

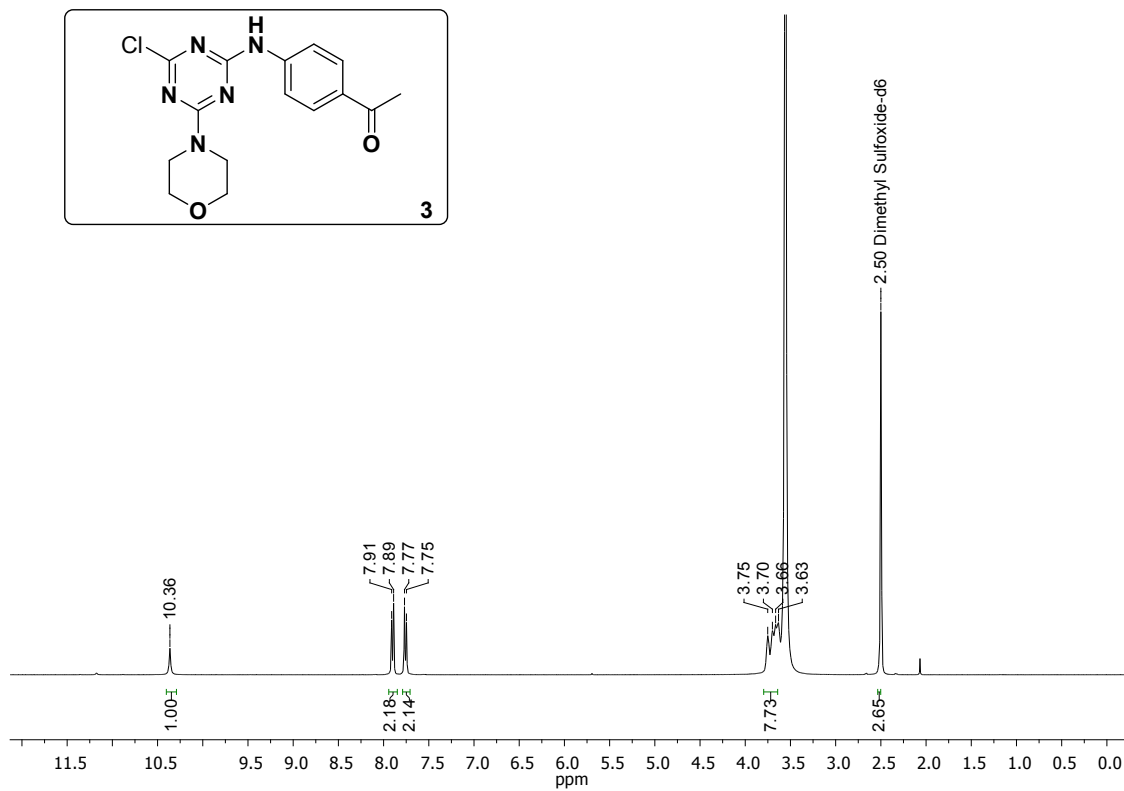
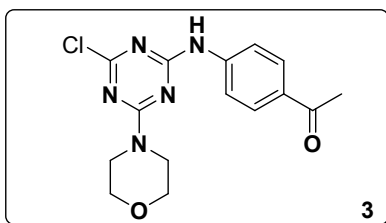
Synthesis, biological evaluation, and *in silico* studies of novel chalcone- and pyrazoline-based 1,3,5-triazine as potential anticancer agents

Leydi M. Moreno,^a Jairo Quiroga,^{a,b} Rodrigo Abonia,^{a,b} Antonino Lauria,^c Annamaria Martorana,^c Henry Insuasty^d and Braulio Insuasty^{*a,b}

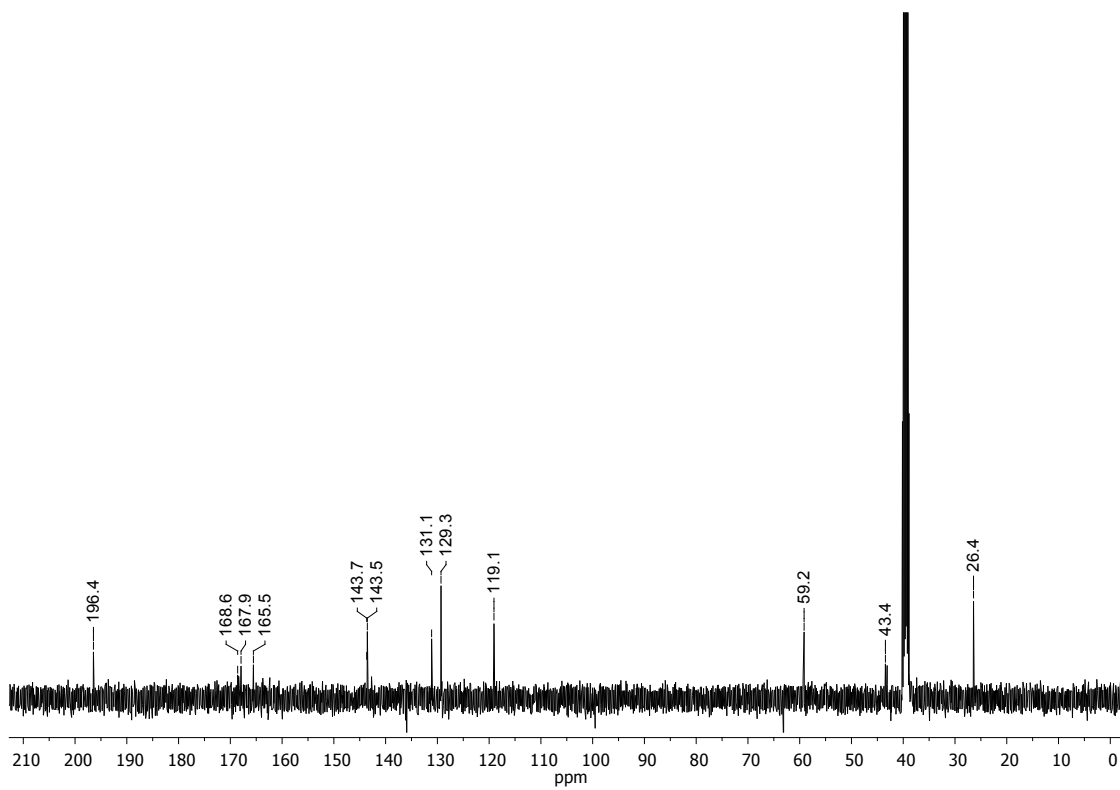
^aHeterocyclic Compounds Research Group, Department of Chemistry, Universidad del Valle, A.A. 25360 Cali, Colombia. E-mail: braulio.insuasty@correounivalle.edu.co. ^bCenter for Bioinformatics and Photonics-CIBioFI, A.A. 25360 Cali, Colombia. ^dDipartimento di Scienze e Tecnologie Biologiche Chimiche e Farmaceutiche "STEBICEF", Università di Palermo, Viale delle Scienze Ed. 17, I-90128 Palermo, Italy. ^eHeterocyclic Compounds Research Group, Department of Chemistry, Universidad de Nariño, A.A. 1175 Pasto, Colombia

Electronic Supplementary Material (ESI)

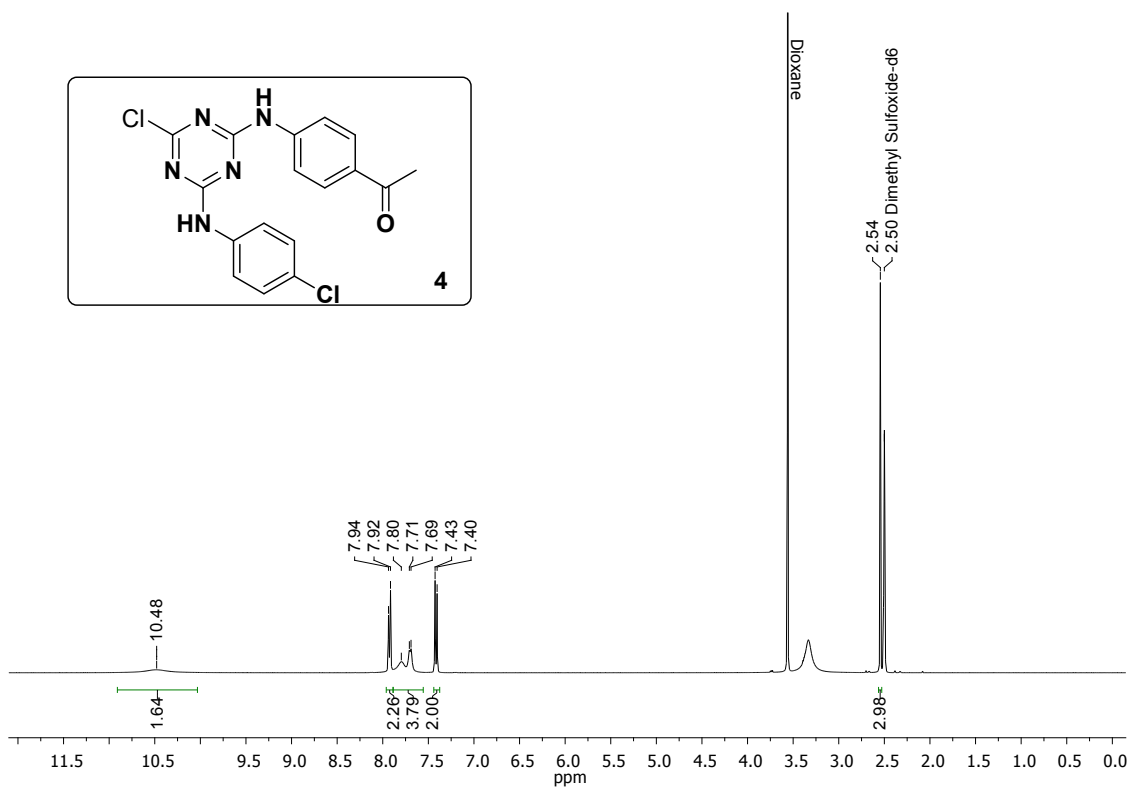
NMR spectra of synthesized compounds.....S2-33



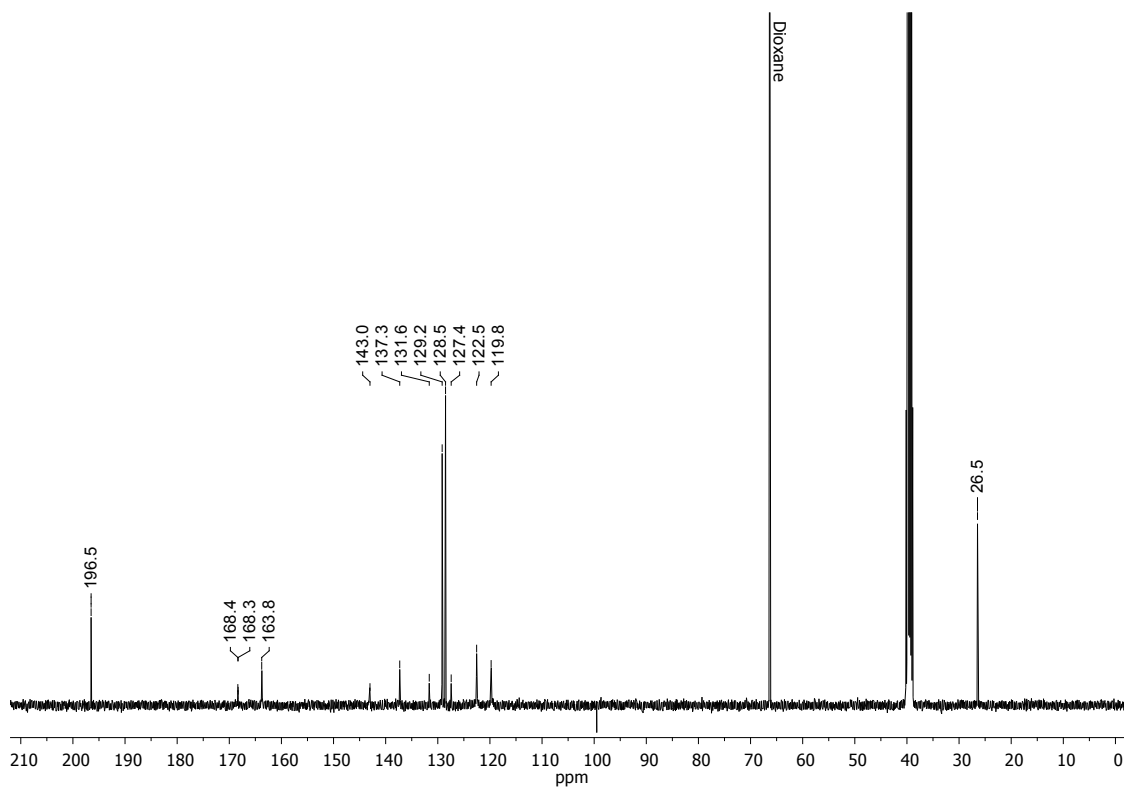
^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of **3**.



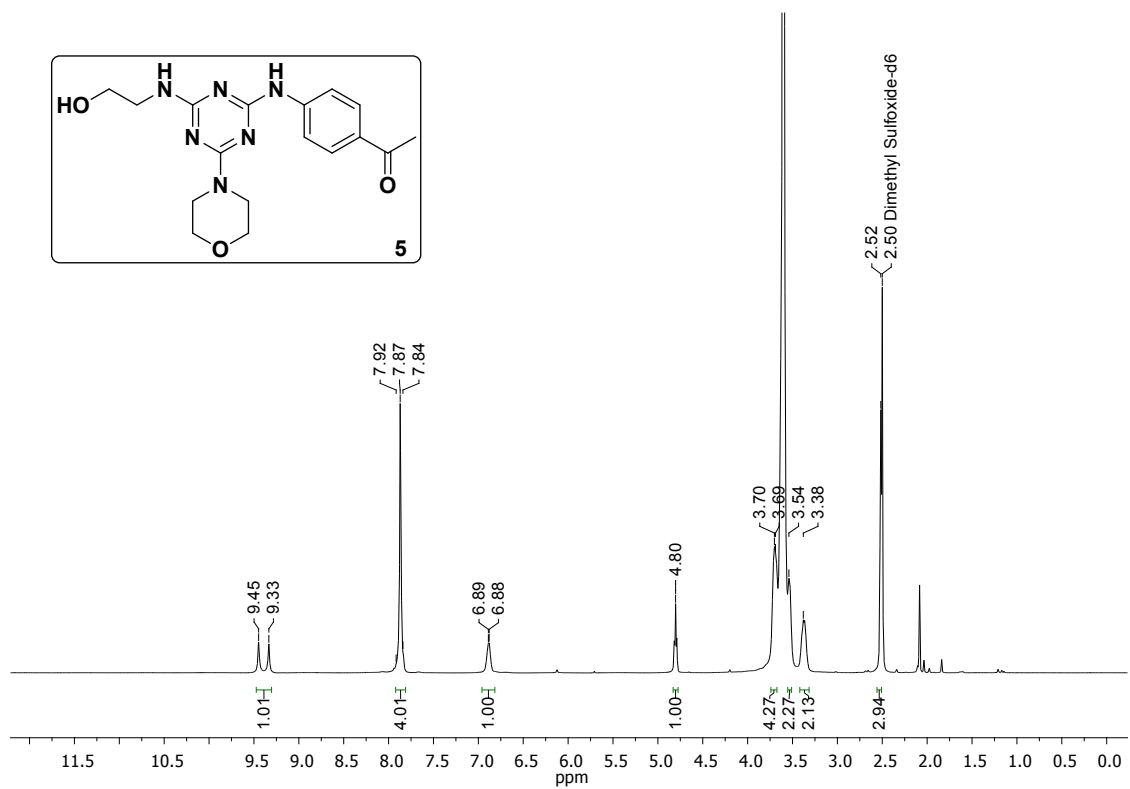
^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of **3**.



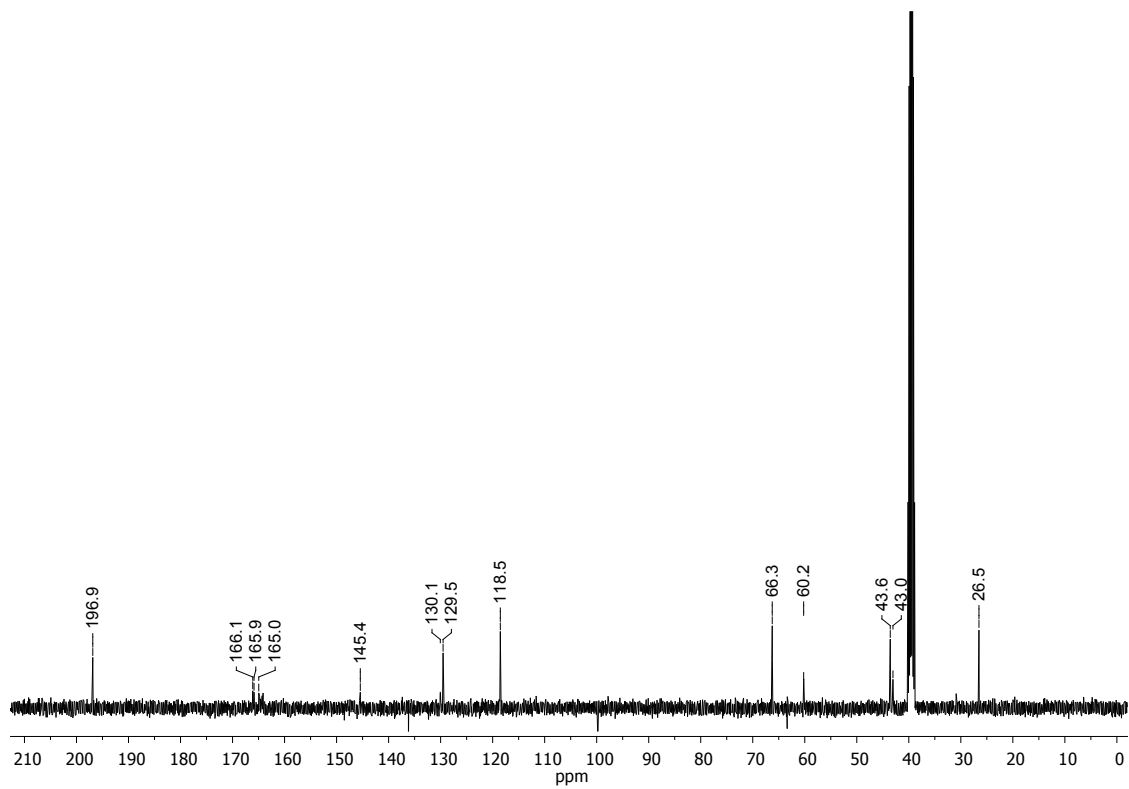
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **4**.



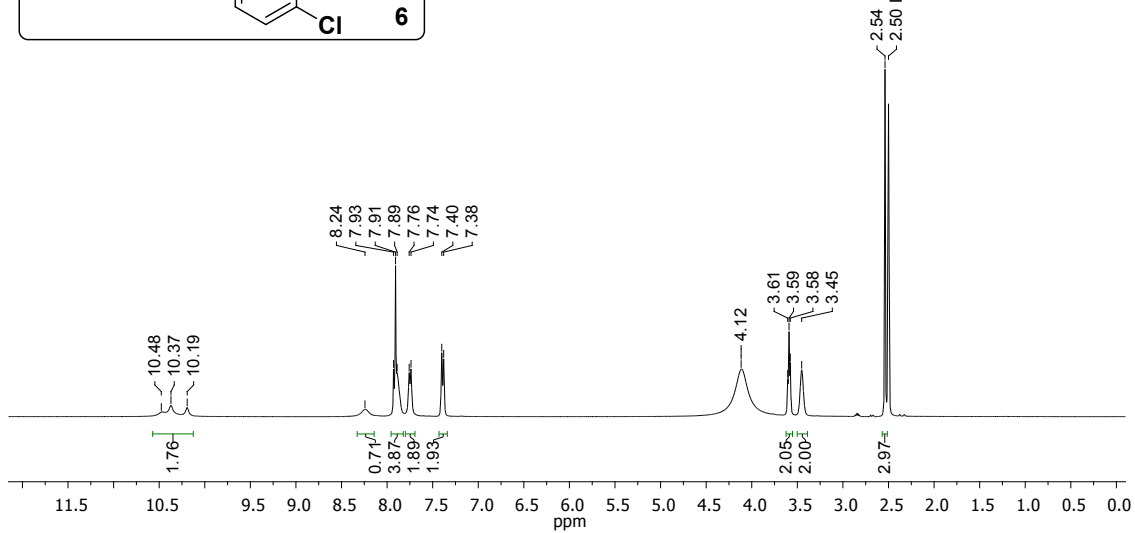
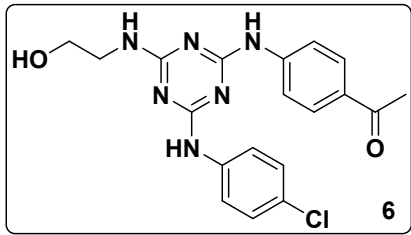
¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of **4**.



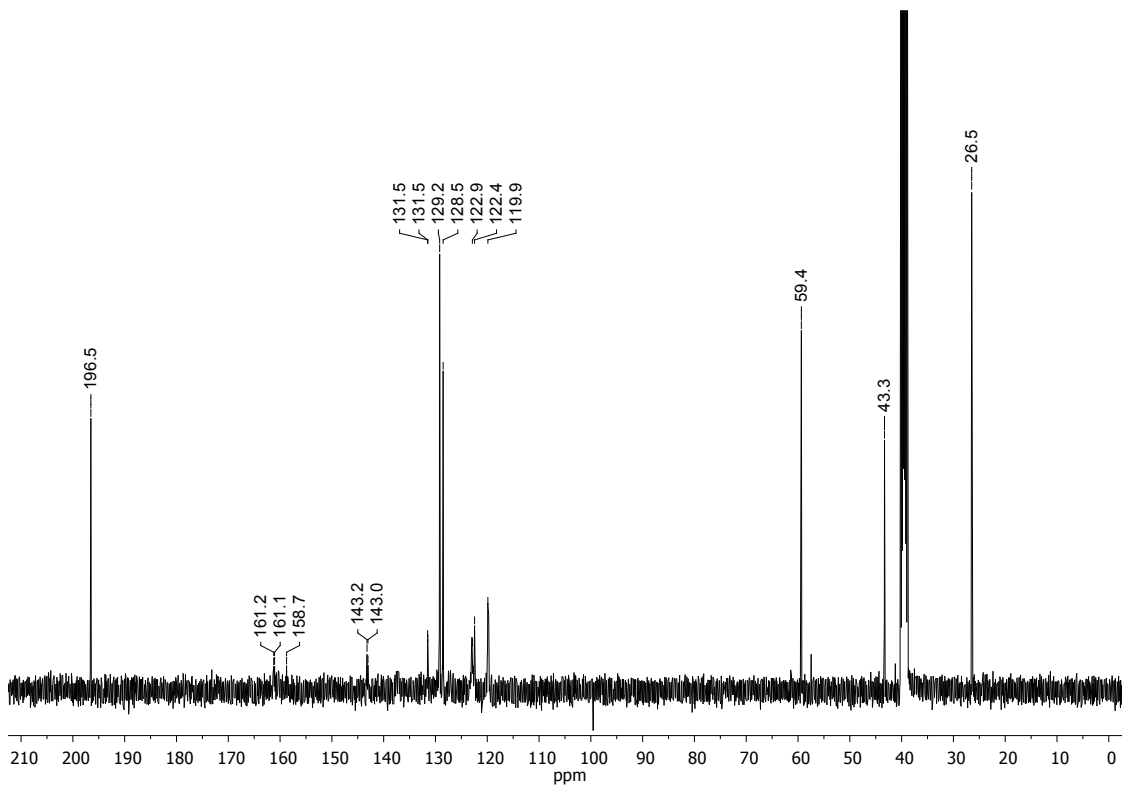
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **5**.



