

Supplementary Materials

Design, Synthesis and Anti-tumor Activity of Novel Benzimidazole-Chalcone Hybrids as Non-Intercalative Topoisomerase II Catalytic Inhibitors

Wei Zhou^{1, *}, Wenjin Zhang¹, Yi Peng¹, Zhi-Hong Jiang², Lanyue Zhang¹, Zhiyun Du^{1, *}

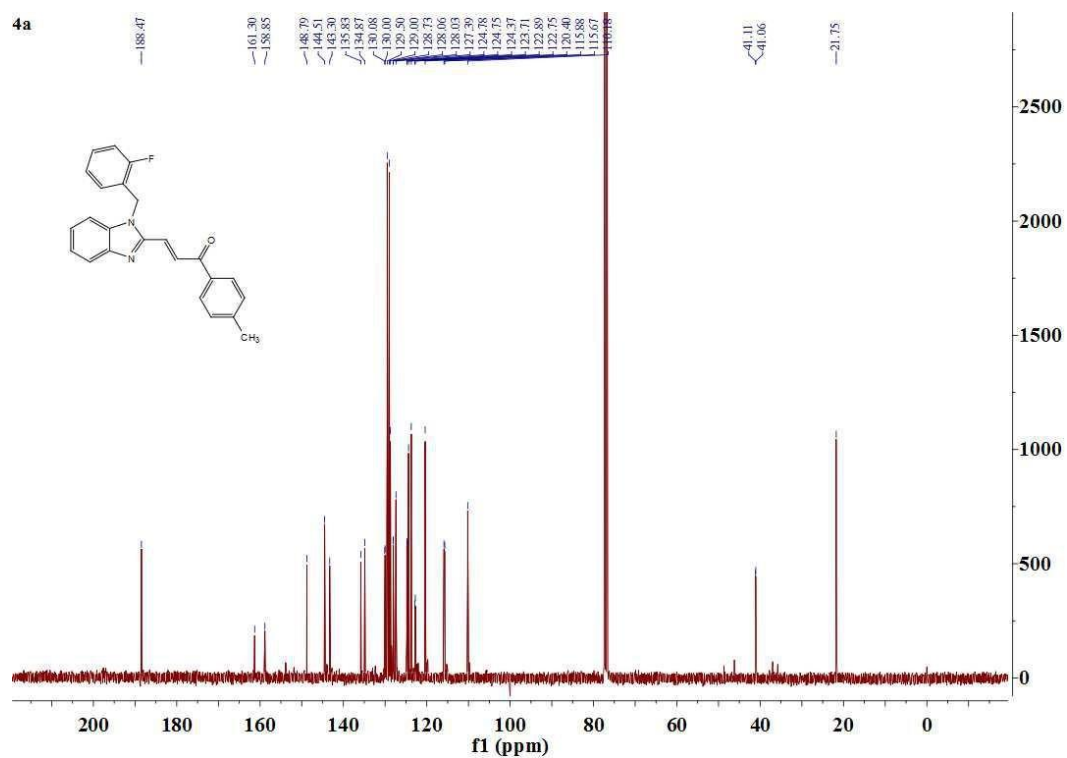
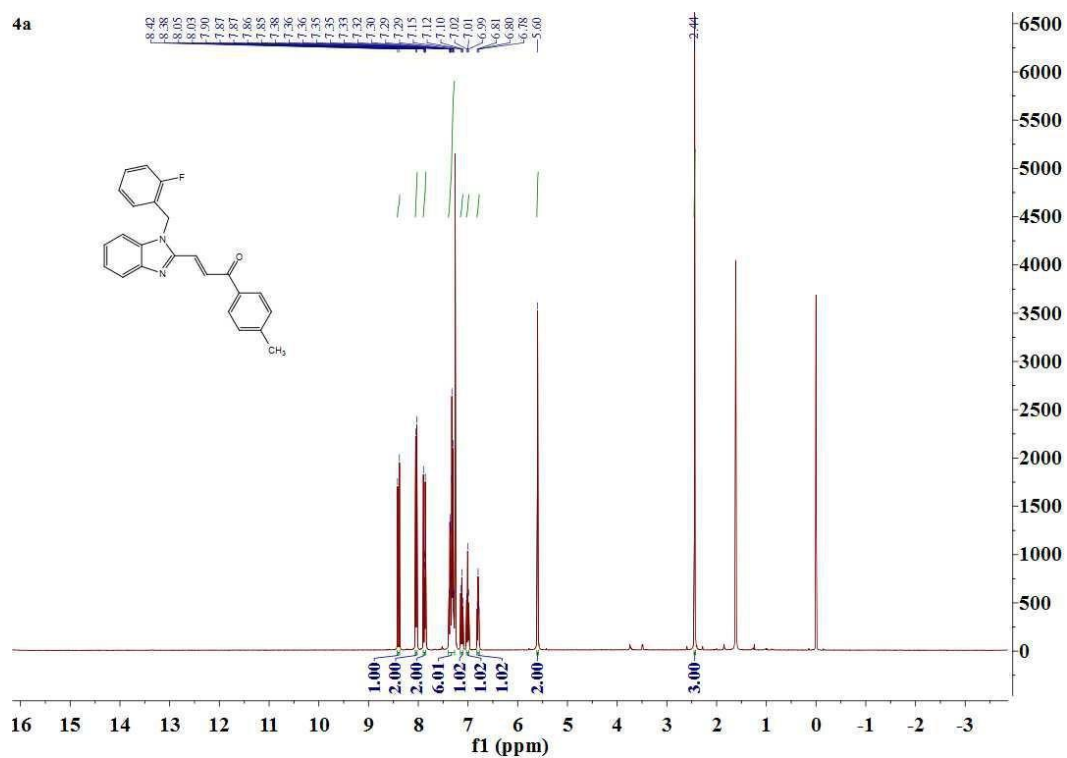
¹ School of Biomedical and Pharmaceutical Sciences, Guangdong University of Technology, Guangzhou 510006, P.R. China

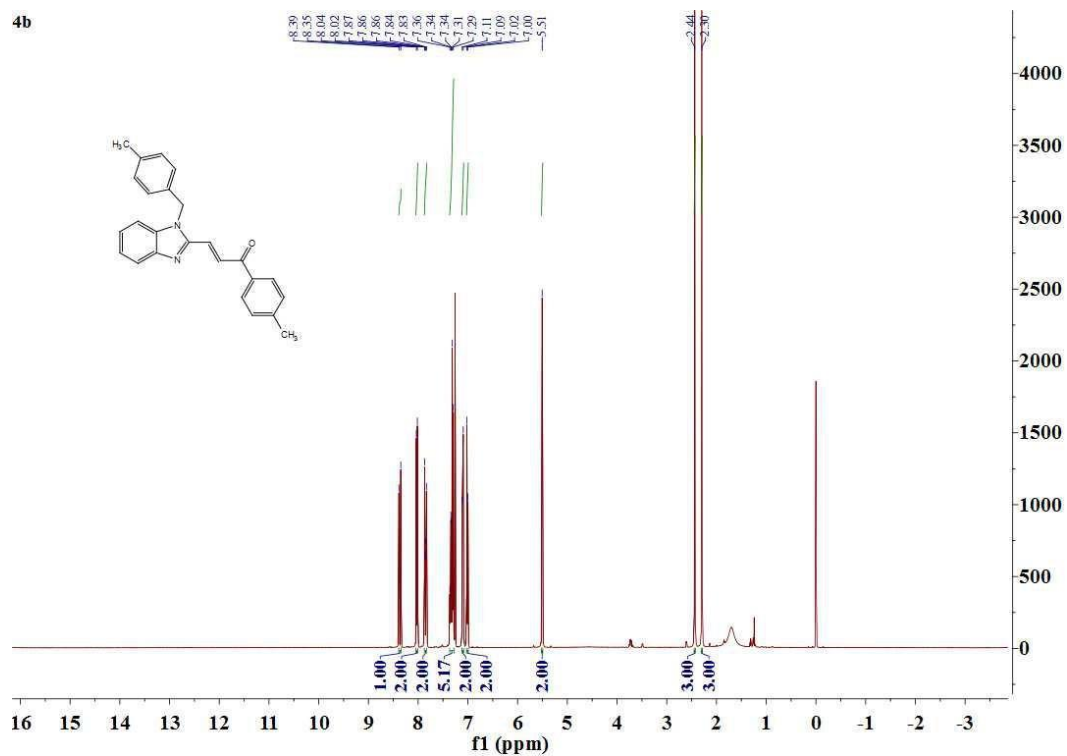
² State Key Laboratory of Quality Research in Chinese Medicine, Macau Institute for Applied Research in Medicine and Health, Macau University of Science and Technology, Avenida Wai Long, Taipa, Macau 999078, P.R. China

* Correspondence: zhou_wei@gdut.edu.cn (W. Z.), zhiyundu@foxmail.com (Z.D.);

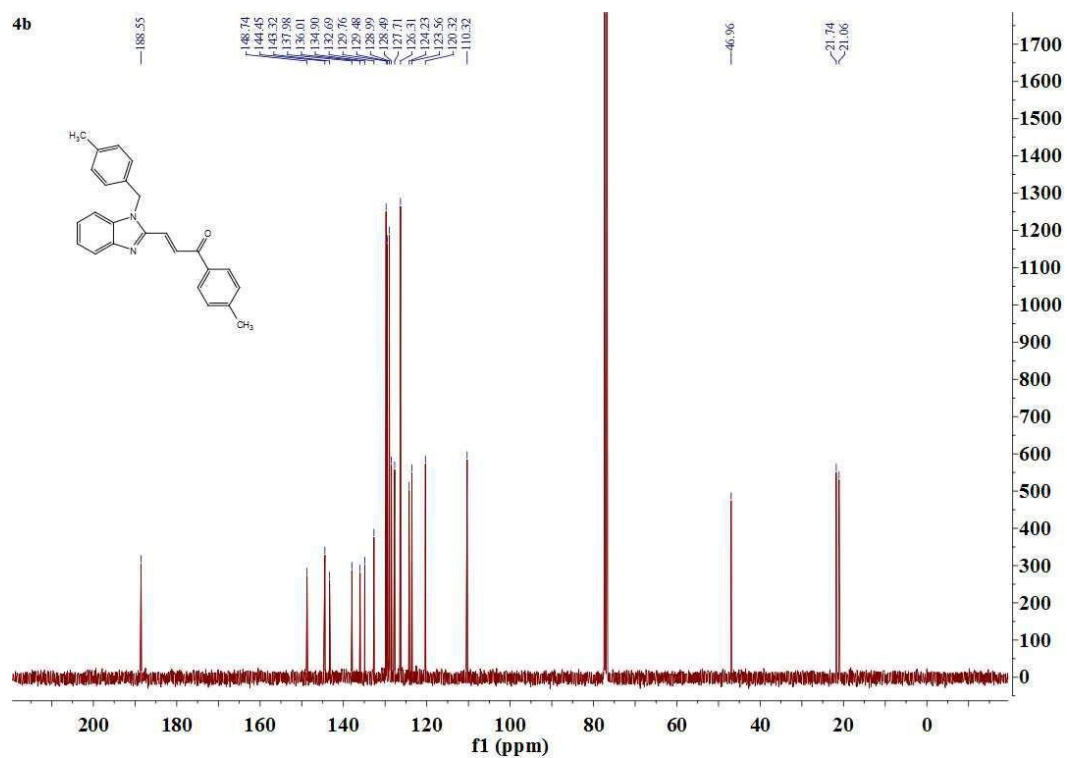
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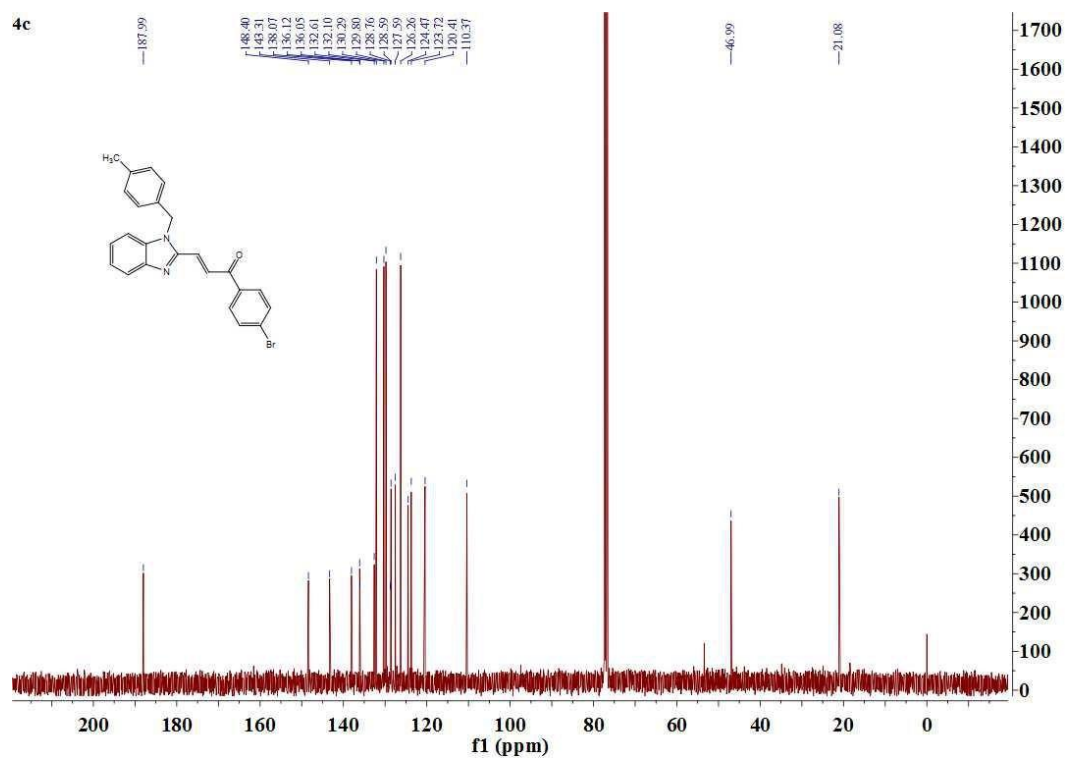
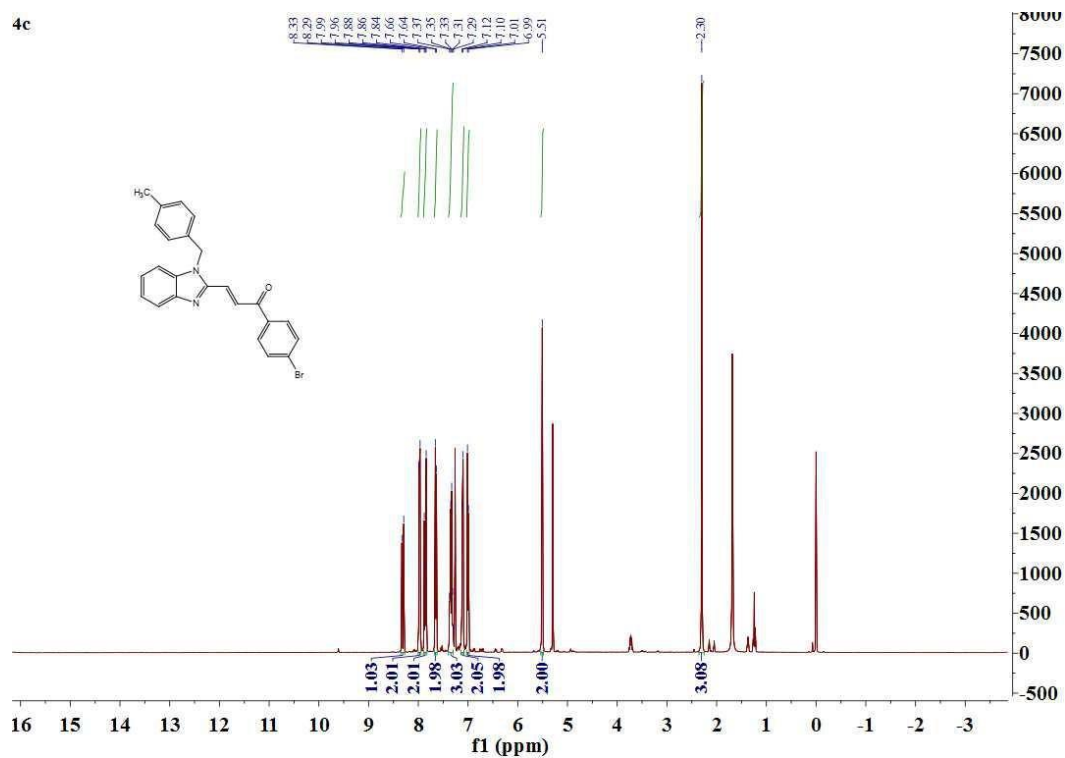




