‘

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.
This journal is © The Royal Society of Chemistry 2014.

Supporting Information:

One pot, oxidative N-S bond formation to access 2-Sulfenylimine Chromenes

Ashok Kale,[a] Madhu Chennapuram,[a] Chiranjeevi Bingi,[a] Jagadeesh Babu Nanubolu[b] and Krishnaiah Atmakur*[a,c]

[a] Division of Crop Protection Chemicals, CSIR-Indian Institute of Chemical Technology, Tarnaka, Hyderabad 500 007, India.

[b] Laboratory of X-ray crystallography, CSIR-Indian Institute of Chemical Technology, Tarnaka, Hyderabad 500 007, India

[c]AcSIR- Indian Institute of Chemical Technology, Tarnaka, Hyderabad 500 007, India.

E-mail: srikrishnua@yahoo.com; Tel: +91- 40-27191436

Content

Spectral data for the known compounds S1-S2.
^{1}H-NMR and ^{13}C-NMR spectra for all compounds S3-S20.

Crystallographic data for 8c

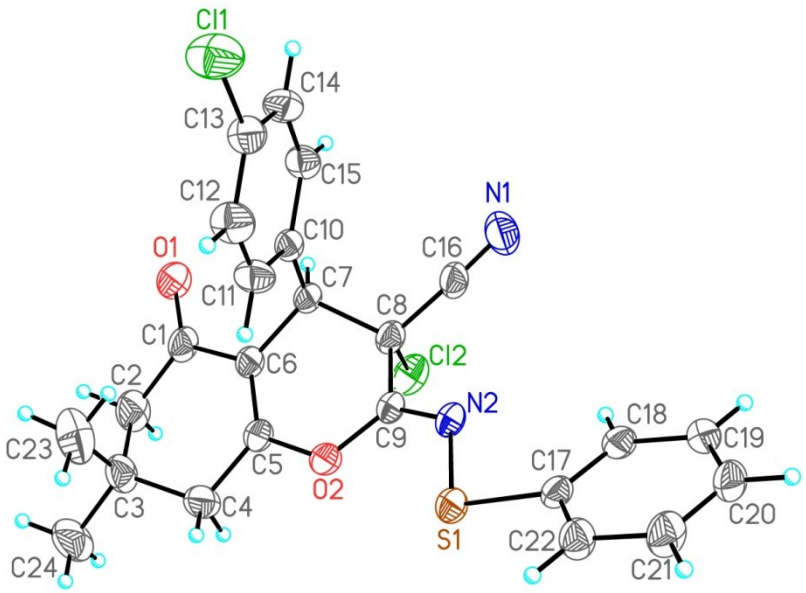


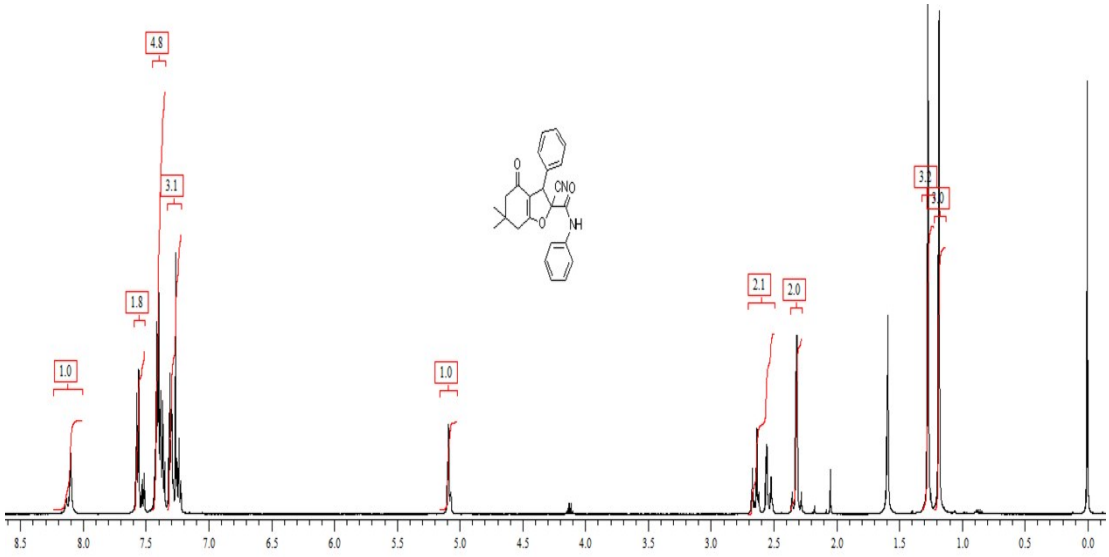
Figure caption: ORTEP diagram of **8c** with the atom-numbering. Displacement thermal ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius. There are two molecules of AY75 compound in the asymmetric unit (Z′=2), however only one is represented in the figure for clarity.

Crystal data for 8c: $C_{24}H_{20}N_2O_2Cl_2S$, M = 471.39, colorless diamond shaped crystal, 0.43 x 0.22 x 0.20 mm^3, monoclinic, space group $P2_1/c$ (No. 14), a = 16.6008(8), b = 13.5612(7), c = 21.8151(11) Å, α = 90, β = 106.926(1), γ = 90°, V = 4698.4(4) Å^3, Z = 8, D_c = 1.333 g/cm^3, F_{000} = 1952, CCD area detector, MoKα radiation, λ = 0.71073 Å, T = 293(2)K, $2\theta_{max}$ = 50.6º, 45900 reflections collected, 8595 unique (R_{int} = 0.042), Final *GooF* = 1.13, *R1* = 0.0633, *wR2* = 0.1452, *R* indices based on 6645 reflections with $I > 2\sigma(I)$ (refinement on F^2), 563 parameters, μ = 0.388 mm^{-1}, minimum and maximum residual density = -0.23 and 0.47 e/Å^3, respectively. **CCDC 1415312** contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

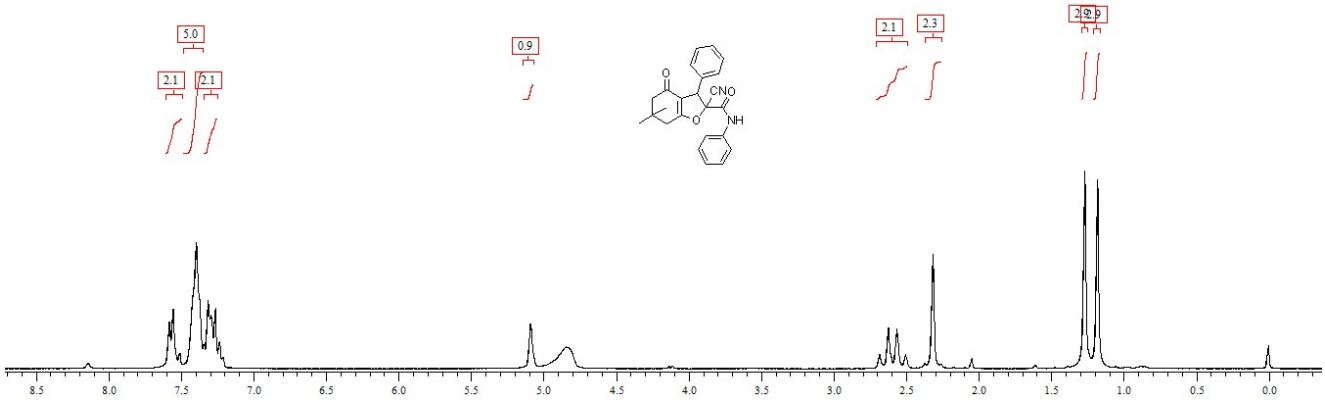
Data collection and Structure solution: X-ray data for **8c** compound were collected at room temperature using the Bruker Smart Apex CCD diffractometer with graphite monochromated MoKα radiation (λ = 0.71073Å) with ω-scan method.[1] Preliminary lattice parameters and orientation matrices were obtained from four sets of frames. Unit cell dimensions were determined using 8332 reflections. Integration and scaling of intensity data were accomplished using SAINT program.[1] The structure was solved by Direct Methods using SHELXS97[2] and refinement was carried out by full-matrix least-squares technique using SHELXL97.[2] 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.

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 SHELXL97, Programs for crystal structure solution and refinement; University of Gottingen: Germany, 1997.

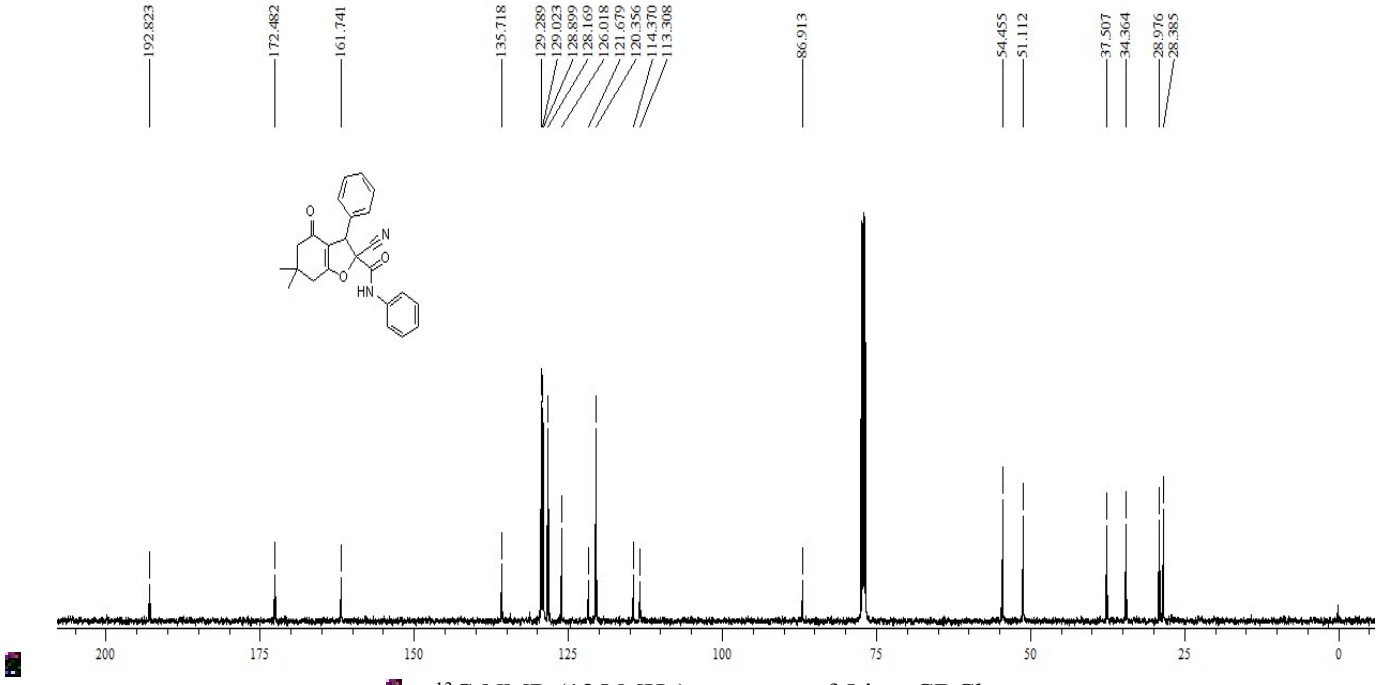
^{1}H and^{13}C NMR spectrums of 5 (a-l):



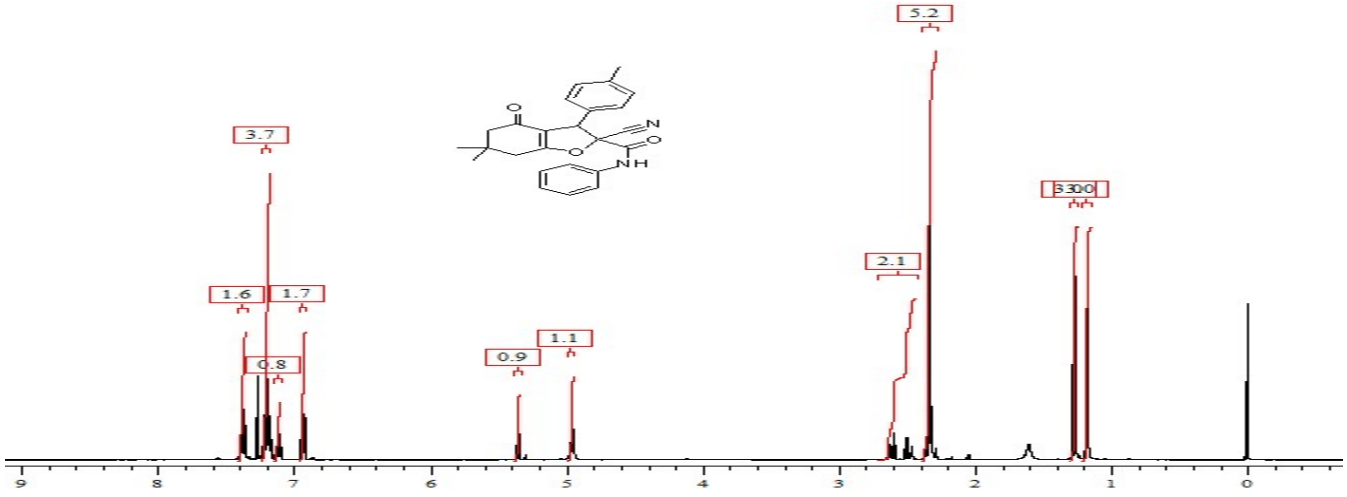
^{1}H-NMR (500 MHz) spectrum of 5 in a $CDCl_3$