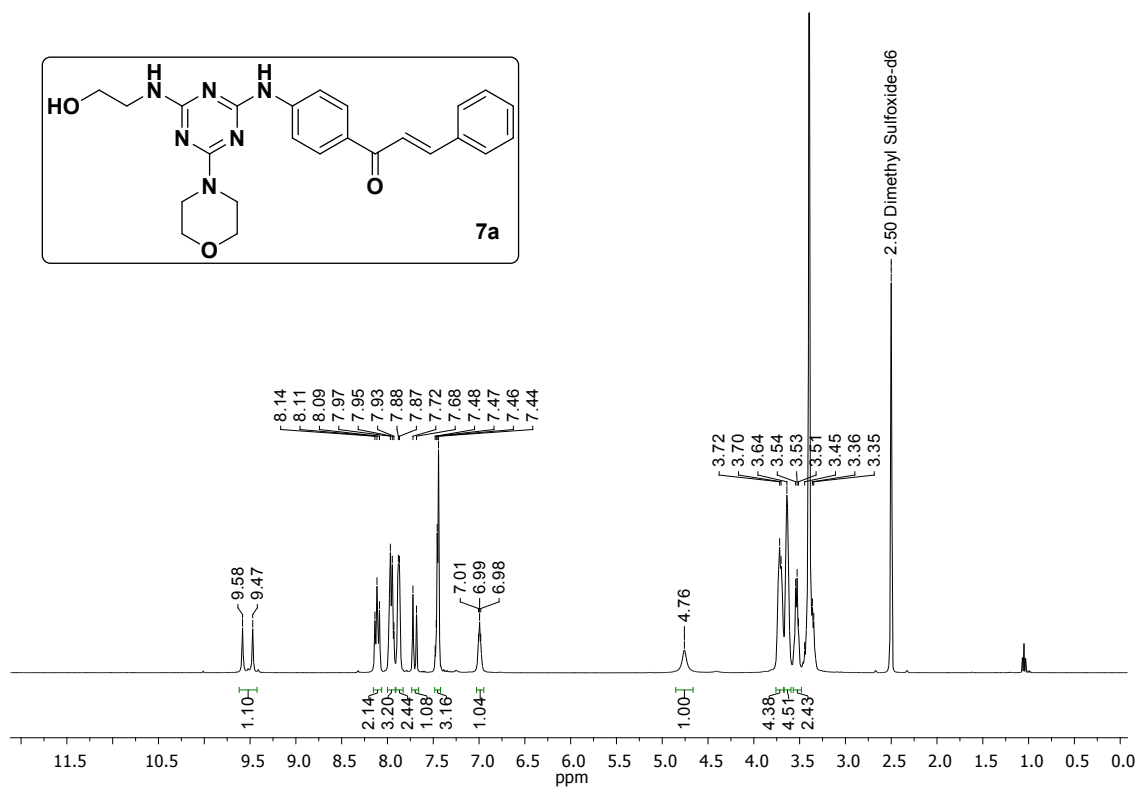
¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of **5**.



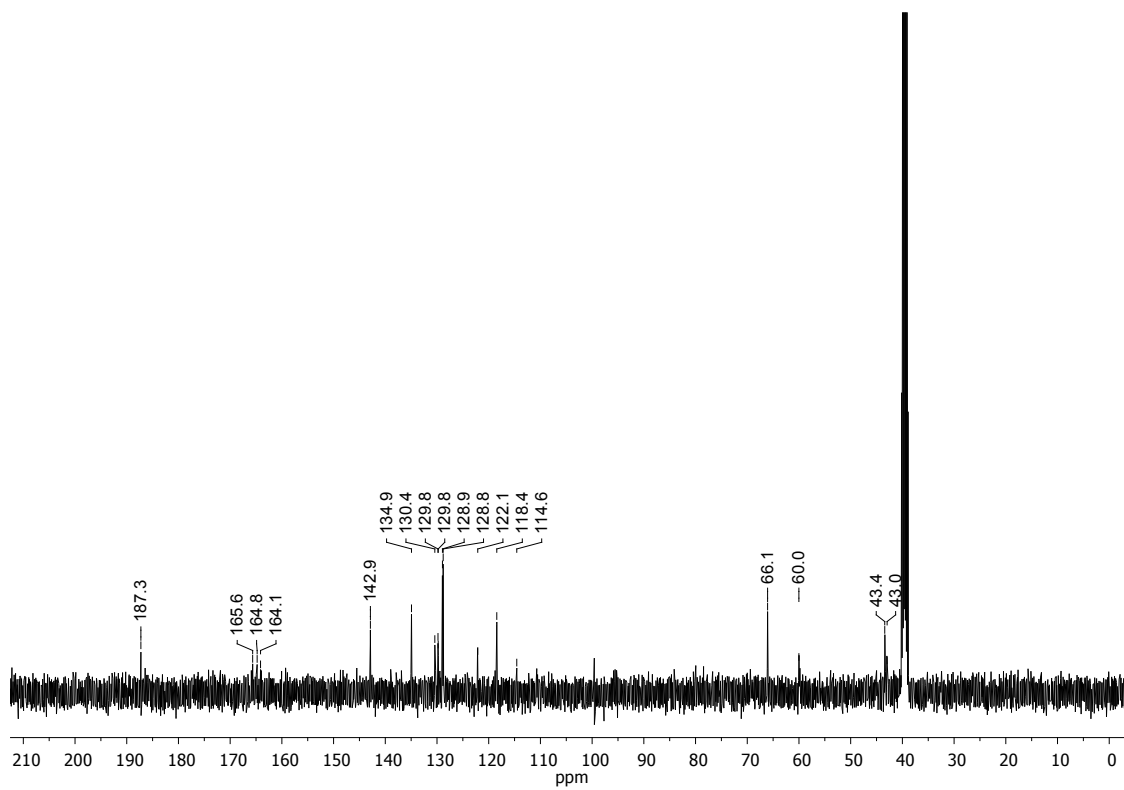
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **6**.



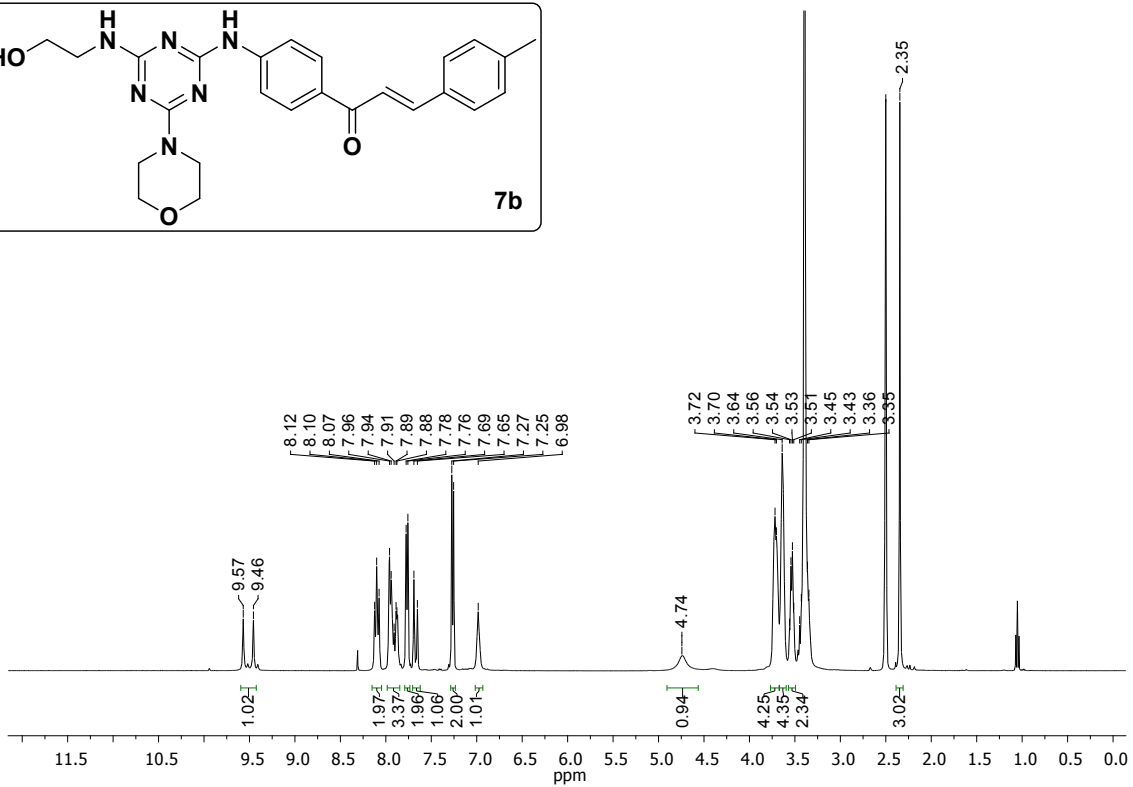
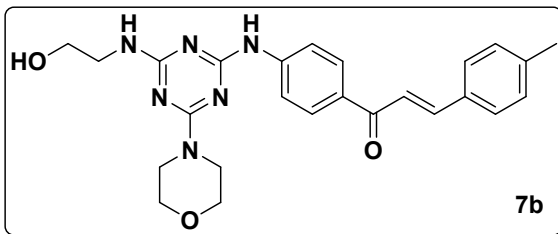
¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of **6**.



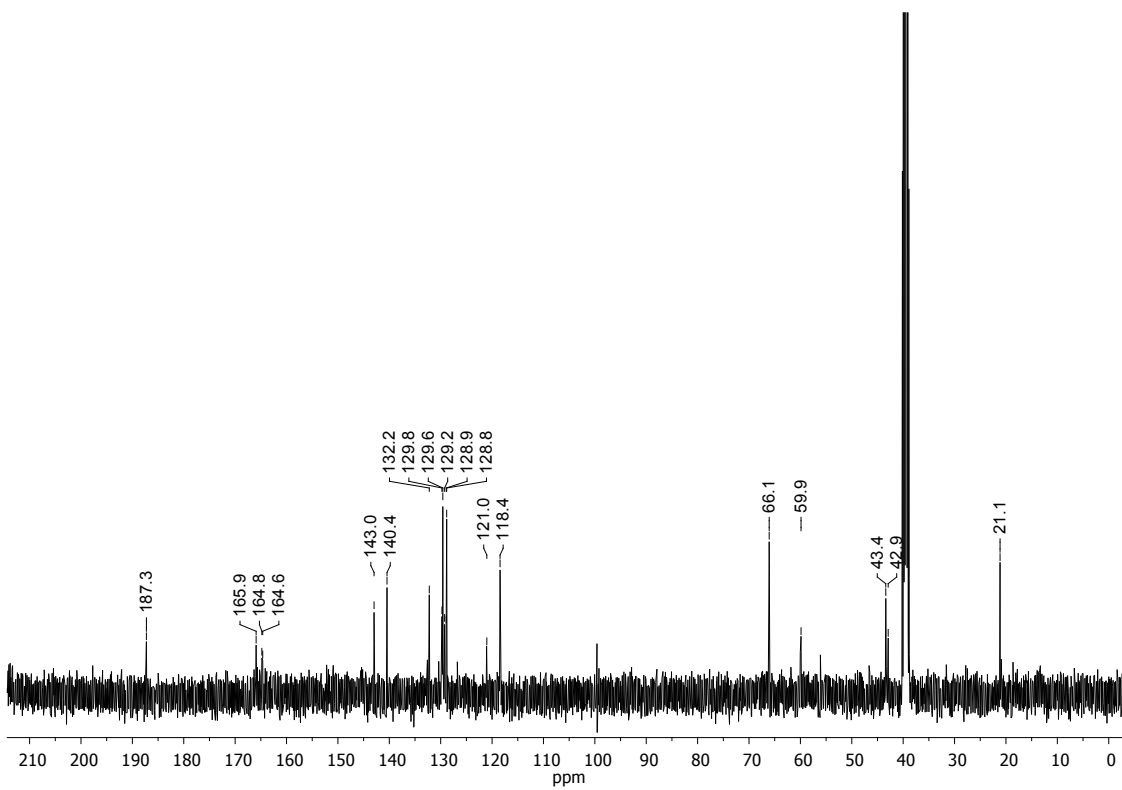
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **7a**.



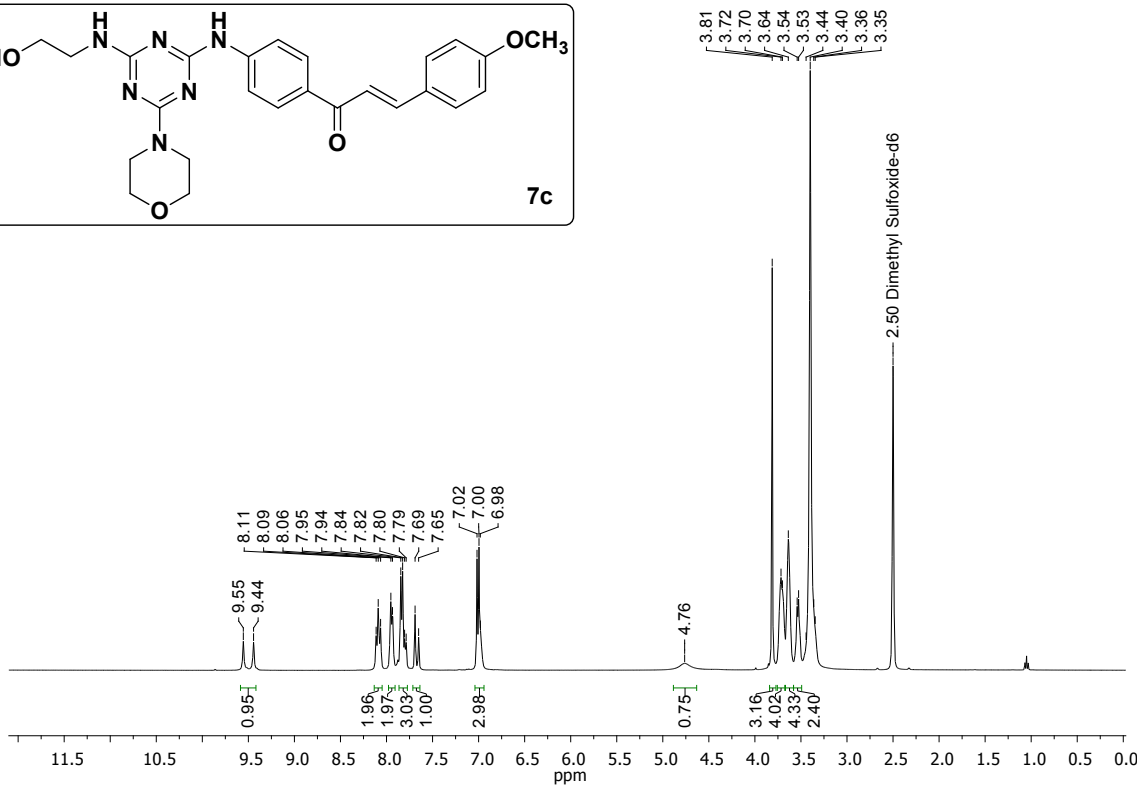
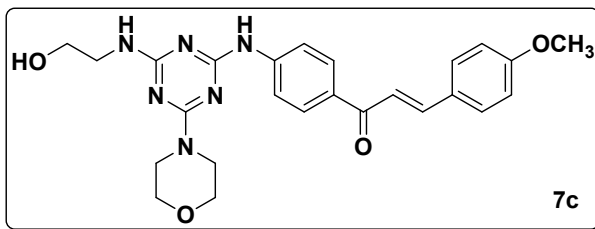
¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of **7a**.



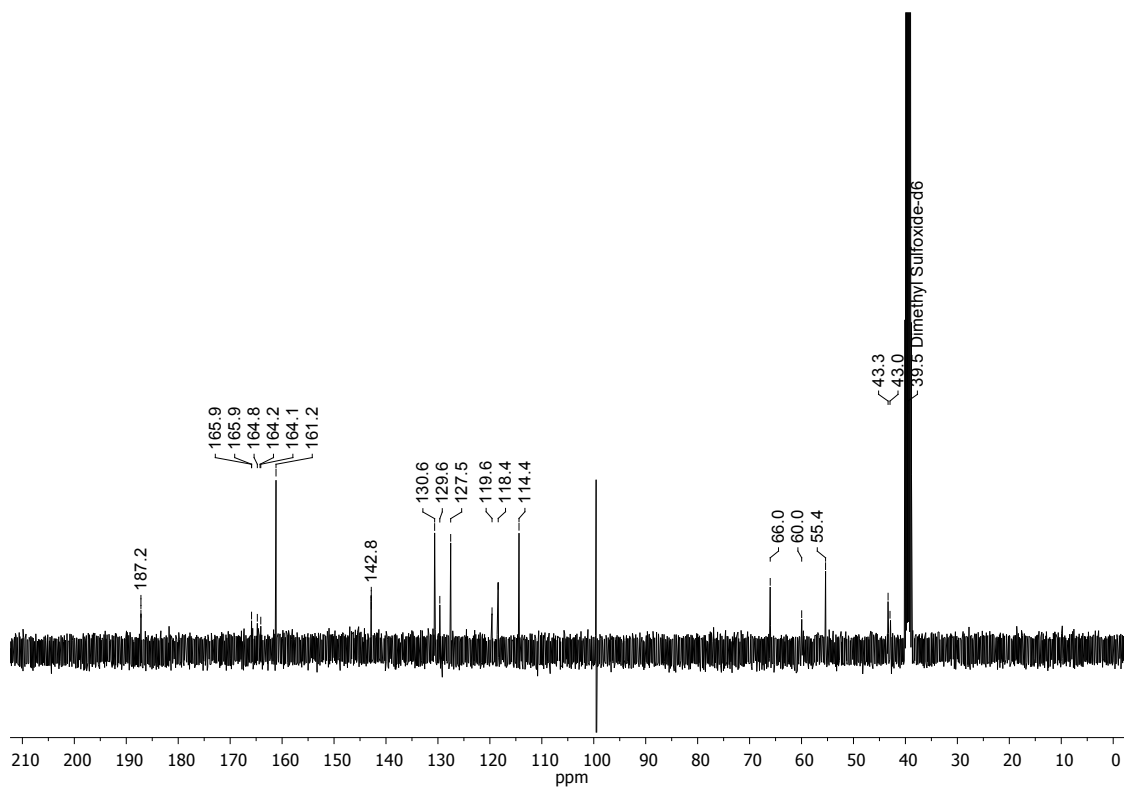
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **7b**.



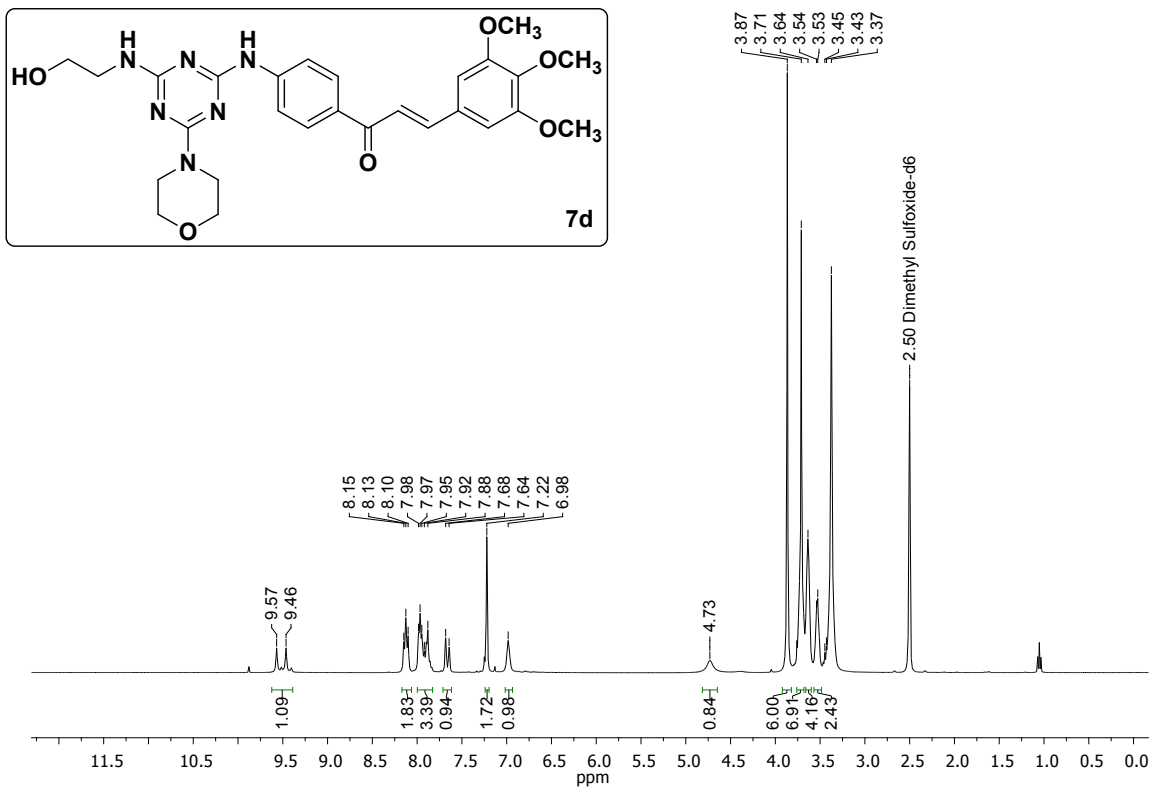
¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of **7b**.



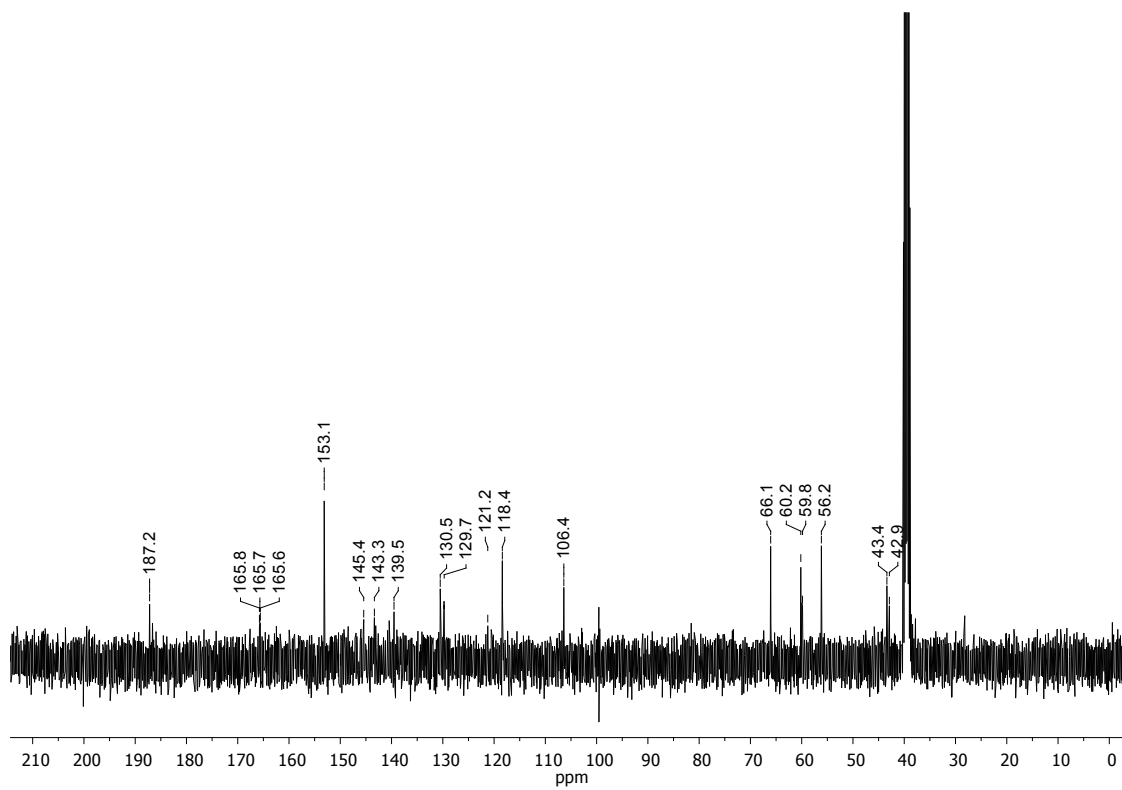
^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of **7c**.