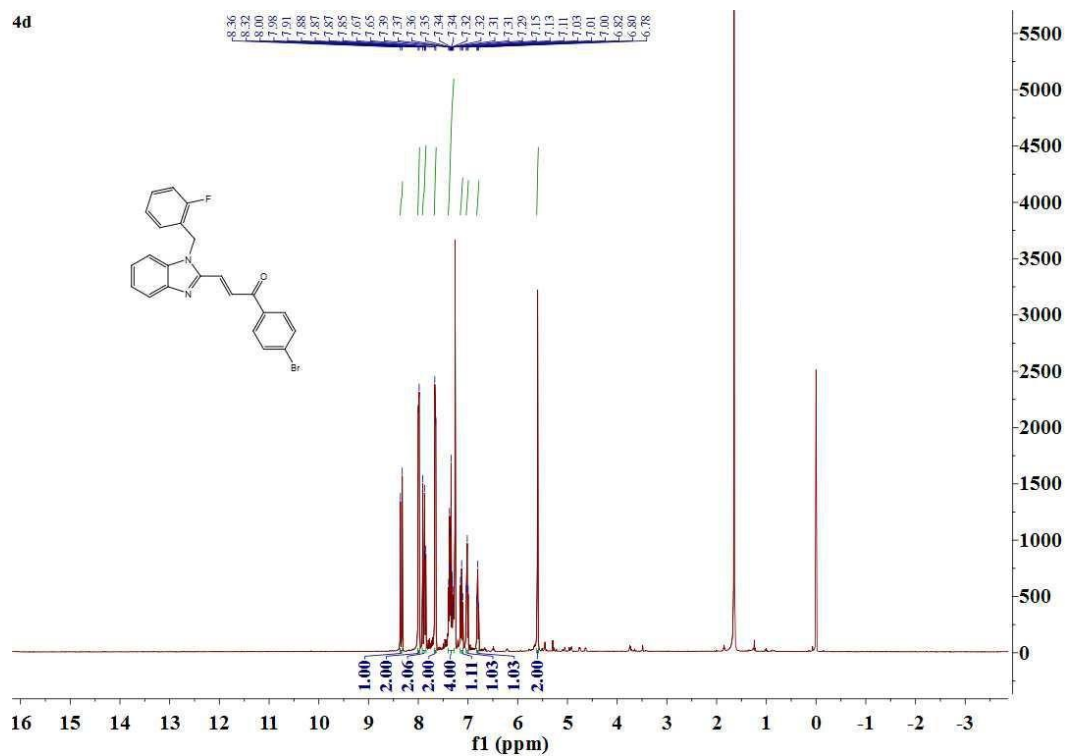
¹H NMR (400 MHz, CDCl₃) of compound **4b**



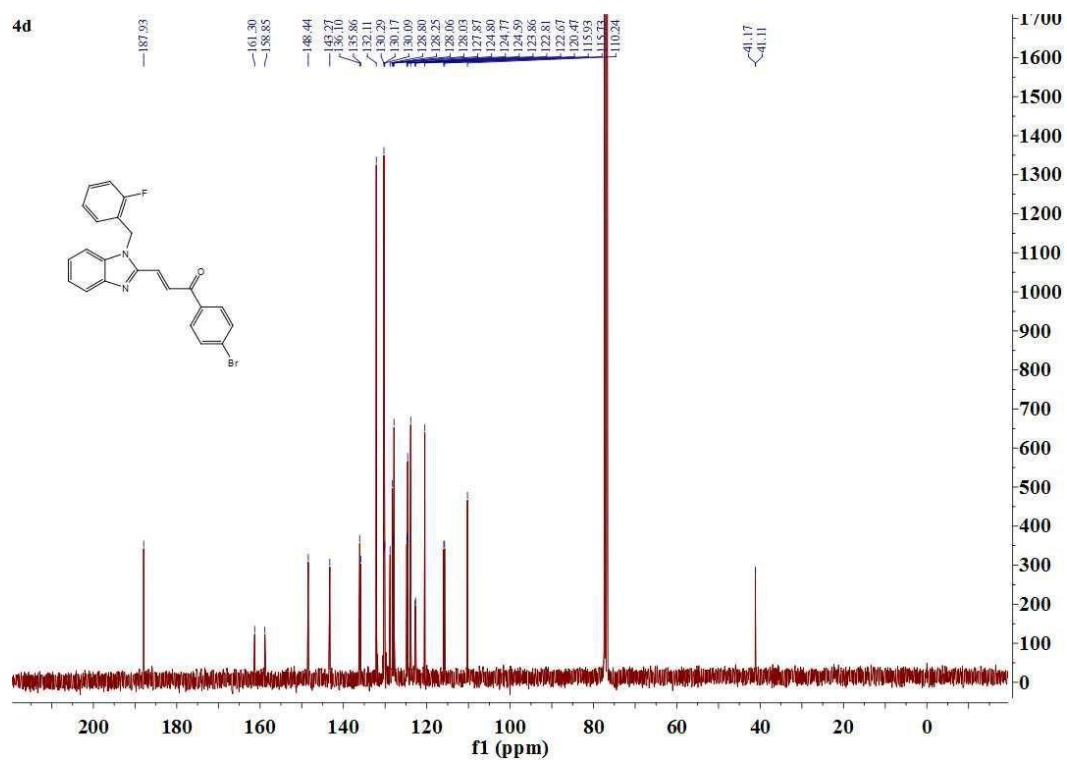
¹³C NMR (101 MHz, CDCl₃) of compound **4b**



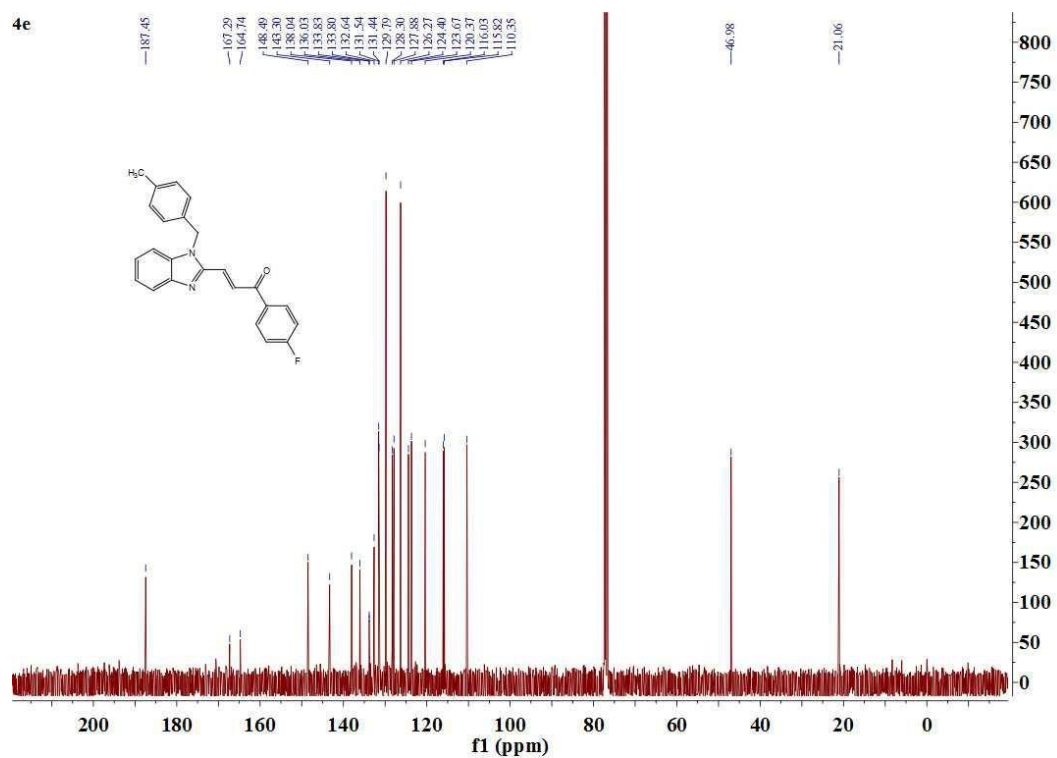
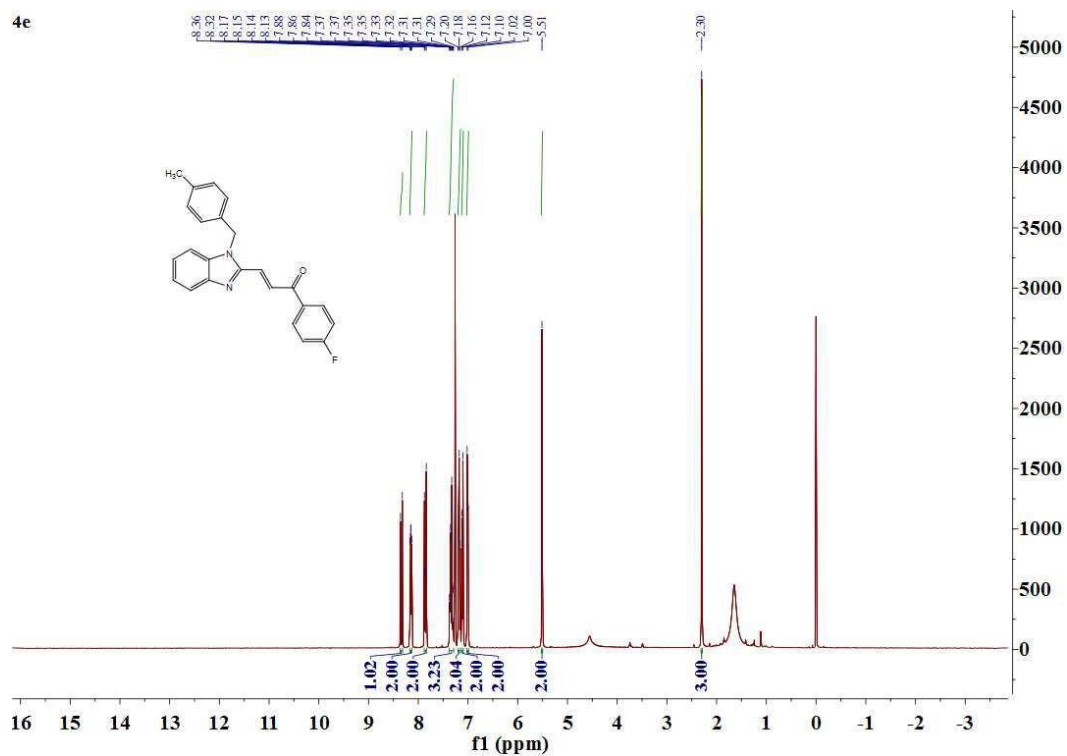
¹³C NMR (101 MHz, CDCl₃) of compound **4c**

