CuI-Catalyzed Cross-Coupling of Diazoacetamide with Terminal Alkynes: An Approach to Substituted Dienamides and 3-Butynamides

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Supporting Information

Contents: Pages

X-Ray Crystallographic Data: CIF in separate file.

Crystallographic data **3c** (CCDC **937191**) has been deposited vat the Cambridge Crystallographic Database Centre and is available on request from the Director, CCDC, 12 Union Road, Cambridge, CB2 1EZ, UK (http//www.ccdc.cam.ac.uk).

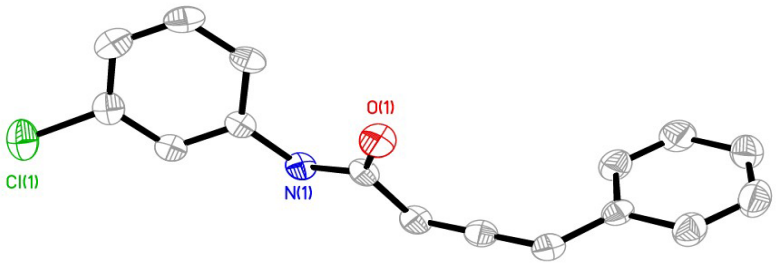
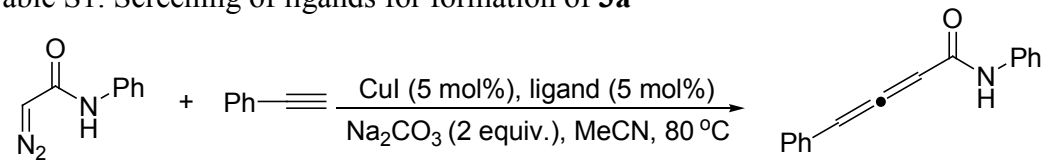
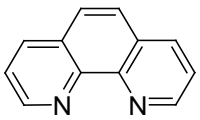
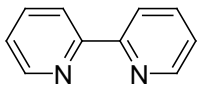
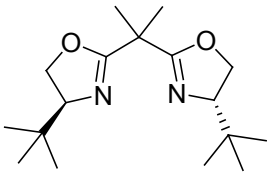
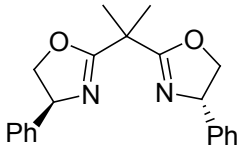
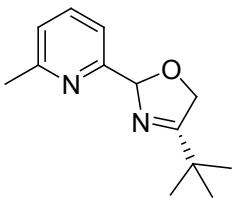
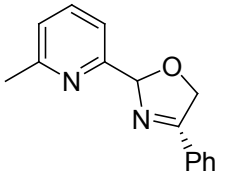


Figure 1 Molecular structure of **3c**

Table S1. Screening of ligands for formation of **3a**[a]

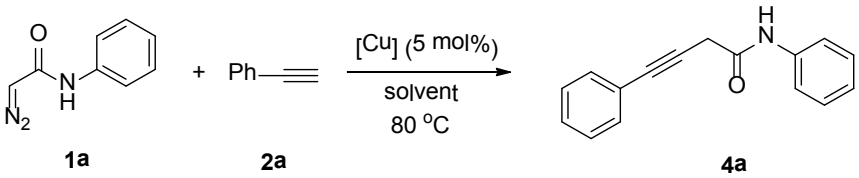


1a **2a** **3a**

		
70% yield [b]	64% yield	74% yield
		
63% yield	67% yield	62% yield

[a] Reaction conditions: **1a** (0.5 mmol), **2a** (0.6 mmol), CuI (5 mol %, 0.025 mmol), ligand (5 mol %, 0.025 mmol), Na_2CO_3 (1 mmol) in MeCN (3 mL) at 80 ºC for 1h under N_2. [b] Isolated yields.

Table S2. Screening of reaction conditions for formation of **4a**[a]



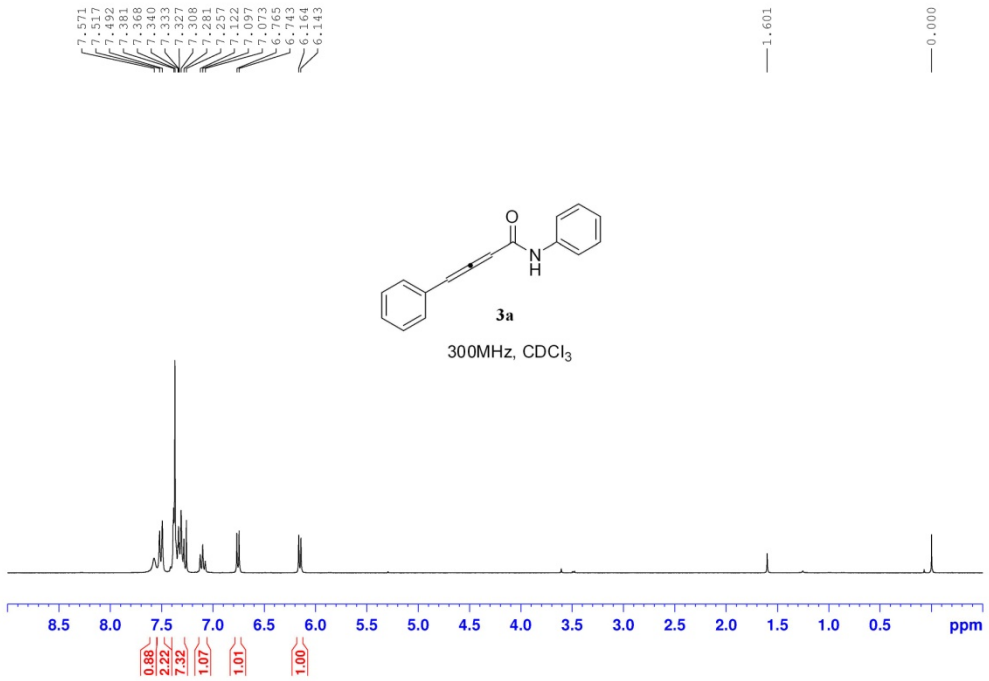
1a **2a** **4a**

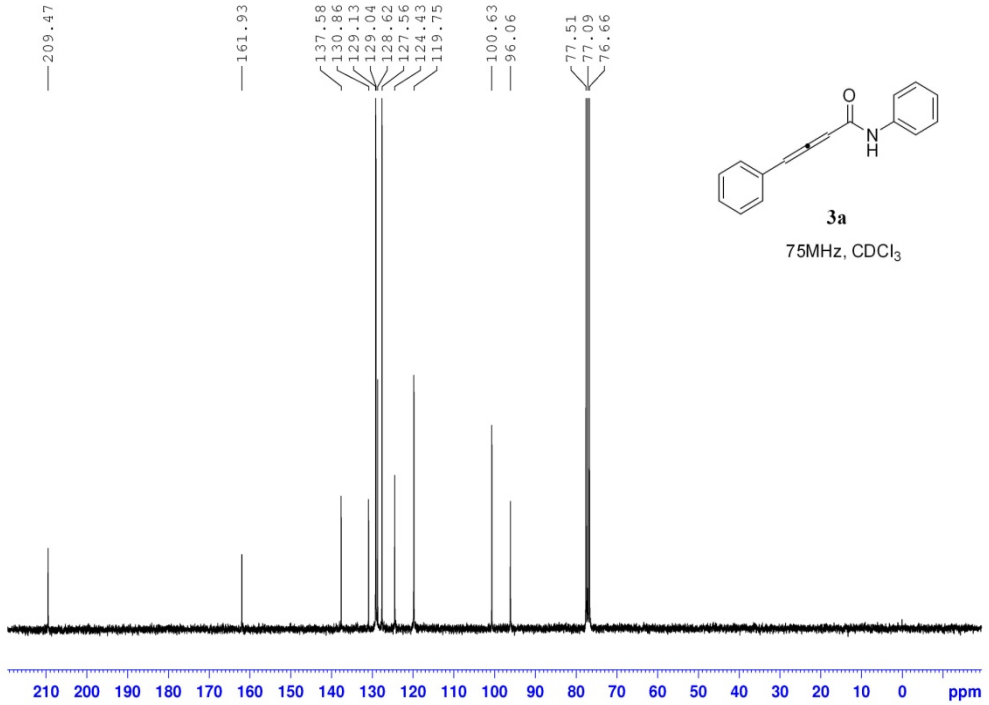
Entry	Catalyst	Solvent	Yield of 4a[b]
1	$Cu(OTf)_2$	MeCN	0
2	$Cu(acac)_2$	MeCN	0
3	CuCl	MeCN	0
4	$Cu[MeCN]_4PF_6$	MeCN	0
5	CuBr	MeCN	46
6	CuI	MeCN	55
7	CuI	Toluene	30
8	CuI	Dioxane	44
9	CuI	1,2-Dichloroethane	39

[a] Reaction condition: 1 (0.5 mmol), 2 (0.6 mmol), catalyst (5 mol%, 0.025 mmol) in solvent (3 mL) at 80 °C for 0.5-3h. [b] Isolated yields.

