

Supporting Information file

DABCO-Catalyzed consecutive one pot four-component protocol for the synthesis of a novel class of (z)-5-(3-hydroxy-2-oxoindolin-3-yl)-2-iminothiazol- idin-4-ones

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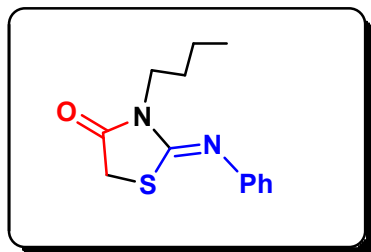
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General procedure for the synthesis of (Z)-3-butyl-5-(3-hydroxy-2-oxoindolin-3-yl)-2-(phenylimino)thiazolidin-4-one (5a):

A mixture of butylamine **2a** (1 mmol), phenylisothiocyanate **3** (1 mmol) and DABCO (30 mol %) in H₂O (5 mL) was stirred for 5 min at room temperature then the ethylbromoacetate **4** (1 mmol) was added and the mixture was stirred at 70 °C for 10 min. After cooling to room temperature, isatin **1** (1 mmol) was added to the reaction mixture and stirred for 10 min at room temperature. After completion of the reaction (monitored by TLC), the product **5a** was extracted with ethylacetate and dried over Na₂SO₄ and the solvent was removed under reduced pressure. The crude product was purified by column chromatography using ethyl acetate/hexane and the product (Z)-3-butyl-5-(3-hydroxy-2-oxoindolin-3-yl)-2-(phenylimino)thiazolidin-4-one **5a** was characterized by NMR, Mass and IR spectroscopic techniques.

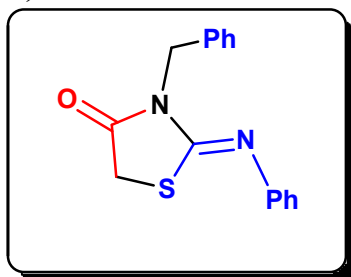
Characterization Data

(Z)-3-butyl-2-(phenylimino)thiazolidin-4-one



Yellow thick liquid; ^1H NMR (300 MHz, CDCl_3): δ 7.37-7.31 (m, 2H), 7.16-7.10 (m, 1H), 6.98-6.93 (m, 2H), 3.85 (t, $J = 7.45$ Hz, 2H), 3.78 (s, 2H), 1.76-1.66 (m, 2H), 1.45-1.34 (m, 2H), 0.96 (t, $J = 7.33$ Hz, 3H) ppm; ^{13}C NMR (75 MHz, CDCl_3): δ 171.1, 153.8, 147.6, 128.6, 123.9, 120.5, 42.3, 32.1, 28.7, 19.5, 13.3 ppm; IR(KBr): $\nu = 2957, 2868, 1724, 1635, 1592, 1384, 1346, 1184, 1124, 770, 696$ cm^{-1} ; MS-ESI: $m/z = 249$ $[\text{M}+1]^+$; HRMS (ESI) calc. $\text{C}_{13}\text{H}_{17}\text{ON}_2\text{S}$: 249.10561, found: 249.10421.

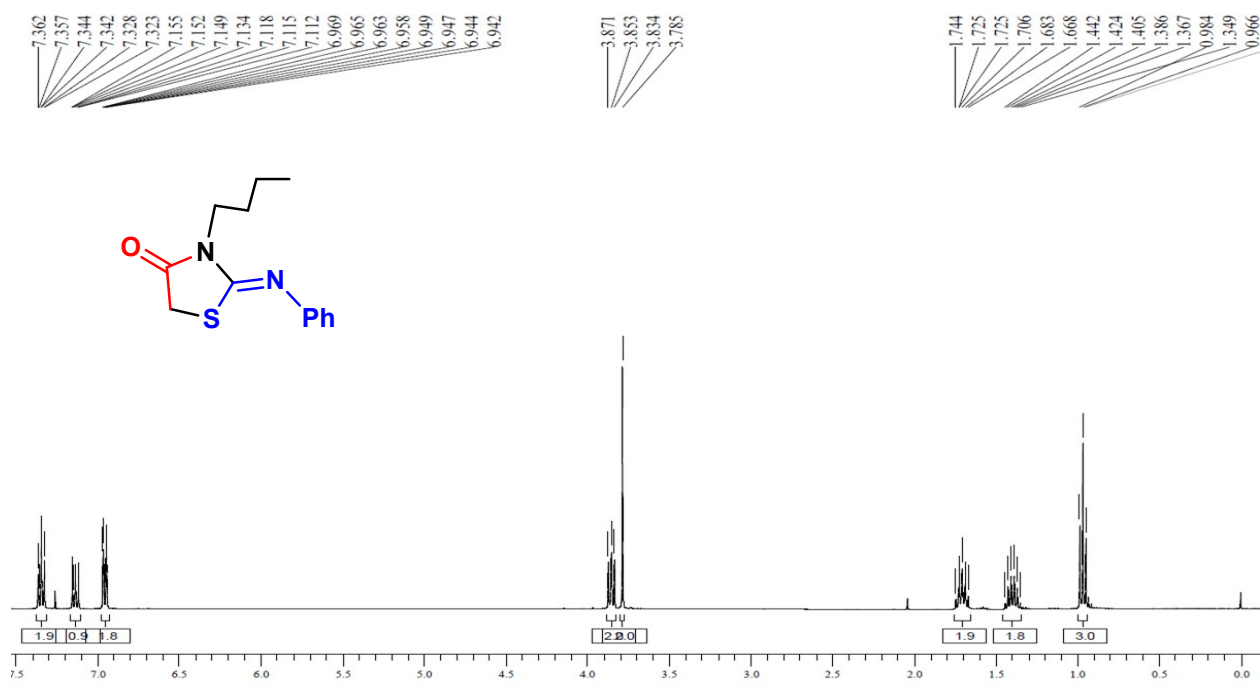
(Z)-3-benzyl-2-(phenylimino)thiazolidin-4-one



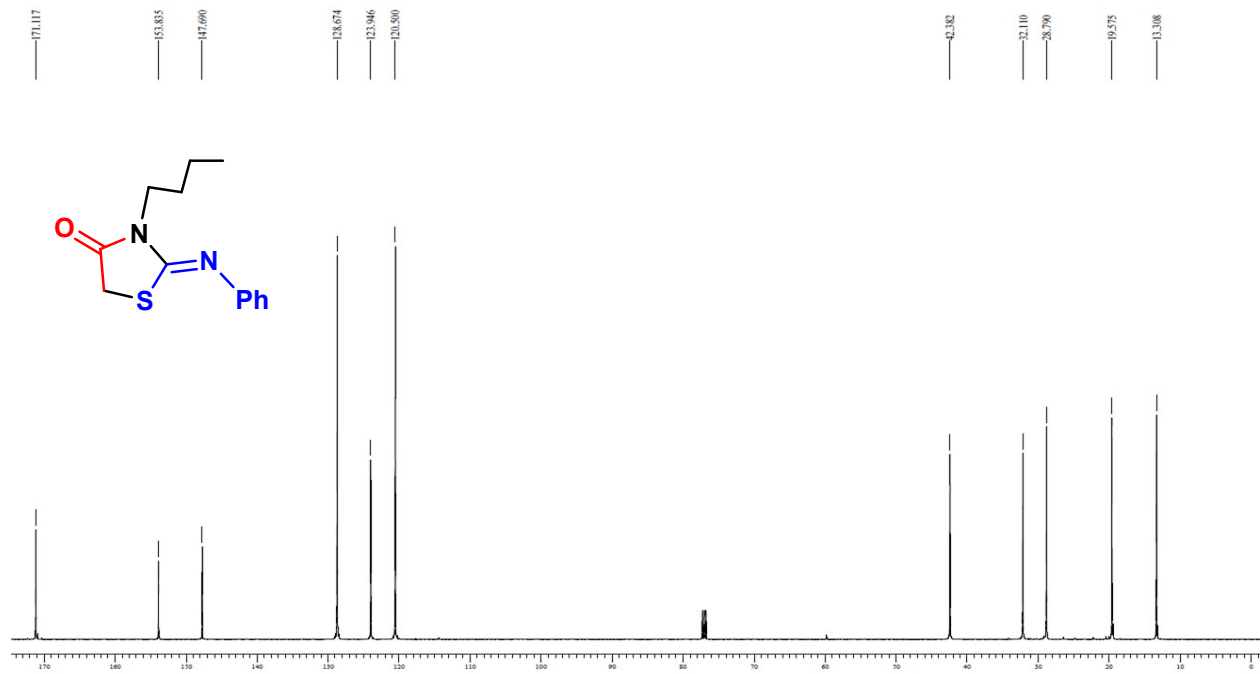
Yellow solid; Mp 111-113 $^{\circ}\text{C}$; ^1H NMR (300 MHz, CDCl_3): δ 7.54-7.50 (m, 2H), 7.37-7.26 (m, 5H), 7.16-7.10 (m, 1H), 6.97-6.92 (m, 2H), 5.02 (s, 2H), 3.79 (s, 2H) ppm; ^{13}C NMR (75 MHz, CDCl_3): δ 171.3, 153.8, 147.7, 135.8, 129.0, 128.8, 128.2, 127.7, 124.4, 120.8, 46.0, 32.4 ppm; IR(KBr): $\nu = 3059, 2945, 1716, 1641, 1588, 1425, 1381, 1319, 1152, 1071, 693$ cm^{-1} ; MS-ESI: $m/z = 283$ $[\text{M}+1]^+$; HRMS (ESI) calc. $\text{C}_{16}\text{H}_{15}\text{ON}_2\text{S}$: 283.08996, found: 283.08914.

^1H NMR and ^{13}C NMR spectra of isolated intermediates

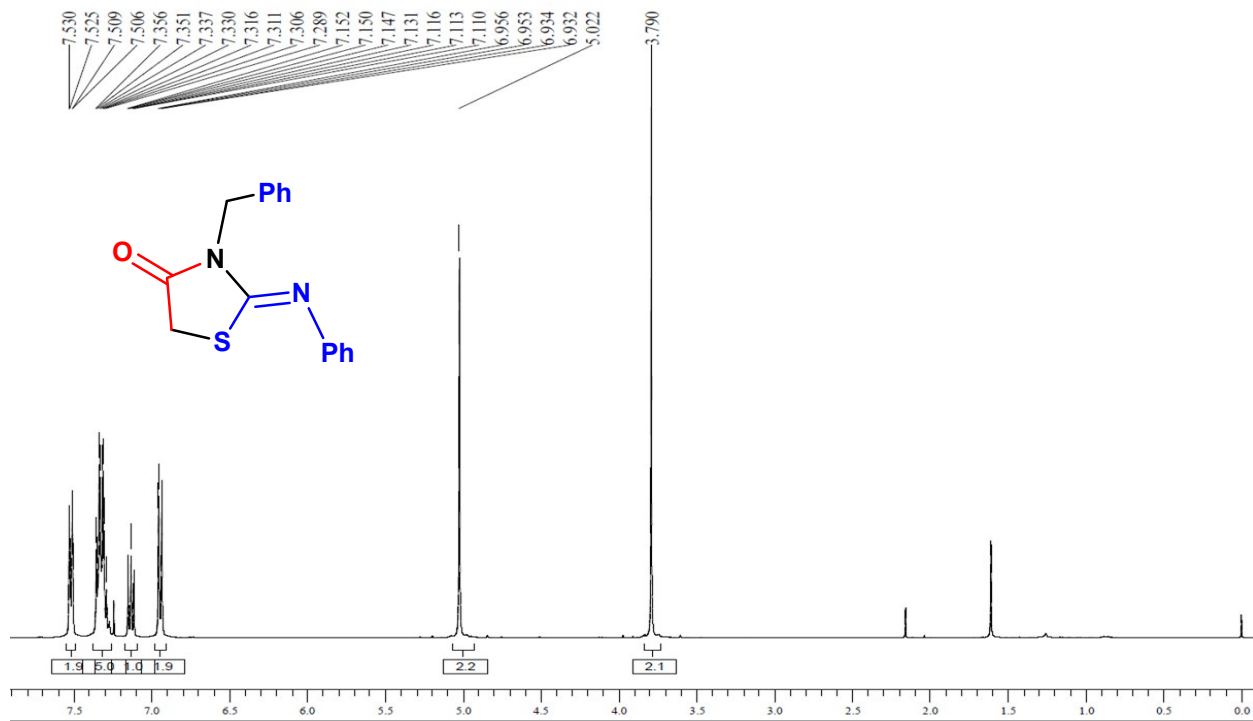
^1H NMR (300 MHz, CDCl_3)



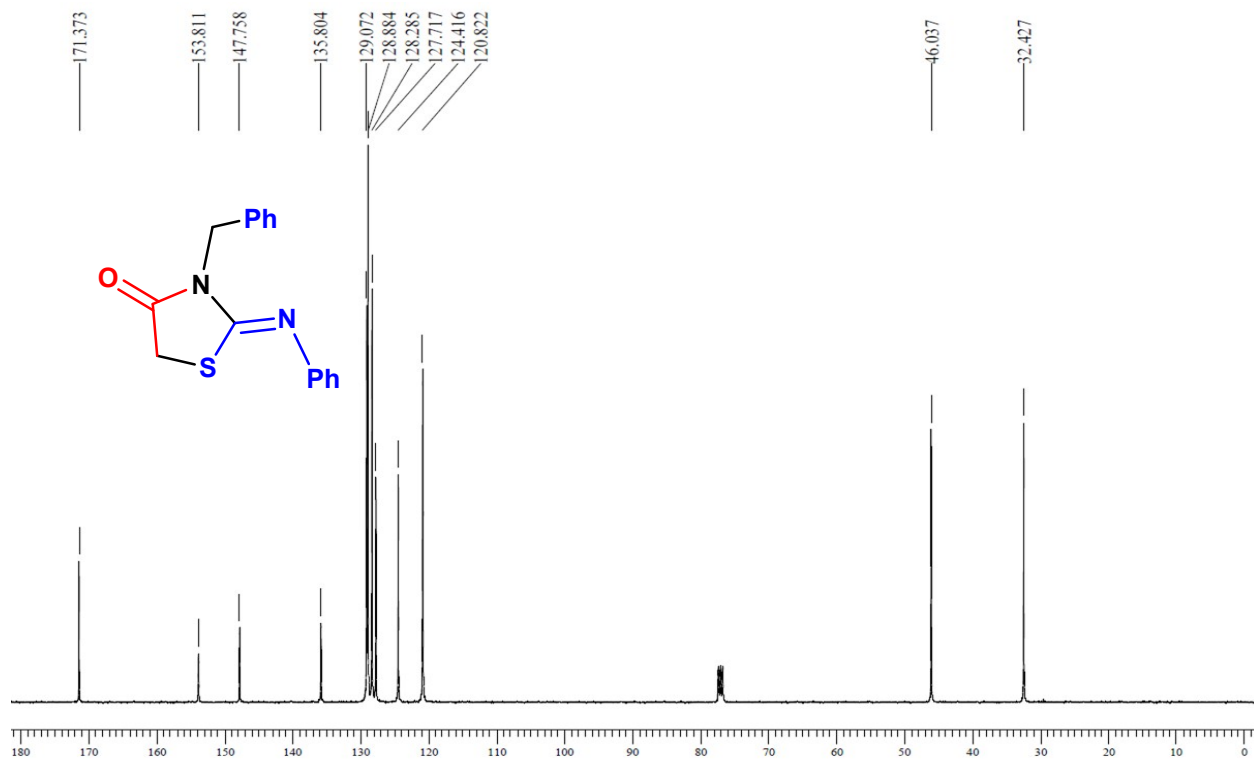
^{13}C NMR (75 MHz, CDCl_3)



¹H NMR (300 MHz, CDCl₃)



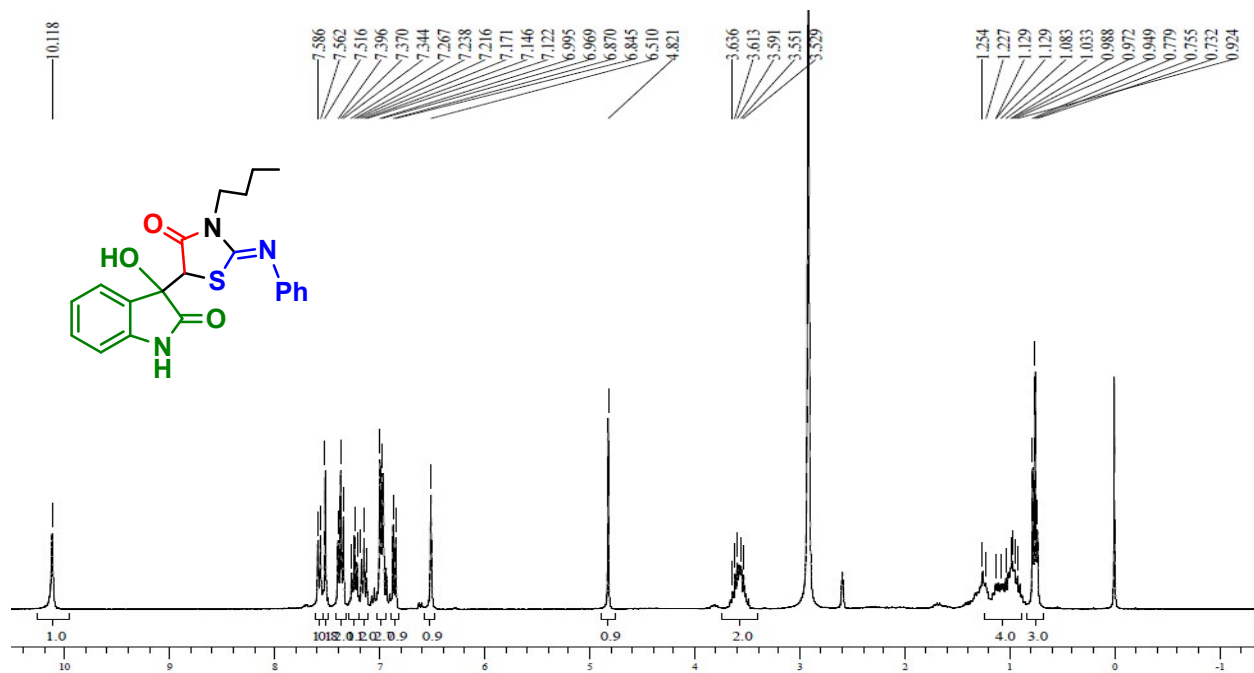
¹³C NMR (75 MHz, CDCl₃)