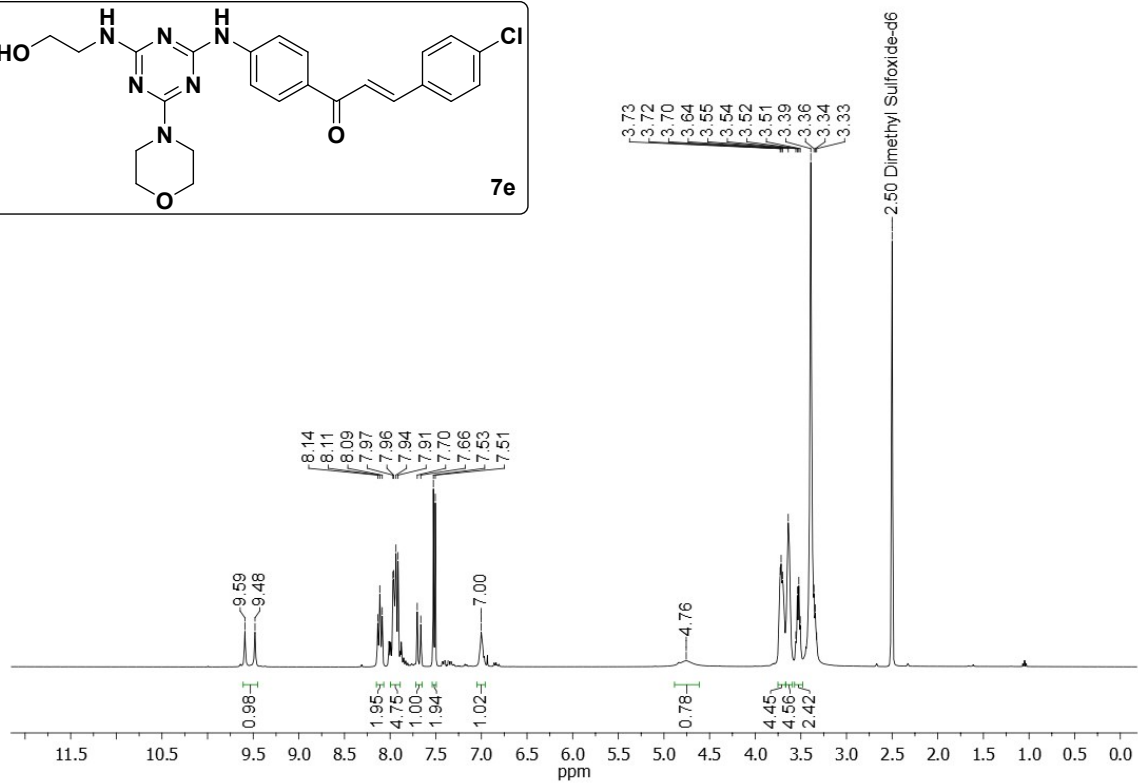
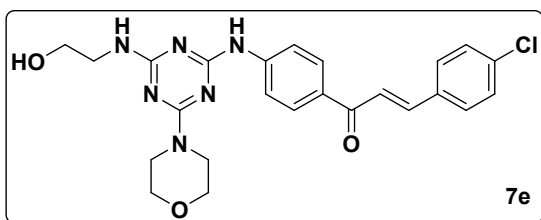
^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of **7c**.



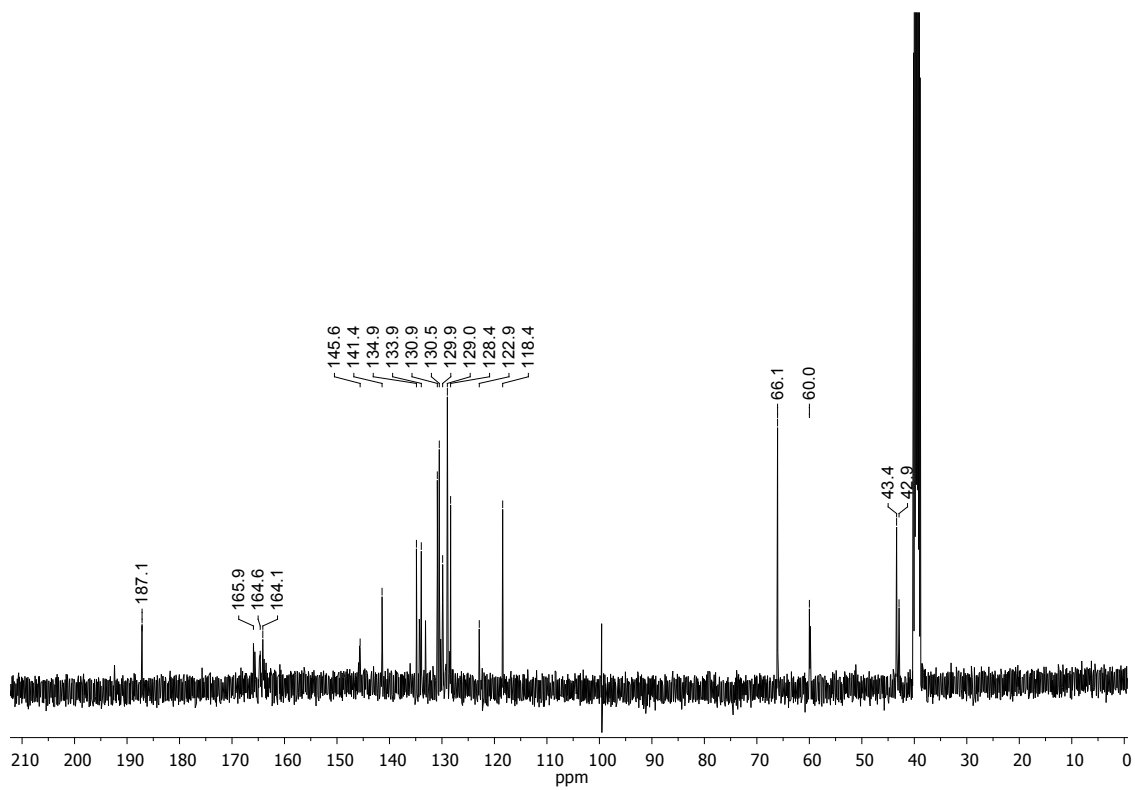
$^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) spectrum of **7d**.



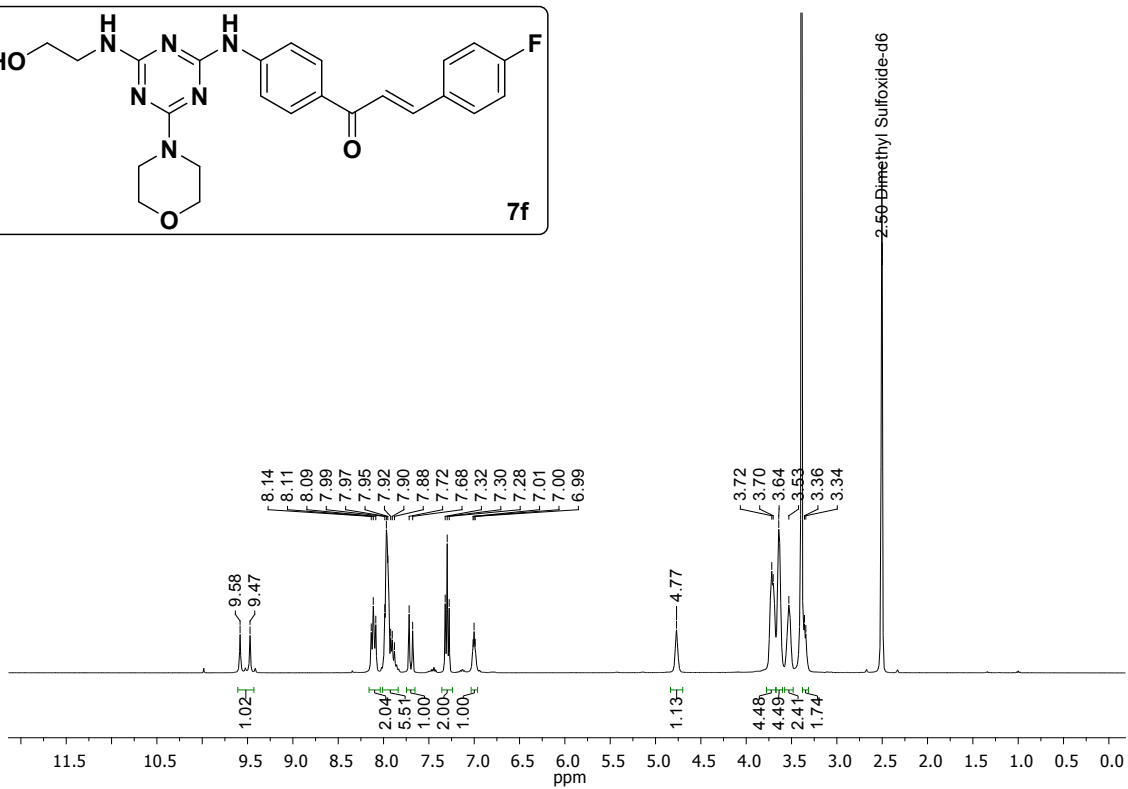
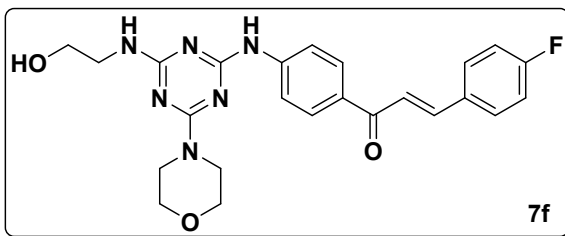
$^{13}\text{C NMR}$ (100 MHz, $\text{DMSO-}d_6$) spectrum of **7d**.



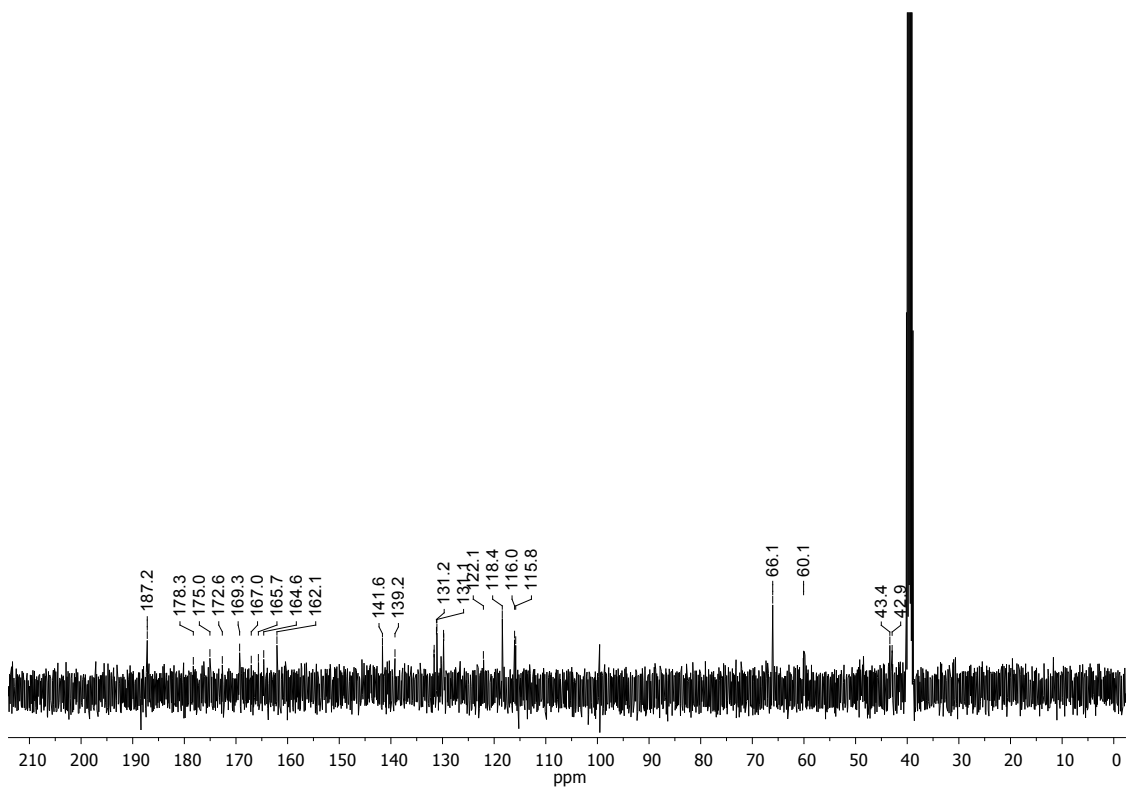
^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of **7e**.



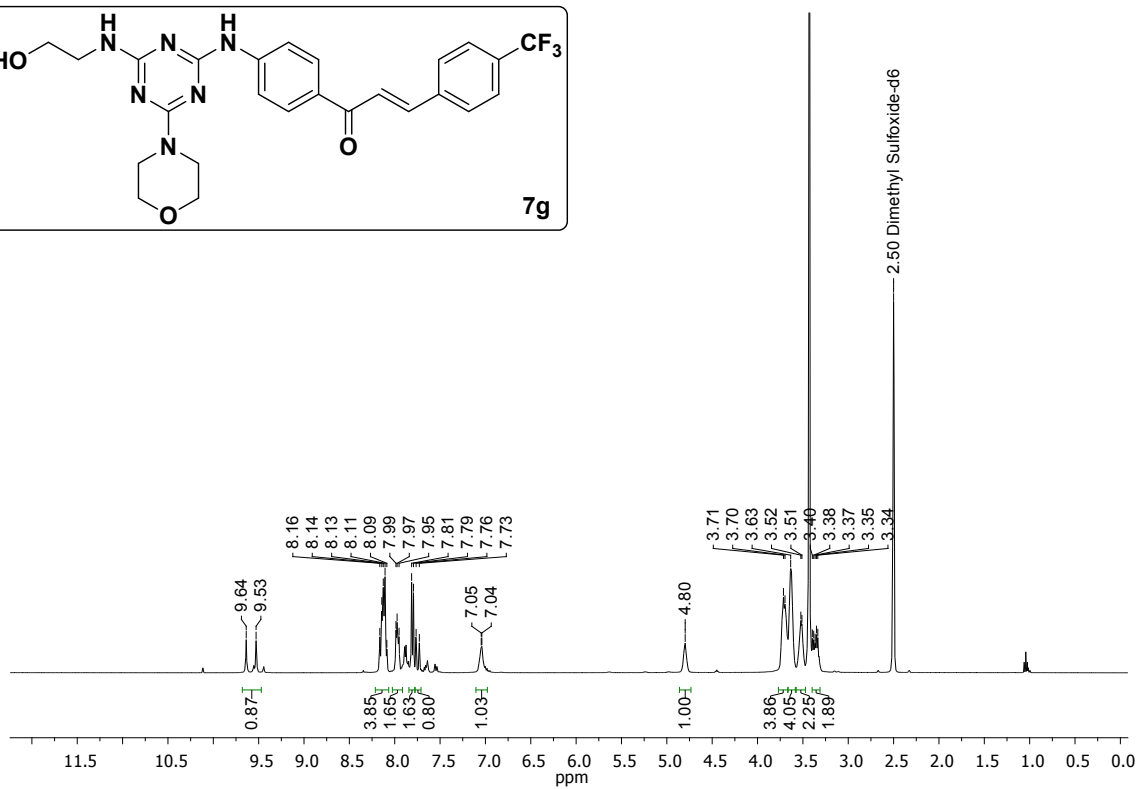
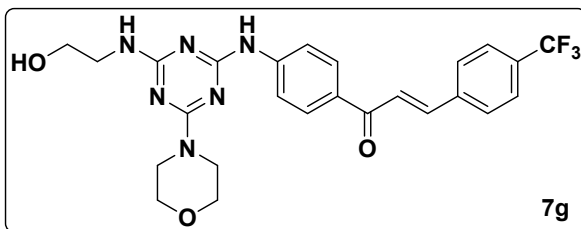
^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of **7e**.



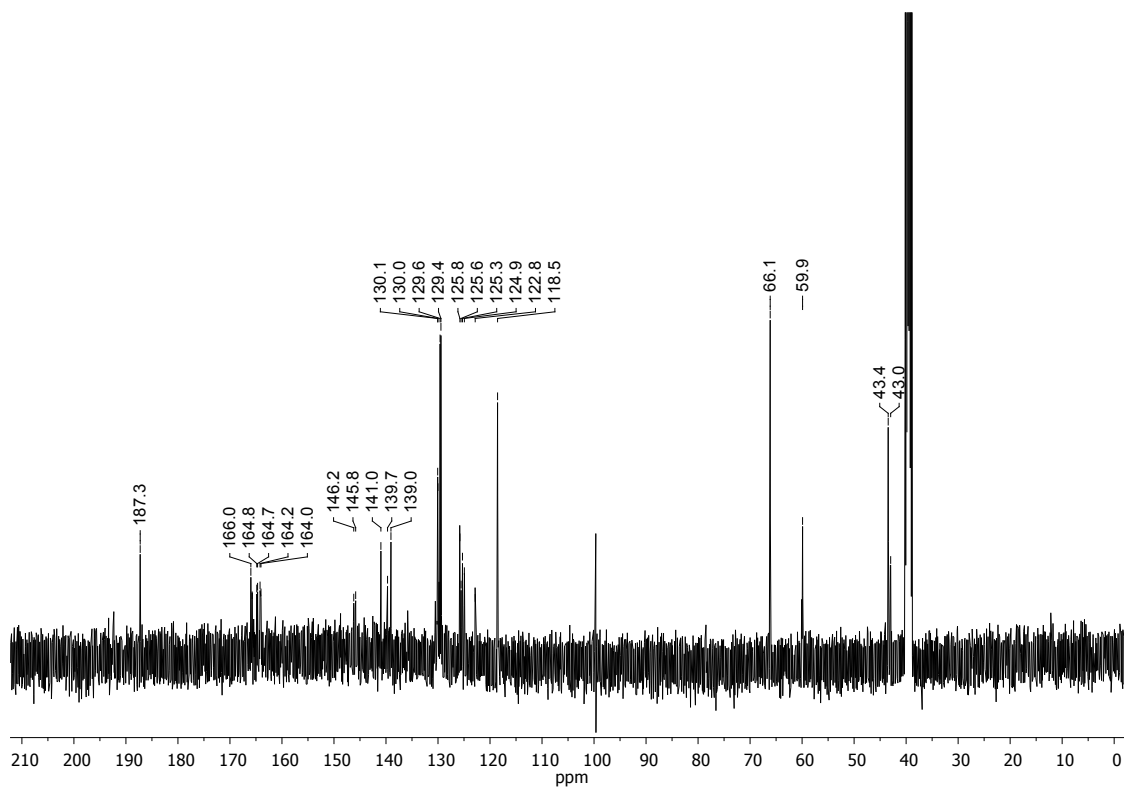
^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of **7f**.



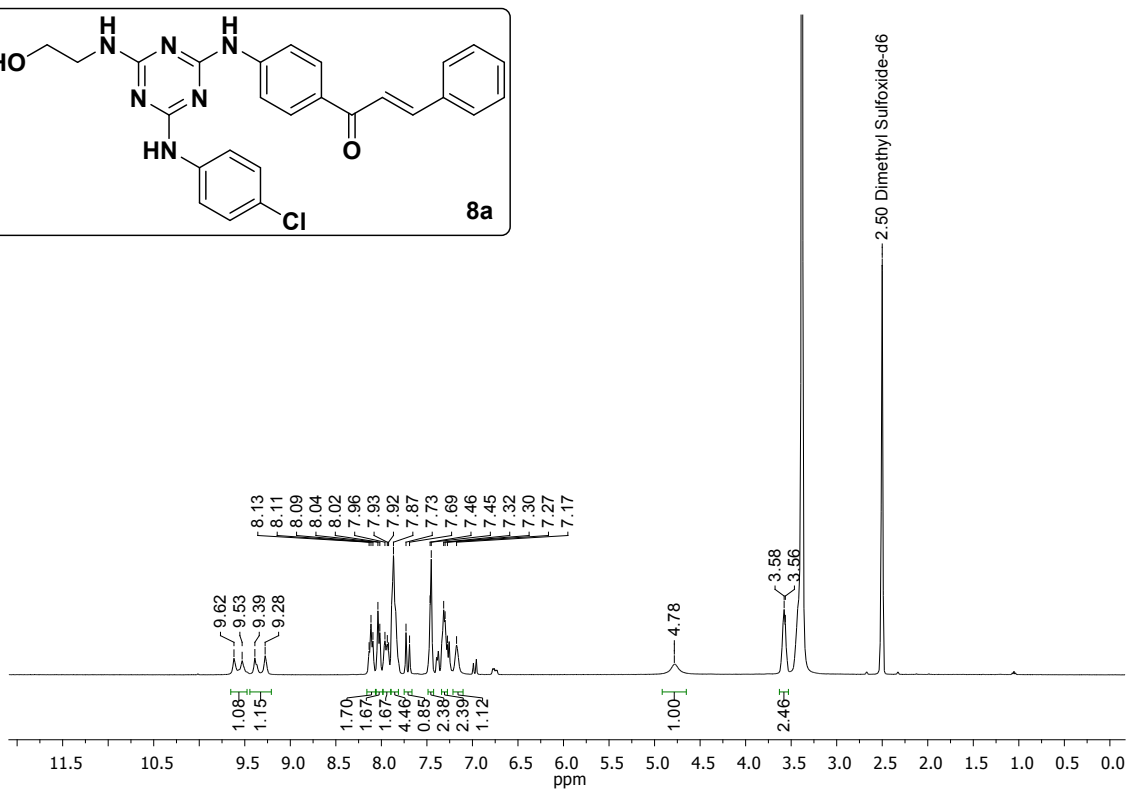
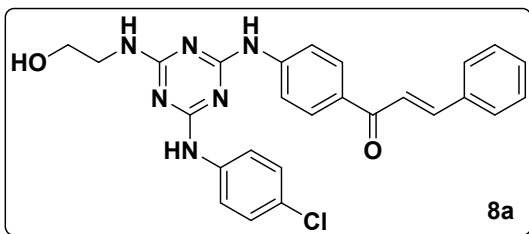
^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of **7f**.