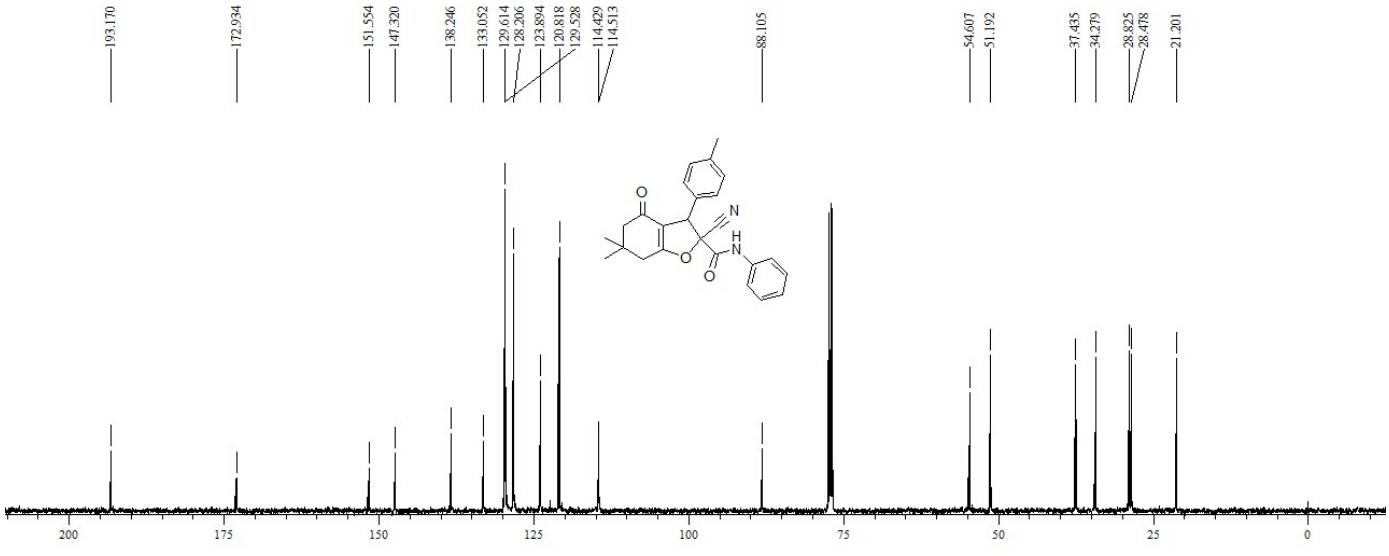
D_2O exchanged ^{1}H-NMR (300 MHz) spectrum of 5 in a $CDCl_3$



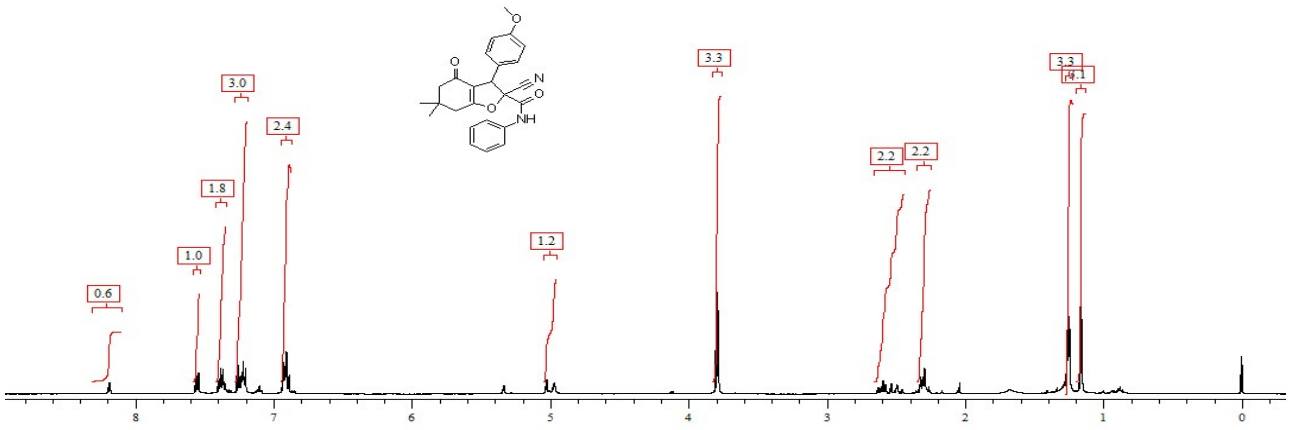
^{13}C-NMR (125 MHz) spectrum of 5 in a $CDCl_3$



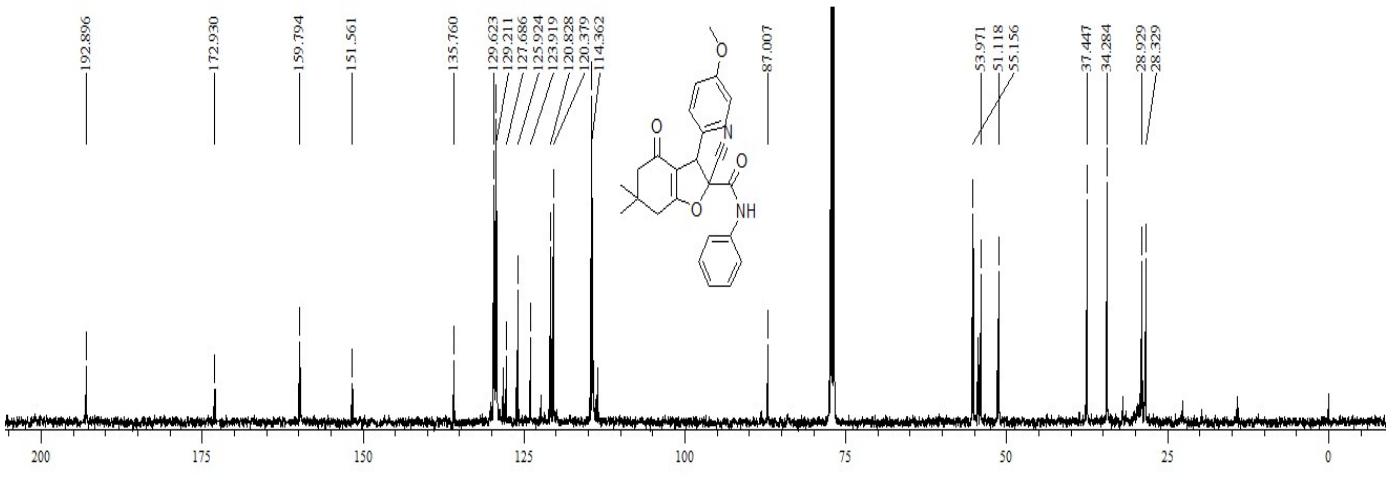
^{1}H-NMR (500 MHz) spectrum of 5a in a $CDCl_3$



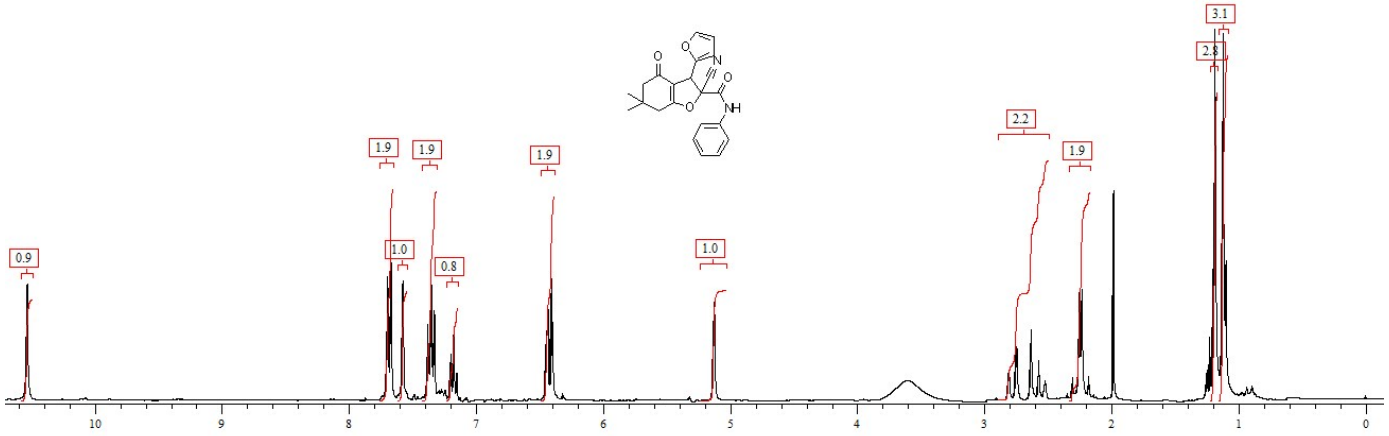
^{13}C-NMR (100 MHz) spectrum of 5a in a $CDCl_3$



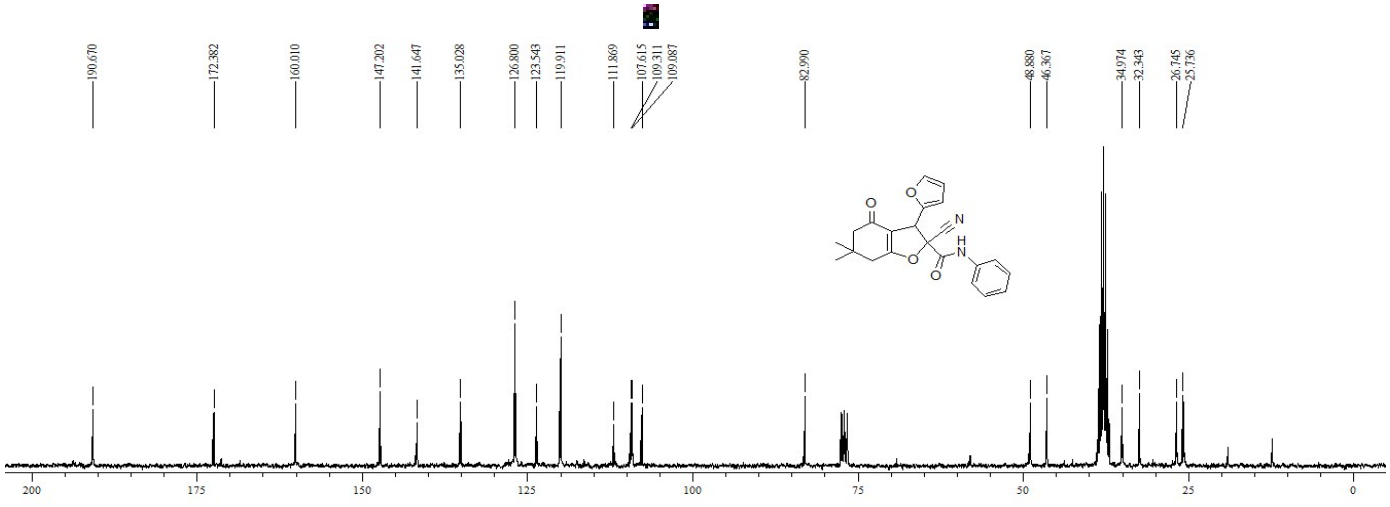
^{1}H-NMR (500 MHz) spectrum of 5b in a $CDCl_3$



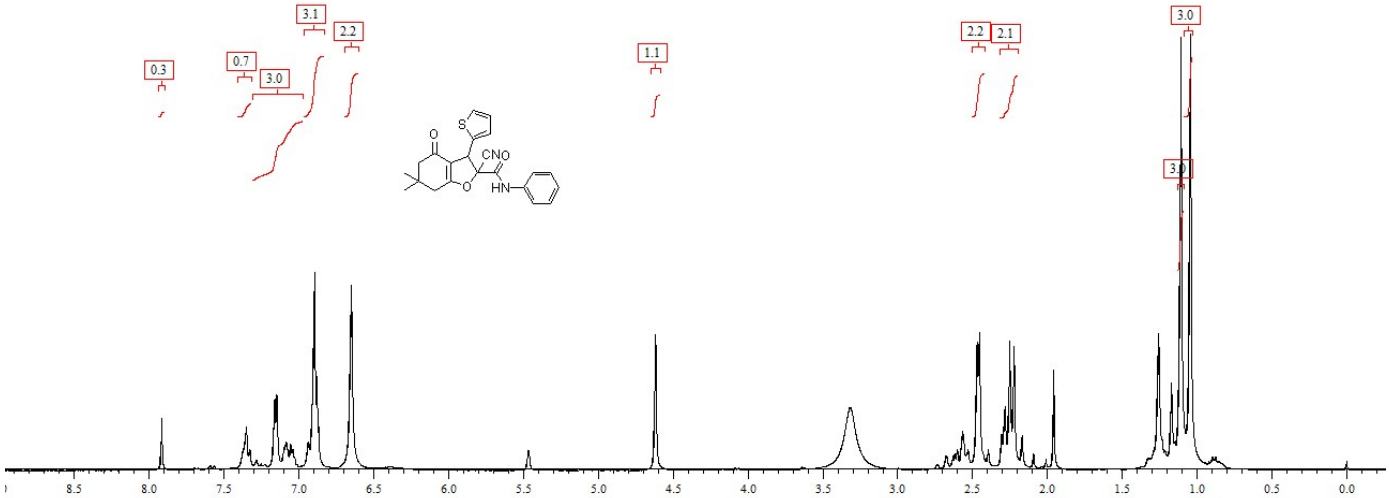
^{13}C-NMR (125 MHz) spectrum of 5b in a $CDCl_3$



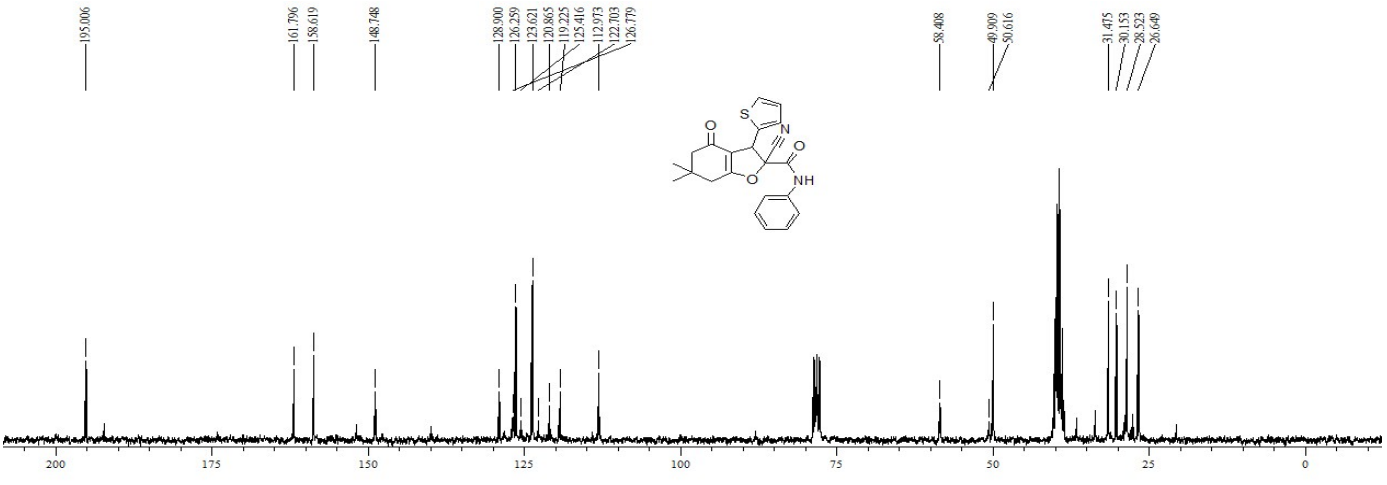
^{1}H-NMR (500 MHz) spectrum of 5c in a $CDCl_3$+DMSO-d_6



