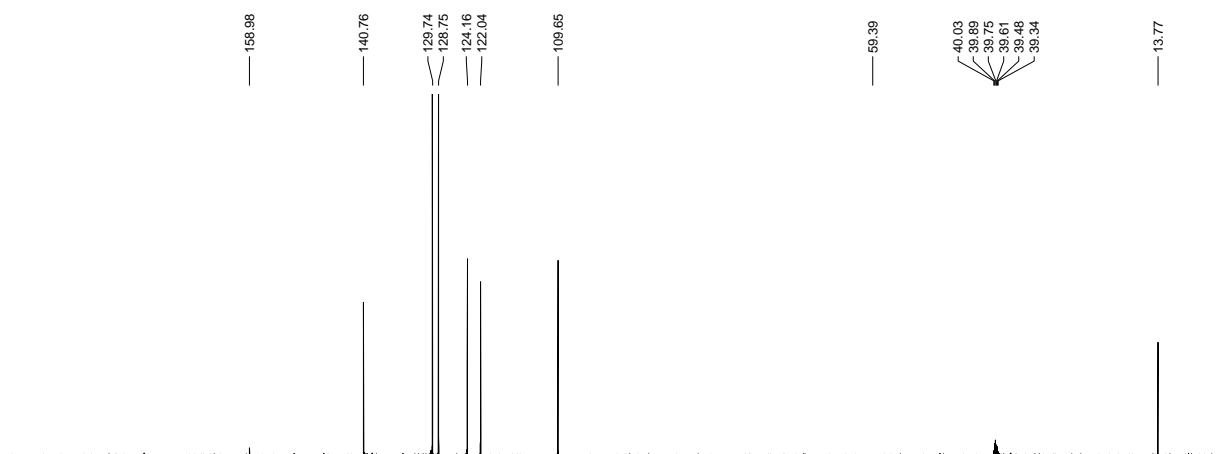


## <sup>13</sup>C NMR in DMSO: 1



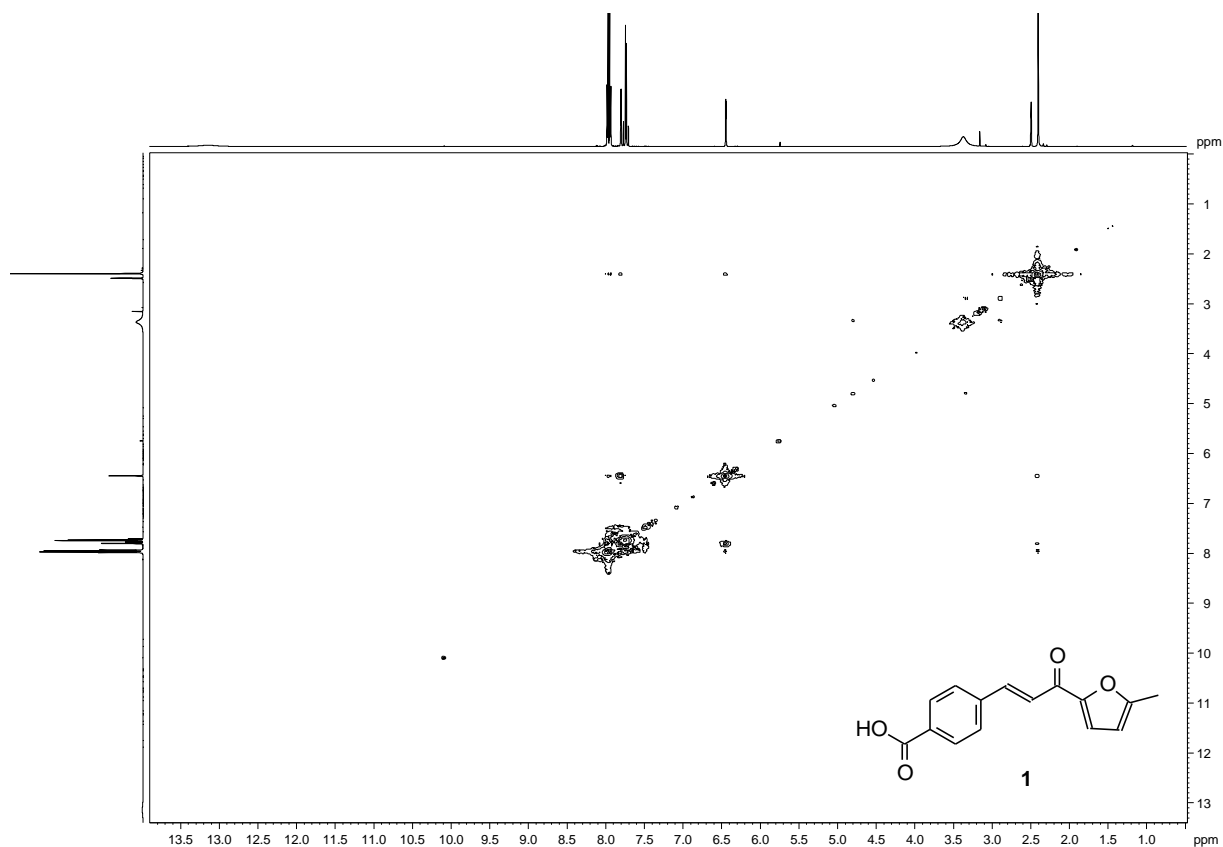
Addendum C – Chapter 5:

DEPT135 in DMSO: **1**



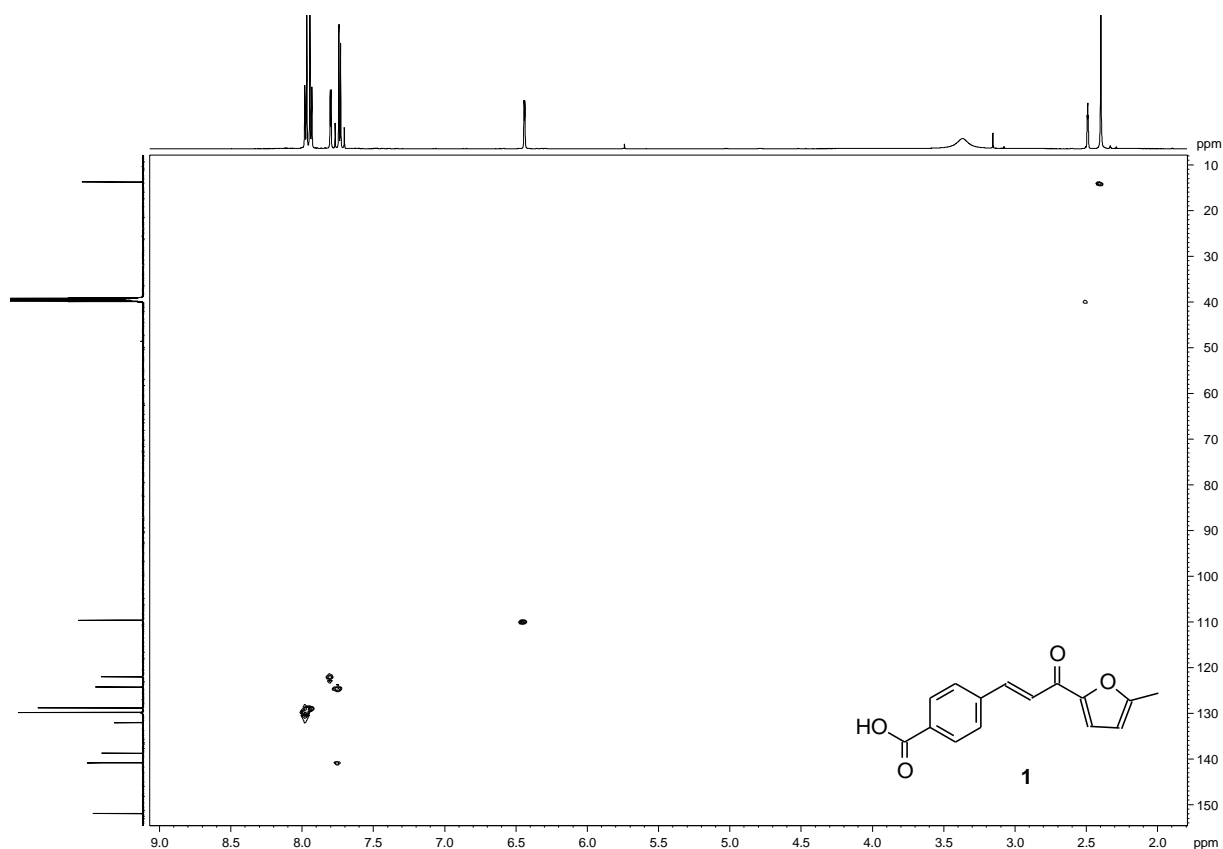
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

COSY in DMSO: **1**



## Addendum C – Chapter 5:

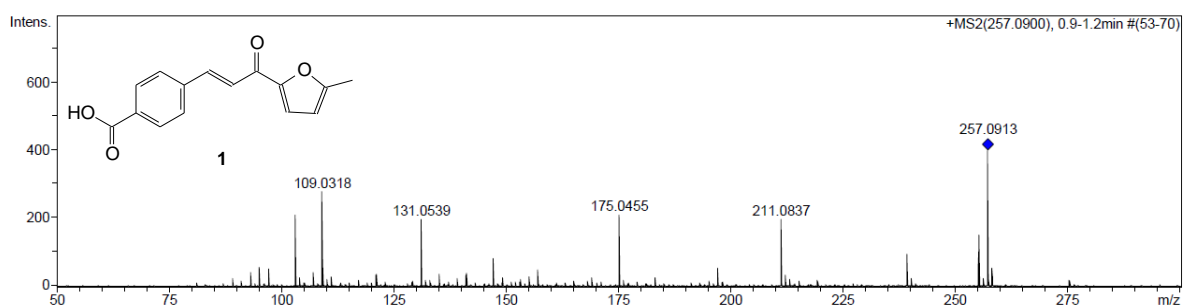
HSQC in DMSO: 1



HRMS: 1

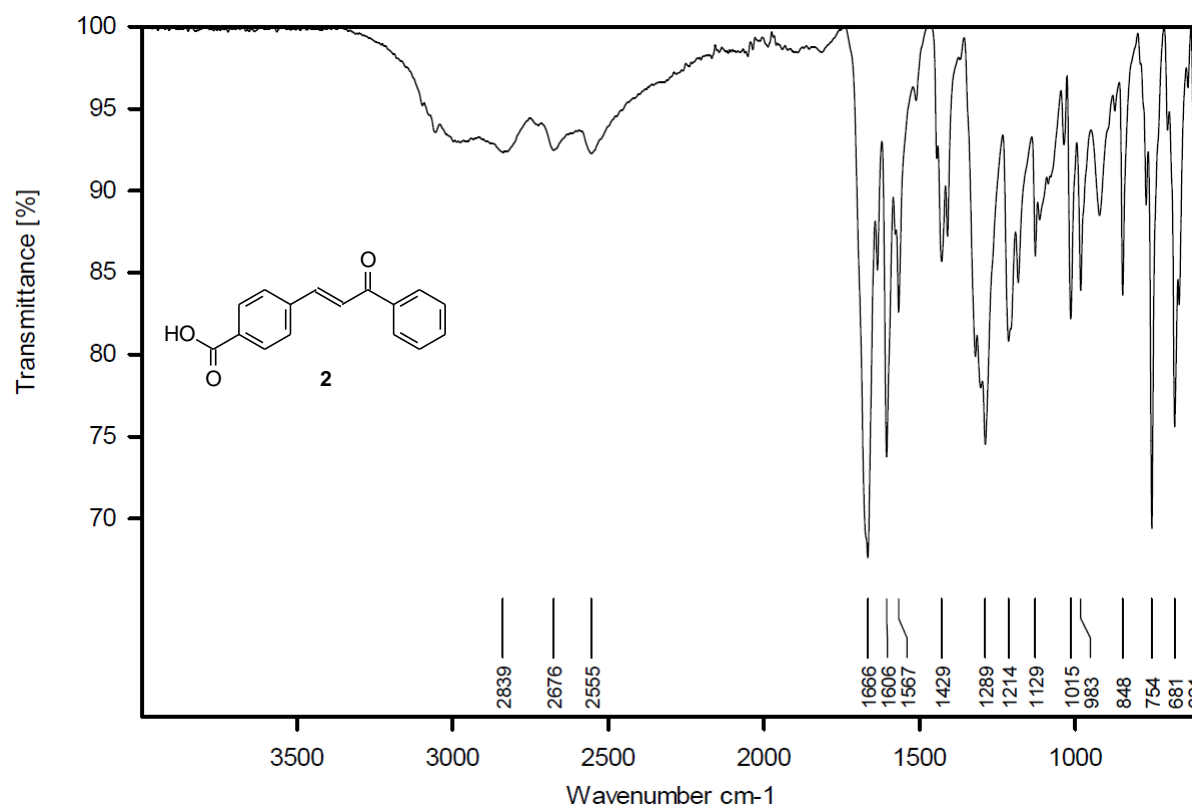
### Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	3000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste

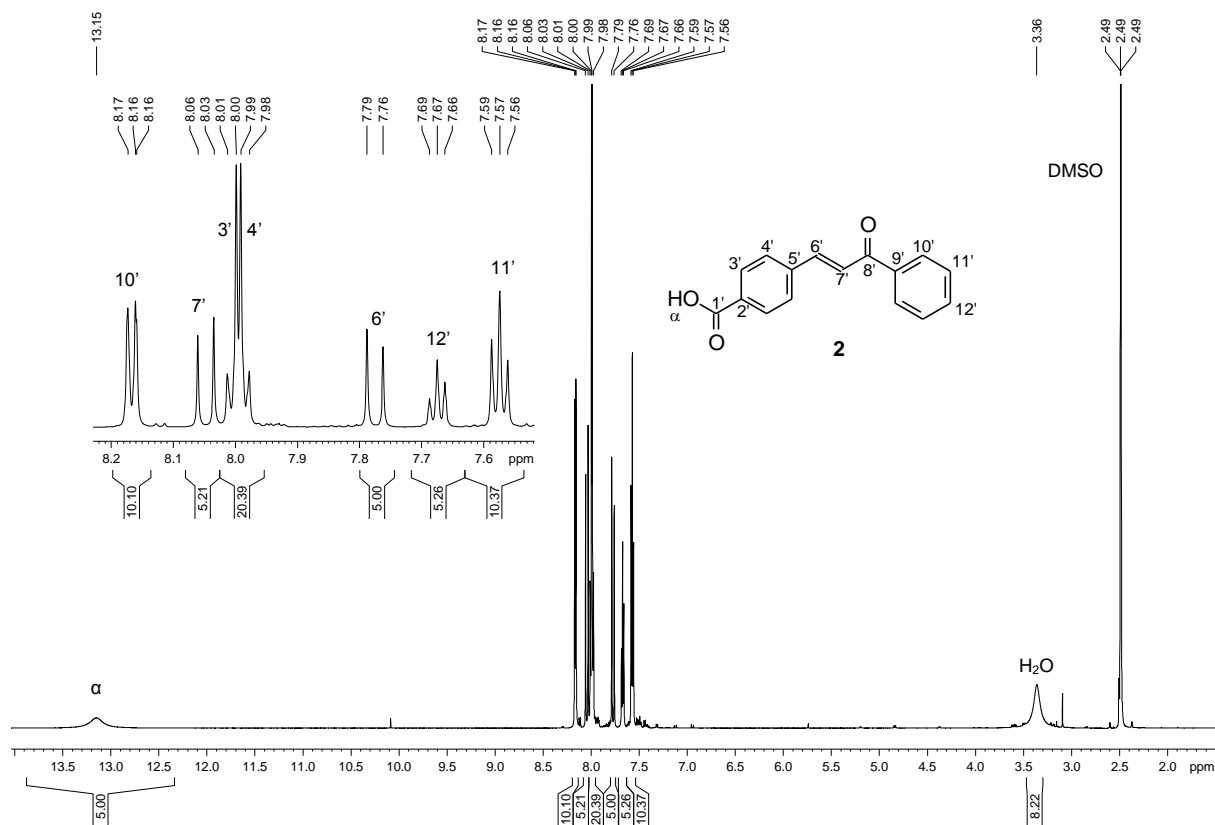


Addendum C – Chapter 5:

IR: 2

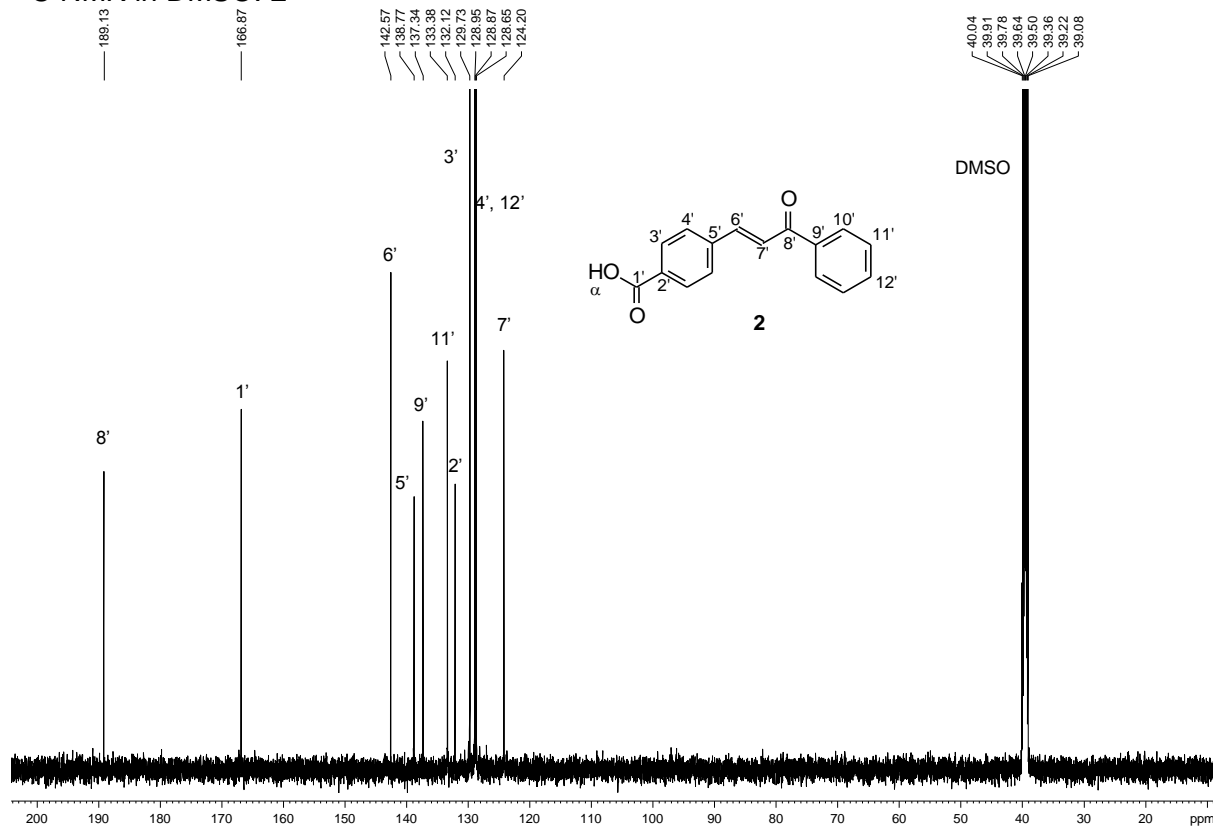


<sup>1</sup>H NMR in DMSO: 2

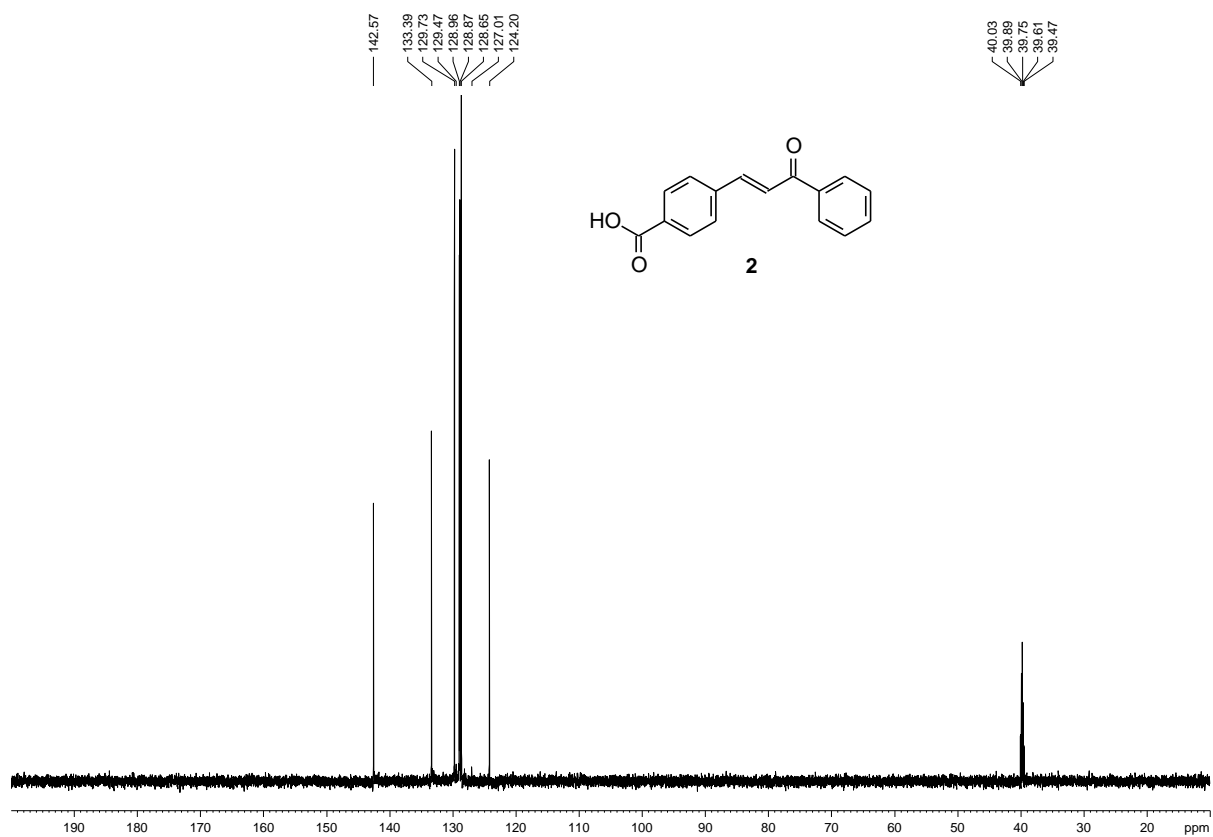


Addendum C – Chapter 5:

<sup>13</sup>C NMR in DMSO: **2**

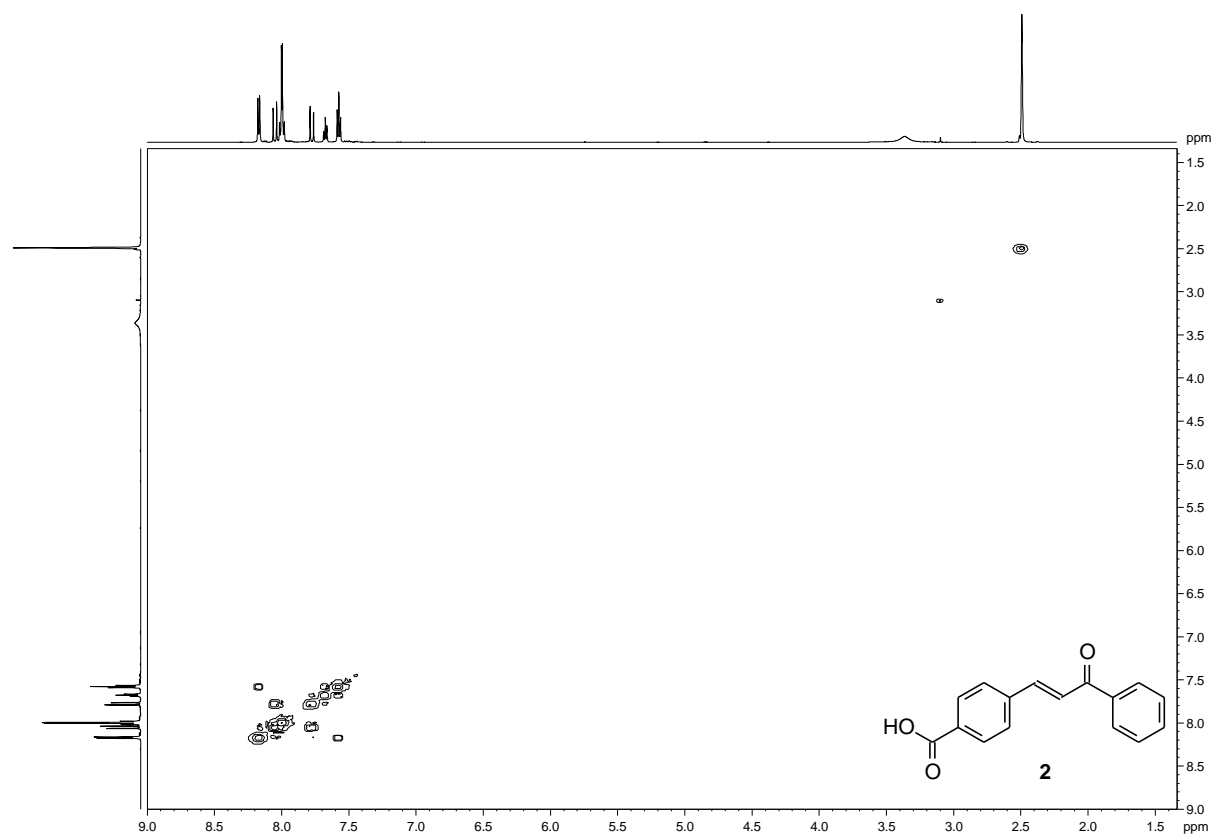


DEPT90 in DMSO: **2**

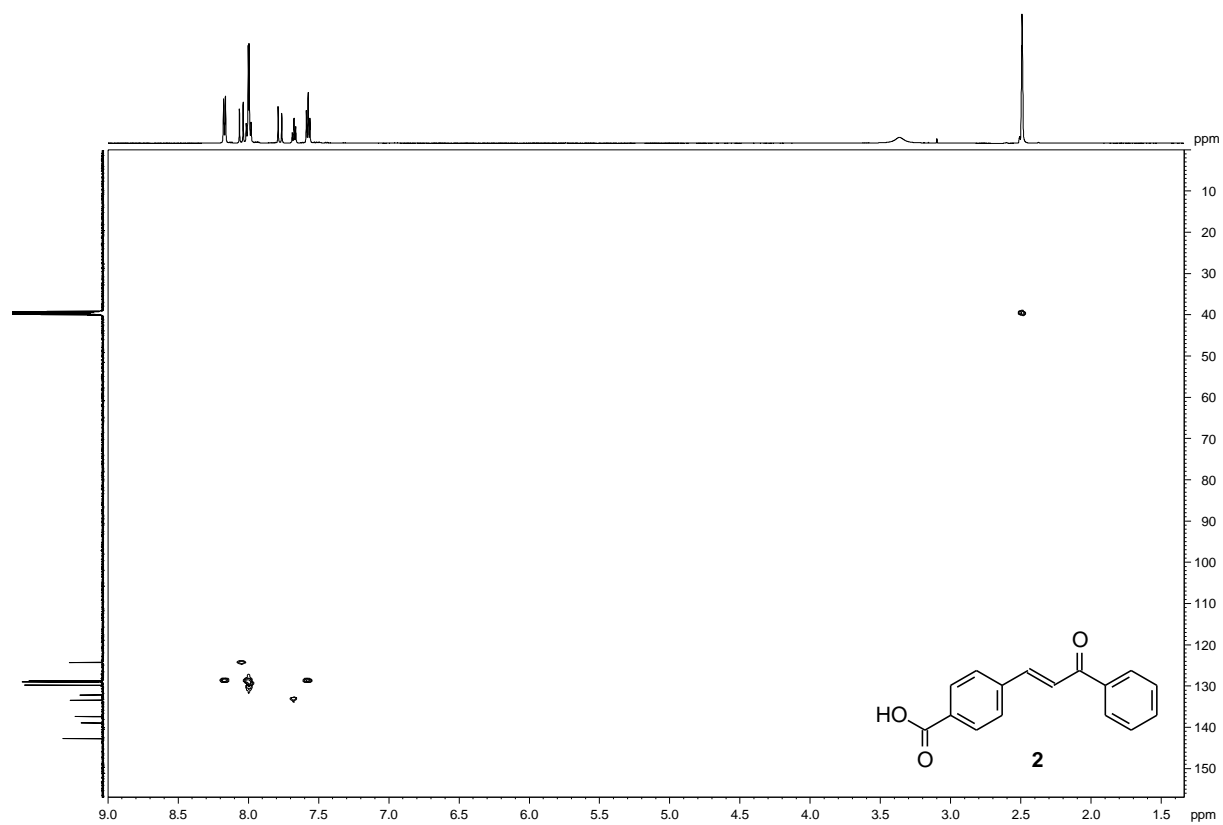


Addendum C – Chapter 5:

COSY in DMSO: 2



HSQC in DMSO: 2

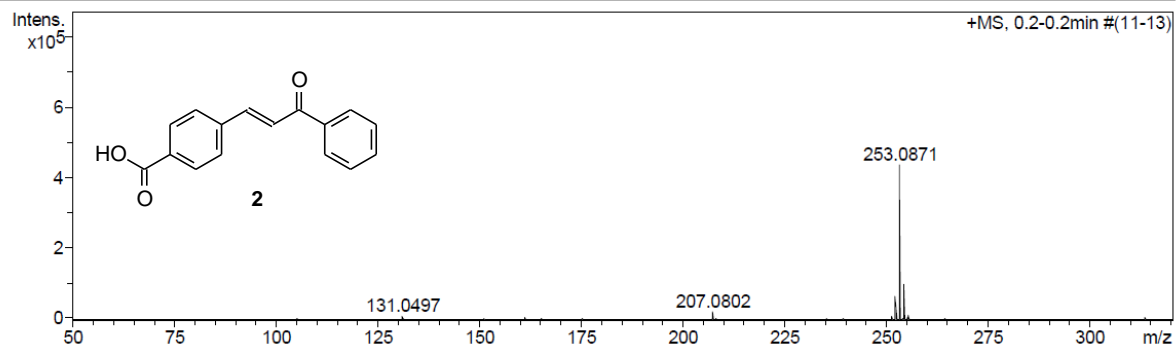


## Addendum C – Chapter 5:

### HRMS: 2

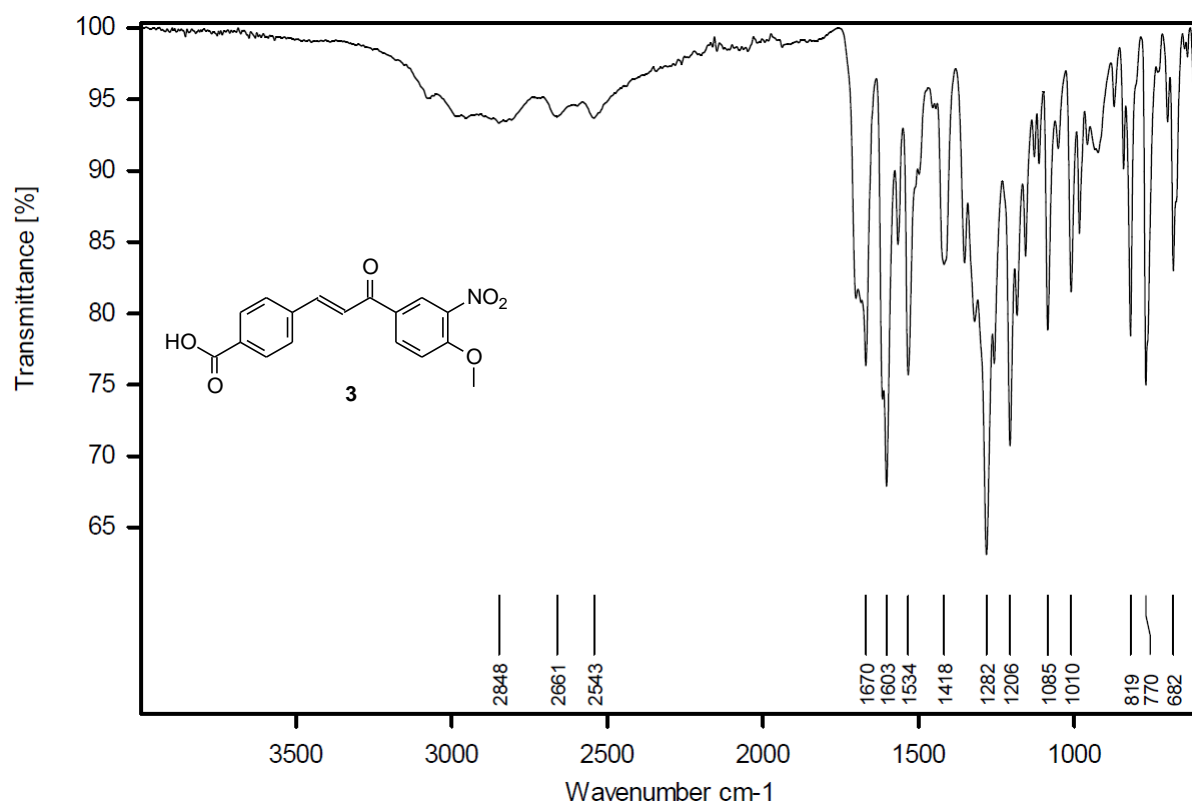
#### Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

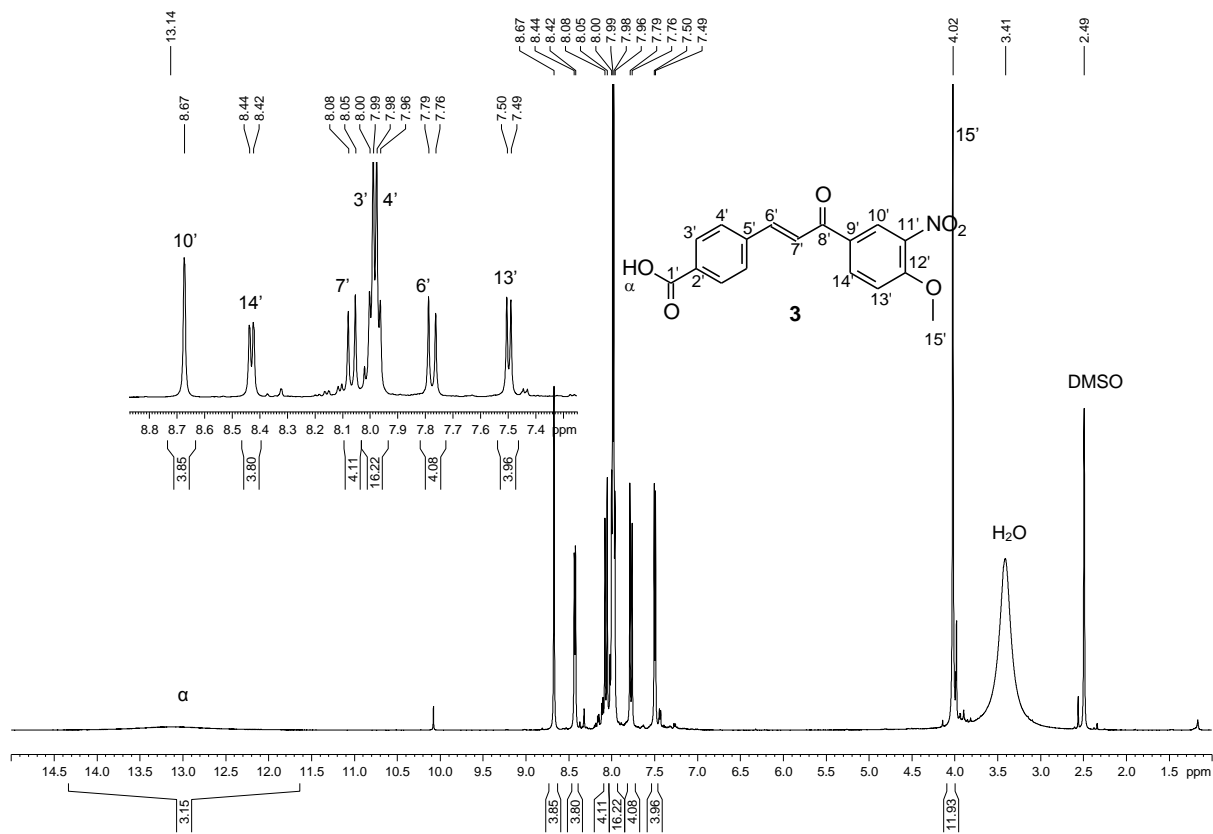


Addendum C – Chapter 5:

IR: **3**

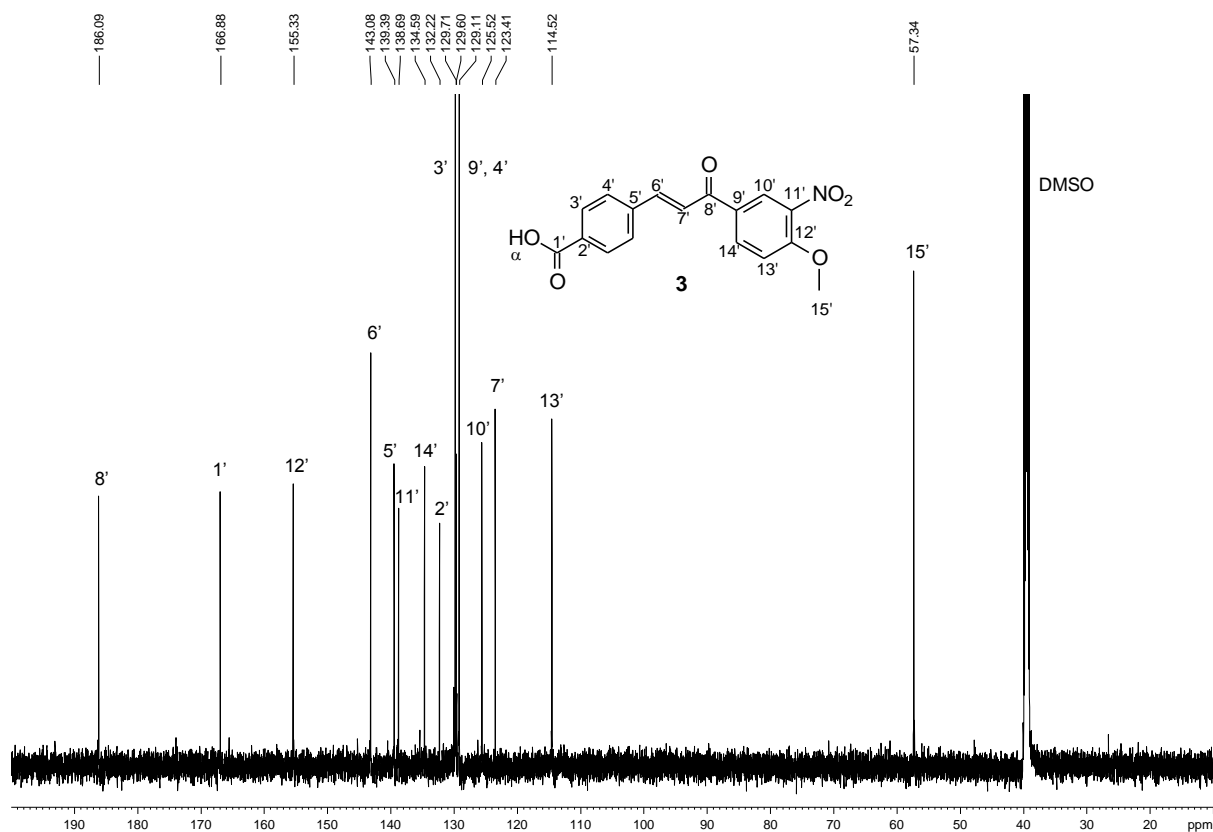


<sup>1</sup>H NMR in DMSO: **3**

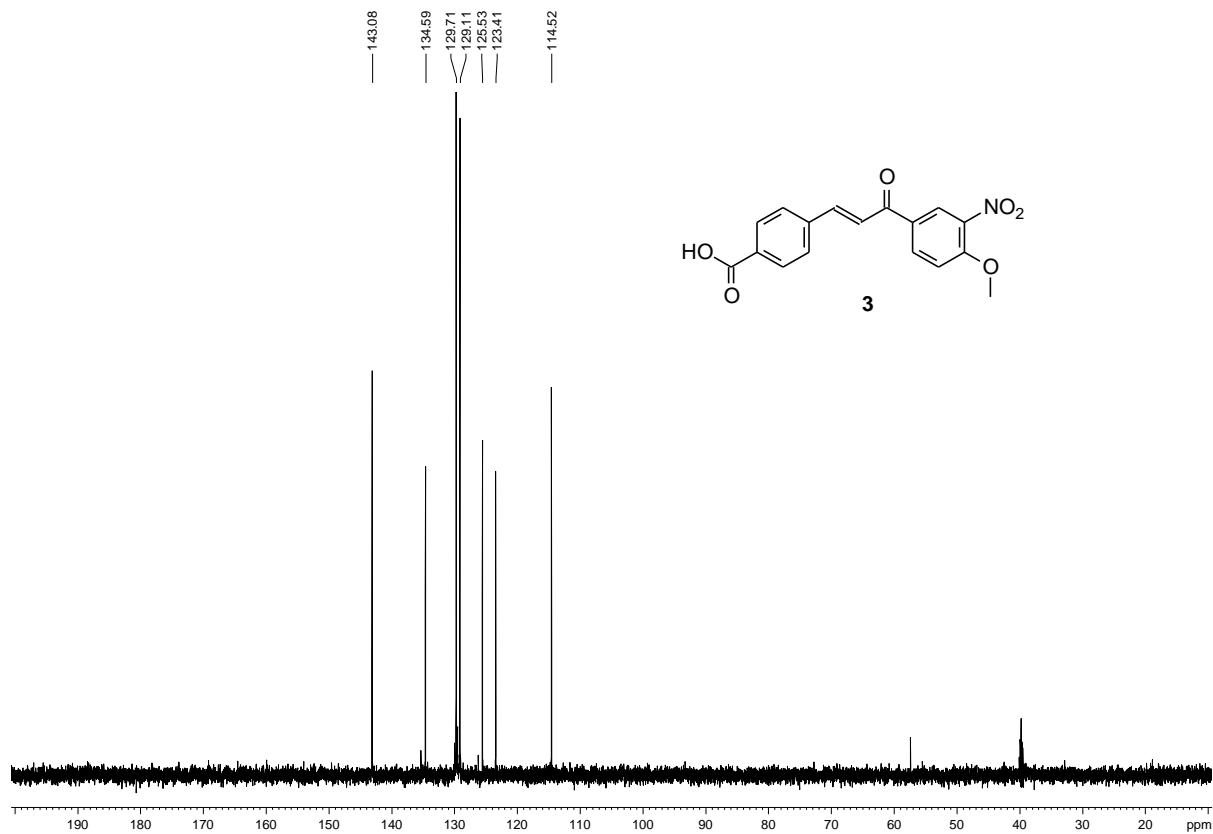


Addendum C – Chapter 5:

<sup>13</sup>C NMR in DMSO: **3**

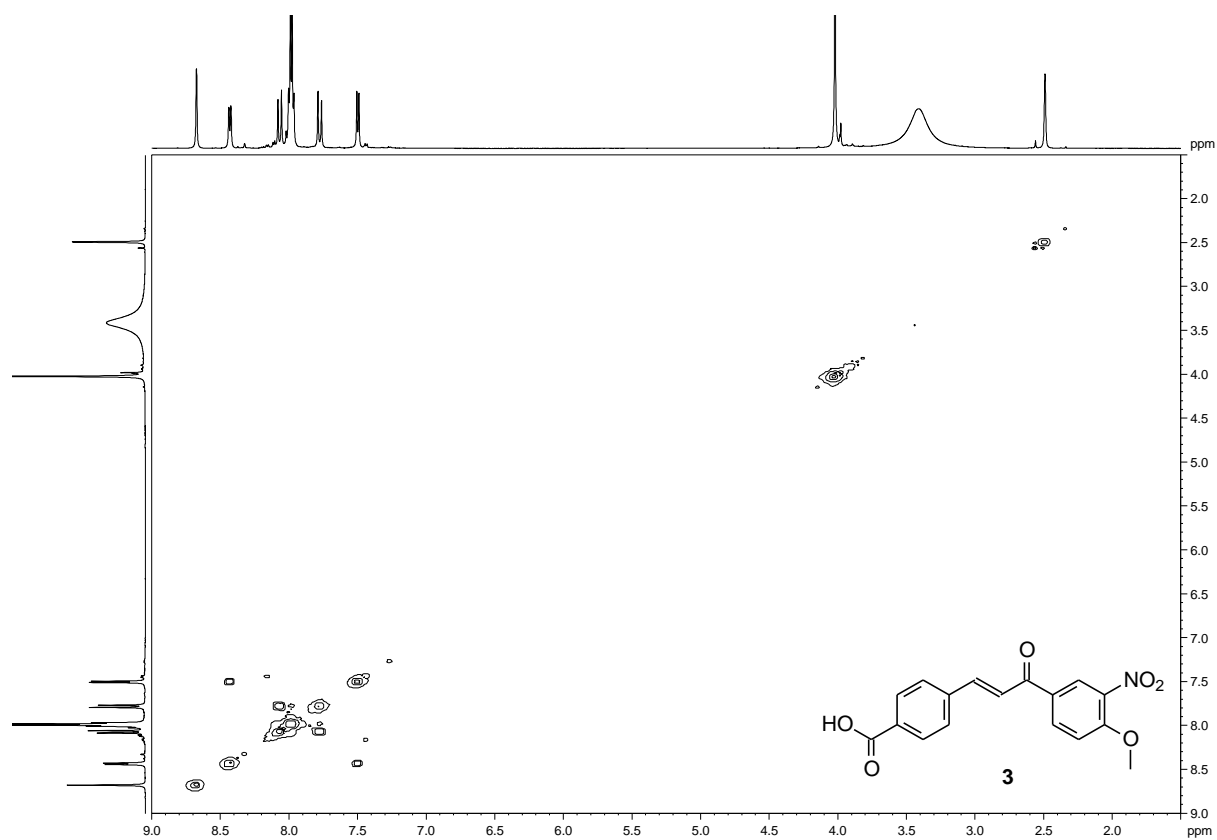


DEPT90 in DMSO: **3**

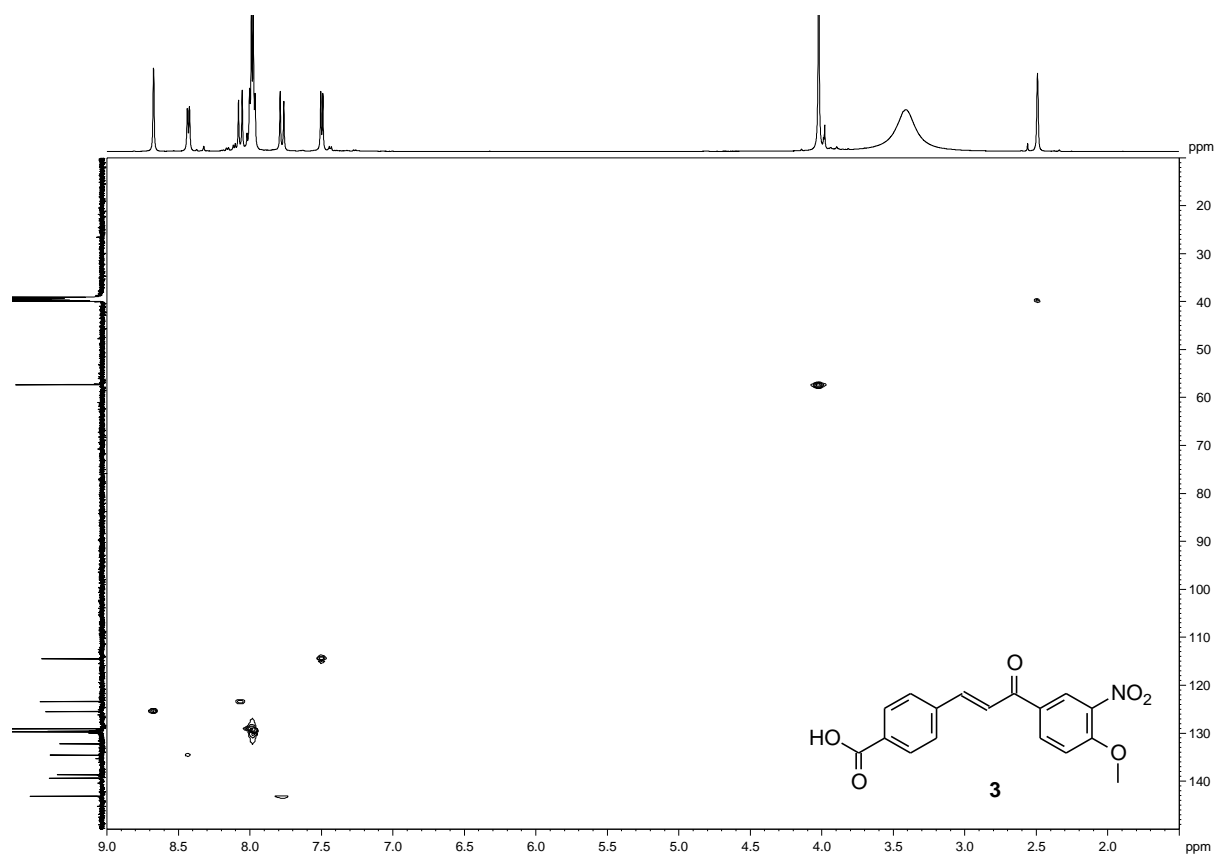


## Addendum C – Chapter 5:

COSY in DMSO: **3**



HSQC in DMSO: **3**

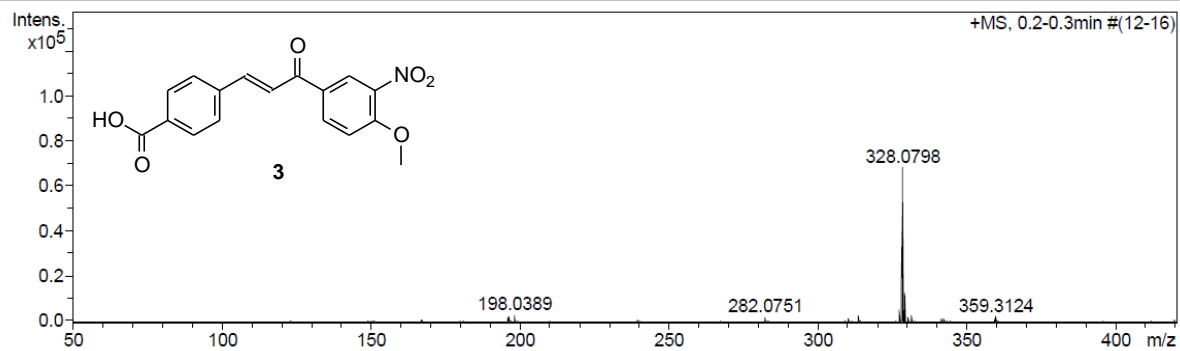


## Addendum C – Chapter 5:

### HRMS: 3

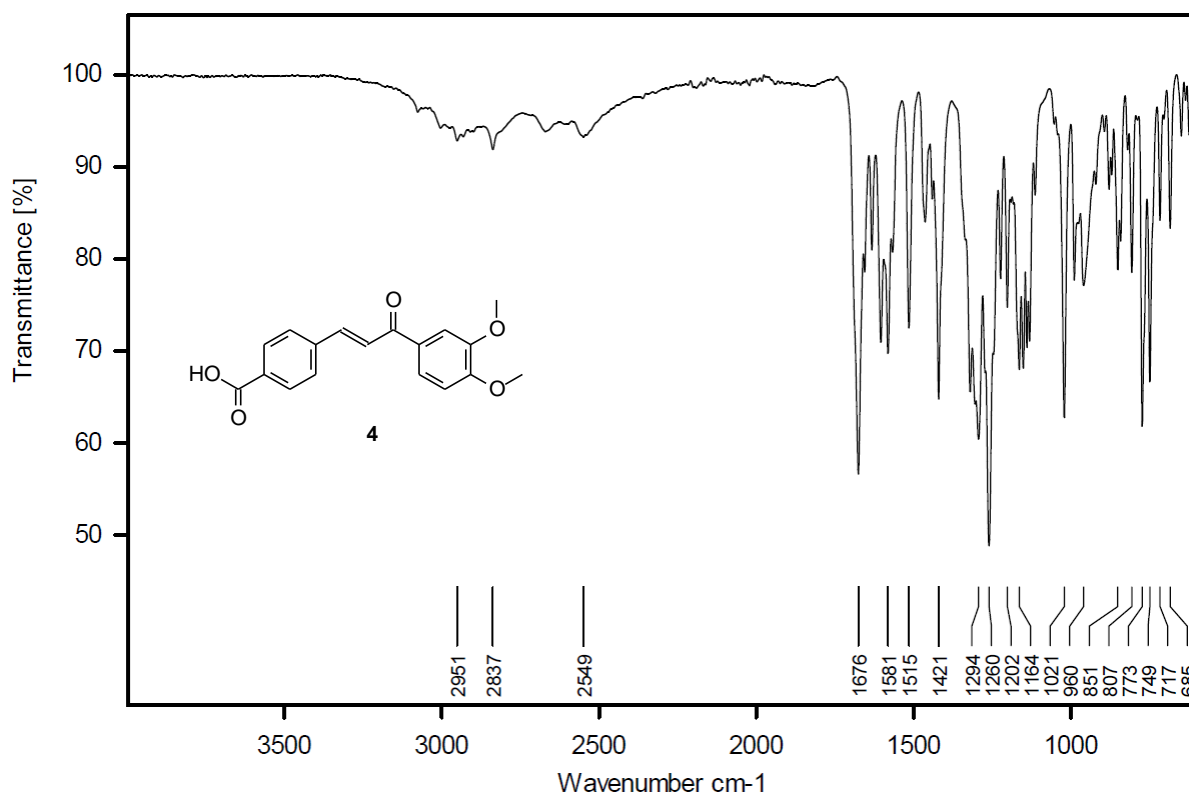
#### Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

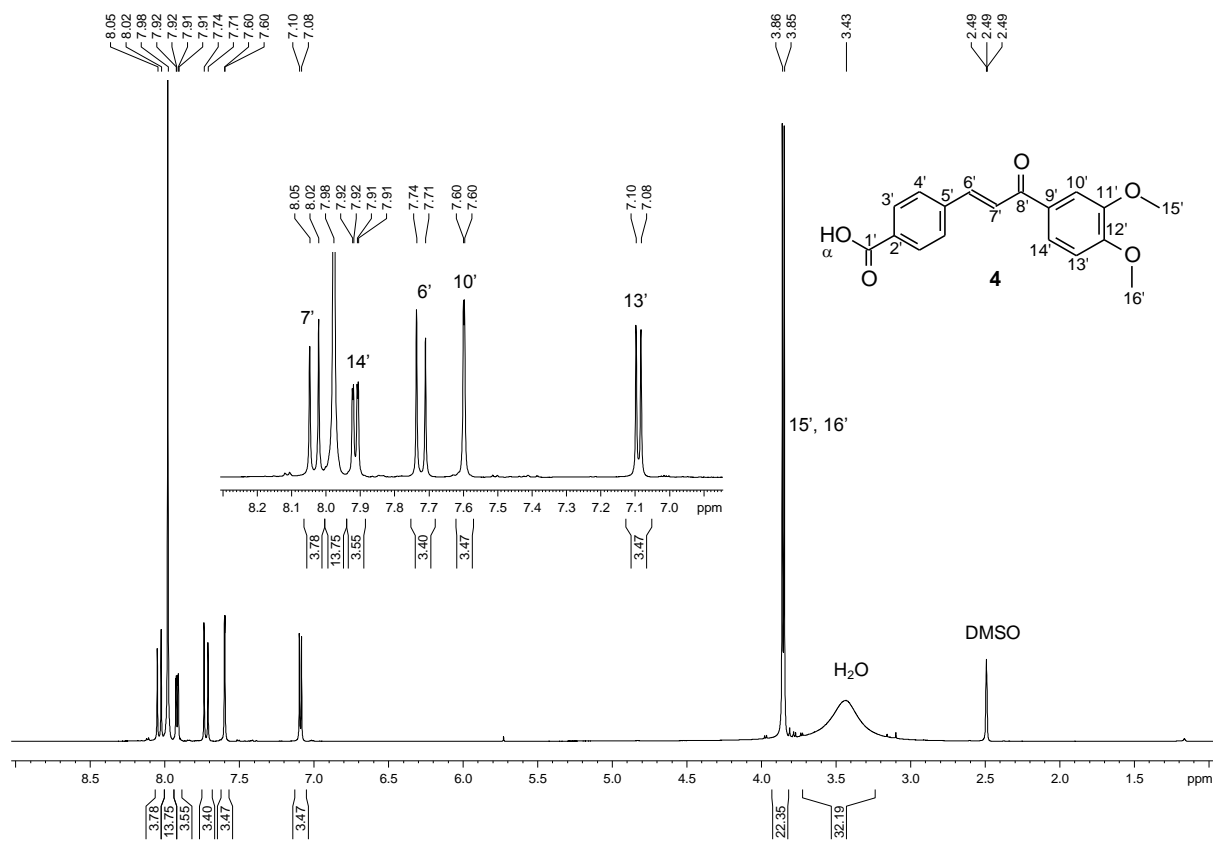


Addendum C – Chapter 5:

IR: 4:

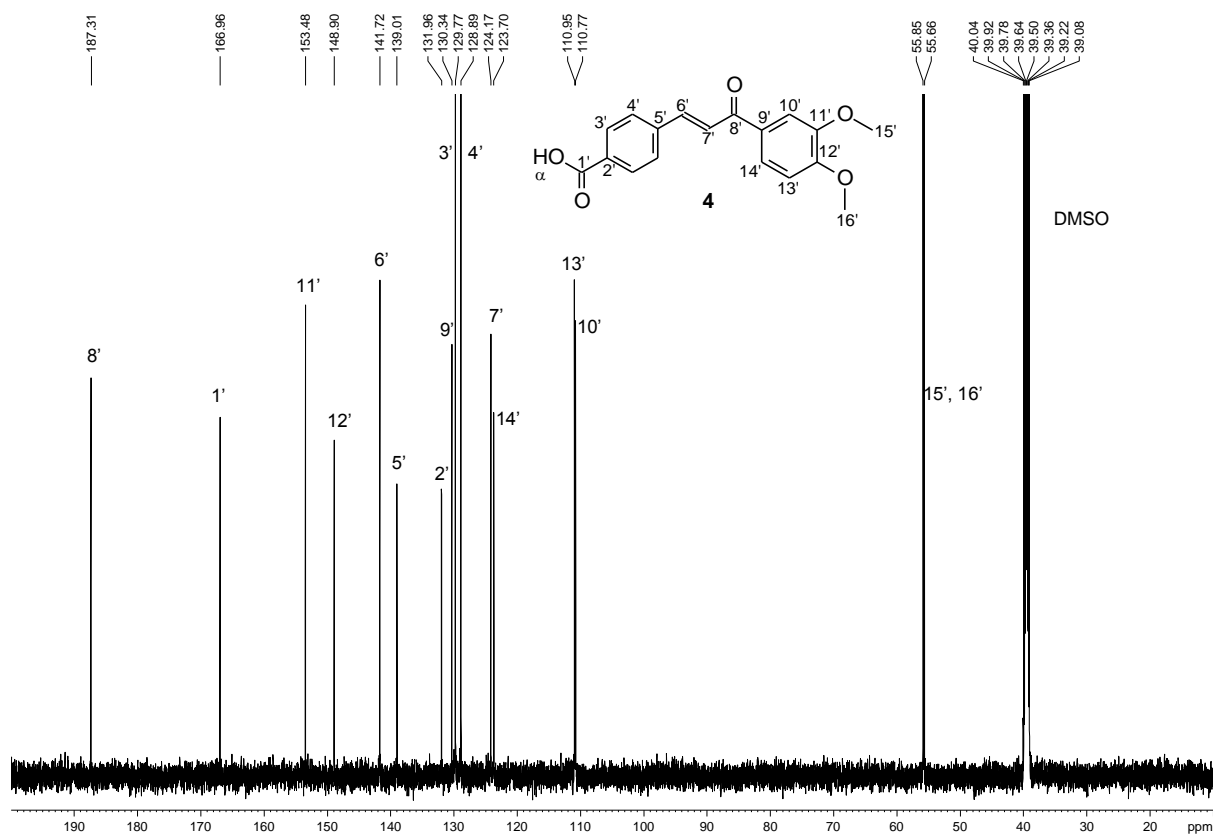


<sup>1</sup>H NMR in DMSO: 4

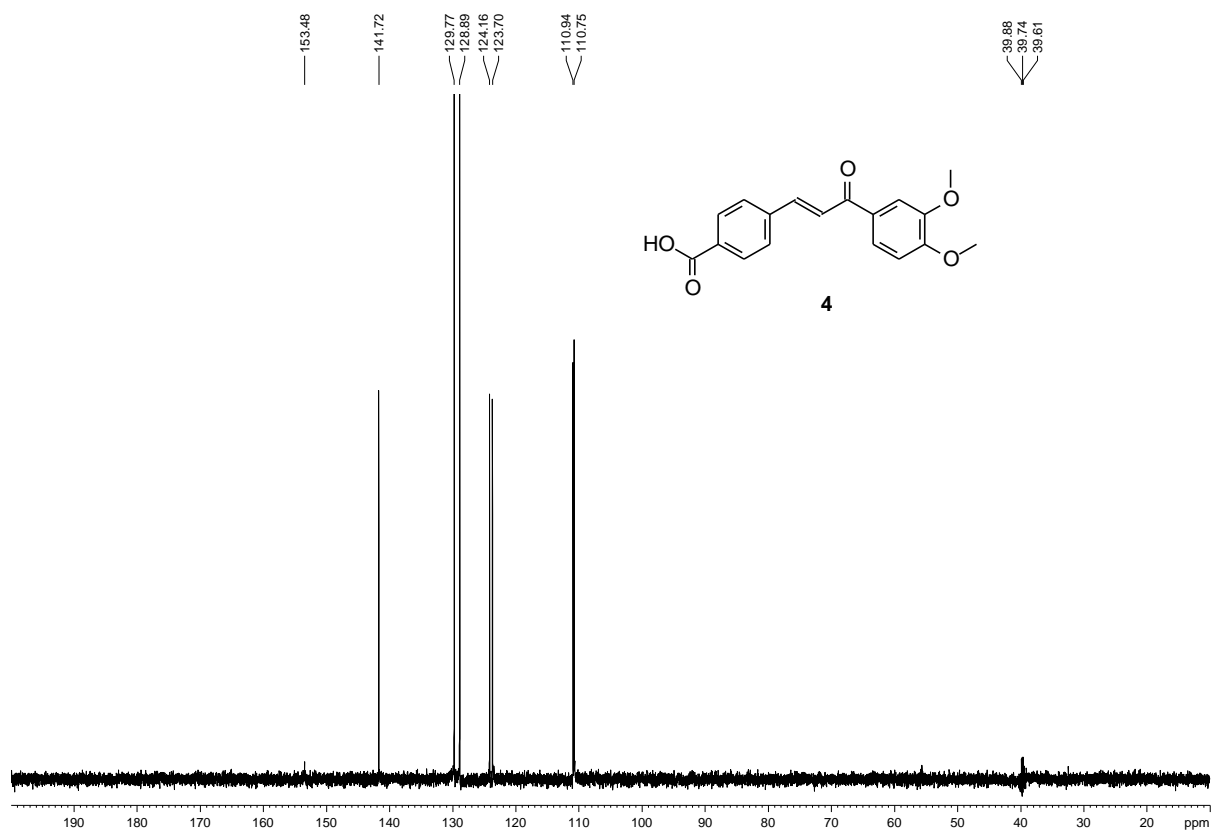


<sup>13</sup>C NMR in DMSO: 4

Addendum C – Chapter 5:

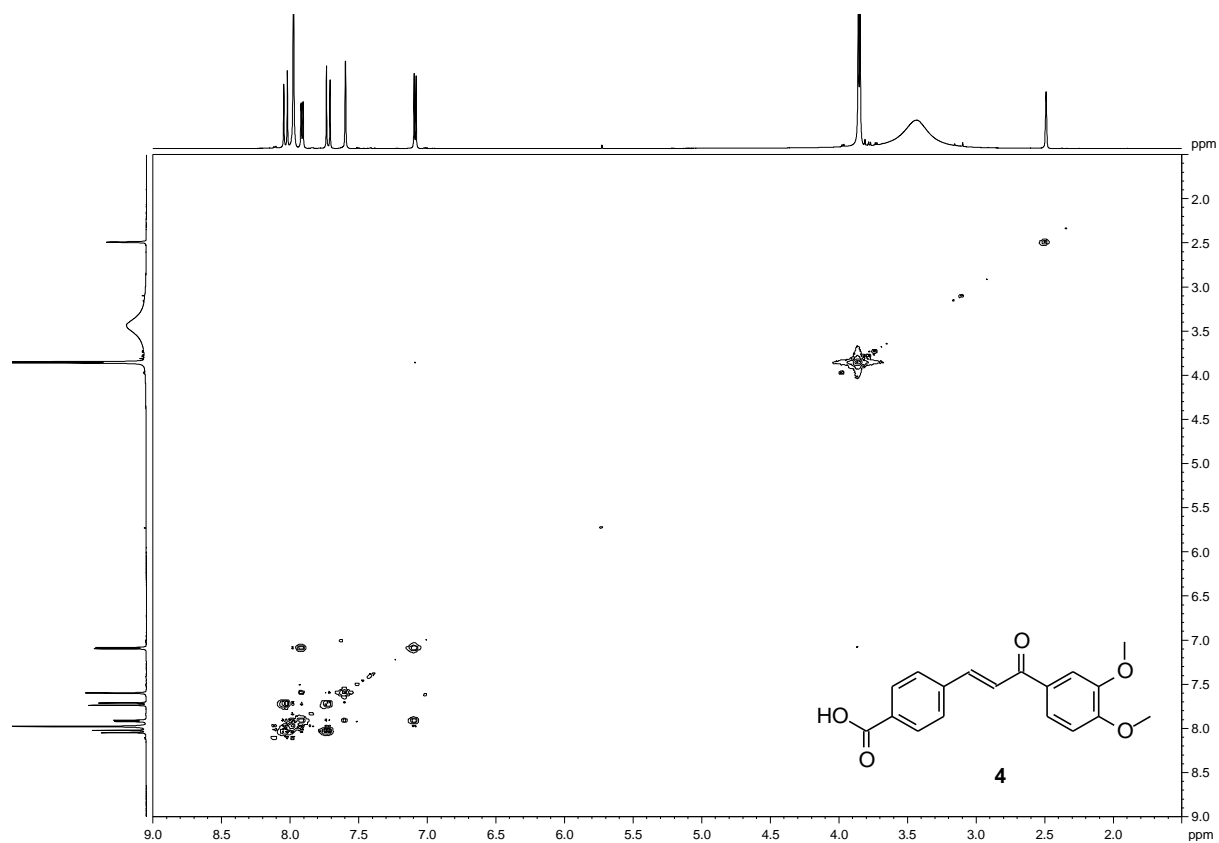


DEPT90 in DMSO: 4

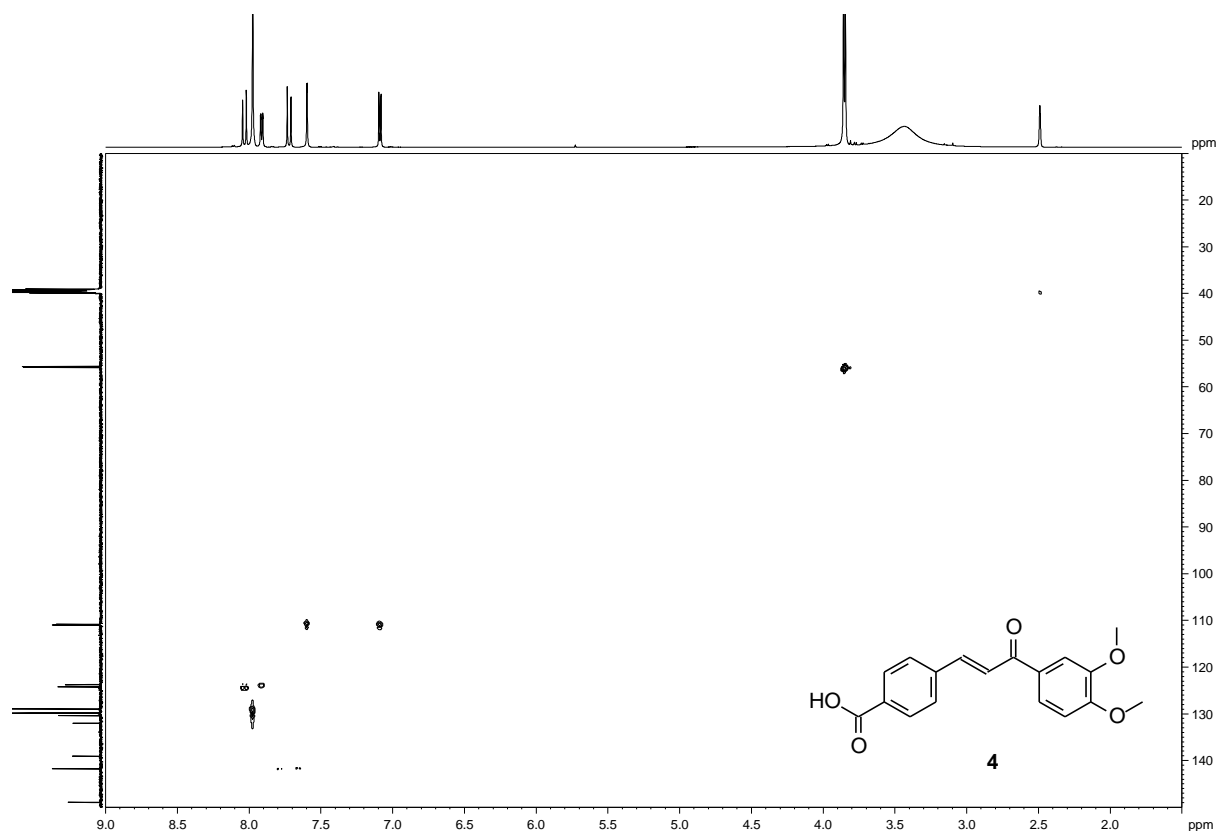


COSY in DMSO: 4

Addendum C – Chapter 5:



HSQC in DMSO: 4

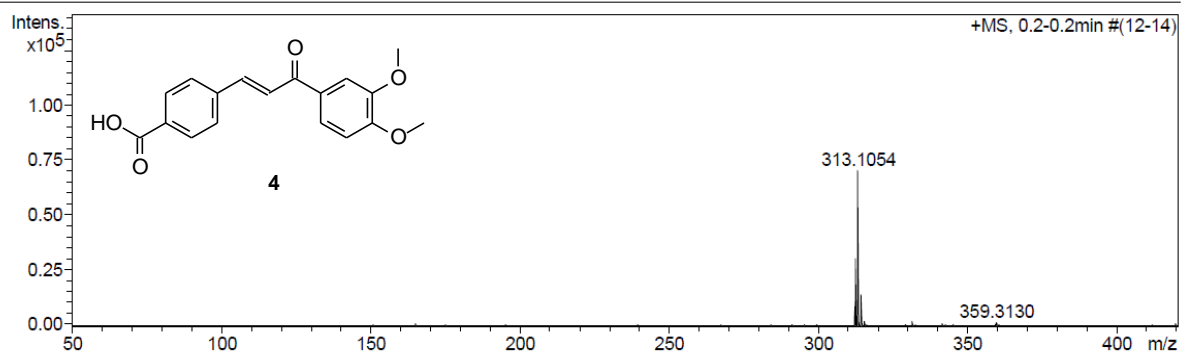


HRMS: 4

## Addendum C – Chapter 5:

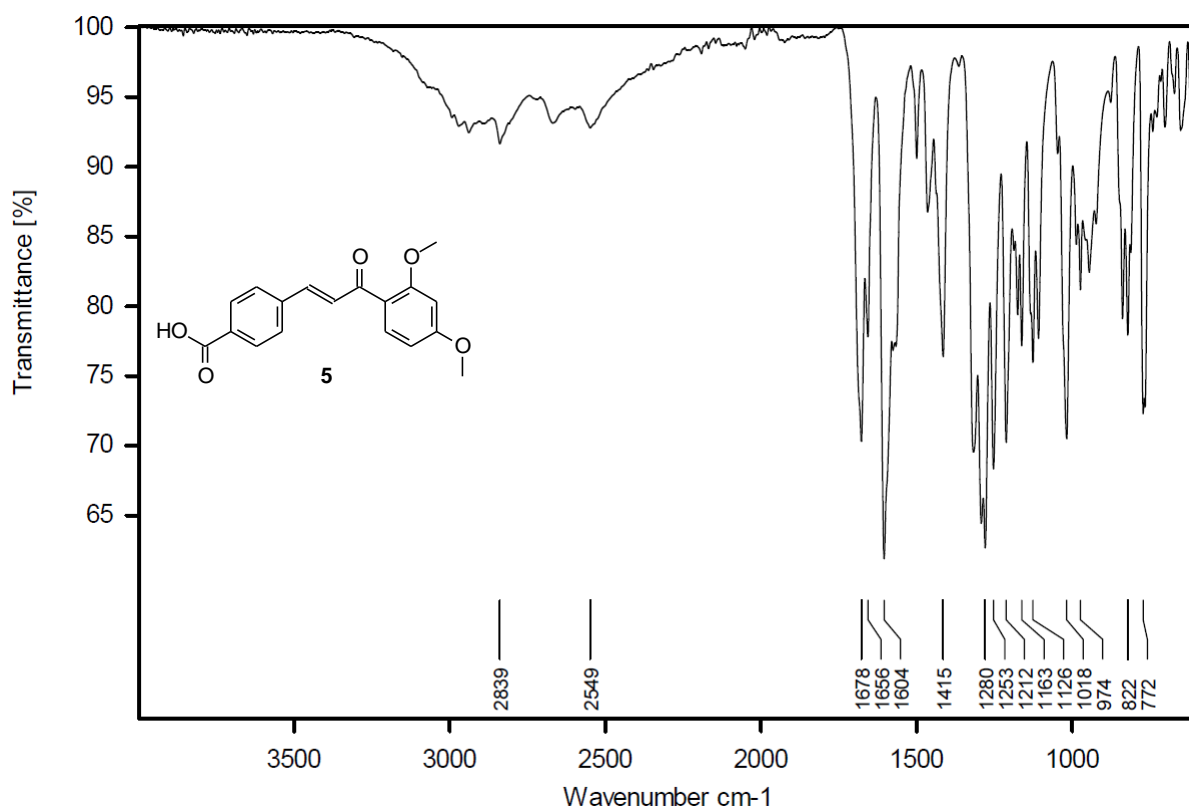
### Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