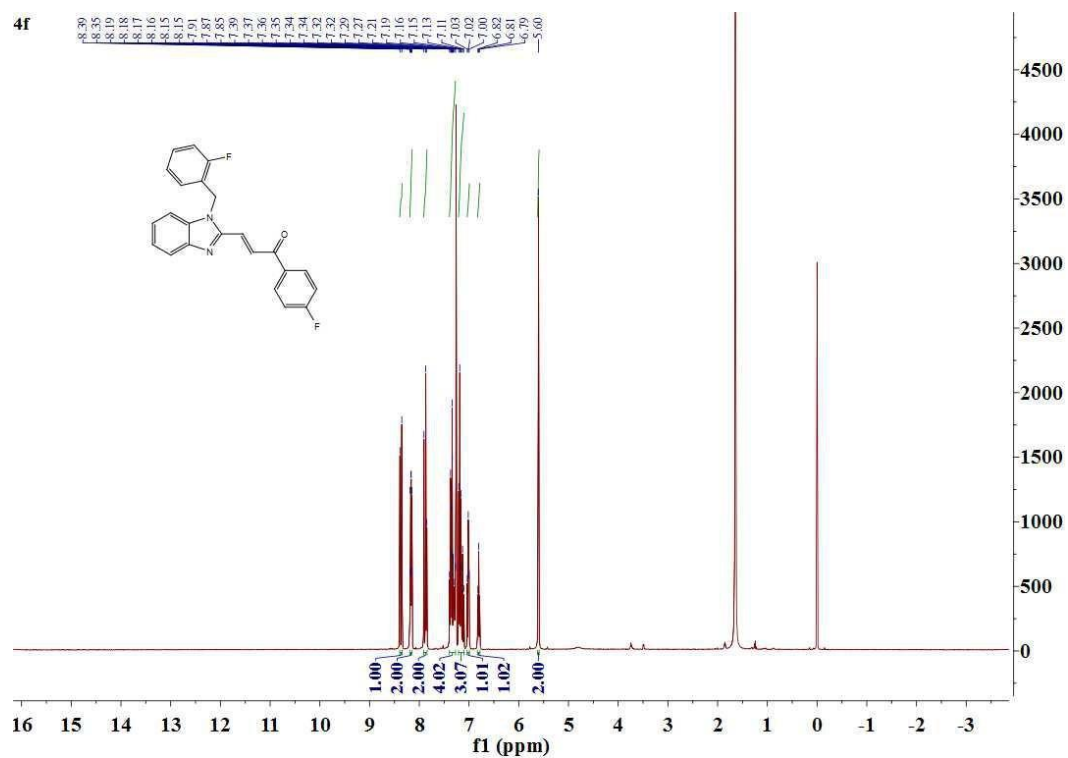


$^1\text{H NMR}$ (400 MHz, CDCl_3) of compound **4d**

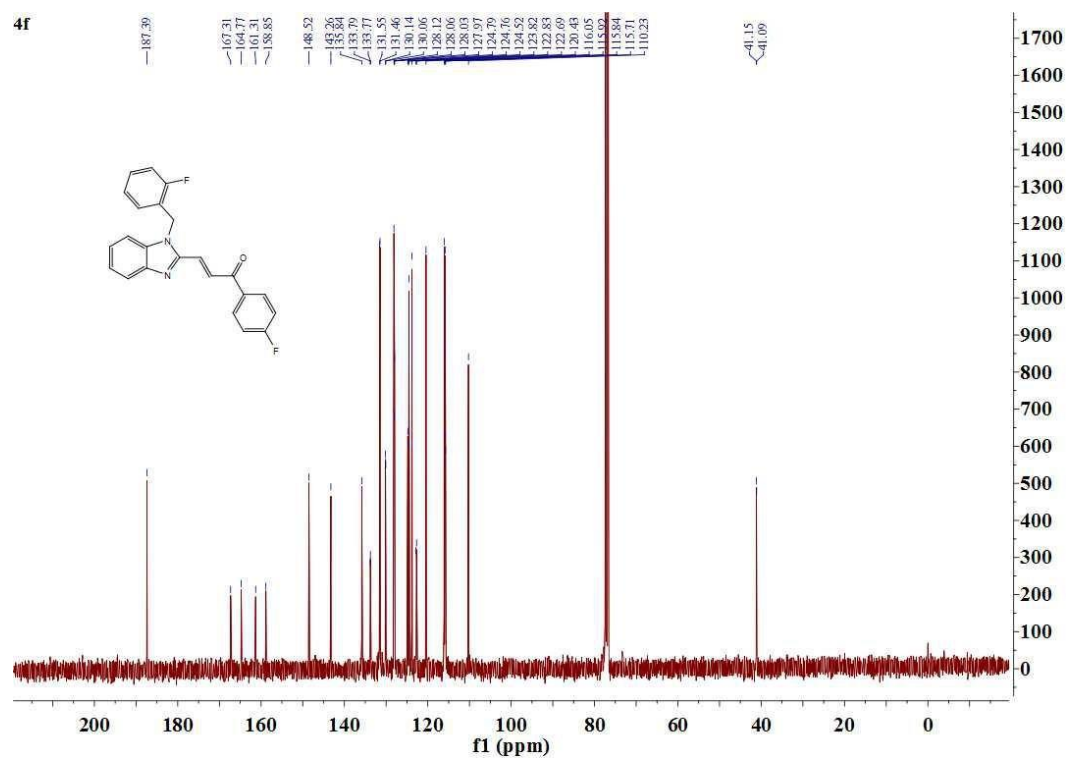


$^{13}\text{C NMR}$ (101 MHz, CDCl_3) of compound **4d**

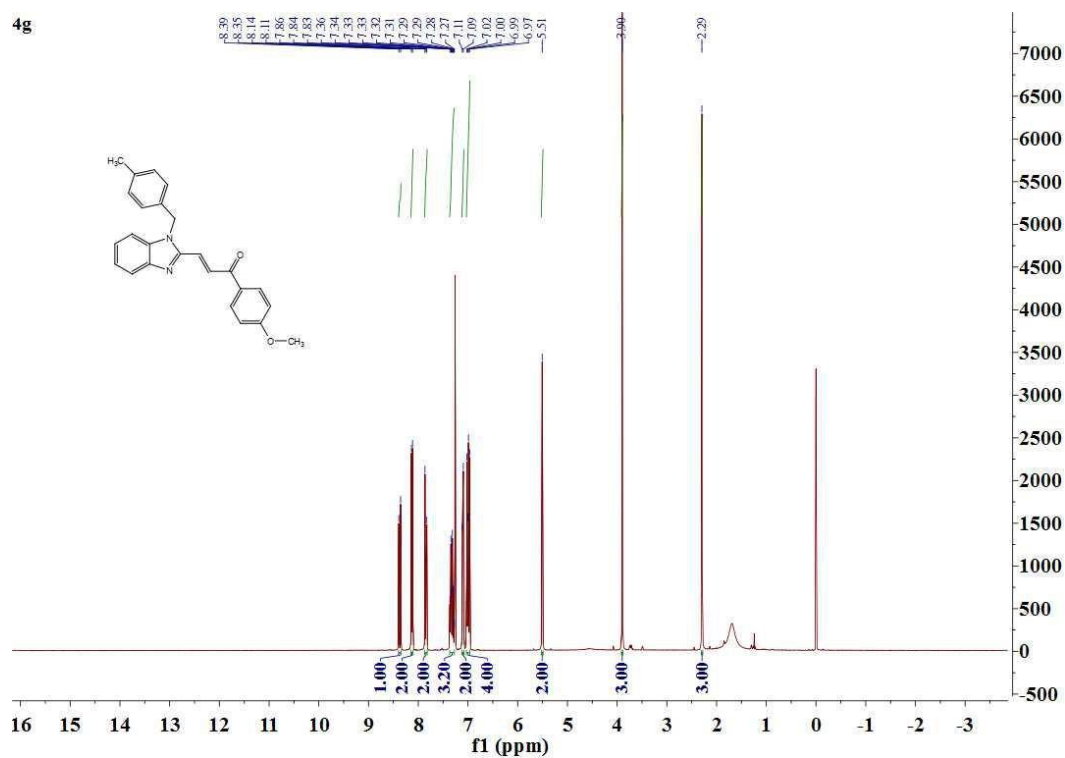




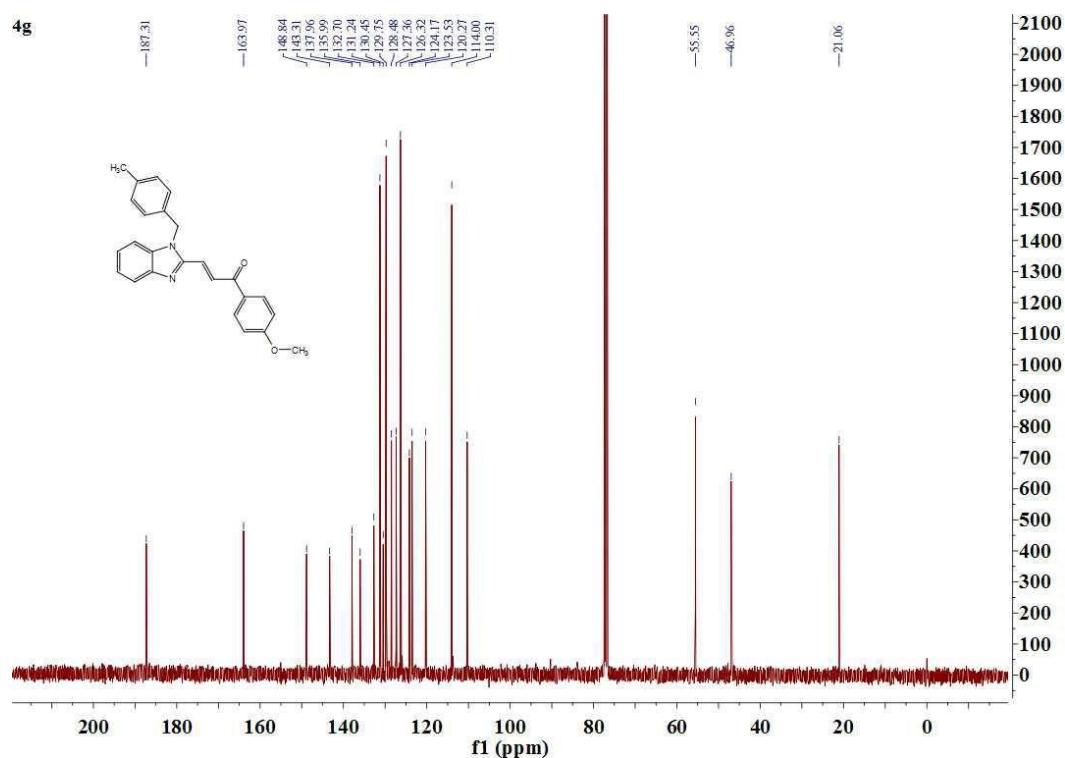
$^1\text{H NMR}$ (400 MHz, CDCl_3) of compound **4f**



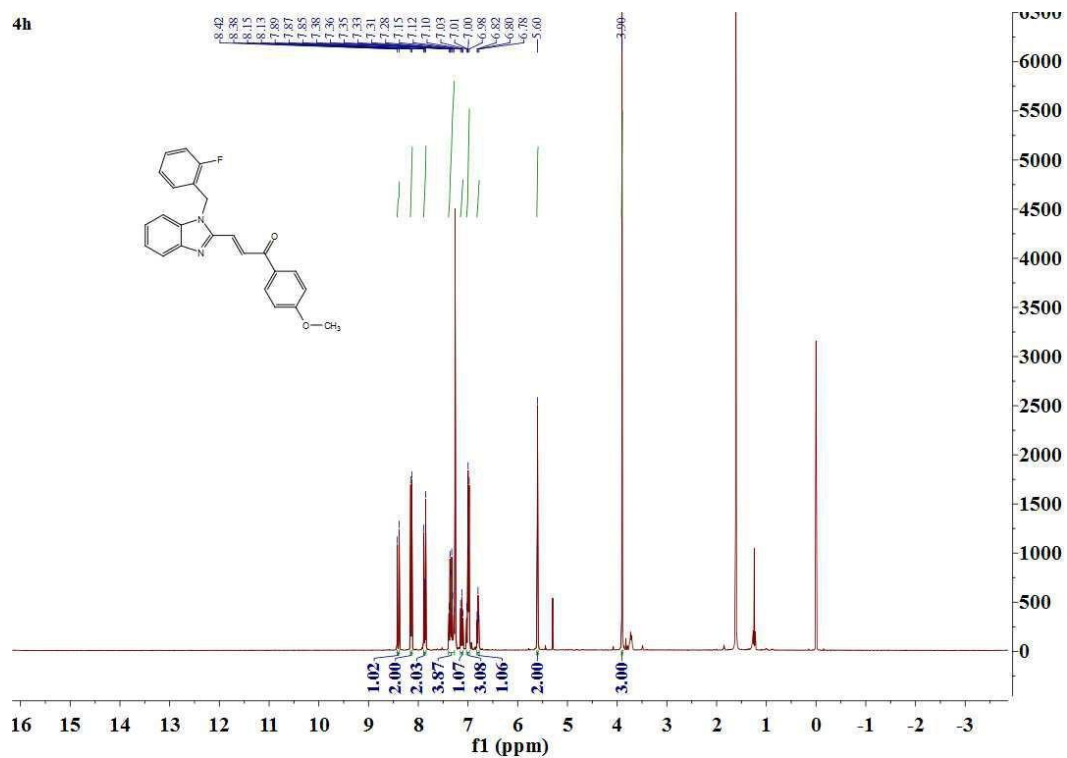
$^{13}\text{C NMR}$ (101 MHz, CDCl_3) of compound **4f**



