Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Photochemical and Photophysical Behavior of Indolyl Anions in Photostimulated Intramolecular Arylation Reactions.

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Supporting Information

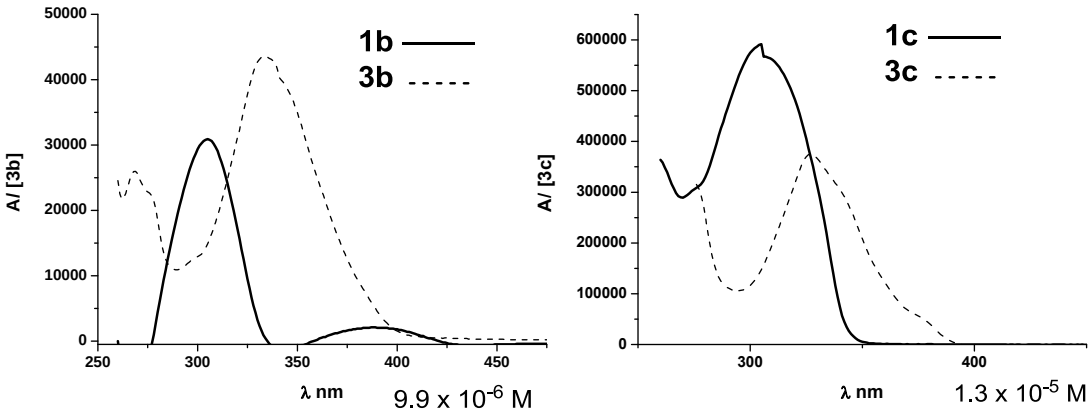


Figure S1: Uv-vis spectra for compounds **1b-c** and anions derivatives **3b-c**. Spectra were performed under N_2 in DMSO. To form the anions, a solution of *t*-BuOK 9.9 x 10^{-4} M was added and the mixture was incubated for 5 min. Solid line: neutral. Dotted line: anion.

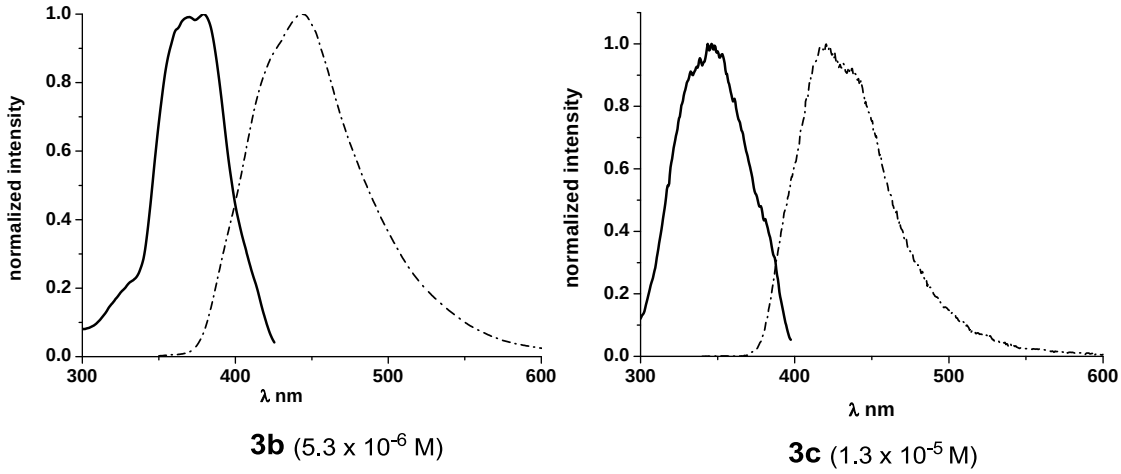
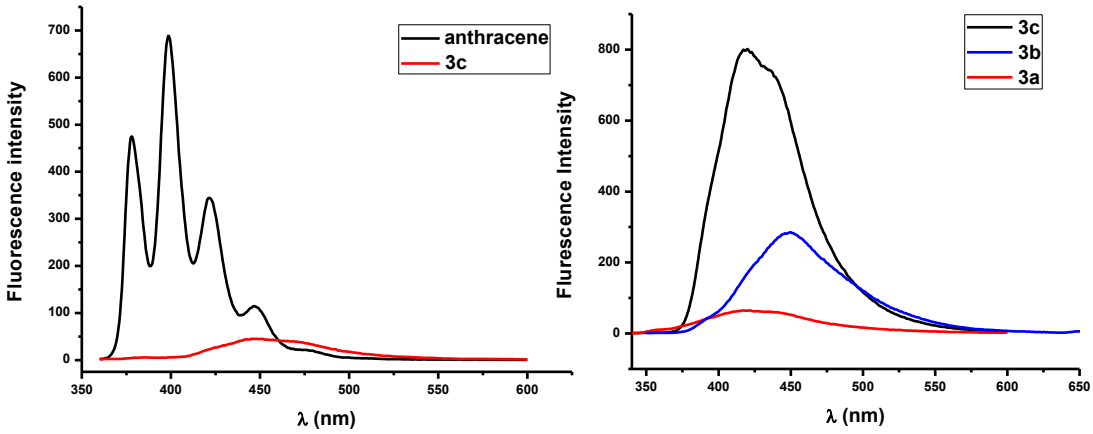


