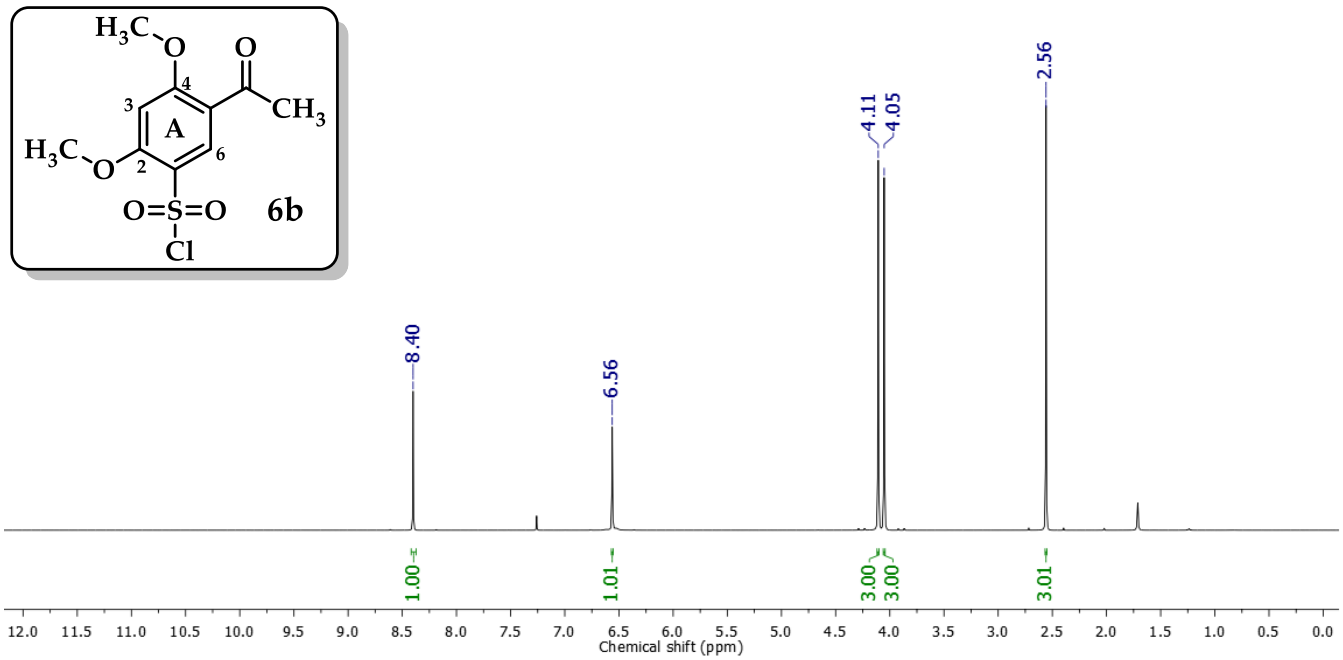
Synthesis, Anticancer and Antitubercular Properties of New Chalcones and Their Nitrogen-Containing Five-Membered Heterocyclic Hybrids Bearing Sulfonamide Moiety

Lina Fernanda Castaño [1], Jairo Quiroga [1,2], Rodrigo Abonia [1,2], Daniel Insuasty [3], Oscar M. Vidal [4], Rosalia Seña [3,4], Vivian Rubio [5], Gloria Puerto [5], Manuel Nogueras [6], Justo Cobo [6], Juan Guzman [7], Alberto Insuasty [8,*] and Braulio Insuasty [1,2,*]

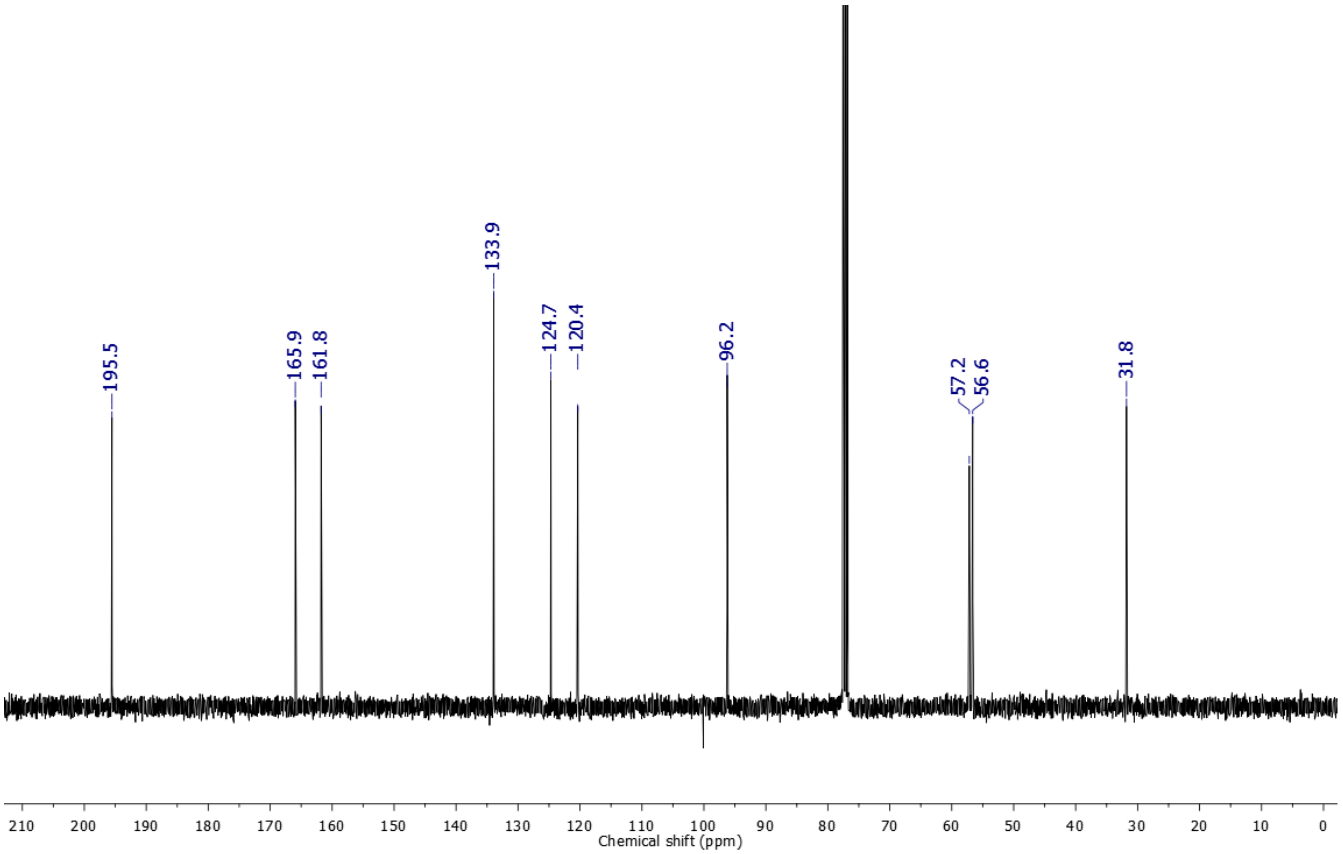
[1] Heterocyclic Compounds Research Group, Department of Chemistry, Universidad del Valle, A.A., Cali 25360, Colombia
[2] Centre for Bioinformatics and Photonics-CIBioFI, Universidad del Valle, A.A., Cali 25360, Colombia
[3] Department of Chemistry and Biology, Basic Sciences Division, Universidad del Norte, Barranquilla 081007, Colombia
[4] Department of Medicine, Health Division, Universidad del Norte, Barranquilla 081007, Colombia
[5] Grupo de Micobacterias, Red TB. Dirección de Investigación en Salud Pública, Instituto Nacional de Salud, Bogotá 111321, Colombia
[6] Department of Inorganic and Organic Chemistry, Universidad de Jaén, 23071 Jaén, Spain
[7] Department of Bioresources, Fraunhofer Institute for Molecular Biology and Applied Ecology, 35392 Giessen, Germany
[8] Nanostructured Functional Materials Research Group, Universidad CESMAG, Pasto 520003, Colombia
* Correspondence: bainsuasty@unicesmag.edu.co (A.I.); braulio.insuasty@correounivalle.edu.co (B.I.)

SUPPORTING INFORMATION

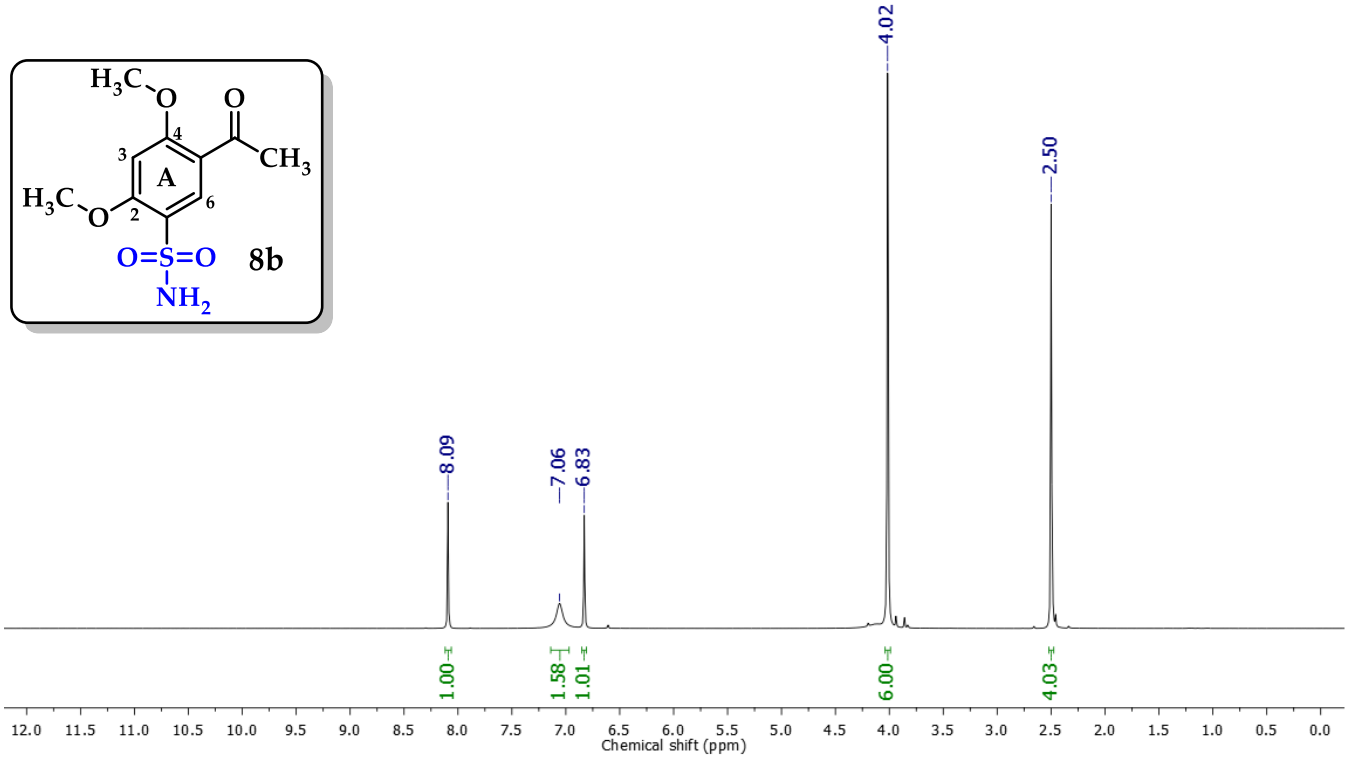
NMR spectra of synthetized compounds …….. File S1
Single Crystal Diffraction Experimental Details……. Table S1



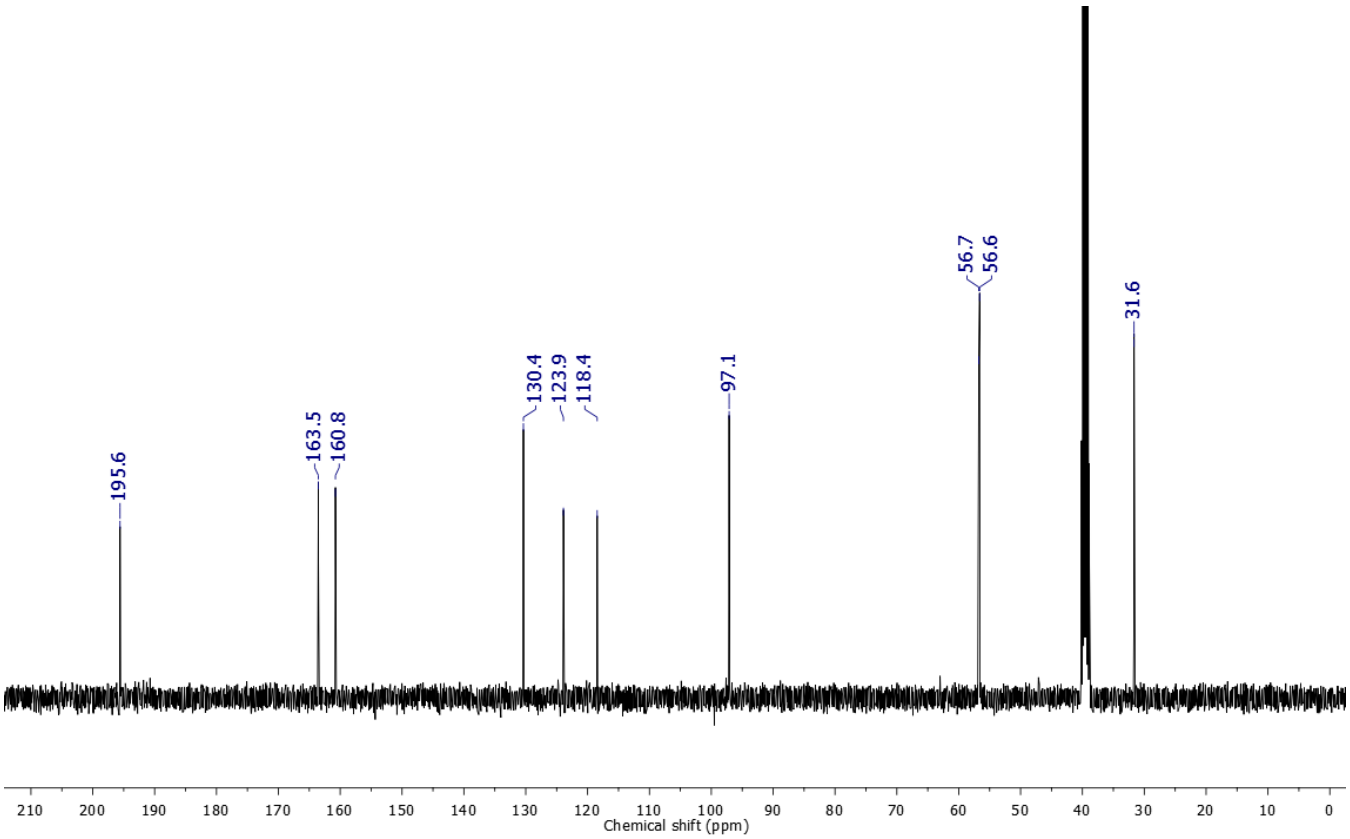
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **6b**.



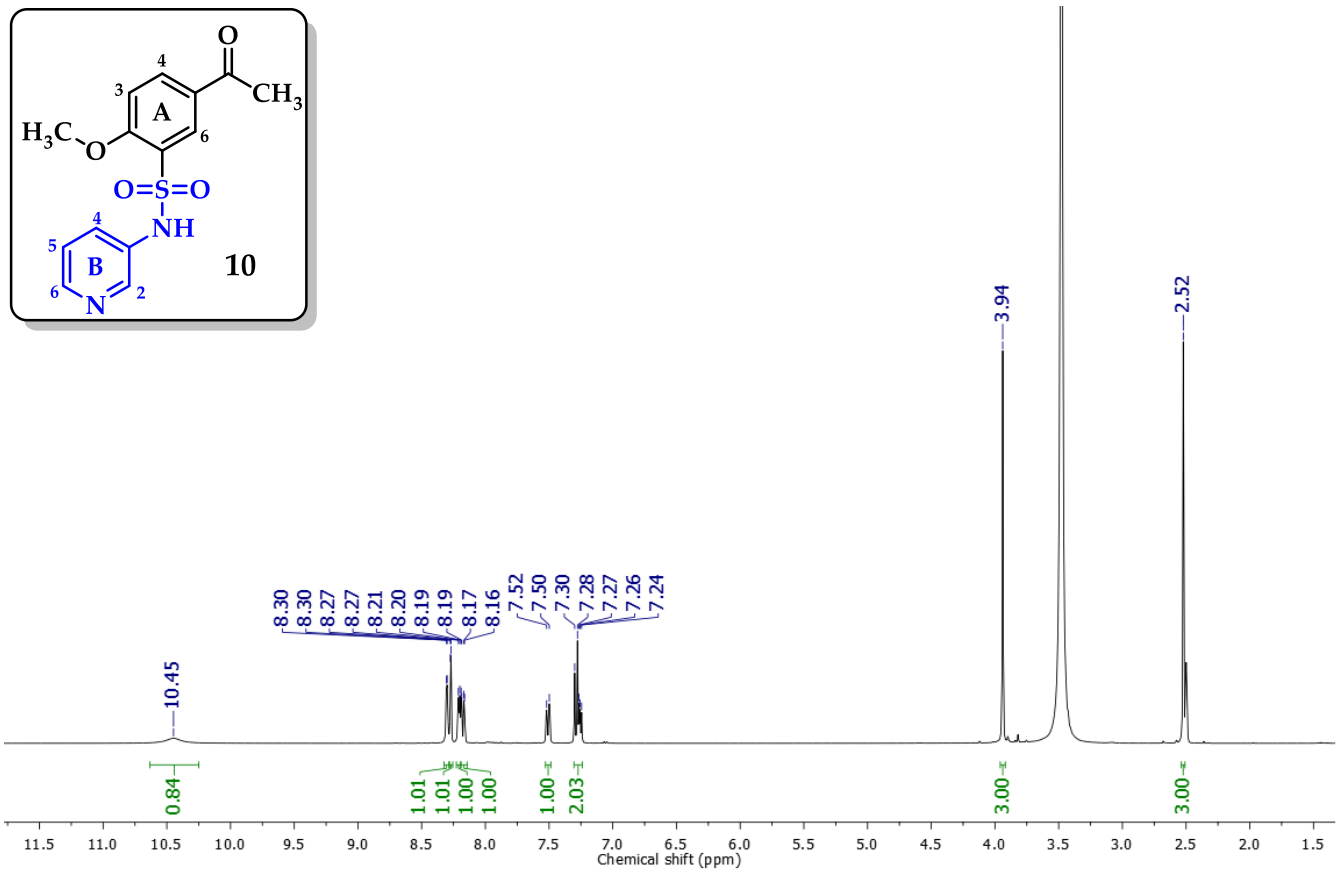
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **6b**.



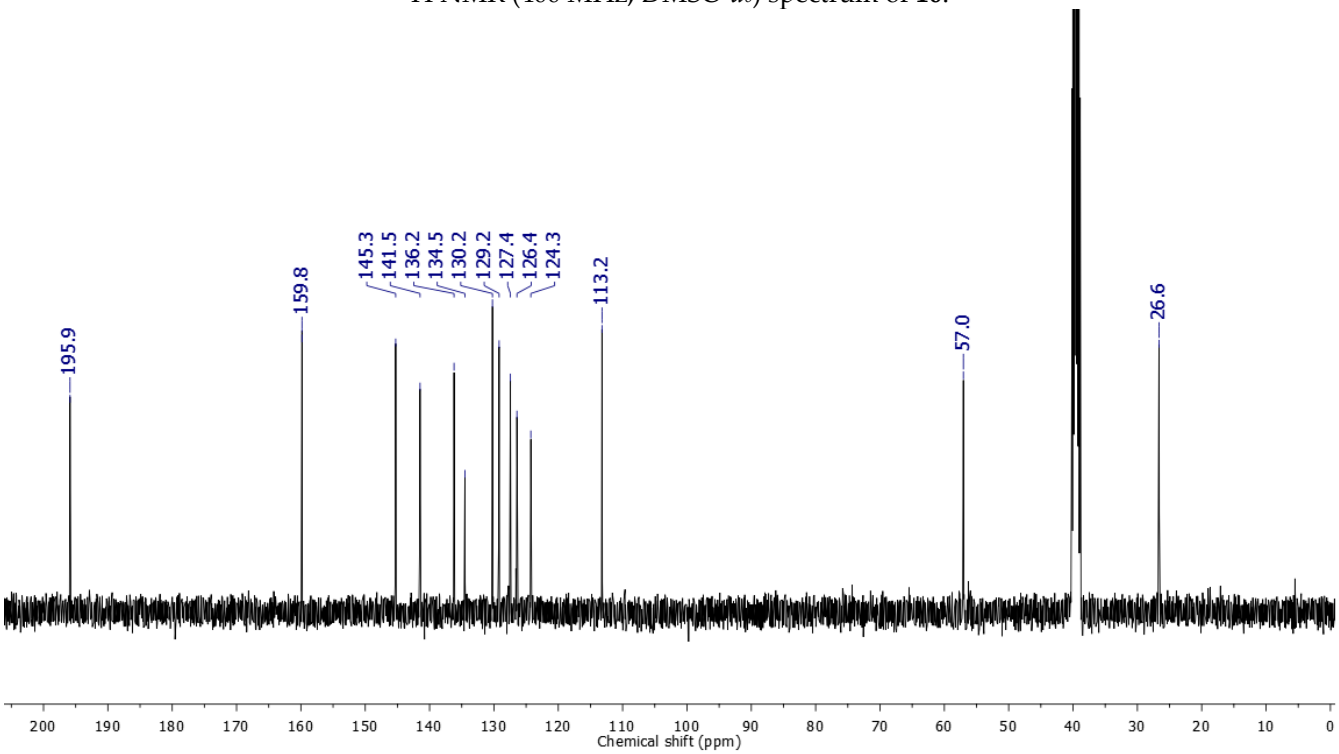
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **8b**.



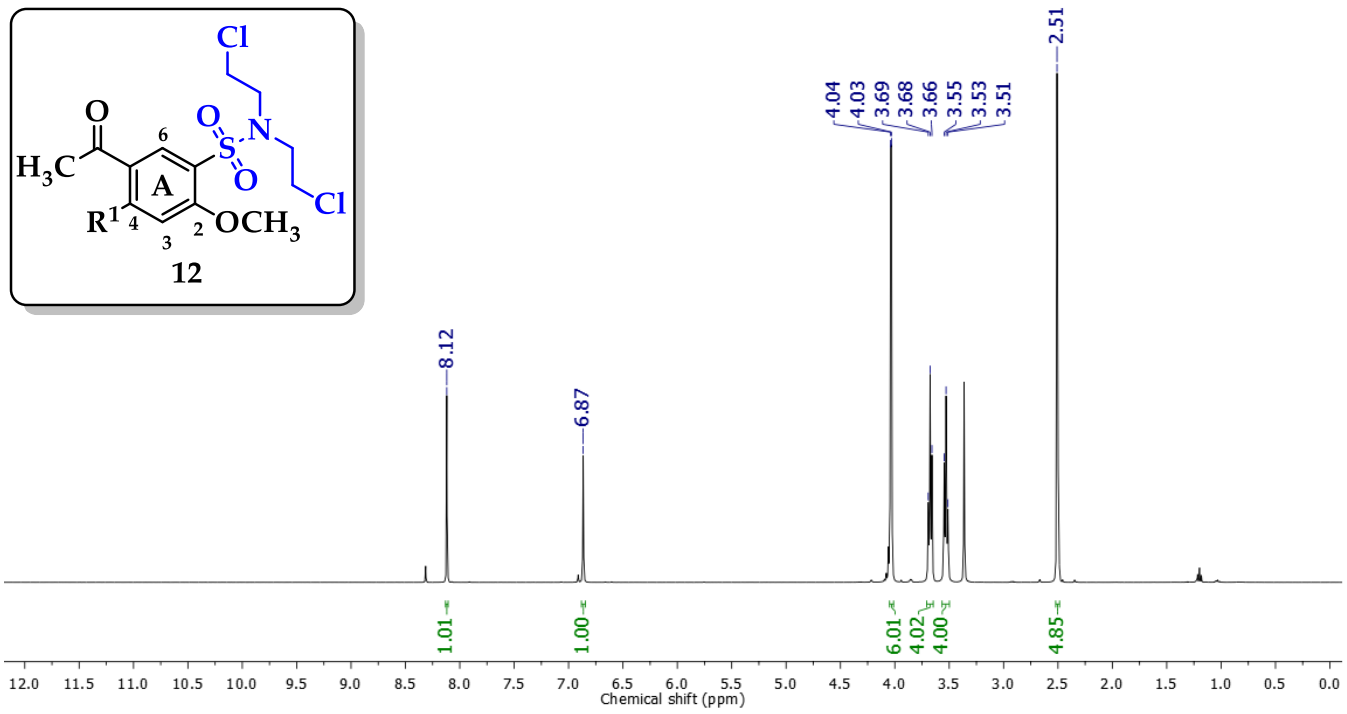
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **8b**.



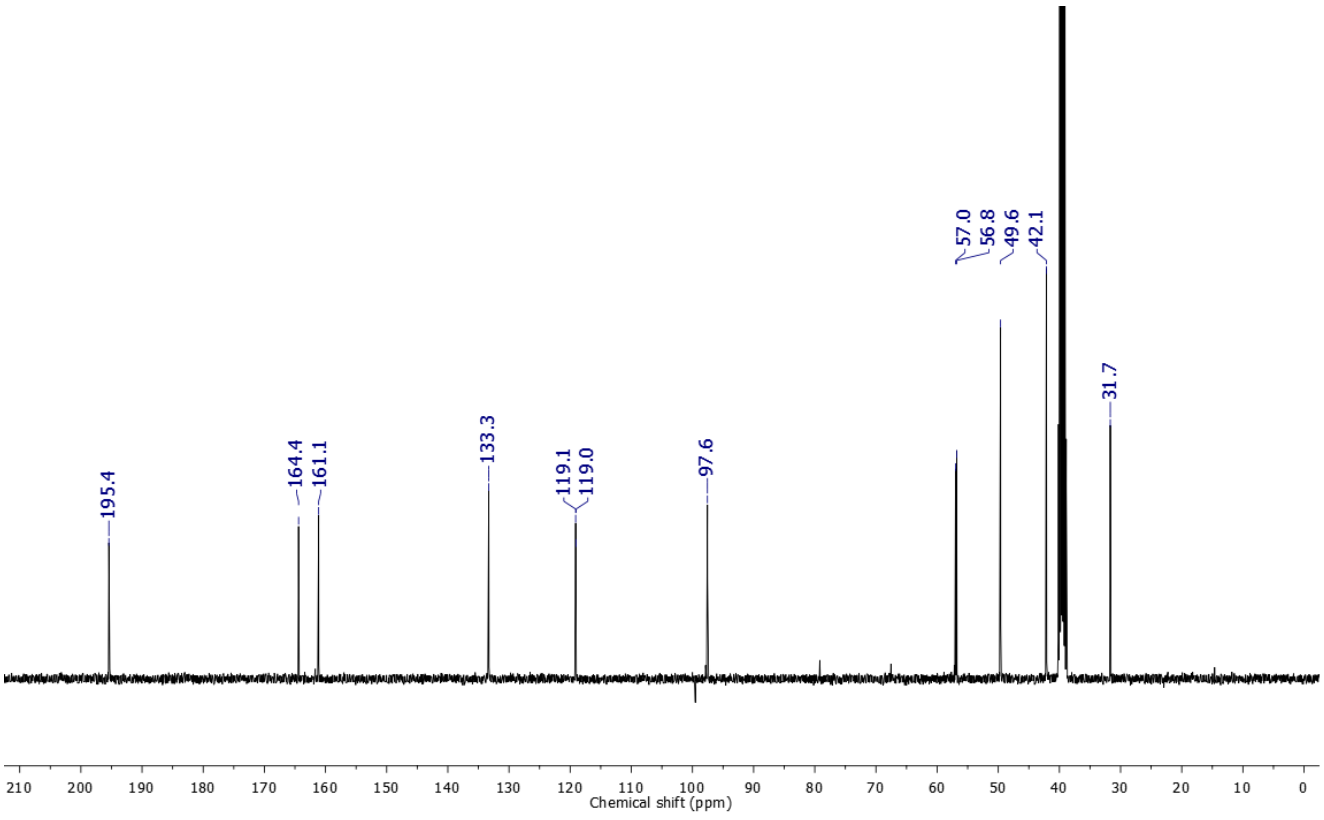
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **10**.



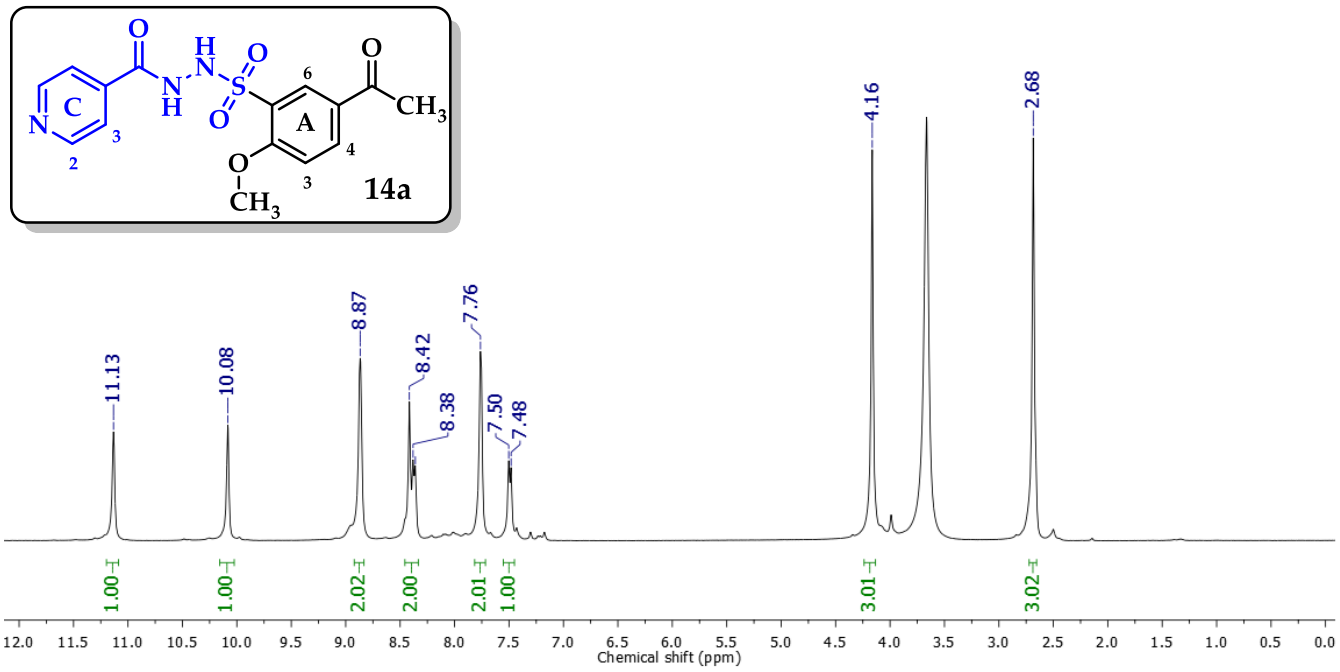
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **10**.



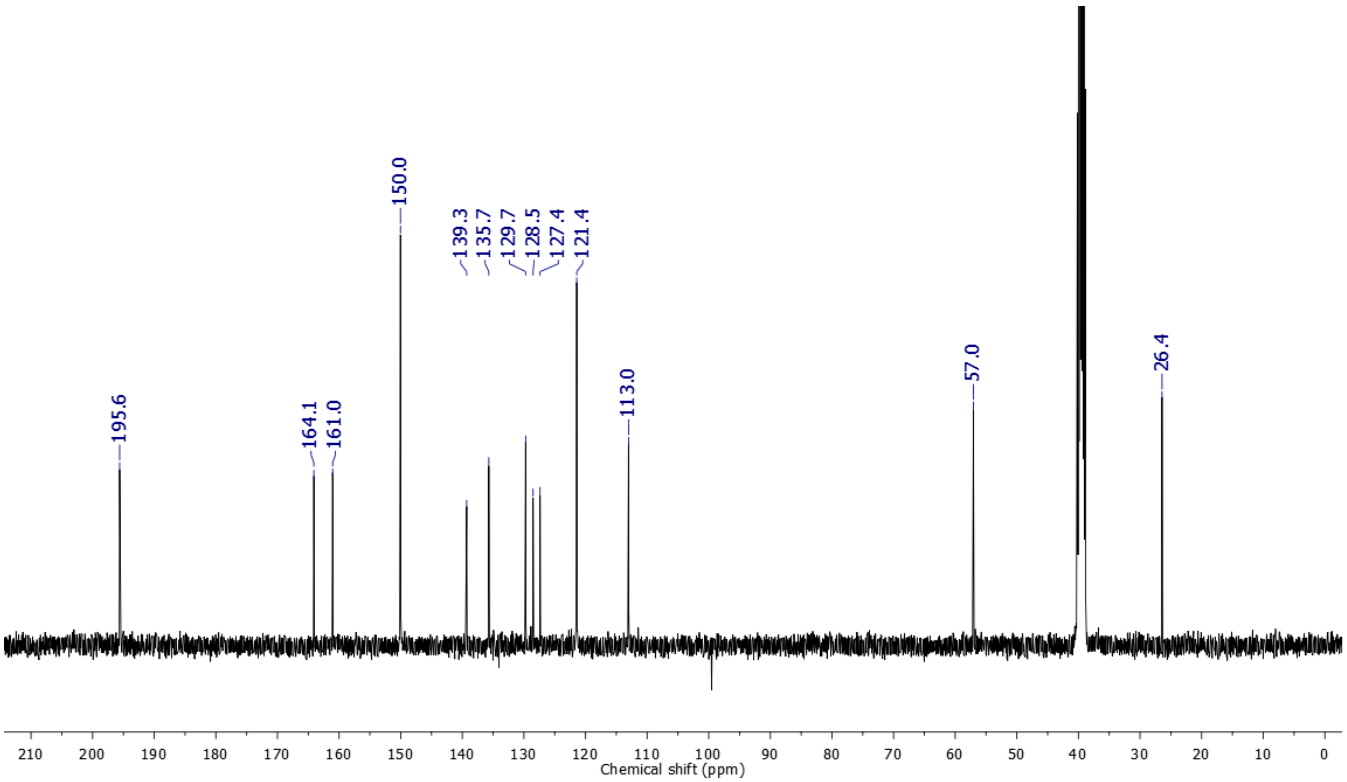
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **12**.



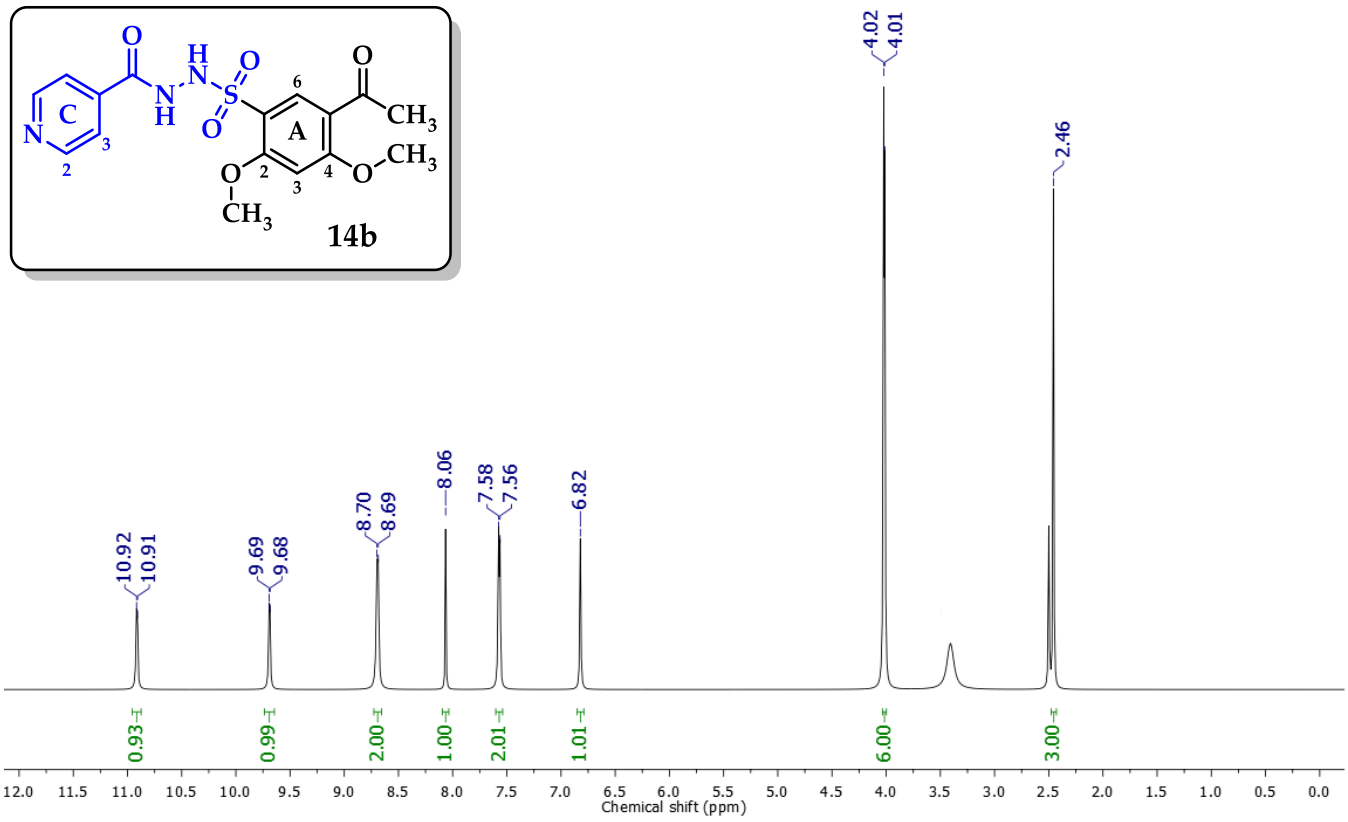
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **12**.



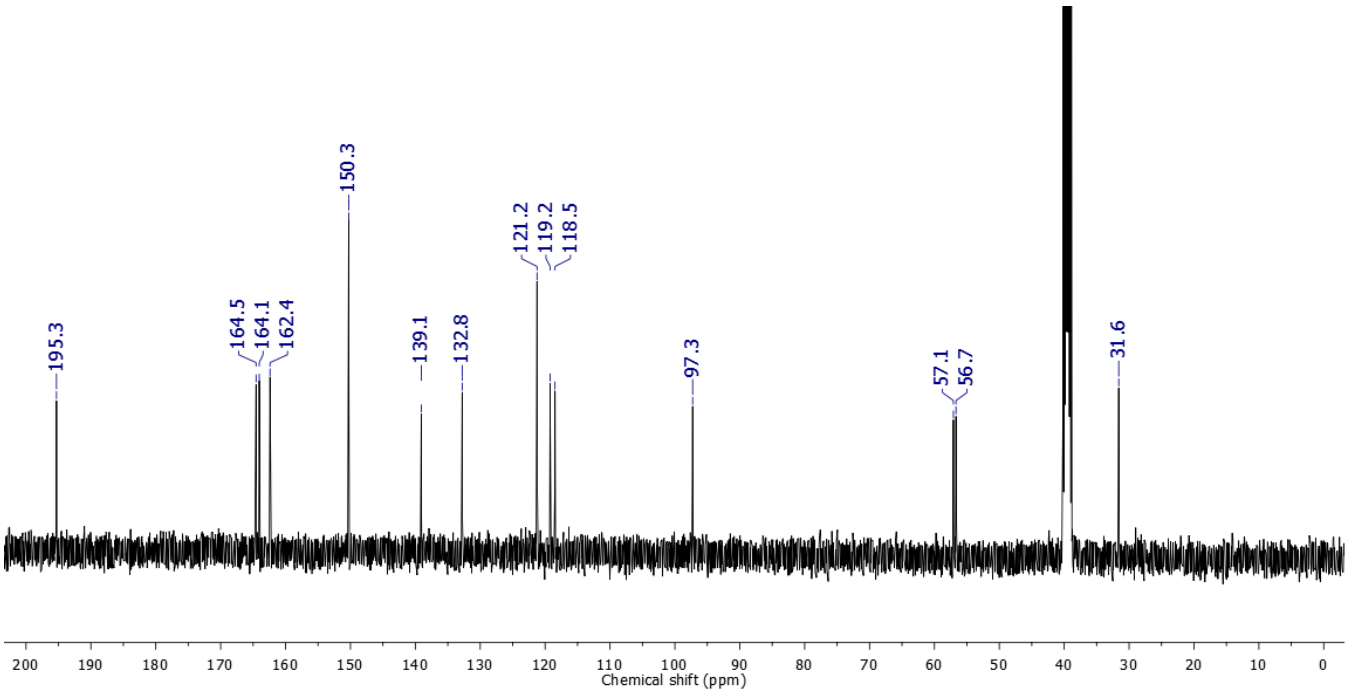
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **14a**.



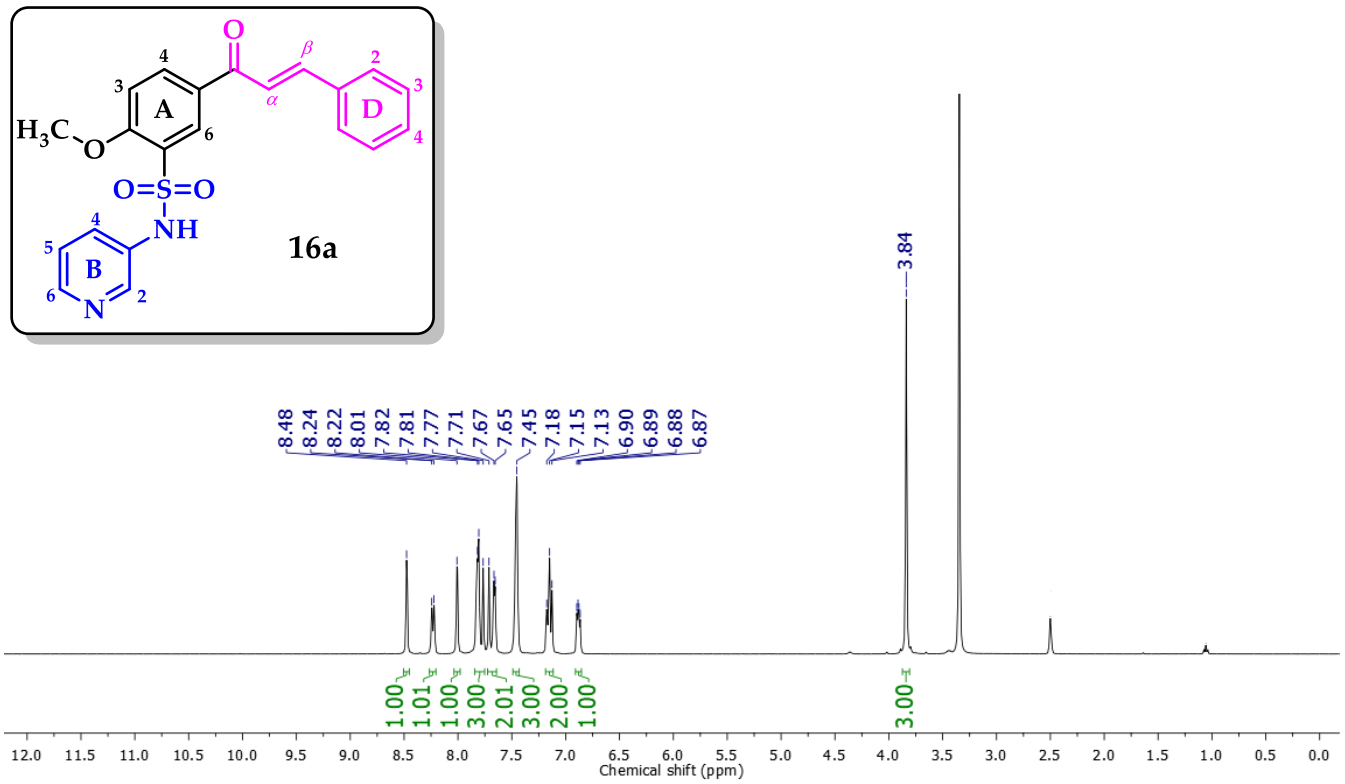
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **14a**.