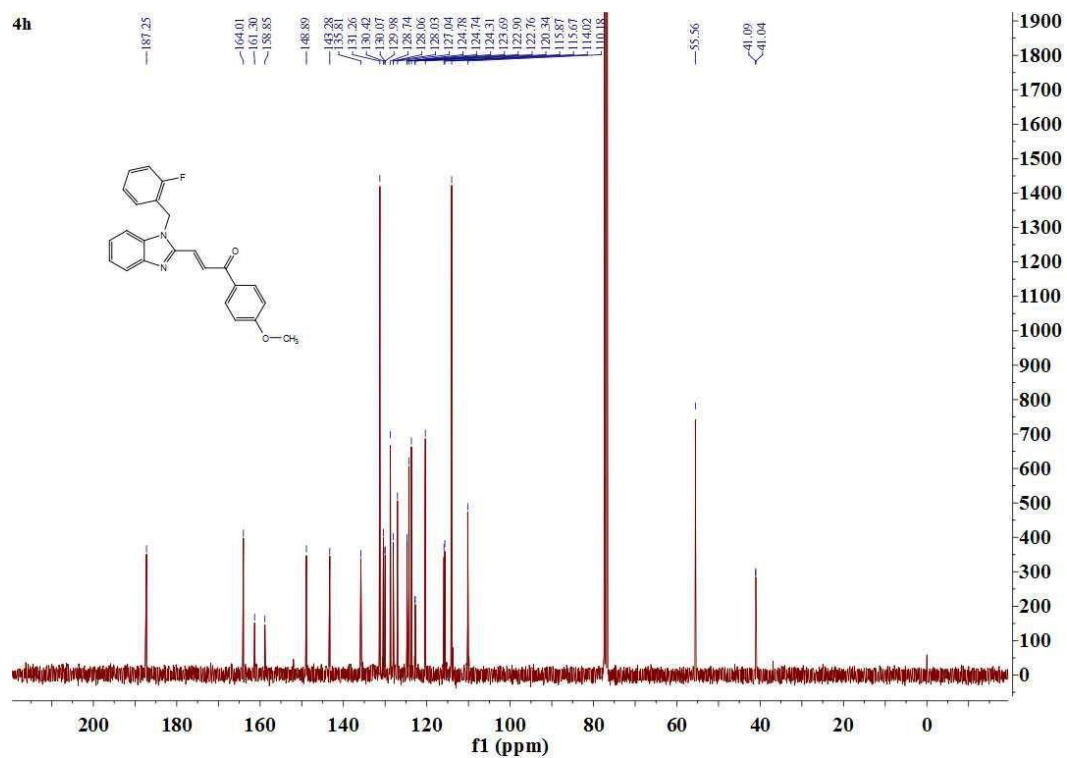
¹H NMR (400 MHz, CDCl₃) of compound 4g



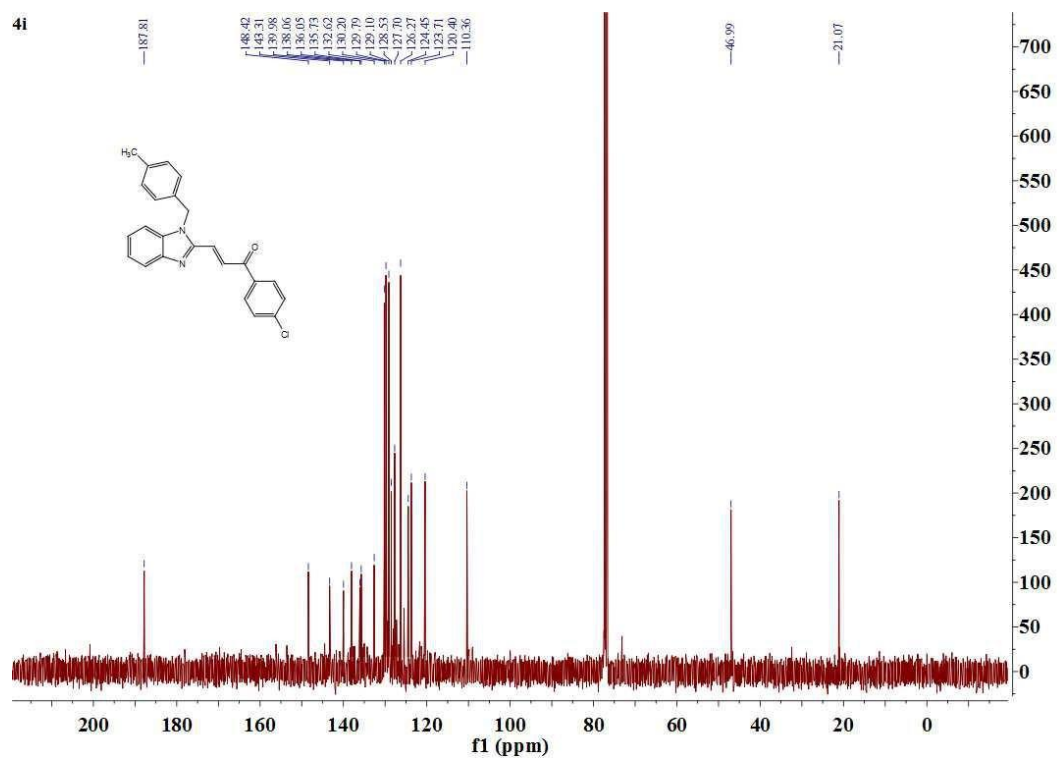
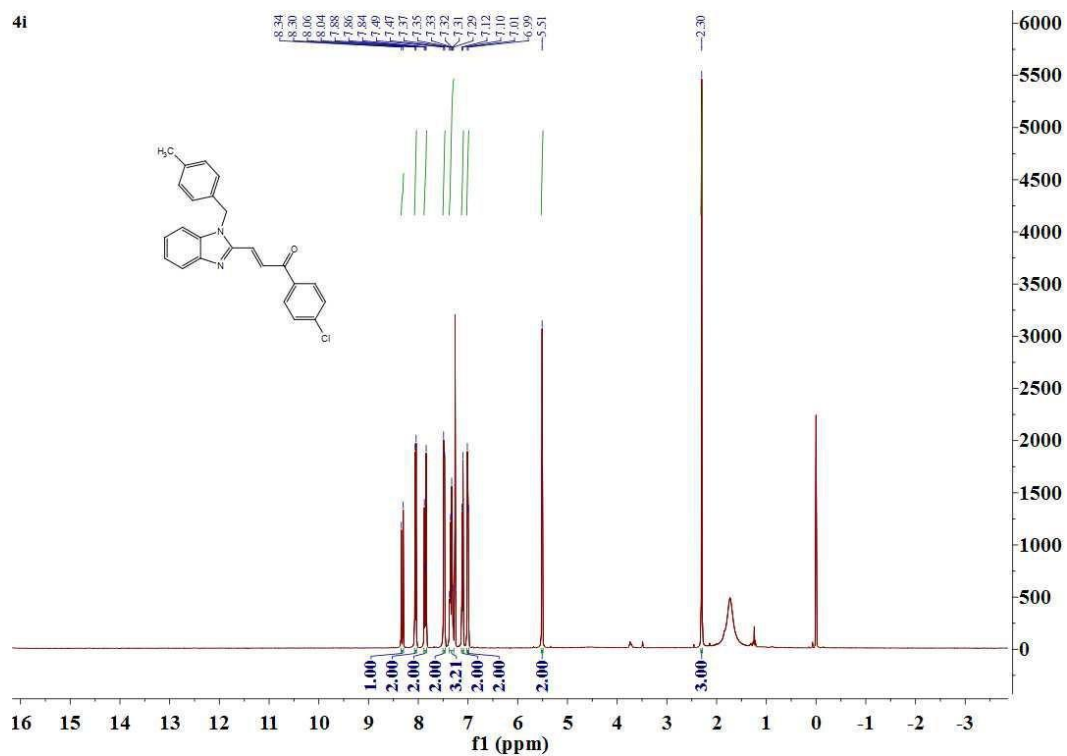
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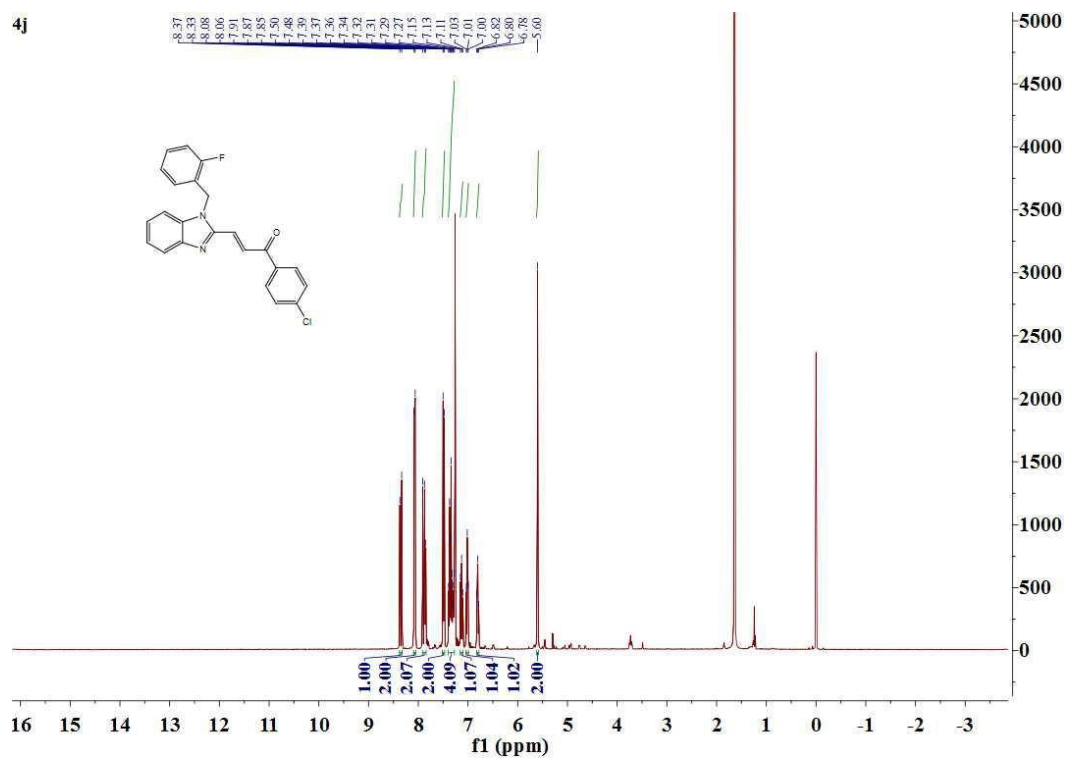


¹H NMR (400 MHz, CDCl₃) of compound **4h**

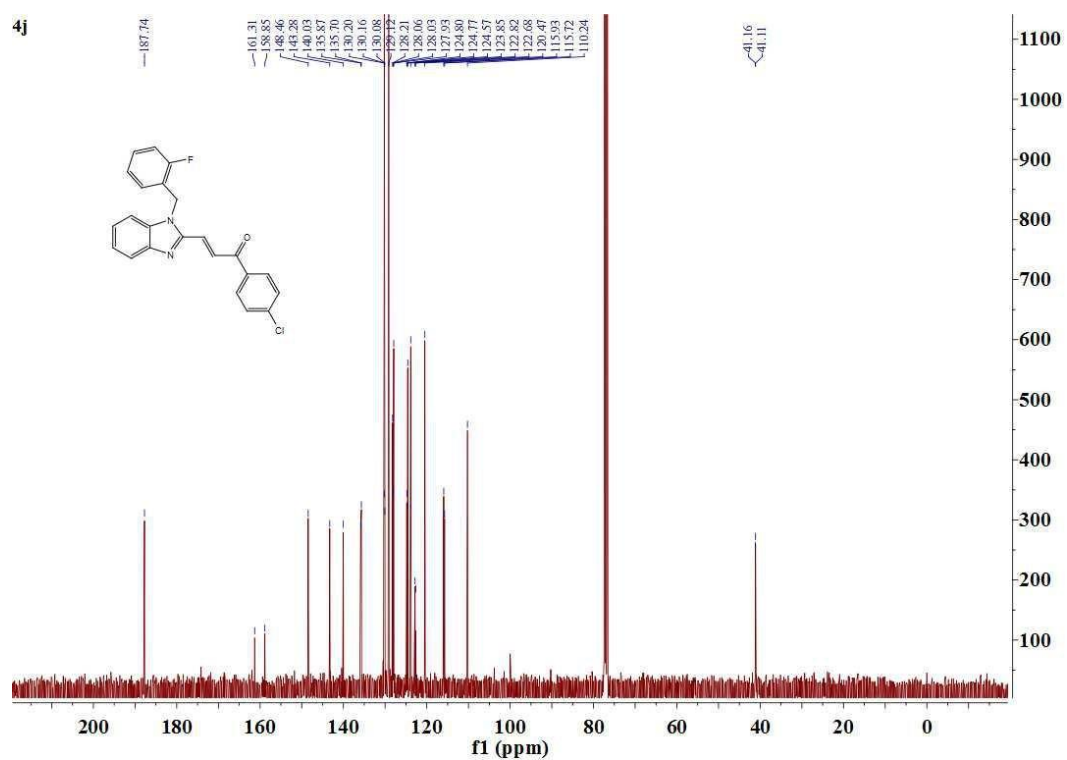


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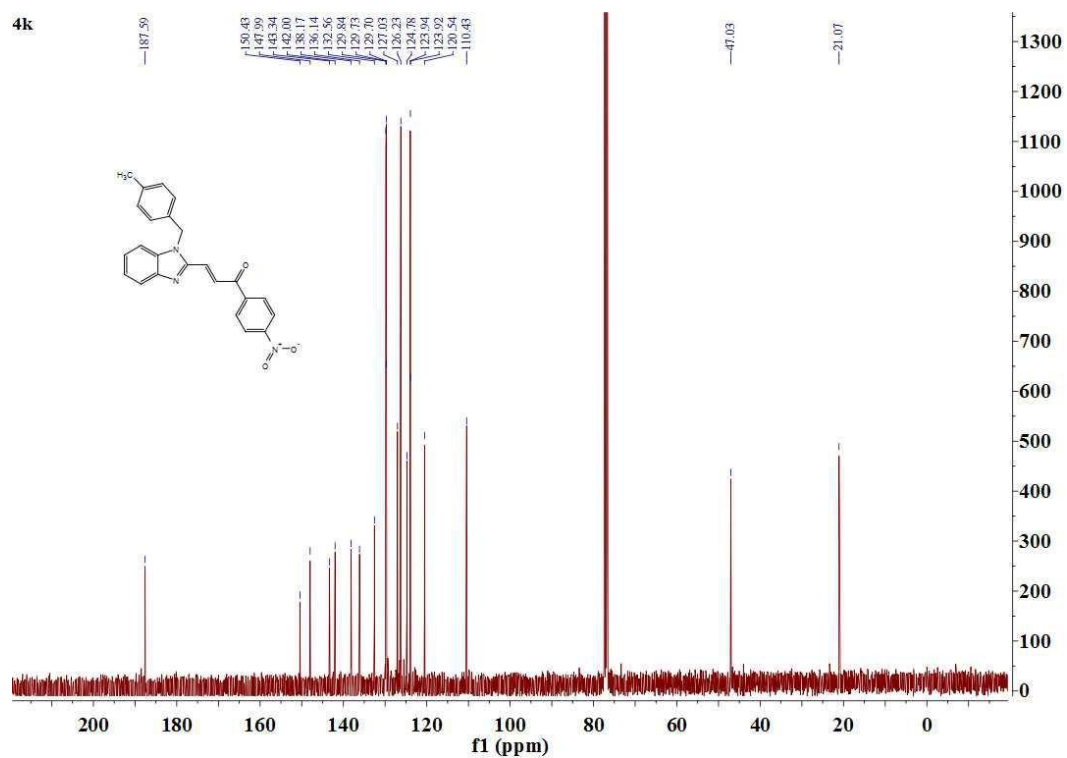
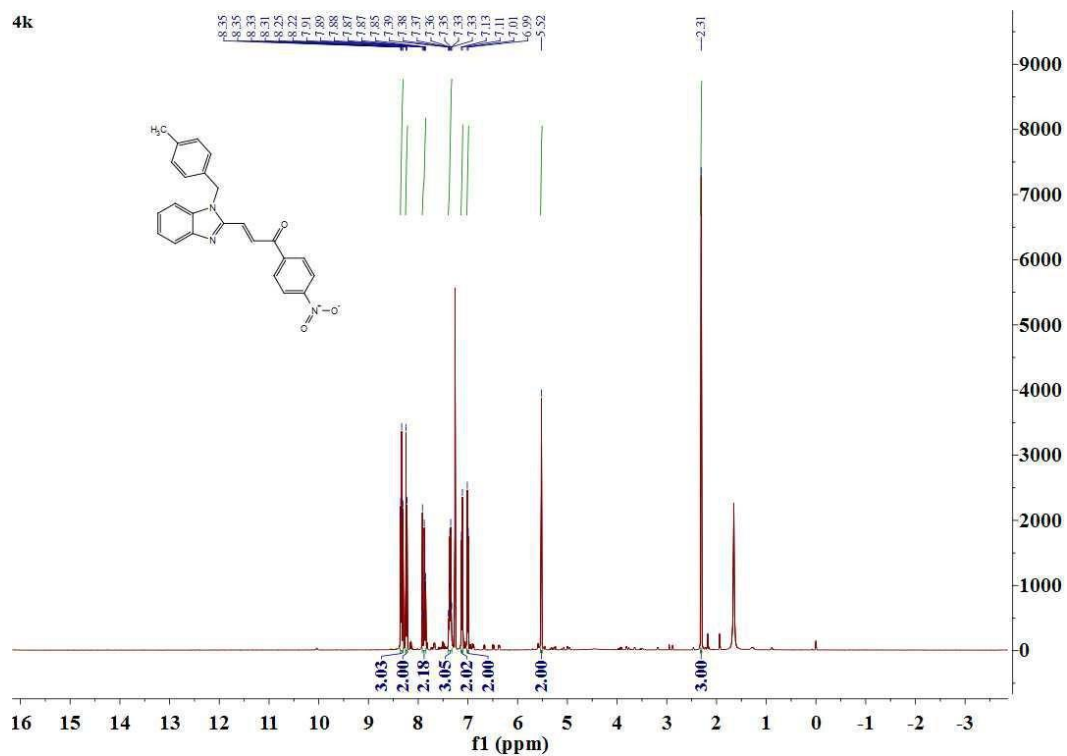


