Supplementary Material

A Synthesis of Pyrrolidin-2-ylidenes and Pyrrol-2-ylidenes *via* 1,3-Dipolar Cycloaddition of H-bond-assisted Azomethine Ylides to Nitrostyrenes
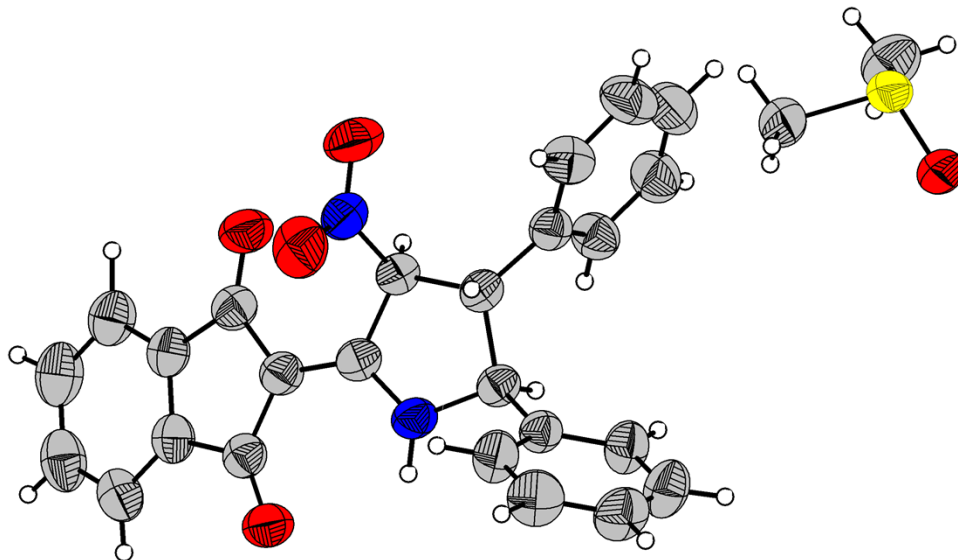
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Supplementary Material- Table of Contents

X-Ray Crystal-Structure Determination of 5a

CCDC 2202656 (**5a**) 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/getstructures.

Table Experimental details of Crystal data

Chemical formula	$C_{25}H_{18}N_2O_4$ [C_2H_6OS]
Mr	488.54
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	290
a, b, c (Å)	14.636 (3), 9.854 (2), 16.905 (3)
β (°)	96.34 (3)
V (Å3)	2423.2 (8)
Z	4

Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.18 mm^{-1}
Crystal size (mm)	0.2 × 0.15 × 0.1 mm

Data collection

Diffractometer	MAR-345dtb
Tmin, Tmax	0.790, 1.221
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17051, 4660, 4339
Rint	0.066
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.616

Refinement

$R[F2 > 2\sigma(F2)]$, $wR(F2)$, S	0.059, 0.161, 1.16
No. of reflections	4660
No. of parameters	390
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho$max, $\Delta\rho$min (e Å^{-3})	0.26, −0.44

Computer programs: MAR345 dtb Program (1.24-4, 2013), Automar software package (3.3a, 2015), *SHELXT* 2018/2 (Sheldrick, 2018), *SHELXL2016*/6
(Sheldrick, 2016), *DIAMOND* (Brandenburg, 1999), *PLATON* (2018).

References

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* 42, 339-341.
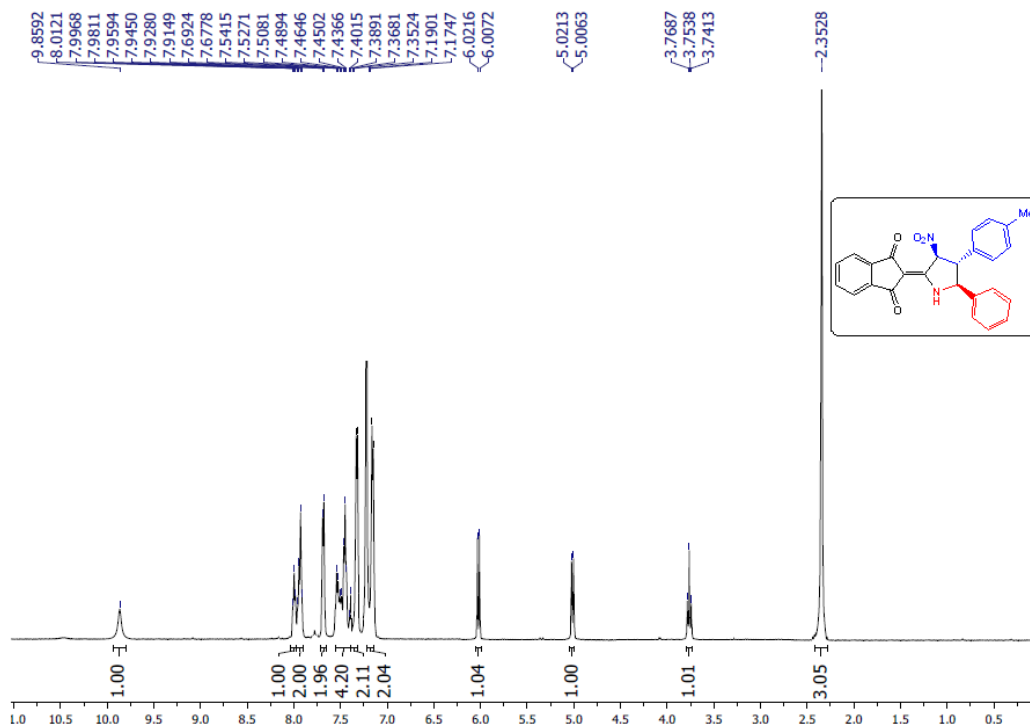Sheldrick, G. M. (2015). *Acta Cryst. C 71*, 3-8.

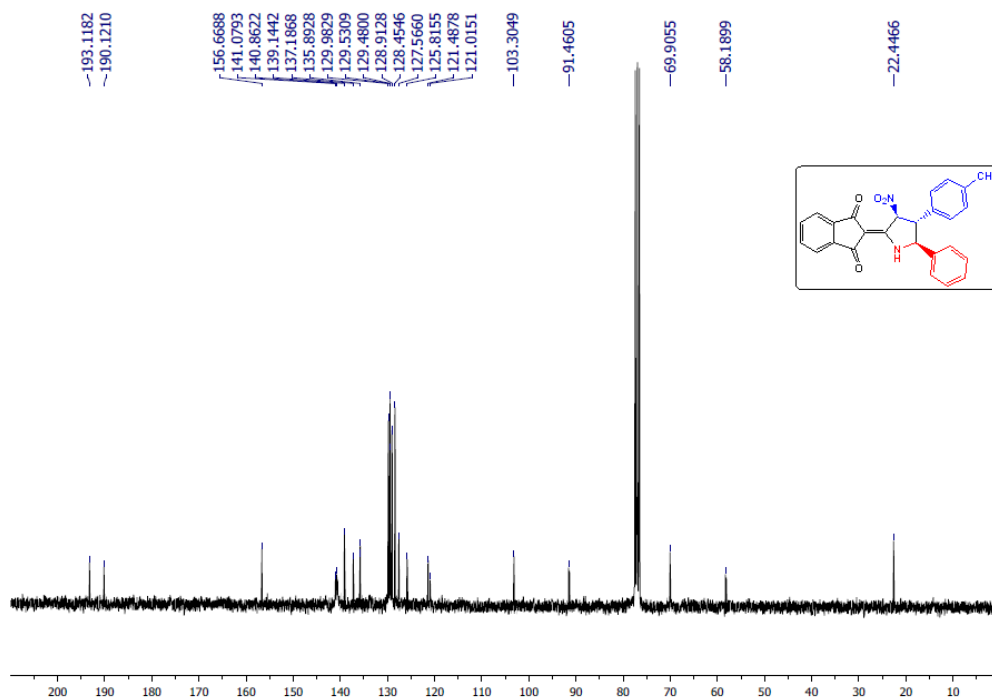**NMR spectra of 2-(3-nitro-4,5-diarylpyrrolidin-2-ylidene)-1*H*-indene-1,3(2*H*)-diones 5a-5n**
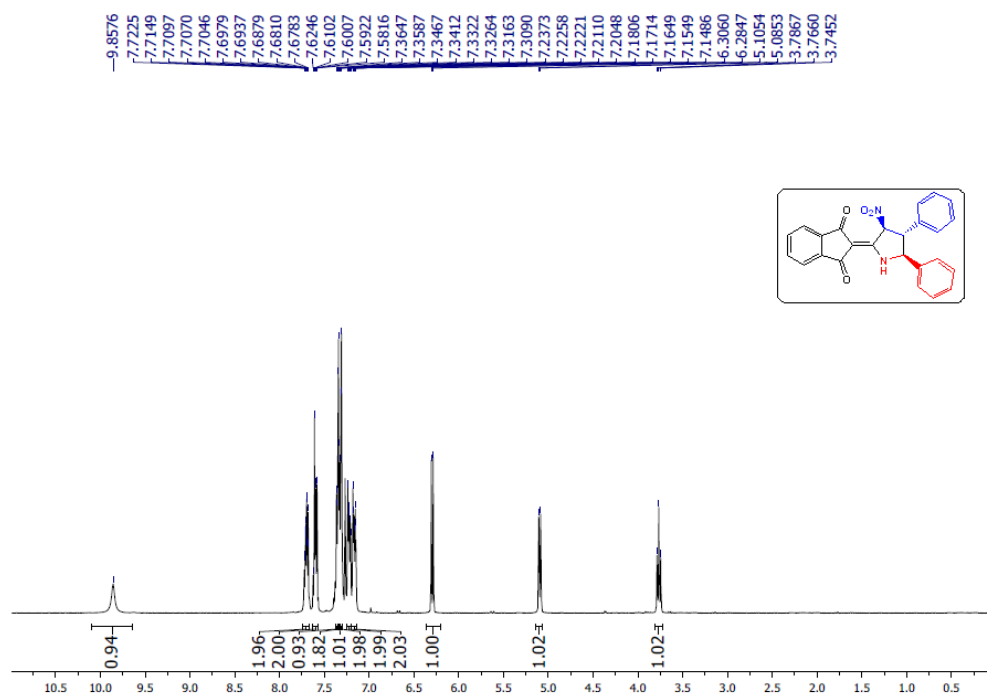
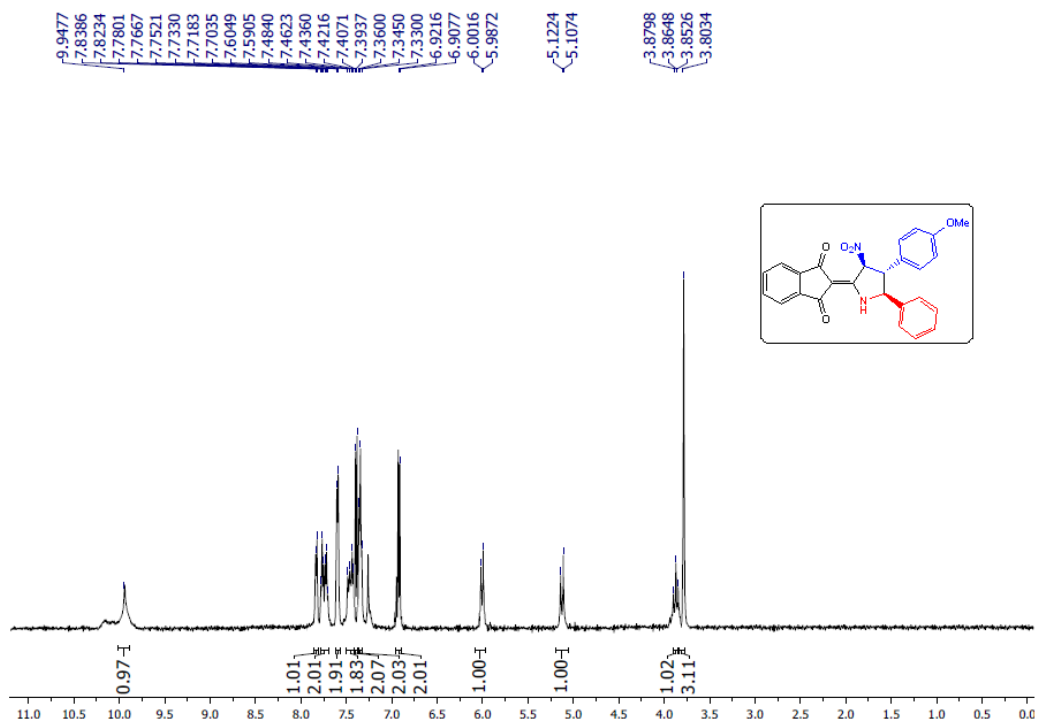¹H NMR (300 MHz) of Compound **5a** in CDCl₃
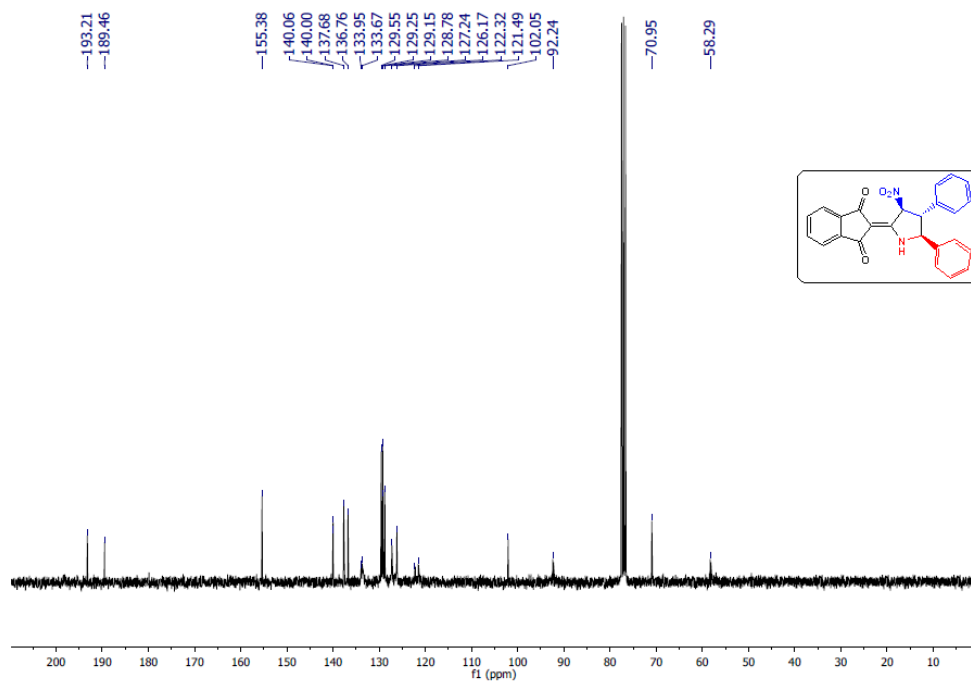
¹³C NMR (75.6 MHz) of Compound **5a** in CDCl₃
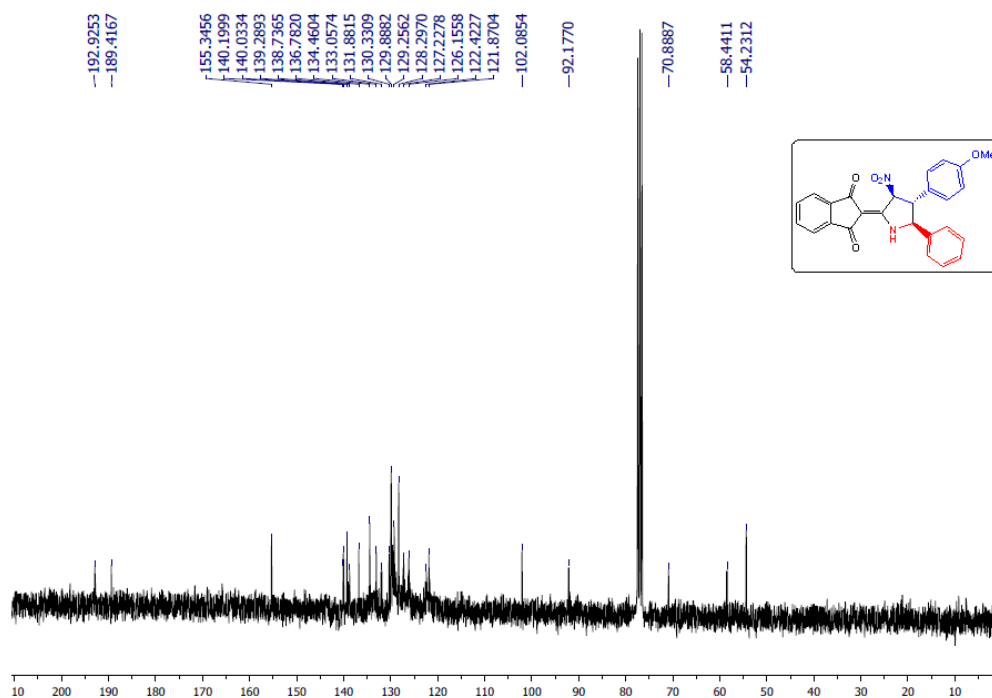
^{1}H NMR (500 MHz) of Compound **5b** in CDCl$_3$
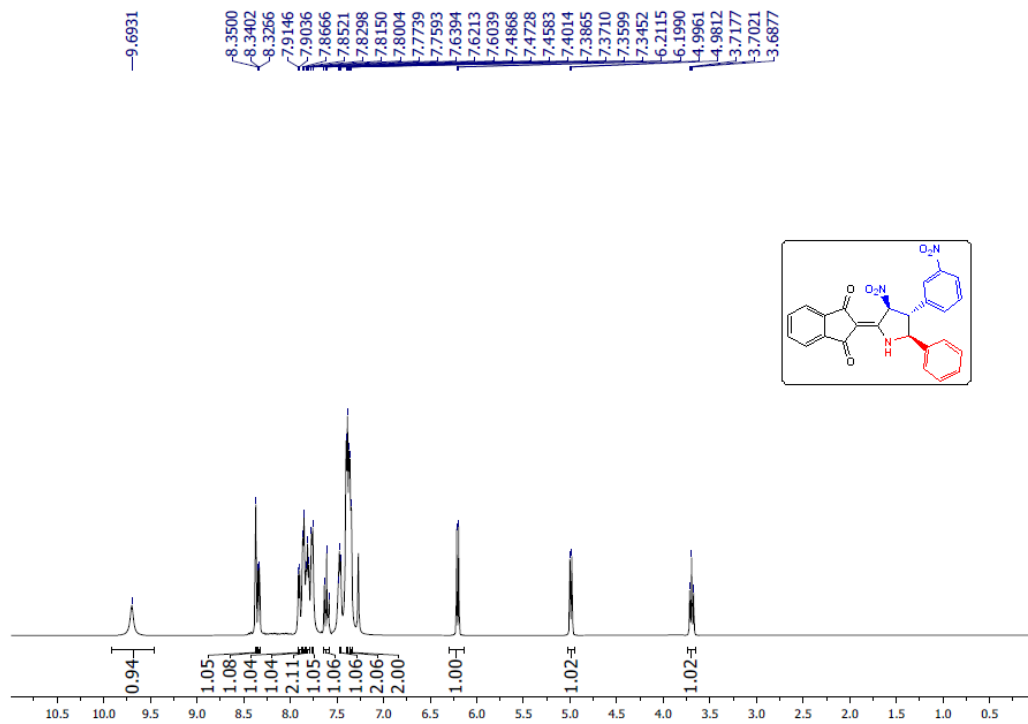