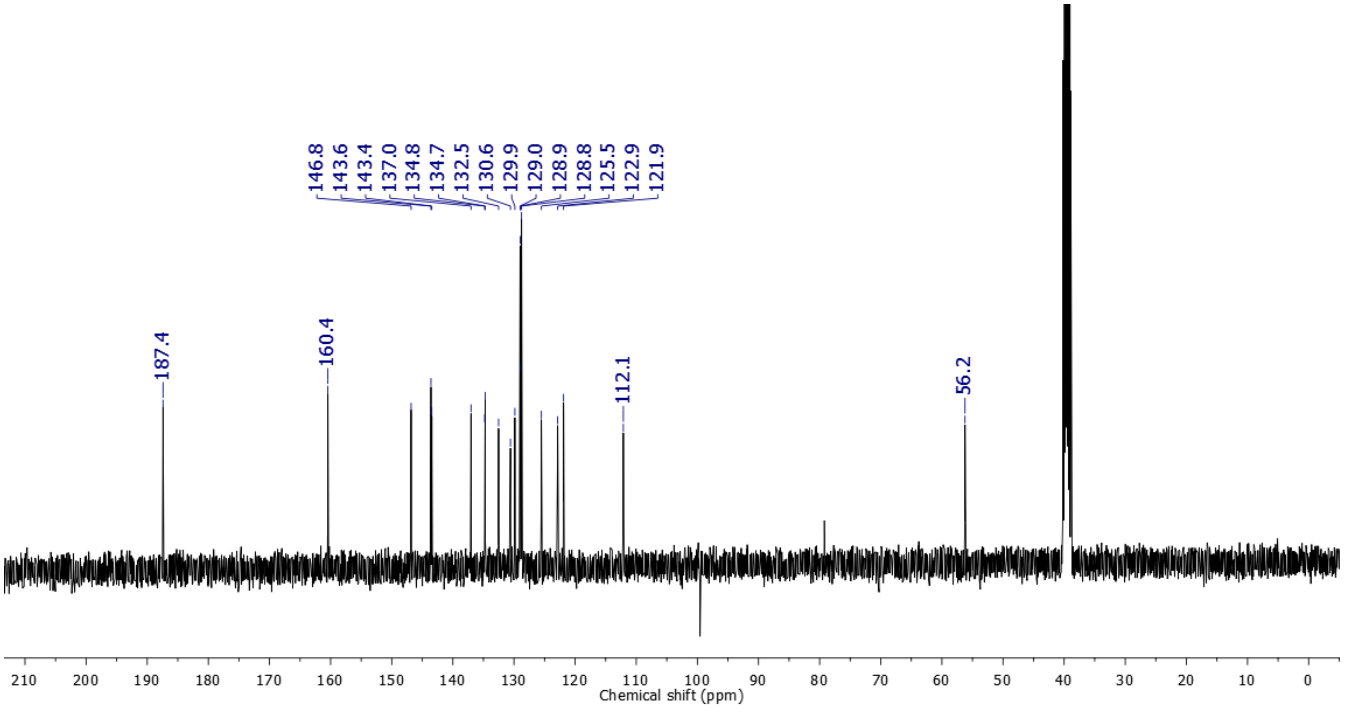
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **14b**.



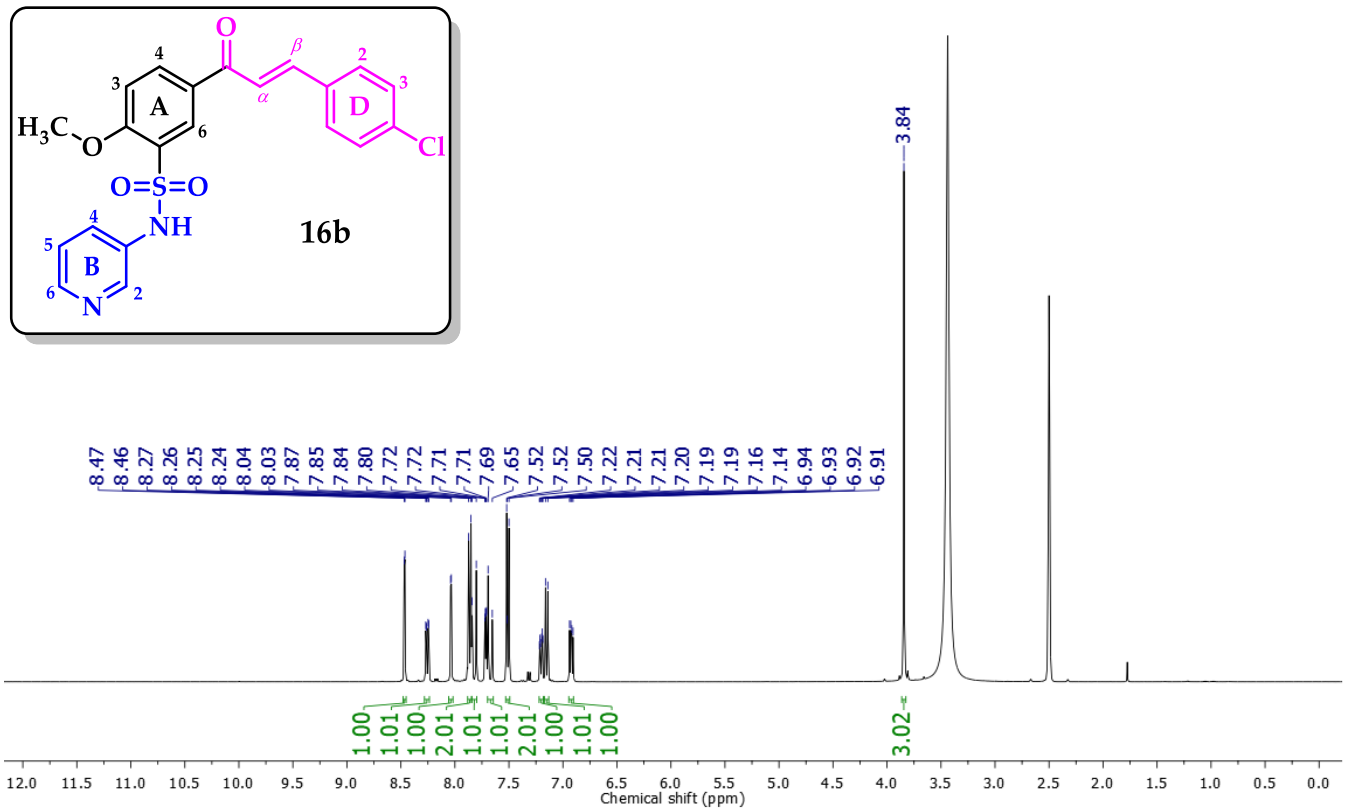
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **14b**.



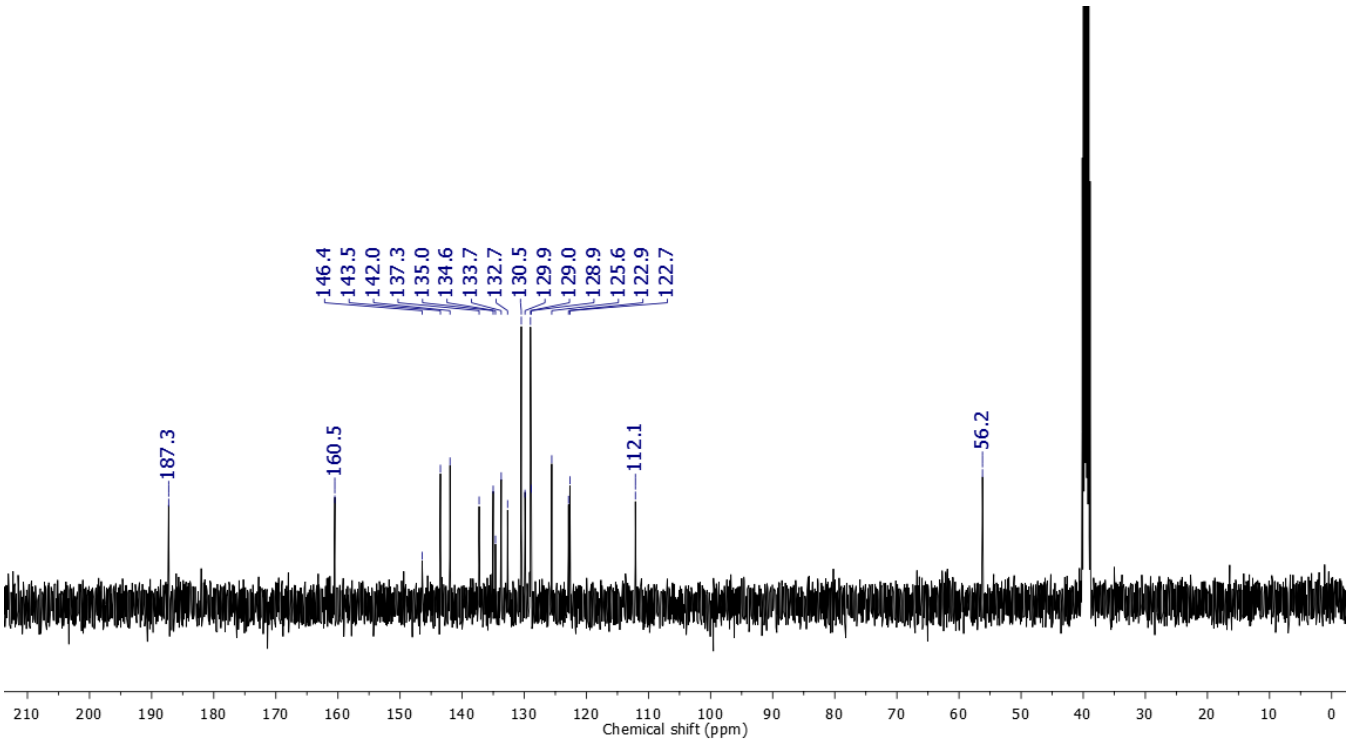
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **16a**.



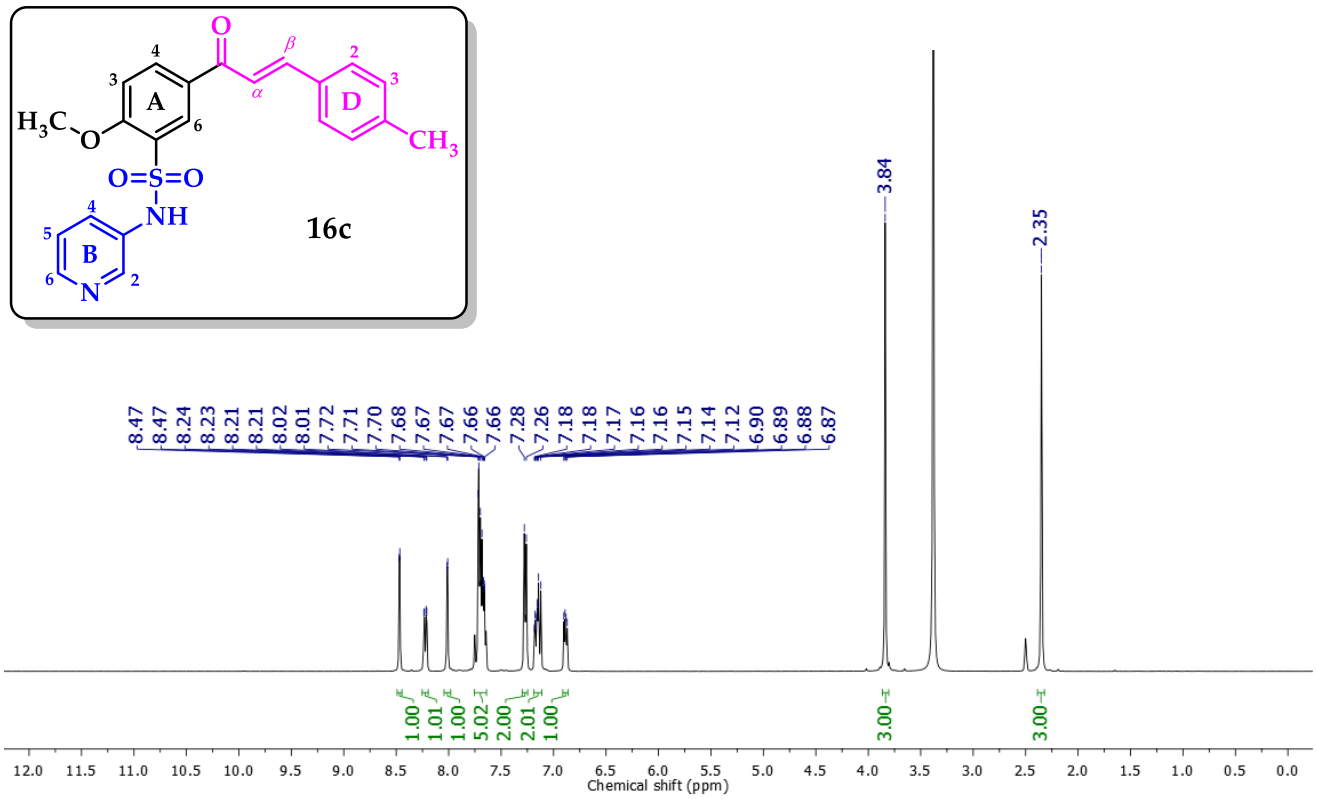
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **16a**.



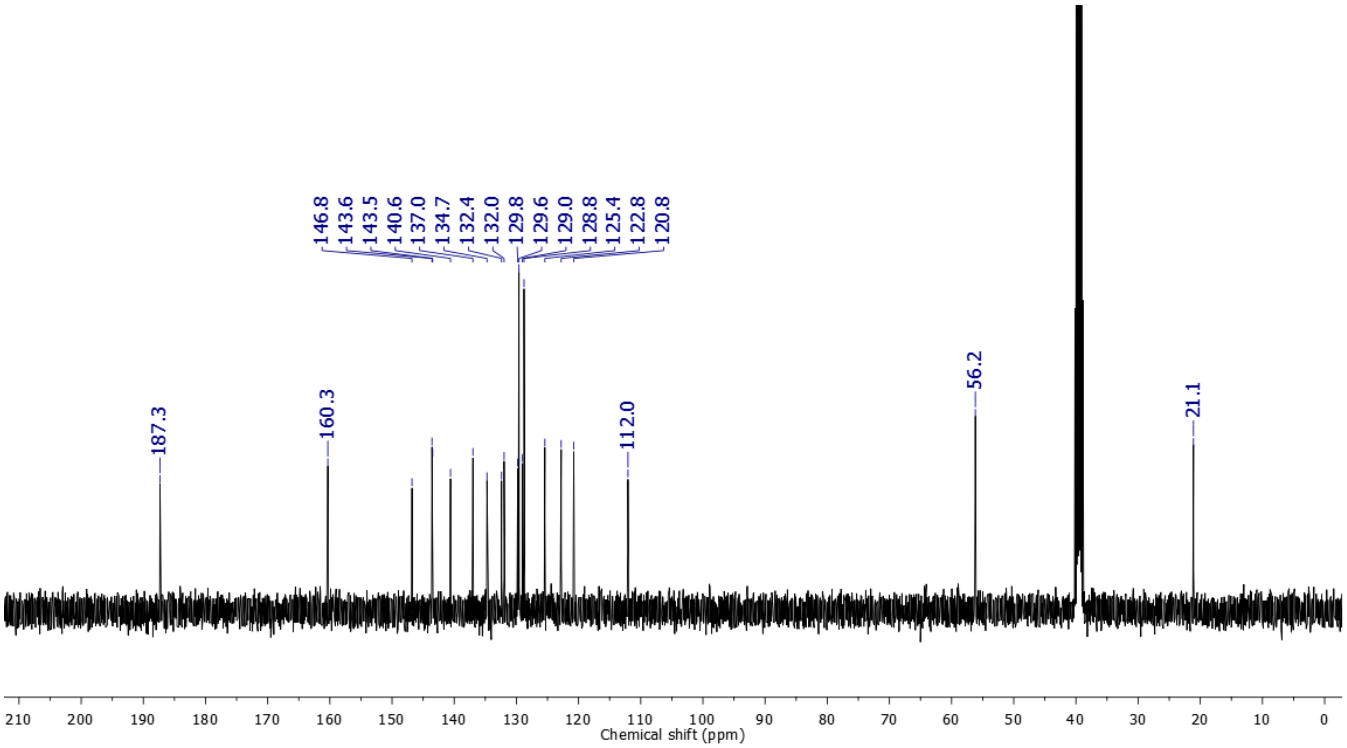
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **16b**.



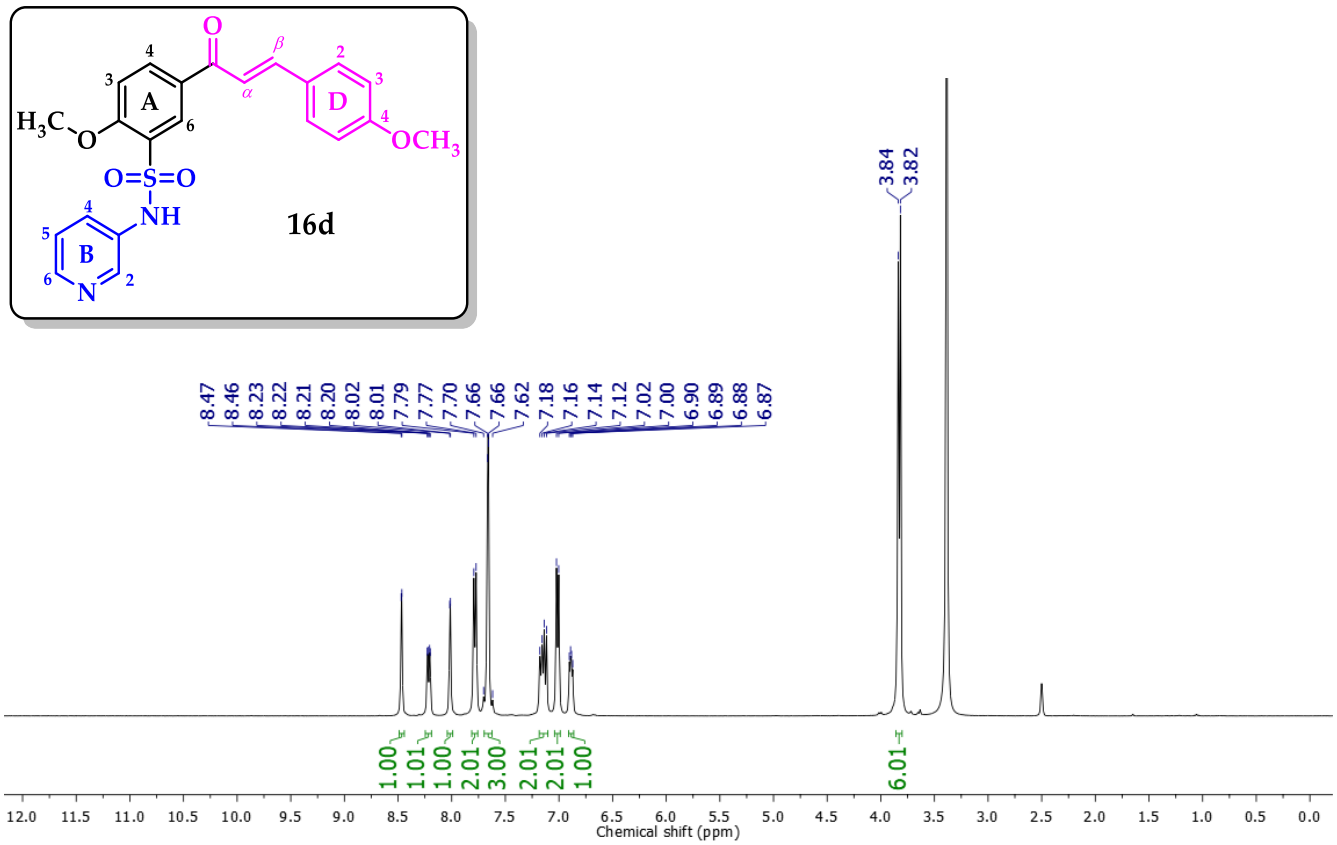
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **16b**.



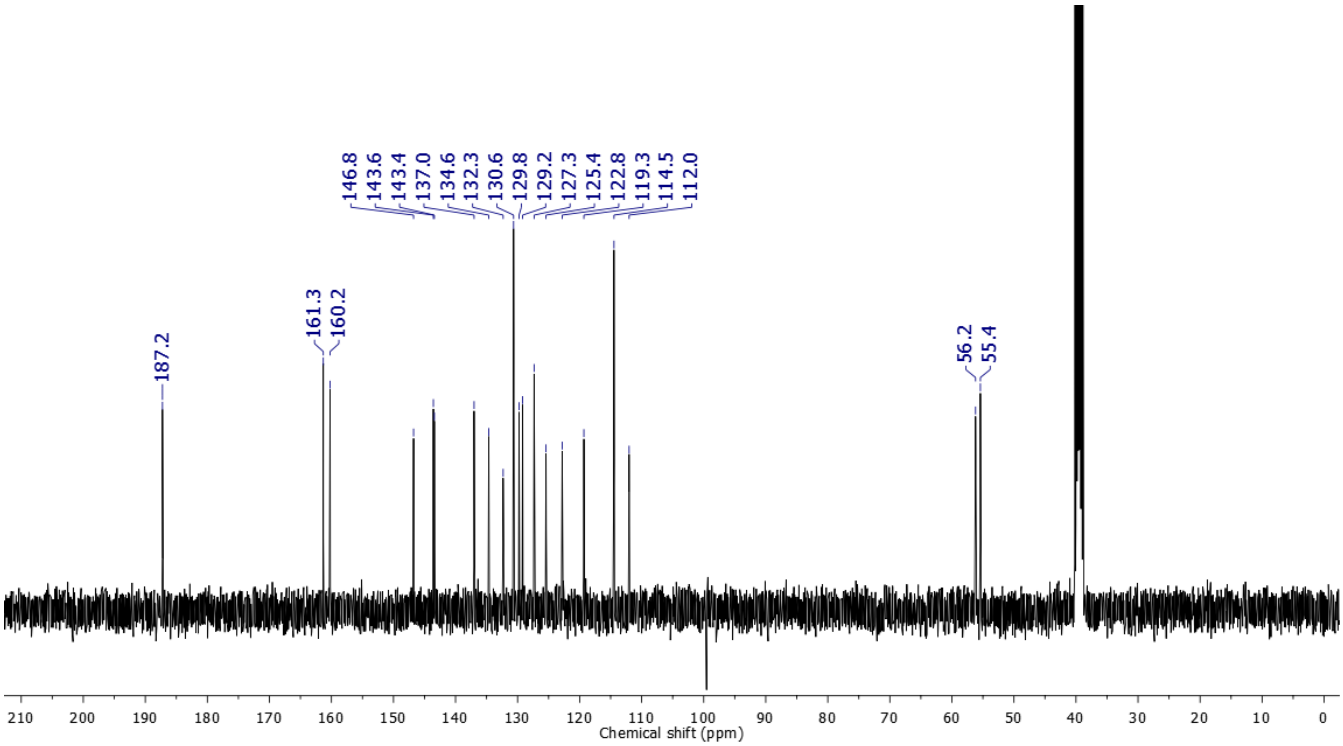
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **16c**.



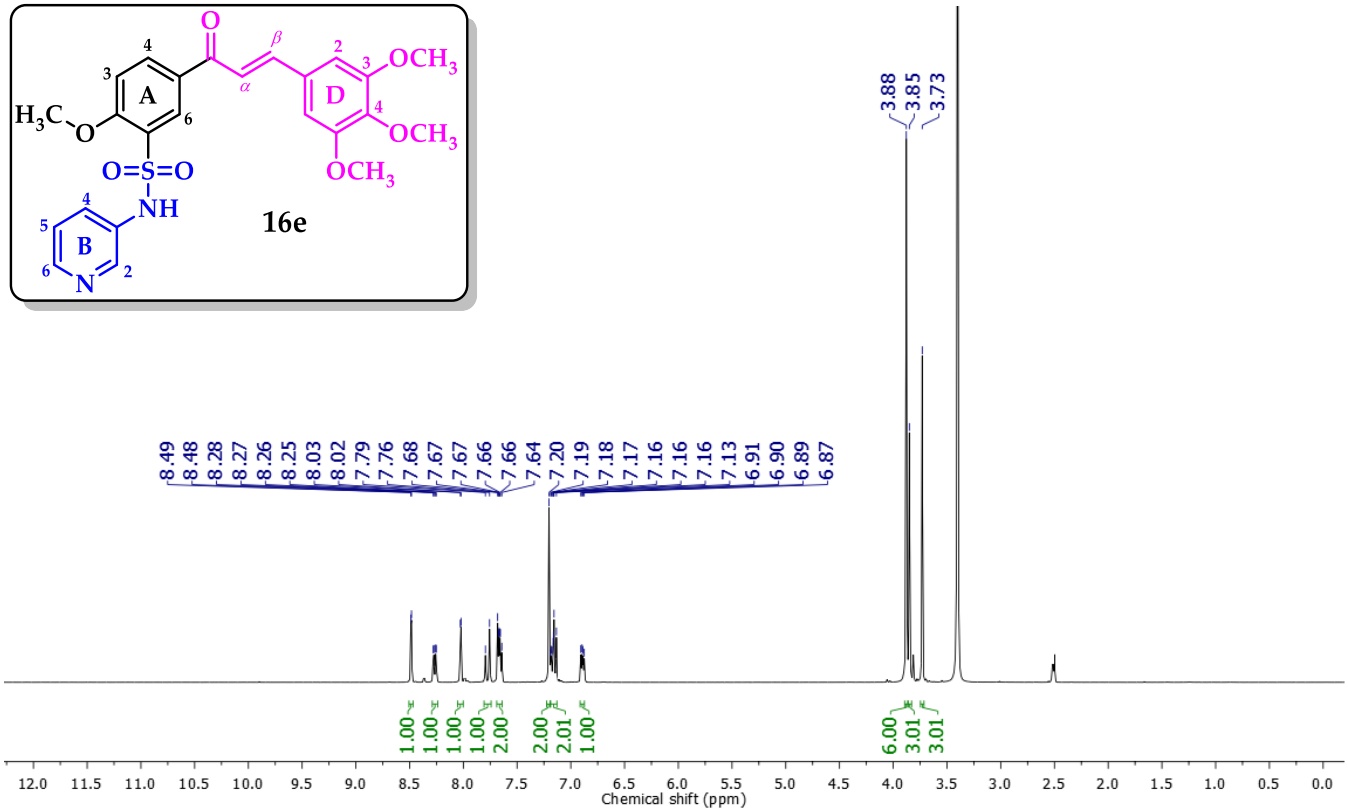
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **16c**.



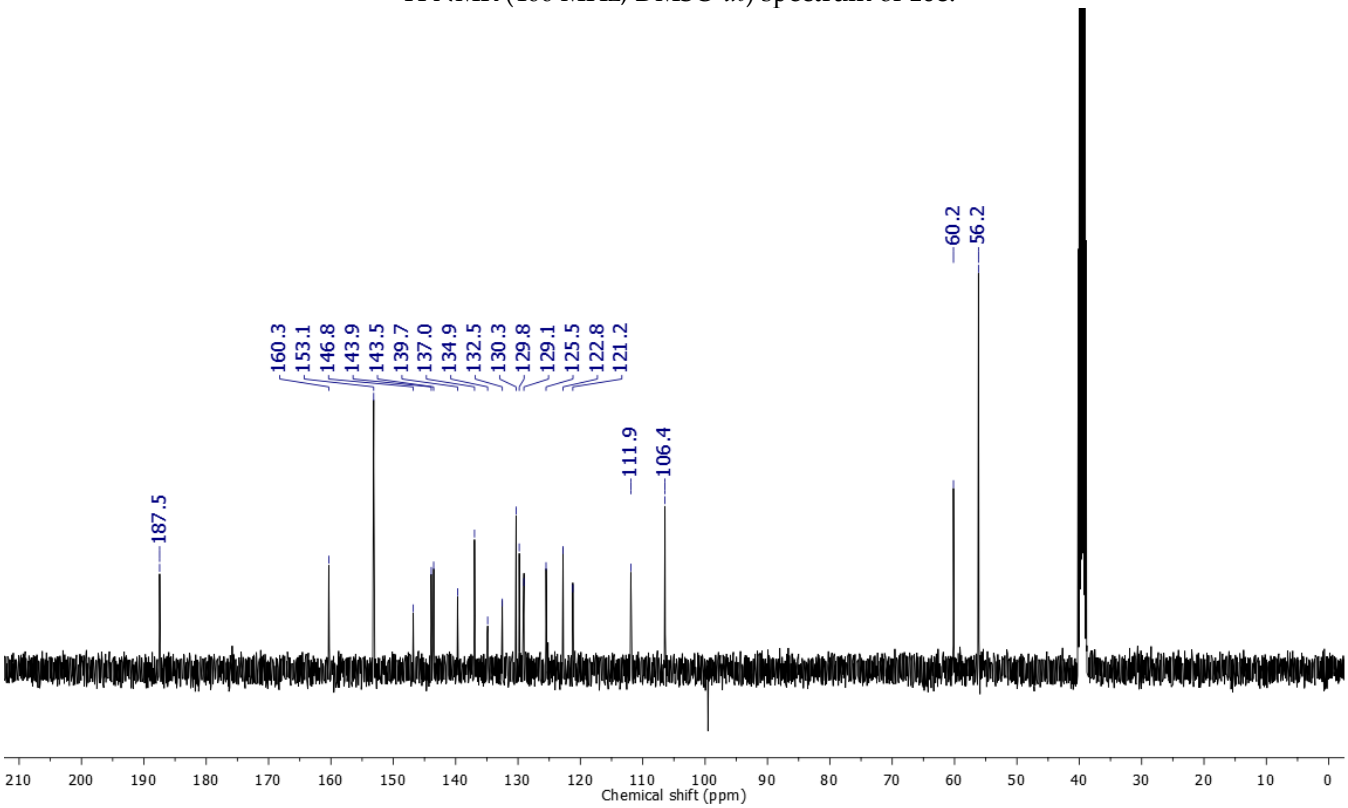
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **16d**.



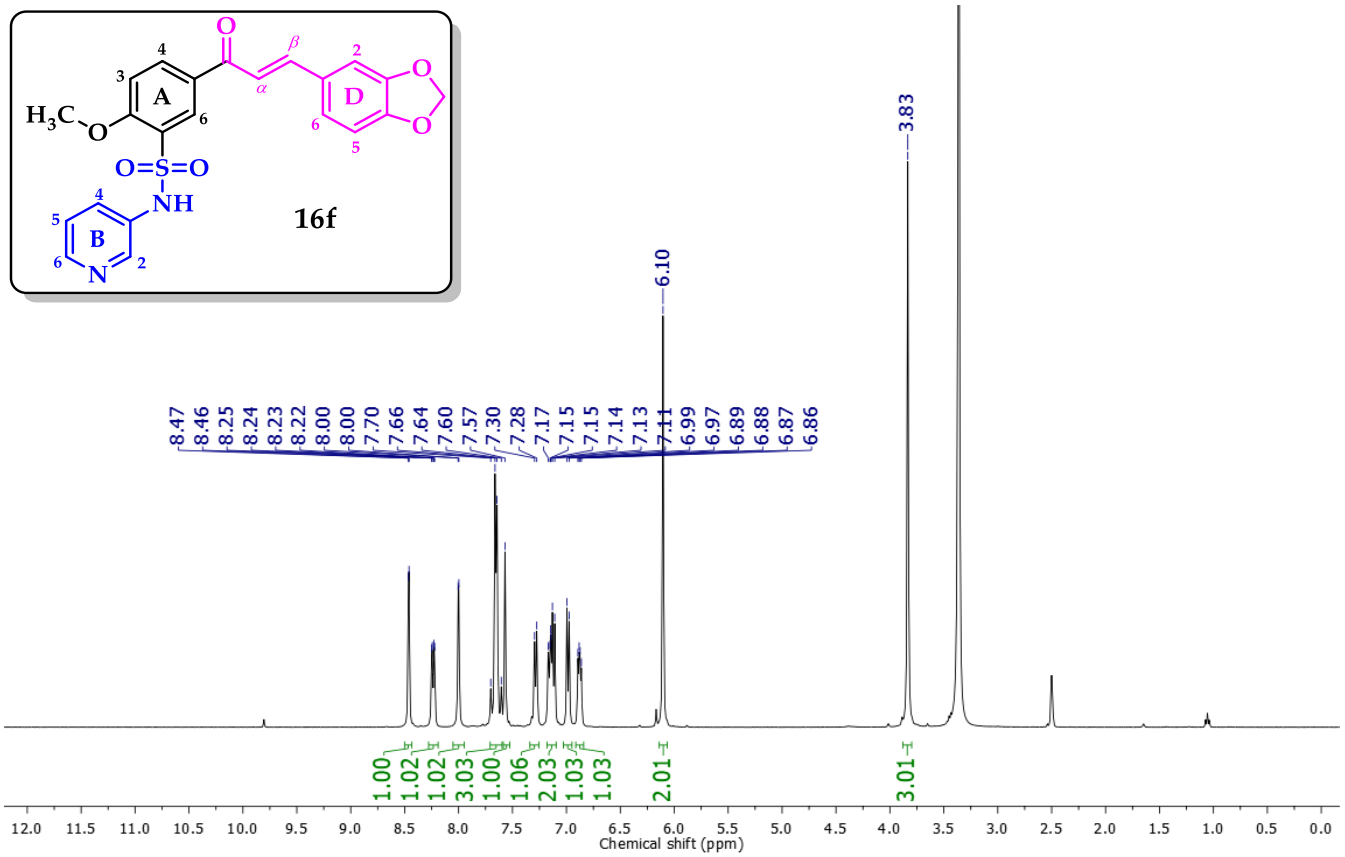
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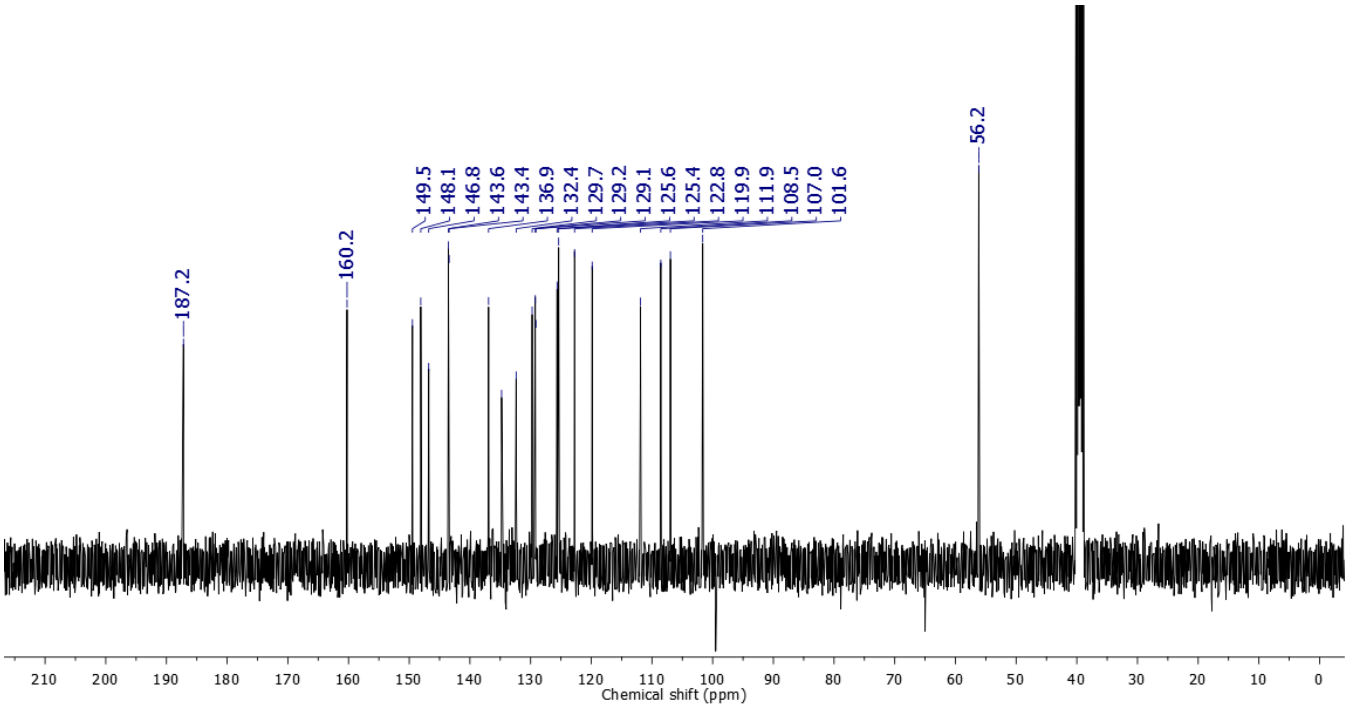
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **16e**.



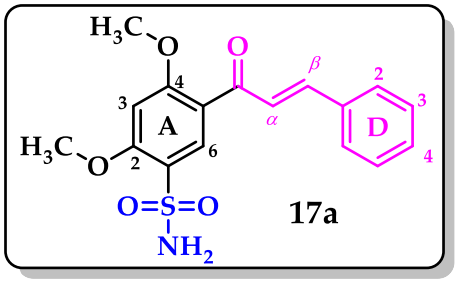
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **16e**.



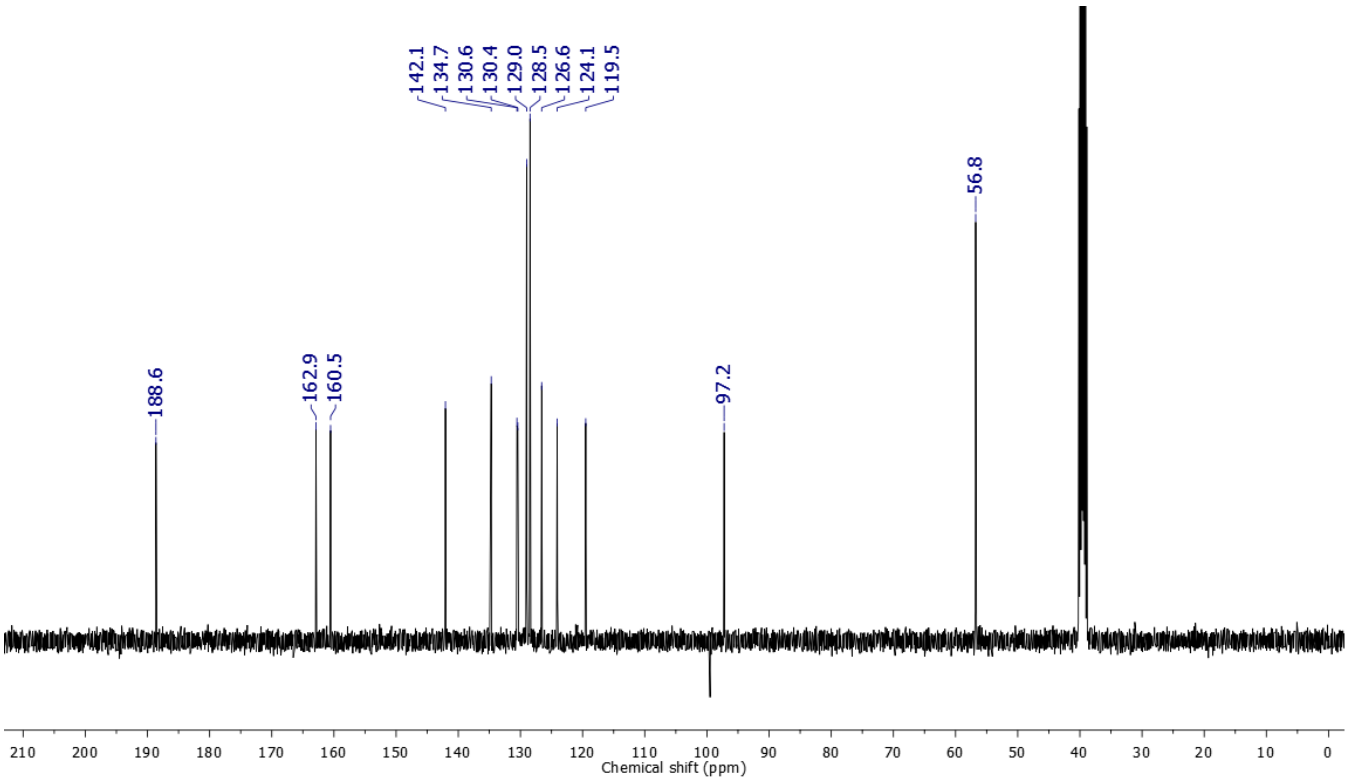
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **16f**.



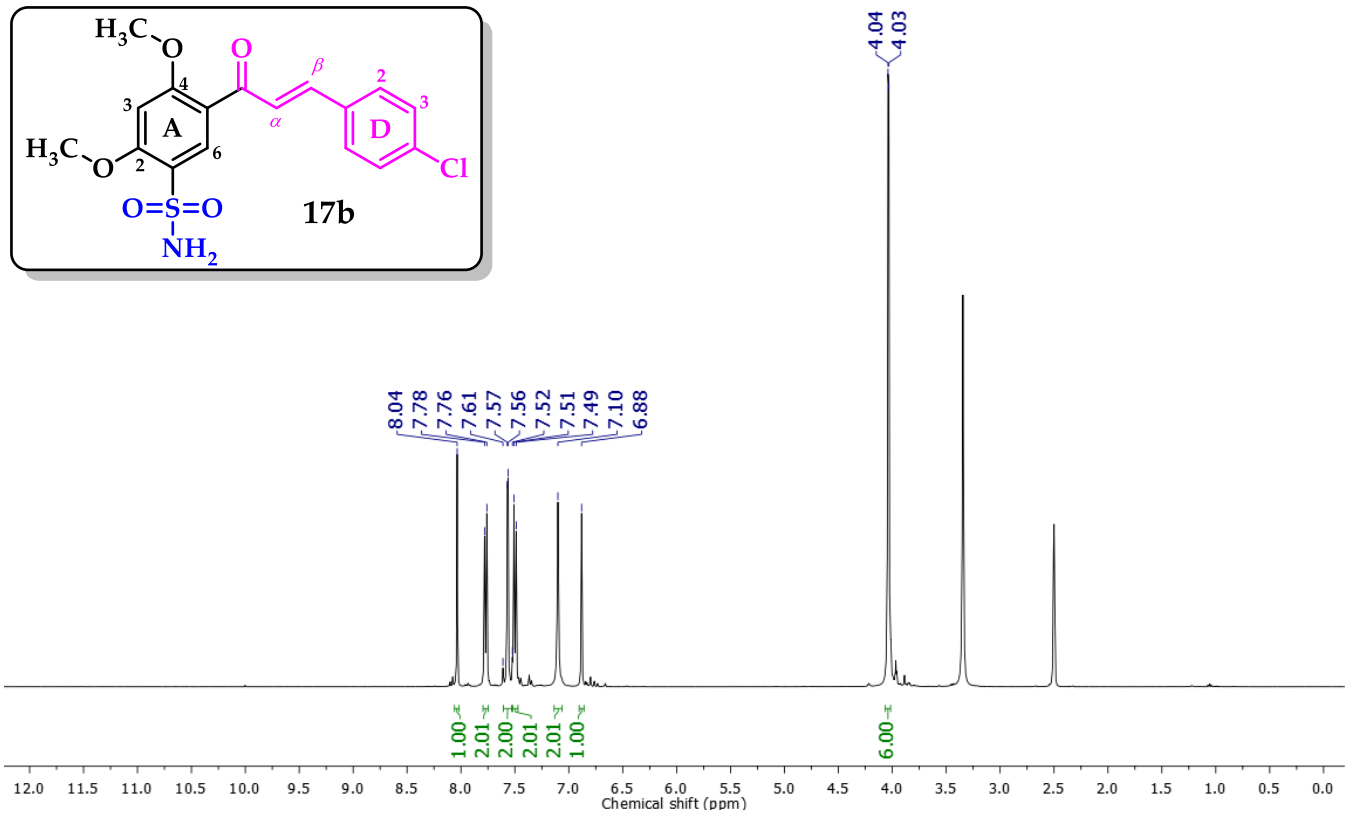
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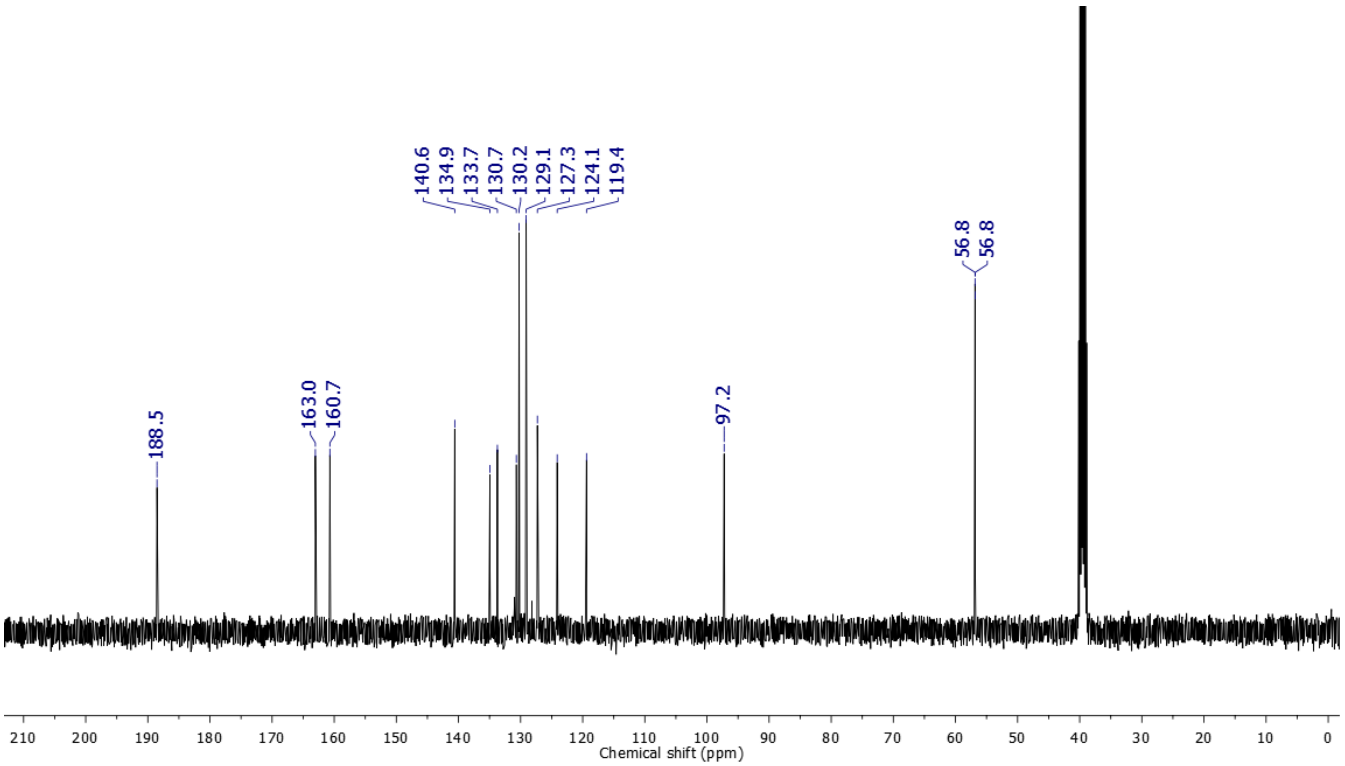
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **17a**.