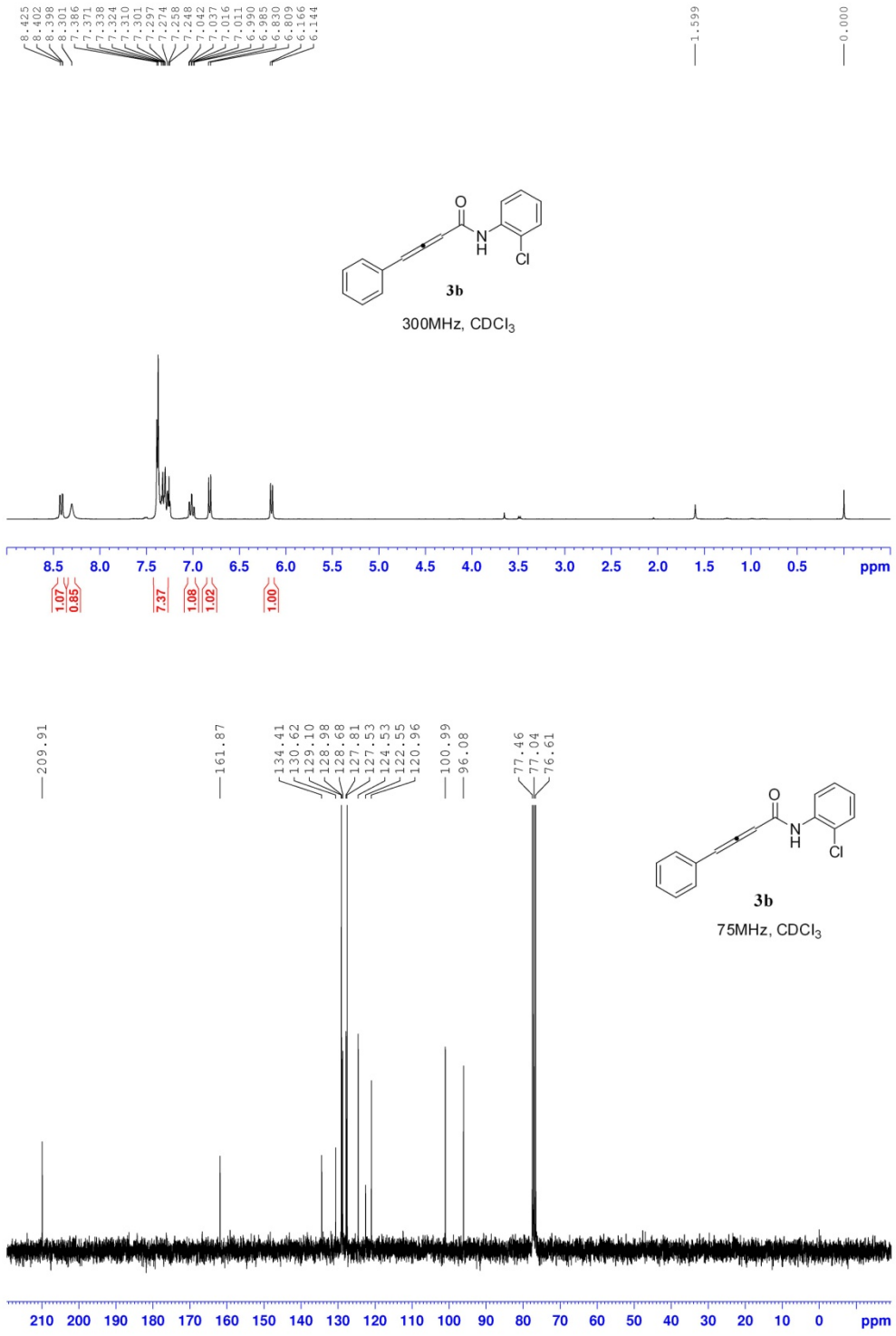
NMR spectra of all new compounds 3 and 4.

NMR spectra of compounds 3a

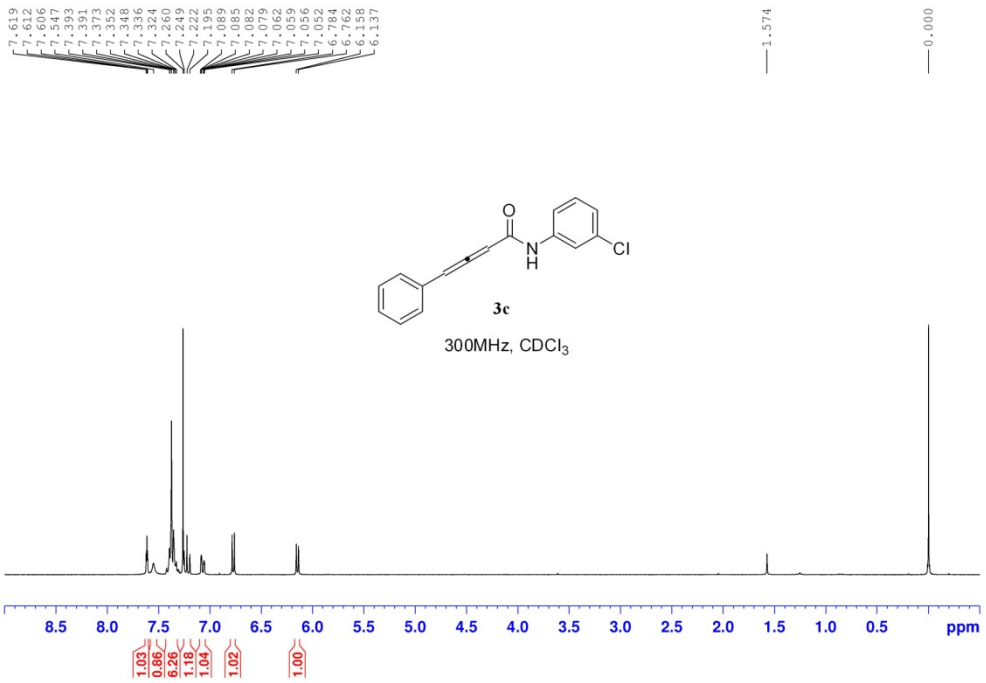


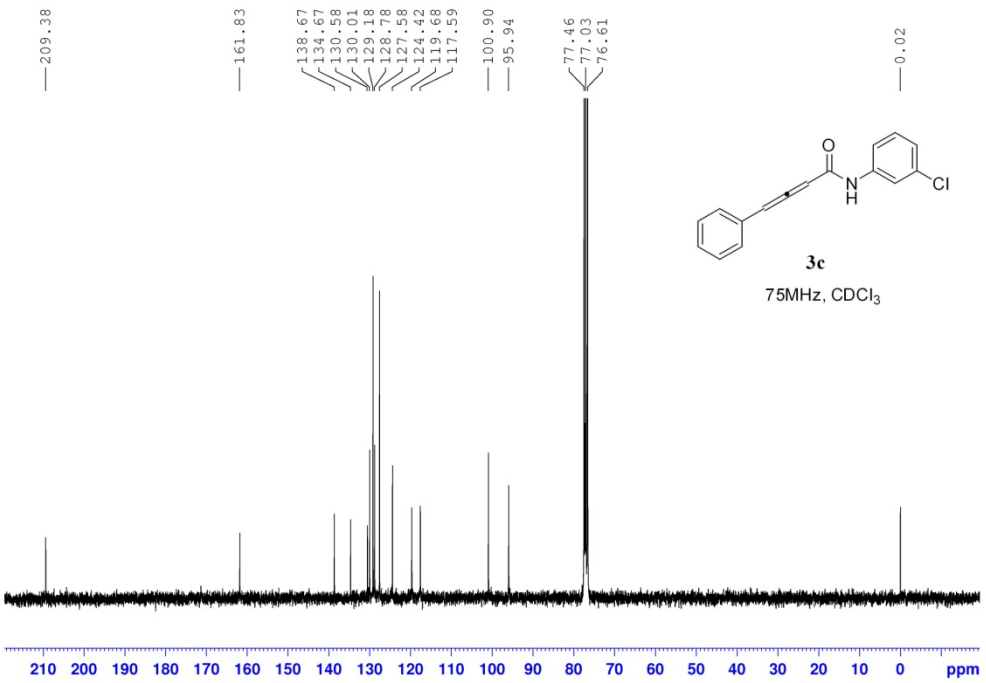


NMR spectra of compounds 3b.