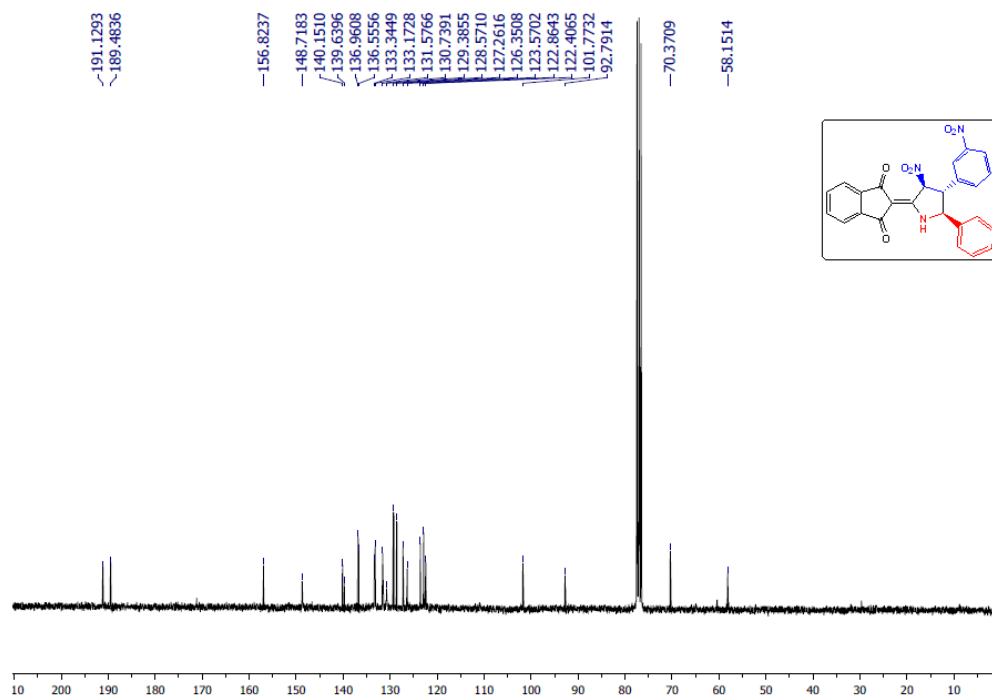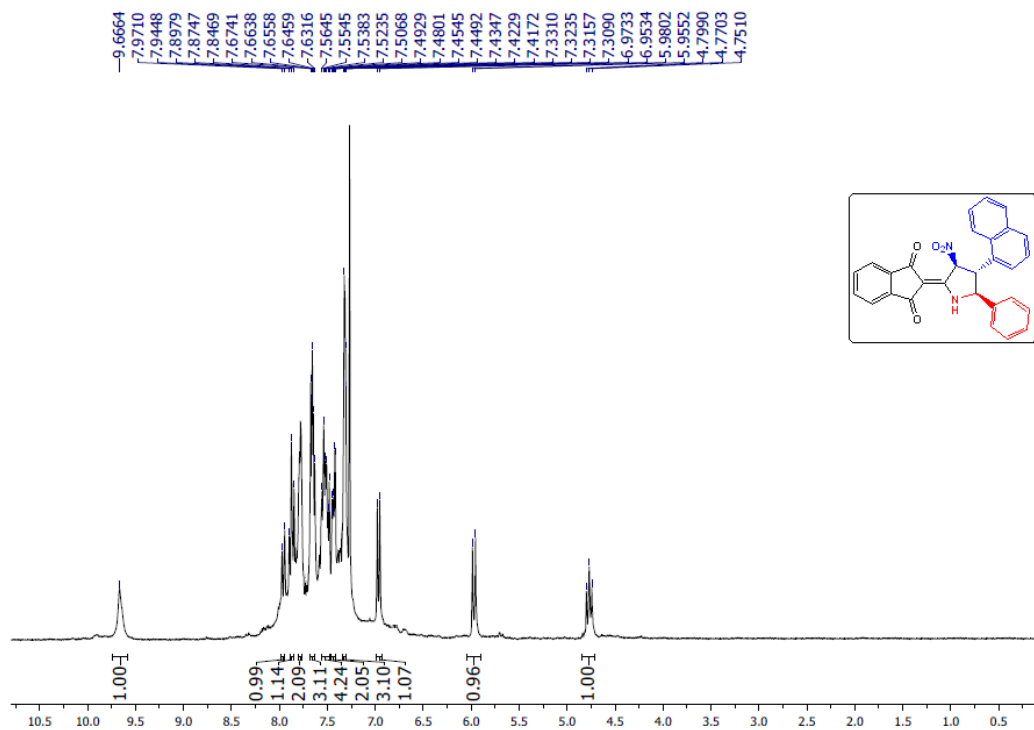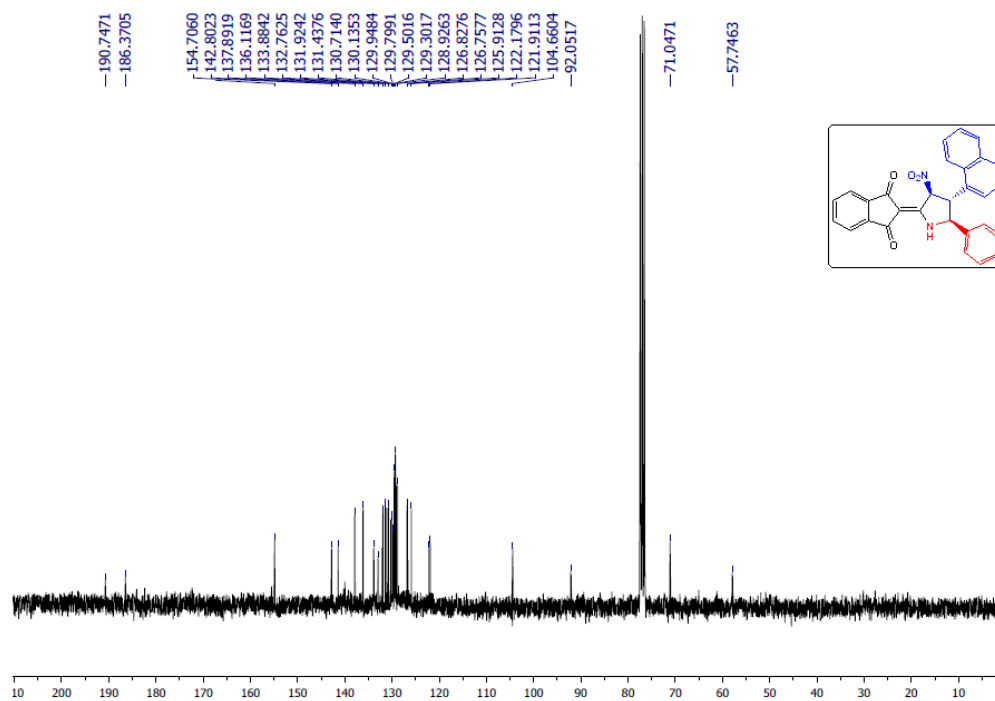^{13}C NMR (126 MHz) of Compound **5b** in CDCl$_3$

