

***In vitro* enzymatic and kinetic studies, and *in silico* drug-receptor interactions and drug-like profiling of the 5-styrylbenzamide derivatives as potential cholinesterase and β -secretase inhibitors with antioxidant properties**

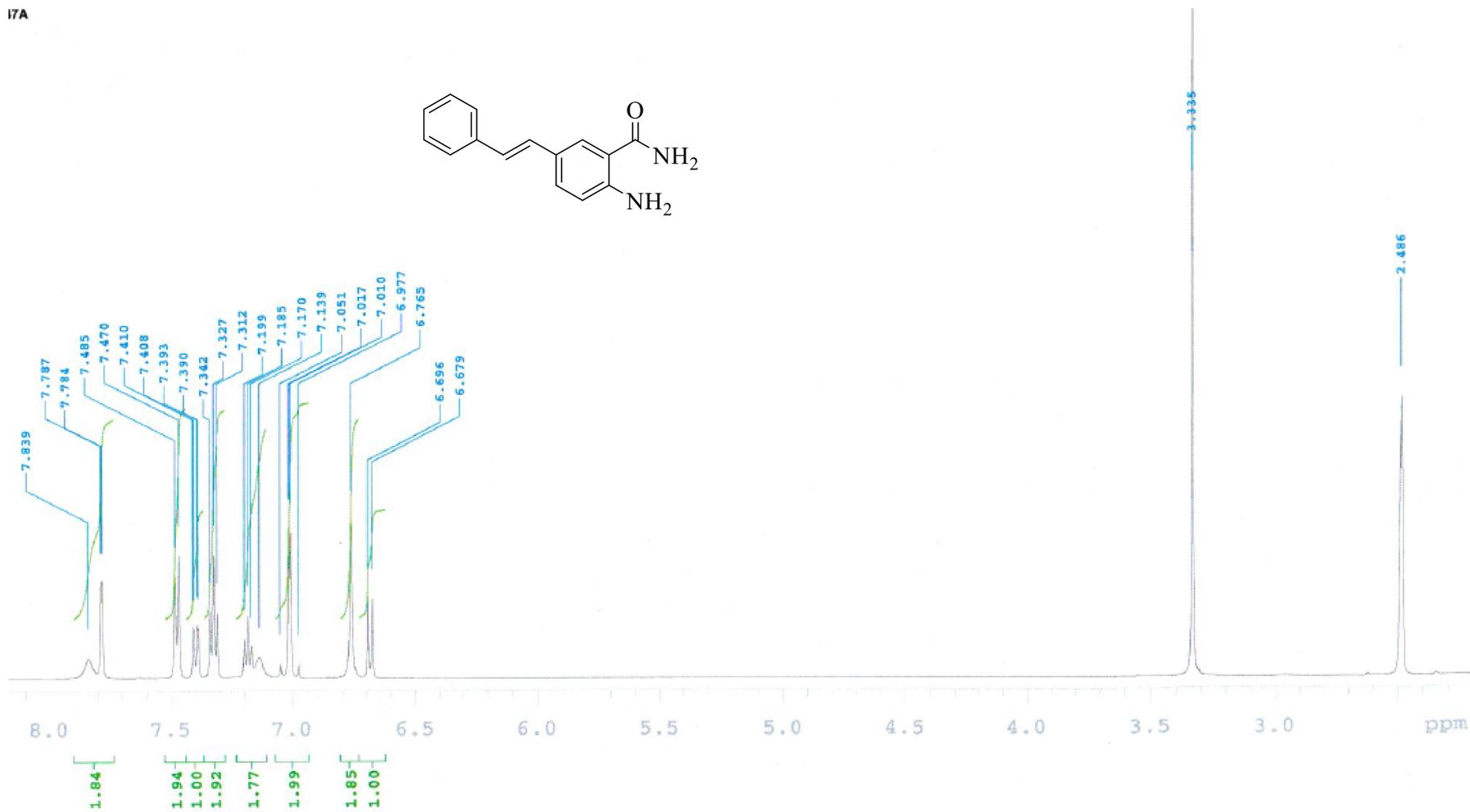
Malose J. Mphahlele,^{1,*} Emmanuel N. Agbo,¹ Garland K. More² and Samantha Gildenhuis²

Figure S1: ¹H- and ¹³C-NMR of compounds 2a–d and 3a–d

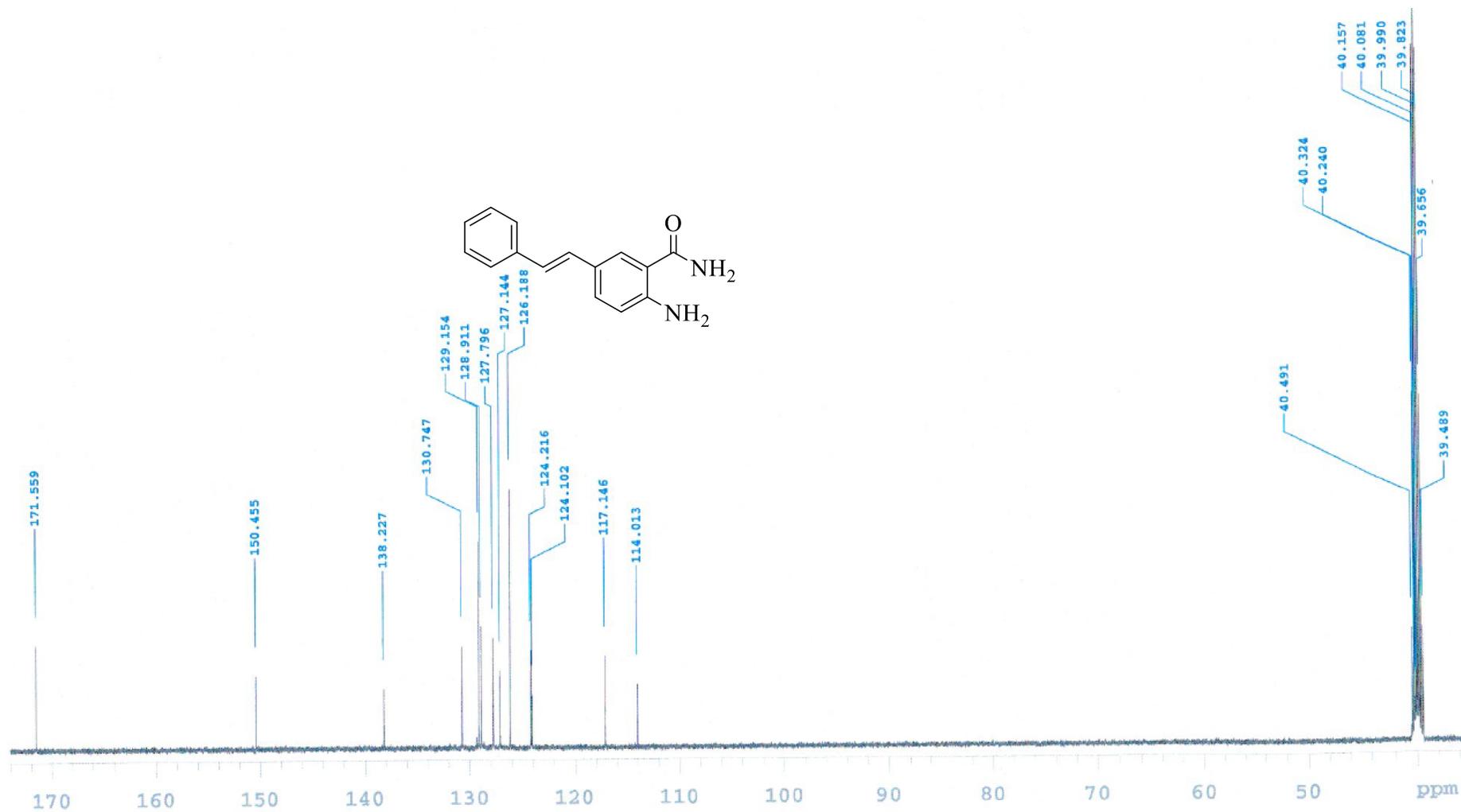
Figure S2: The 2-dimensional (2D) plots of docking results for donepezil into AChE and BChE

Figure S1: ¹H- and ¹³C-NMR of compounds 2 and 3.

