Supporting Information

Copper-Catalyzed Domino Addition, Hydroamination and Cyclization: A Multicomponent Approach to Spiro Oxazolidinone Derivatives

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1. Crystal structure analysis of compound 4e (#CCDC **1863694)**

Table S1 Crystal data and structure refinement for compound 4e.

Identification code	KA409MF
Empirical formula	$C_{24}H_{17}ClN_2O_3$
Formula weight	416.84
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	6.16338(8)
b/Å	33.2578(5)
c/Å	9.94383(14)
α/°	90
β/°	100.2051(8)
γ/°	90
Volume/Å^3	2006.05(5)
Z	4
ρ_{calc}g/cm^3	1.380
μ/mm^{-1}	0.220
F(000)	864.0
Crystal size/mm^3	0.300 × 0.210 × 0.150
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.338 to 55
Index ranges	-8 ≤ h ≤ 8, -43 ≤ k ≤ 43, -12 ≤ l ≤ 12
Reflections collected	19219
Independent reflections	4589 [R_{int} = 0.0370, R_{sigma} = 0.0323]
Data/restraints/parameters	4589/6/270
Goodness-of-fit on F^2	1.128
Final R indexes [I>=2σ (I)]	R_1 = 0.0506, wR_2 = 0.1467
Final R indexes [all data]	R_1 = 0.0697, wR_2 = 0.1603

Largest diff. peak/hole / e Å^{-3}	0.26/-0.43

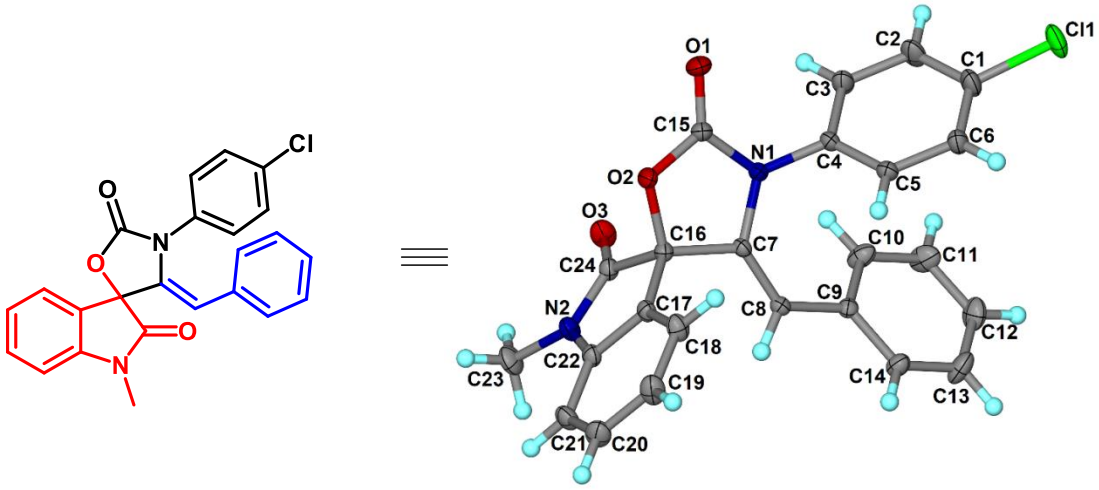


Figure S1. X-ray crystal structure of compound 4e

Figure S1: X-ray crystal structure of compound 4e with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius. Only major component of the disordered atoms is shown for clarity.

3. Crystal structure analysis of compound 6f (#CCDC 1863695)

Table S2 Crystal data and structure refinement for compound 6f.

Identification code	KA471MF
Empirical formula	$C_{21}H_{20}ClNO_2$
Formula weight	353.83
Temperature/K	293(2)
Crystal system	monoclinic
Space group	C2/c
a/Å	27.583(2)
b/Å	13.6001(10)
c/Å	10.2013(10)
α/°	90
β/°	104.589(4)
γ/°	90

Volume/Å^3	3703.5(5)
Z	8
ρ_{calc}g/cm^3	1.269
μ/mm^{-1}	0.220
F(000)	1488.0
Crystal size/mm^3	0.400 × 0.360 × 0.320
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.016 to 49.98
Index ranges	-32 ≤ h ≤ 32, -16 ≤ k ≤ 16, -12 ≤ l ≤ 11
Reflections collected	21907
Independent reflections	3261 [R_{int} = 0.0611, R_{sigma} = 0.0393]
Data/restraints/parameters	3261/240/290
Goodness-of-fit on F^2	1.066
Final R indexes [I>=2σ (I)]	R_1 = 0.0550, wR_2 = 0.1412
Final R indexes [all data]	R_1 = 0.0921, wR_2 = 0.1641
Largest diff. peak/hole / e Å^{-3}	0.15/-0.28

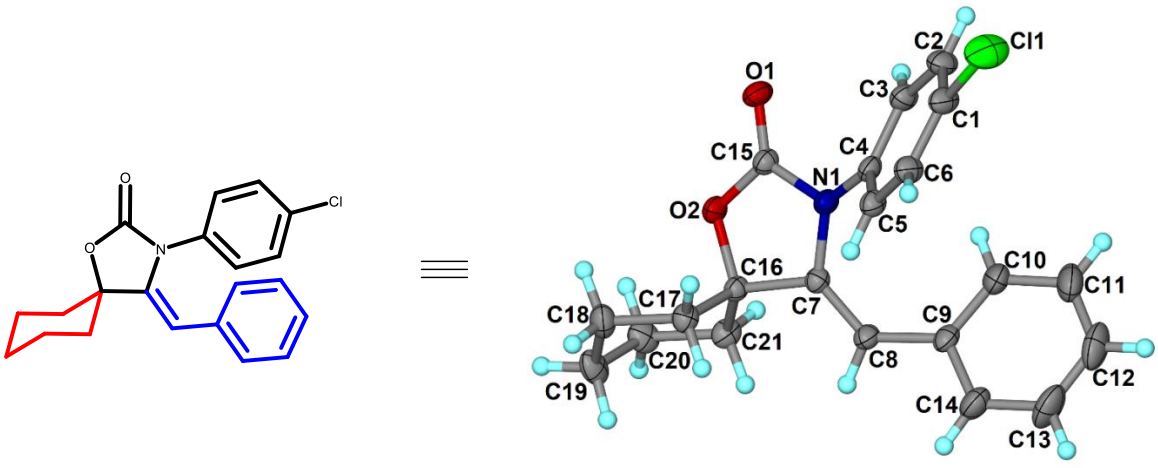


Figure S2. X-ray crystal structure of compound 6f

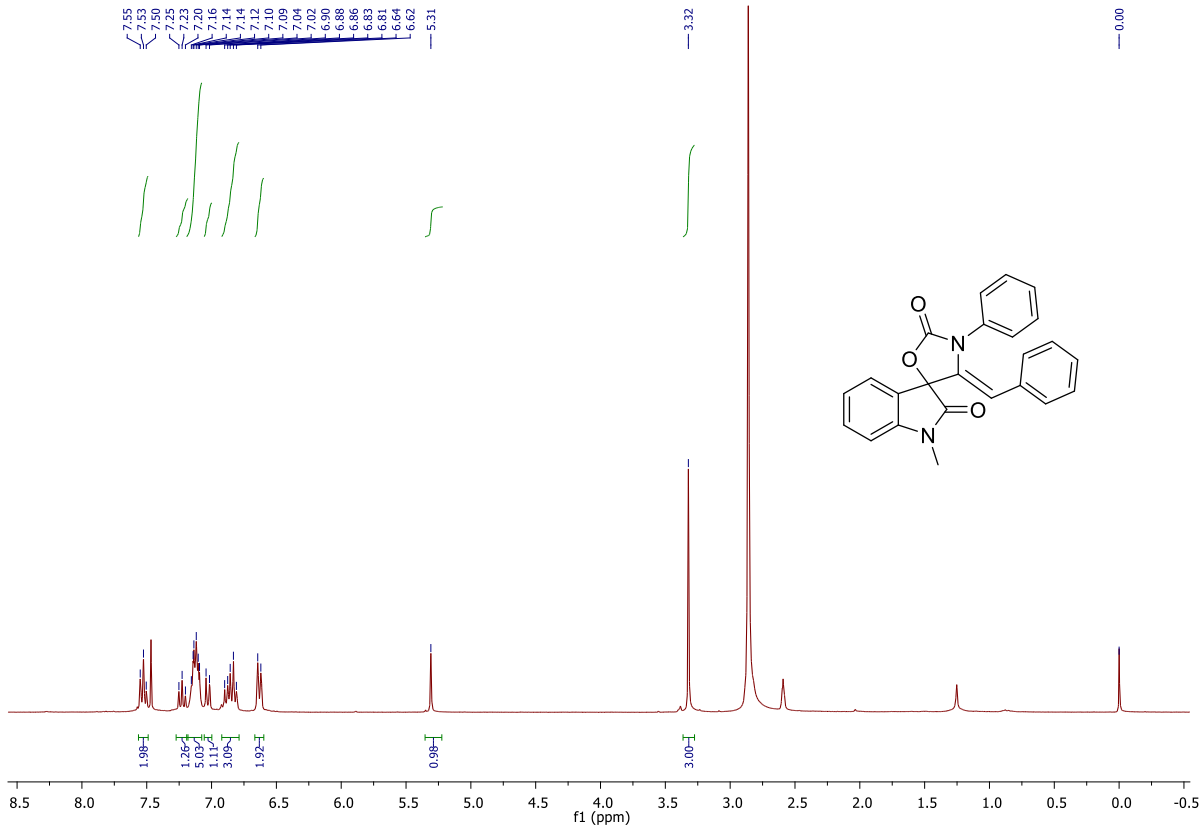
Figures S2: X-ray crystal structure of compound 6f with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius. Only major component of the disorder atoms is shown for clarity.

#CCDC **1863694 & 1863695** contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures/

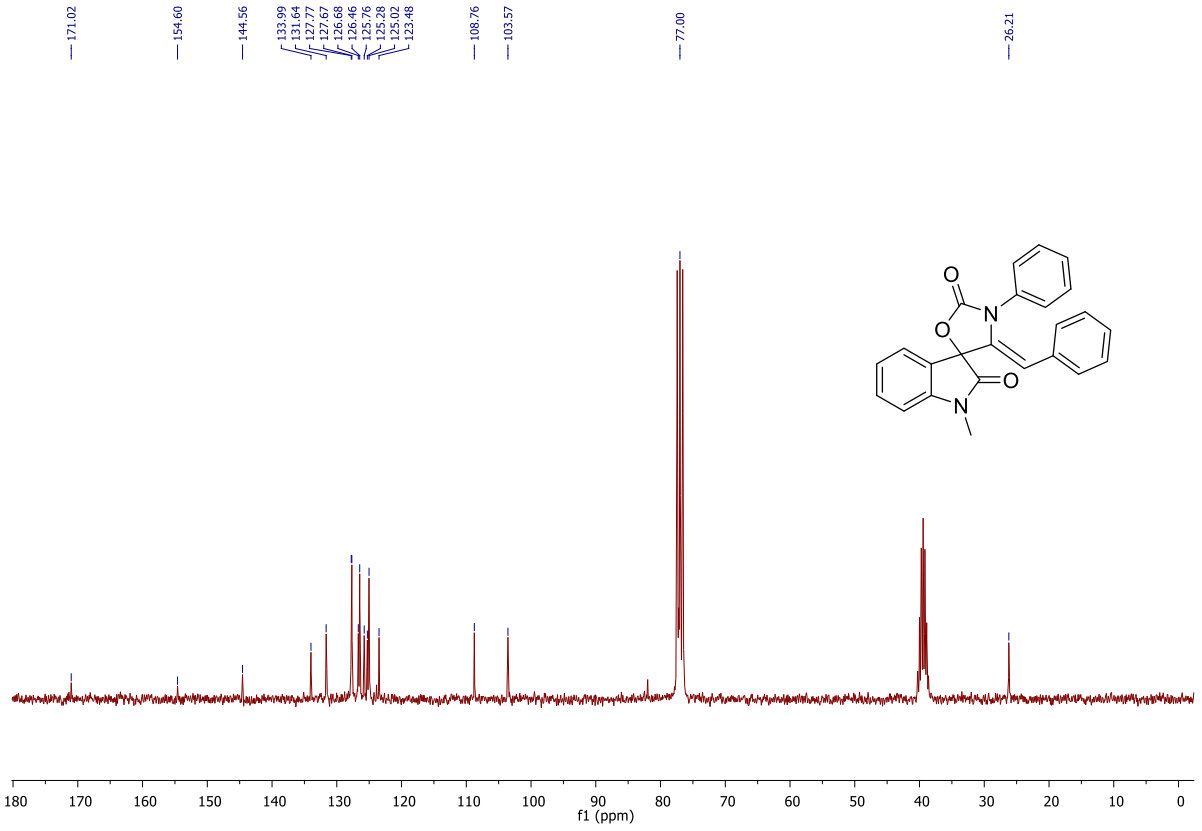
Data collection and structure solution of 4e (KA409) and 6f (KA471): Single crystal X-ray data for two compounds were collected at room temperature on a Bruker D8 QUEST equipped with a four-circle kappa diffractometer and Photon 100 detector. An Iμs microfocus Mo source (λ=0.71073Å) supplied the multi-mirror monochromated incident beam. A combination of Phi and Omega scans were used to collect the necessary data. Unit cell dimensions were determined using 7490 reflections for KA409 & 5607 reflection for KA417 data sets. Integration and scaling of intensity data were accomplished using SAINT program.[1] The structures were solved by Direct Methods using SHELXS97[2] and refinement was carried out by full-matrix least-squares technique using SHELXL-2014/7.[2-3] Anisotropic displacement parameters were included for all non-hydrogen atoms. All H atoms were positioned geometrically and treated as riding on their parent C atoms with C-H distances of 0.93--0.97 Å, and with $U_{iso}(H) = 1.2U_{eq}$ (C) or $1.5U_{eq}$ for methyl atoms. In KA409, the chlorine atom on the phenyl ring was disordered over two sites, with the site occupancy factor of 0.57(2) for Cl1 atom (major component) & 0.43(2) for Cl1D atom (minor component). In KA416, the chlorophenyl ring was disordered over two sites, with the site occupancy factor of 0.52(2) for Cl1/C1/C2/C3/C4/C5/C6 atoms (major component) & 0.48(2) for Cl1D/C1D/C2D/C3D/C4D/C5D/C6D atoms (minor component). The anisotropic displacement parameters of the disordered carbon atoms were restrained to be similar (SIMU instruction) and the direction of motion along the axis between these atoms was also restrained (DELU instruction).[3] The C-C bond distances of disordered ethyl groups were restrained to their expected values with DFIX instruction and performed the final cycle of refinement. The phenyl ring atoms were also treated as split models joining isopropyl group major and minor components respectively.

1. SMART & SAINT. Software Reference manuals. Versions 6.28a & 5.625, Bruker Analytical X-ray Systems Inc., Madison, Wisconsin, U.S.A., 2001.
2. Sheldrick, G. M. SHELXS97 and SHELXL Version 2014/7, http://shelx.uni-ac.gwdg.de/SHELX/index.php
3. Muller, P, Herbst-Imer, R, Spek, A. L, Schneider, T. R, and Sawaya, M. R. Crystal Structure Refinement: A Crystallographer's Guide to SHELXL. Muller, P. Ed. 2006 Oxford University Press: Oxford, New York, pp. 57–91

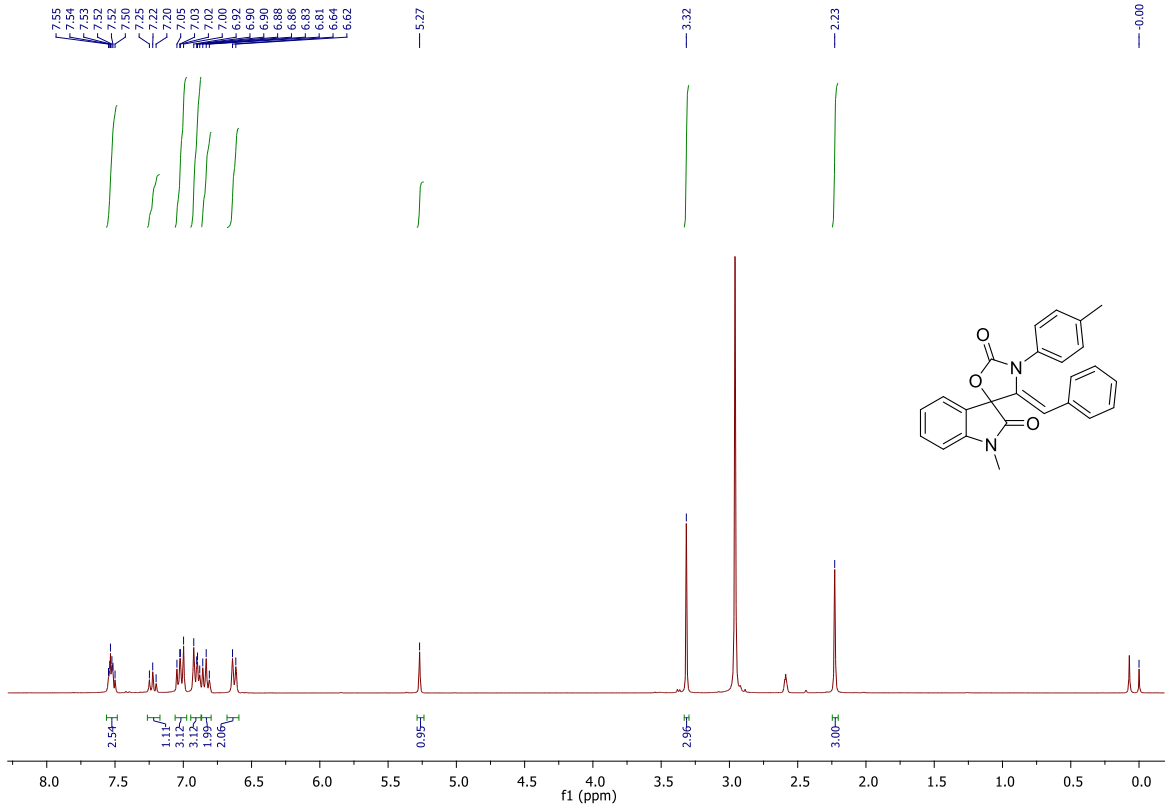
^{1}H NMR (300 MHz, $CDCl_3$+DMSO-d_6**) spectrum of compound 4a**



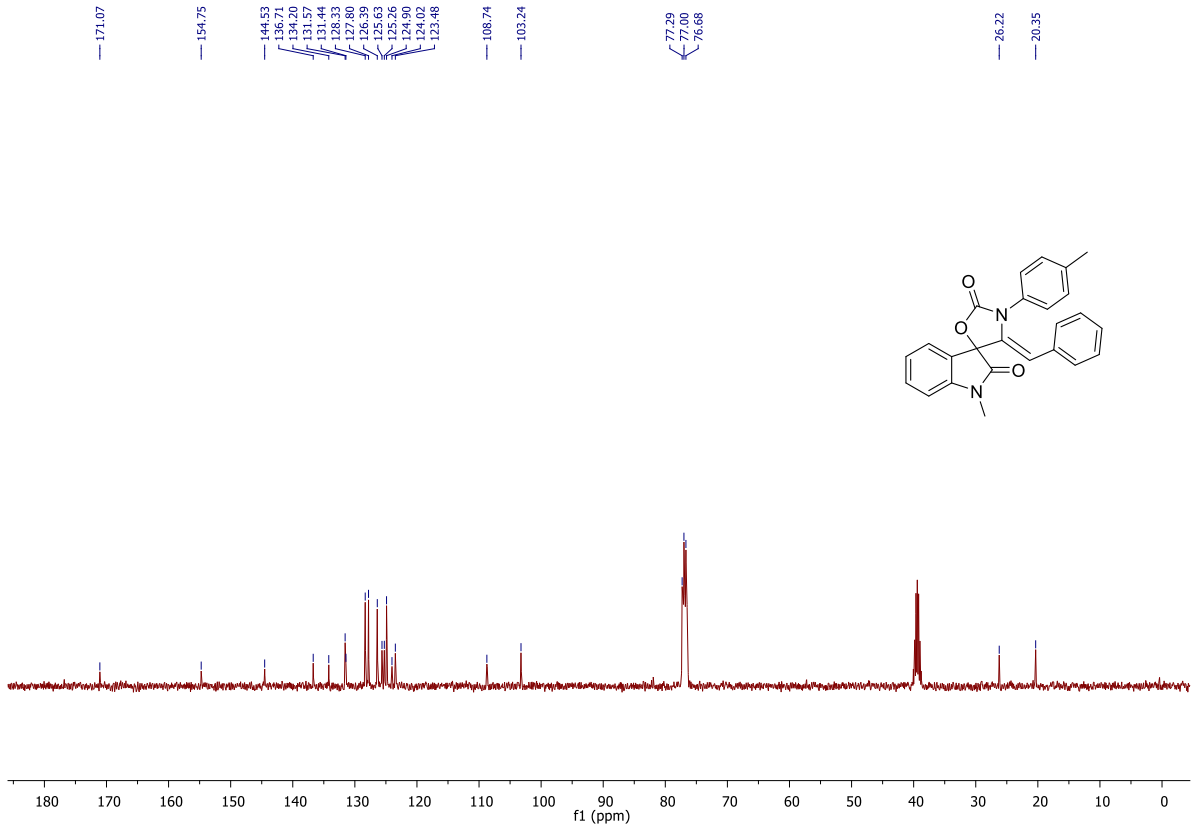
^{13}C NMR (75 MHz, $CDCl_3$+DMSO-d_6**) spectrum of compound 4a**