^{1}H NMR (500 MHz) of Compound **5c** in CDCl$_3$

^{13}C NMR (126 MHz) of Compound **5c** in CDCl$_3$
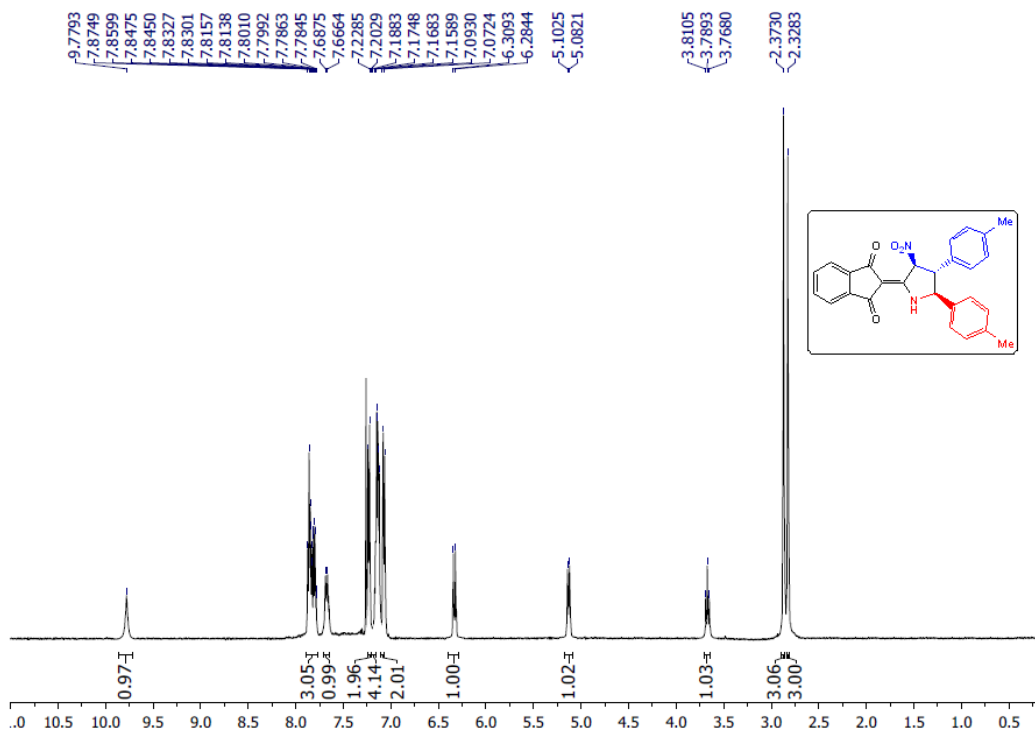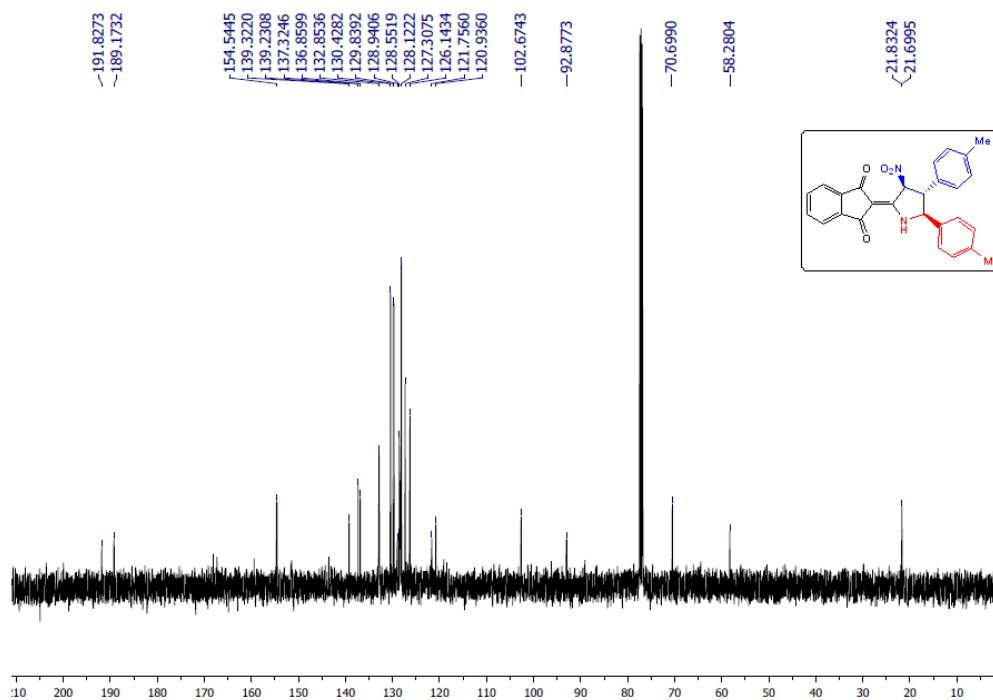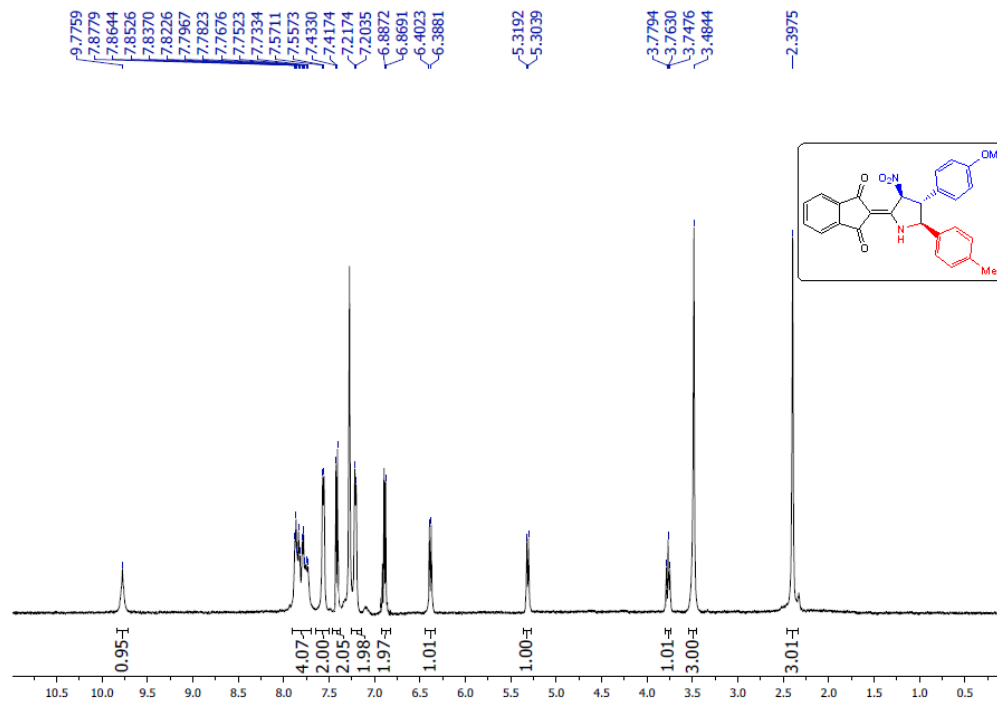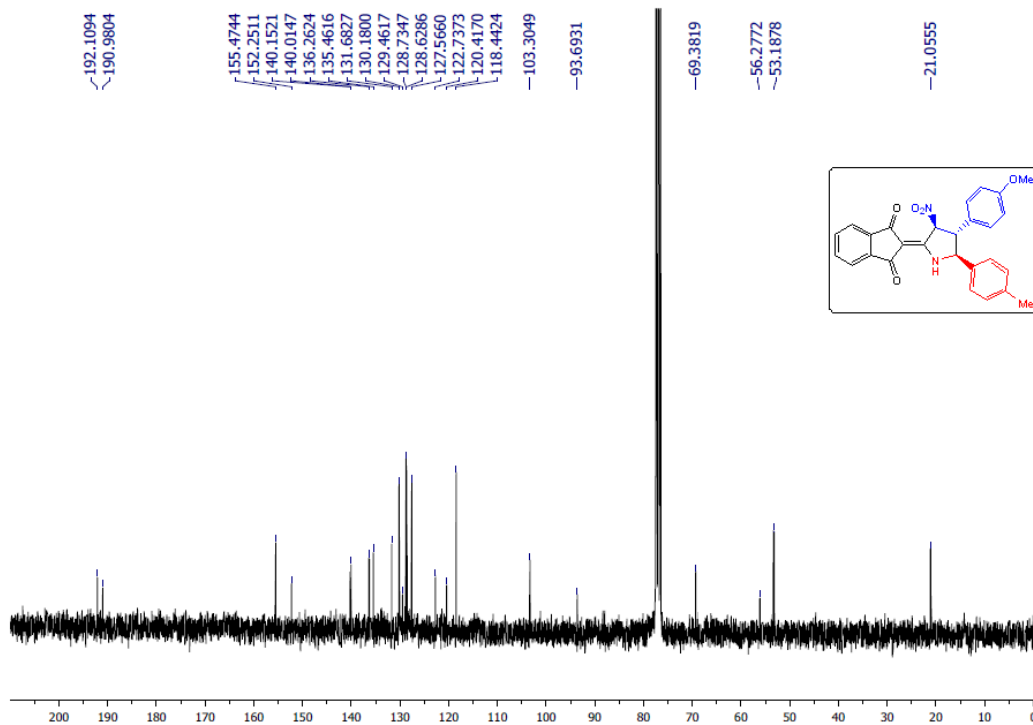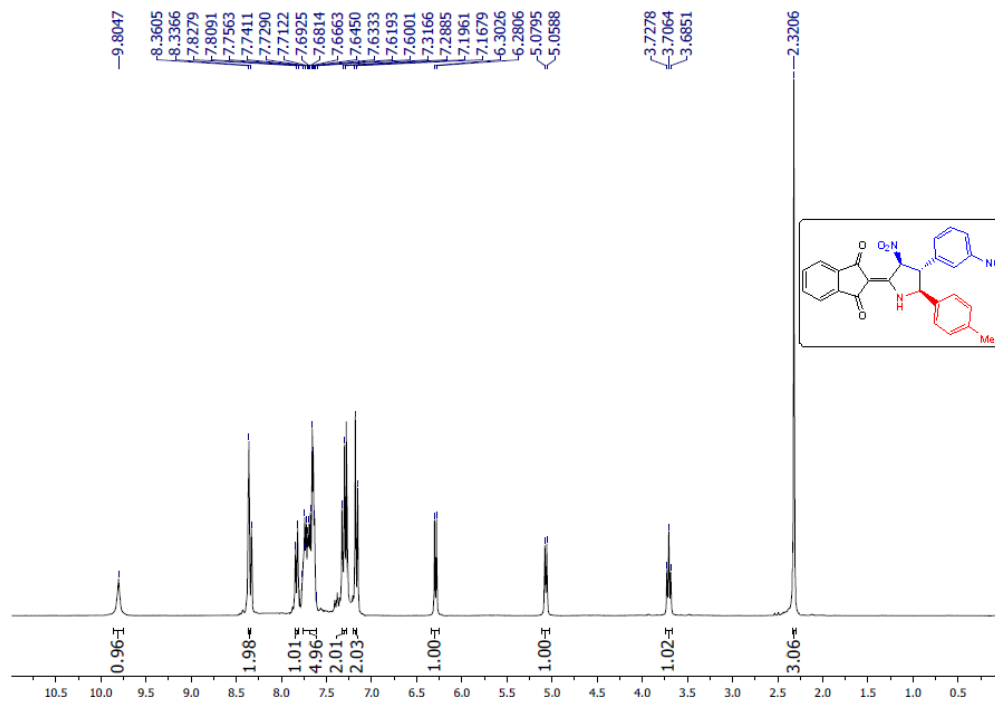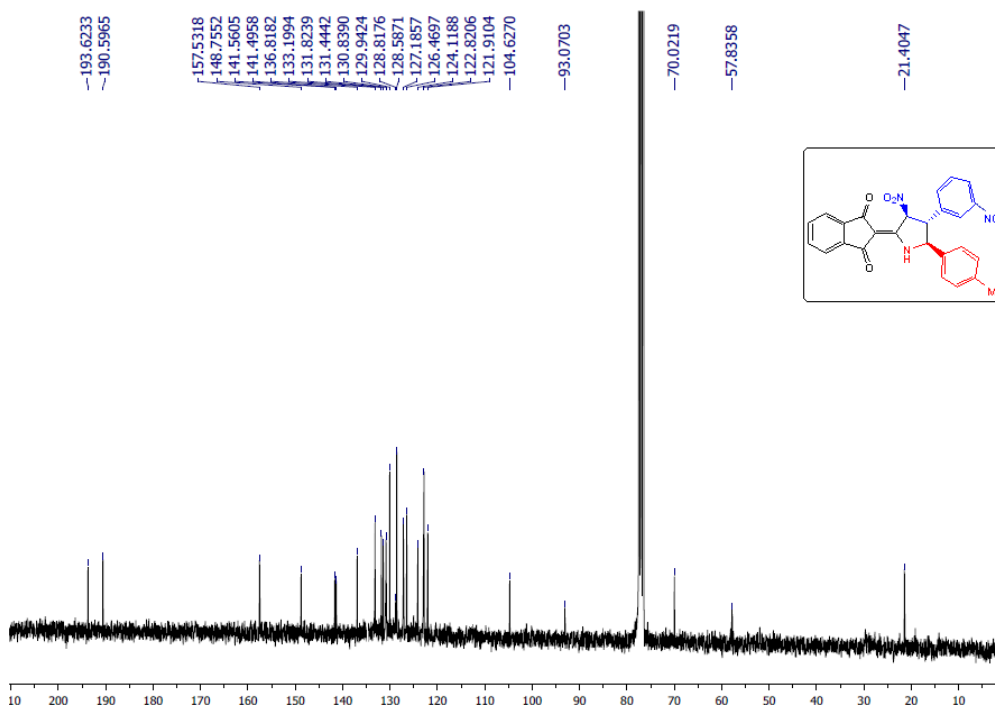
^{1}H NMR (500 MHz) of Compound **5d** in CDCl$_3$