17A

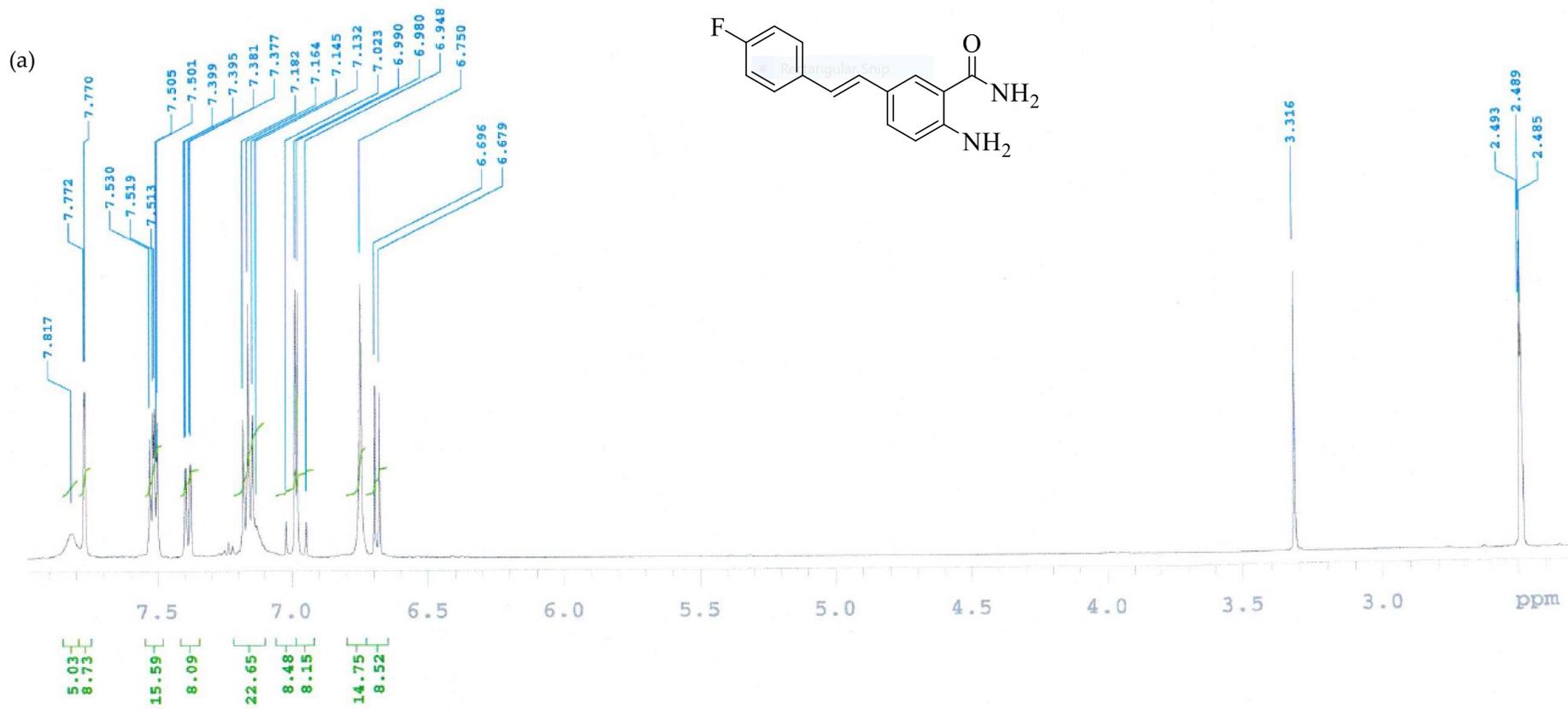


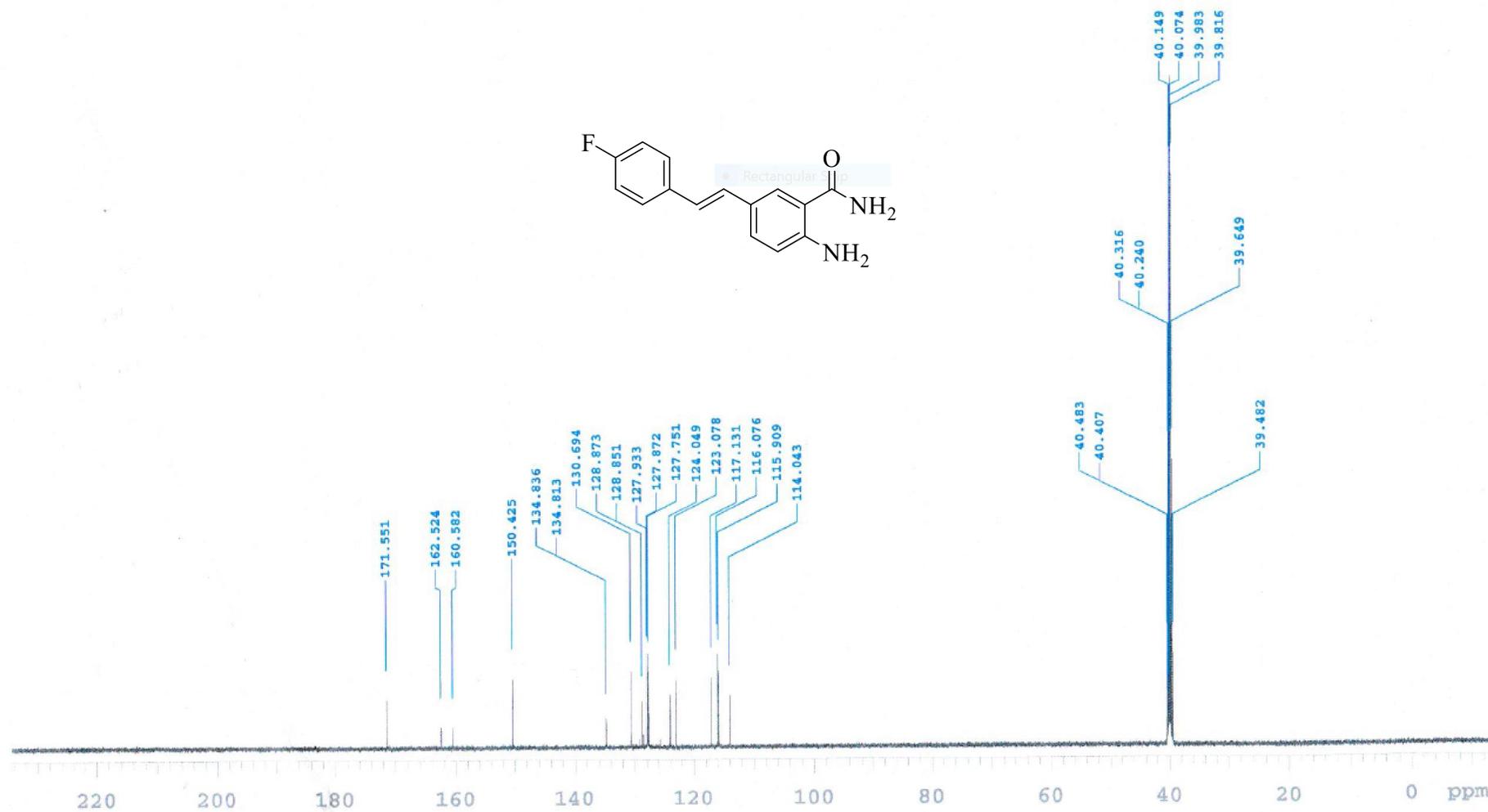
(a)



(b)

Figure S1.1: ^1H - and ^{13}C -NMR of **2a** in $\text{DMSO-}d_6$ at 500 MHz (a) and 125 MHz (b), respectively.