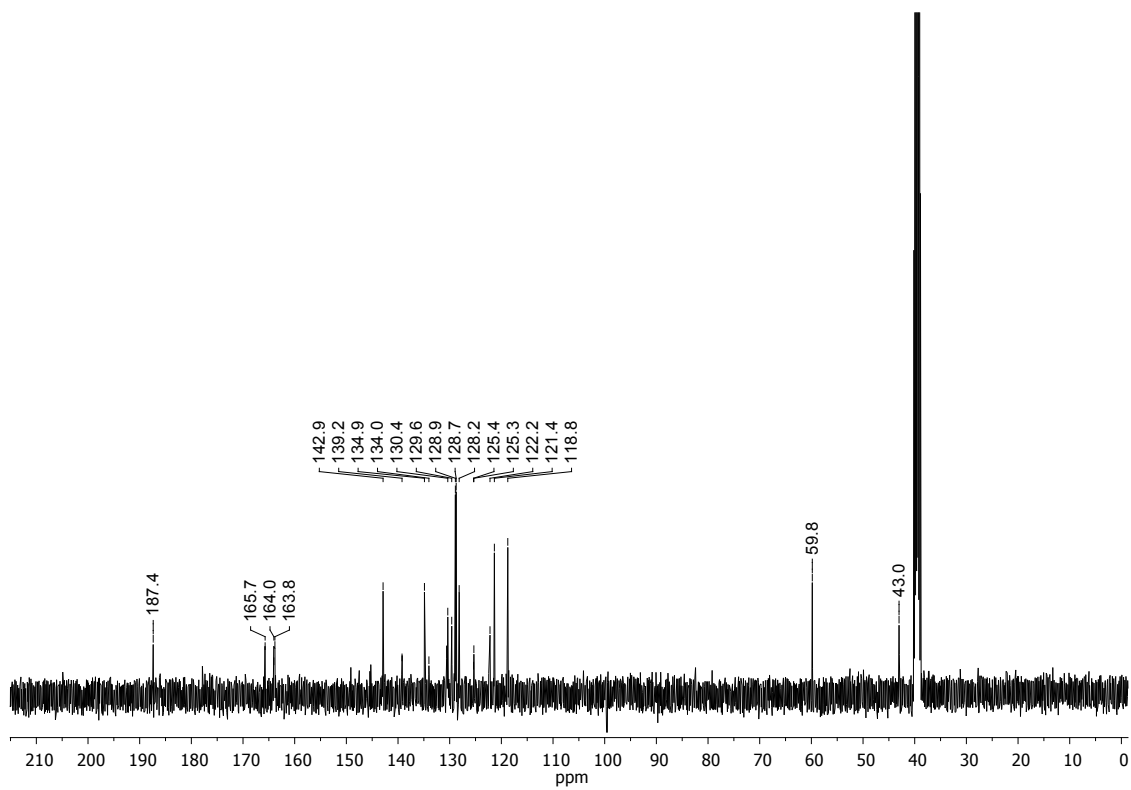
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **7g**.



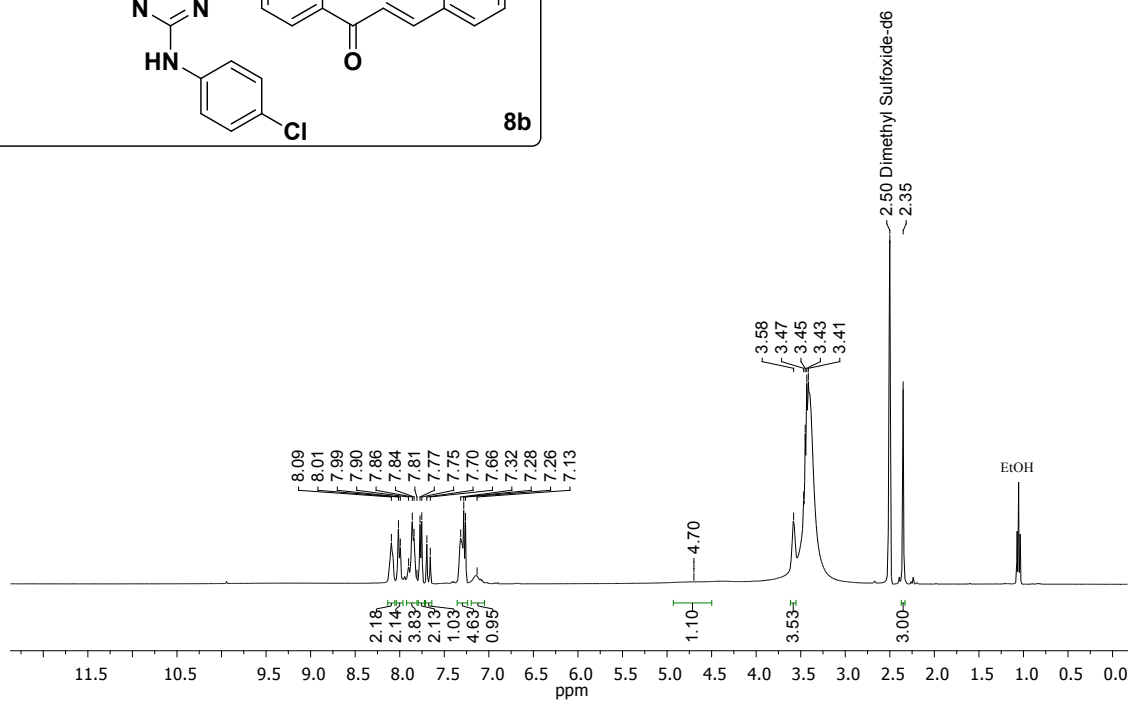
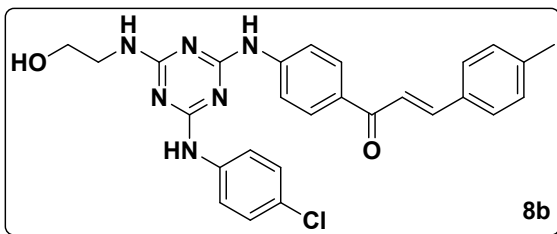
¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of **7g**.



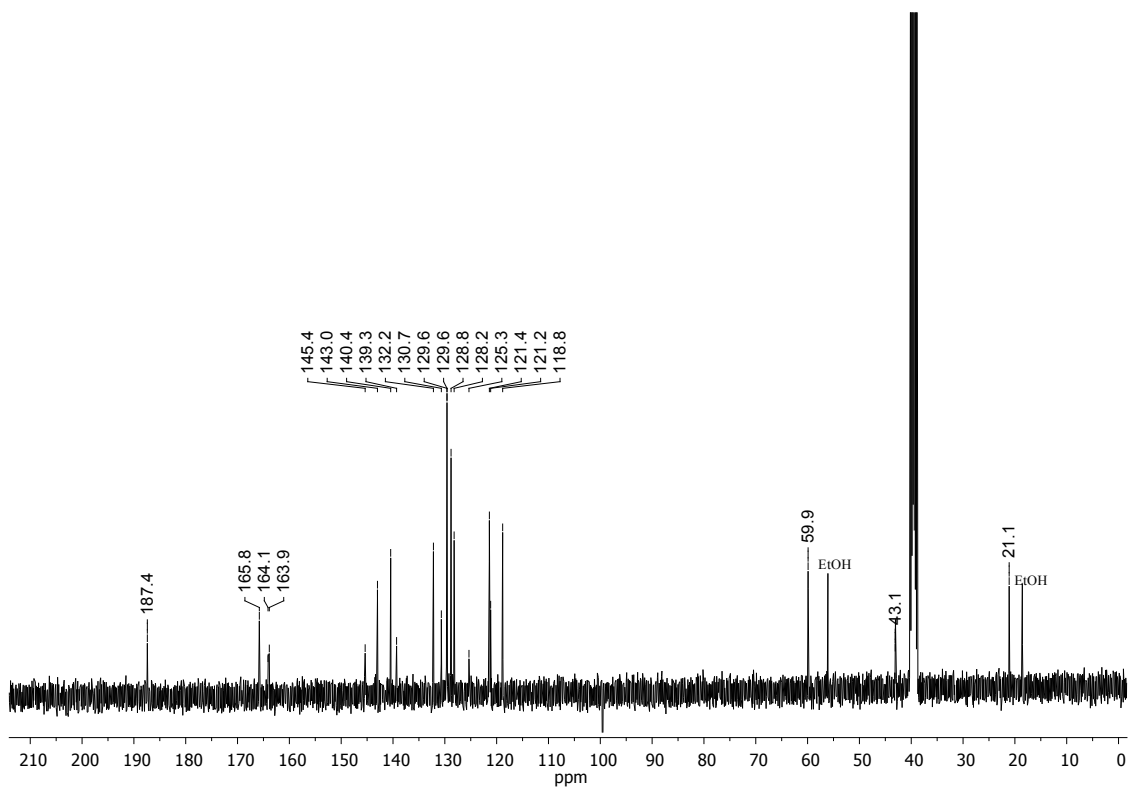
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **8a**.



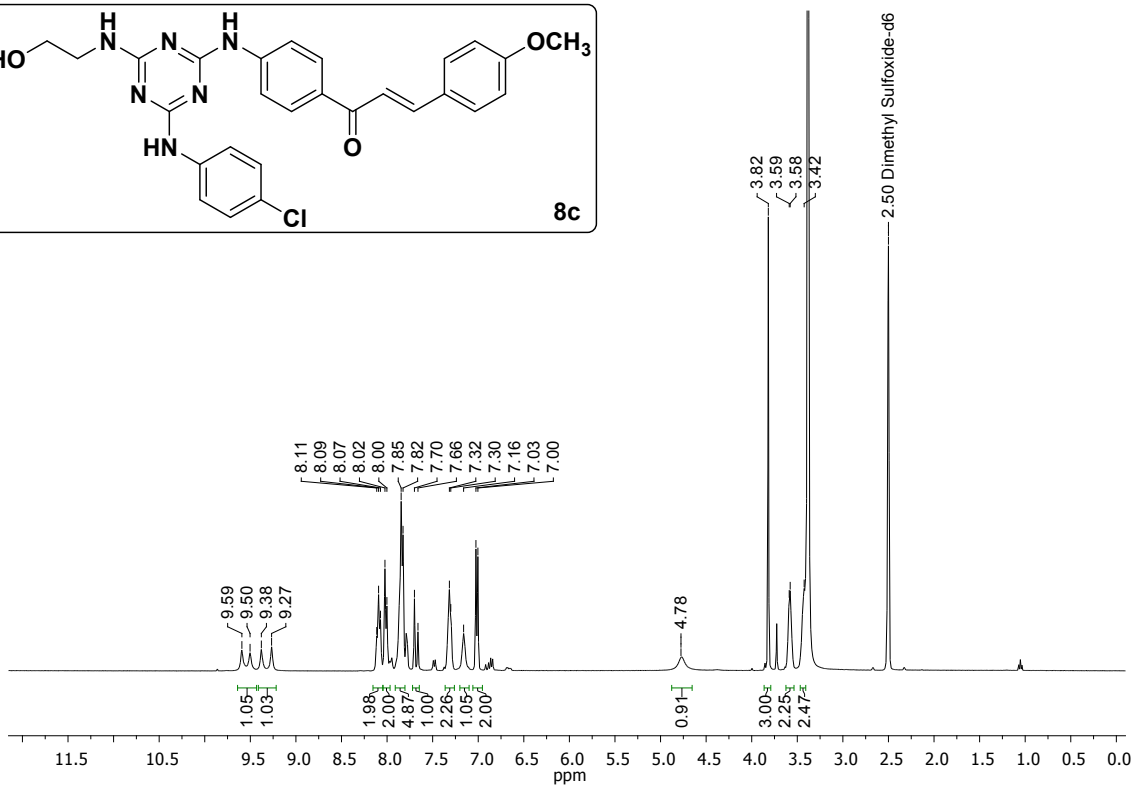
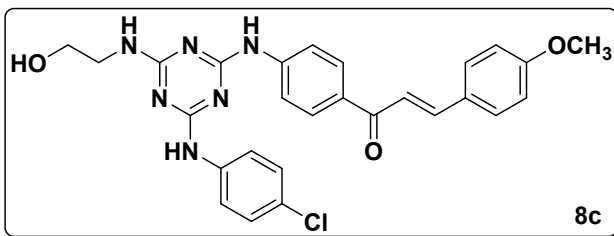
¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of **8a**.



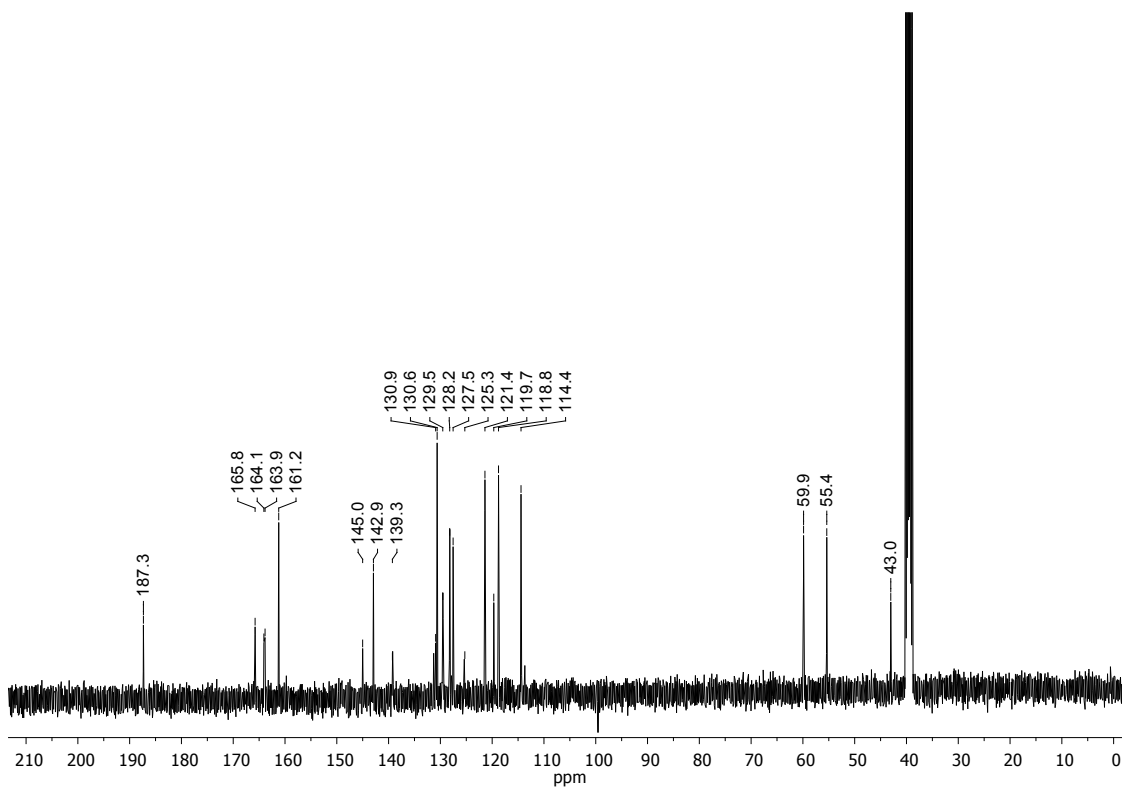
^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of **8b**.



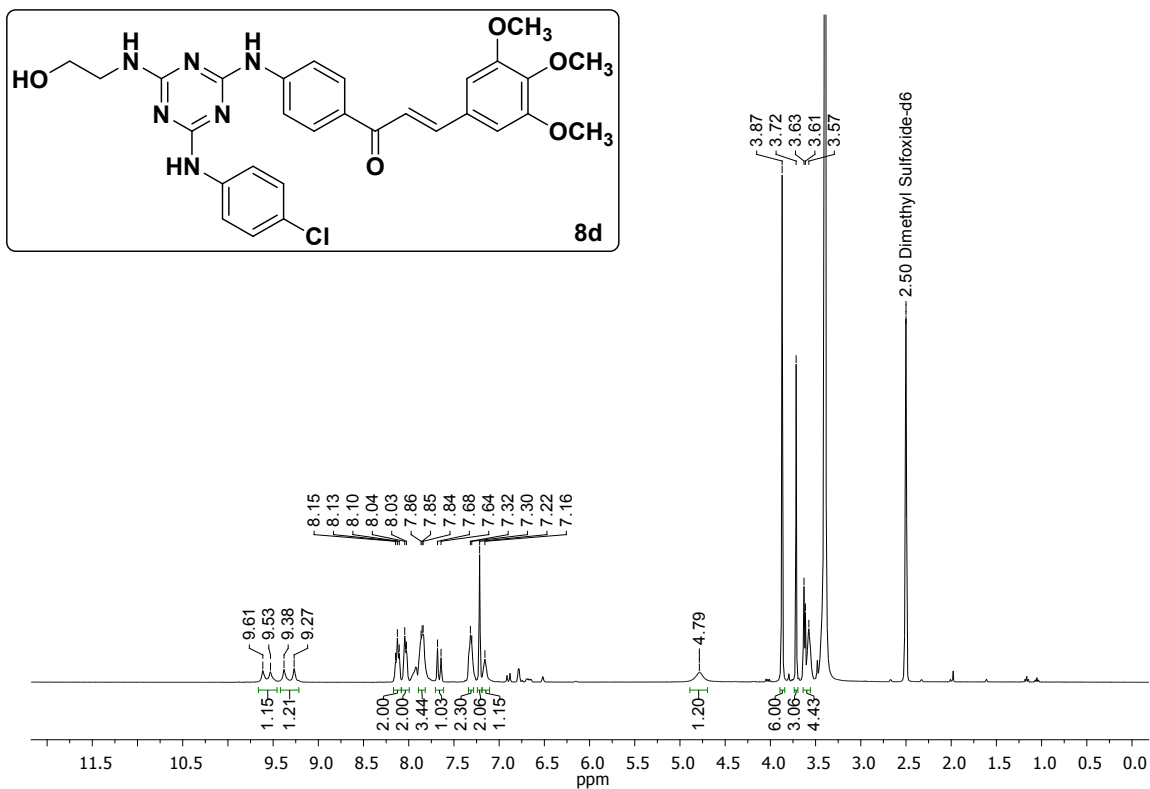
^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of **8b**.



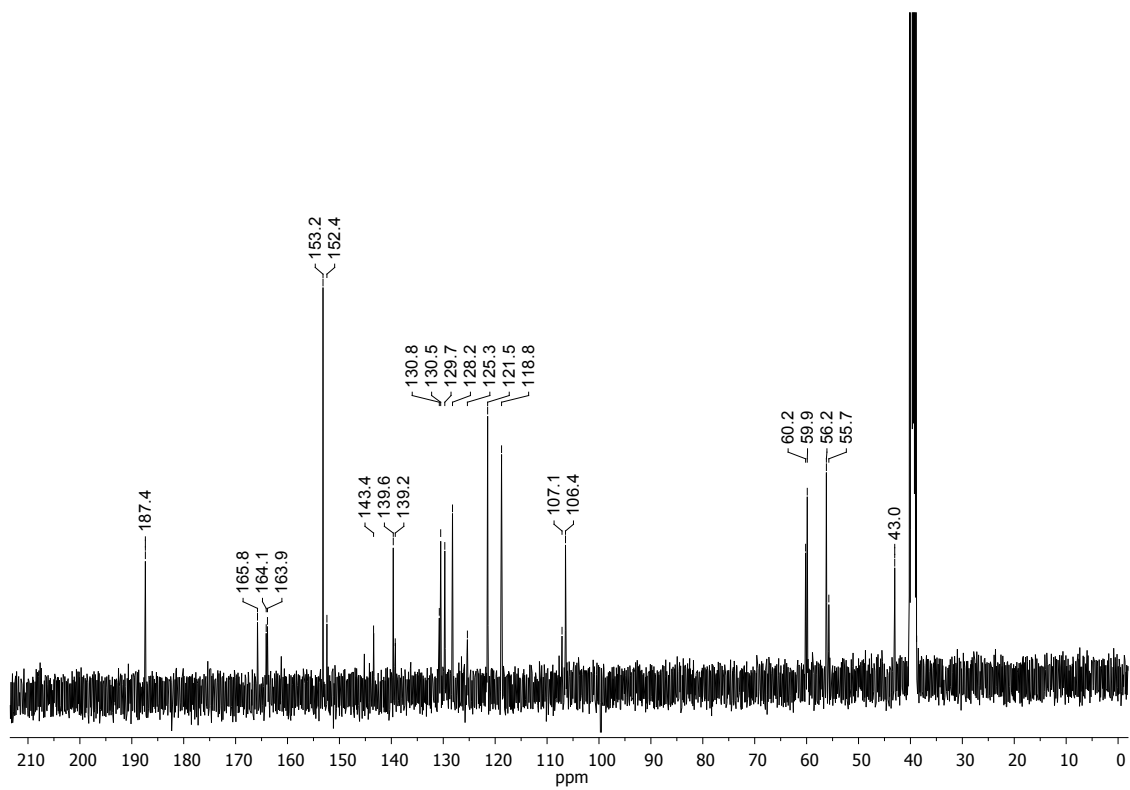
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **8c**.



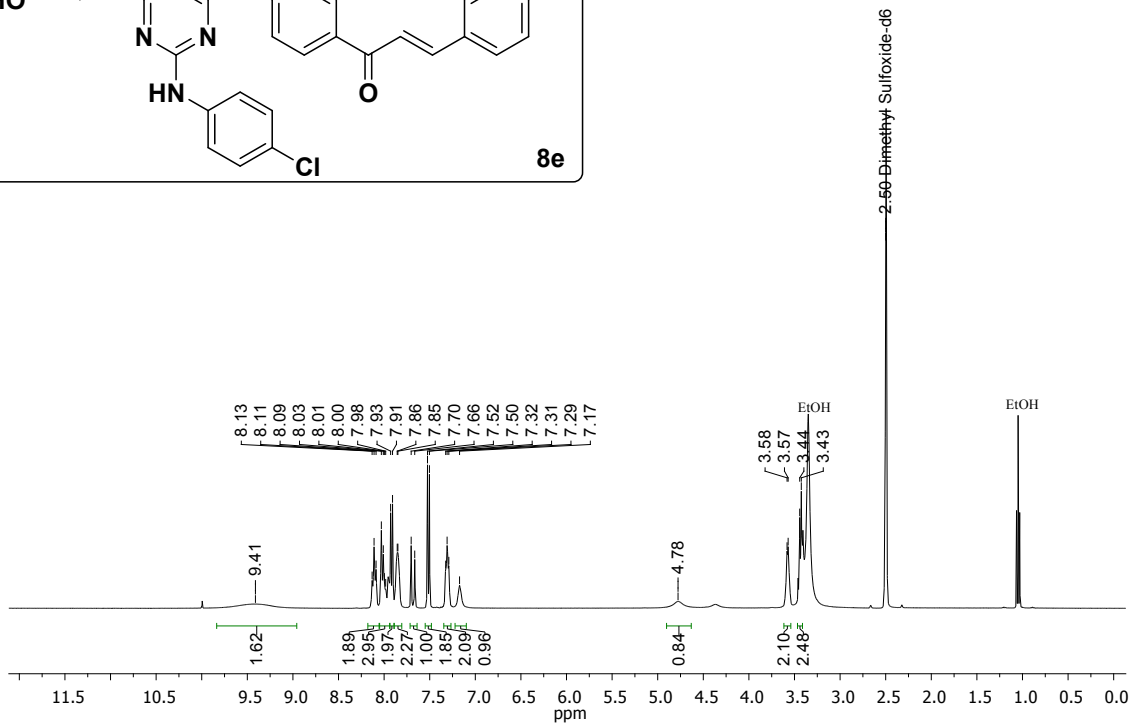
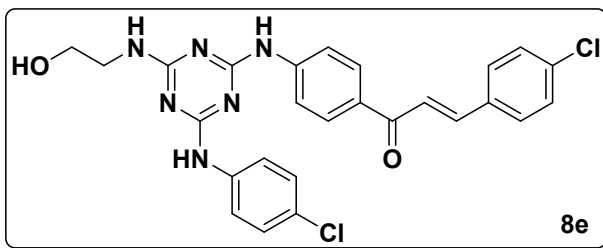
¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of **8c**.