^{13}C NMR (126 MHz) of Compound **5d** in CDCl$_3$

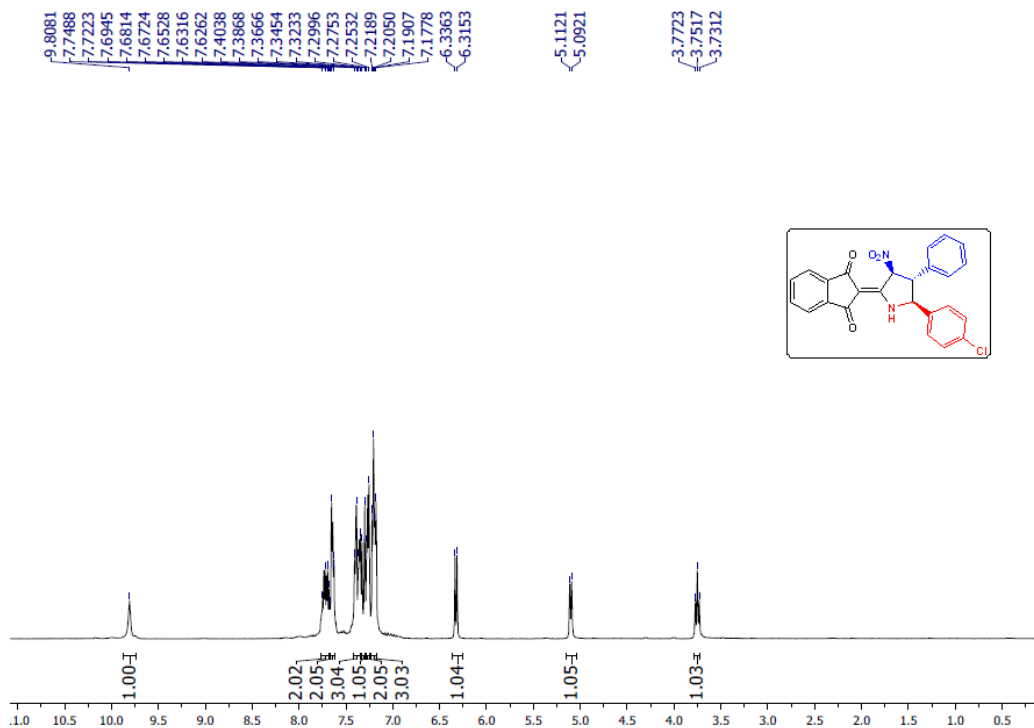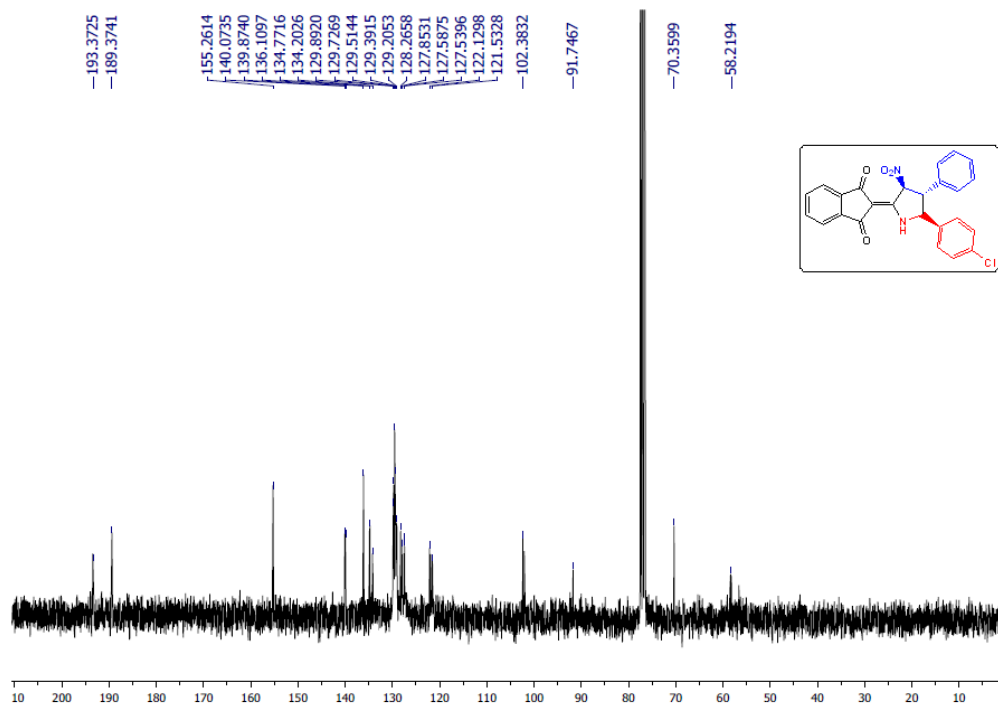^{1}H NMR (500 MHz) of compound **5e** in CDCl$_3$

^{13}C NMR (126 MHz) of compound **5e** in CDCl$_3$

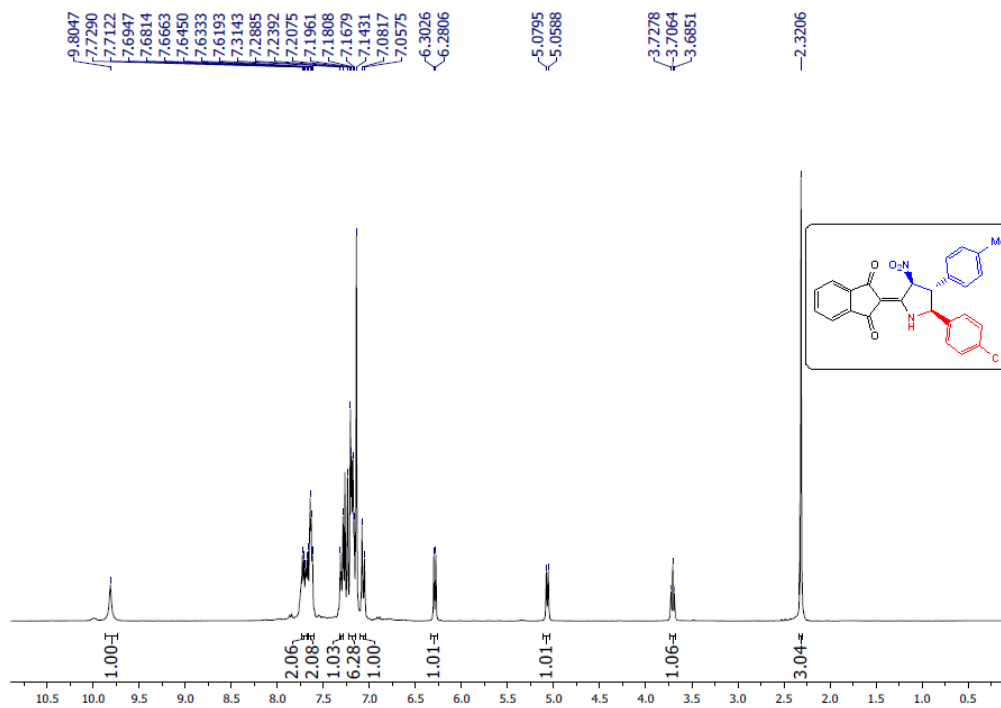^{1}H NMR (300 MHz) of compound **5f** in CDCl$_3$
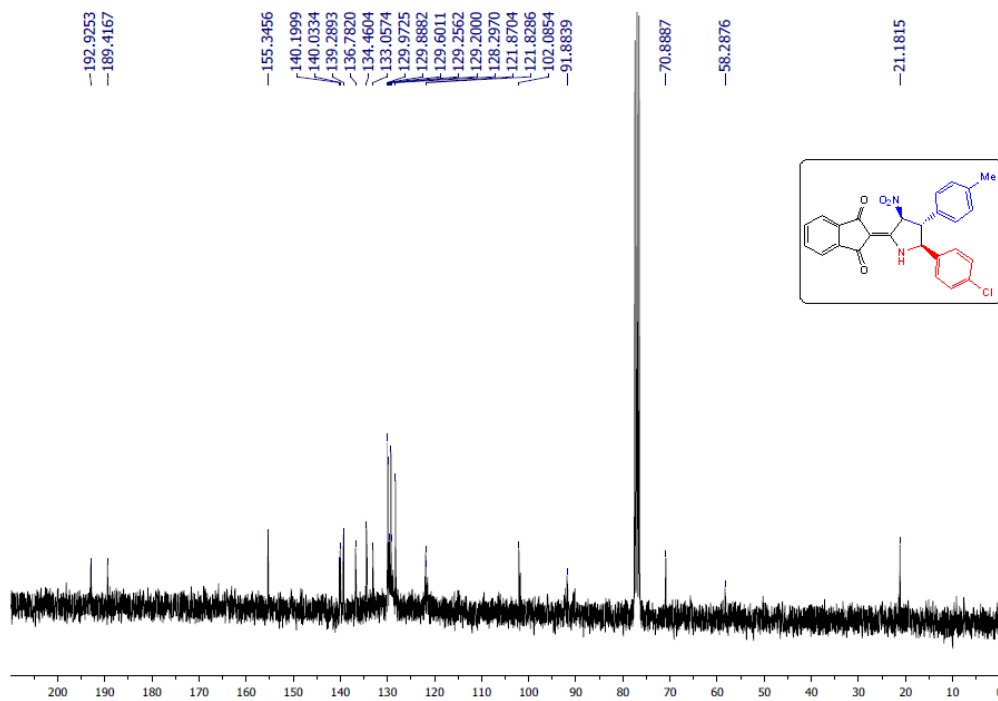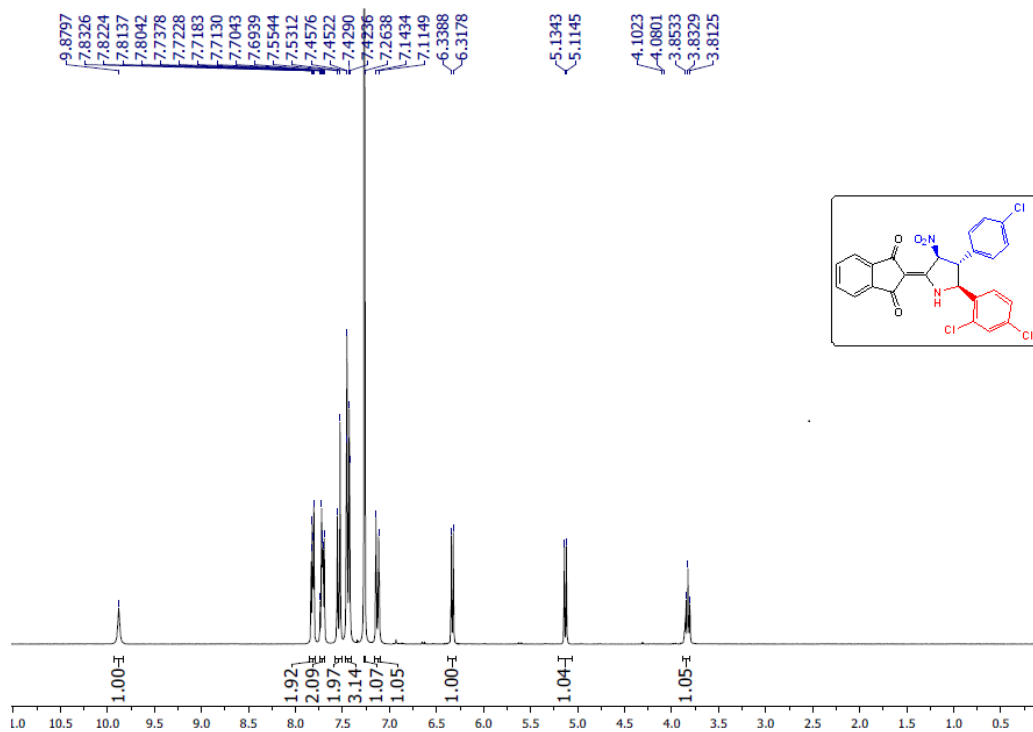

^{13}C NMR (75.6 MHz) of compound **5f** in CDCl$_3$

9.7759
7.8879
7.8644
7.8526
7.8370
7.8226
7.7967
7.7823
7.7676
7.7523
7.7334
7.5711
7.5573
7.4330
7.4174
7.2174
7.2035
6.8872
6.8691
6.4023
6.3881
5.3192
5.3039
3.7794
3.7630
3.7476
3.4844
2.3975

0.95
4.07
2.00
2.05
1.98
1.97
1.01
1.00
1.01
3.00
3.01

10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5

^{1}H NMR (500 MHz) of compound **5g** in CDCl$_3$

192.1094
190.9804
155.4744
152.2511
140.1521
140.0147
136.2624
135.4616
131.6827
130.1800
129.4617
128.7347
128.6286
127.5660
122.7373
120.4170
118.4424
103.3049
93.6931
69.3819
56.2772
53.1878
21.0555

