

Supporting Information

Palladium-catalyzed three-component cascade arylthiolation with aryldiazonium salts as S-arylation sources

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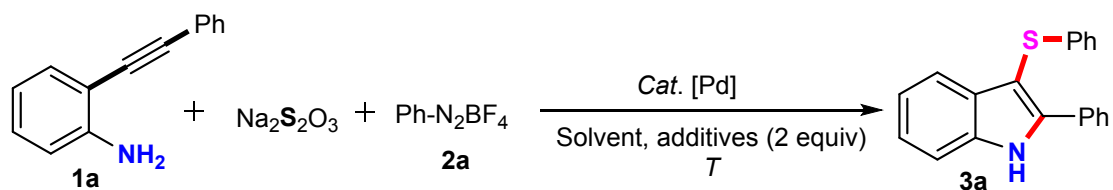
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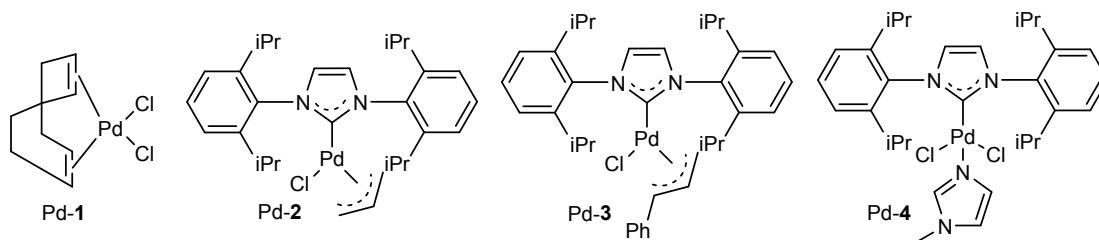
Optimization of the reaction conditions ^a



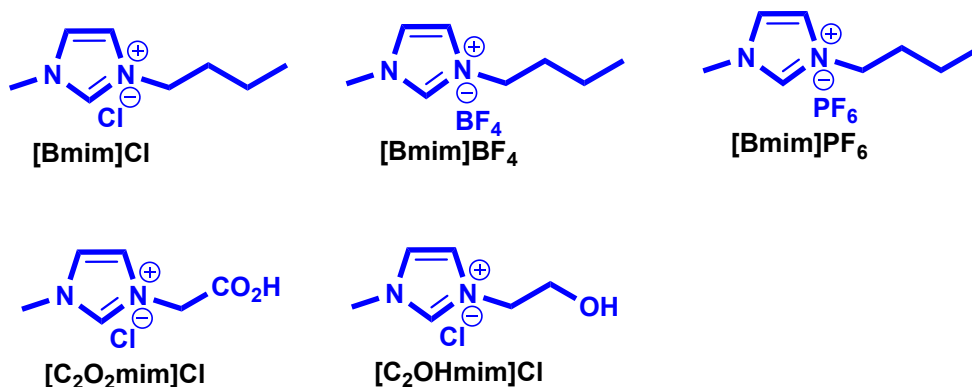
Entry	Catalyst	Additives	Solvent	Yield/ % ^b
1	$\text{Pd}(\text{OAc})_2$	nBu_4NBr	DMF	N.D.
2	$\text{Pd}(\text{TFA})_2$	nBu_4NBr	DMF	trace
3	PdCl_2	nBu_4NBr	DMF	trace
4	$\text{Pd}(\text{PhCN})_2\text{Cl}_2$	nBu_4NBr	DMF	11
5	$[\text{Pd}(\eta^3\text{-C}_3\text{H}_5)\text{Cl}]_2$	nBu_4NBr	DMF	34
6	Pd-1	nBu_4NBr	DMF	28
7	Pd-2	nBu_4NBr	DMF	45
8	Pd-3	nBu_4NBr	DMF	57
9	Pd-4	nBu_4NBr	DMF	35
10	Pd-3	nBu_4NI	DMF	40
11	Pd-3	nBu_4NCl	DMF	43
12	Pd-3	$[\text{Bmim}]\text{Cl}$	DMF	50
13	Pd-3	$[\text{Bmim}]\text{BF}_4$	DMF	trace
14	Pd-3	$[\text{Bmim}]\text{PF}_6$	DMF	trace
15	Pd-3	$[\text{C}_2\text{OHmim}]\text{Cl}$	DMF	68
16	Pd-3	$[\text{C}_2\text{O}_2\text{mim}]\text{Cl}$	DMF	49
17	Pd-3	$[\text{C}_2\text{OHmim}]\text{Cl}$	DMSO	70
18	Pd-3	$[\text{C}_2\text{OHmim}]\text{Cl}$	Toluene	26
19	Pd-3	$[\text{C}_2\text{OHmim}]\text{Cl}$	PEG-200	89 (82)
20	Pd-3	$[\text{C}_2\text{OHmim}]\text{Cl}$	PEG-400	74
21 ^c	Pd-3	$[\text{C}_2\text{OHmim}]\text{Cl}$	PEG-200	67
22 ^d	Pd-3	$[\text{C}_2\text{OHmim}]\text{Cl}$	PEG-200	89

23 ^e	Pd-3	[C ₂ OHmim]Cl	PEG-200	89
24	-	[C ₂ OHmim]Cl	PEG-200	0

^a Reactions were performed with **1a** (0.10 mmol), **2a** (0.12 mmol), Na₂S₂O₃ (0.20 mmol), catalyst (2 mol %), additives (0.20 mmol), solvent (1 mL) at 100 °C for 16 h; ^b Determined by GC using dodecane as the internal standard; The value in parentheses is the yield of isolated product; ^c At 80 °C; ^d At 110 °C. ^e 1 mol% Pd-3 was used.



The full names and structural formula of ionic liquids:



[Bmim]Cl: 1-butyl-3-methylimidazolium chloride

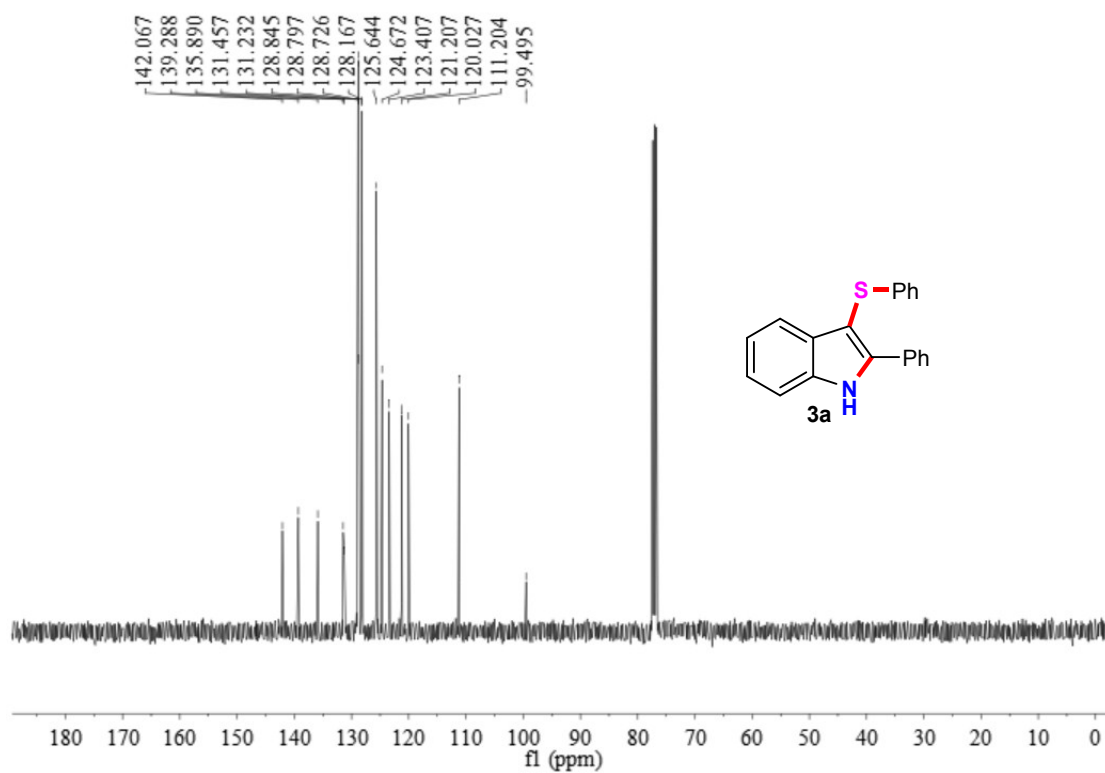
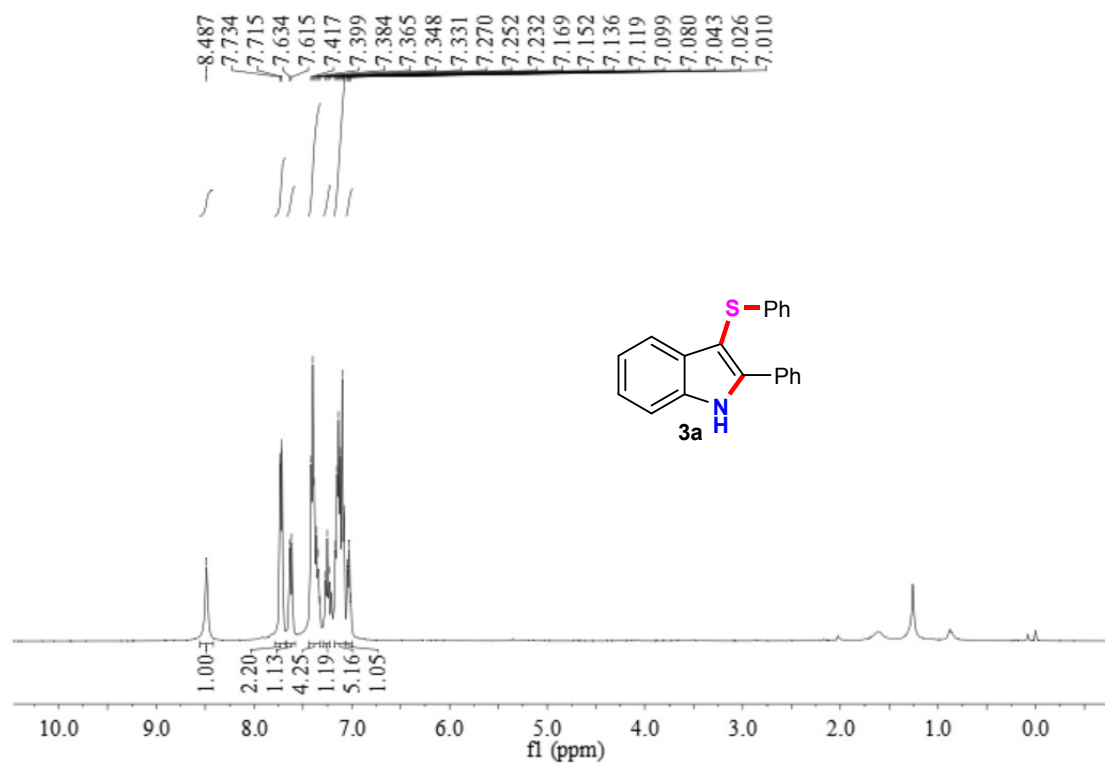
[Bmim]BF₄: 1-butyl-3-methylimidazolium tetrafluoroborate