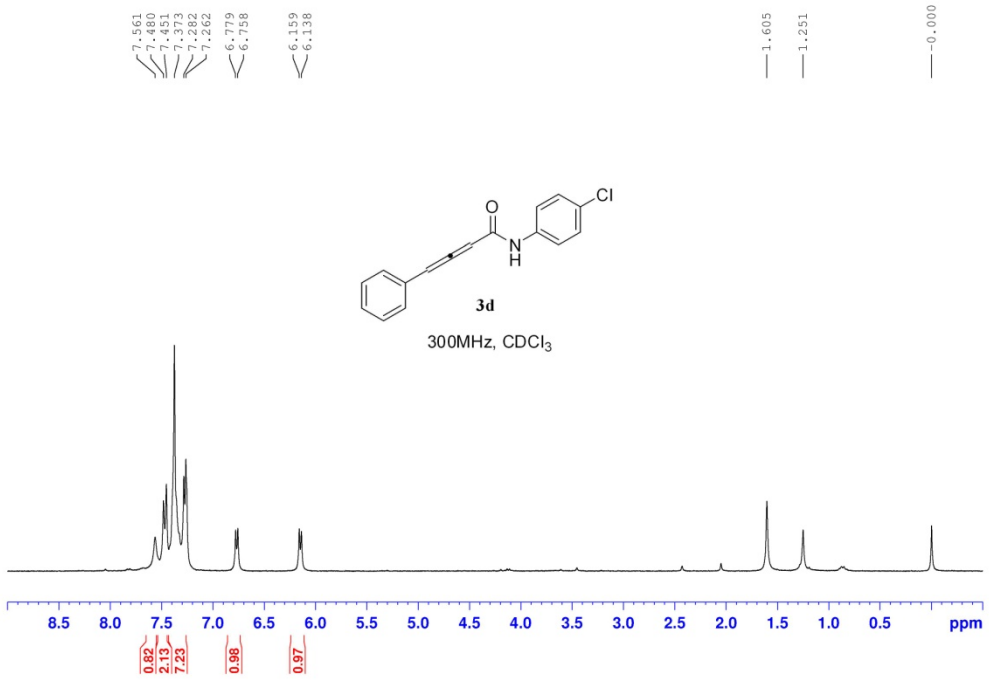


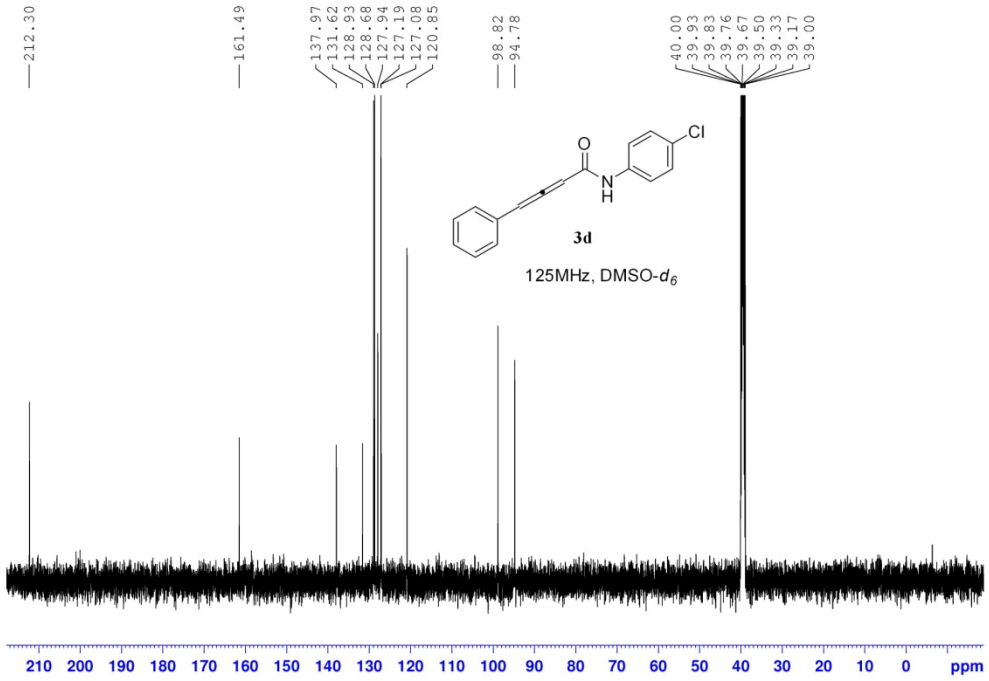
NMR spectra of compounds 3c



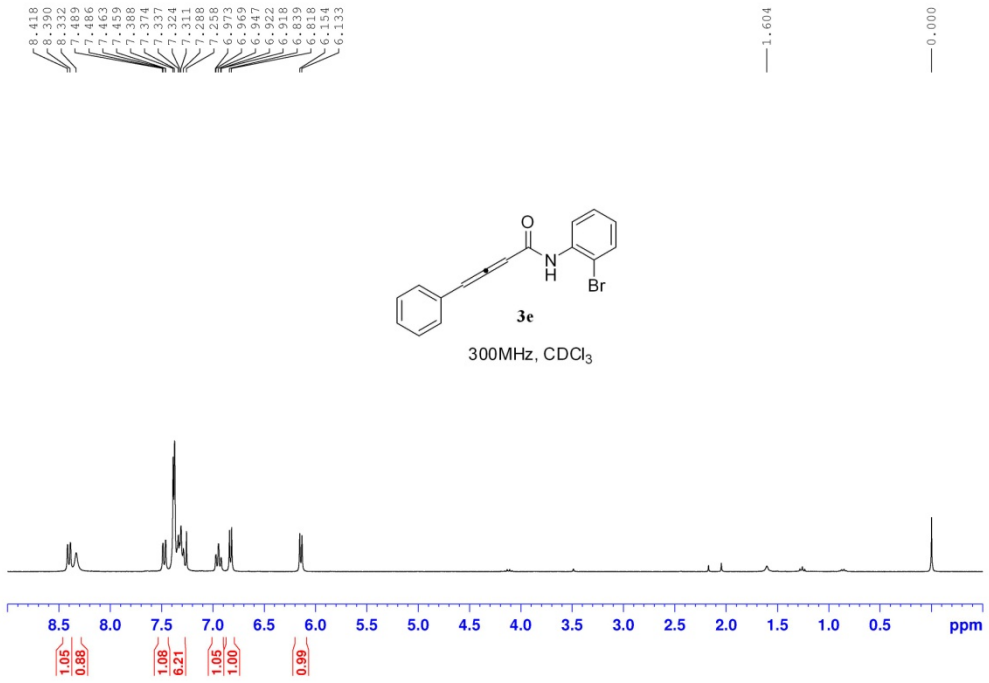


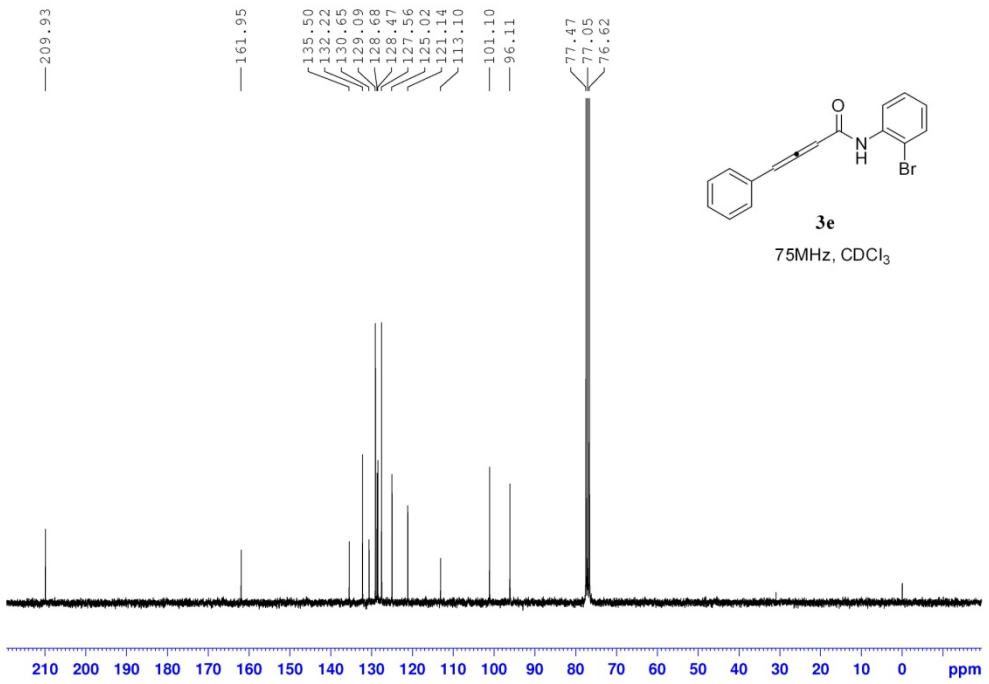
NMR spectra of compounds 3d