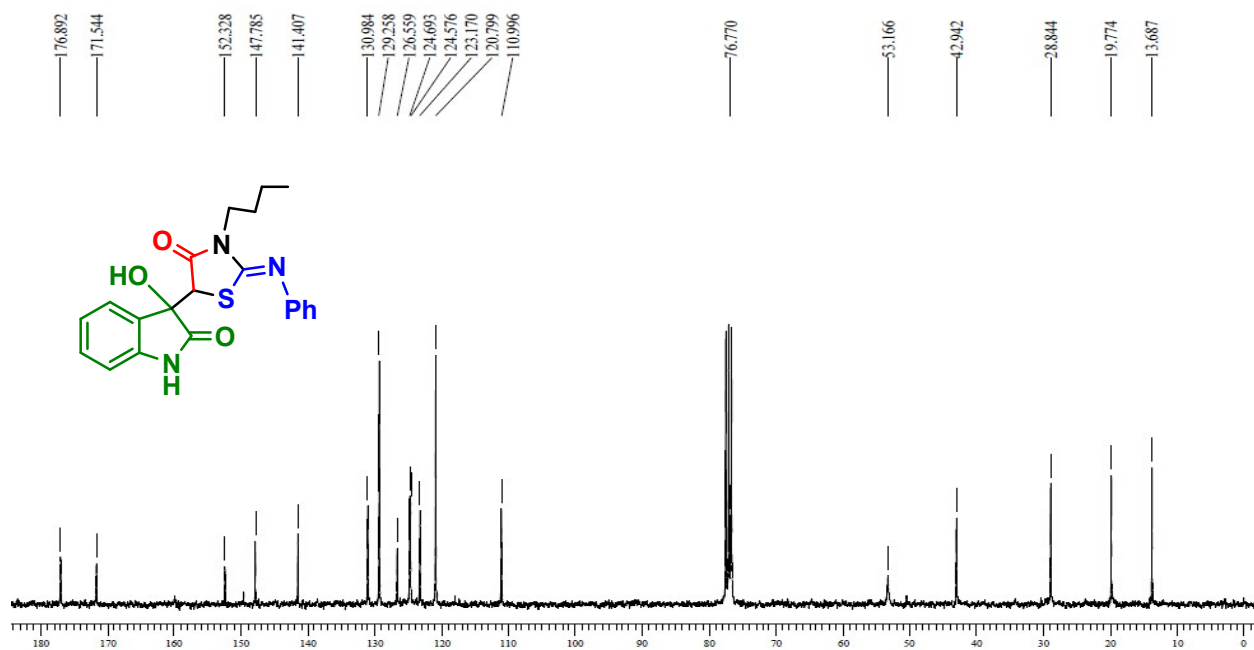
¹H NMR and ¹³C NMR spectra

Compound 5a

¹H NMR (300 MHz, CDCl₃)

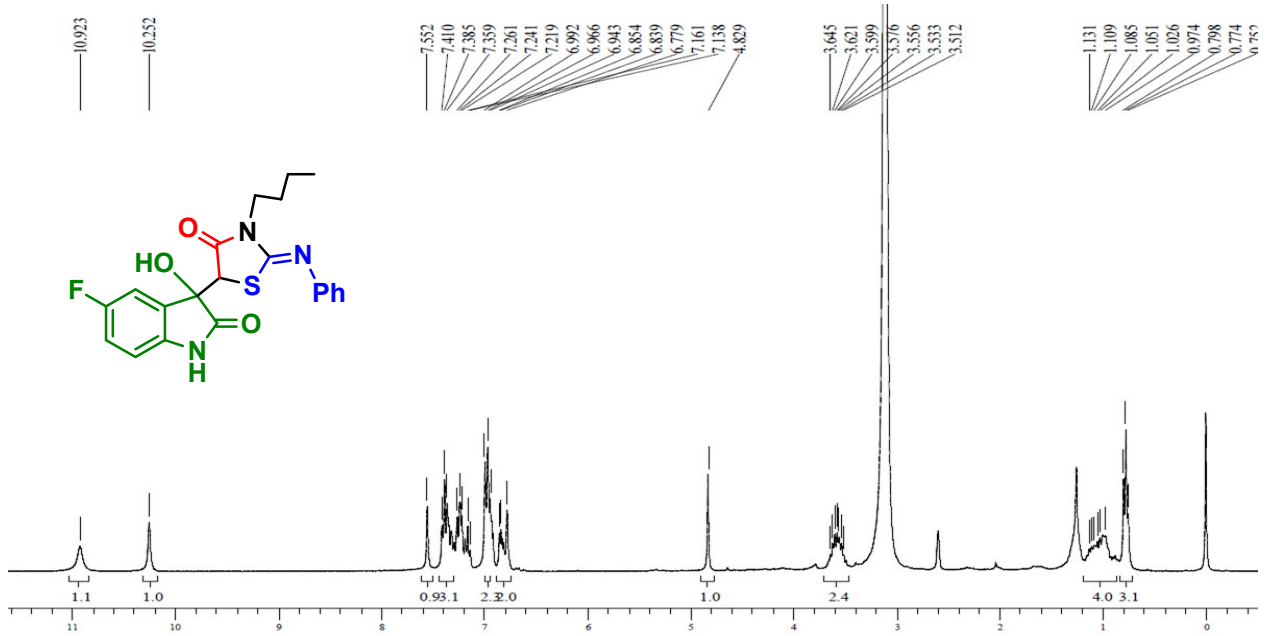


¹³C NMR (75 MHz, CDCl₃)

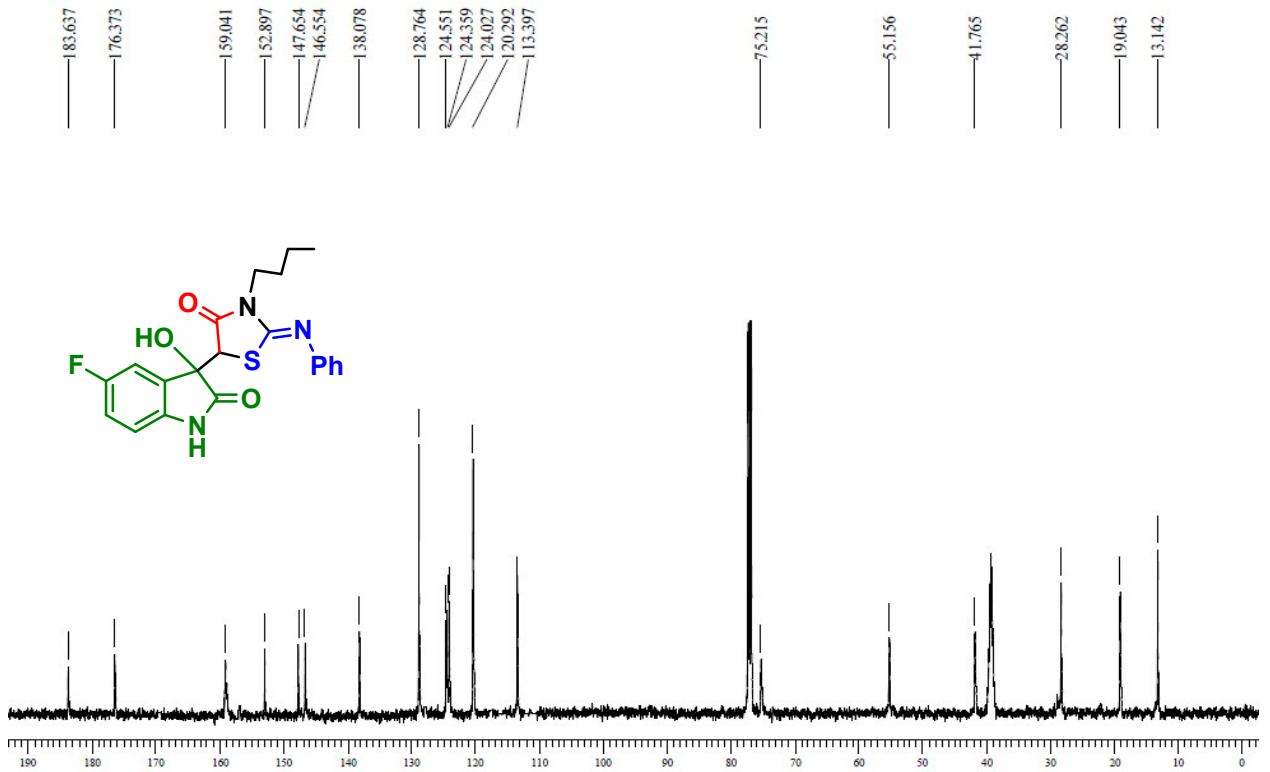


Compound 5b

^1H NMR (300 MHz, CDCl_3)

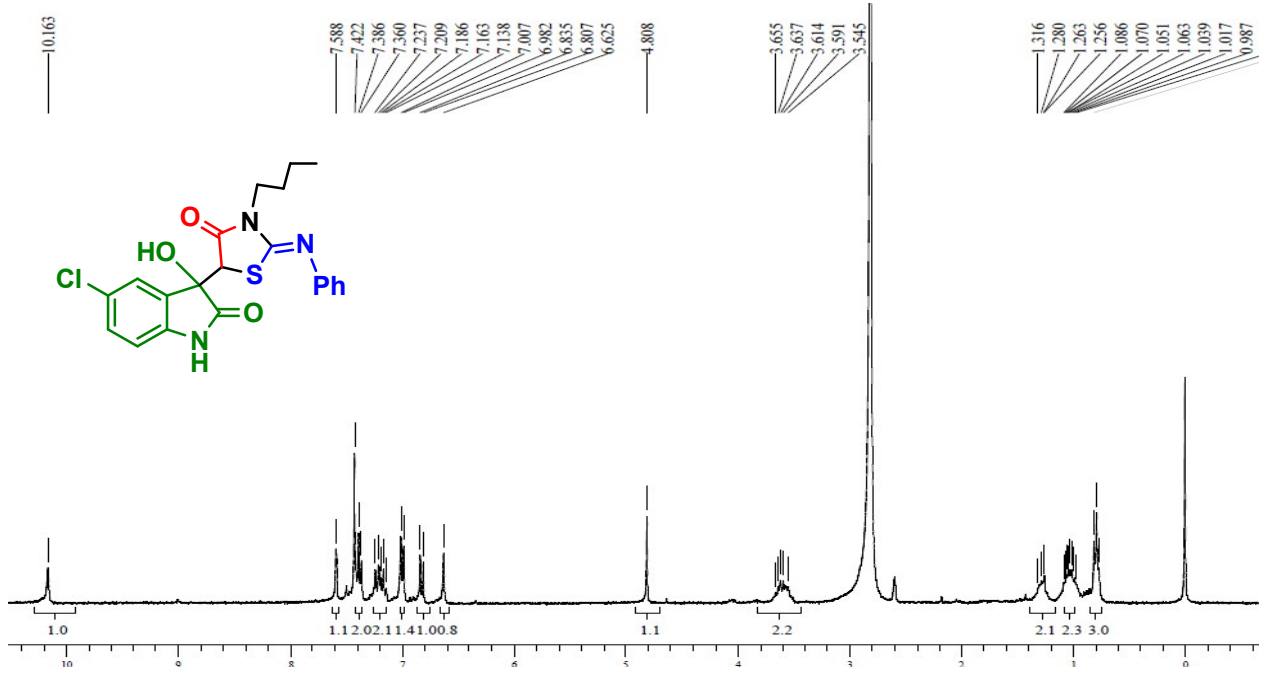


^{13}C NMR (75 MHz, CDCl_3)

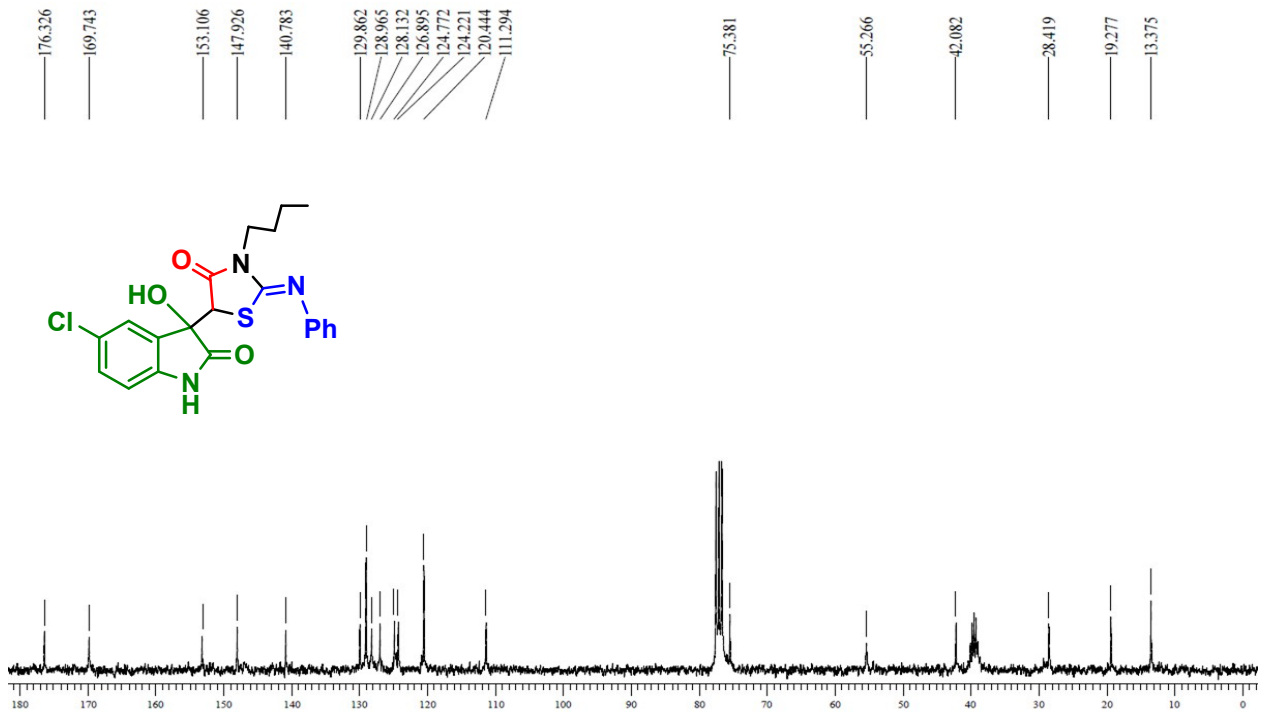


Compound 5c

^1H NMR (300 MHz, CDCl_3)

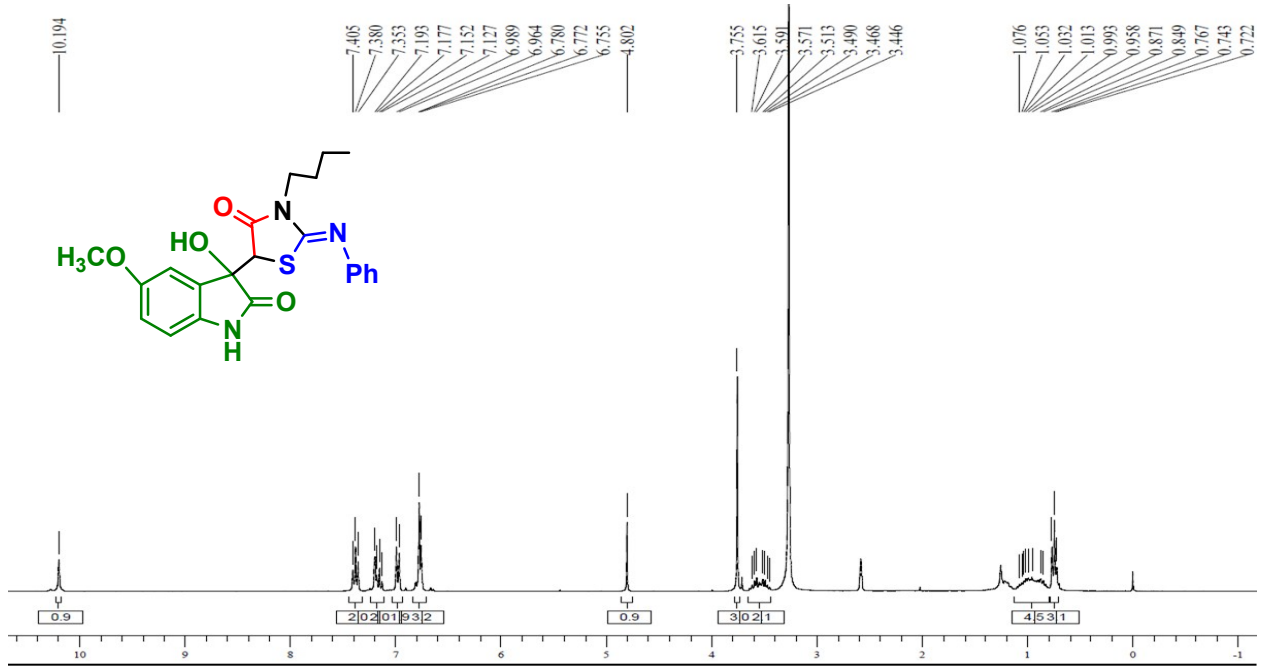


^{13}C NMR (75 MHz, CDCl_3)

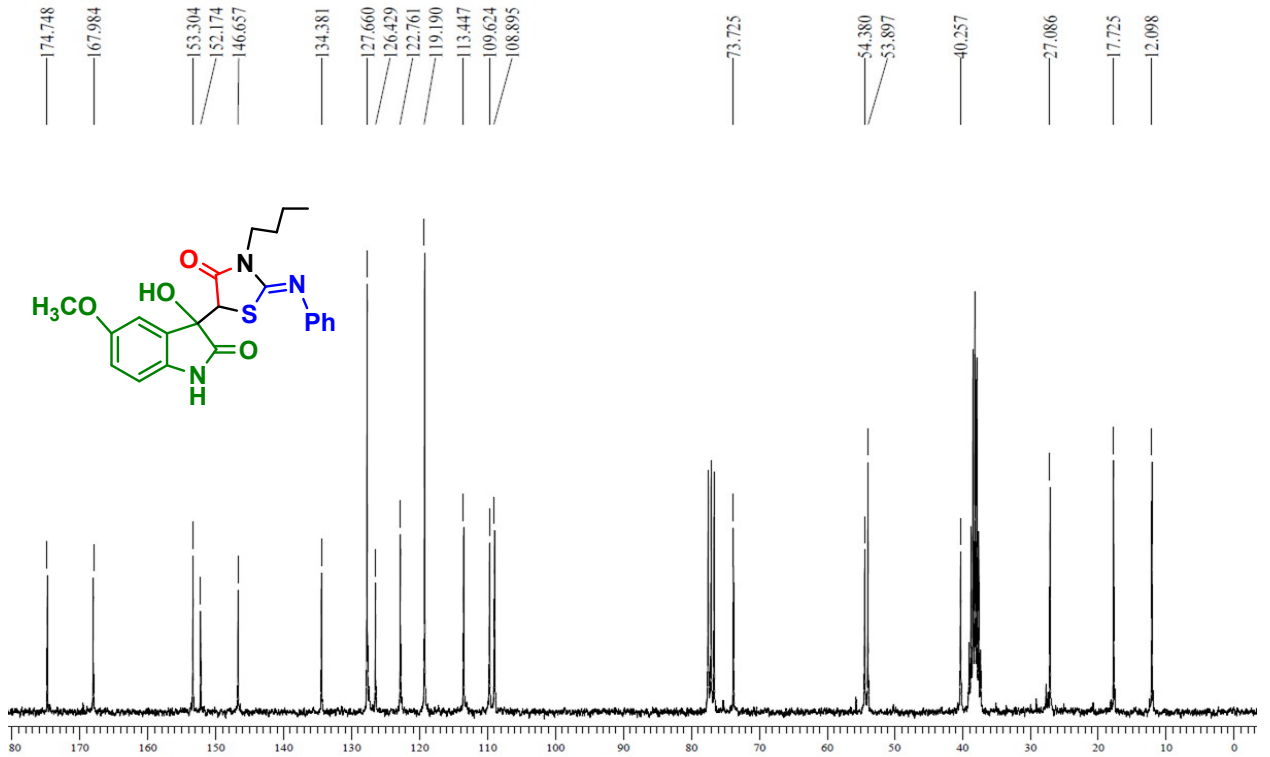


Compound 5d

¹H NMR (300 MHz, CDCl₃)