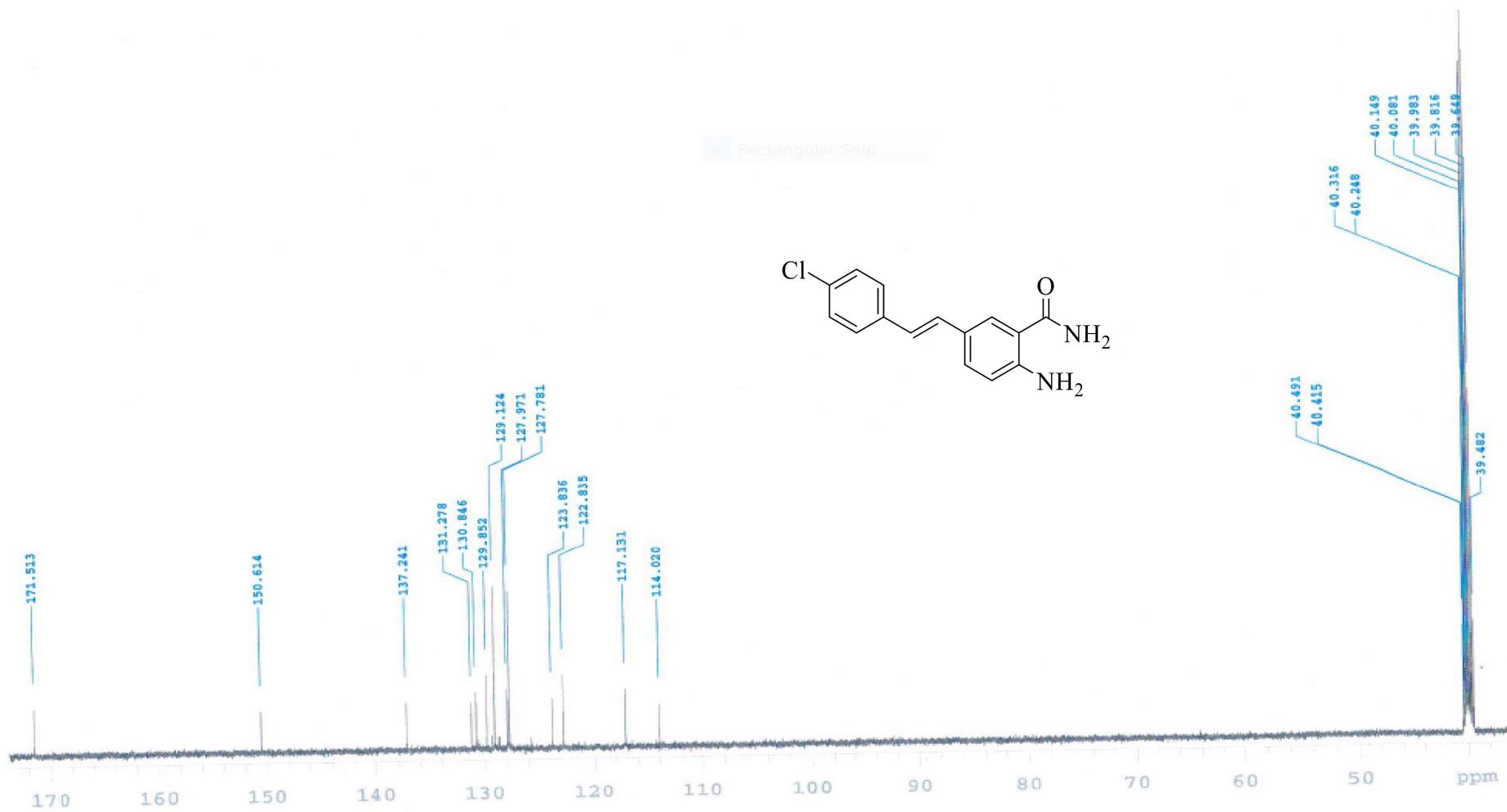
(b)

Figure S1.2: ¹H- and ¹³C-NMR of 2b in DMSO-*d*₆ at 500 MHz (a) and 125 MHz (b), respectively.

Rectangular Snip

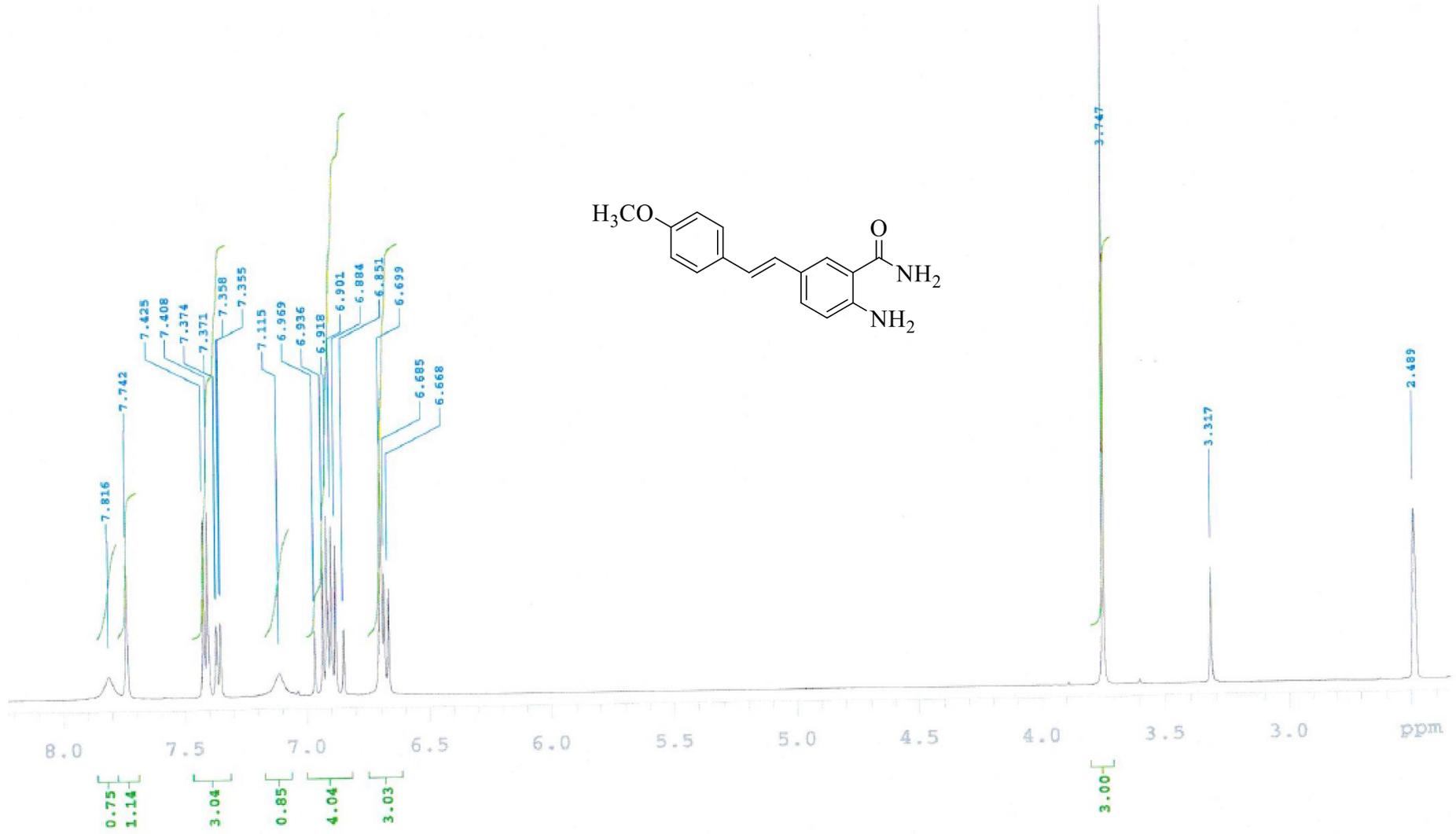


(a)