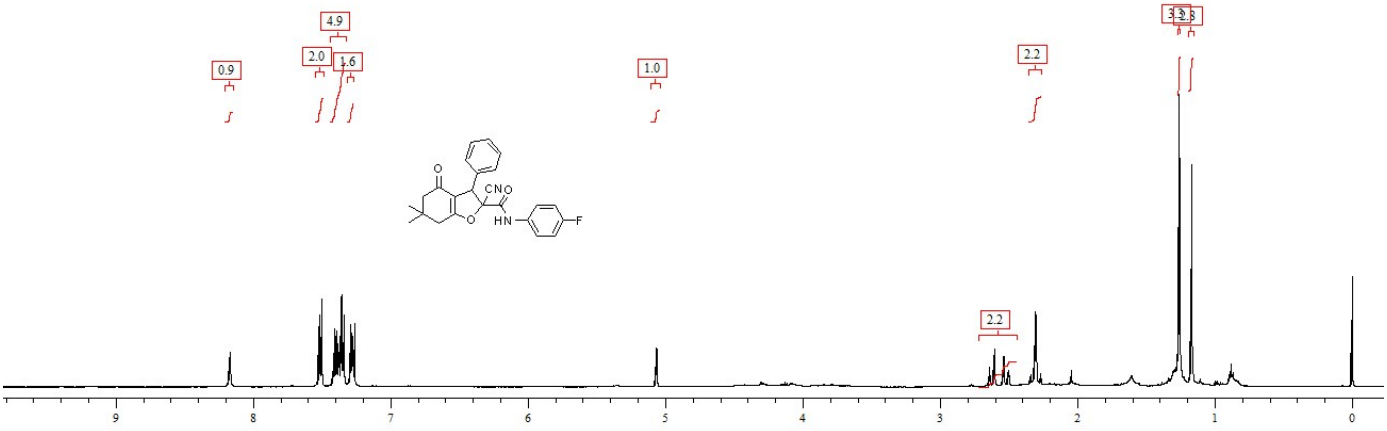
^{13}C-NMR (75 MHz) spectrum of 5c in a $CDCl_3$+DMSO-d_6



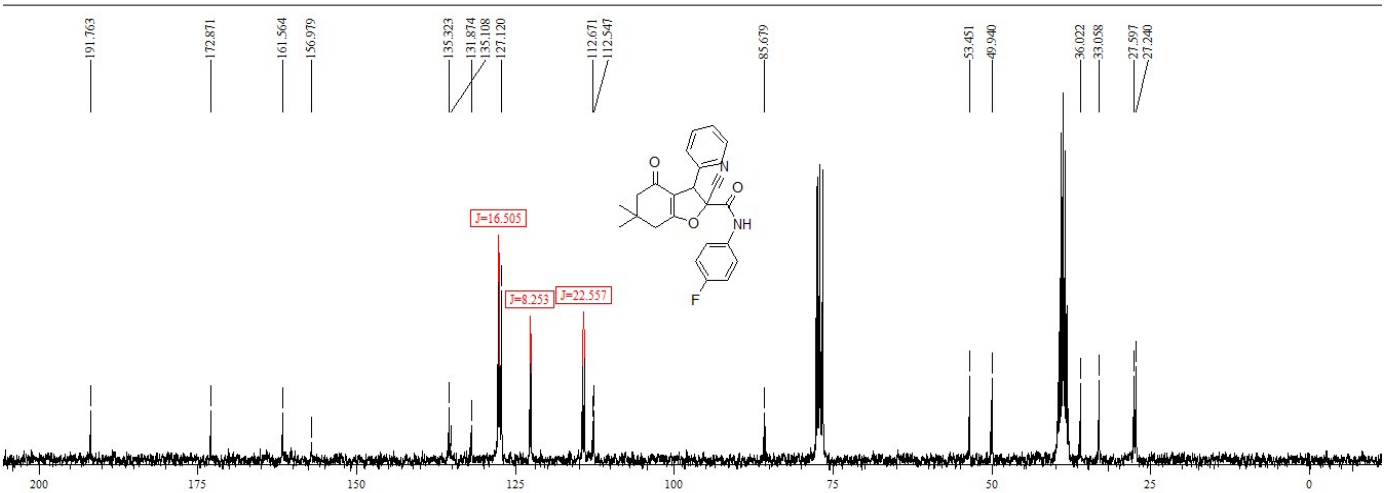
^{1}H-NMR (300 MHz) spectrum of 5d in a $CDCl_3$+DMSO-d_6



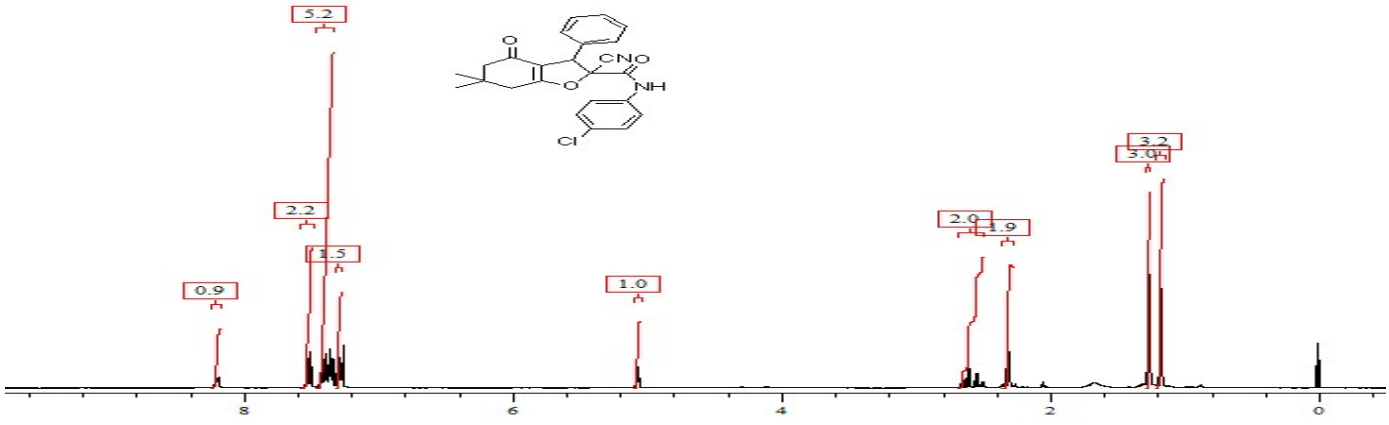
^{13}C-NMR (75 MHz) spectrum of 5d in a $CDCl_3$+DMSO-d_6



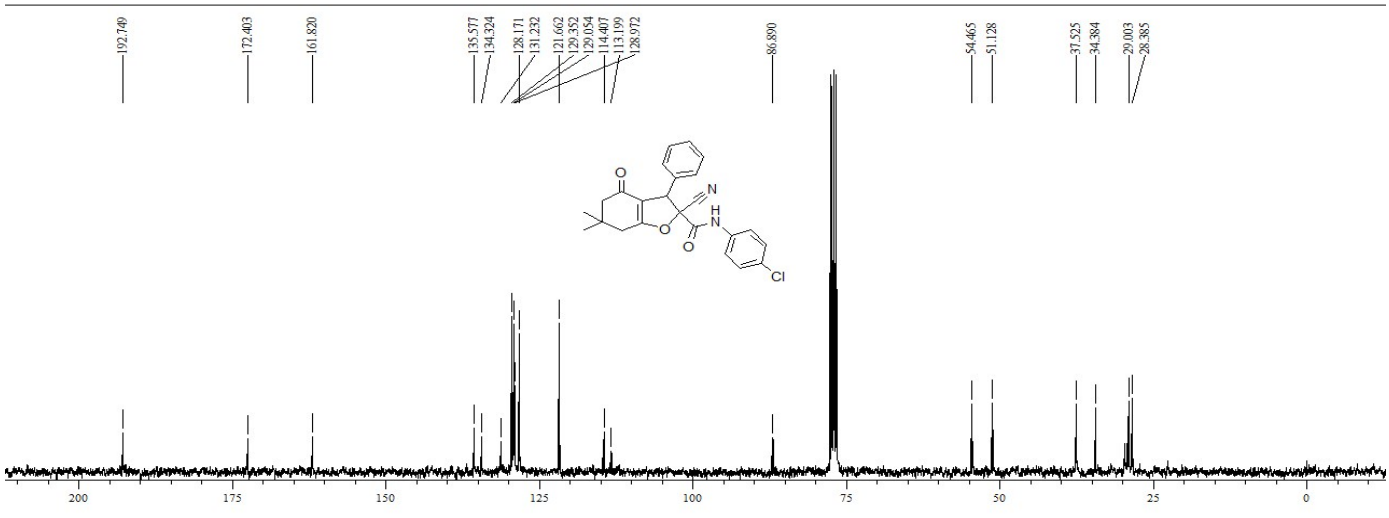
^{1}H-NMR (500 MHz) spectrum of 5e in a $CDCl_3$



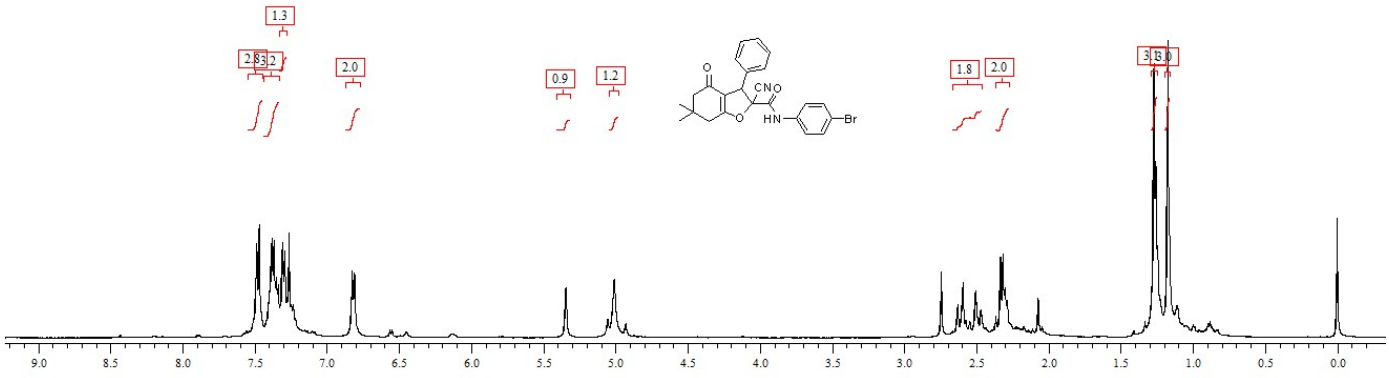
^{13}C-NMR (75 MHz) spectrum of 5e in a $CDCl_3$+DMSO-d_6



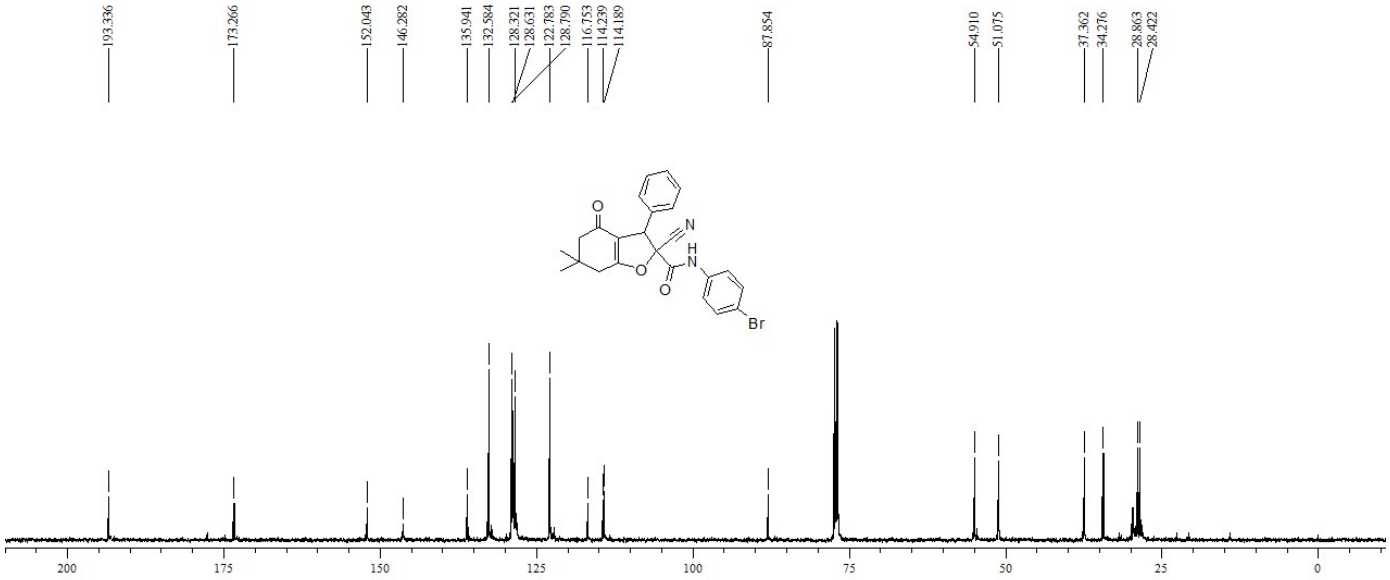
^{1}H-NMR (400 MHz) spectrum of 5f in a $CDCl_3$



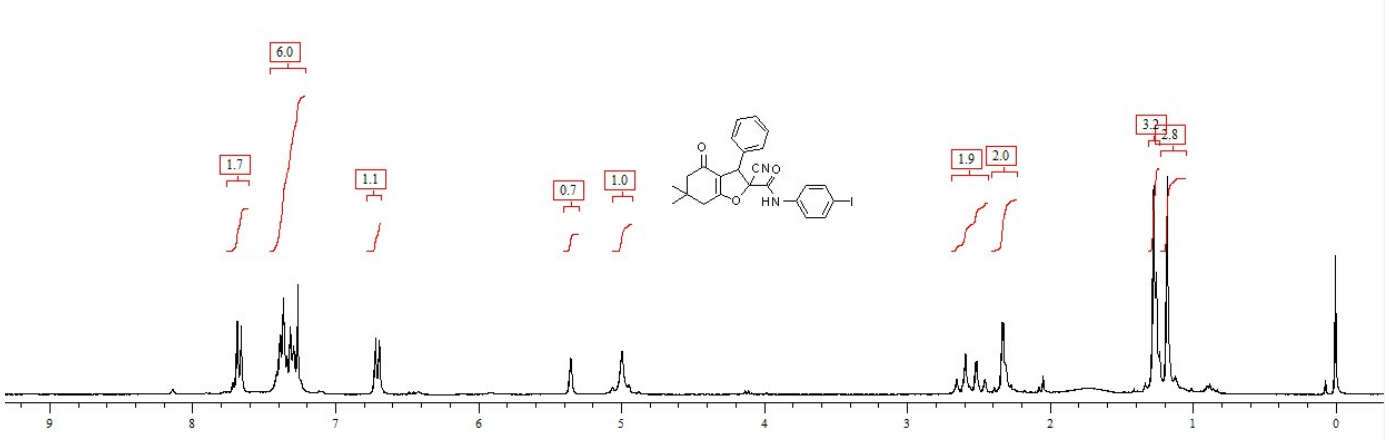
^{13}C-NMR (75 MHz) spectrum of 5f in a $CDCl_3$