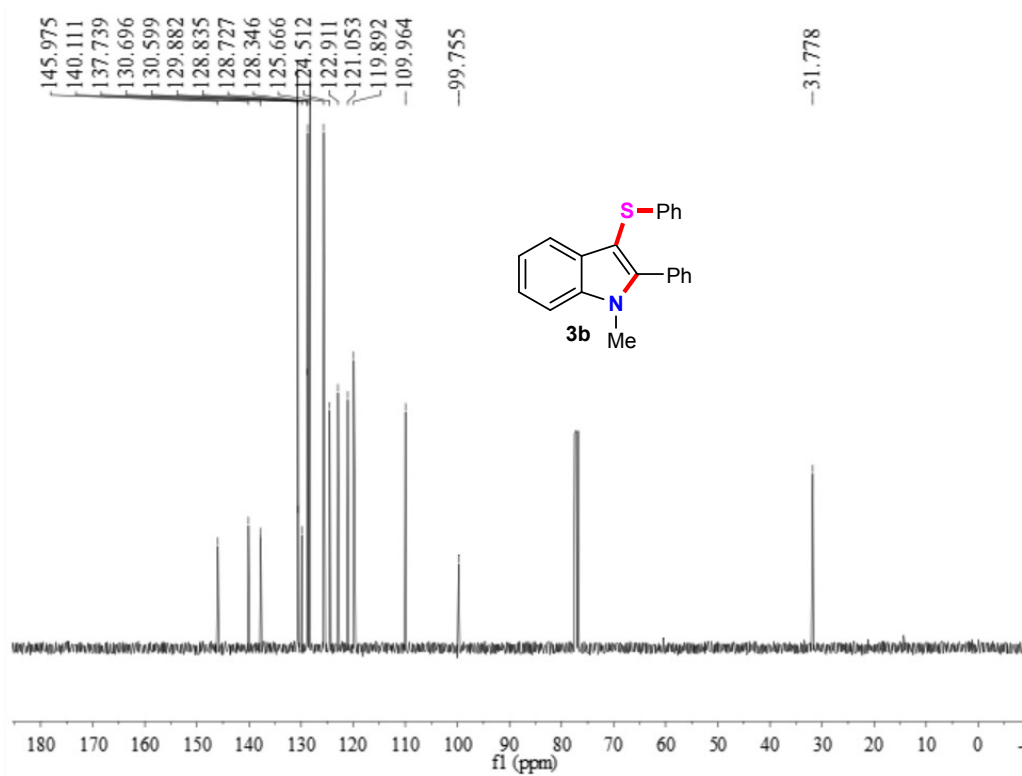
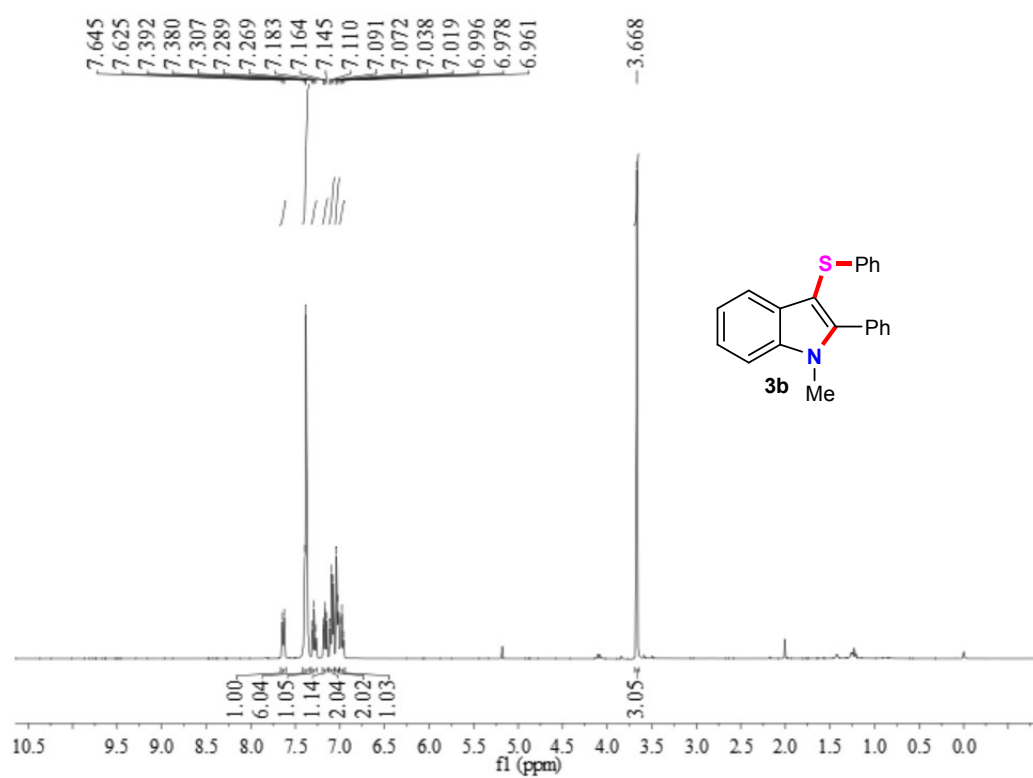
[Bmim]PF₆: 1-butyl-3-methylimidazolium hexafluorophosphate

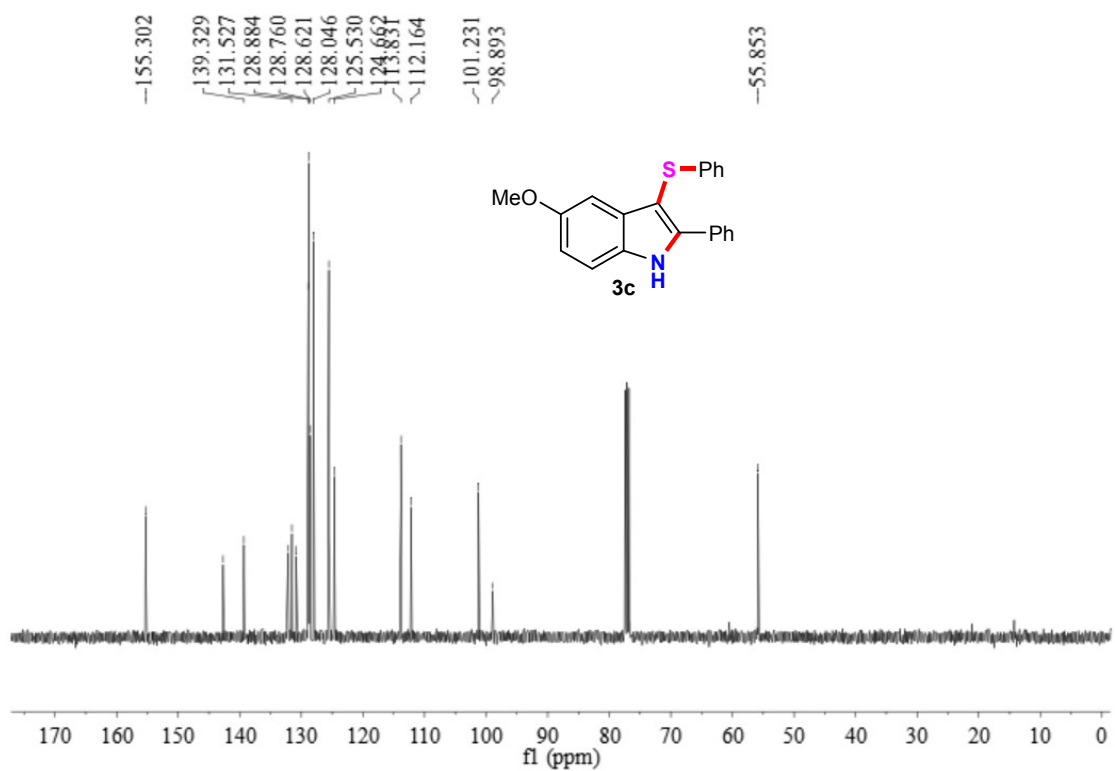
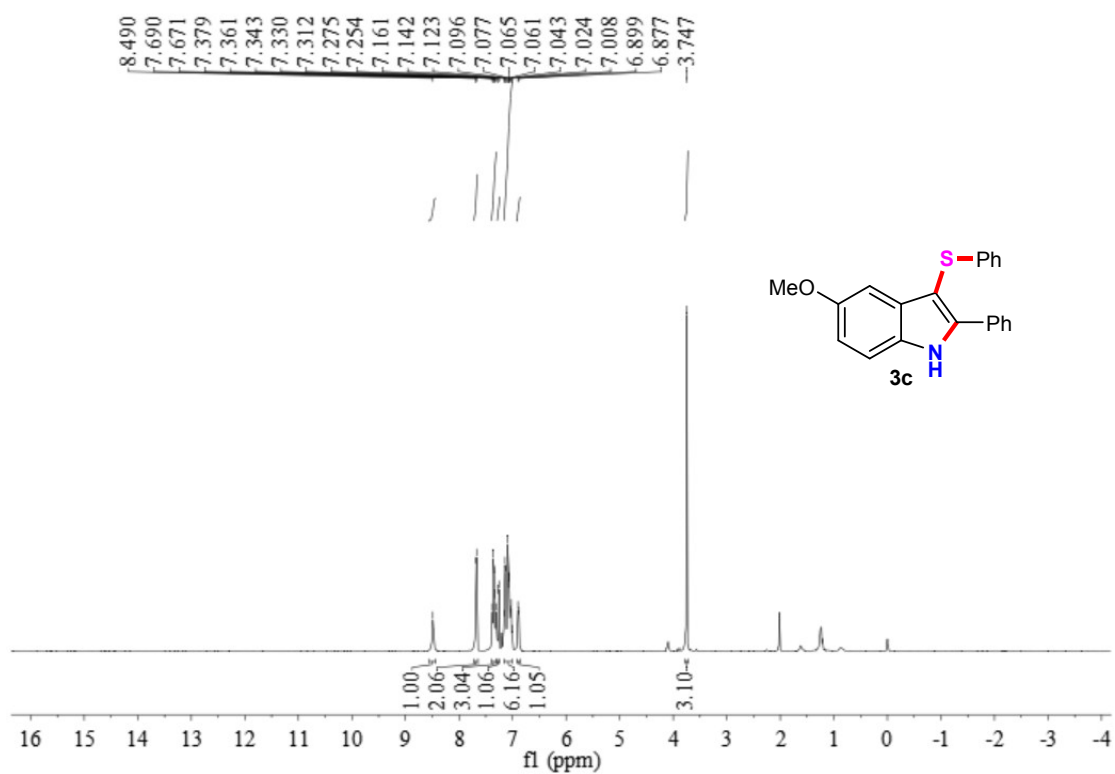
[C₂OHmim]Cl: 1-hydroxyethyl-3-methylimidazolium chloride