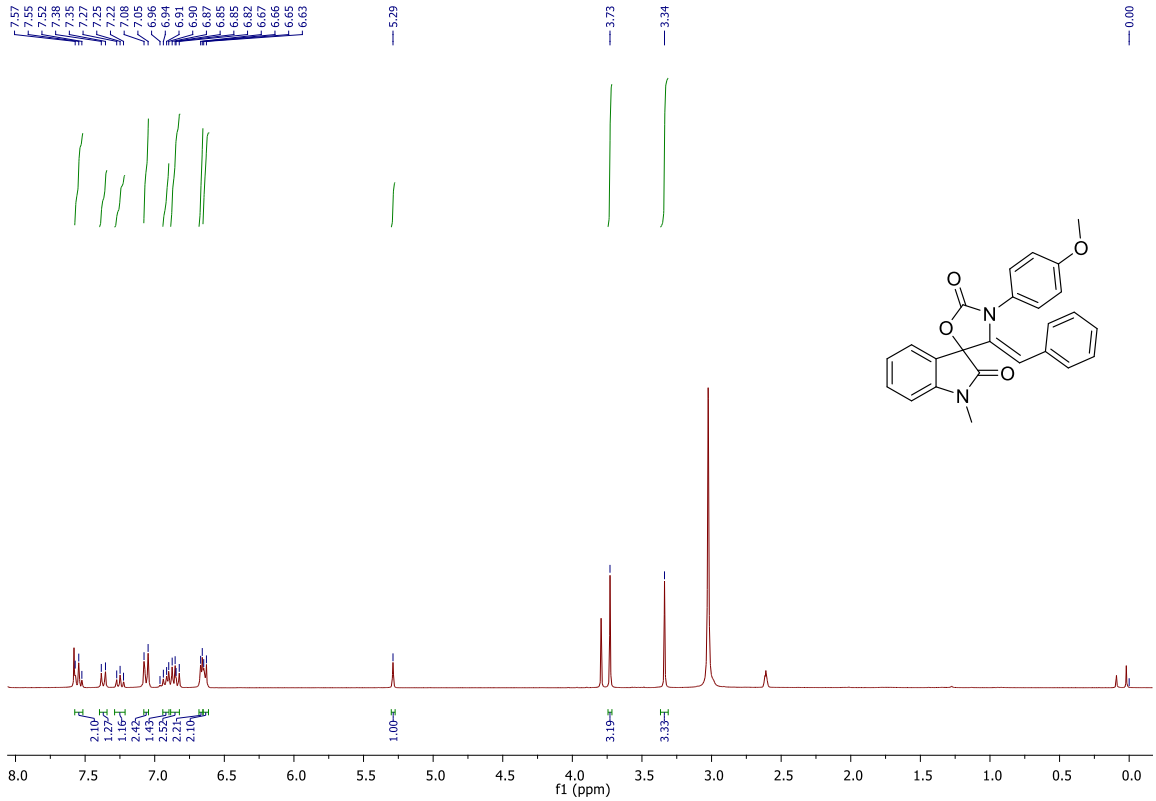
^{1}H NMR (300 MHz, $CDCl_3$+DMSO-d_6**) spectrum of compound 4b**



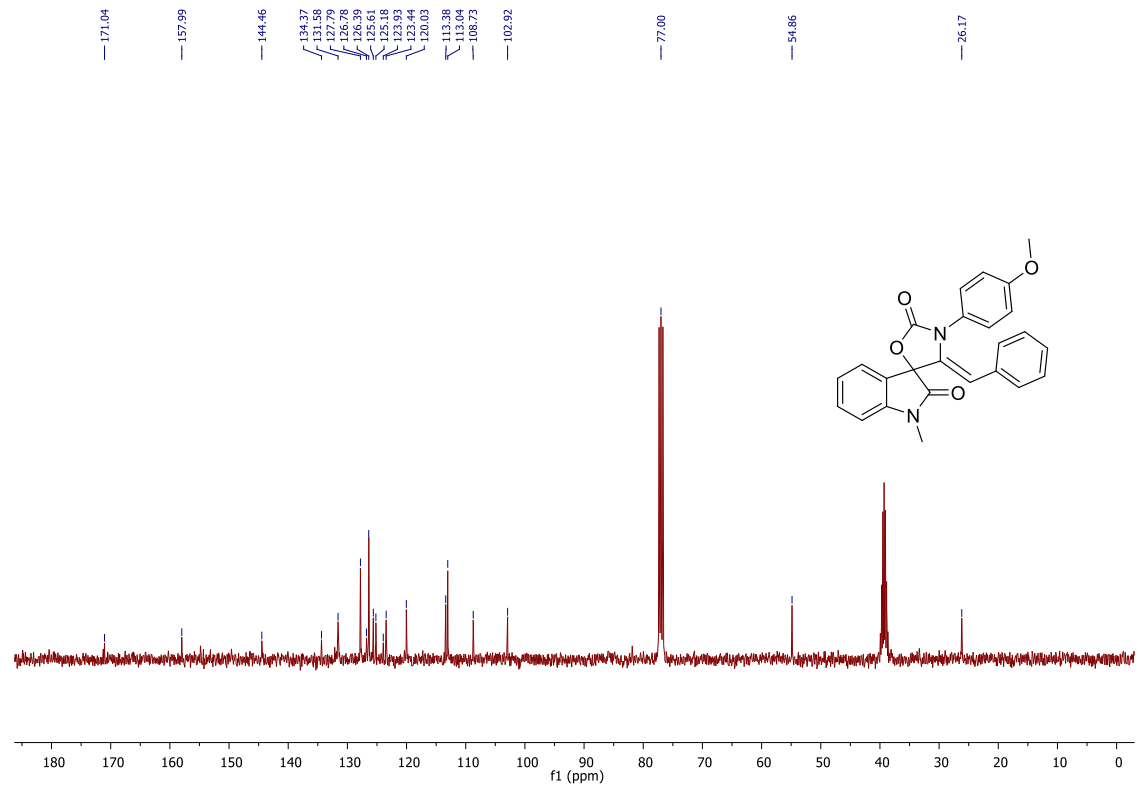
^{13}C NMR (100 MHz, $CDCl_3$+DMSO-d_6**) spectrum of compound 4b**



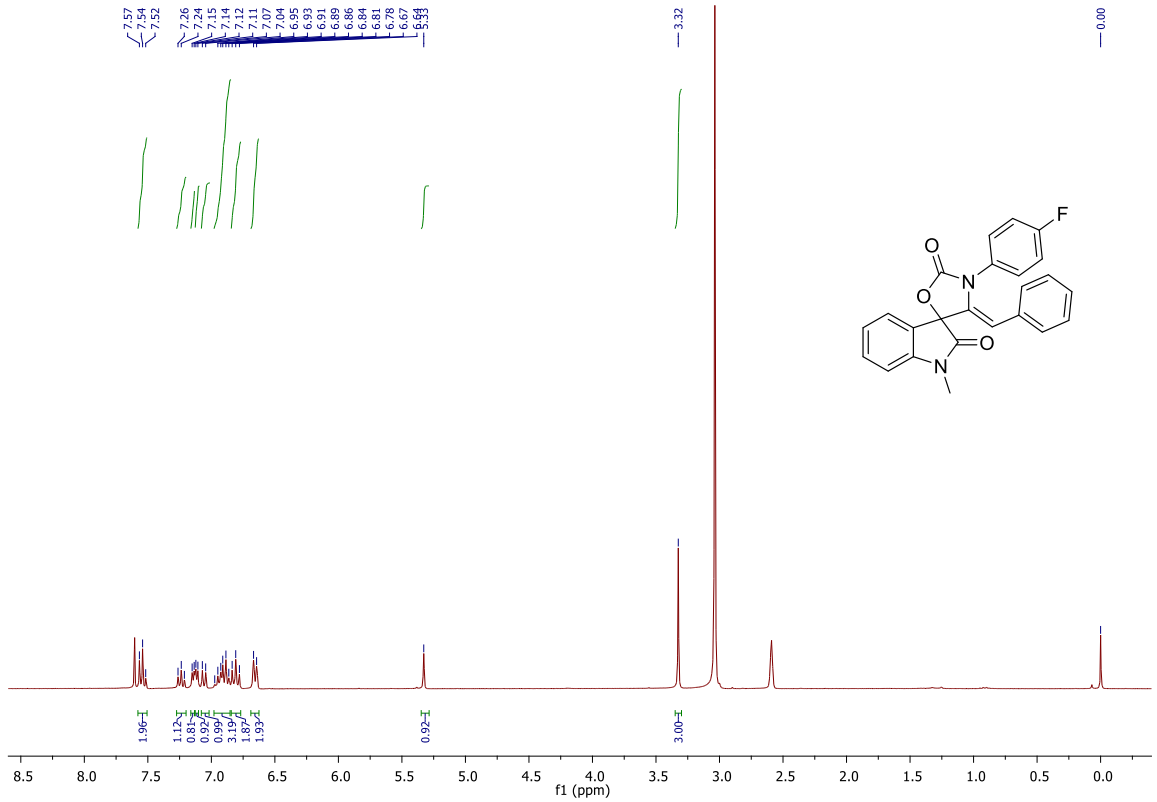
^{1}H NMR (300 MHz, $CDCl_3$+DMSO-d_6**) spectrum of compound 4c**



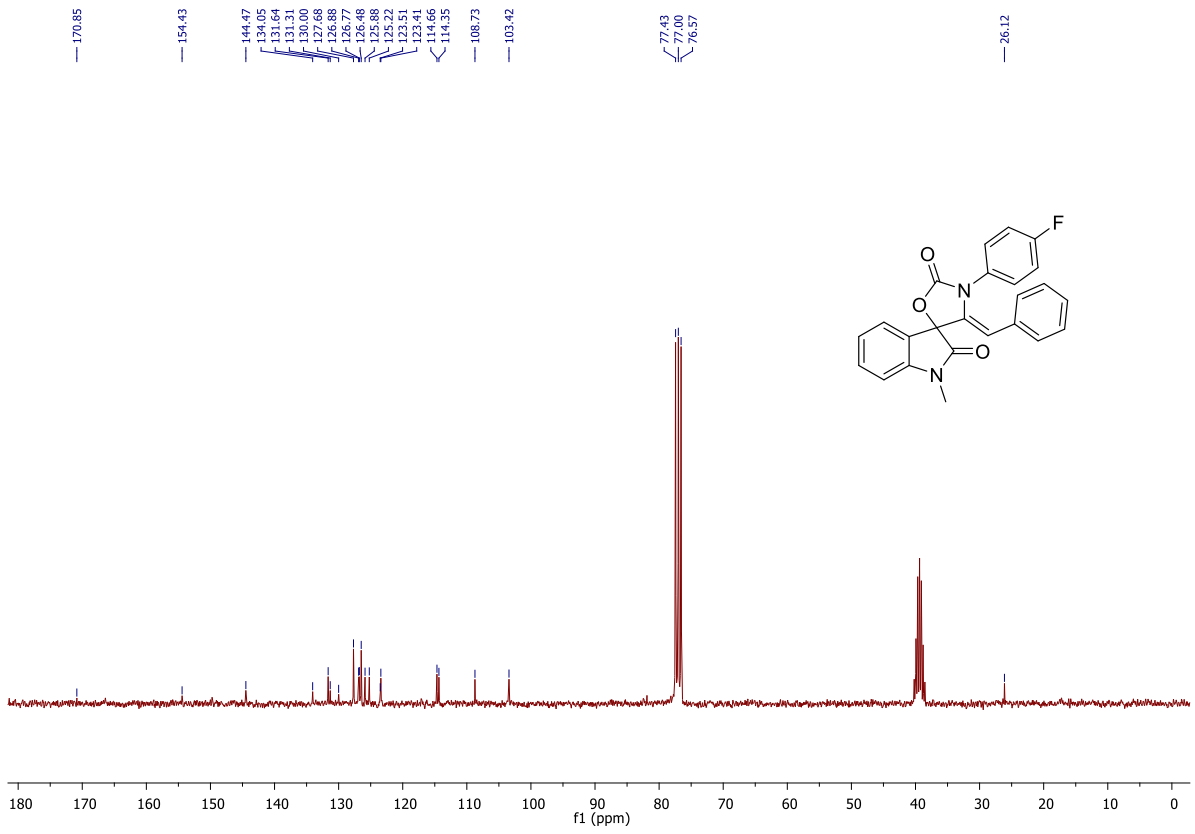
^{13}C NMR (100 MHz, $CDCl_3$+DMSO-d_6**) spectrum of compound 4c**



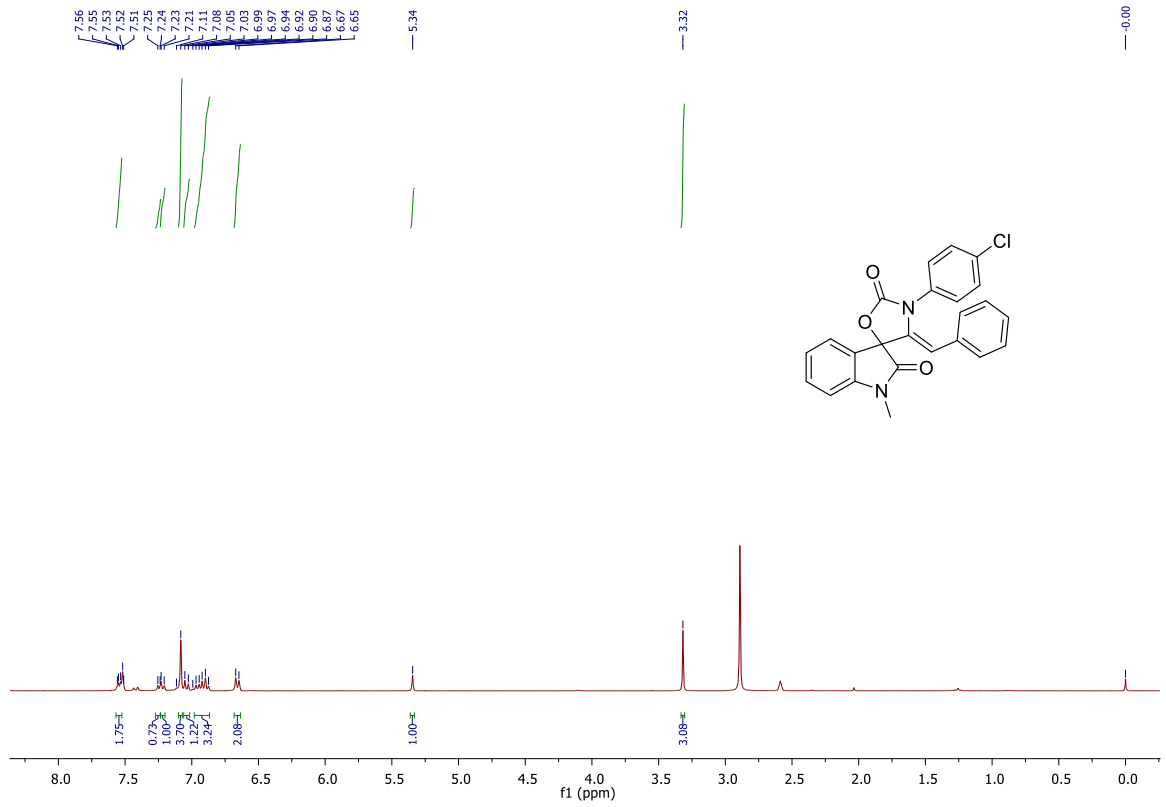
^{1}H NMR (300 MHz, $CDCl_3$+DMSO-d_6**) spectrum of compound 4d**



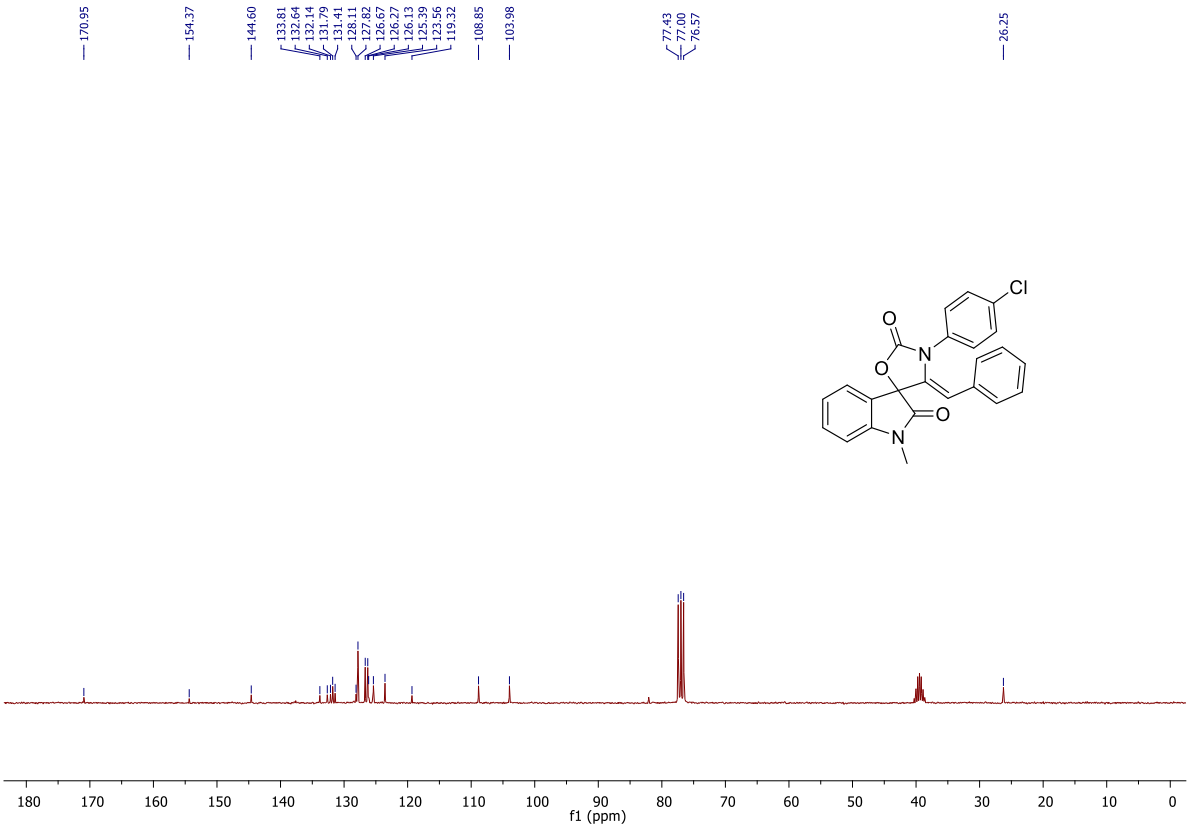
^{13}C NMR (75 MHz, $CDCl_3$+DMSO-d_6**) spectrum of compound 4d**



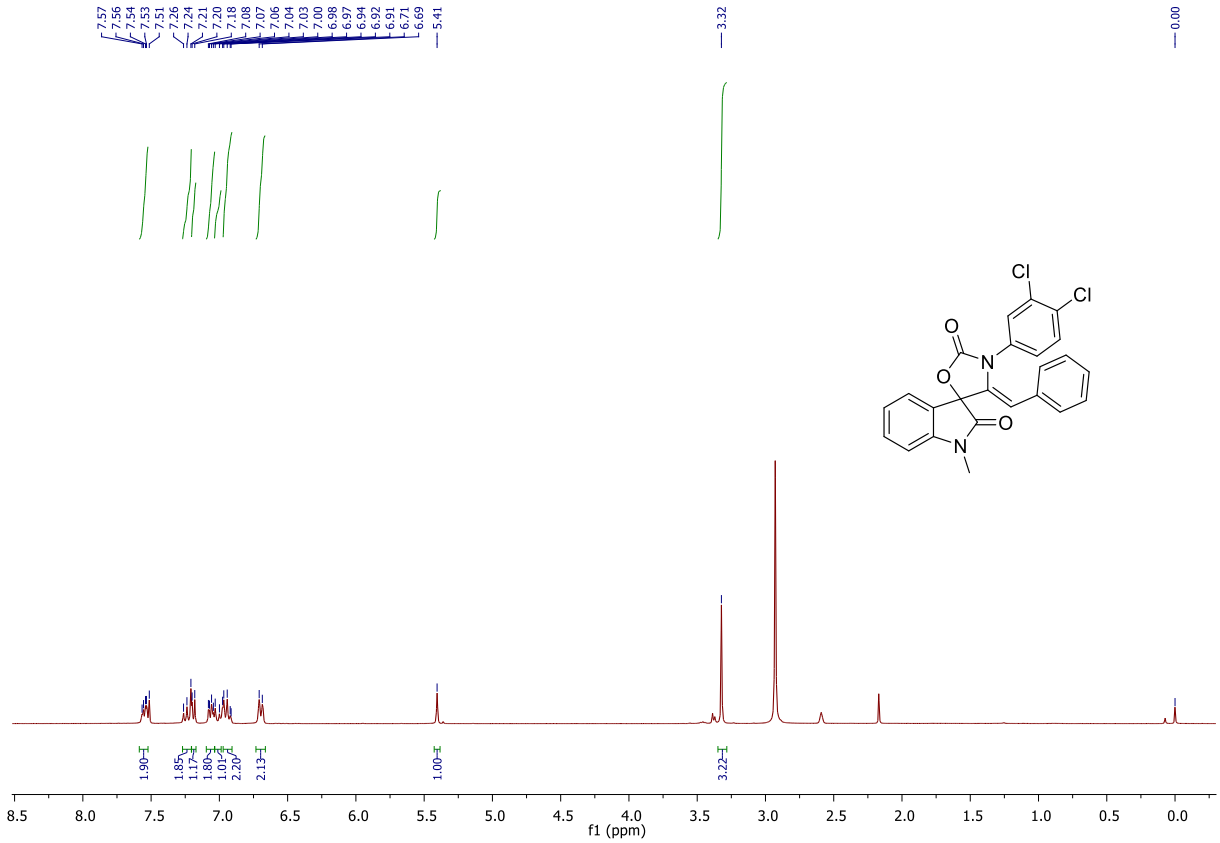
^{1}H NMR (300 MHz, $CDCl_3$+DMSO-d_6) spectrum of compound 4e