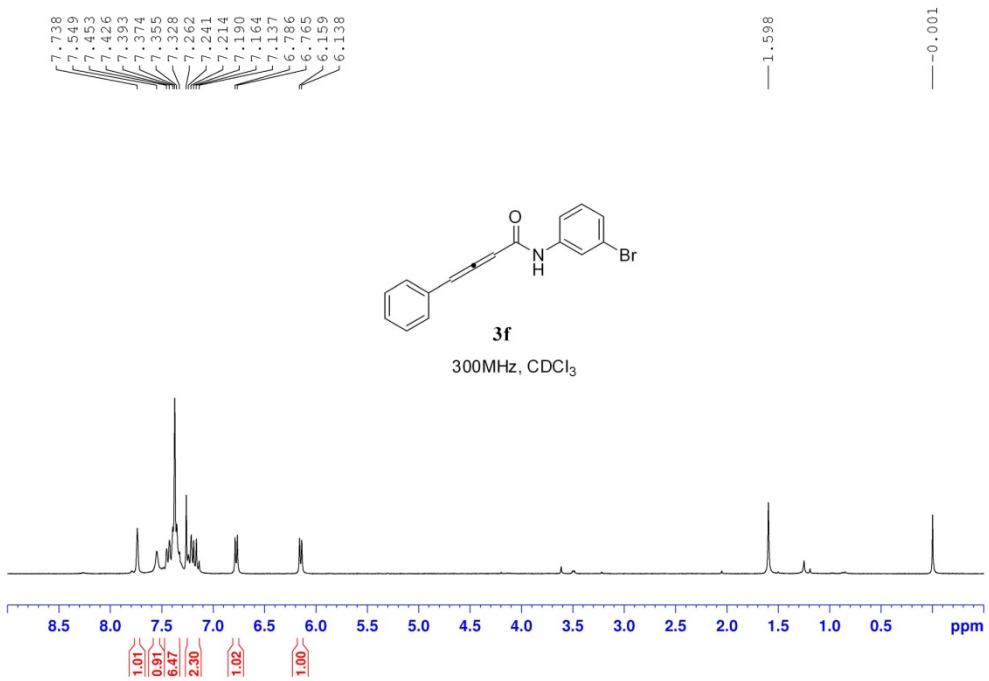


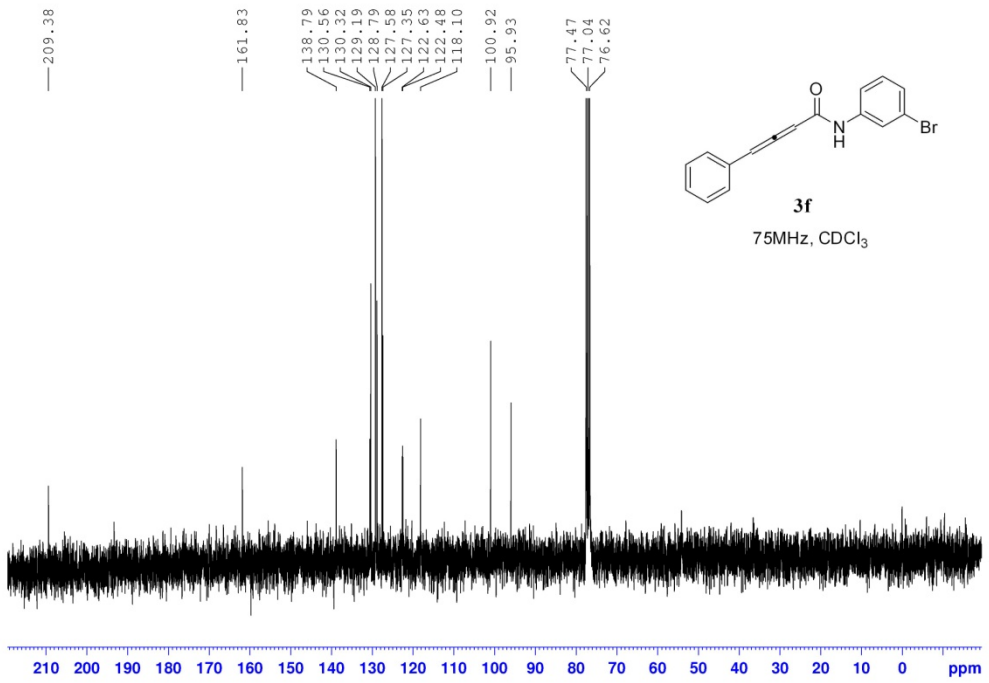
NMR spectra of compounds 3e



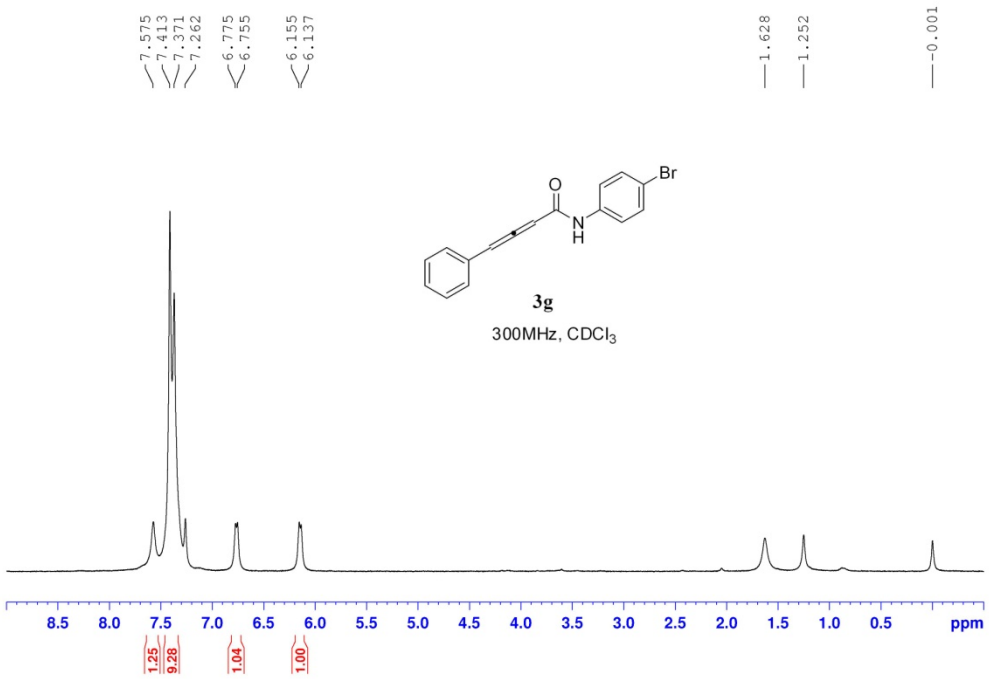


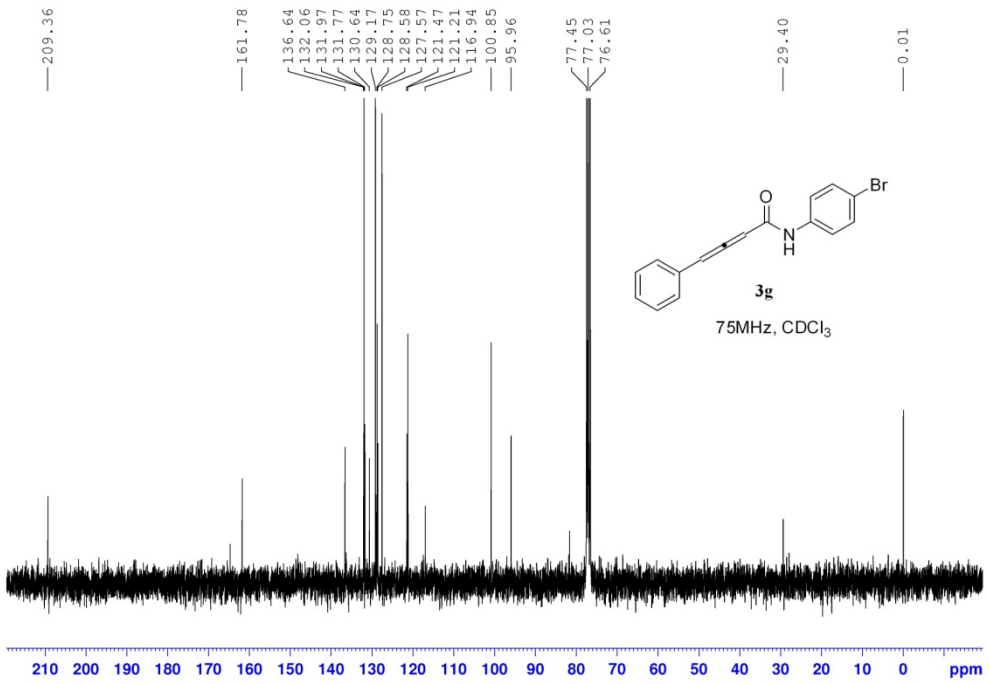
NMR spectra of compounds 3f



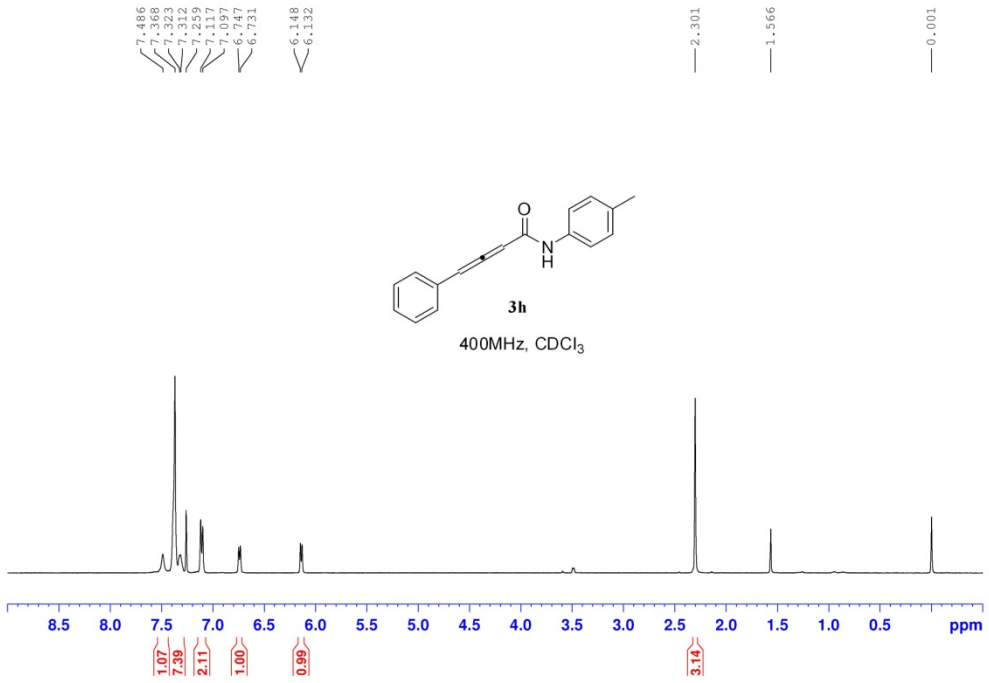