Figure S2: Excitation (solid line——) and fluorescence (dotted line **….**) spectra for **3b-c**. Spectra were performed under N_2 in DMSO. To form anions, a solution of *t*-BuOK 9.9 x 10^{-4} M was added and the mixture was incubated for 5 min.



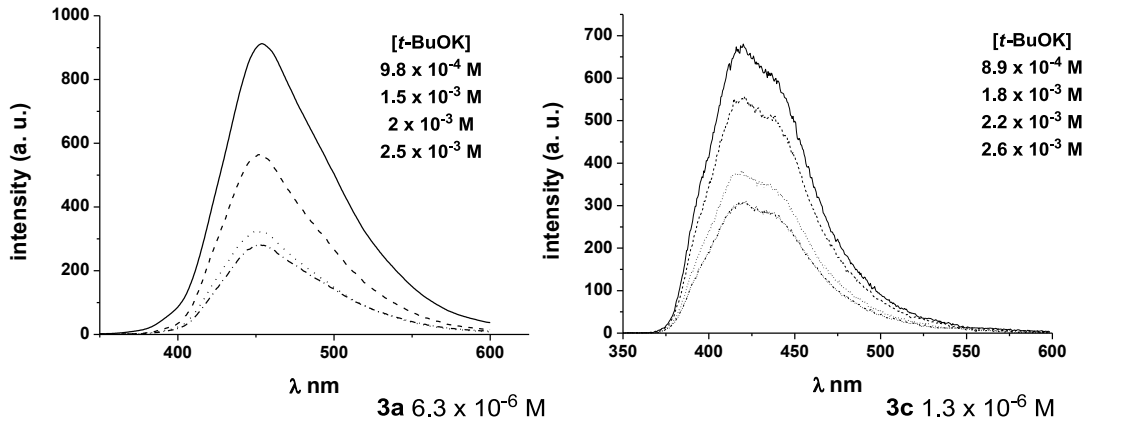
	anthracene	3c[b]	3b[b]	3a[b]
concentration (M)	3,1 x 10^{-5}	4,61 x 10^{-6}	5,26 x 10^{-6}	6,31 x 10^{-6}
λ max. (nm)	356	327	332	339
solvent	EtOH 95 %	DMSO	DMSO	DMSO
RI solvent	1,3611	1,4768	1,4768	1,4768
absorbance	0,124	0,140	0,128	0,127

[a]Measurements were performed under N_2, in fluorimeter Perkin Elmer LS55 Fluorescence Spectrometers. [b]To form anions **3a-c**, *t*-BuOK was added (final concentration: 9,9 x 10^{-4} M.