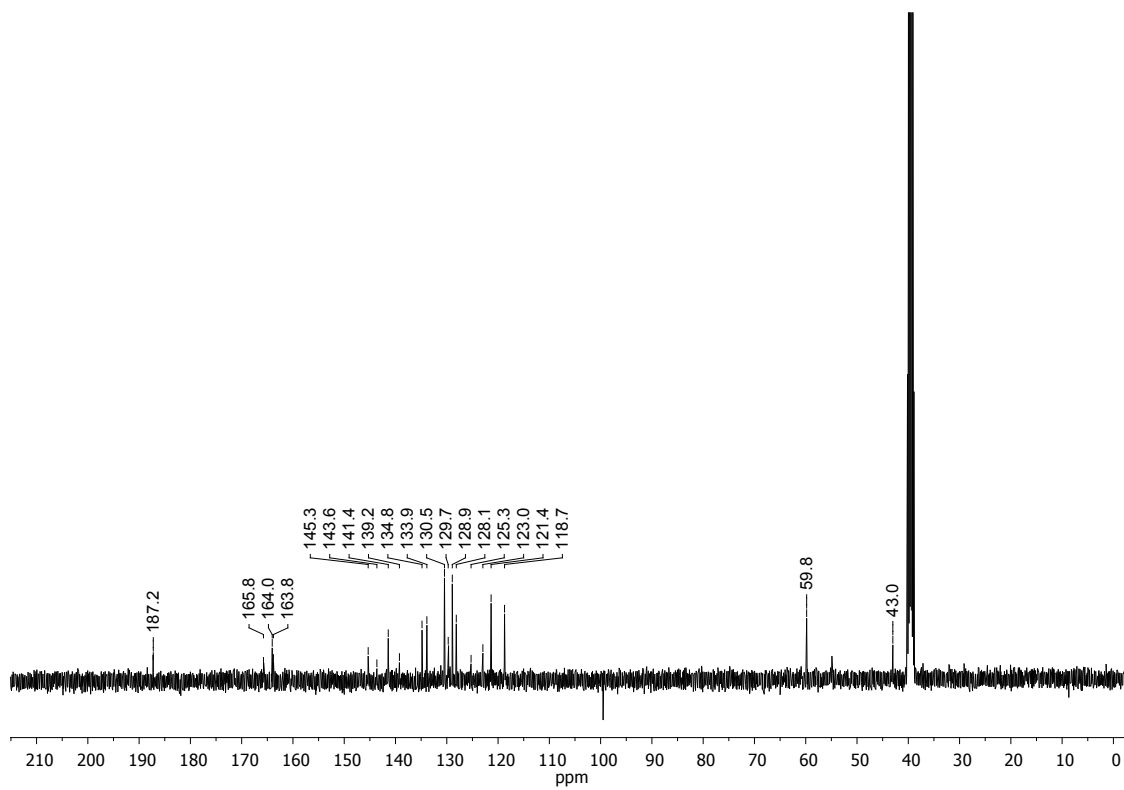
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **8d**.



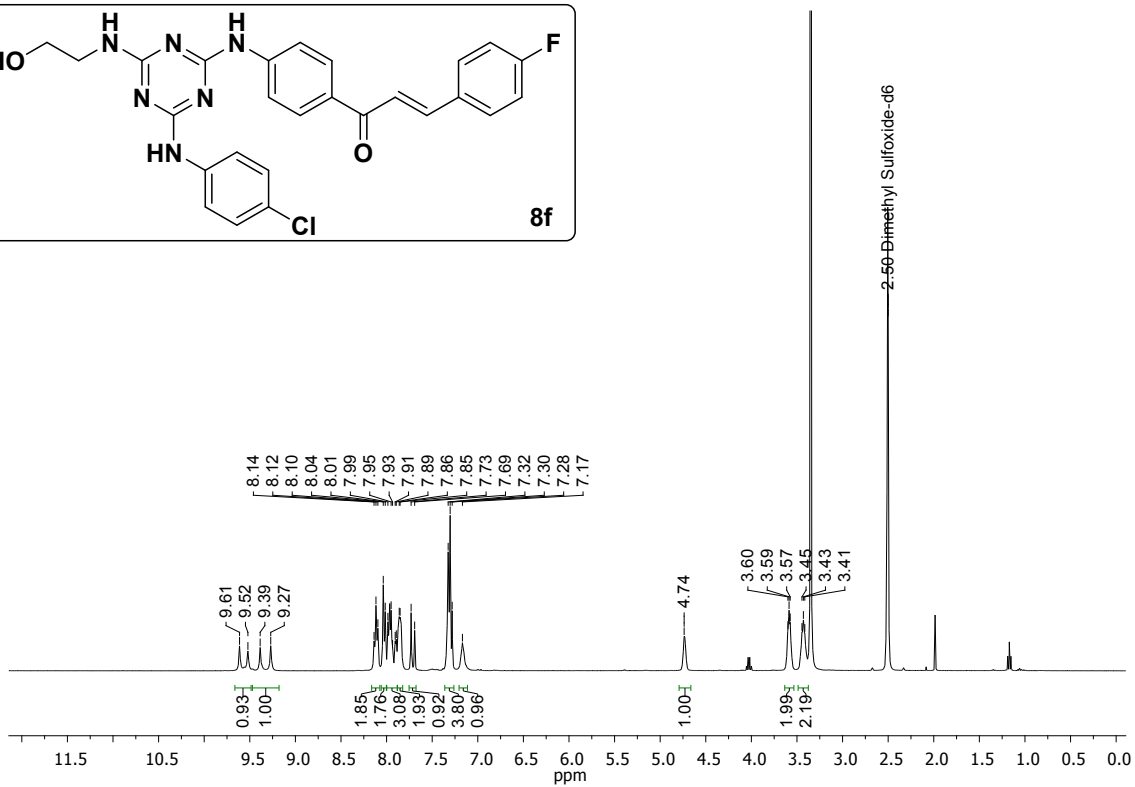
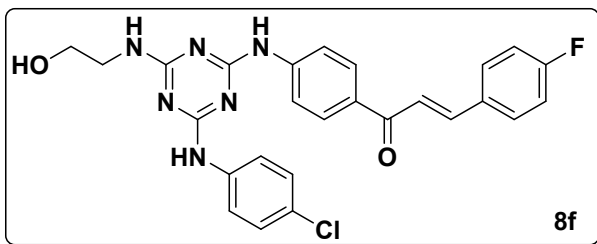
¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of **8d**.



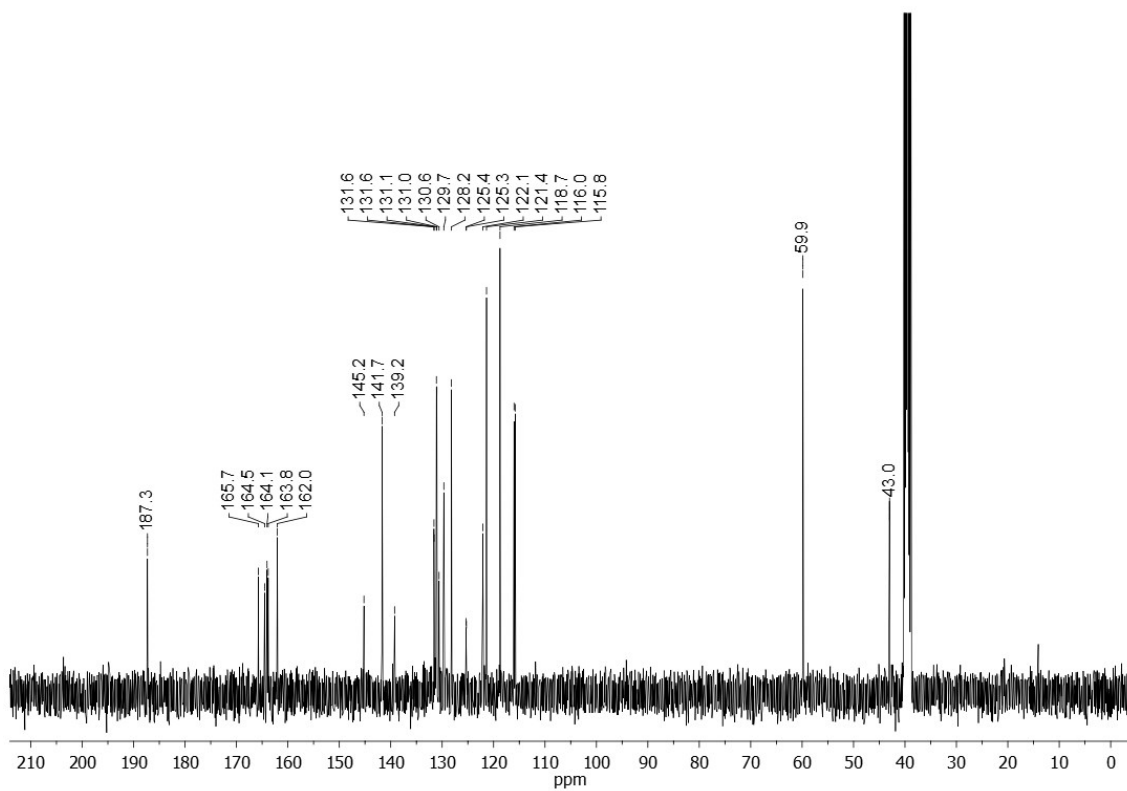
^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of **8e**.



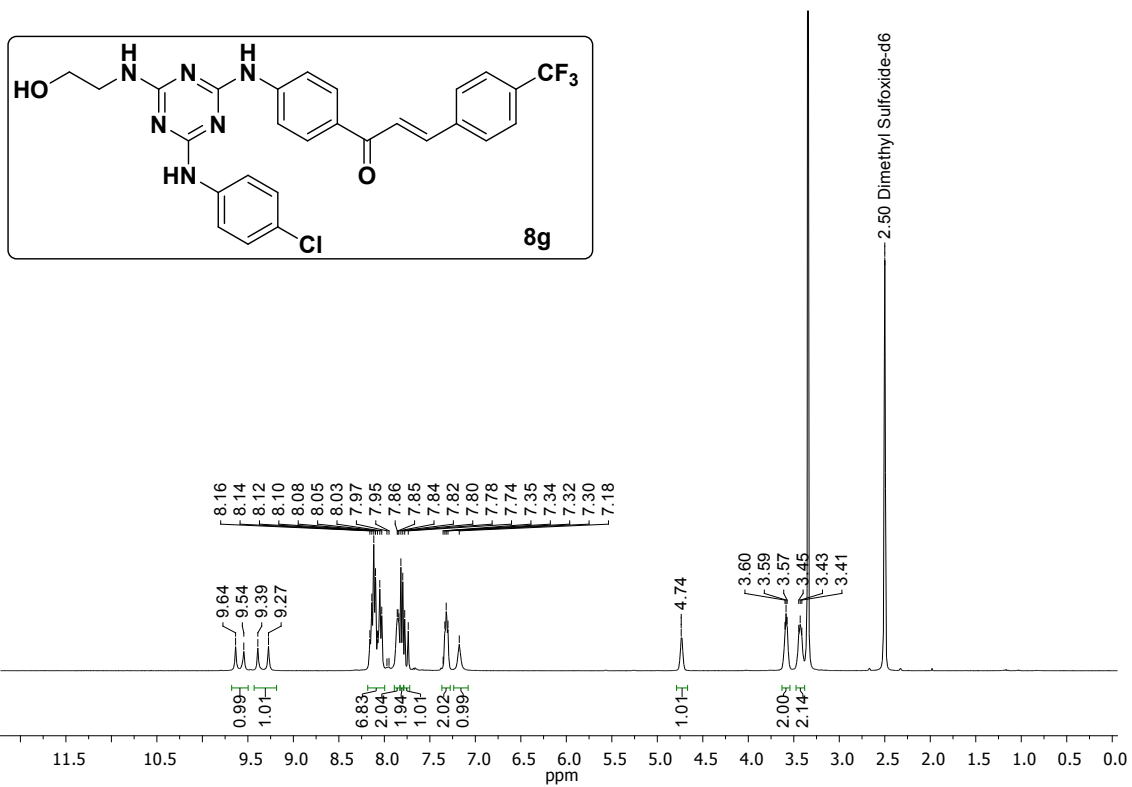
^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of **8e**.



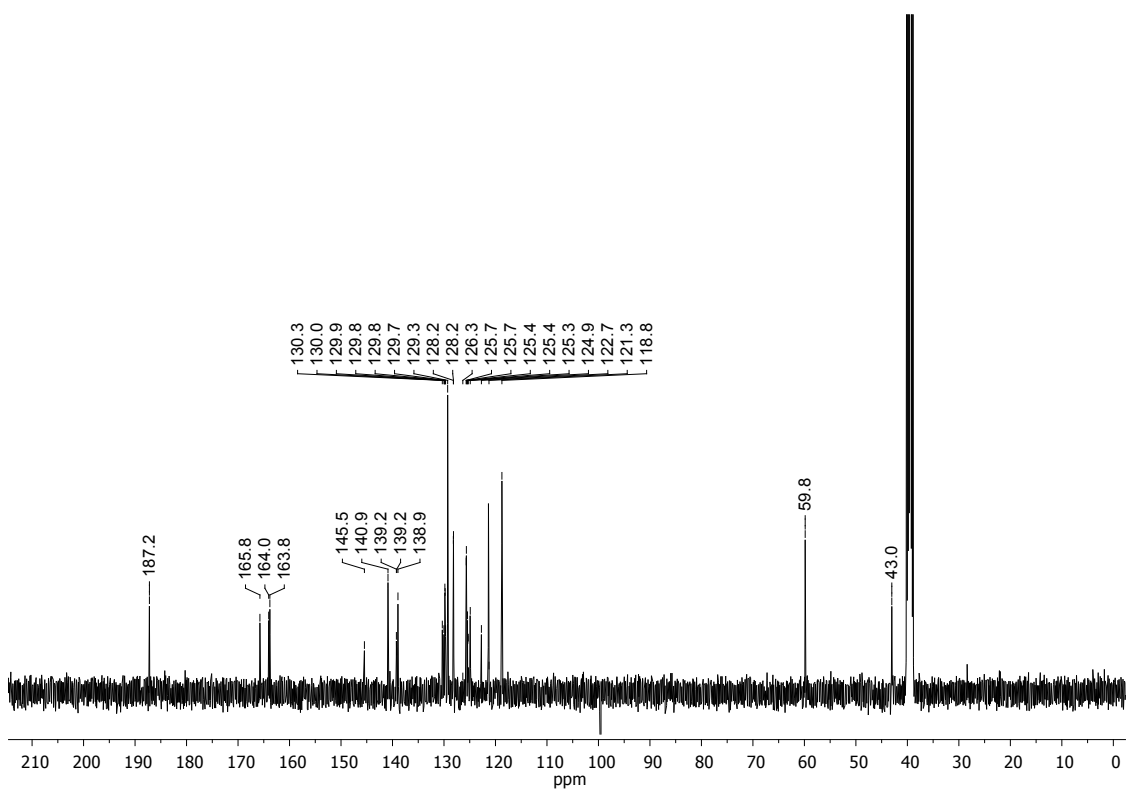
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **8f**.



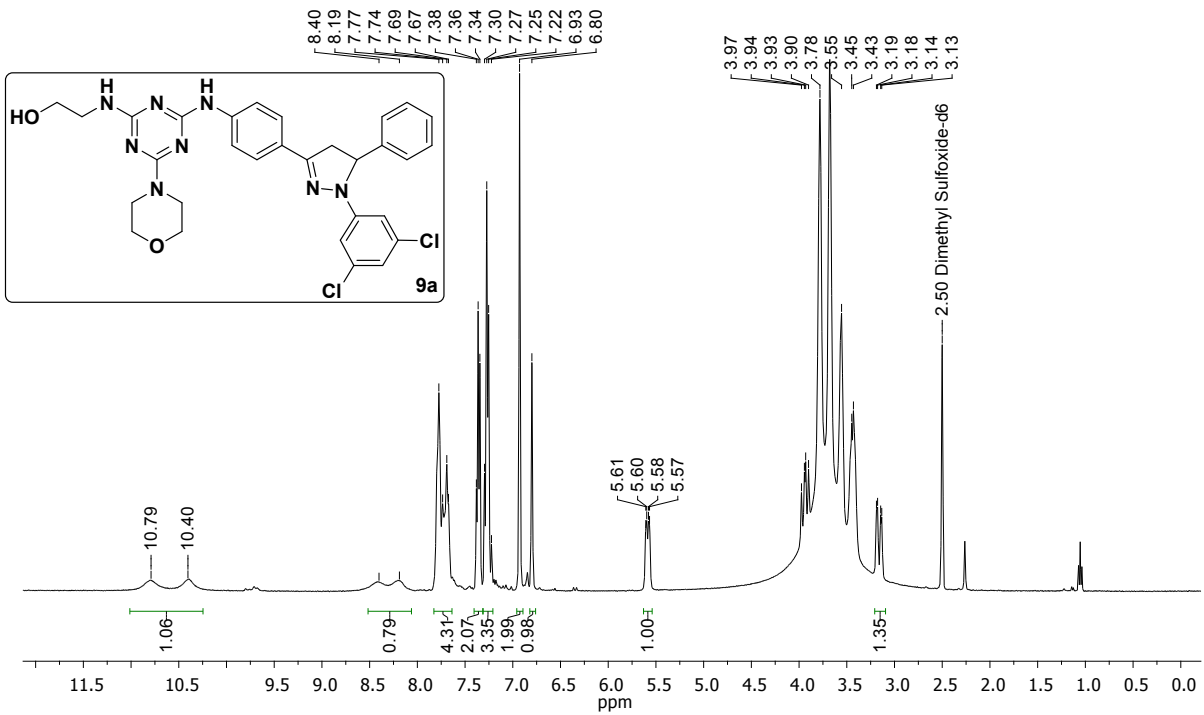
¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of **8f**.



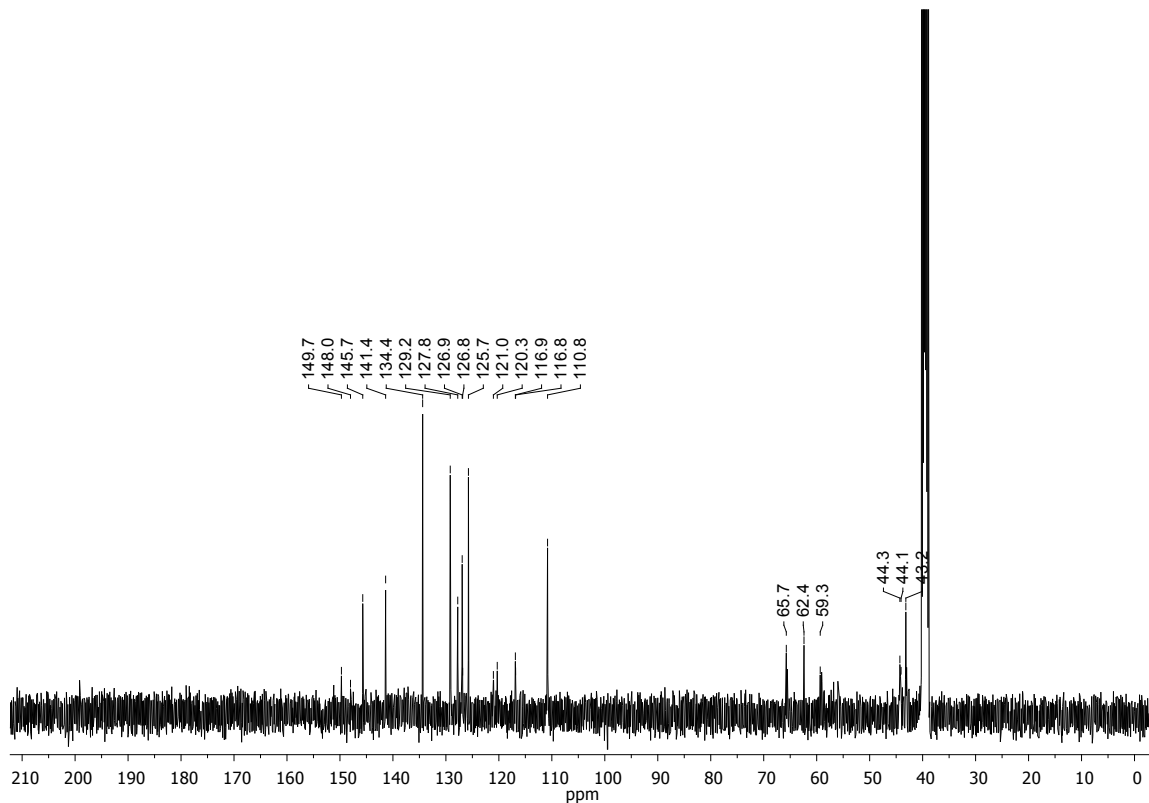
^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of **8g**.



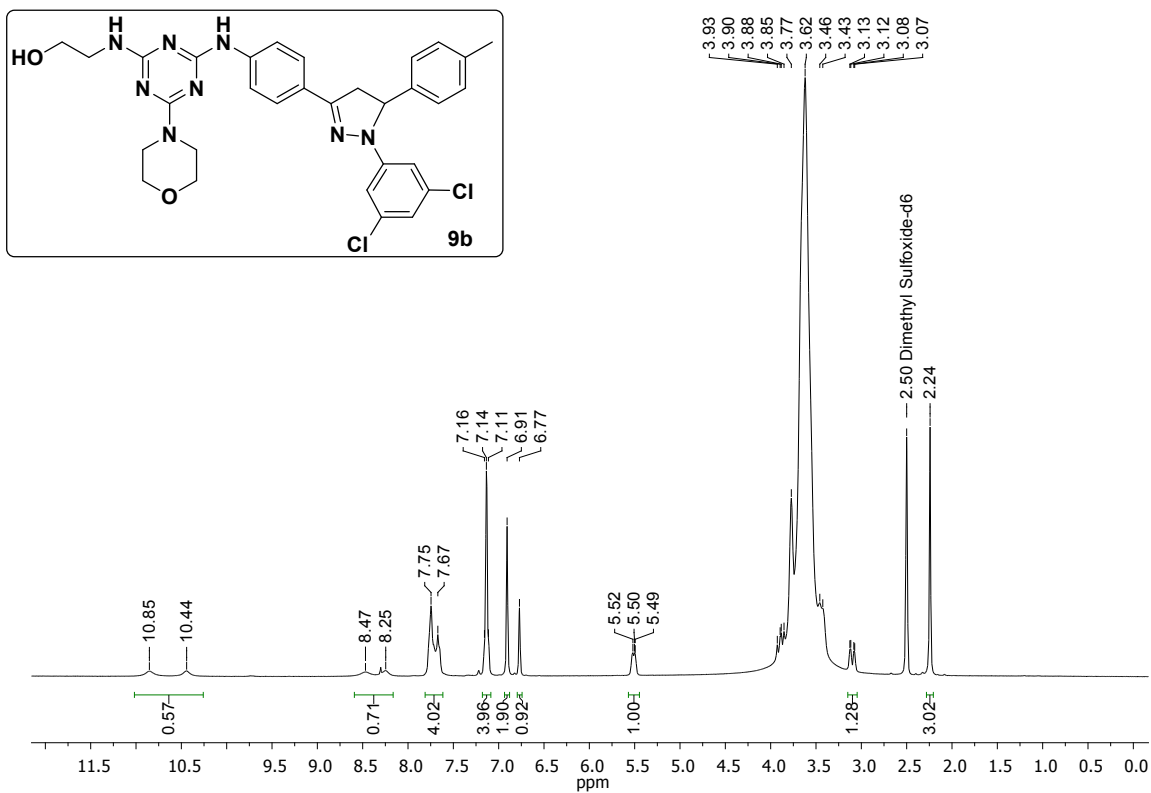
^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of **8g**.