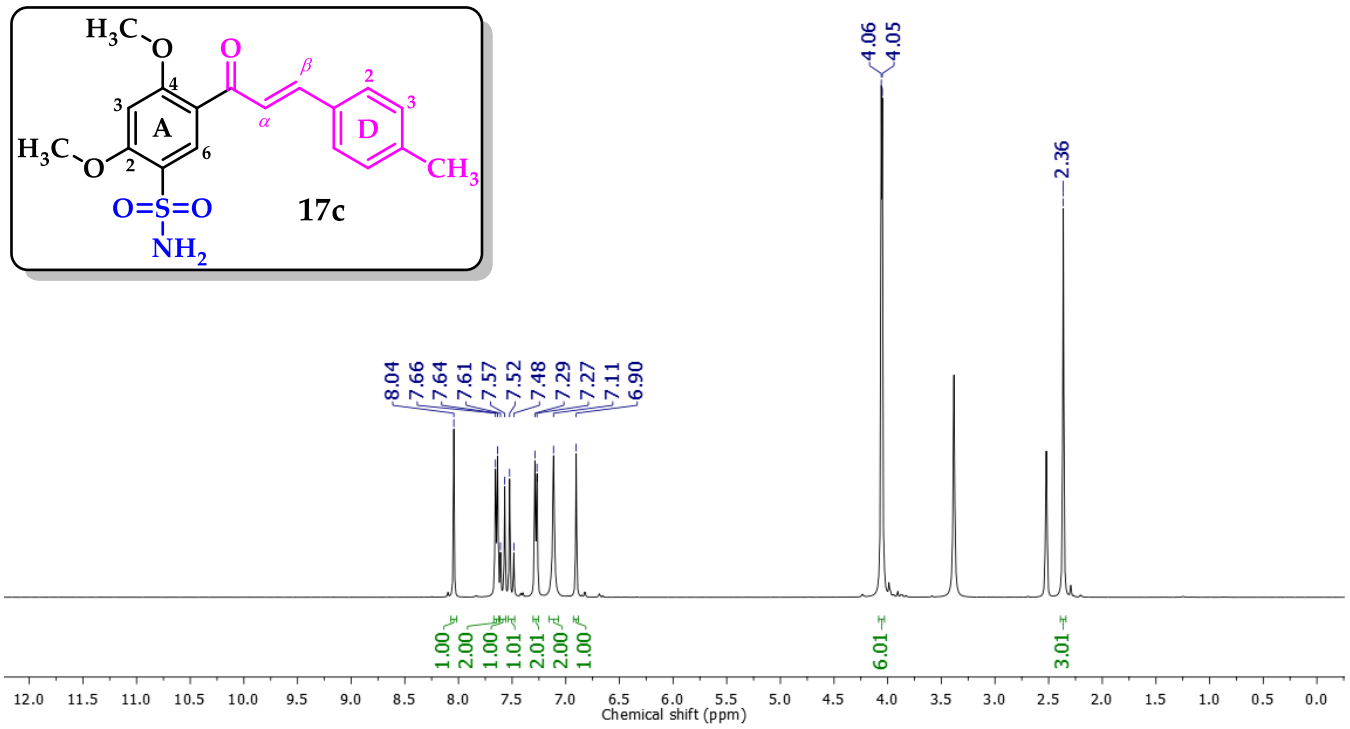
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **17a**.



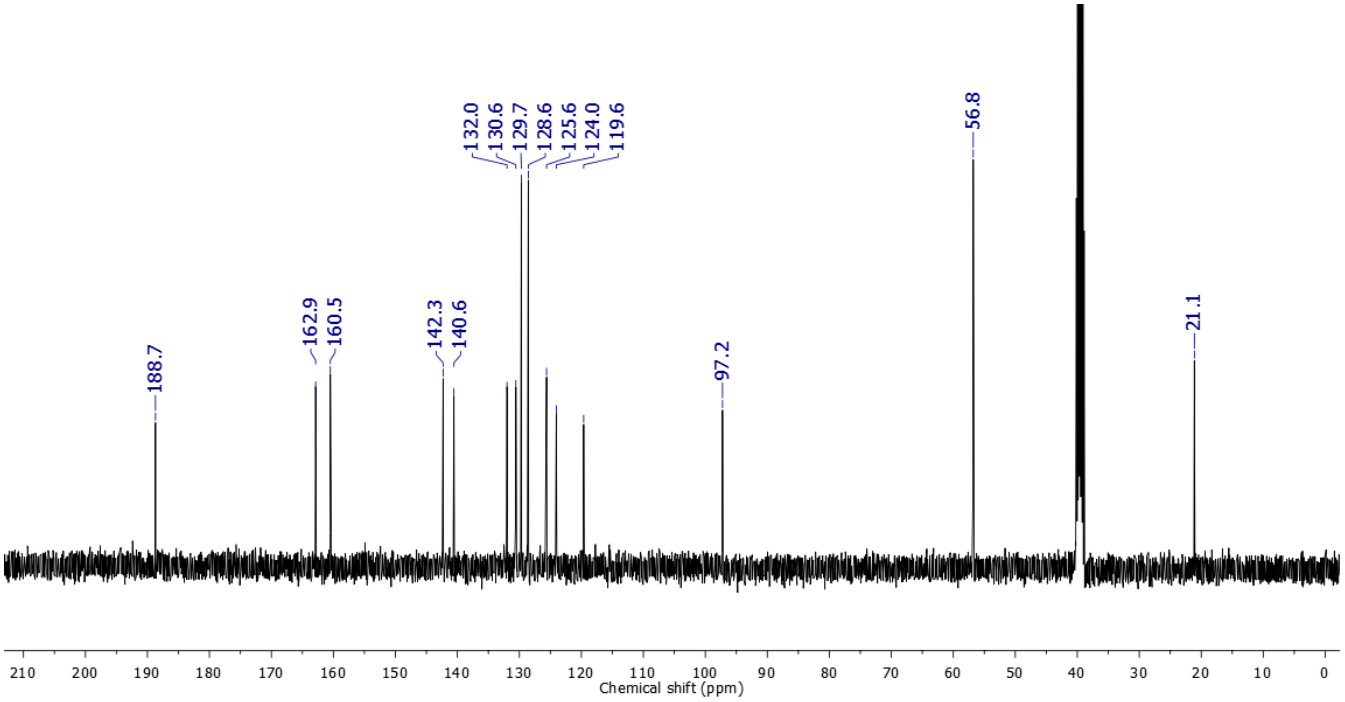
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **17b**.



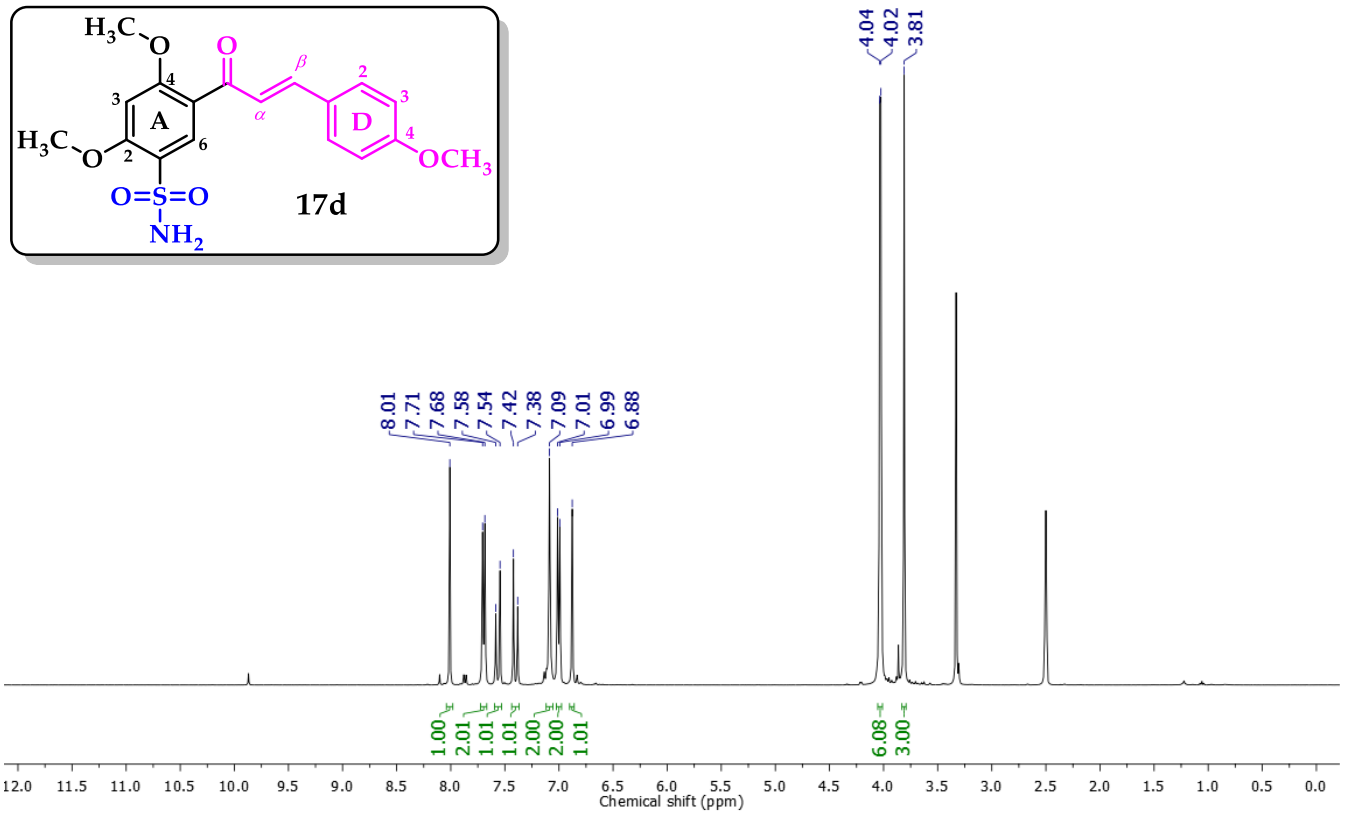
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **17b**.



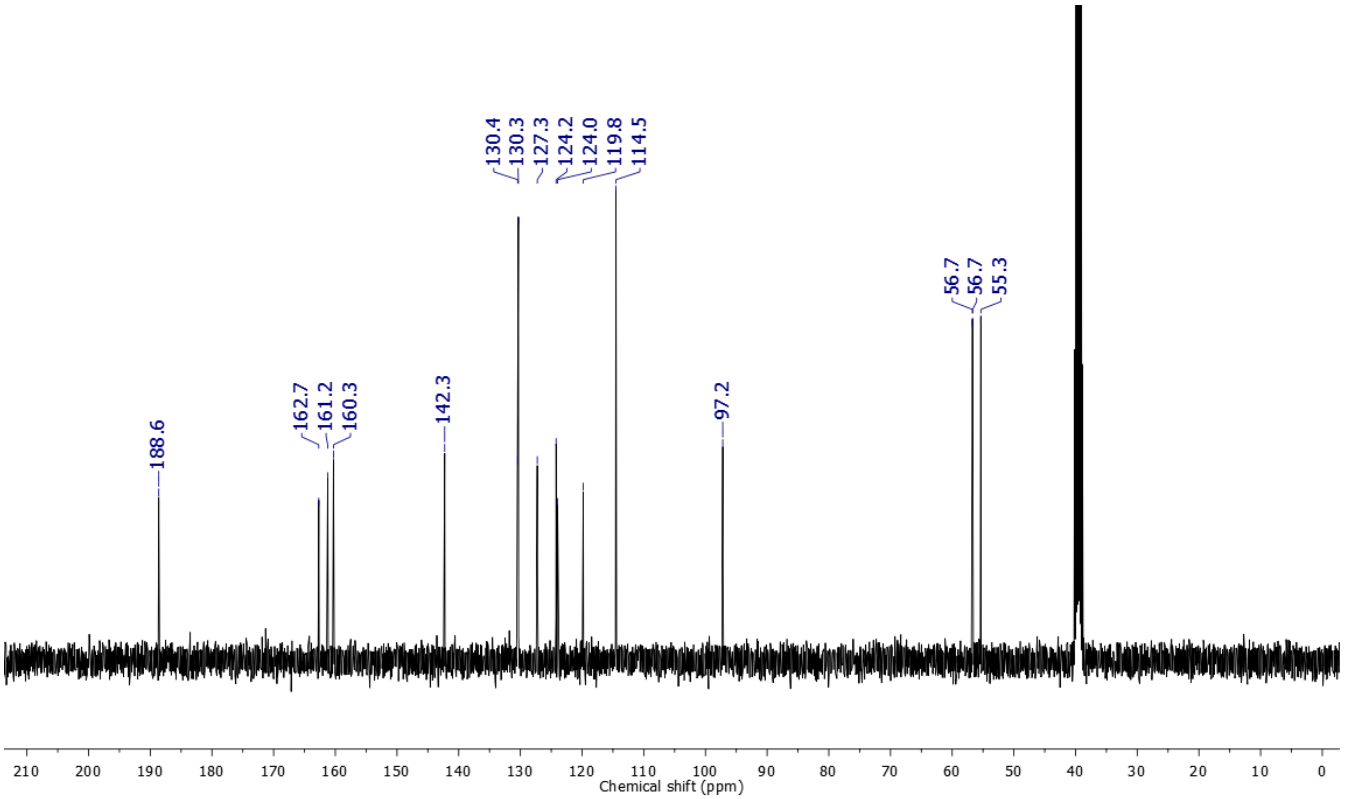
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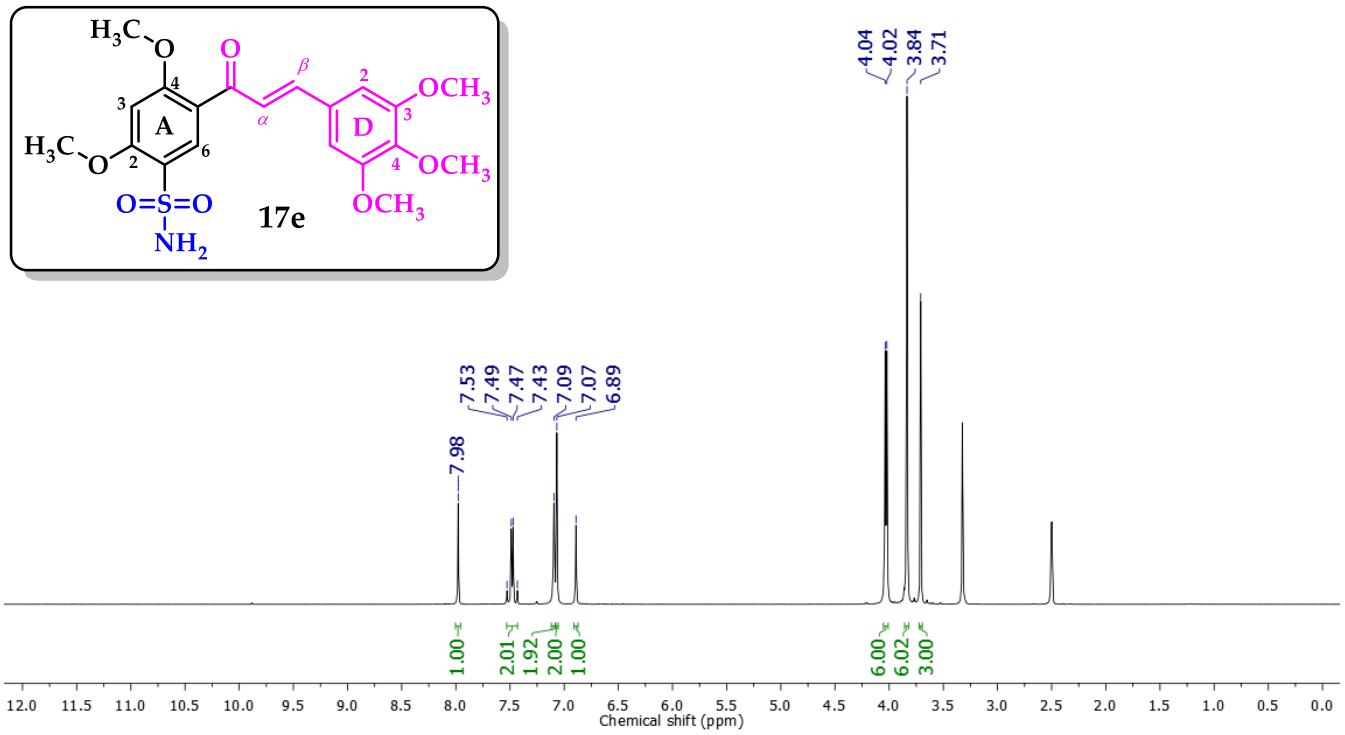
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **17c**.



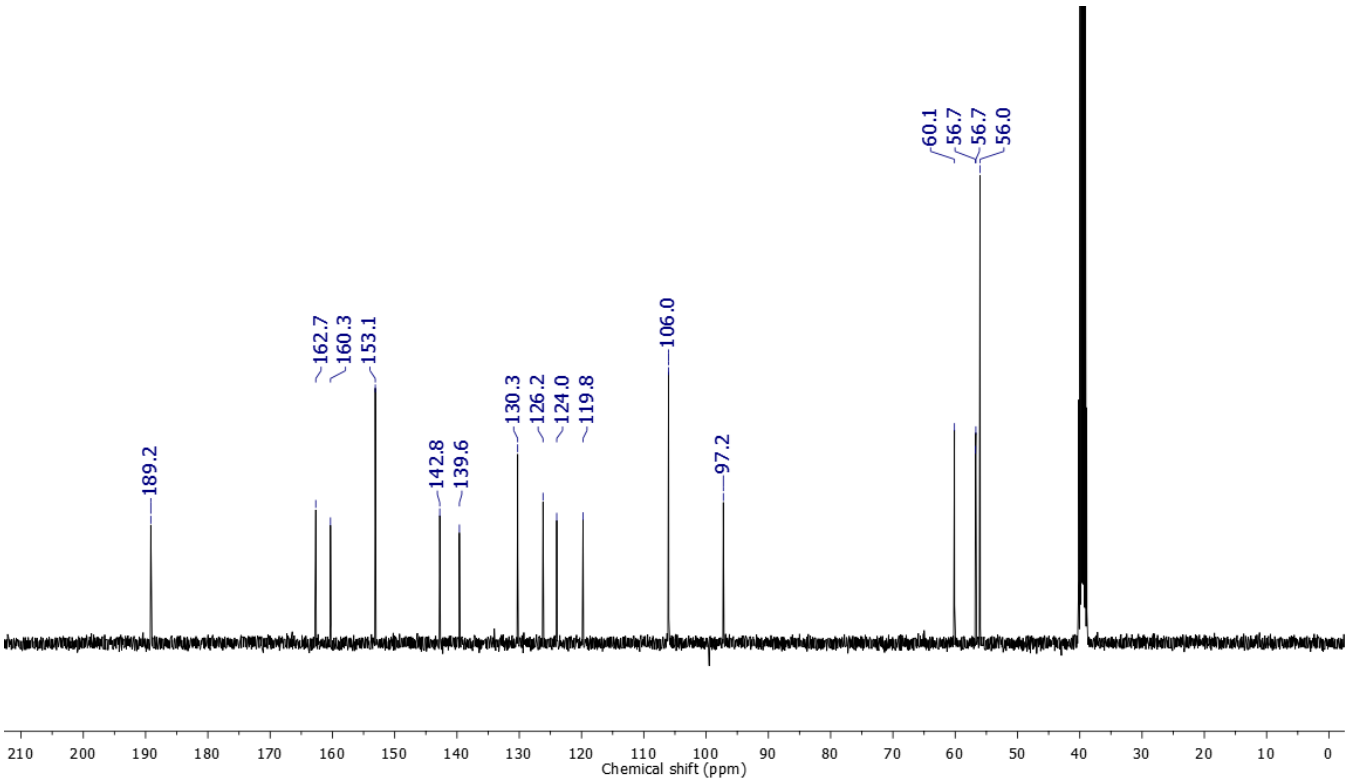
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **17d**.



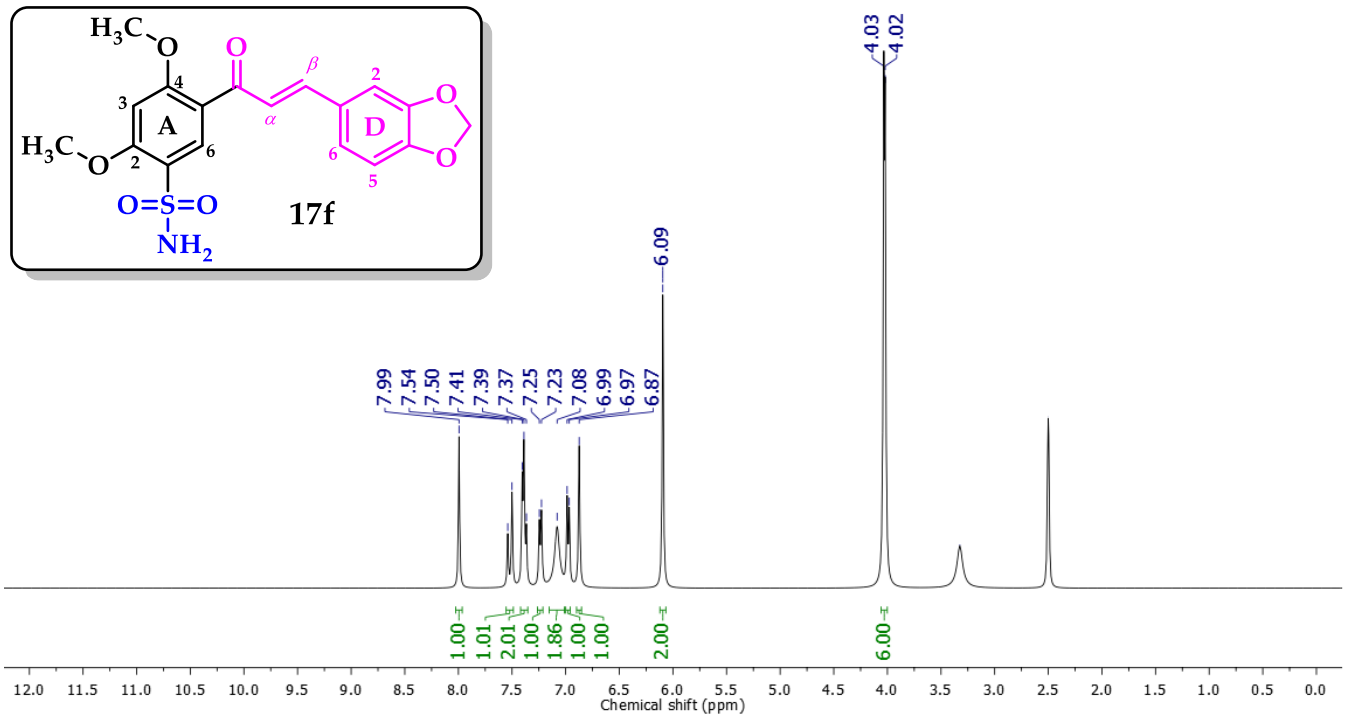
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **17d**.



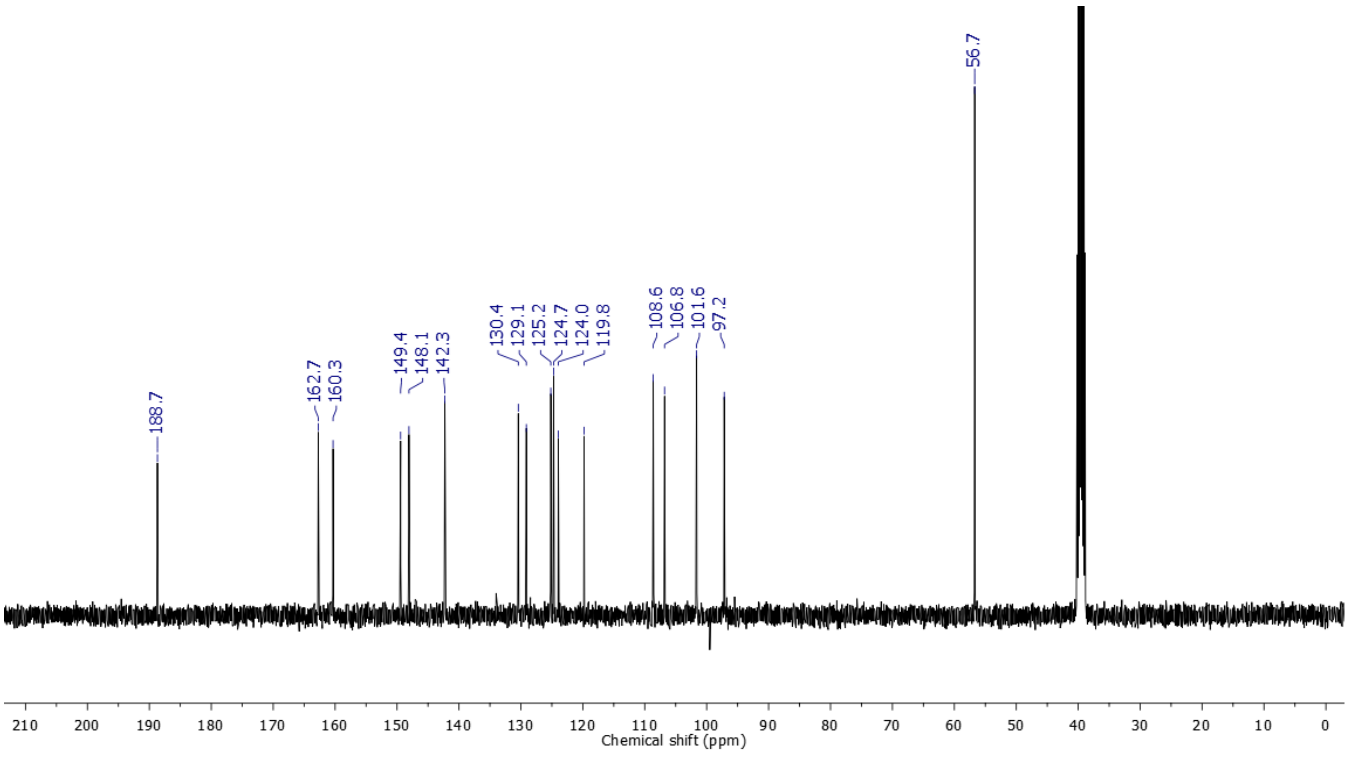
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **17e**.



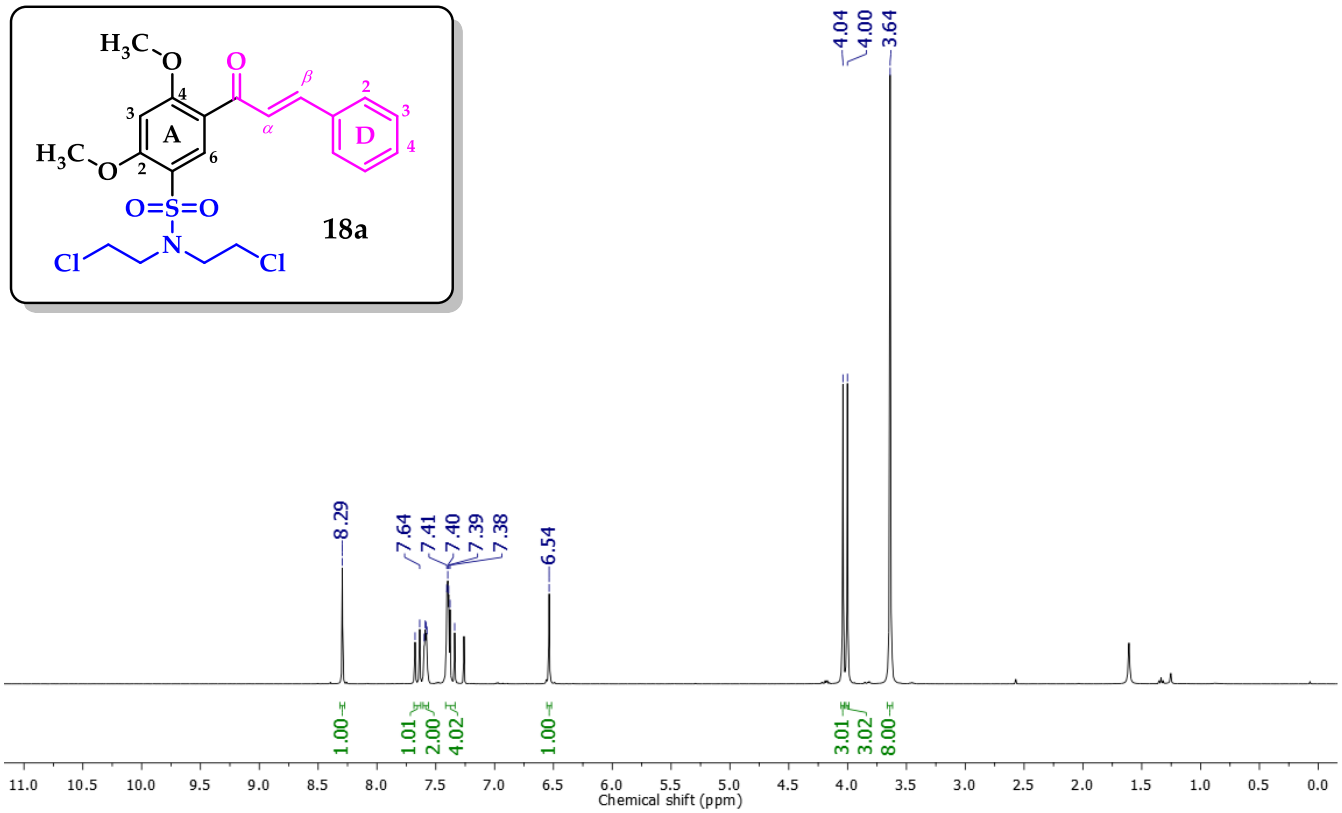
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **17e**.



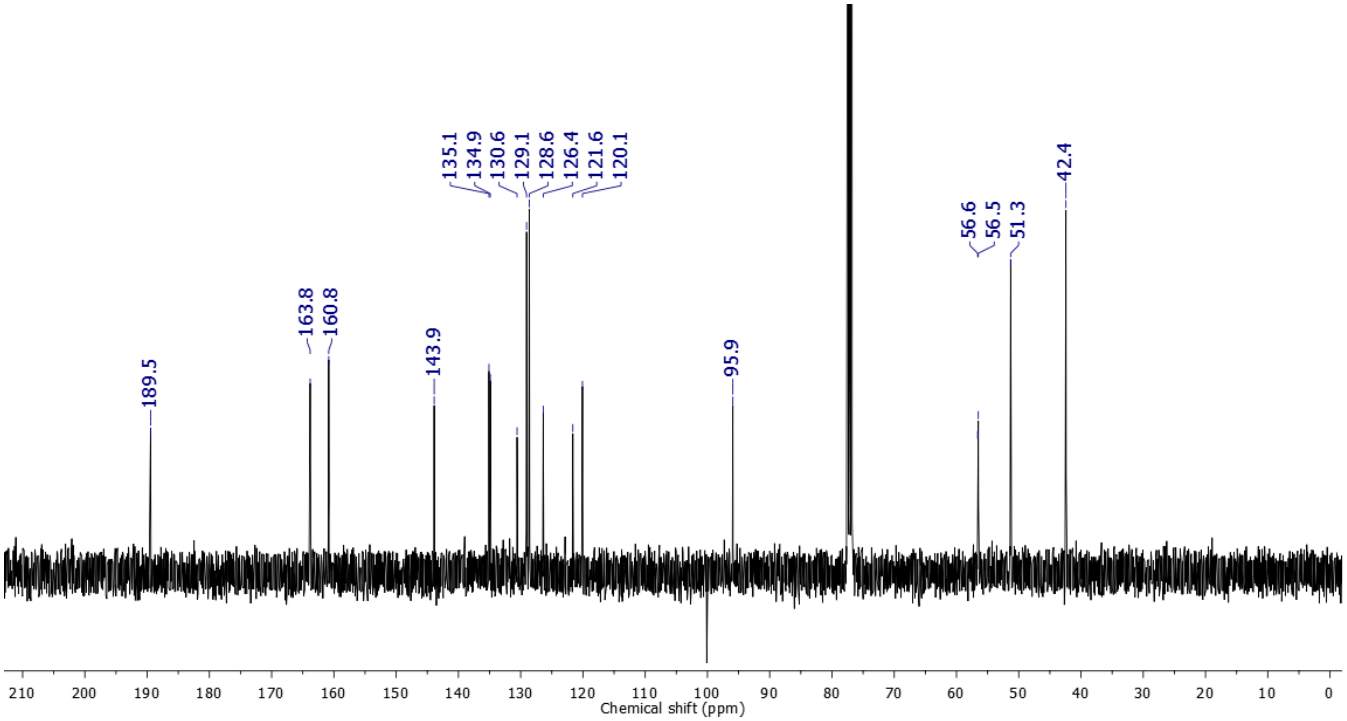
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **17f**.



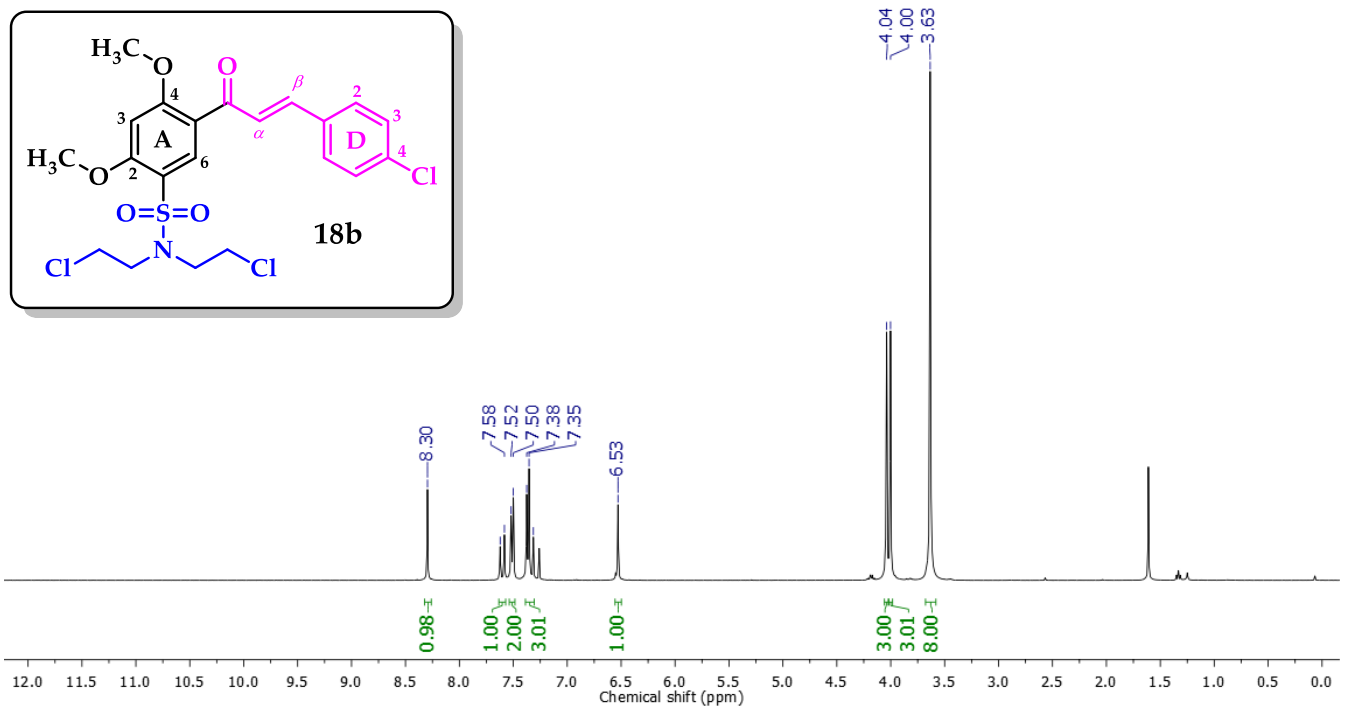
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **17f**.



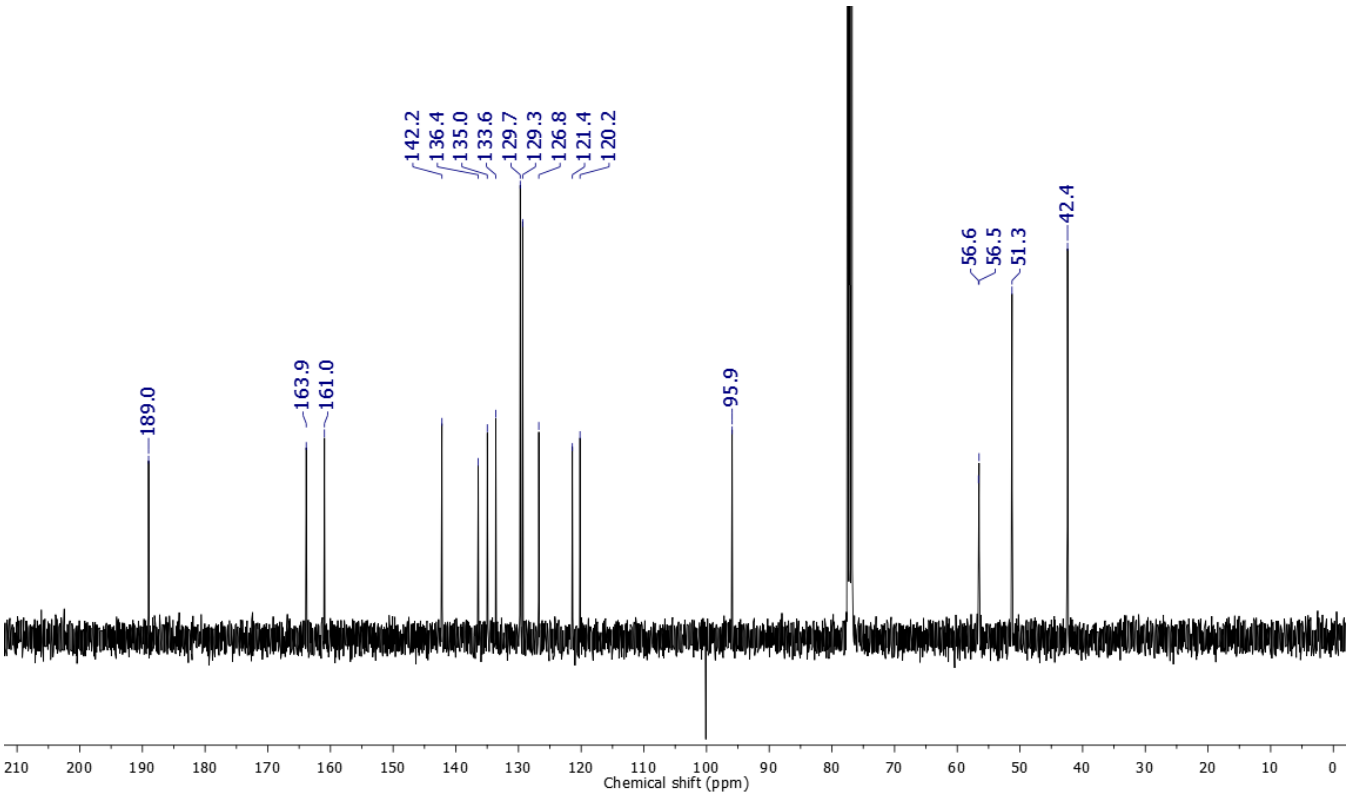
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **18a**.



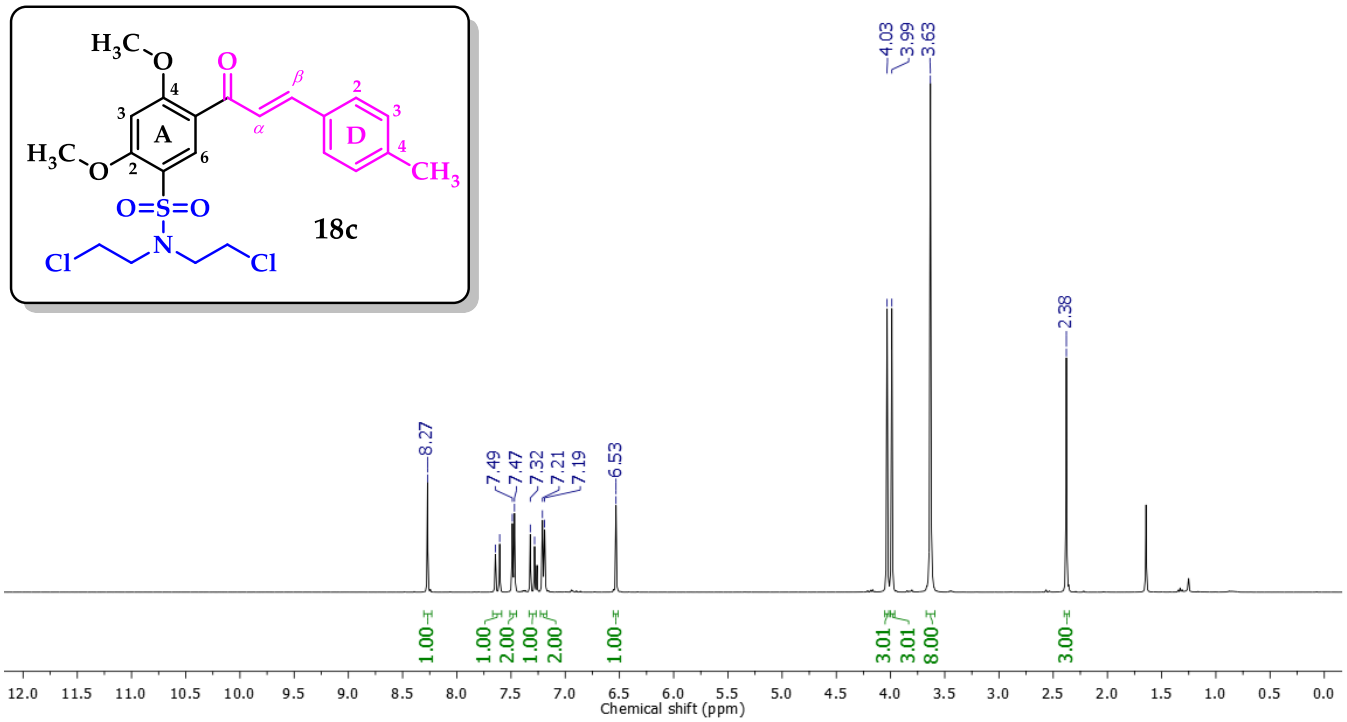
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **18a**.