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

^{13}C NMR (126 MHz) of compound **5g** in CDCl$_3$
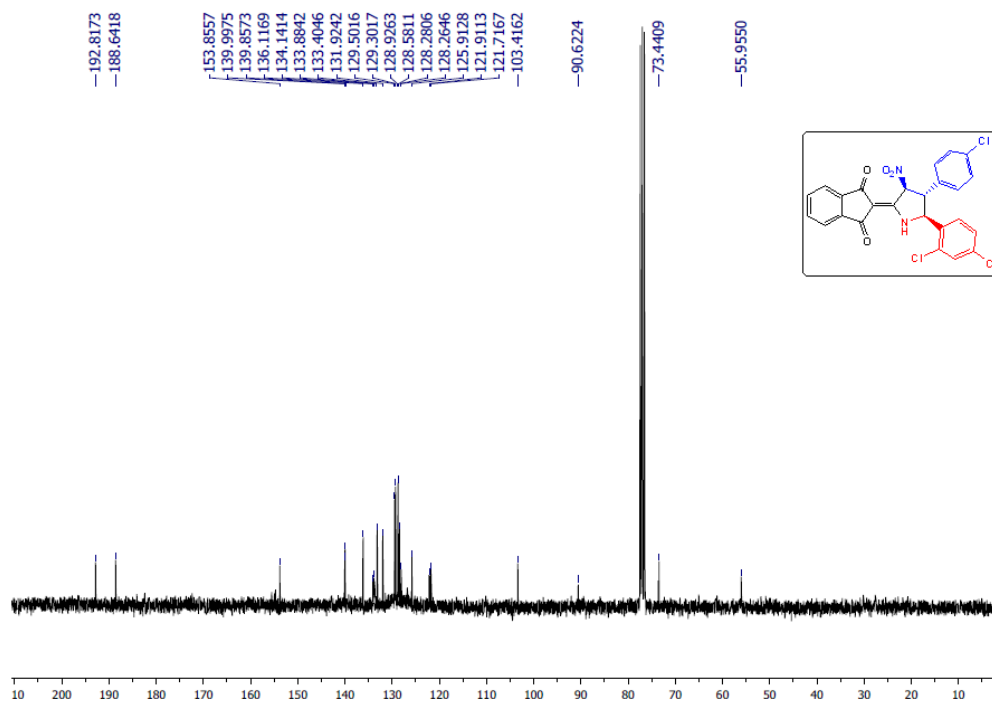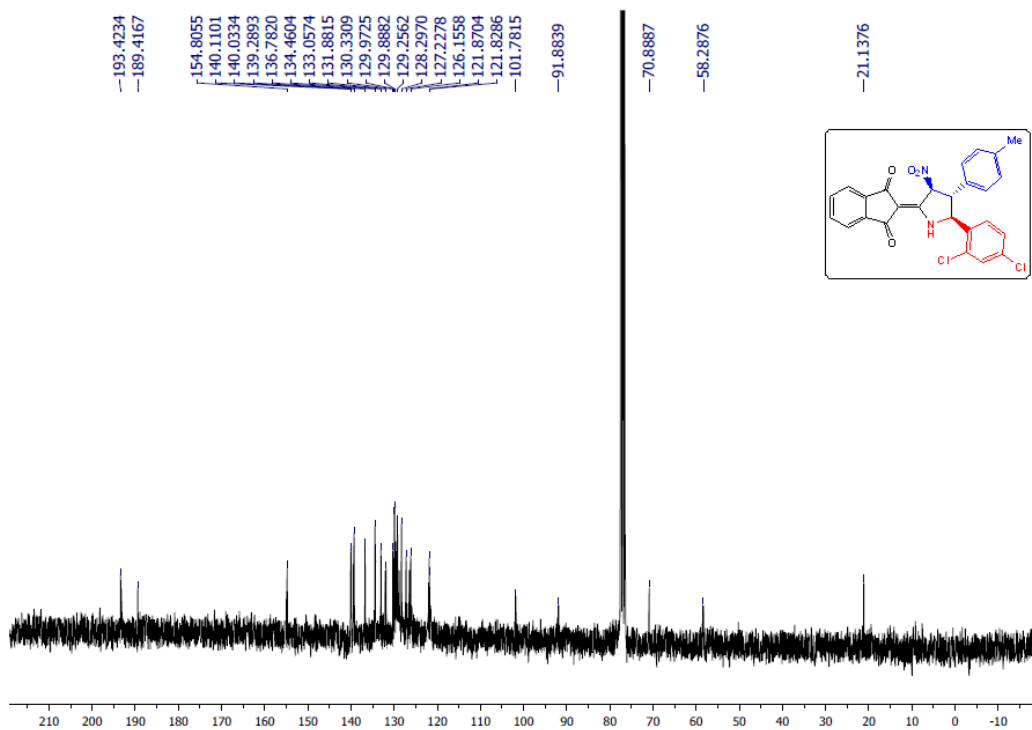
^{1}H NMR (300 MHz) of compound **5h** in CDCl$_3$

^{13}C NMR (75.6 MHz) of compound **5h** in CDCl$_3$

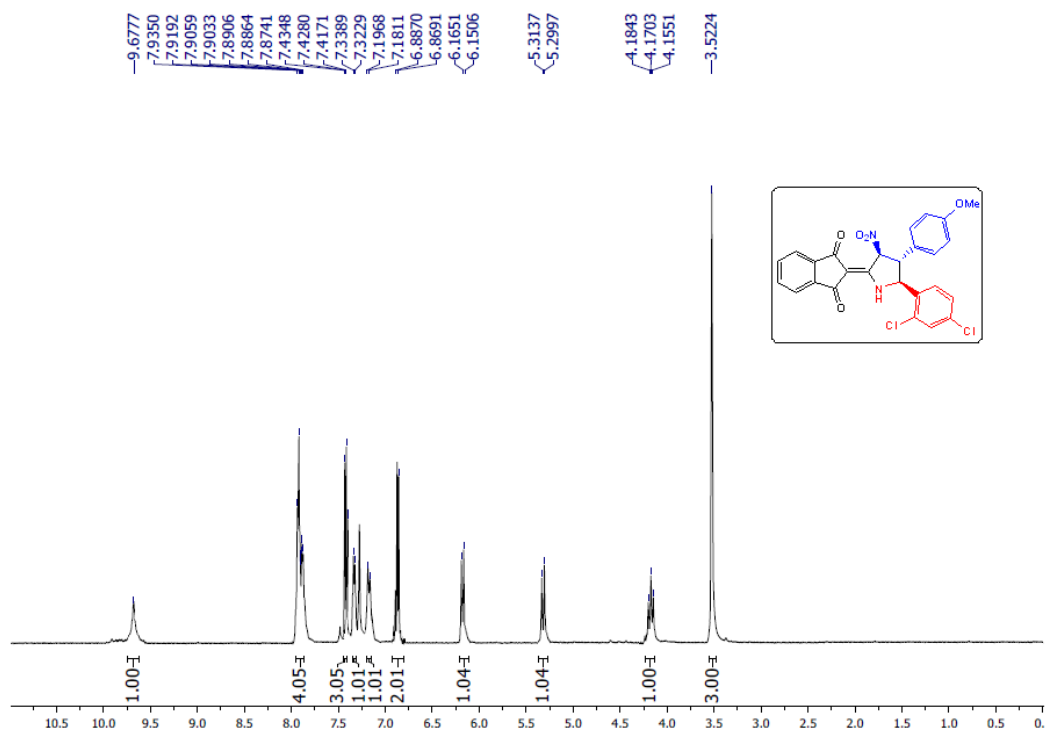^{1}H NMR (300 MHz) of compound **5i** in CDCl$_3$
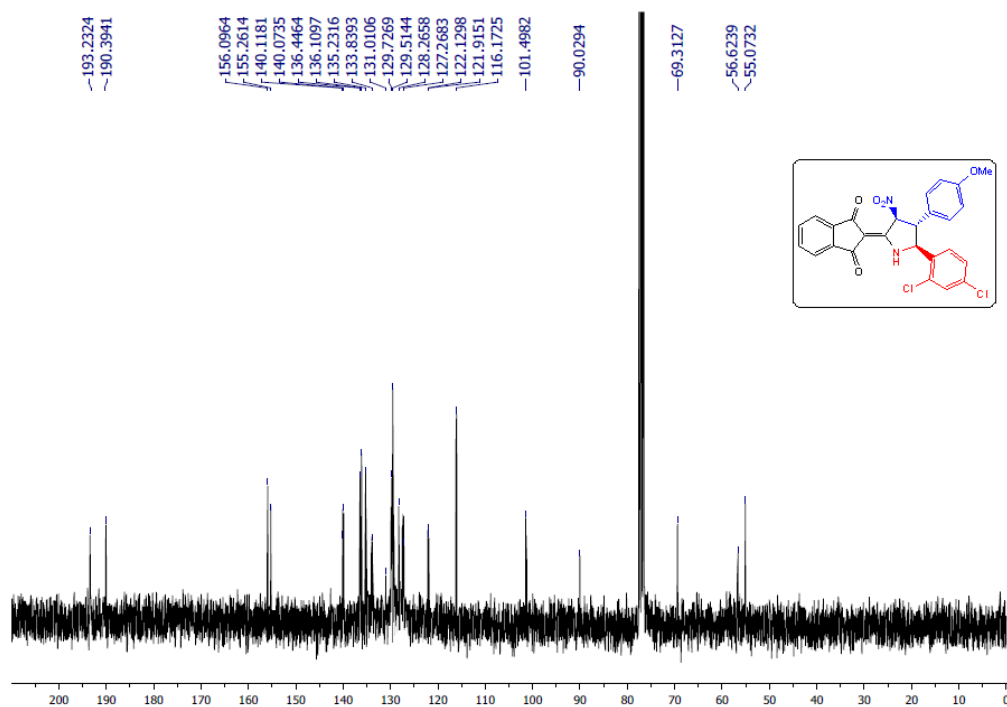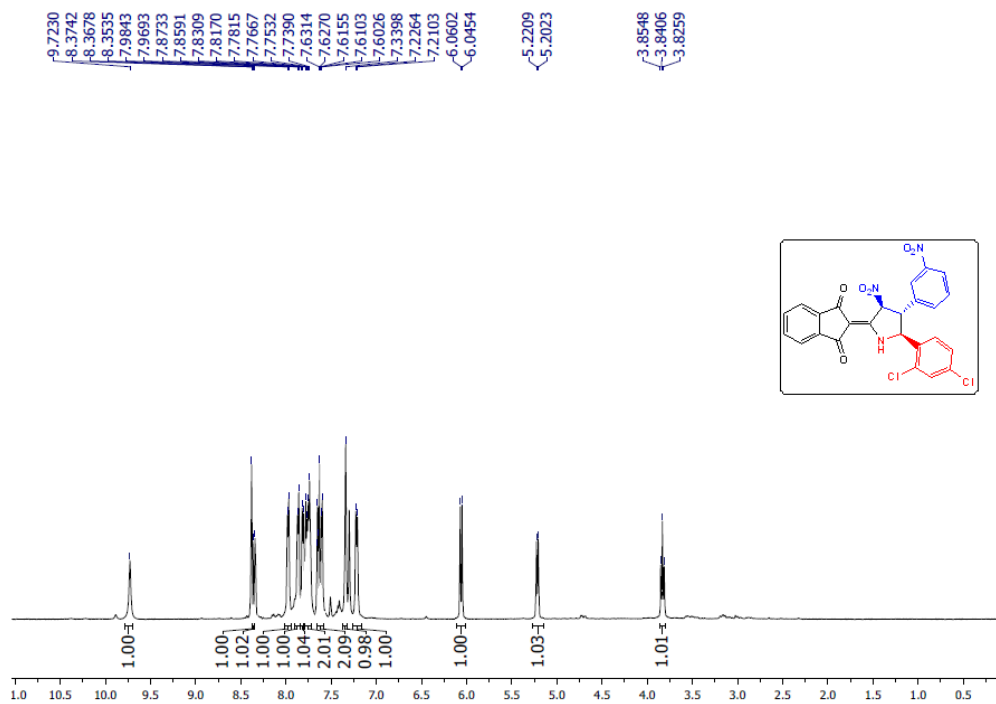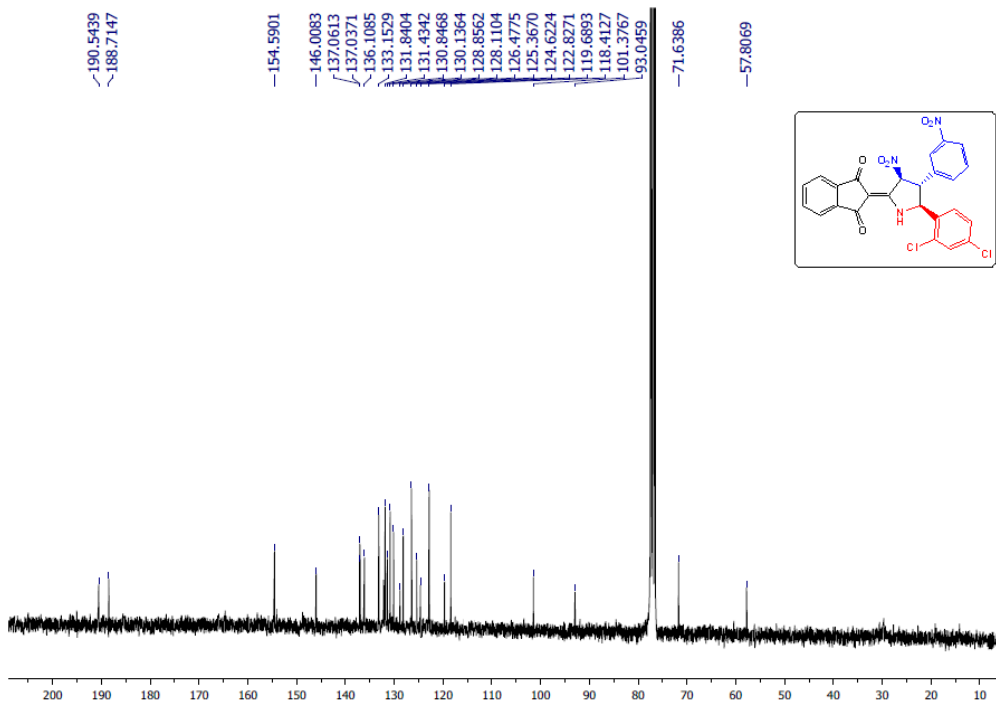