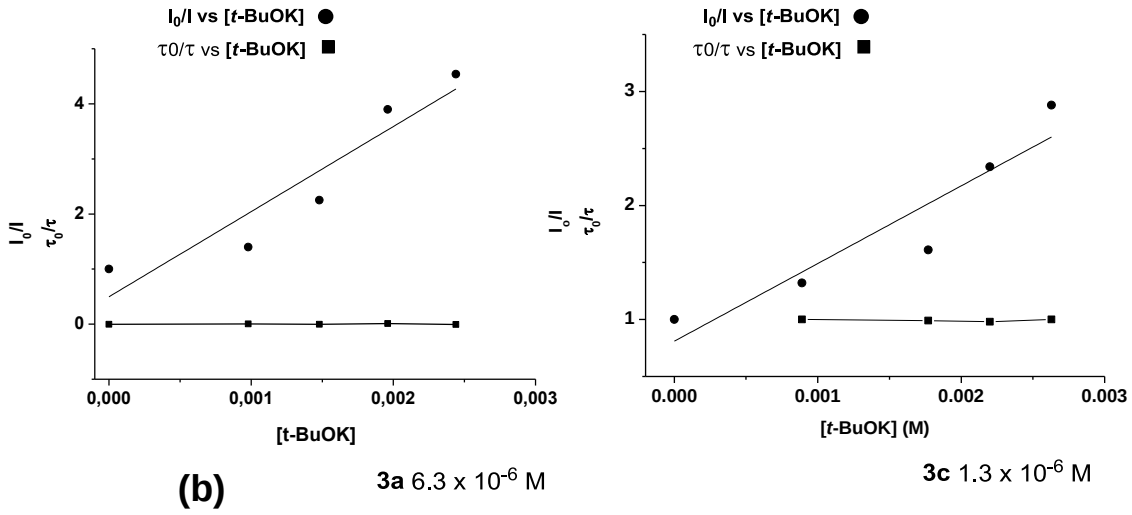
Fluorescence quantum yields were calculated according the following equation,

$$\Phi_{f\,3} = \Phi_{reference} \times \frac{area_3}{area_{reference}} \times \frac{Abs_{reference}}{Abs_3} \times \frac{(RI_3)^2}{(RI_{reference})^2}$$

Where $\Phi_{reference}$ is the fluorescence quantum yield of the reference, area is the integrated area under the fluorescence spectra of compound **3** and the reference, Abs are the absorbance of **3** and the reference, RI is the refractive index of the solvent employed. To determine values of Φf for **3a-b**, **3c** was used as reference using the same equation.



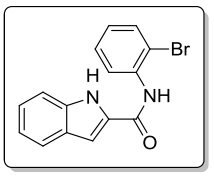
(a)