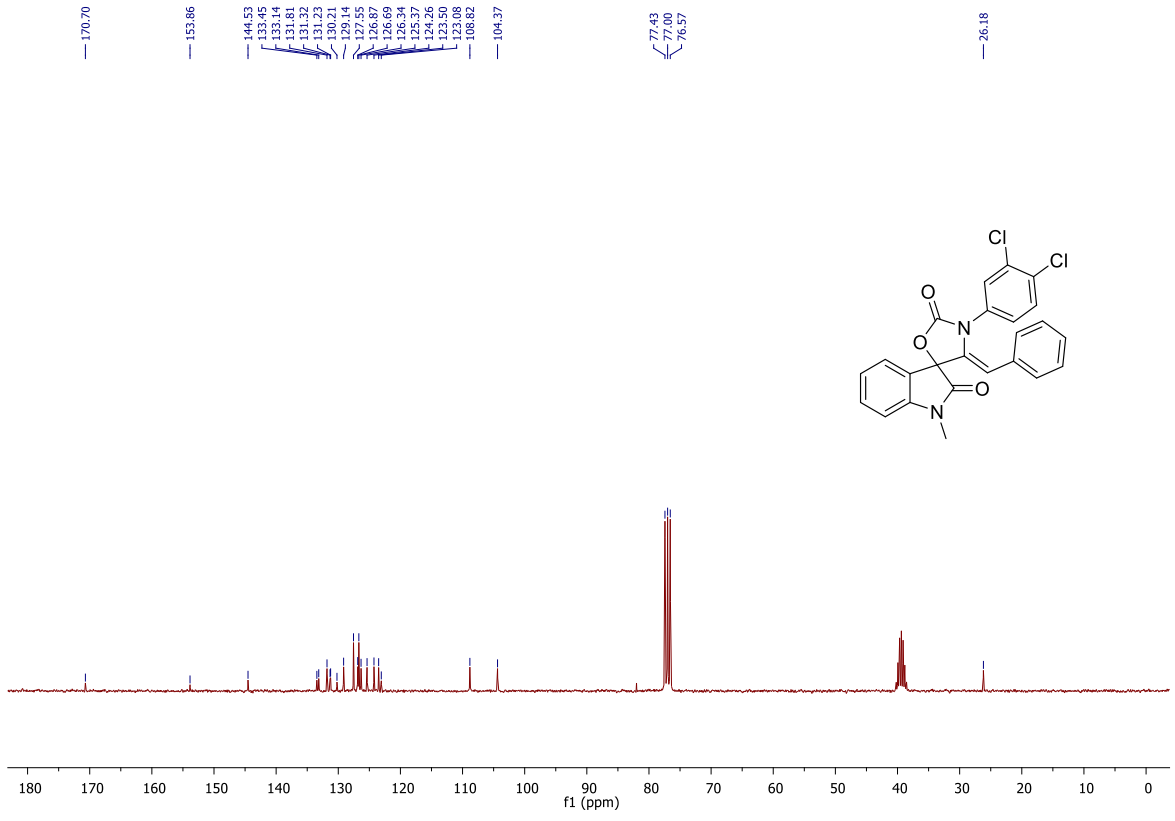
^{13}C NMR (75 MHz, $CDCl_3$+DMSO-d_6) spectrum of compound 4e



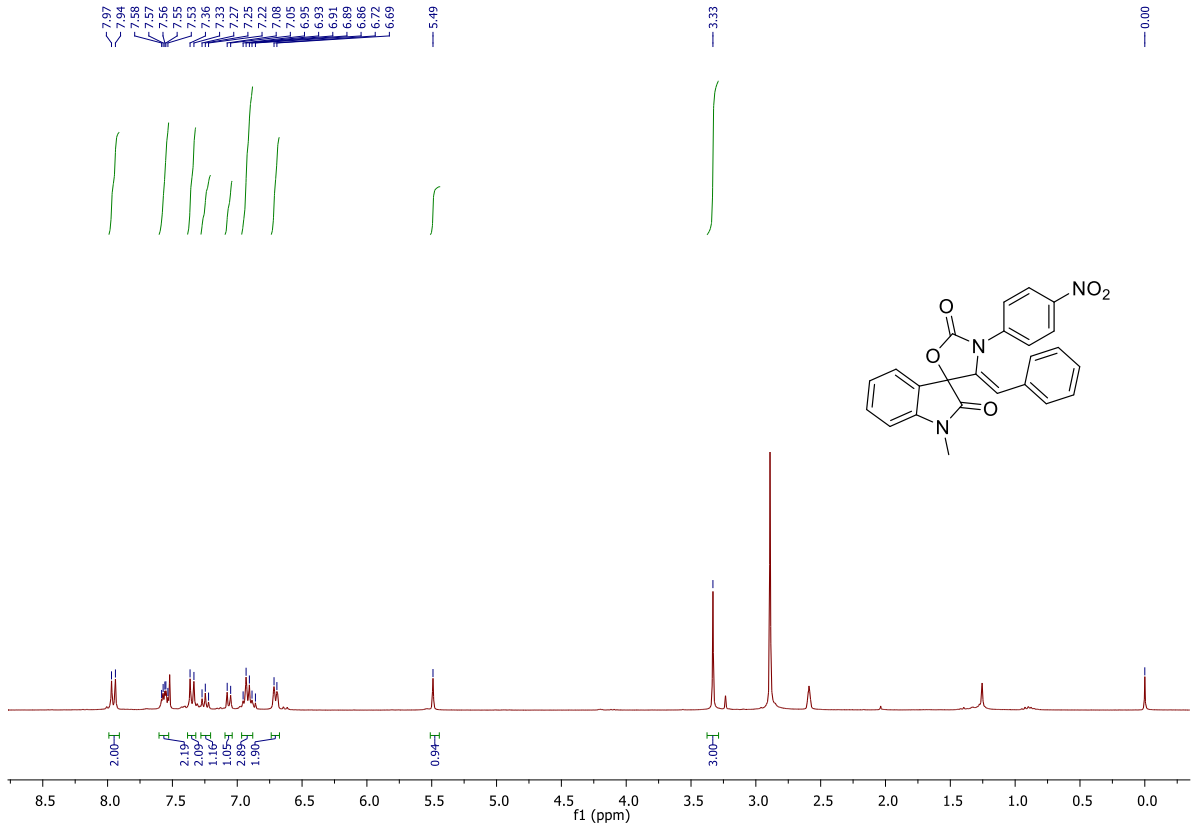
^{1}H NMR (300 MHz, $CDCl_3$+DMSO-d_6**) spectrum of compound 4f**



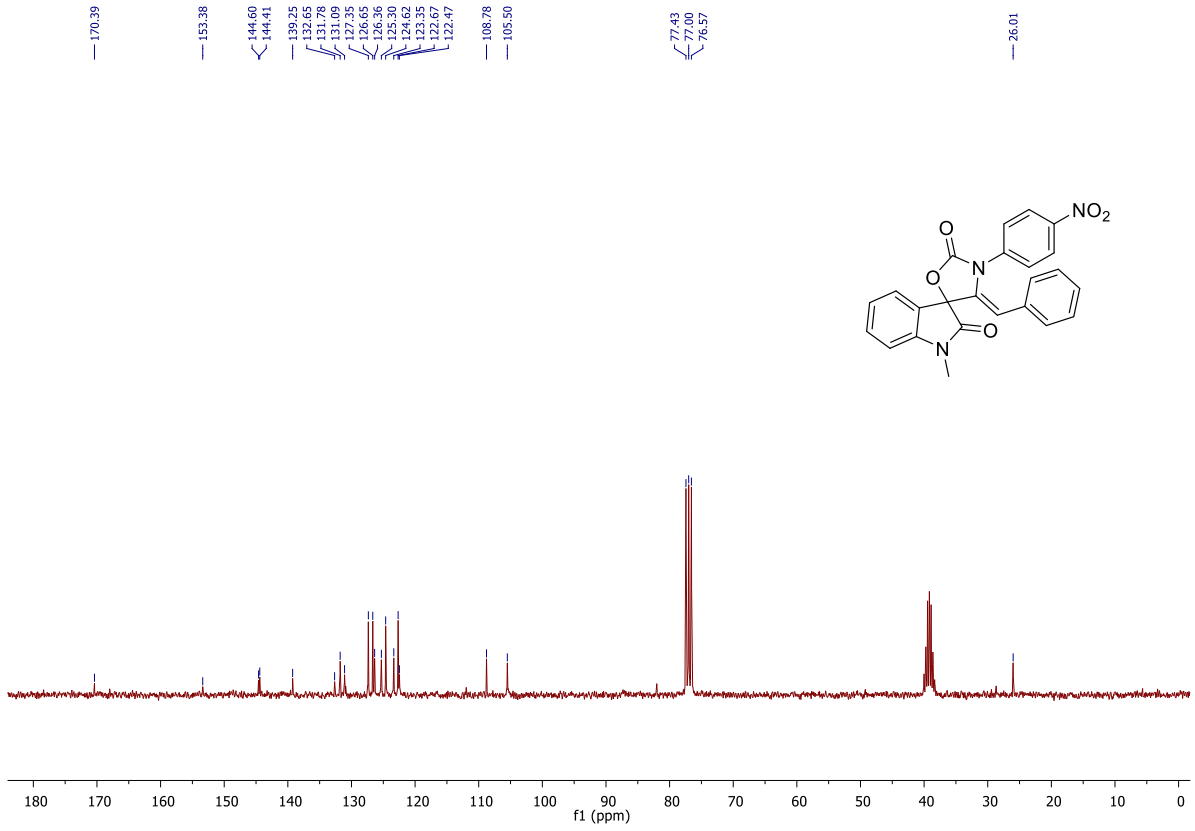
^{13}C NMR (75 MHz, $CDCl_3$+DMSO-d_6**) spectrum of compound 4f**



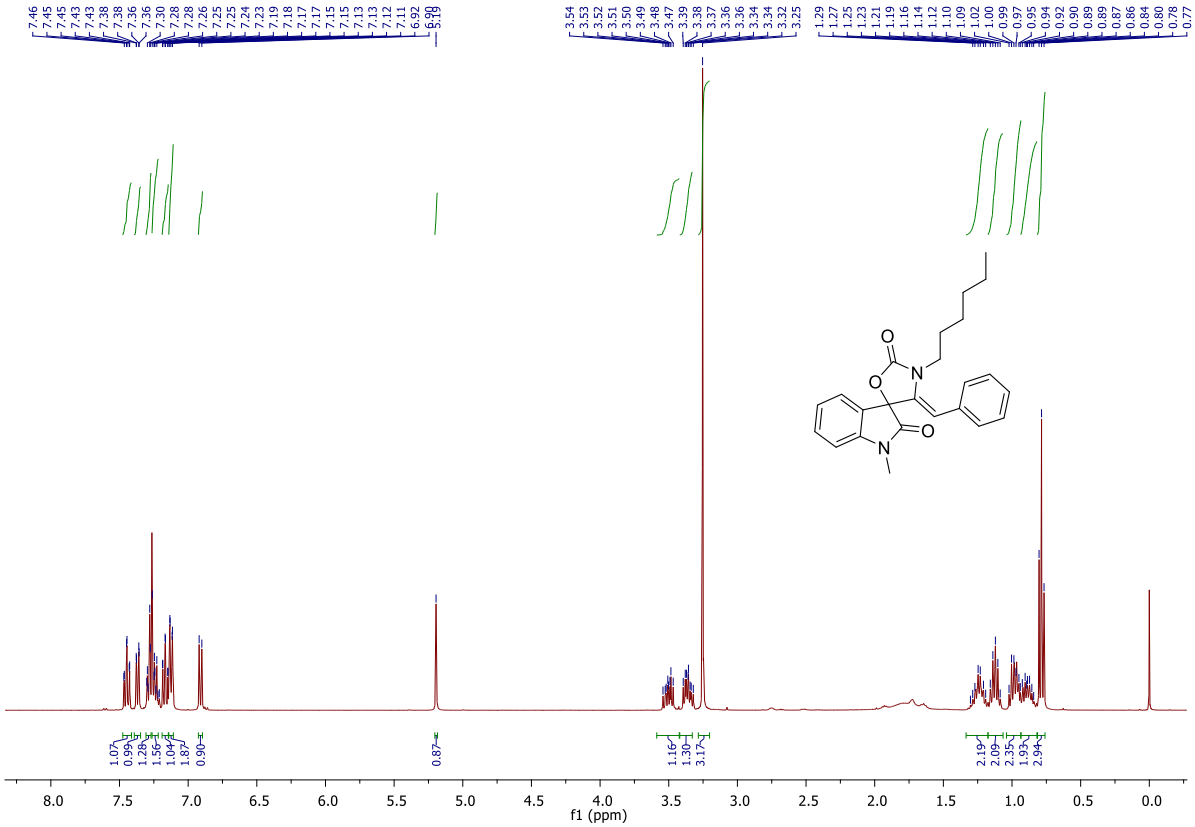
^{1}H NMR (300 MHz, $CDCl_3$+DMSO-d_6**) spectrum of compound 4g**



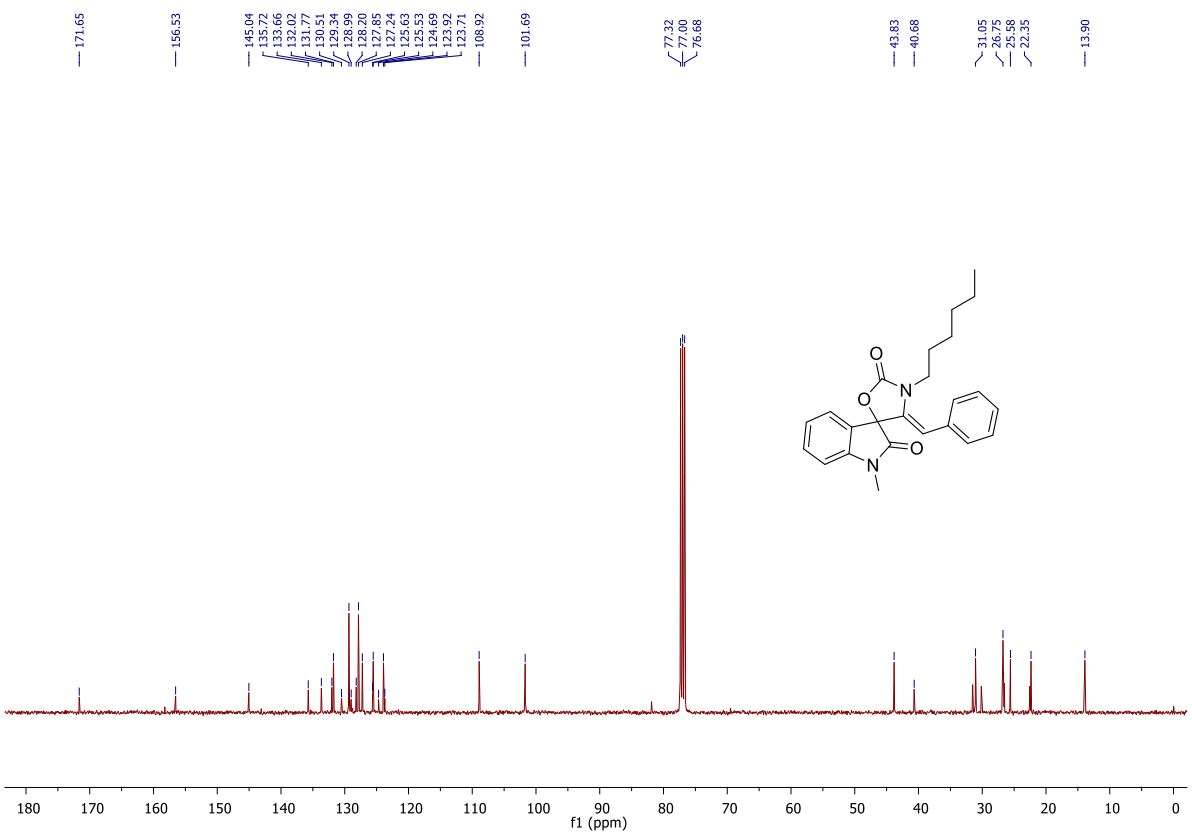
^{13}C NMR (75 MHz, $CDCl_3$+DMSO-d_6**) spectrum of compound 4g**



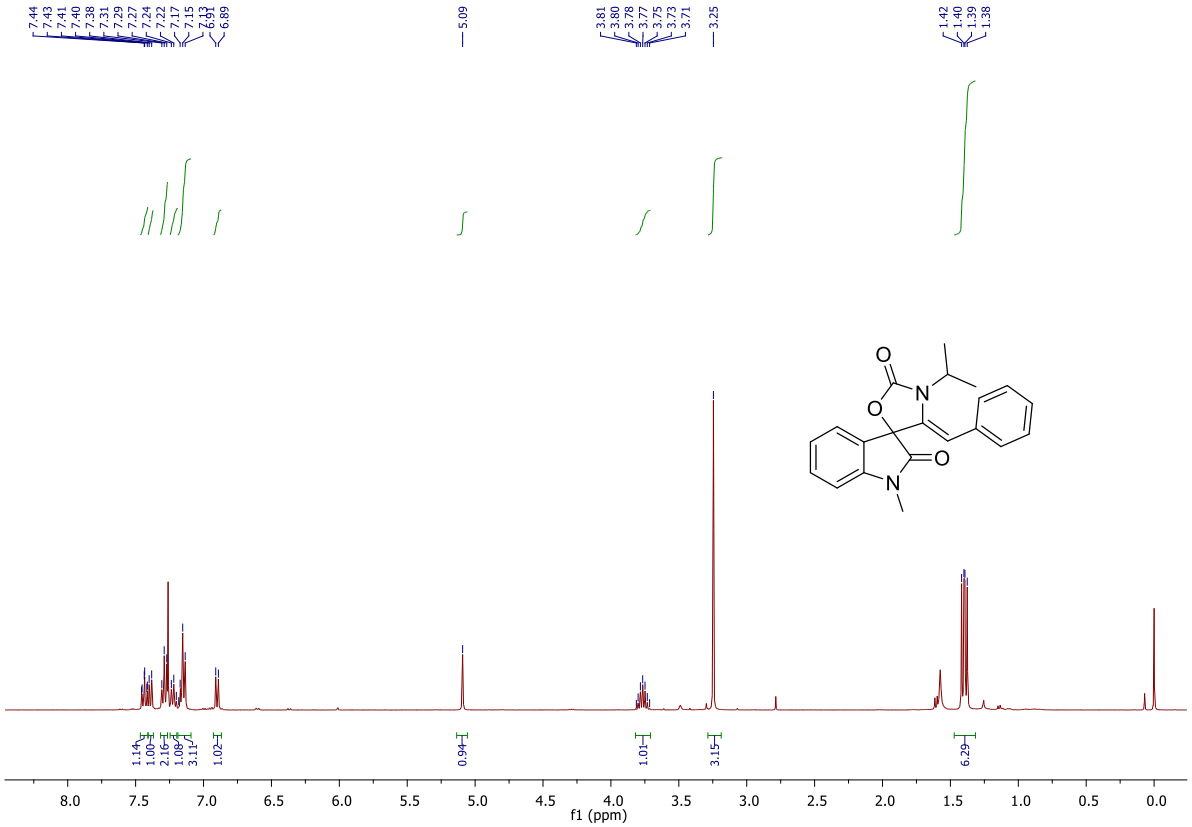
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 4h



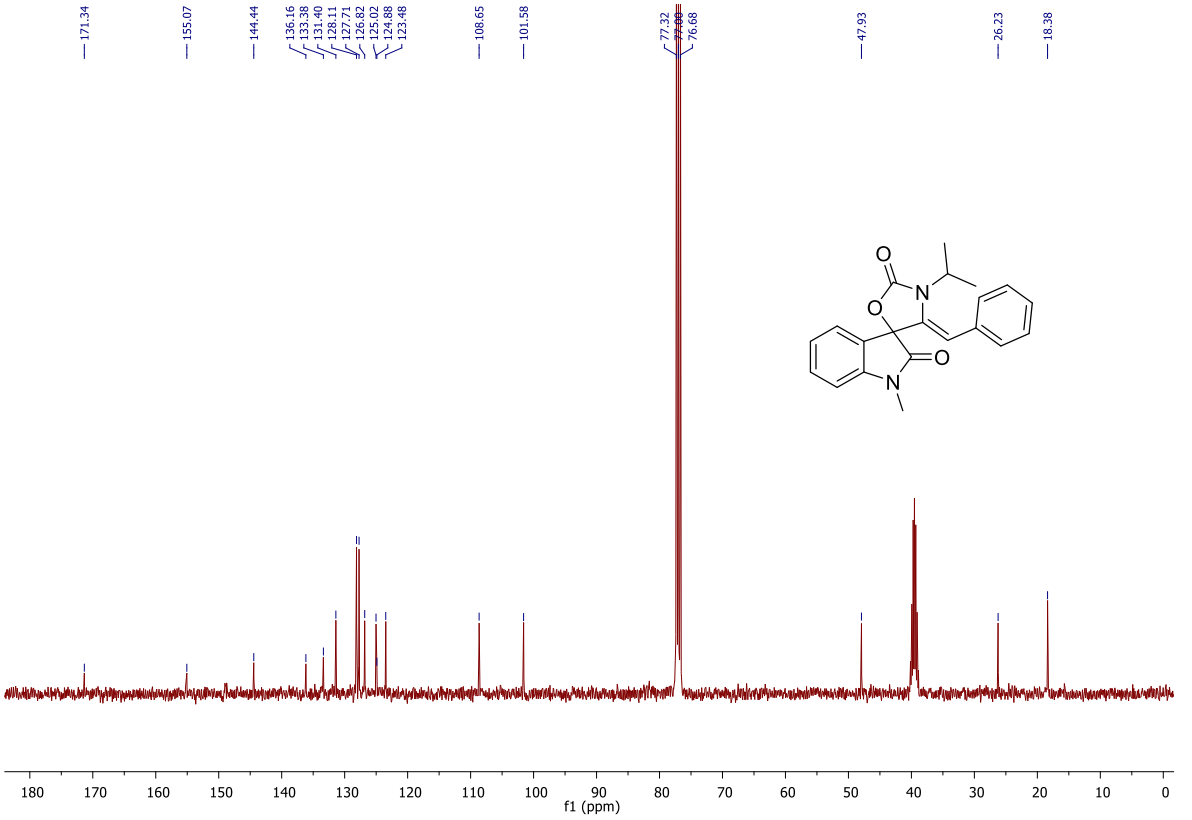
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 4h