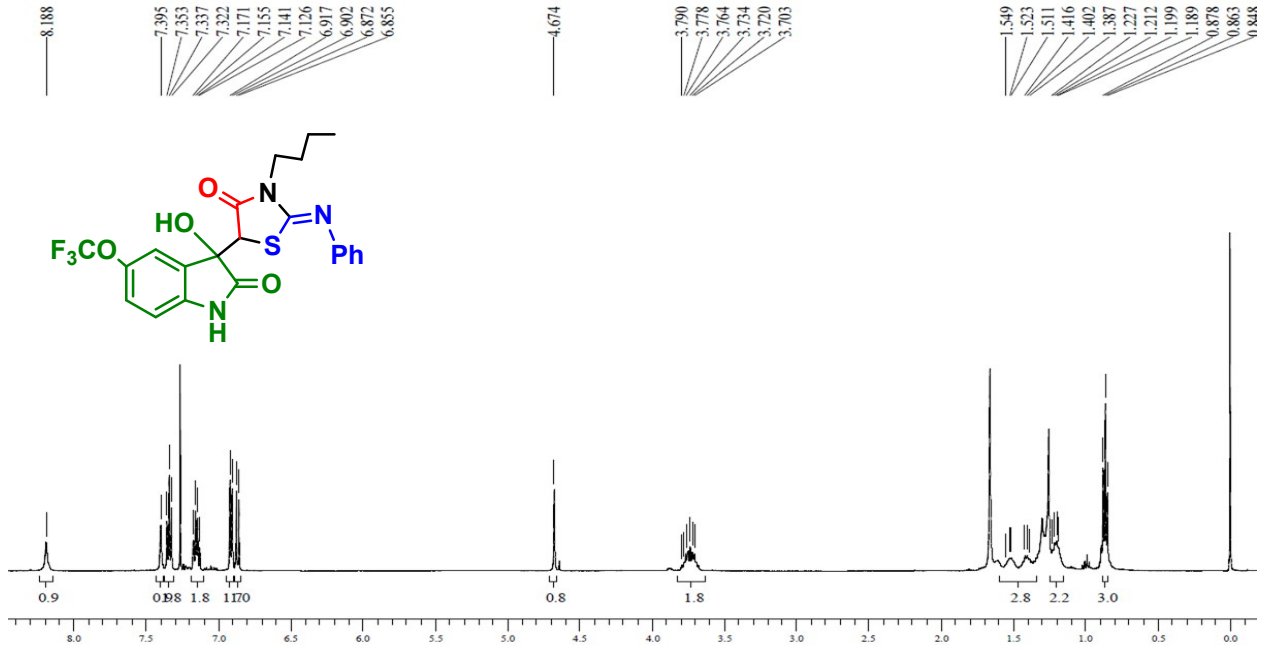


¹³C NMR (75 MHz, CDCl₃)

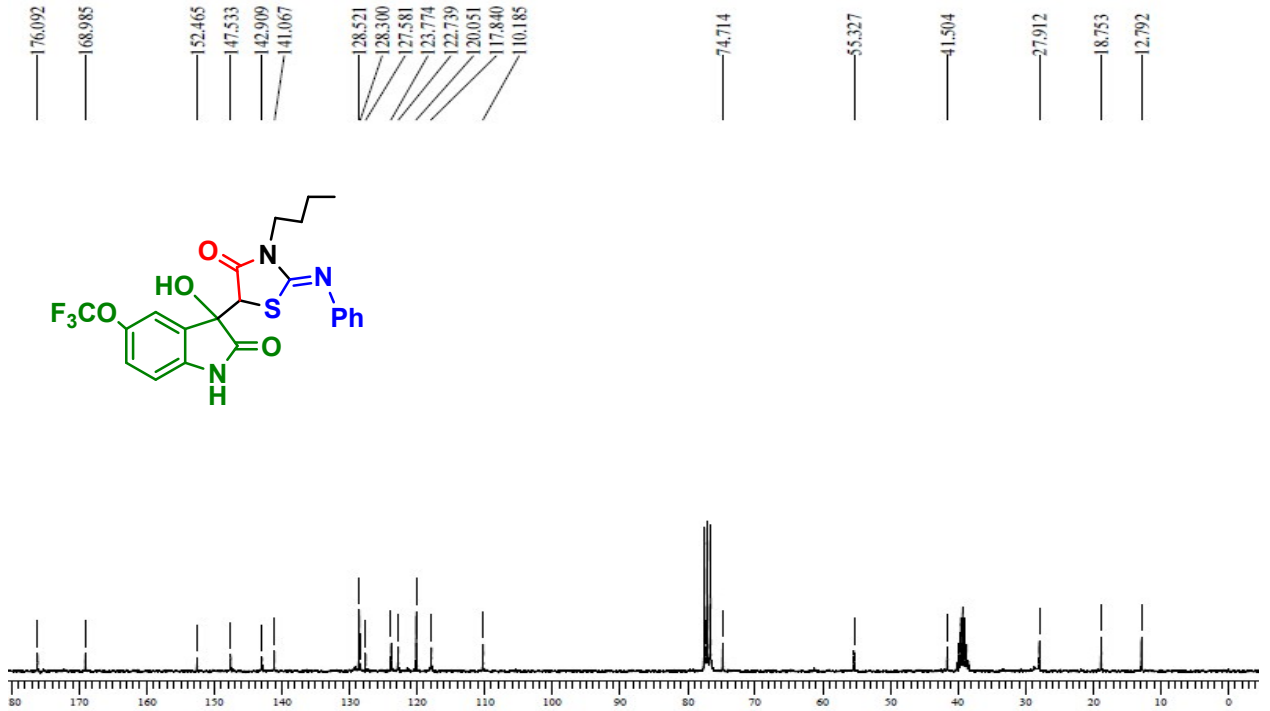


Compound 5e

¹H NMR (300 MHz, CDCl₃)

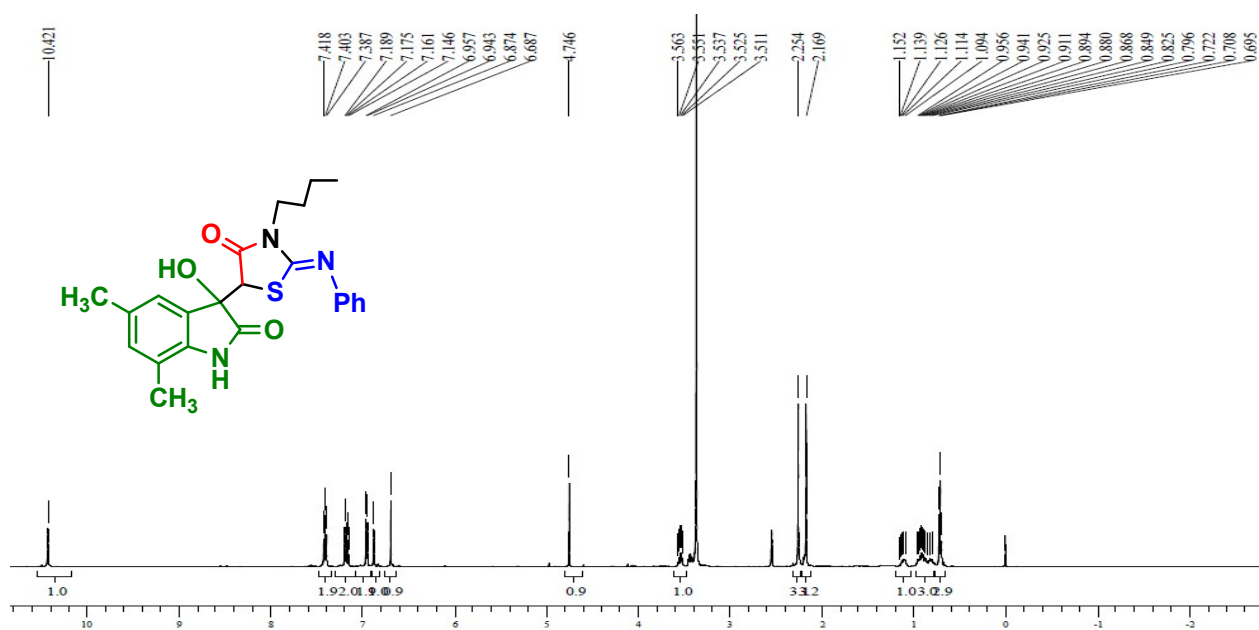


¹³C NMR (75 MHz, CDCl₃)

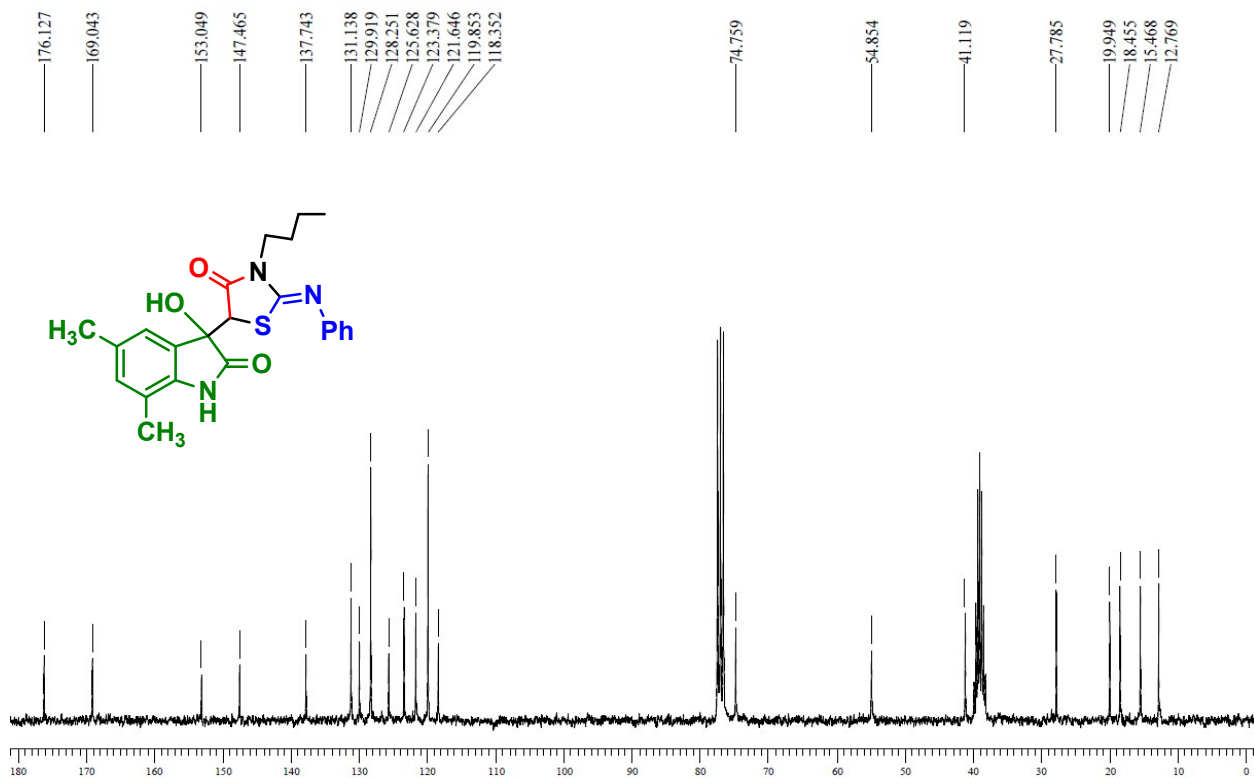


Compound 5f

¹H NMR (300 MHz, CDCl₃)

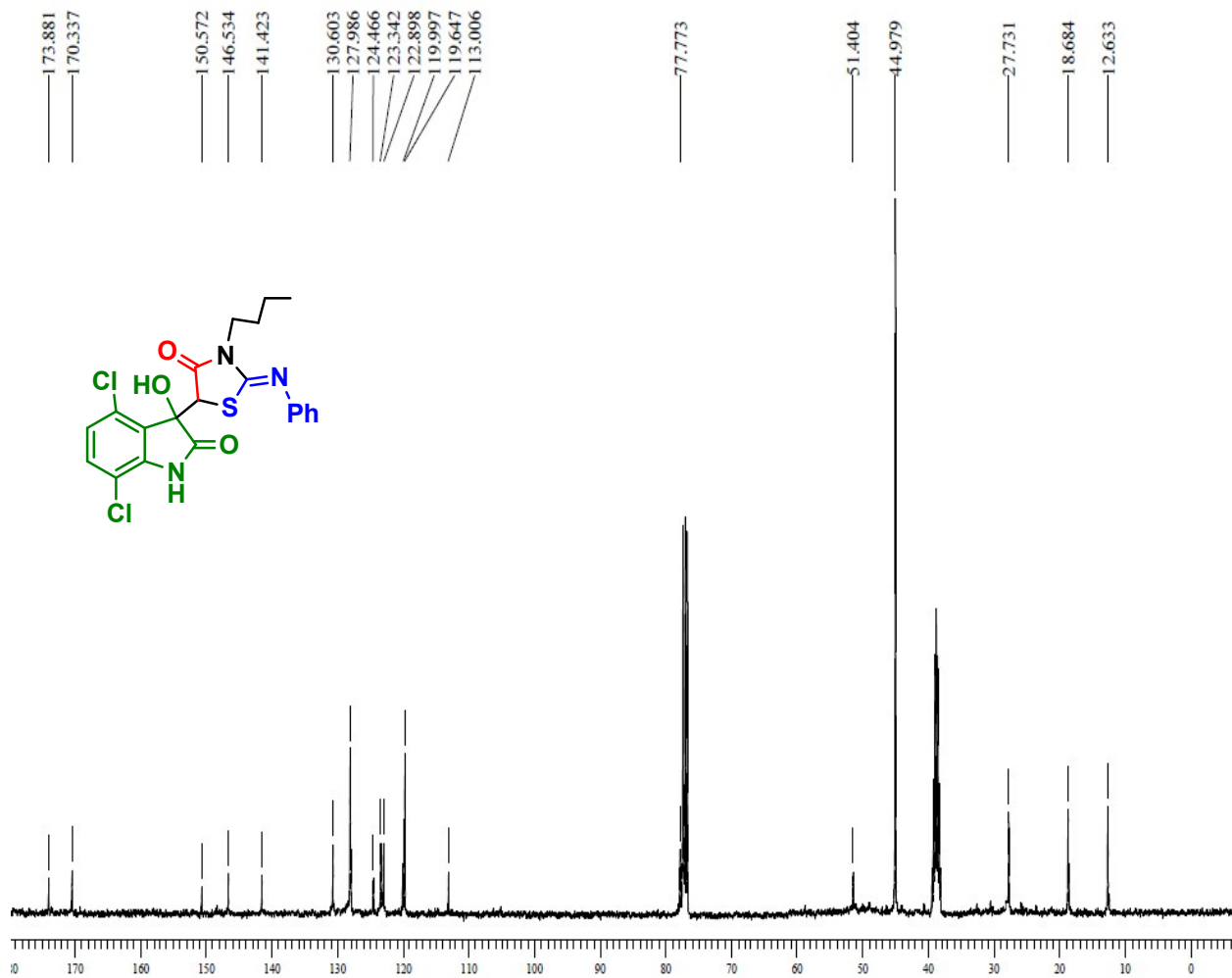


¹³C NMR (75 MHz, CDCl₃)



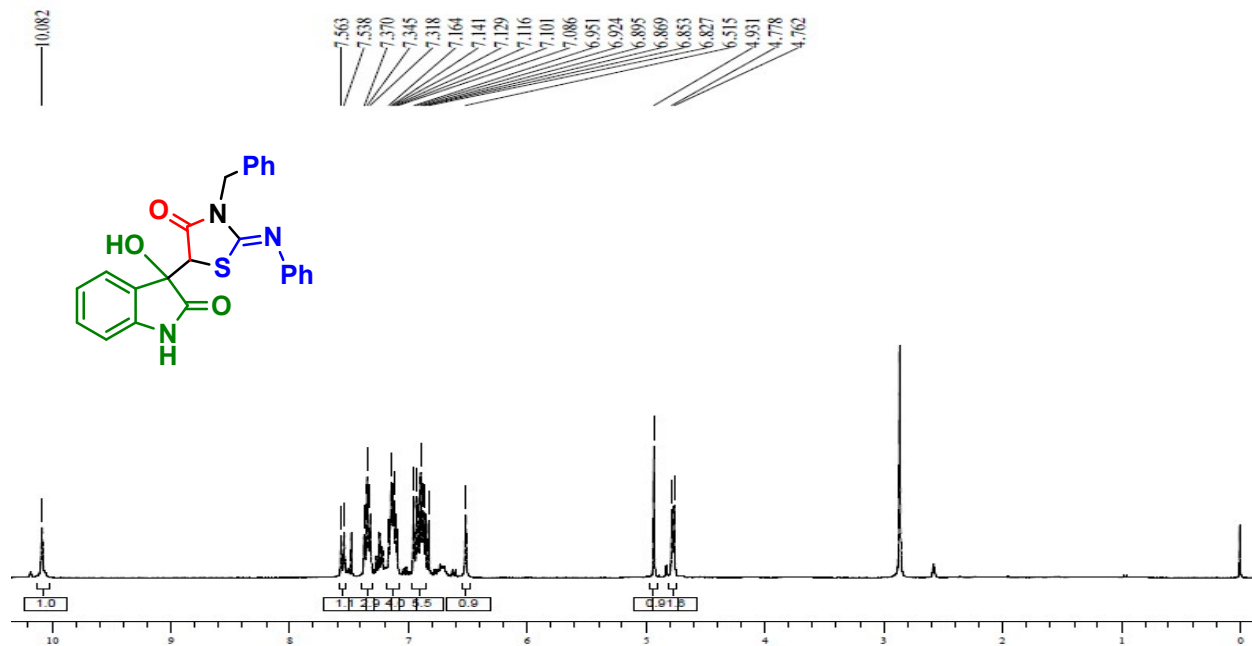
Compound 5g

^{13}C NMR (75 MHz, CDCl_3)