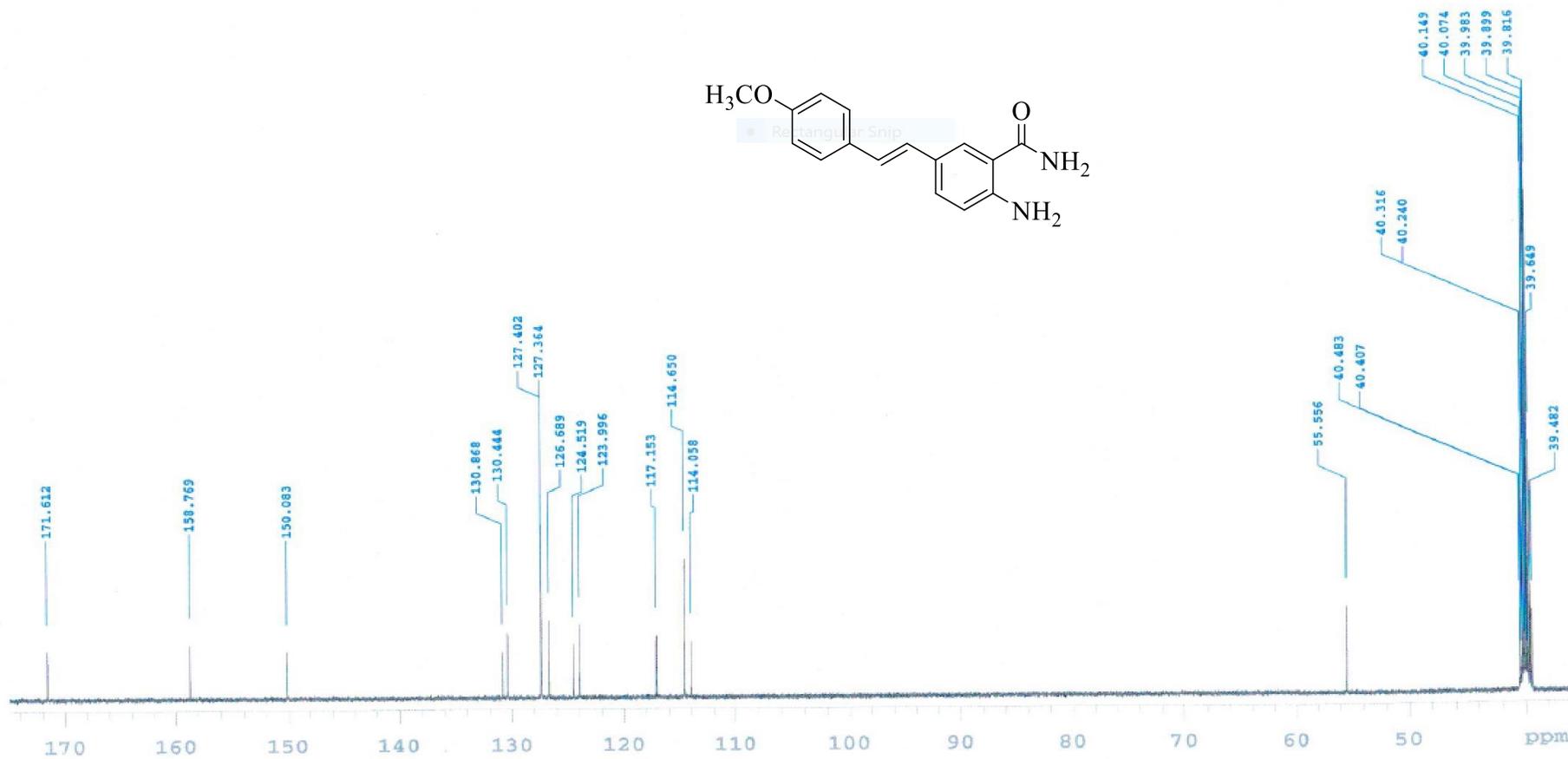


(b)

Figure S1.3: ¹H- and ¹³C-NMR of 2c in DMSO-*d*₆ at 500 MHz (a) and 125 MHz (b), respectively.

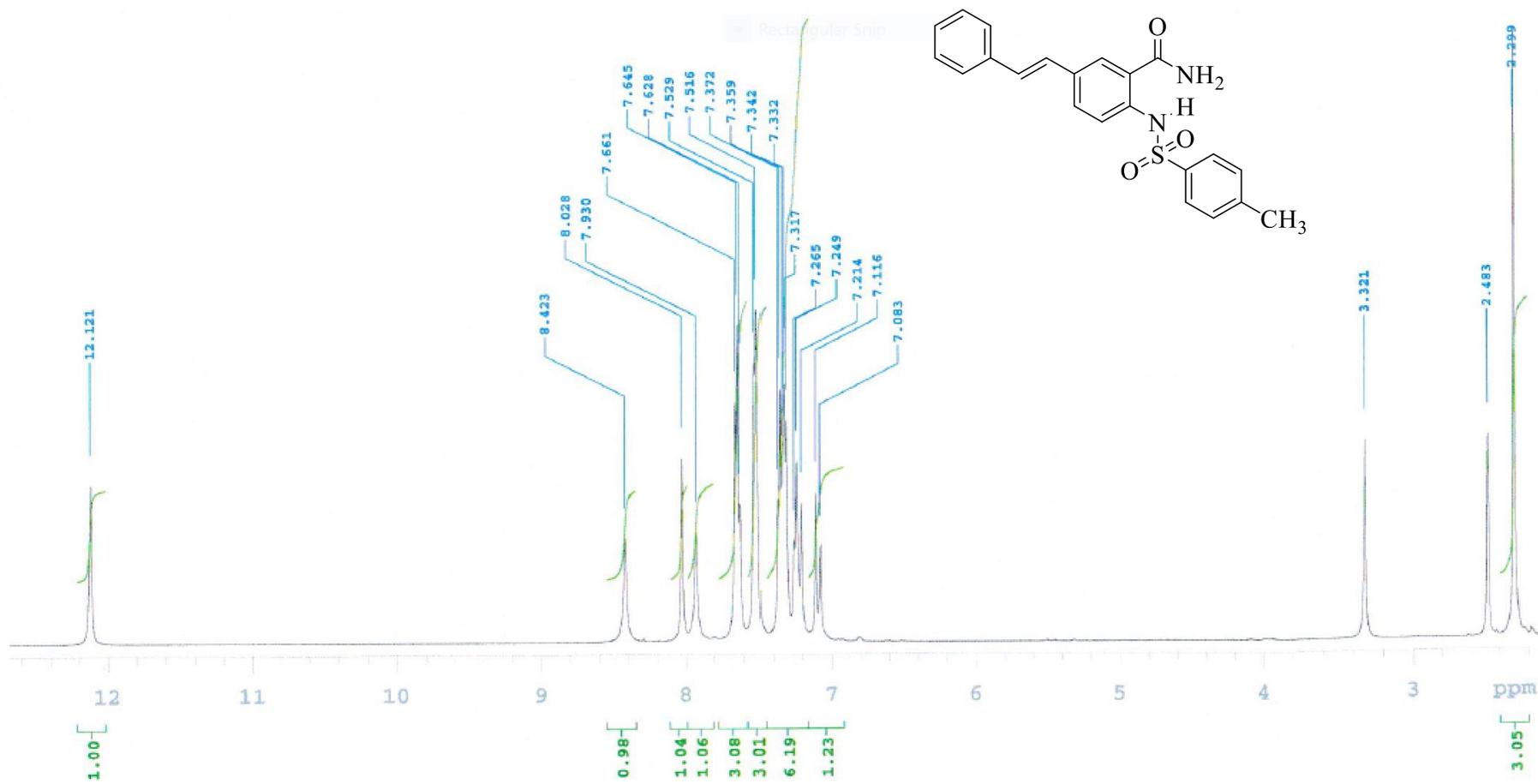


(a)