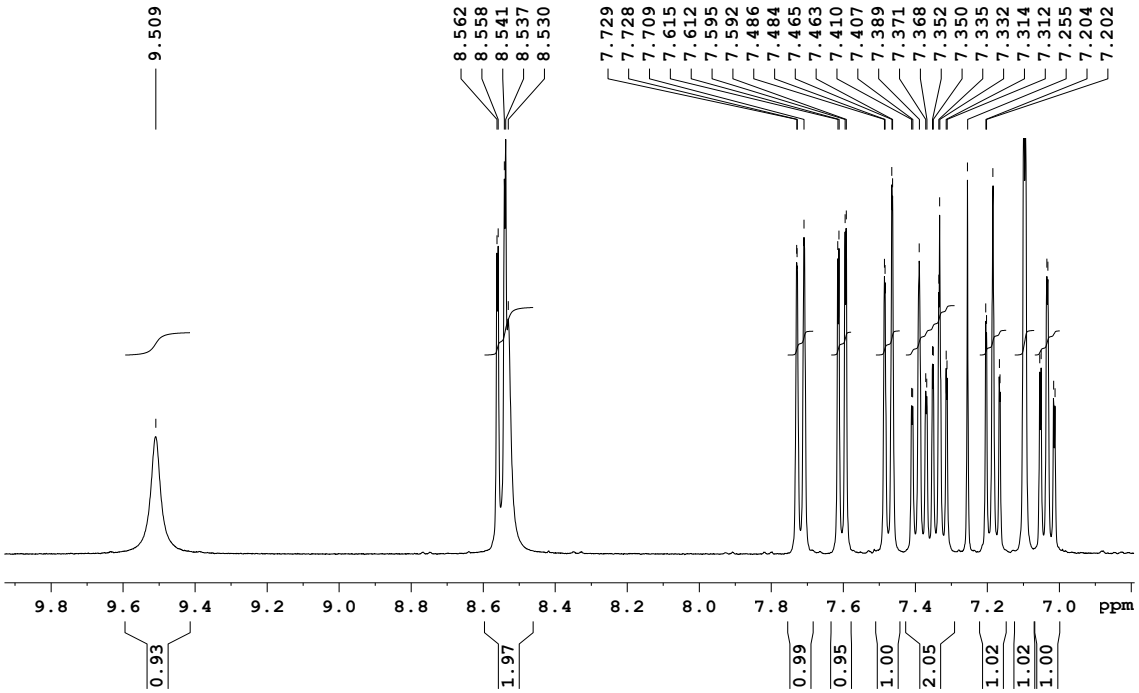


(b)

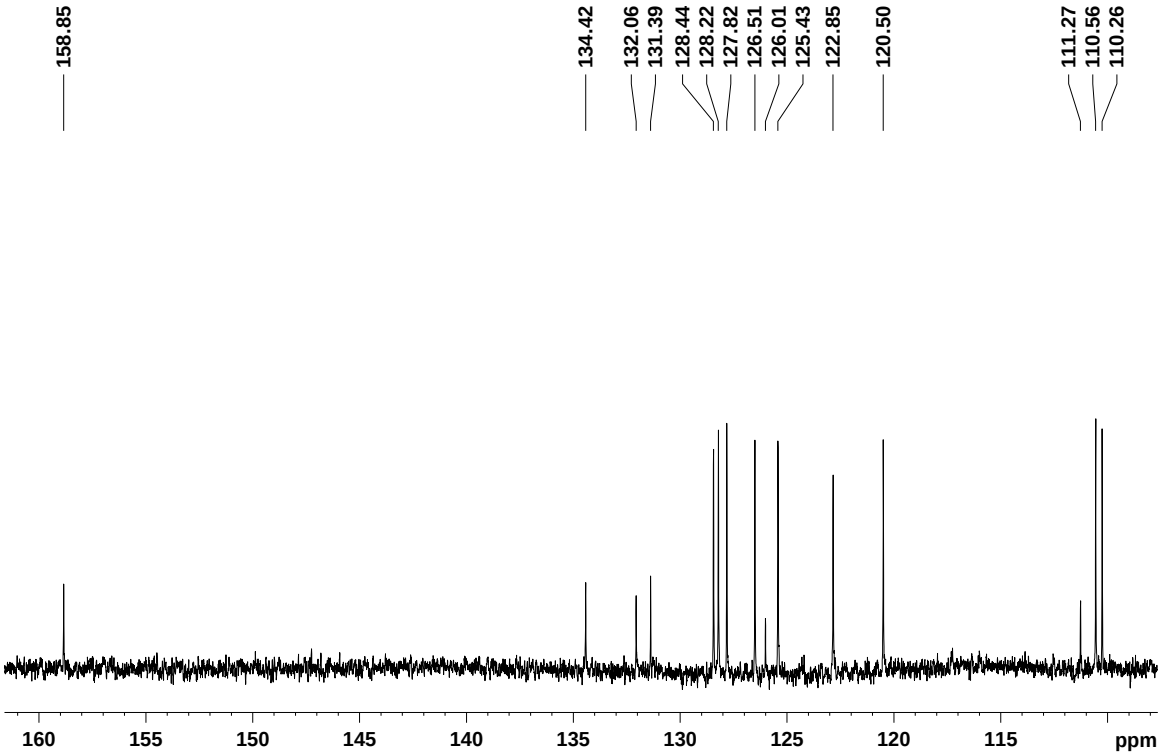
Figure S3: (a) Fluorescence quenching to **3a** and **3c** by successive additions of increasing concentrations of *t*-BuOK. **(b)** Stern-Volmer plots to **3a** and **3c** (static quenching).