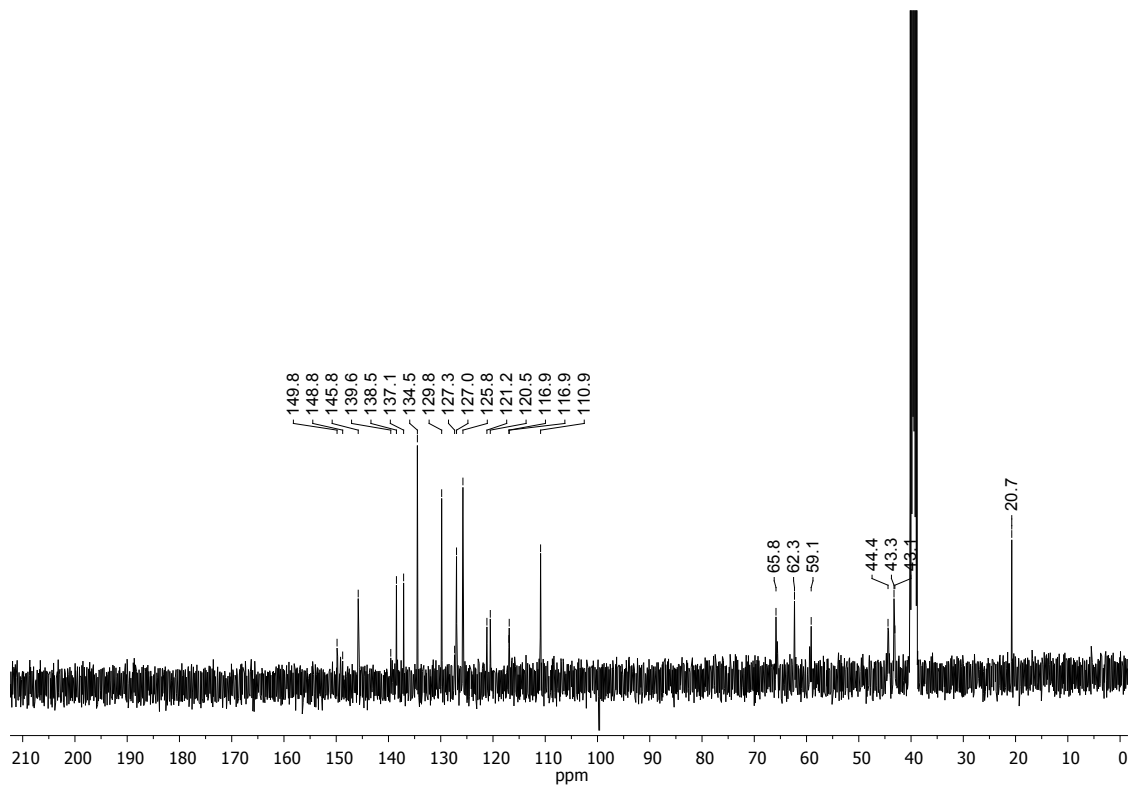
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **9a**.



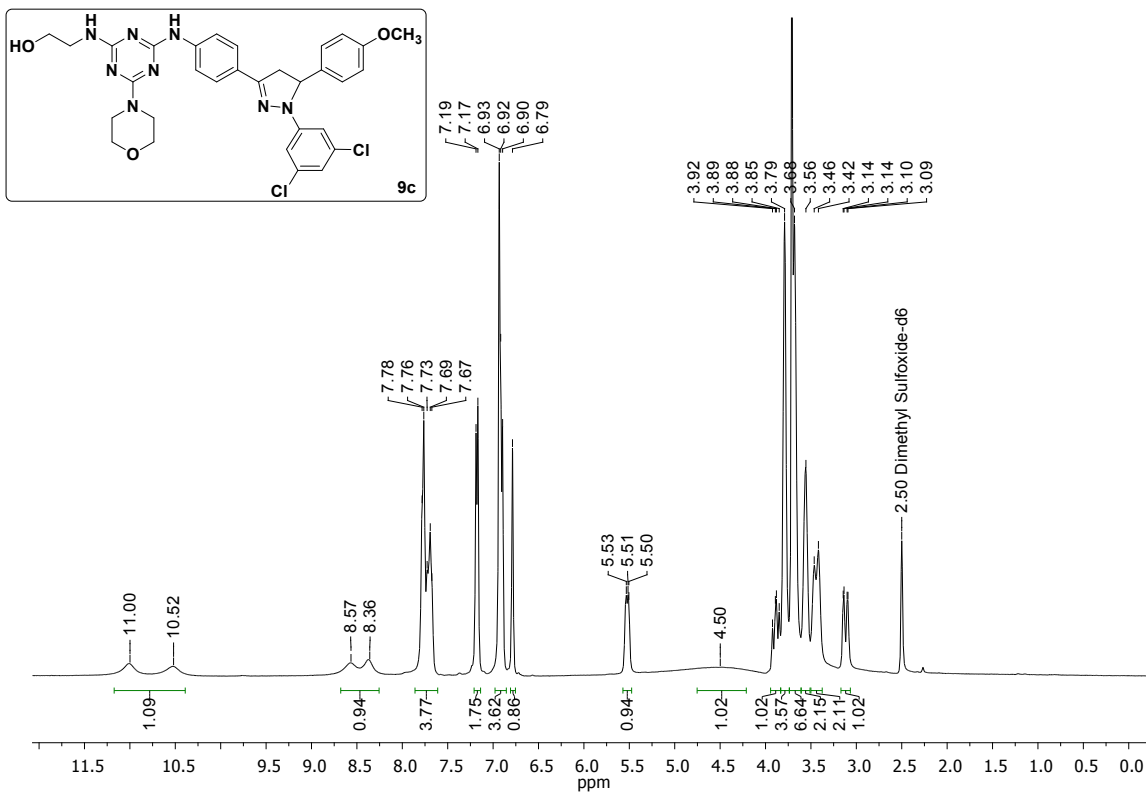
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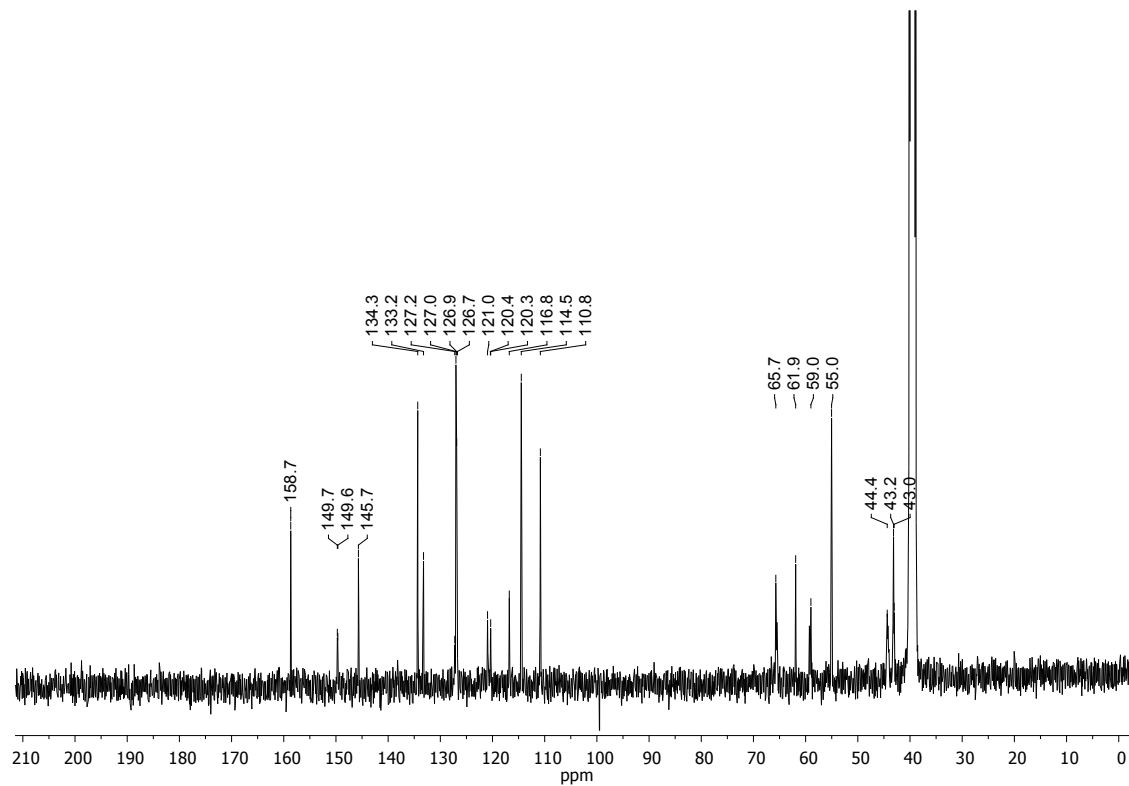
^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of **9b**.



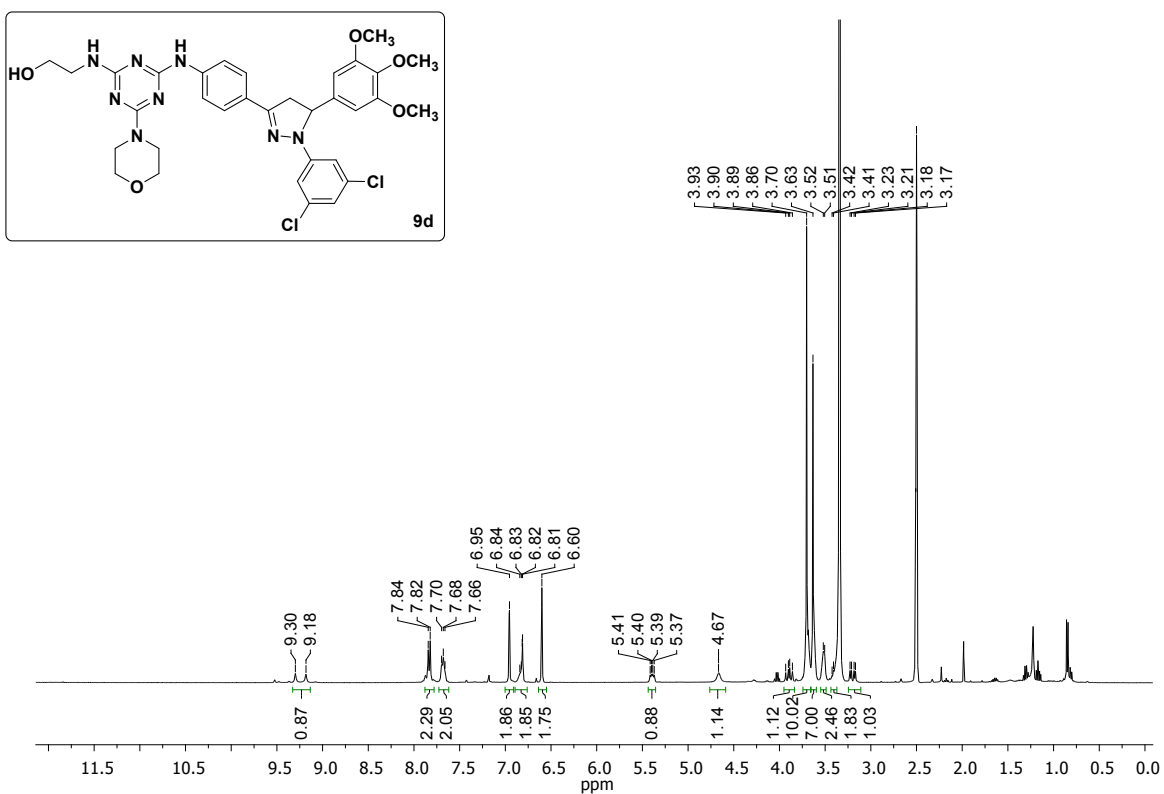
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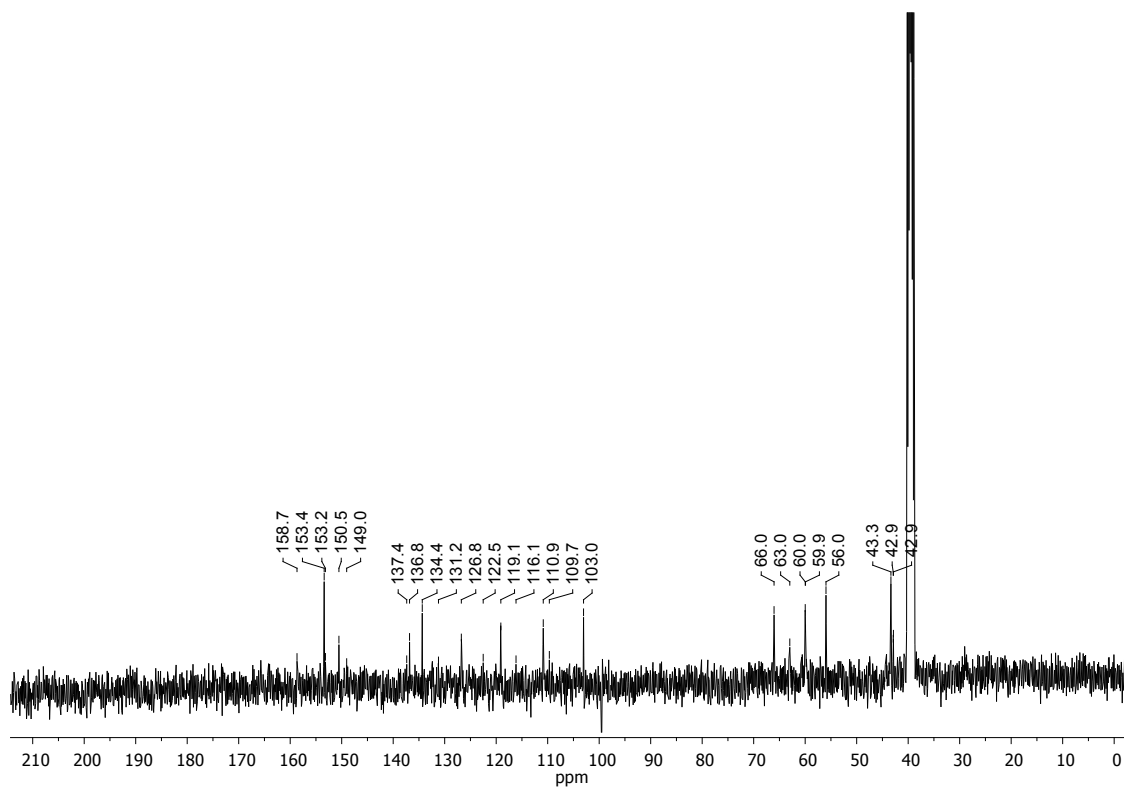
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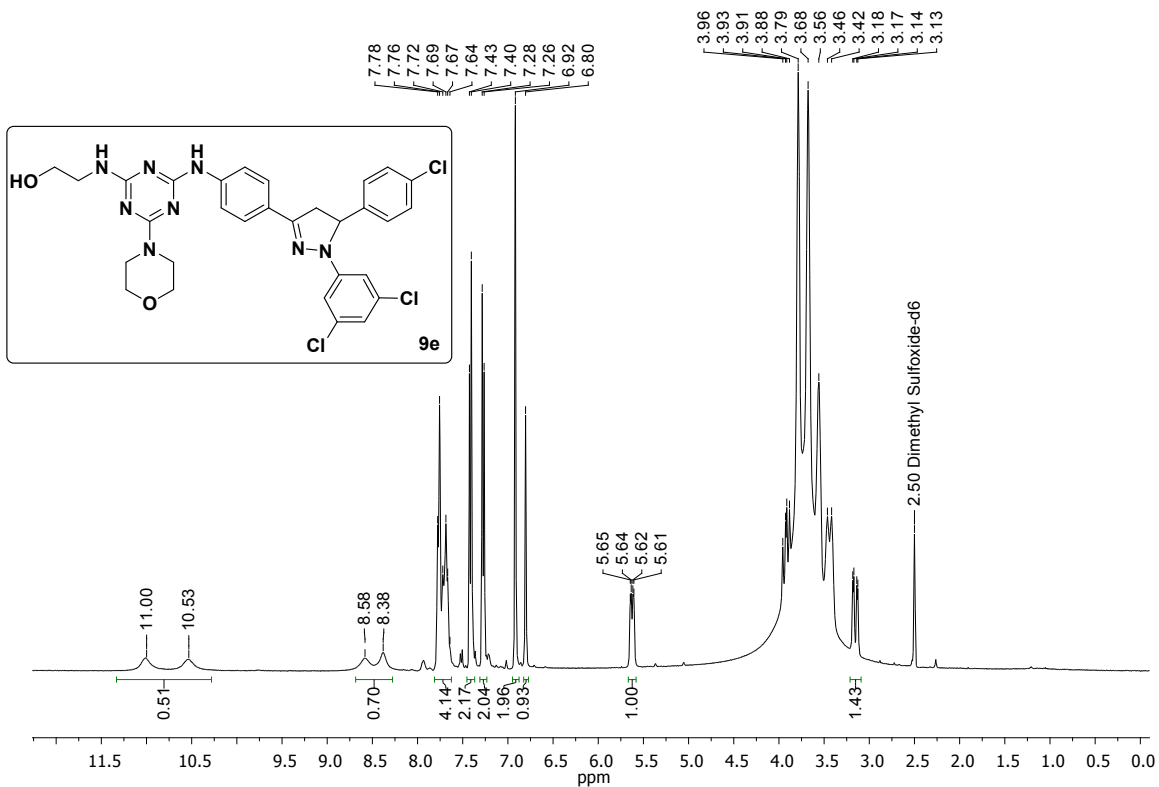
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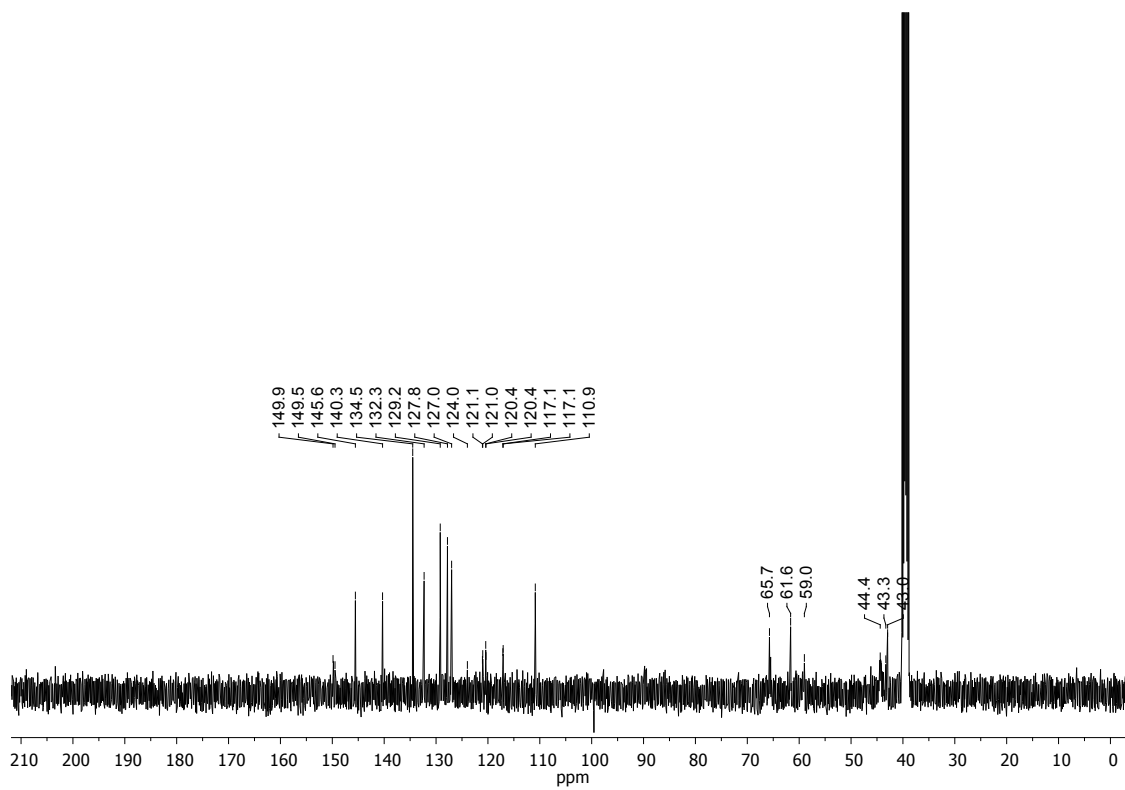
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **9d**.