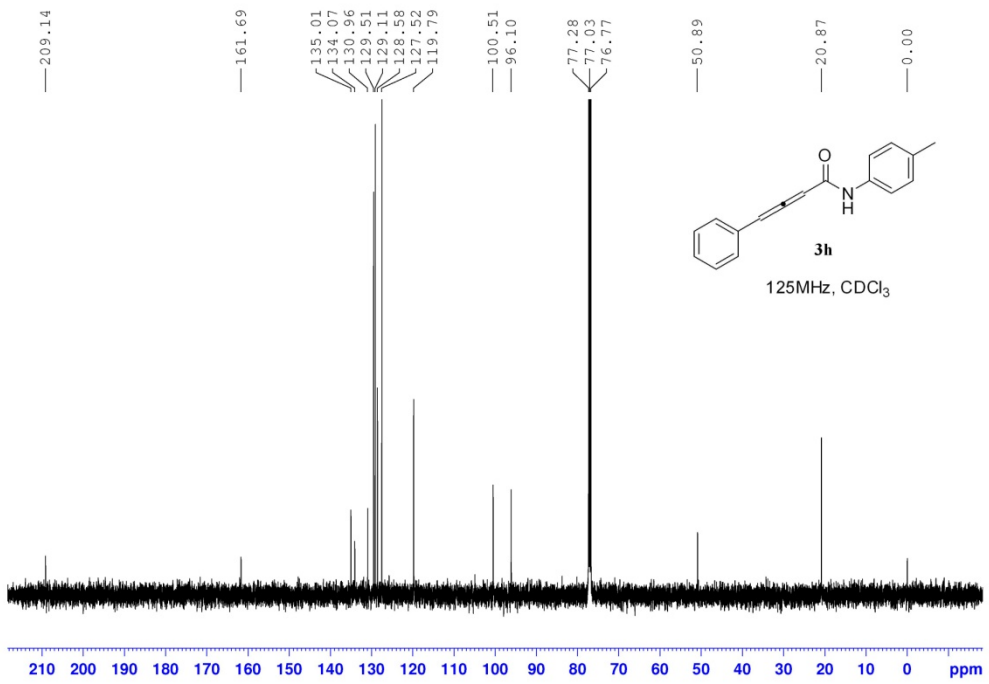
NMR spectra of compounds 3g



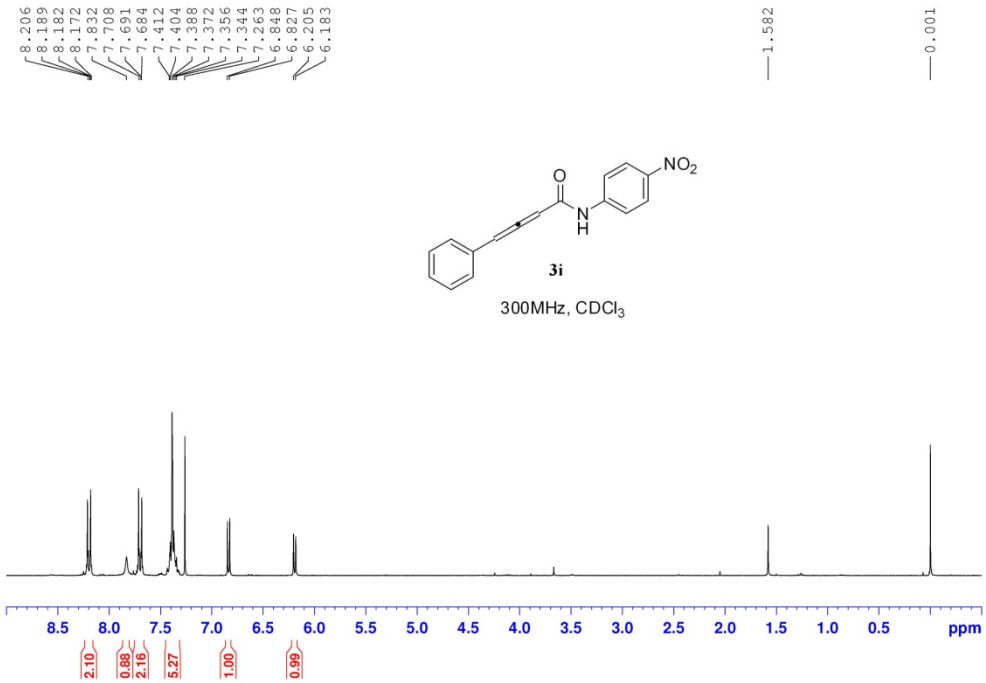


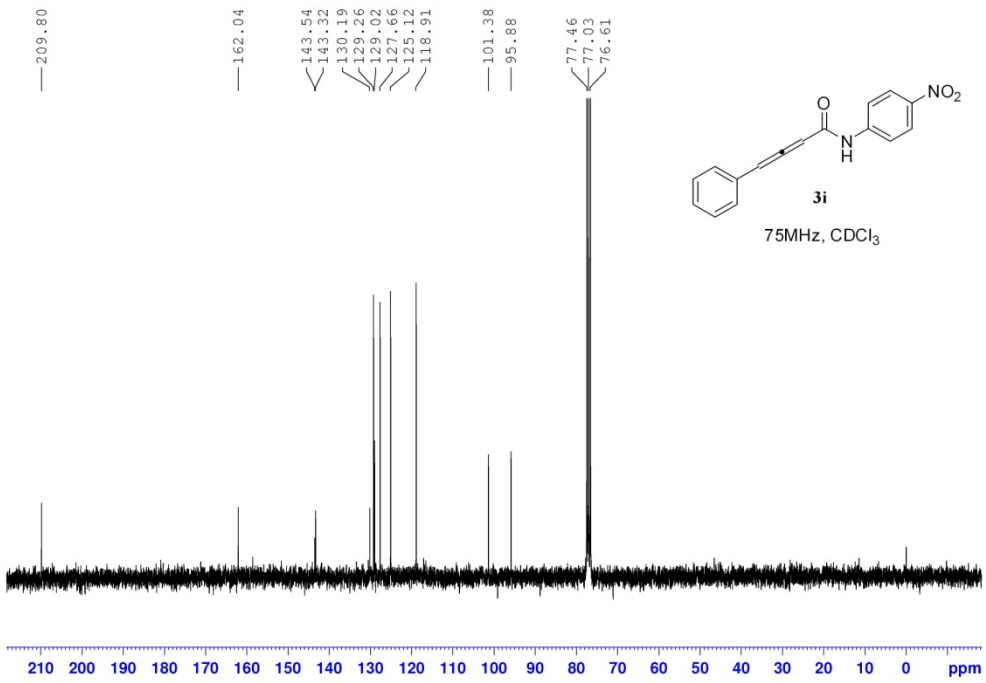
NMR spectra of compounds 3h



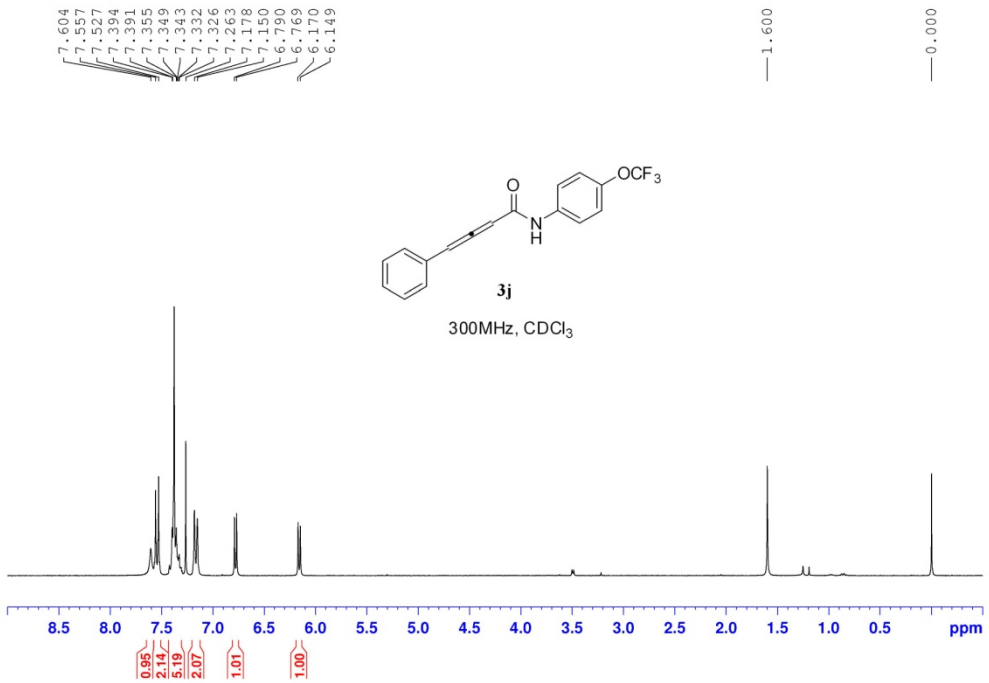