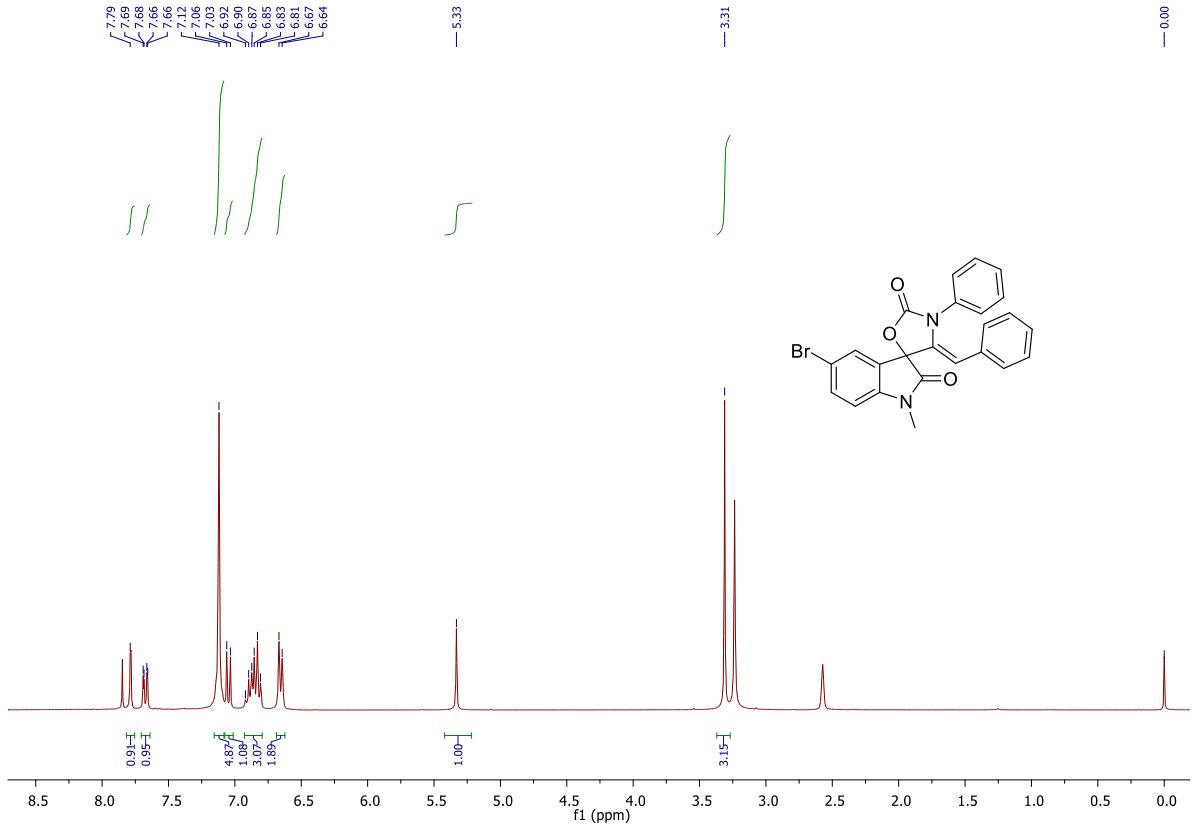
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 4i



^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 4i



^{1}H NMR (300 MHz, $CDCl_3$+DMSO-d_6) spectrum of compound 4j



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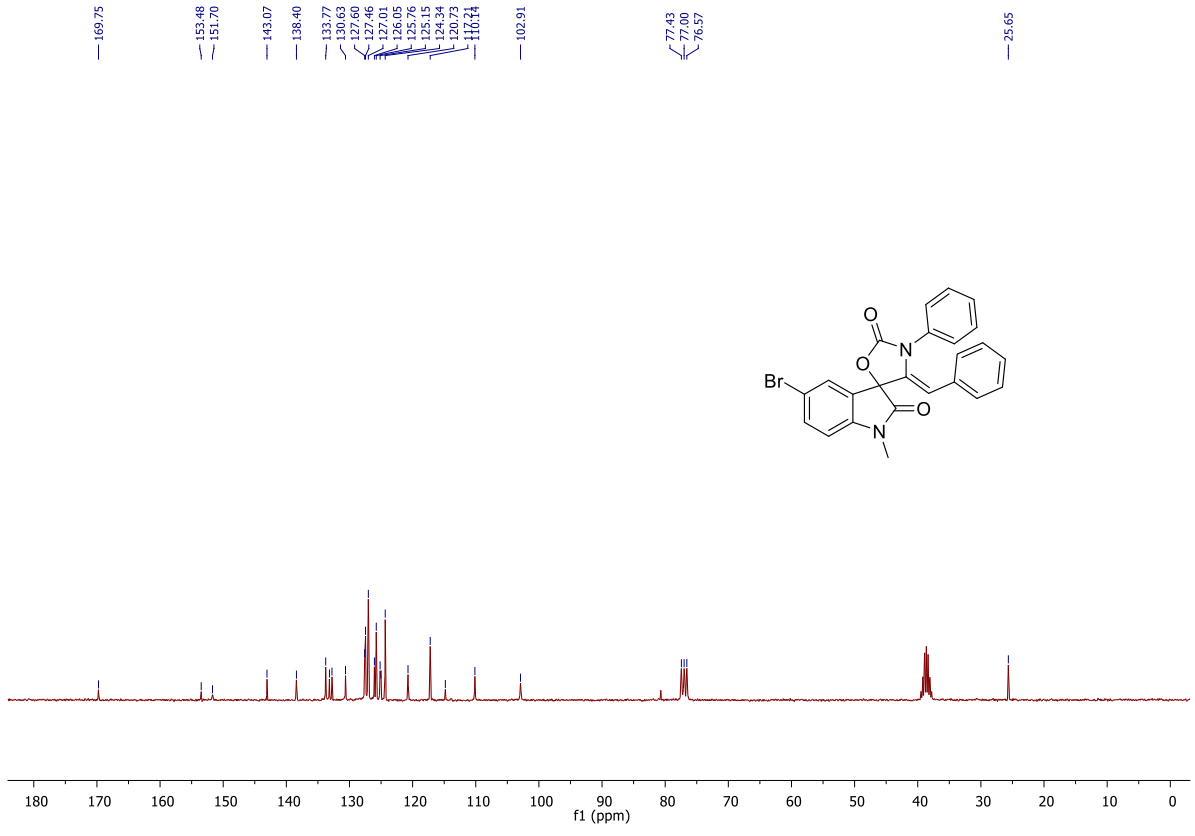
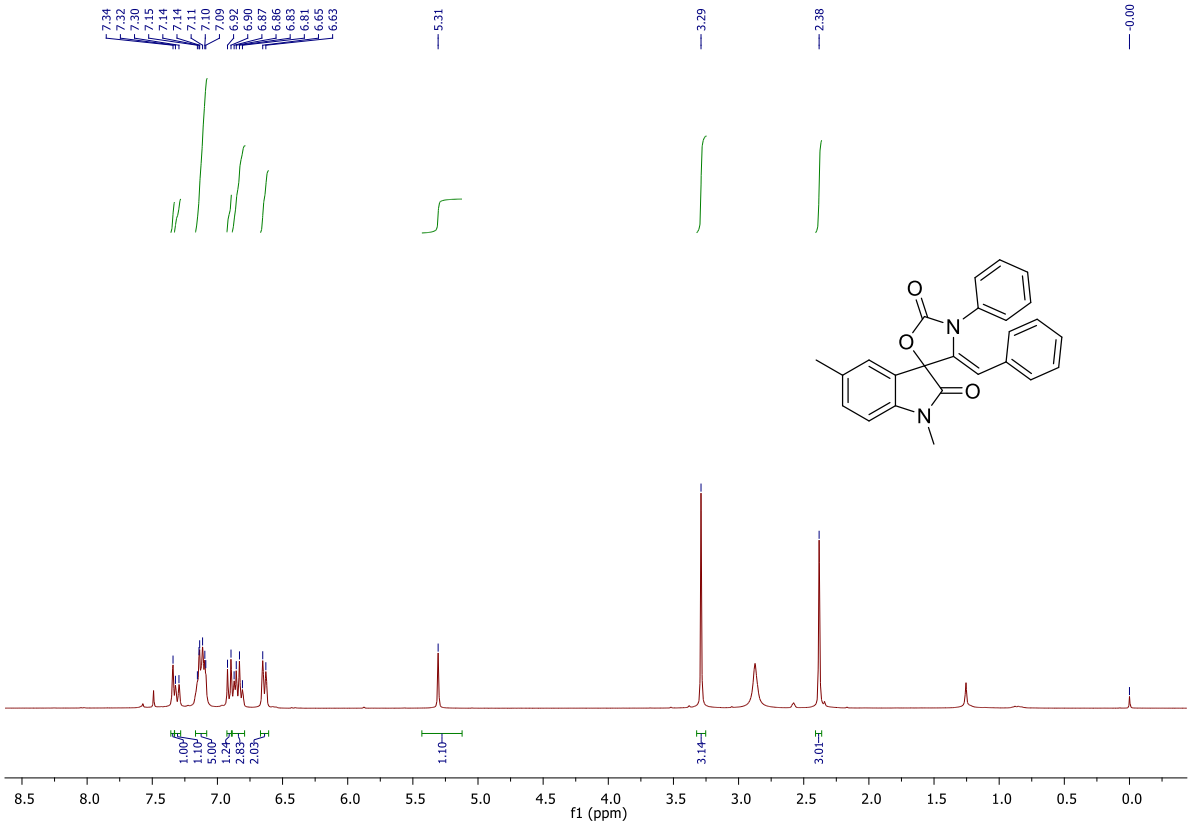
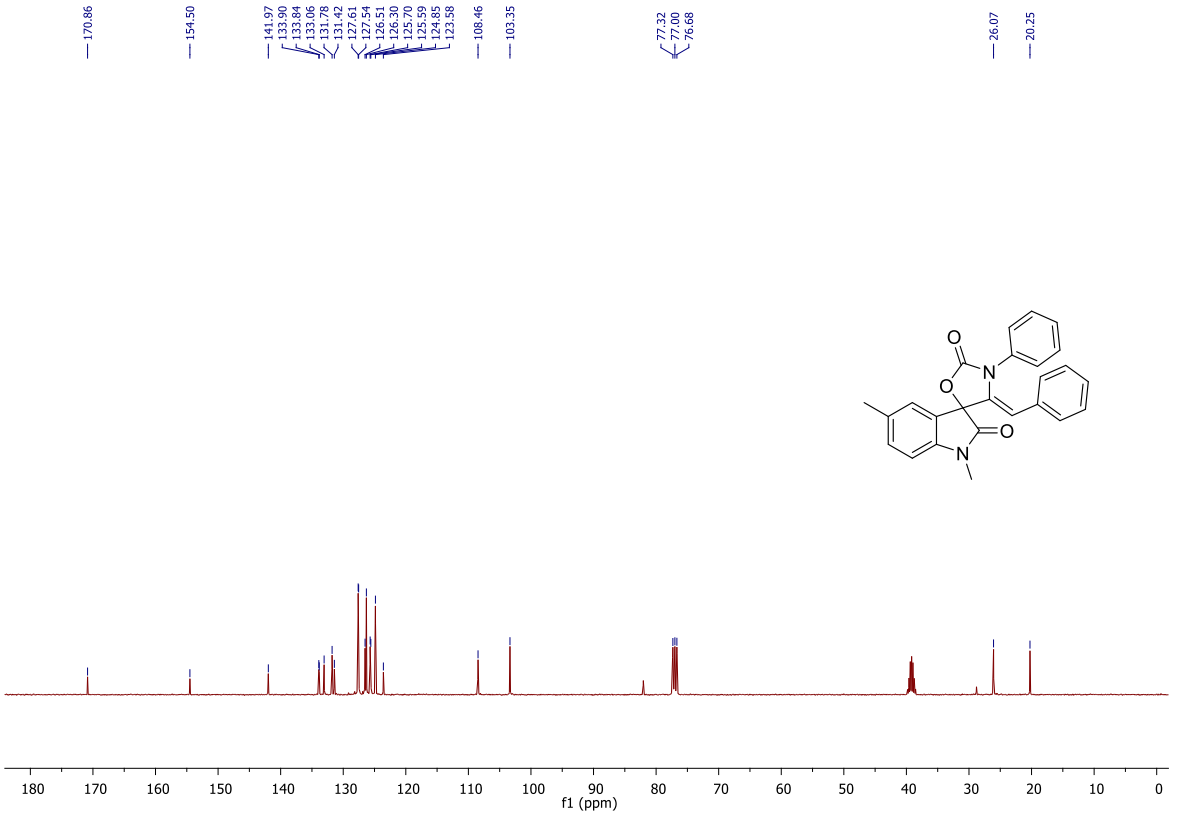


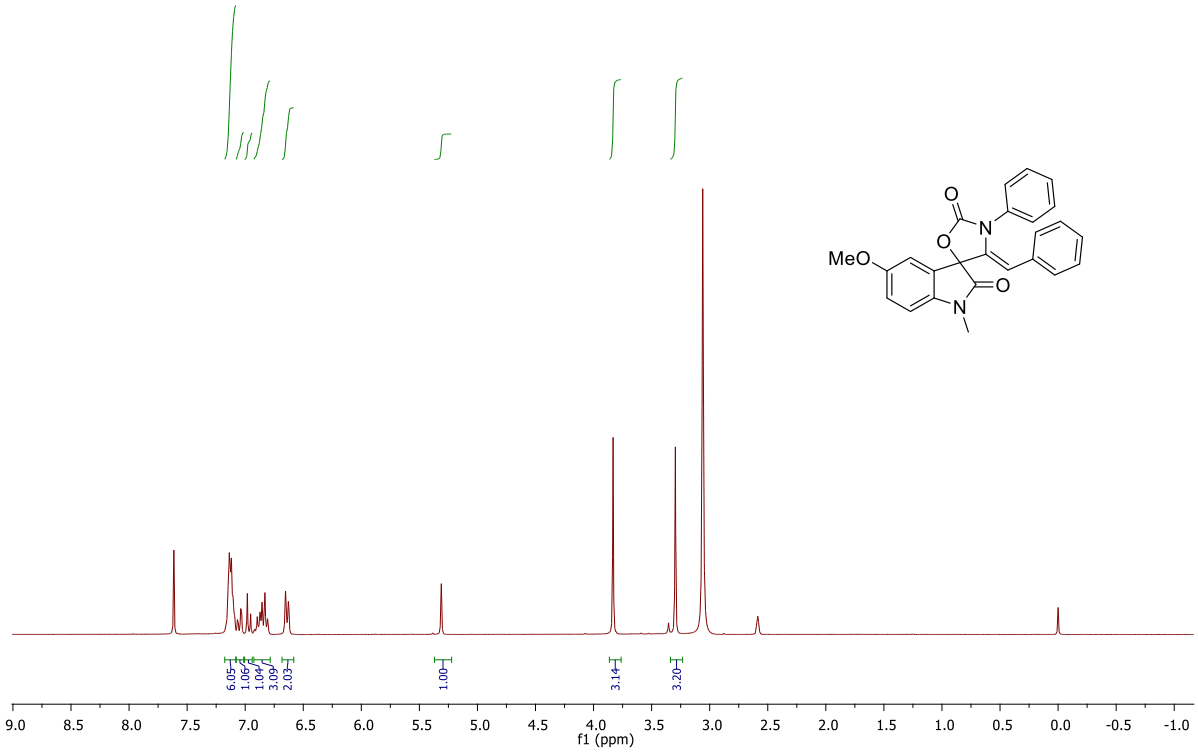
^{1}H NMR (300 MHz, $CDCl_3$+DMSO-d_6**) spectrum of compound 4k**



^{13}C NMR (75 MHz, $CDCl_3$+DMSO-d_6**) spectrum of compound 4k**



^{1}H NMR (300 MHz, $CDCl_3$+DMSO-d_6) spectrum of compound 4l



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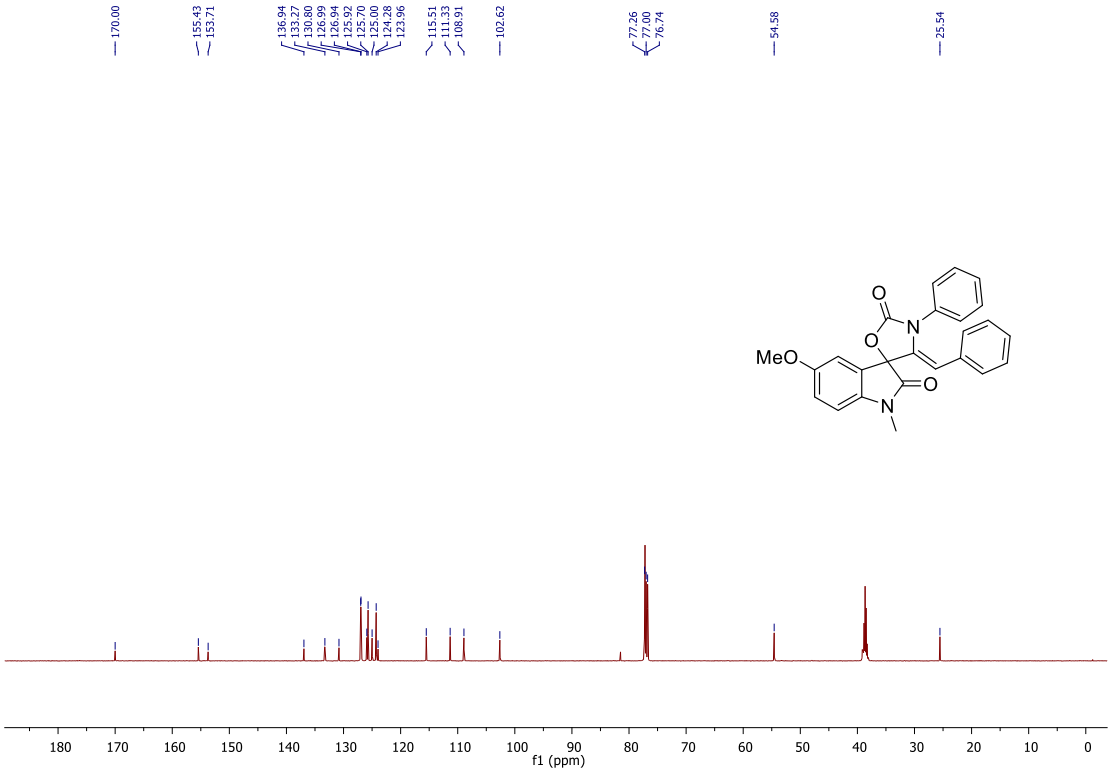
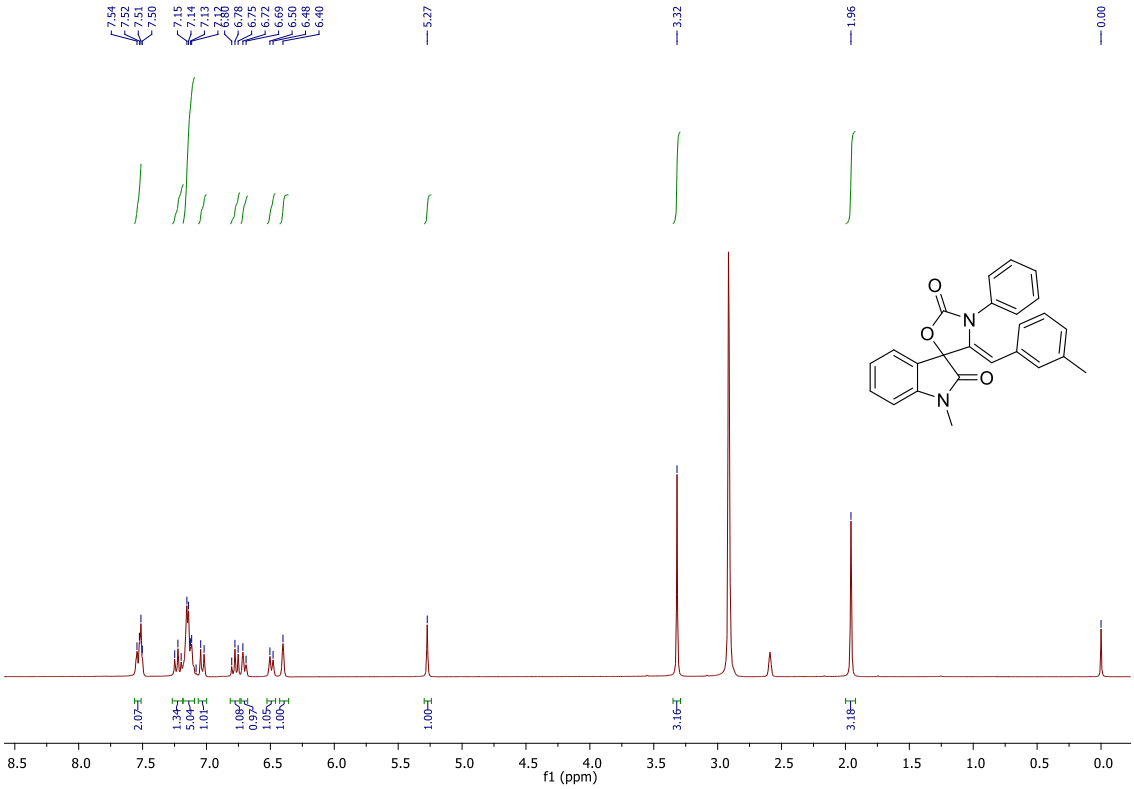
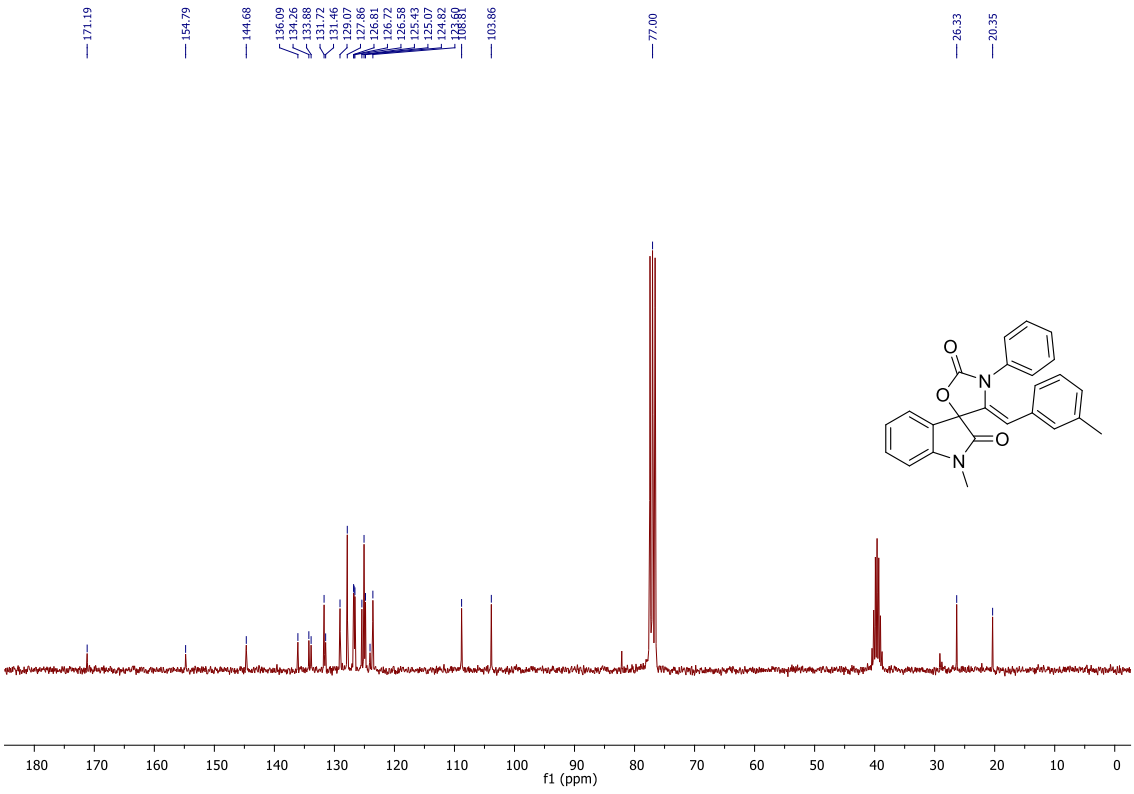