^{1}H NMR *N*-(2-bromophenyl)-1*H*-indole-2-carboxamide ($CDCl_3$) **1a**

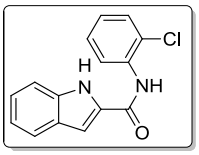


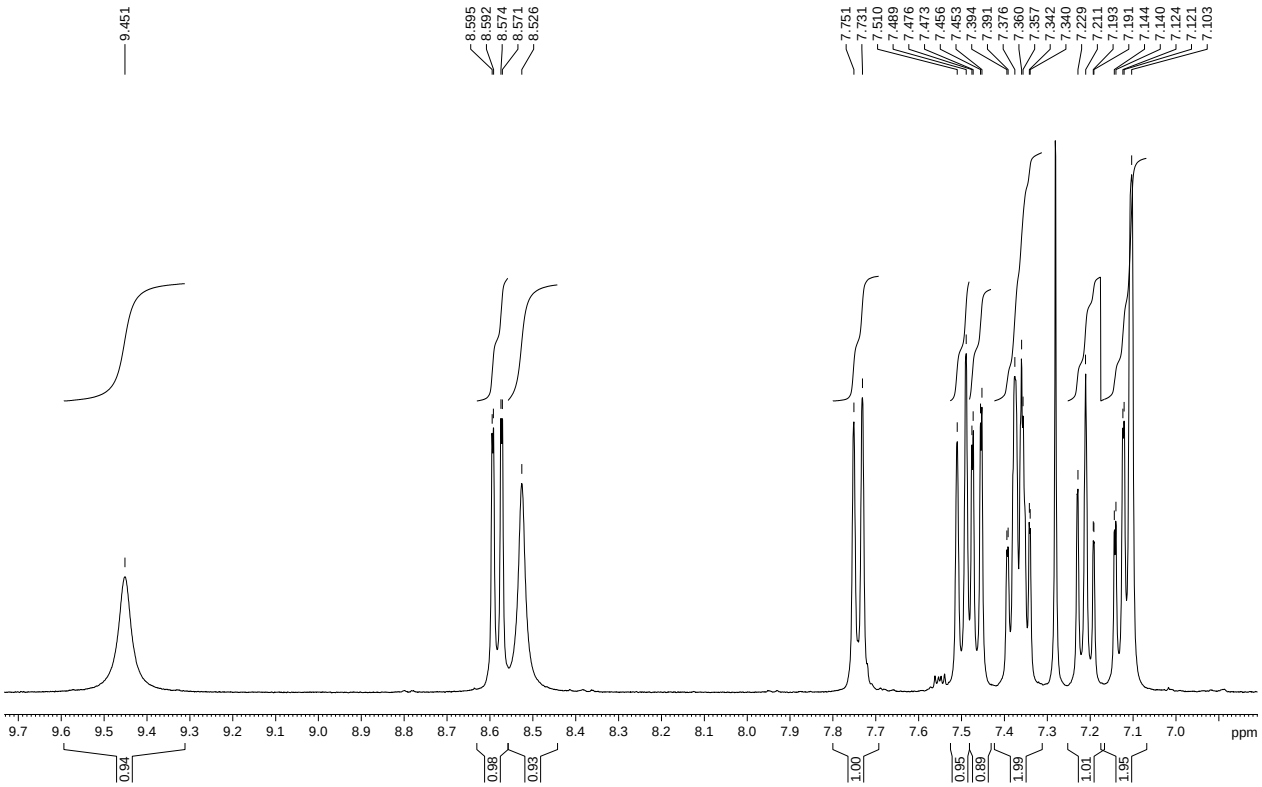


^{13}C NMR *N*-(2-bromophenyl)-1*H*-indole-2-carboxamide ($CDCl_3$) **1a**