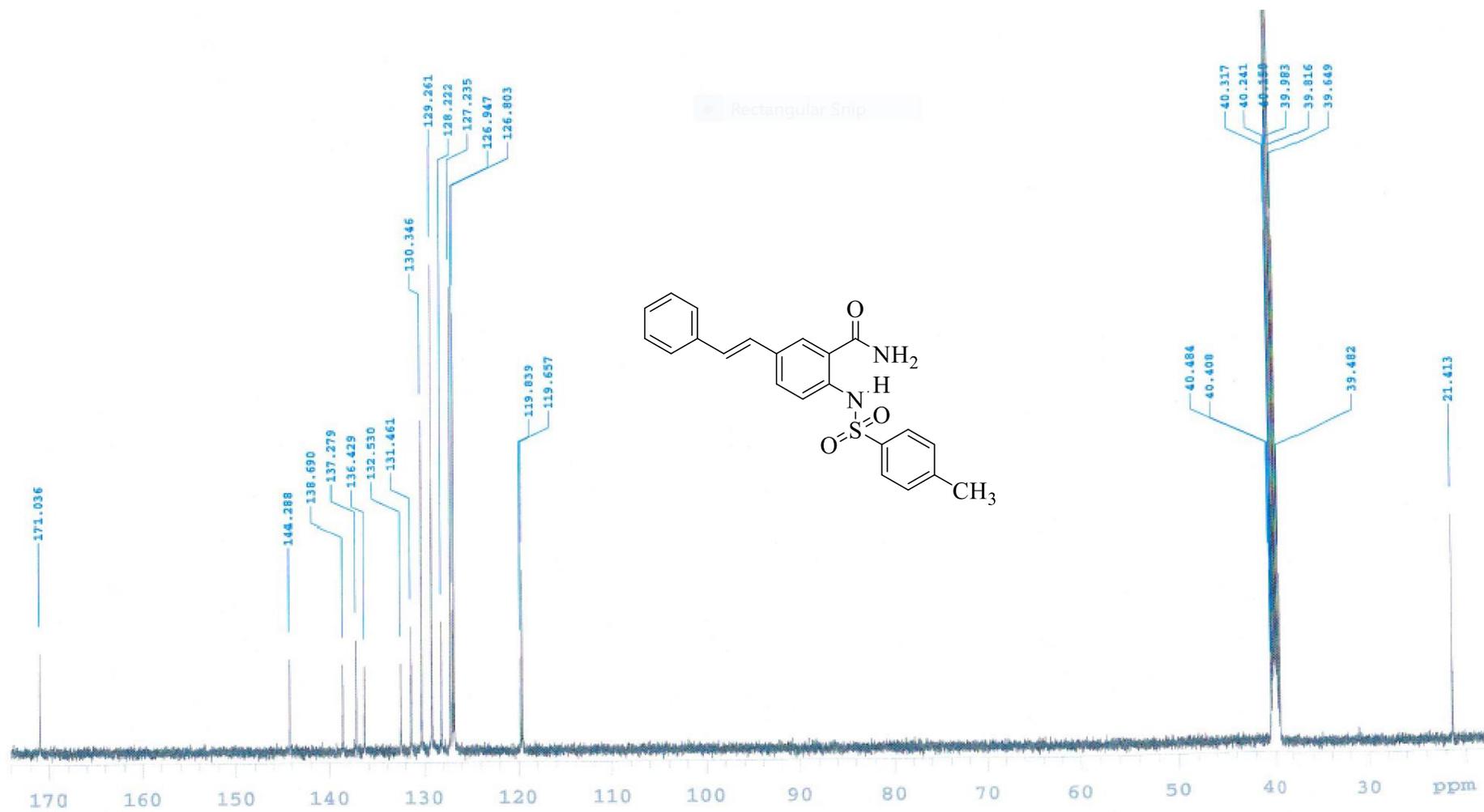


(b)

Figure S1.4: ¹H- and ¹³C-NMR of **2d** in DMSO-*d*₆ at 500 MHz (a) and 125 MHz (b), respectively.

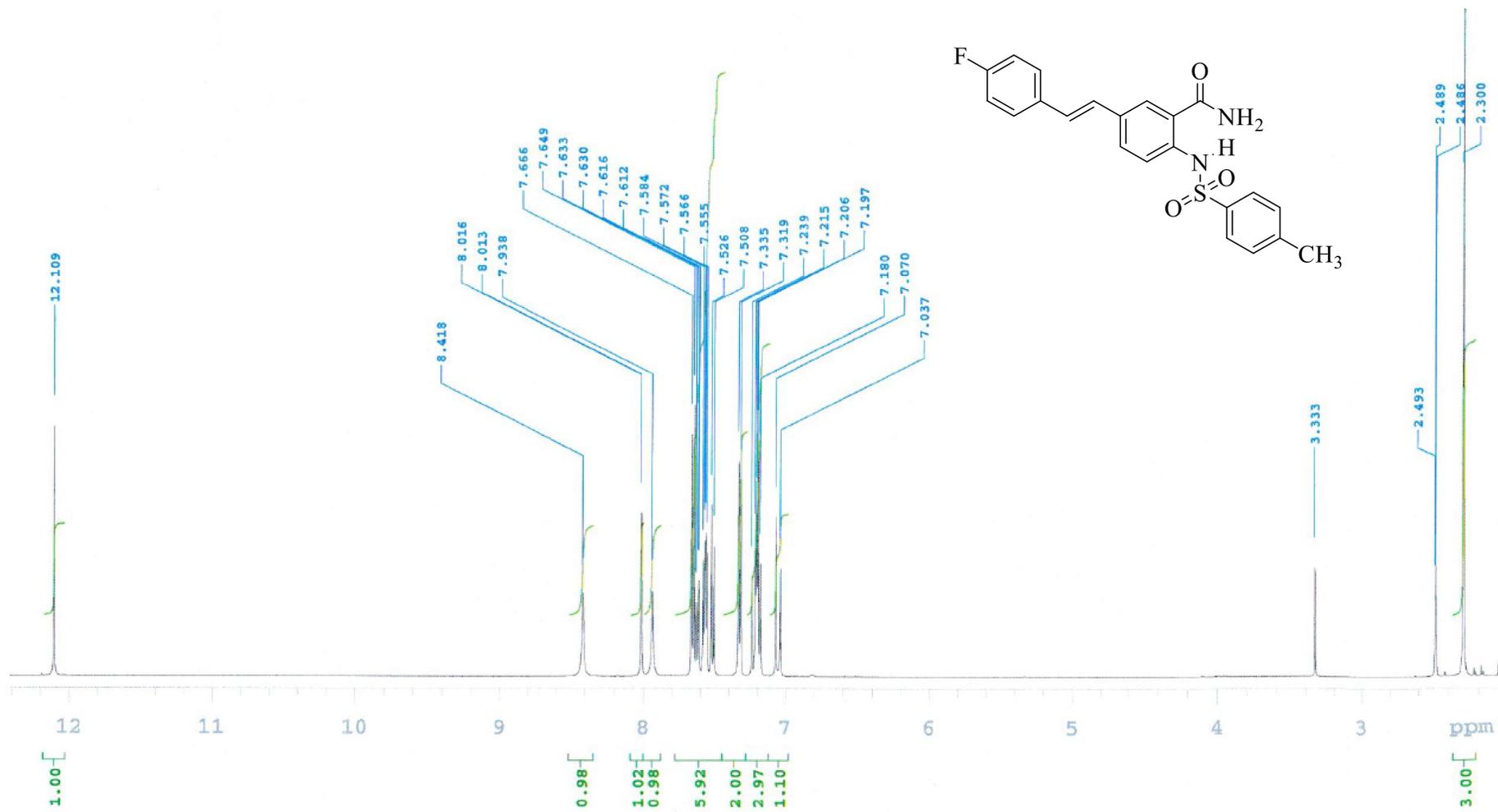


(a)