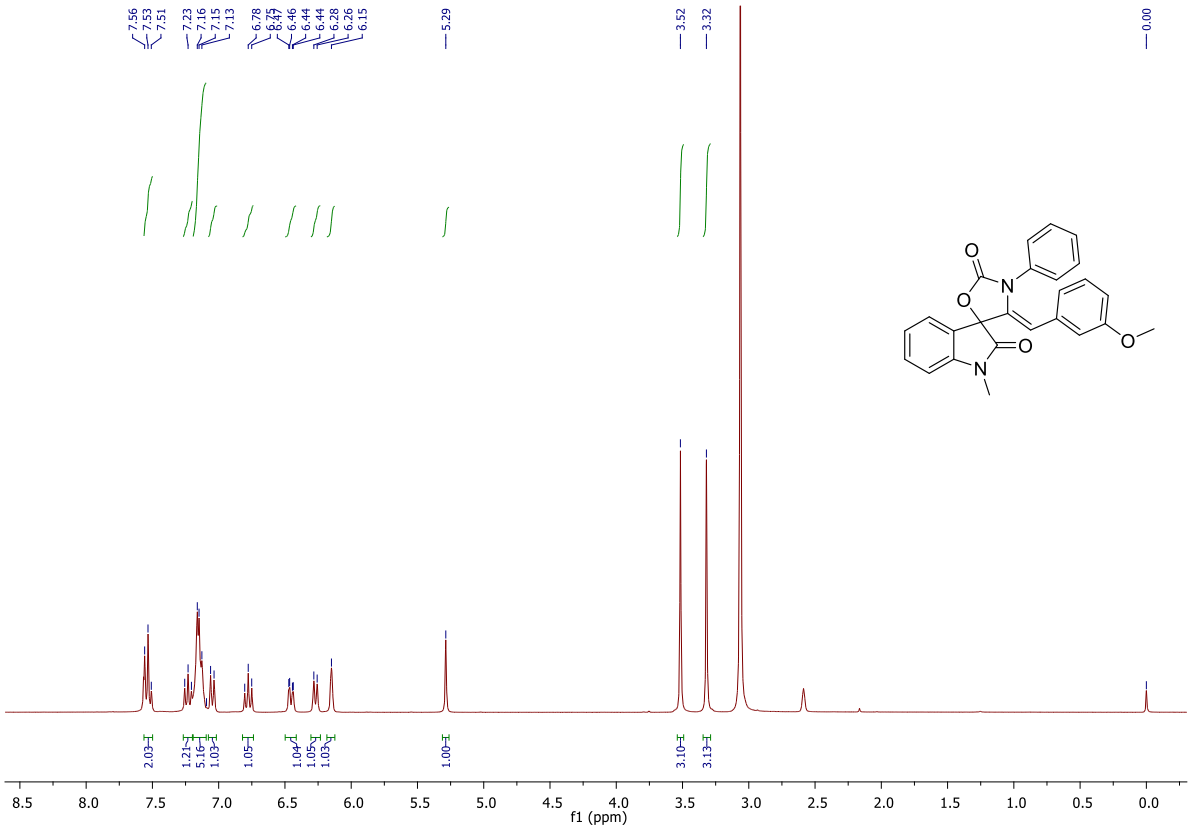
^{1}H NMR (300 MHz, $CDCl_3$+DMSO-d_6) spectrum of compound 4m



^{13}C NMR (75 MHz, $CDCl_3$+DMSO-d_6) spectrum of compound 4m



^{1}H NMR (300 MHz, $CDCl_3$+DMSO-d_6) spectrum of compound 4n



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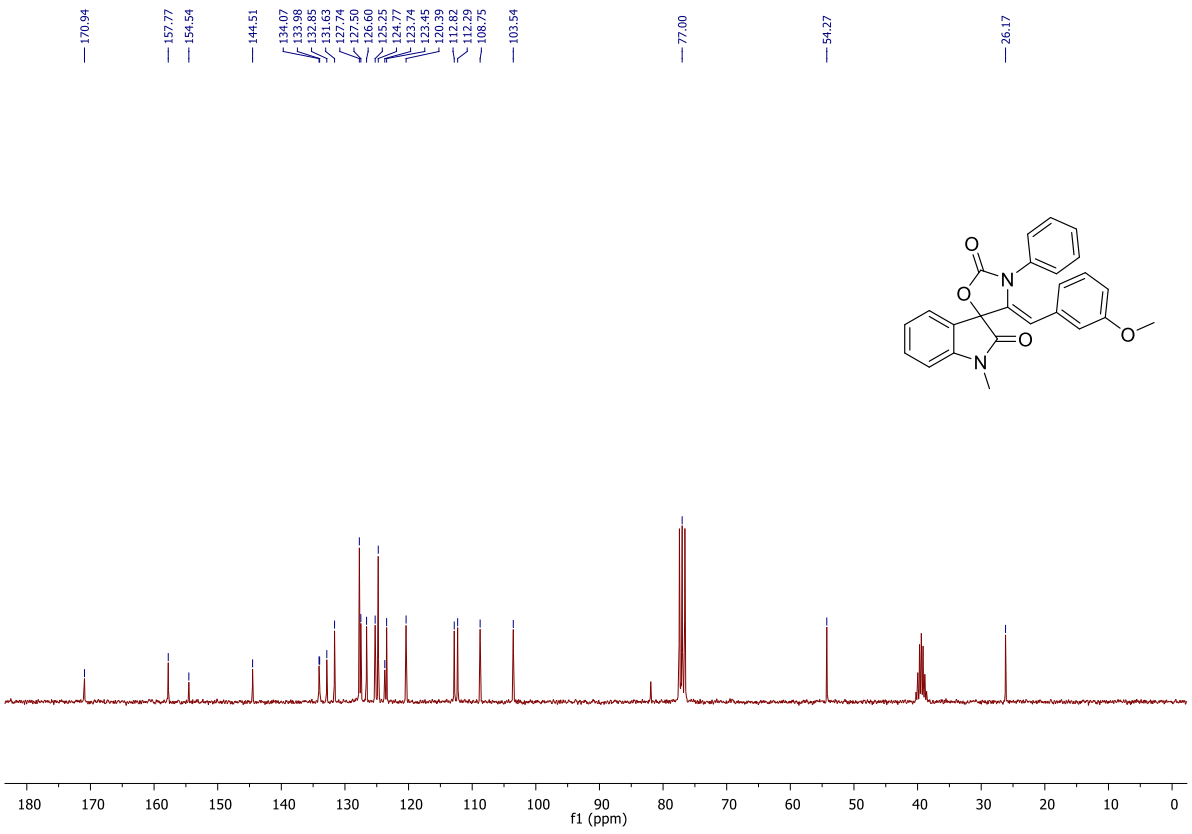
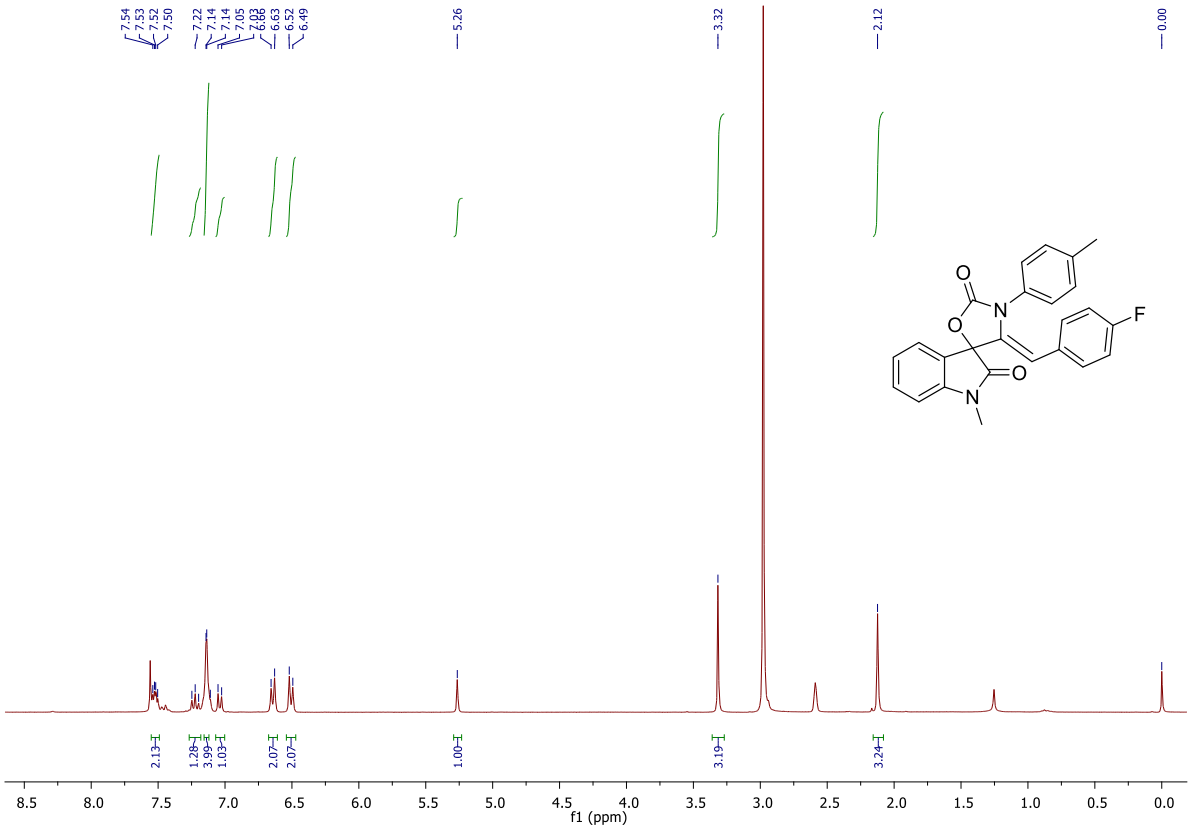
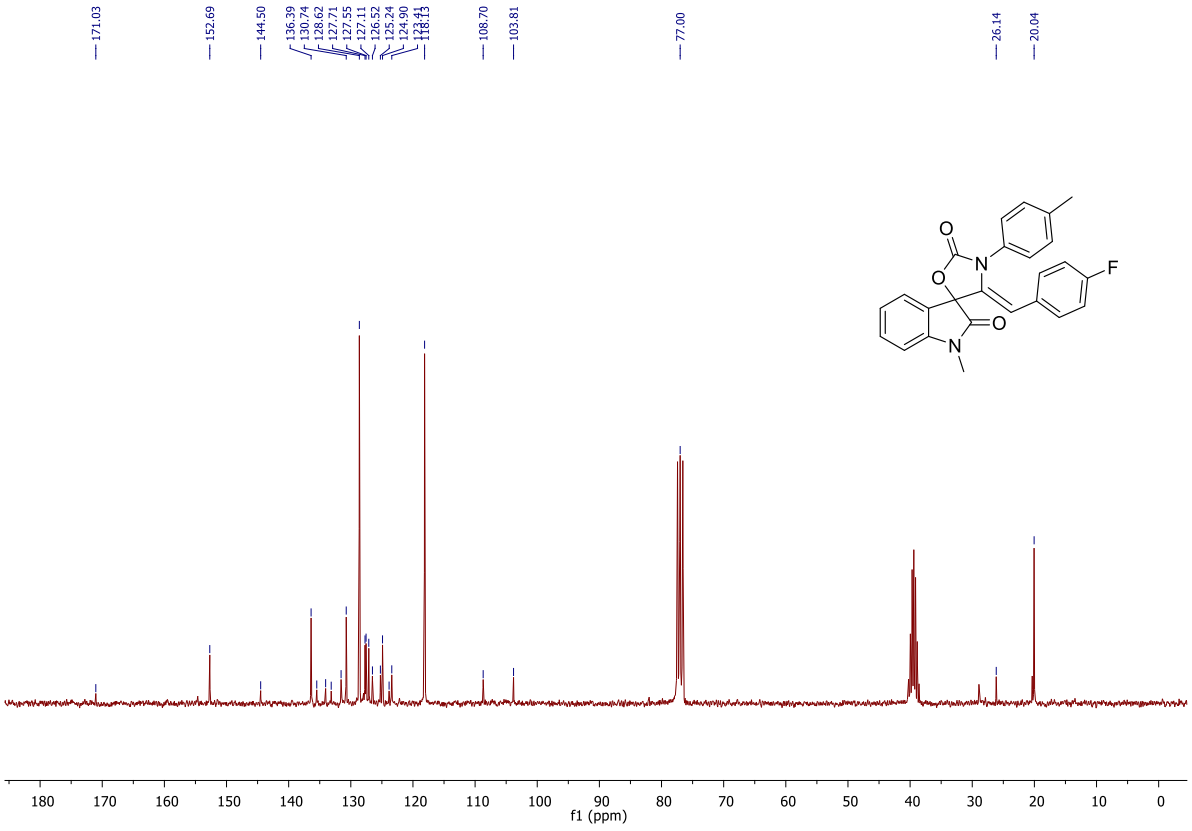


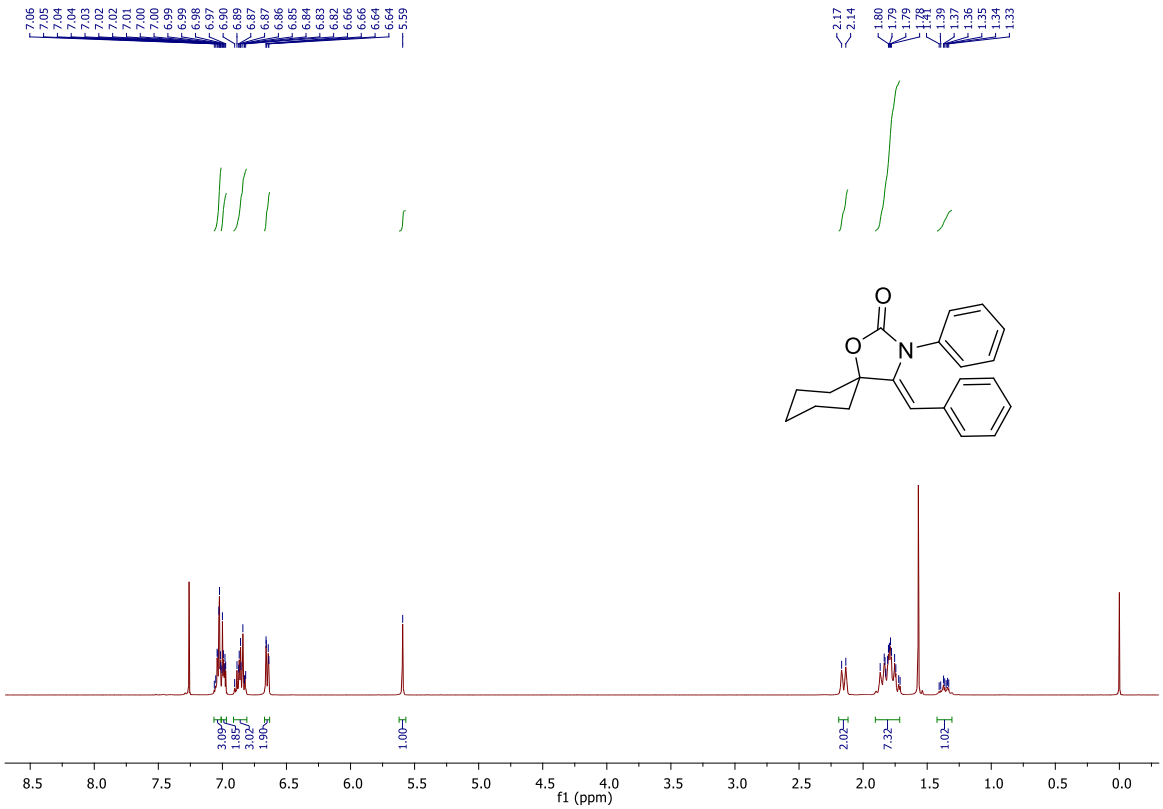
^{1}H NMR (300 MHz, $CDCl_3$+DMSO-d_6**) spectrum of compound 4o**



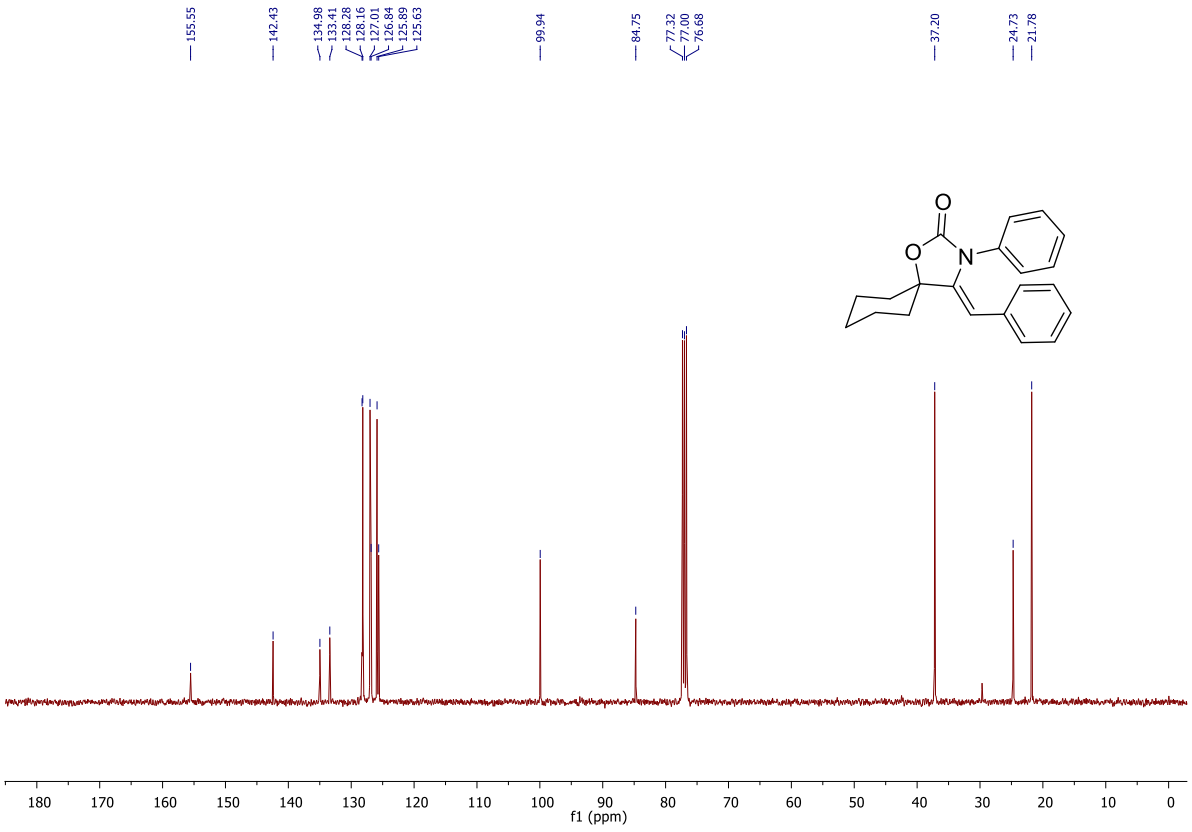
^{13}C NMR (75 MHz, $CDCl_3$+DMSO-d_6**) spectrum of compound 4o**