^{13}C NMR (75.6 MHz) of compound **5i** in CDCl$_3$

^{1}H NMR (300 MHz) of compound **5j** in CDCl$_3$
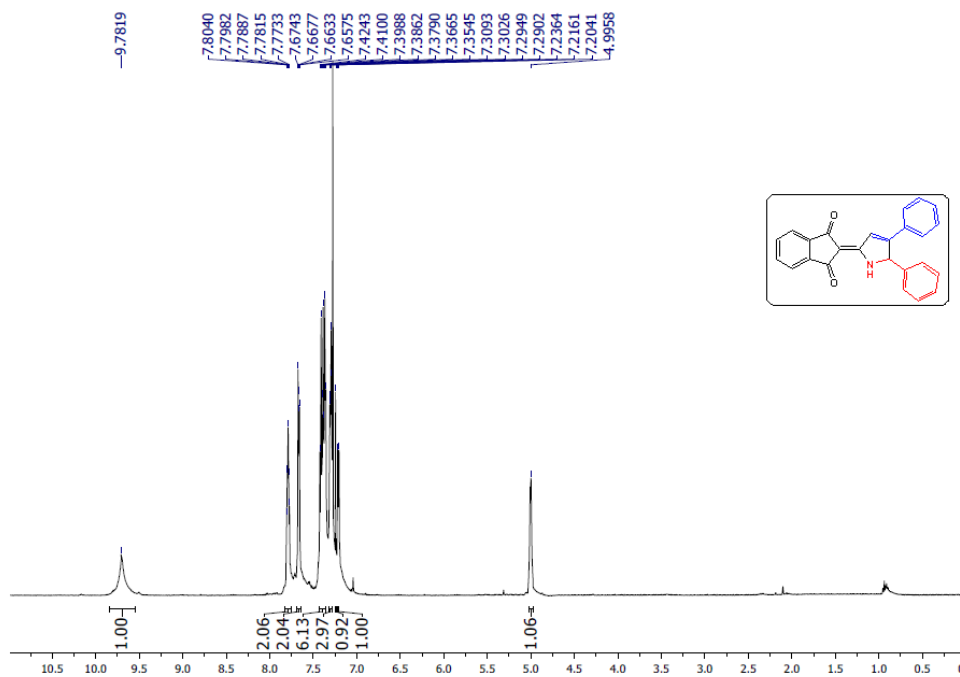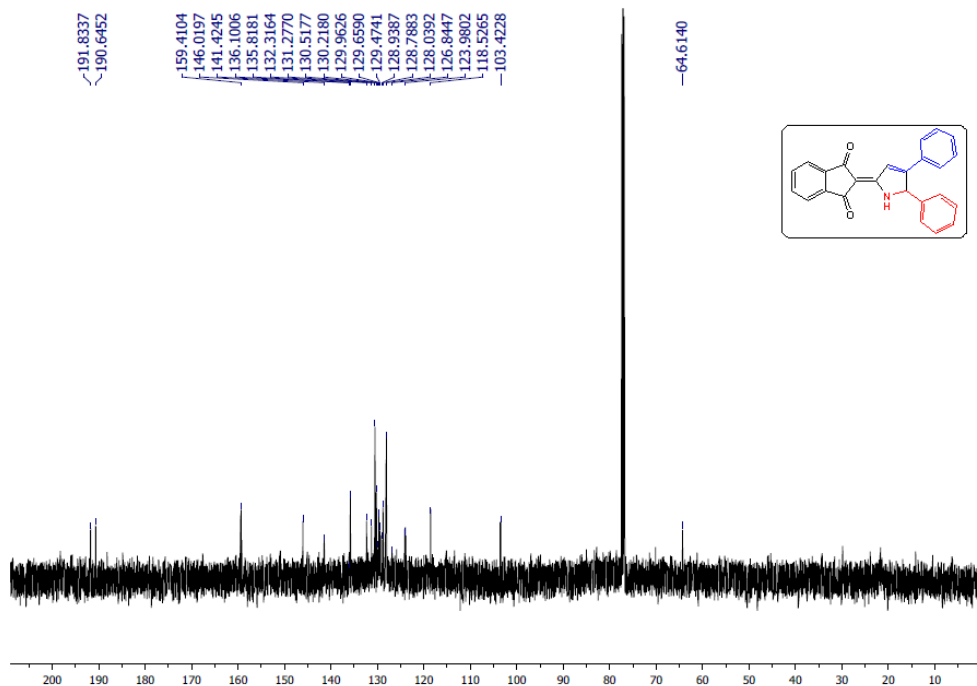

^{13}C NMR (75.6 MHz) of compound **5j** in CDCl$_3$

^{1}H NMR (300 MHz) of compound **5k** in CDCl$_3$

^{13}C NMR (75.6 MHz) of compound **5k** in CDCl$_3$

^{1}H NMR (500 MHz) of compound **5l** in CDCl$_3$

^{13}C NMR (126 MHz) of compound **5l** in CDCl$_3$

^{1}H NMR (500 MHz) of compound **5m** in CDCl$_3$

^{13}C NMR (126 MHz) of compound **5m** in CDCl$_3$

^{1}H NMR (500 MHz) of compound **5n** in CDCl$_3$

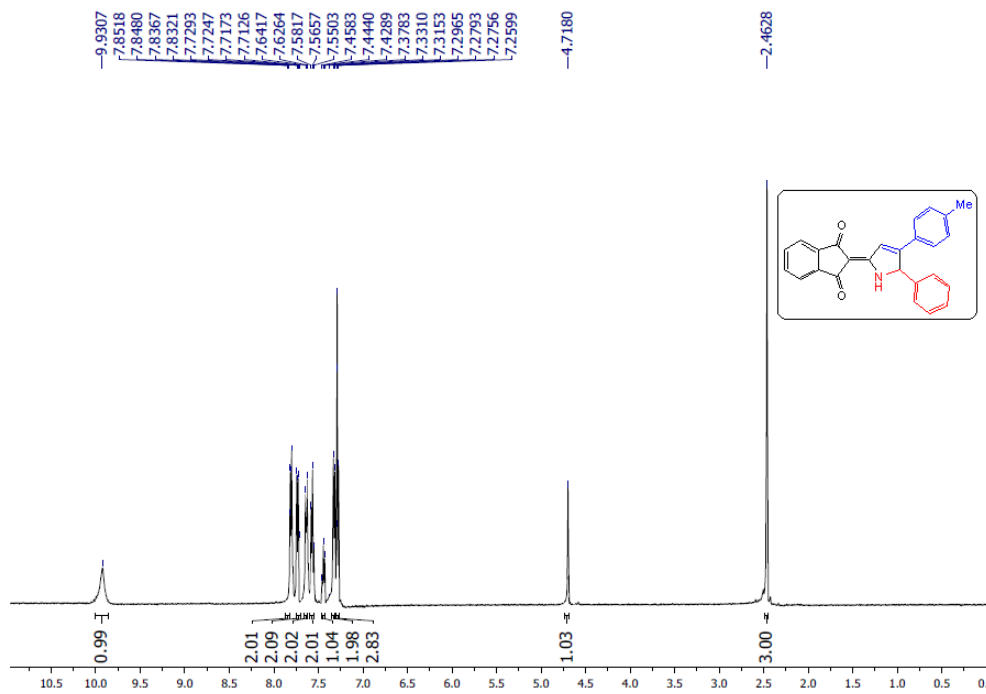^{13}C NMR (126 MHz) of compound **5n** in CDCl$_3$