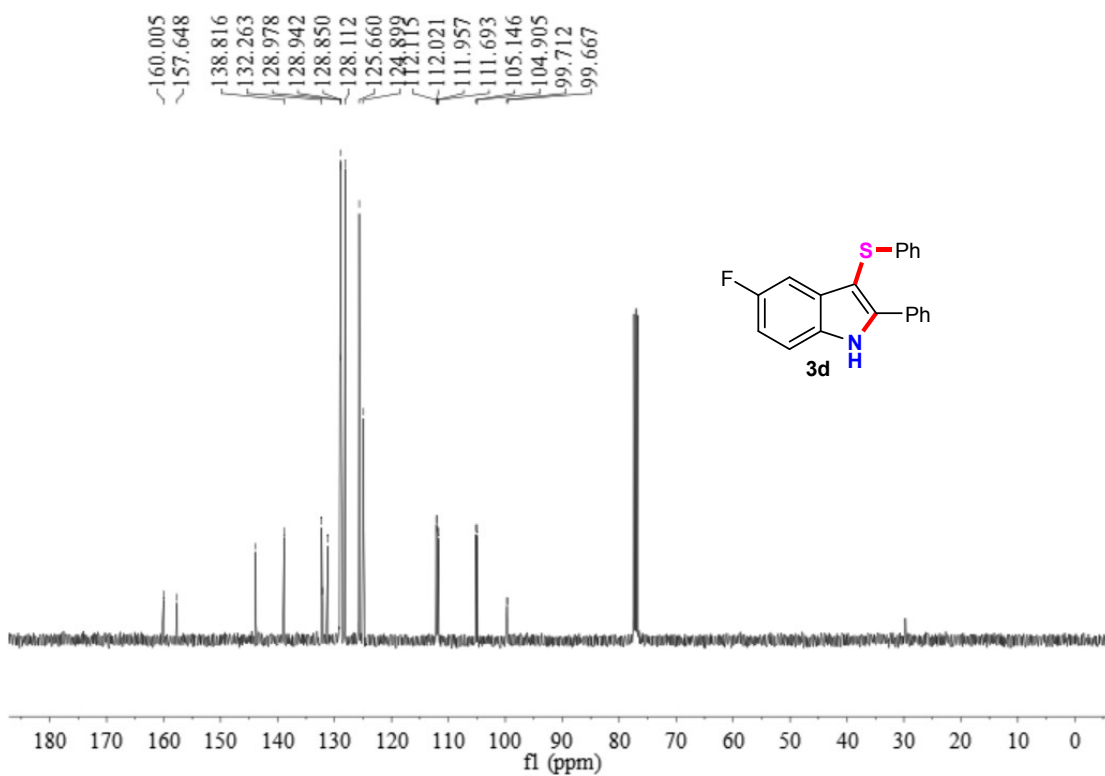
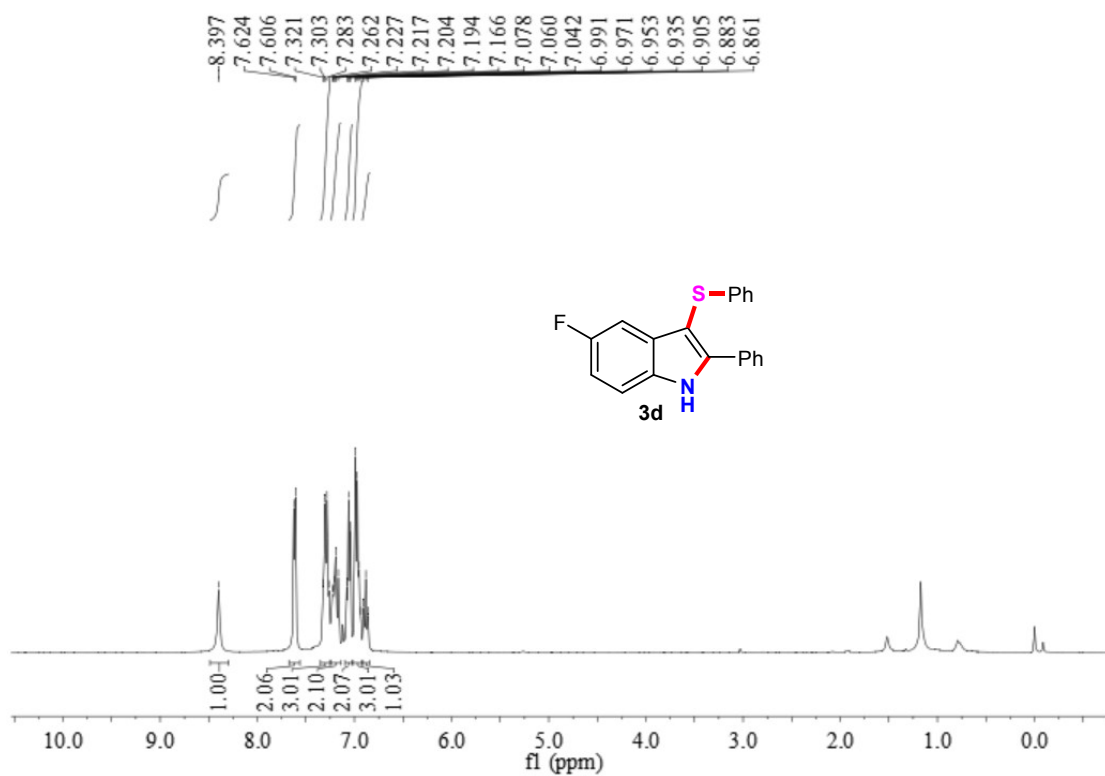
[C₂O₂mim]Cl: 1-carboxymethyl-3-methylimidazolium chloride

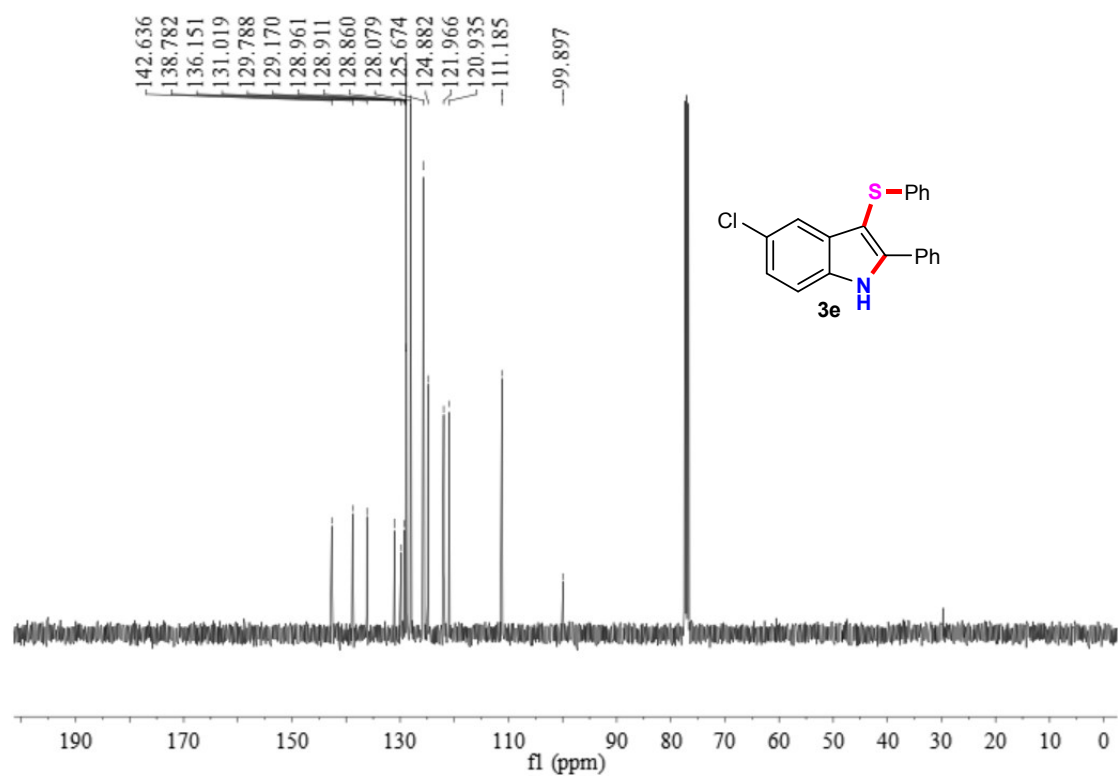
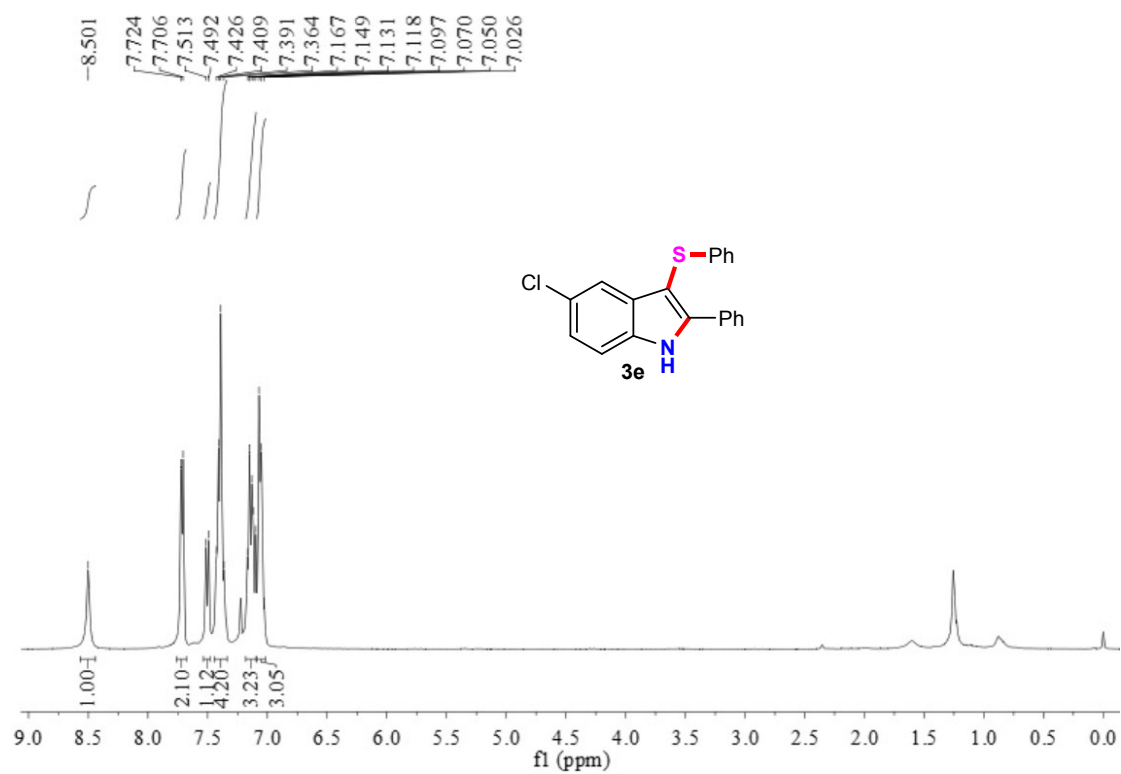
¹H and ¹³C NMR spectra of compounds 3