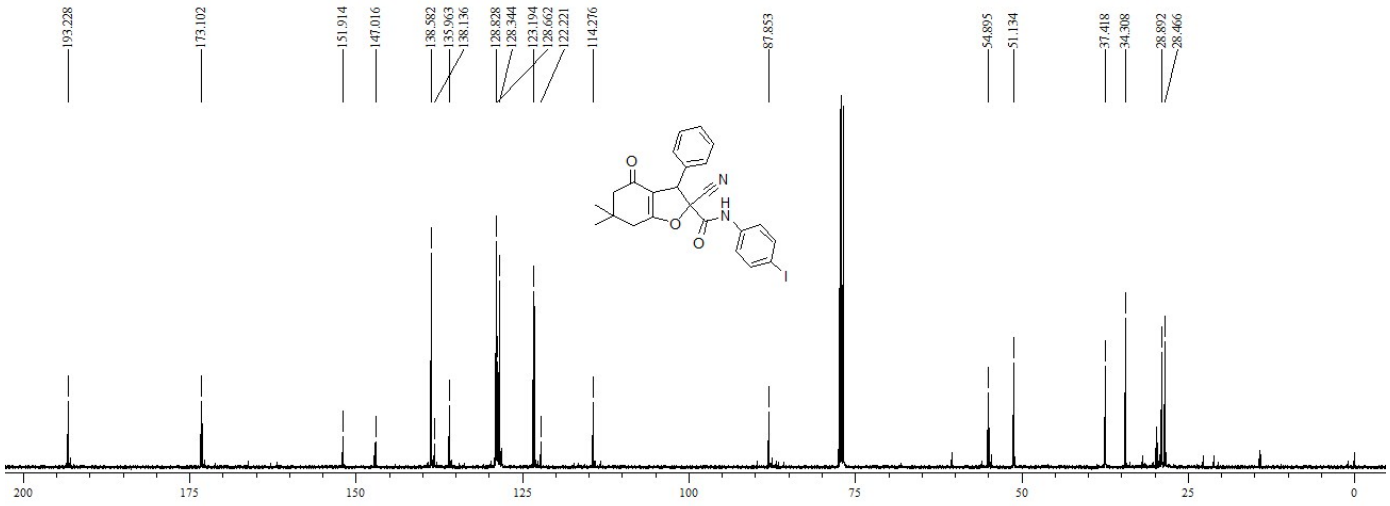
^{1}H-NMR (500 MHz) spectrum of 5g in a $CDCl_3$



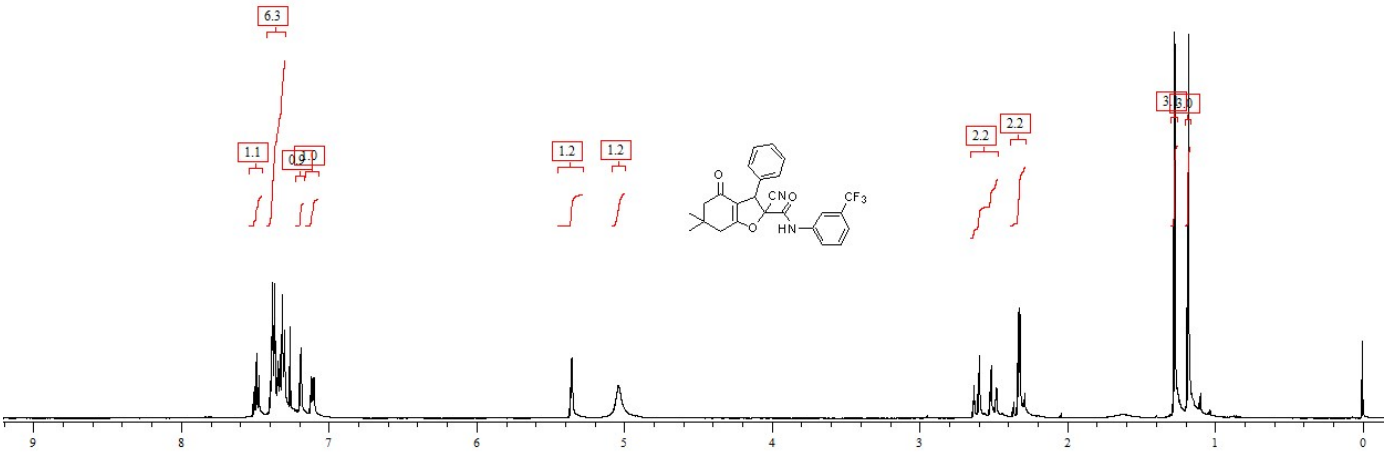
^{13}C-NMR (125 MHz) spectrum of 5g in a $CDCl_3$



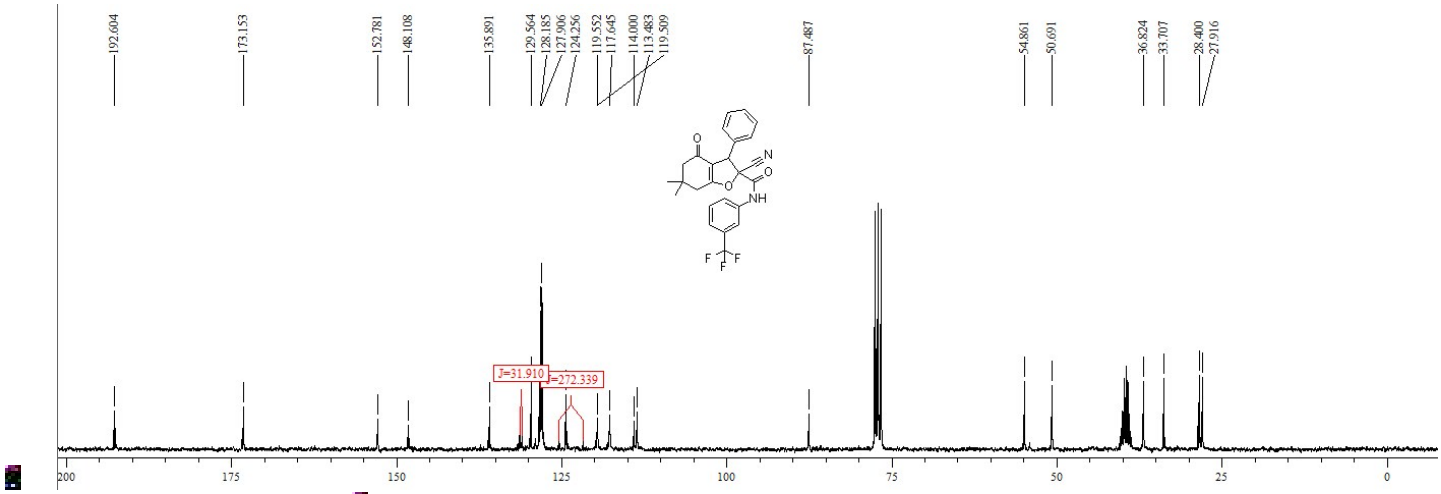
^{1}H-NMR (500 MHz) spectrum of 5h in a $CDCl_3$



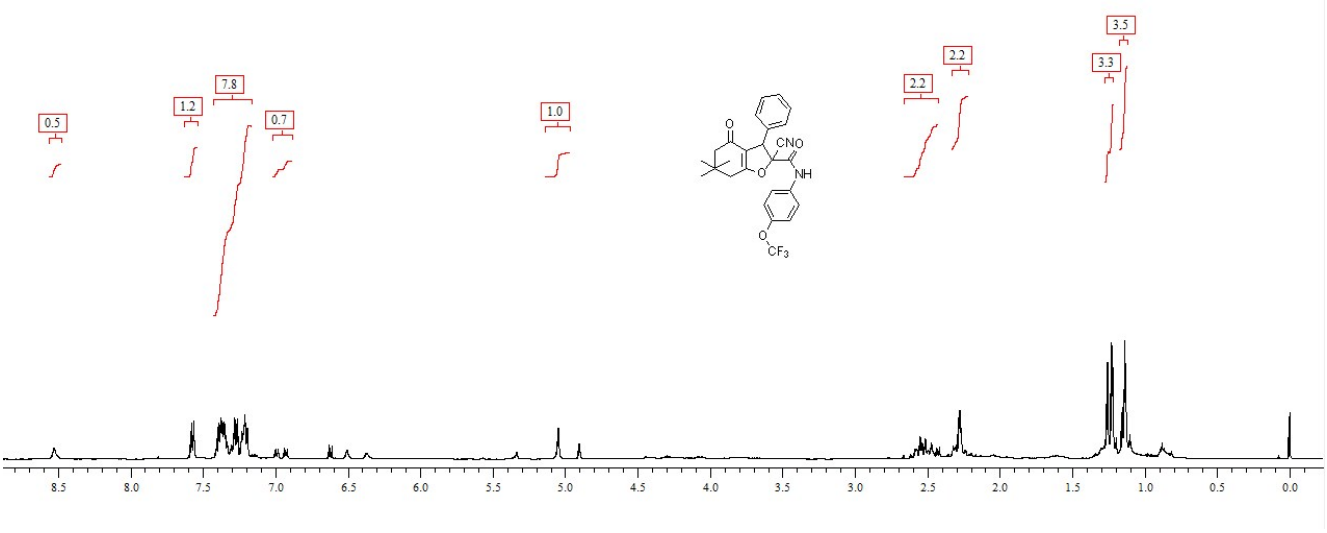
^{13}C-NMR (125 MHz) spectrum of 5h in a $CDCl_3$



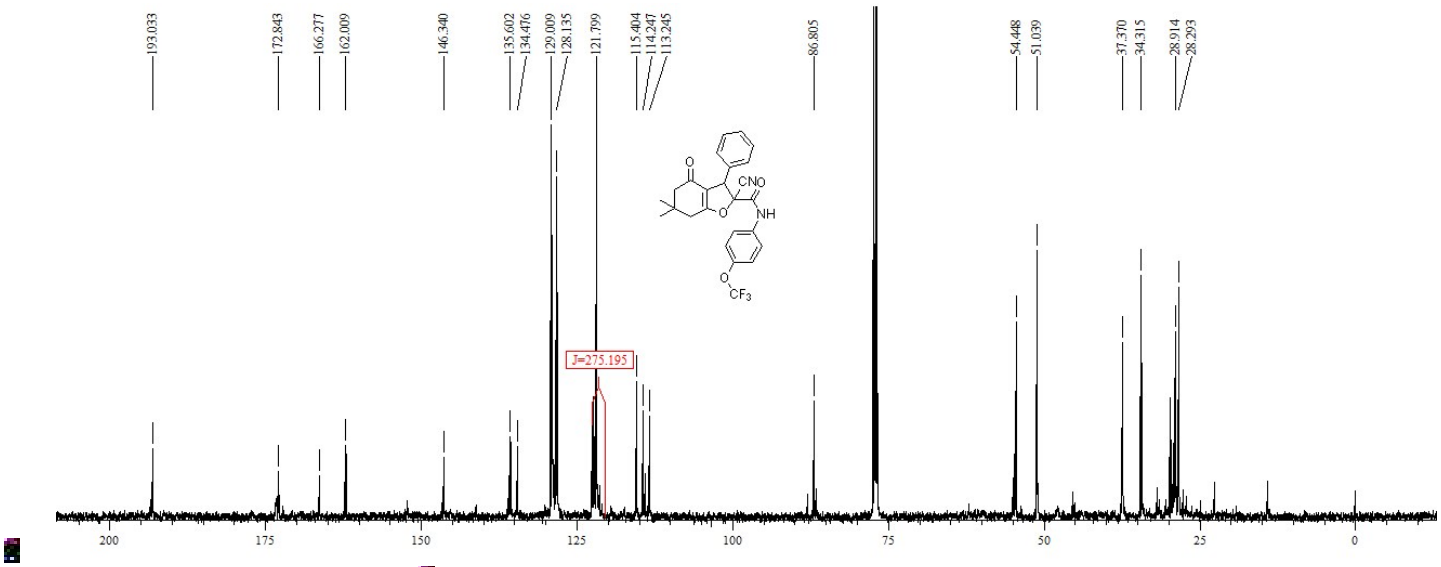
^{1}H-NMR (500 MHz) spectrum of 5i in a $CDCl_3$



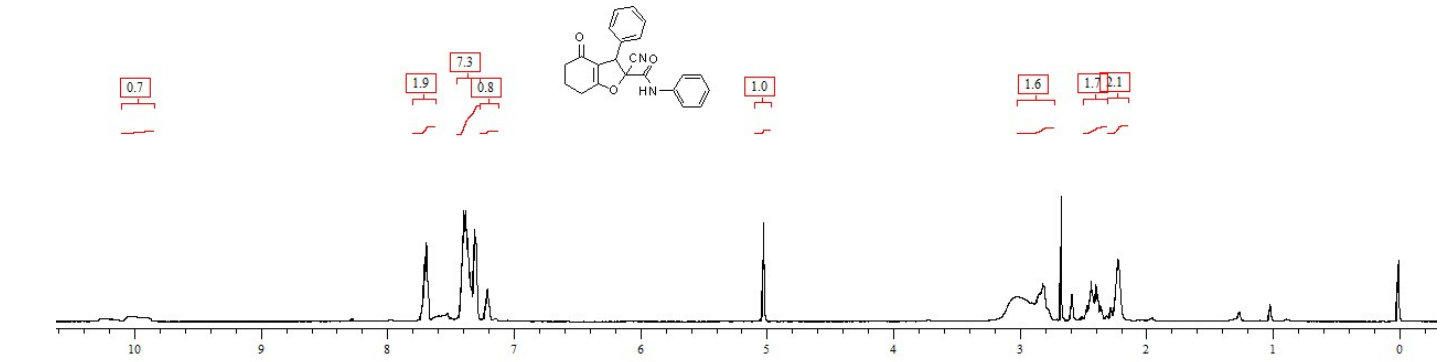
^{13}C-NMR (75 MHz) spectrum of 5i in a $CDCl_3$+DMSO-d_6