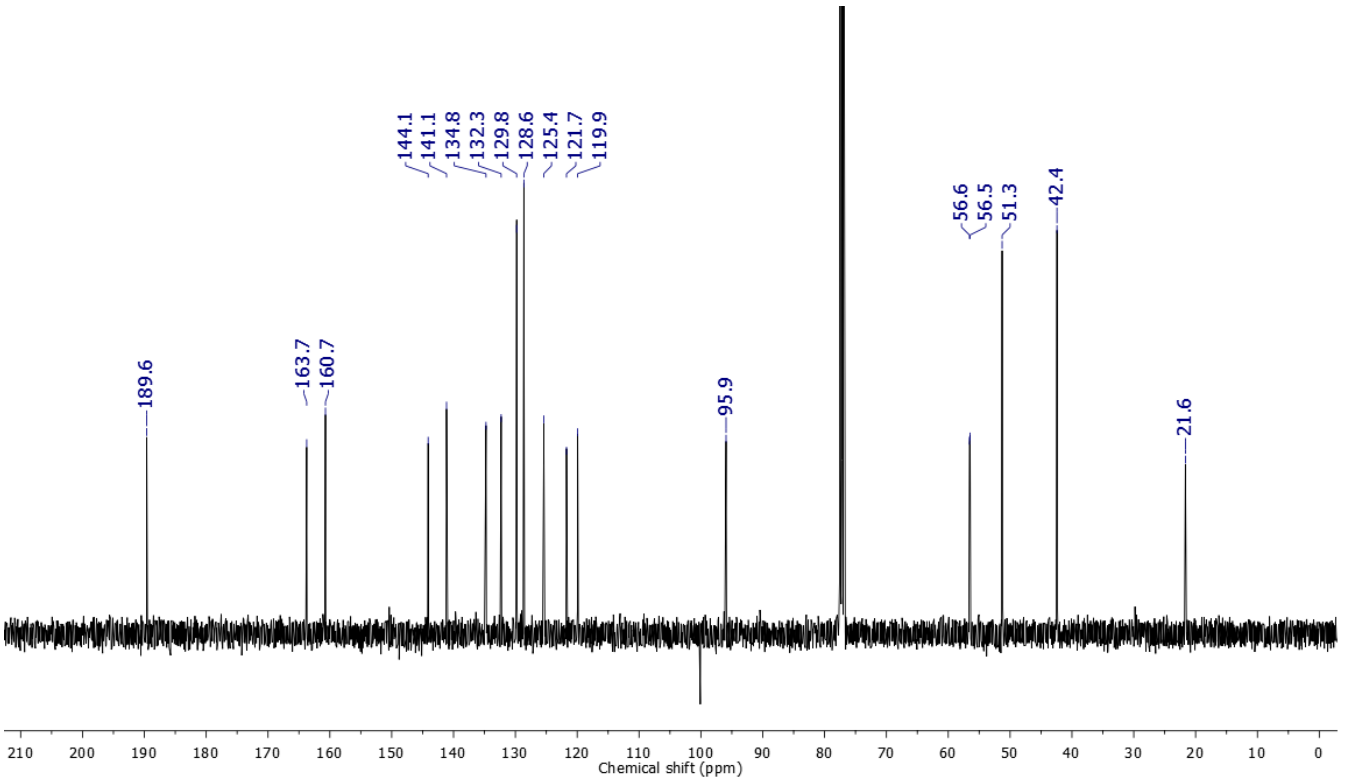
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **18b**.



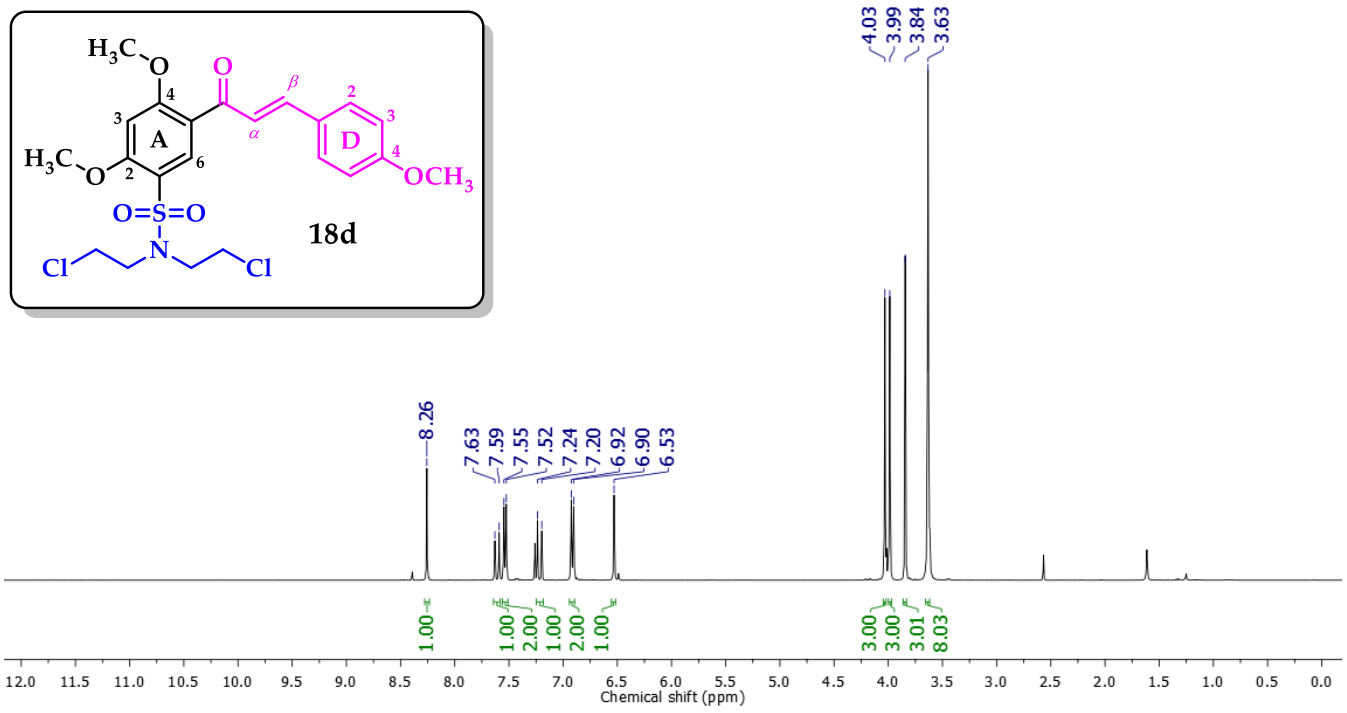
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **18b**.



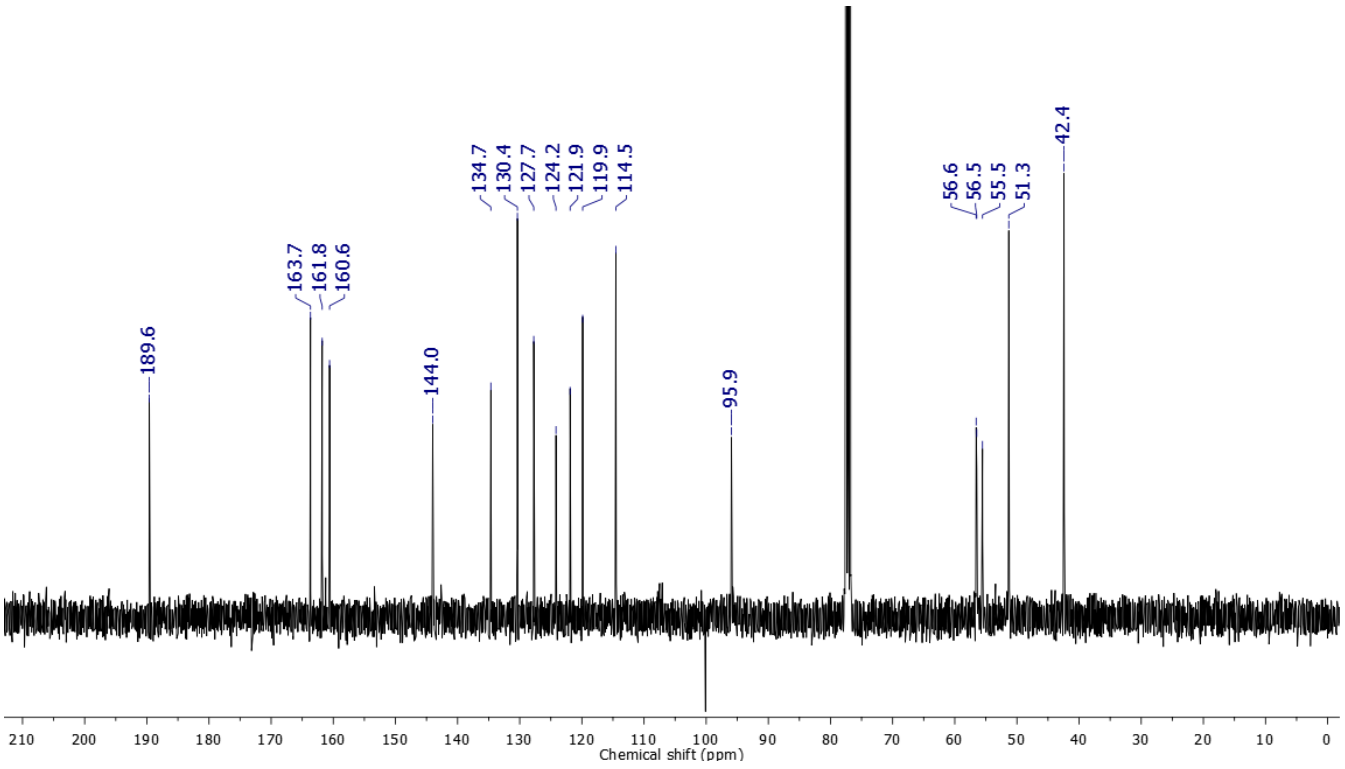
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **18c**.



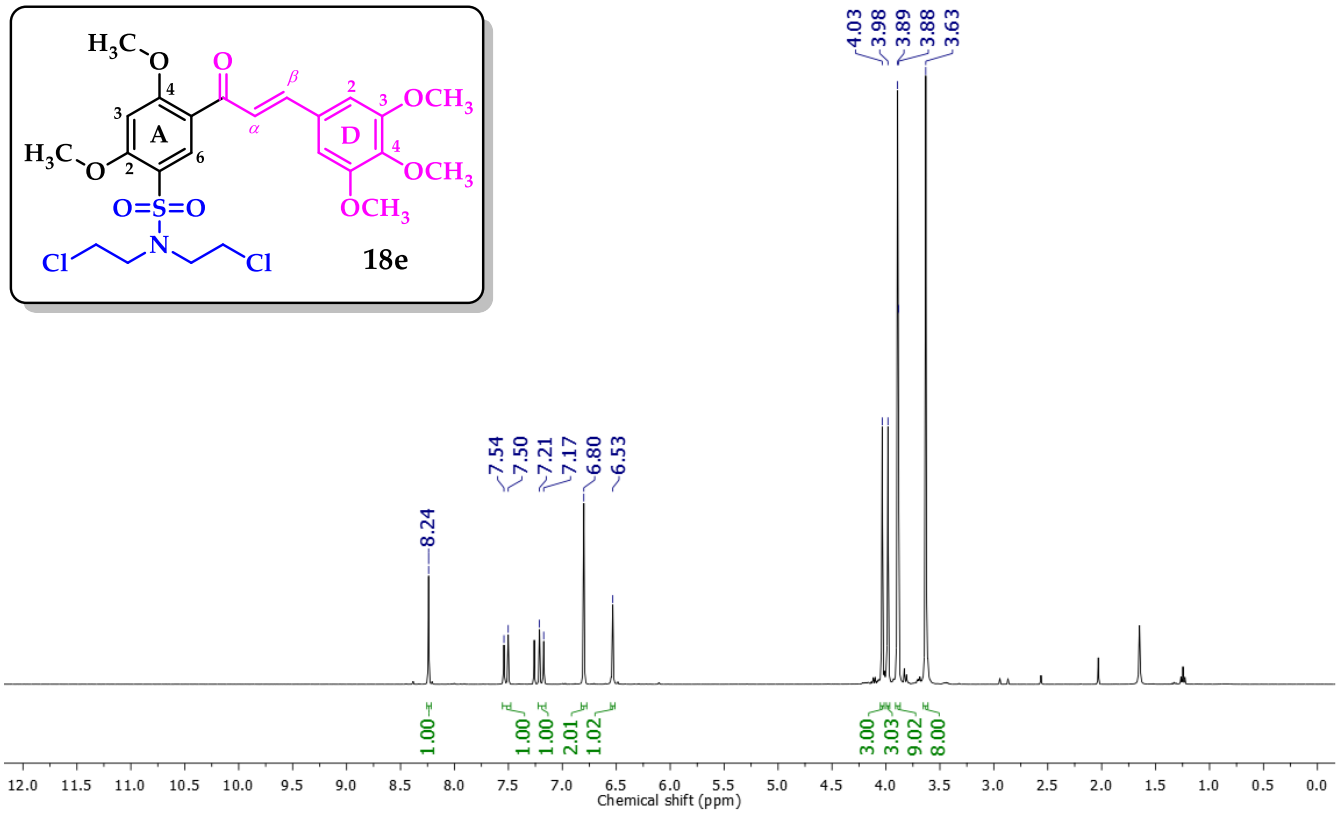
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **18c**.



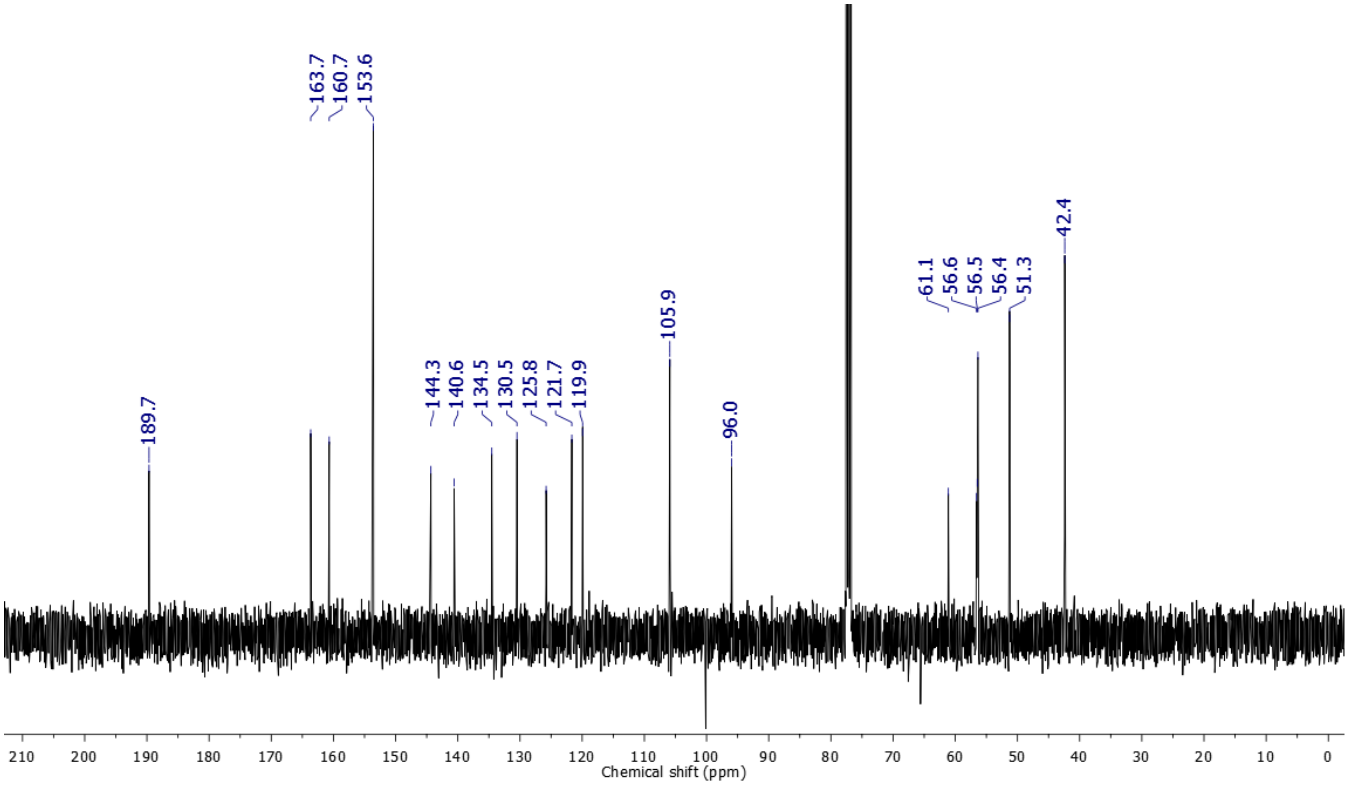
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **18d**.



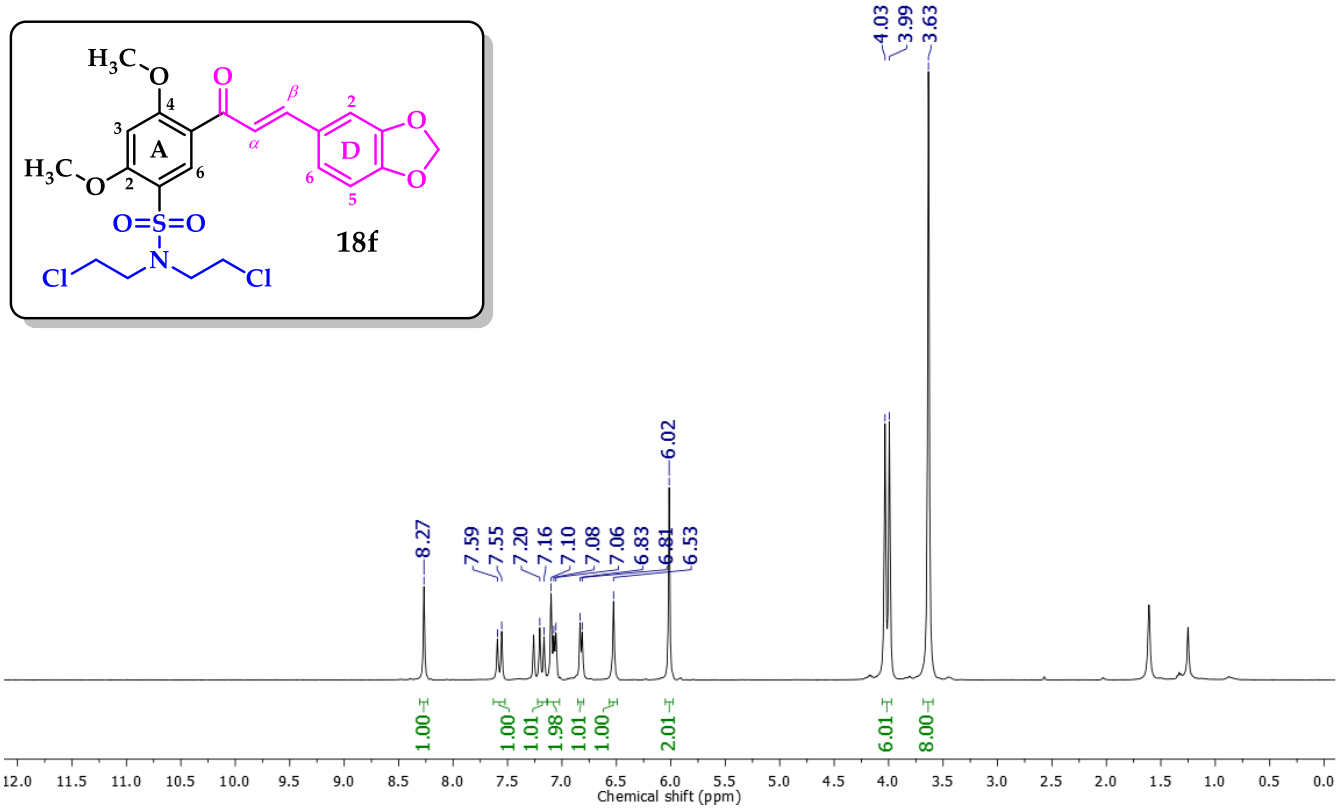
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **18d**.



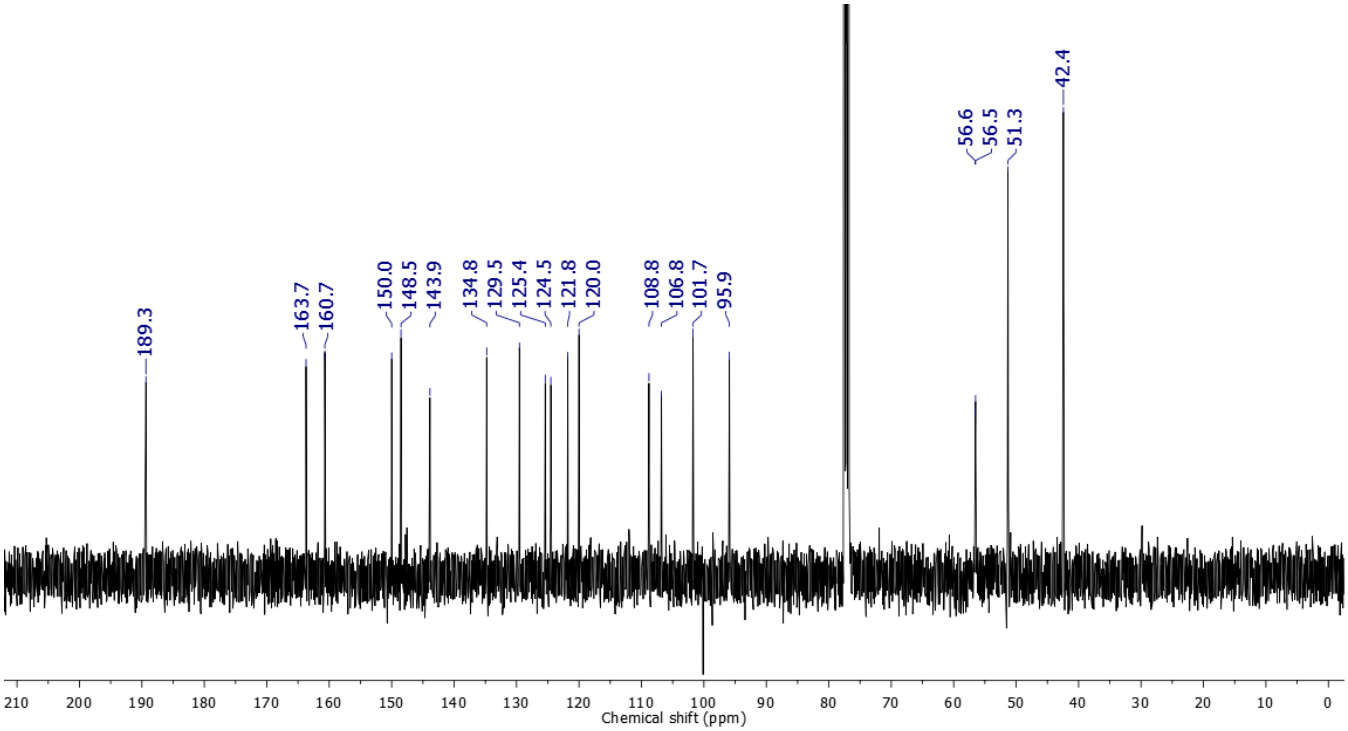
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **18e**.



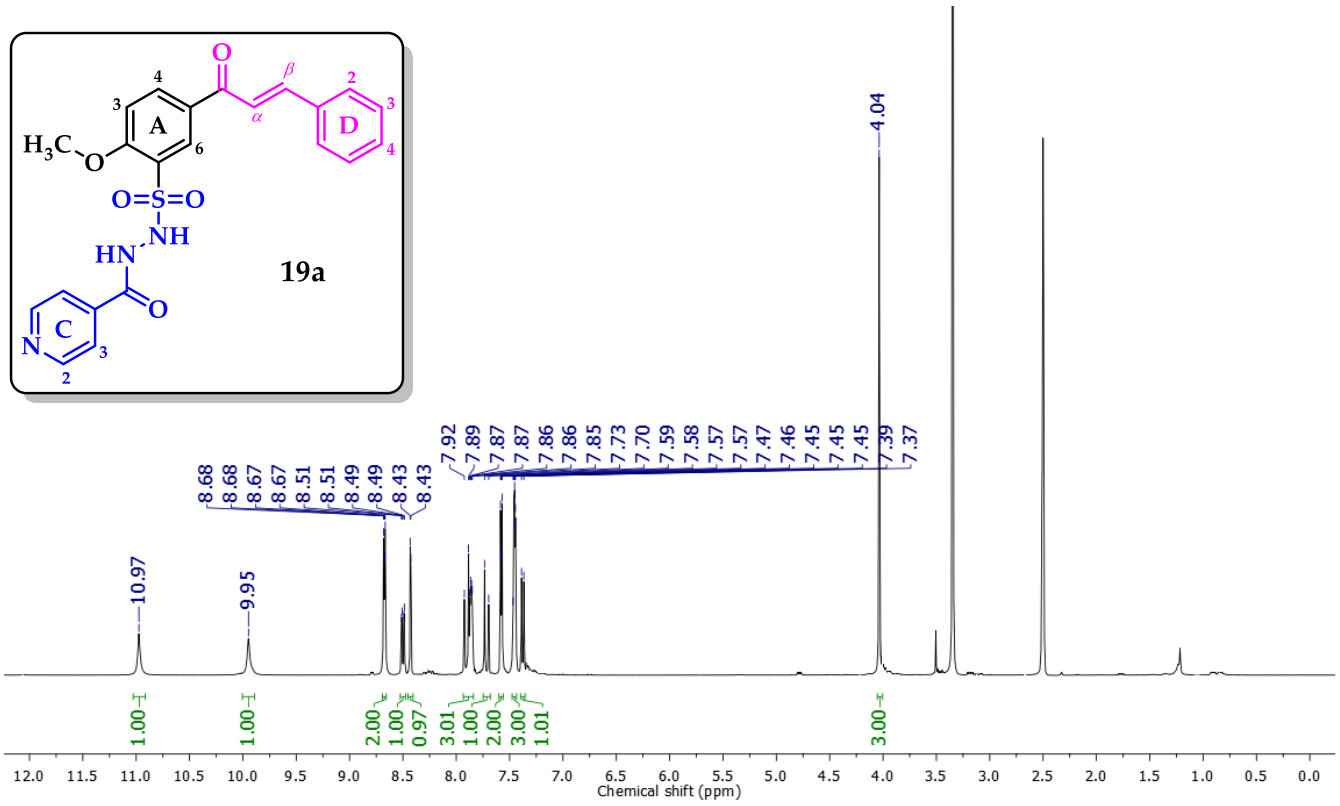
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **18e**.



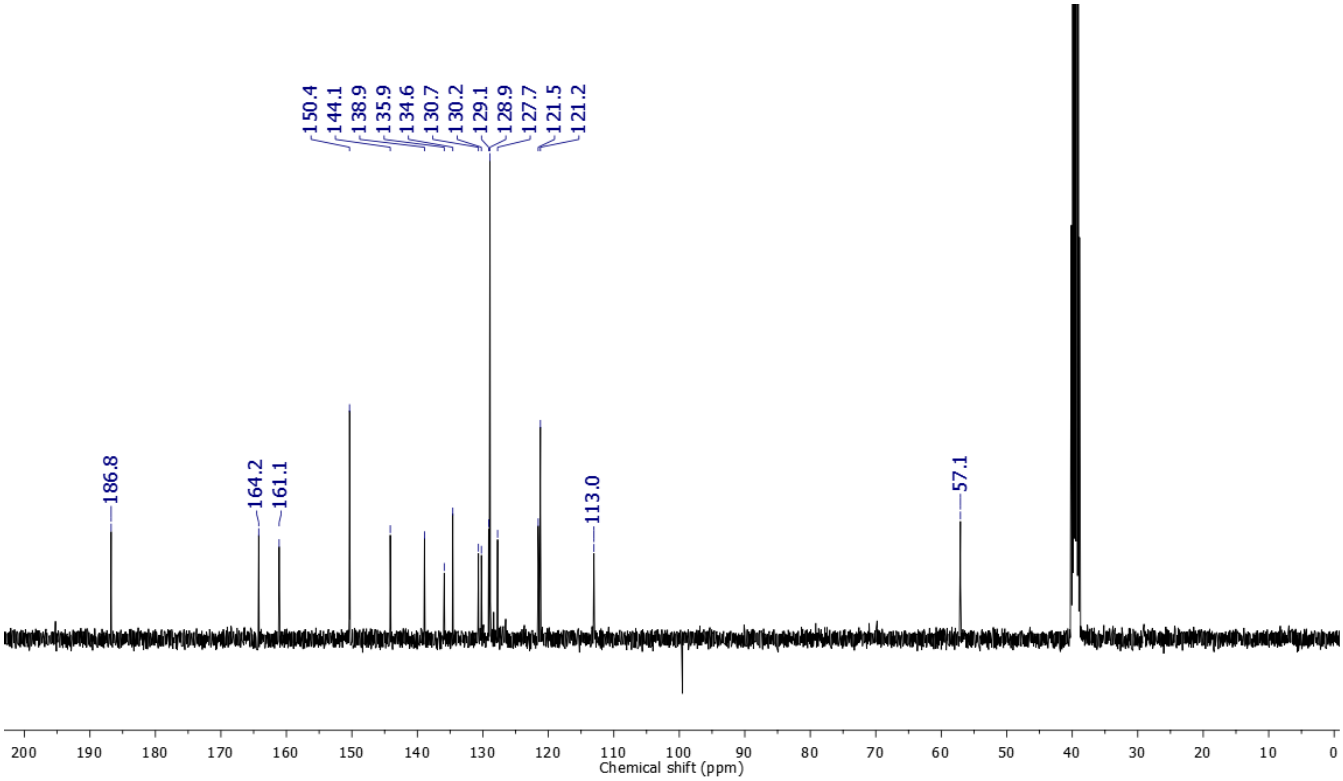
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **18f**.



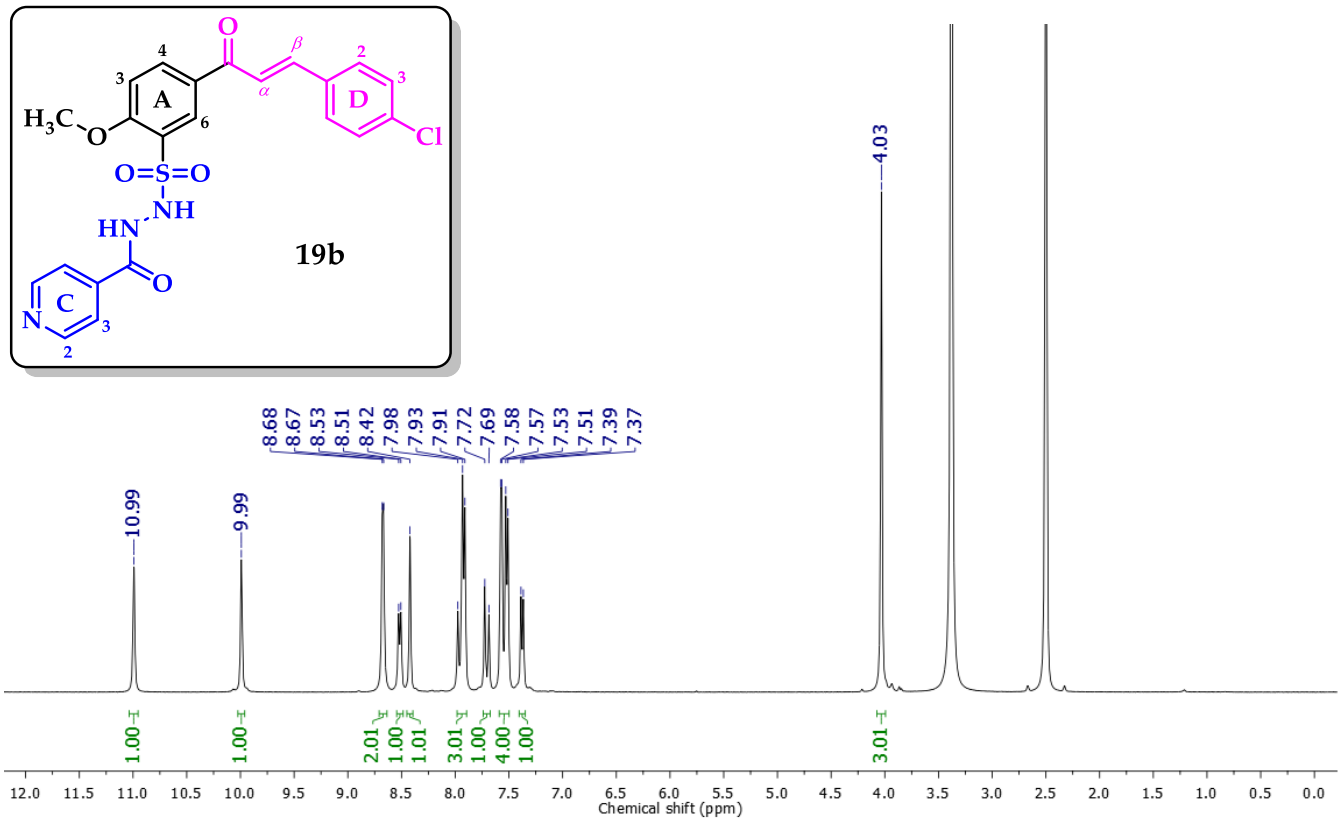
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **18f**.



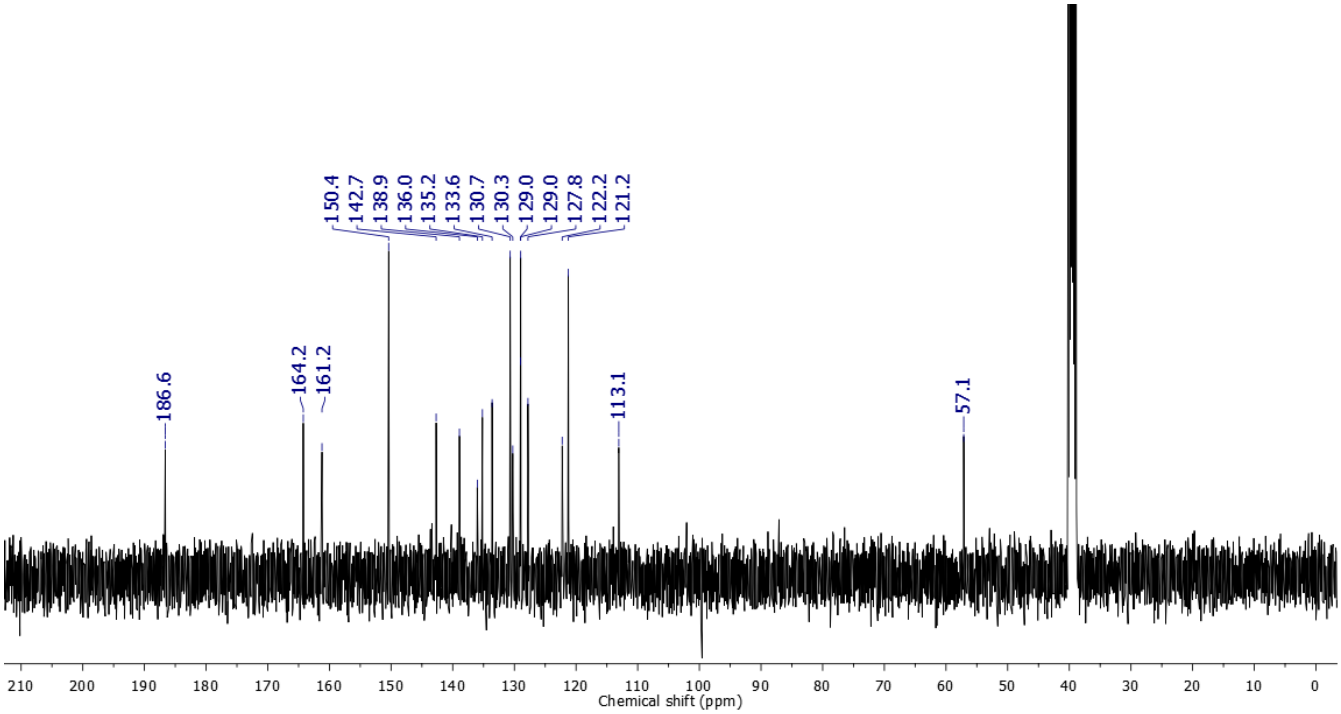
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **19a**.



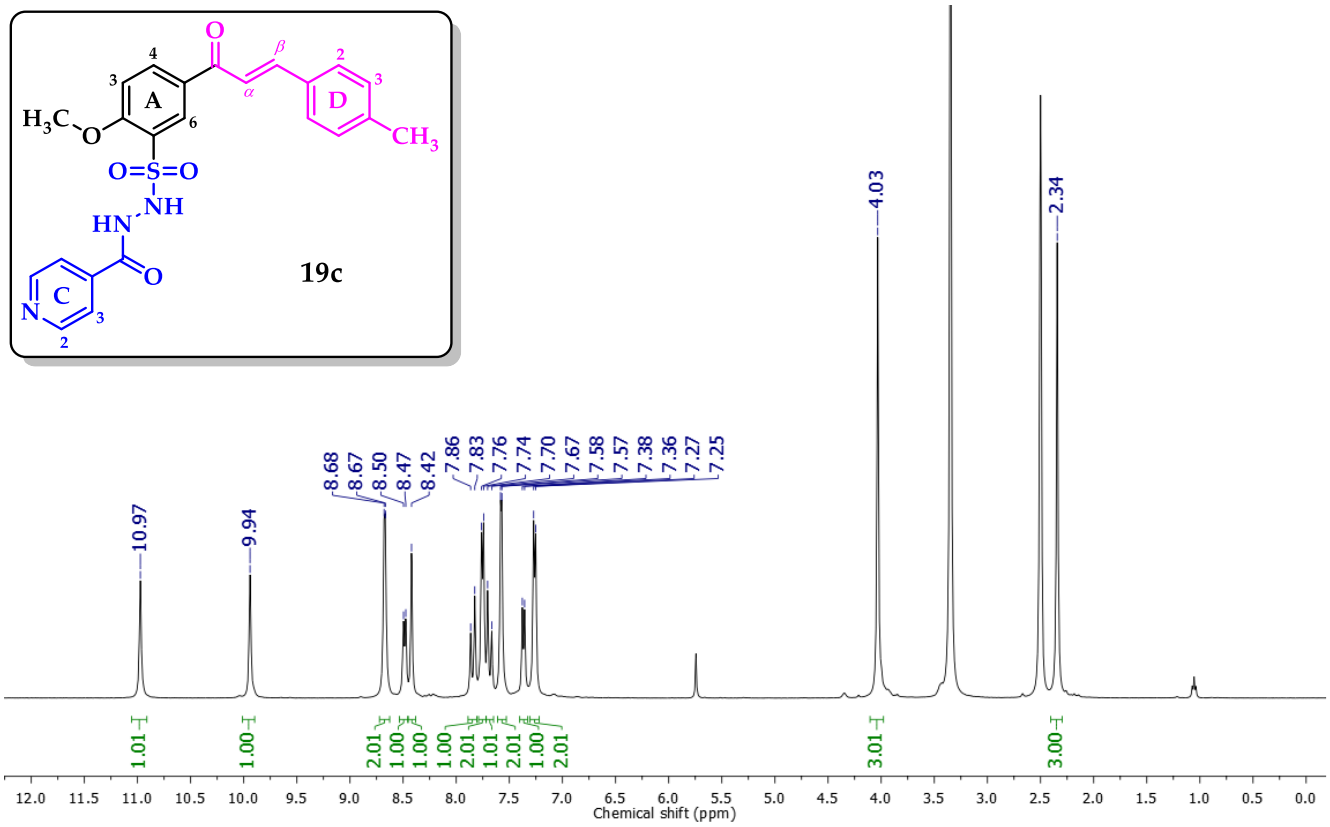
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **19a**.



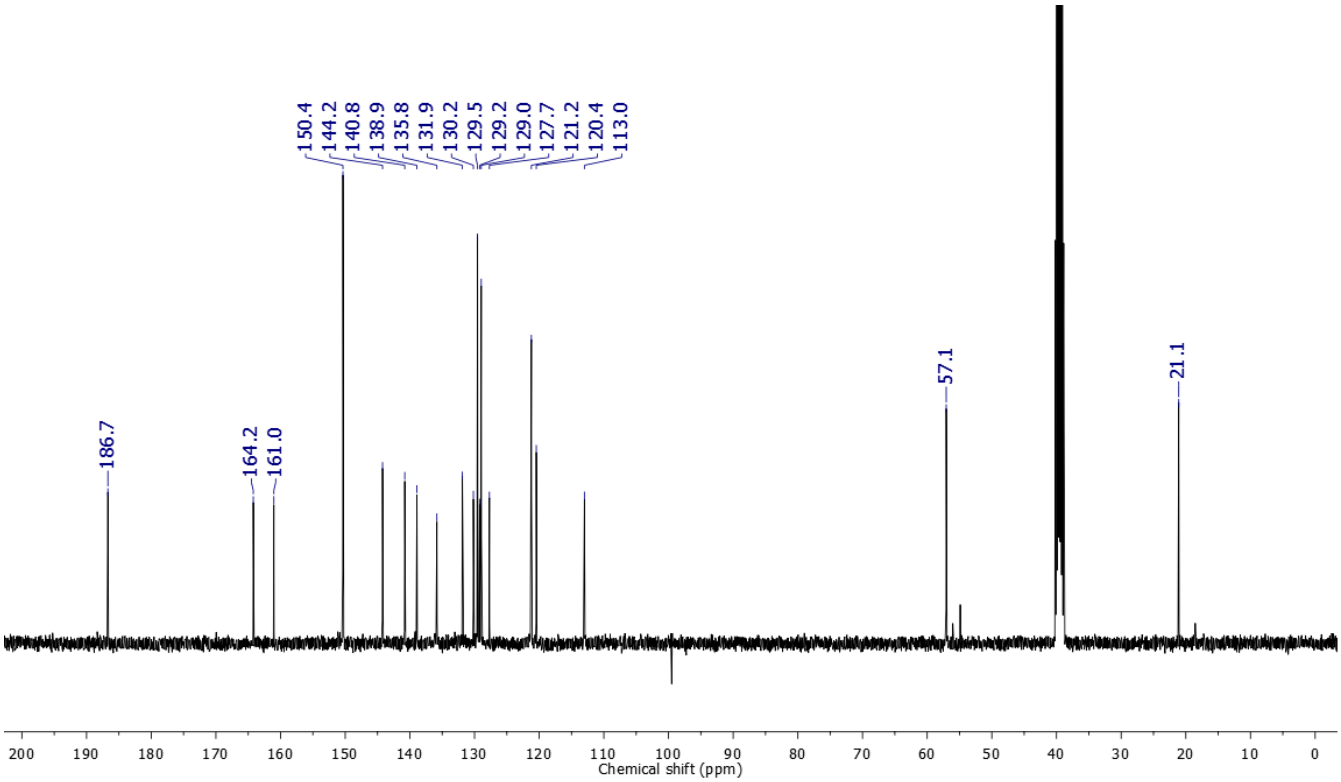
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **19b**.



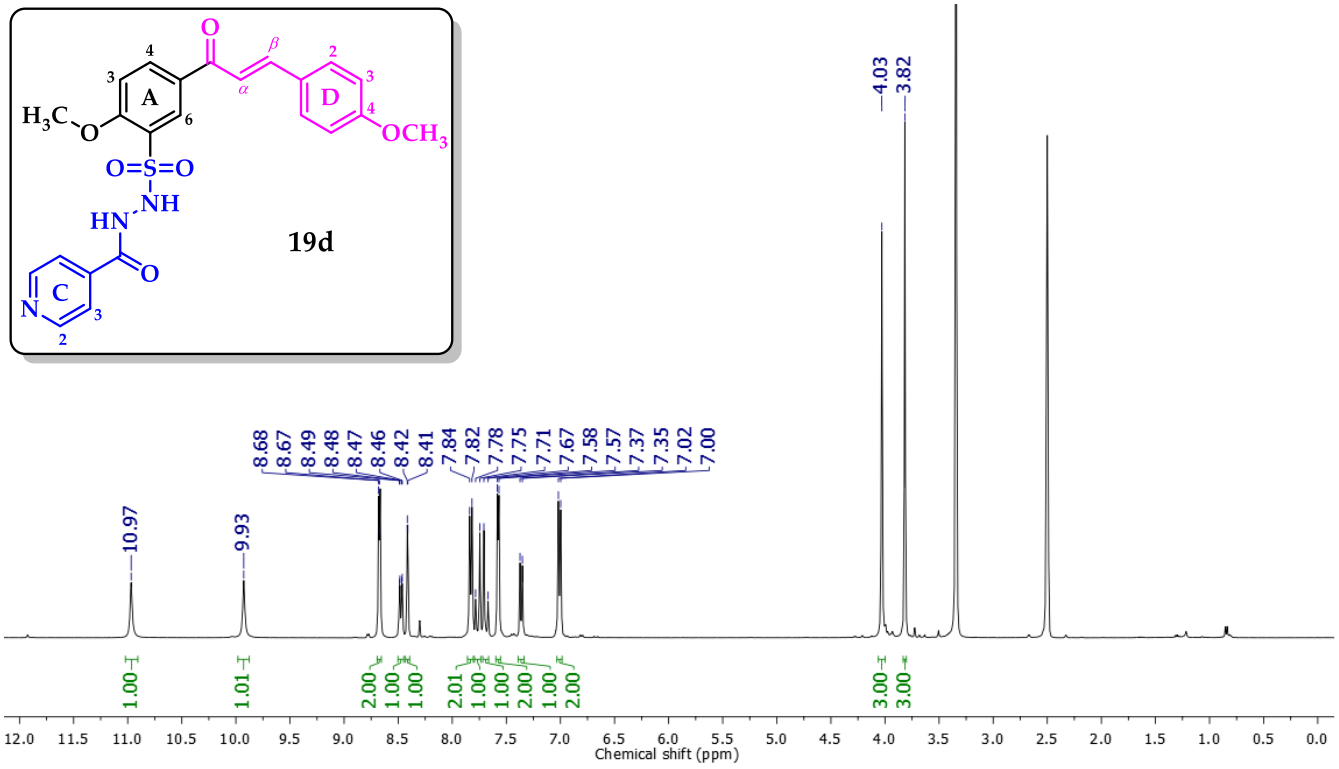
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **19b**.