NMR spectra of 2-(4,5-diaryl-1,5-dihydro-2*H*-pyrrol-2-ylidene)-1*H*-indene-1,3(2*H*)-diones 10a-10i
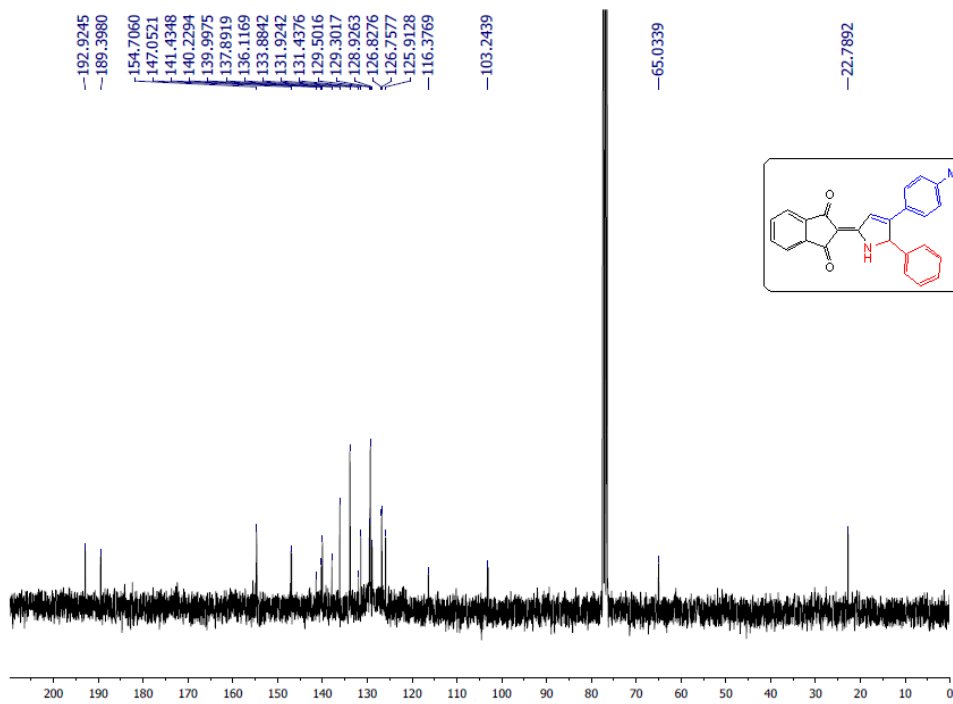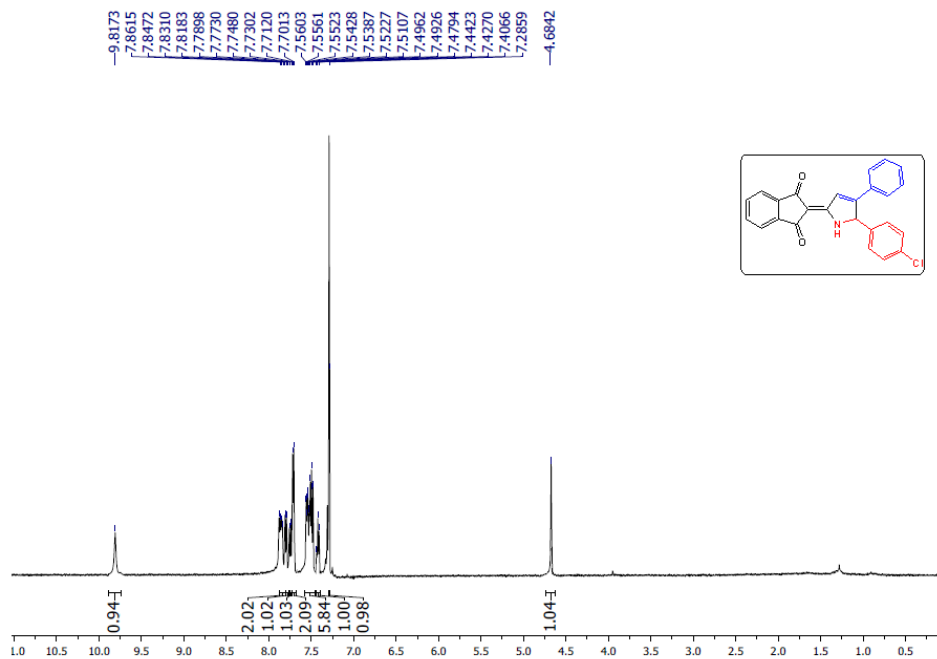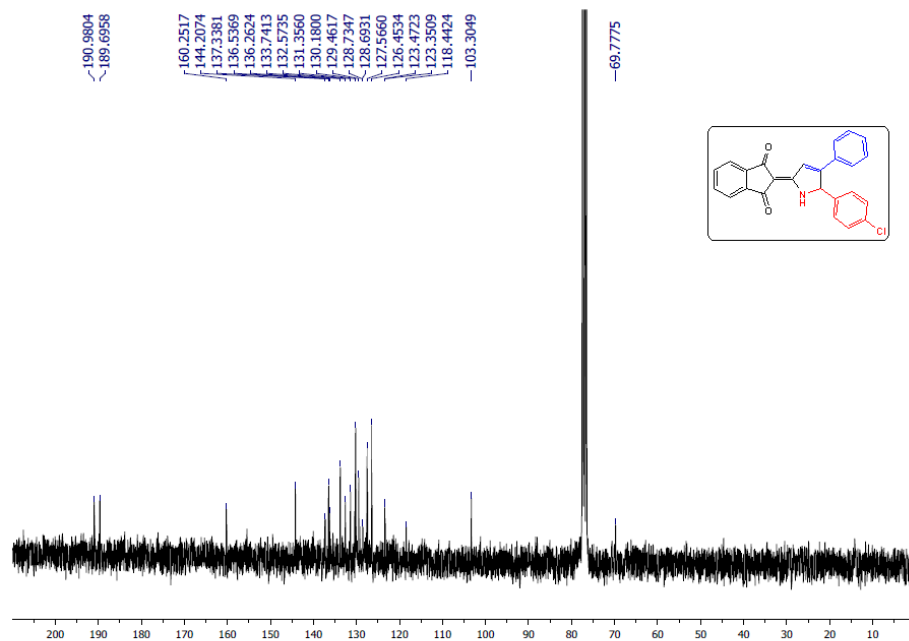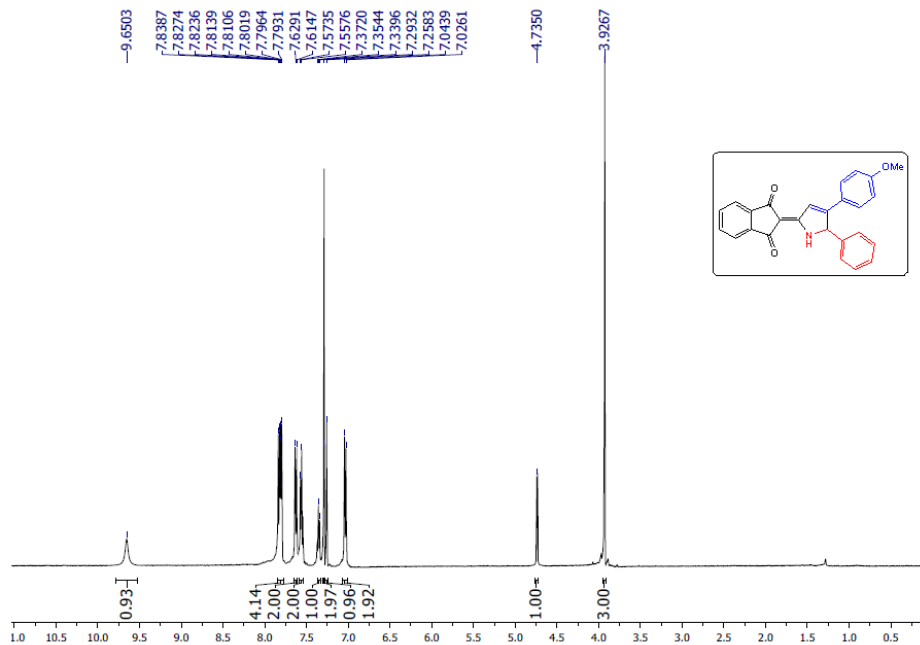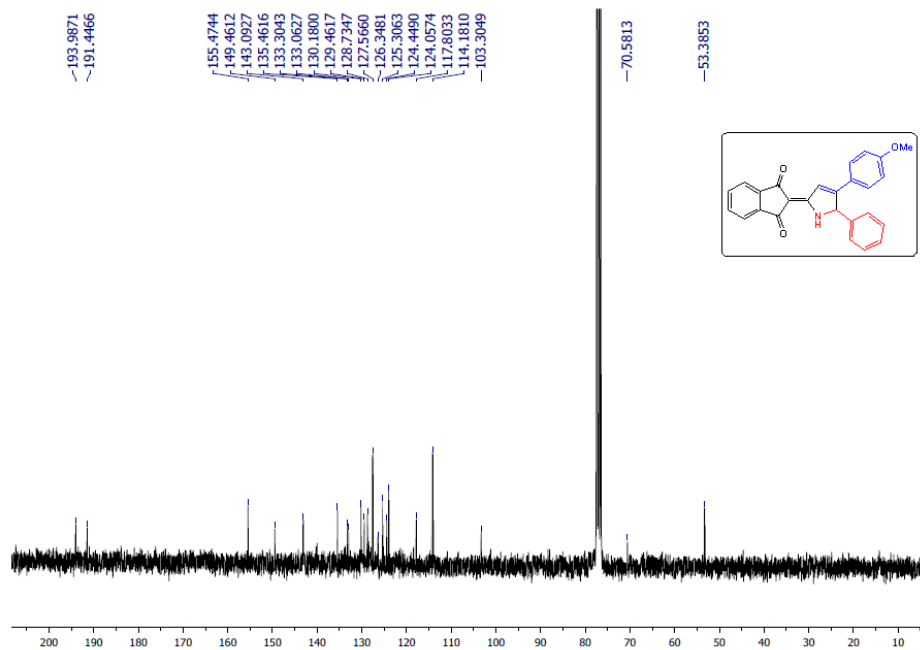

^{1}H NMR (500 MHz) of compound **10a** in CDCl$_3$

^{13}C NMR (126 MHz) of compound **10a** in CDCl$_3$

^{1}H NMR (500 MHz) of compound **10b** in CDCl$_3$

^{13}C NMR (126 MHz) of compound **10b** in CDCl$_3$
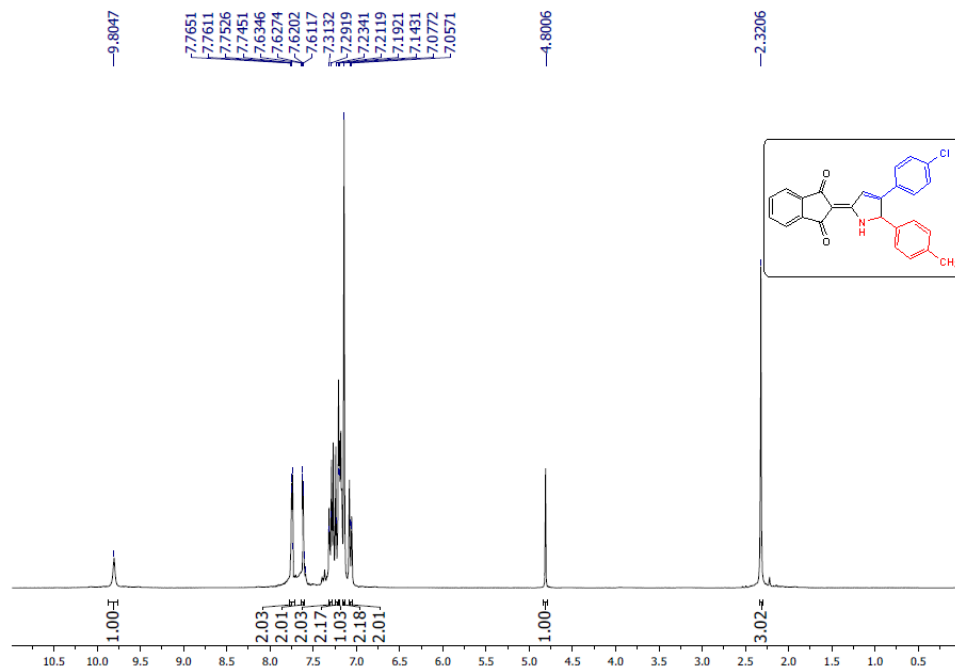
^{1}H NMR (500 MHz) of compound **10c** in CDCl$_3$

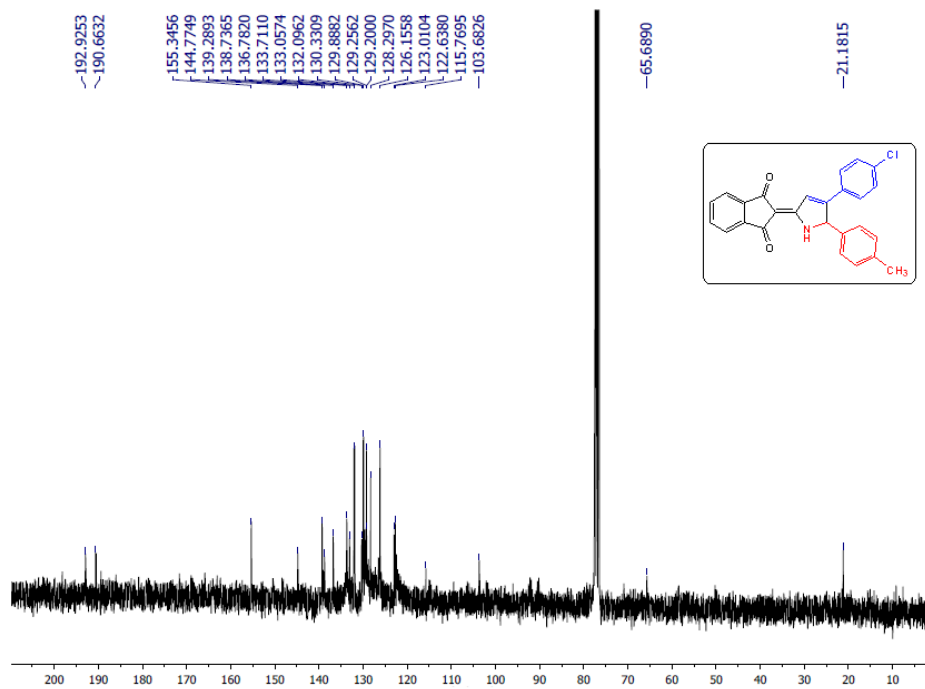

^{13}C NMR (126 MHz) of compound **10c** in CDCl$_3$

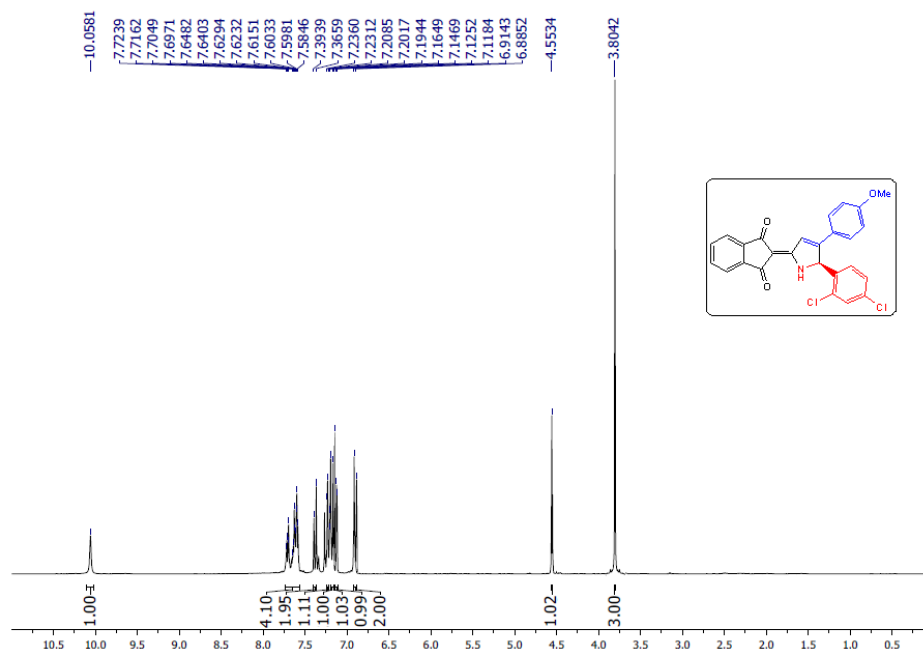^{1}H NMR (500 MHz) of compound **10d** in CDCl$_3$

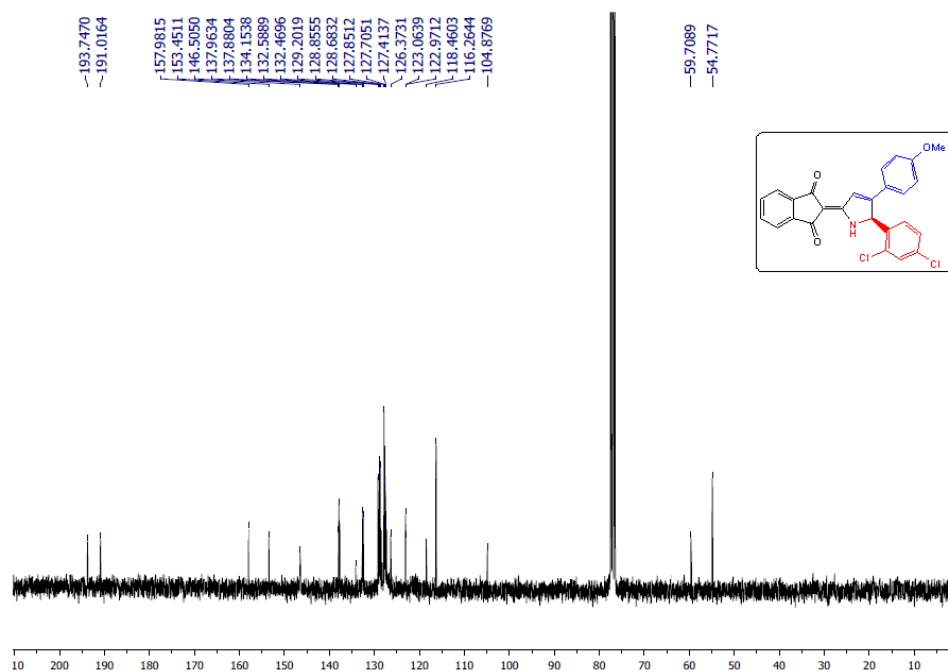^{13}C NMR (126 MHz) of compound **10d** in CDCl$_3$