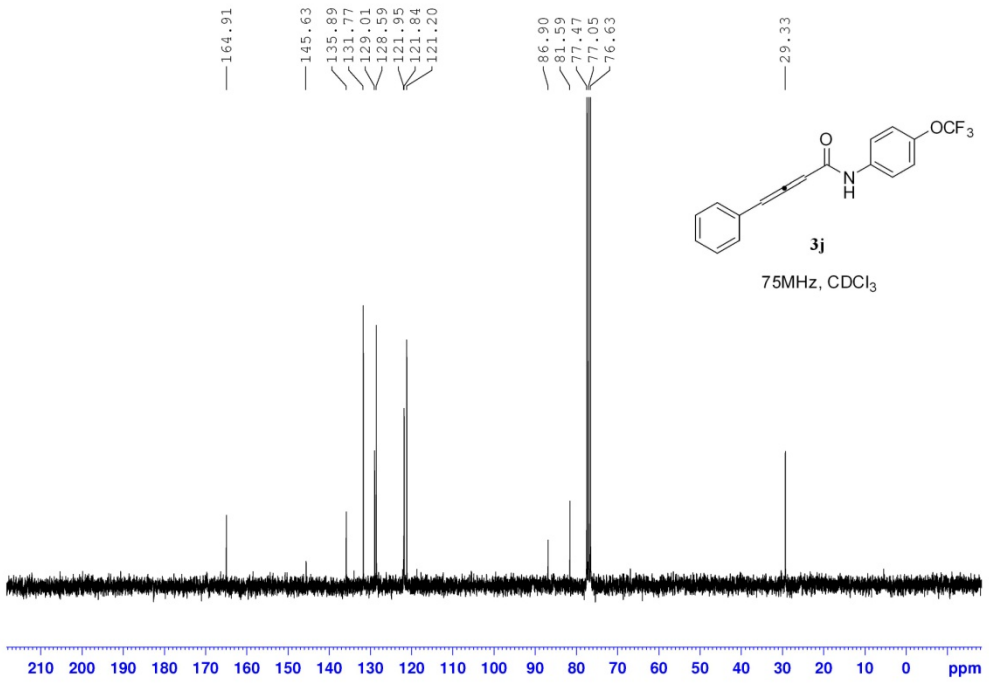
NMR spectra of compounds 3i



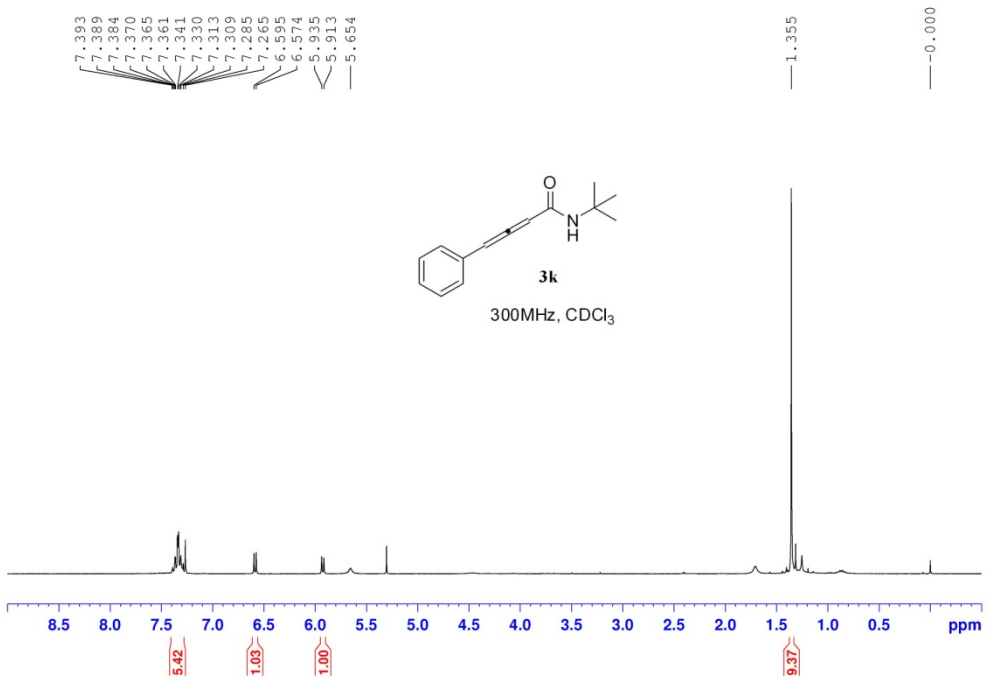


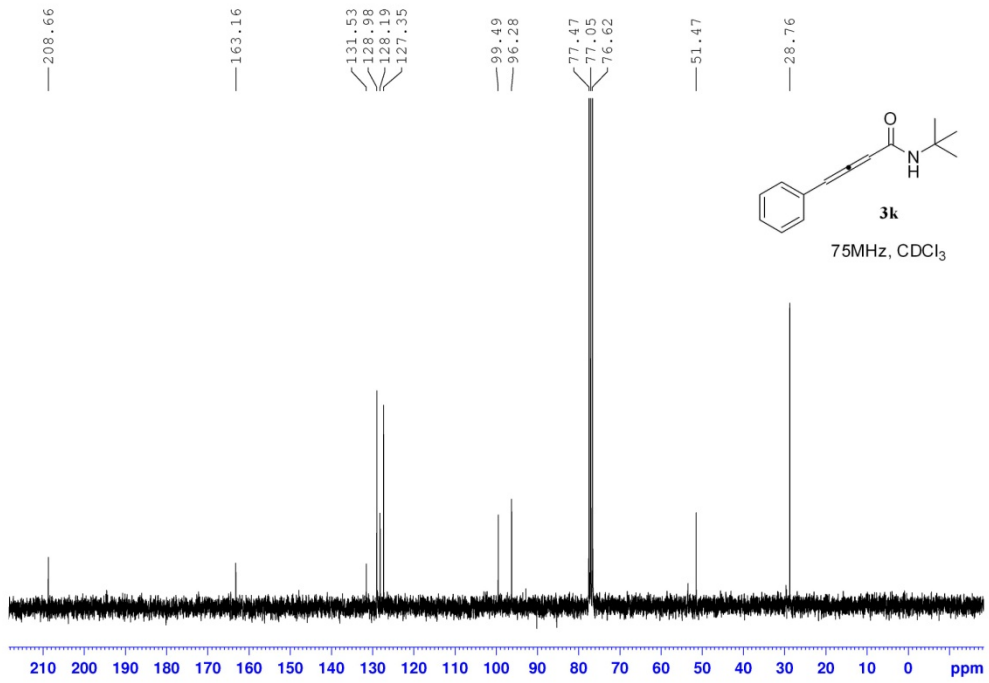
NMR spectra of compounds 3j



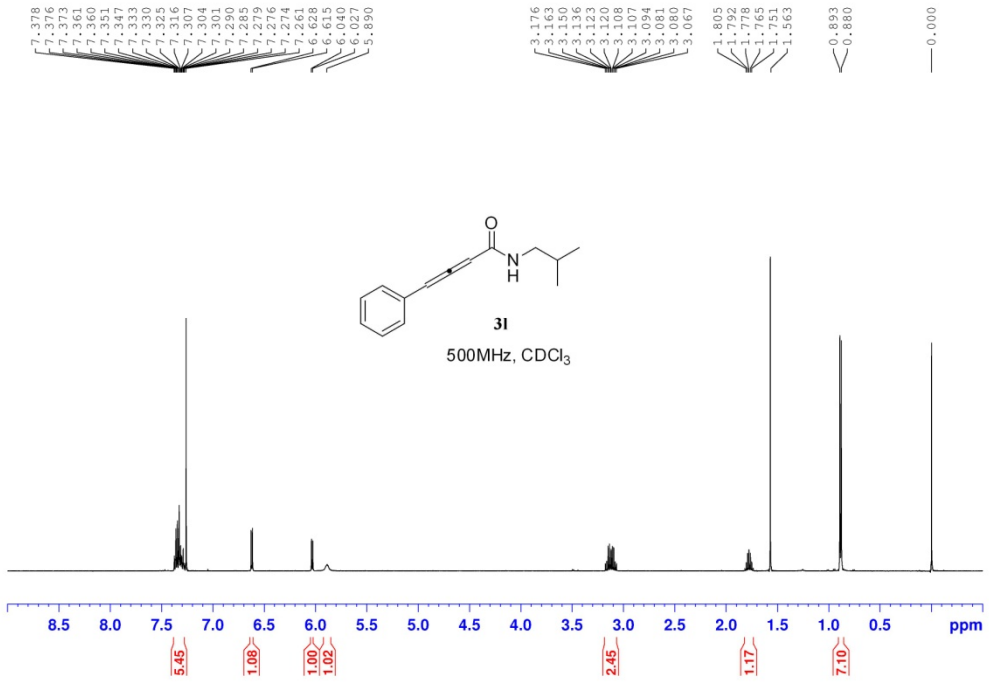


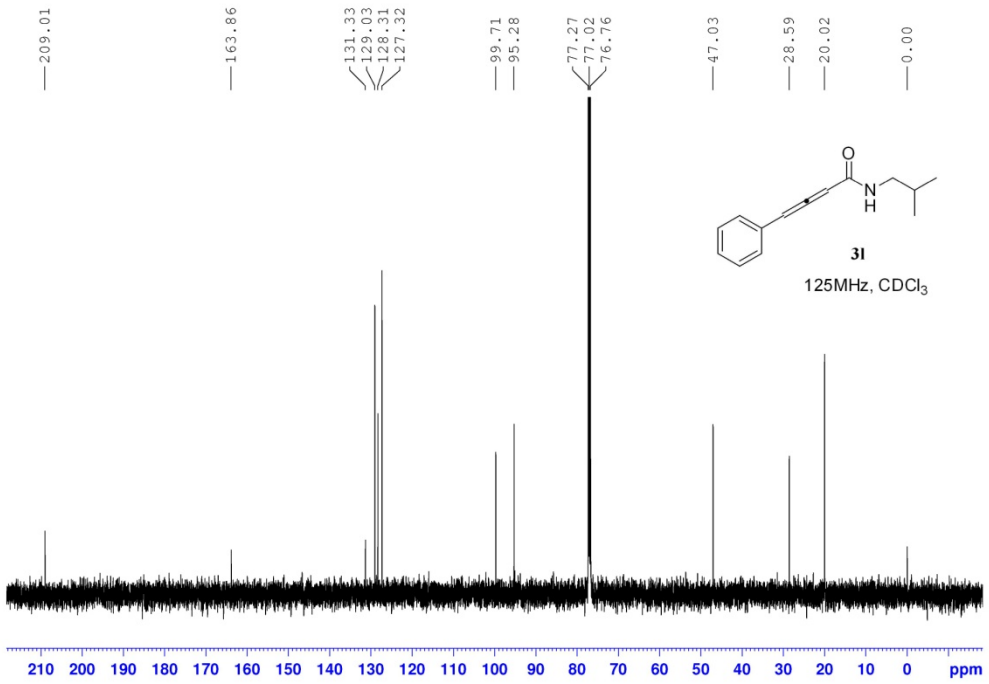