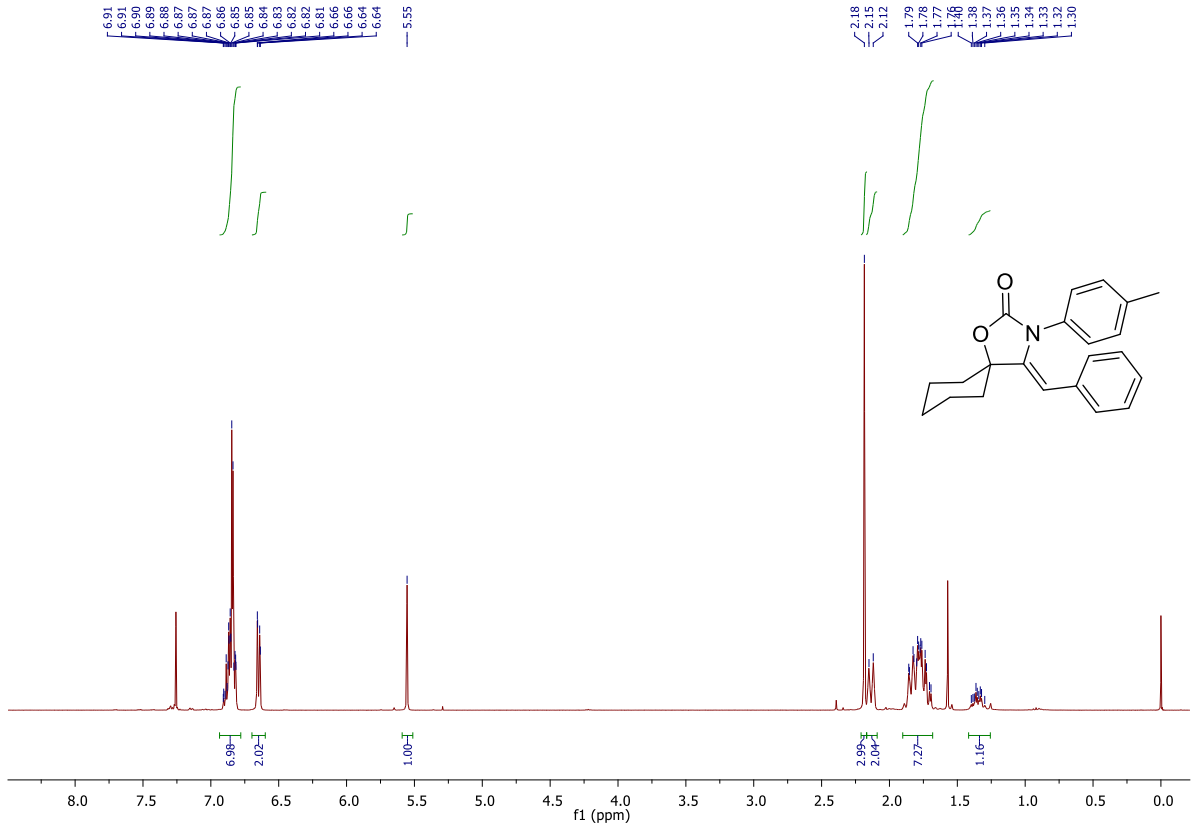
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 6a



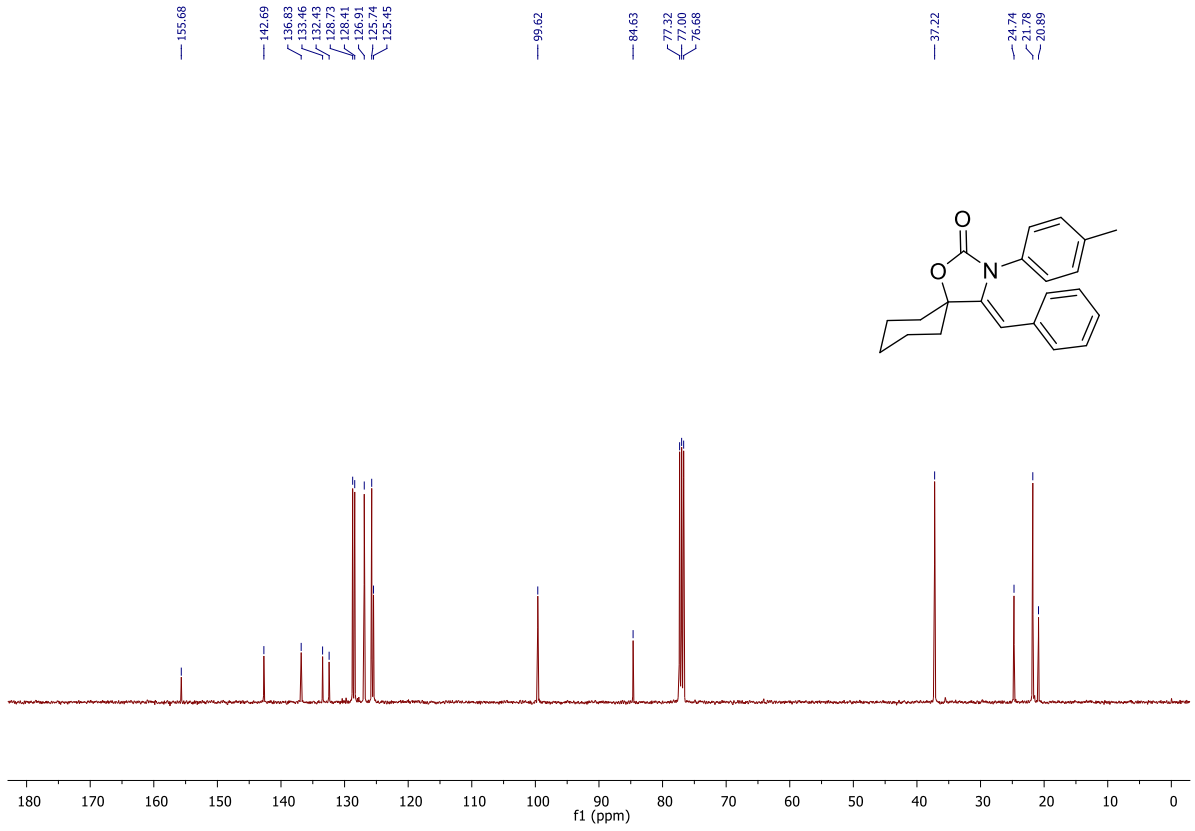
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 6a



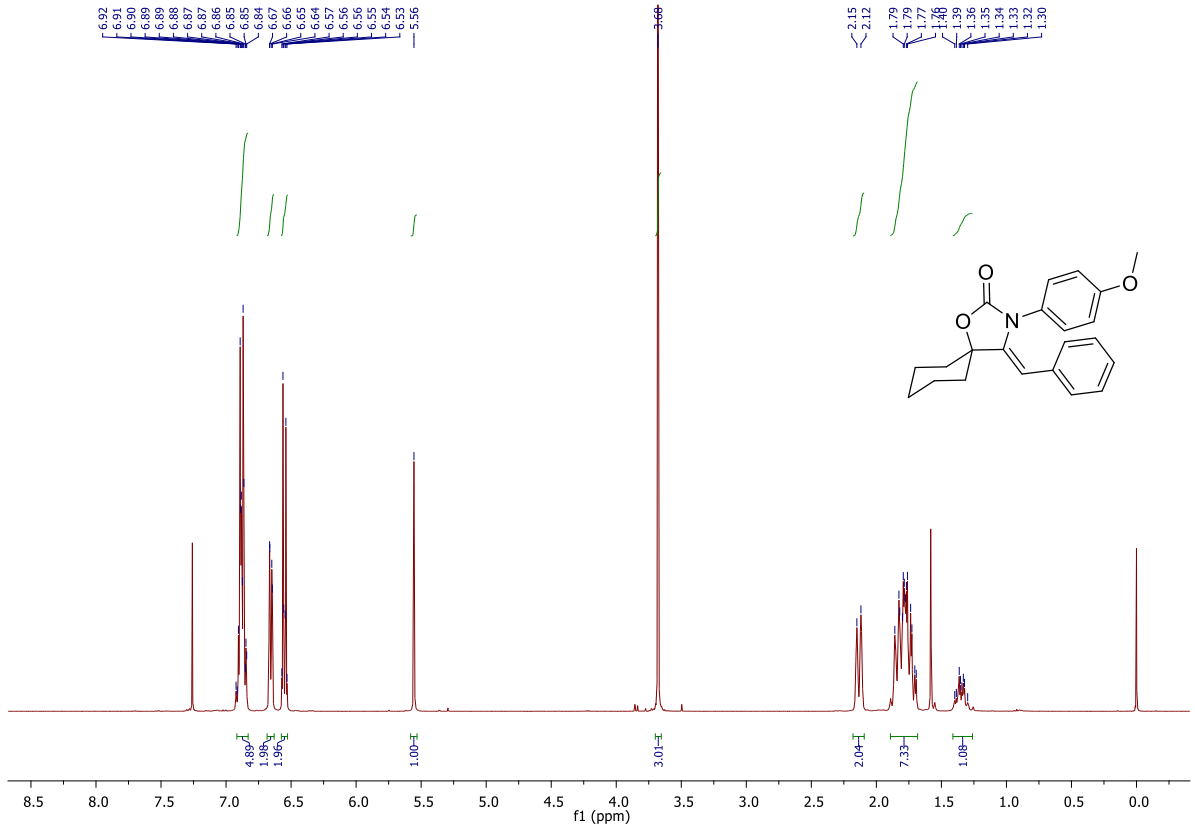
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 6b



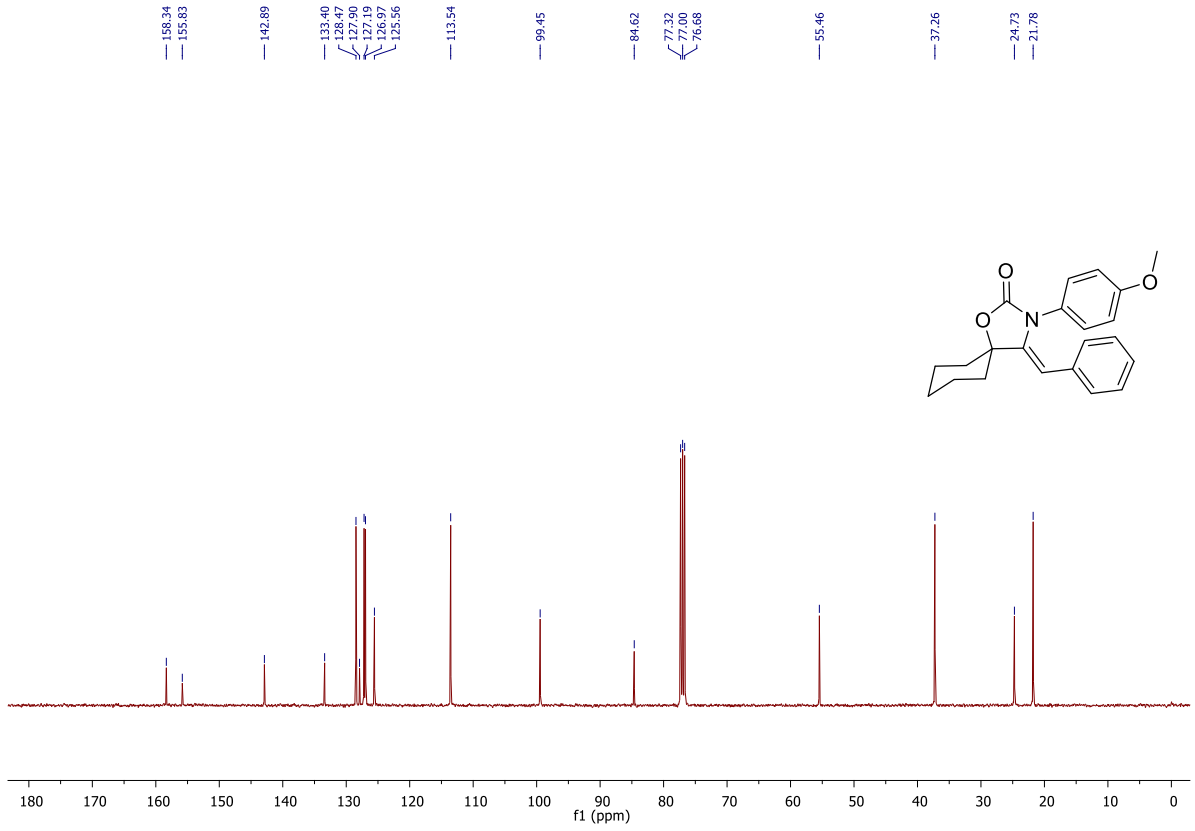
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 6b



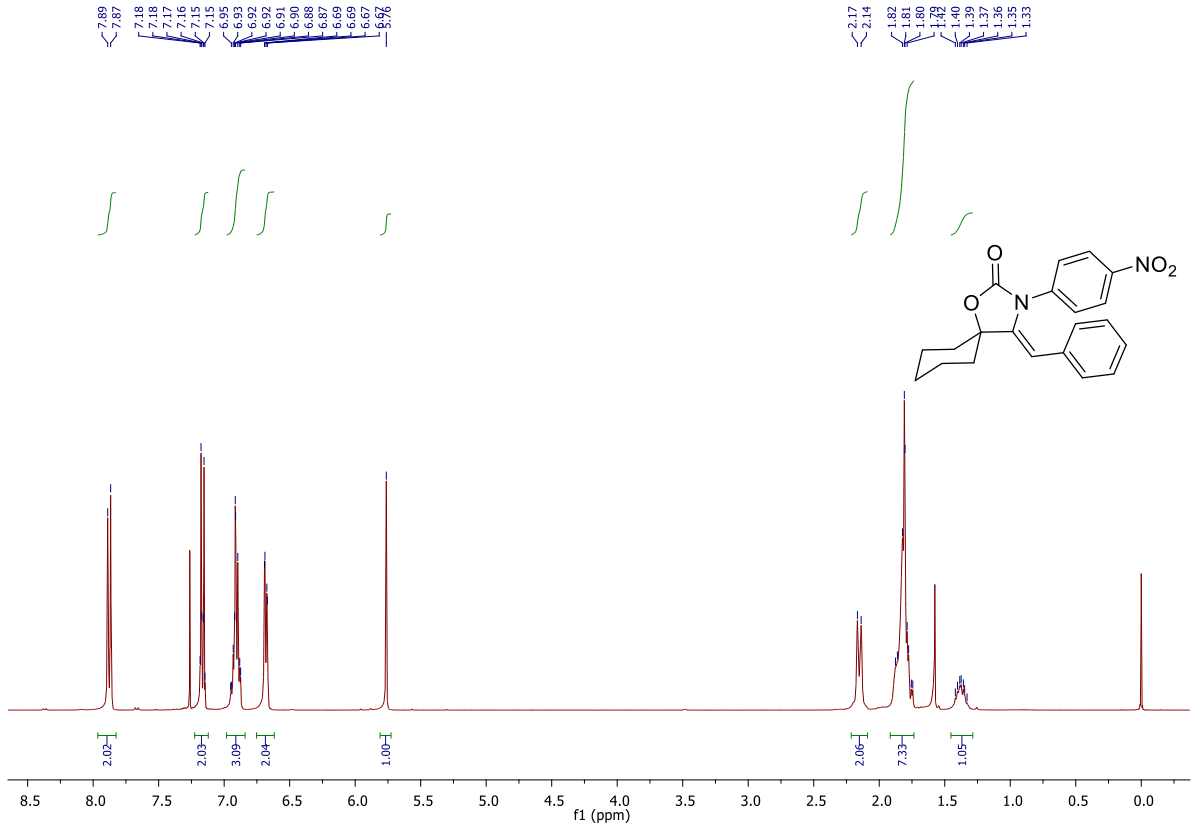
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 6c



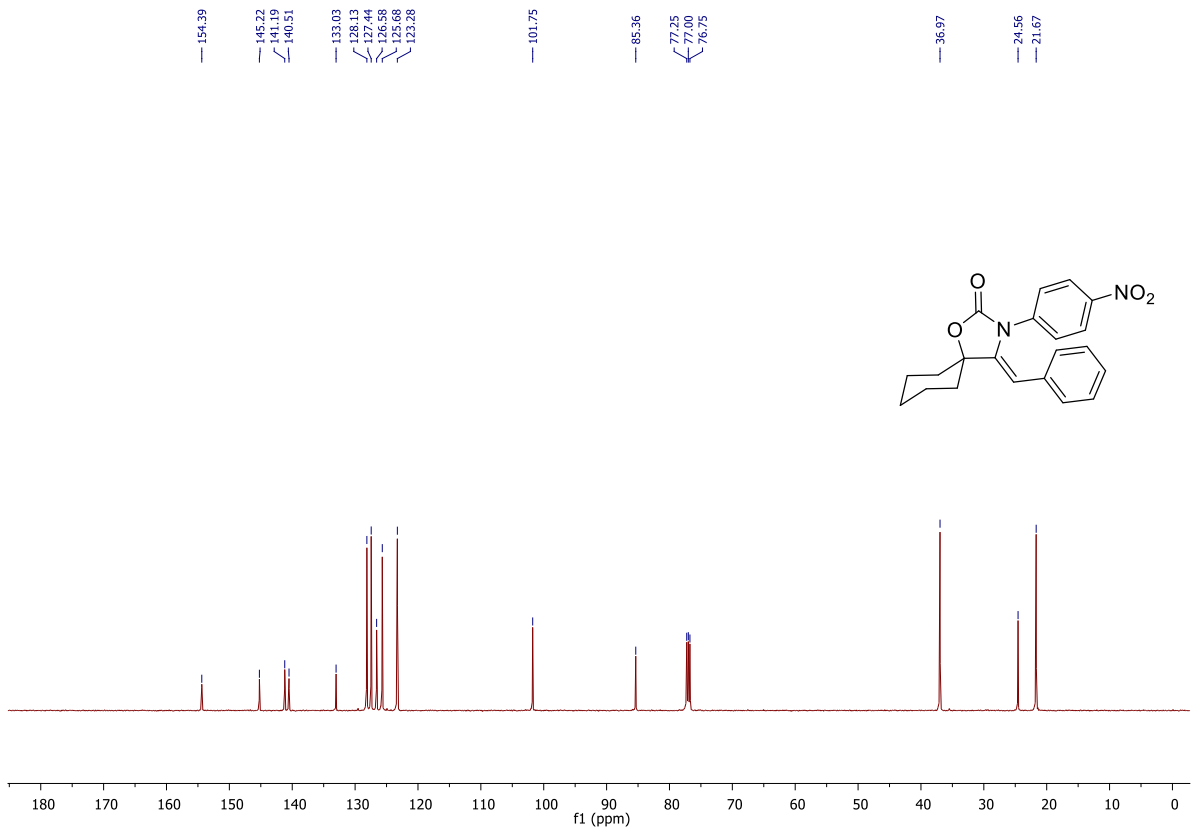
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 6c



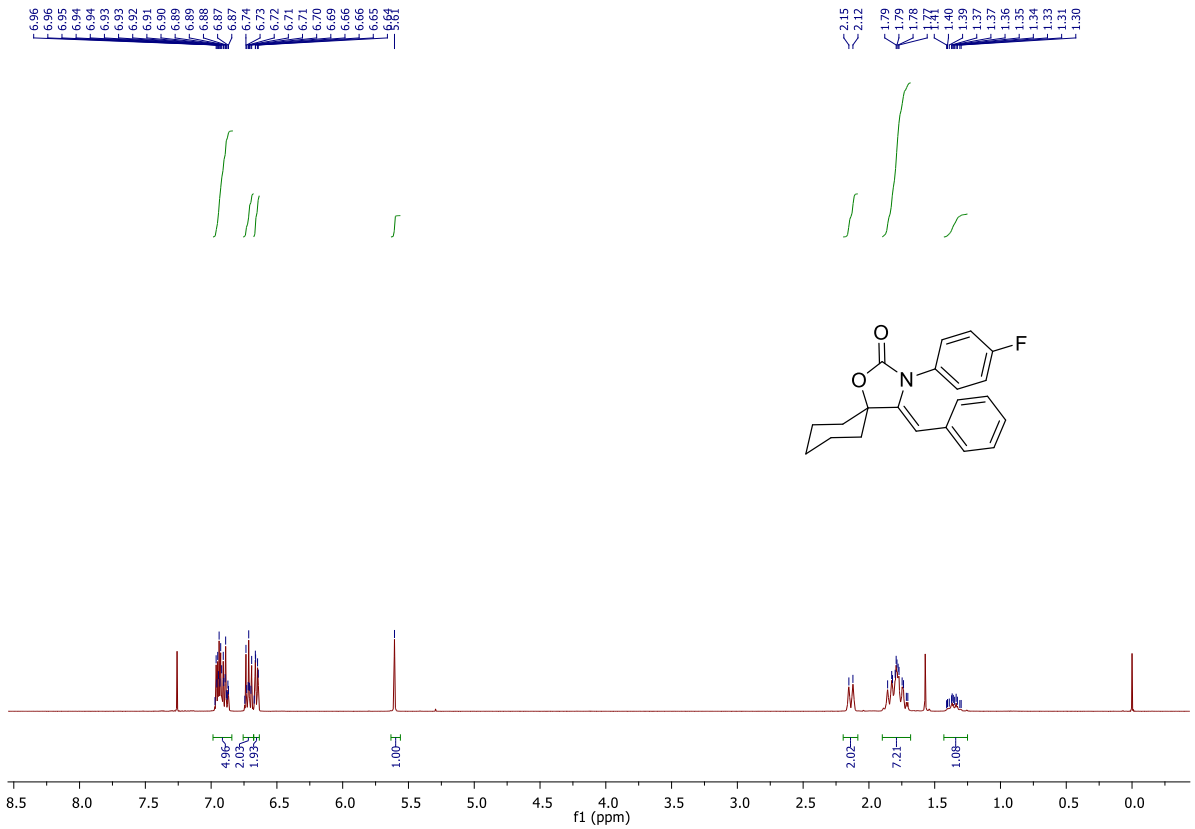
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 6d