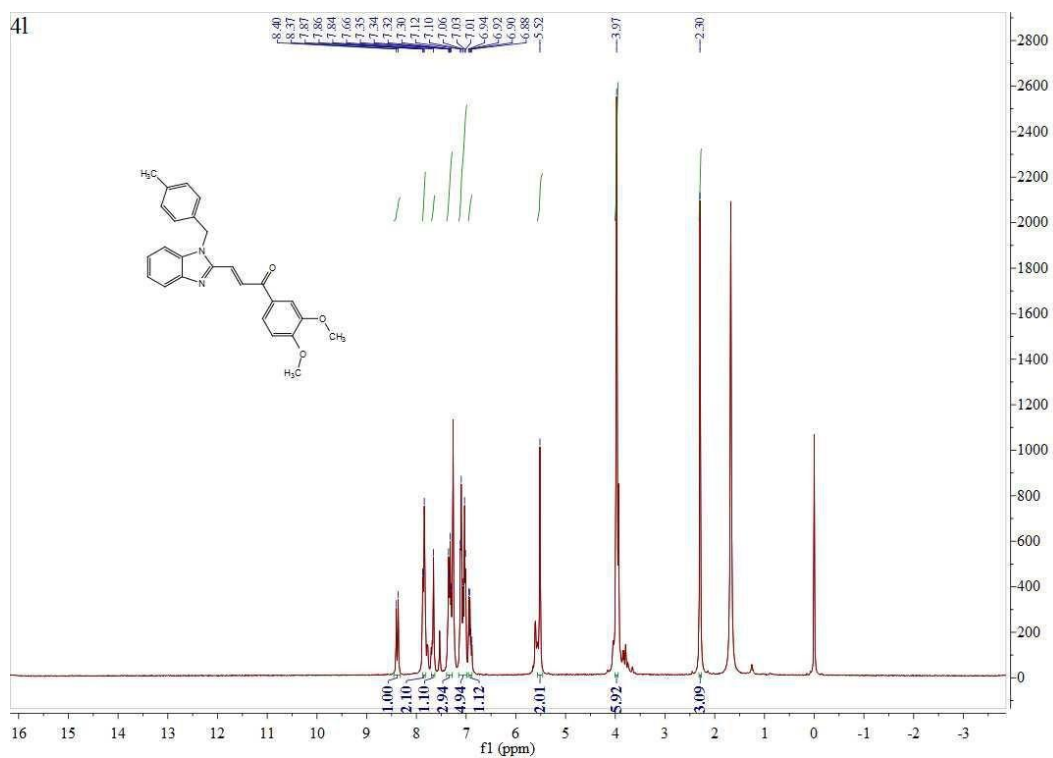


¹H NMR (400 MHz, CDCl₃) of compound **4j**

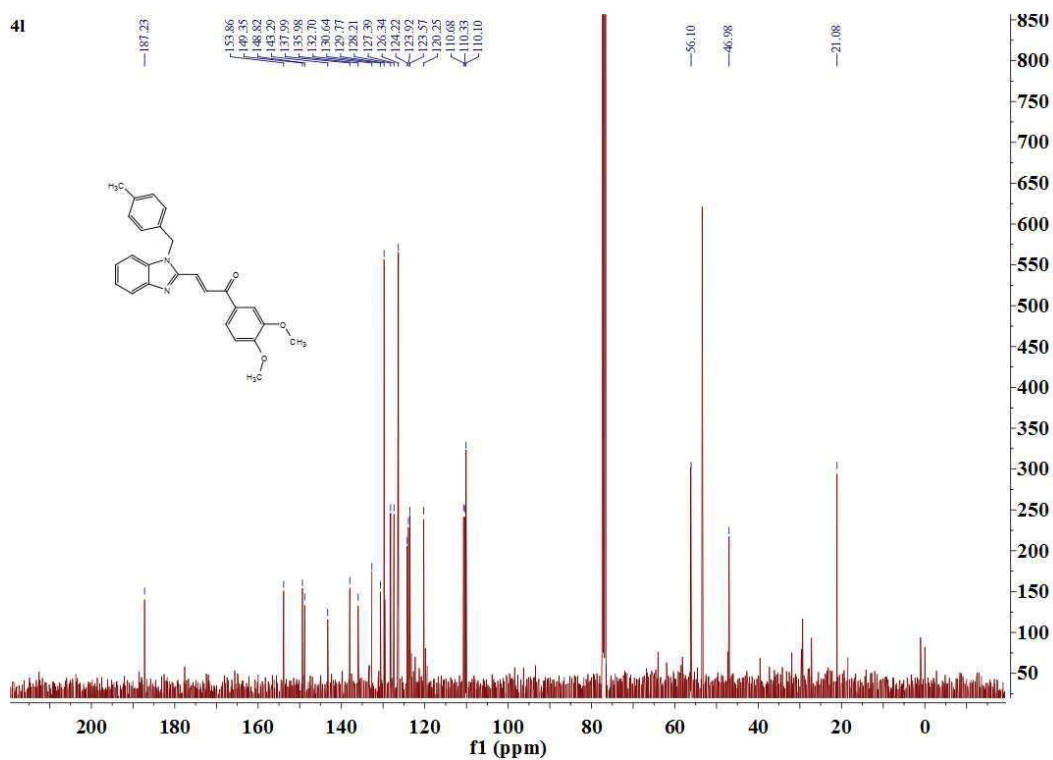


¹³C NMR (101 MHz, CDCl₃) of compound **4j**

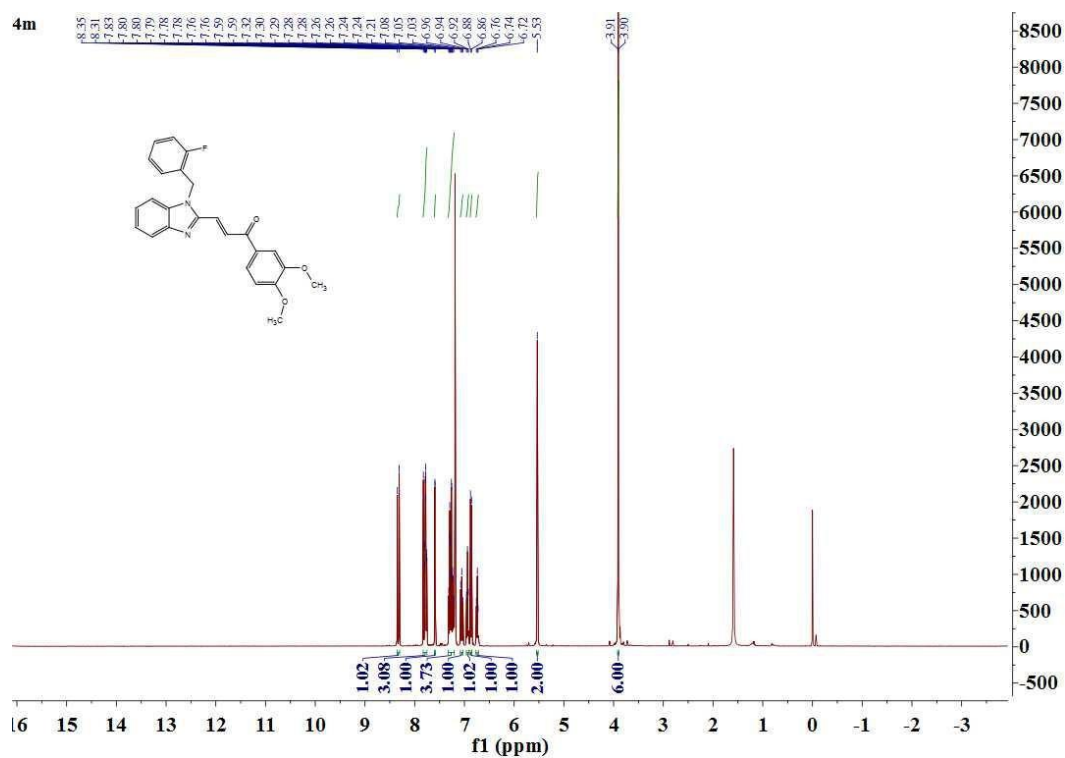




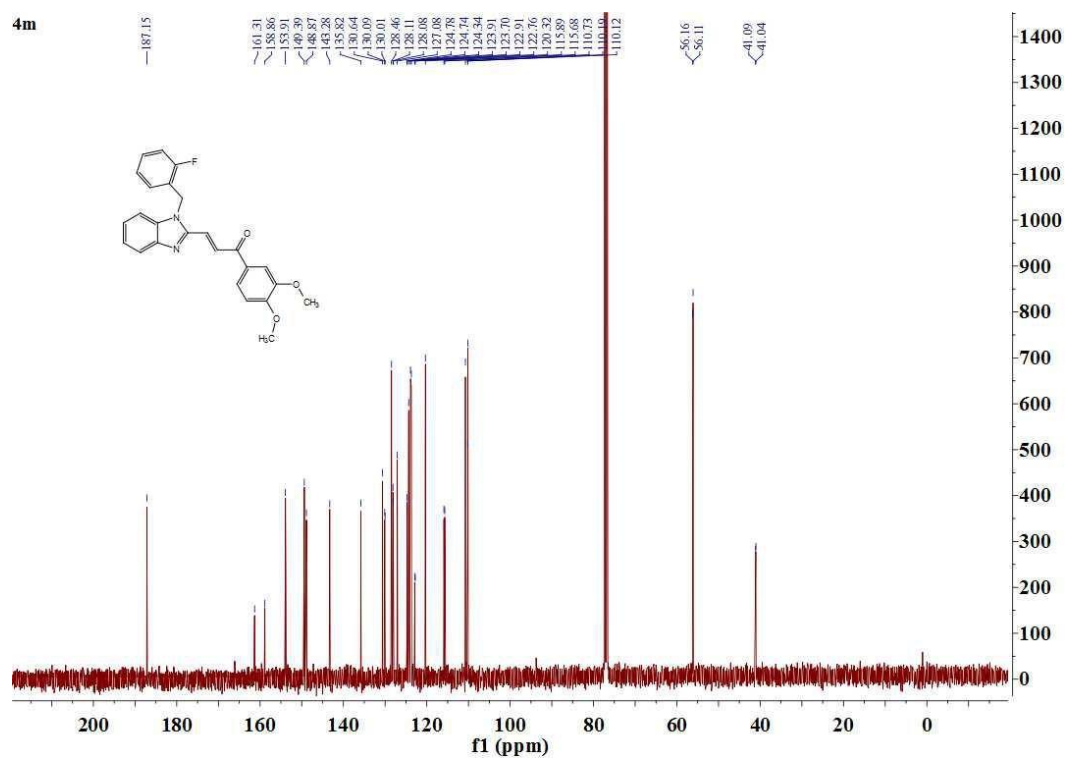
^1H NMR (400 MHz, CDCl_3) of compound **41**