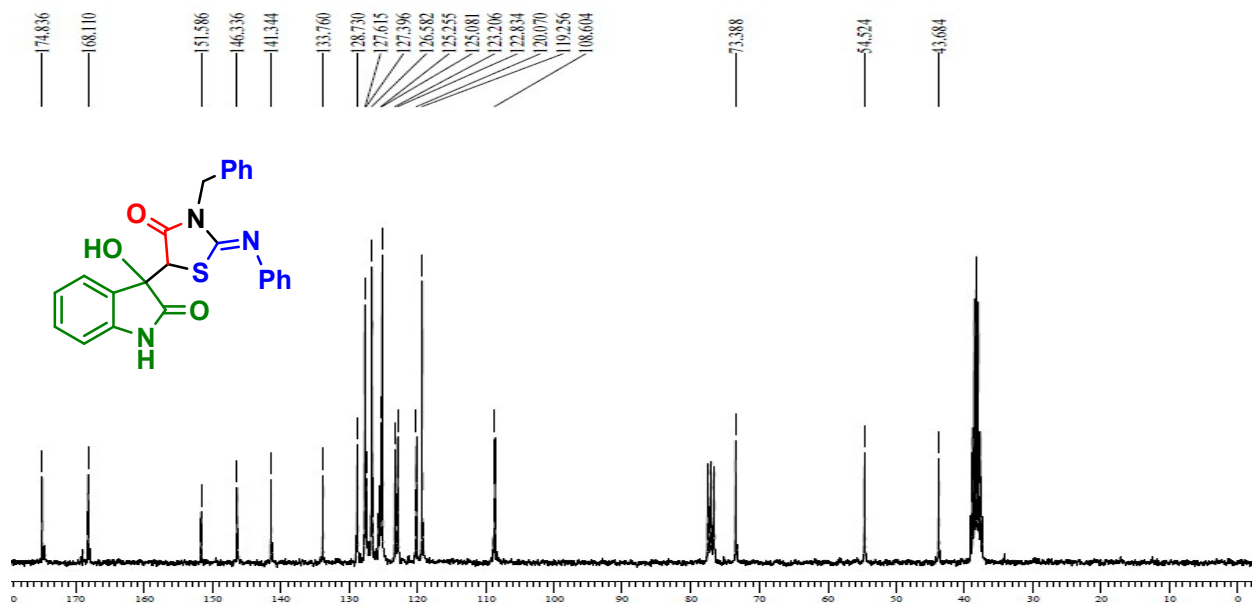


Compound 5h

¹H NMR (300 MHz, CDCl₃)

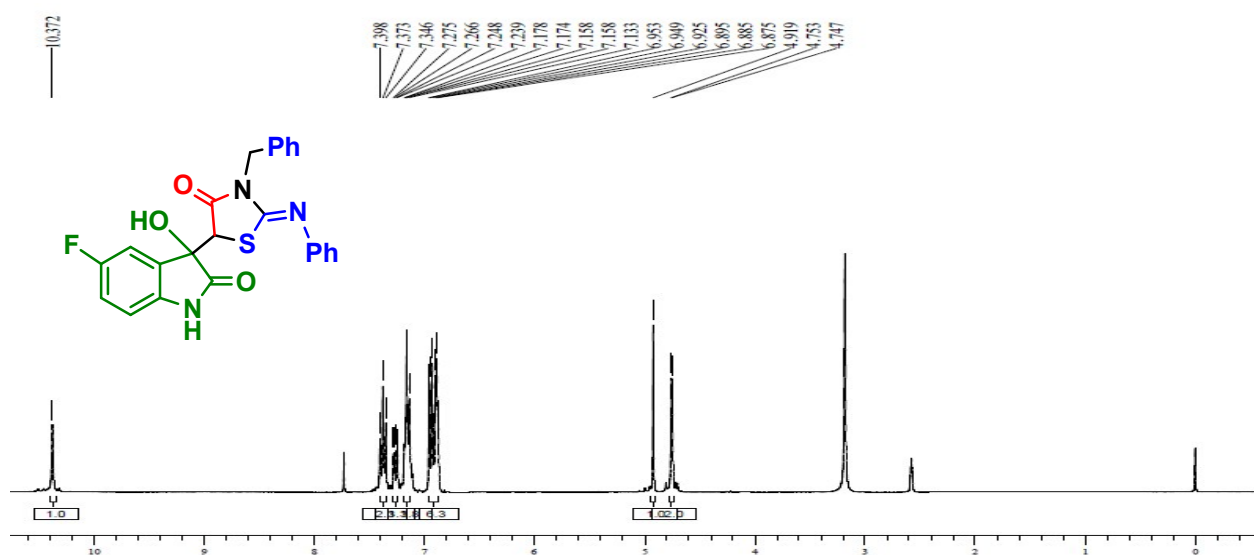


¹³C NMR (75 MHz, CDCl₃)

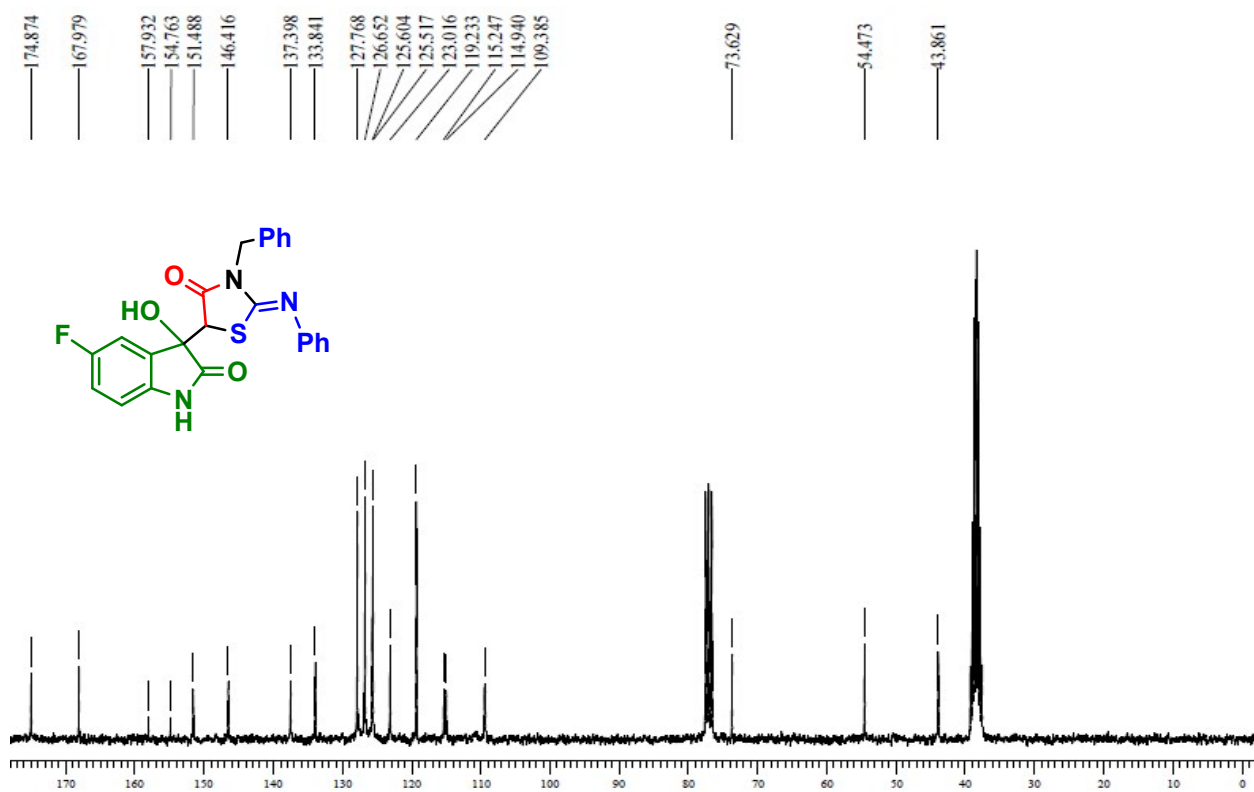


Compound 5i

¹H NMR (300 MHz, CDCl₃)

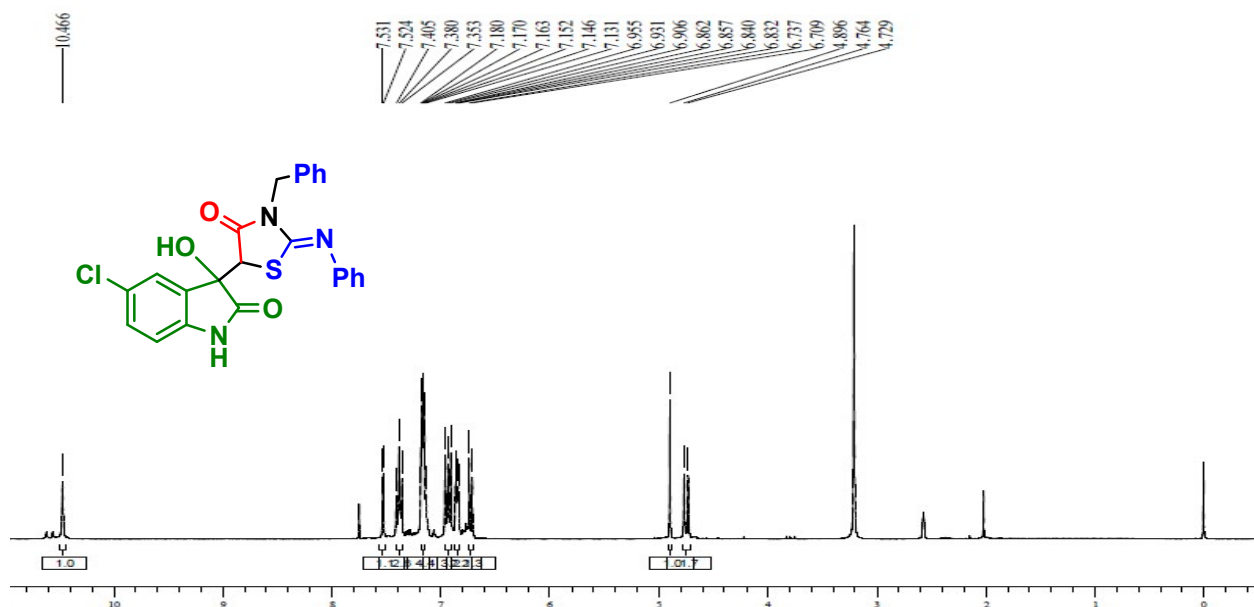


¹³C NMR (75 MHz, CDCl₃)

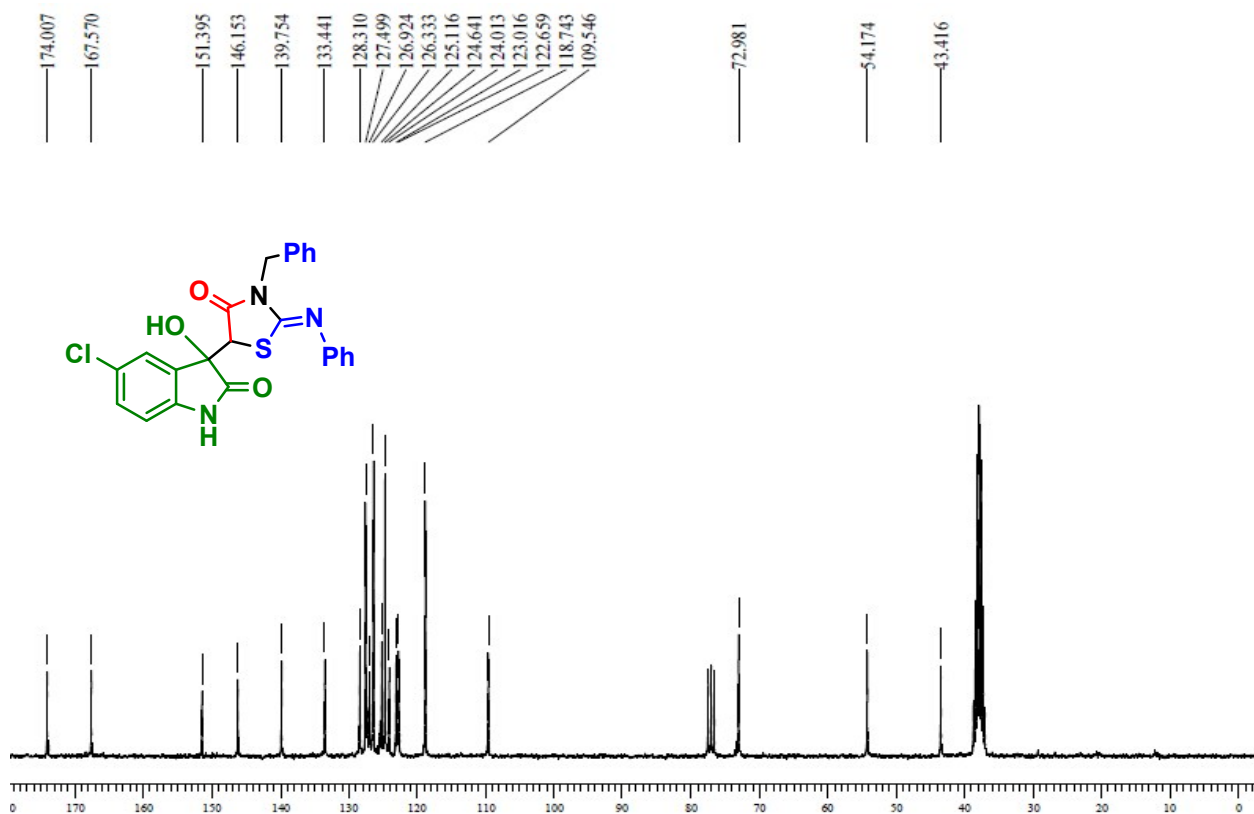


Compound 5j

¹H NMR (300 MHz, CDCl₃)

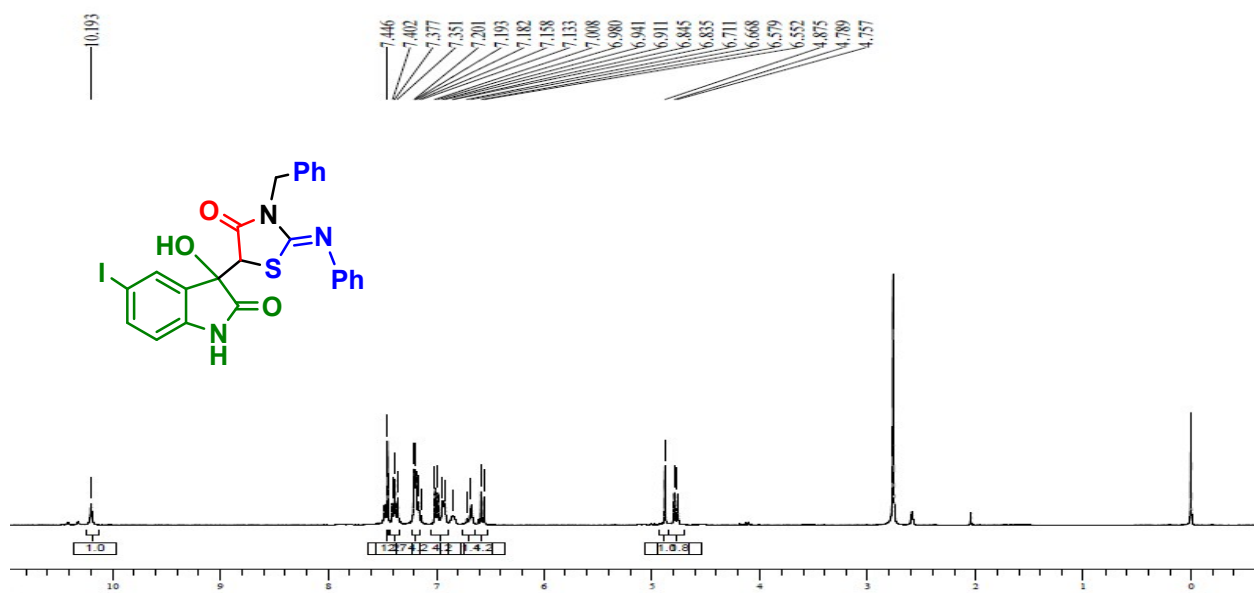


¹³C NMR (75 MHz, CDCl₃)

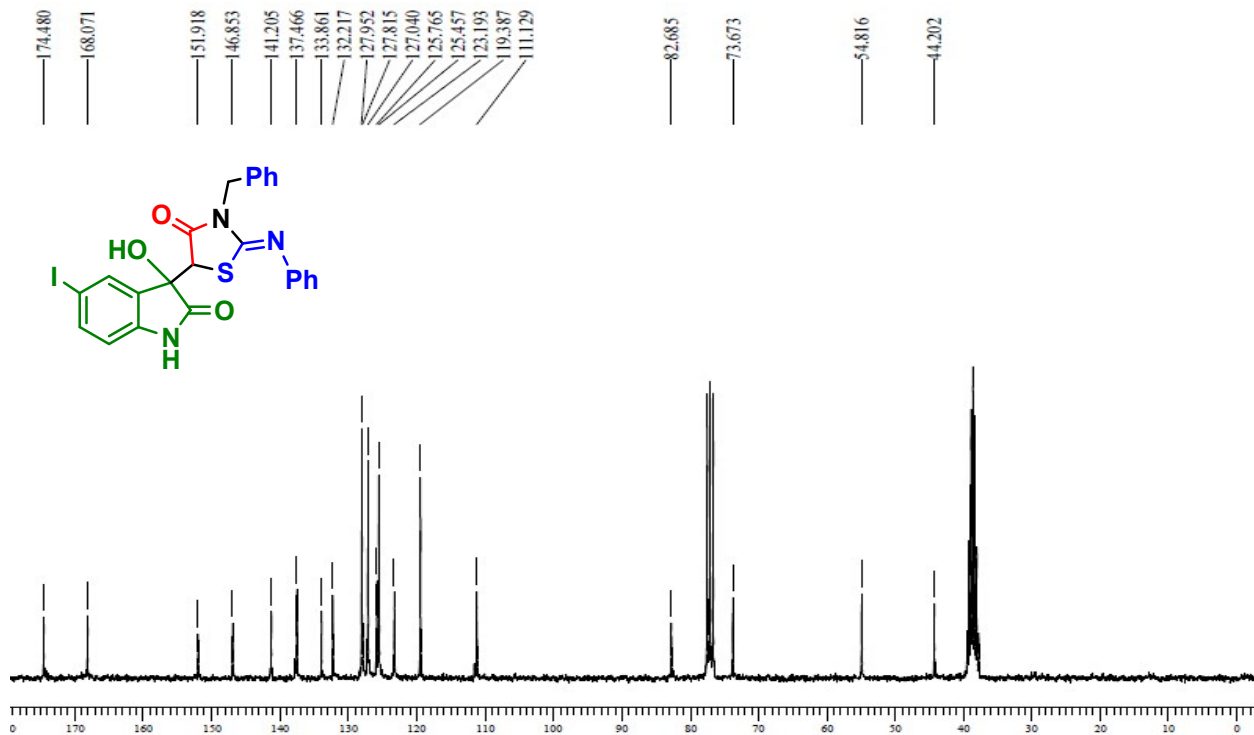


Compound 5k

^1H NMR (300 MHz, CDCl_3)