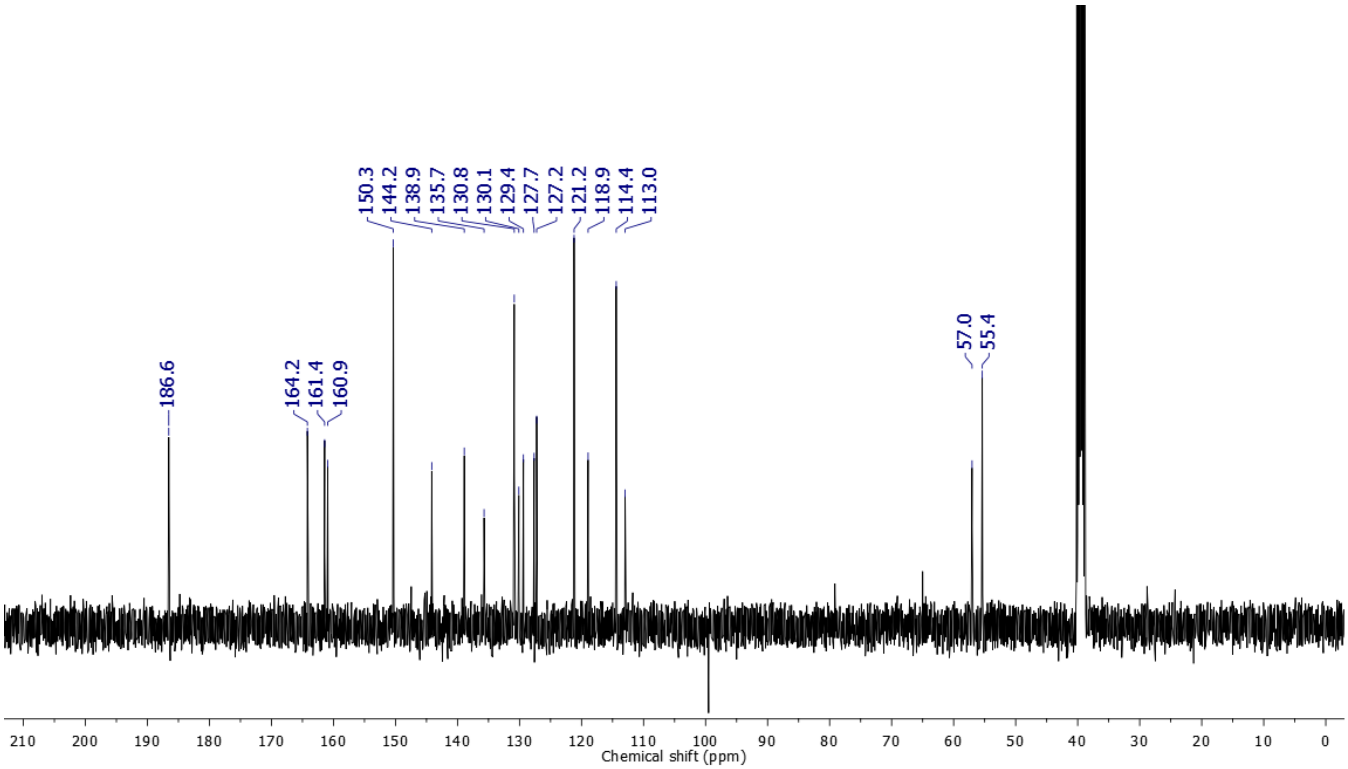
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **19c**.



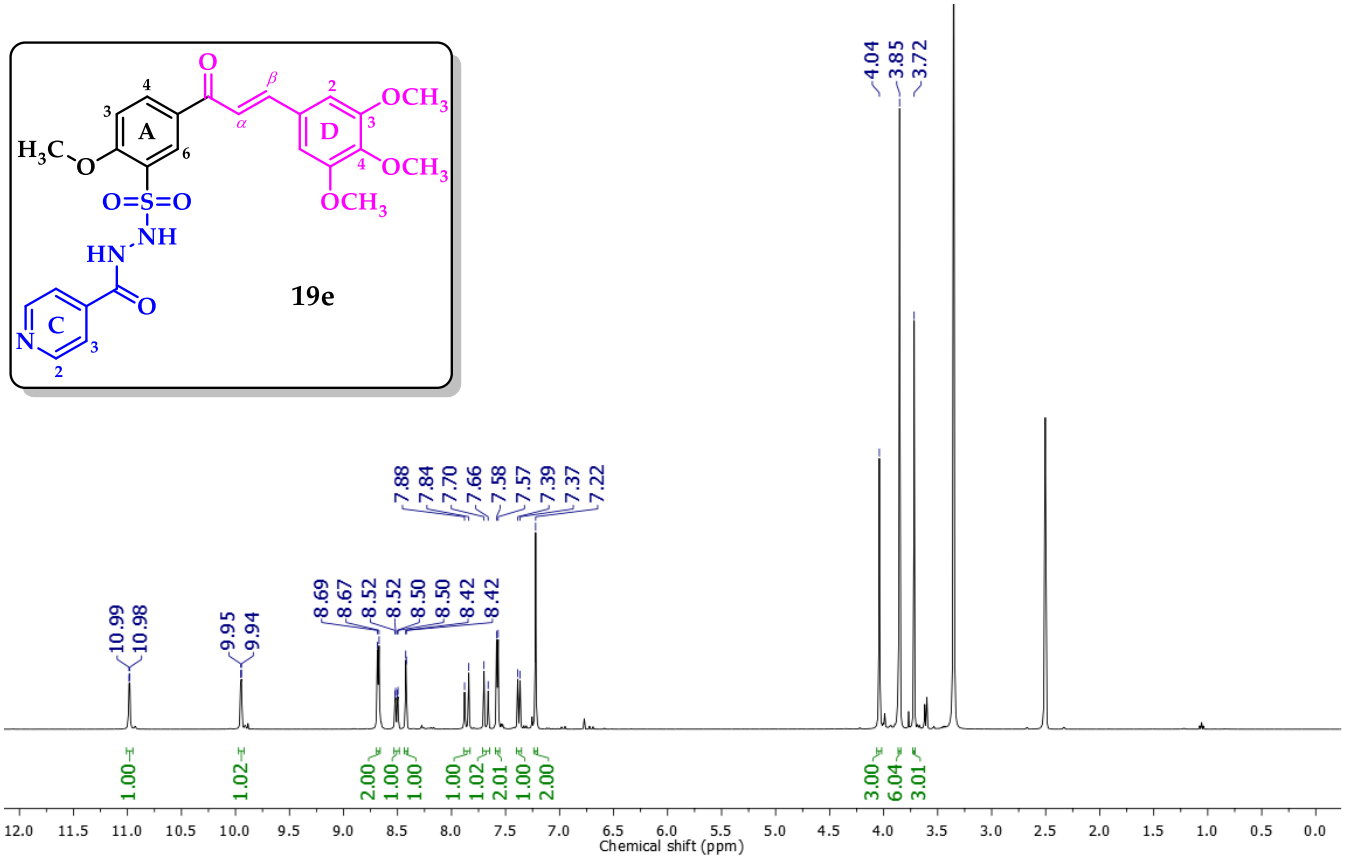
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **19c**.



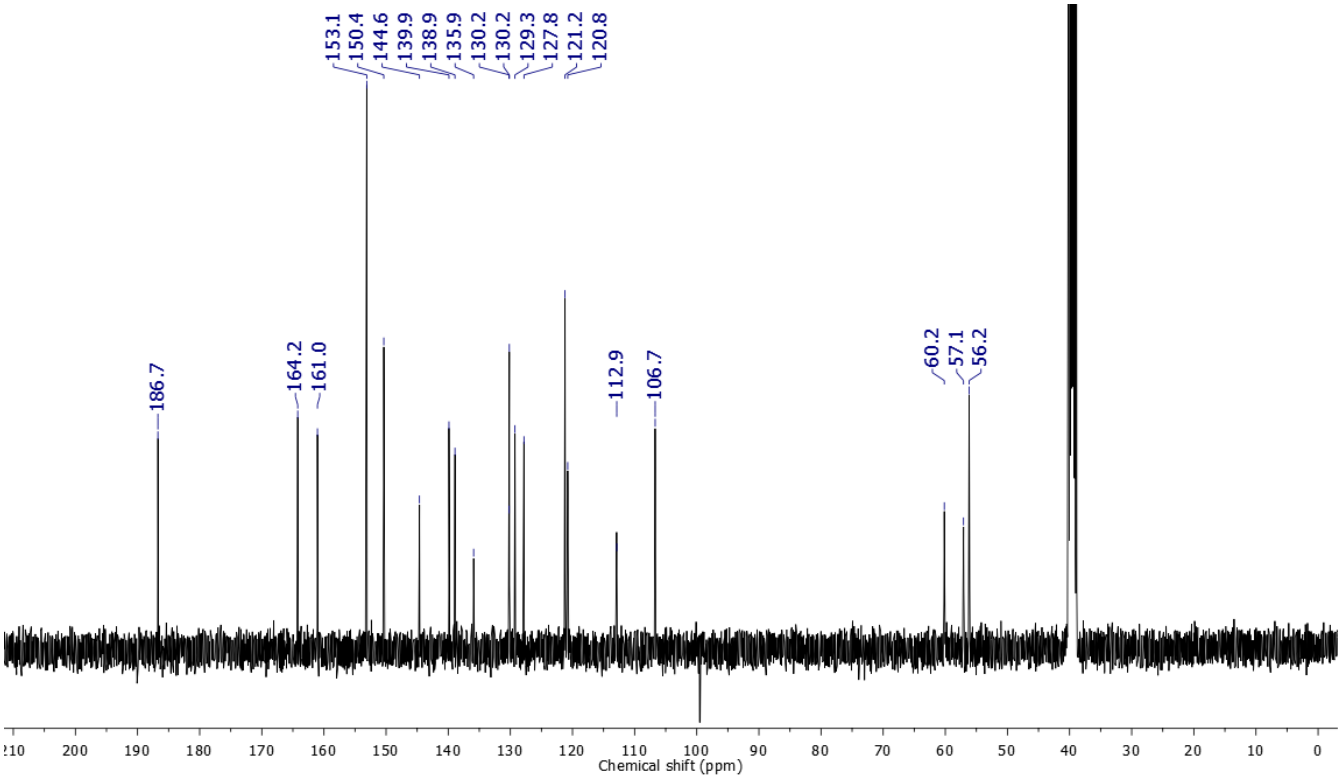
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **19d**.



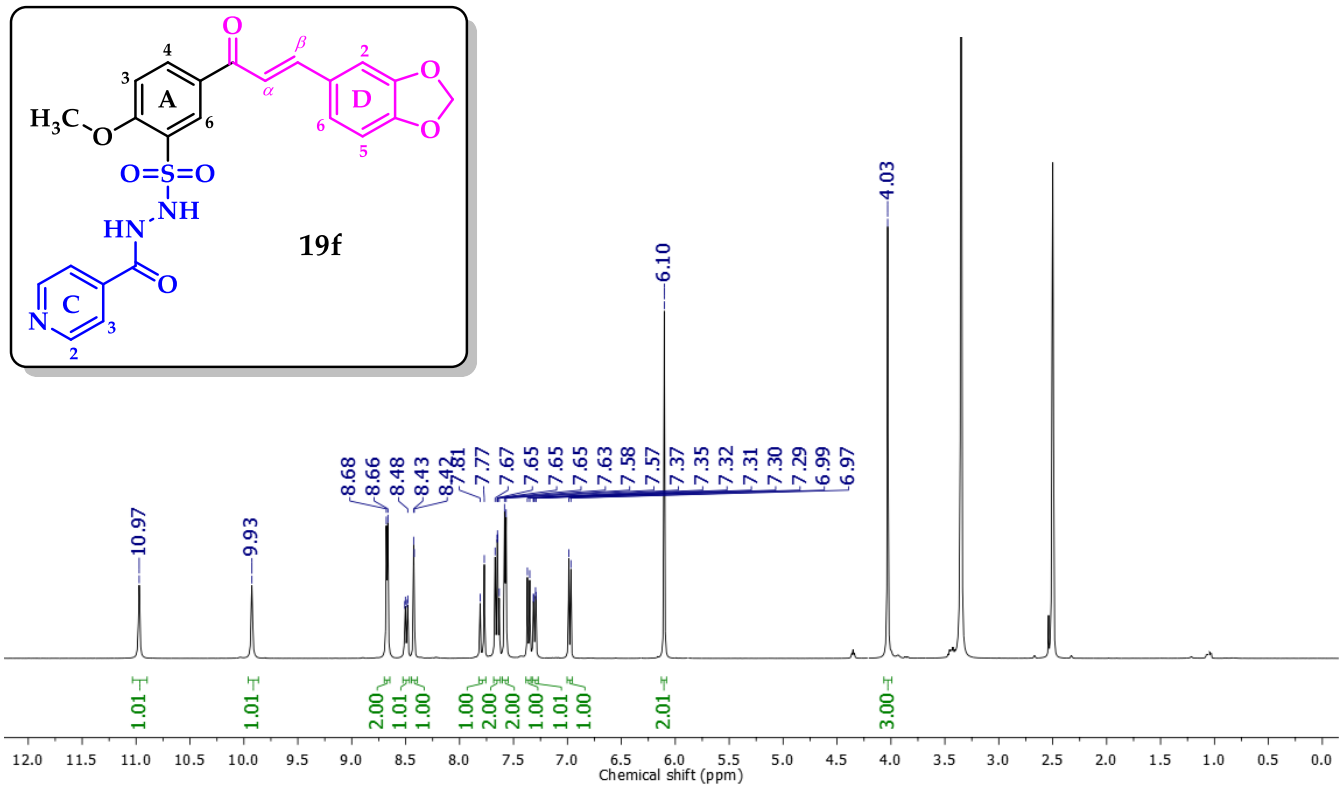
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **19d**.



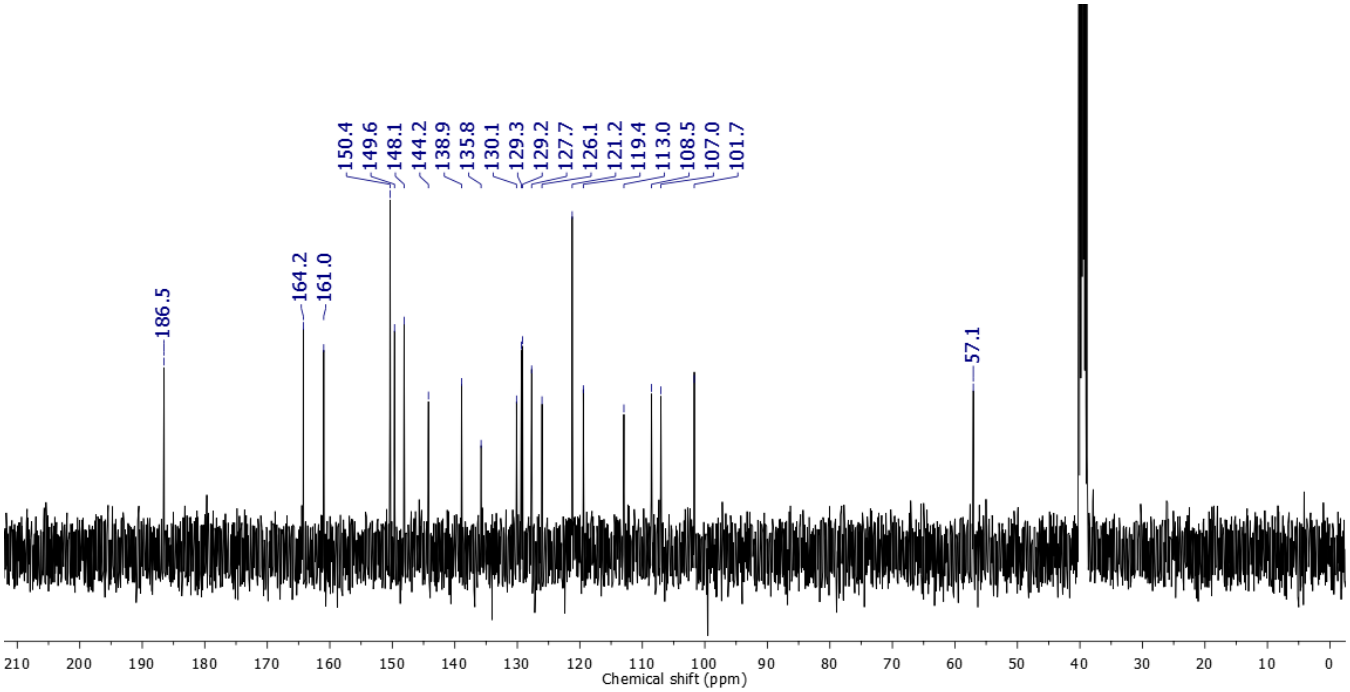
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **19e**.



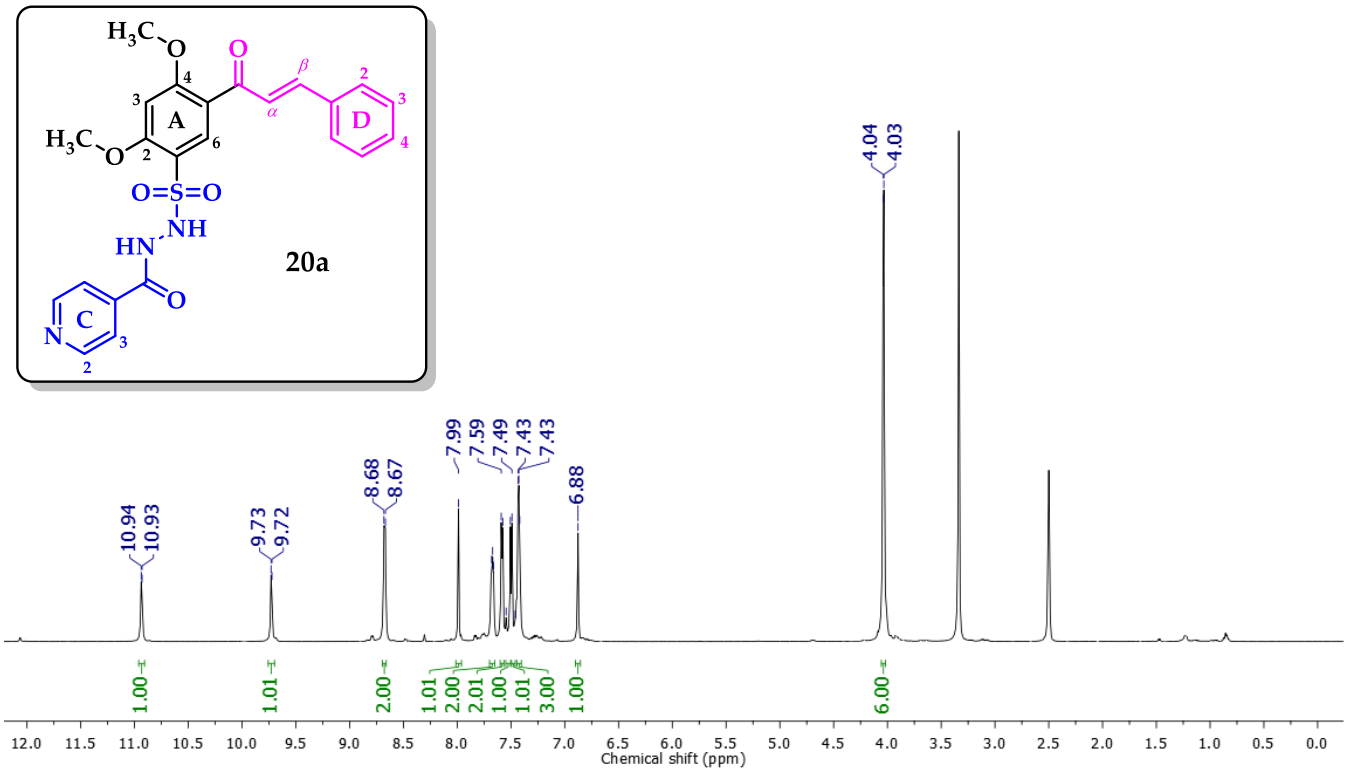
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **19e**.



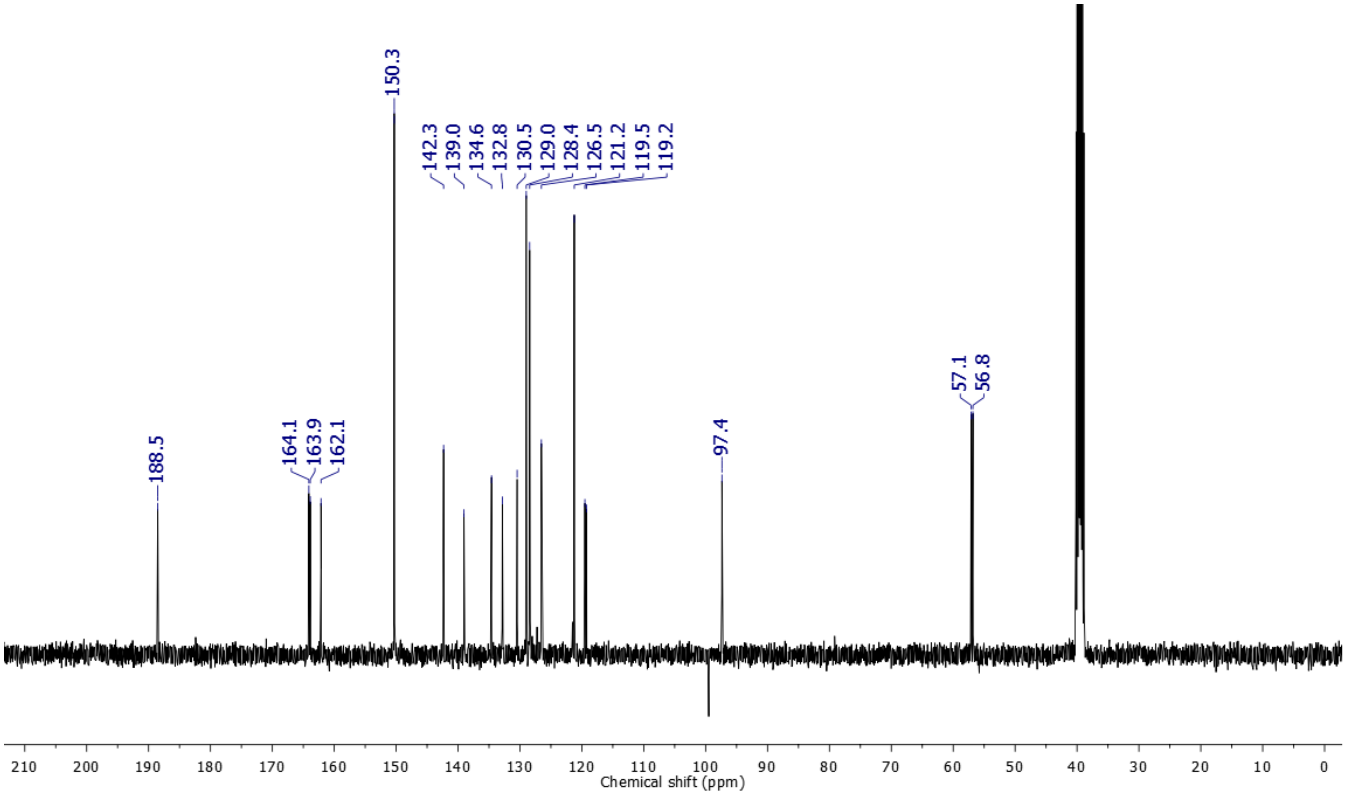
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **19f**.



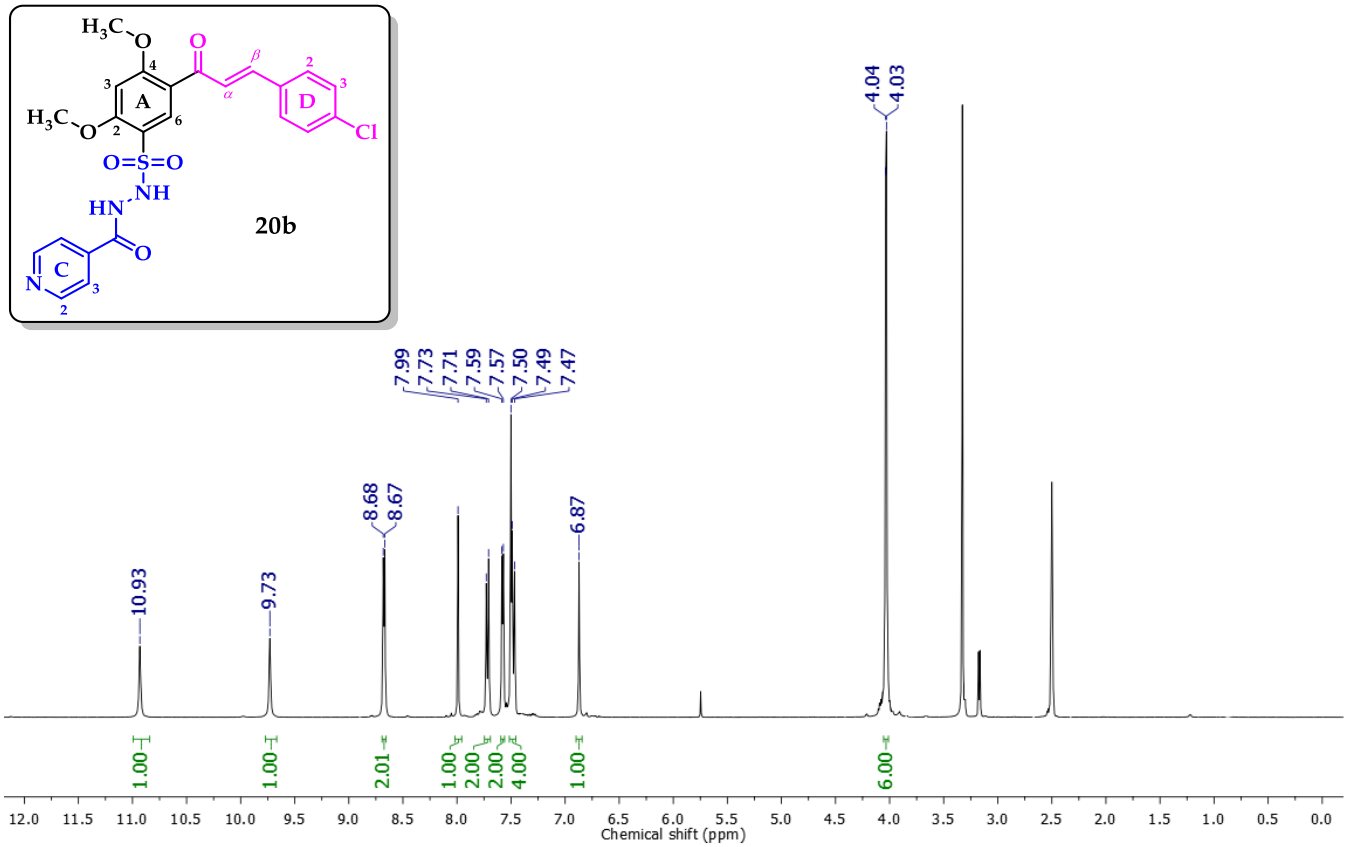
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **19f**.



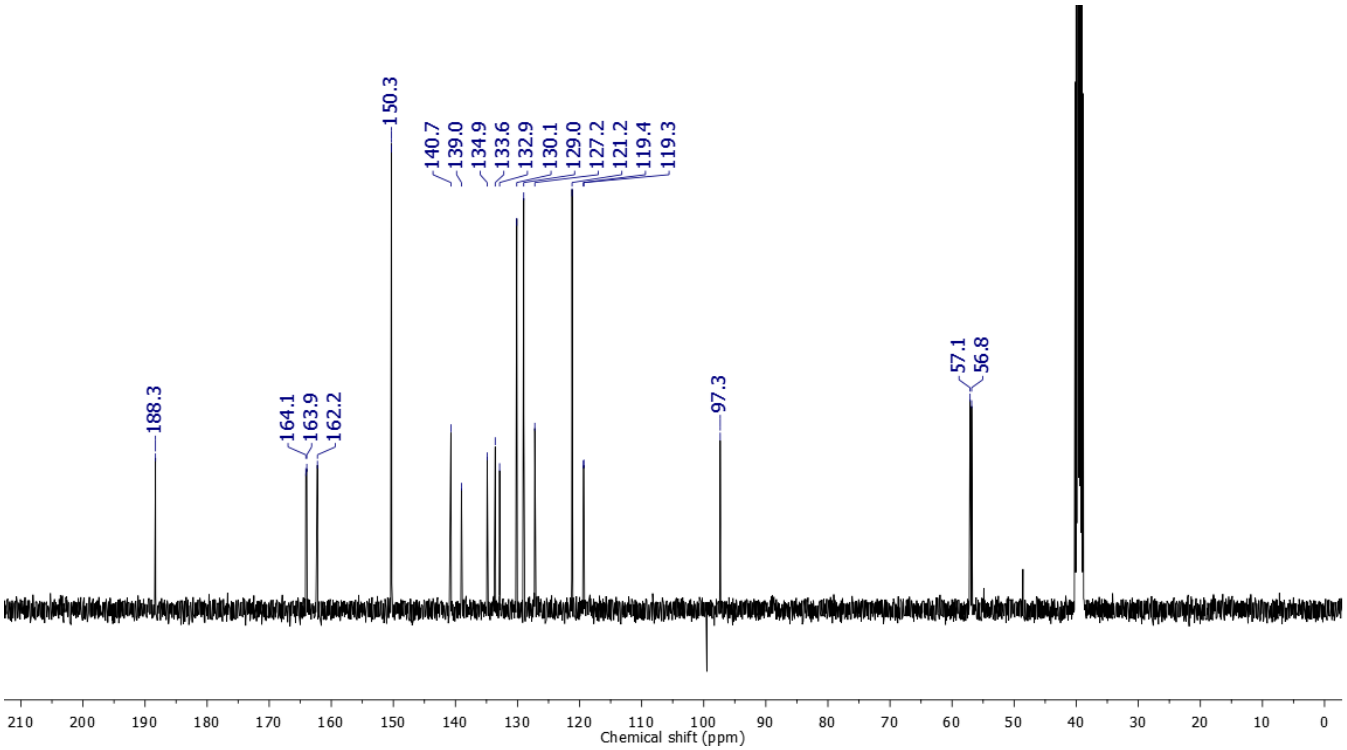
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **20a**.



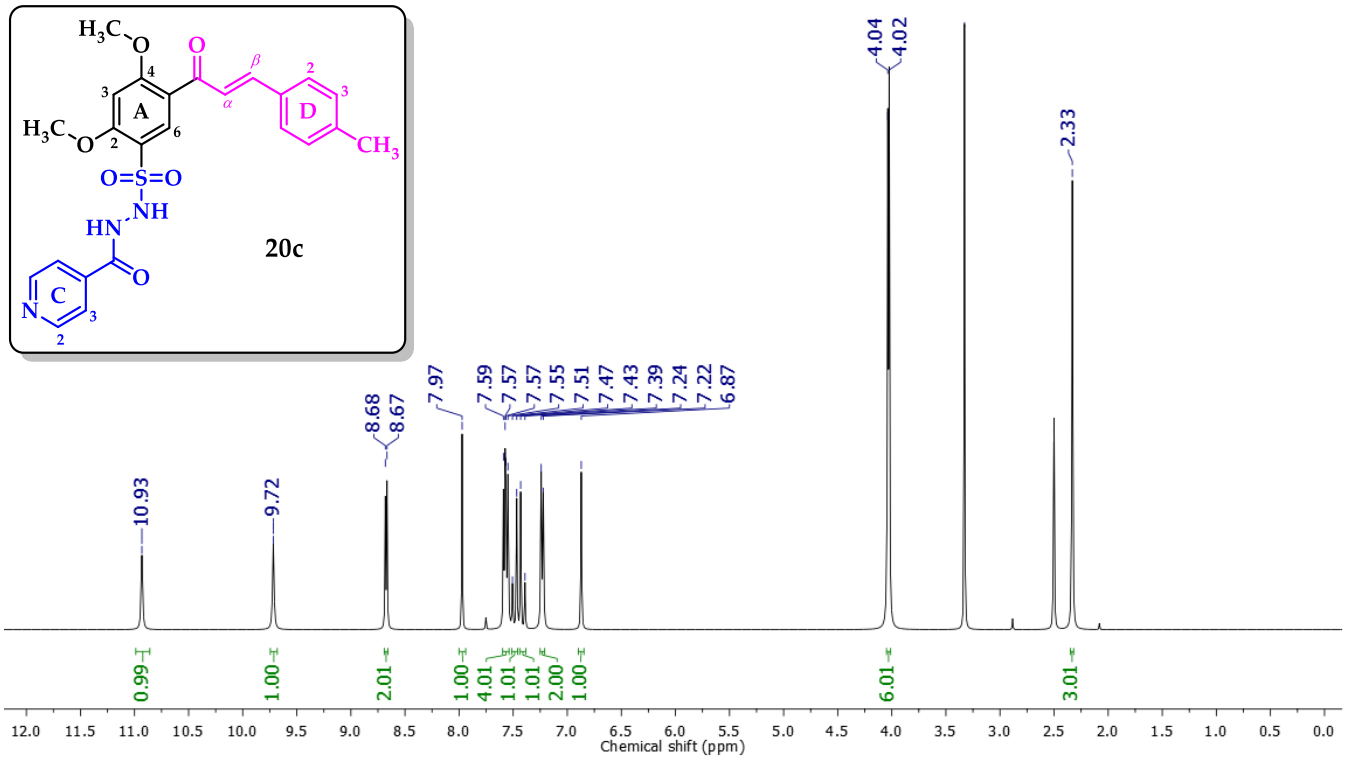
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **20a**.



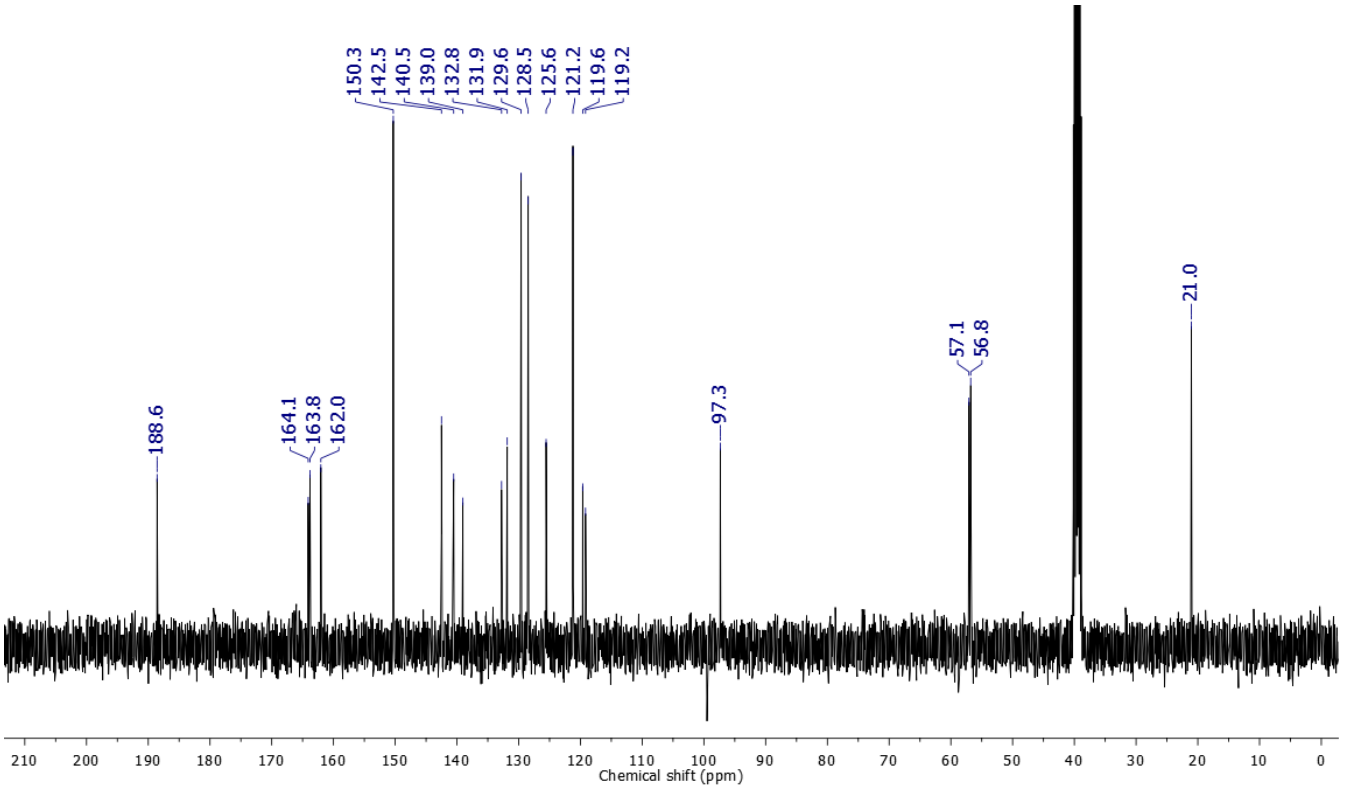
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **20b**.



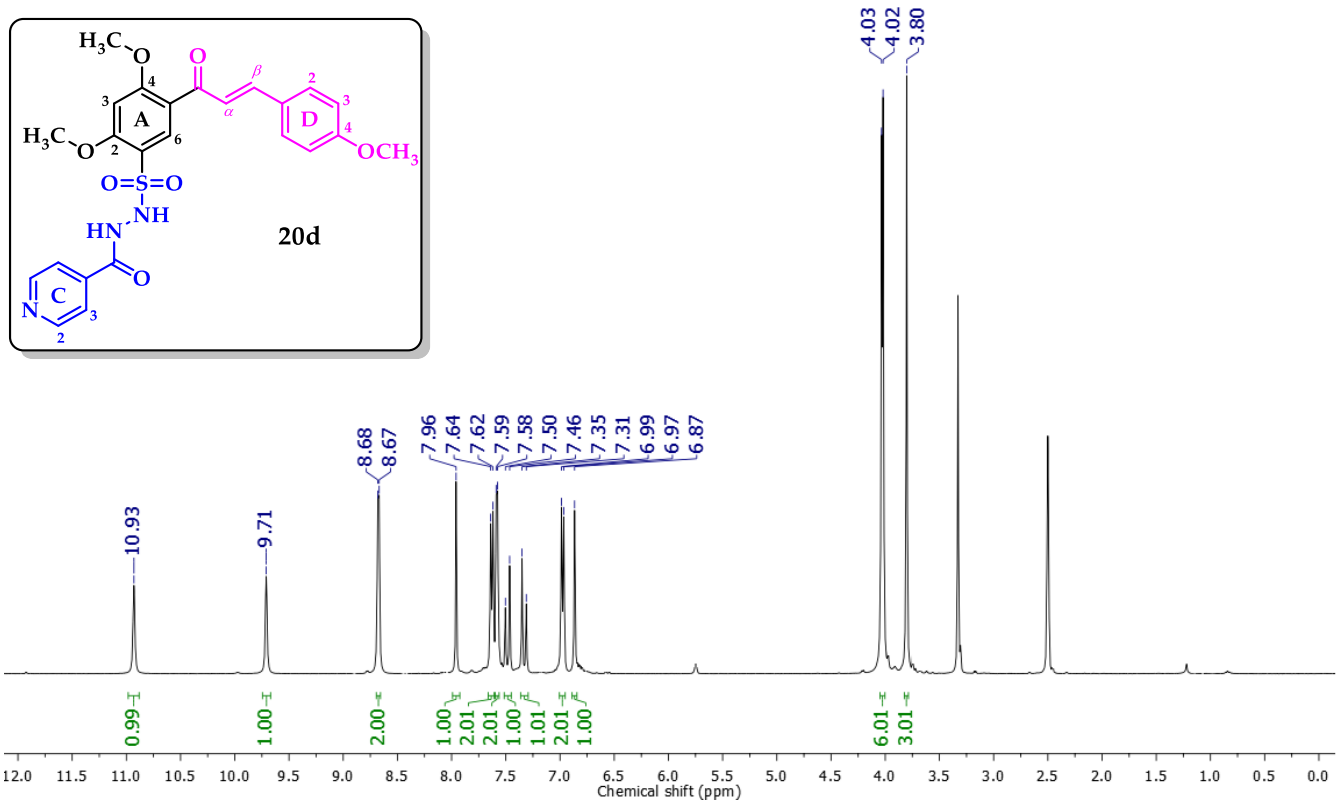
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **20b**.



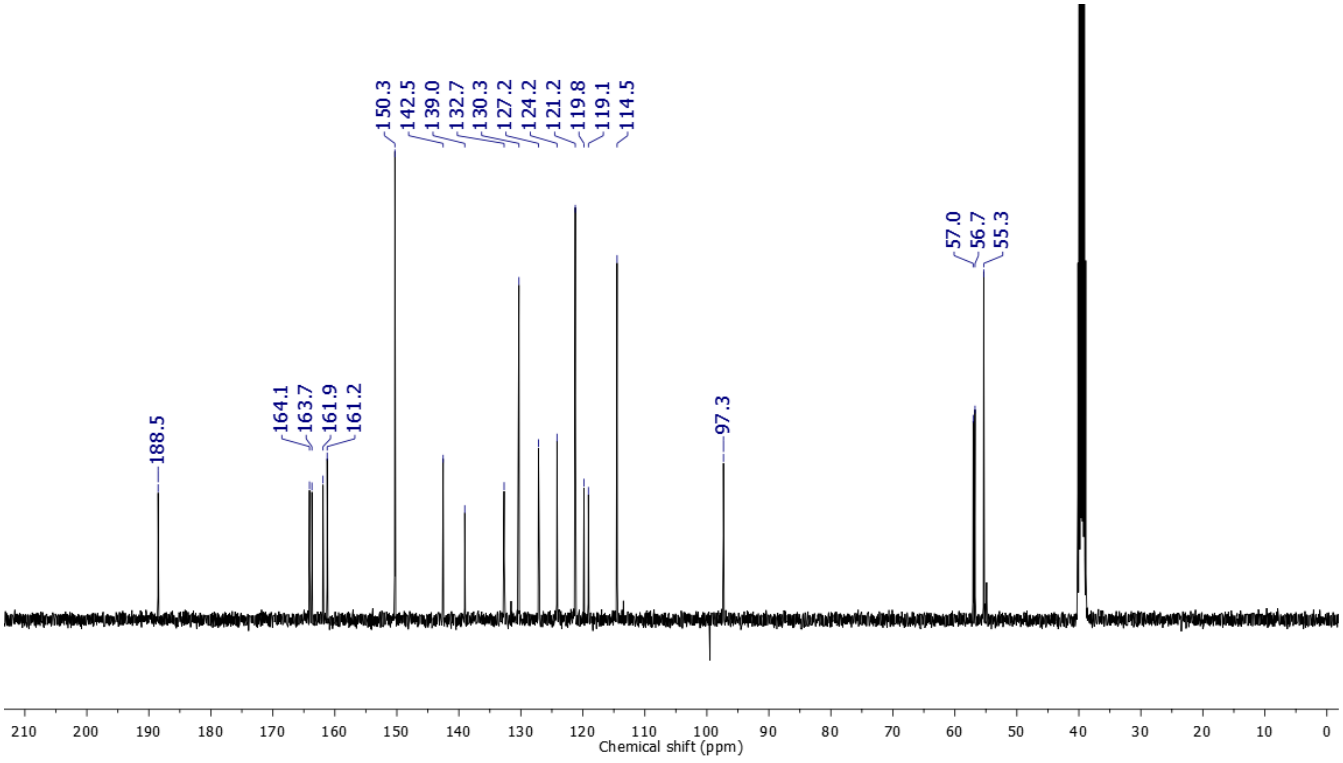
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **20c**.