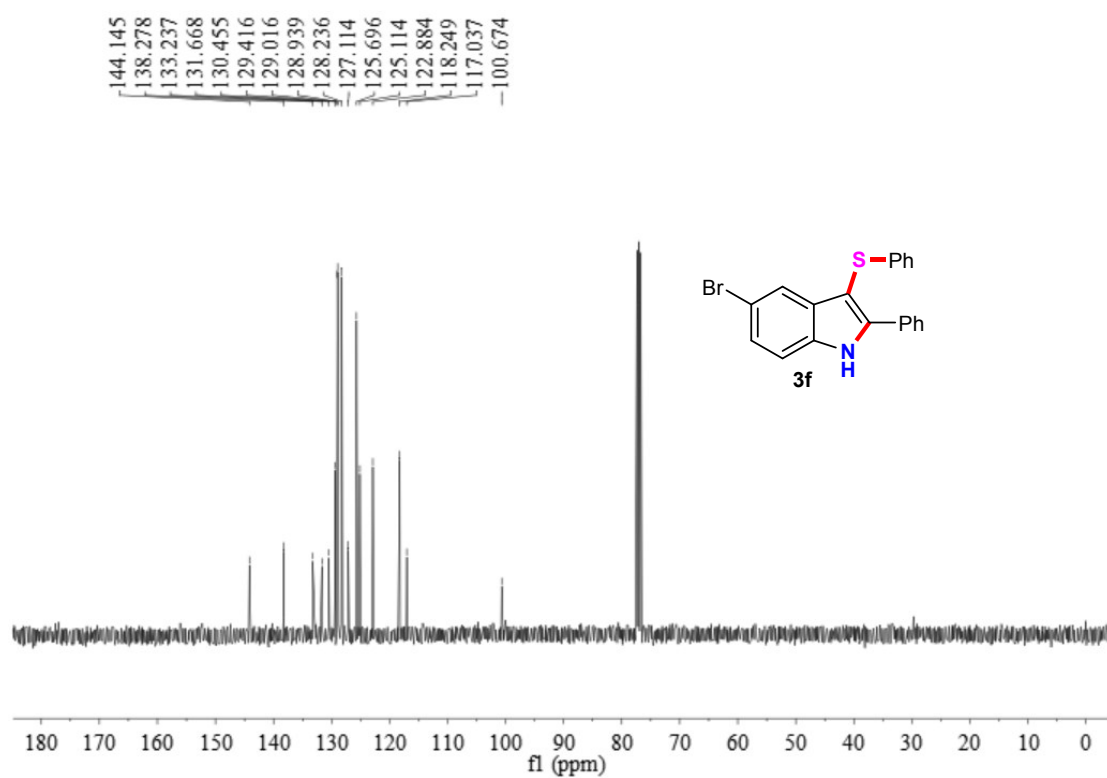
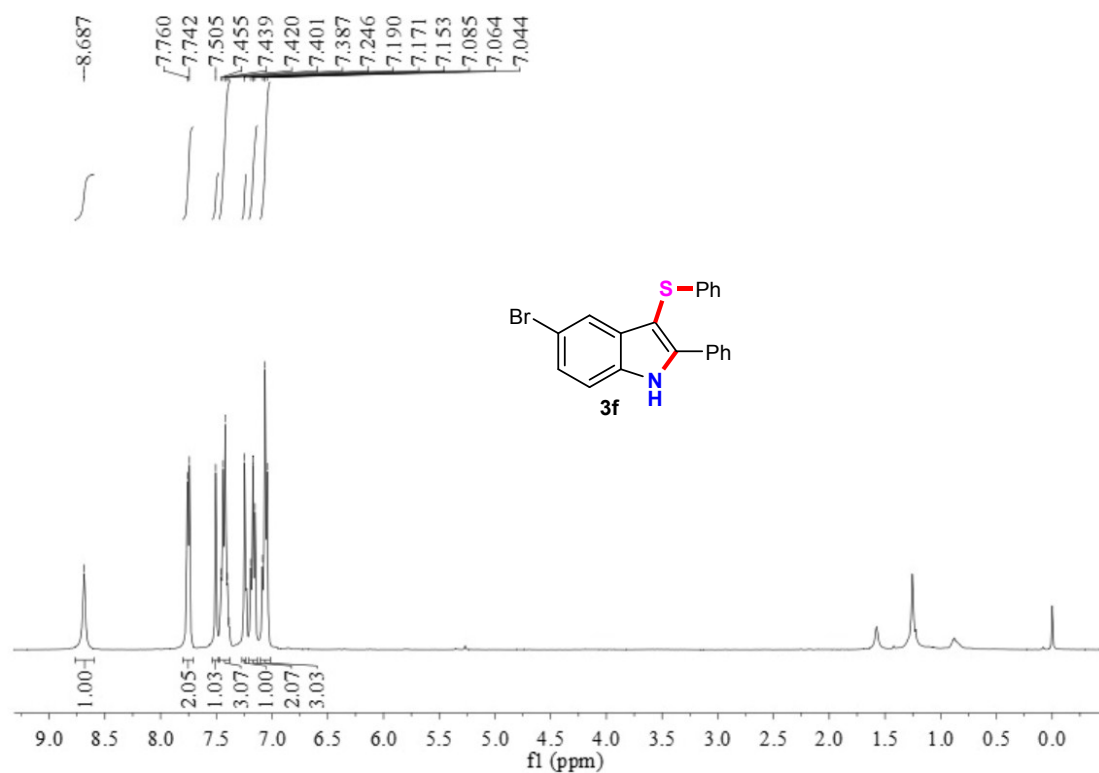


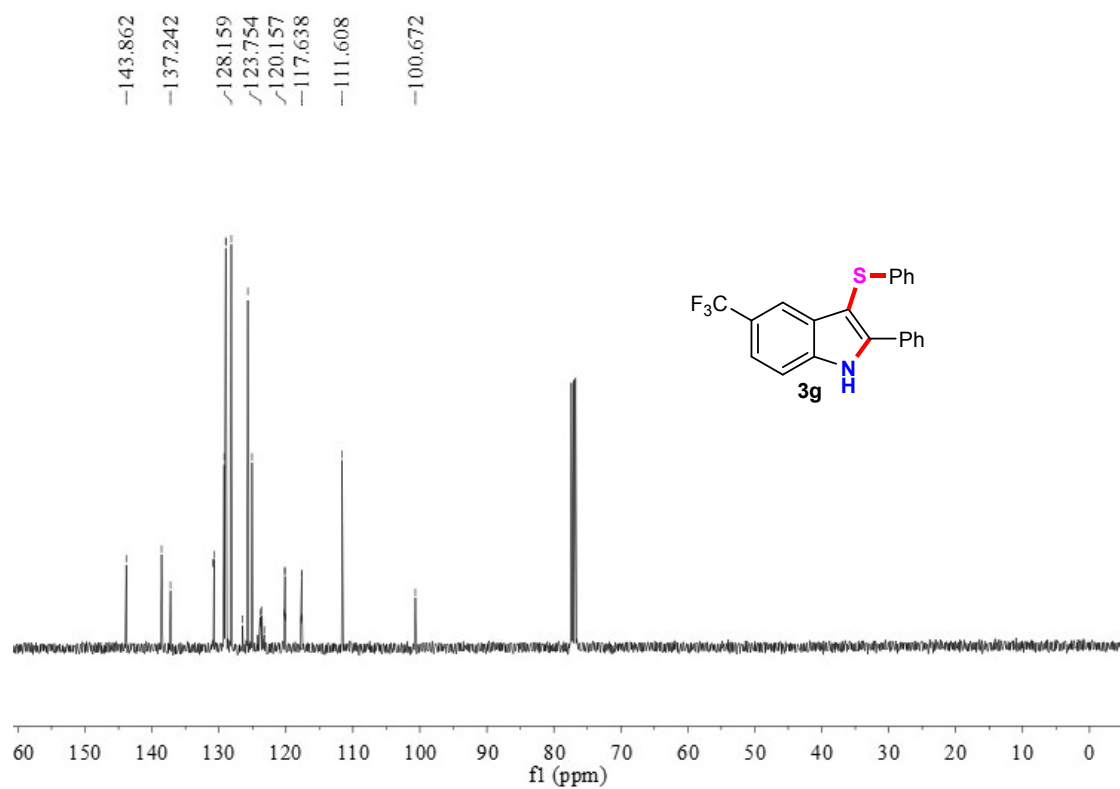
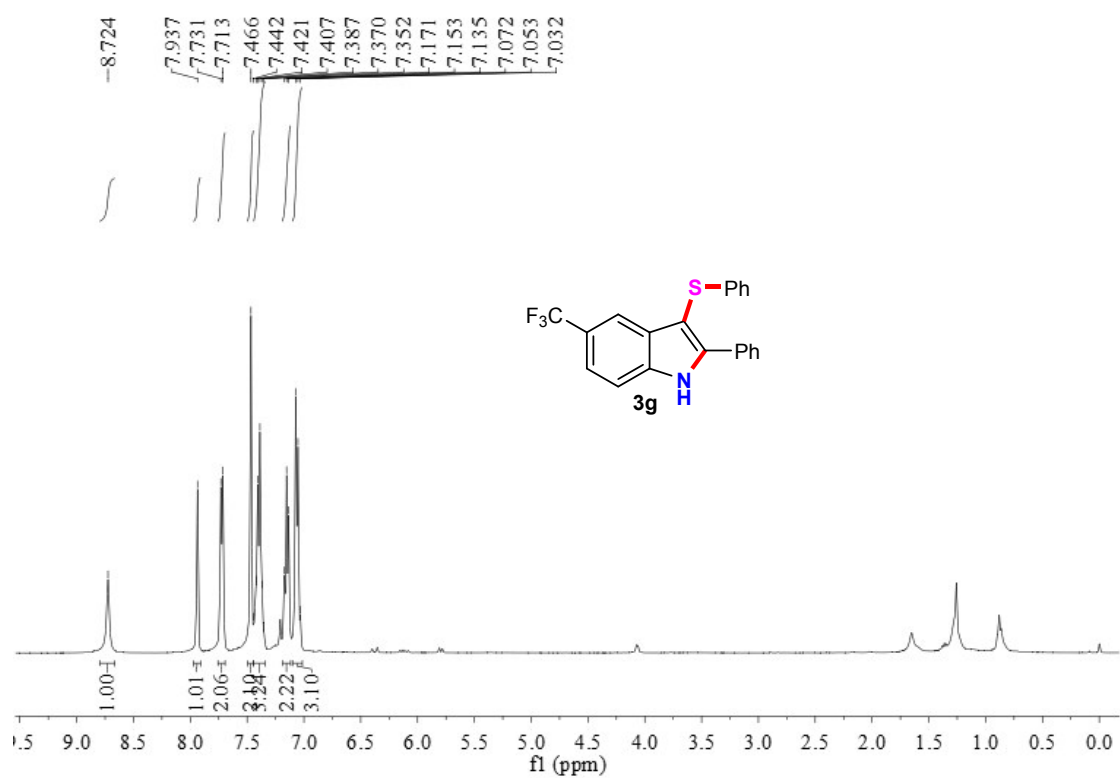