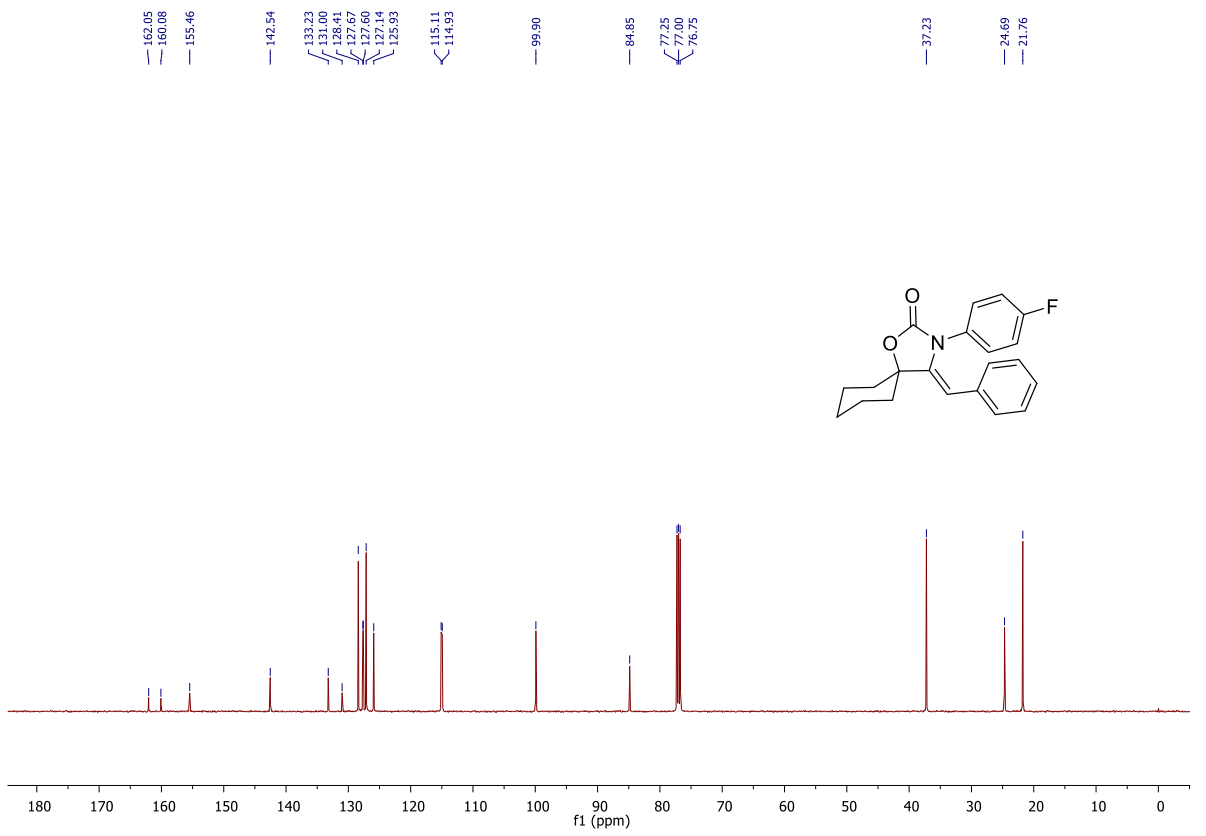
^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound 6d



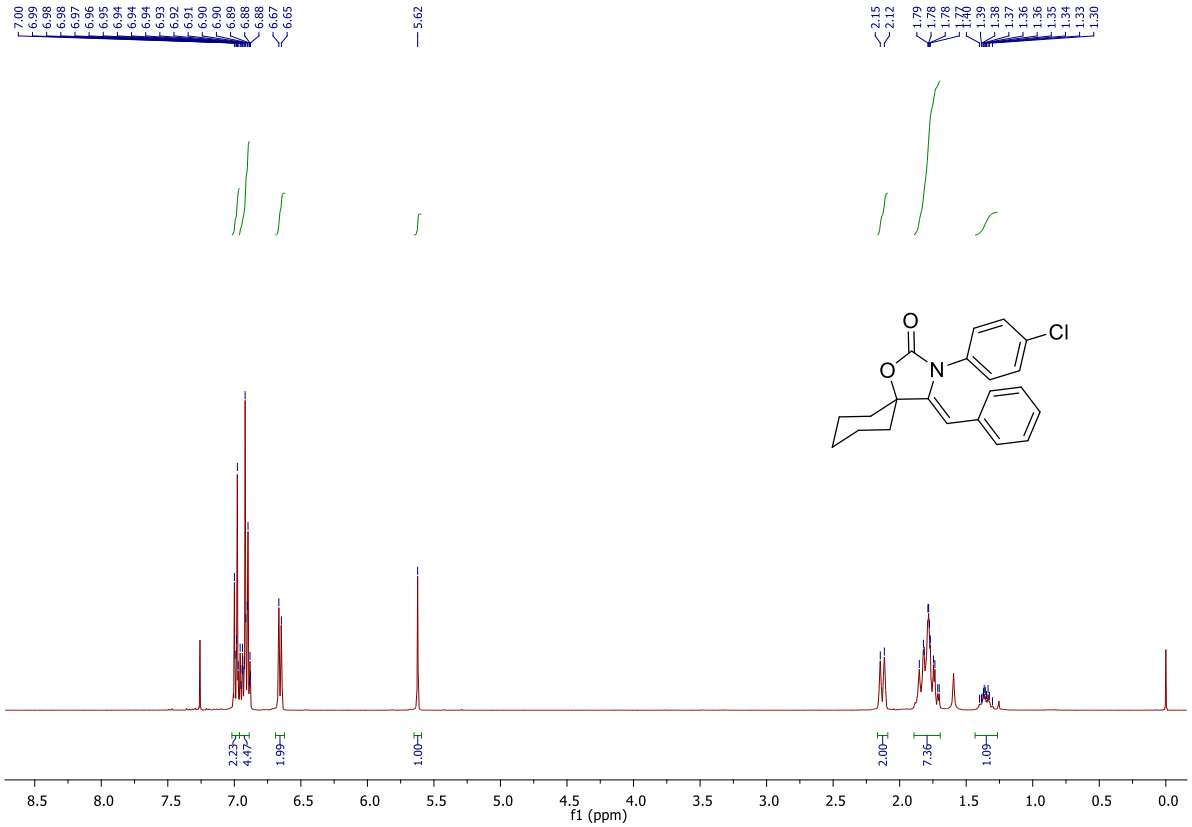
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 6e



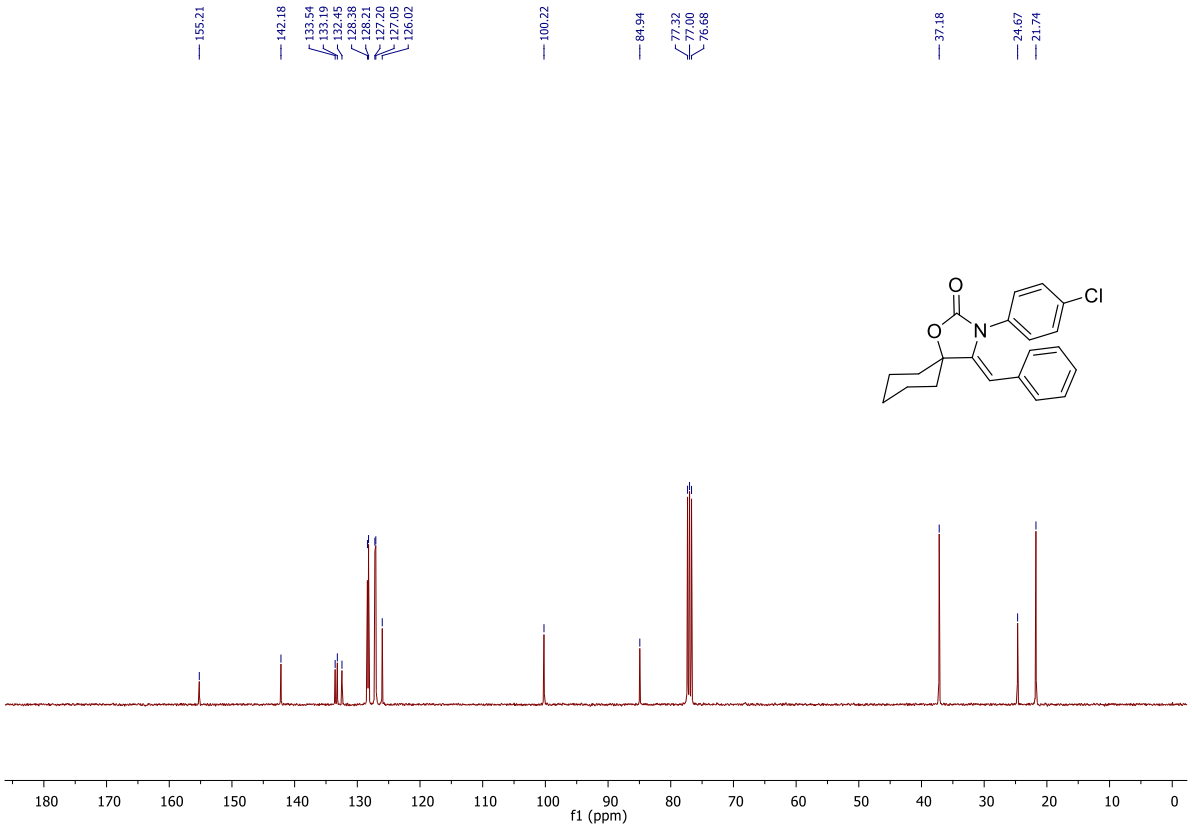
^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound 6e



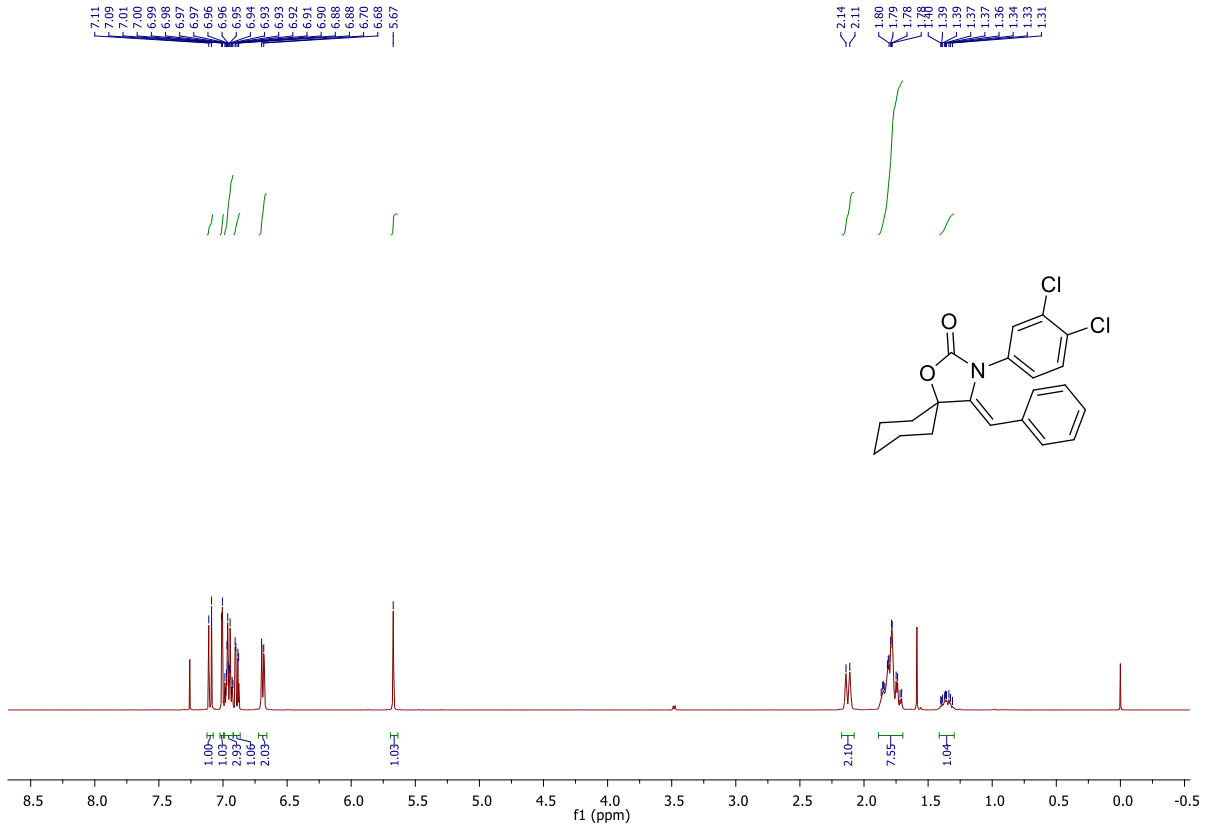
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 6f



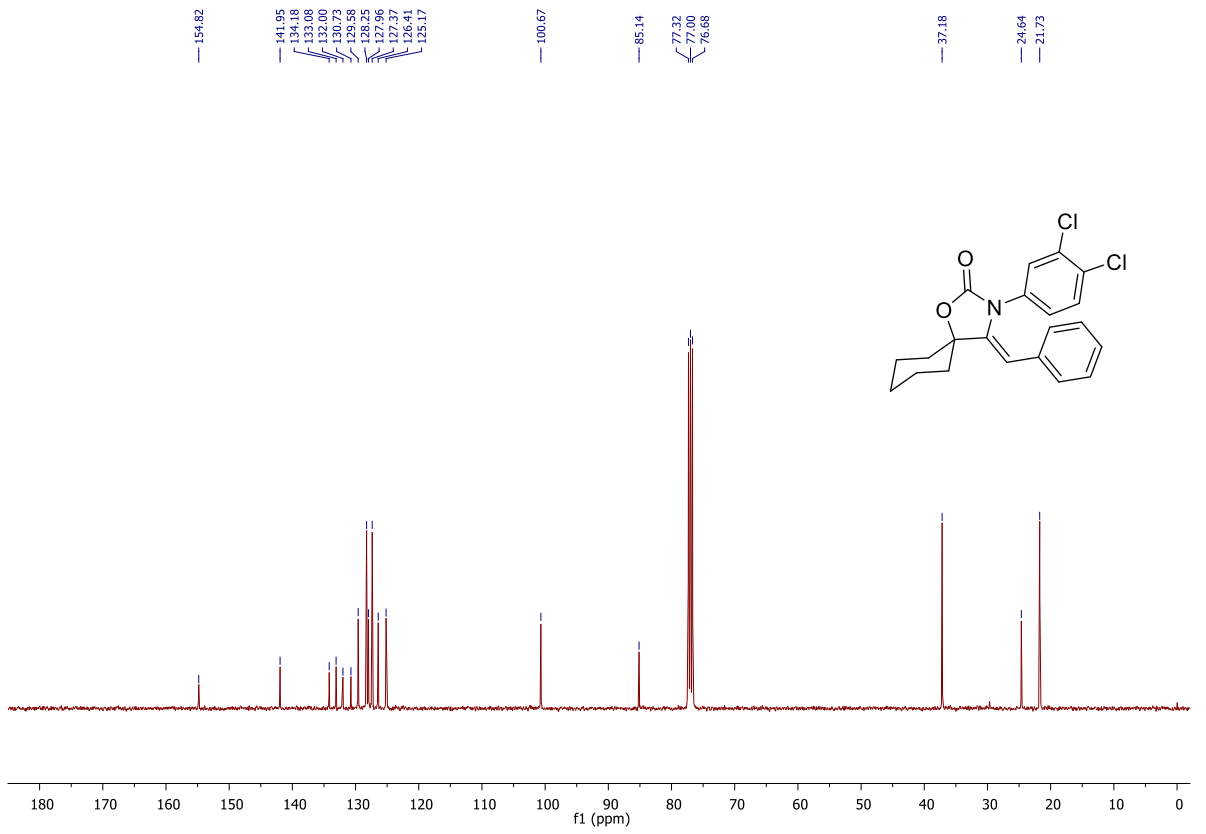
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 6f



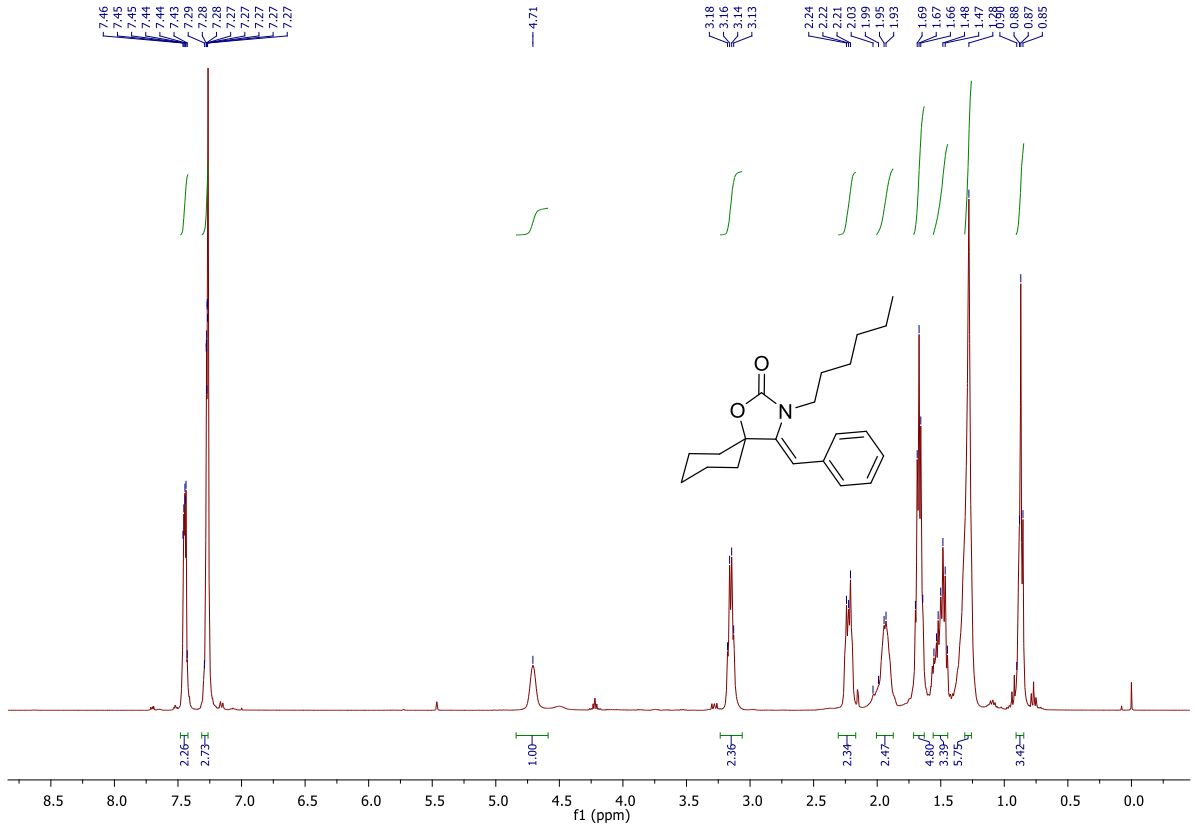
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 6g



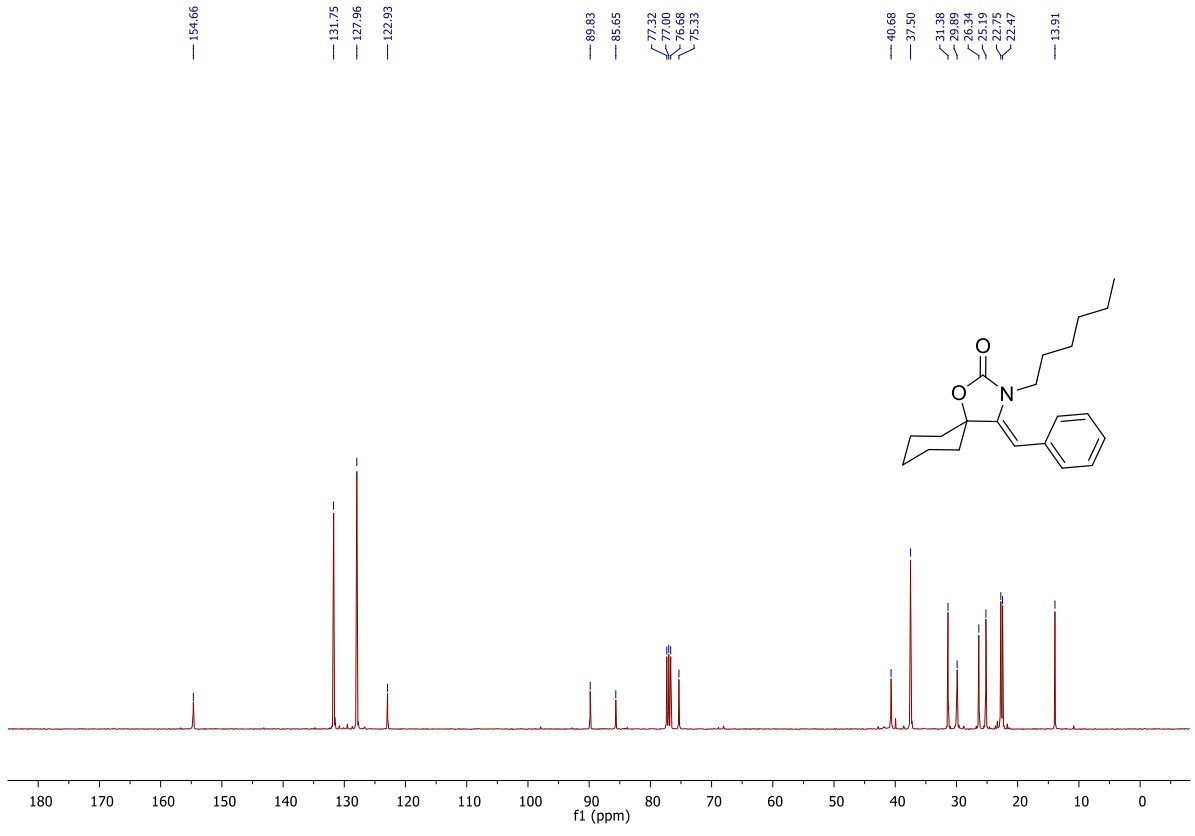
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 6g