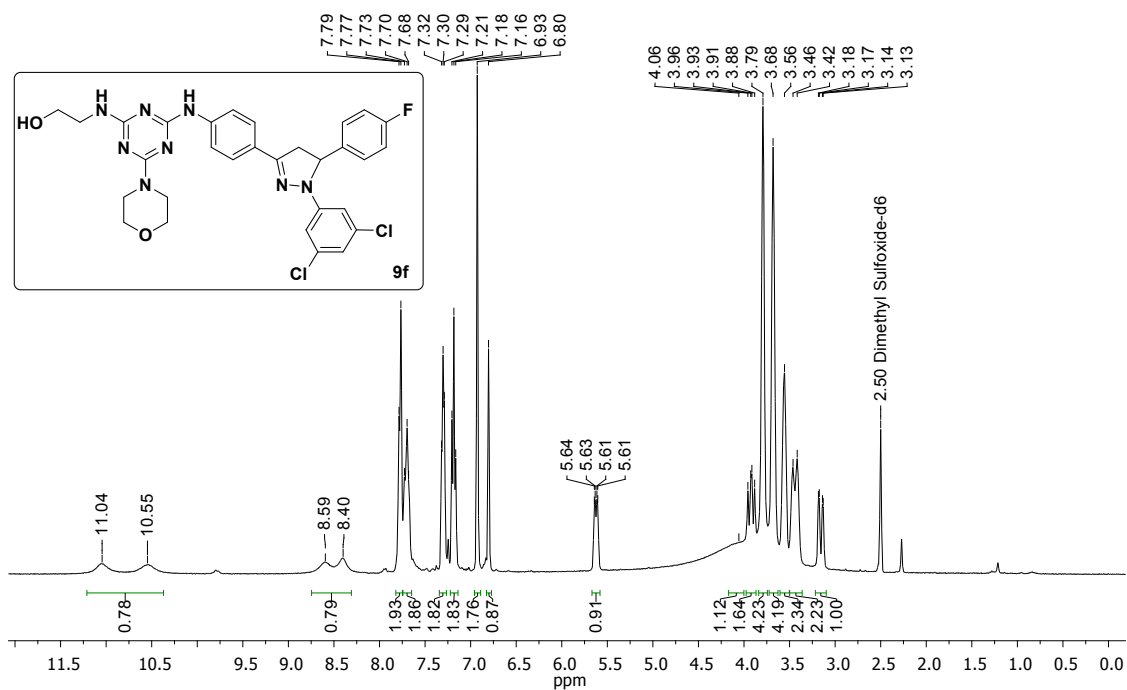
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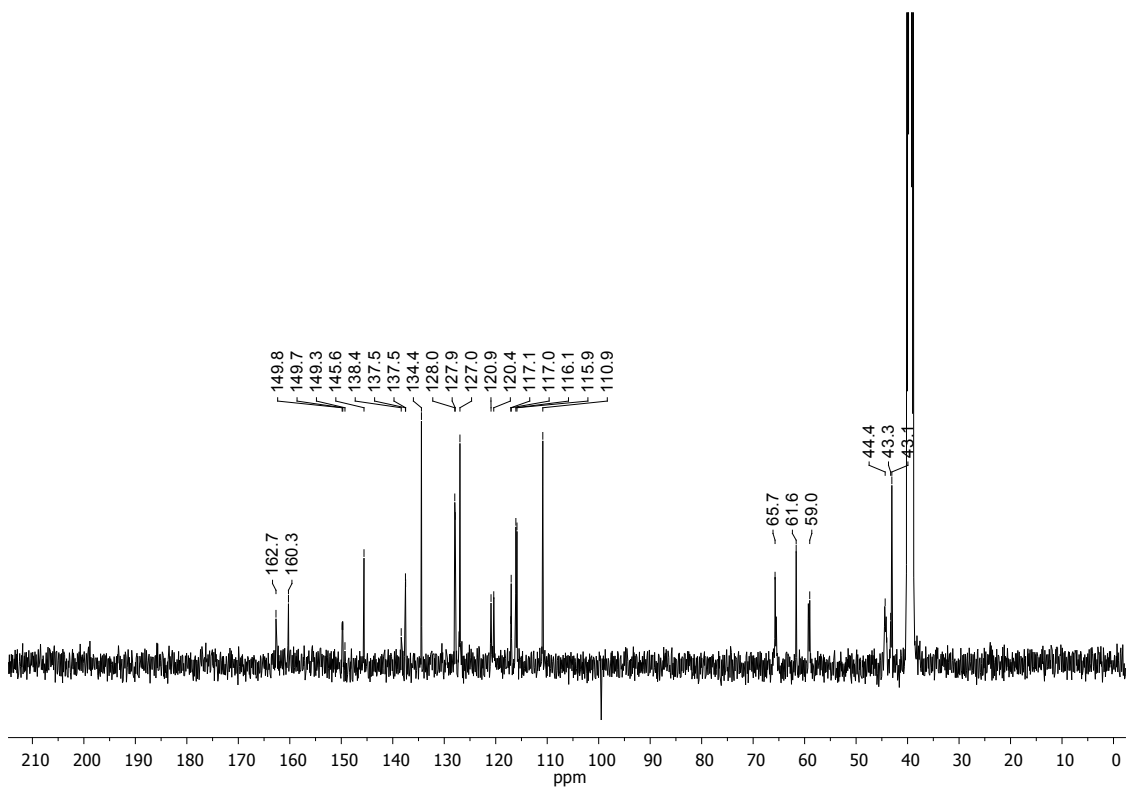
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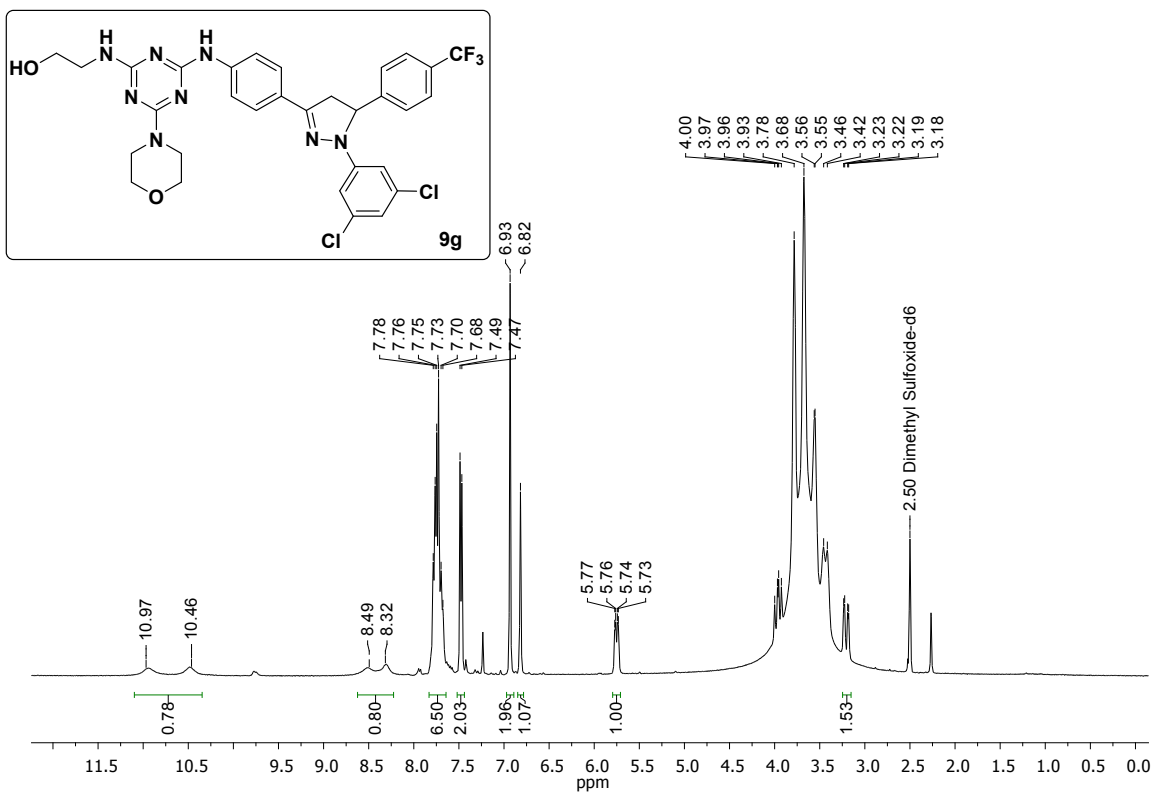
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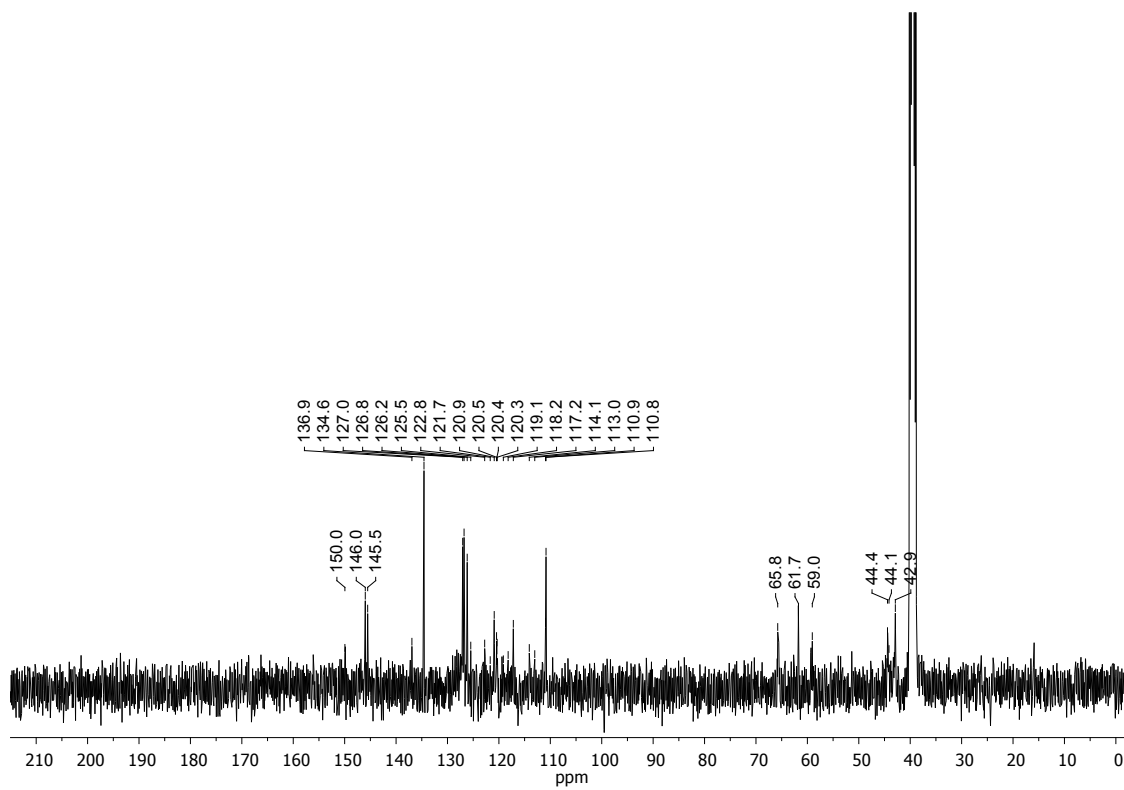
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **9f**.



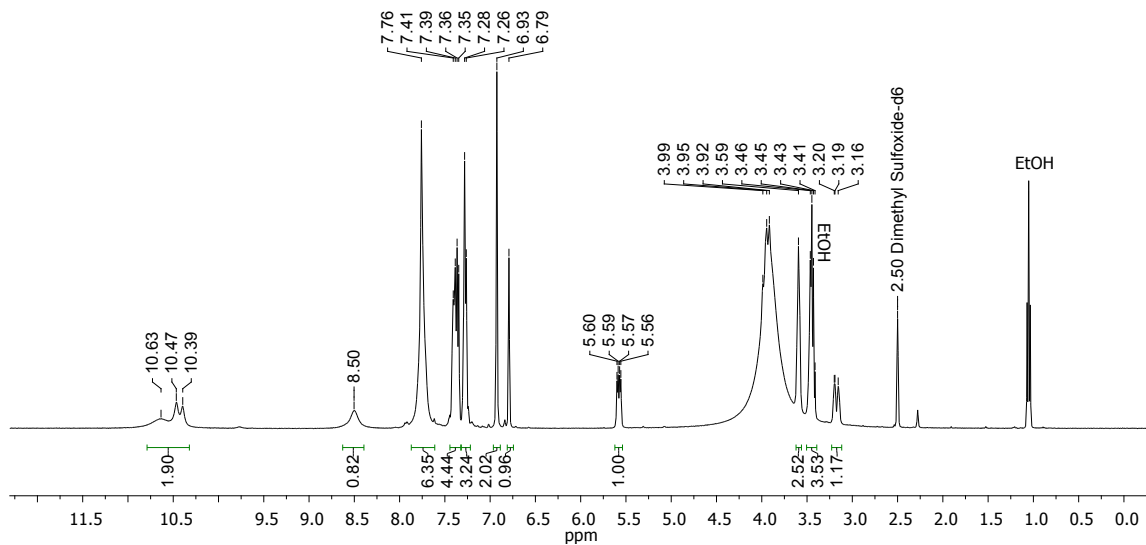
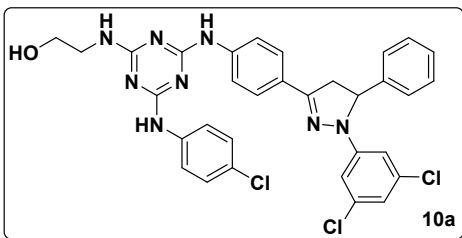
¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of **9f**.



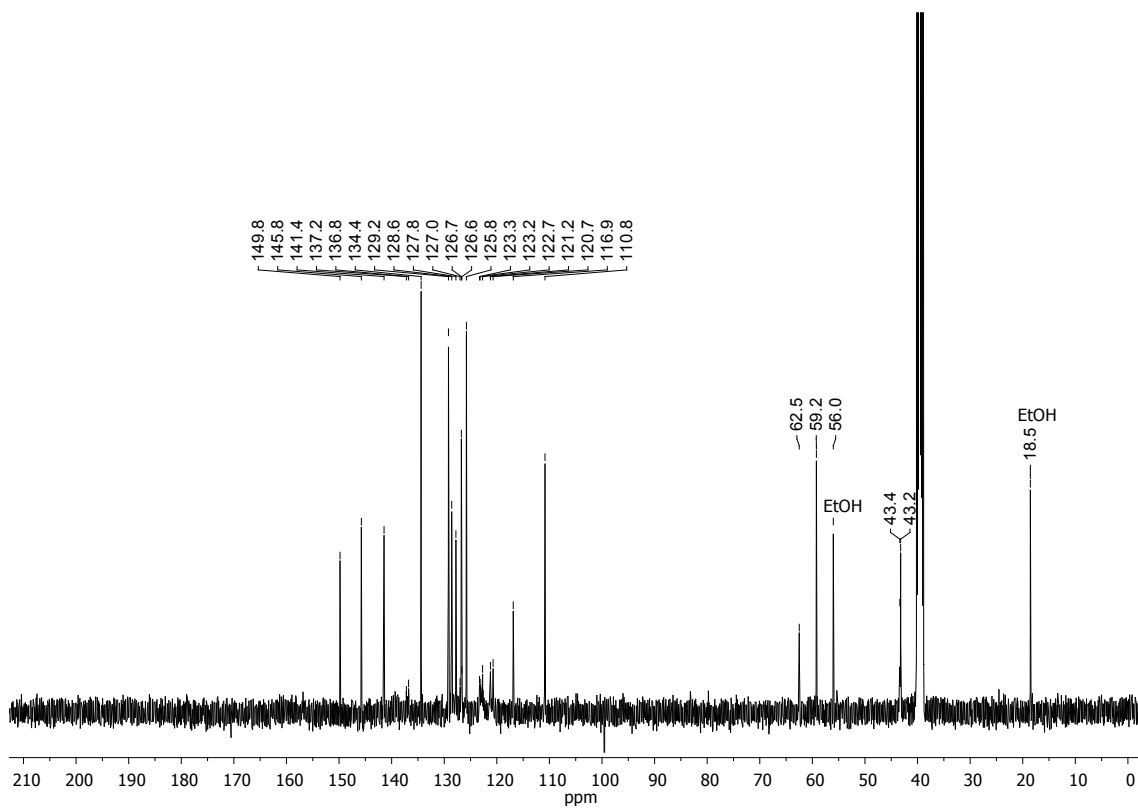
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **9g**.



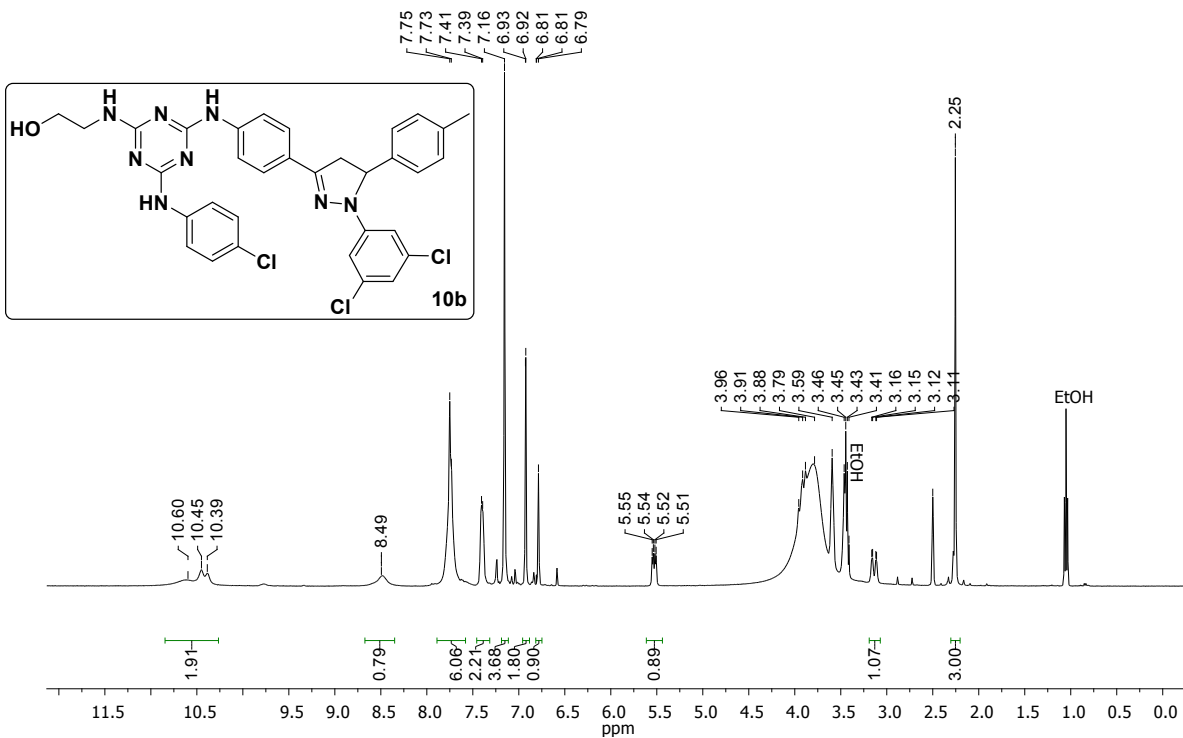
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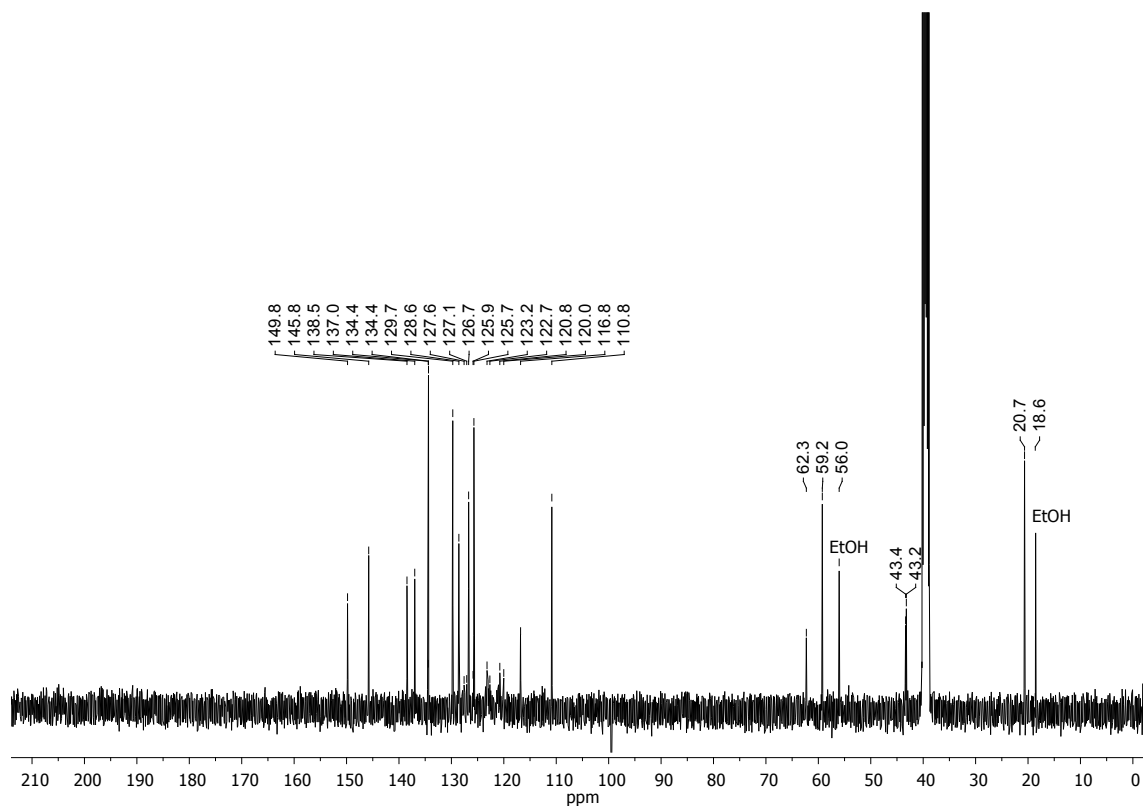
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **10a**.



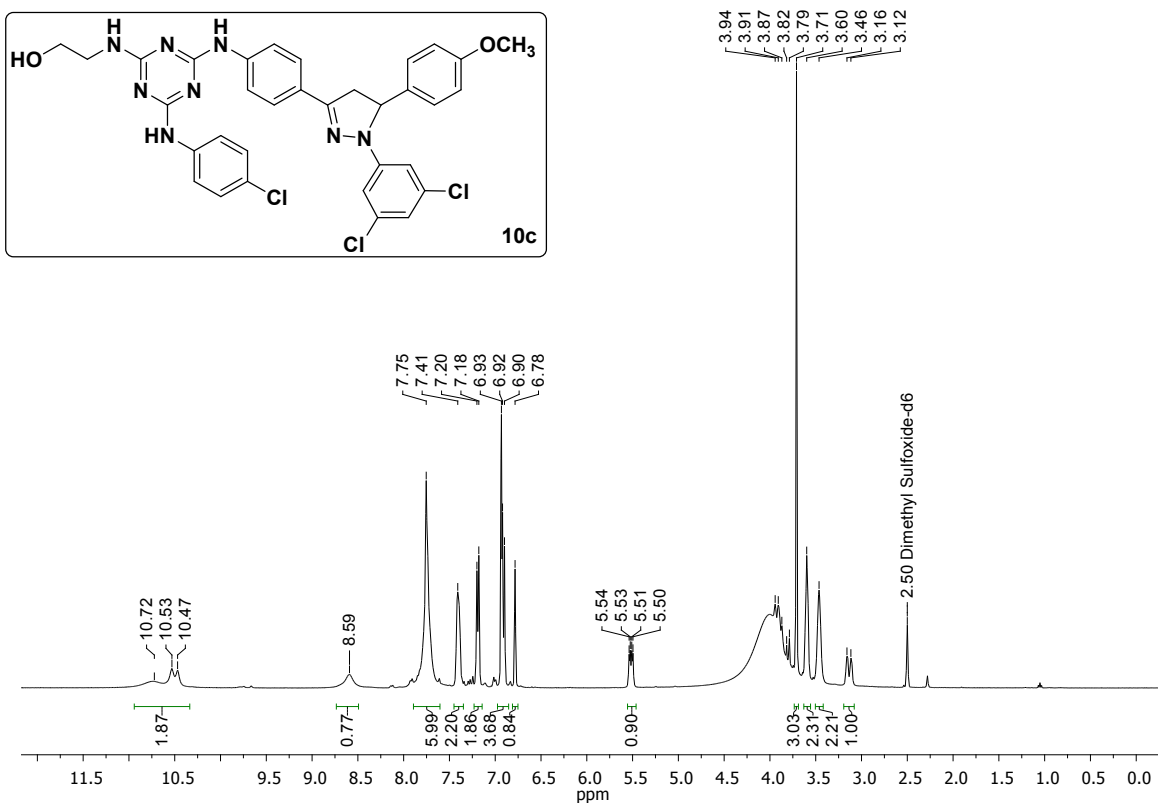
¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of **10a**.



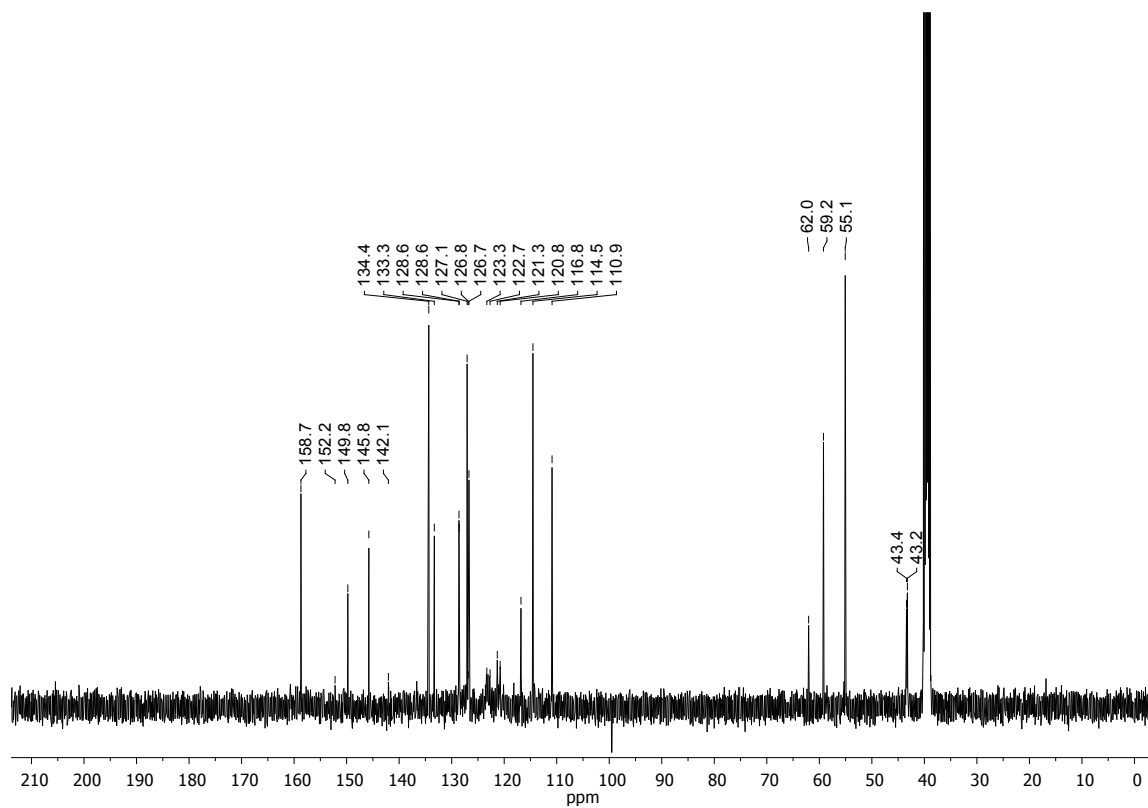
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **10b**.