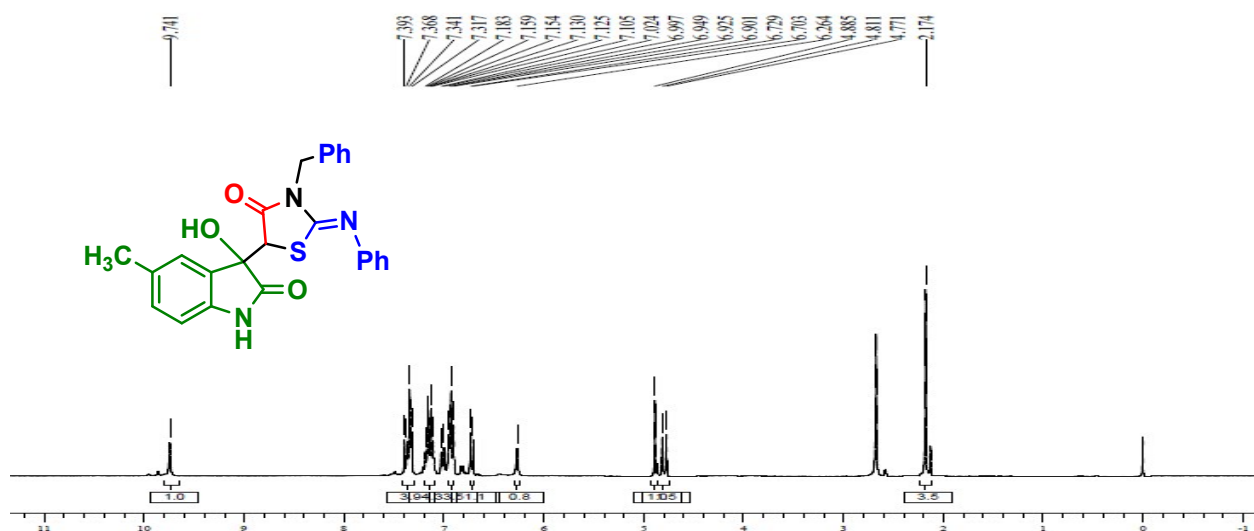


^{13}C NMR (75 MHz, CDCl_3)

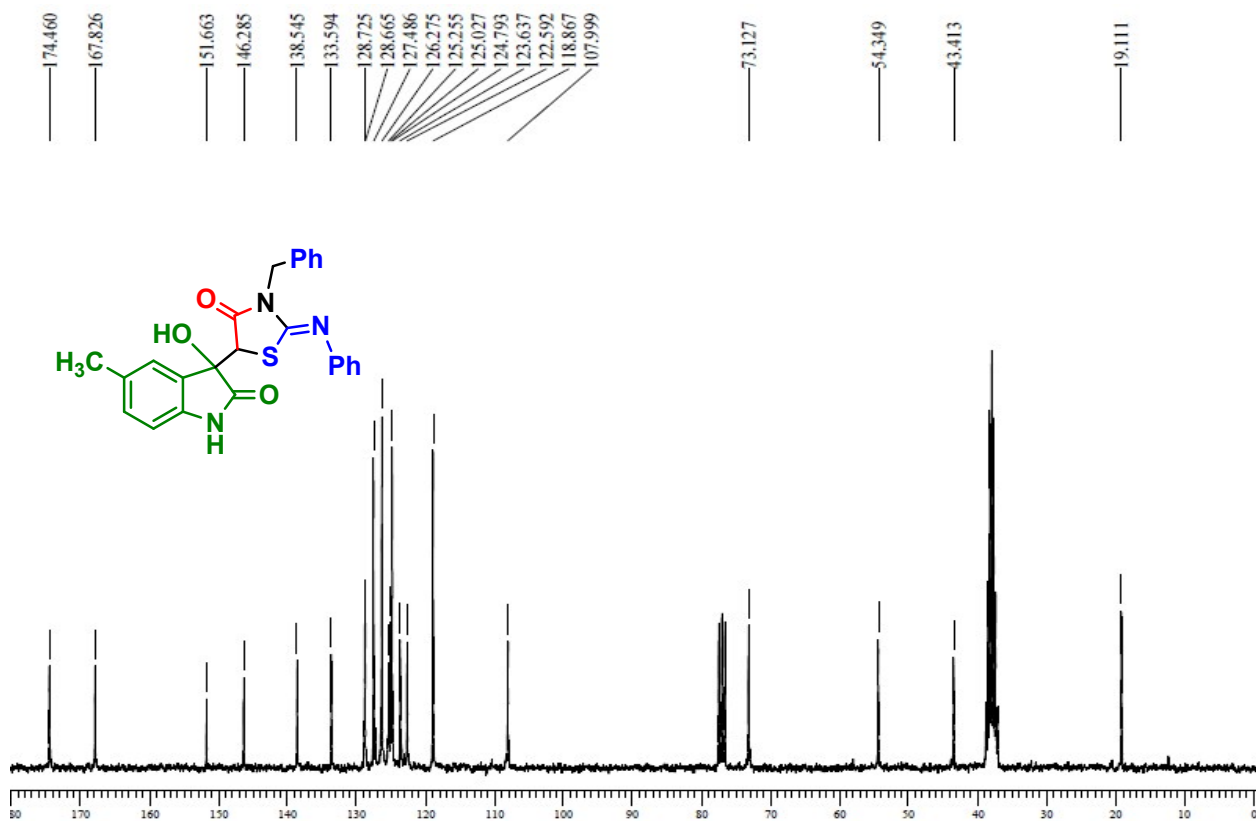


Compound 5l

¹H NMR (300 MHz, CDCl₃)

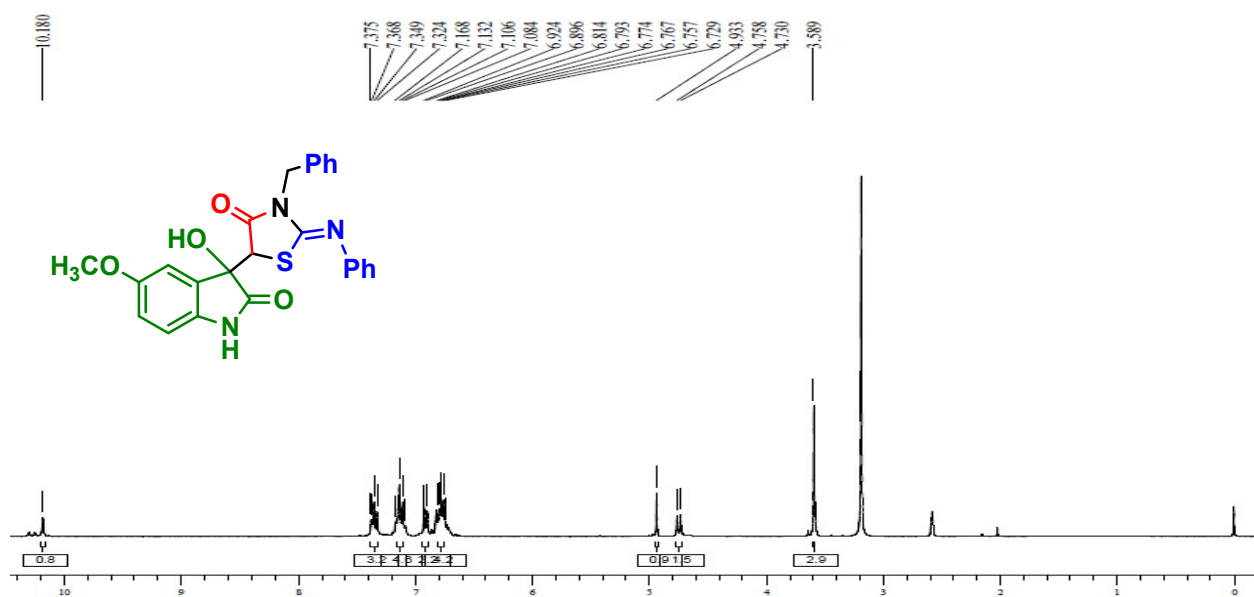


¹³C NMR (75 MHz, CDCl₃)

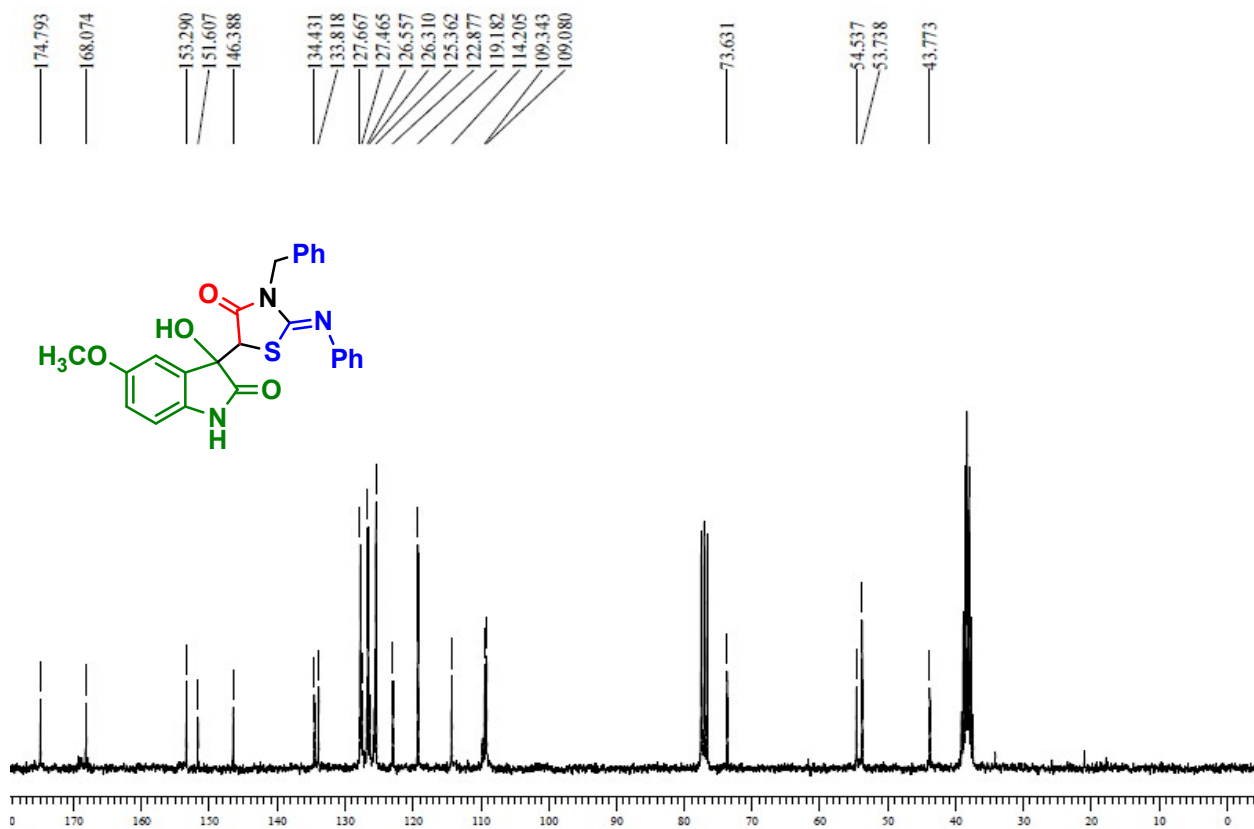


Compound 5m

¹H NMR (300 MHz, CDCl₃)

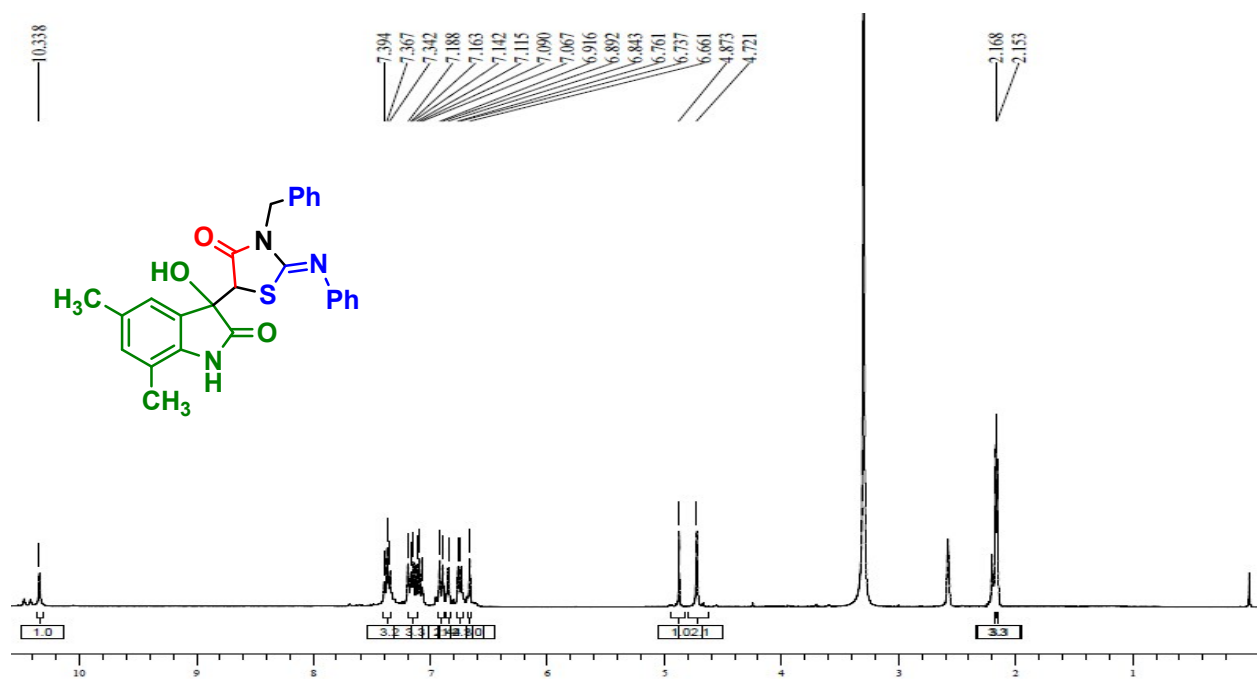


¹³C NMR (75 MHz, CDCl₃)

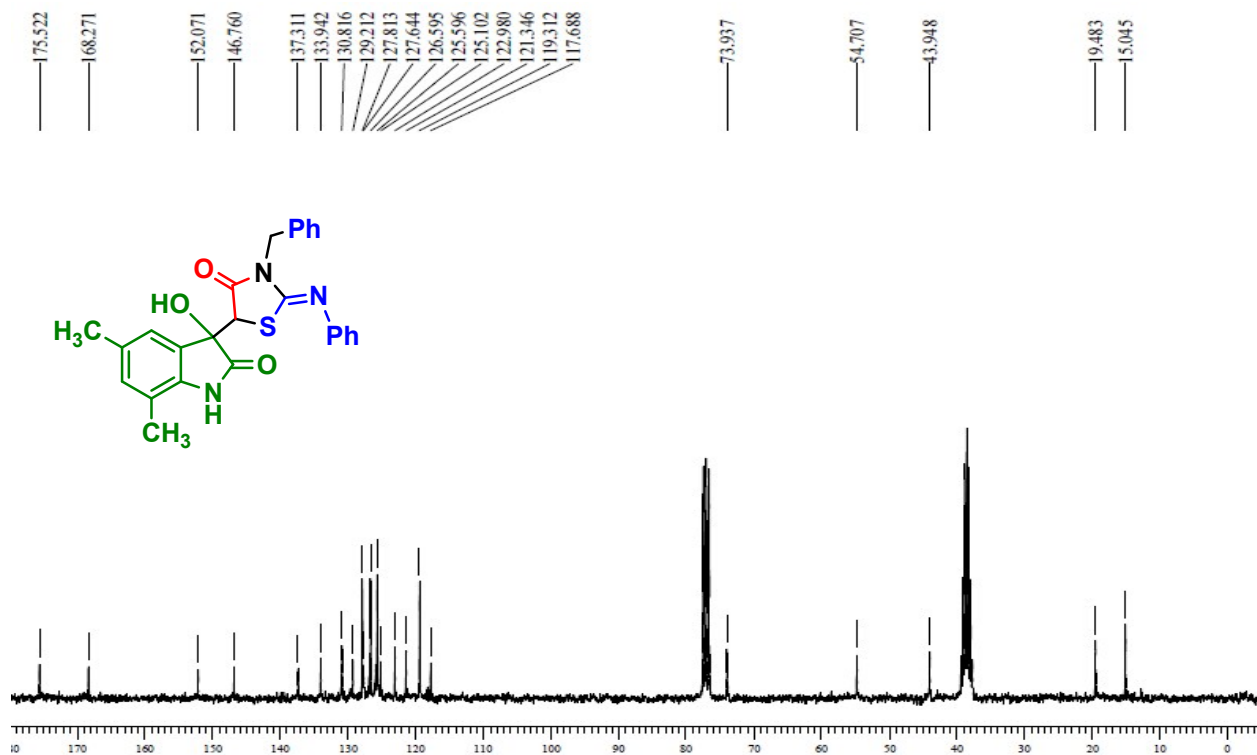


Compound 5n

^1H NMR (300 MHz, CDCl_3)