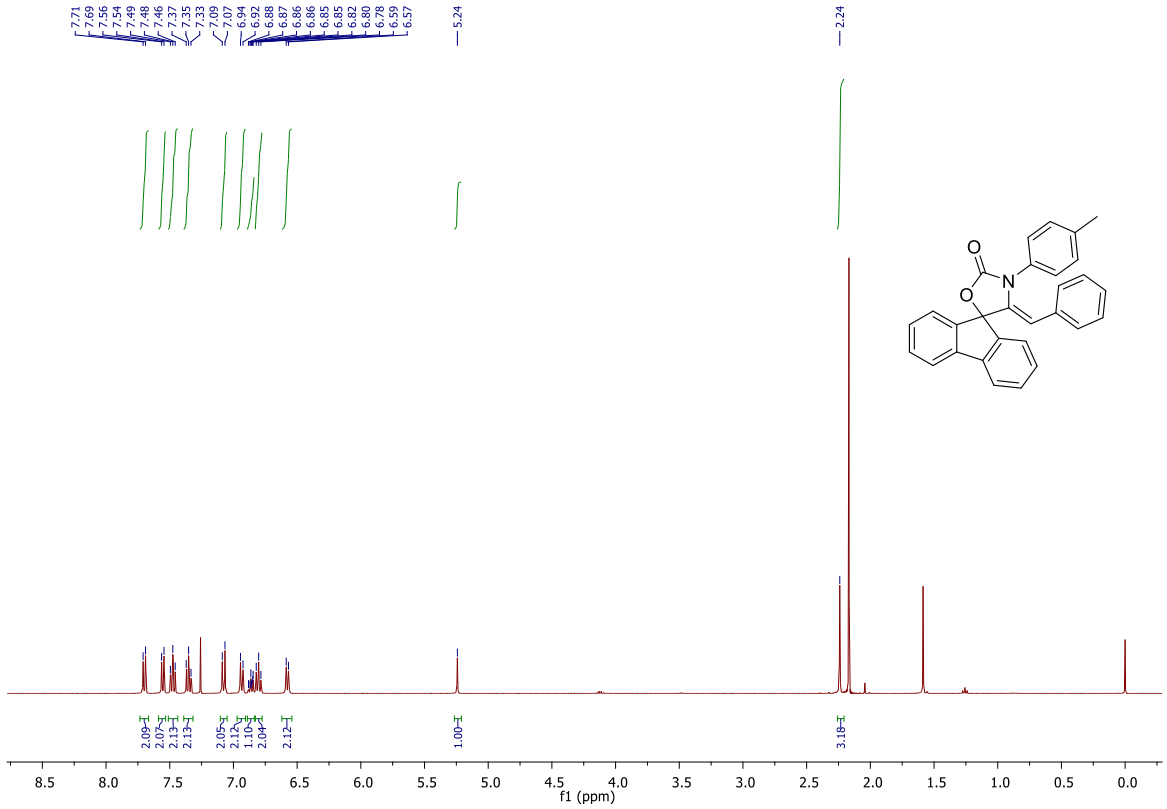
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 6h



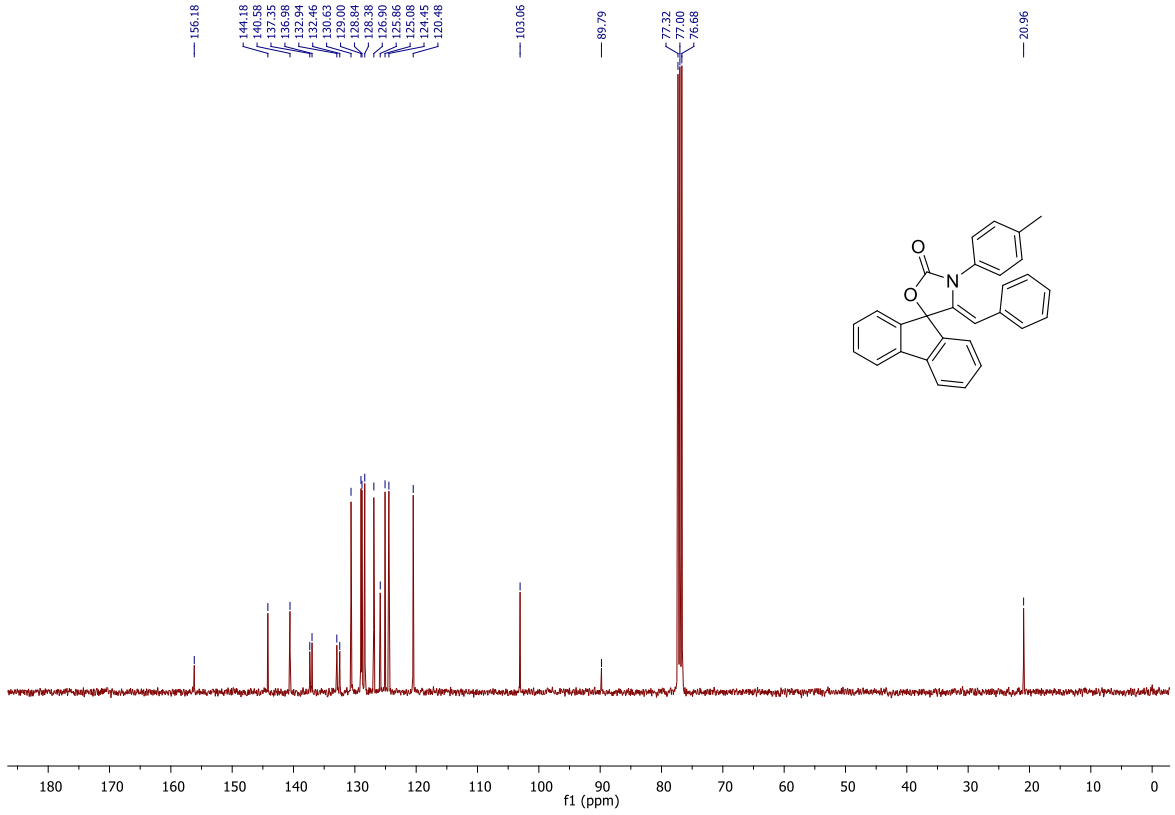
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 6h



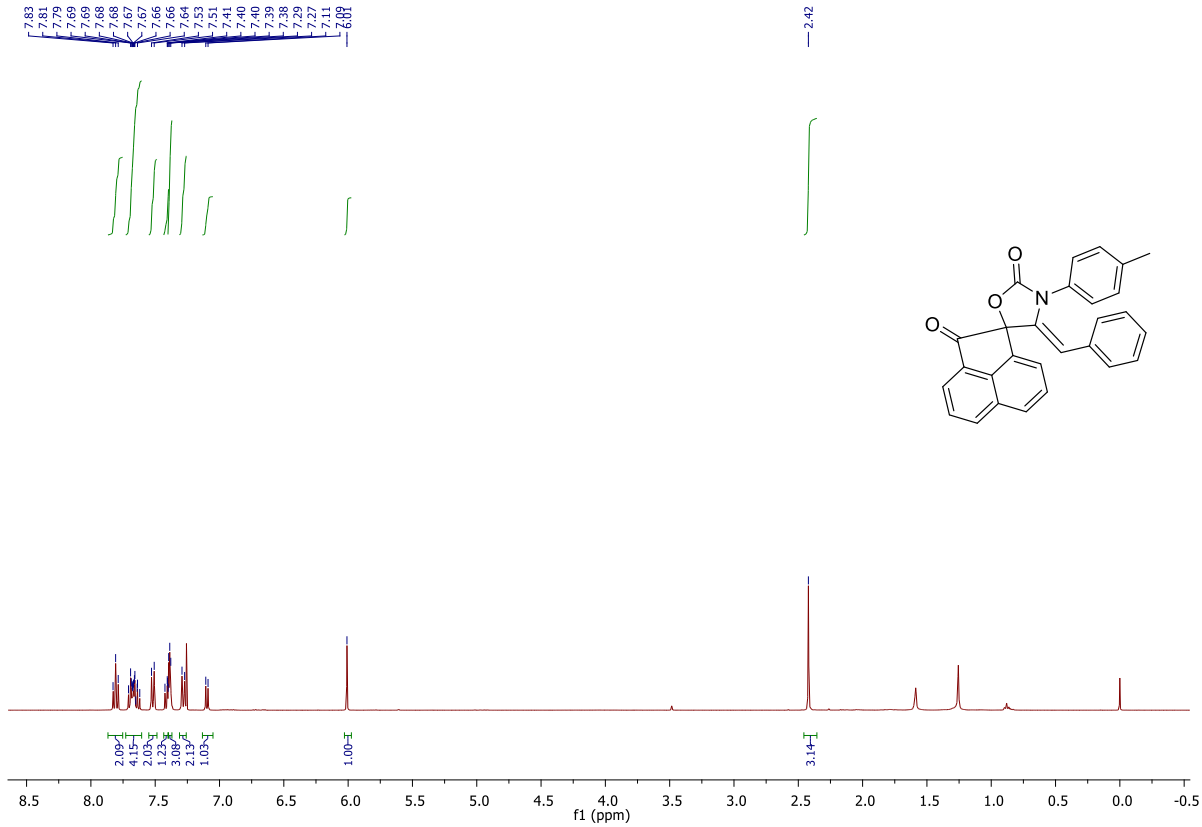
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 8a



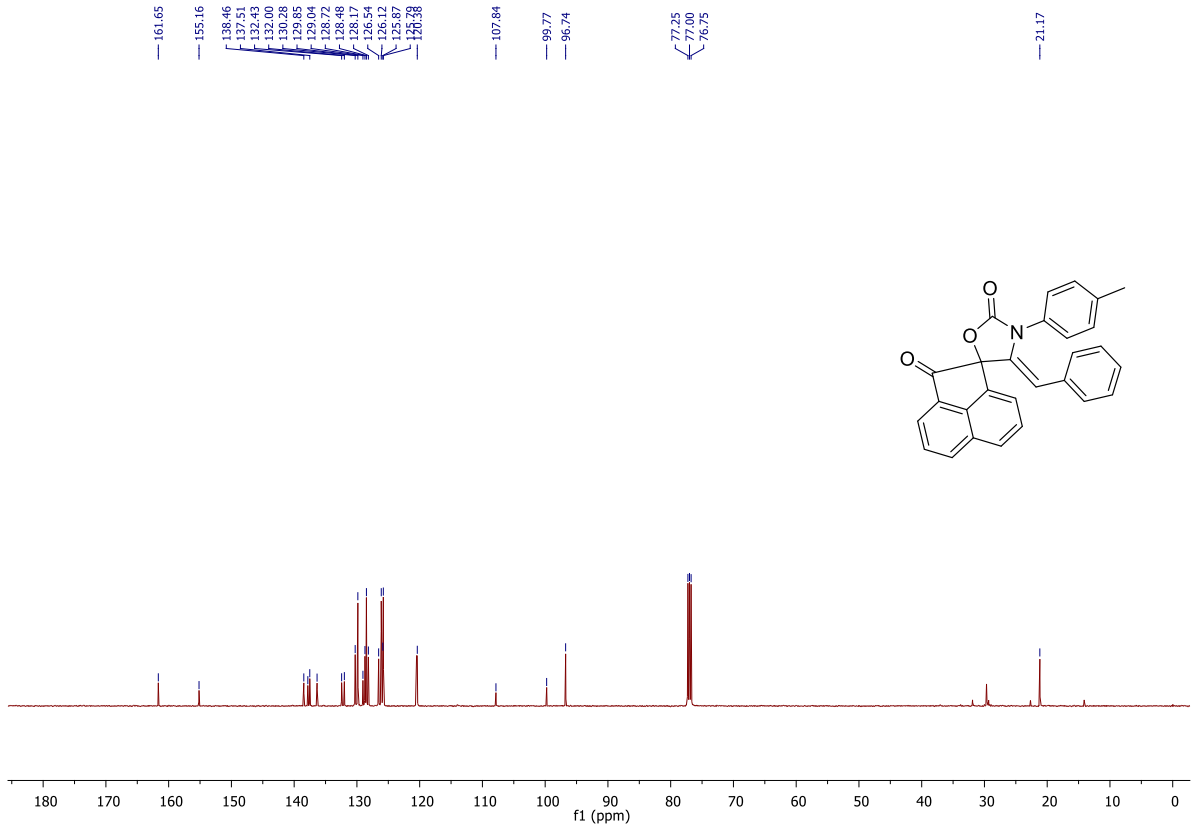
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 8a



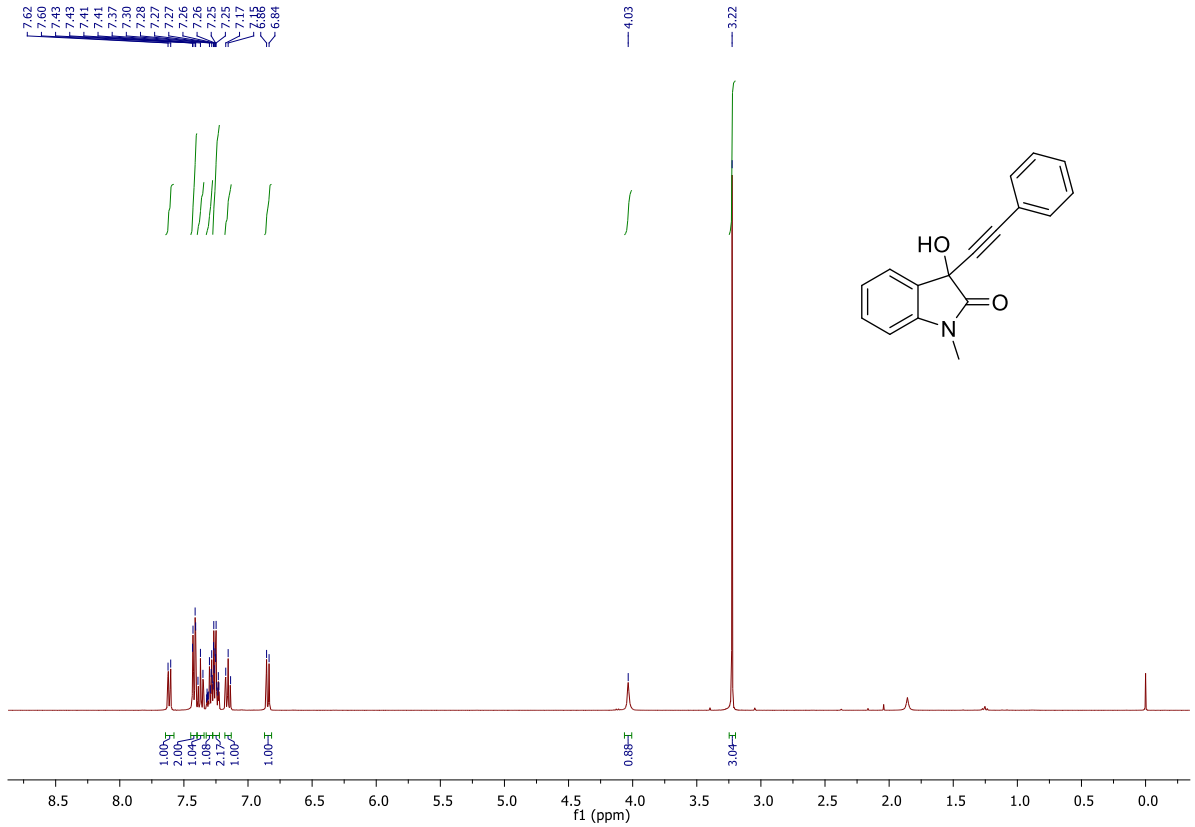
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 10a



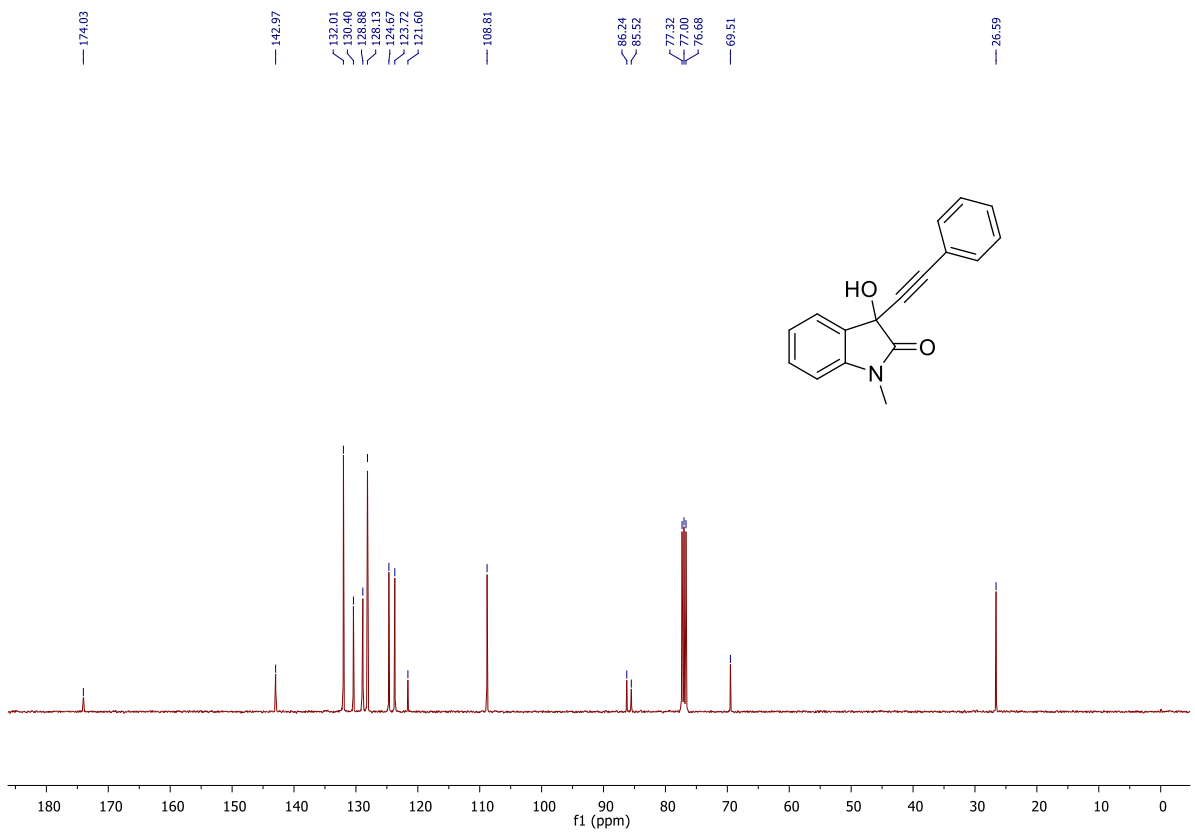
^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound 10a



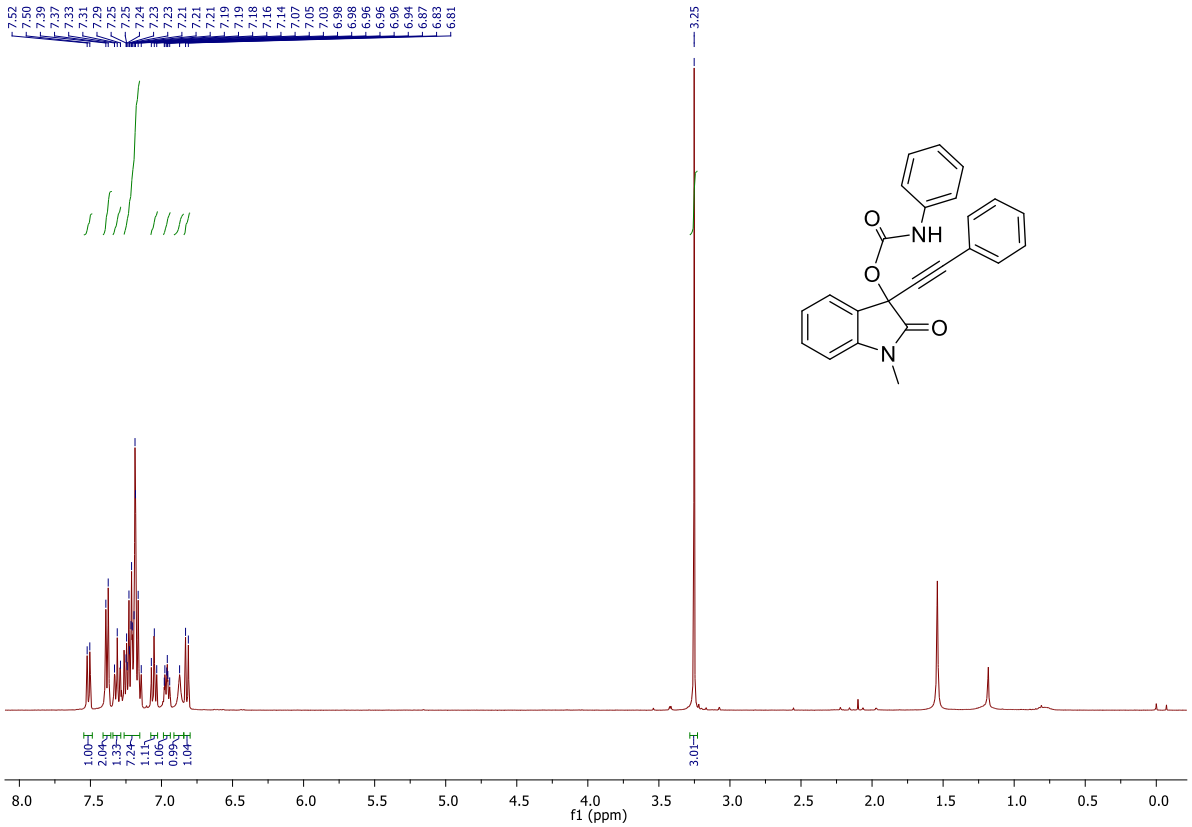
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 11



^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 11



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 12



^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 12