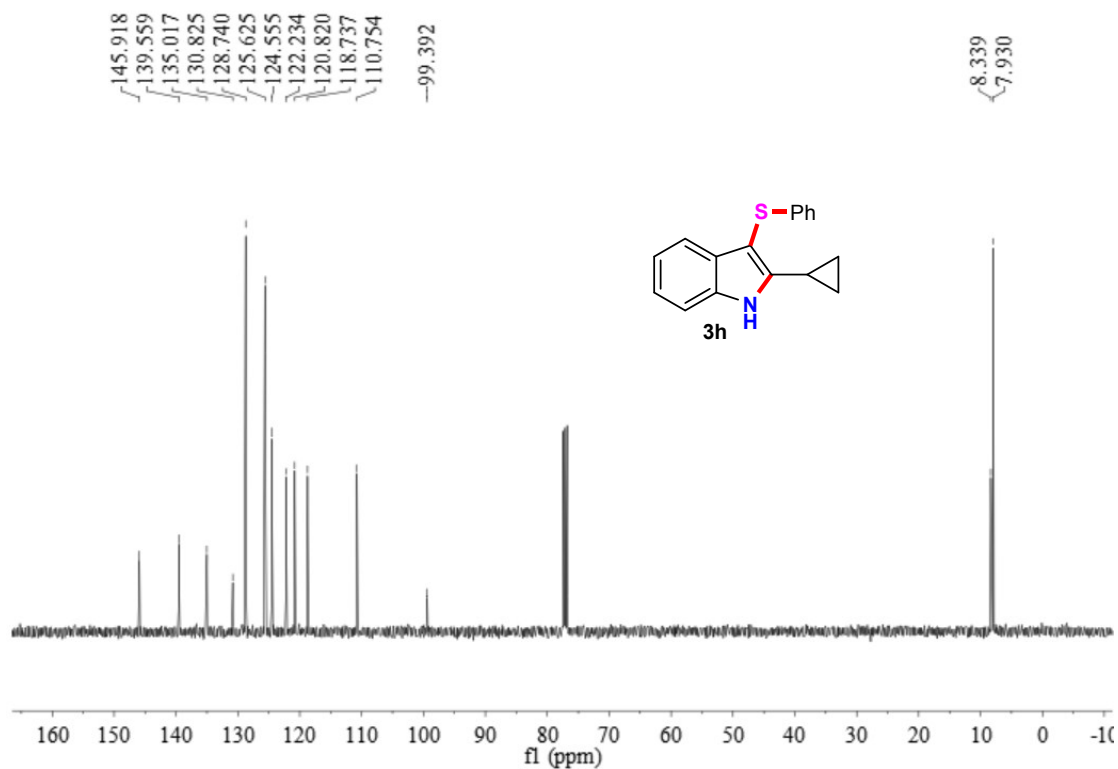
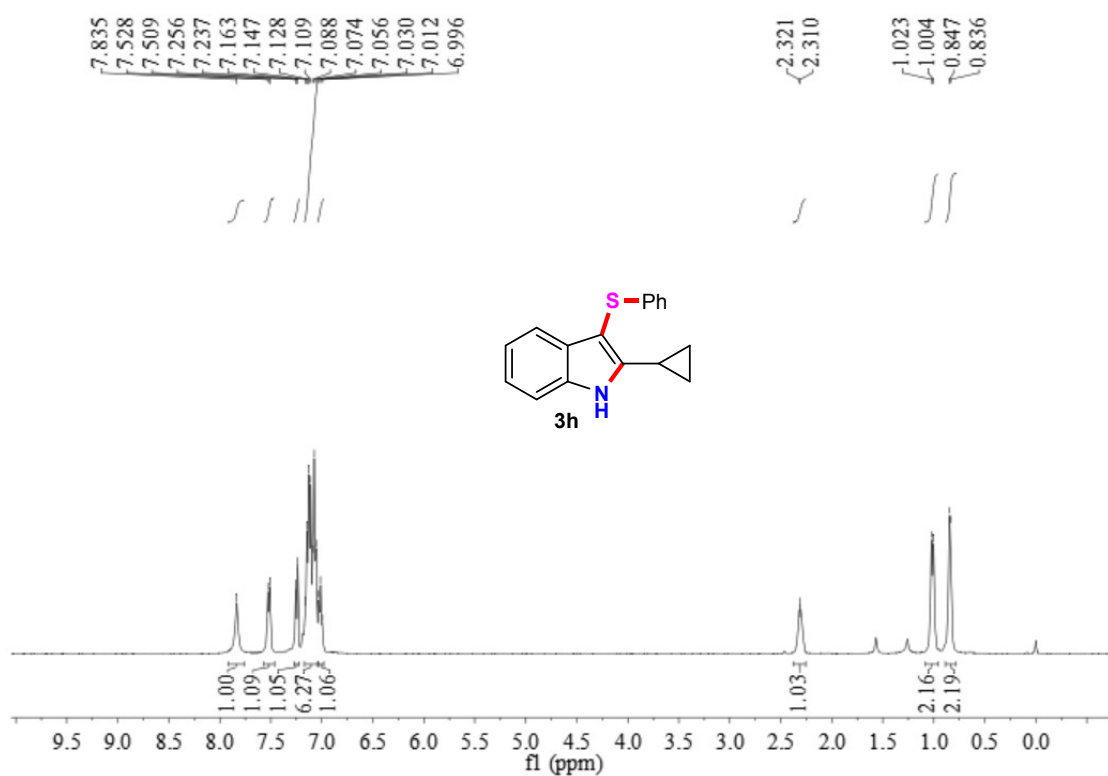


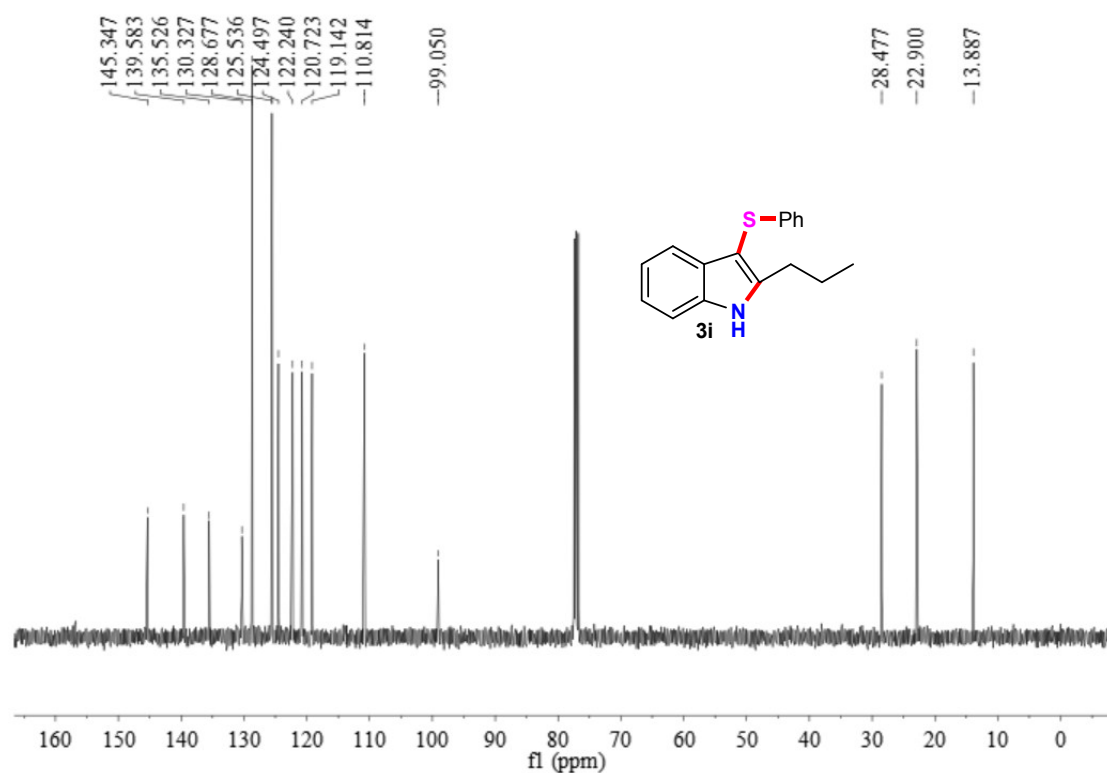
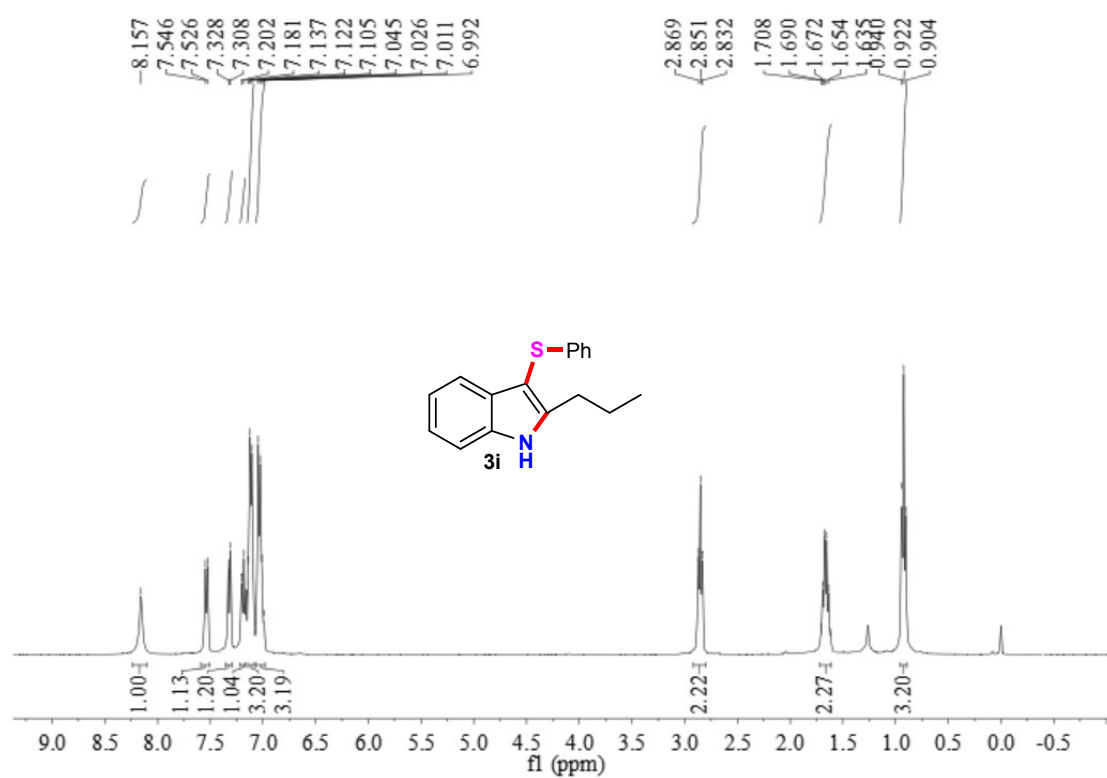