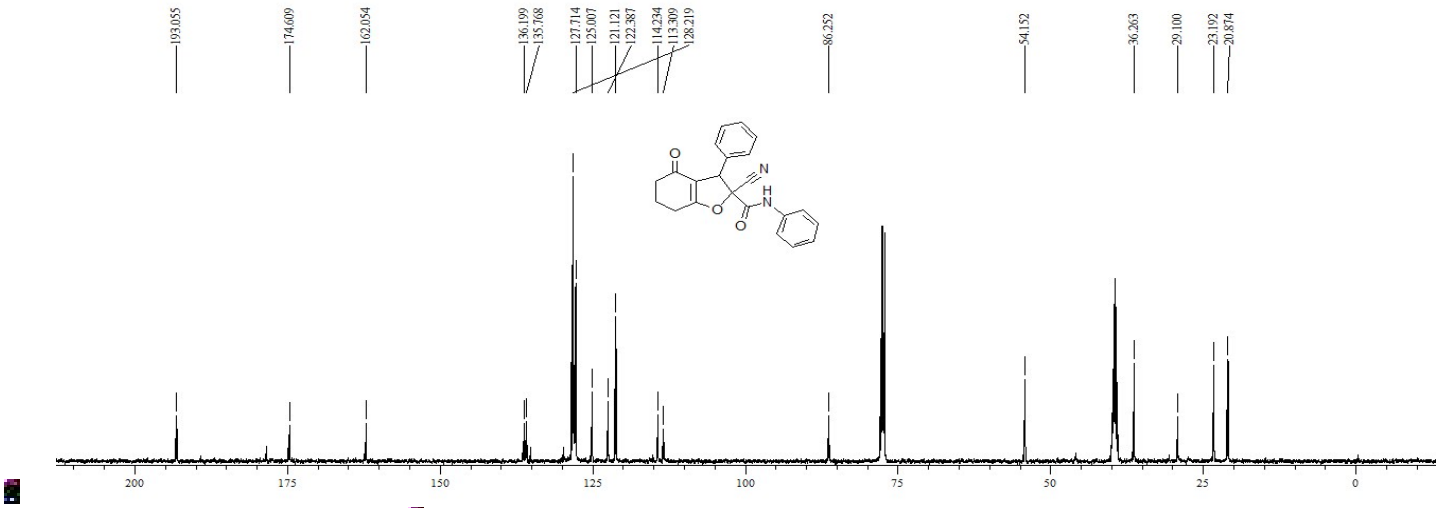
^{1}H-NMR (500 MHz) spectrum of 5j in a $CDCl_3$



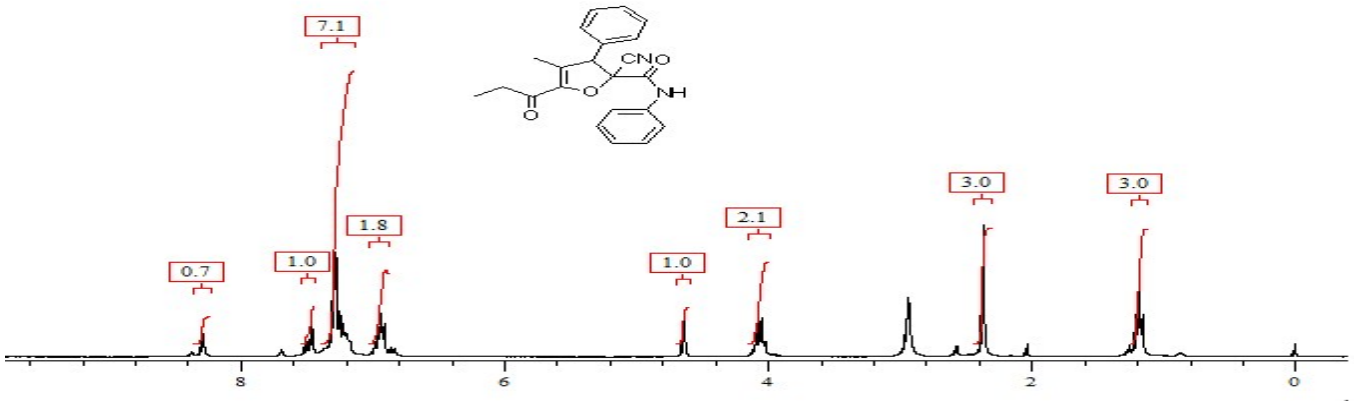
^{13}C-NMR (75 MHz) spectrum of 5j in a $CDCl_3$



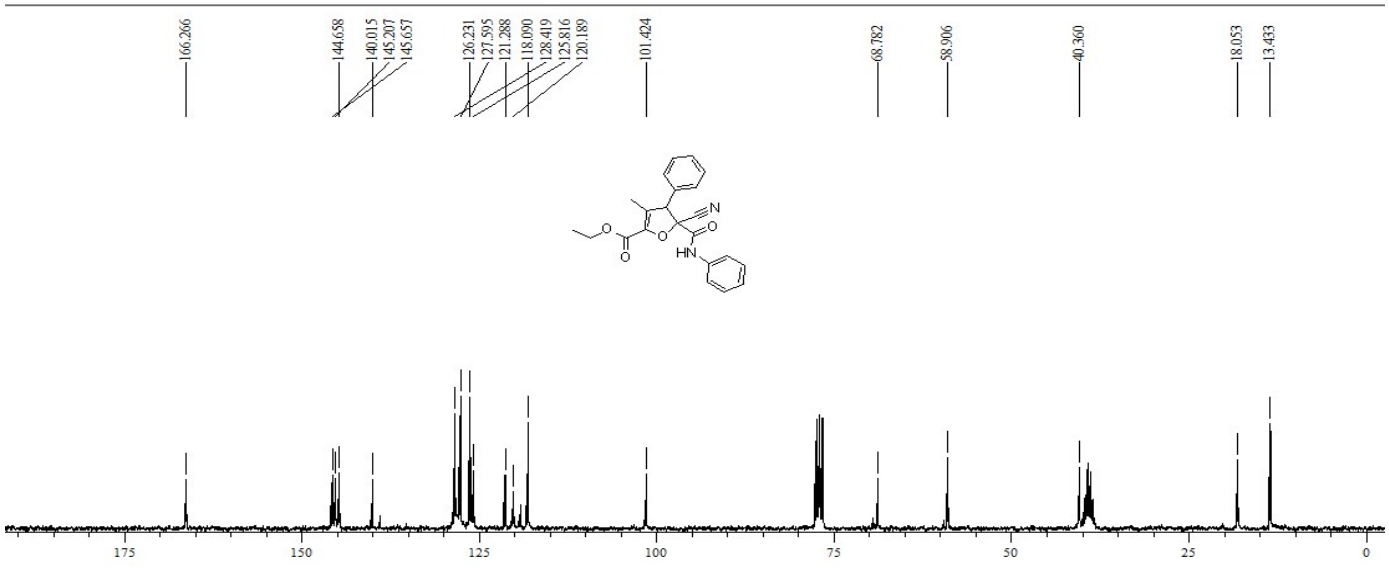
^{1}H-NMR (300 MHz) spectrum of 5k in a $CDCl_3$+DMSO-d_6



^{13}C-NMR (500 MHz) spectrum of 5k in a $CDCl_3$

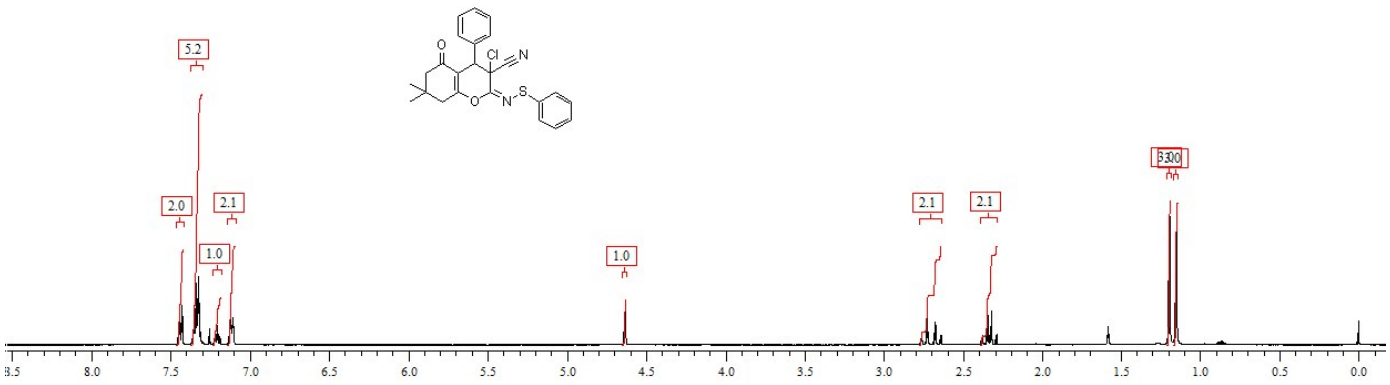


^{1}H-NMR (300 MHz) spectrum of 5l in a $CDCl_3$+DMSO-d_6

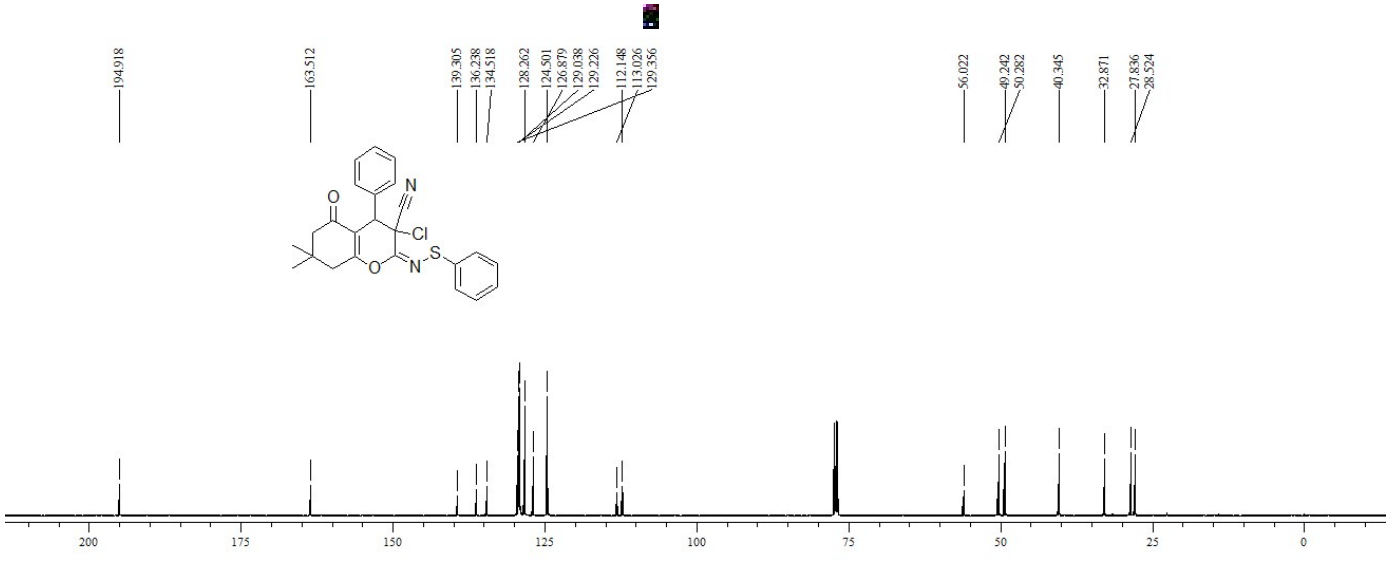


^{13}C-NMR (75 MHz) spectrum of 5l in a $CDCl_3$+DMSO-d_6

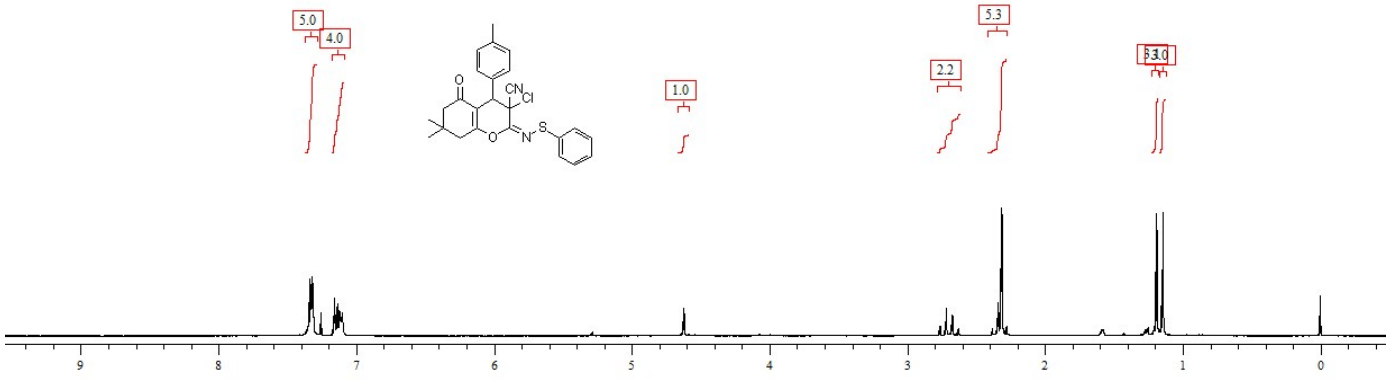
^{1}H and^{13}C NMR spectrums of 8 (a-k) :



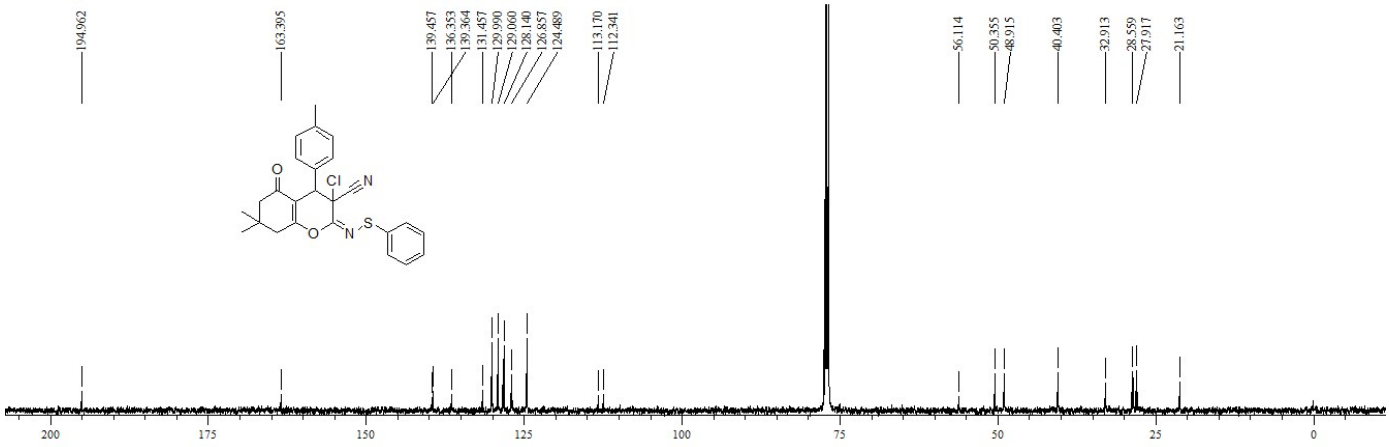
^{1}H-NMR (500 MHz) spectrum of 8 in a $CDCl_3$