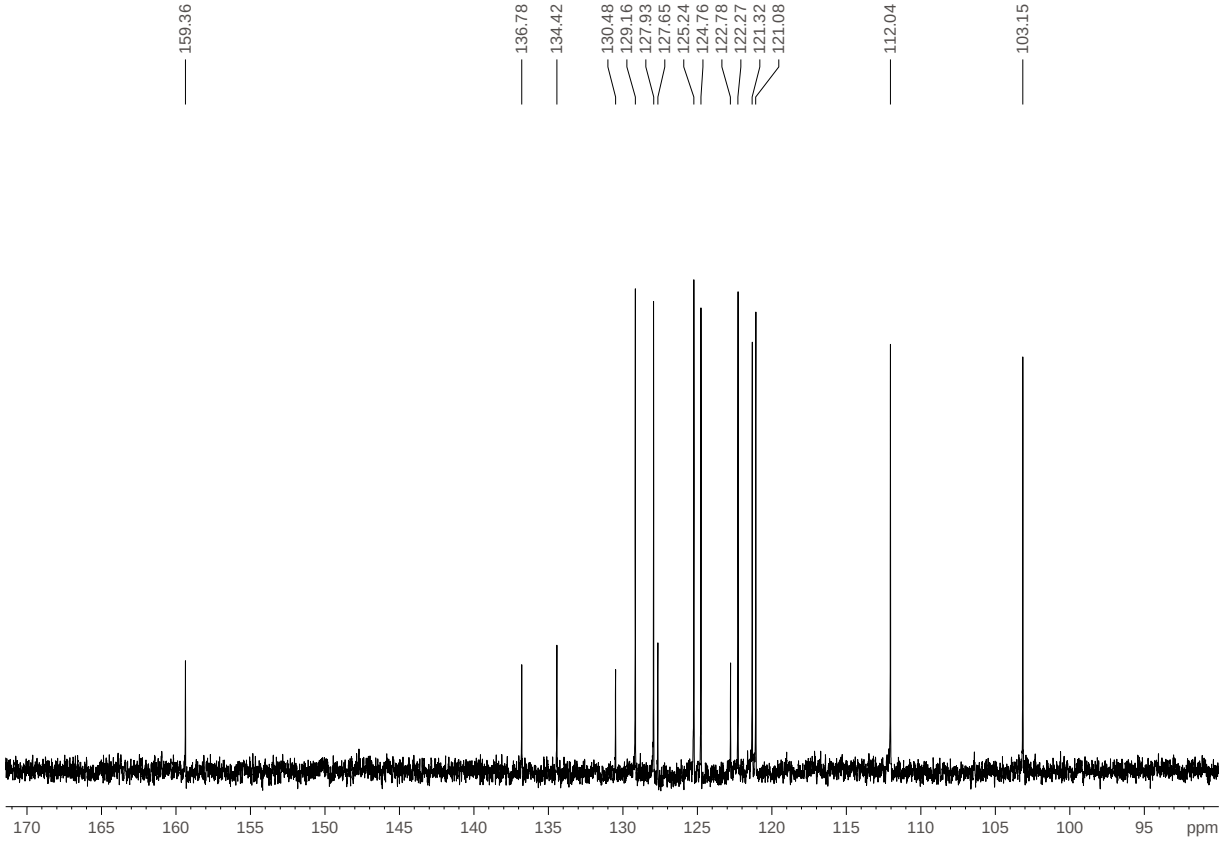


^{1}H NMR *N*-(2-chlorophenyl)-1*H*-indole-2-carboxamide ($CDCl_3$) **1b.**

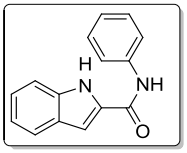


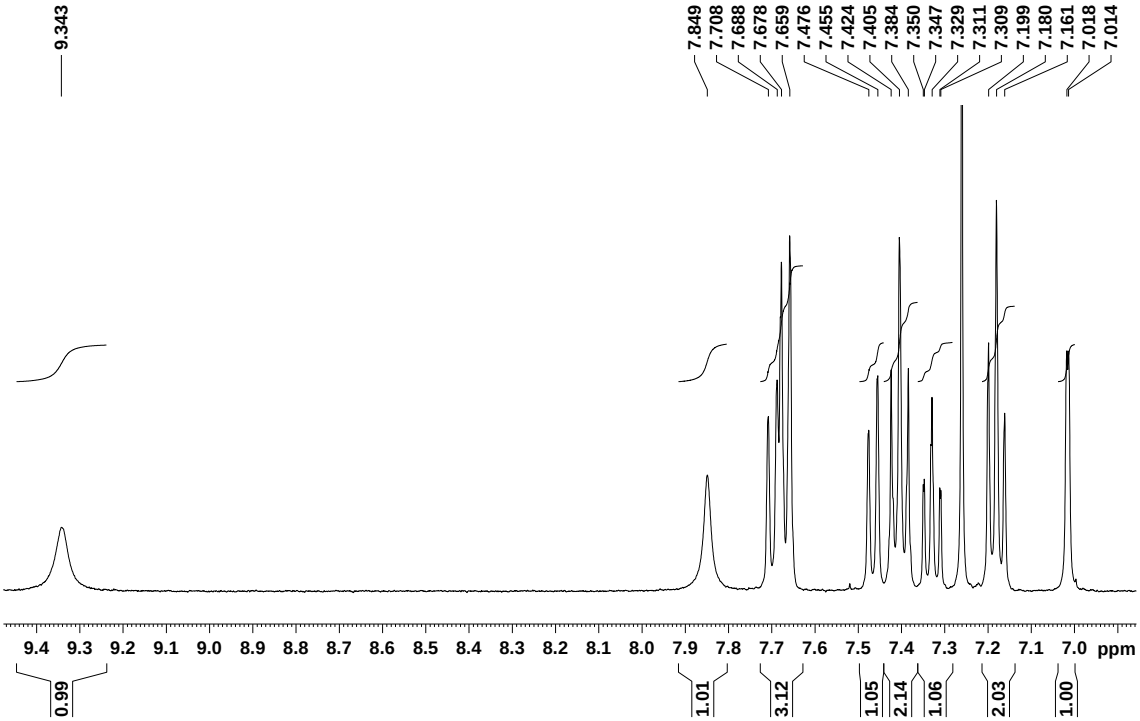