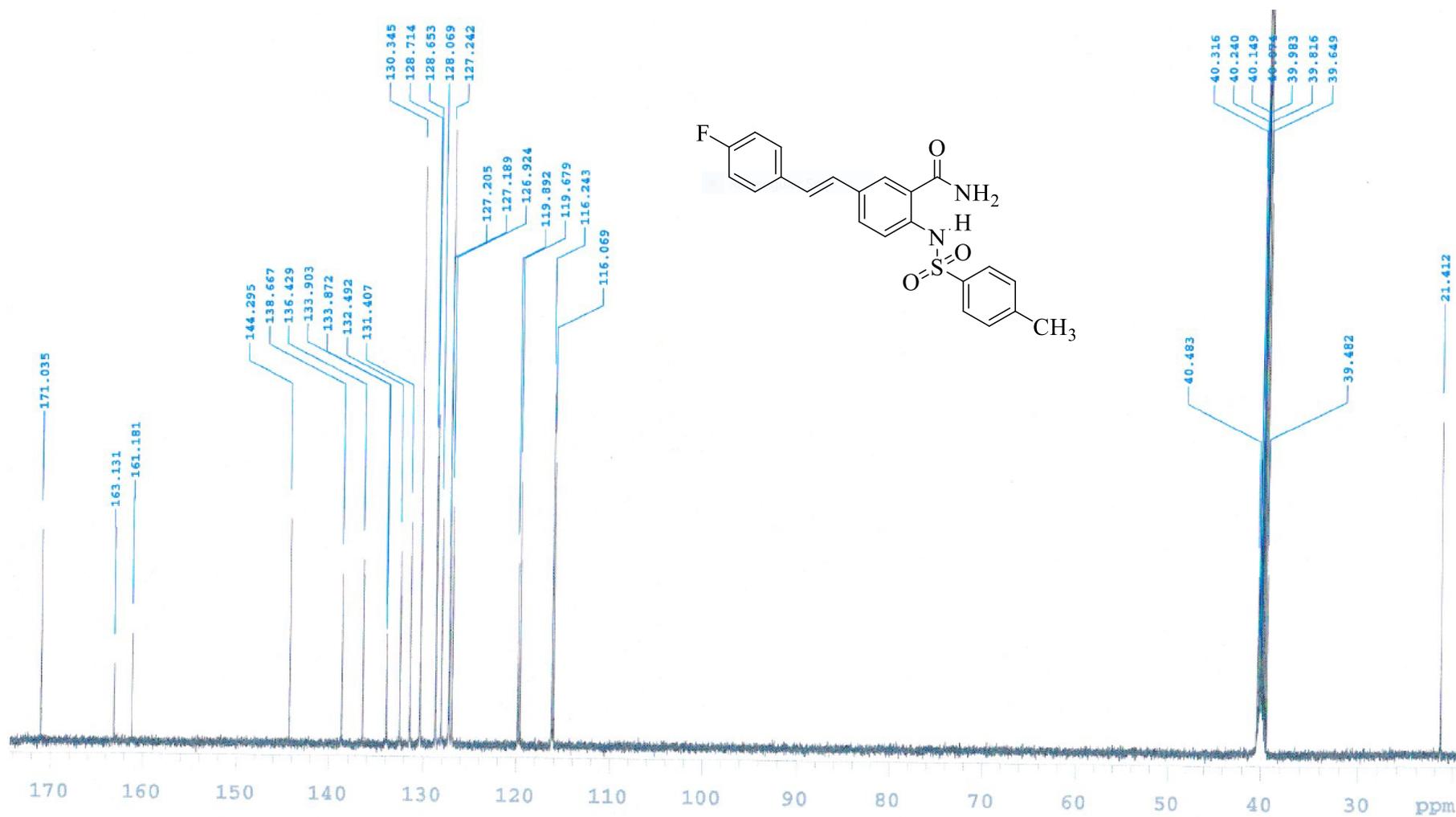


(b)

Figure S1.5: ^1H - and ^{13}C -NMR of **3a** in $\text{DMSO-}d_6$ at 500 MHz and 125 MHz, respectively.

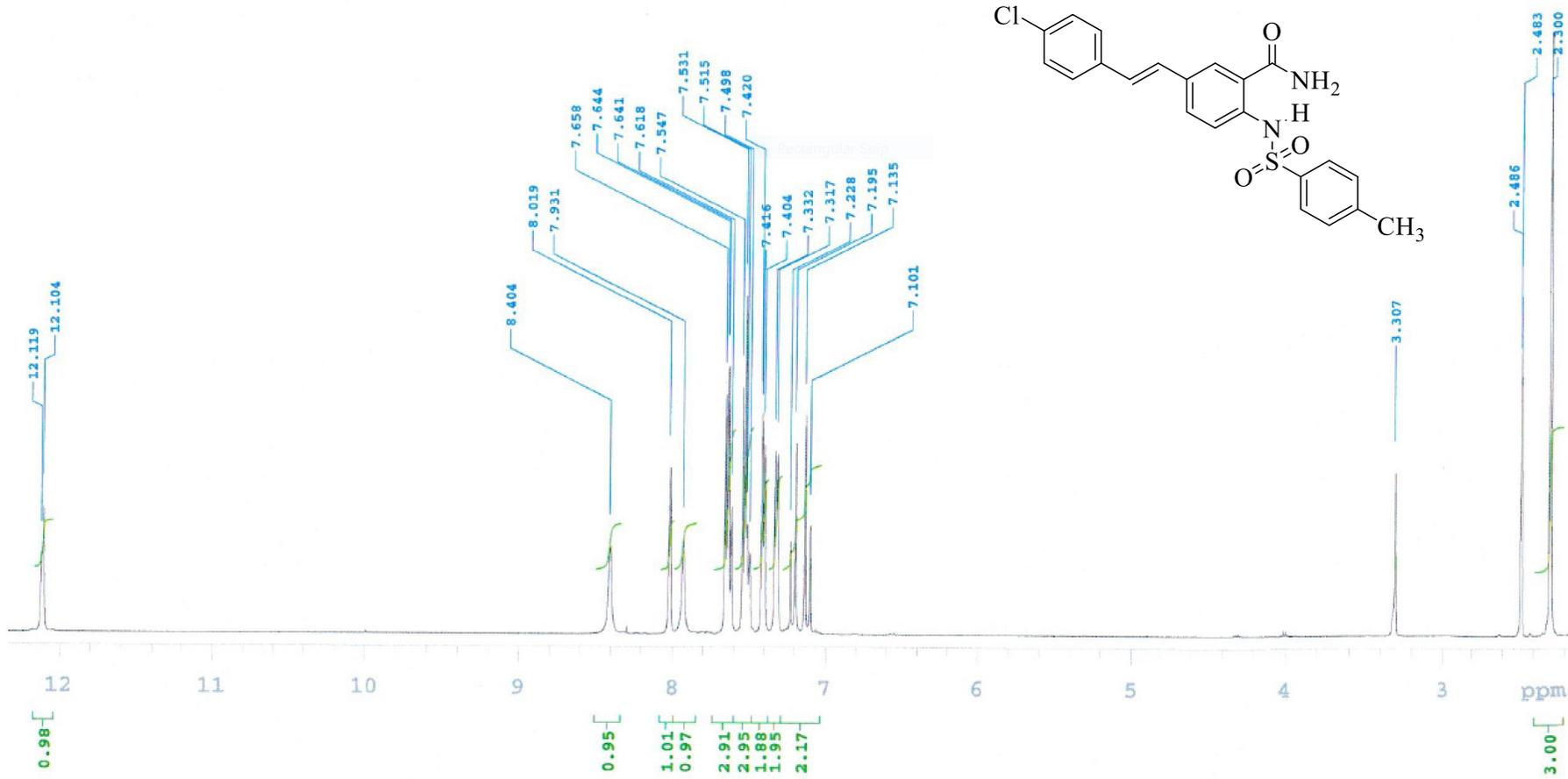


(a)