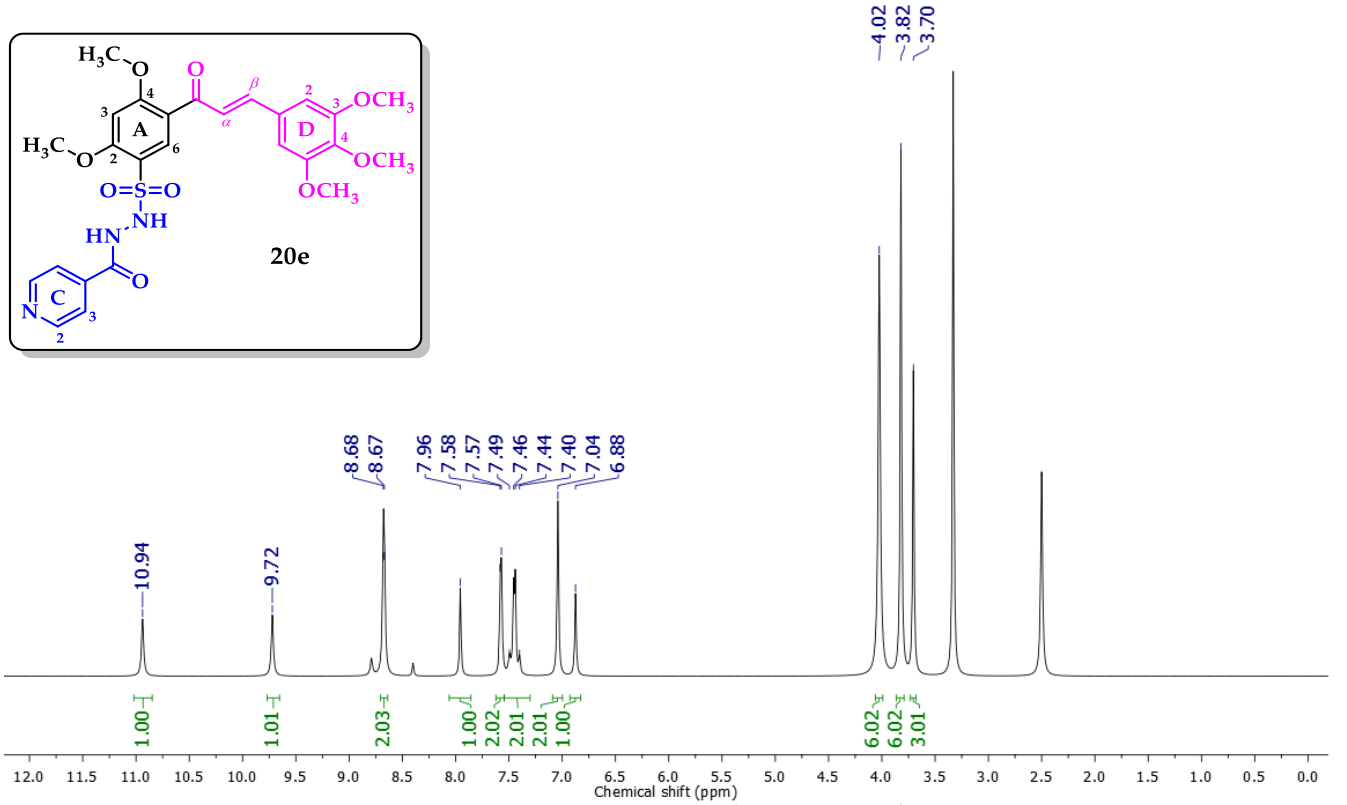
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **20c**.



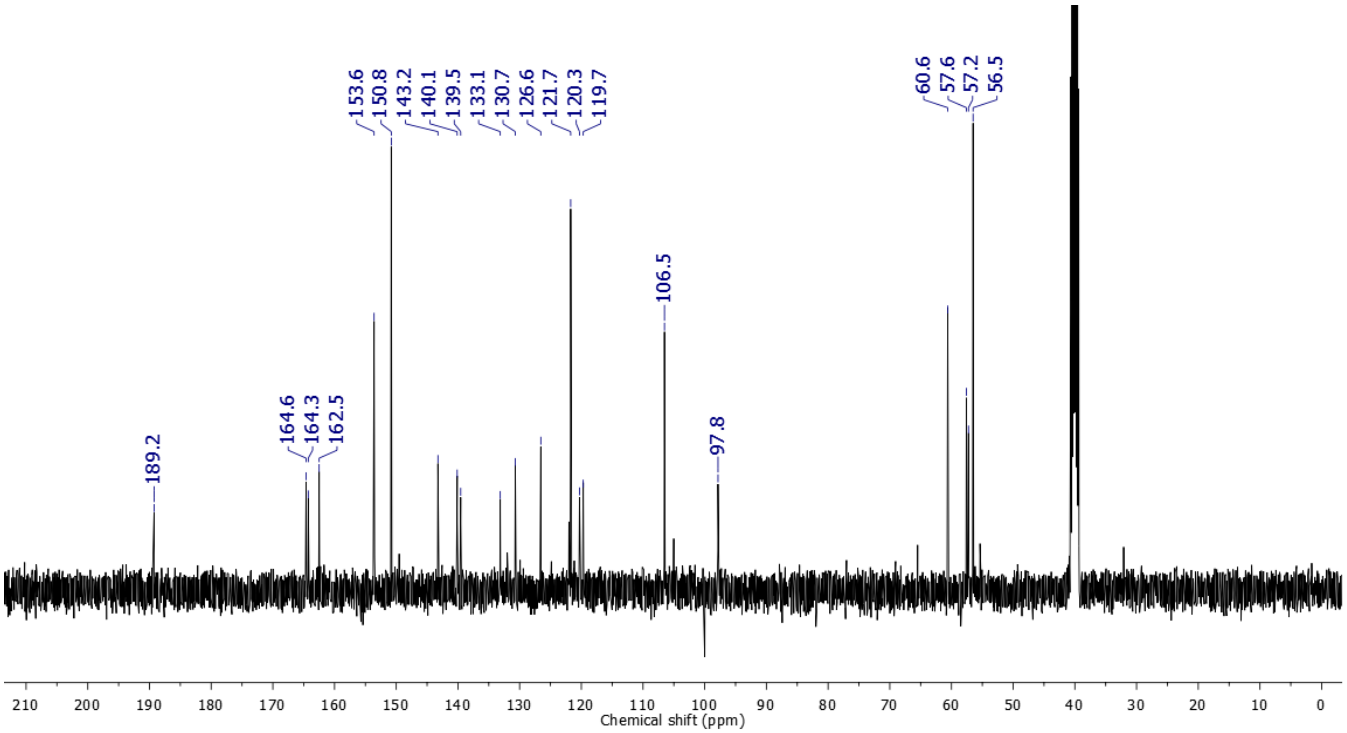
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **20d**.



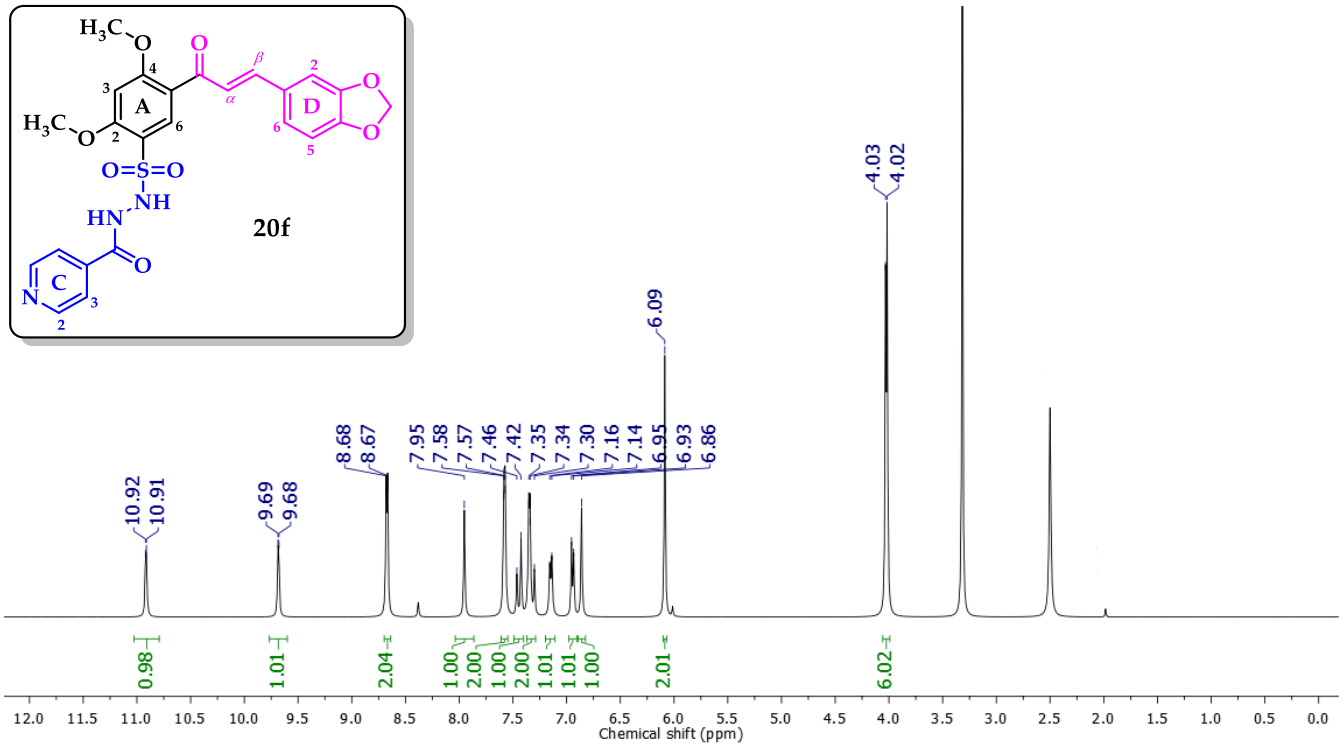
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **20d**.



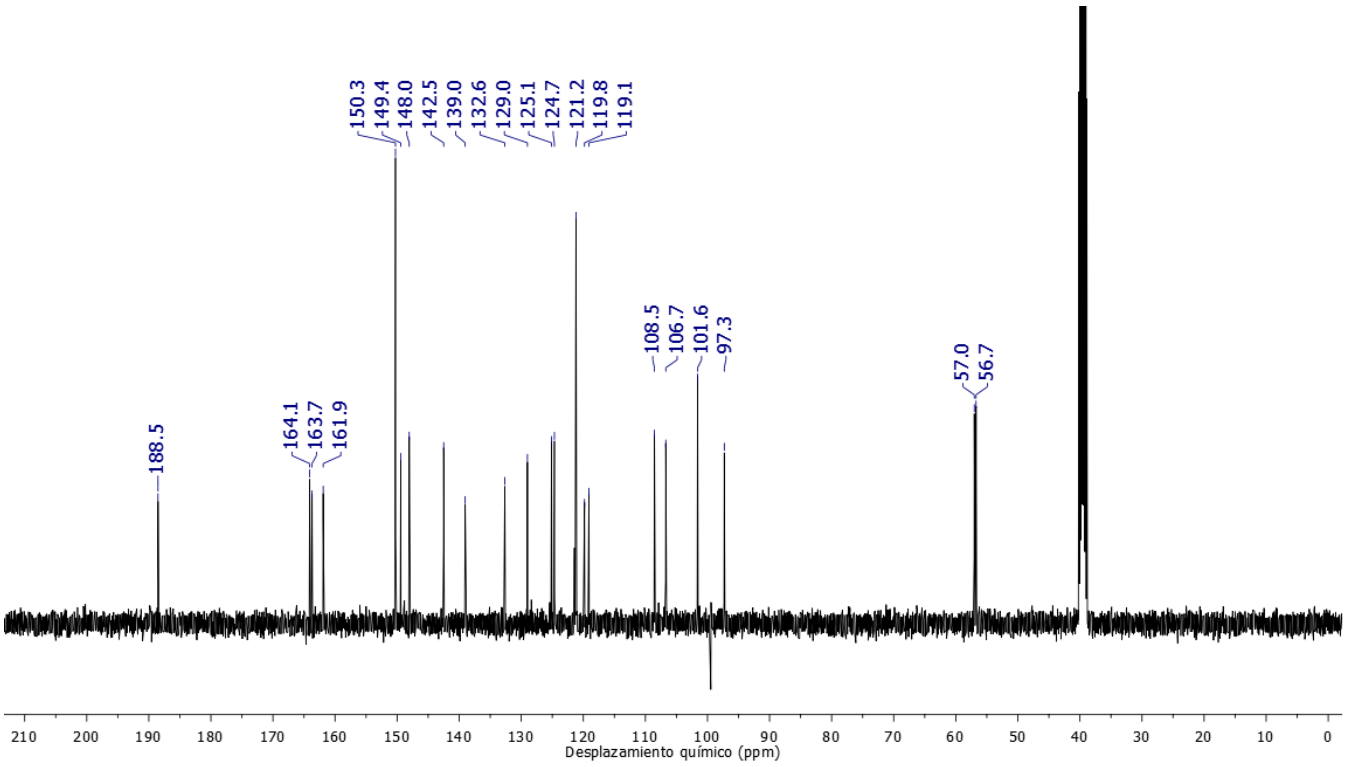
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **20e**.



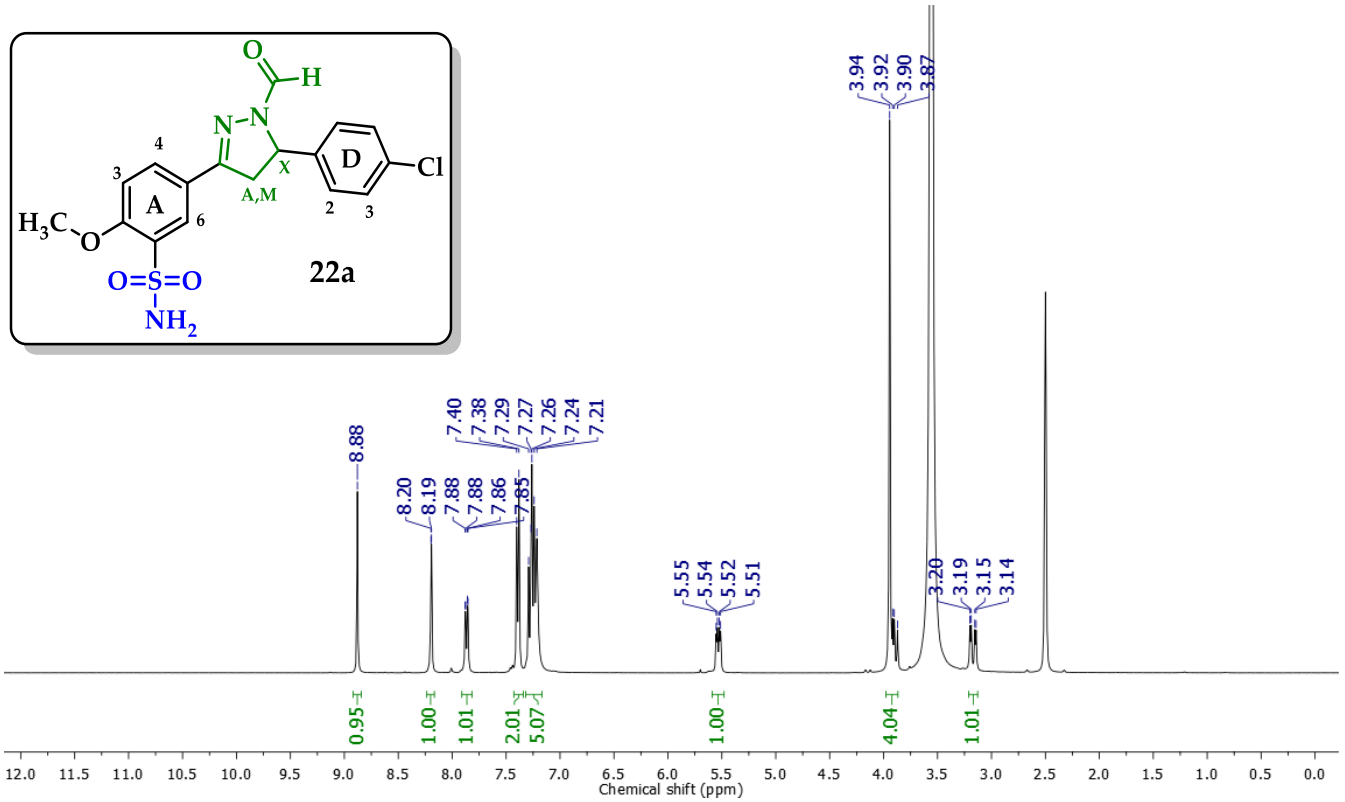
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **20e**.



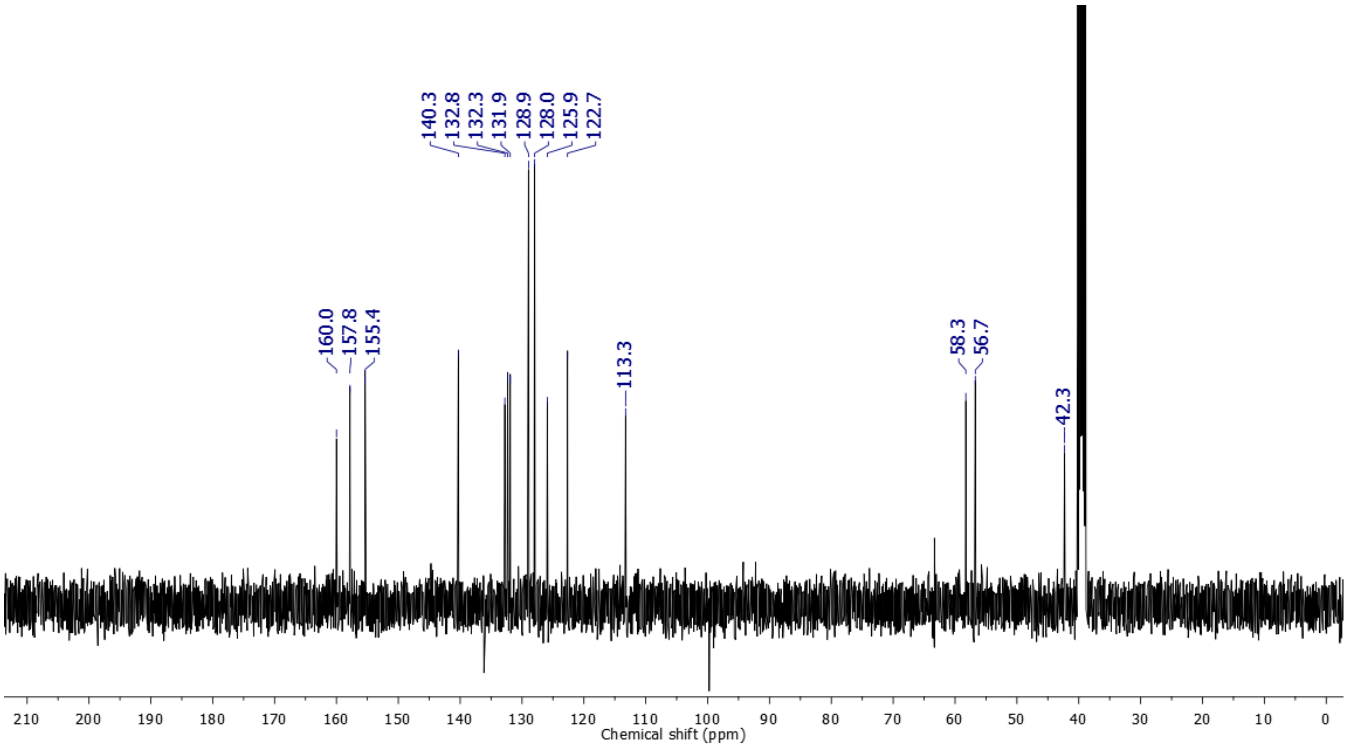
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **20f**.



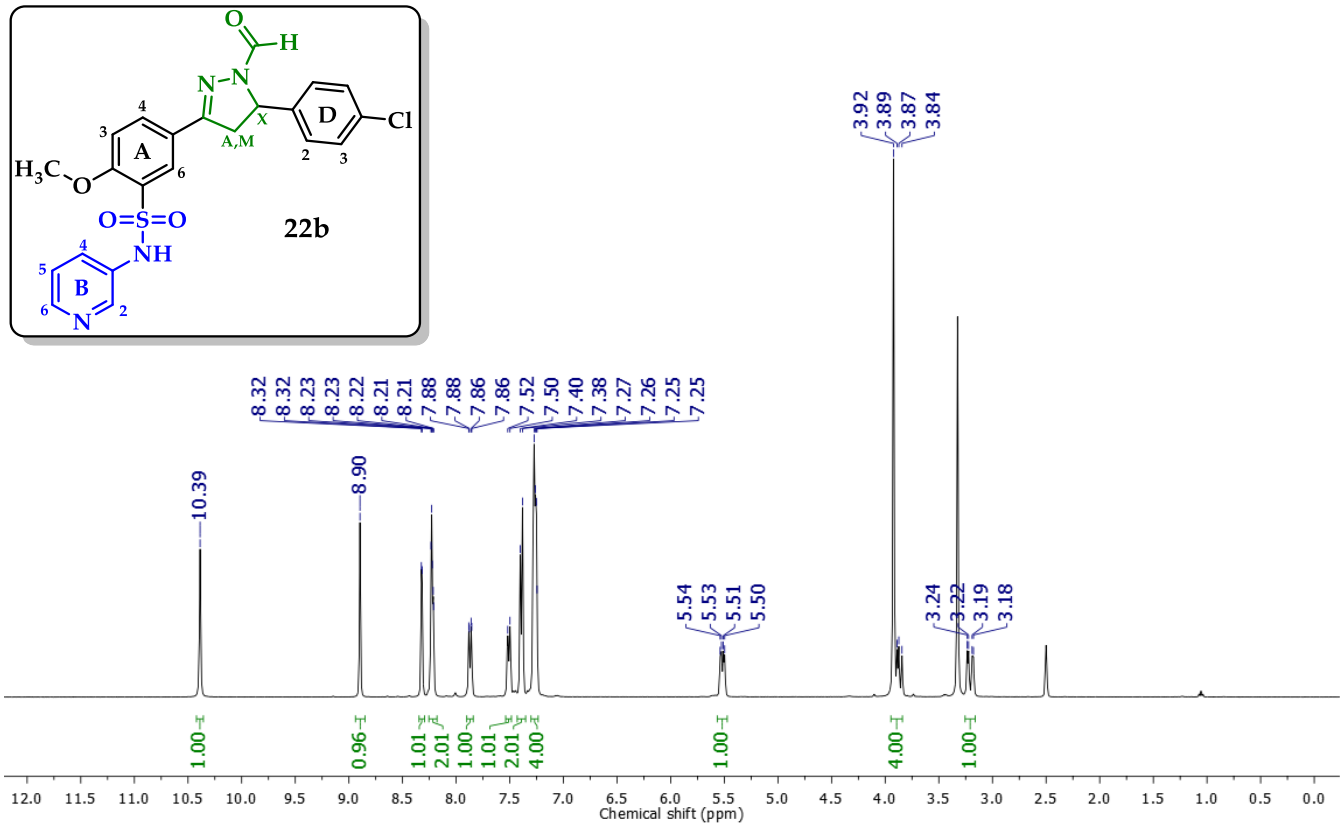
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **20f**.



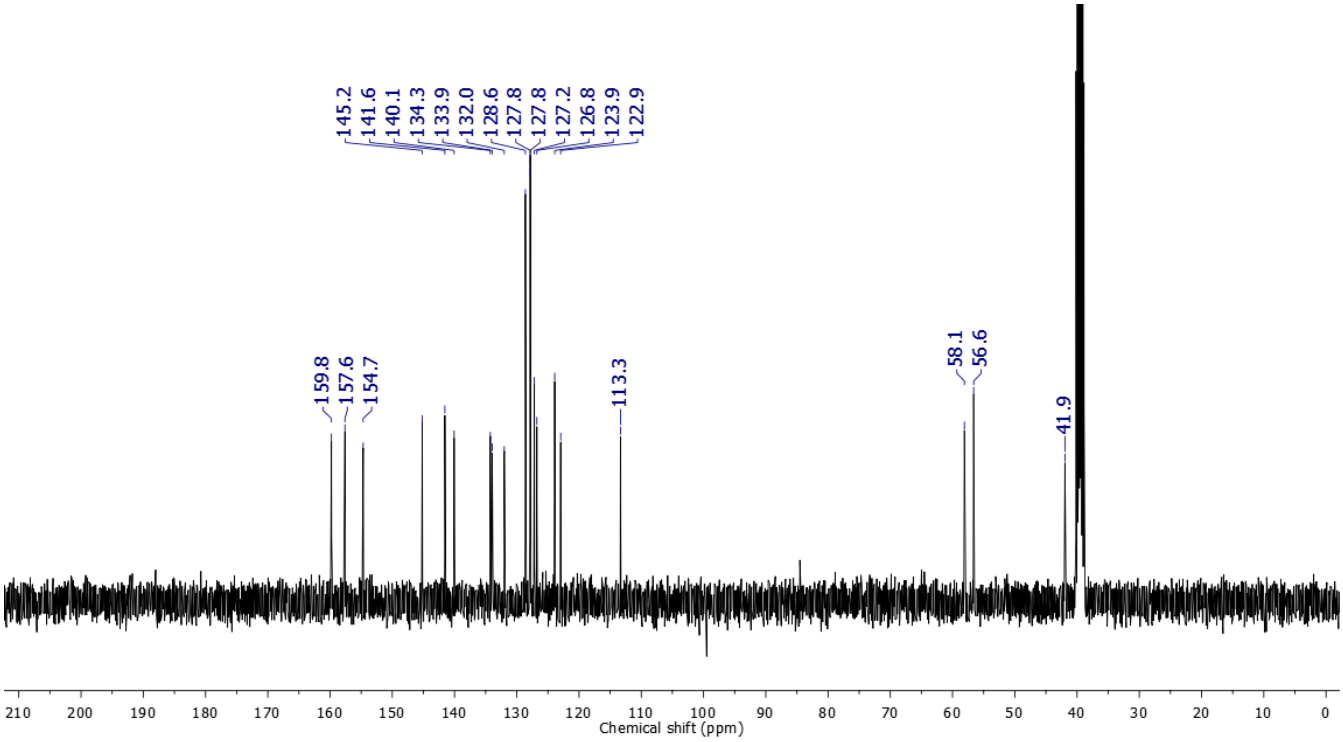
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **22a**.



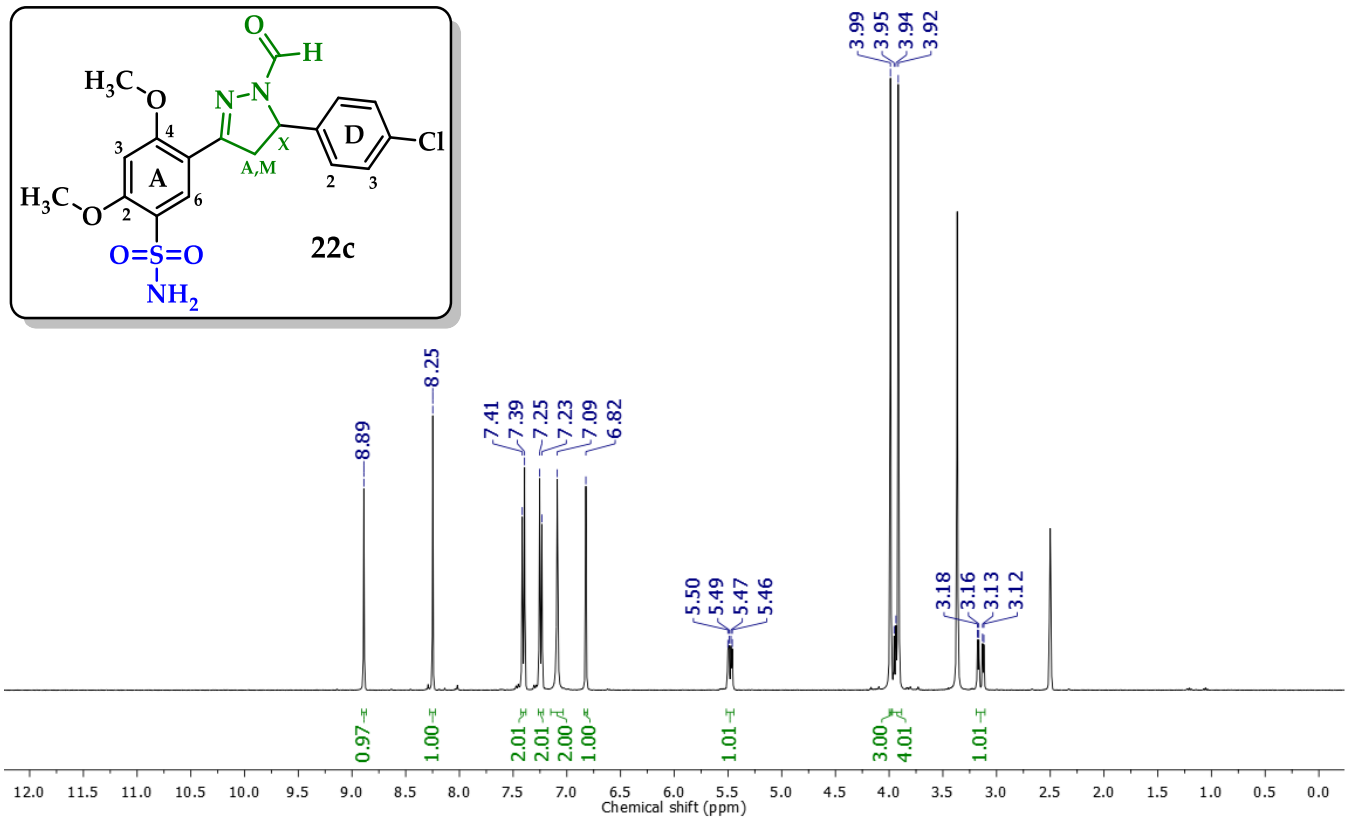
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **22a**.



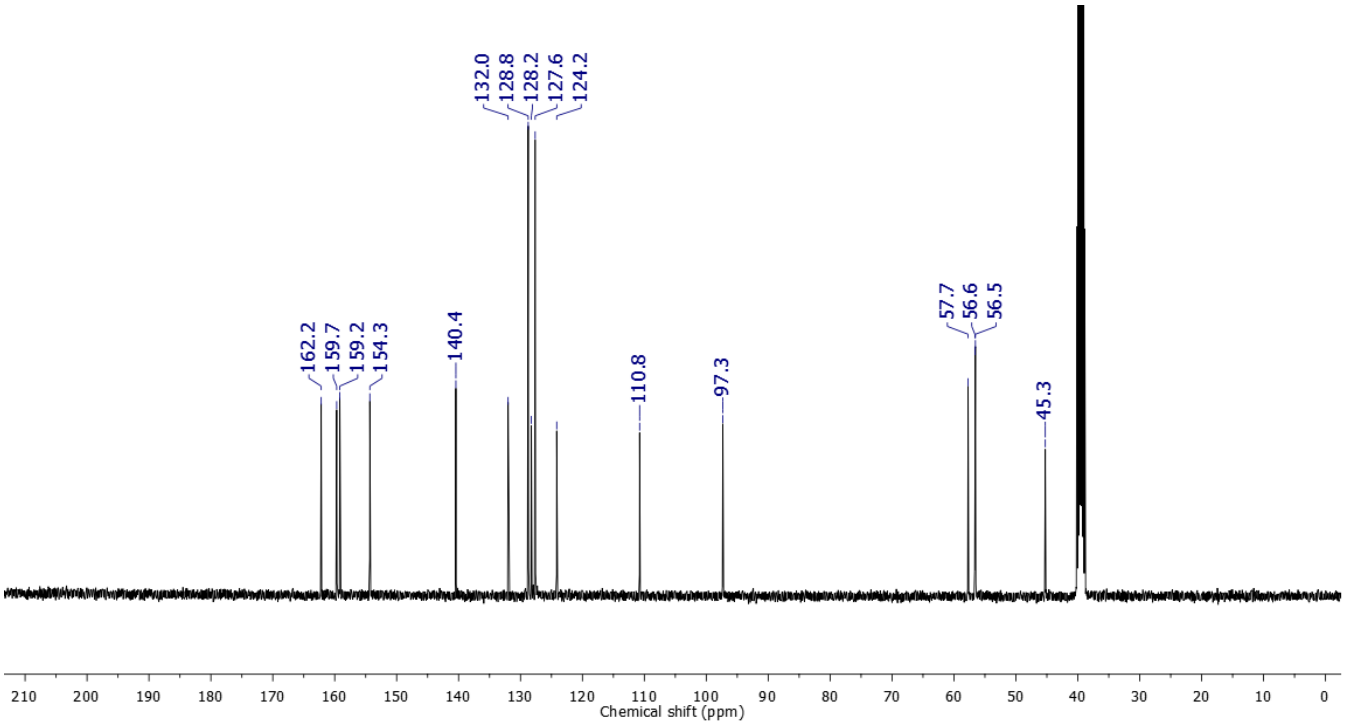
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **22b**.



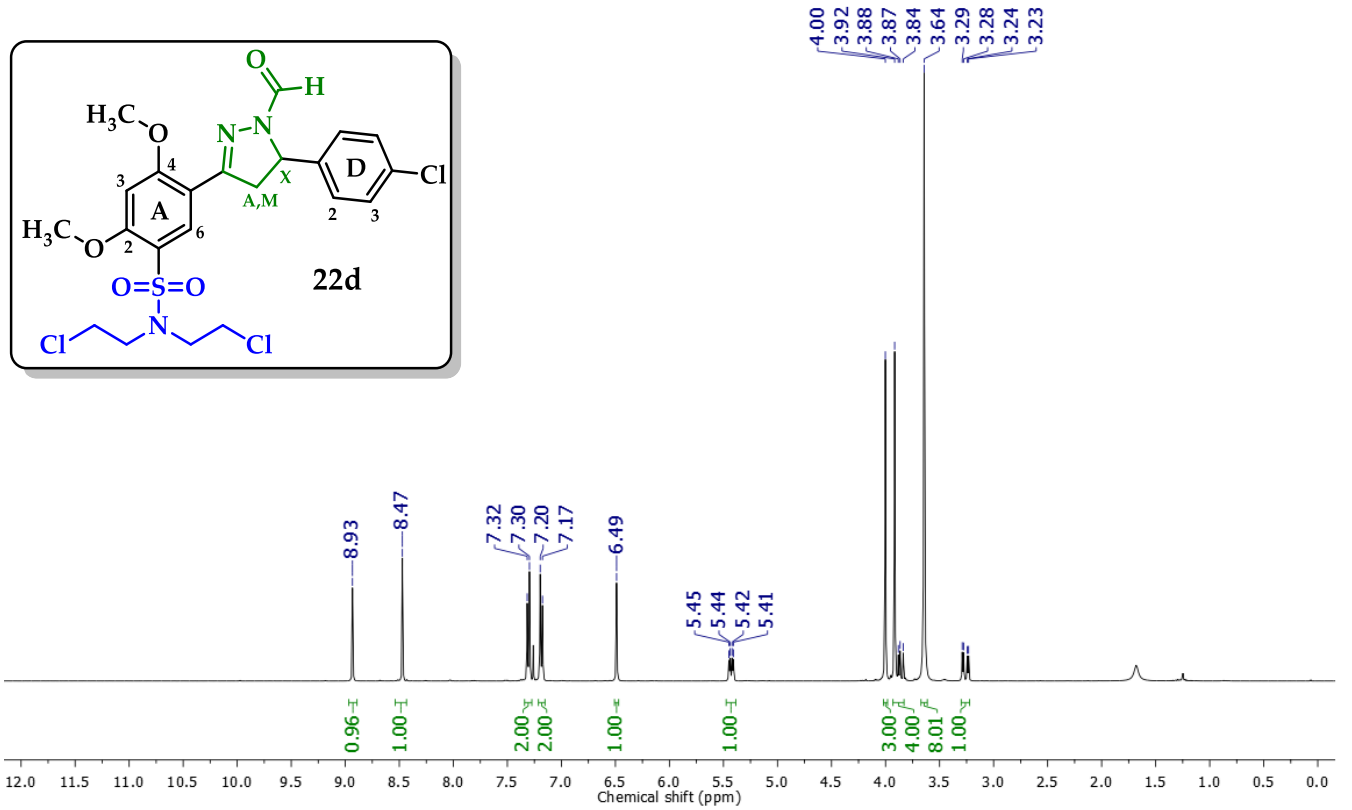
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **22b**.



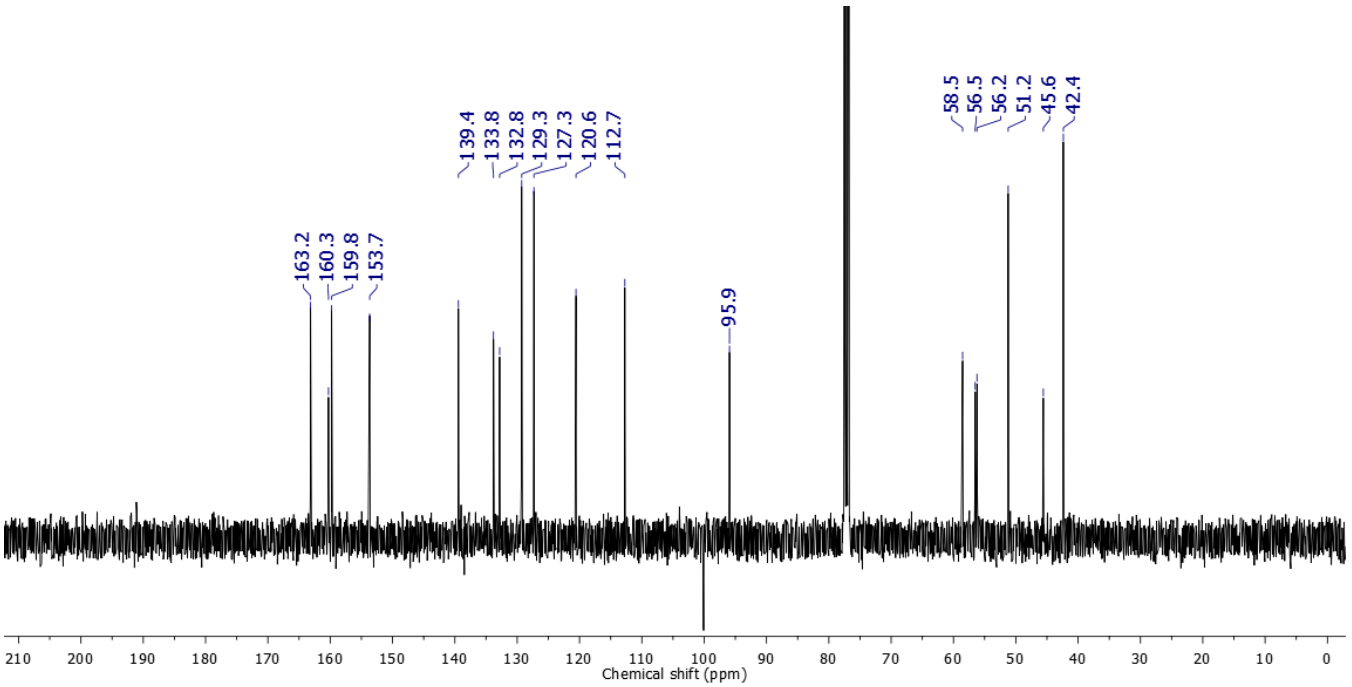
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **22c**.



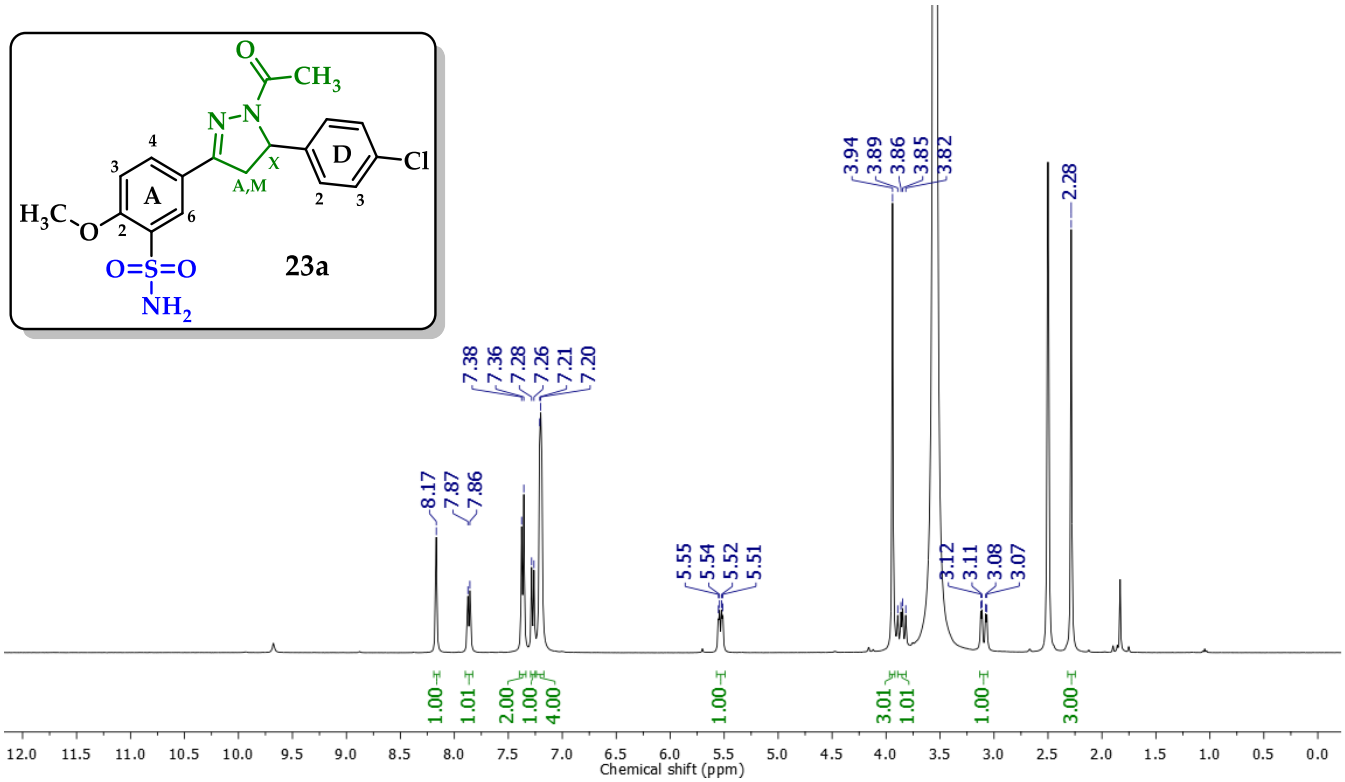
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **22c**.



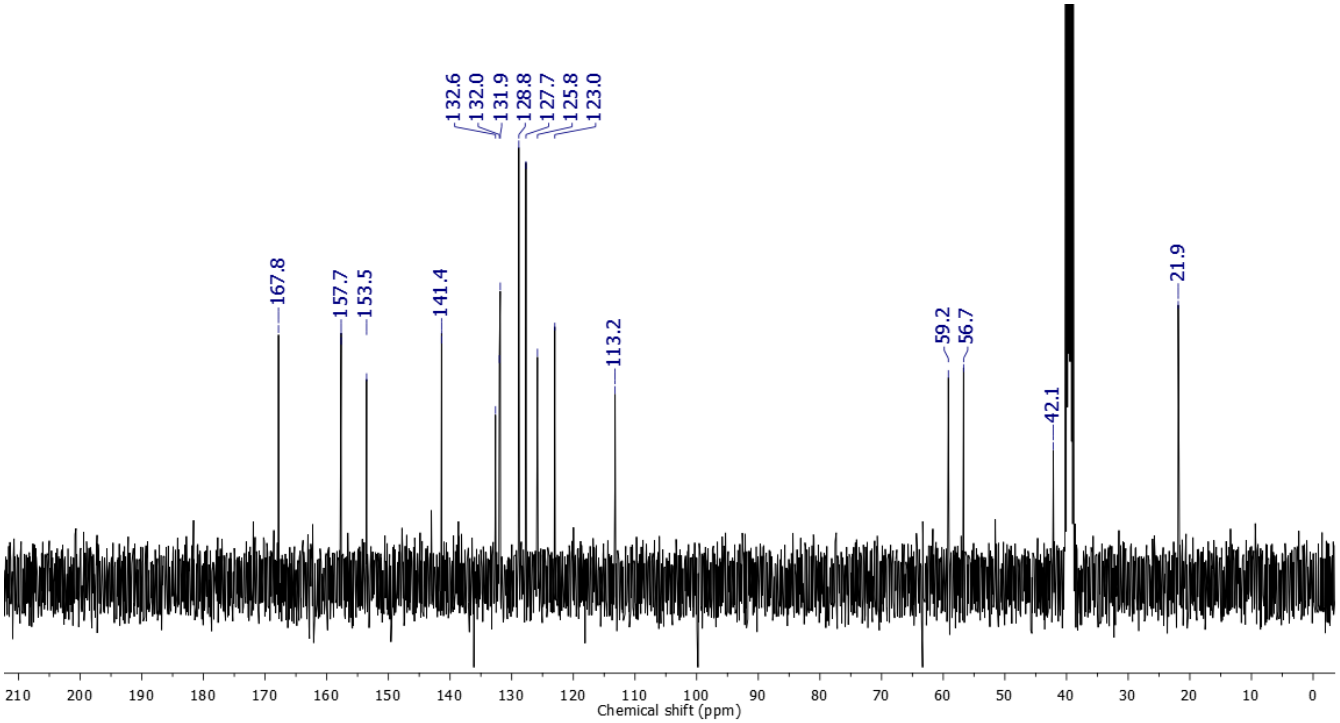
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **22d**.