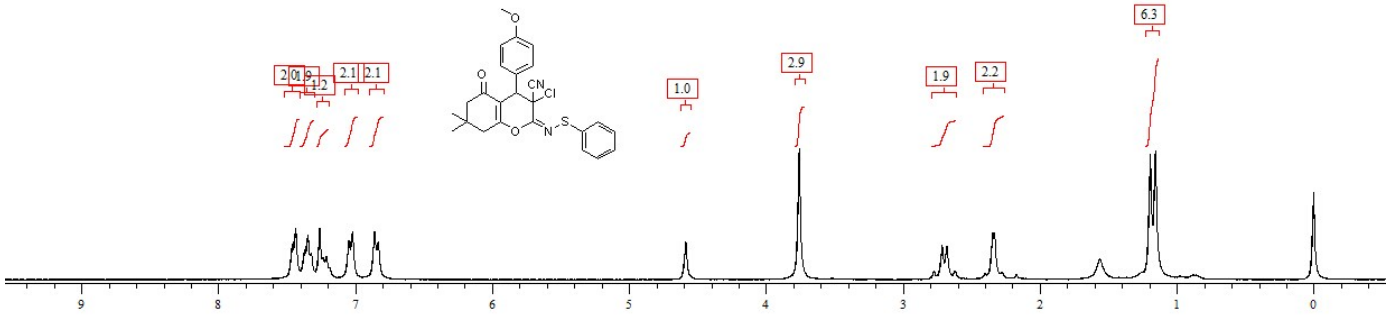
^{13}C-NMR (125 MHz) spectrum of 8 in a $CDCl_3$



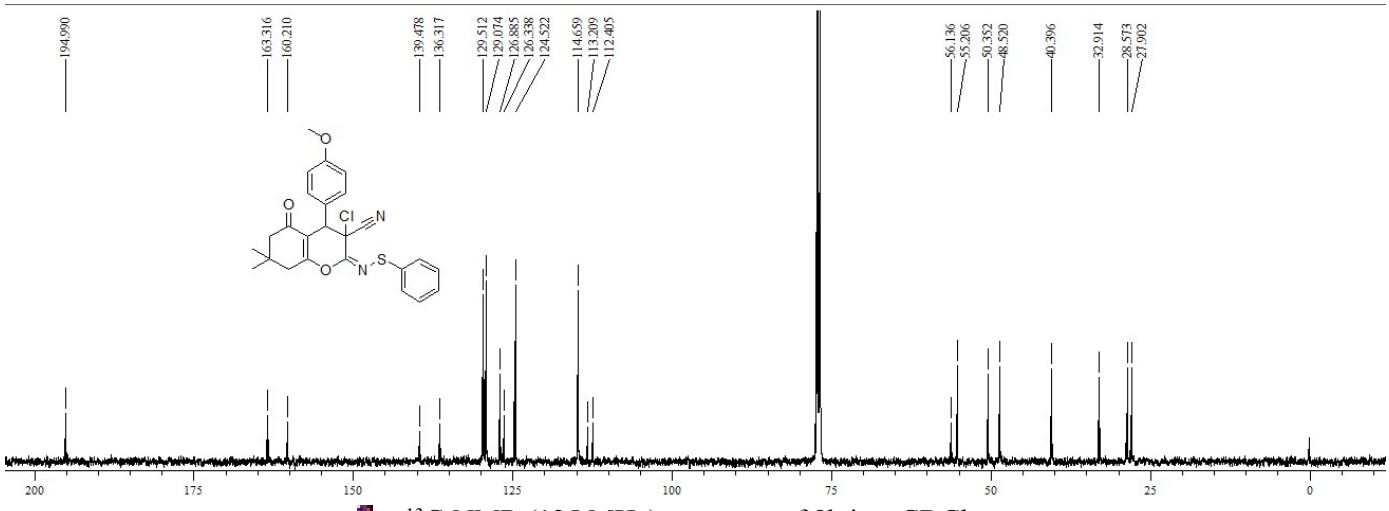
^{1}H-NMR (500 MHz) spectrum of 8a in a $CDCl_3$



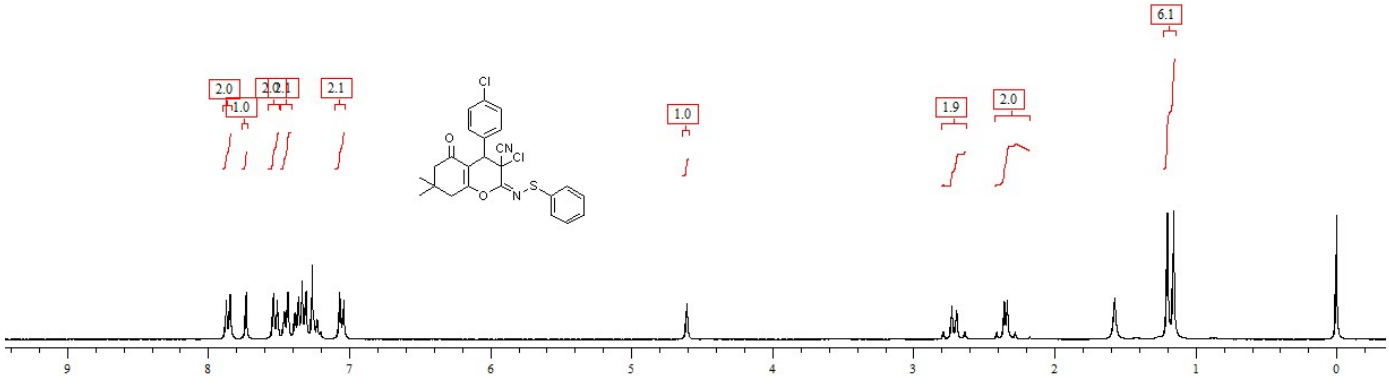
^{13}C-NMR (100 MHz) spectrum of 8a in a $CDCl_3$



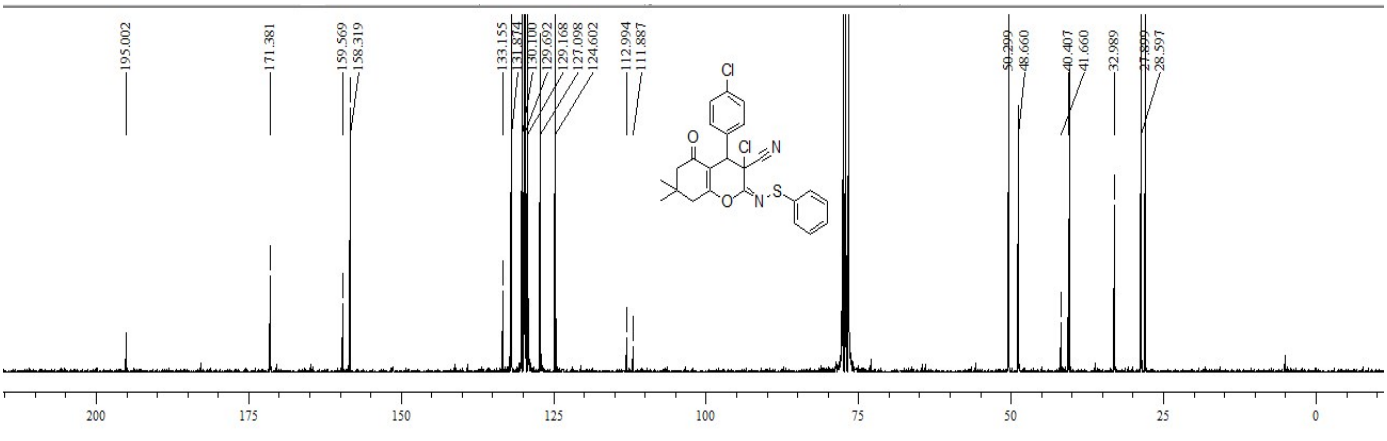
^{1}H-NMR (300 MHz) spectrum of 8b in a $CDCl_3$



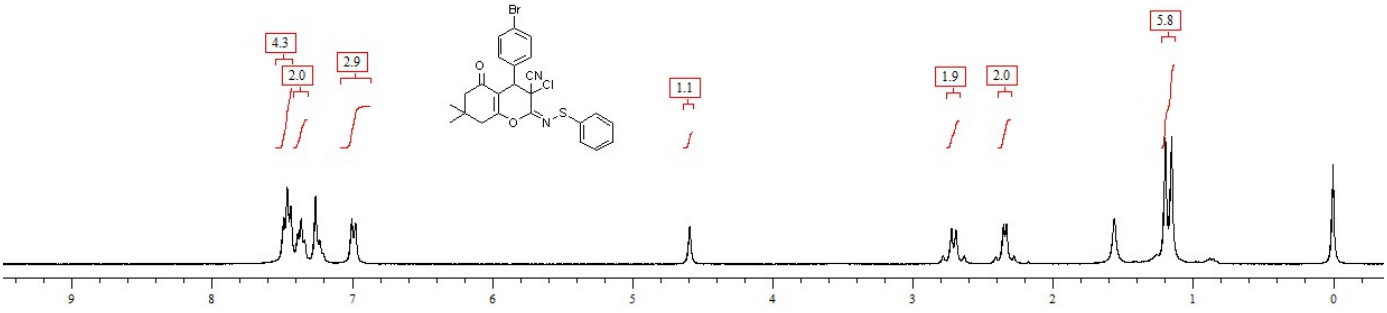
^{13}C-NMR (125 MHz) spectrum of 8b in a $CDCl_3$



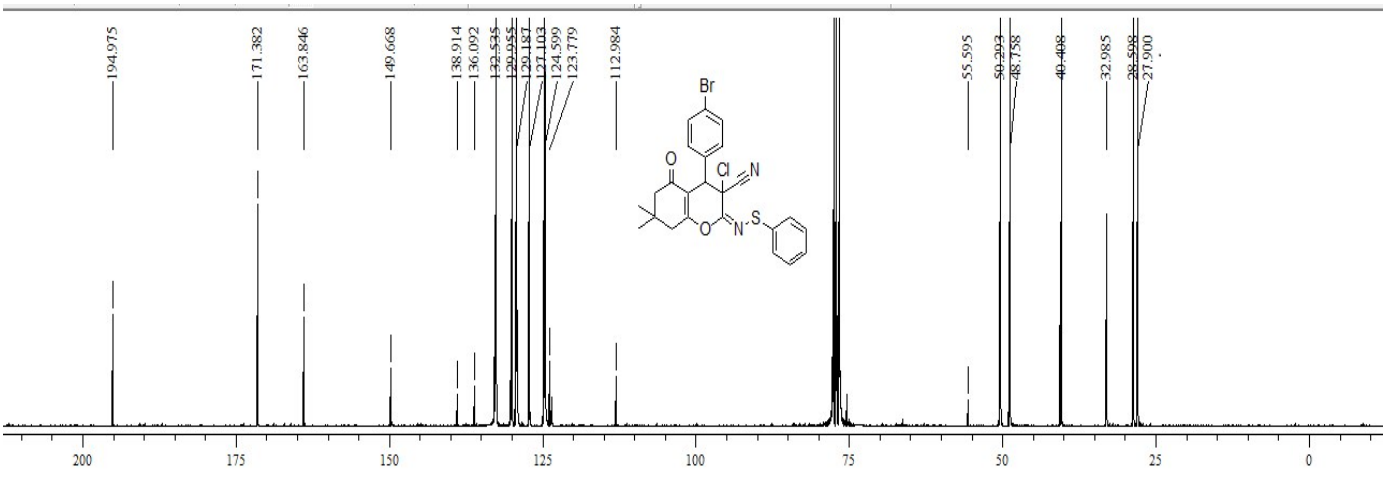
^{1}H-NMR (300 MHz) spectrum of 8c in a $CDCl_3$



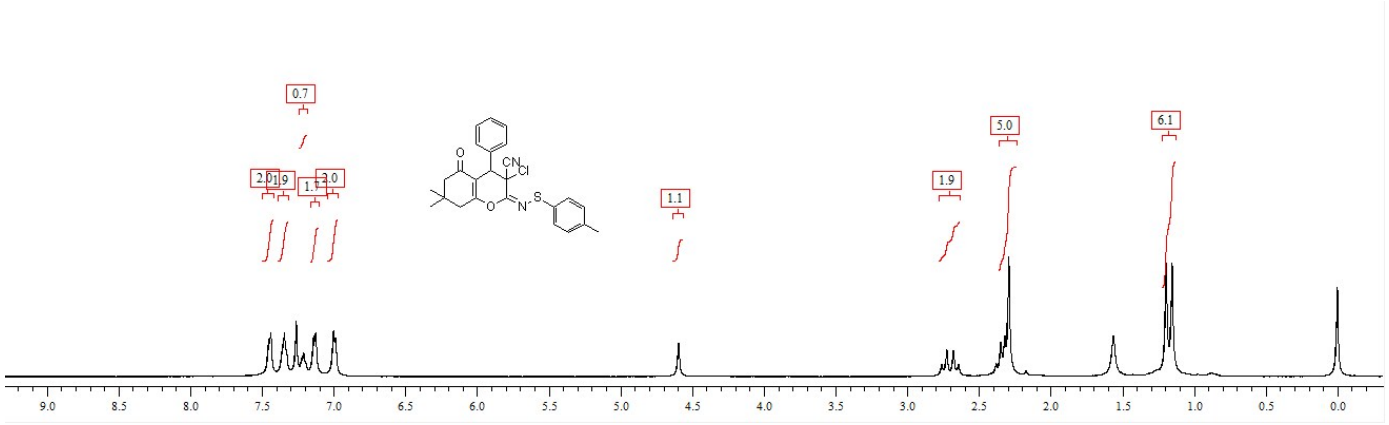
^{13}C-NMR (125 MHz) spectrum of 8c in a $CDCl_3$