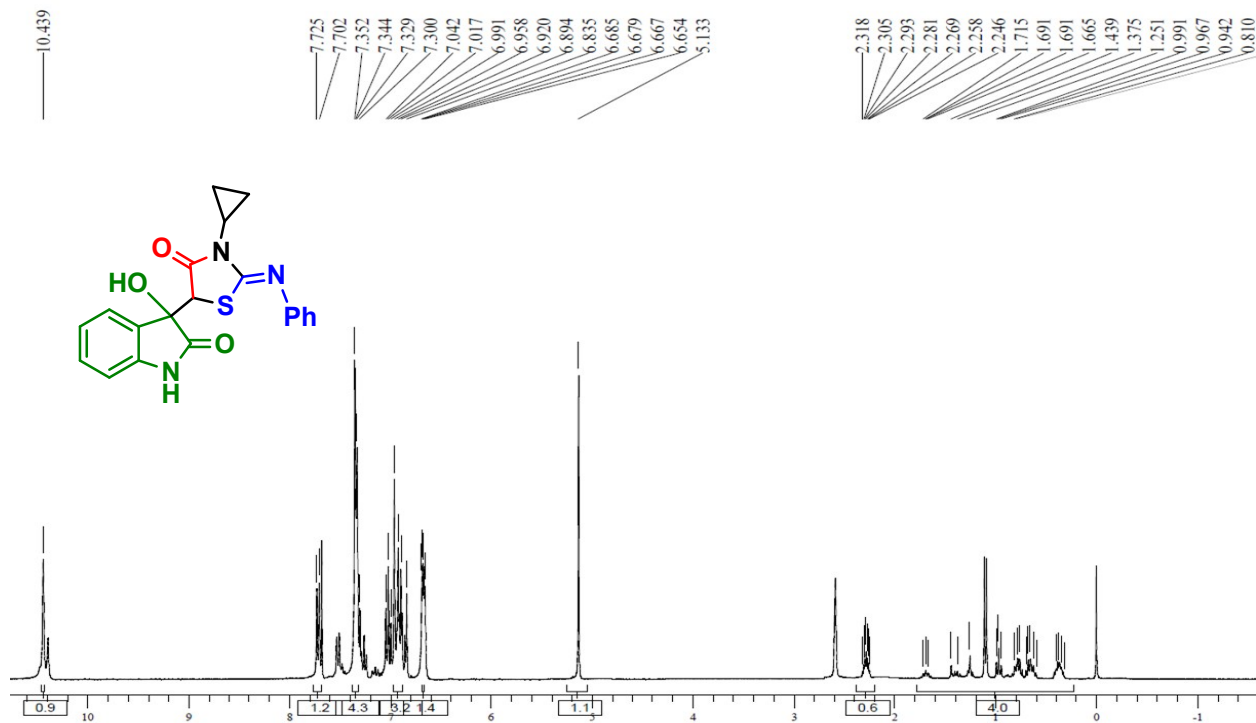


^{13}C NMR (75 MHz, CDCl_3)

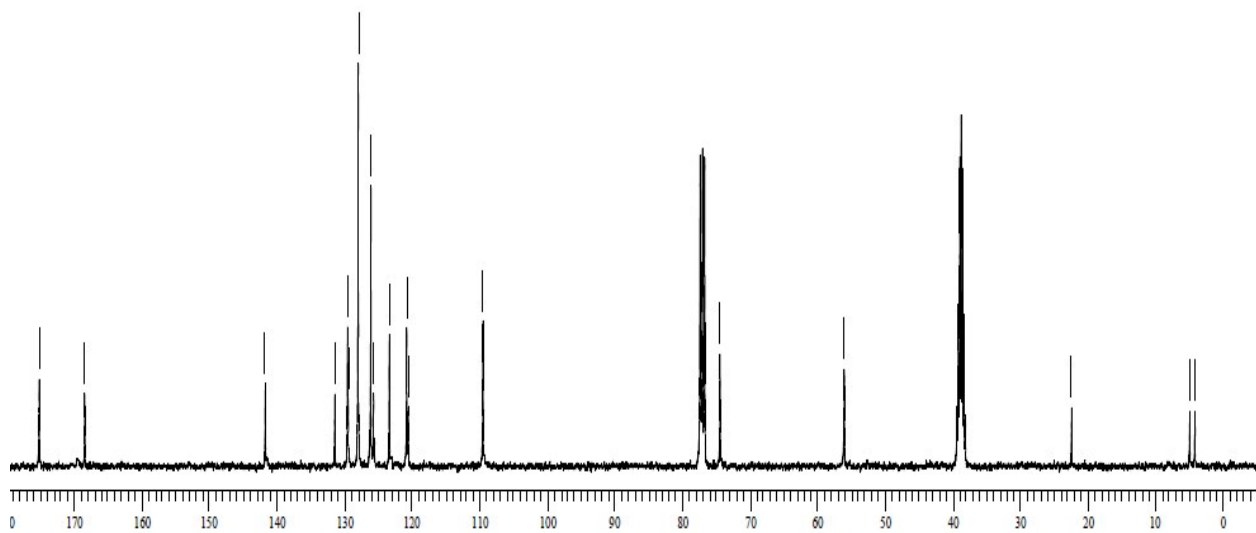
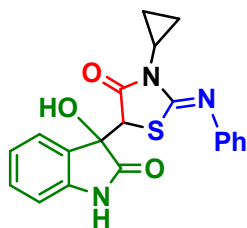


Compound 5o

^1H NMR (300 MHz, CDCl_3)

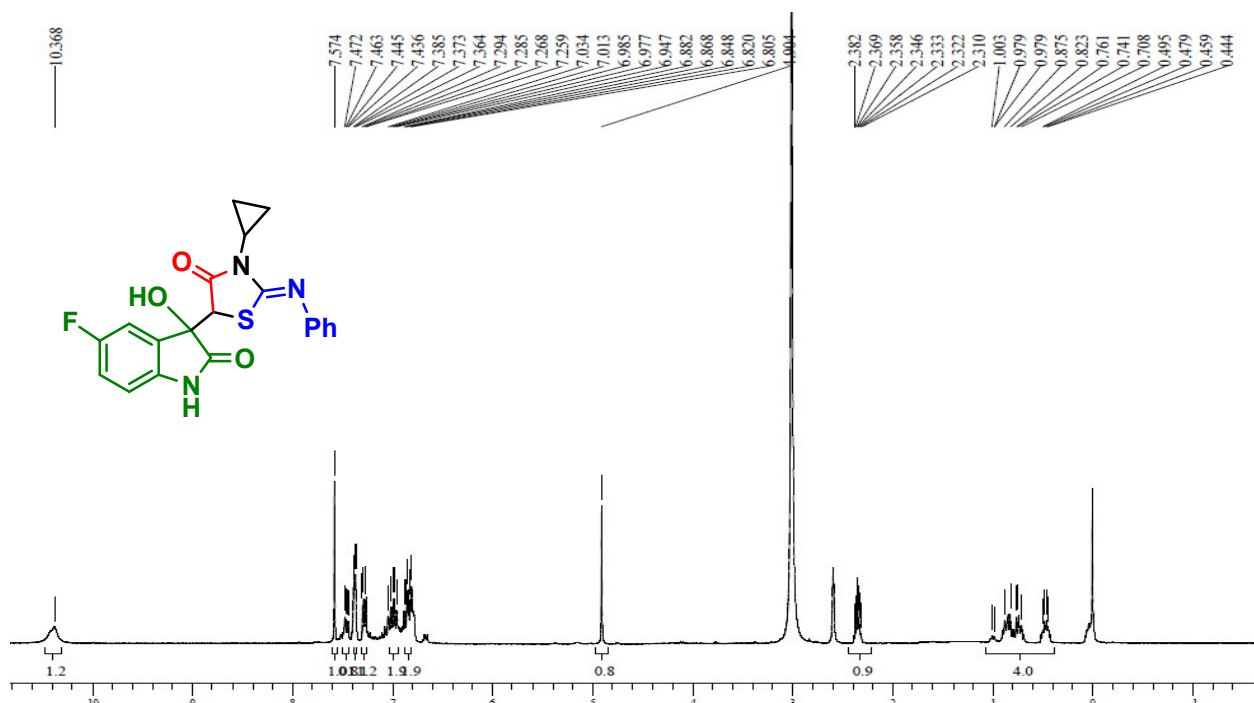


^{13}C NMR (75 MHz, CDCl_3)

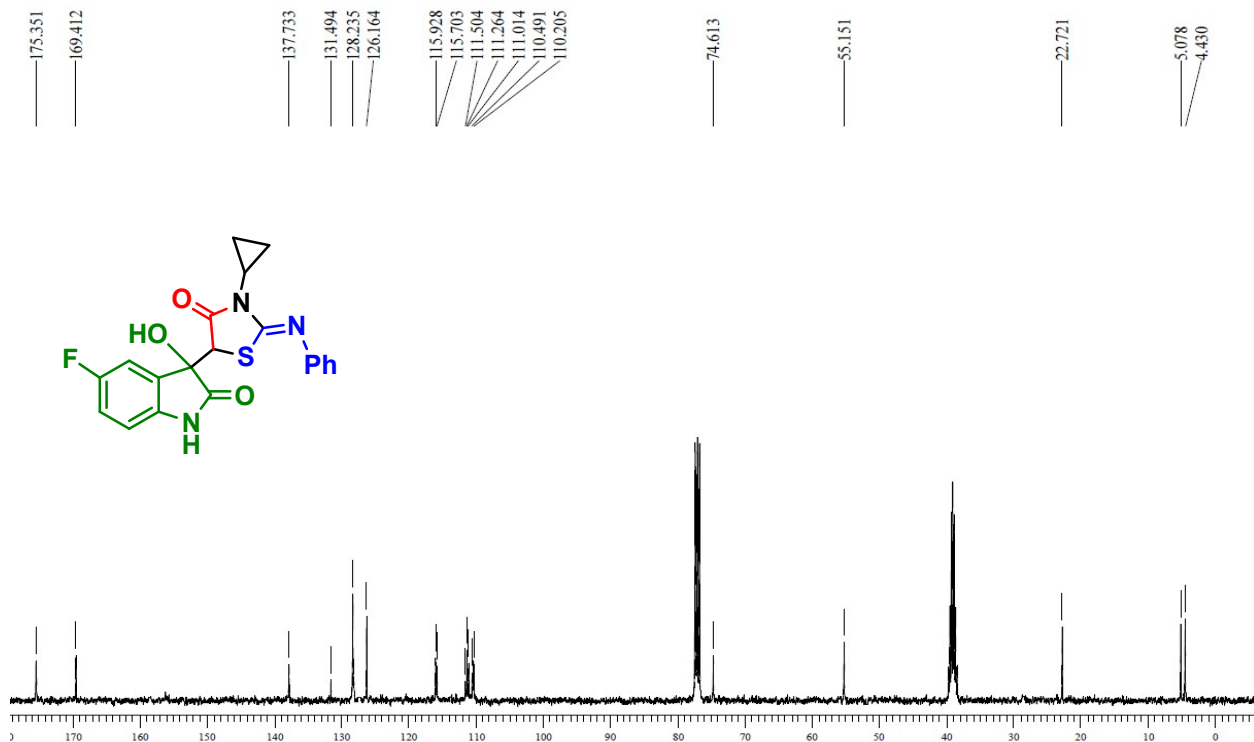


Compound 5p

^1H NMR (300 MHz, CDCl_3)

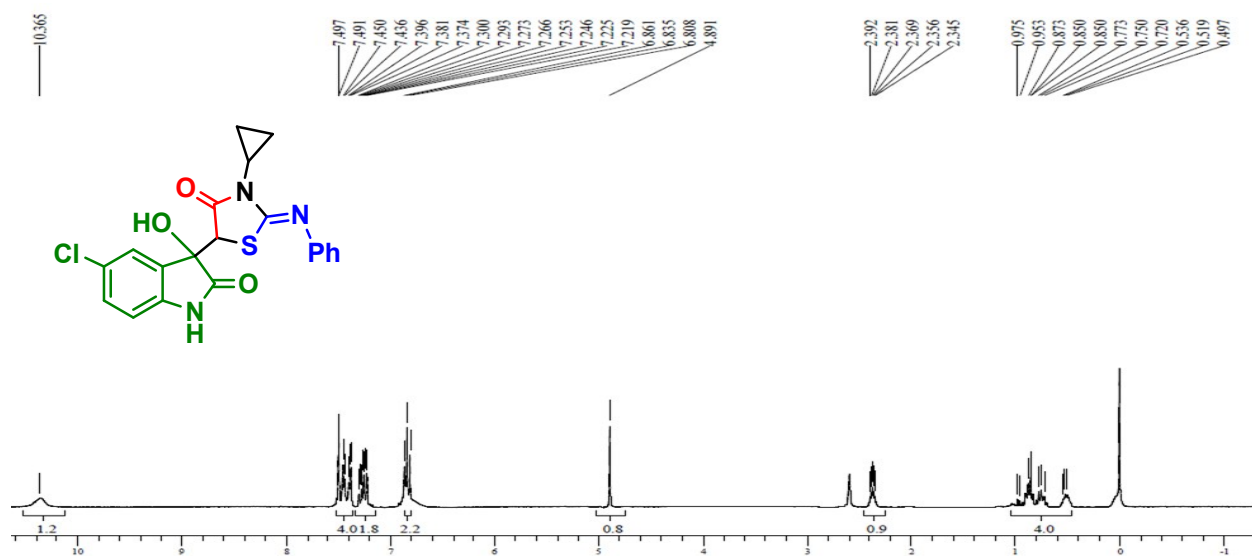


^{13}C NMR (75 MHz, CDCl_3)

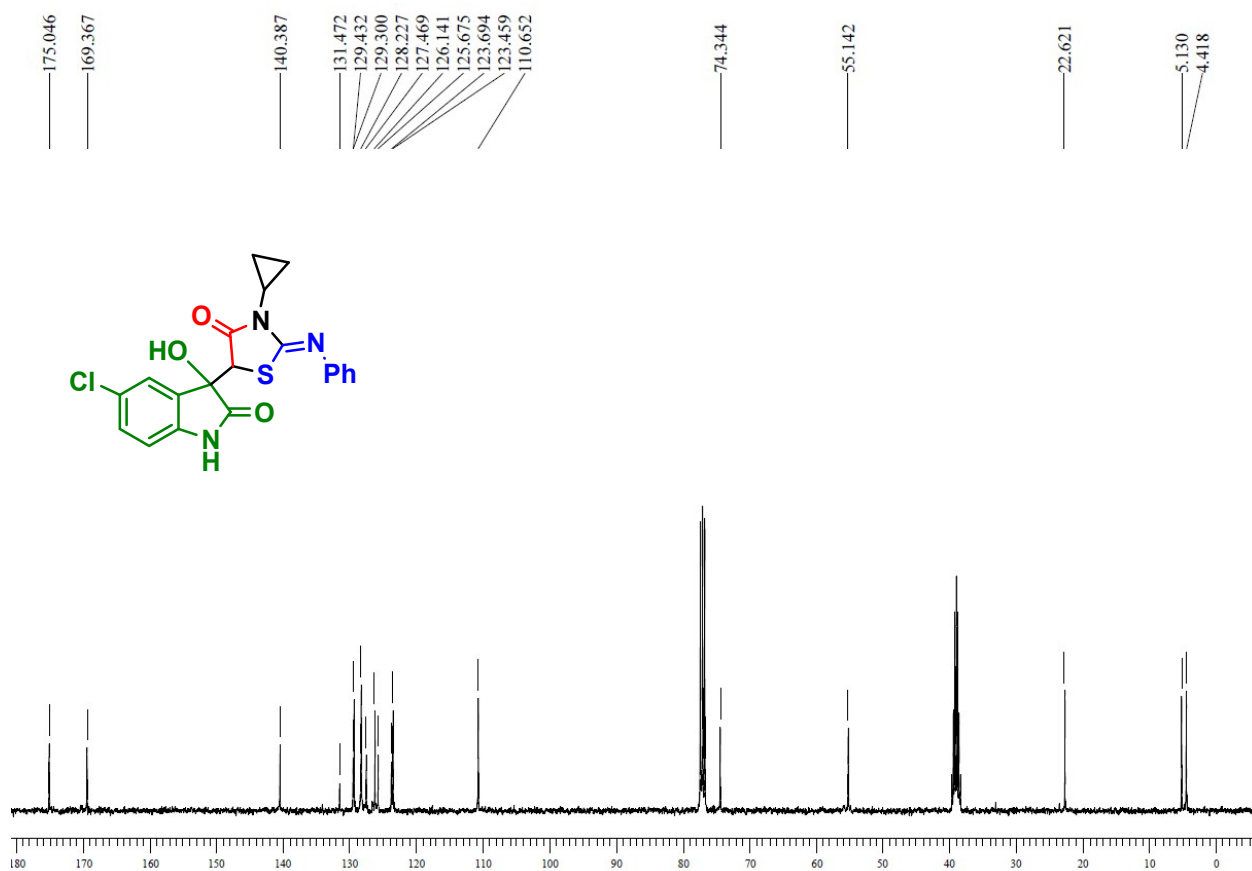


Compound 5q

^1H NMR (300 MHz, CDCl_3)

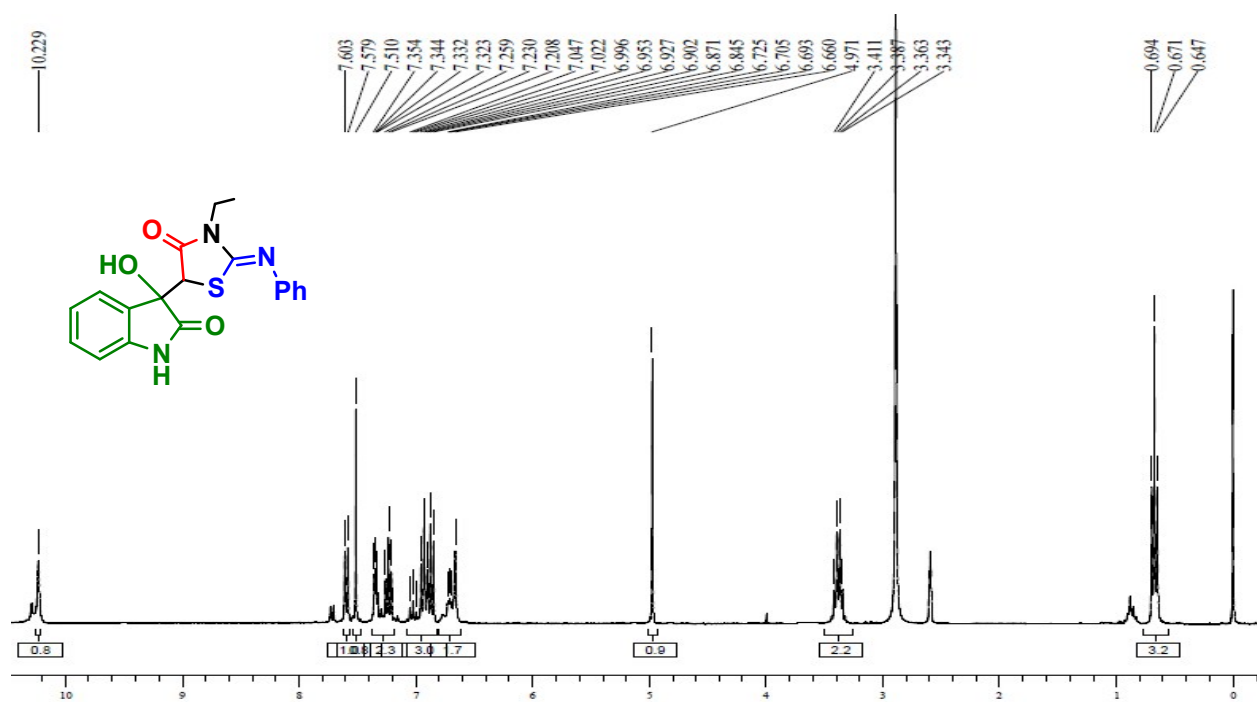


^{13}C NMR (75 MHz, CDCl_3)