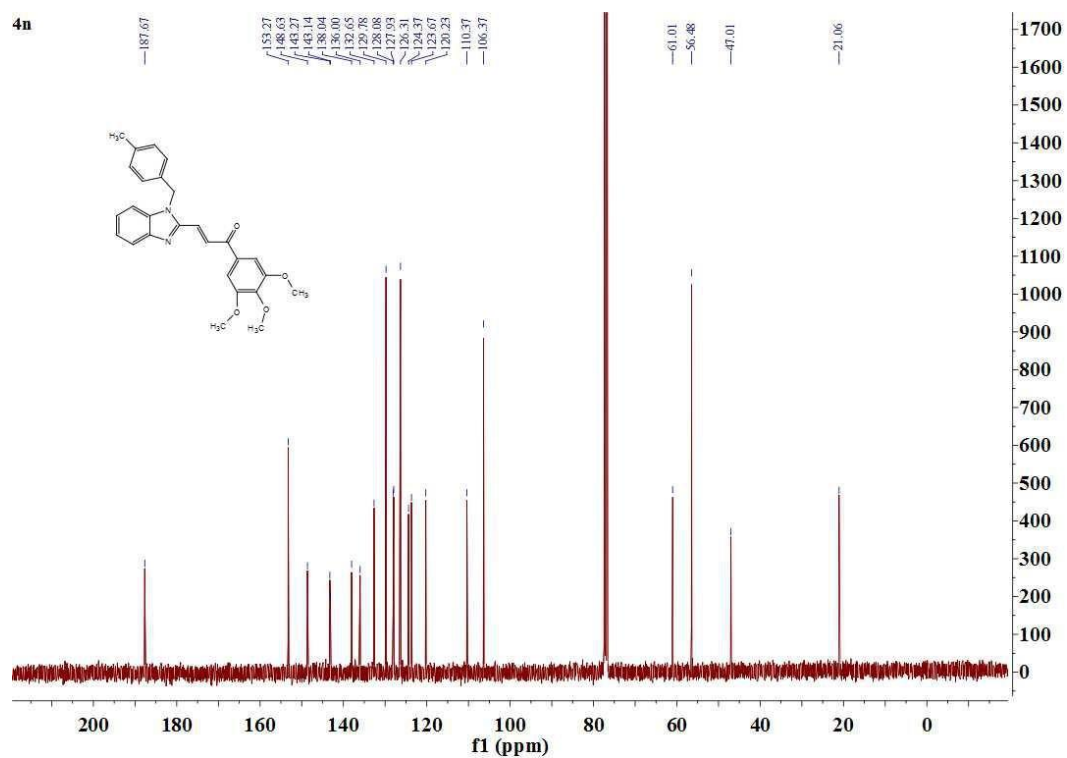
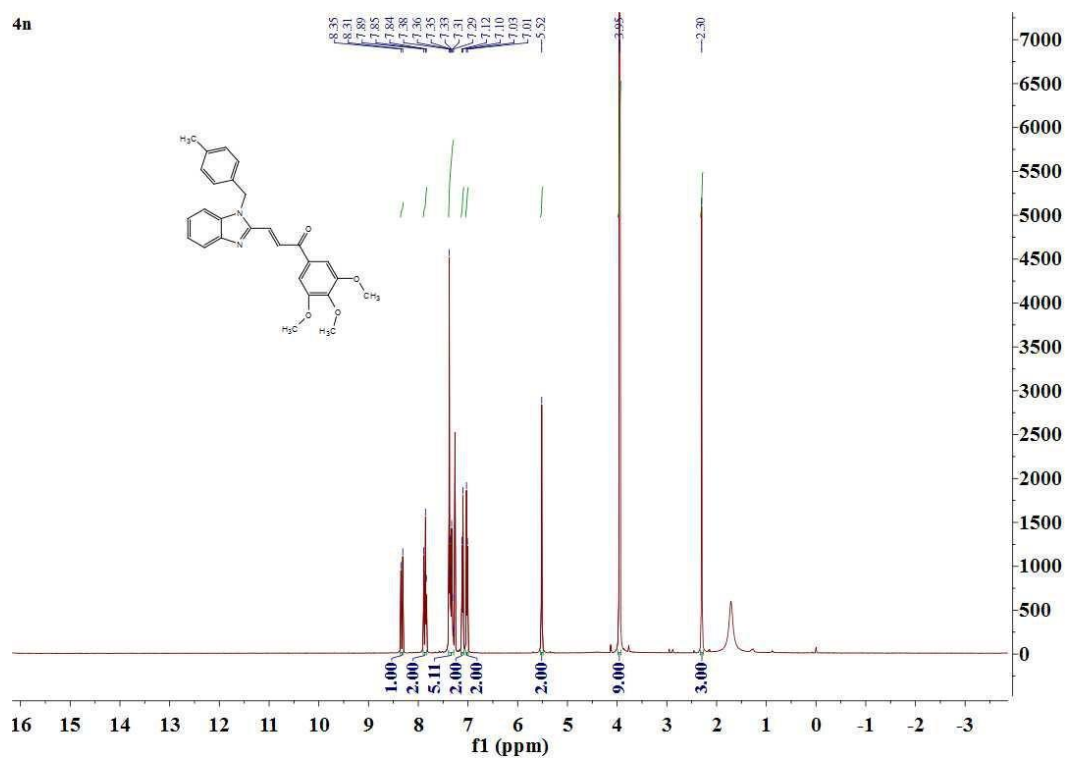
^{13}C NMR (101 MHz, CDCl_3) of compound **41**

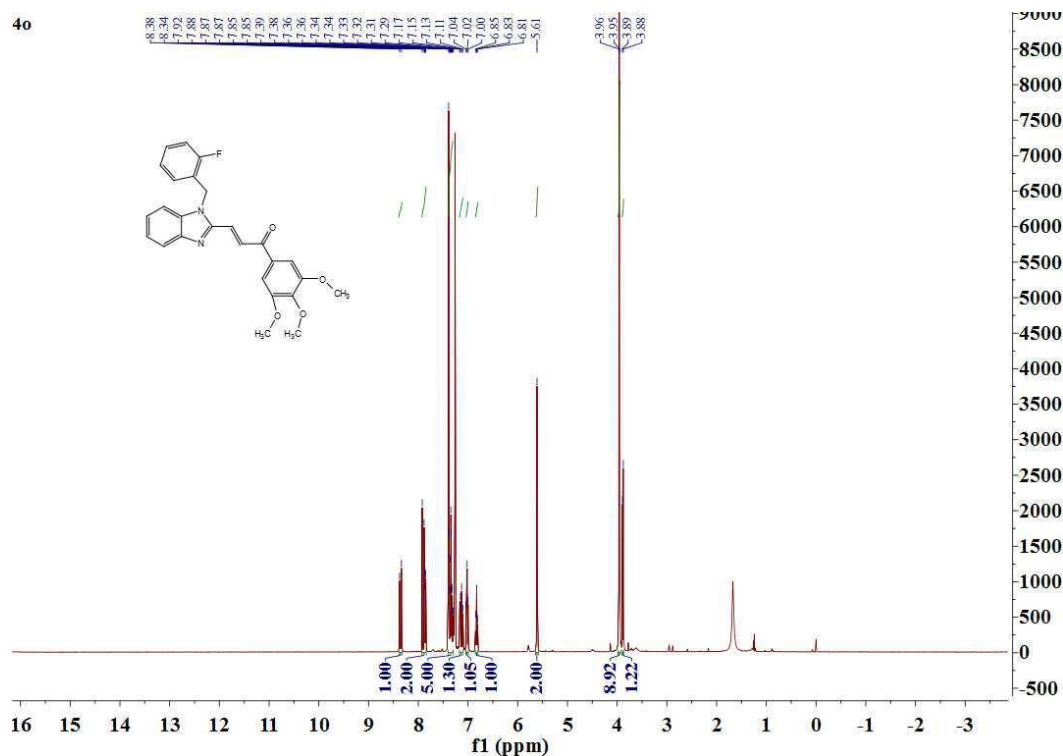


¹H NMR (400 MHz, CDCl₃) of compound **4m**

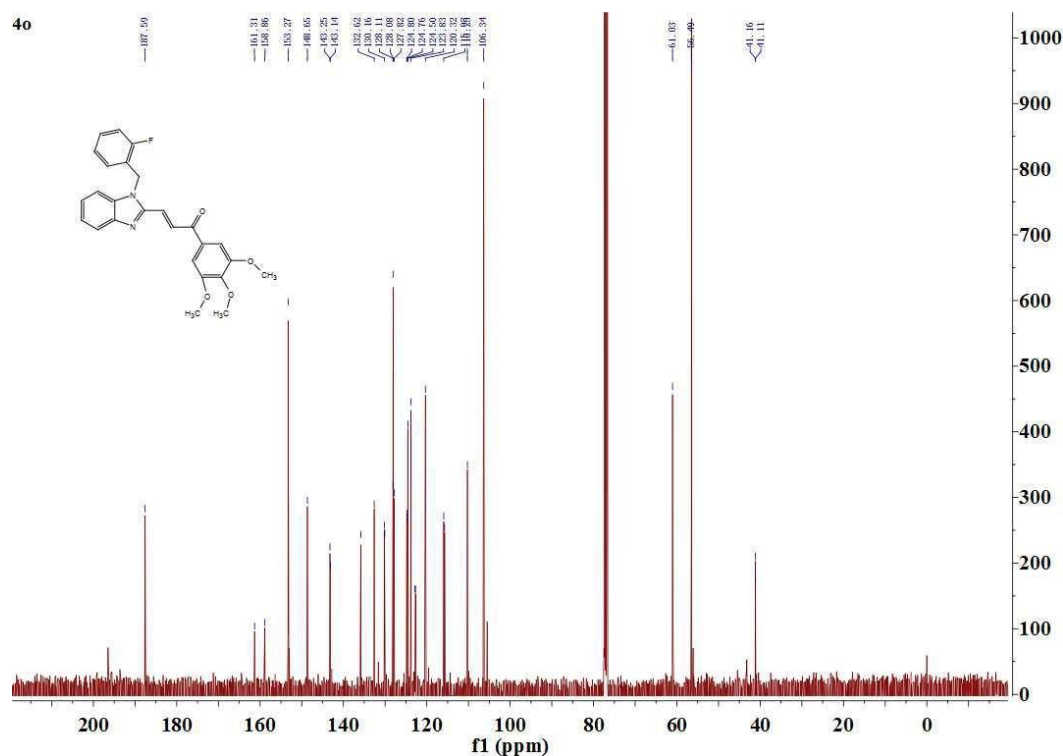


¹³C NMR (101 MHz, CDCl₃) of compound **4m**

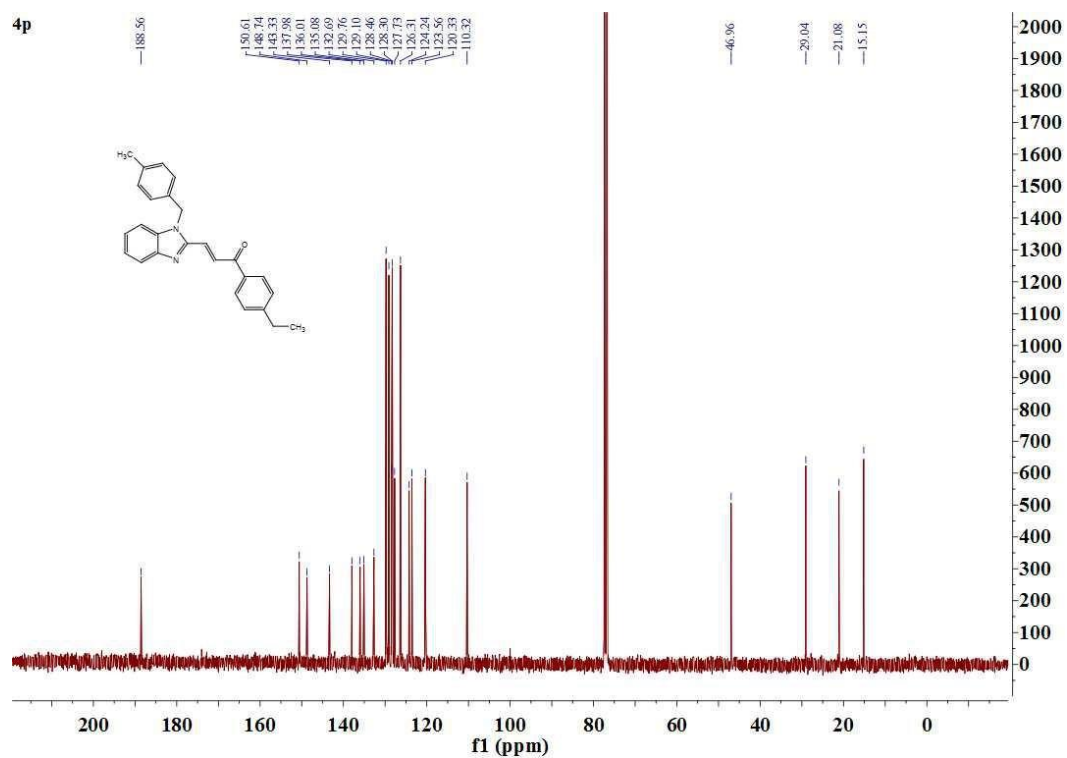
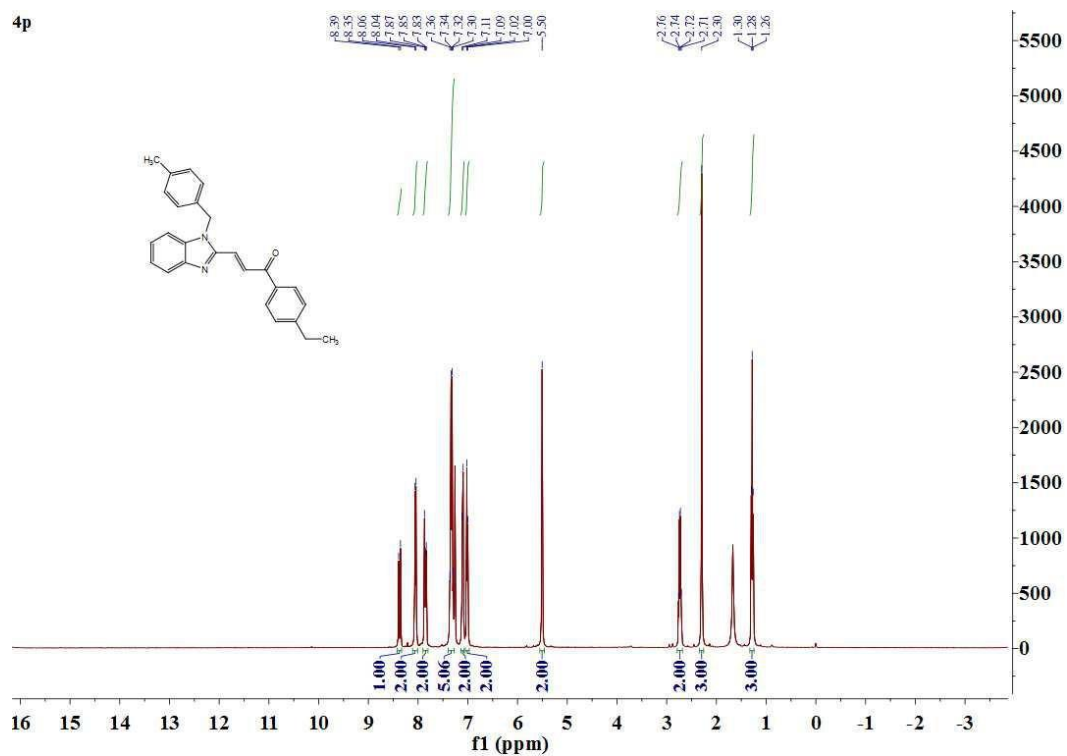