^{13}C NMR *N*-(2-chlorophenyl)-1*H*-indole-2-carboxamide ($CDCl_3$) **1b.**

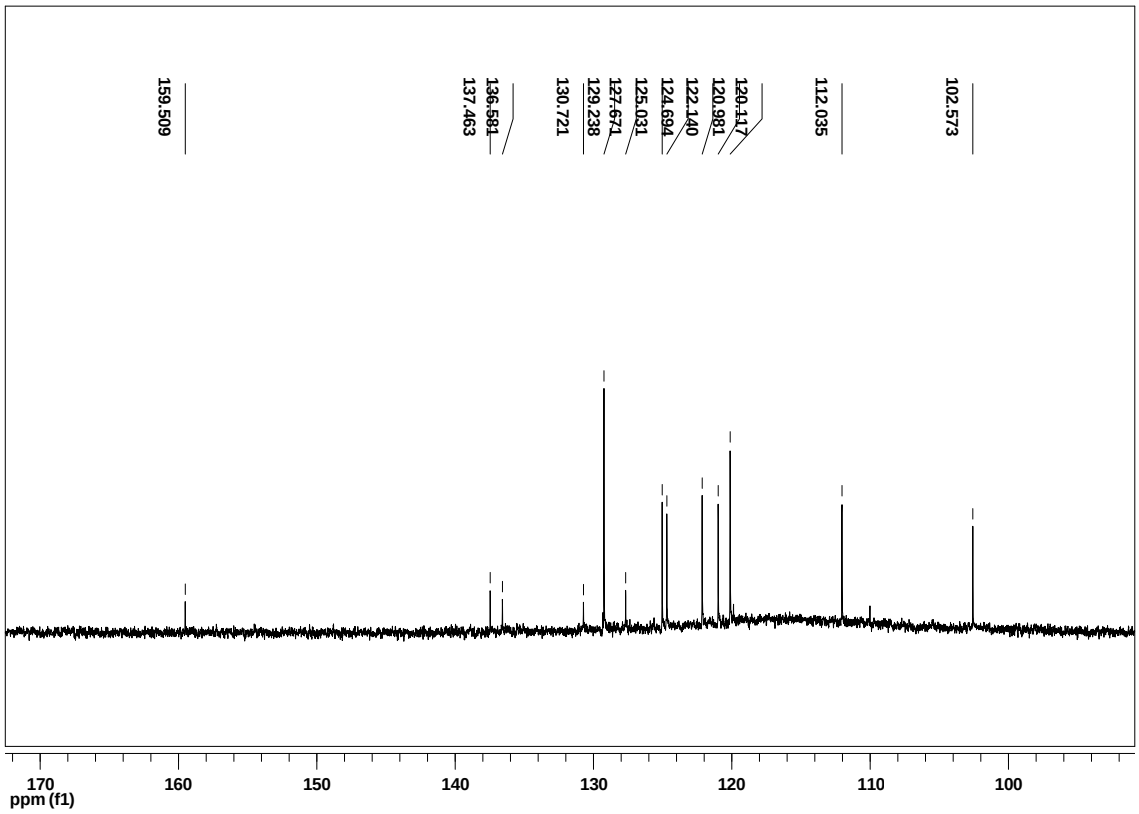


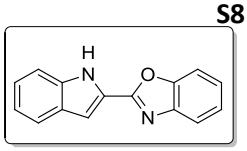
^{1}H NMR *N*-phenyl-1H-indole-2-carboxamide ($CDCl_3$) **1c.**