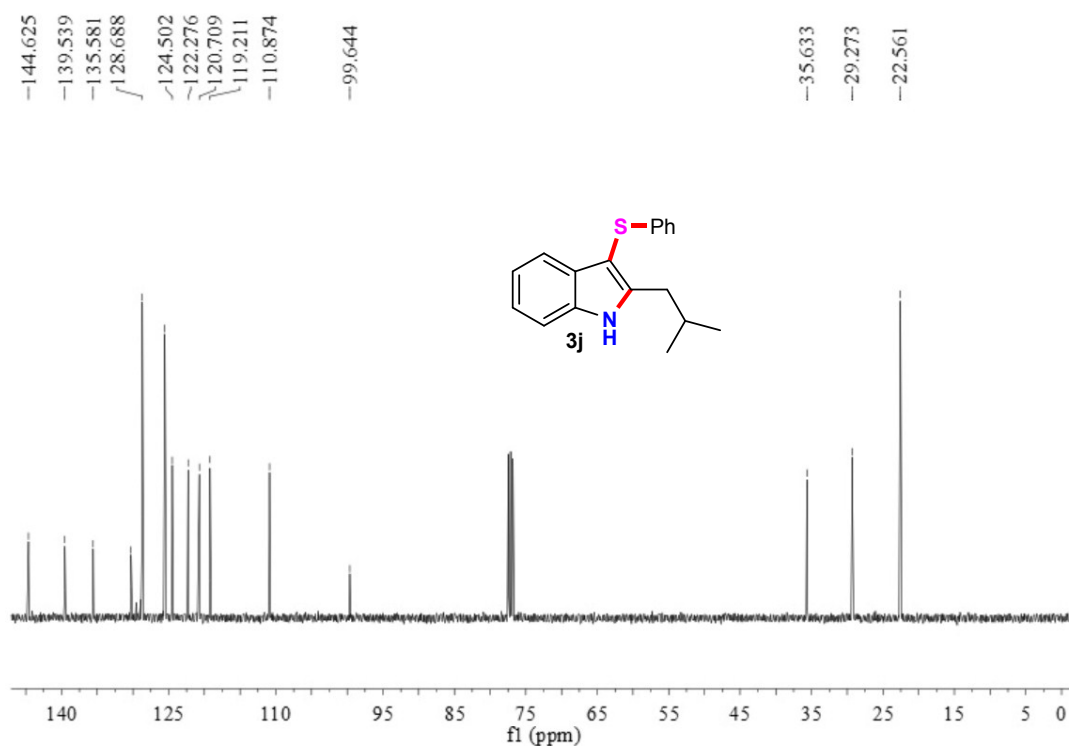
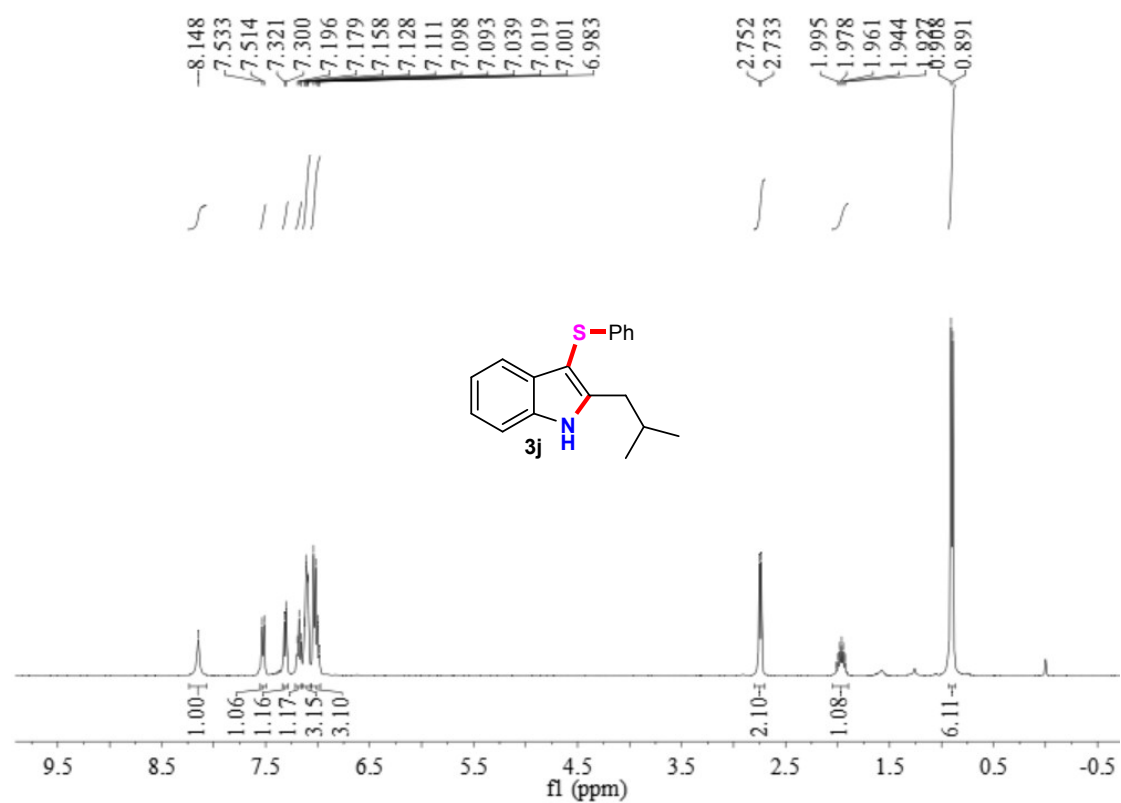


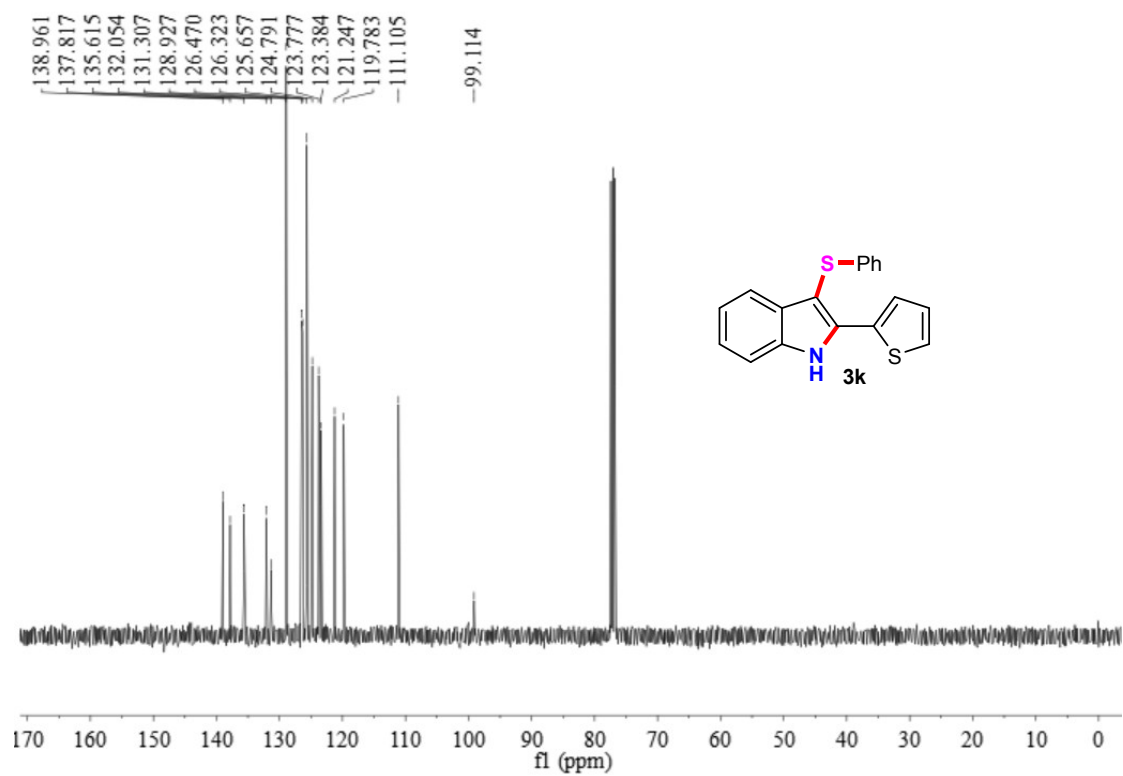
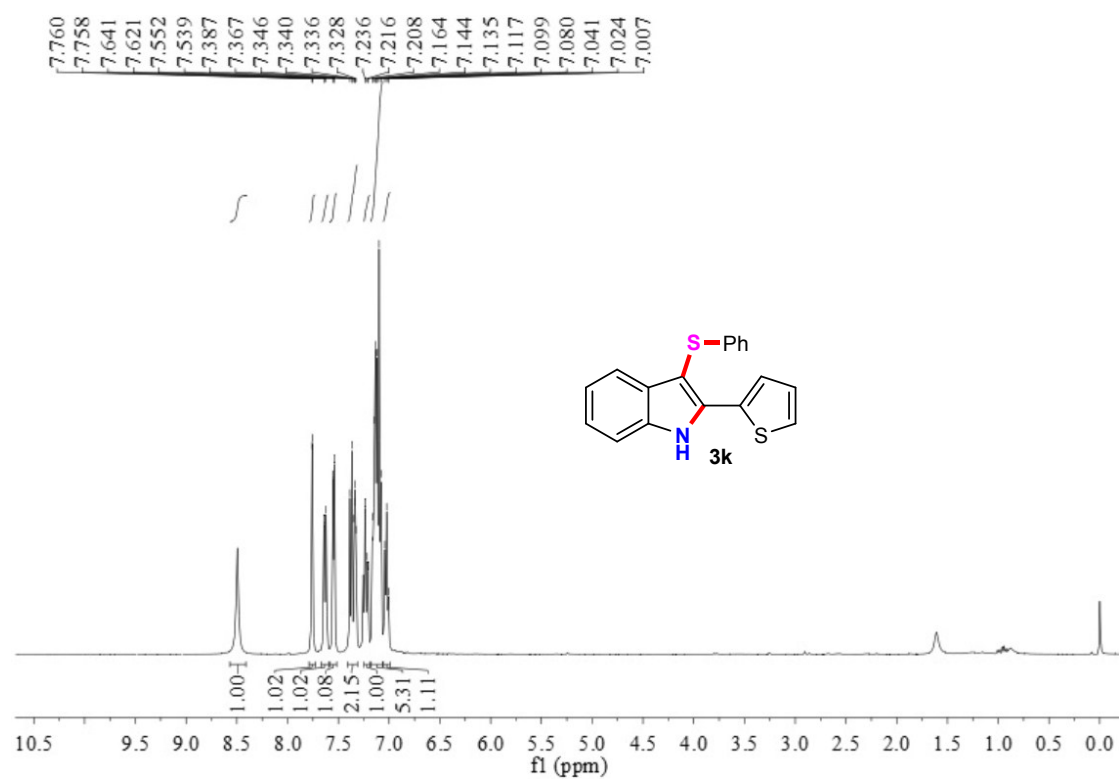