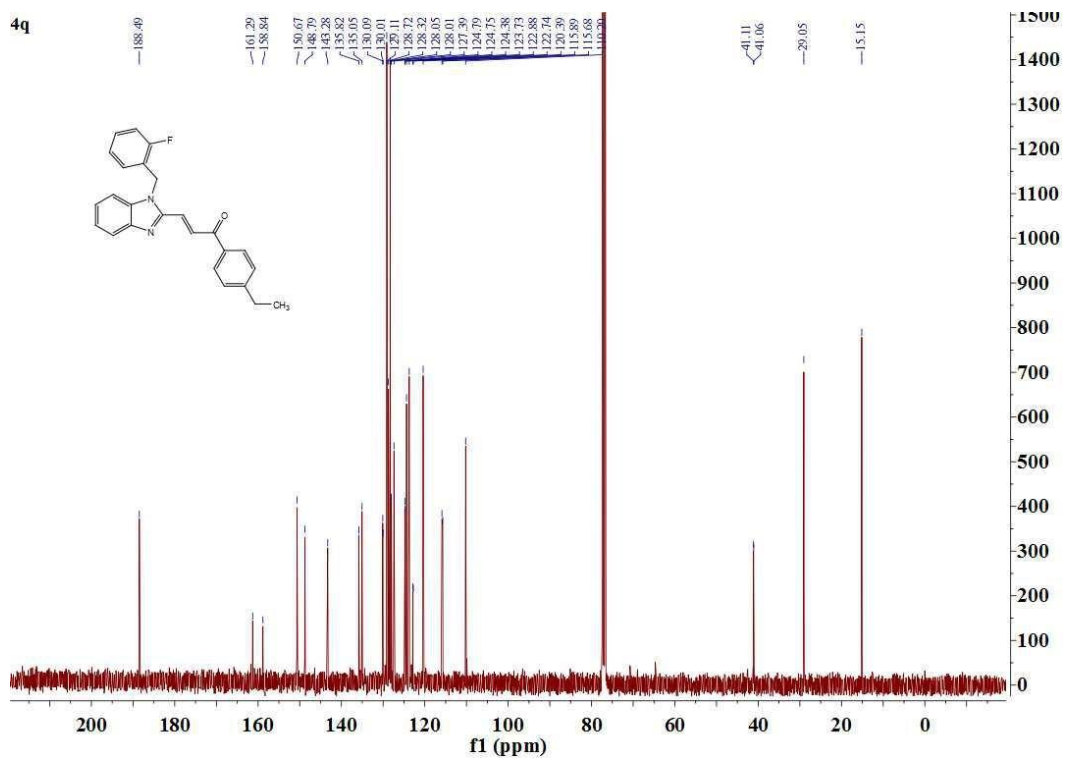
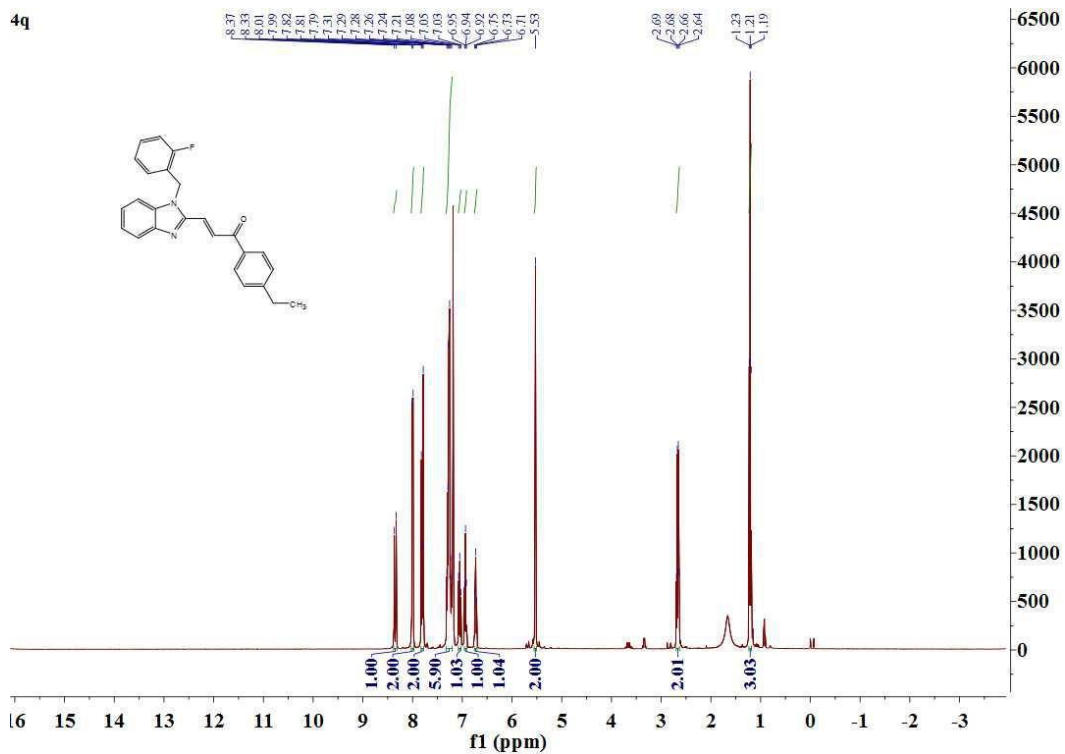


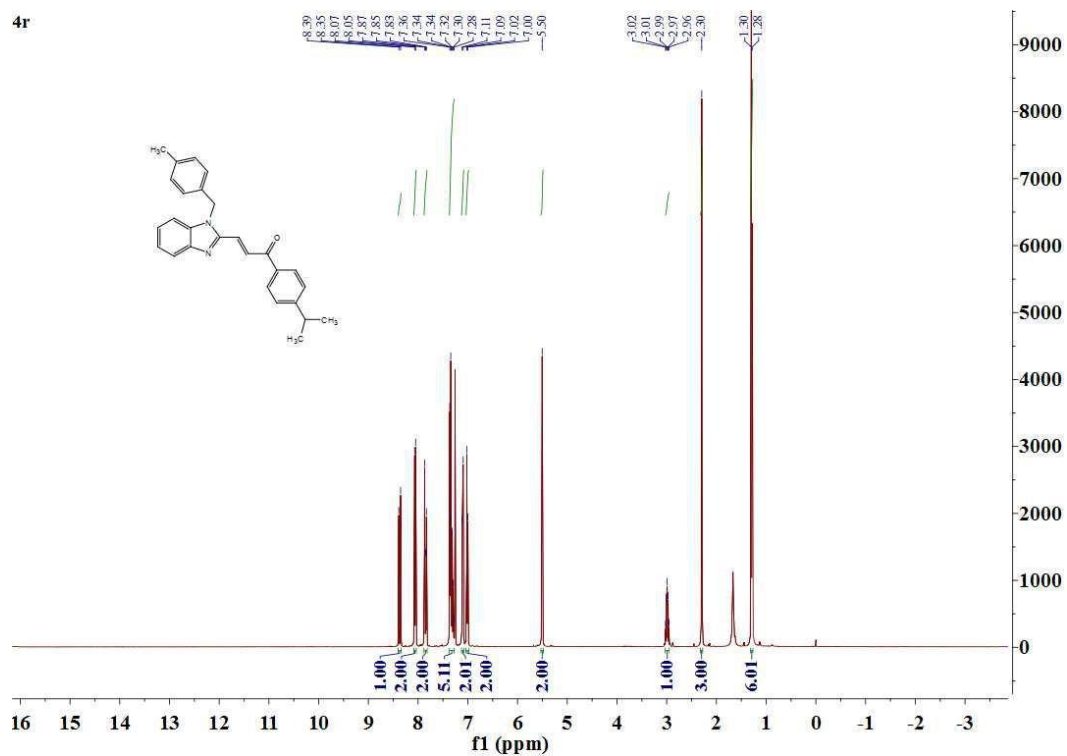
¹H NMR (400 MHz, CDCl₃) of compound **4o**



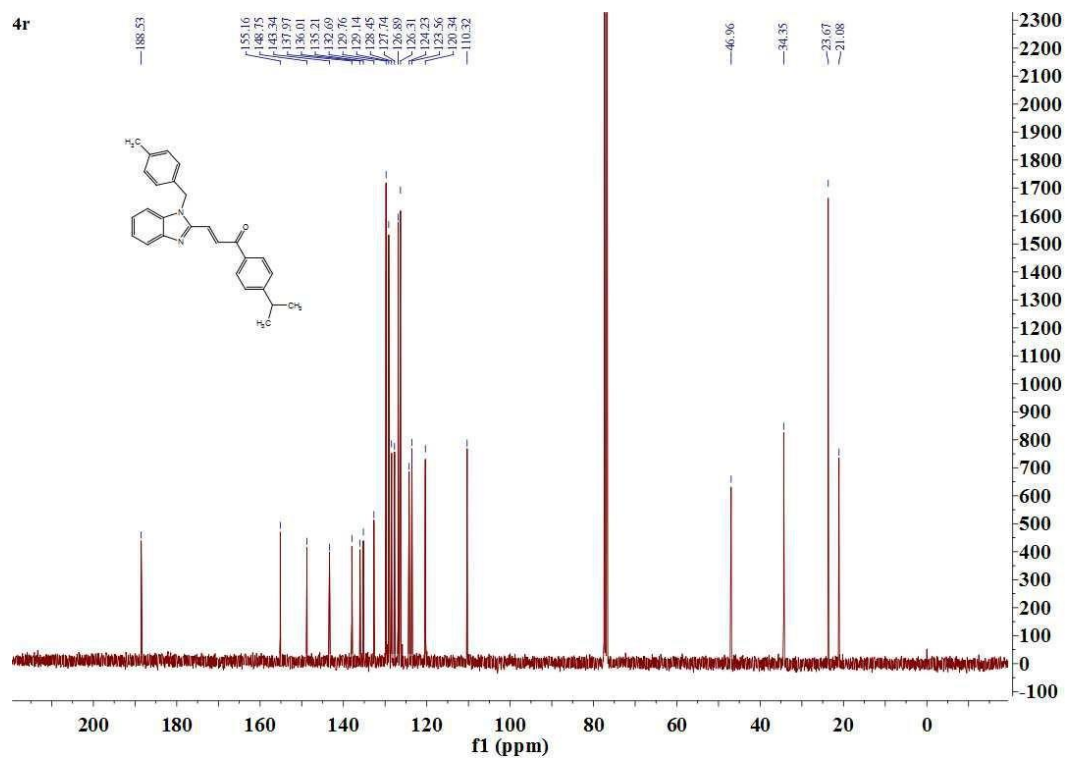
¹³C NMR (101 MHz, CDCl₃) of compound **4o**



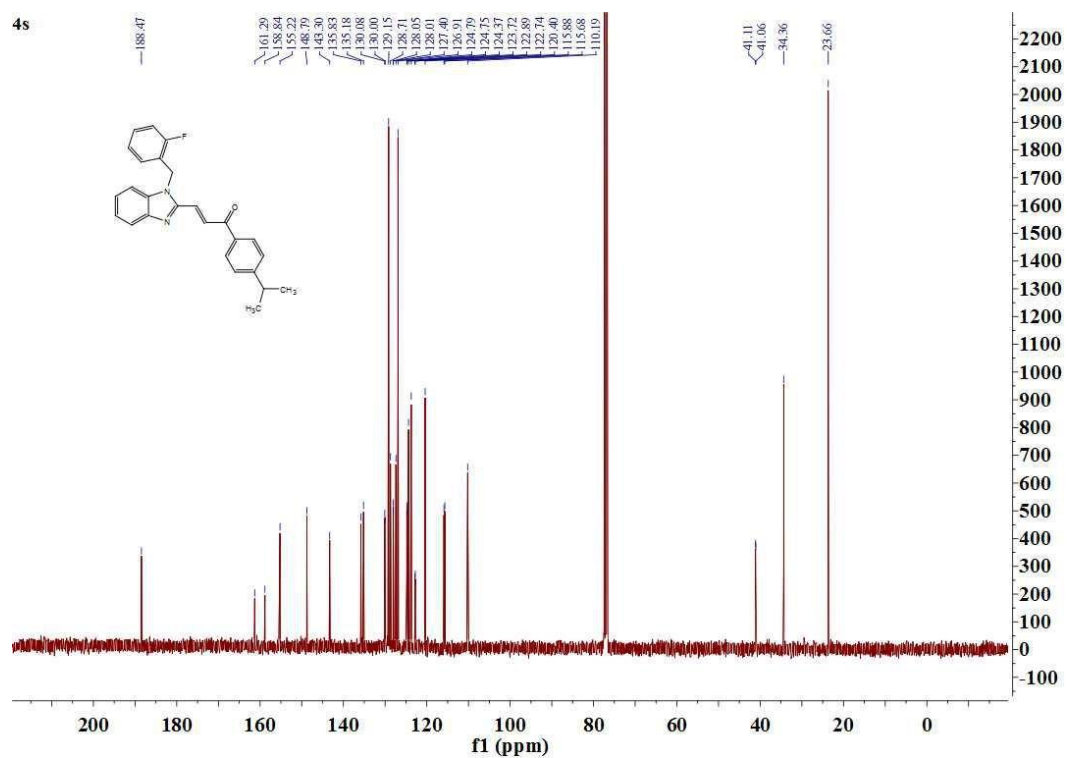
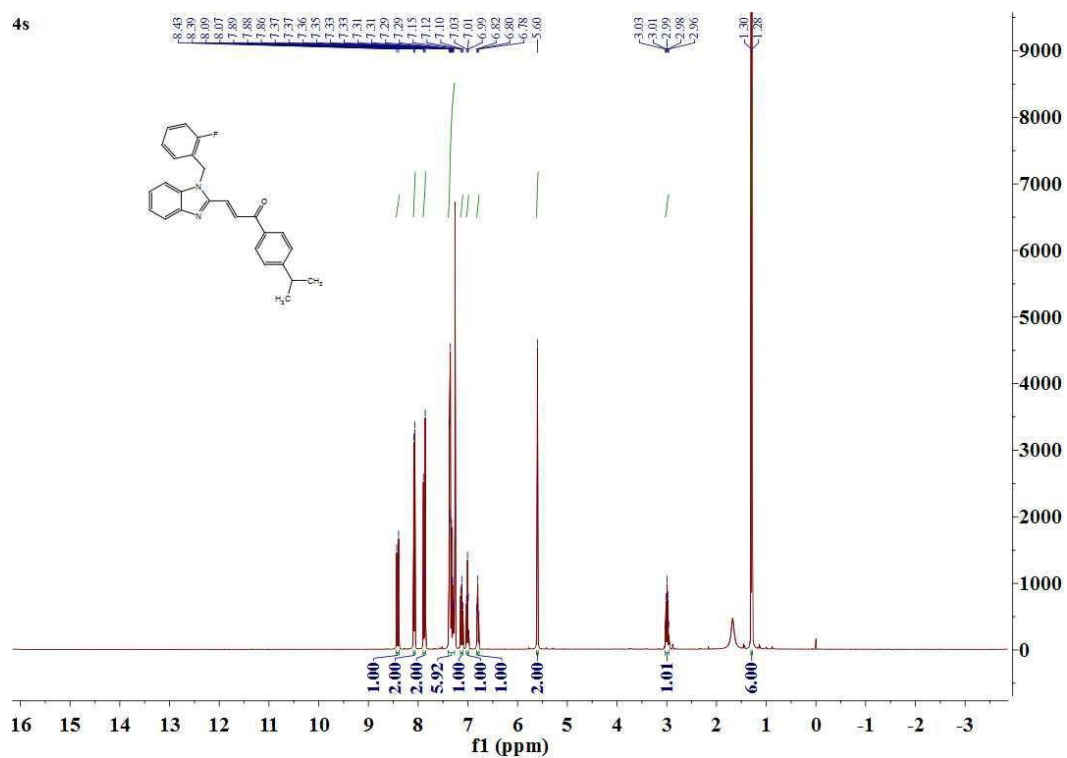