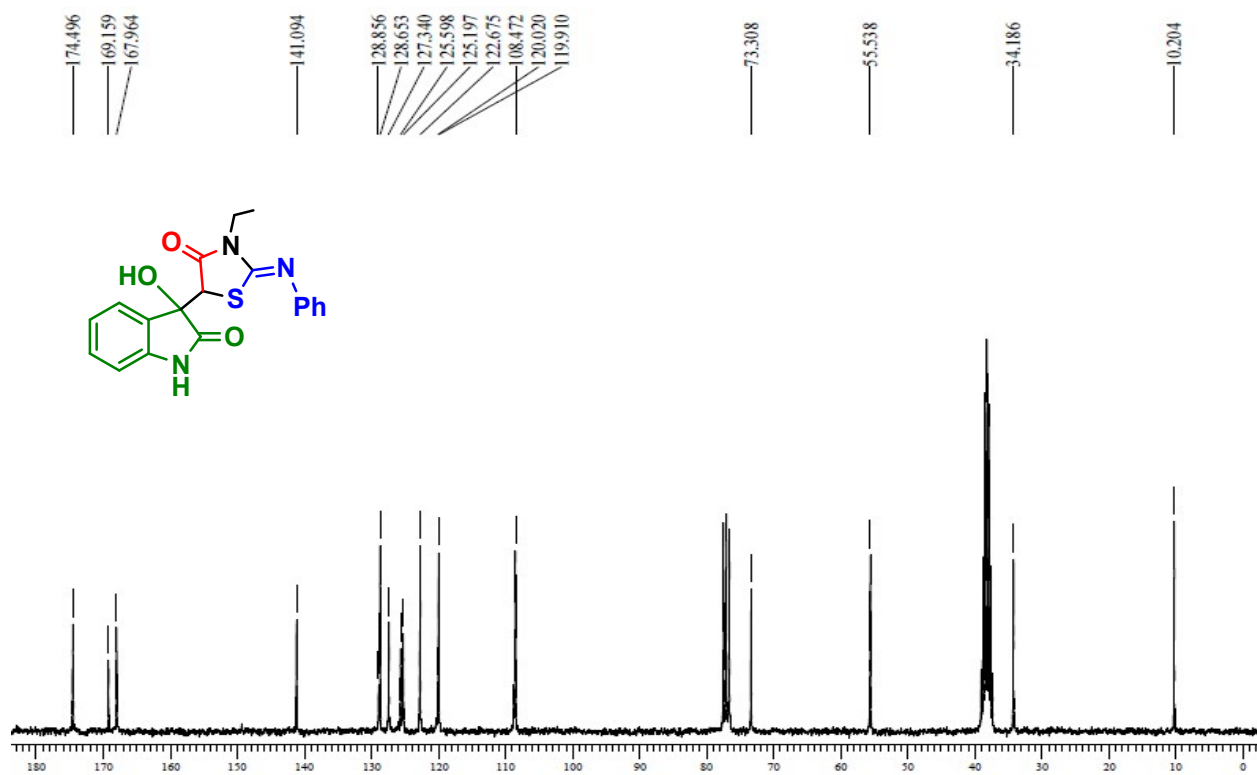


Compound 5r

¹H NMR (300 MHz, CDCl₃)

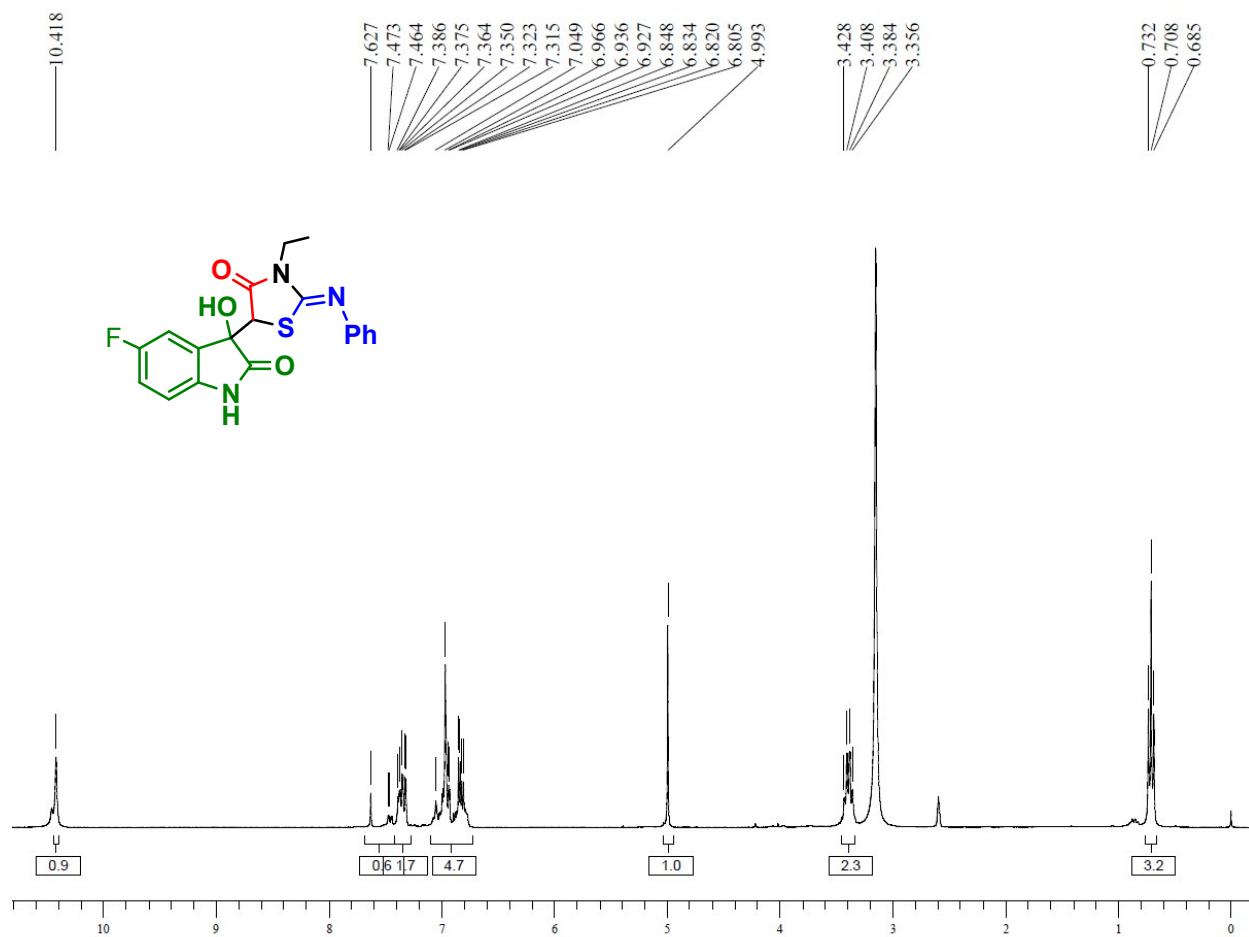


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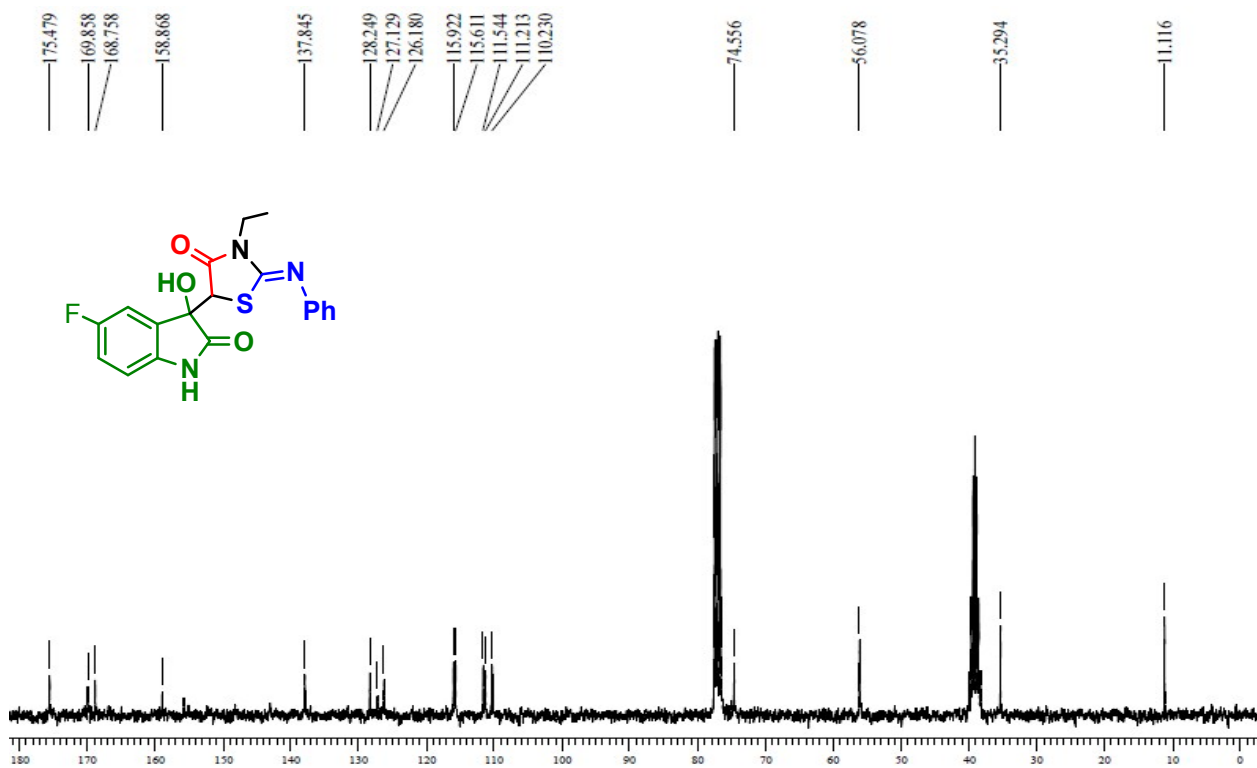


Compound 5s

^1H NMR (300 MHz, CDCl_3)

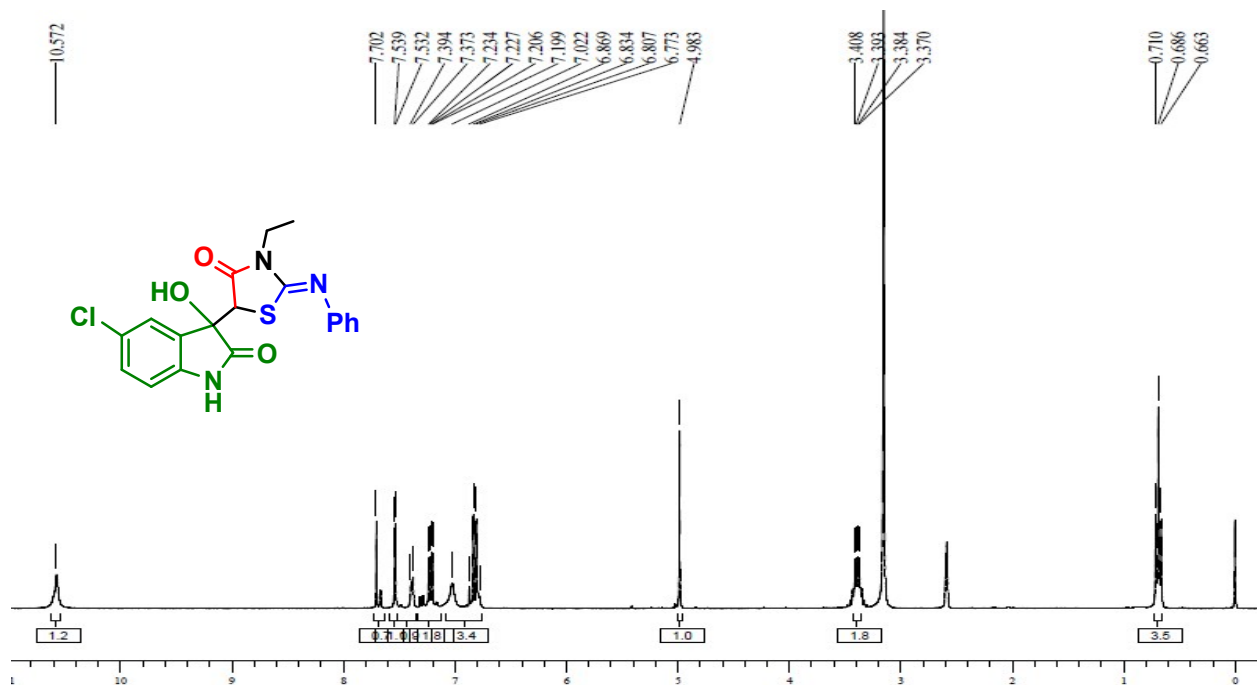


^{13}C NMR (75 MHz, CDCl_3)

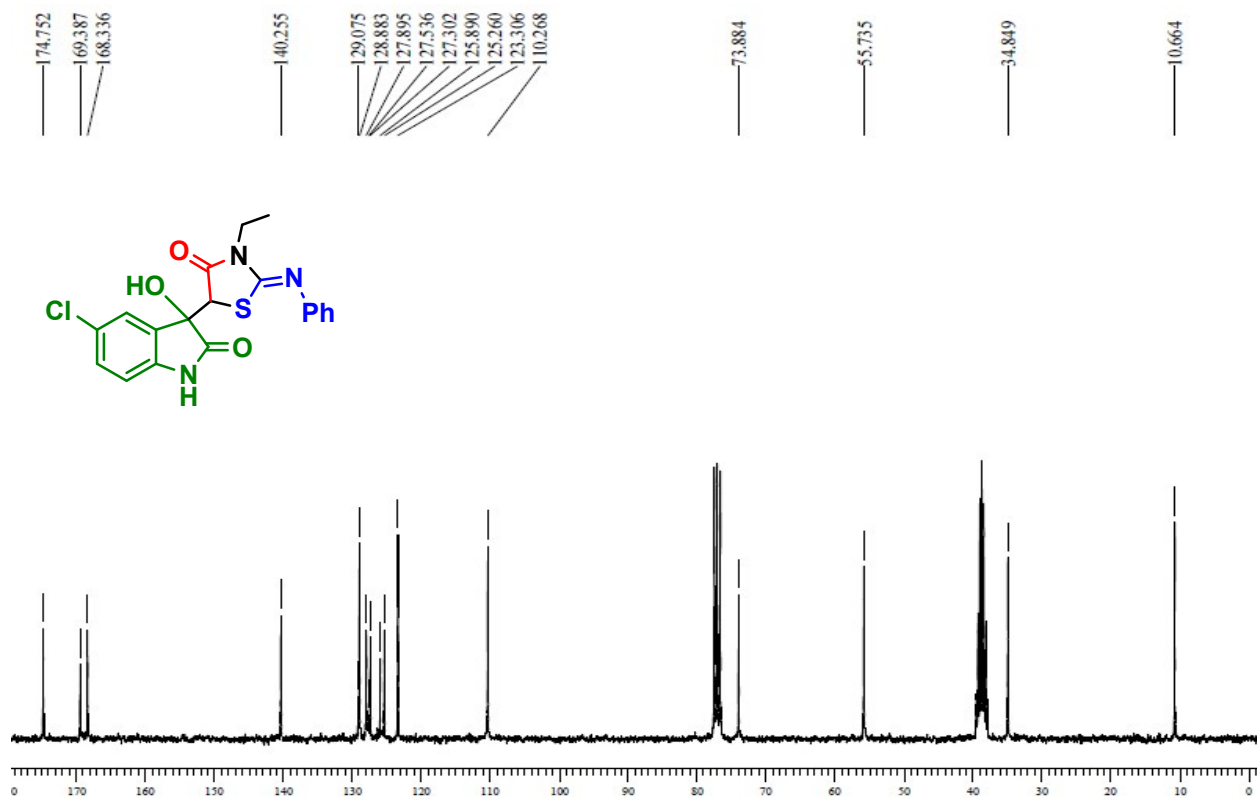


Compound 5t

¹H NMR (300 MHz, CDCl₃)