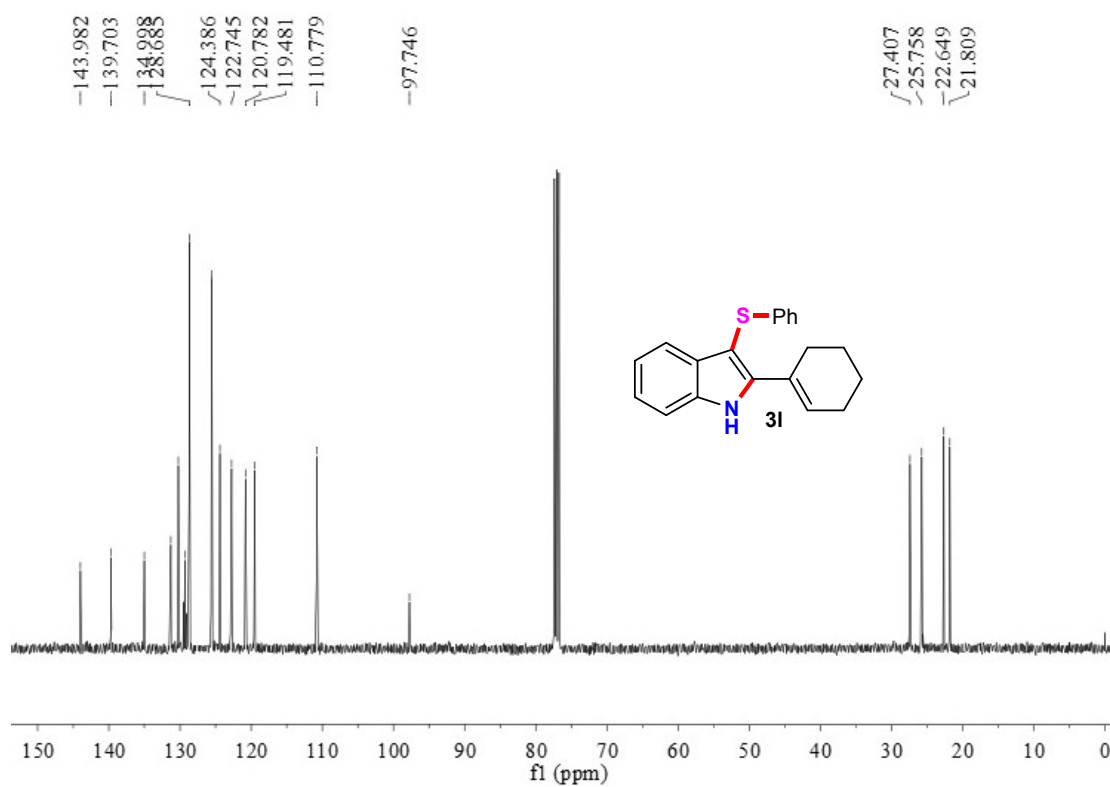
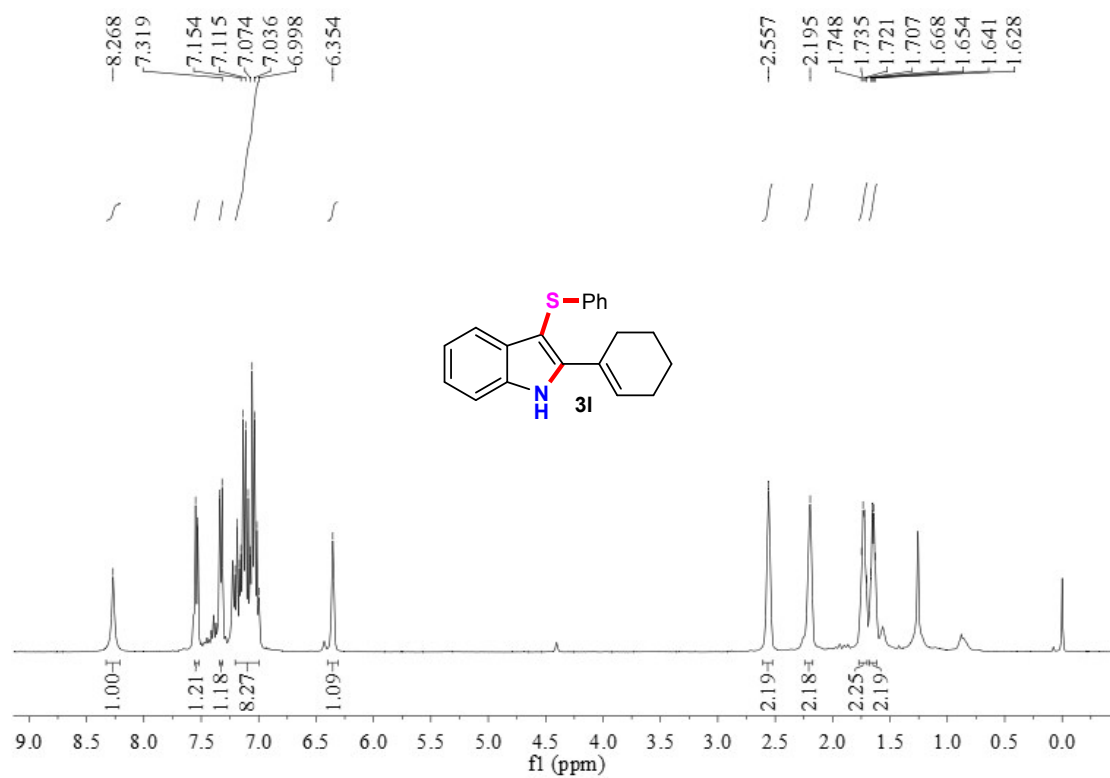


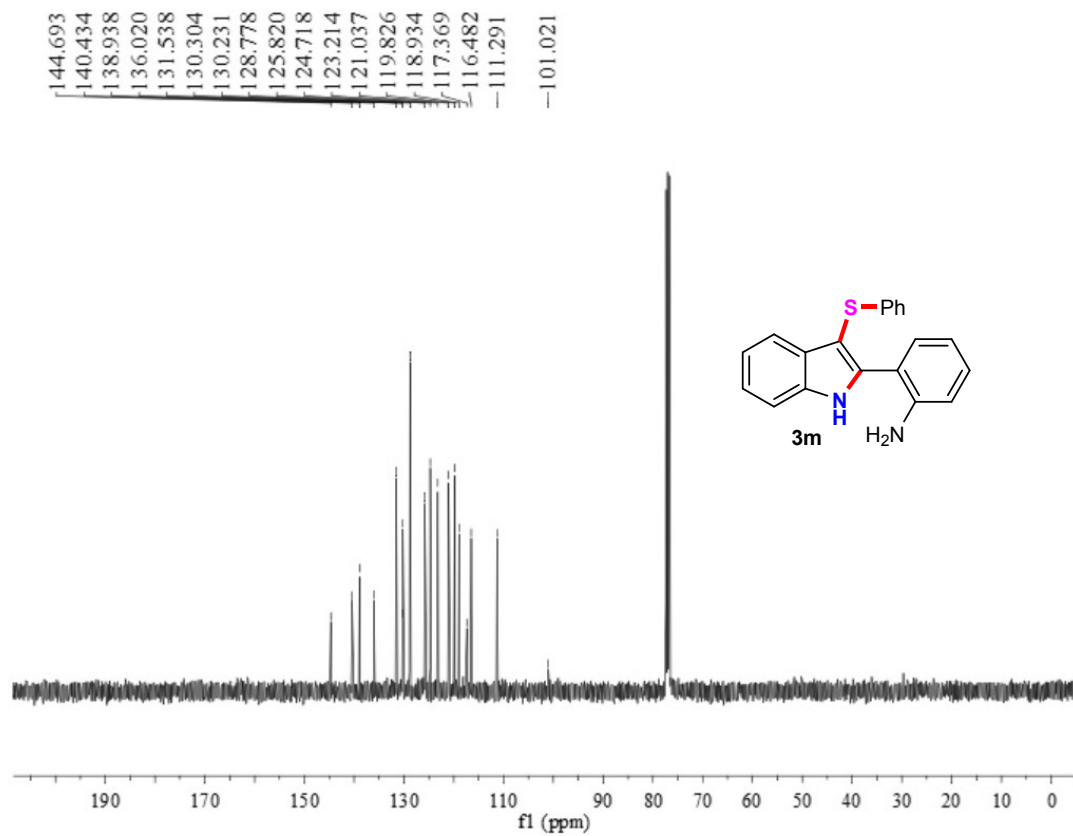
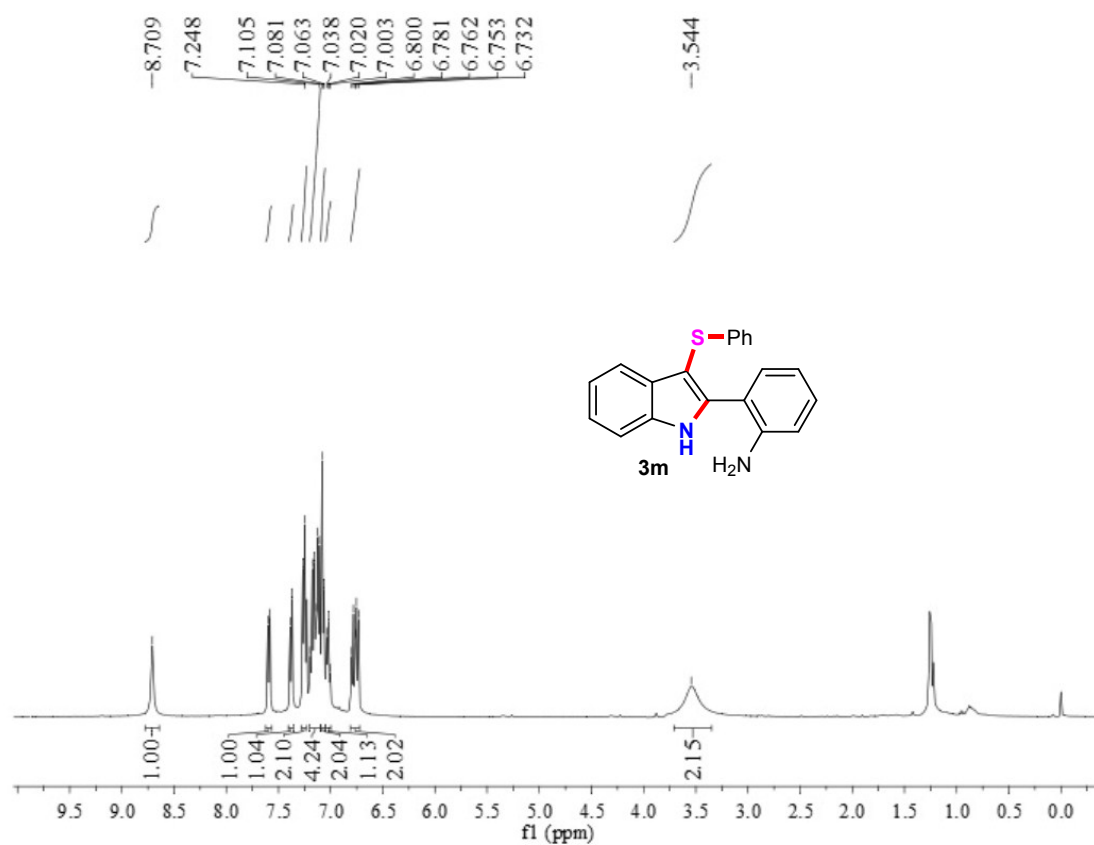