NMR spectra of compounds 3k



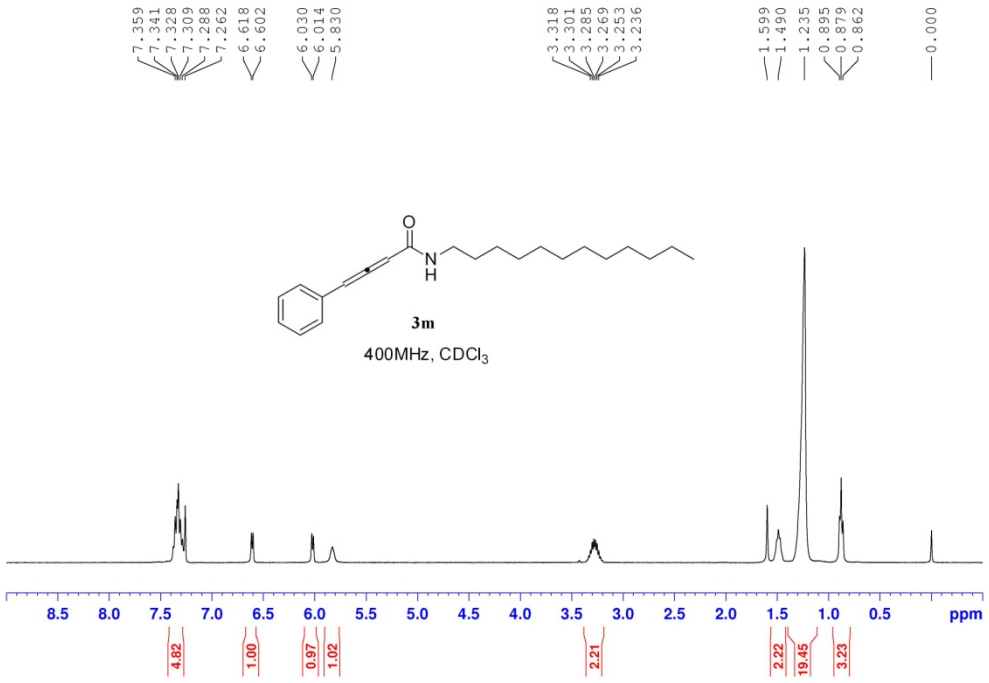


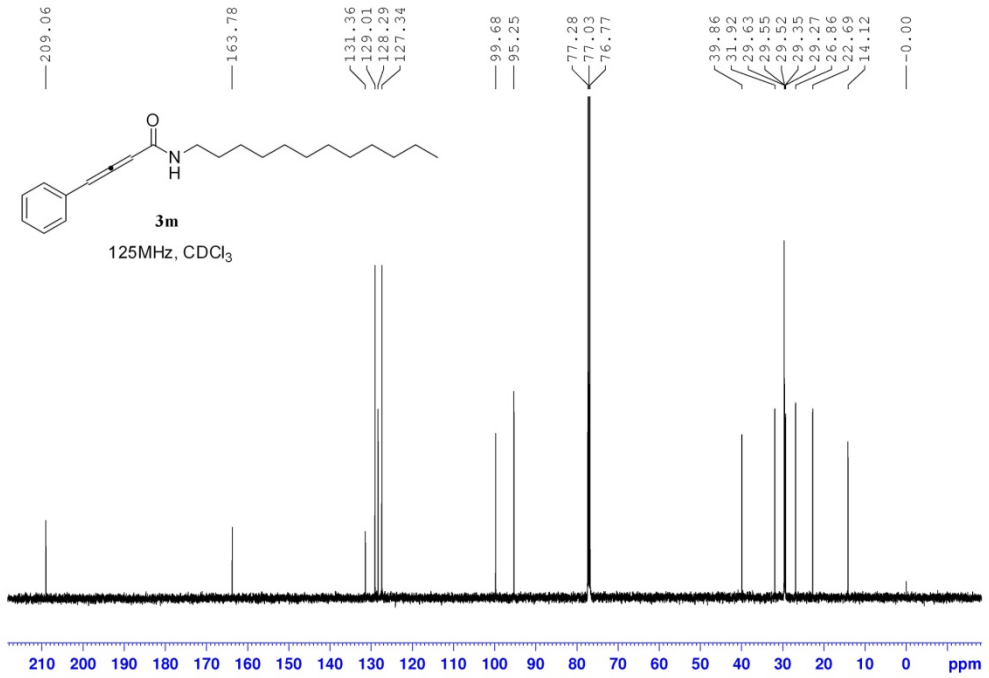
NMR spectra of compounds 3l



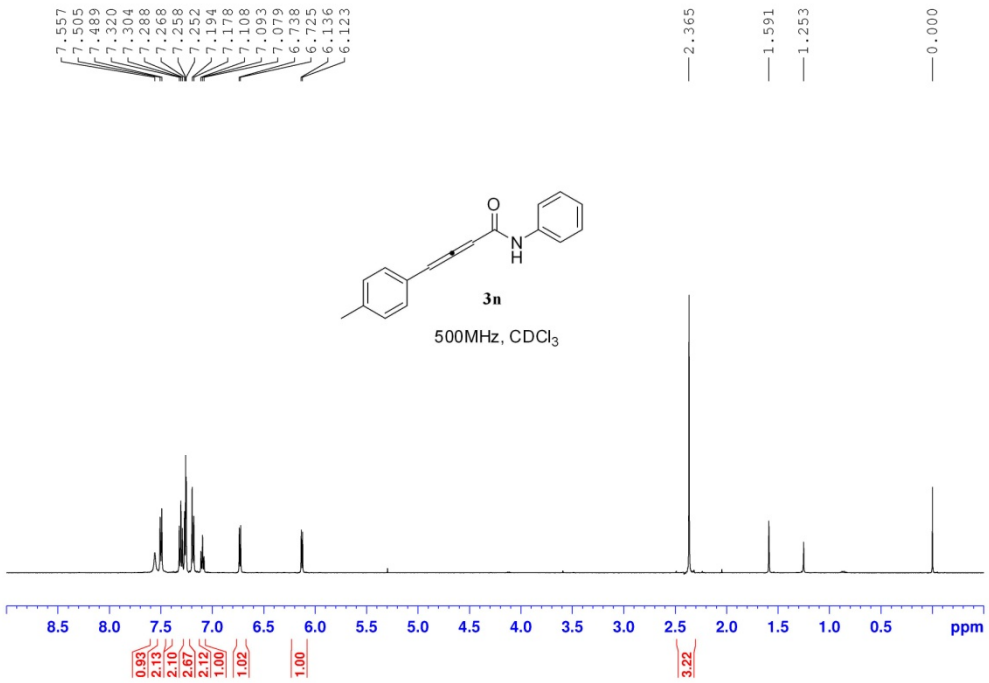


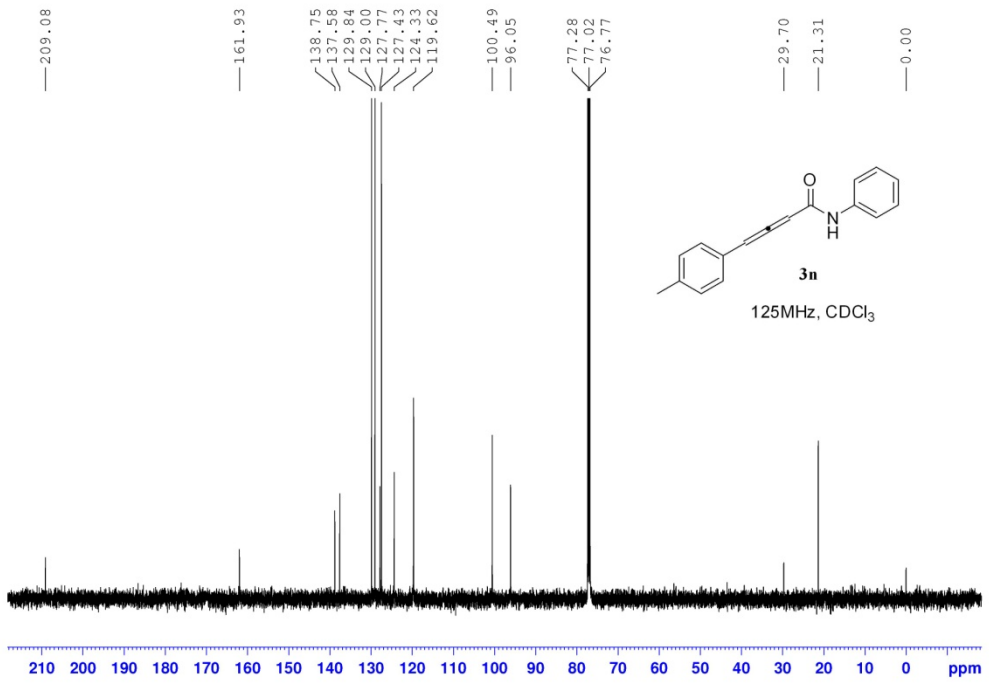