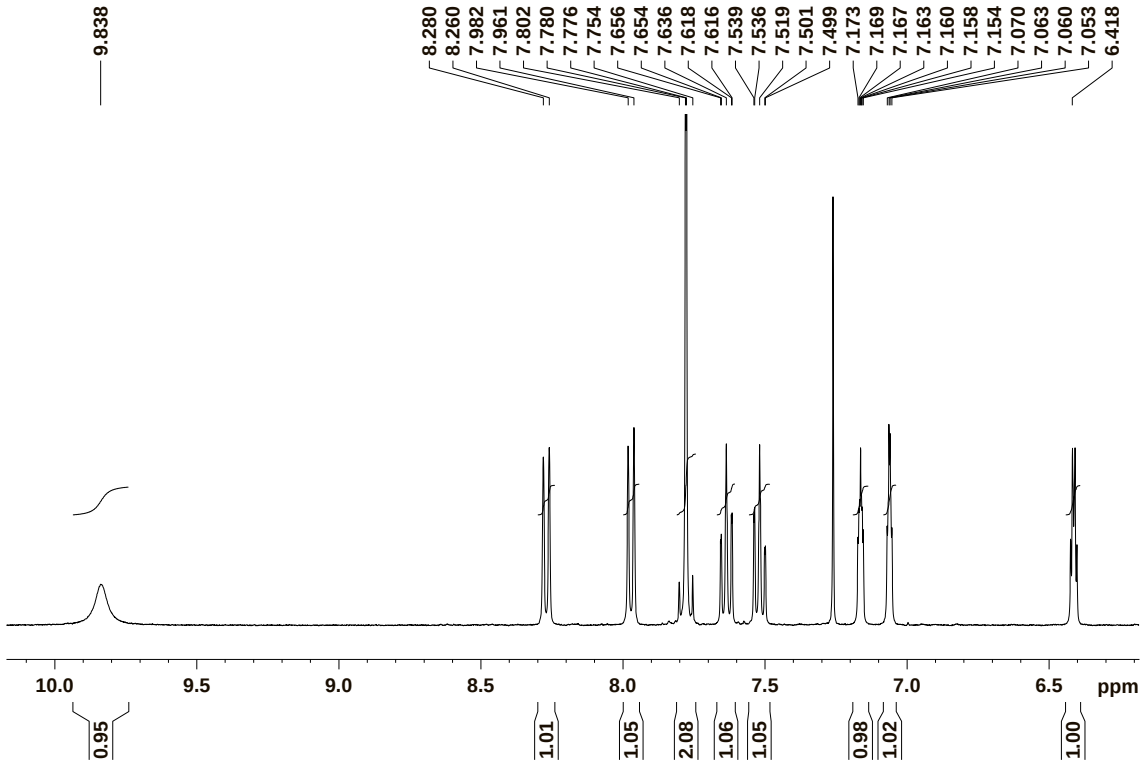


^{13}C NMR *N*-phenyl-1H-indole-2-carboxamide ($CDCl_3$) **1c.**





^{1}H NMR 2-(1*H*-indol-2-yl)benzo[*d*]oxazole ($CDCl_3$) **2**.



^{13}C NMR 2-(1*H*-indol-2-yl)benzo[*d*]oxazole ($CDCl_3$) **2**.