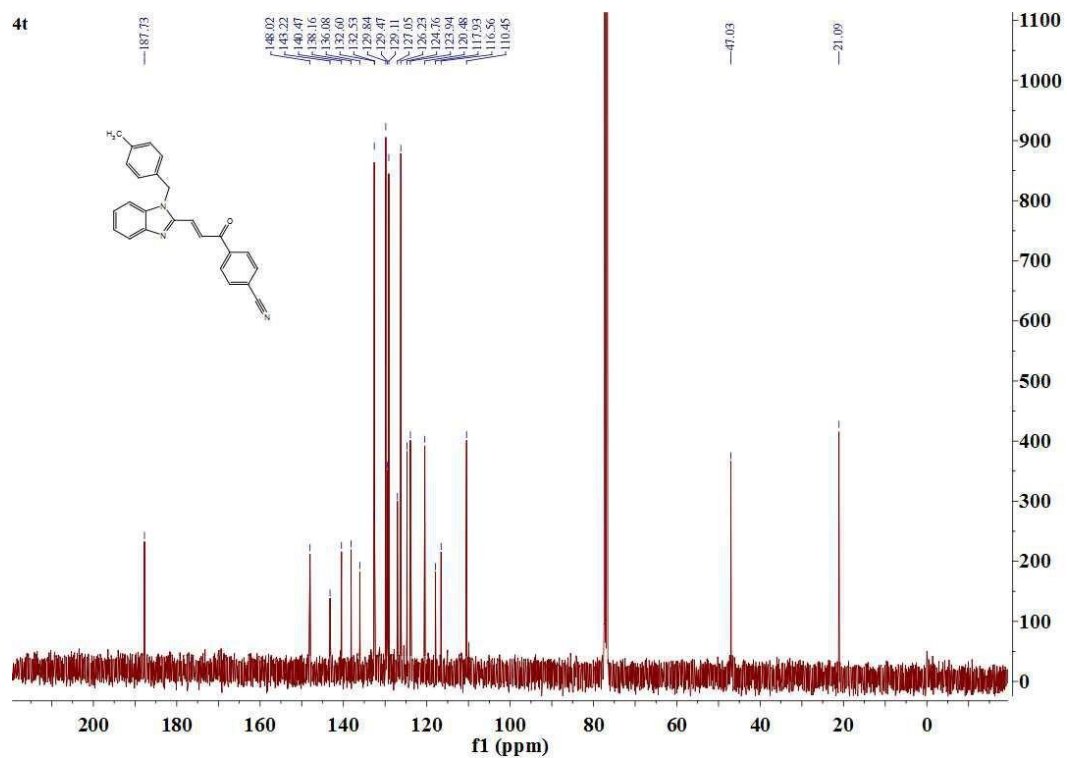
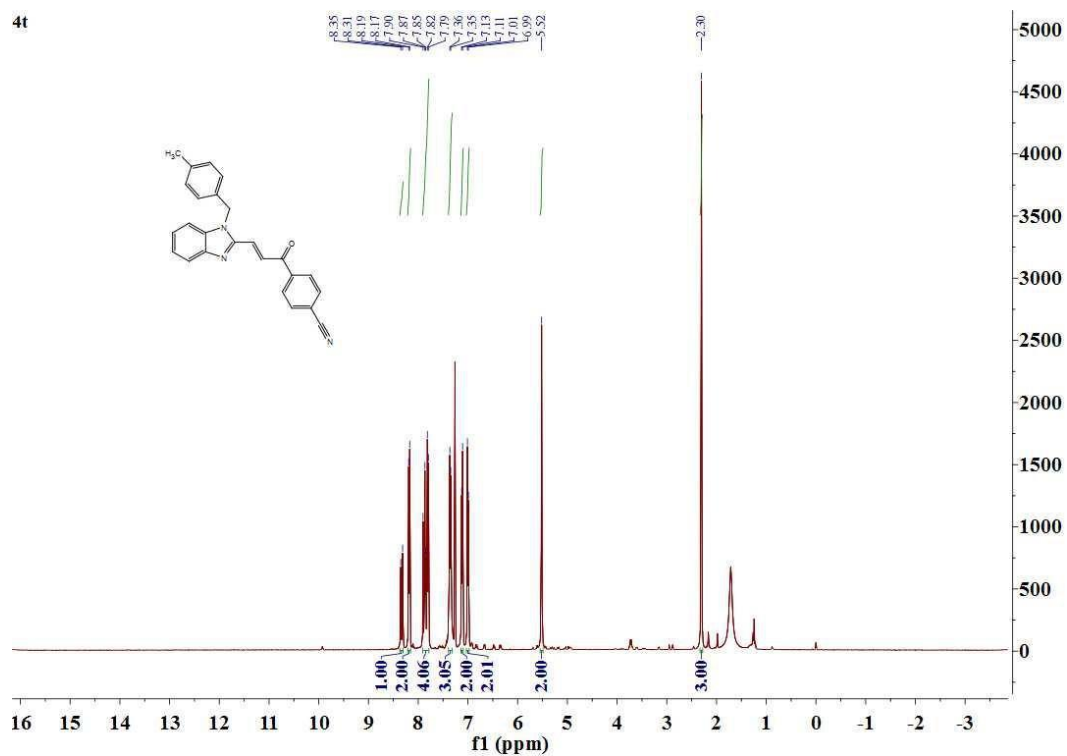


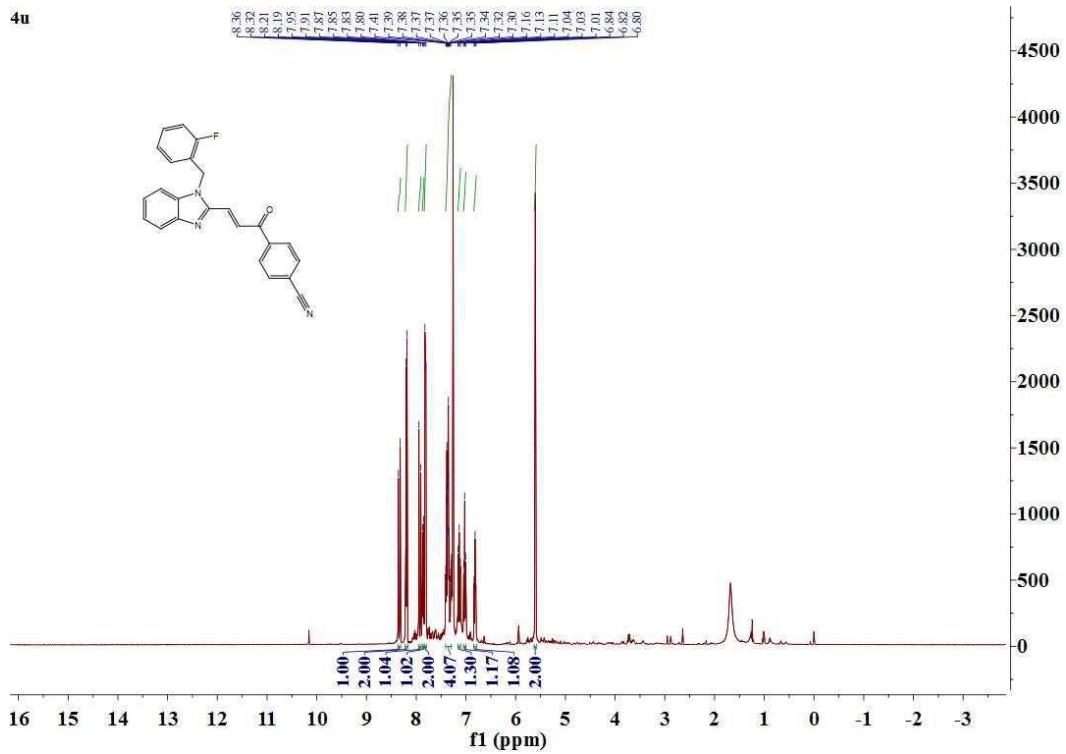
¹H NMR (400 MHz, CDCl₃) of compound **4r**



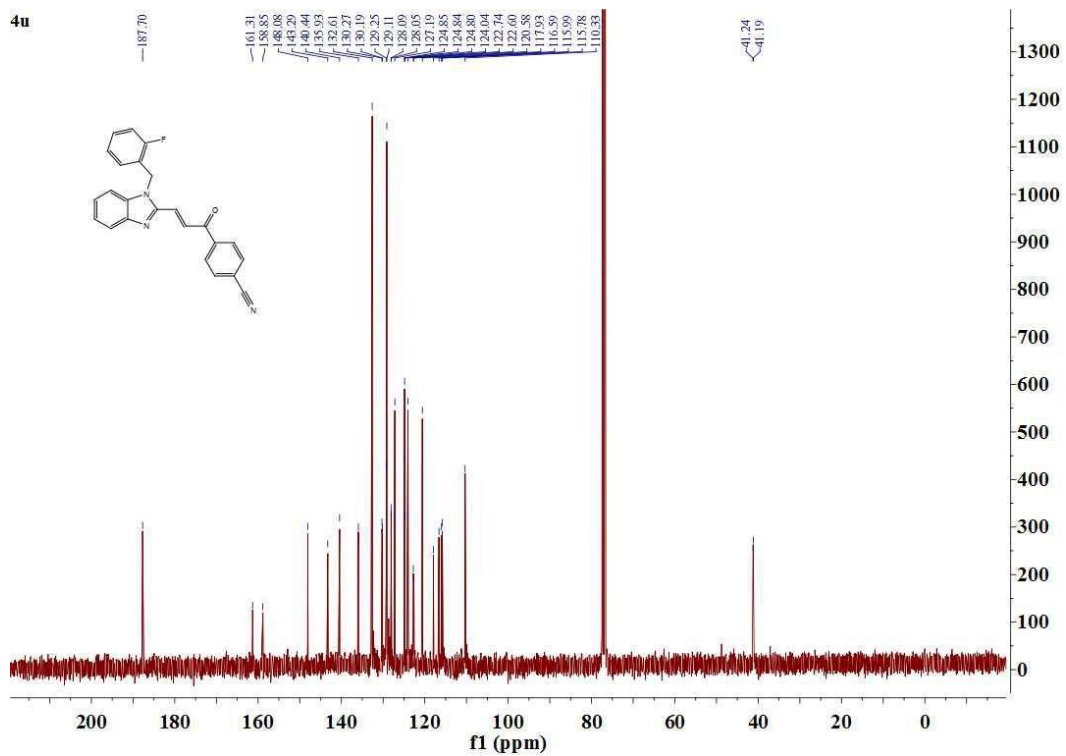
¹³C NMR (101 MHz, CDCl₃) of compound **4r**







¹H NMR (400 MHz, CDCl₃) of compound **4u**

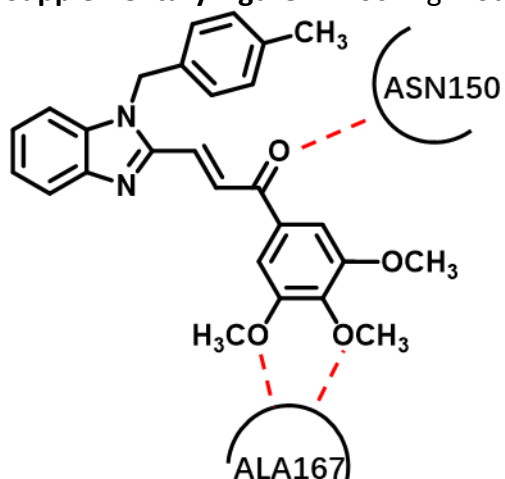


¹³C NMR (101 MHz, CDCl₃) of compound **4u**

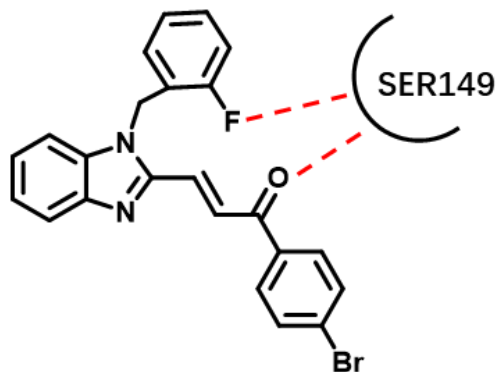
Supplementary Table 1: Total scores of 4n, 4d and original ligand of Topo II (1ZXM)

Spreadsheet			1: Total_Score	2: Crash	3: Polar	4: D_SCORE	5: PMF_SCORE	6: G_SCORE	7: CHEMScore	8: CSCORE	9: GLOBAL_CSCORE
1	<input checked="" type="checkbox"/>	1zxm_ligand_000	12.31	-2.42	8.96	-160.575	-76.006	-369.724	-22.601	4	3
2	<input checked="" type="checkbox"/>	4n_000	9.62	-3.74	1.28	-191.591	46.253	-311.829	-30.155	3	4
3	<input checked="" type="checkbox"/>	4d_000	6.53	-0.63	1.12	-130.878	5.300	-180.310	-28.311	2	1
4	<input checked="" type="checkbox"/>	334-18-9.mo_000	6.52	-7.83	2.52	-208.135	-0.424	-403.241	-34.455	1	3

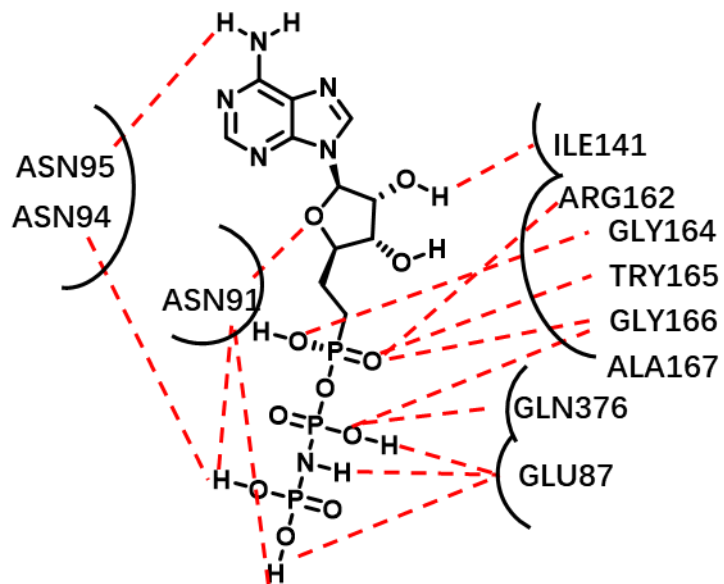
Supplementary Figure 1: Docking model of 4n with Topo II protein (1ZXM)



Supplementary Figure 2: Docking model of 4d with Topo II protein (1ZXM)



Supplementary Figure 3: Docking model of Topo II protein (1ZXM) with its original ligand



Supplementary Figure 4: Docking result of Topo II protein (1ZXM) with its original ligand