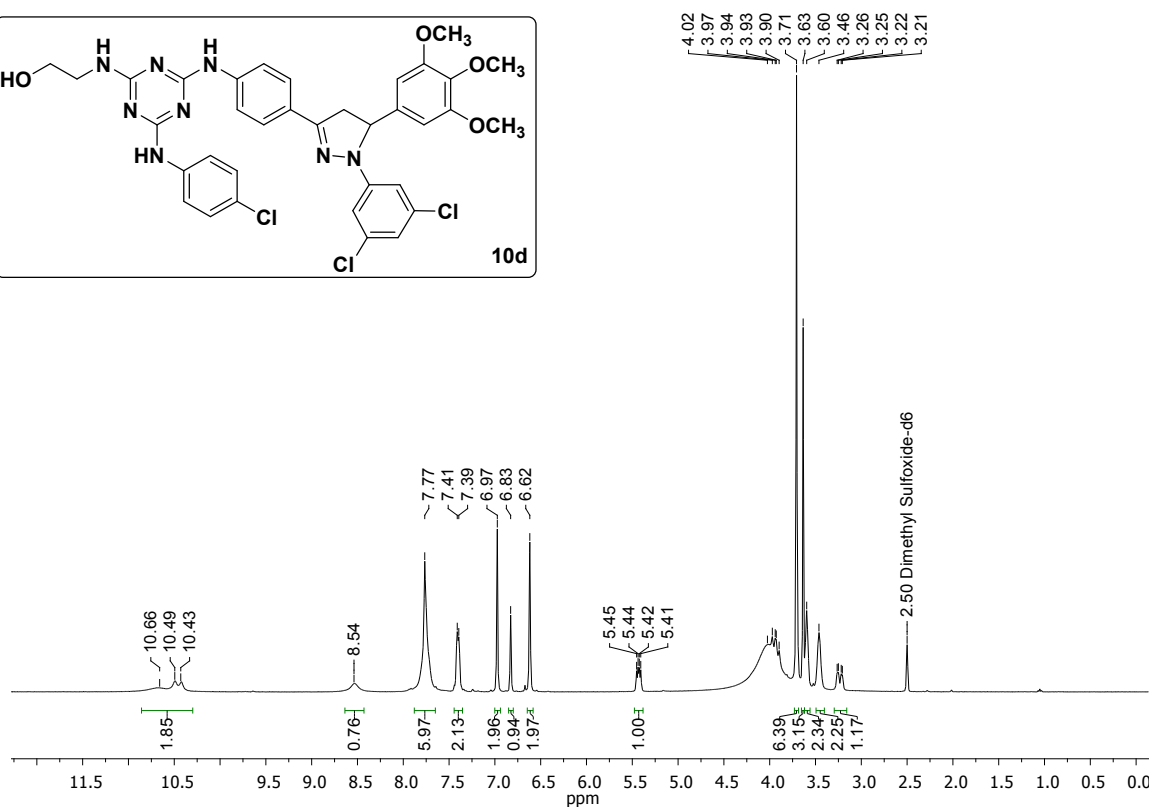
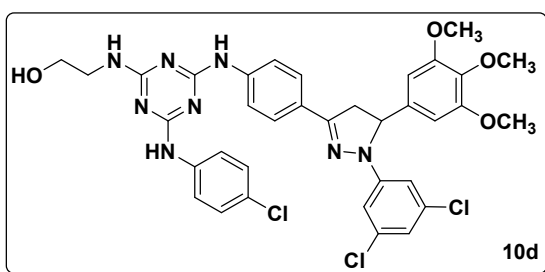
¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of **10b**.



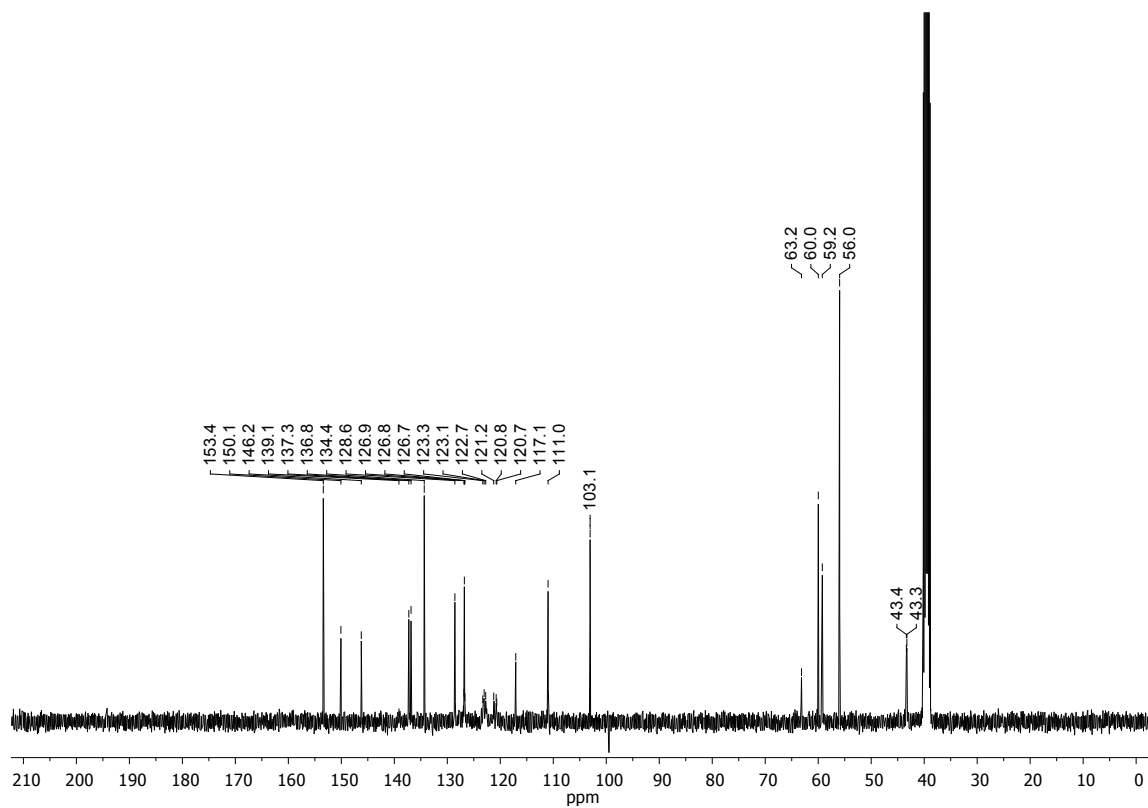
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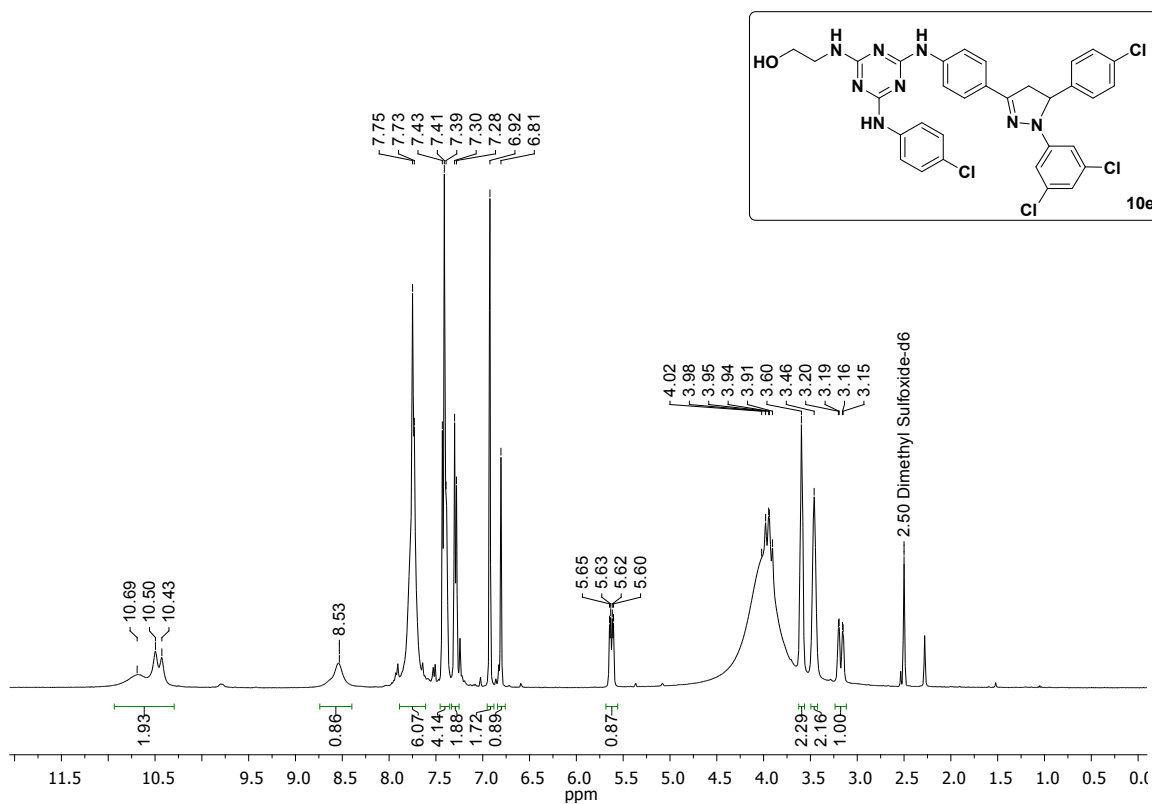
¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of **10c**.



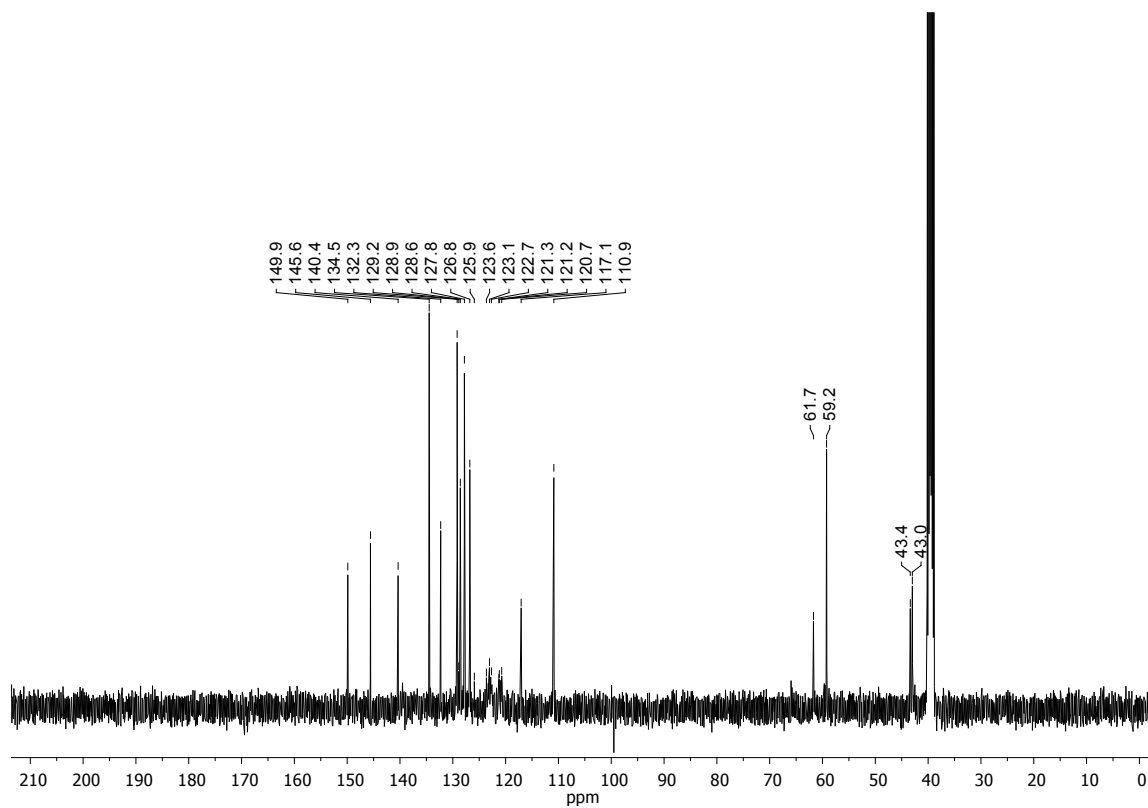
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **10d**.



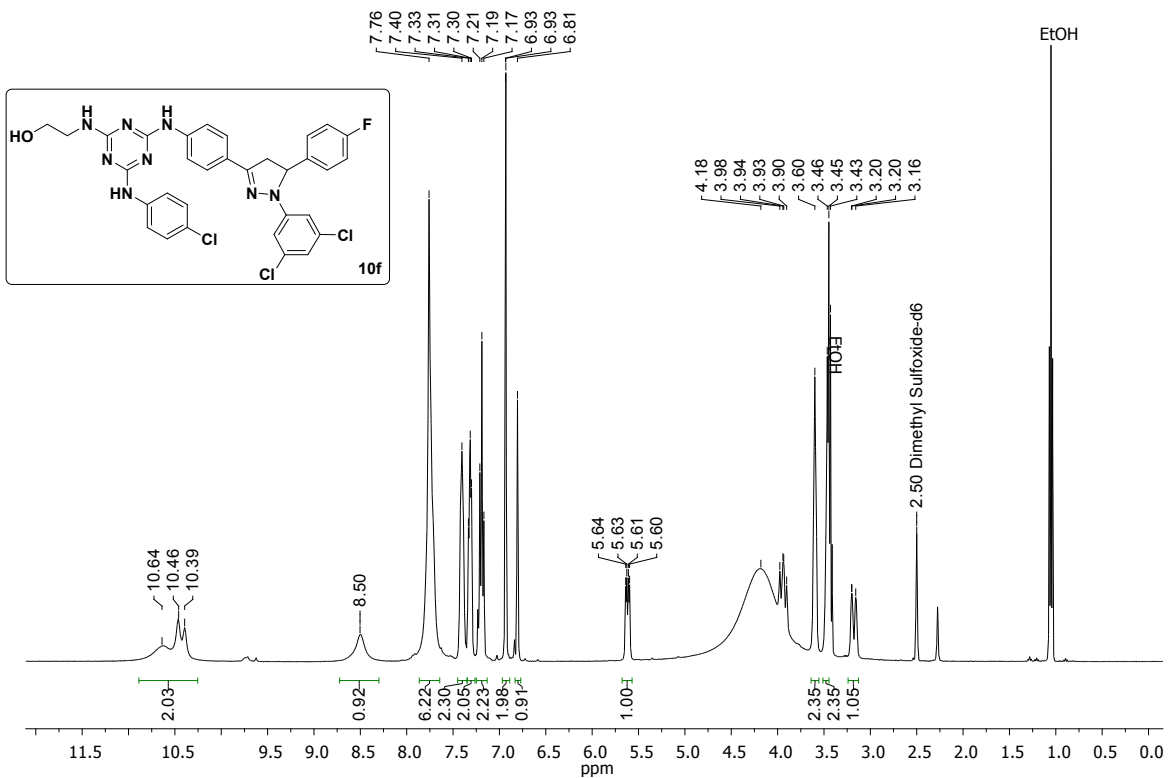
¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of **10d**.



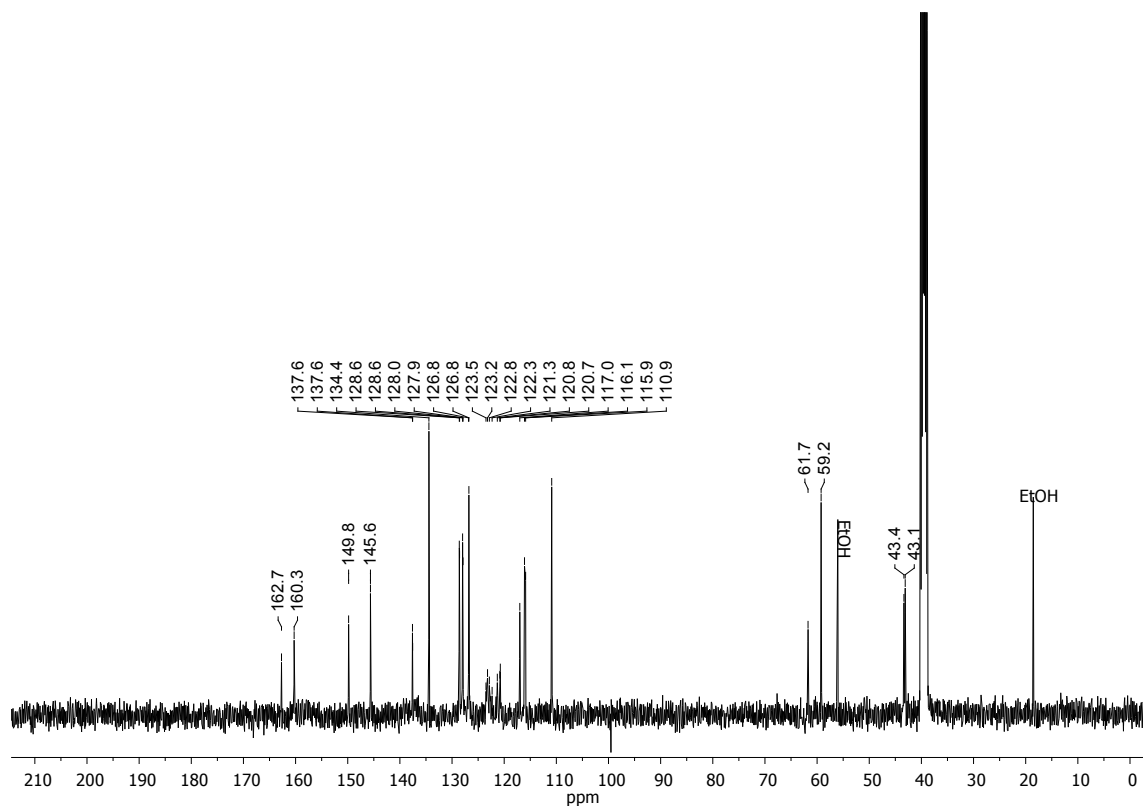
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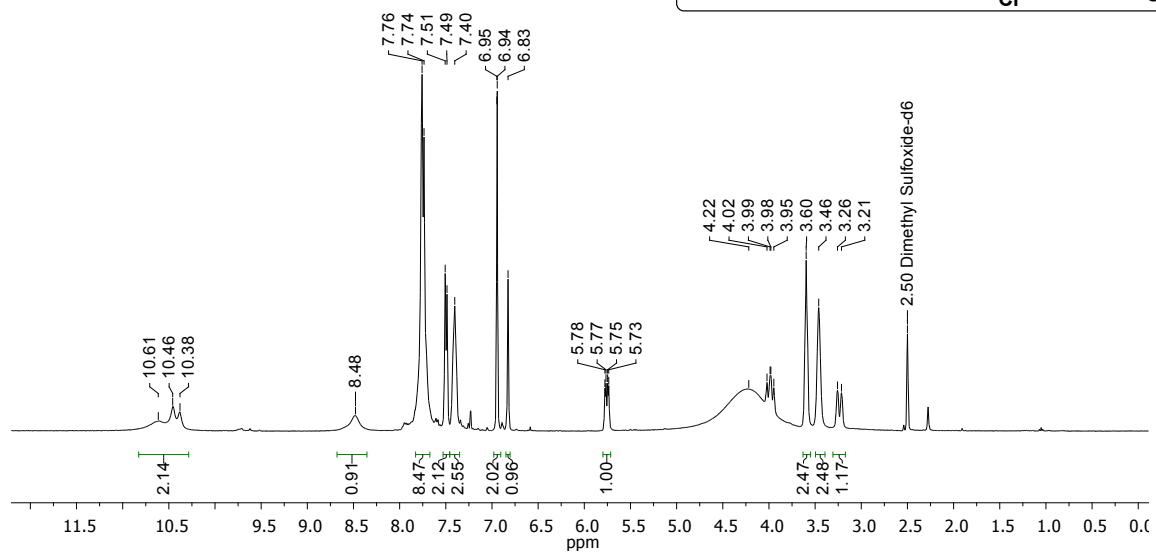
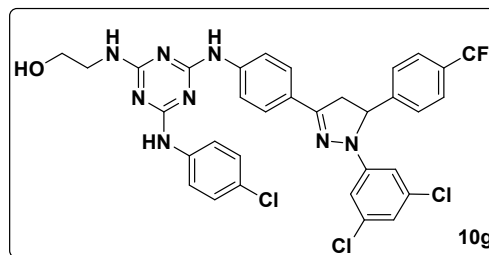
¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of **10e.**



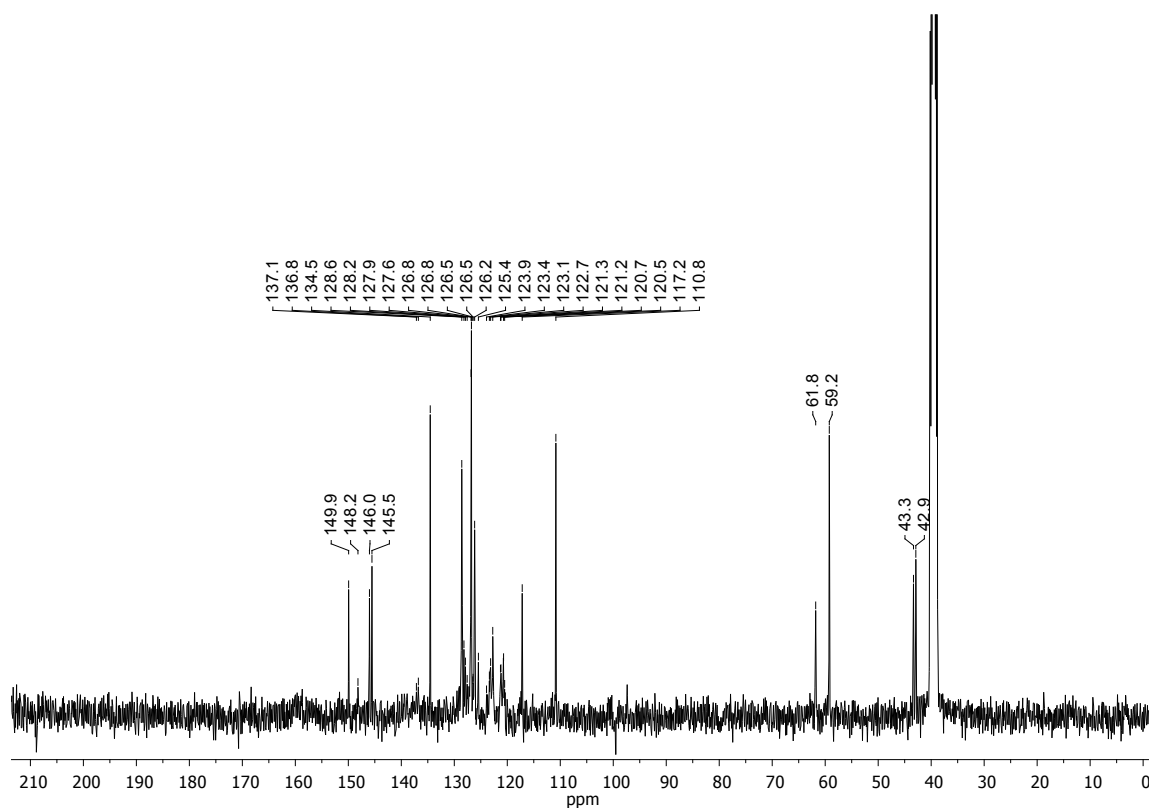
¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **10f**.



¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of **10f**.



¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **10g**.



¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of **10g**.