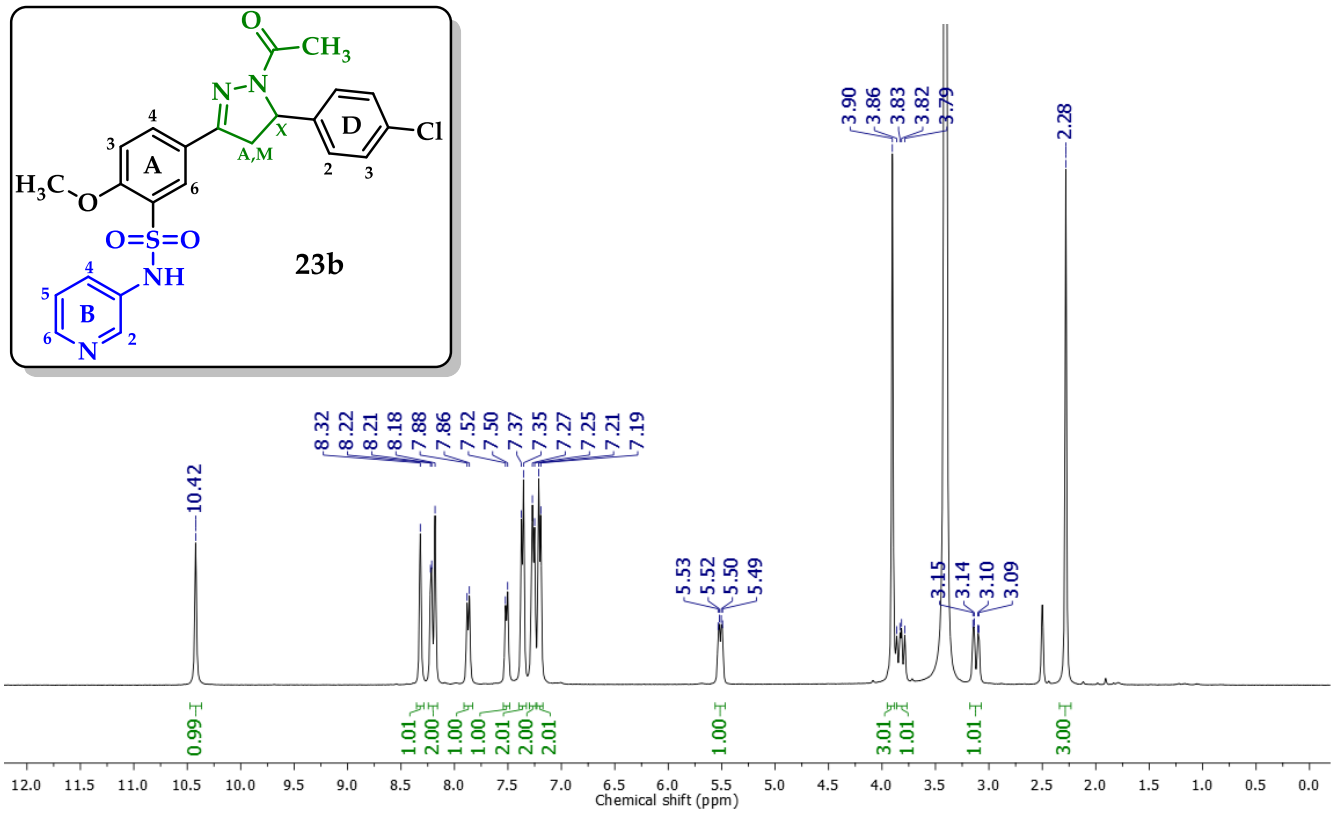
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **22d**.



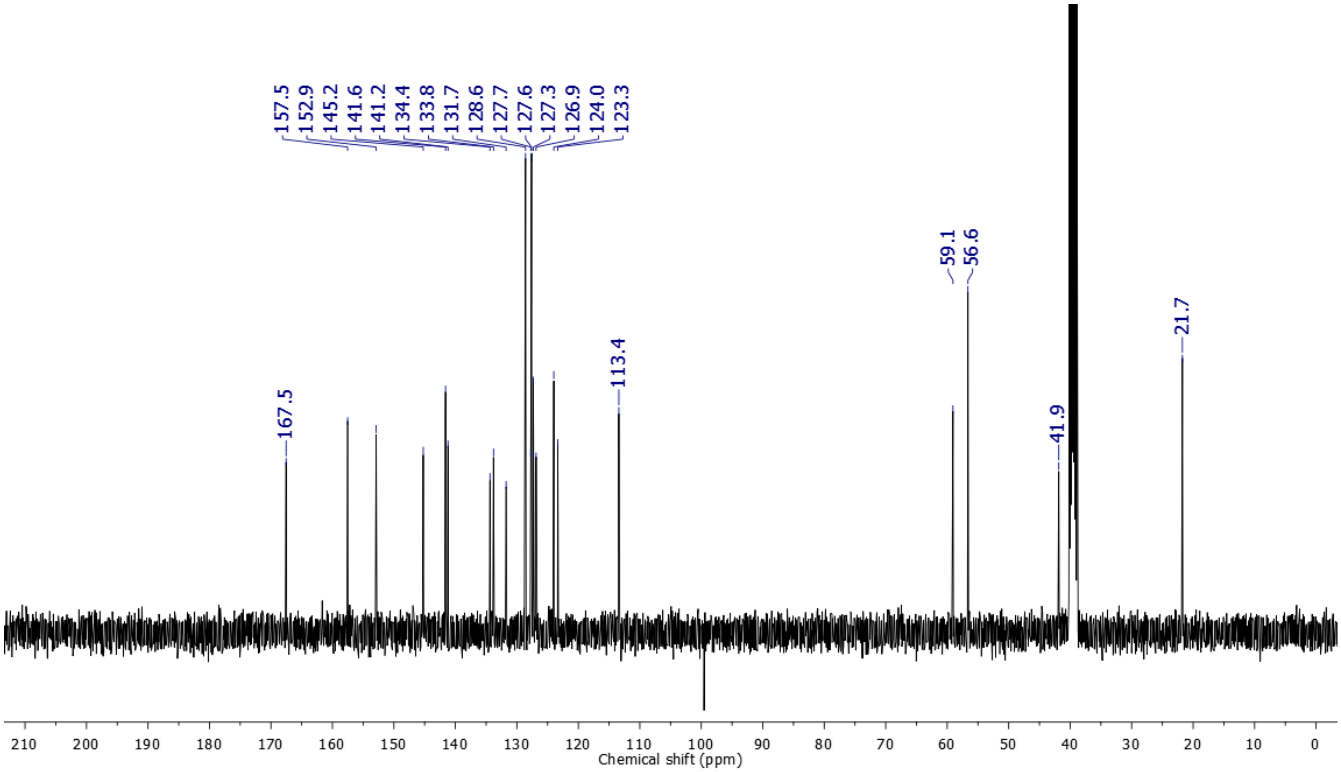
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **23a**.



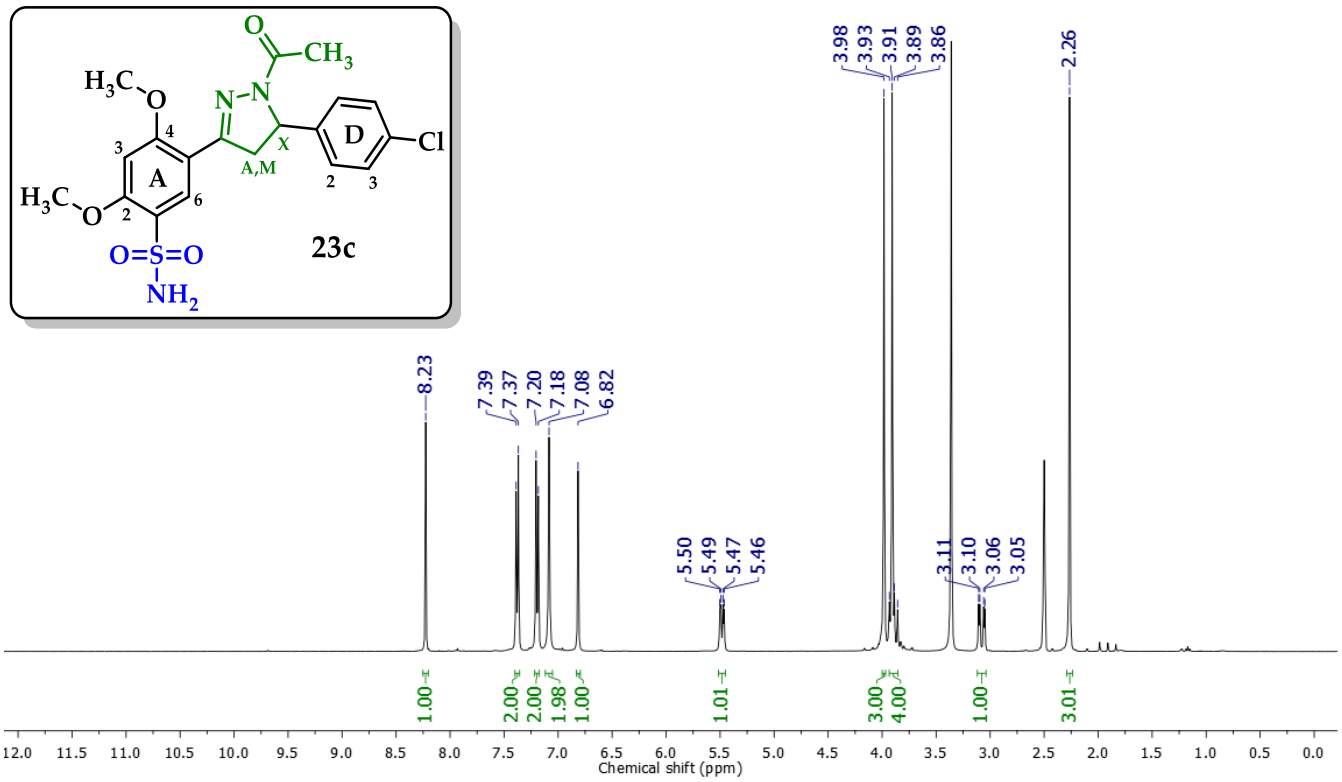
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **23a**.



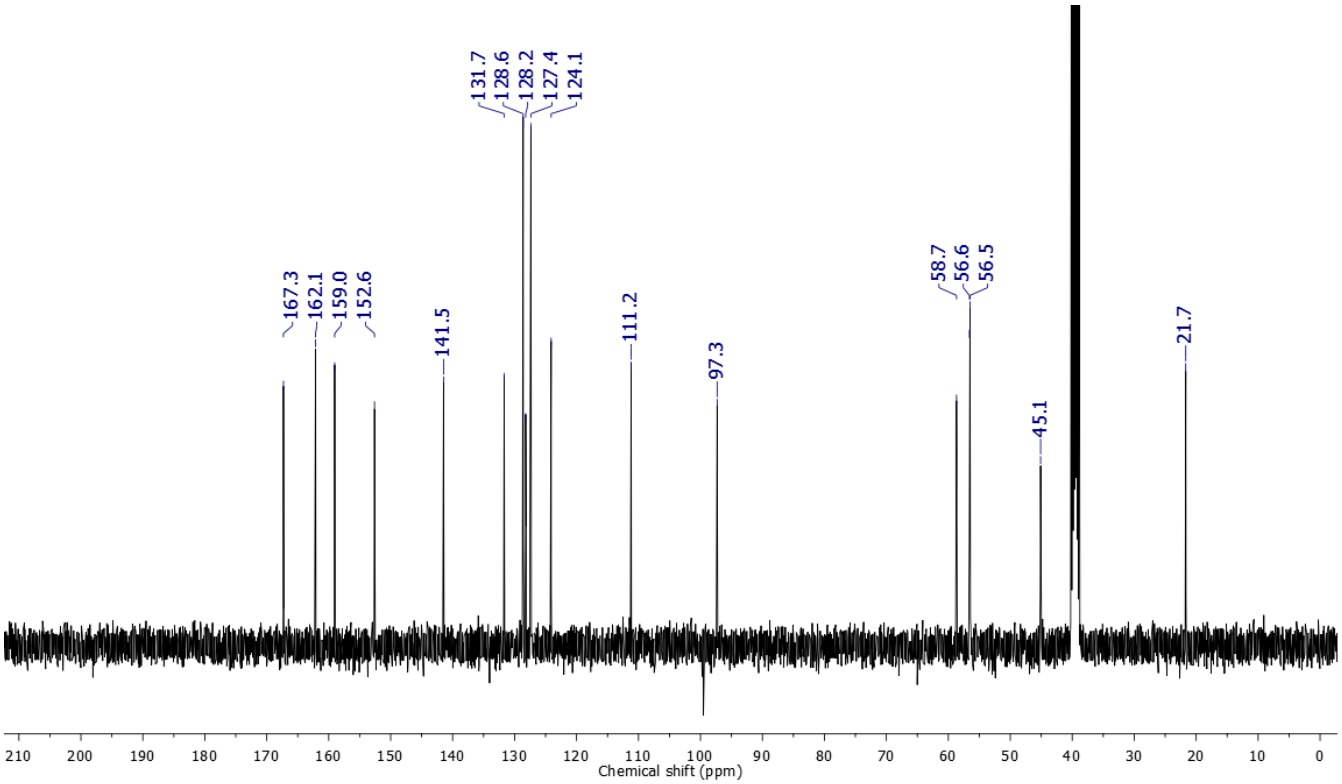
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **23b**.



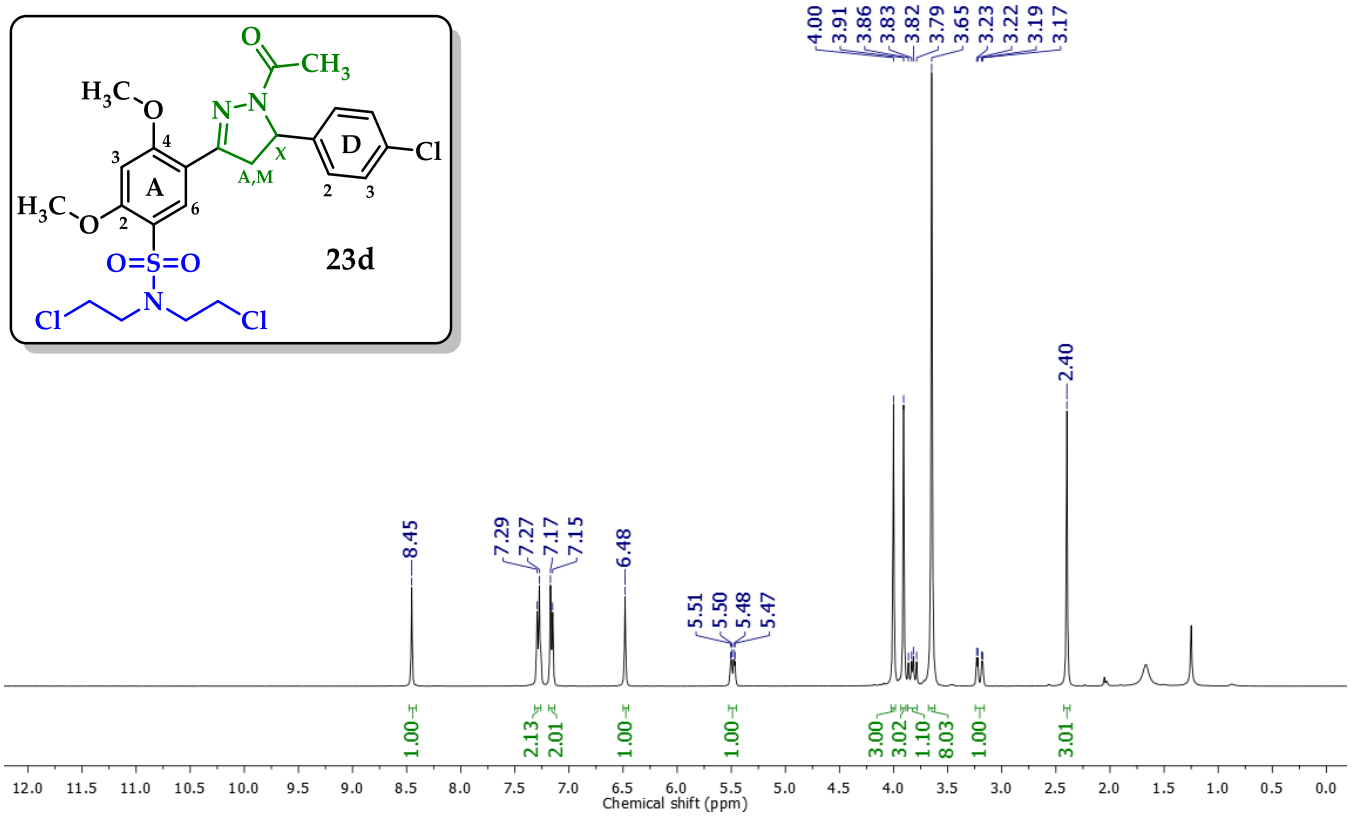
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **23b**.



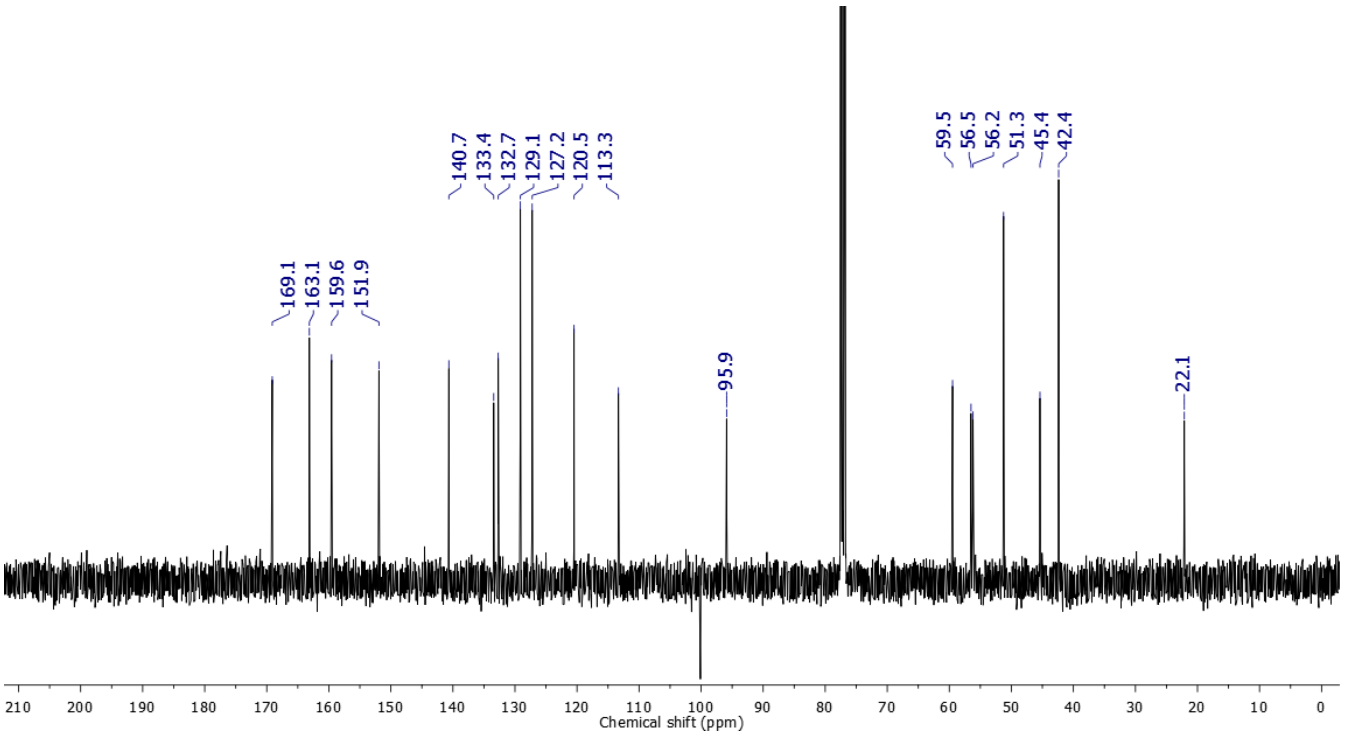
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **23c**.



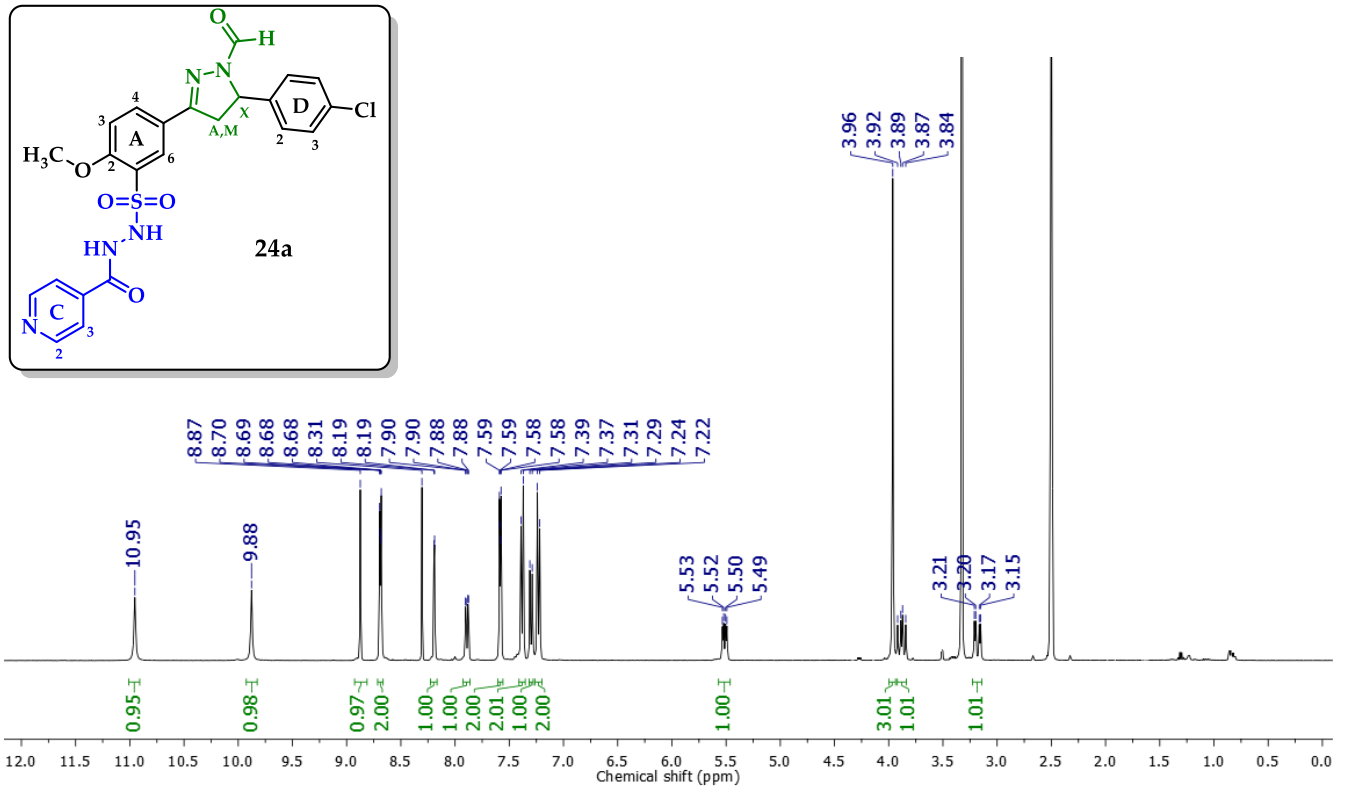
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **23c**.



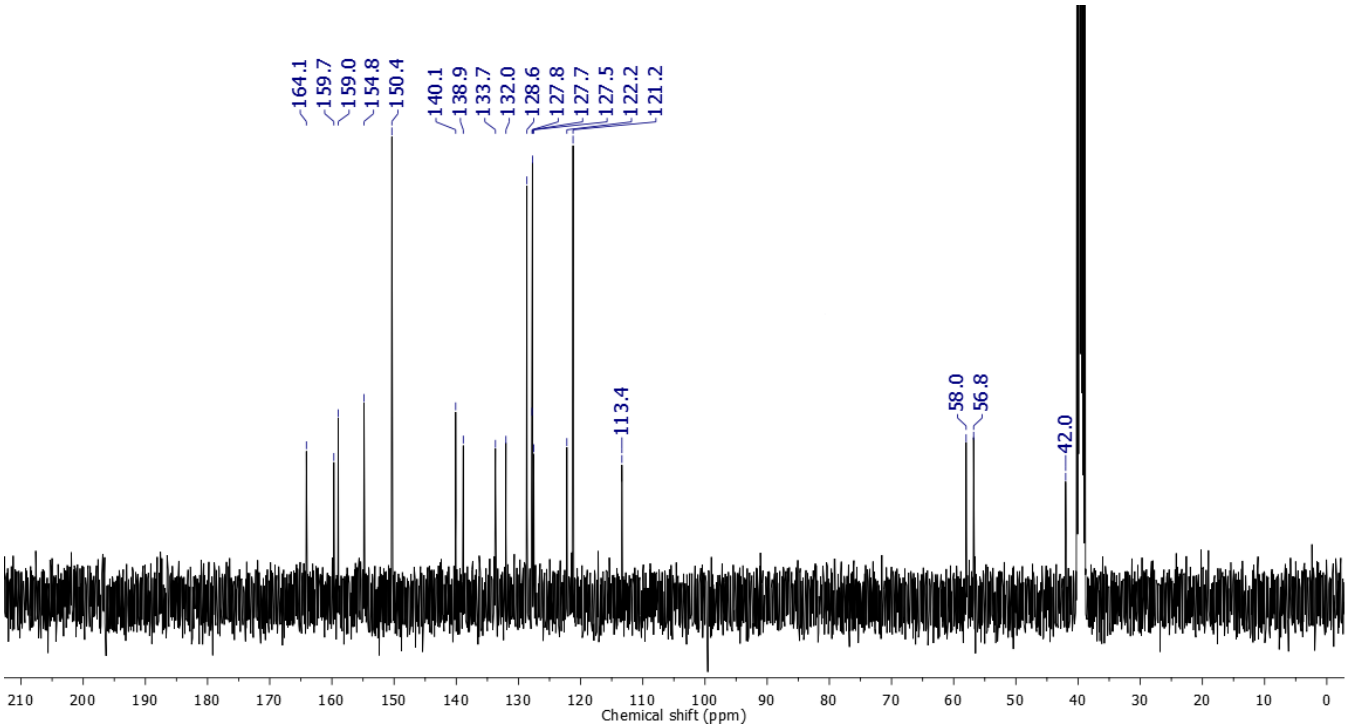
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **23d**.



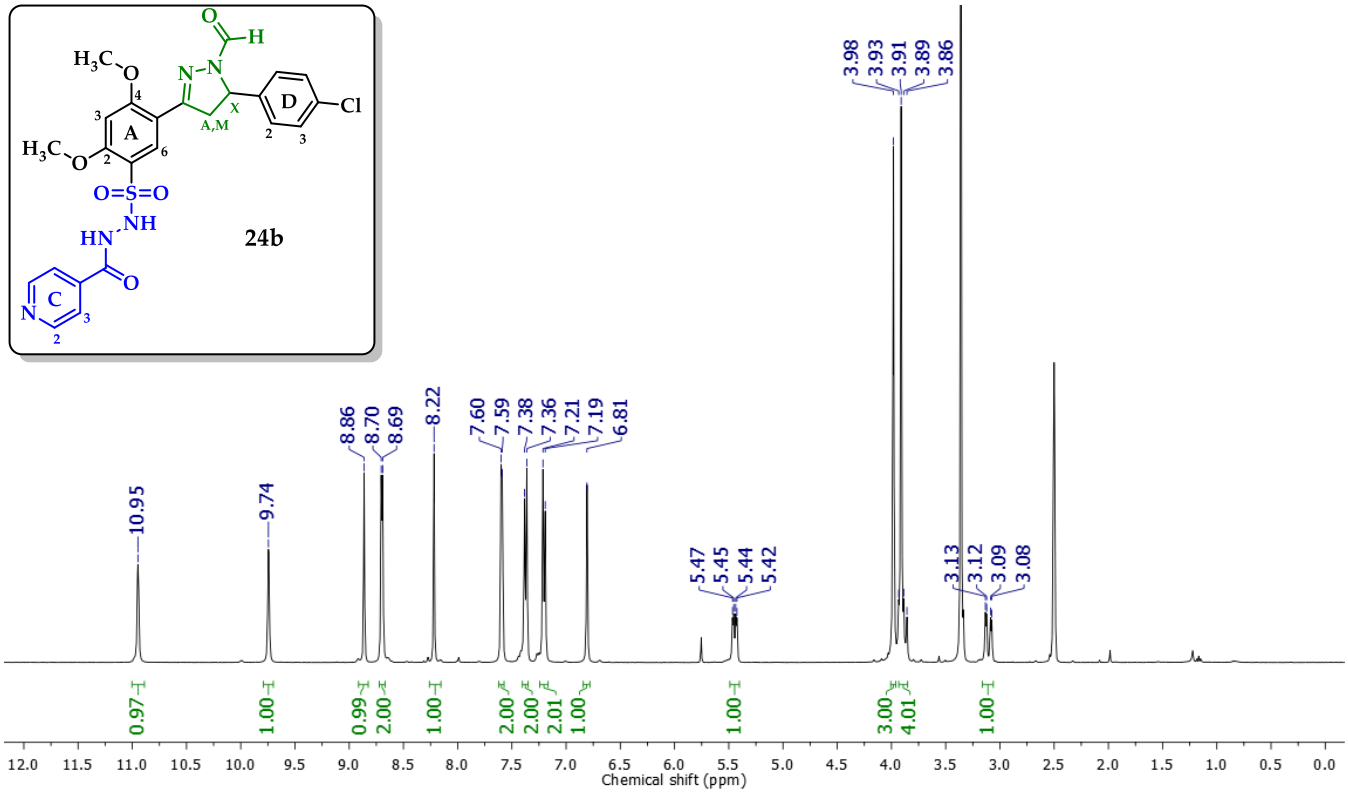
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **23d**.



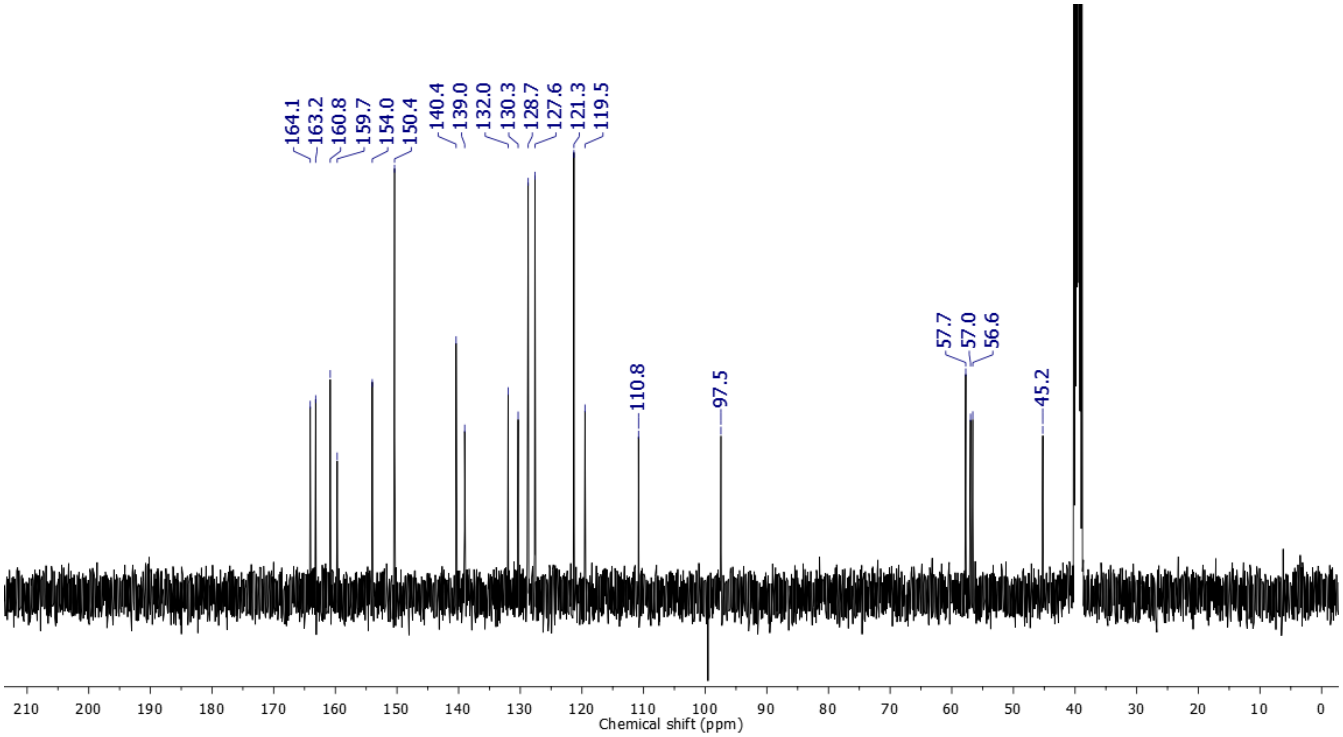
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **24a**.



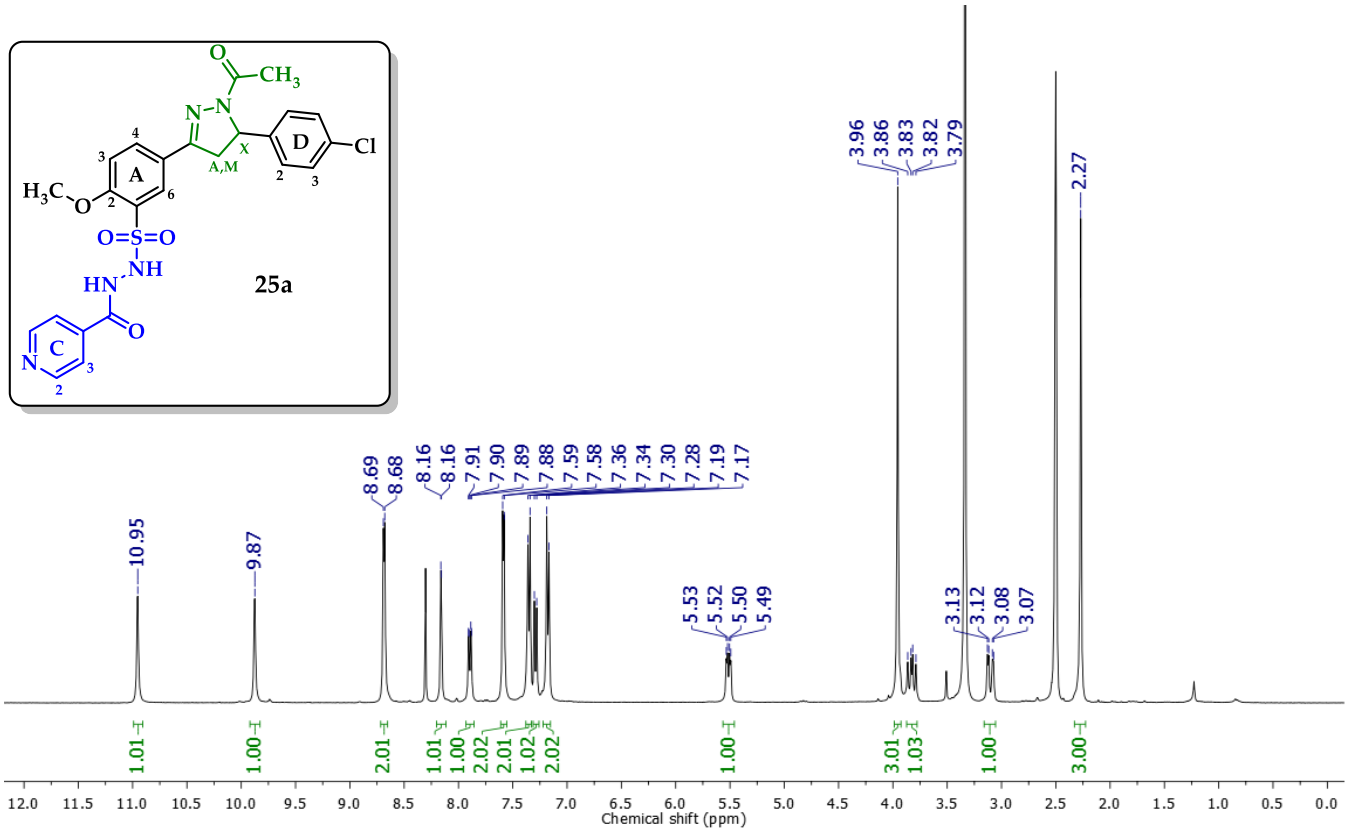
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **24a**.



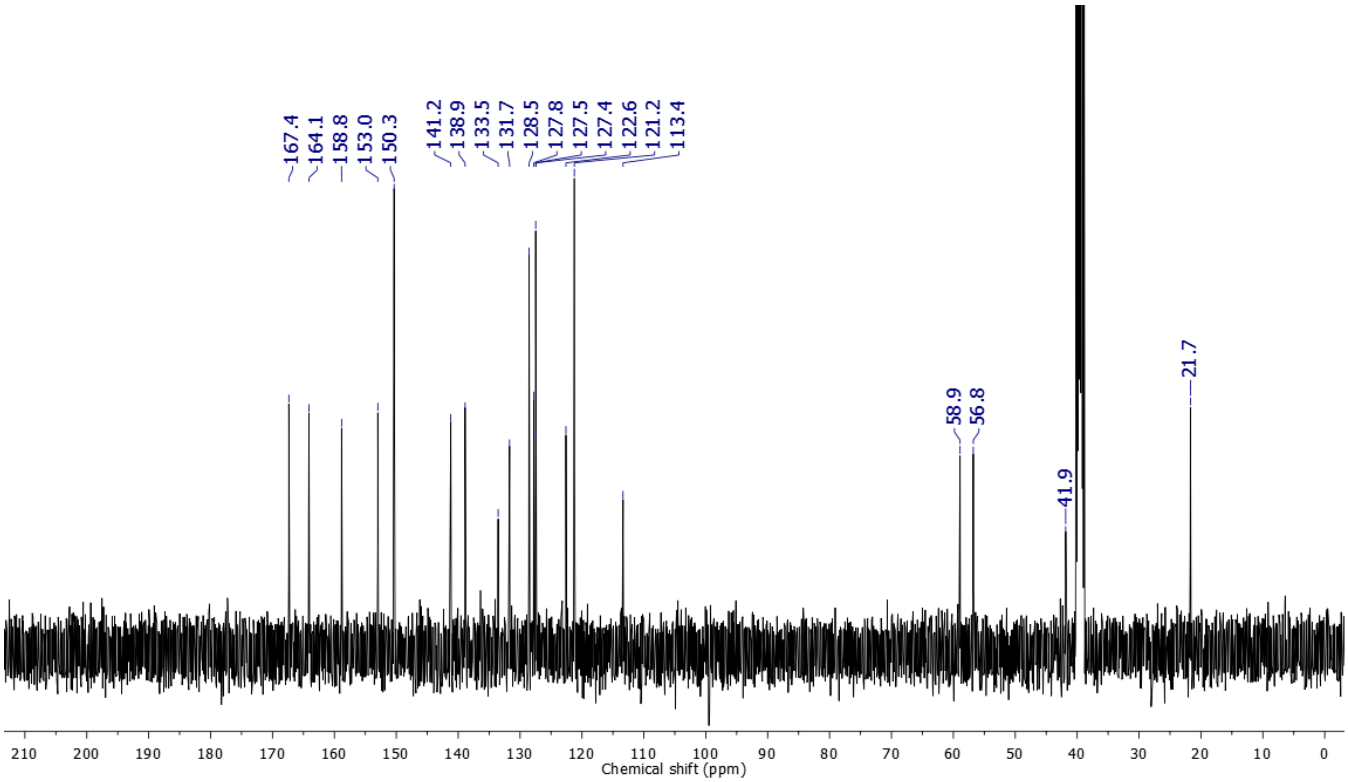
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **24b**.



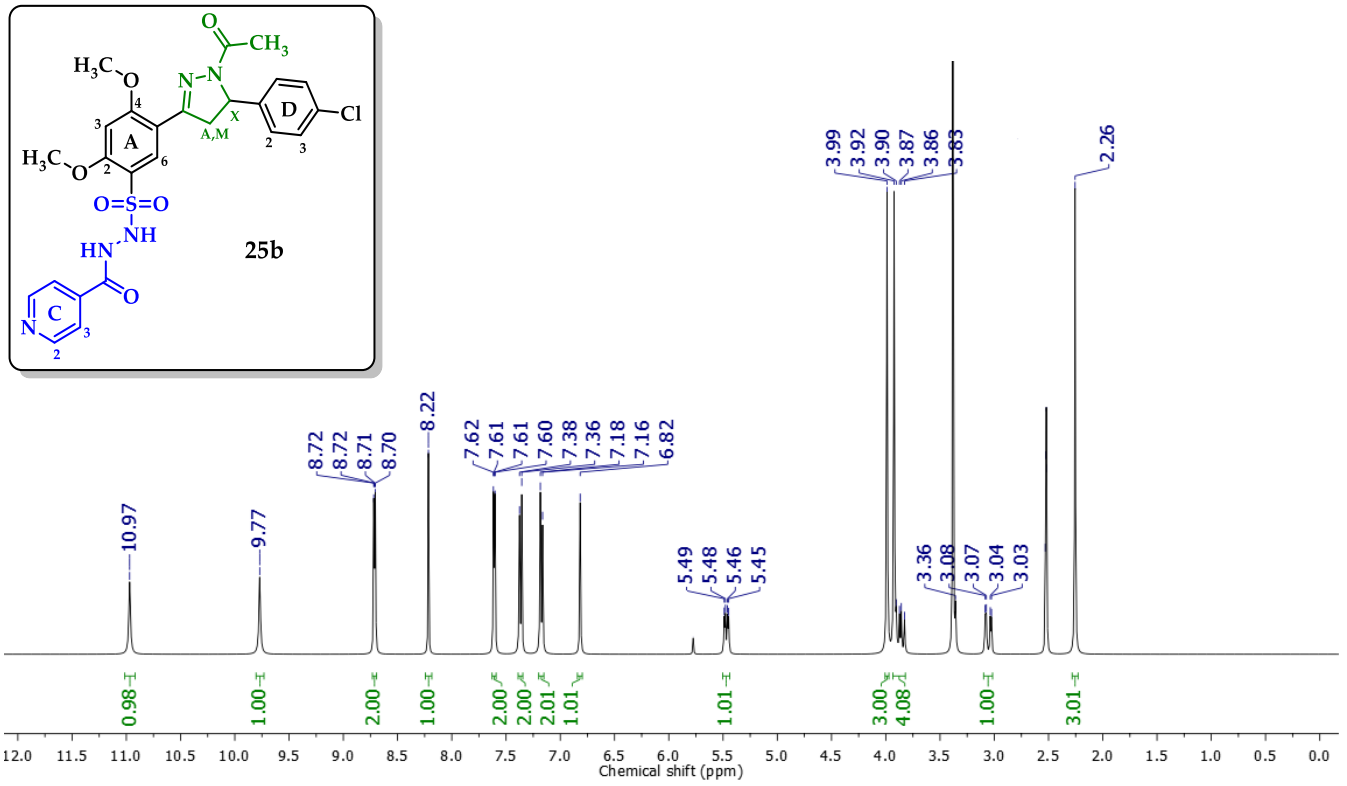
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **24b**.