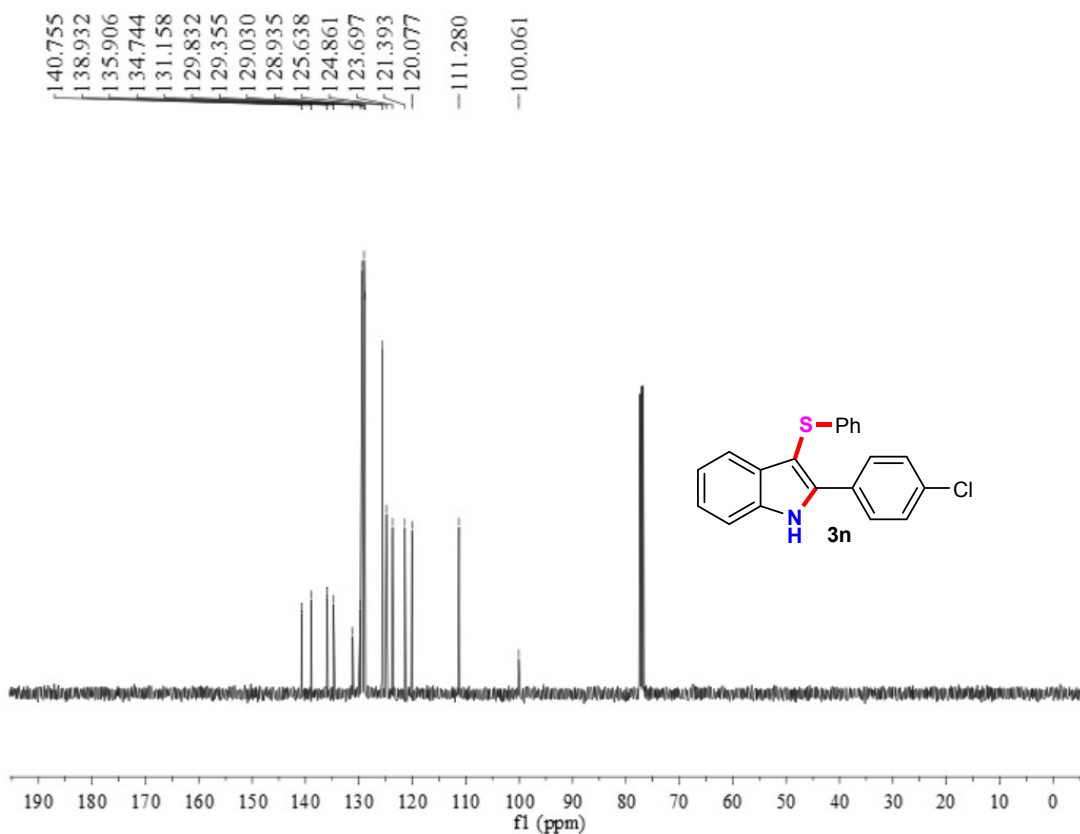
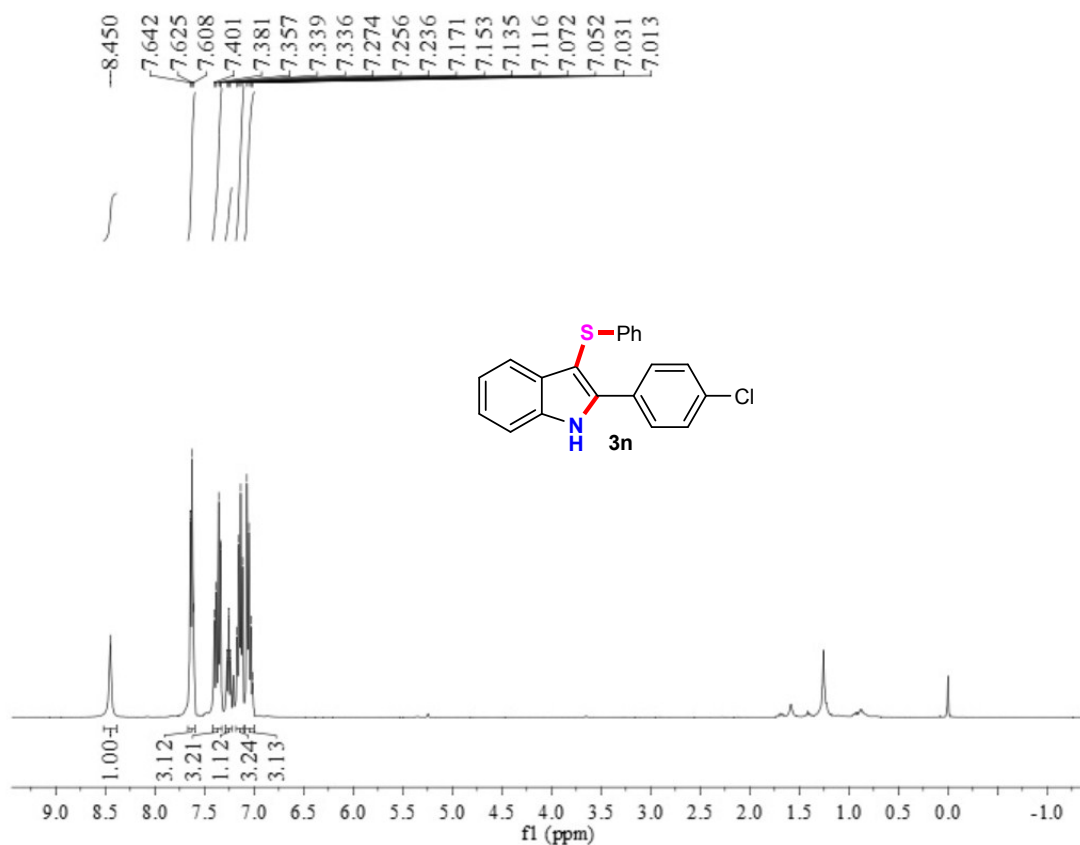


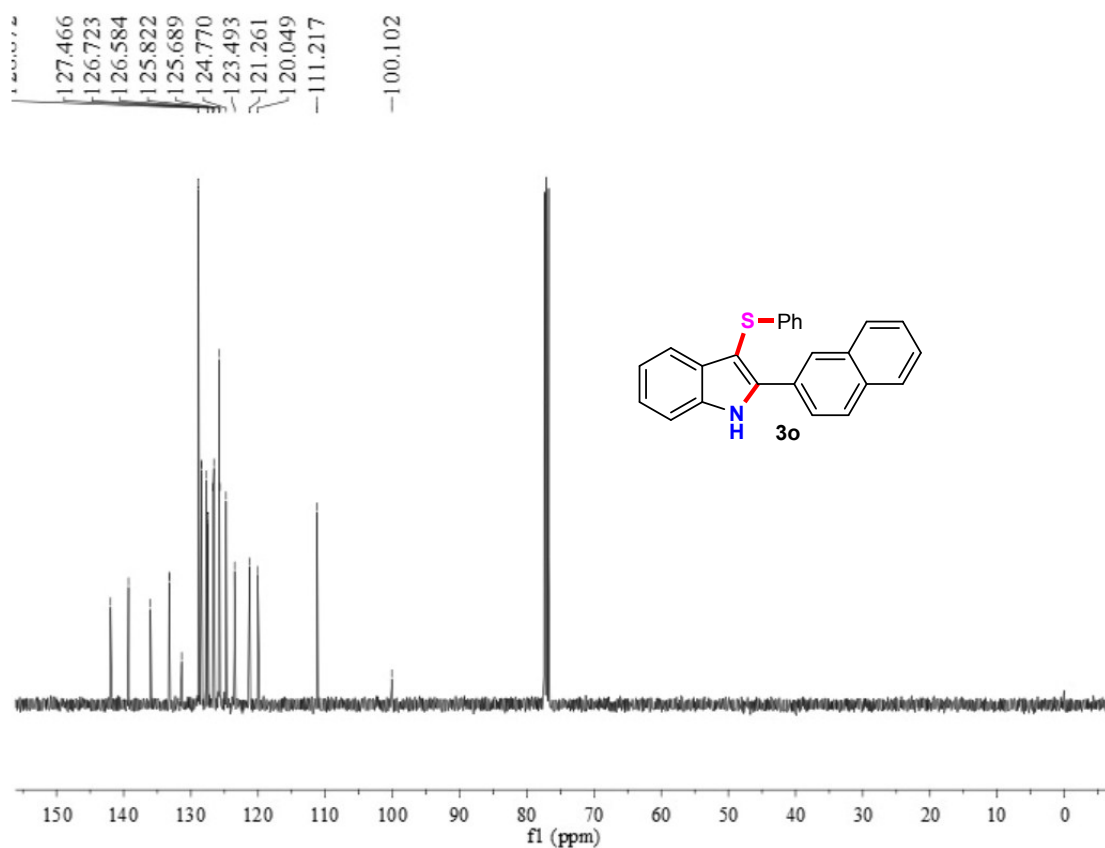
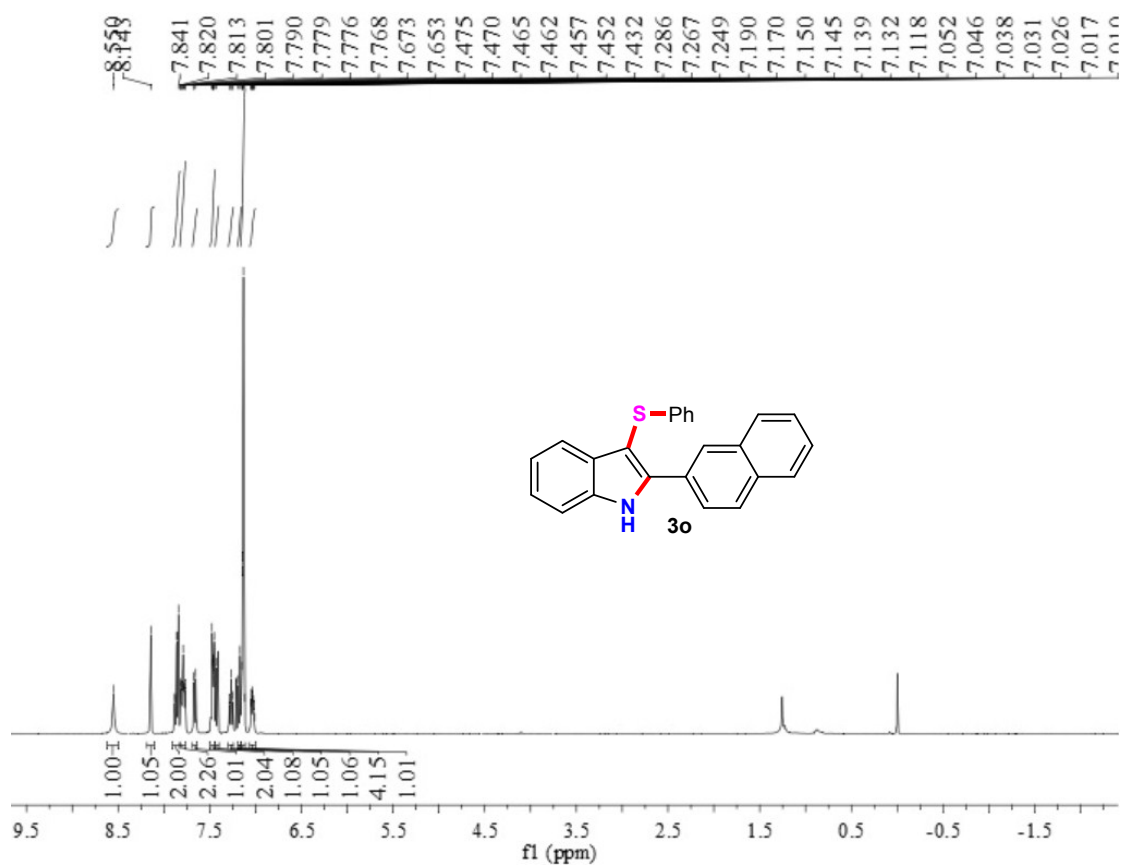












^1H and ^{13}C NMR spectra of compounds 5