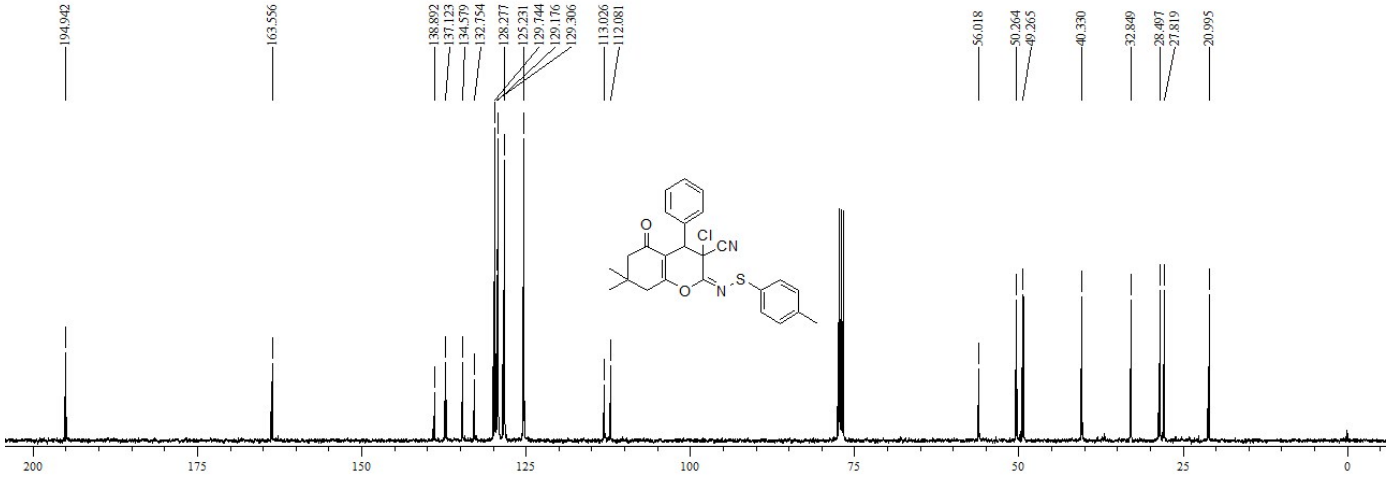
^{1}H-NMR (300 MHz) spectrum of 8d in a $CDCl_3$



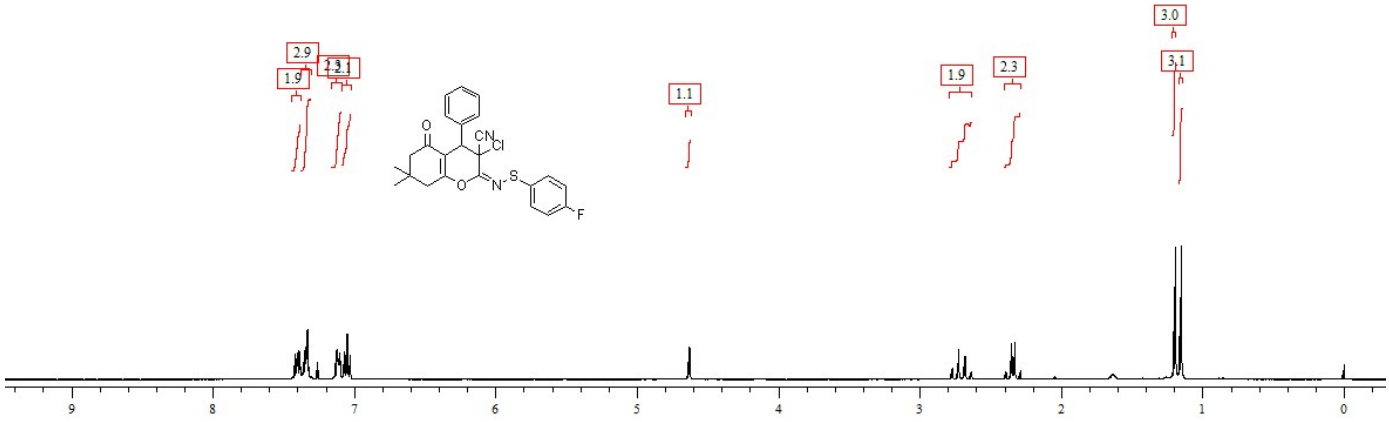
^{13}C-NMR (125 MHz) spectrum of 8d in a $CDCl_3$



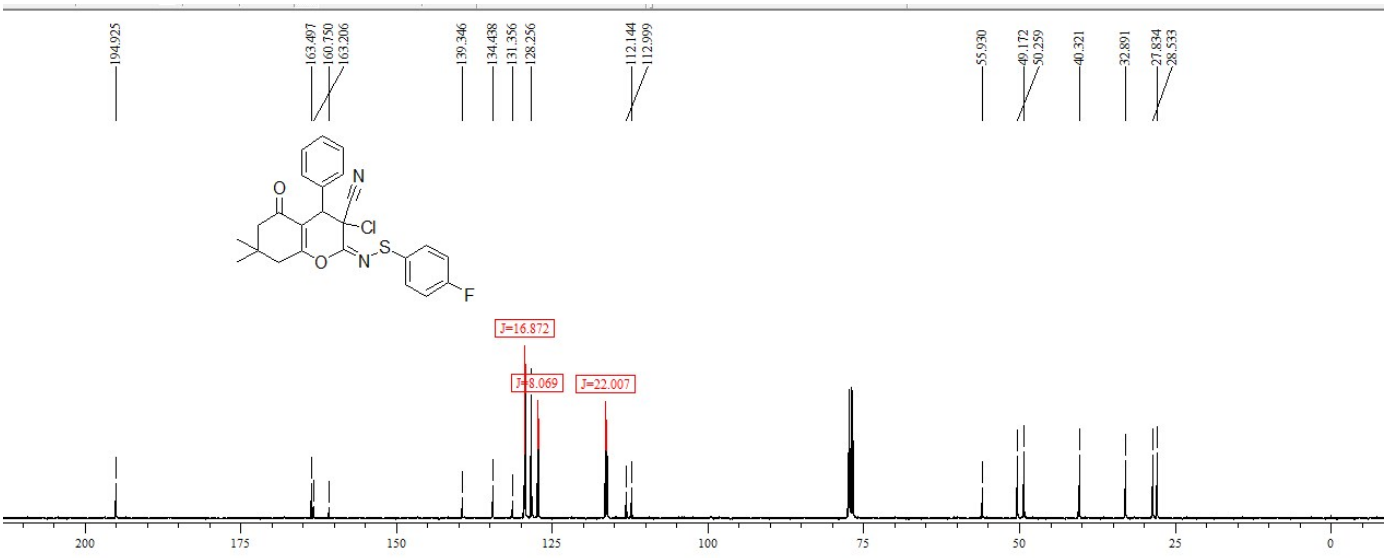
^{1}H-NMR (500 MHz) spectrum of 8e in a $CDCl_3$



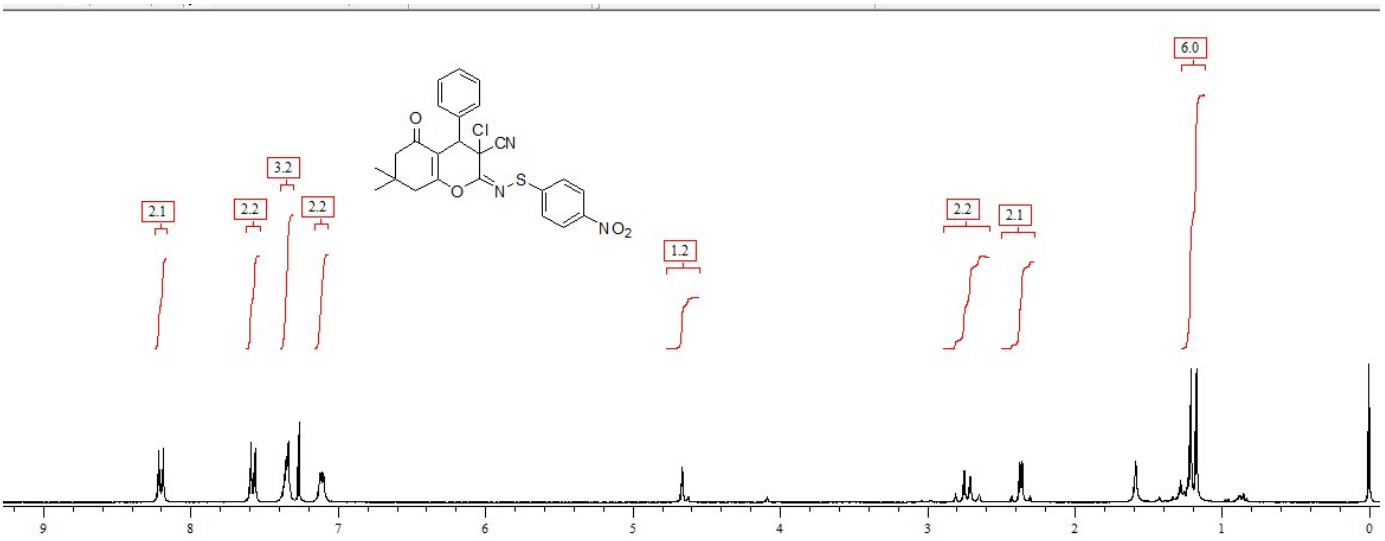
^{13}C-NMR (125 MHz) spectrum of 8e in a $CDCl_3$



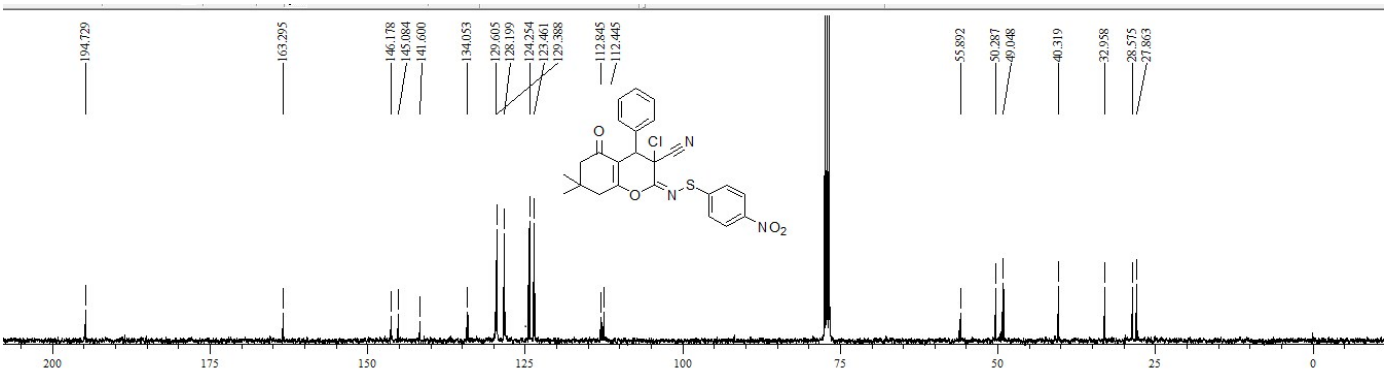
^{1}H-NMR (400 MHz) spectrum of 8f in a $CDCl_3$



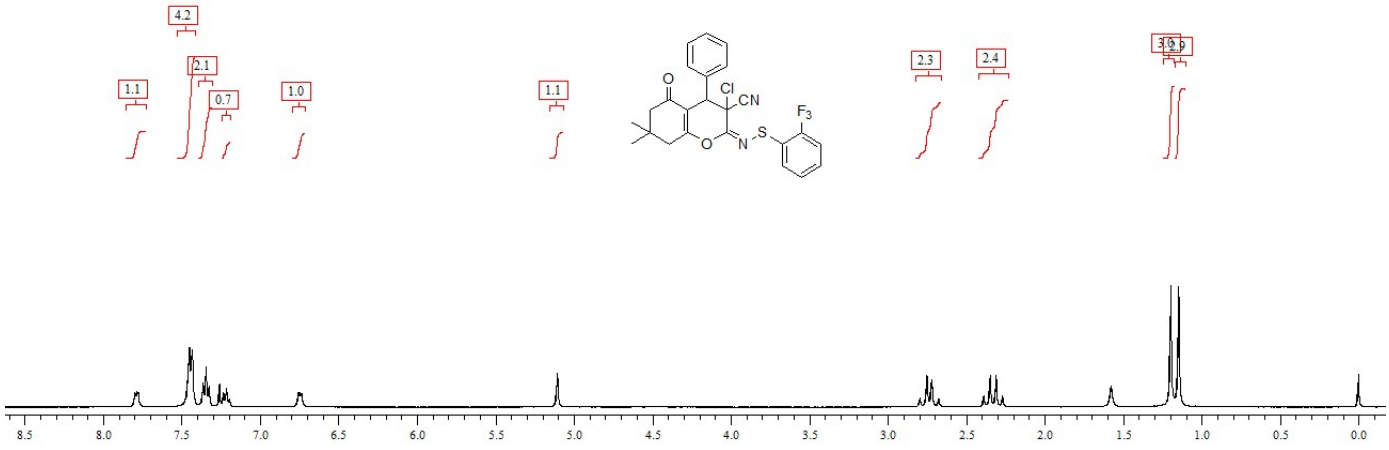
^{13}C-NMR (100 MHz) spectrum of 8f in a $CDCl_3$



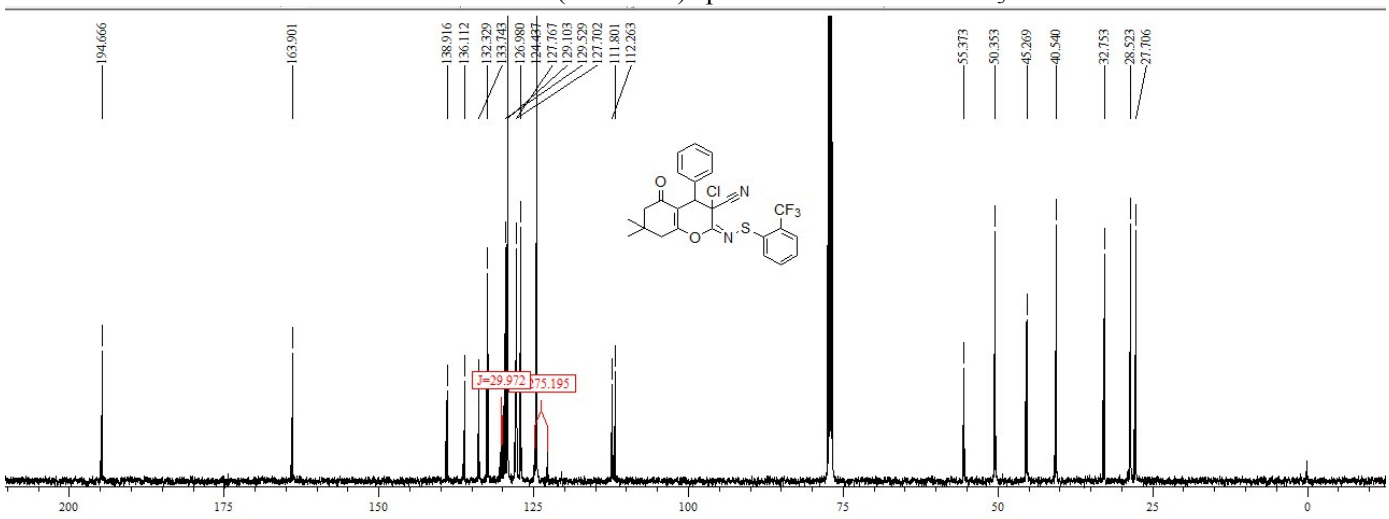
^{1}H-NMR (500 MHz) spectrum of 8g in a $CDCl_3$