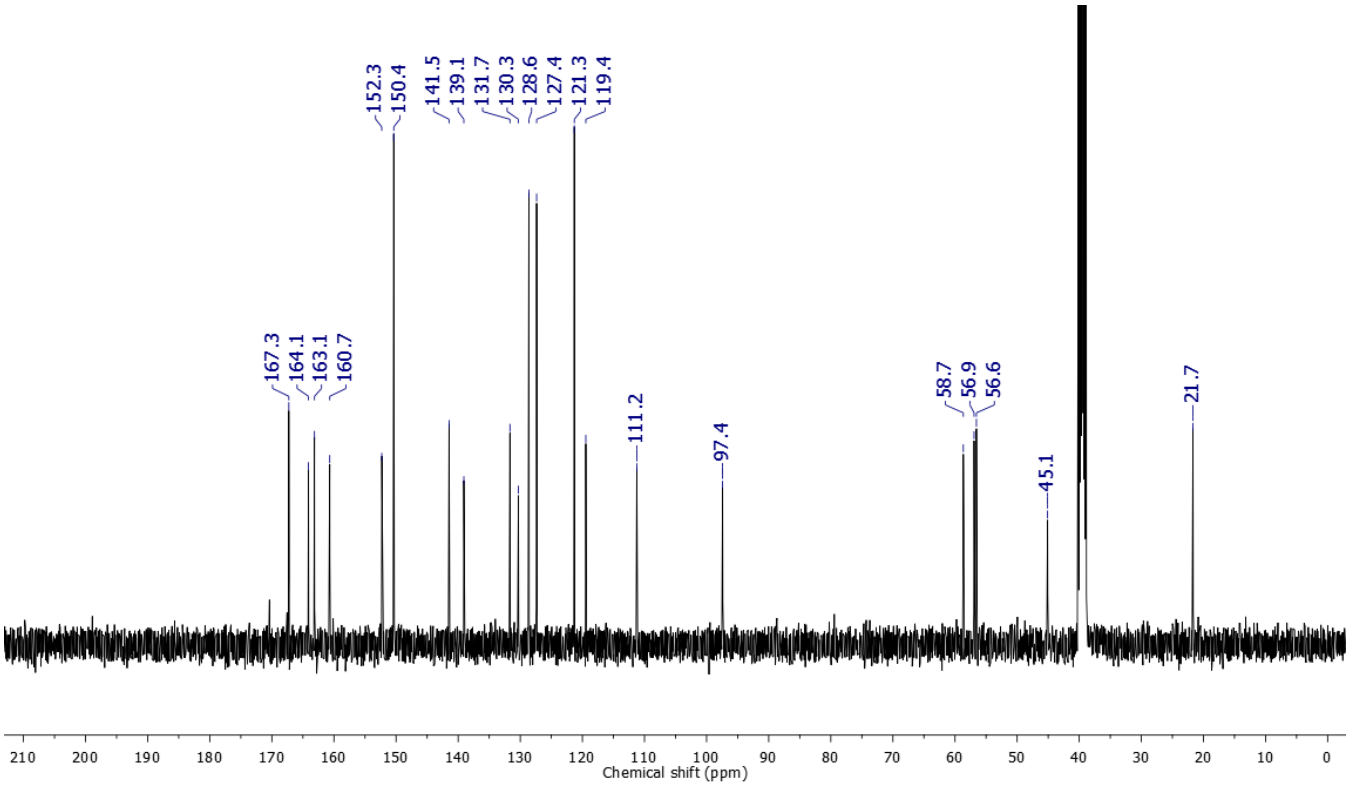
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **25a**.



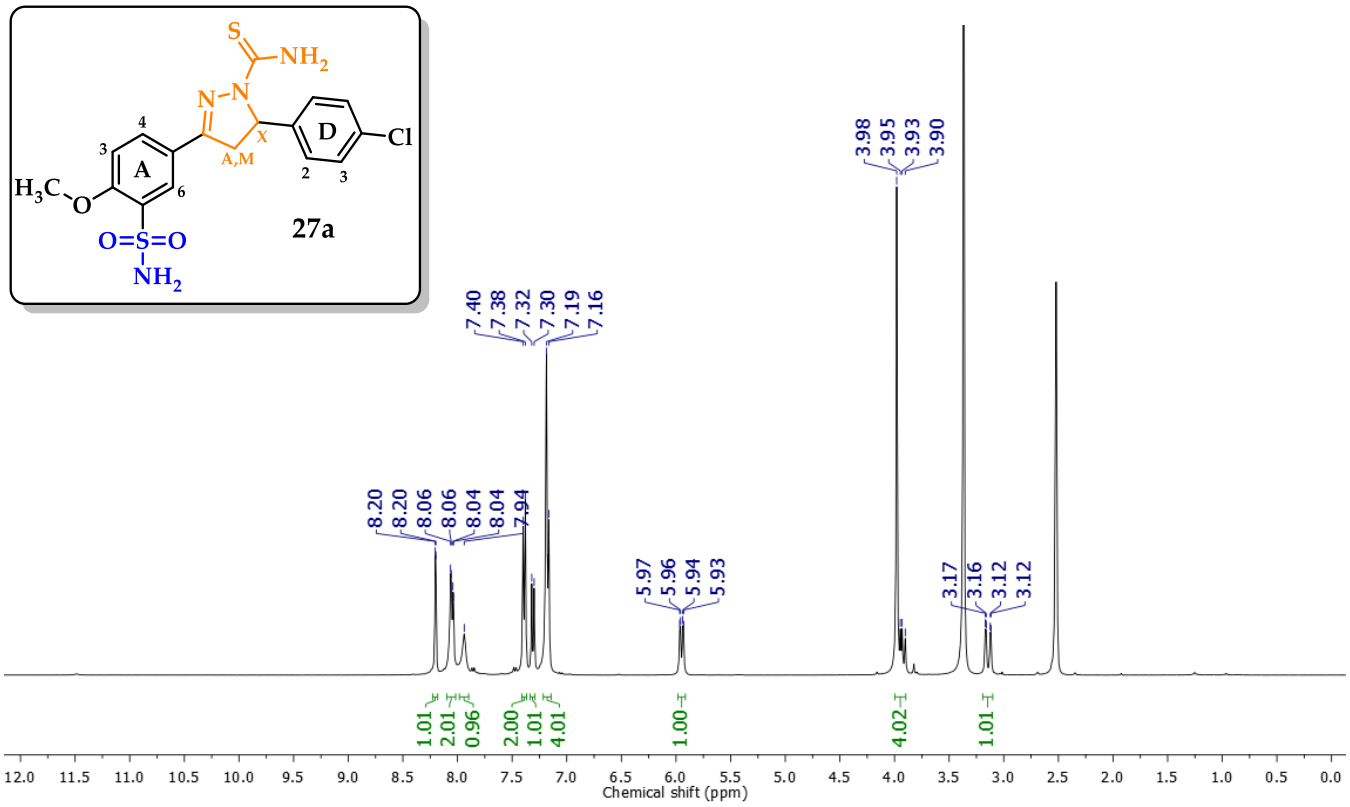
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **25a**.



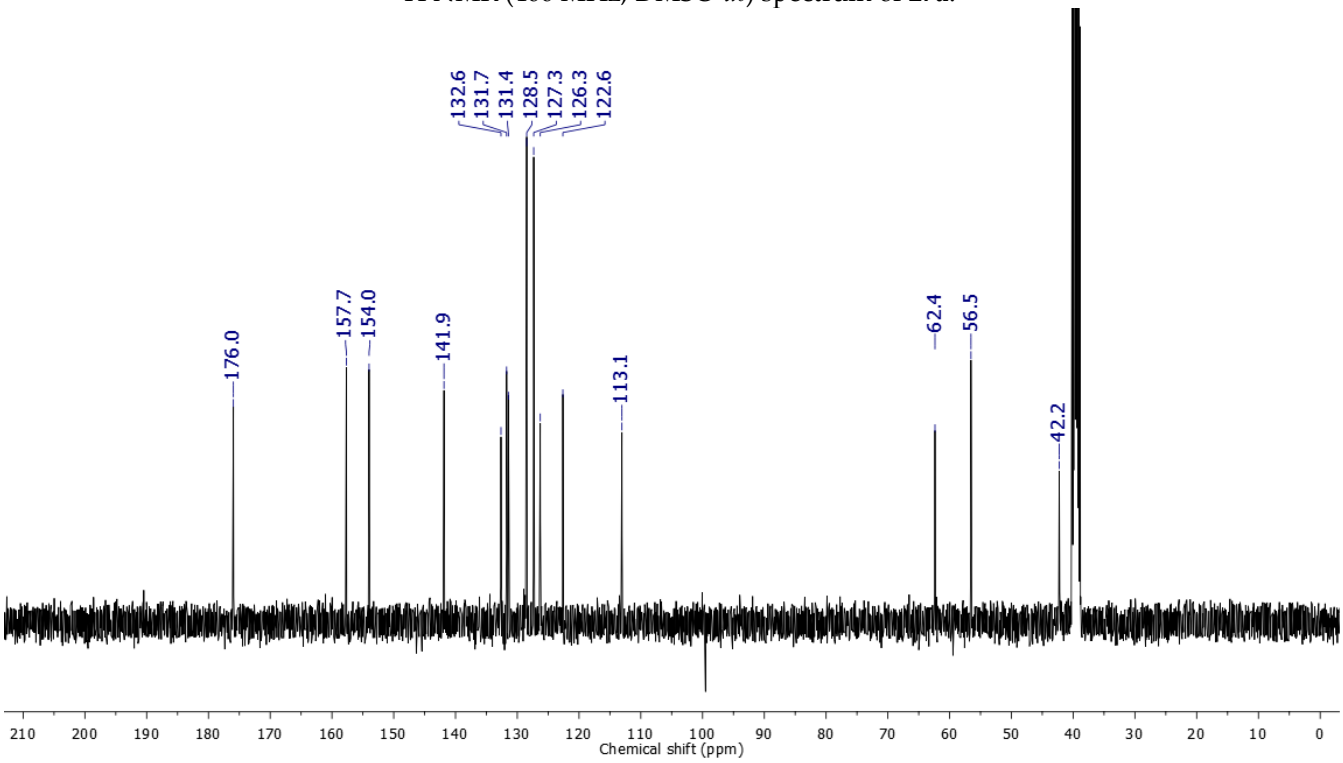
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **25b**.



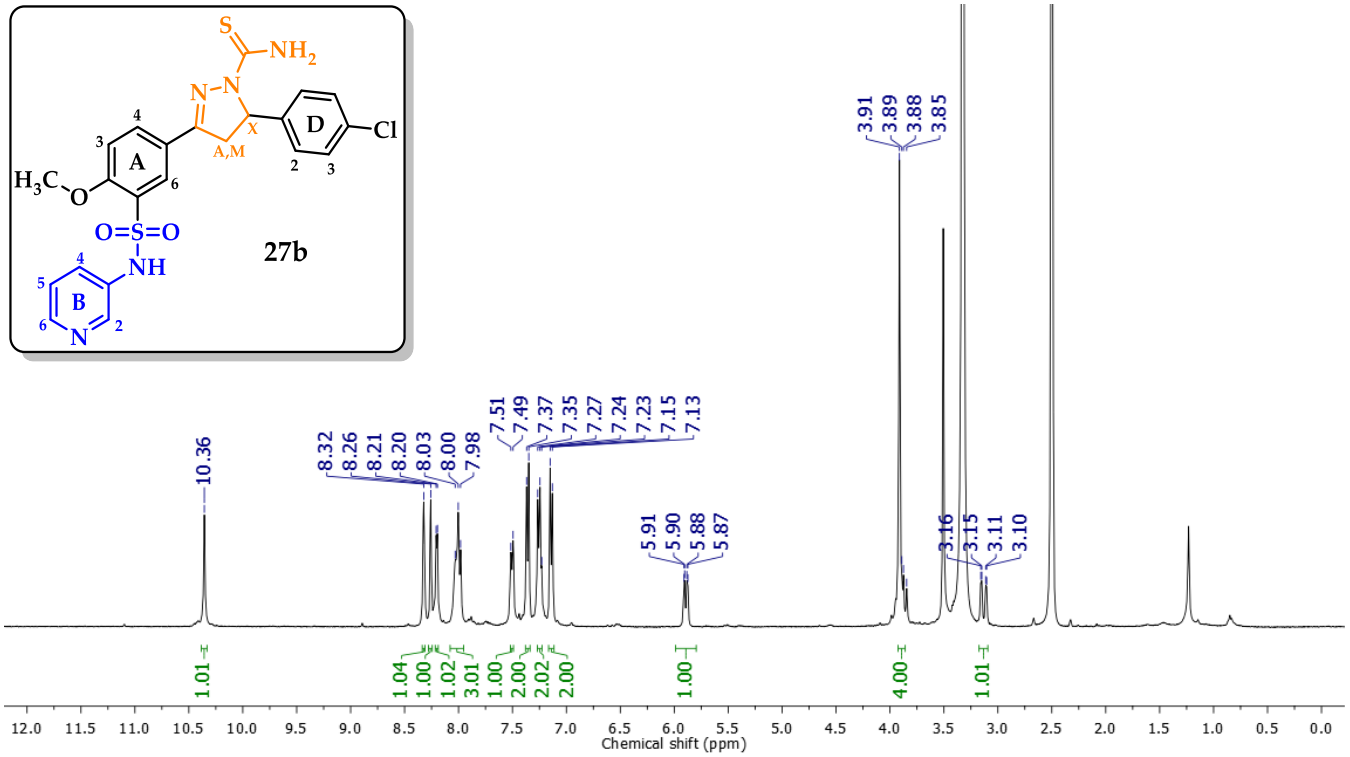
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **25b**.



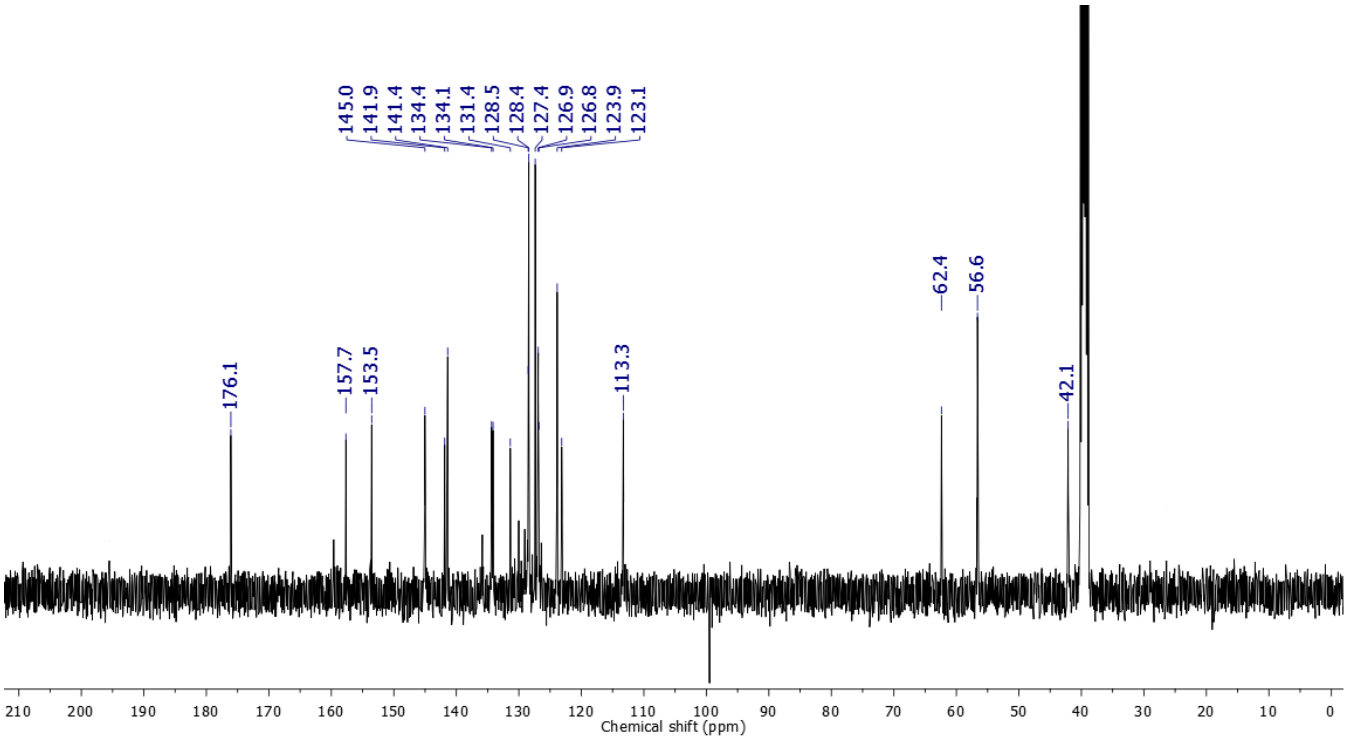
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **27a**.



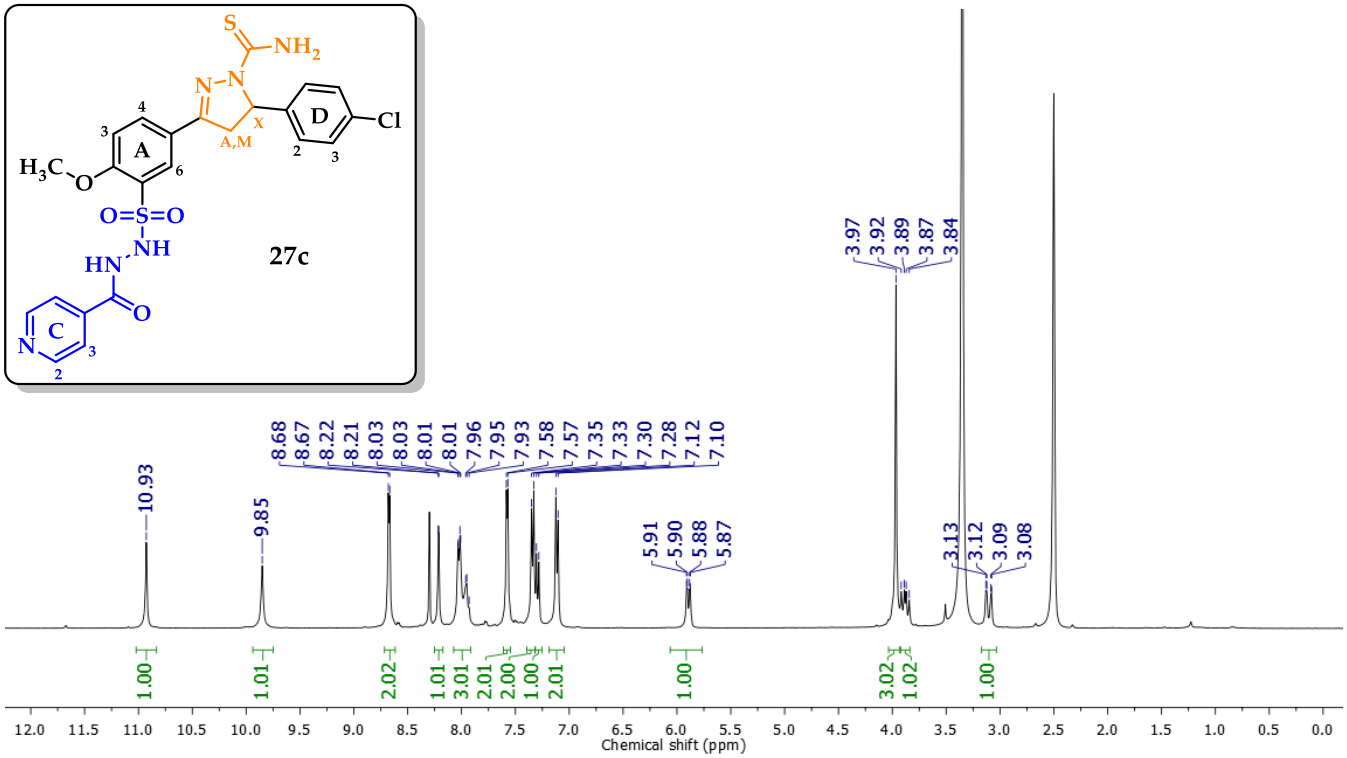
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **27a**.



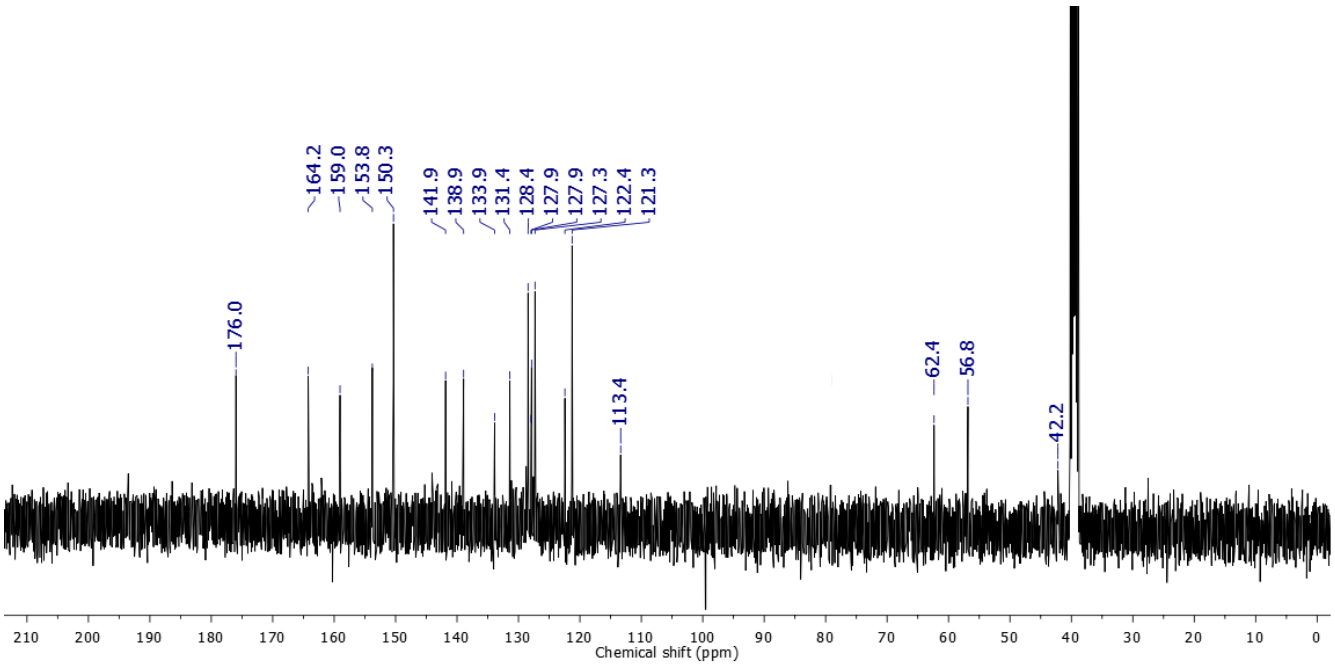
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **27b**.



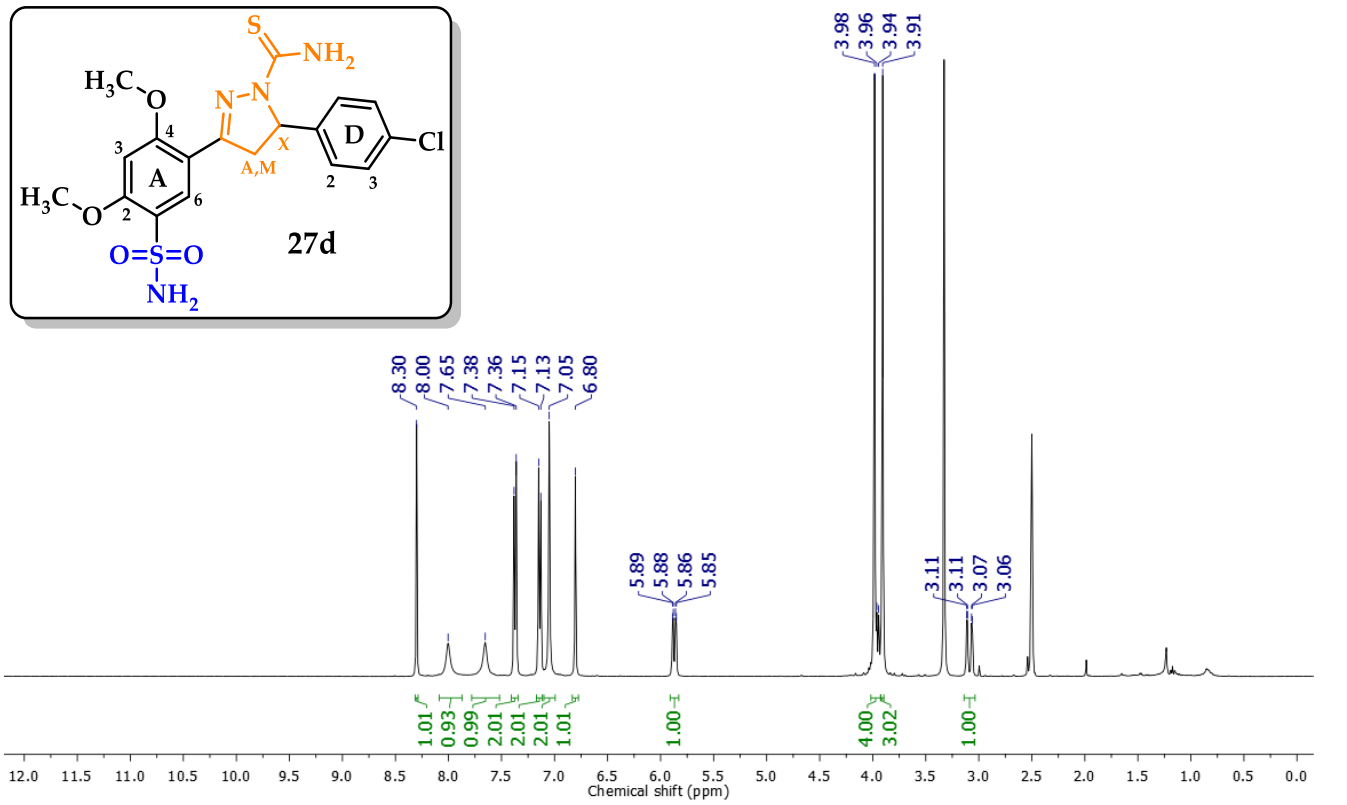
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **27b**.



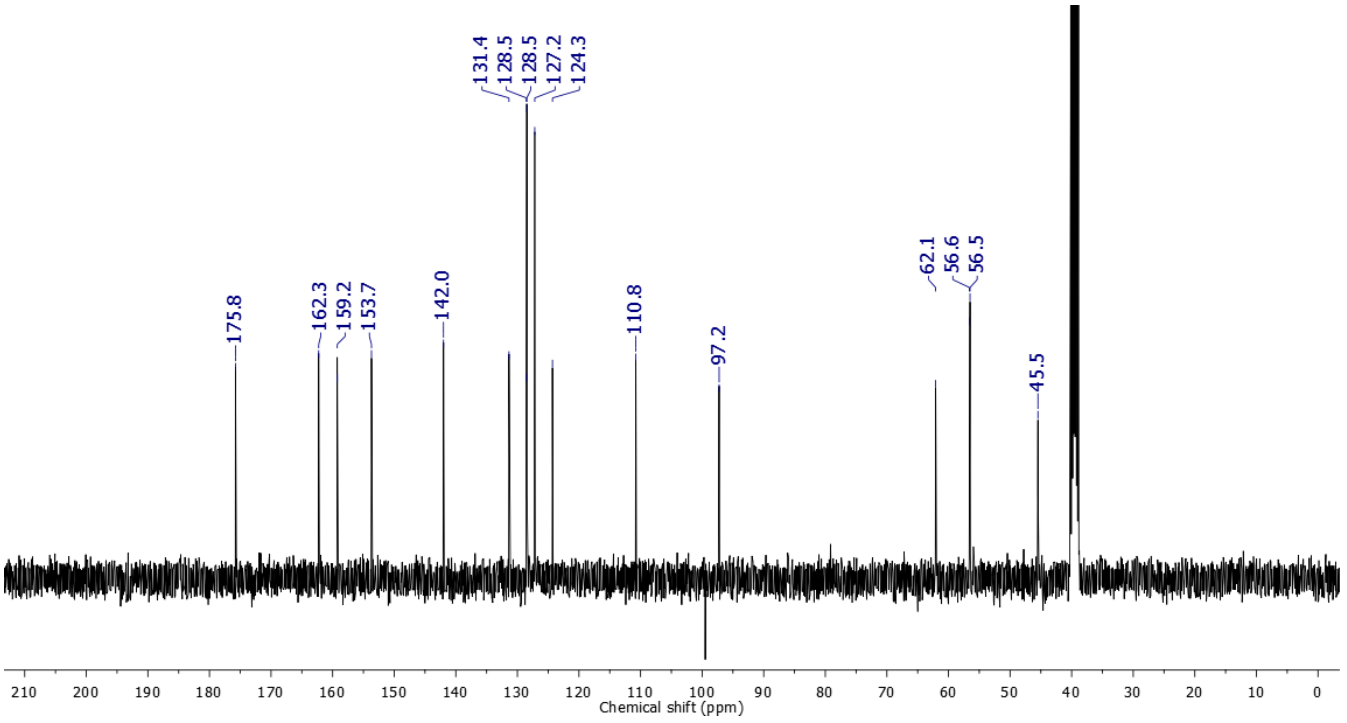
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **27c**.



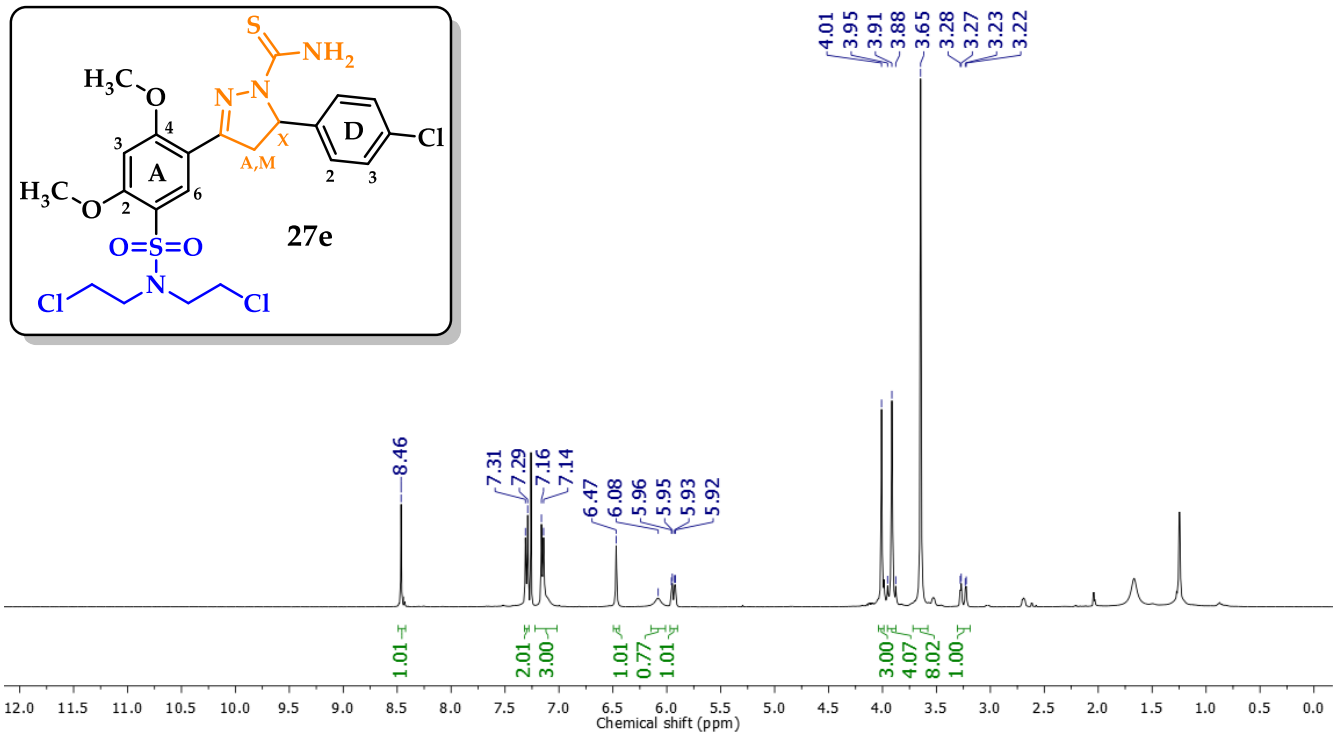
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **27c**.



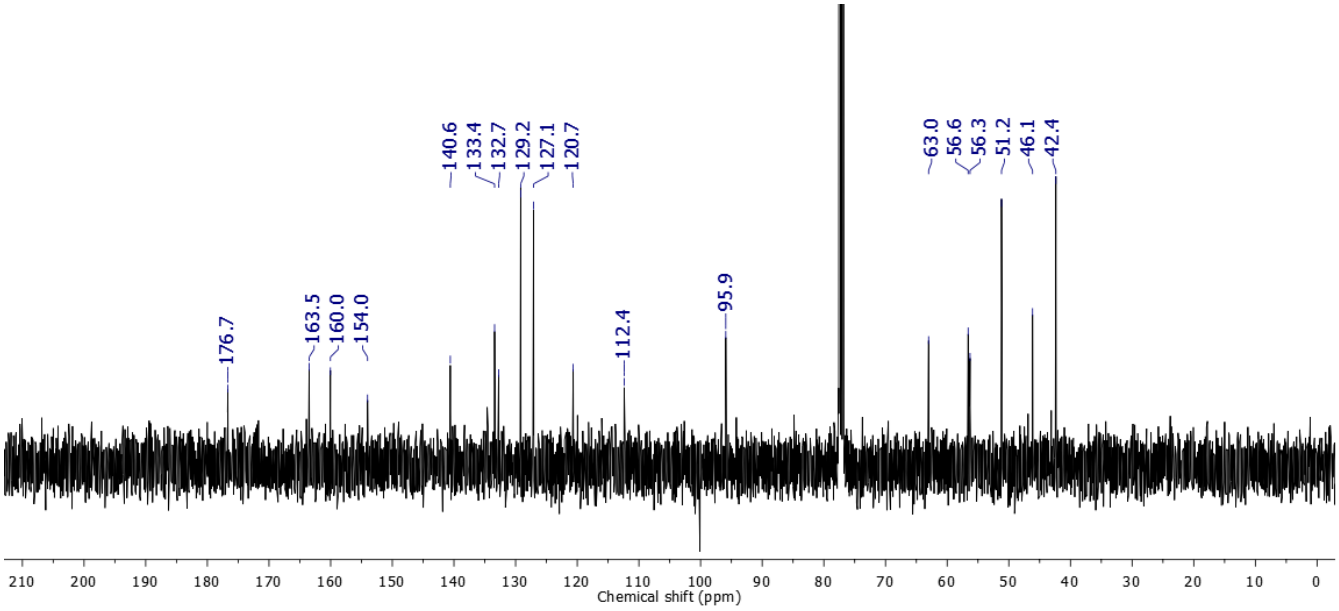
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **27d**.



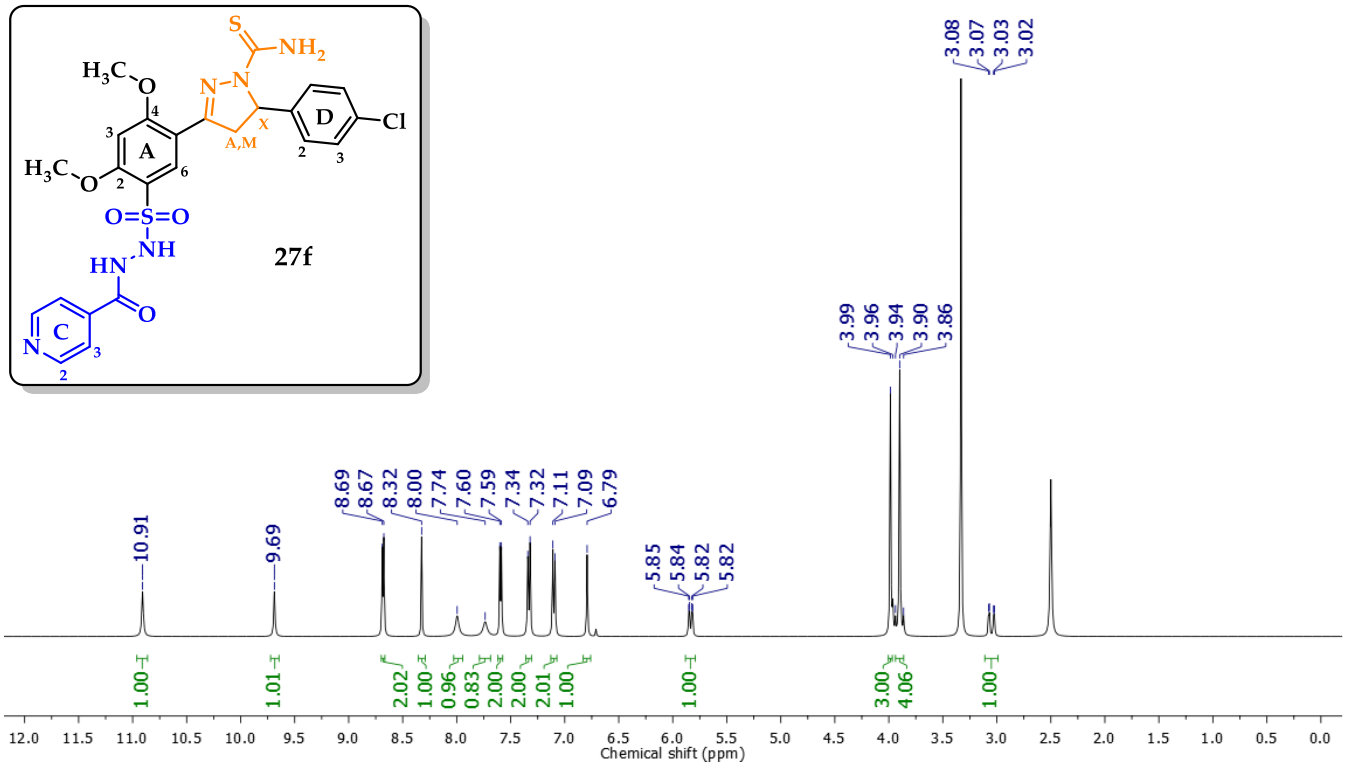
^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **27d**.



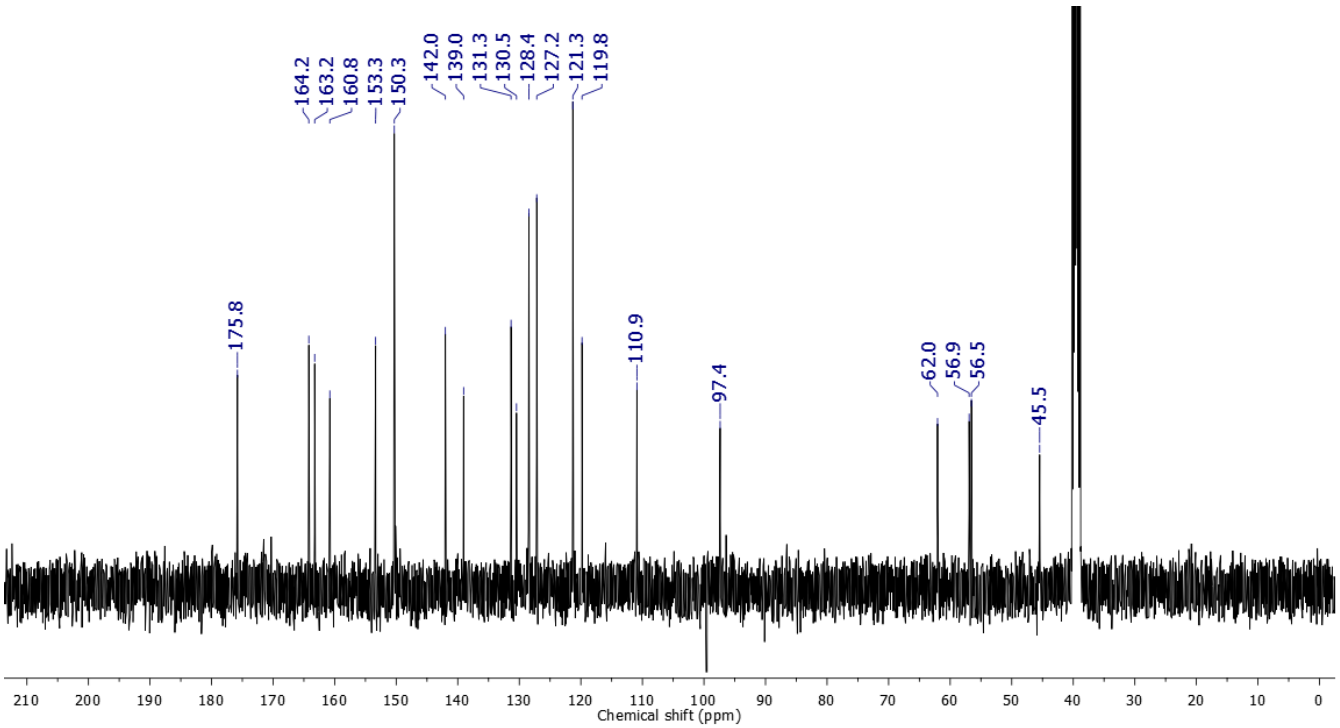
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **27e**.



^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **27e**.



^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **27f**.



^{13}C NMR (101 MHz, DMSO-d_6) spectrum of **27f**.

Table S1. Single Crystal Diffraction Experimental Details

Compound	**8b**	**14a**	**14b**
CCDC code	*2191609*	*2191607*	*2191610*
Crystal data			
Chemical formula	$C_{10}H_{13}NO_5S$	$C_{15}H_{15}N_3O_5S$	$C_{16}H_{17}N_3O_6S{\cdot}H_2O$
M_r	259.27	349.36	397.40
Crystal system, space group	Monoclinic, $P2_1/c$	Triclinic, $P\bar{1}$	Triclinic, $P\bar{1}$
Temperature (K)	100	100	100
a, b, c (Å)	10.1290 (3), 7.8633 (3), 15.0022 (6)	8.1469 (4), 8.6691 (5), 11.2683 (6)	10.4346 (4), 13.3686 (6), 19.7728 (8)
α, β, γ (°)	90, 104.850 (1), 90	94.600 (2), 95.040 (2), 105.641 (2)	84.686 (2), 87.900 (2), 73.780 (2)
V (Å^3)	1154.98 (7)	758.92 (7)	2636.89 (19)
Z	4	2	6
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.29	0.25	0.23
Crystal size (mm)	0.25 × 0.12 × 0.07	0.28 × 0.28 × 0.16	0.15 × 0.14 × 0.13
Data collection			
Diffractometer	Bruker D8 Venture		
Absorption correction	MULTISCAN; SADABS 2016/2		
T_{min}, T_{max}	0.619, 0.746	0.708, 0.746	0.708, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25007, 2651, 2356	38280, 3489, 2991	121286, 12120, 10461
R_{int}	0.047	0.063	0.044
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.650	0.650	0.650
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.029, 0.076, 1.05	0.035, 0.095, 1.10	0.032, 0.100, 1.05
No. of reflections	2651	3489	12120
No. of parameters	157	219	787
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.31, -0.42	0.36, -0.44	0.37, -0.49

Compound	**17d**	**20f**	**17c**
CCDC code	2191609	2191607	2191610
Crystal data			
Chemical formula	$C_{18}H_{19}NO_6S$	$C_{24}H_{23}N_3O_9S$	$C_{18}H_{19}NO_5S$
M_r	377.40	529.51	361.40
Crystal system, space group	Monoclinic, $P2_1/n$	Triclinic, $P\bar{1}$	Orthorhombic, *Pbcn*
Temperature (K)	100	100	100
a, *b*, *c* (Å)	8.7129 (3), 15.0324 (5), 13.6114 (4)	8.1544 (4), 12.3336 (7), 12.7882 (7)	10.4991 (3), 10.1829 (3), 32.3481 (9)
α, β, γ (°)	90, 107.554 (1), 90	86.224 (2), 71.888 (2), 89.788 (2)	90, 90, 90
V (Å^3)	1699.75 (10)	1219.58 (11)	3458.38 (17)
Z	4	2	8
Radiation type	Mo *K*α	Mo *K*α	Mo *K*α
μ (mm^{-1})	0.23	0.19	0.22
Crystal size (mm)	0.24 × 0.20 × 0.12	0.34 × 0.21 × 0.18	0.20 × 0.15 × 0.14
Data collection			
Diffractometer	Bruker D8 Venture		
Absorption correction	MULTISCAN; SADABS 2016/2		
T_{min}, T_{max}	0.691, 0.746	0.705, 0.746	0.683, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28650, 3910, 3325	55766, 5603, 5018	29731, 3966, 3484
R_{int}	0.051	0.039	0.045
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.650	0.650	0.650
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.032, 0.087, 1.04	0.039, 0.109, 1.04	0.035, 0.093, 1.05
No. of reflections	3910	5603	3966
No. of parameters	238	336	229, 2 restraints
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.34, -0.42	1.52, -0.34	0.42, -0.47

Computer programs: *APEX3* v2019.1-0 (Bruker Nano Inc., 2019), *SAINT* V8.38A (Bruker AXS Inc., 2017), *SHELXT*–2014/5 (Sheldrick, 2014), *SHELXL*–2018/2 (Sheldrick, 2018).