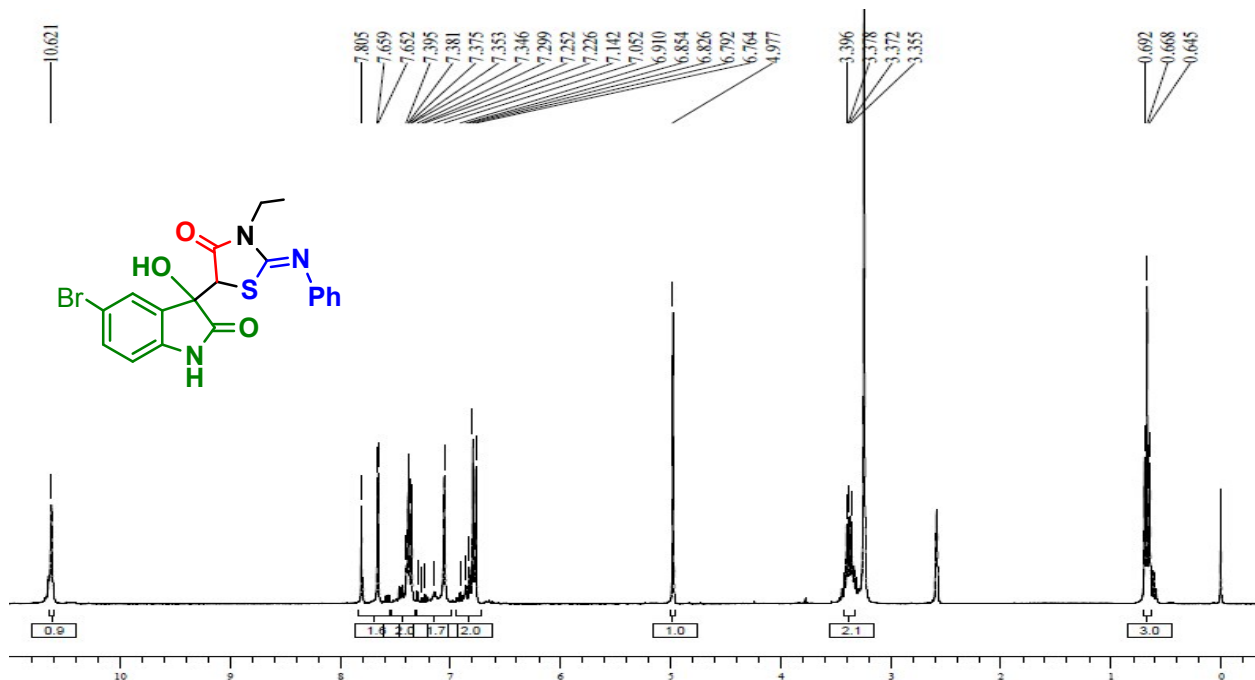


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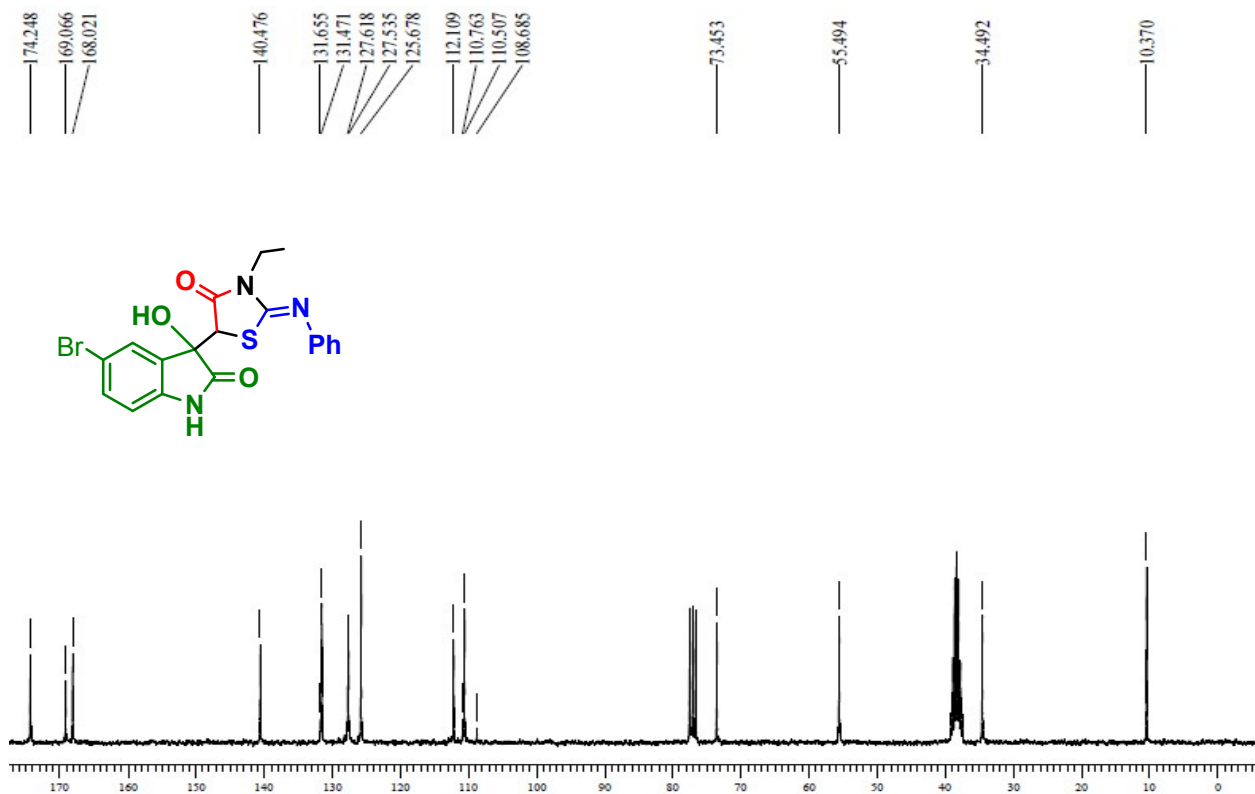


Compound 5u

¹H NMR (300 MHz, CDCl₃)

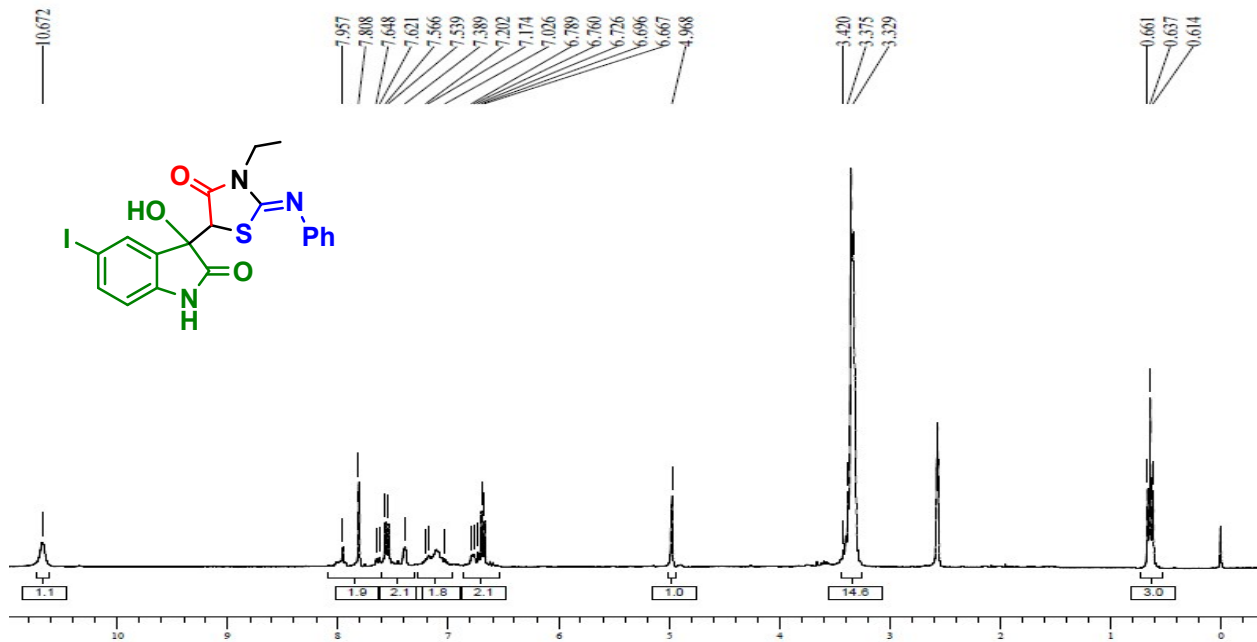


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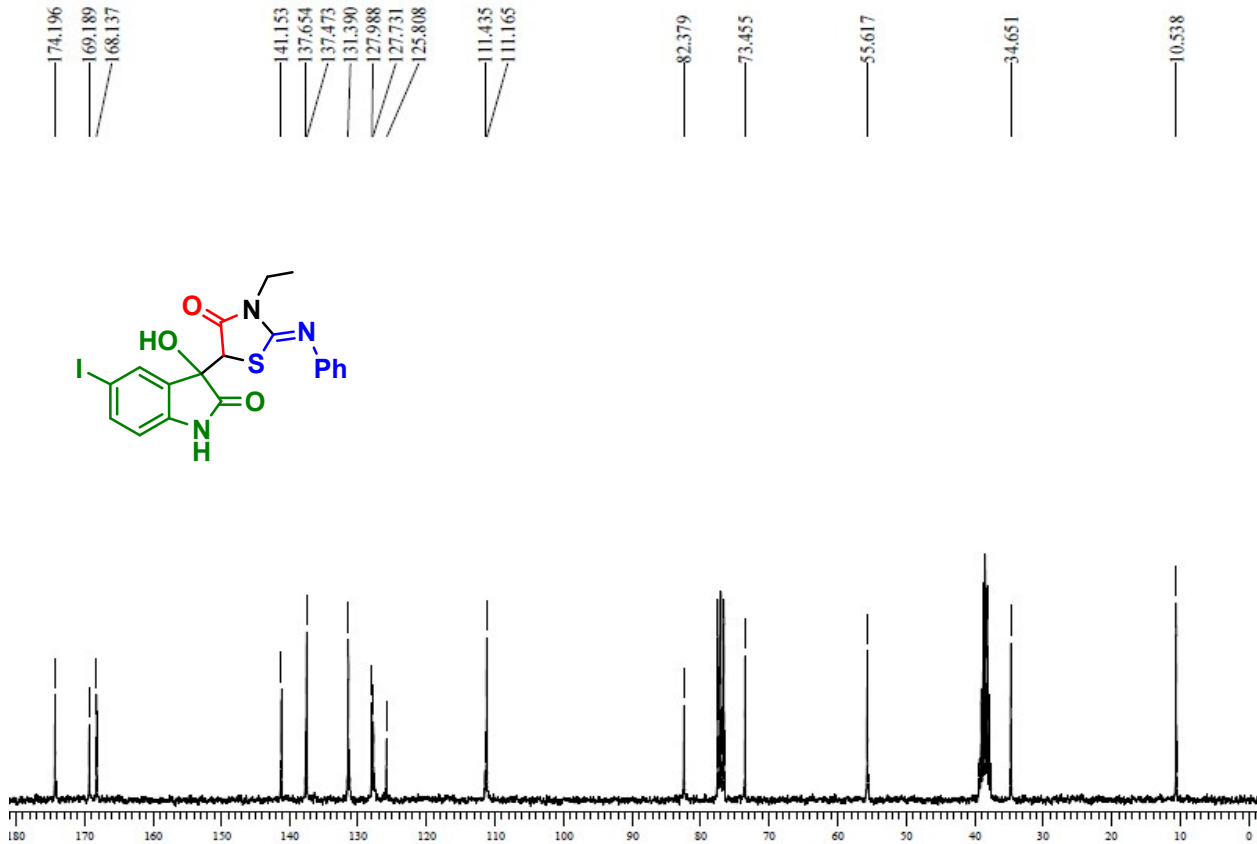


Compound 5v

¹H NMR (300 MHz, CDCl₃)

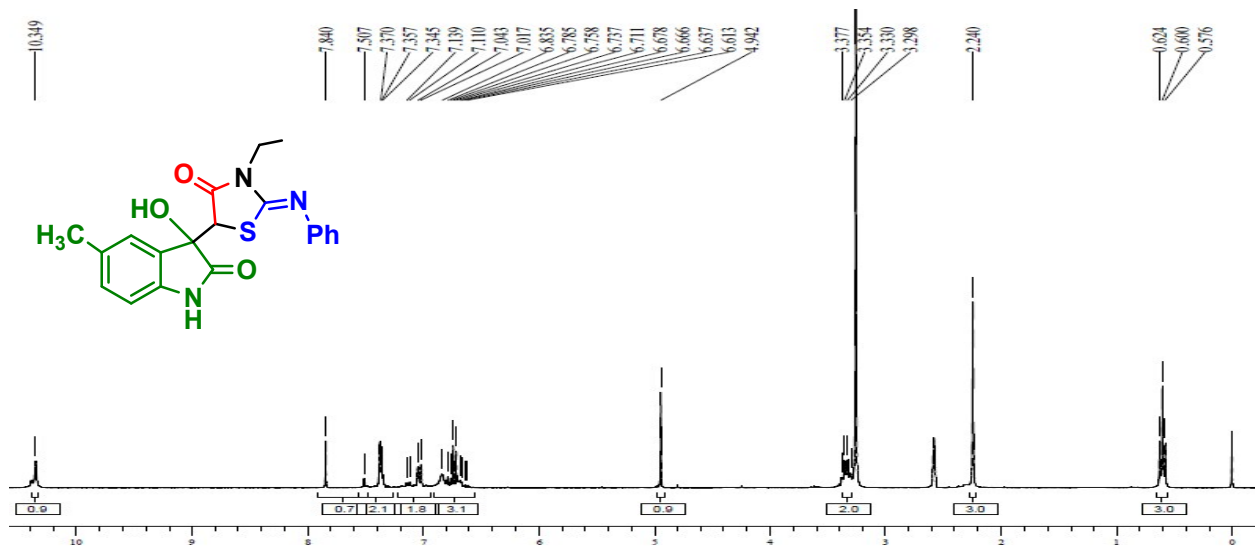


¹³C NMR (75 MHz, CDCl₃)

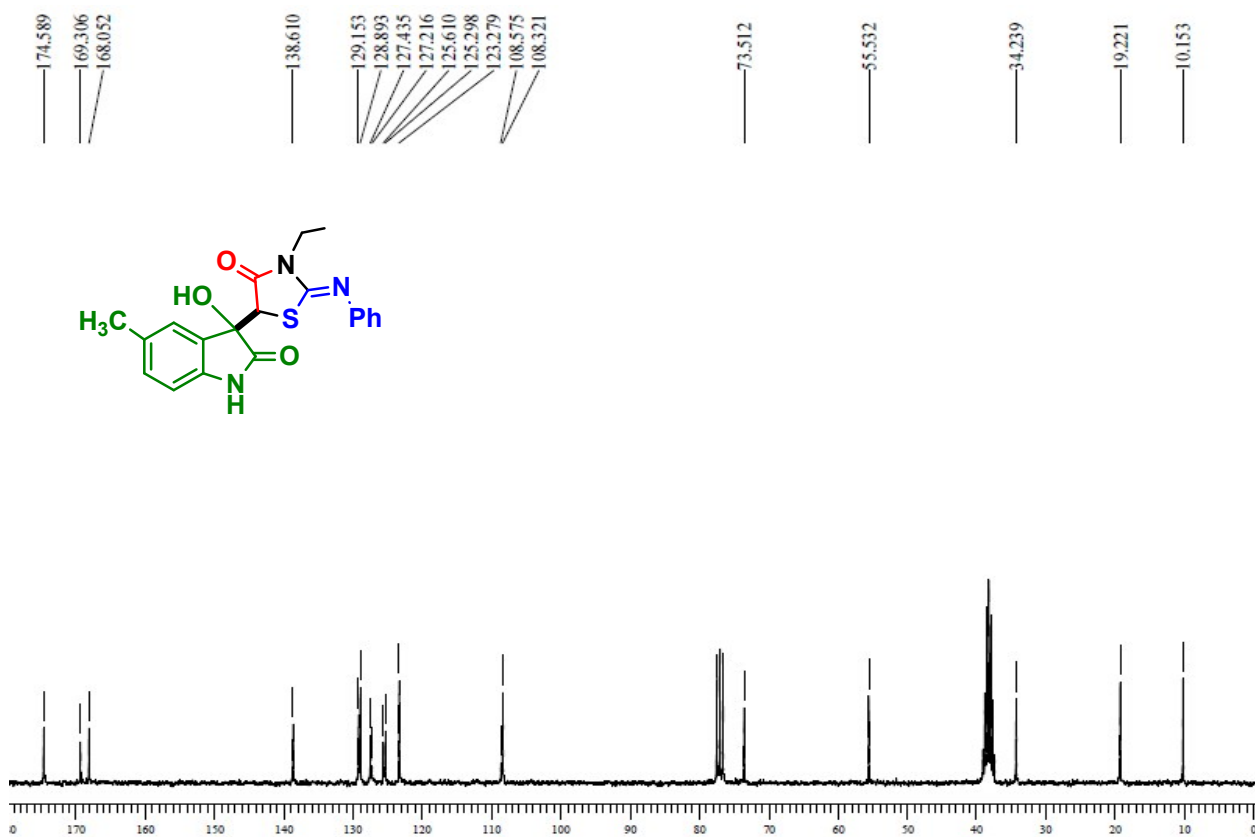


Compound 5w

¹H NMR (300 MHz, CDCl₃)

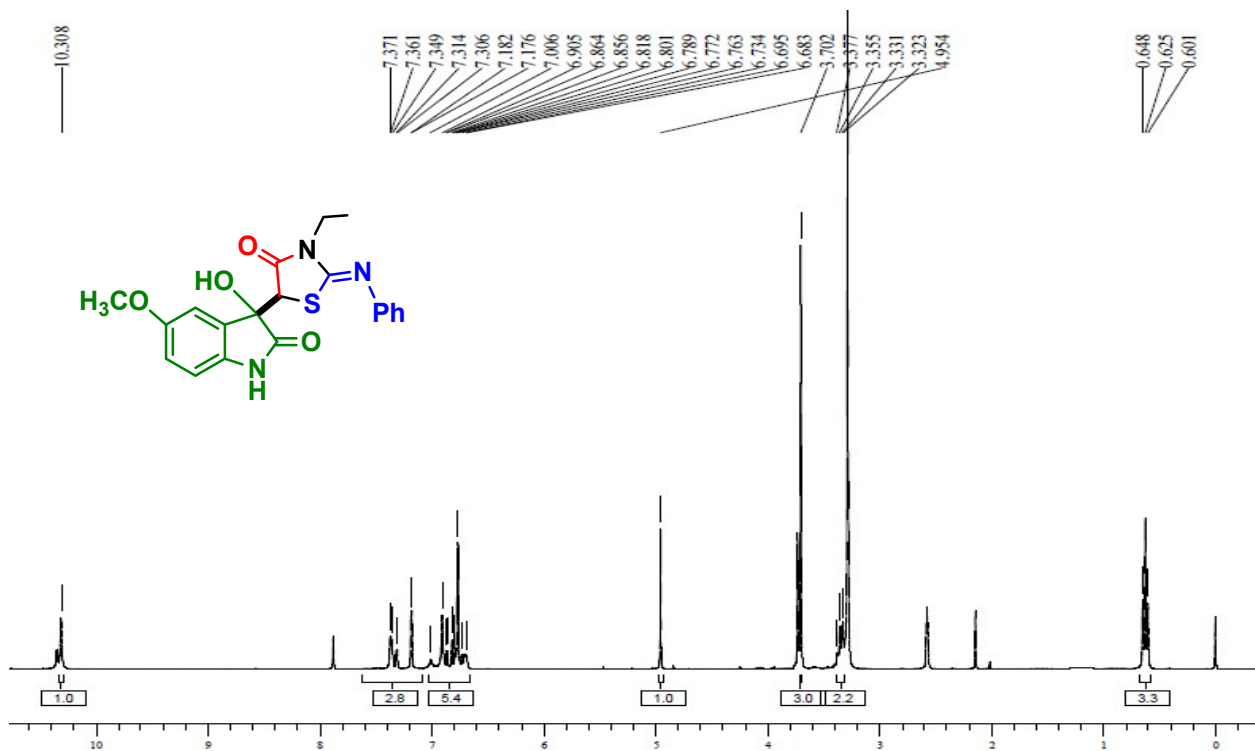


¹³C NMR (75 MHz, CDCl₃)



Compound 5x

¹H NMR (300 MHz, CDCl₃)



¹³C NMR (75 MHz, CDCl₃)