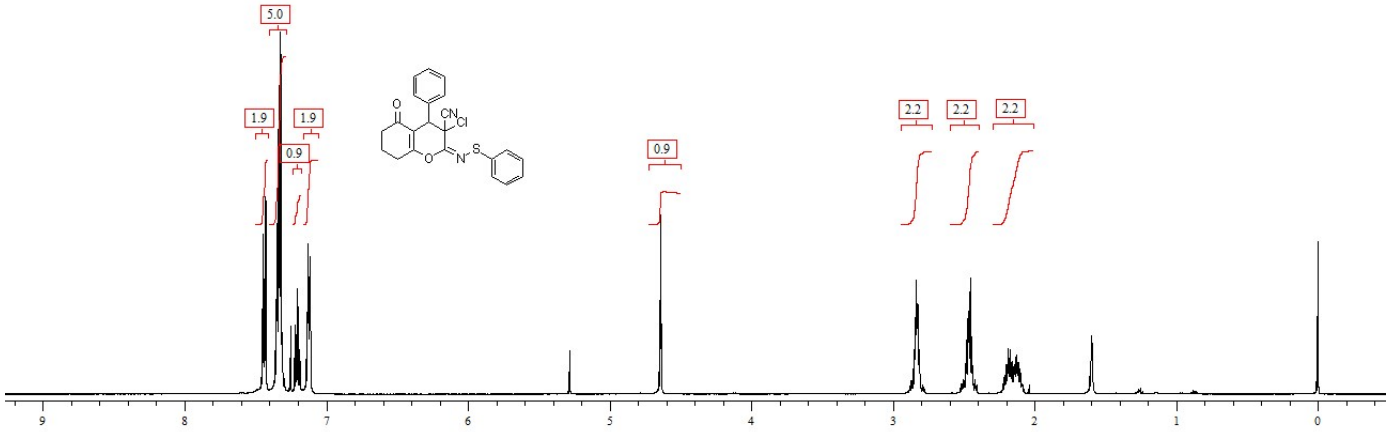
^{13}C-NMR (100 MHz) spectrum of 8g in a $CDCl_3$



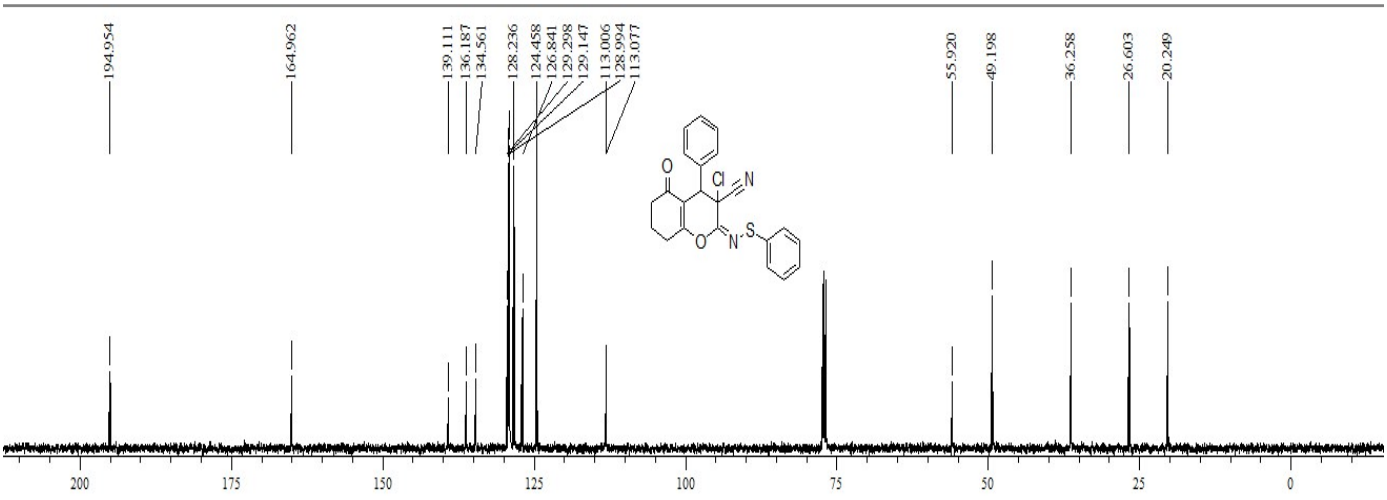
^{1}H-NMR (400 MHz) spectrum of 8h in a $CDCl_3$



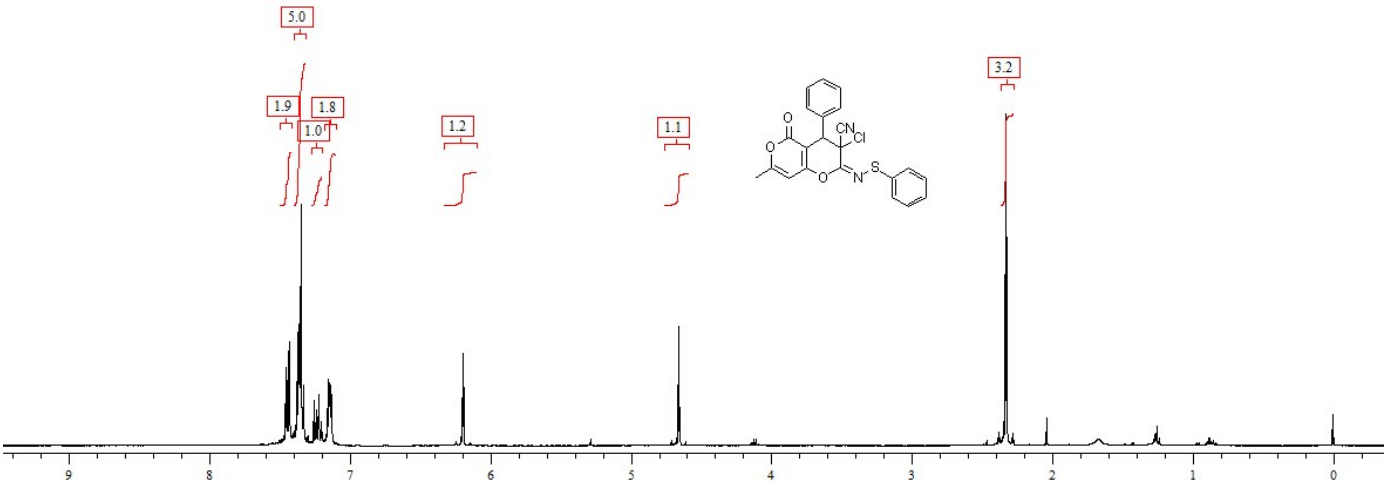
^{13}C-NMR (125 MHz) spectrum of 8h in a $CDCl_3$



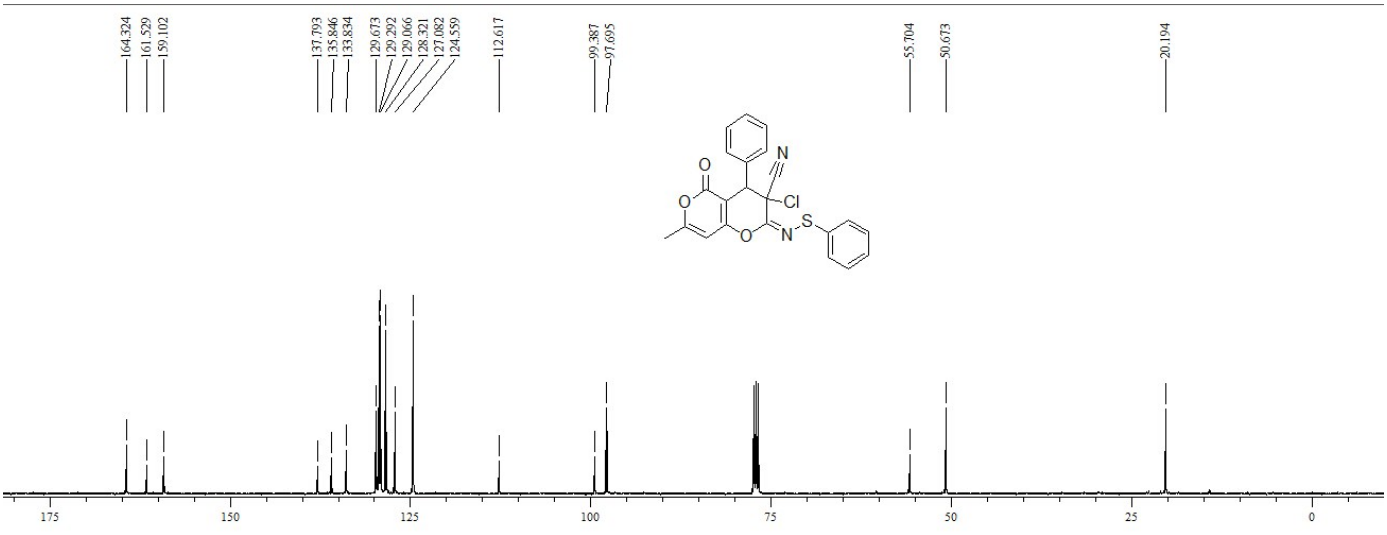
^{1}H-NMR (500 MHz) spectrum of 8i in a $CDCl_3$



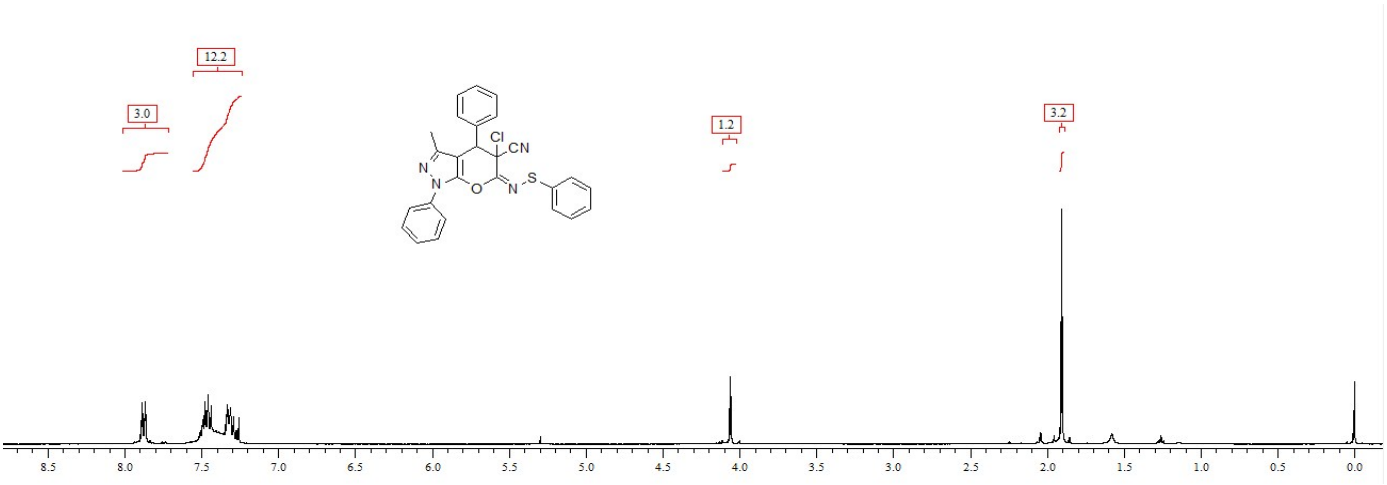
^{13}C-NMR (125 MHz) spectrum of 8i in a $CDCl_3$



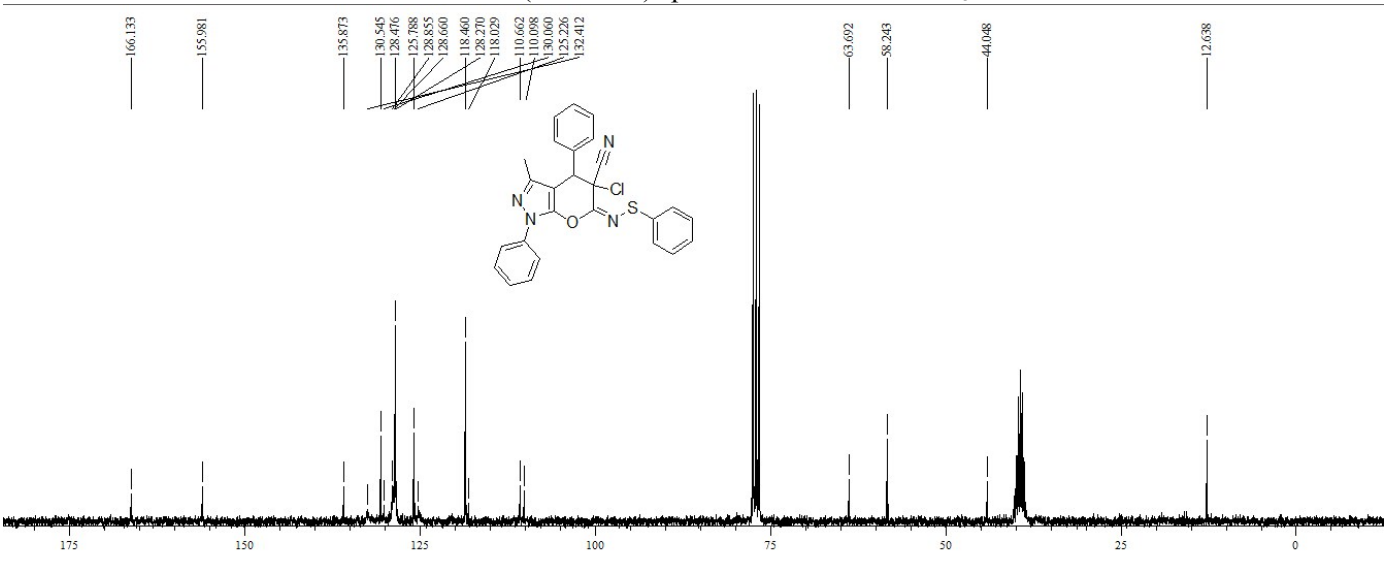
^{1}H-NMR (500 MHz) spectrum of 8j in a $CDCl_3$



^{13}C-NMR (125 MHz) spectrum of 8j in a $CDCl_3$



^{1}H-NMR (500 MHz) spectrum of 8k in a $CDCl_3$



^{13}C-NMR (125 MHz) spectrum of 8k in a $CDCl_3$+DMSO-d_6