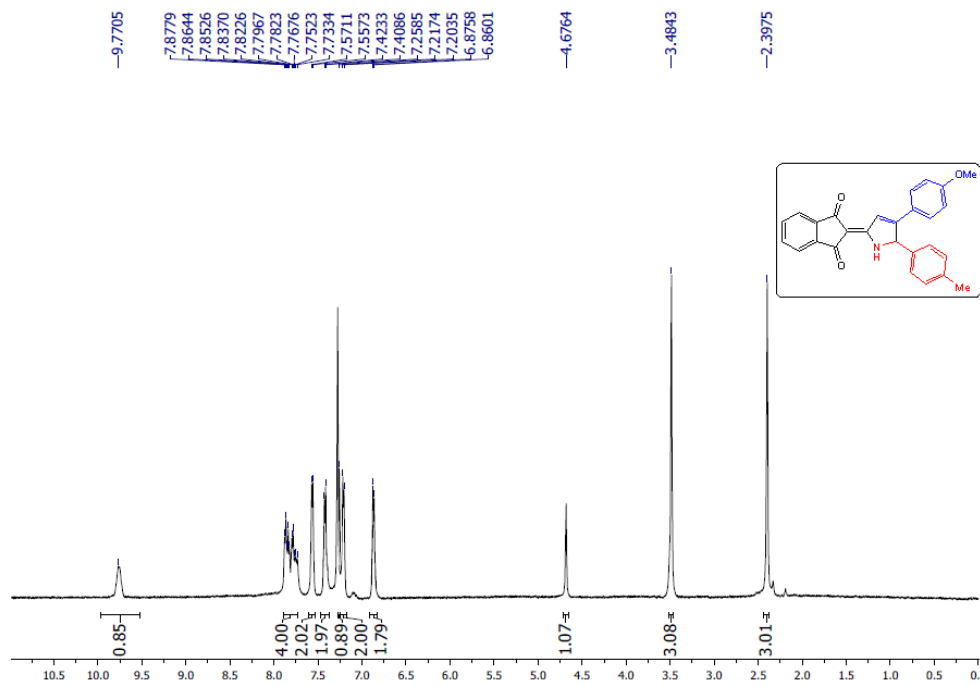^{1}H NMR (500 MHz) of compound **10e** in CDCl$_3$
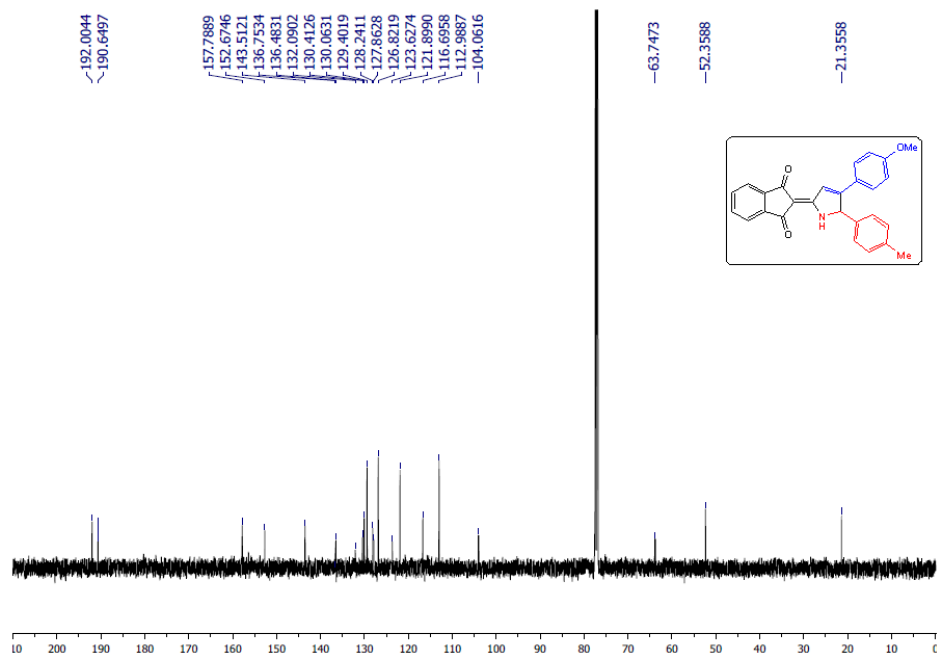

^{13}C NMR (126 MHz) of compound **10e** in CDCl$_3$

^{1}H NMR (300 MHz) of compound **10f** in CDCl$_3$

^{13}C NMR (75.6 MHz) of compound **10f** in CDCl$_3$

^{1}H NMR (500 MHz) of compound **10g** in CDCl$_3$

^{13}C NMR (126 MHz) of compound **10g** in CDCl$_3$

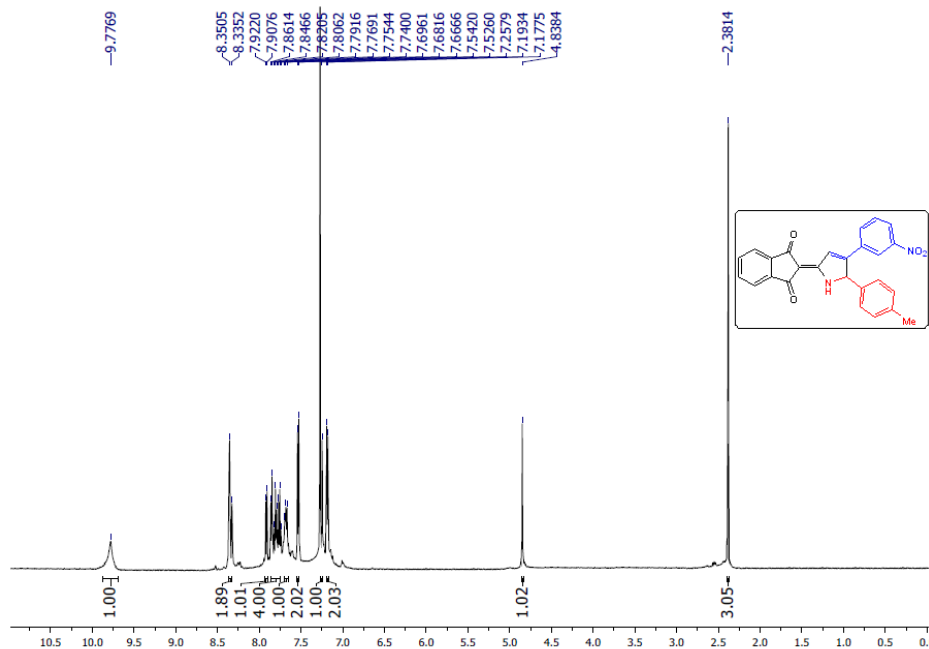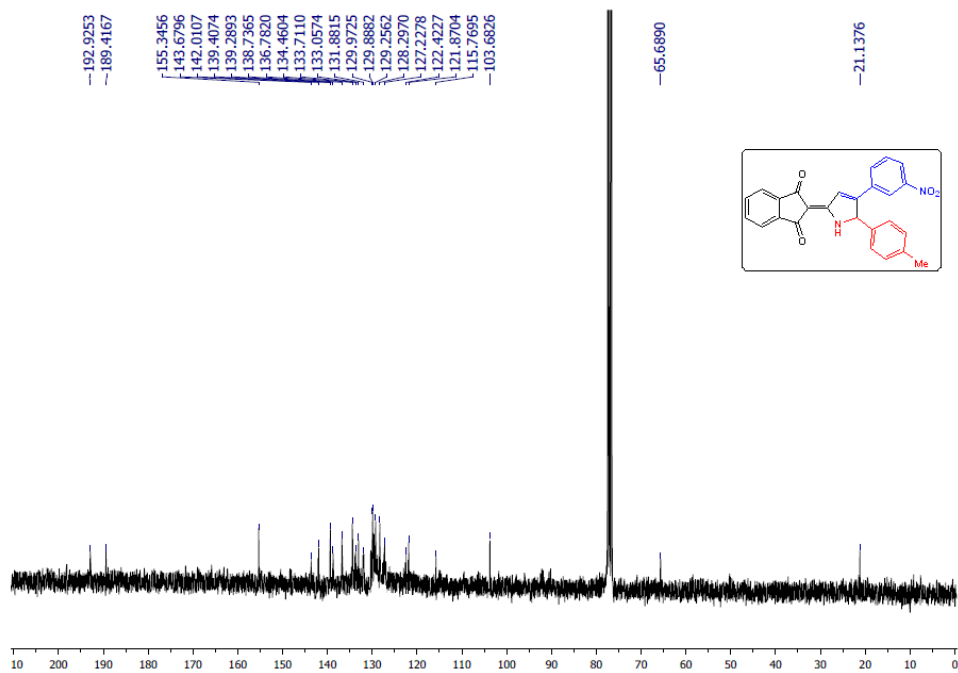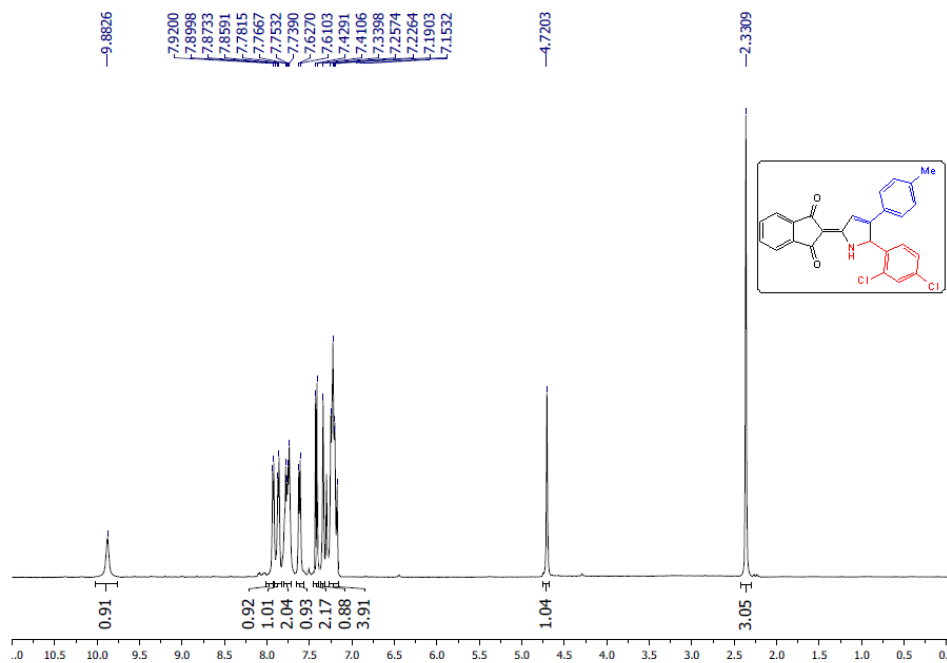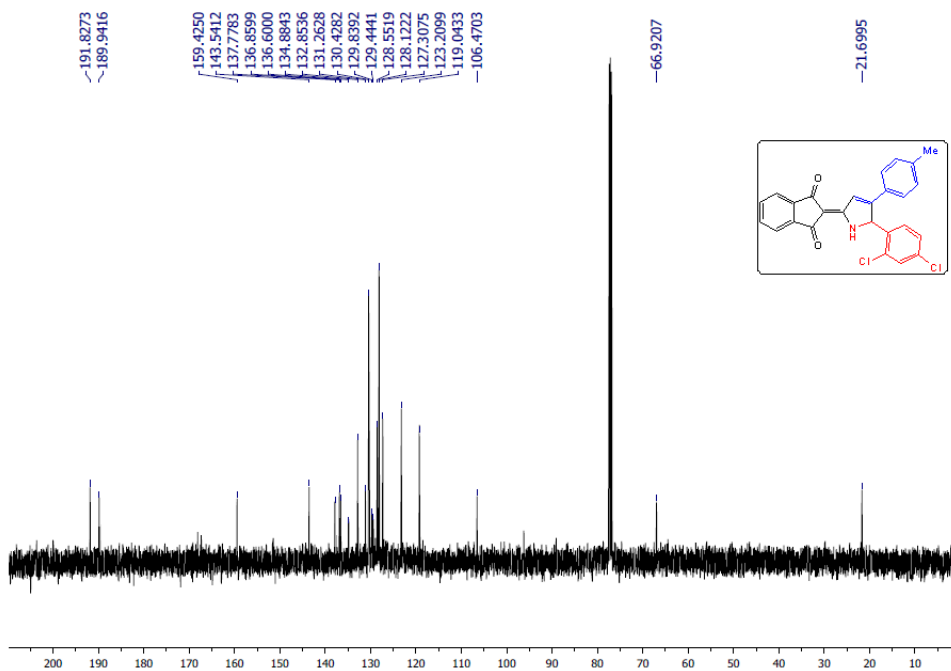^{1}H NMR (500 MHz) of compound **10h** in CDCl$_3$

^{13}C NMR (126 MHz) of compound **10h** in CDCl$_3$

^{1}H NMR (500 MHz) of compound **10i** in CDCl$_3$

^{13}C NMR (126 MHz) of compound **10i** in CDCl$_3$