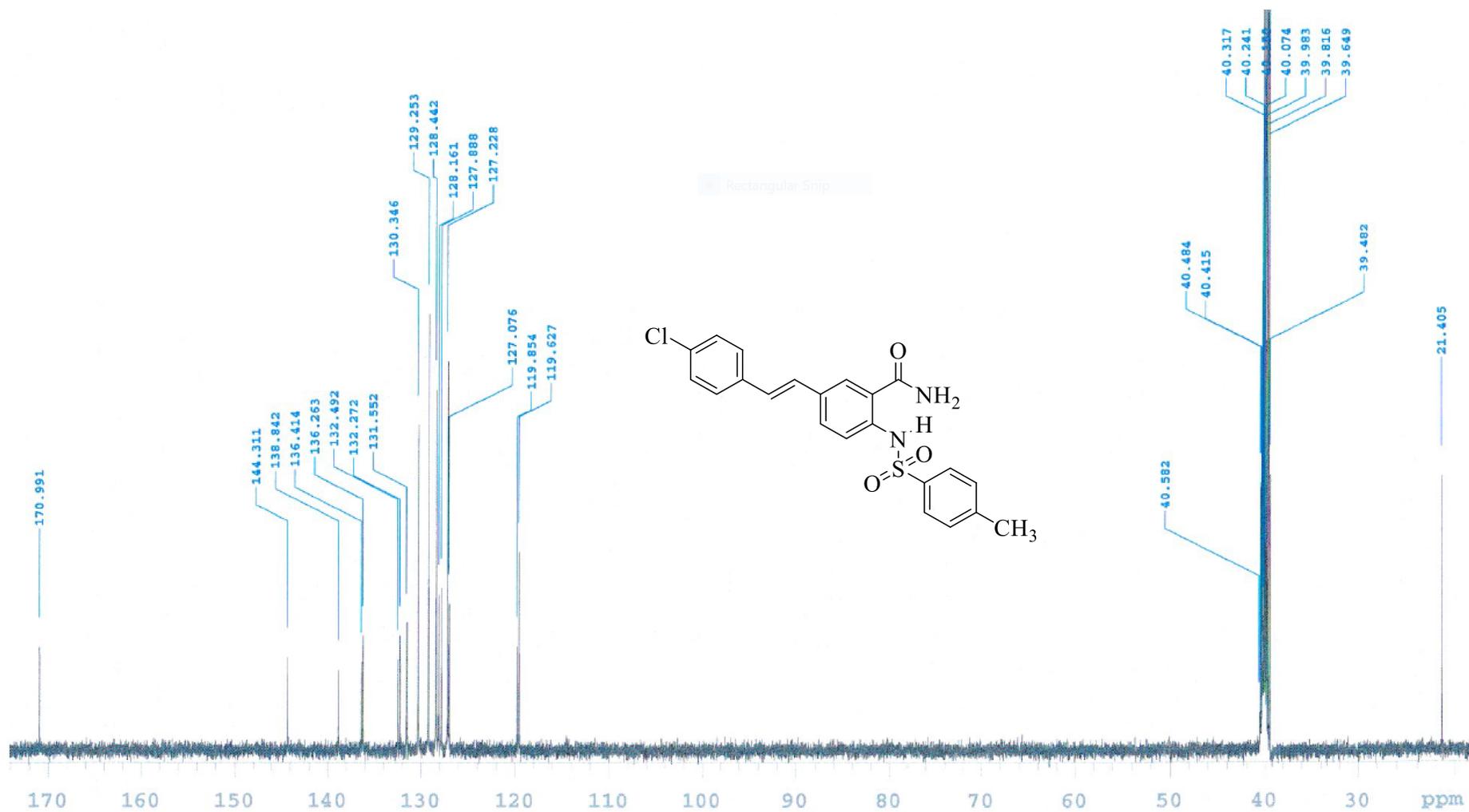


(b)

Figure S1.6: ¹H- and ¹³C-NMR of **3b** in DMSO-*d*₆ at 500 MHz (a) and 125 MHz (b), respectively.

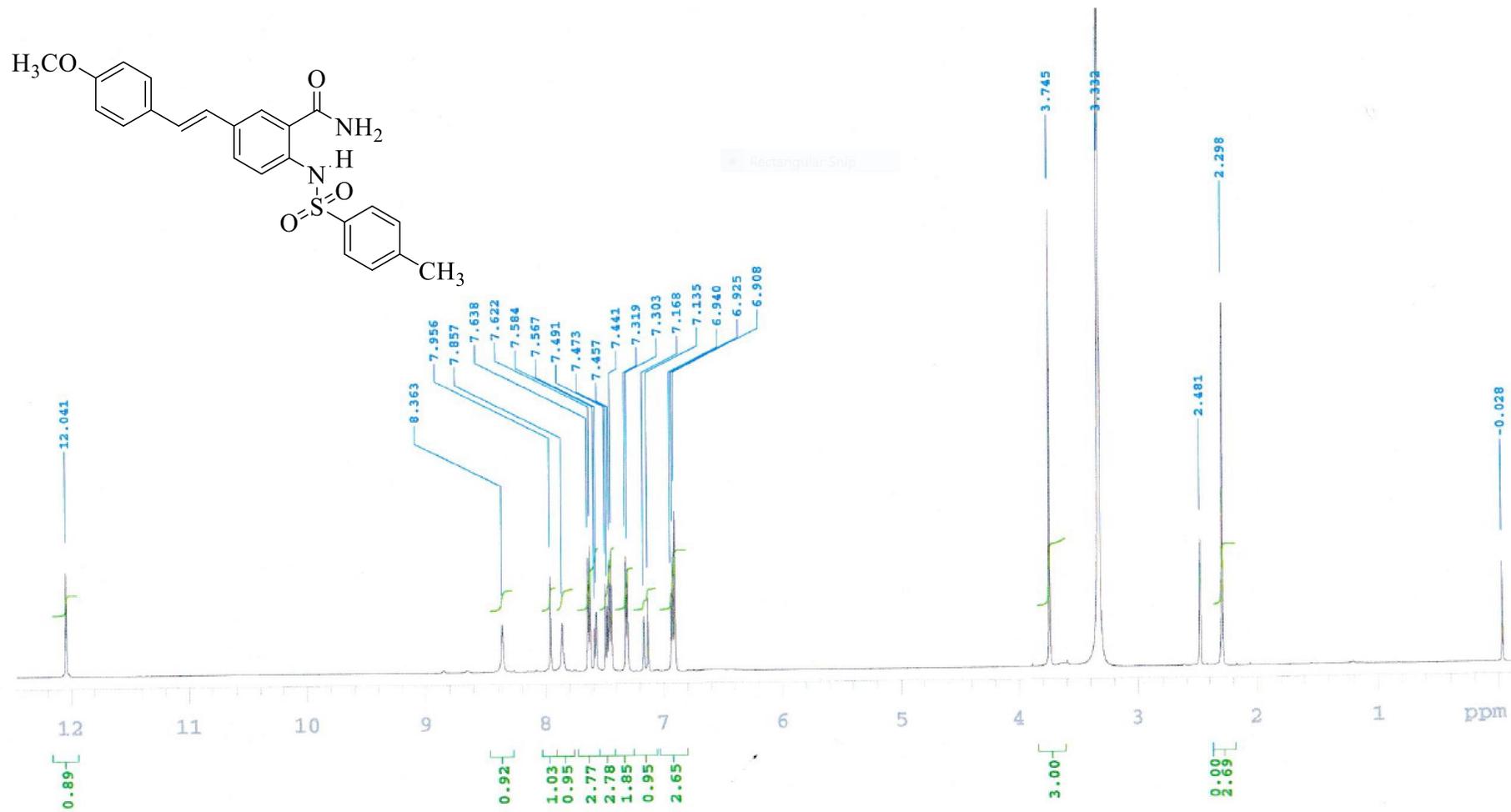


(a)