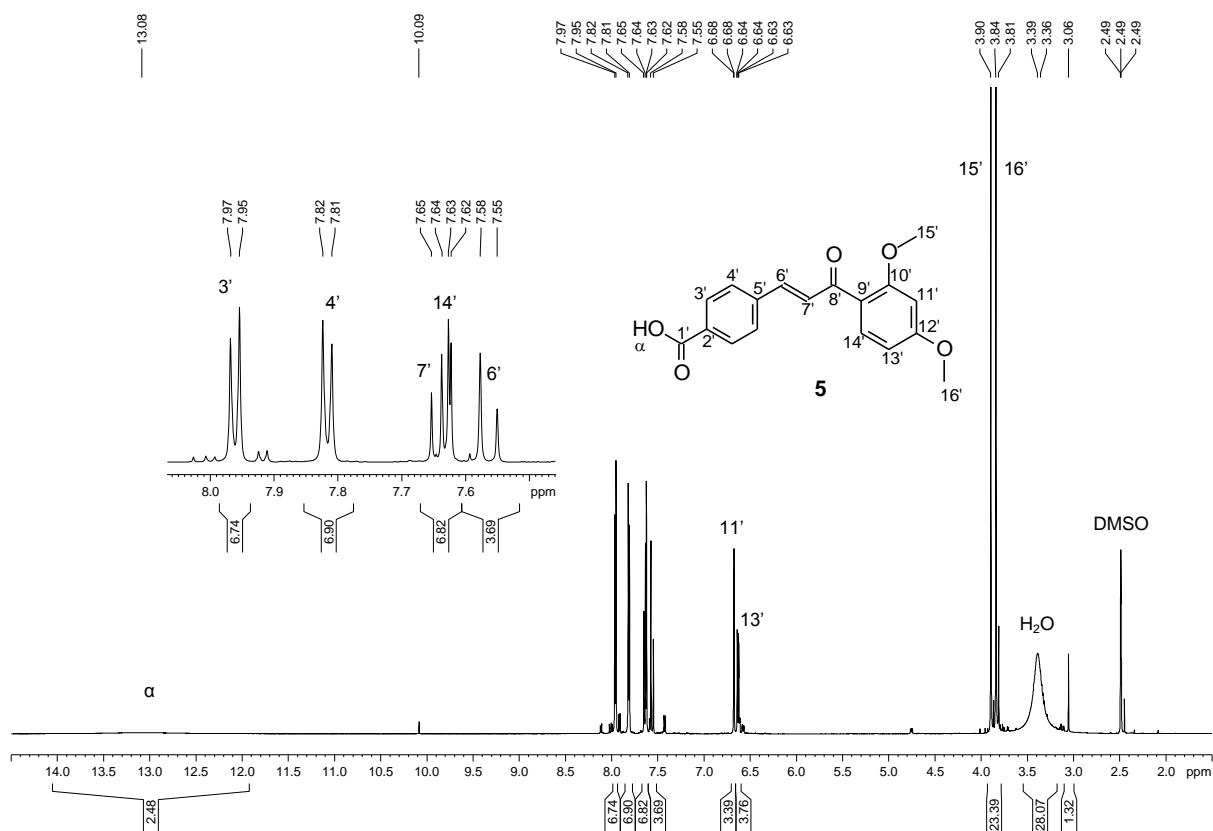


Addendum C – Chapter 5:

IR: 5:

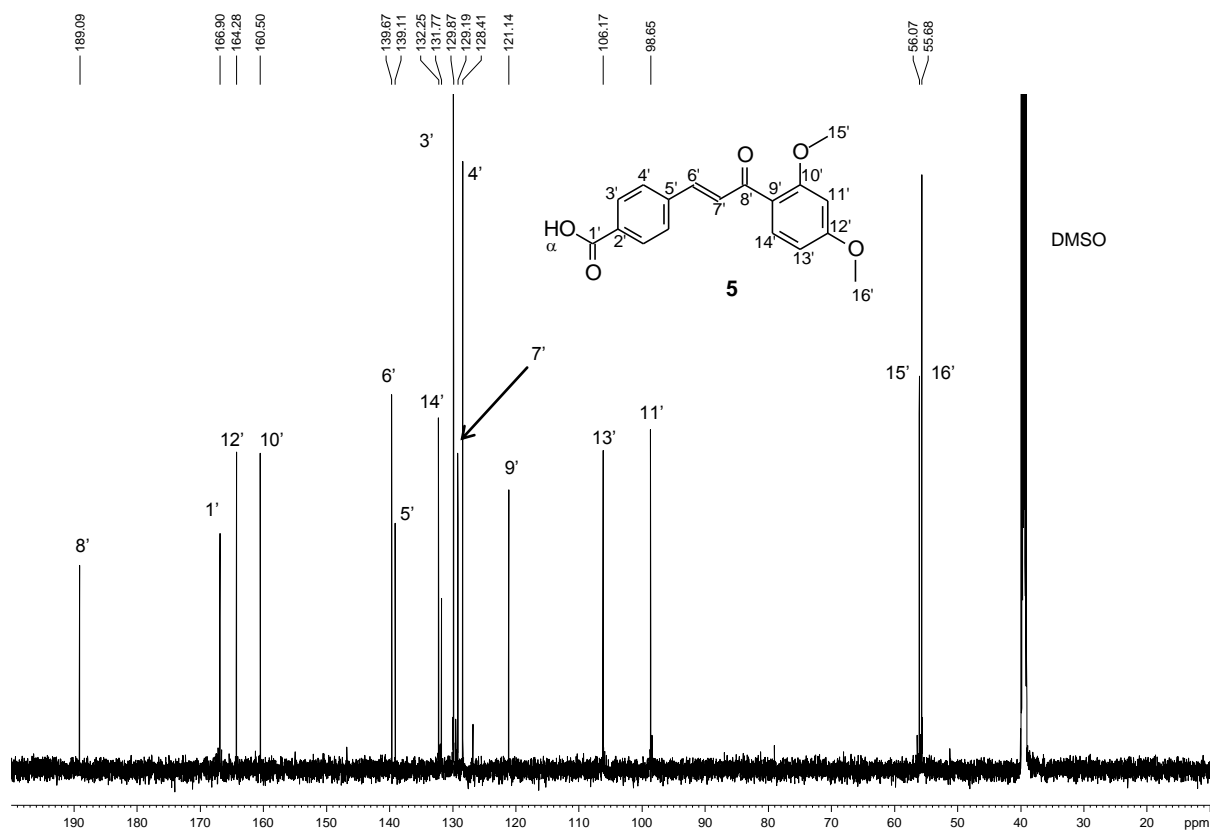


<sup>1</sup>H NMR in DMSO: 5

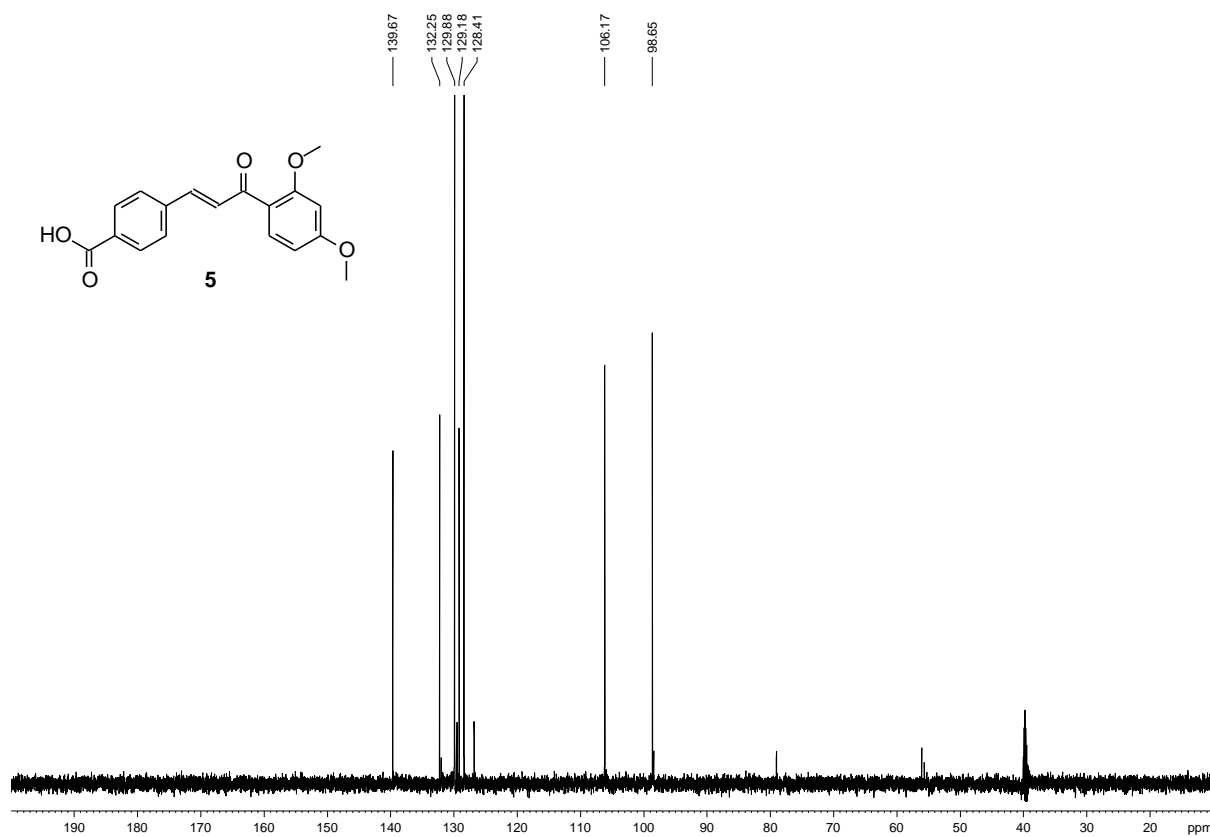


# Addendum C – Chapter 5:

## <sup>13</sup>C NMR in DMSO: 5

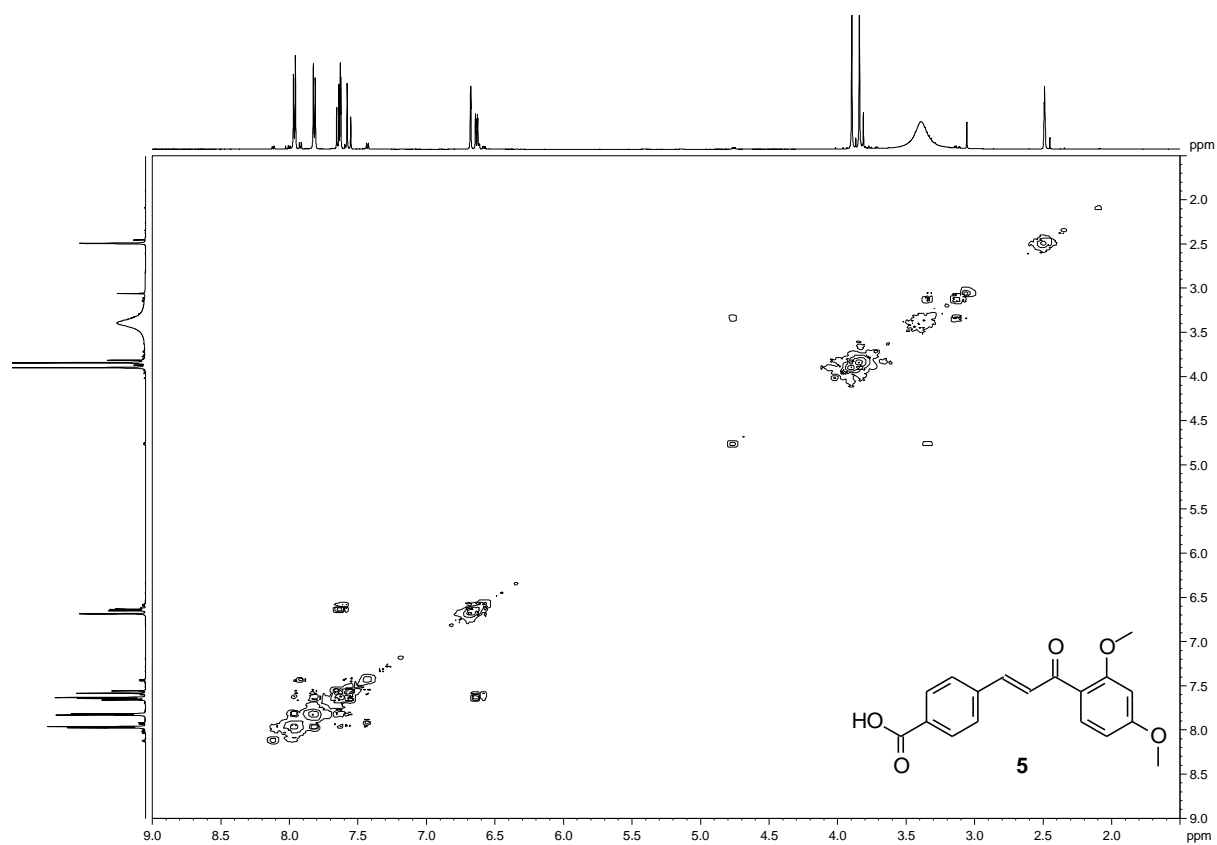


## DEPT90 in DMSO: 5

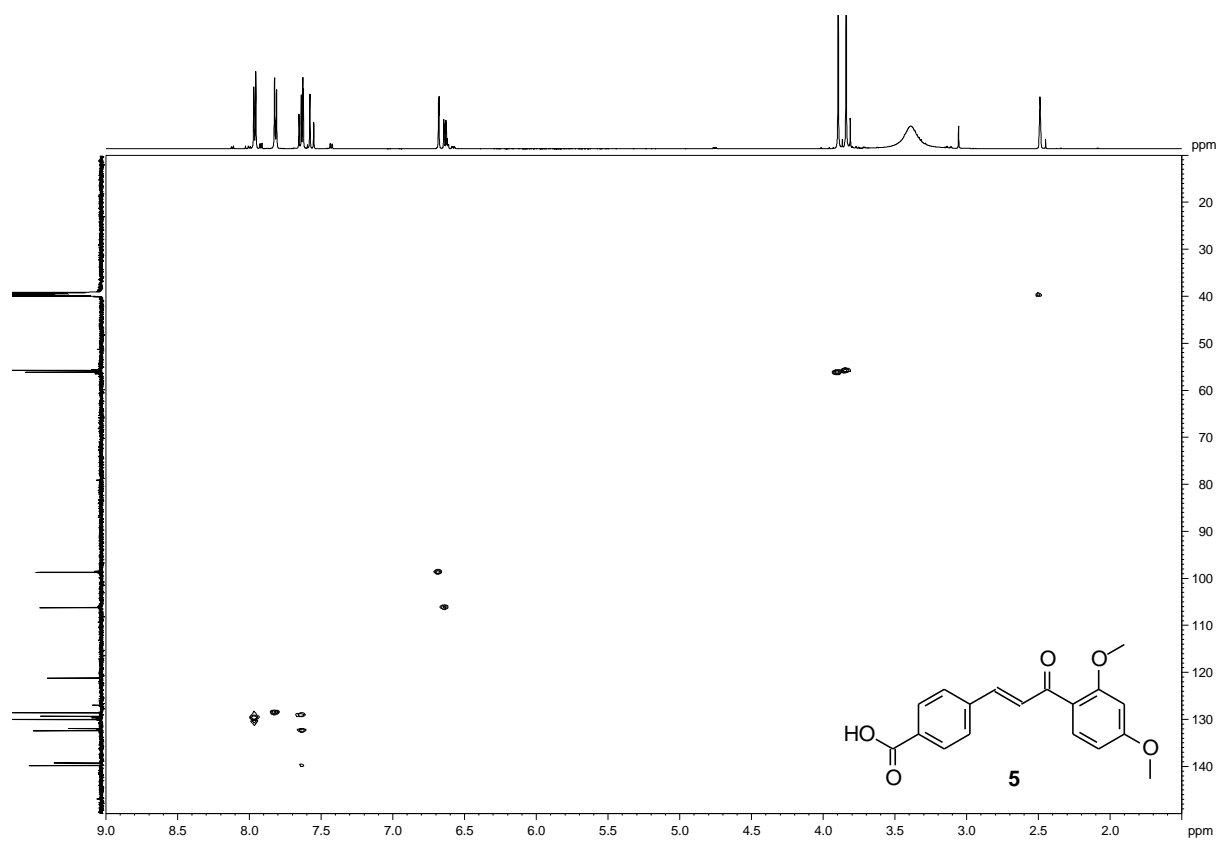


Addendum C – Chapter 5:

COSY in DMSO: 5



HSQC in DMSO: 5

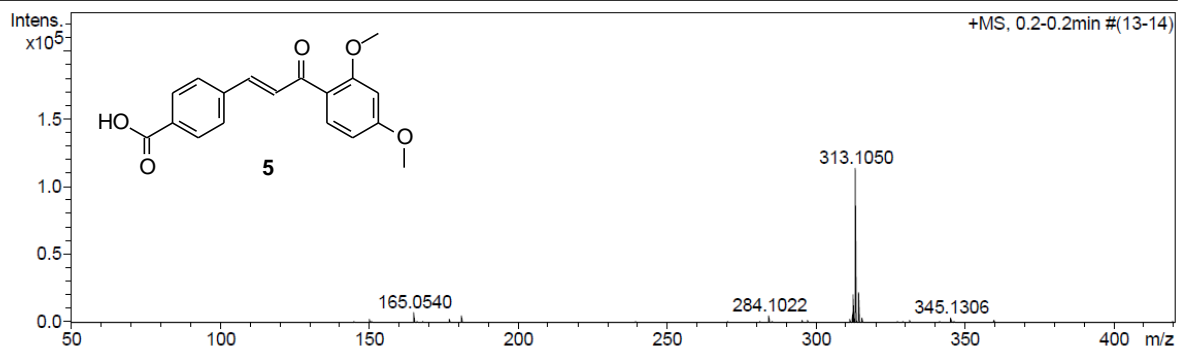


## Addendum C – Chapter 5:

### HRMS: 5

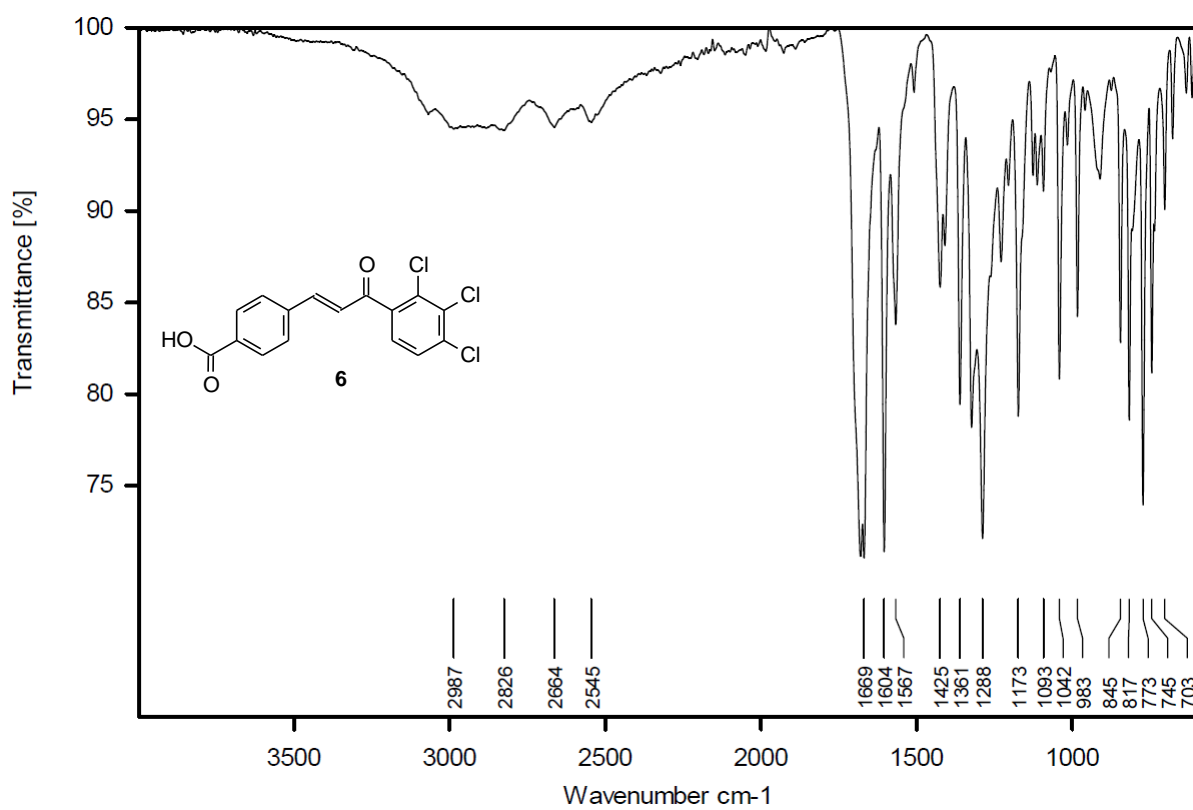
#### Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

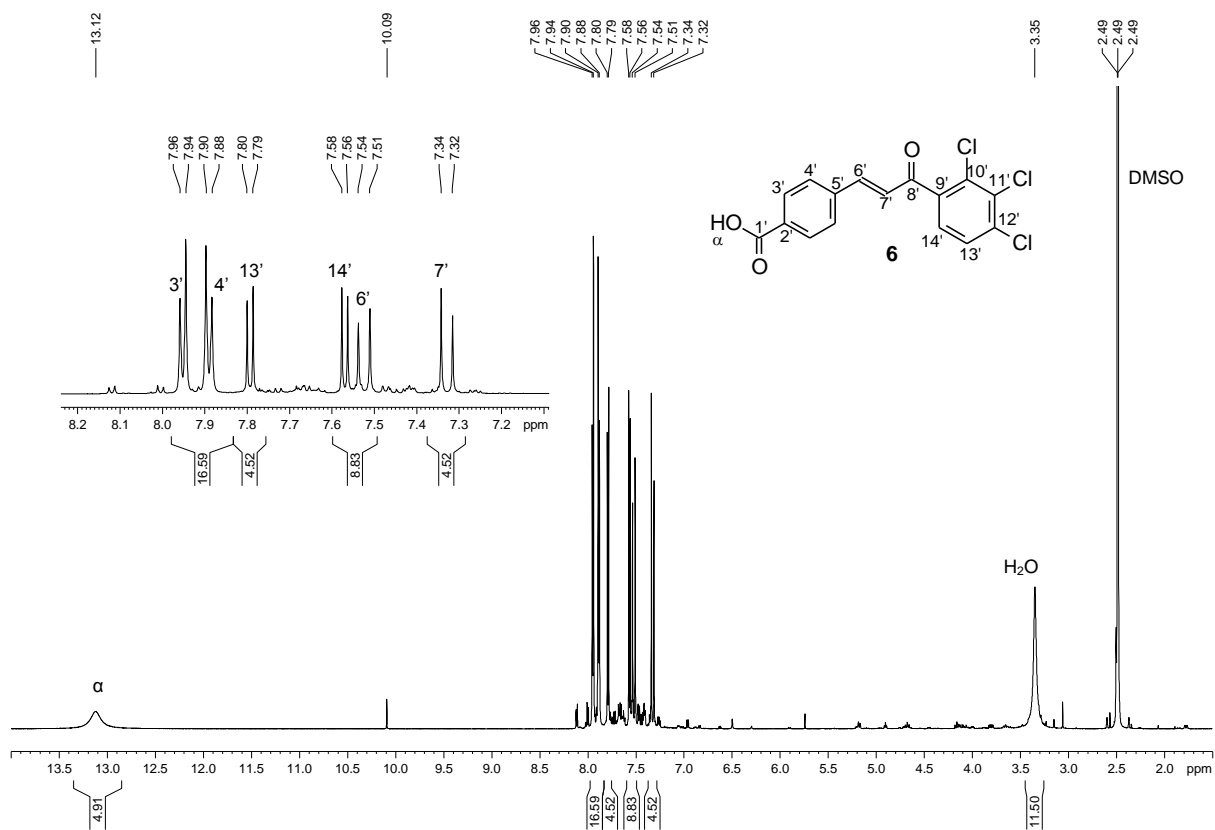


Addendum C – Chapter 5:

IR: 6:

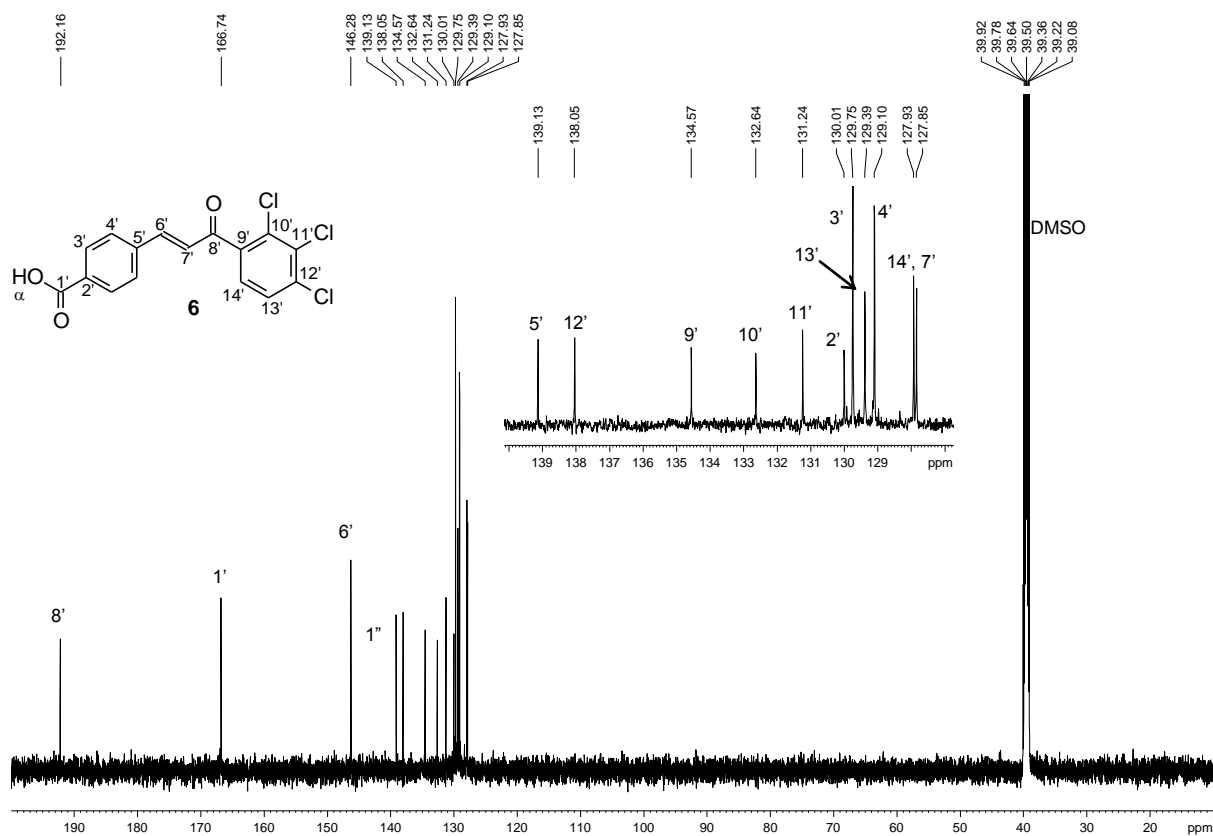


<sup>1</sup>H NMR in DMSO: 6

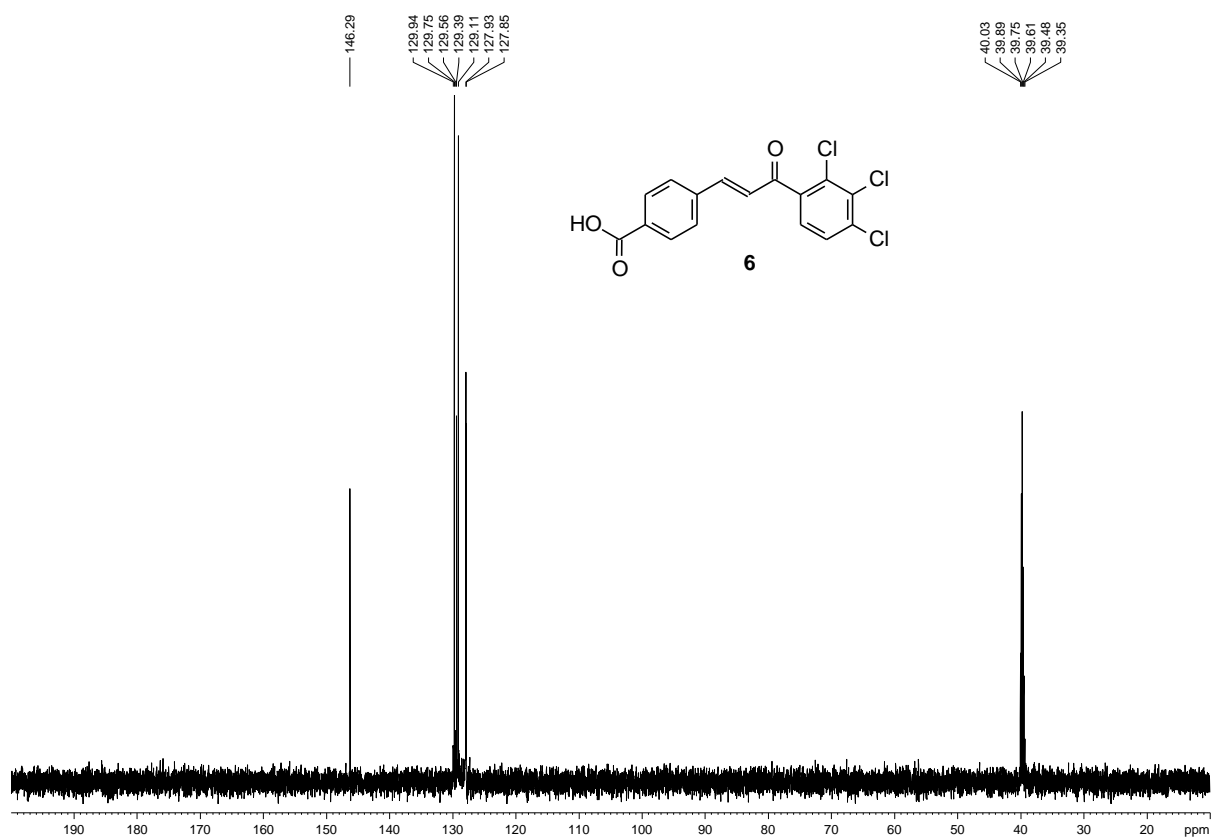


# Addendum C – Chapter 5:

## <sup>13</sup>C NMR in DMSO: 6

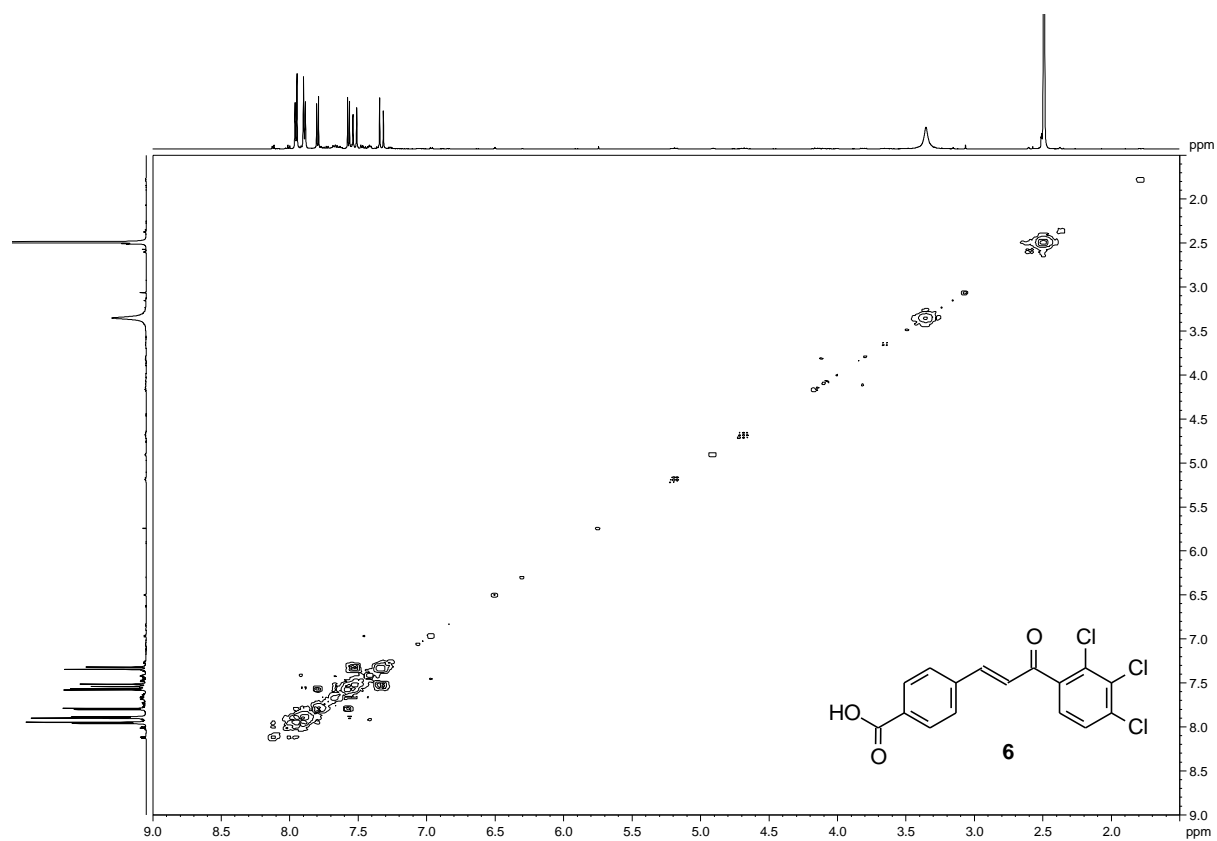


## DEPT90 in DMSO: 6

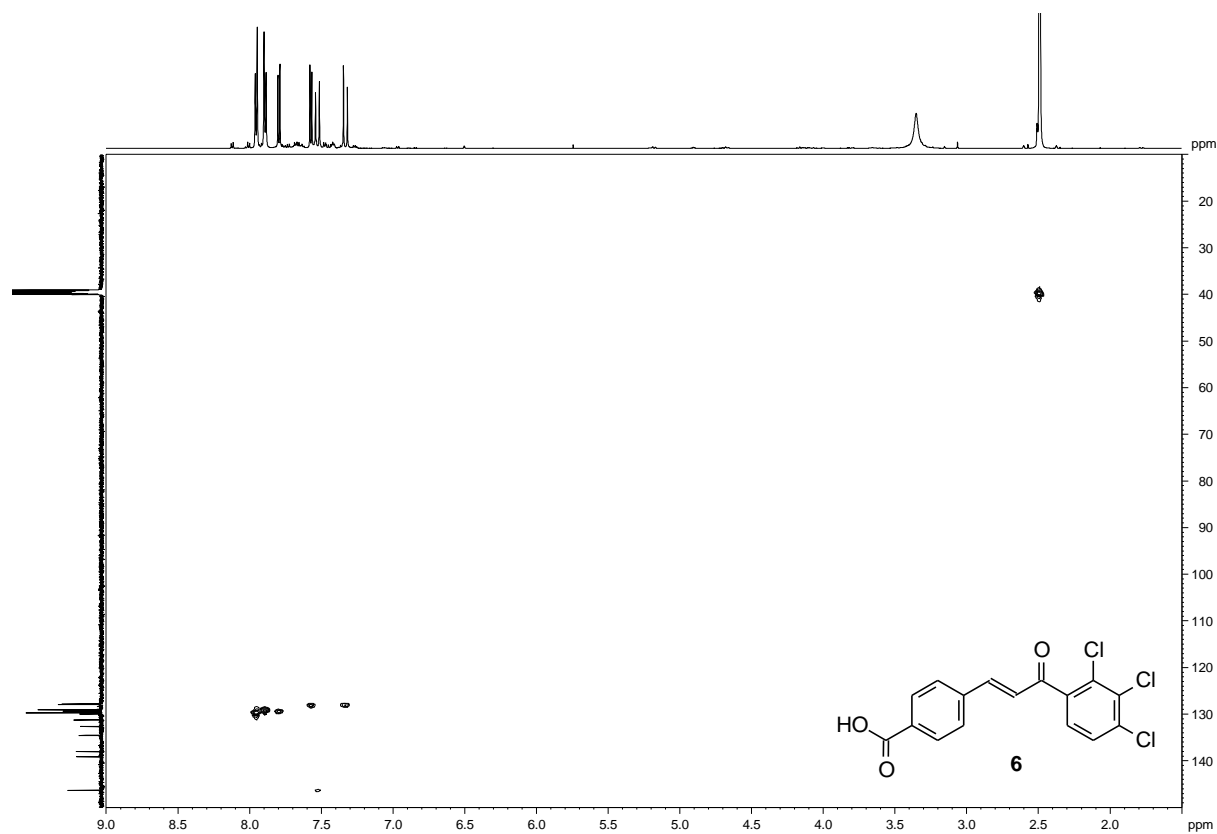


Addendum C – Chapter 5:

COSY in DMSO: **6**



HSCQ in DMSO: **6**

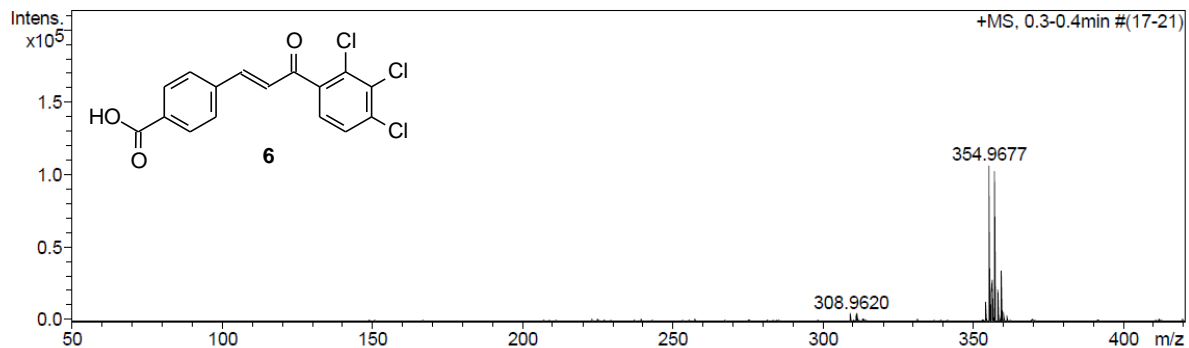


## Addendum C – Chapter 5:

### HRMS: 6

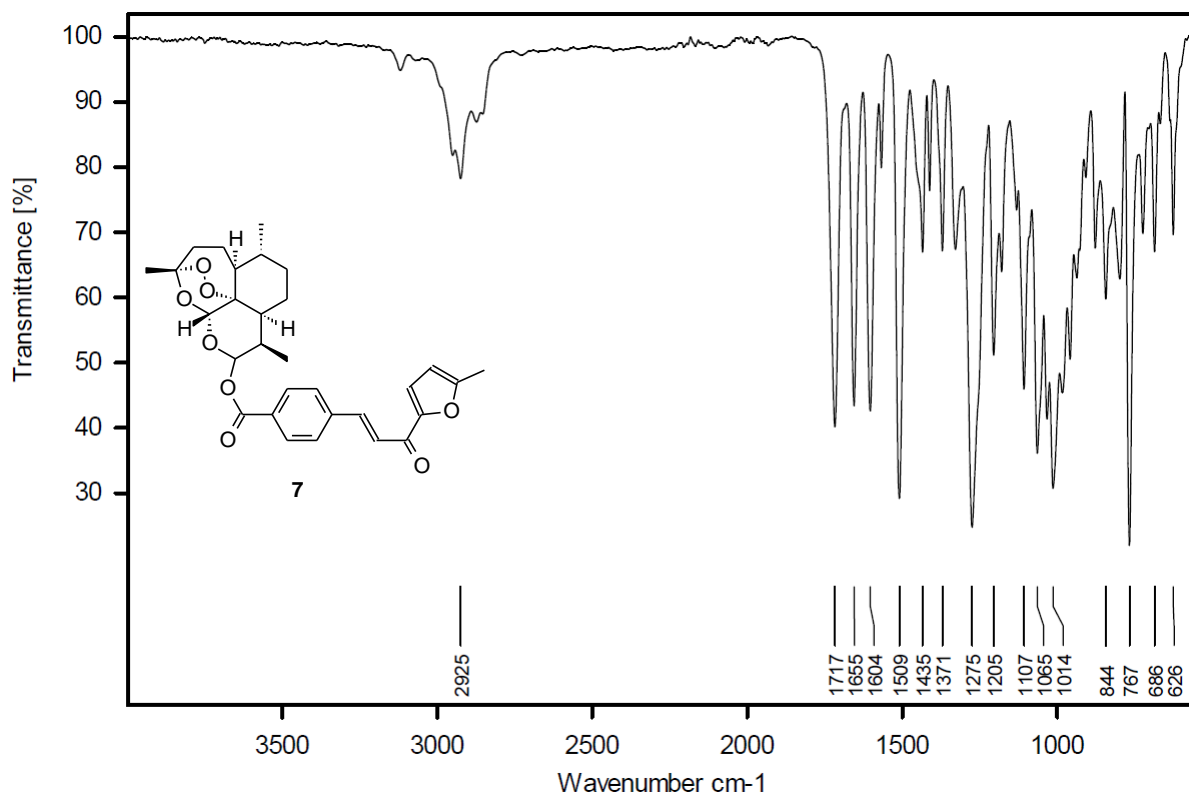
#### Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

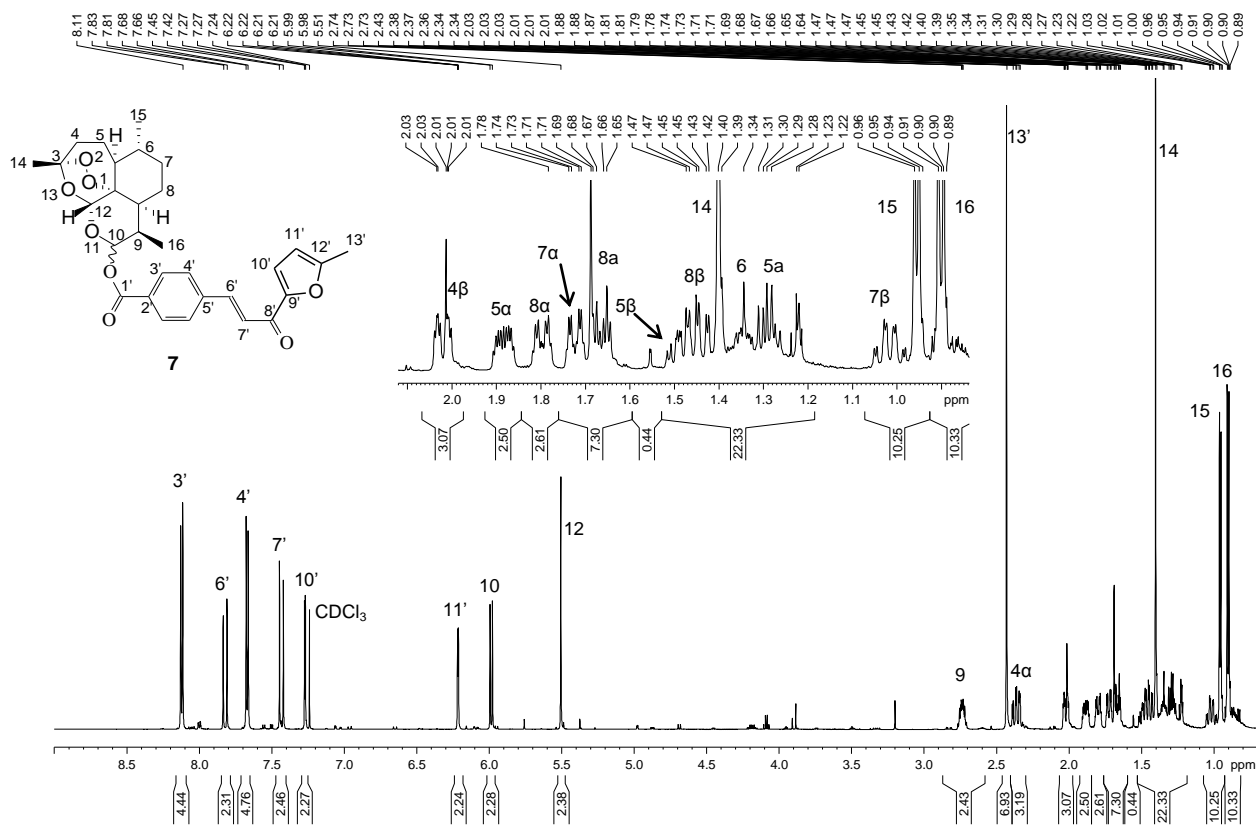


Addendum C – Chapter 5:

IR: 7

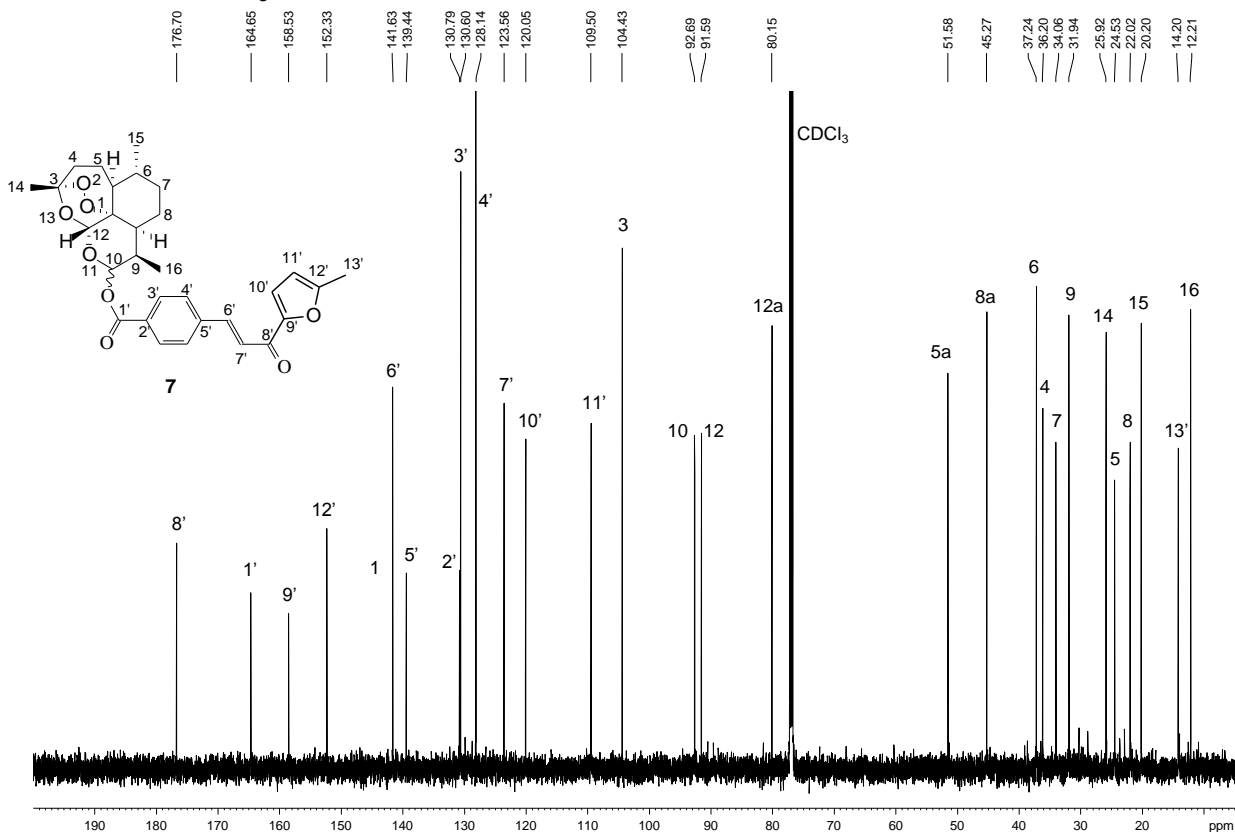


<sup>1</sup>H NMR in CDCl<sub>3</sub>: 7

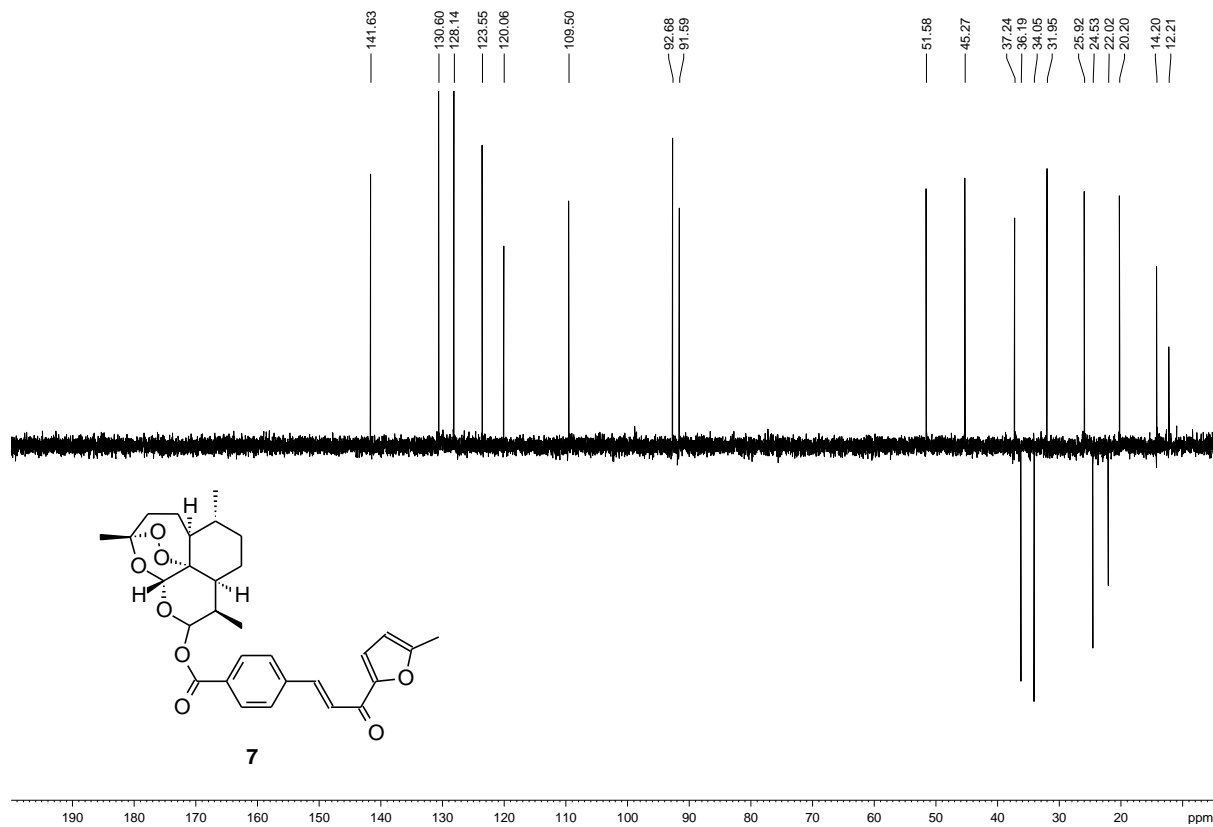


# Addendum C – Chapter 5:

## <sup>13</sup>C NMR in CDCl<sub>3</sub>: 7

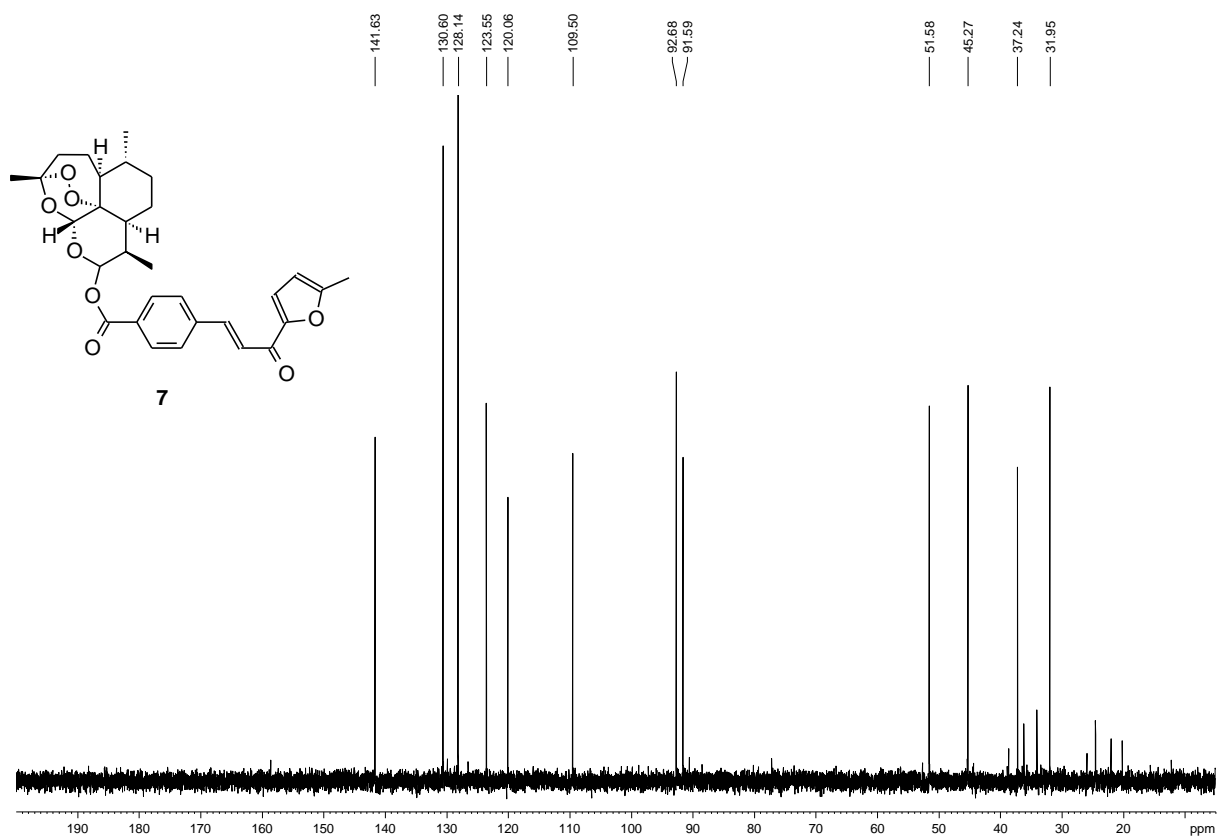


## DEPT135 in CDCl<sub>3</sub>: 7

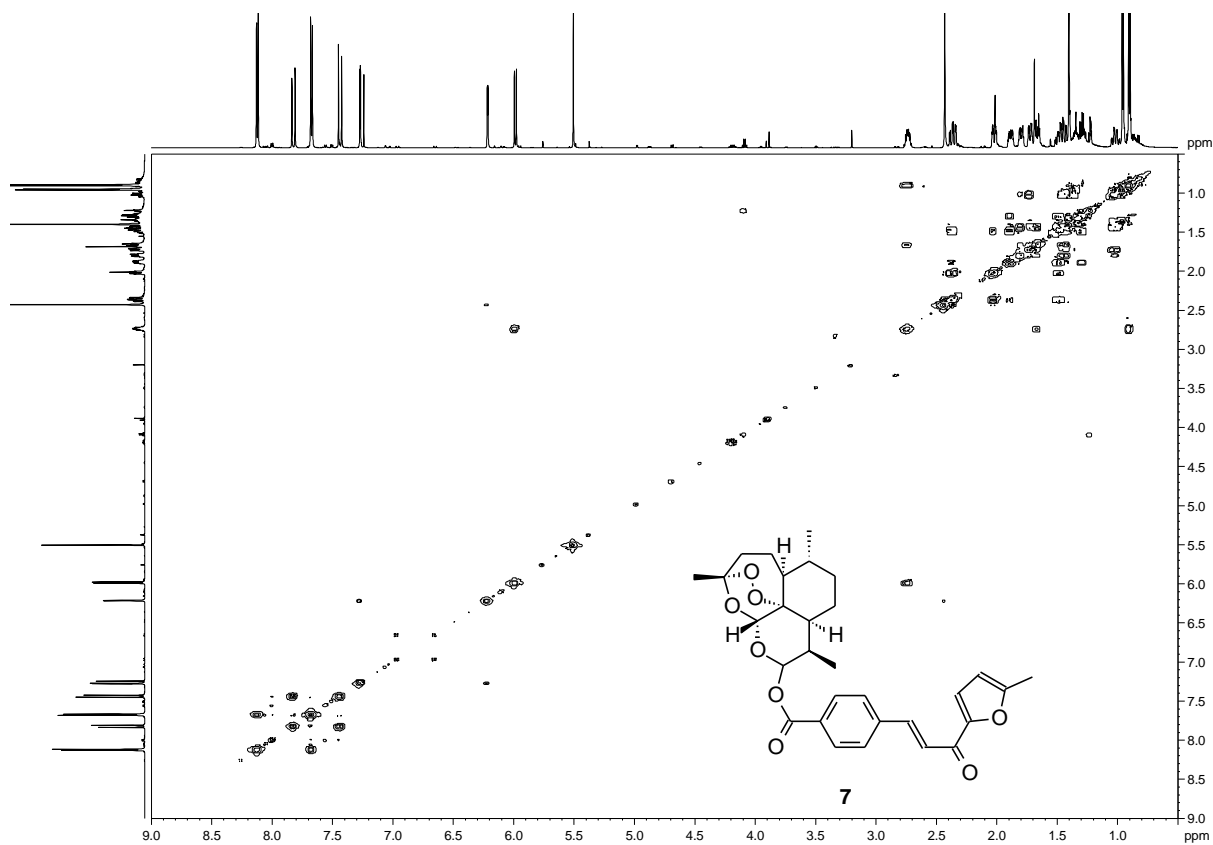


# Addendum C – Chapter 5:

## DEPT90 in CDCl<sub>3</sub>: 7

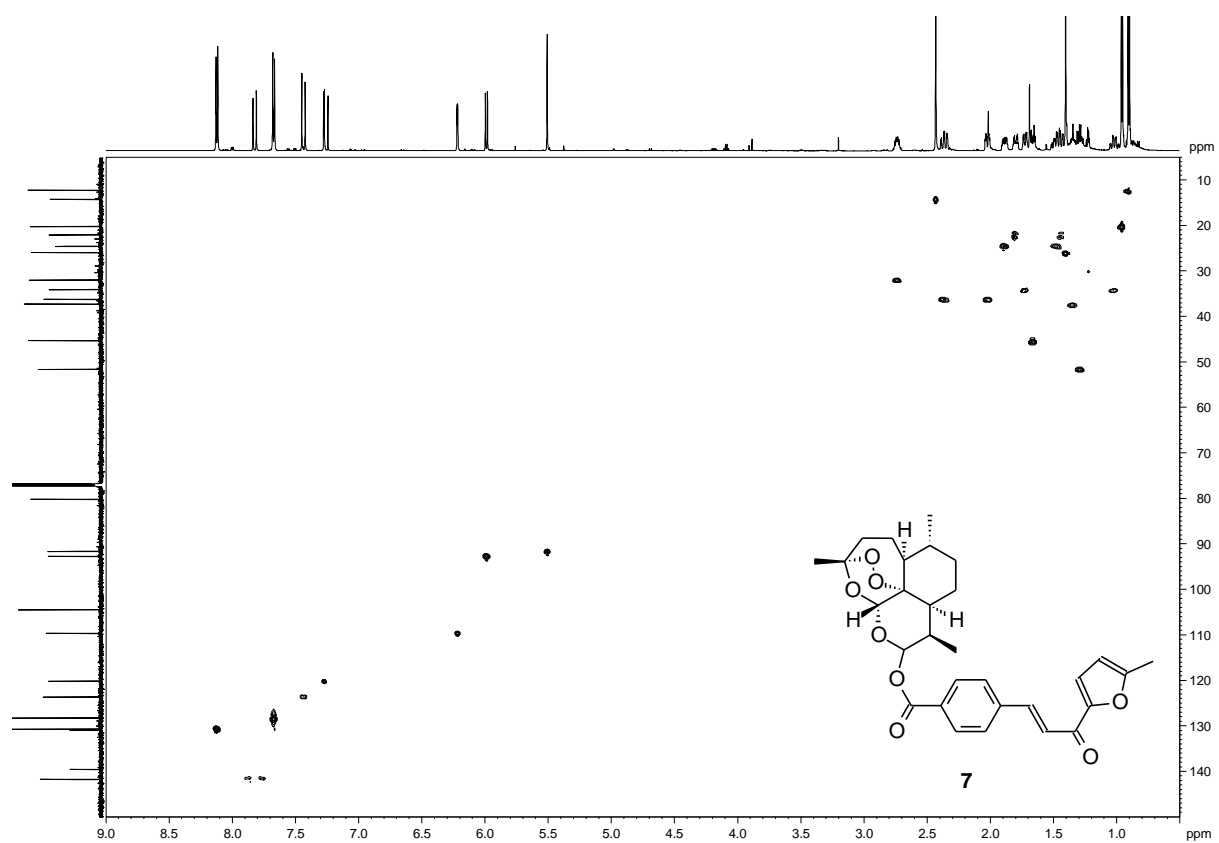


## COSY in CDCl<sub>3</sub>: 7



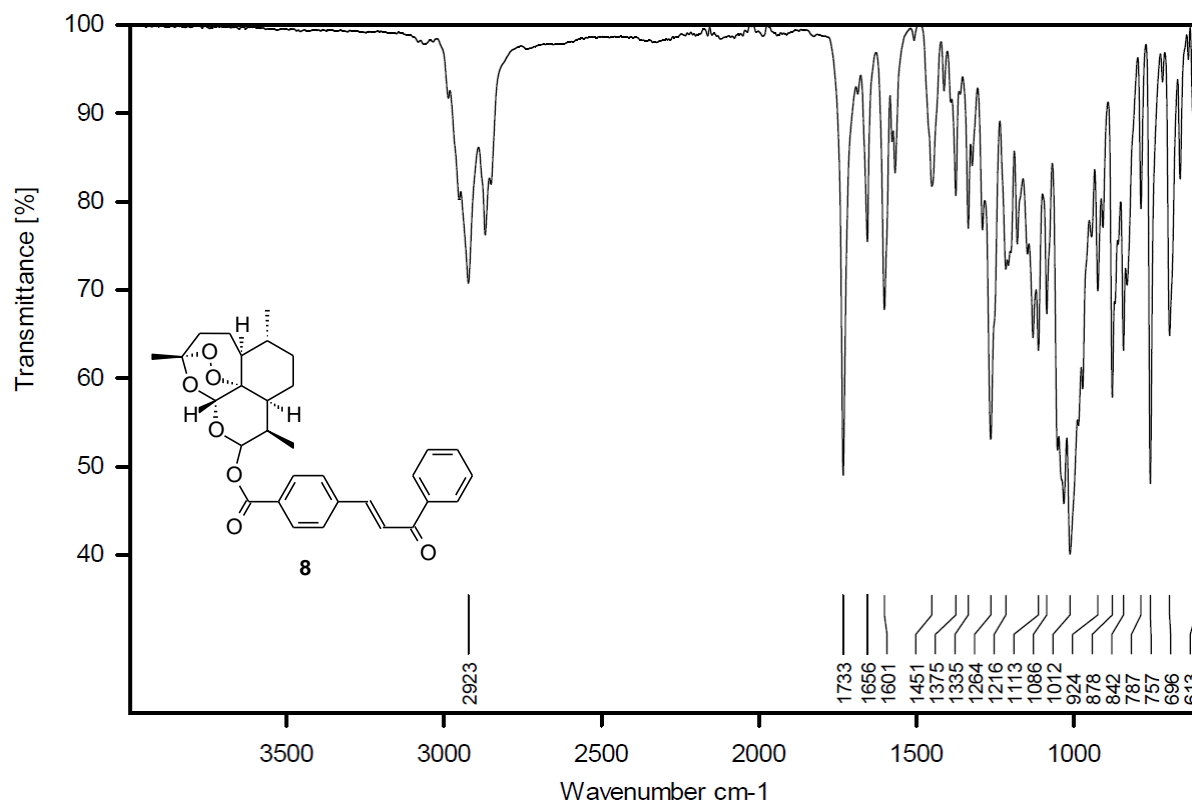
Addendum C – Chapter 5:

HSQC in CDCl<sub>3</sub>: 7

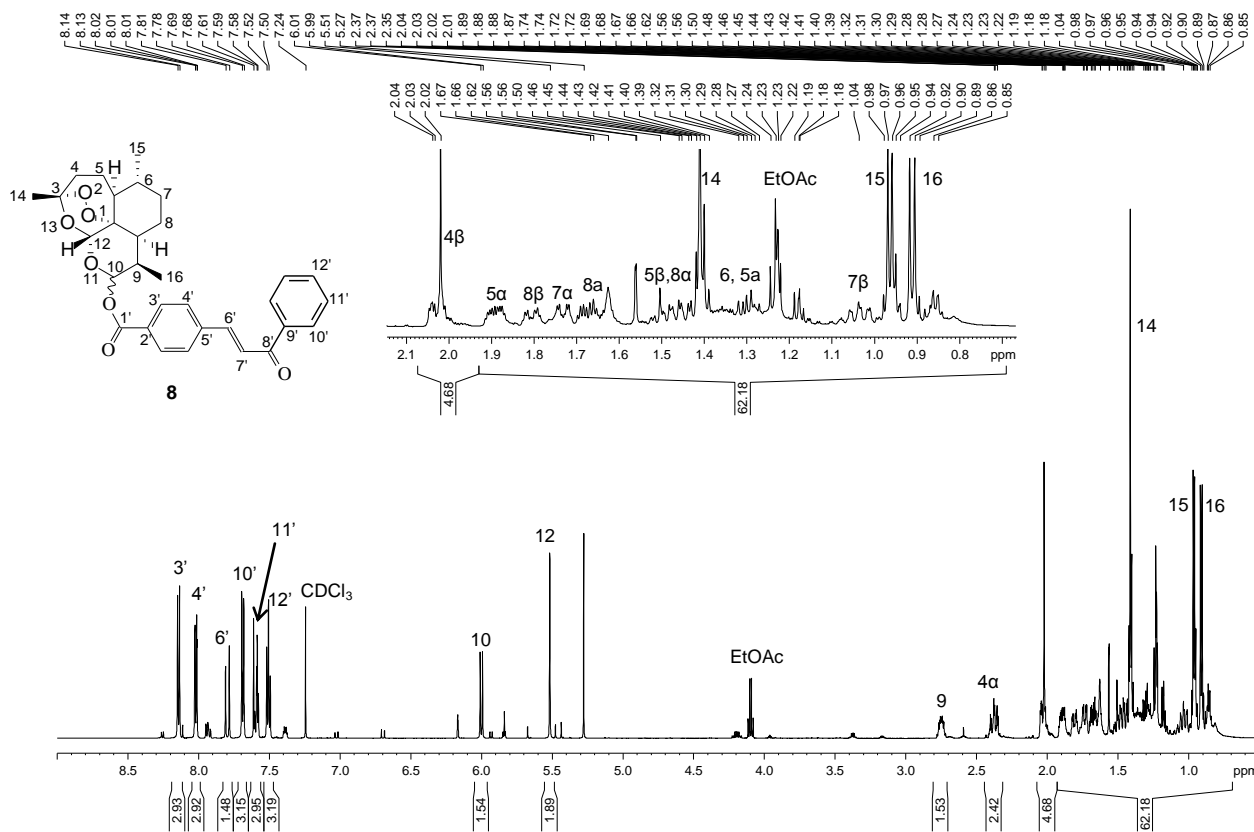


Addendum C – Chapter 5:

IR: 8

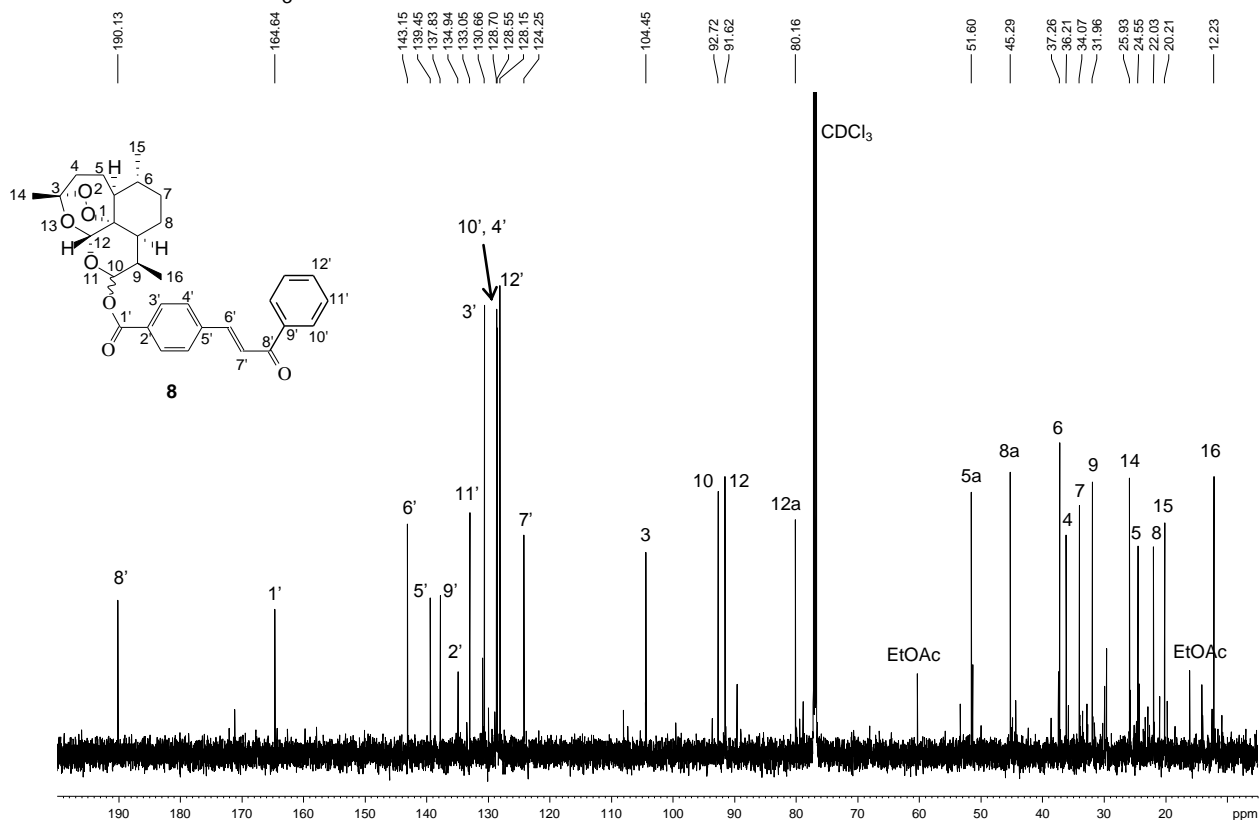


<sup>1</sup>H NMR in CDCl<sub>3</sub>: 8

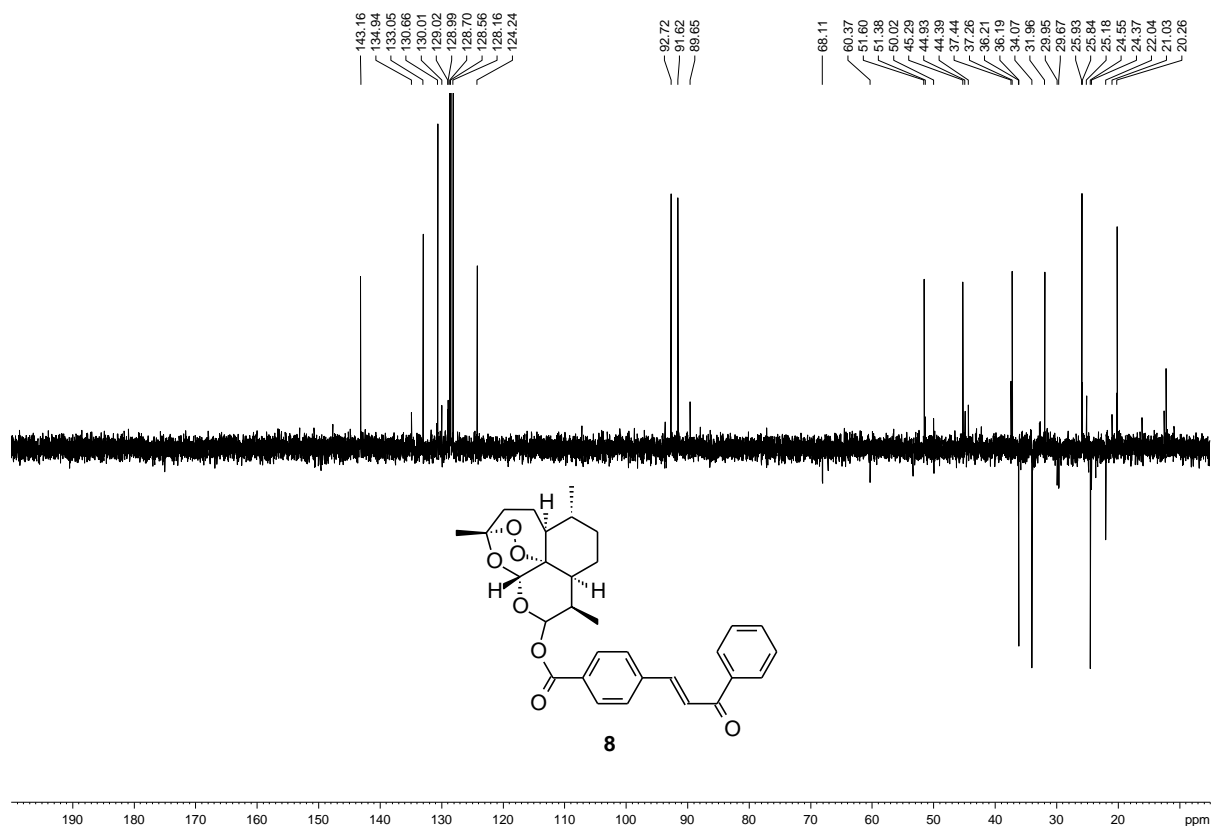


# Addendum C – Chapter 5:

## <sup>13</sup>C NMR in CDCl<sub>3</sub>: 8

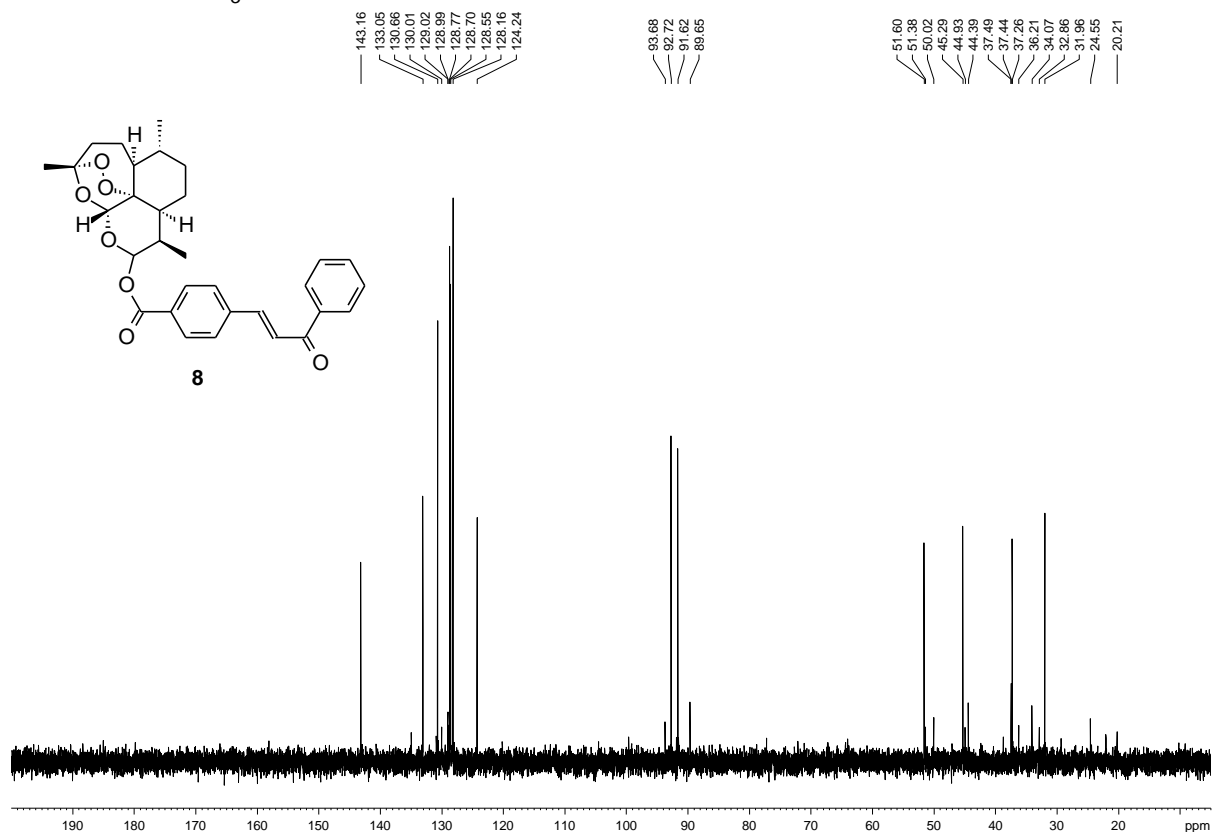


## DEPT135 in CDCl<sub>3</sub>: 8

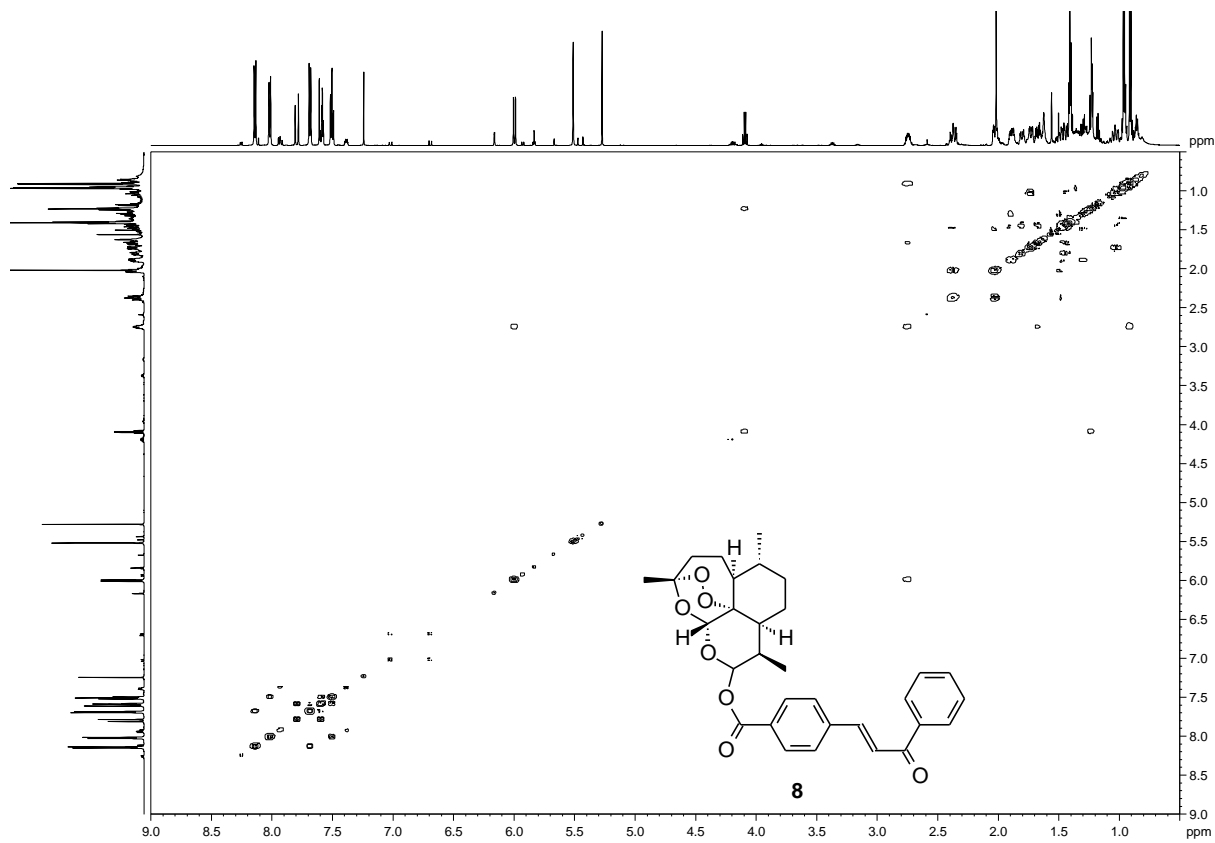


Addendum C – Chapter 5:

DEPT90 in CDCl<sub>3</sub>: **8**

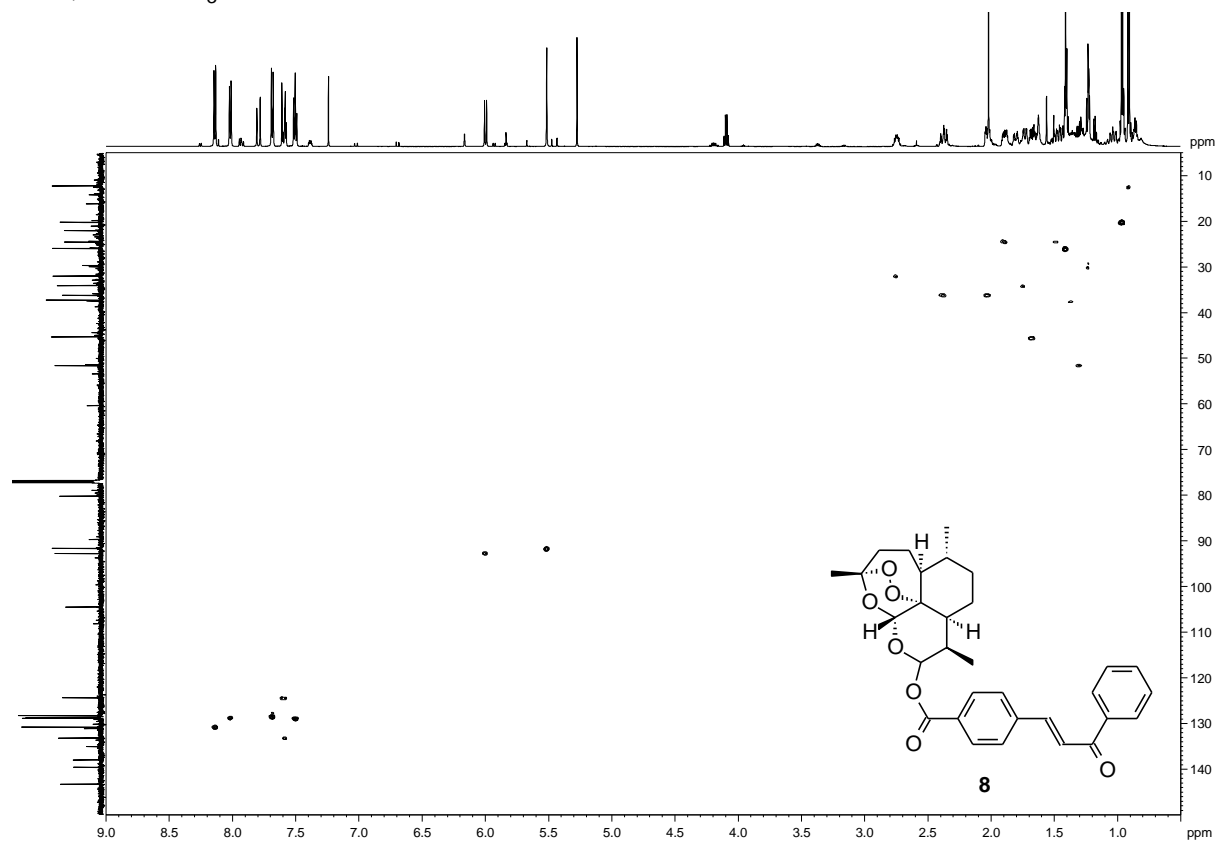


COSY in CDCl<sub>3</sub>: **8**



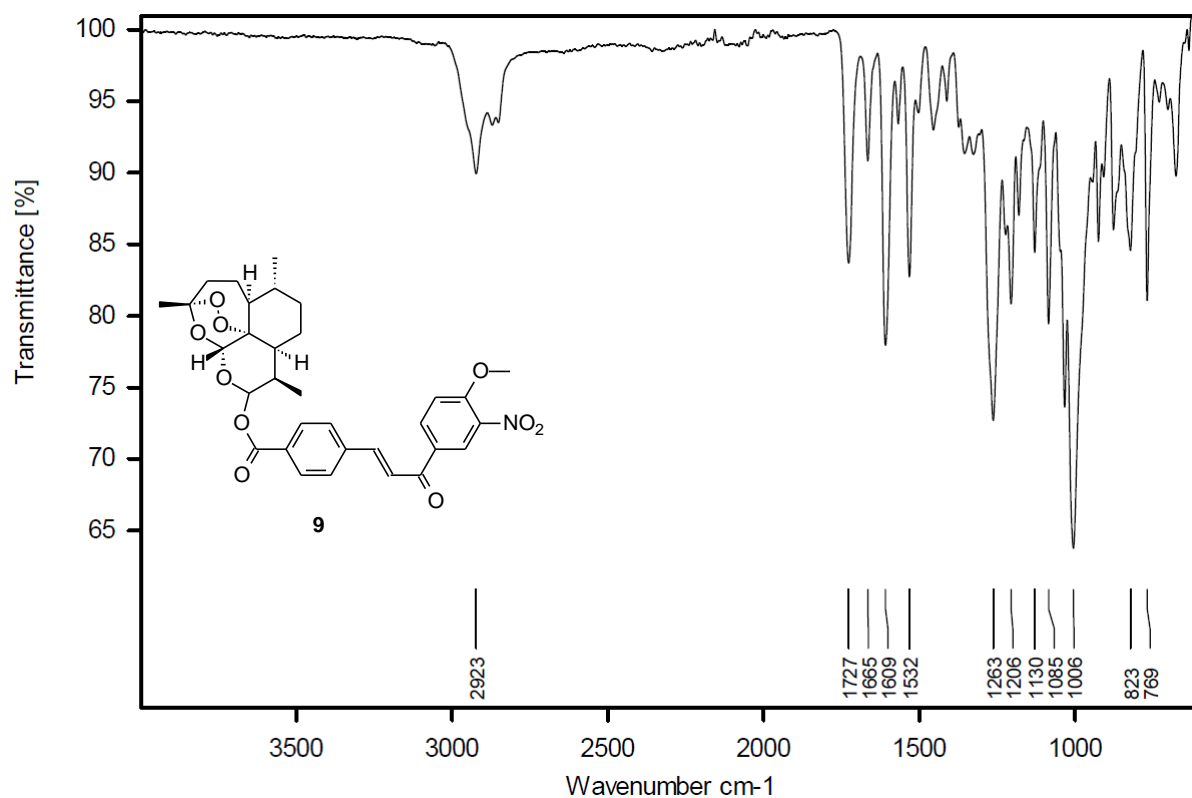
Addendum C – Chapter 5:

HSQC in CDCl<sub>3</sub>: **8**

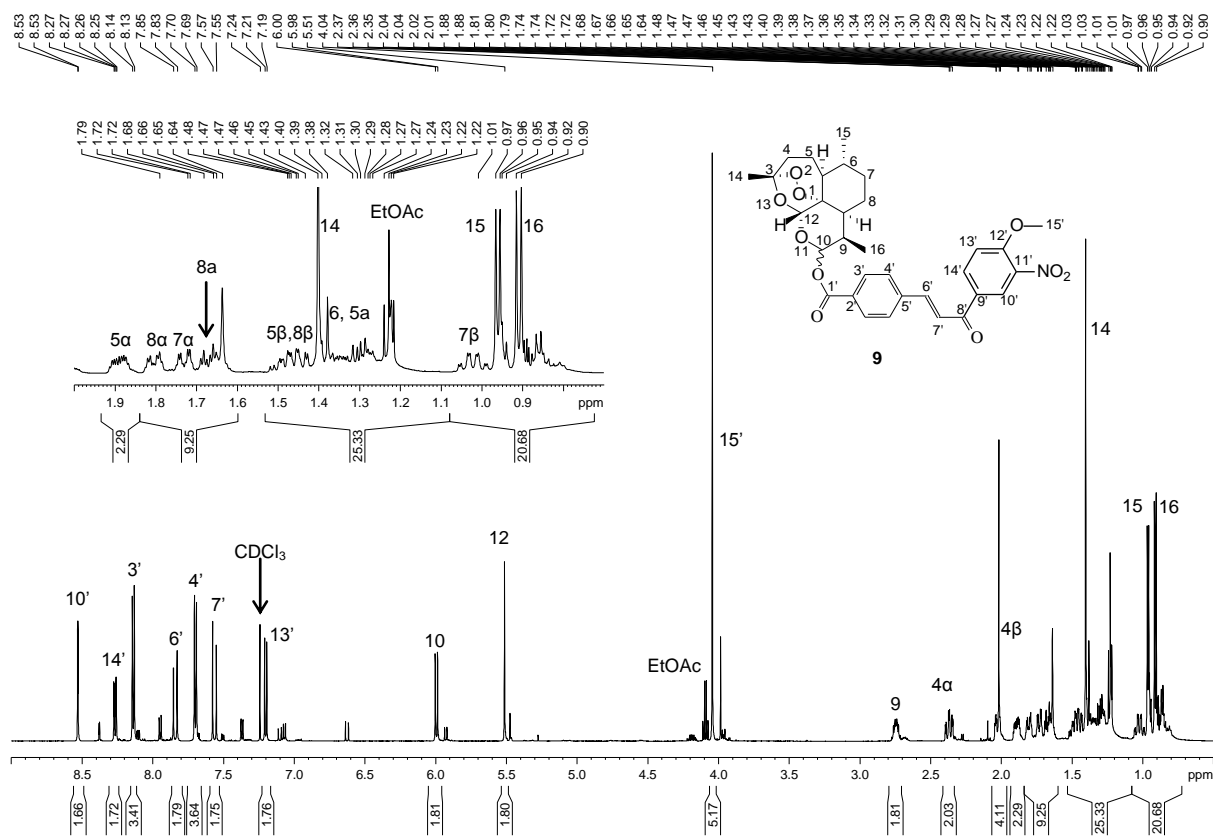


Addendum C – Chapter 5:

IR: 9

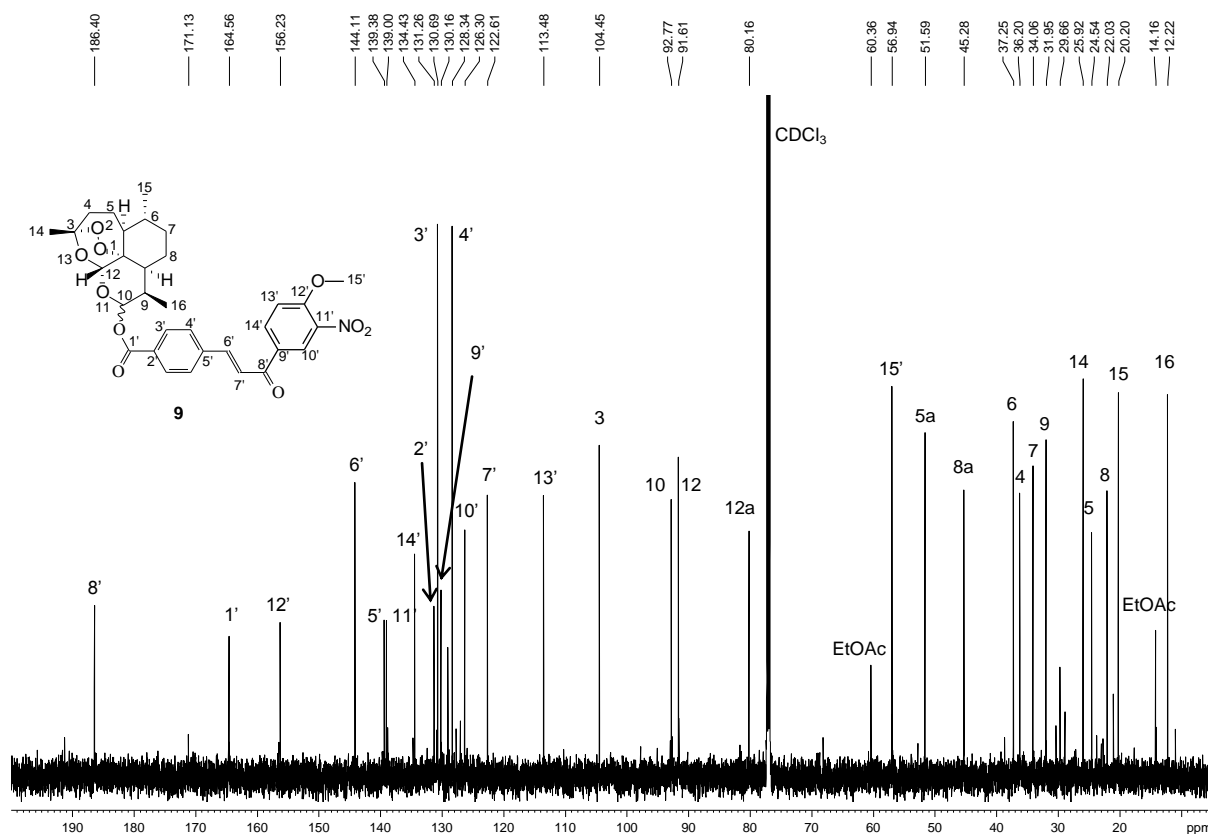


<sup>1</sup>H NMR in CDCl<sub>3</sub>: 9

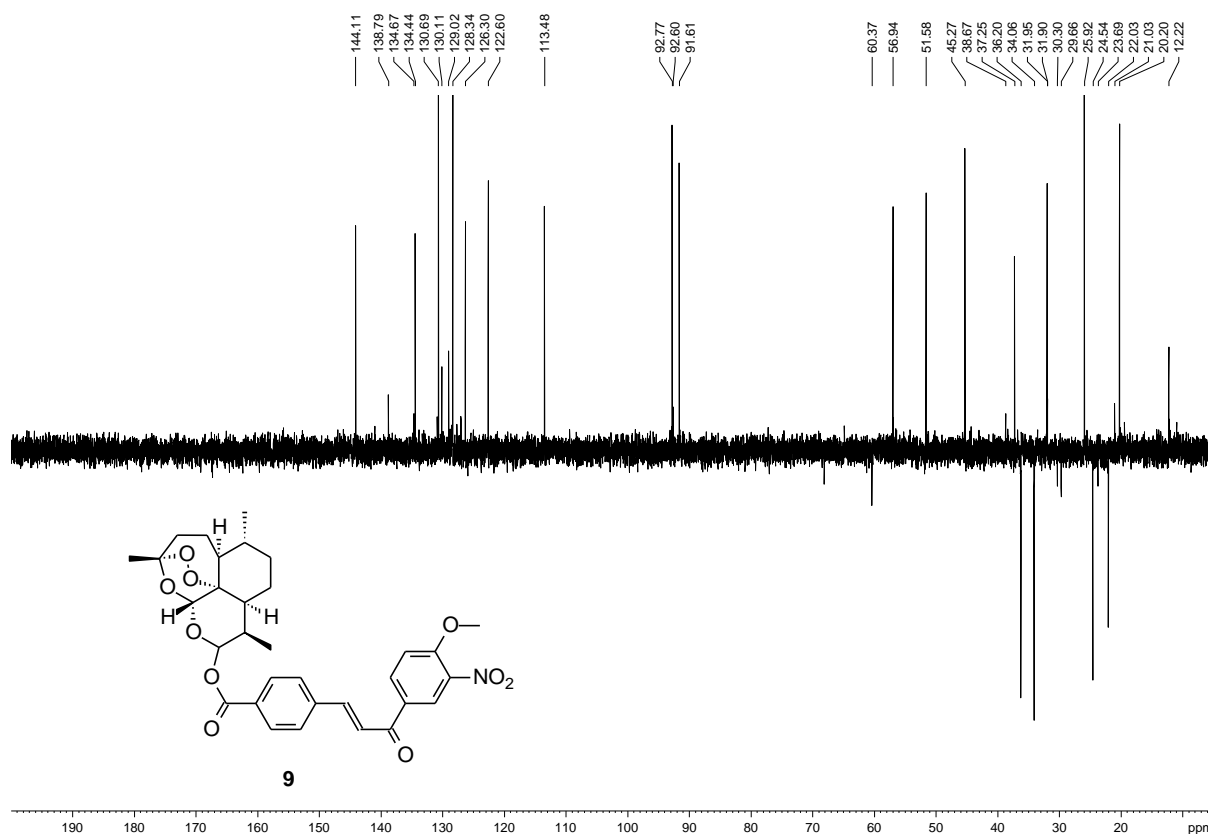


# Addendum C – Chapter 5:

## <sup>13</sup>C NMR in CDCl<sub>3</sub>: 9

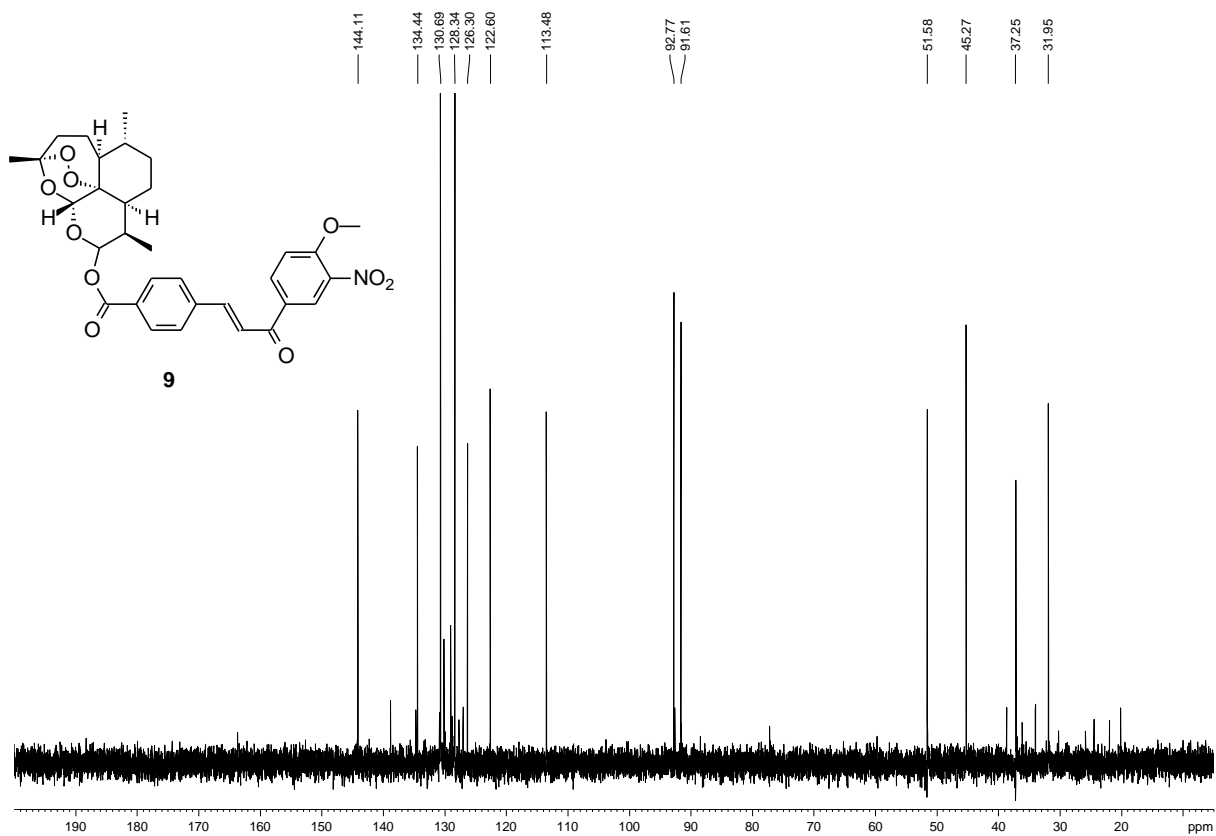


## DEPT135 in CDCl<sub>3</sub>: 9

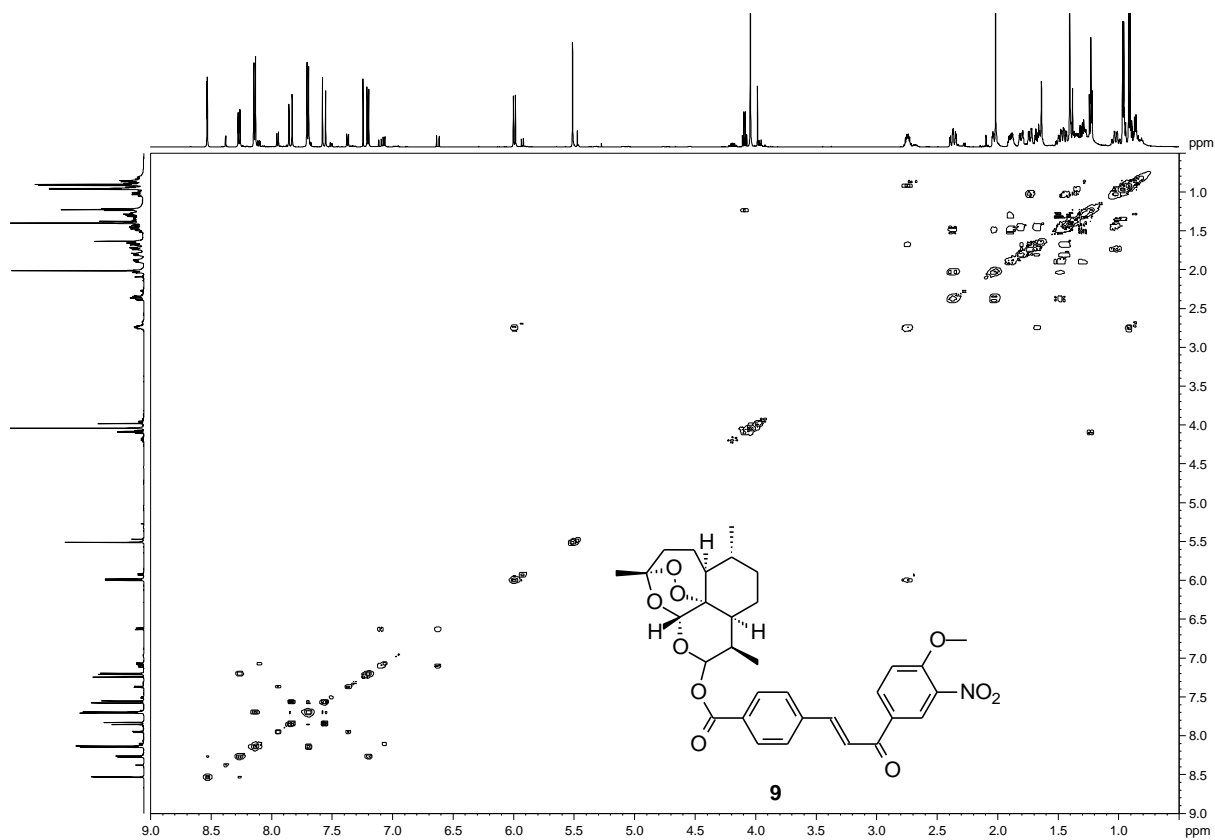


# Addendum C – Chapter 5:

## DEPT90 in CDCl<sub>3</sub>: **9**

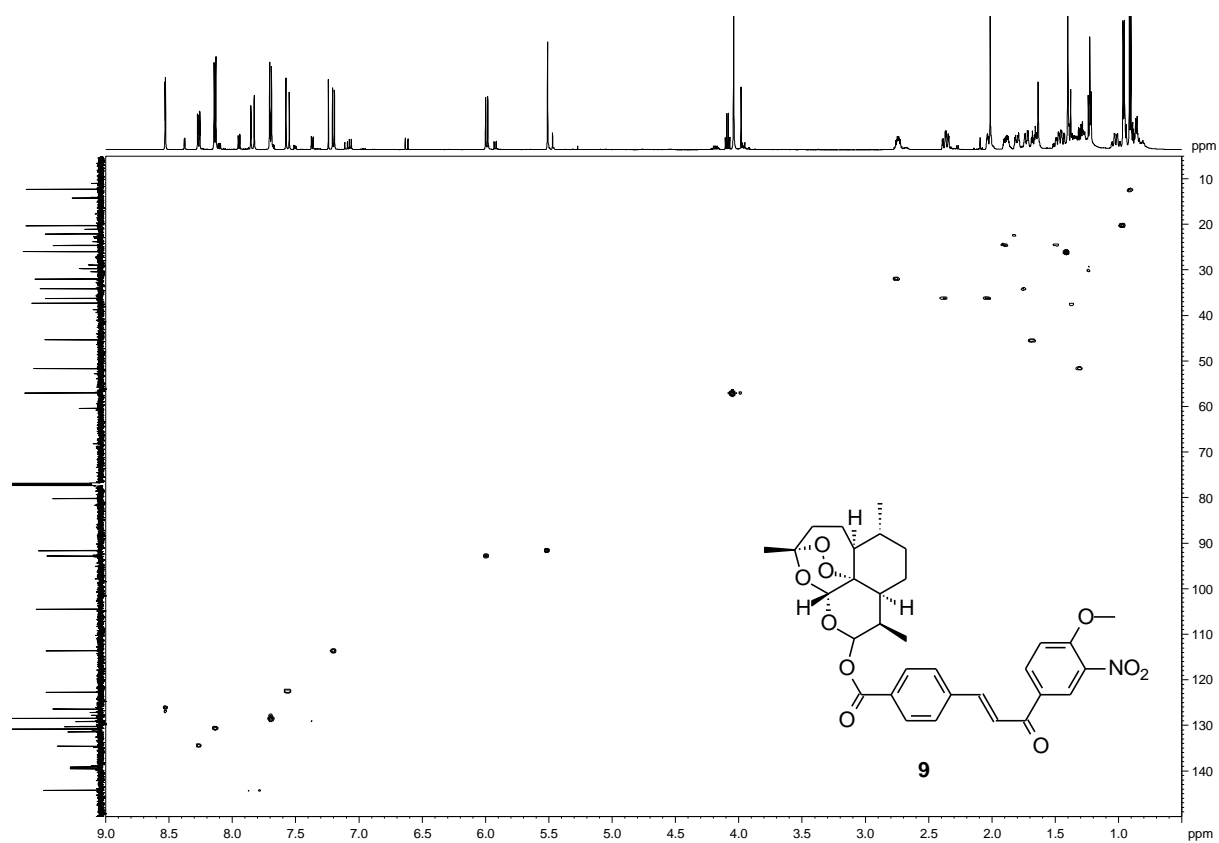


## COSY in CDCl<sub>3</sub>: **9**



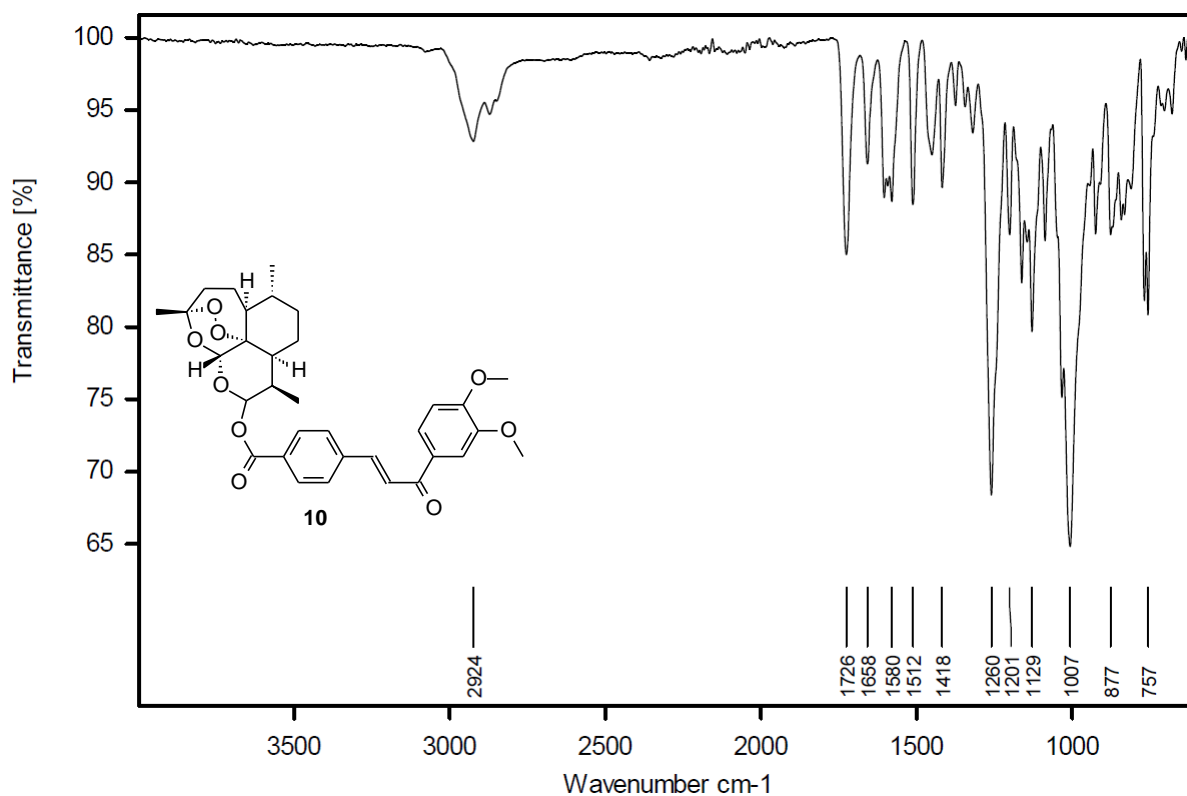
Addendum C – Chapter 5:

HSQC in CDCl<sub>3</sub>: **9**

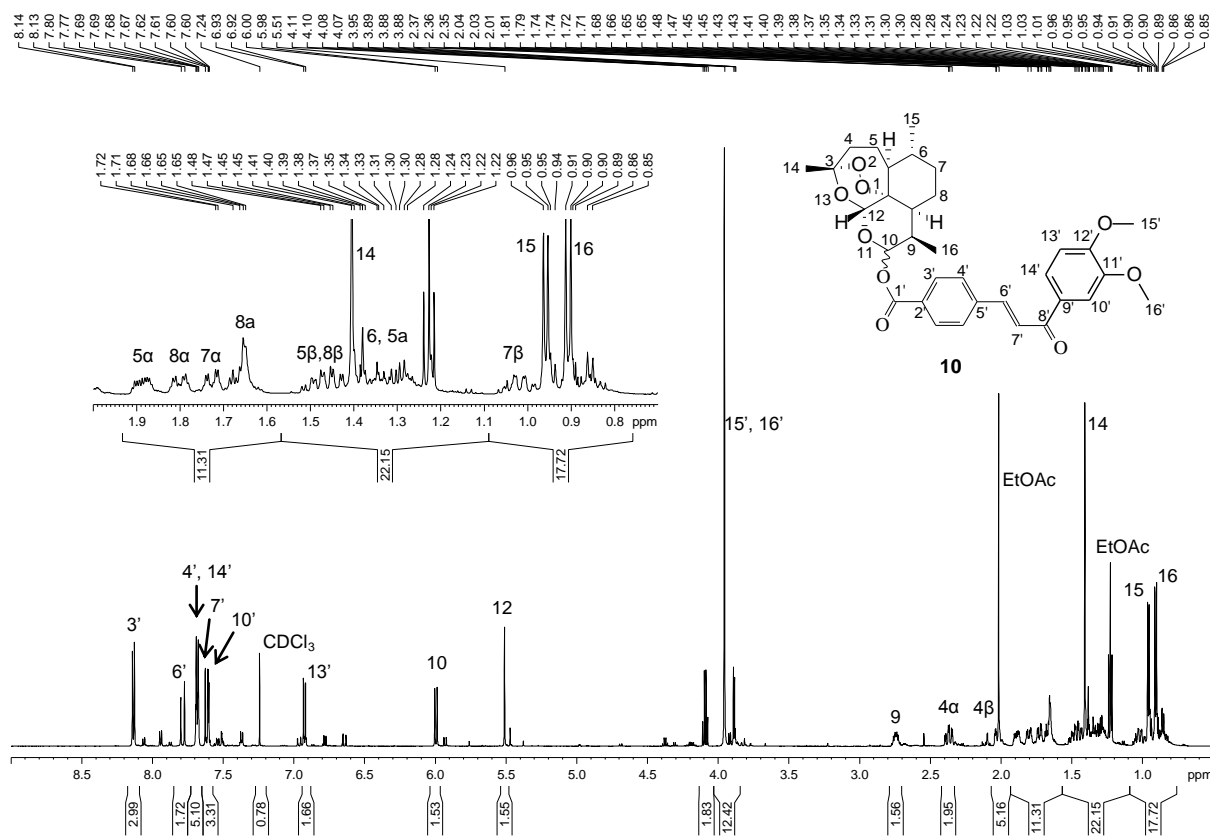


Addendum C – Chapter 5:

IR: 10

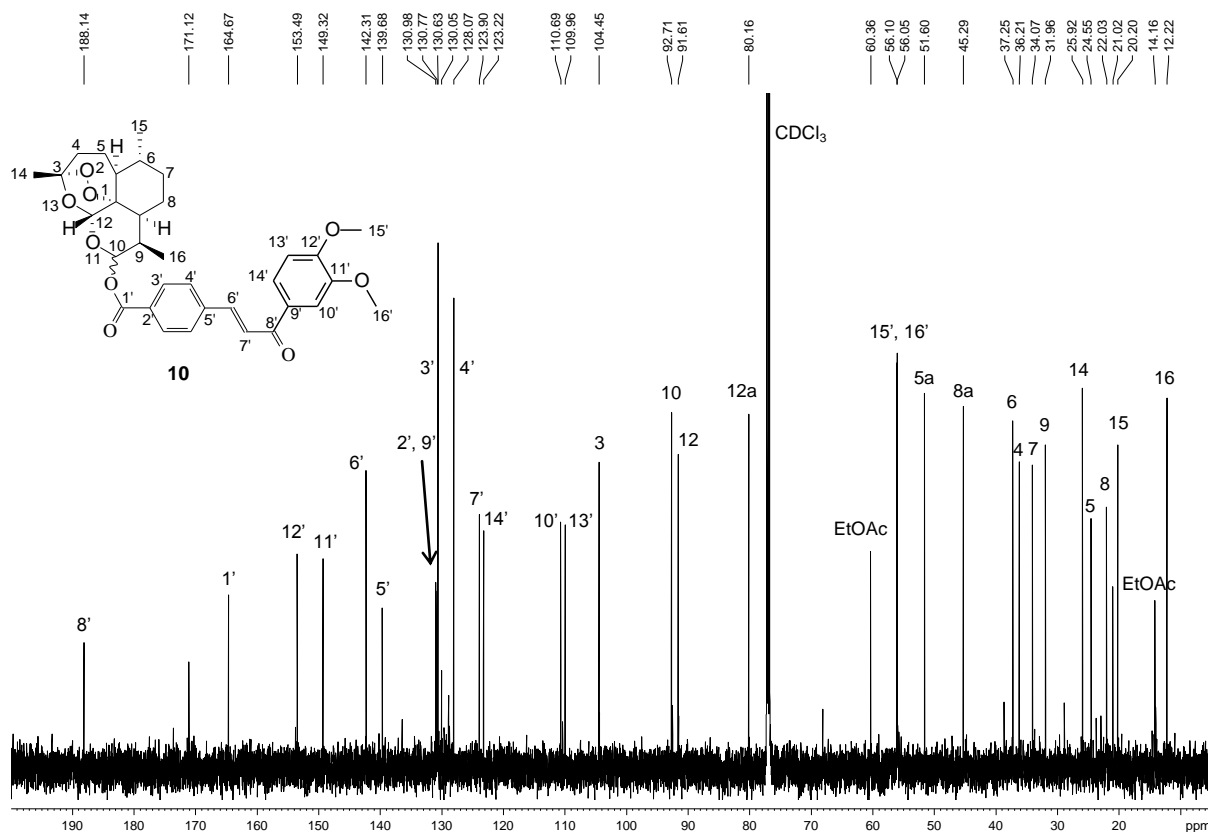


<sup>1</sup>H NMR in CDCl<sub>3</sub>: 10

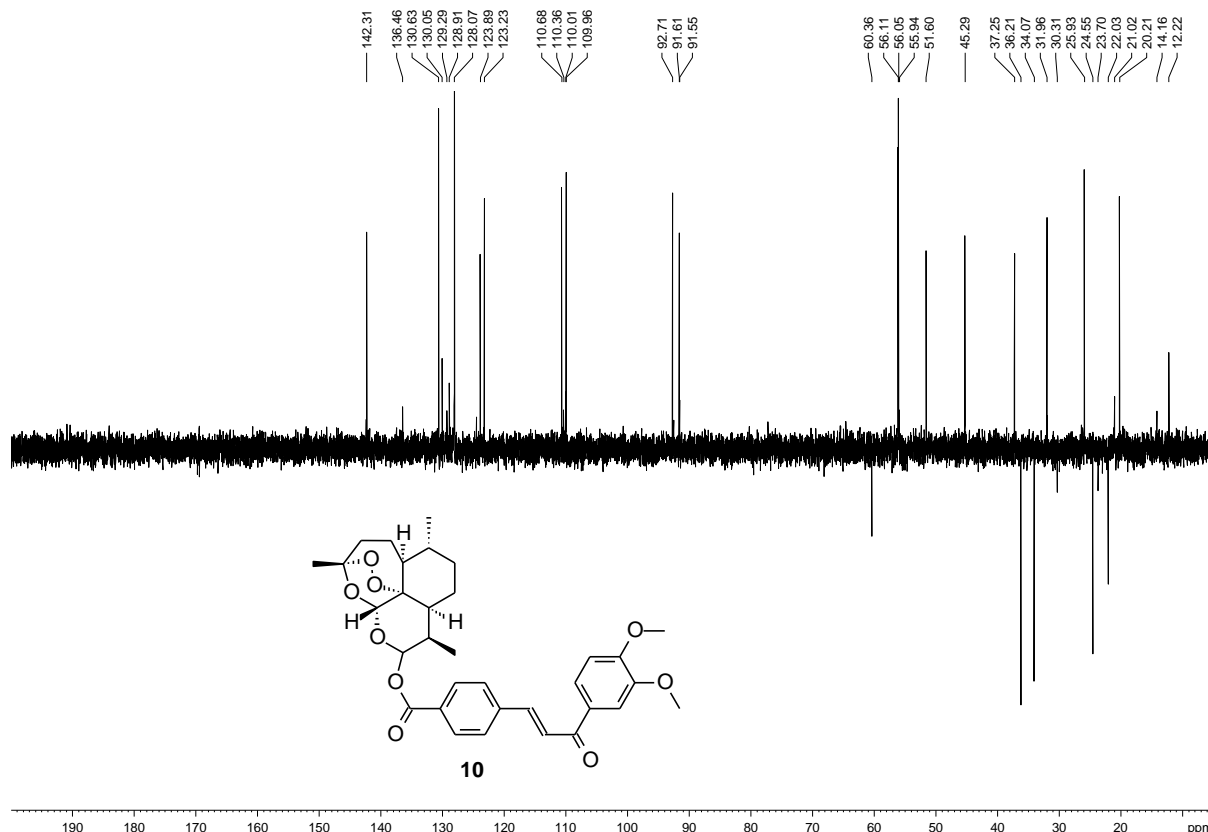


# Addendum C – Chapter 5:

## <sup>13</sup>C NMR in CDCl<sub>3</sub>: 10

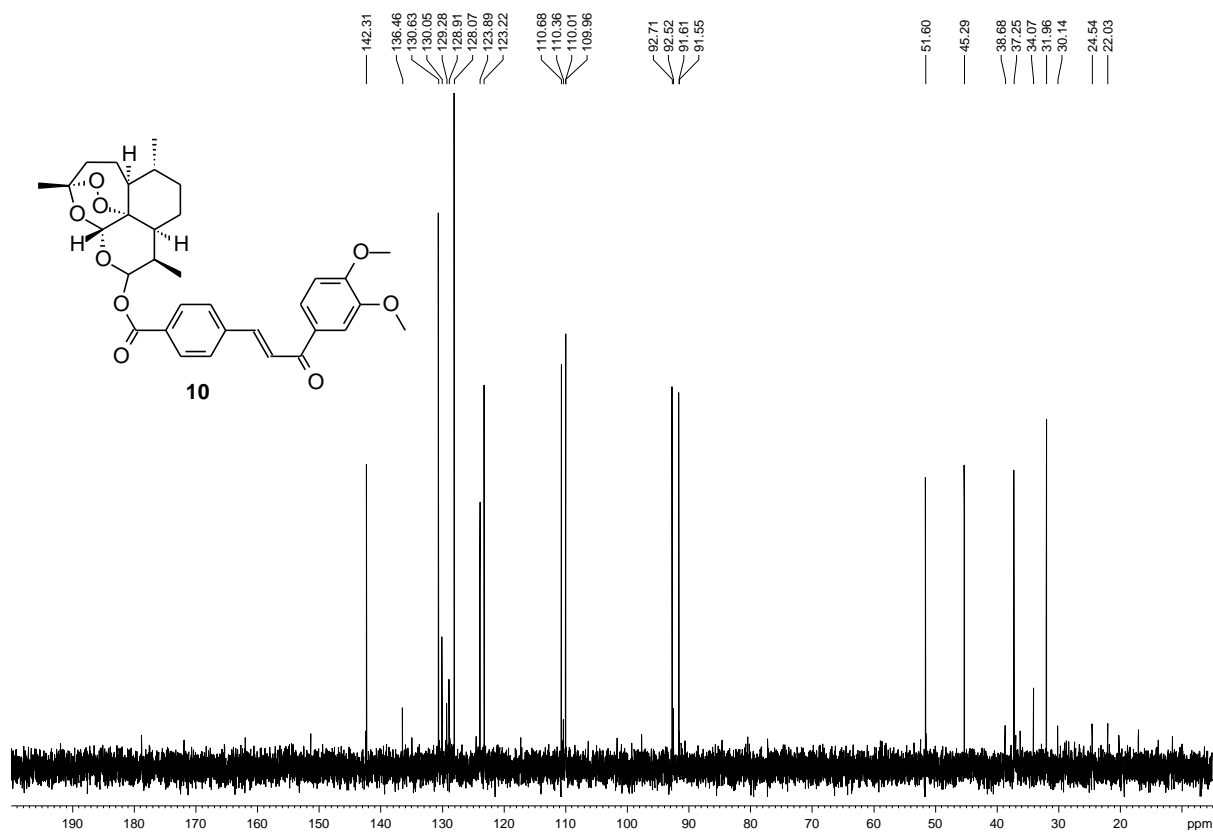


## DEPT135 in CDCl<sub>3</sub>: 10

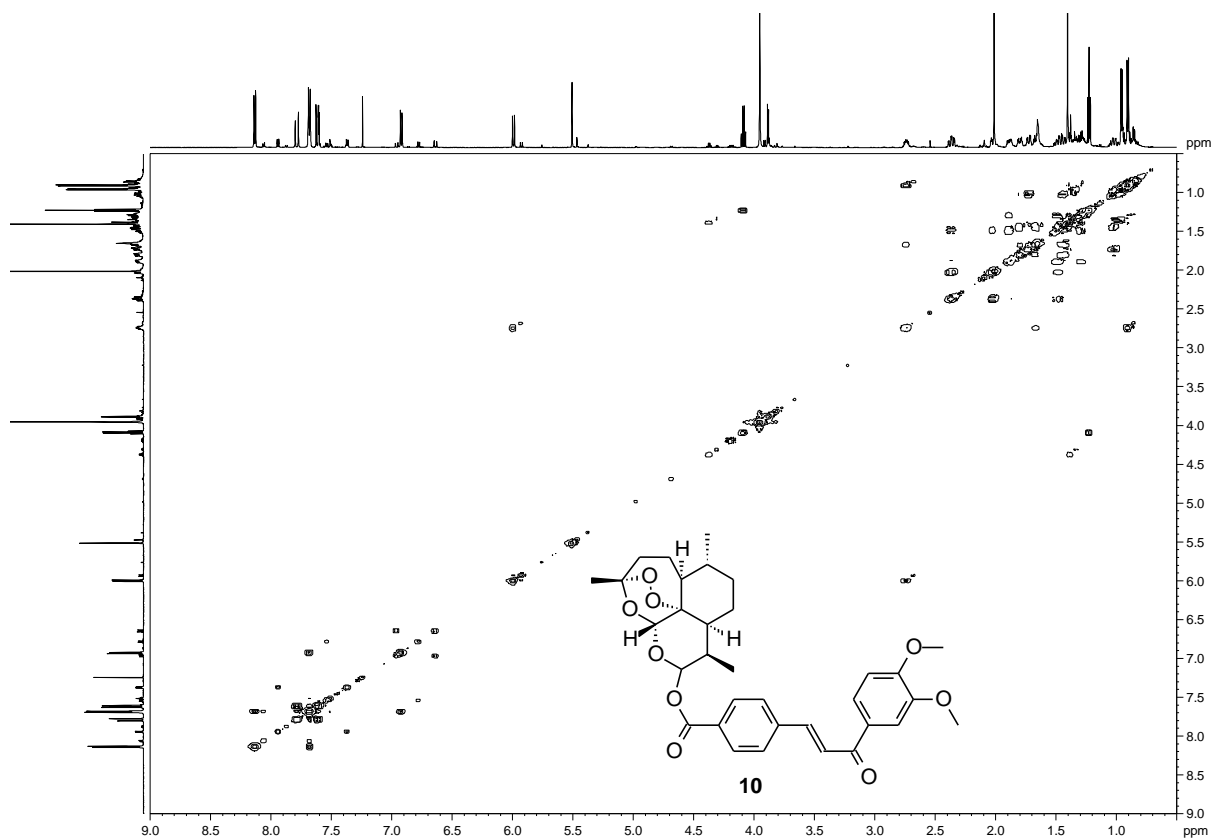


Addendum C – Chapter 5:

DEPT90 in CDCl<sub>3</sub>: **10**

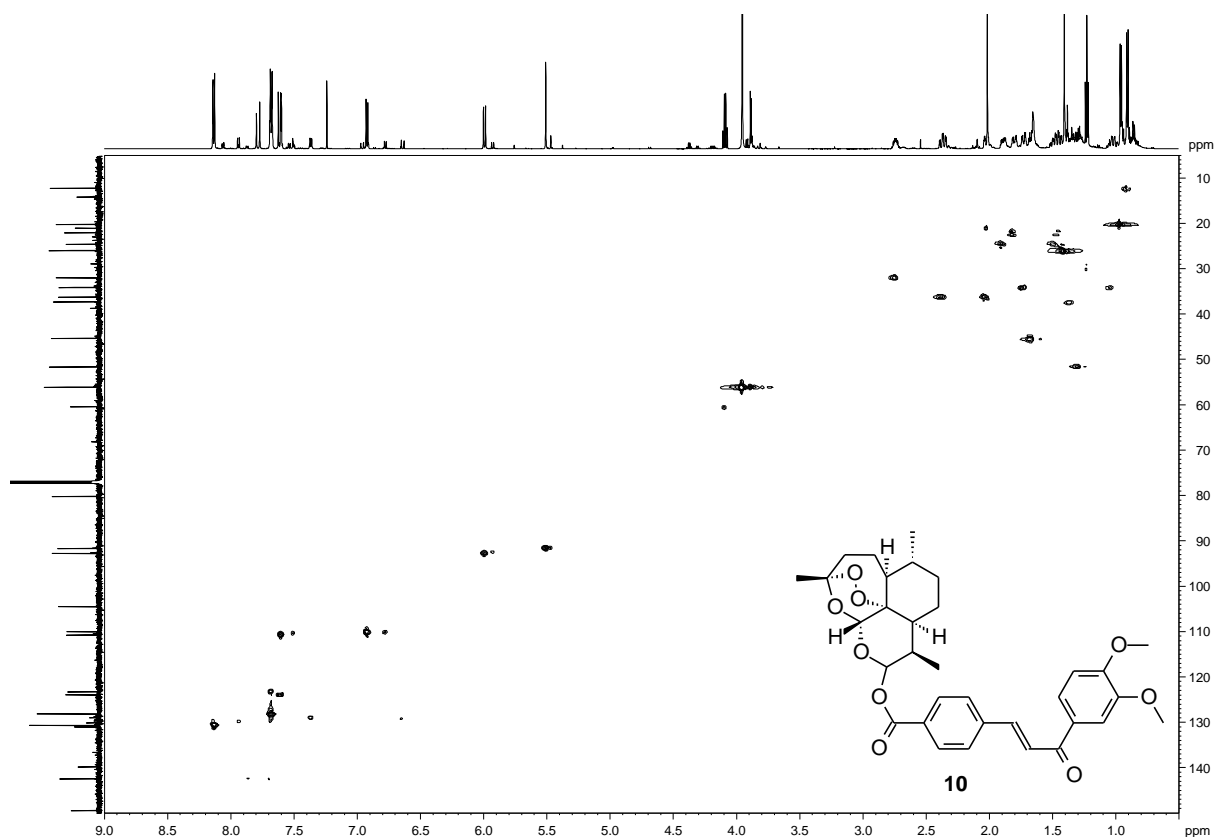


COSY in CDCl<sub>3</sub>: **10**



## Addendum C – Chapter 5:

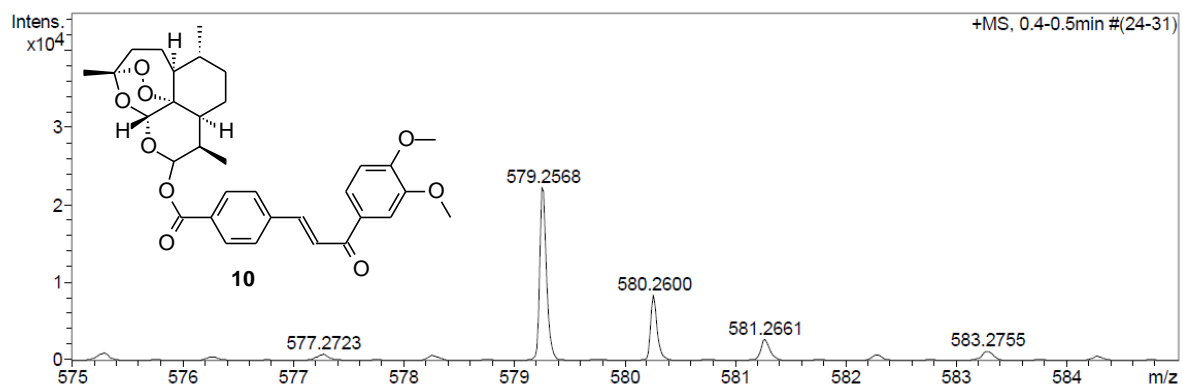
HSQC in CDCl<sub>3</sub>: **10**



HRMS: **10**

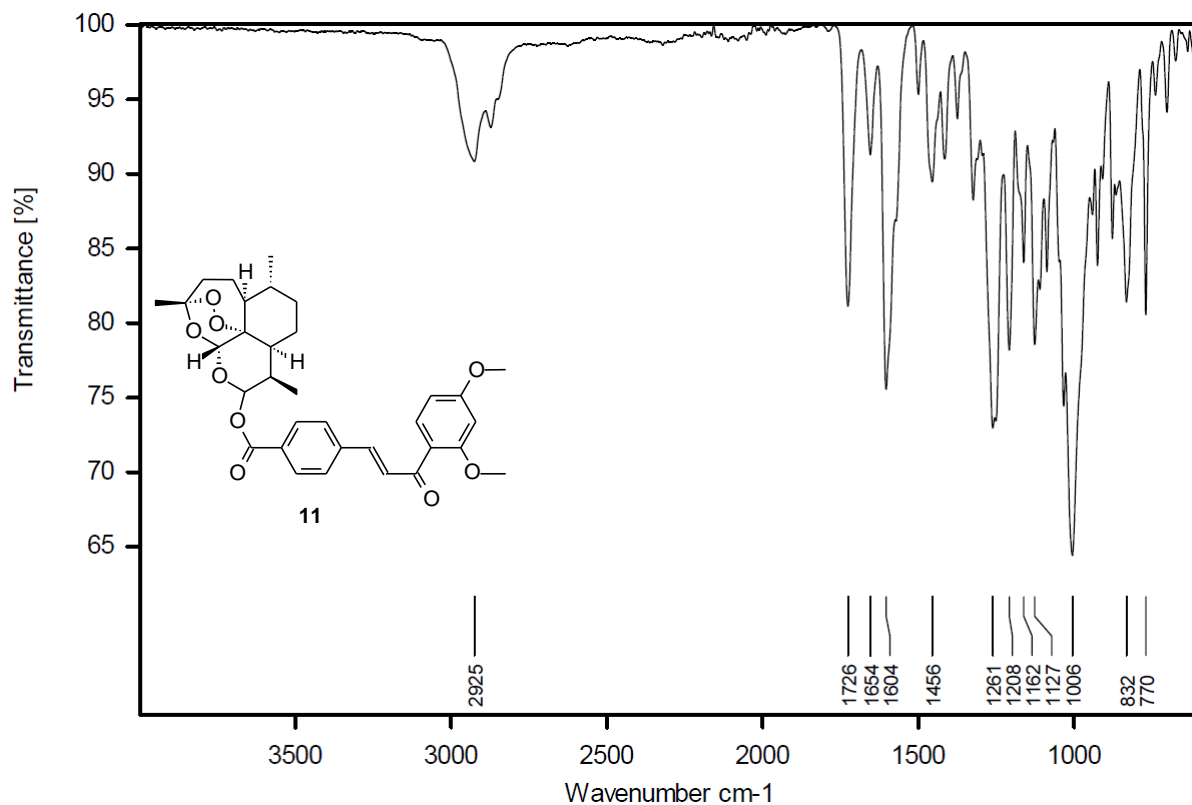
### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste

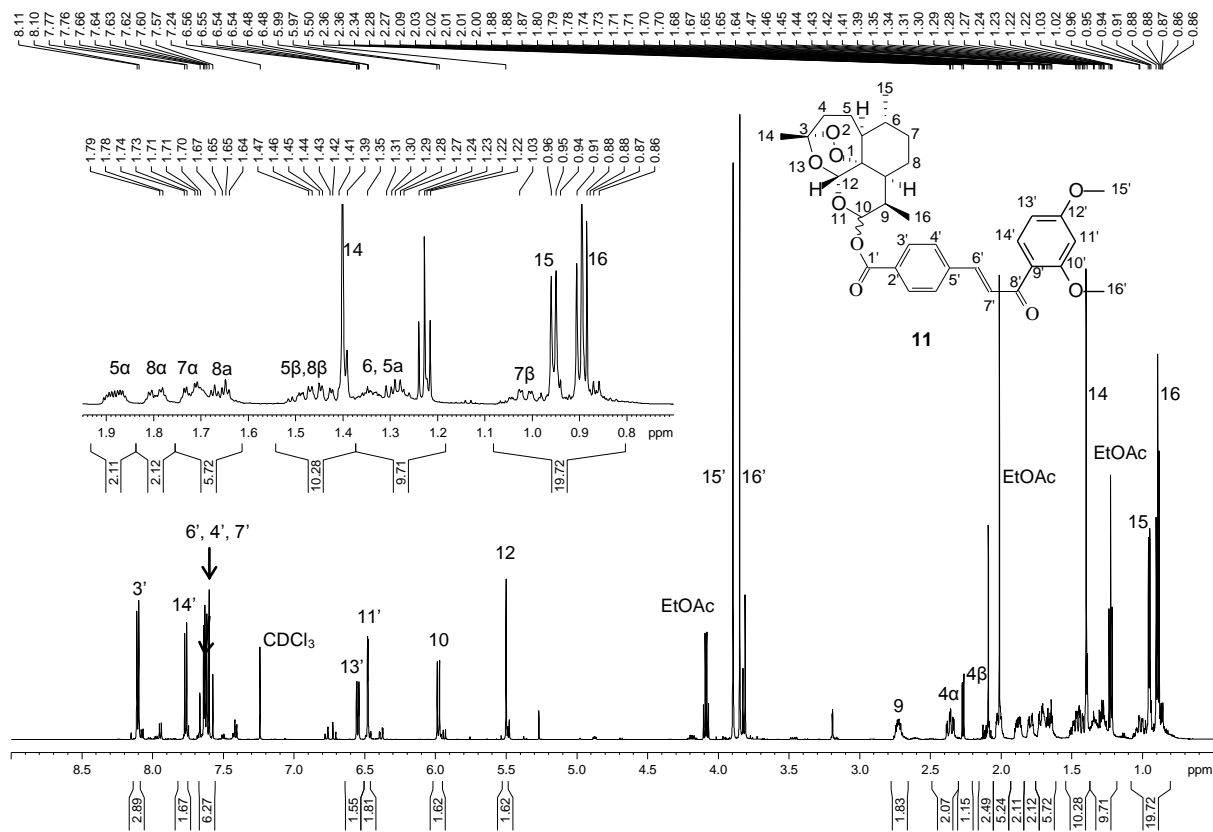


Addendum C – Chapter 5:

IR: 11

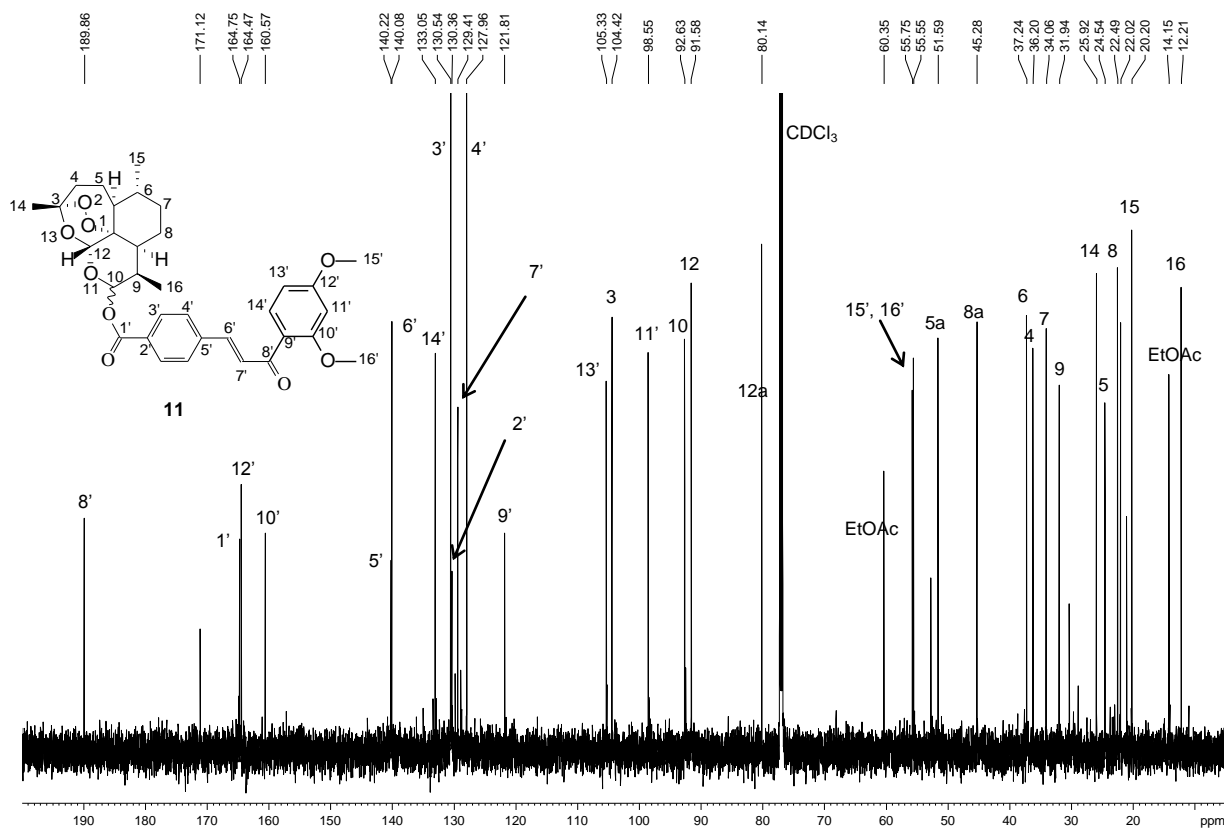


<sup>1</sup>H NMR in CDCl<sub>3</sub>: 11

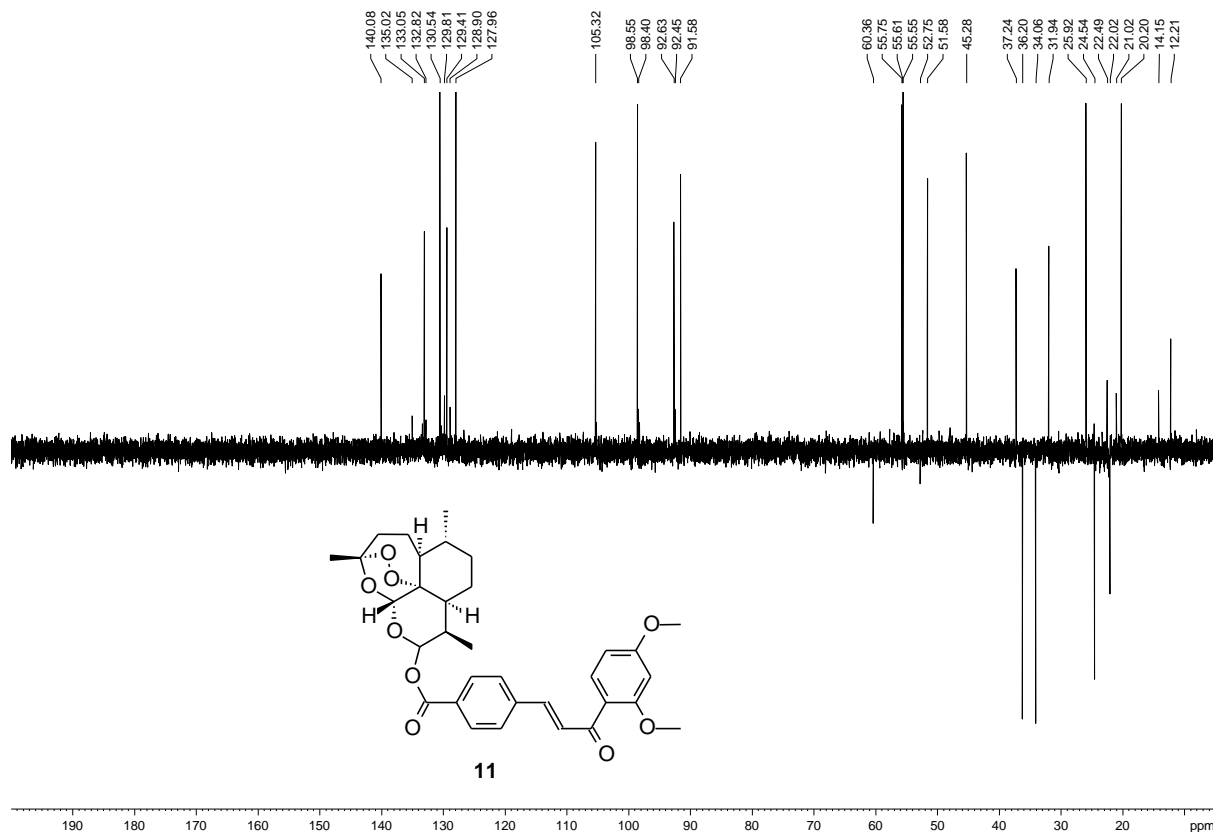


# Addendum C – Chapter 5:

## $^{13}\text{C}$ in $\text{CDCl}_3$ : 11

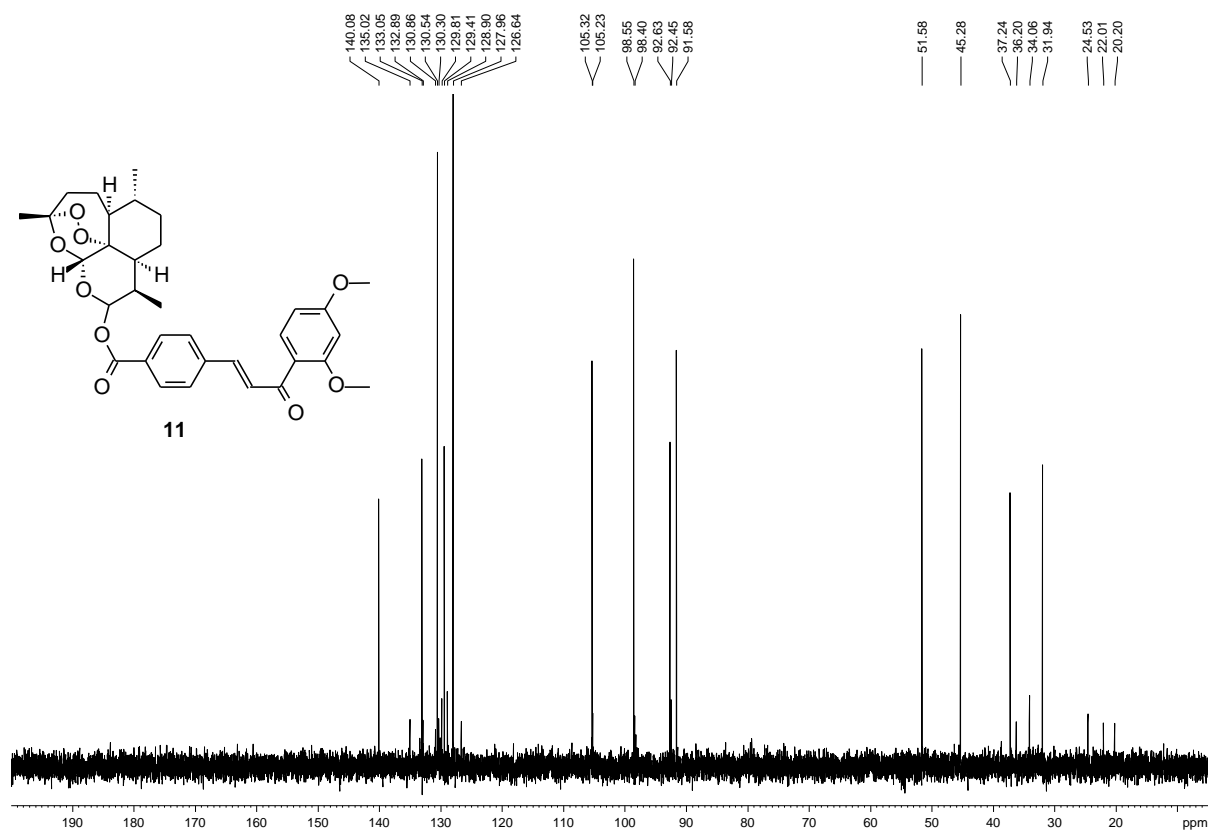


## DEPT135 in $\text{CDCl}_3$ : 11

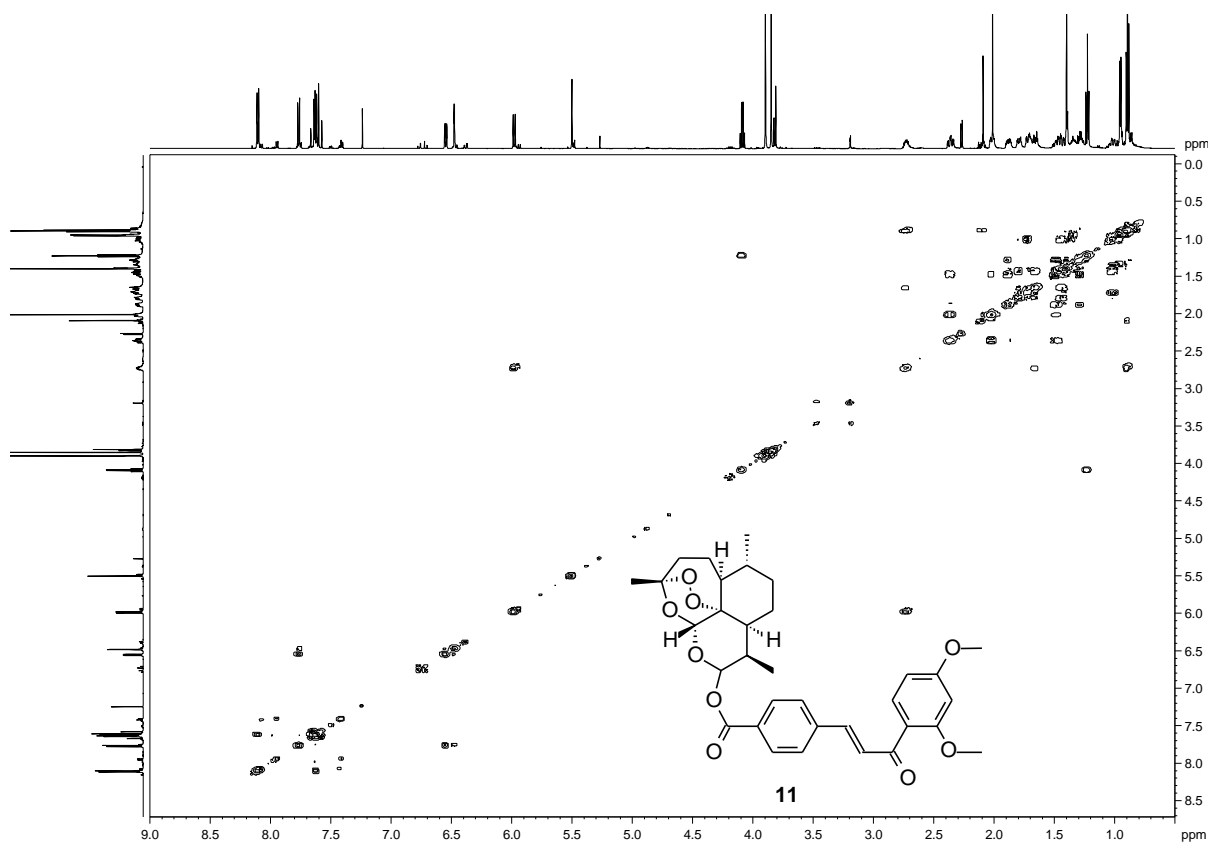


Addendum C – Chapter 5:

DEPT90 in CDCl<sub>3</sub>: 11

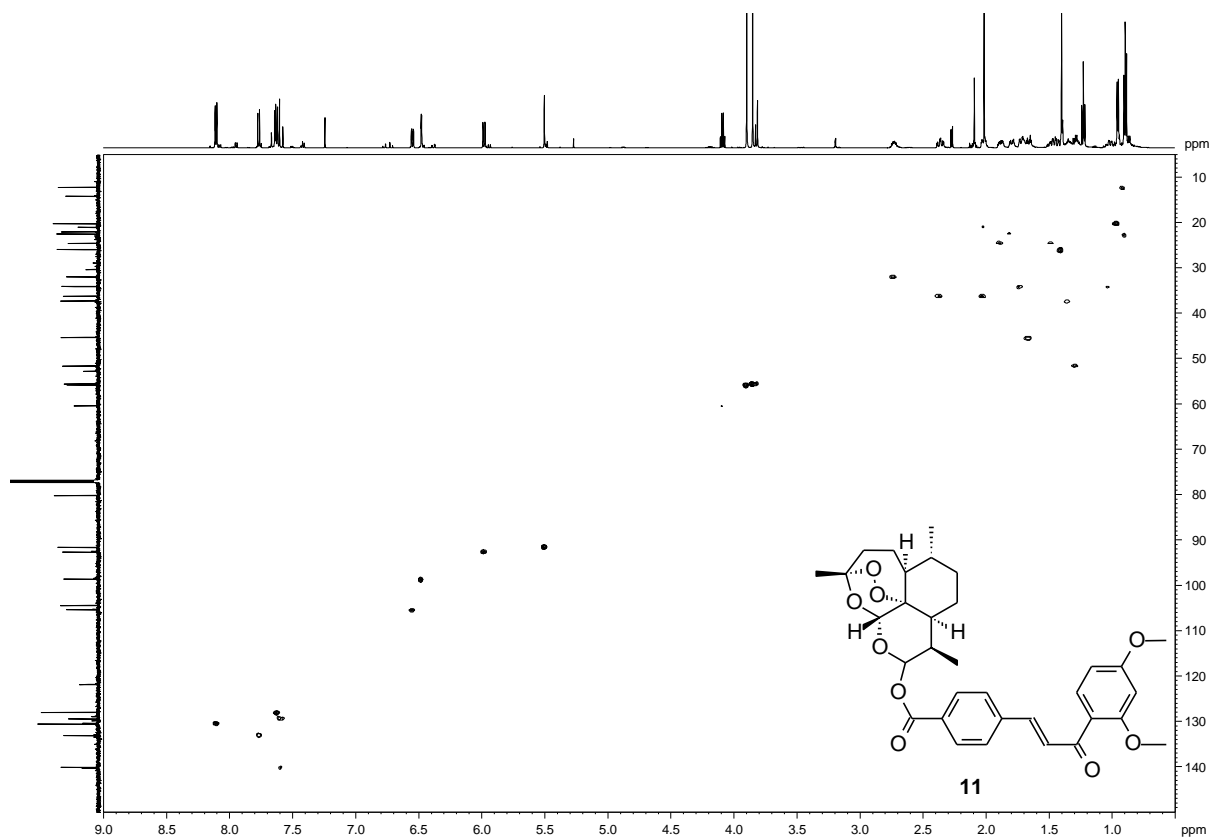


COSY in CDCl<sub>3</sub>: 11



# Addendum C – Chapter 5:

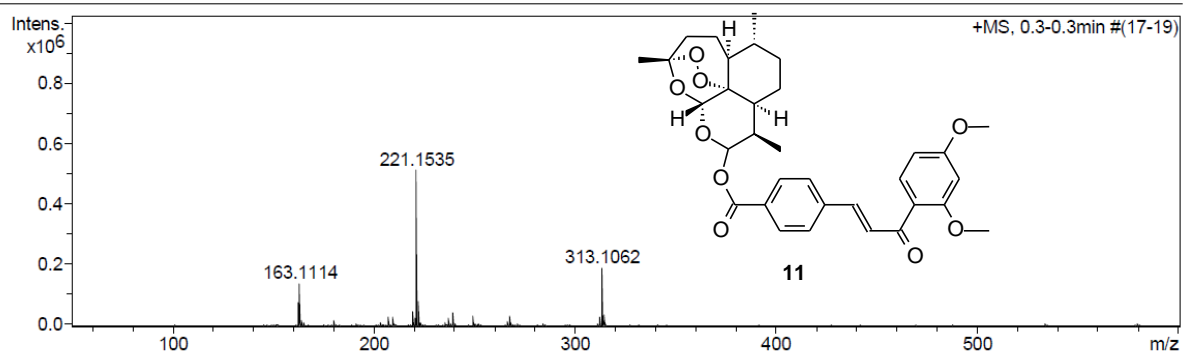
## HMBC in CDCl<sub>3</sub>: 11



## HRMS: 11

### Acquisition Parameter

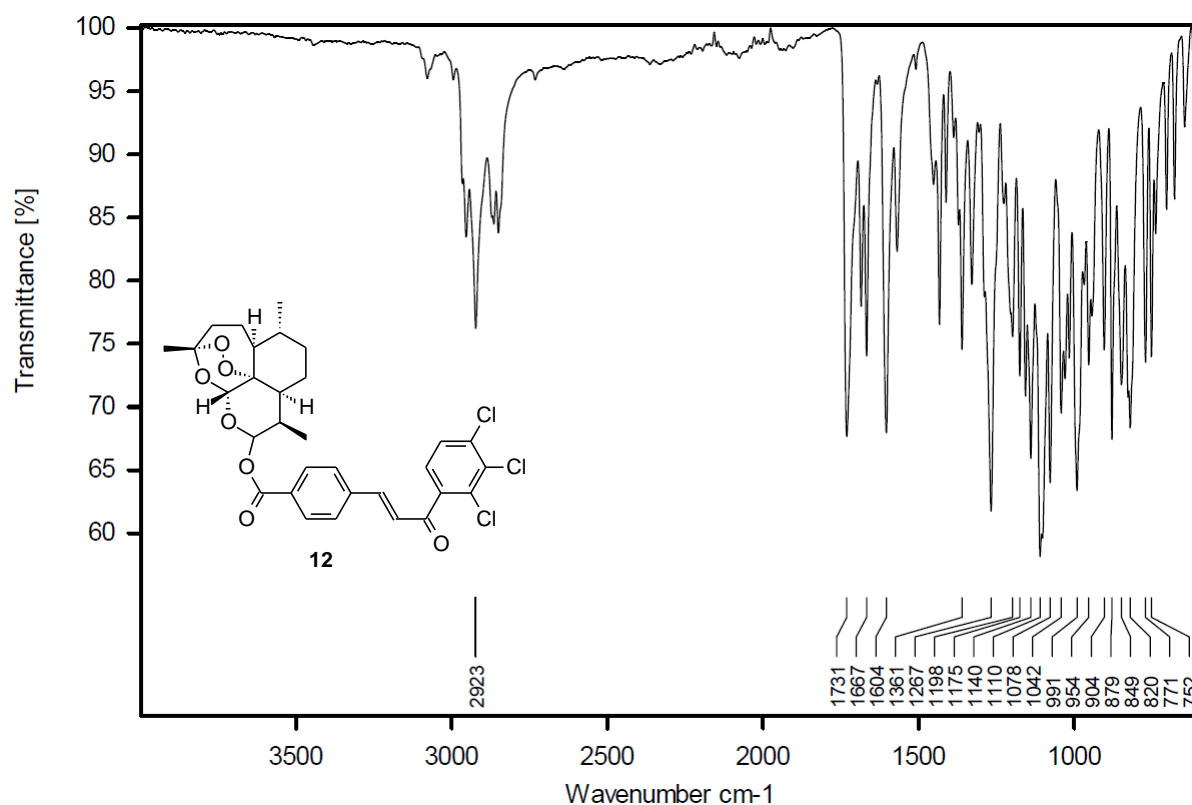
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste



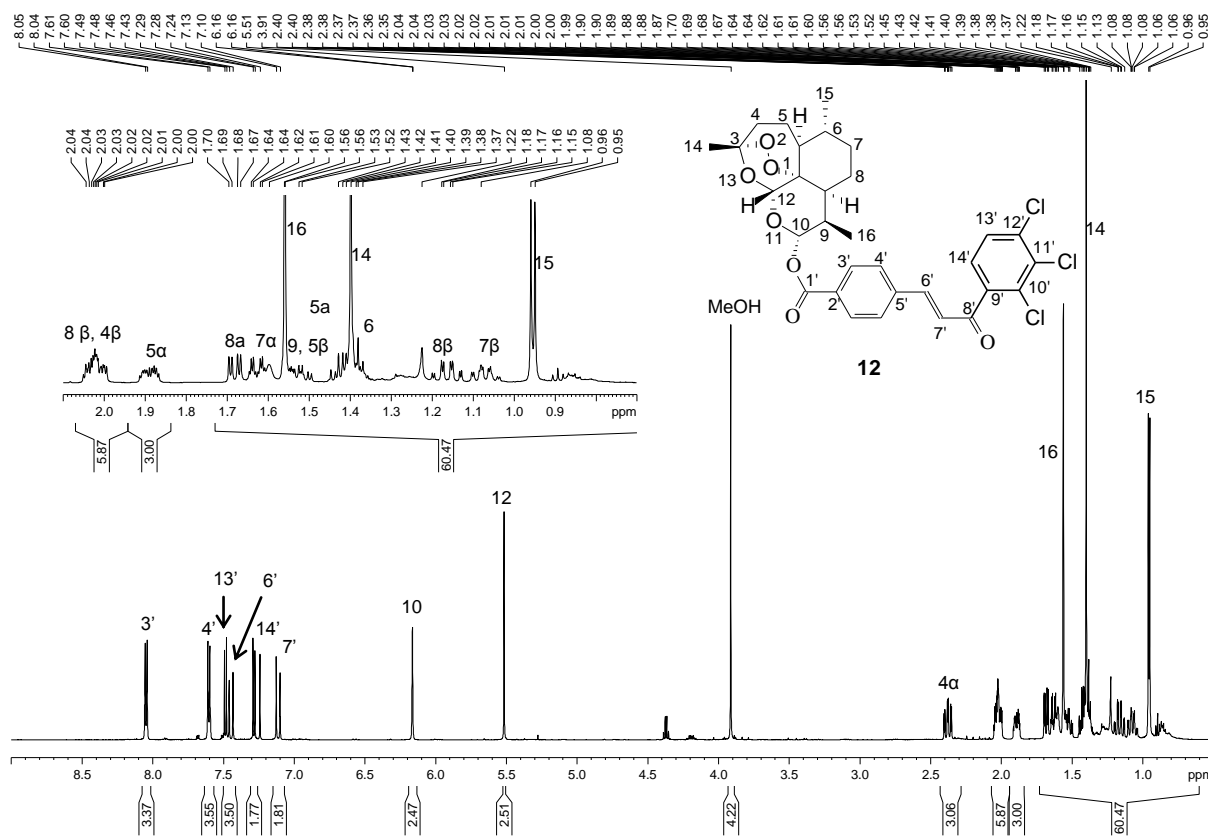
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	N-Rule	e <sup>-</sup> Conf
579.2560	1	C <sub>33</sub> H <sub>39</sub> O <sub>9</sub>	60.97	579.2589	2.8	4.8	18.5	14.5	ok	even

Addendum C – Chapter 5:

IR: 12

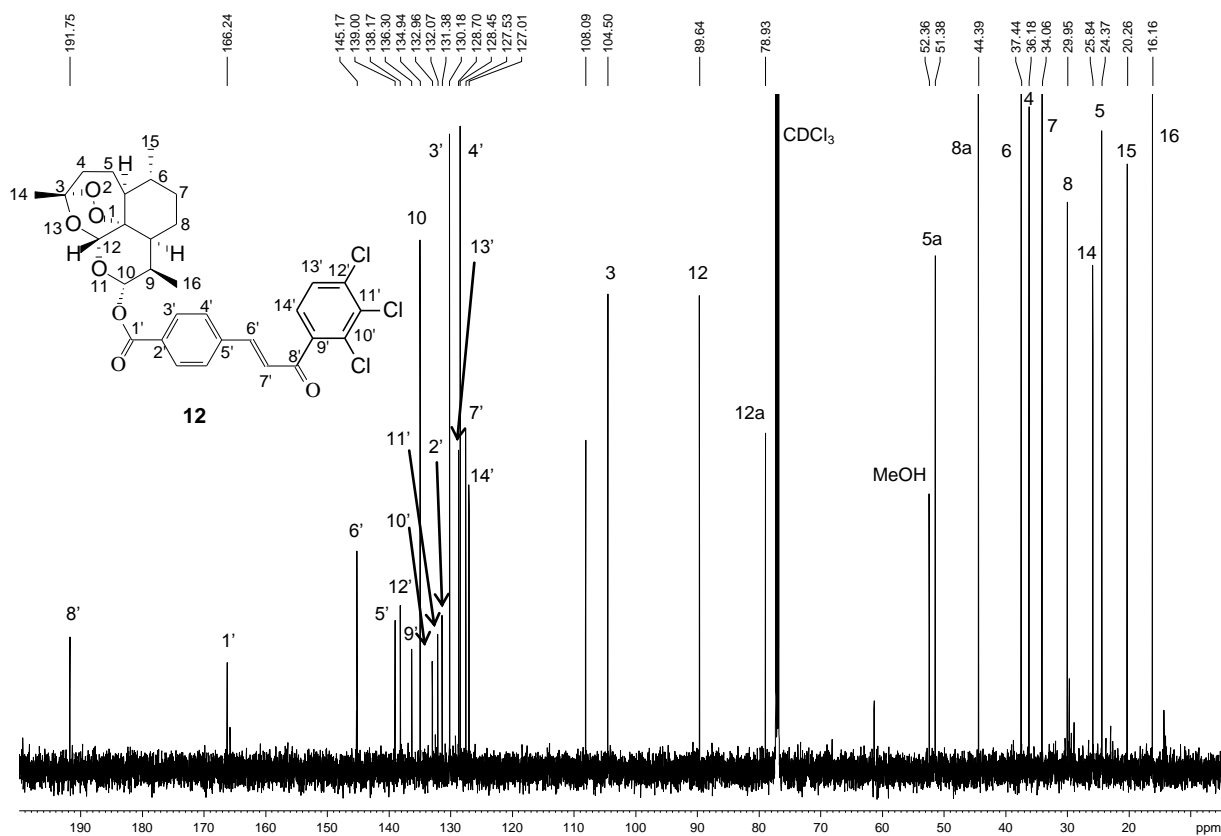


<sup>1</sup>H NMR in CDCl<sub>3</sub>: 12

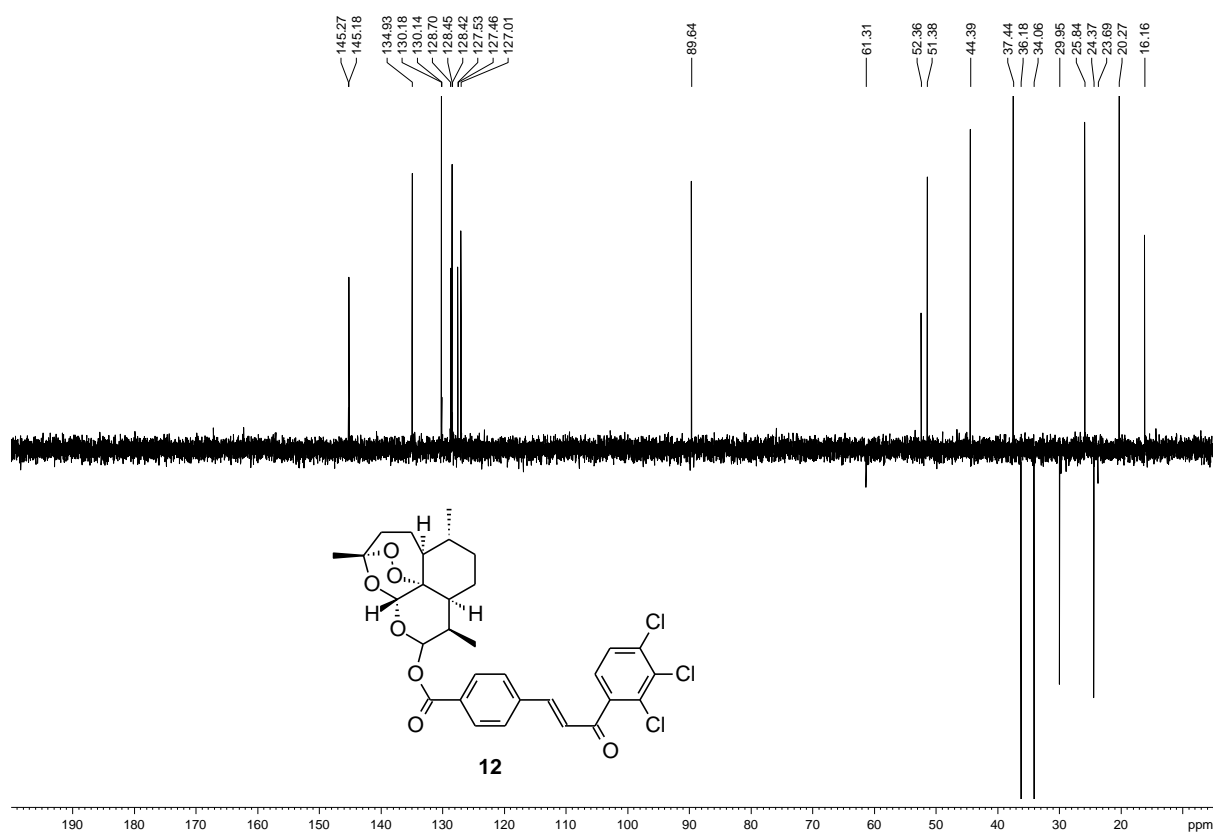


# Addendum C – Chapter 5:

## <sup>13</sup>C NMR in CDCl<sub>3</sub>: 12

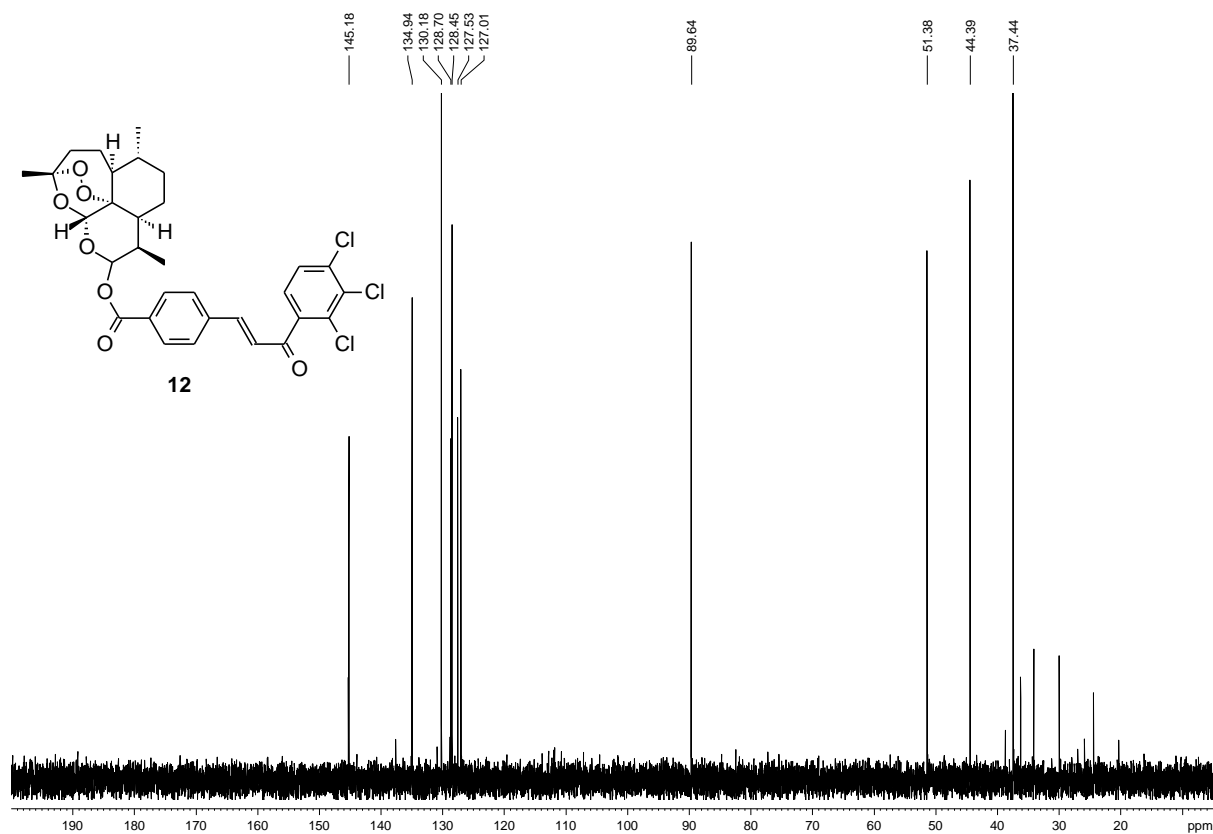


## DEPT135 in CDCl<sub>3</sub>: 12

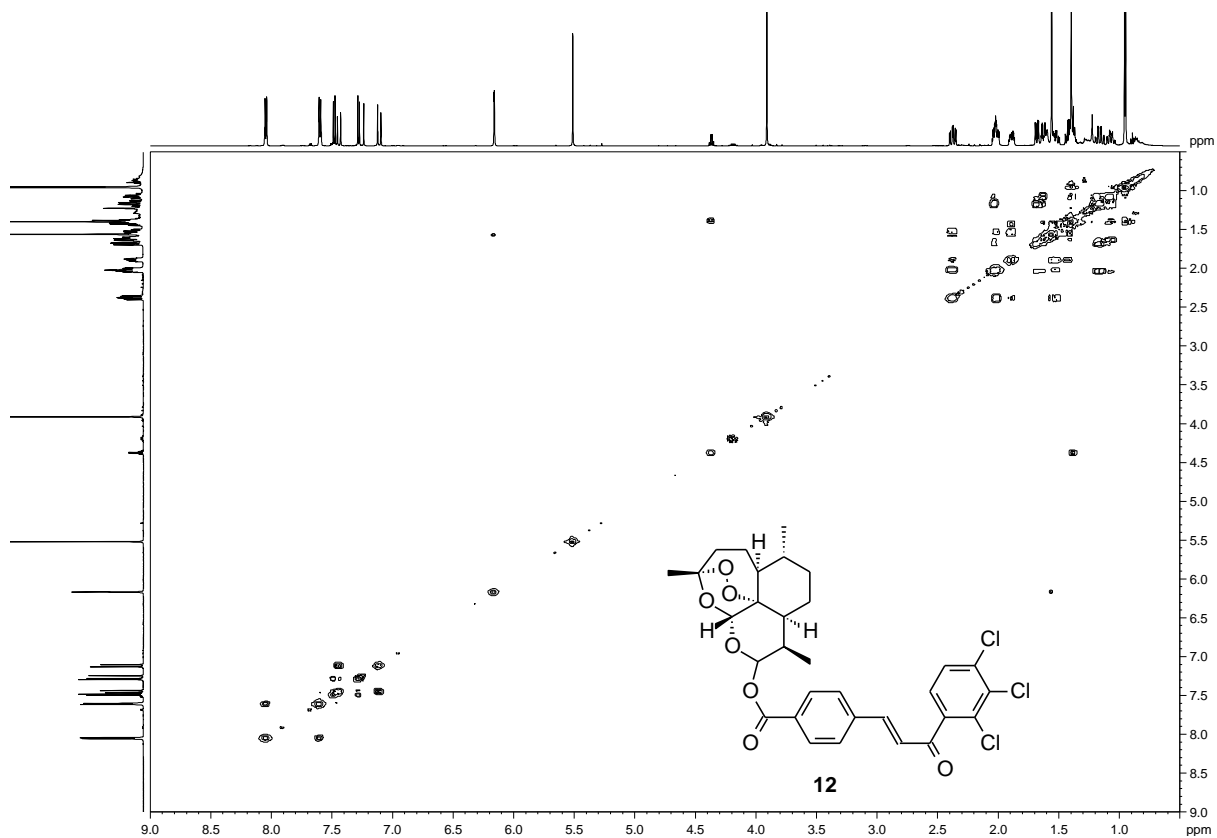


Addendum C – Chapter 5:

DEPT90 in CDCl<sub>3</sub>: **12**

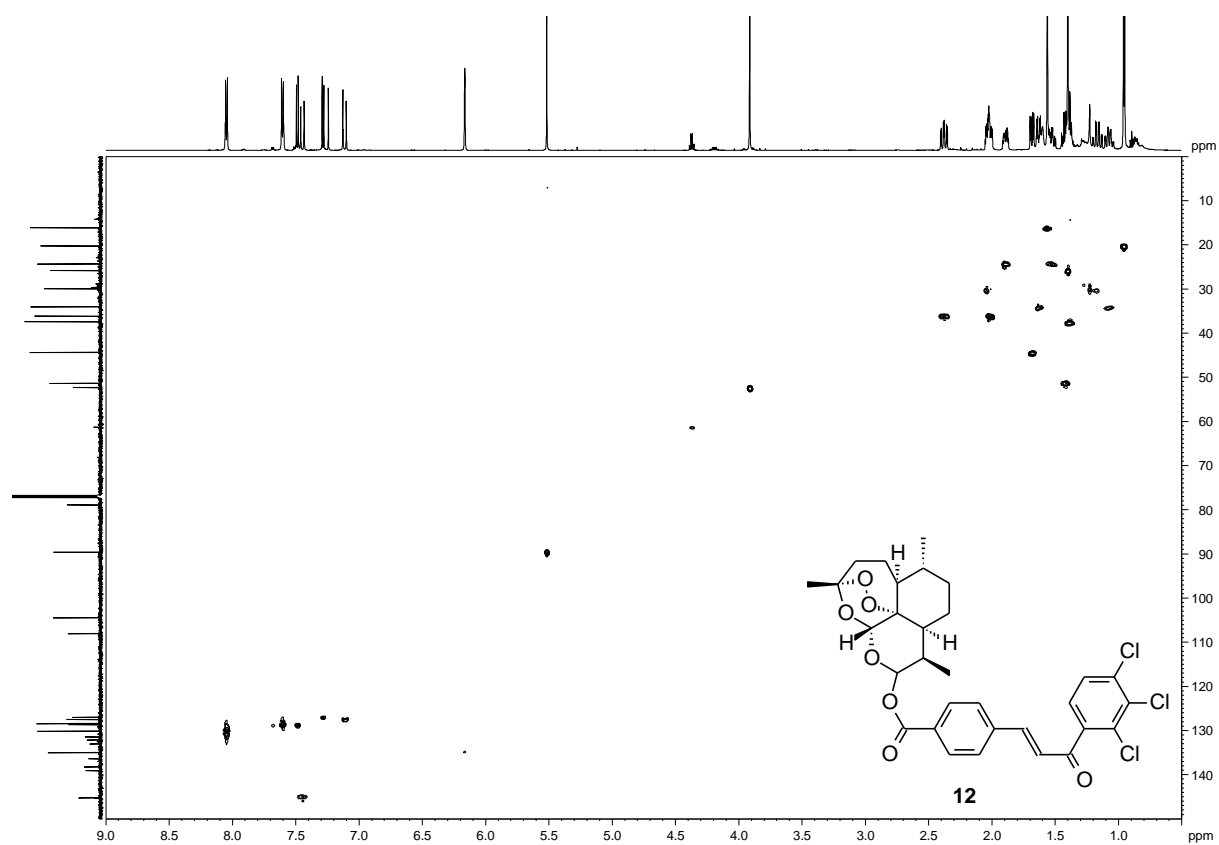


COSY in CDCl<sub>3</sub>: **12**



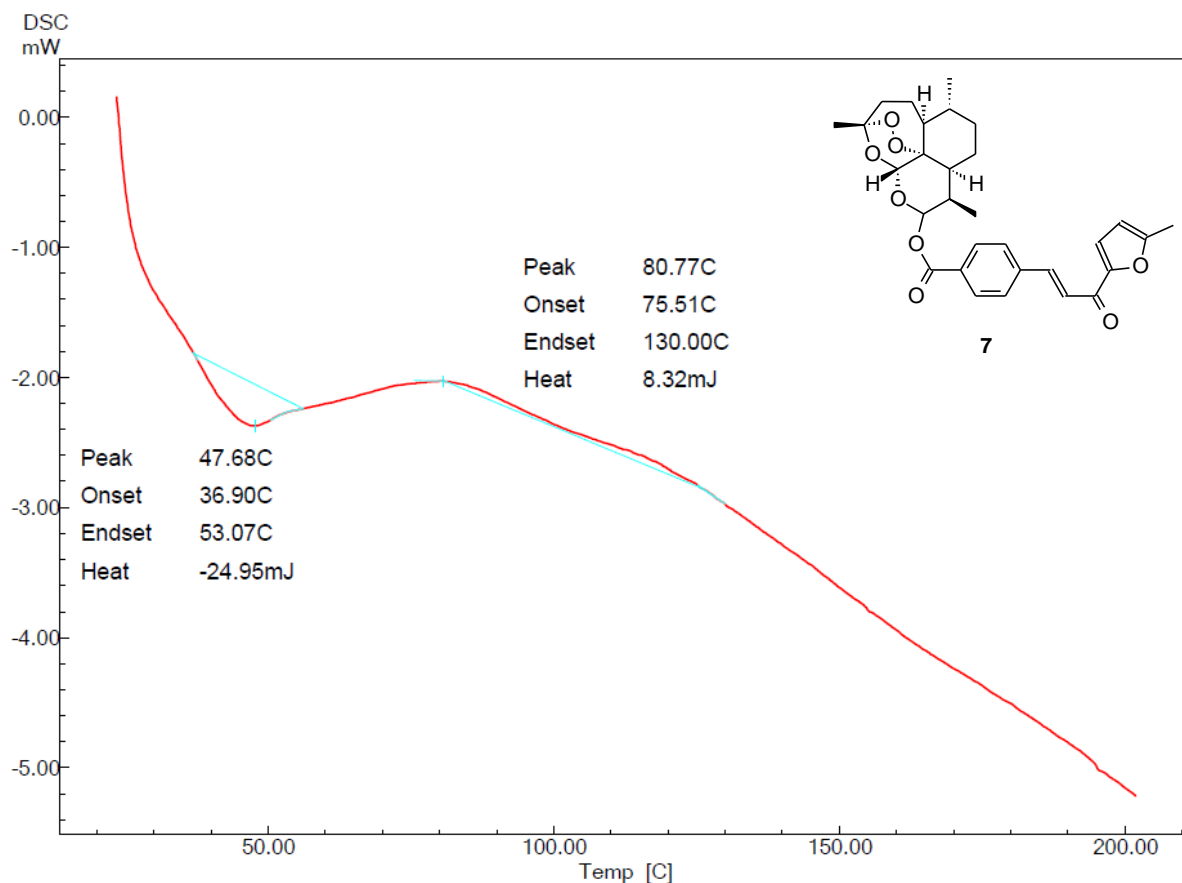
Addendum C – Chapter 5:

HSQC in CDCl<sub>3</sub>: 12

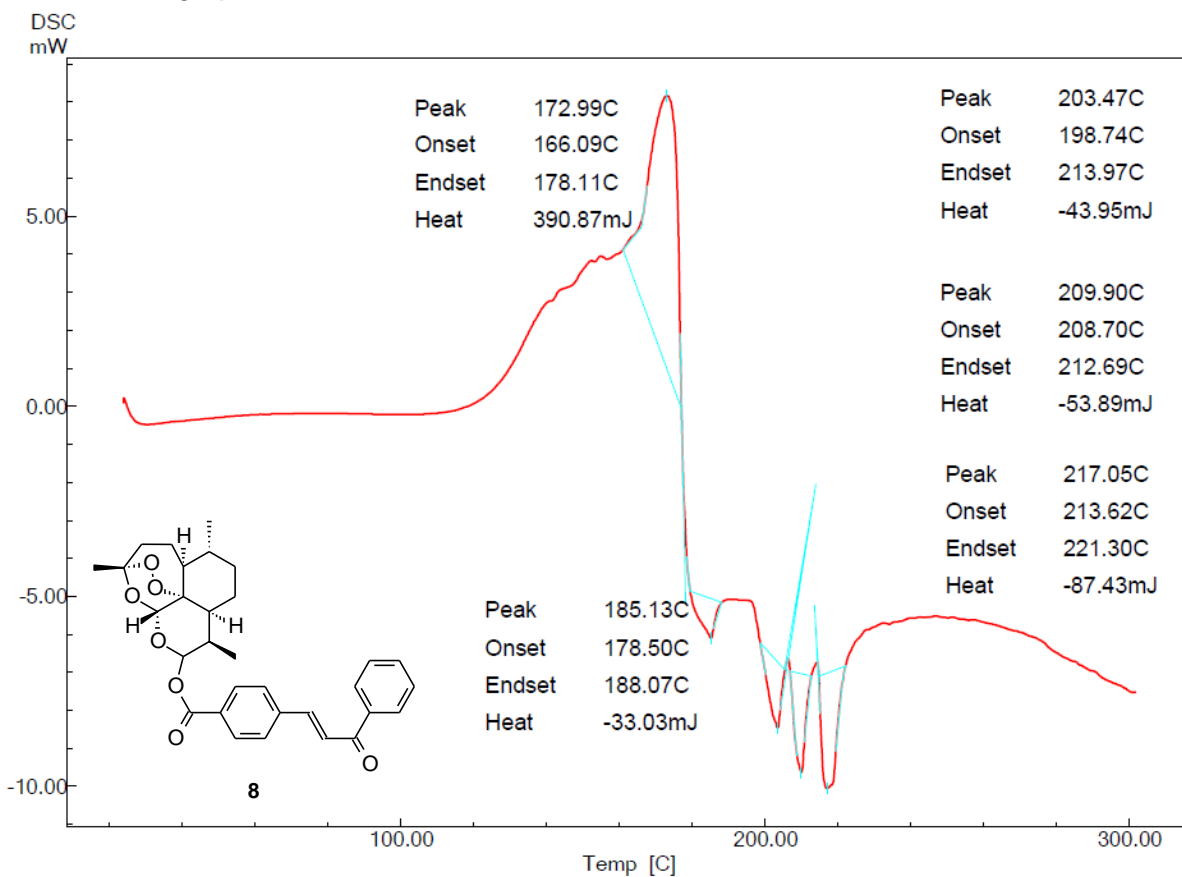


Addendum C – Chapter 5:

DSC Thermograph: 7

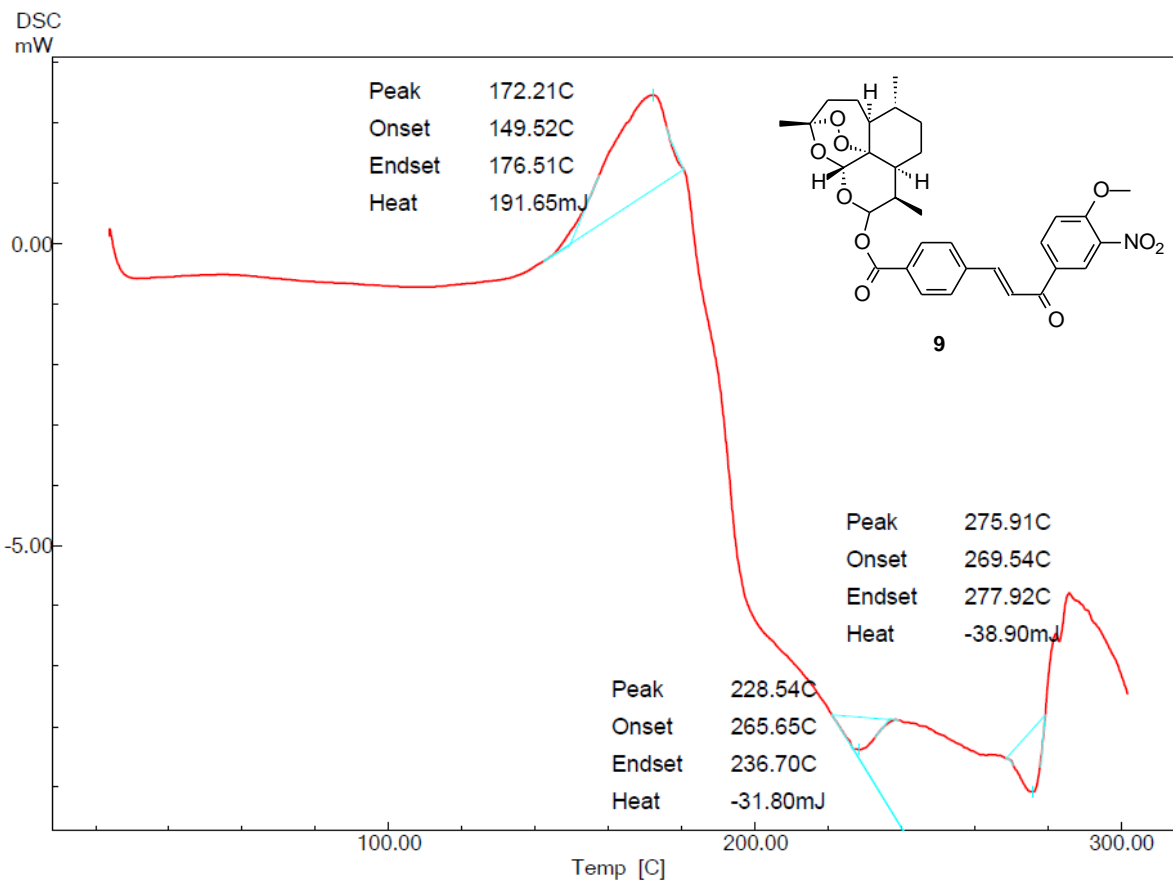


DSC Thermograph: 8

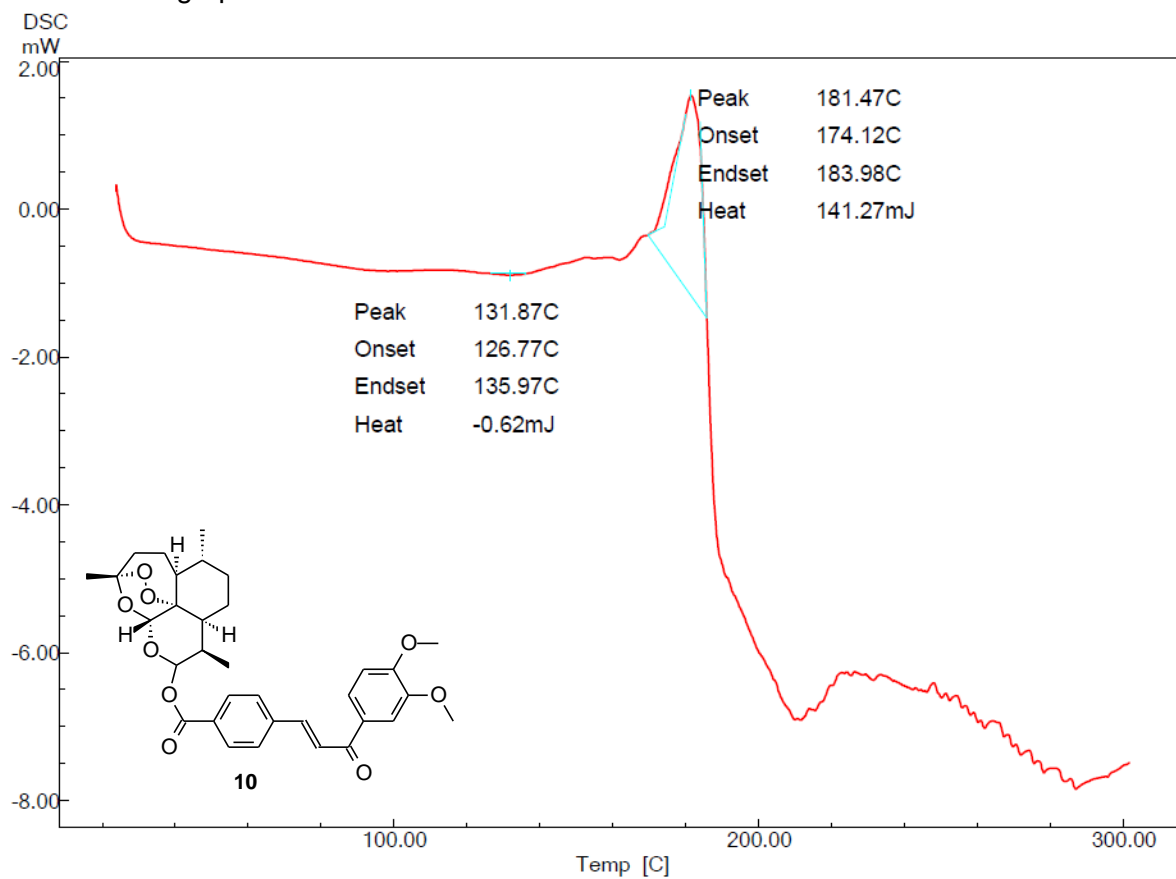


## Addendum C – Chapter 5:

### DSC Thermograph: 9

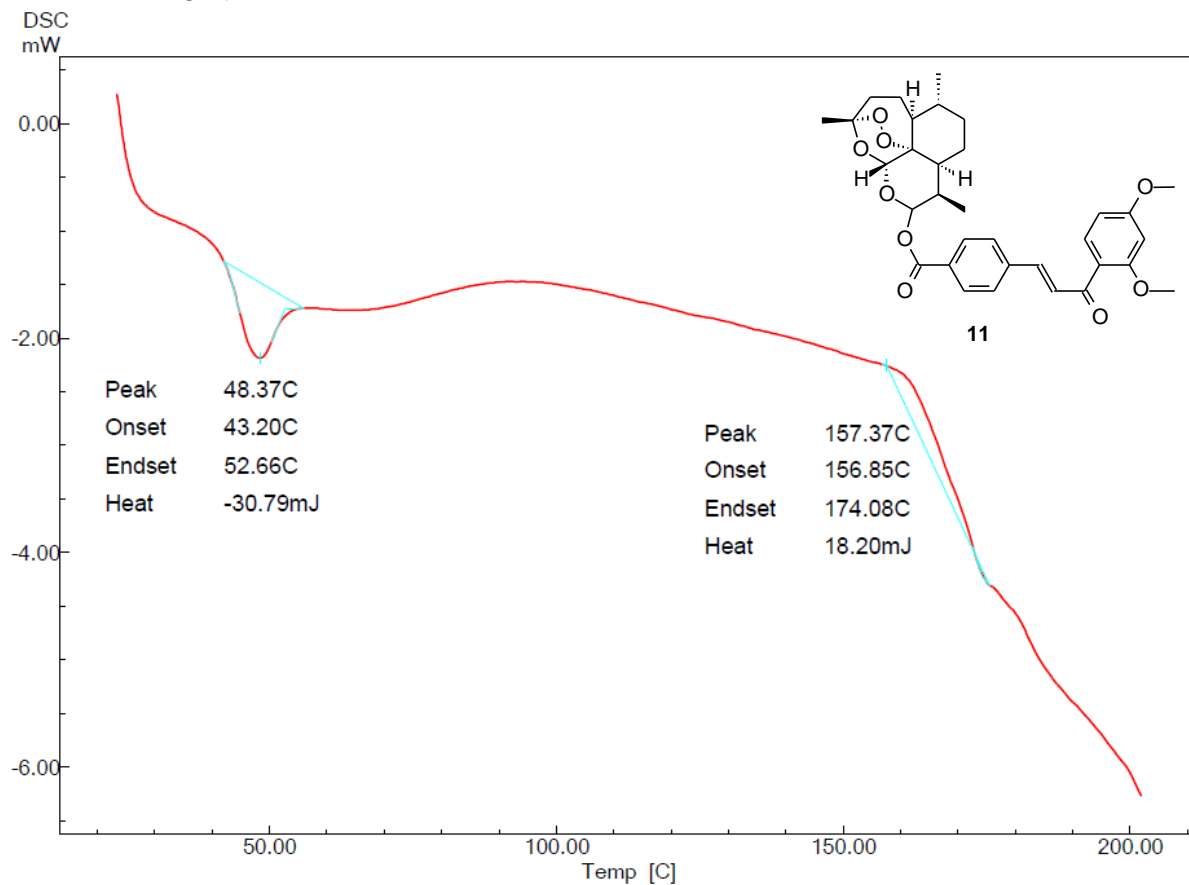


### DSC Thermograph: 10

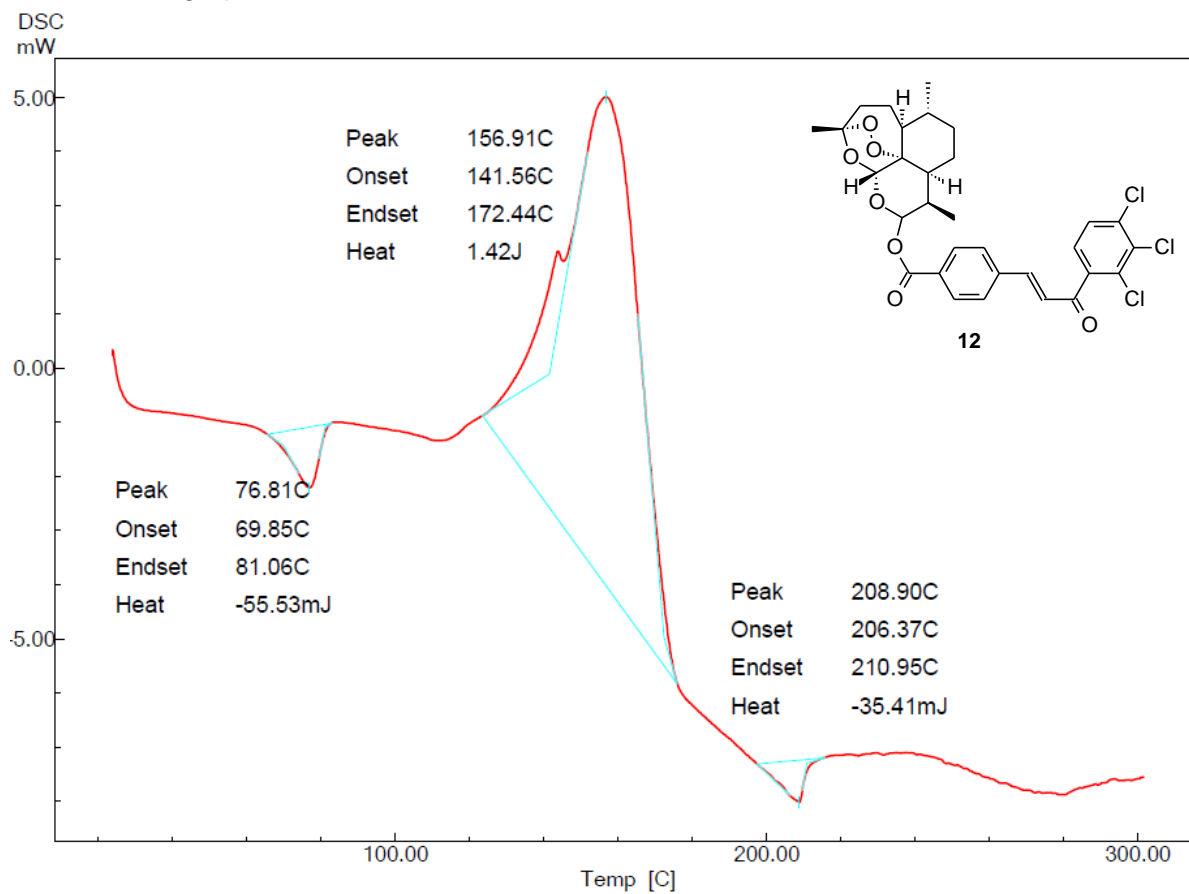


**Addendum C – Chapter 5:**

**DSC Thermograph: 11**

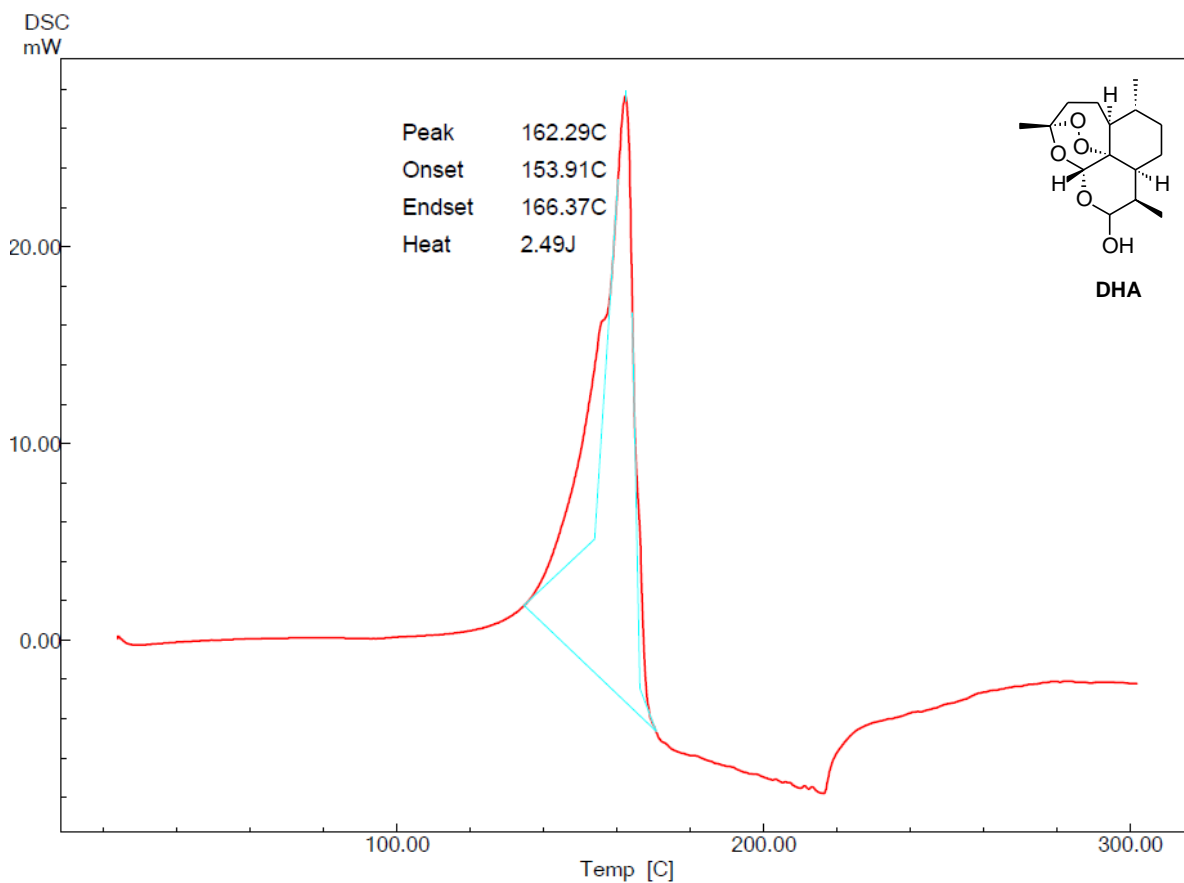


**DSC Thermograph: 12**

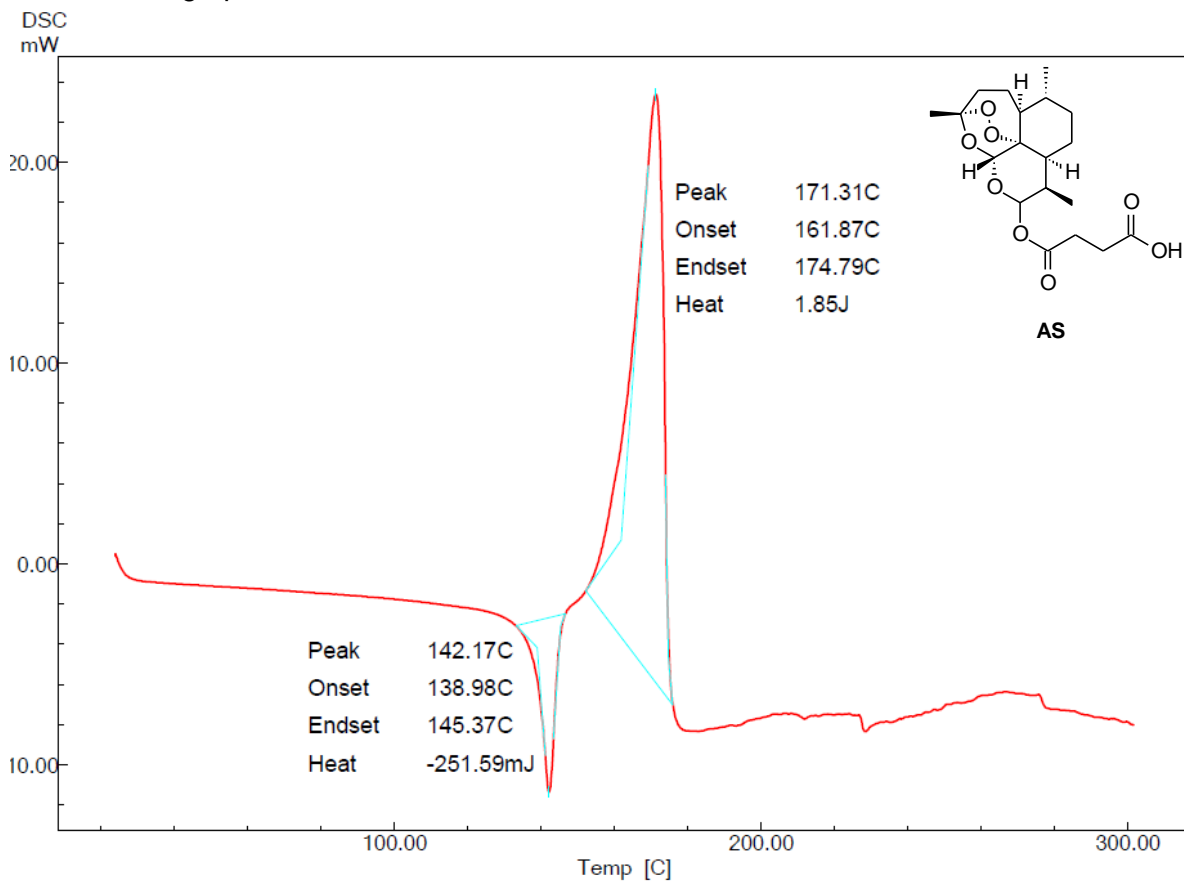


## Addendum C – Chapter 5:

### DSC Thermograph: DHA

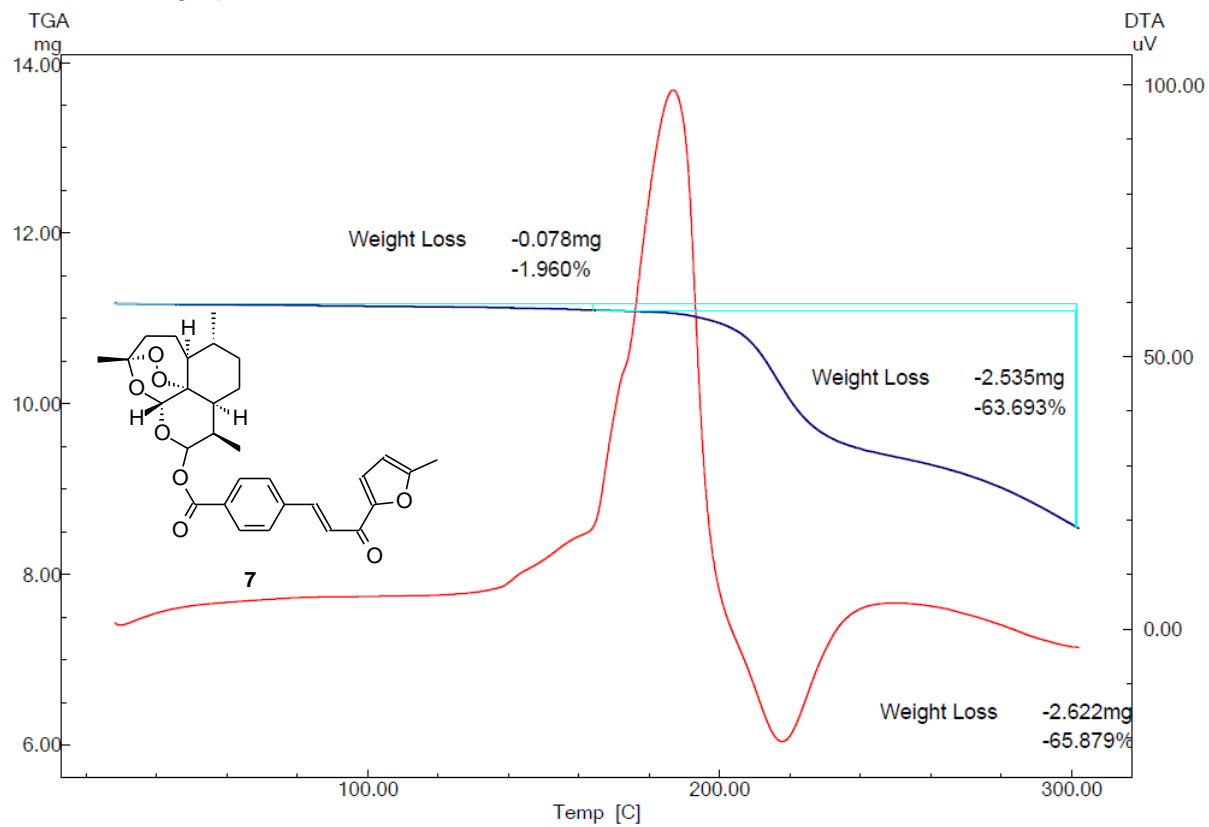


### DSC Thermograph: AS

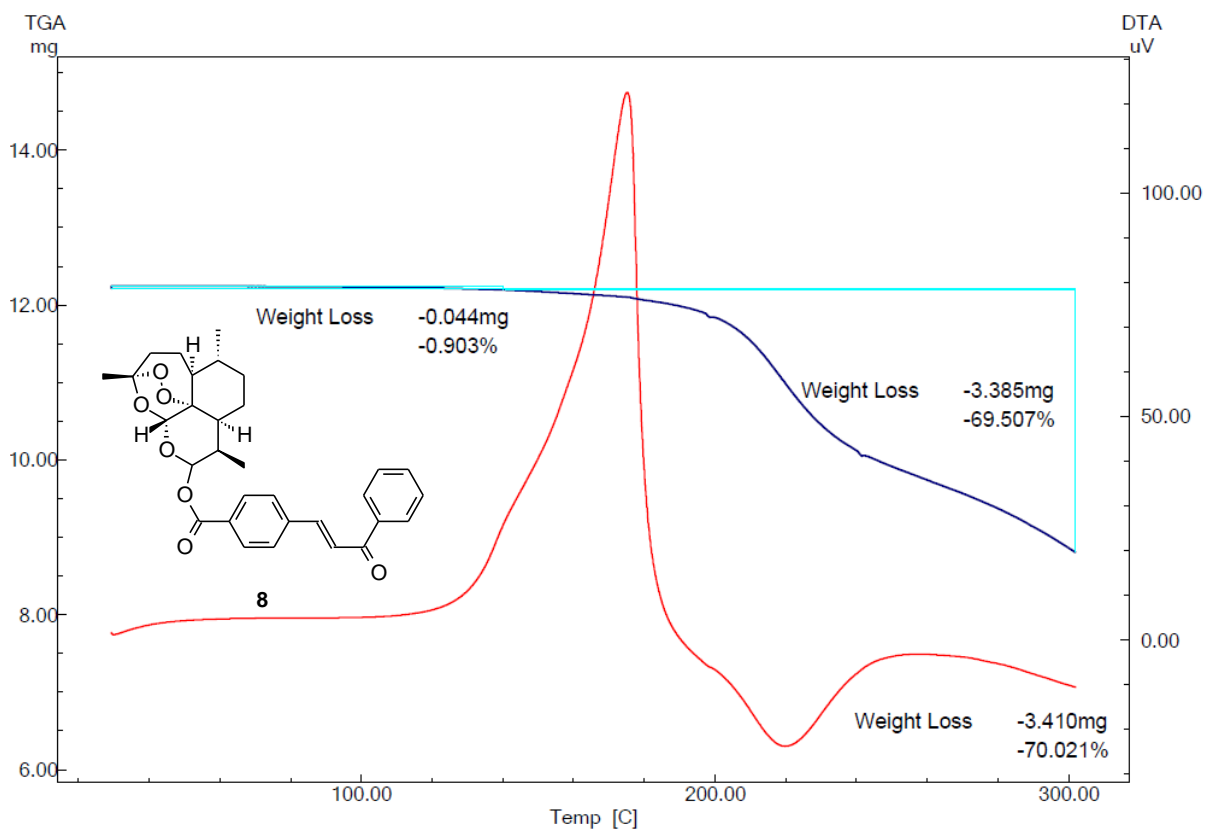


## Addendum C – Chapter 5:

### TGA Thermograph: 7

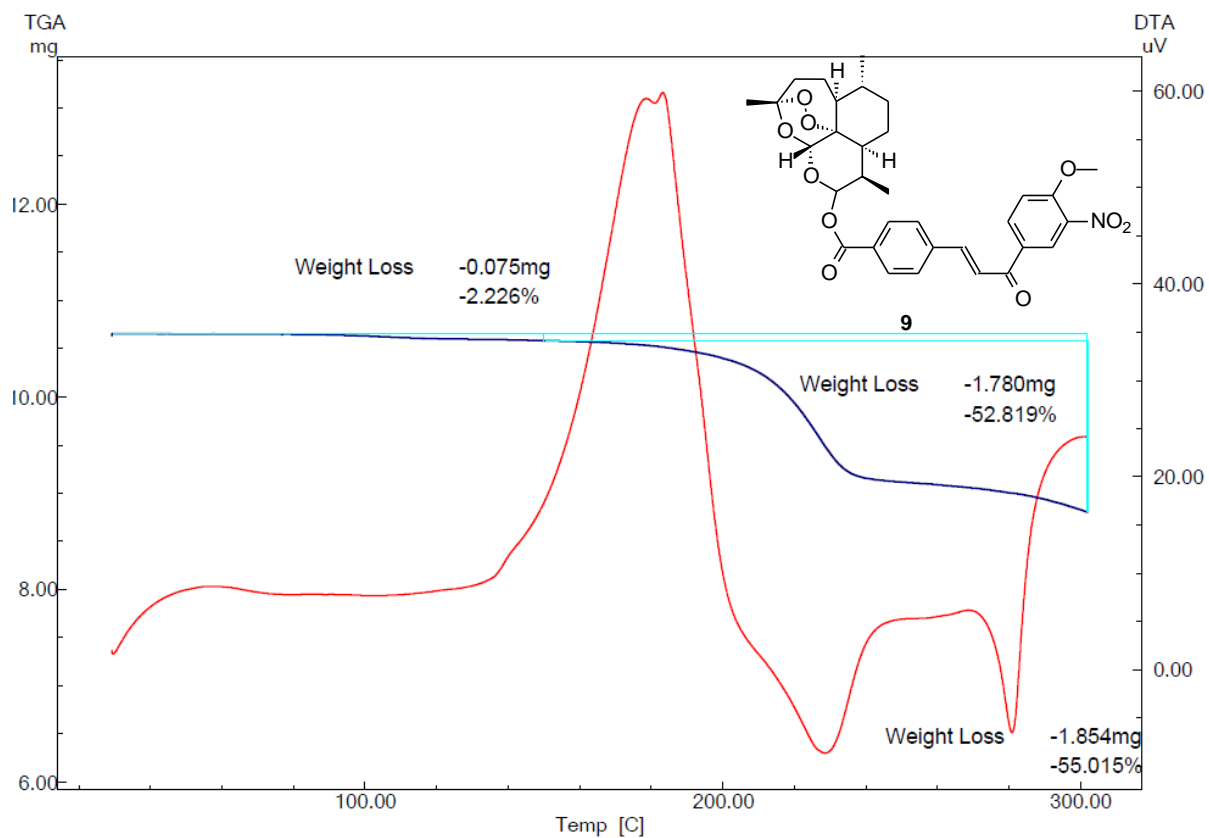


### TGA Thermograph: 8

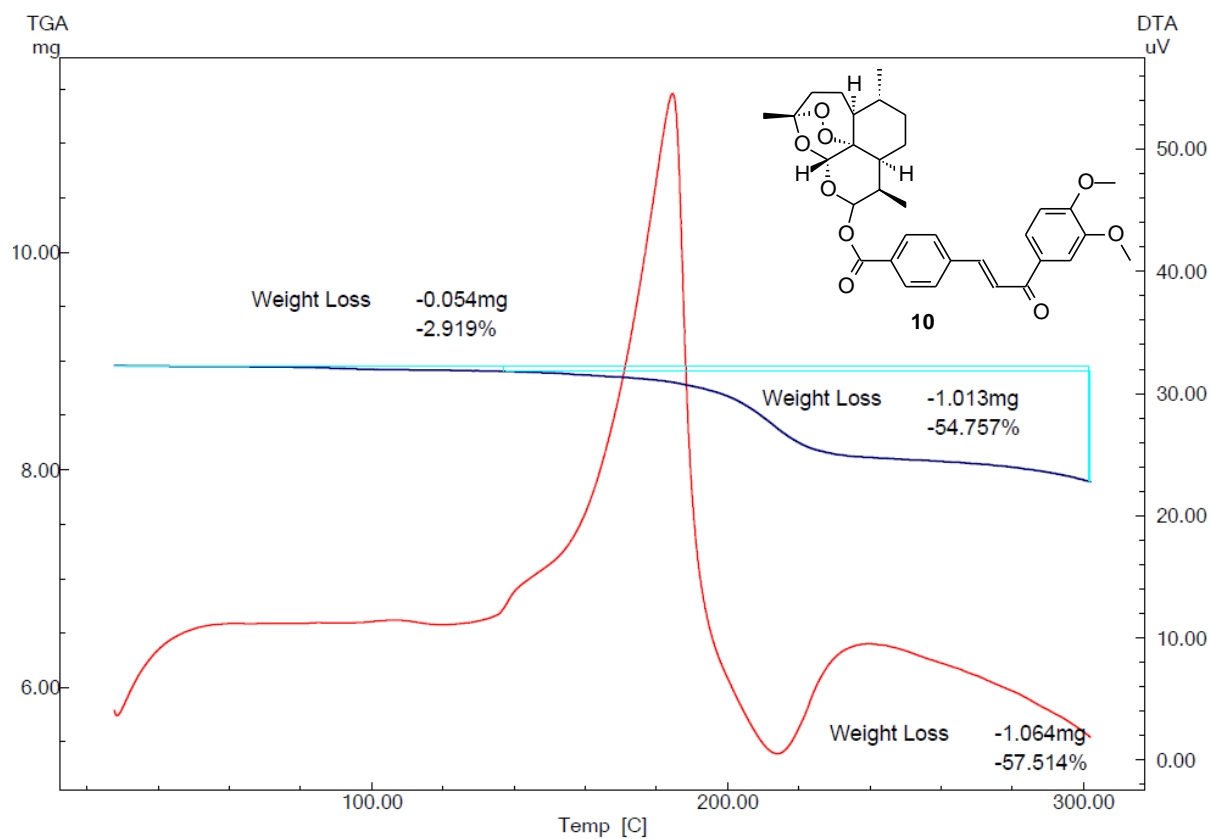


# Addendum C – Chapter 5:

## TGA Thermograph: 9

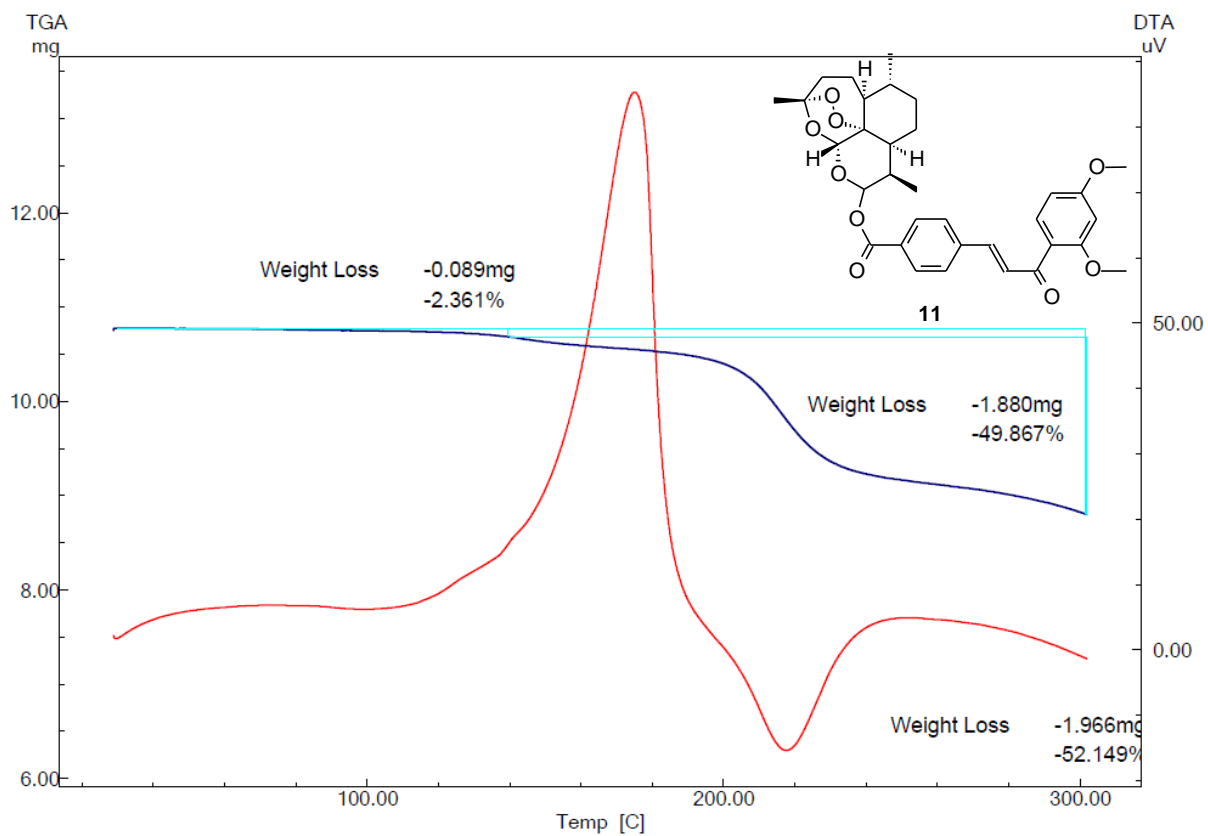


## TGA Thermograph: 10

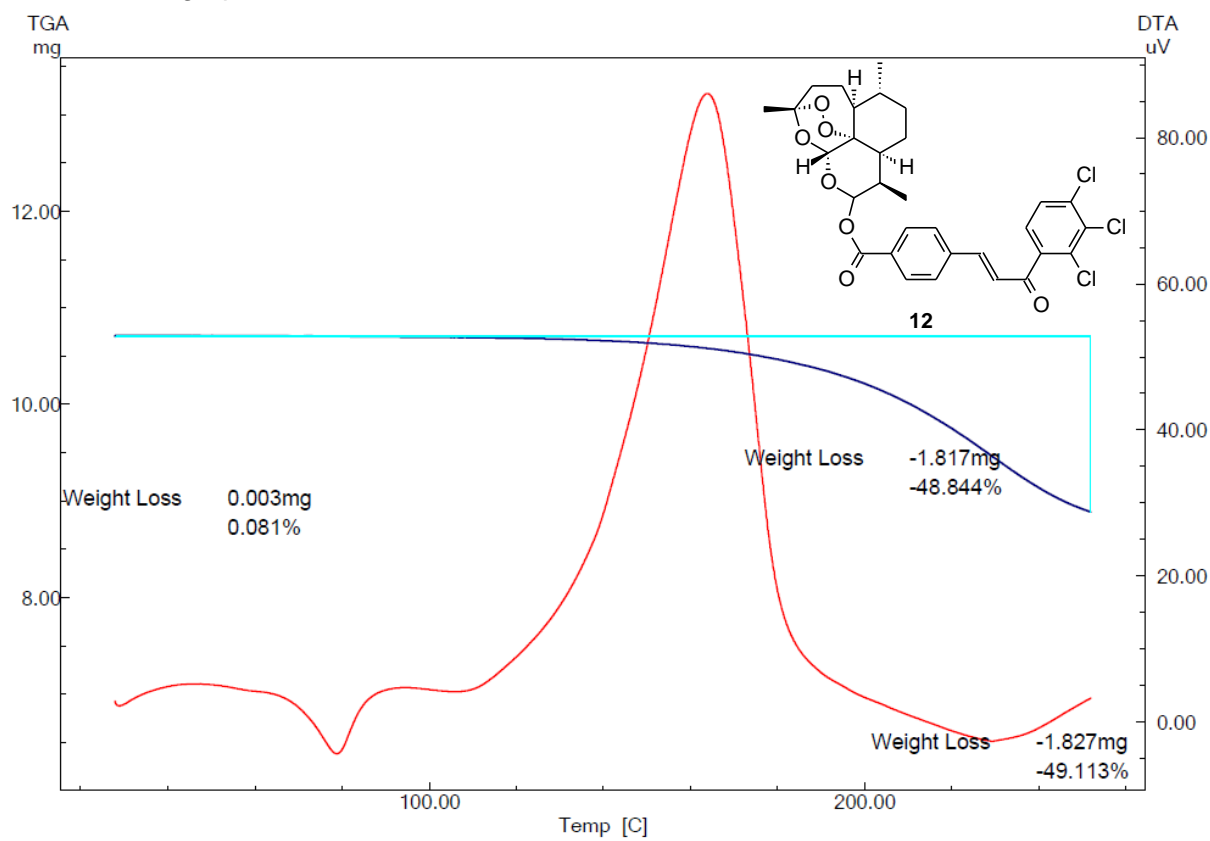


## Addendum C – Chapter 5:

### TGA Thermograph: 11

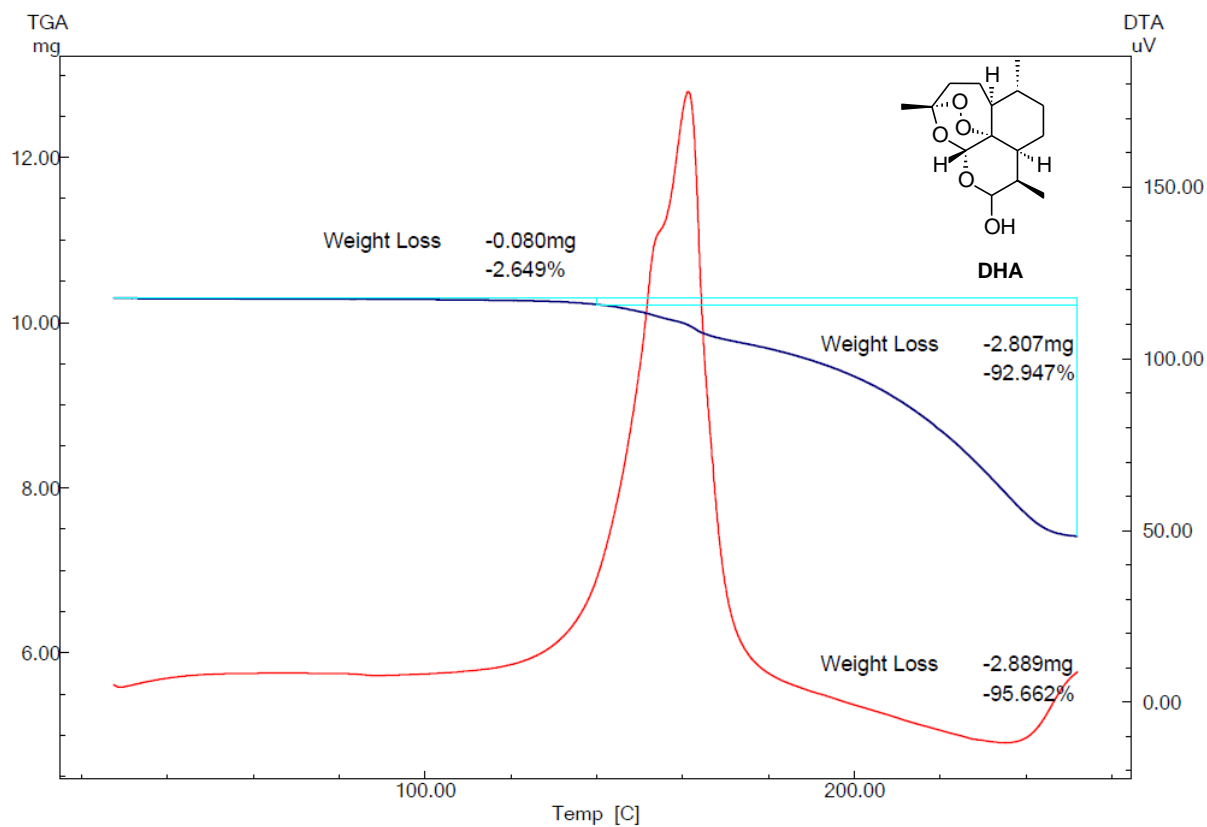


### TGA Thermograph: 12



## Addendum C – Chapter 5:

### TGA Thermograph: DHA



### TGA Thermograph: AS