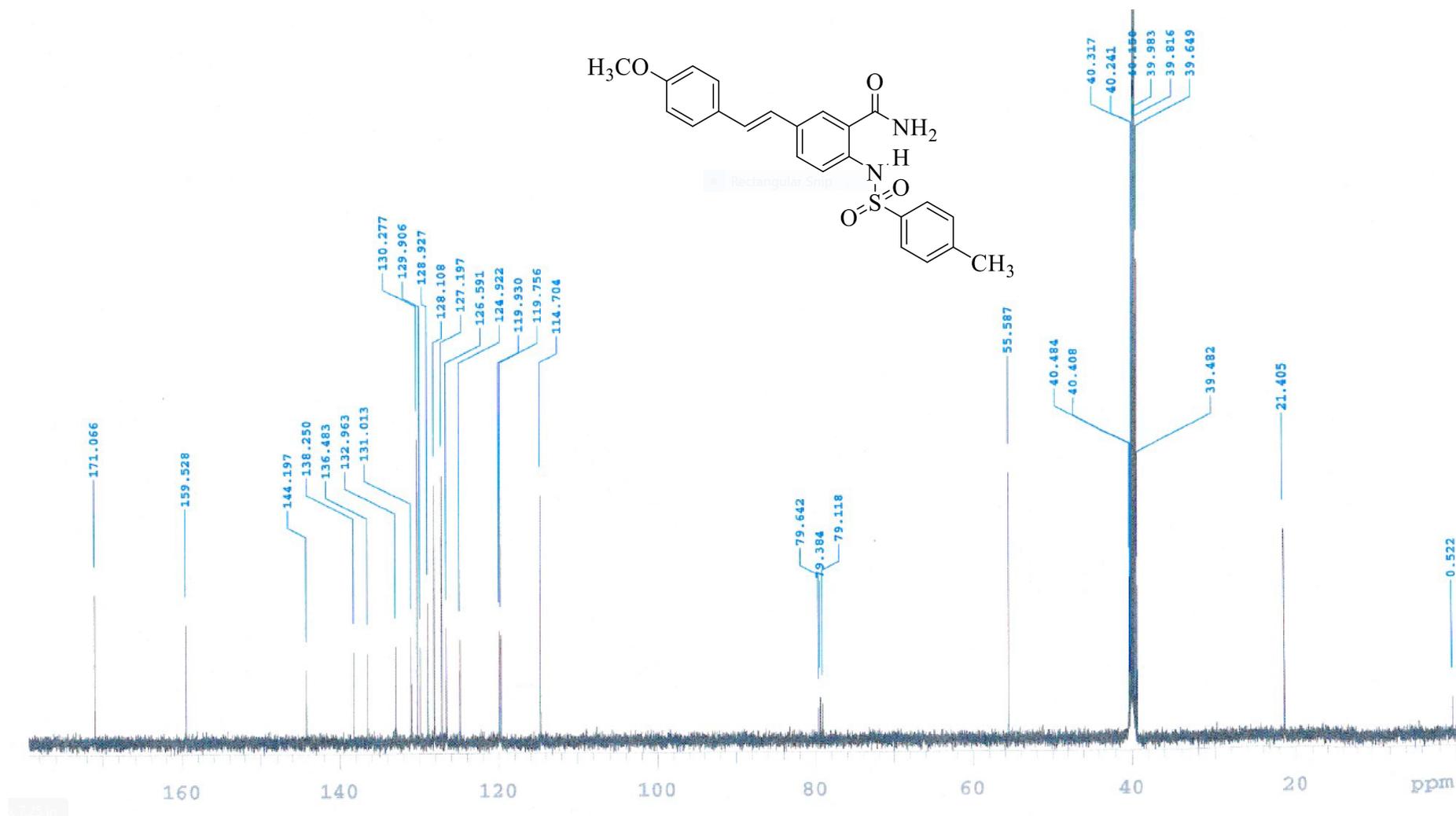


(b)

Figure S1.7: ¹H- and ¹³C-NMR of 3c in DMSO-*d*₆ at 500 MHz (a) and 125 MHz (b), respectively

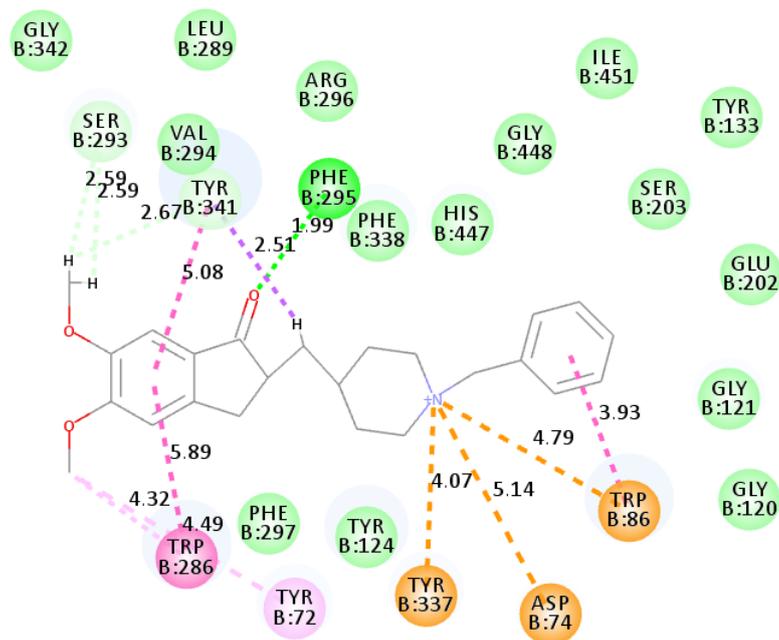


(a)



(b)

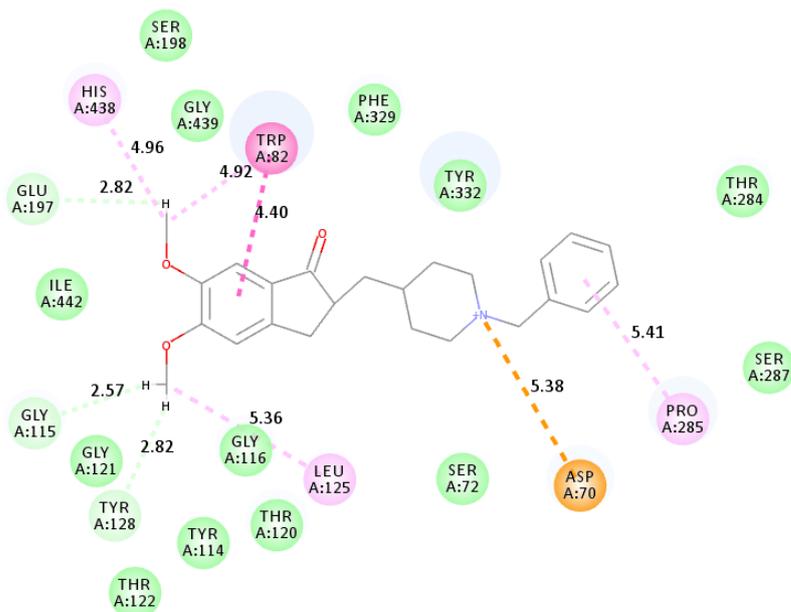
Figure S1.8: ¹H- and ¹³C-NMR of 3d in DMSO-*d*₆ at 500 MHz (a) and 125 MHz (b), respectively.



Interactions

- | | |
|----------------------------|---------------|
| van der Waals | Pi-Cation |
| Attractive Charge | Pi-Sigma |
| Conventional Hydrogen Bond | Pi-Pi Stacked |
| Carbon Hydrogen Bond | Pi-Alkyl |

(a)



Interactions

- | | |
|----------------------|---------------|
| van der Waals | Pi-Pi Stacked |
| Attractive Charge | Alkyl |
| Carbon Hydrogen Bond | Pi-Alkyl |

(b)

Figure S2: The 2-dimensional (2D) plots of docking results for donepezil into AChE (**a**) and BChE (**b**), including bonding interaction distances and colour codes for various interactions.