NMR spectra of compounds 3m



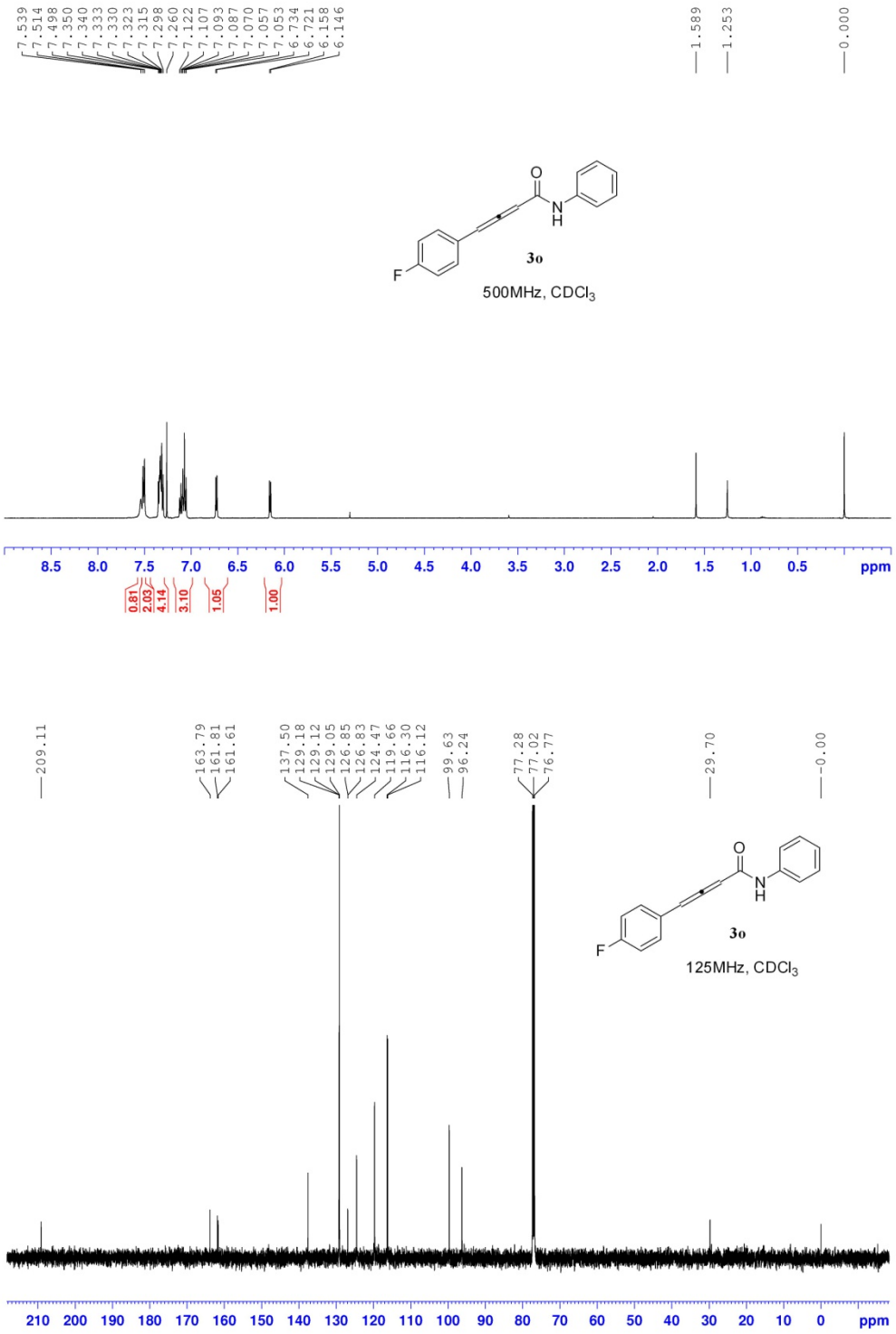


NMR spectra of compounds 3n

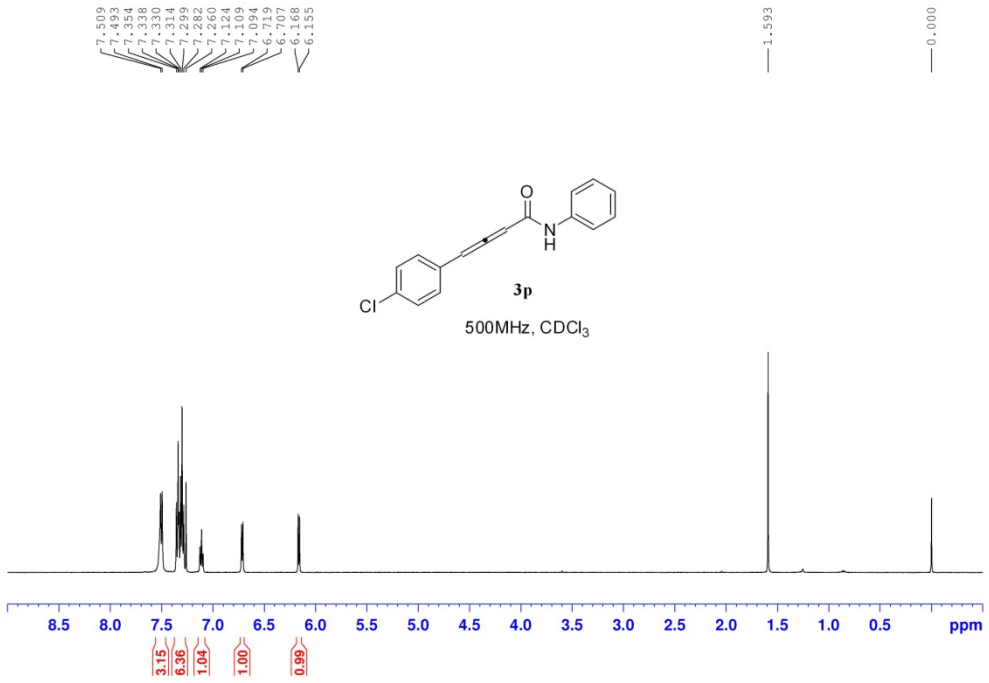


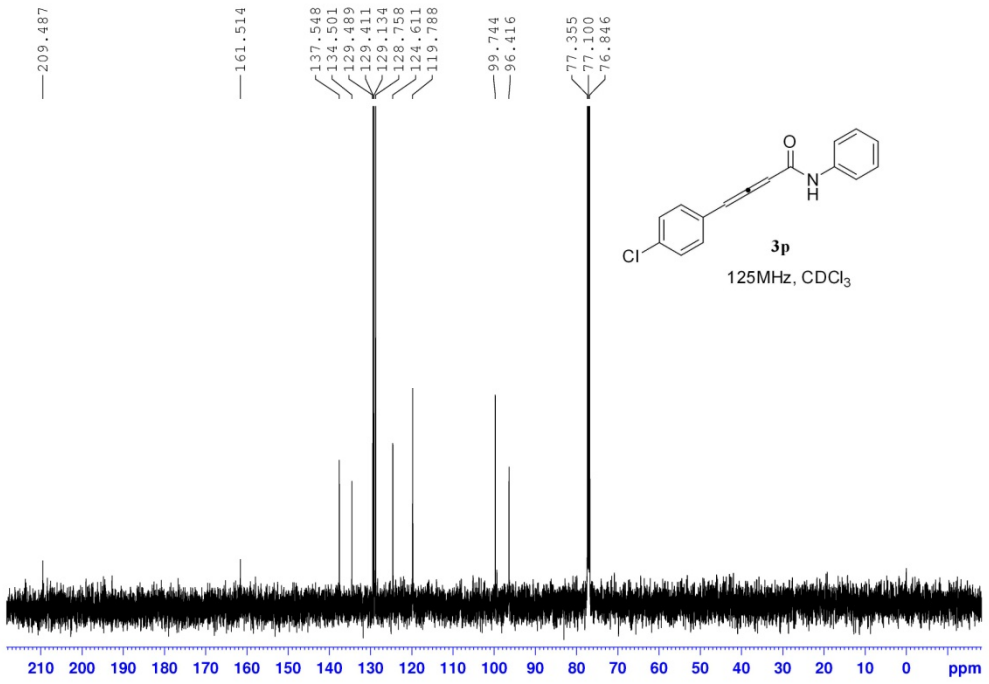


NMR spectra of compounds 3o

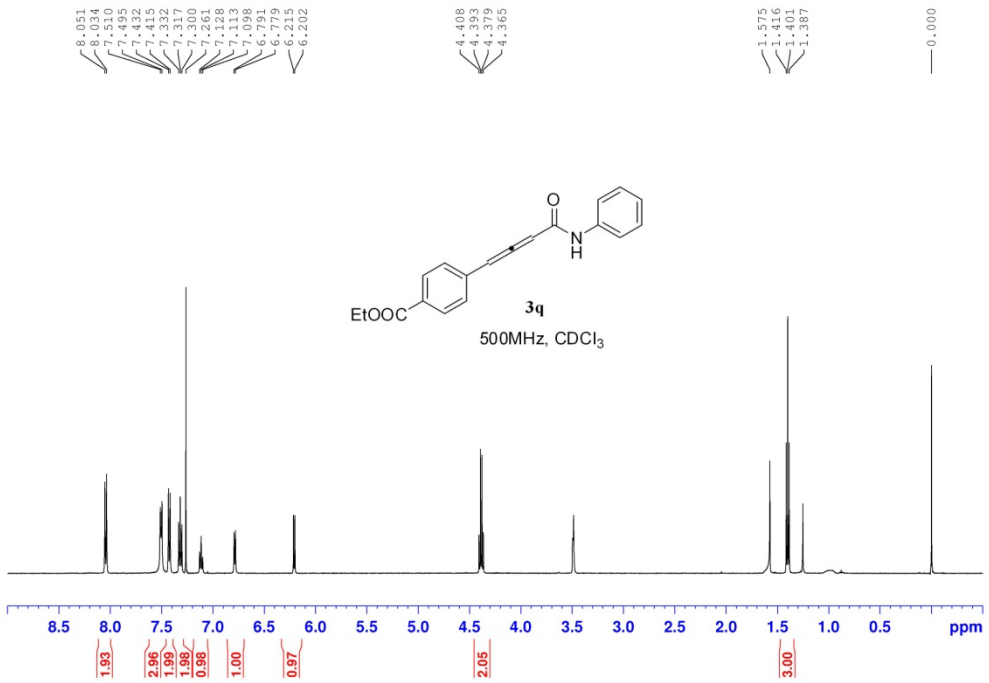


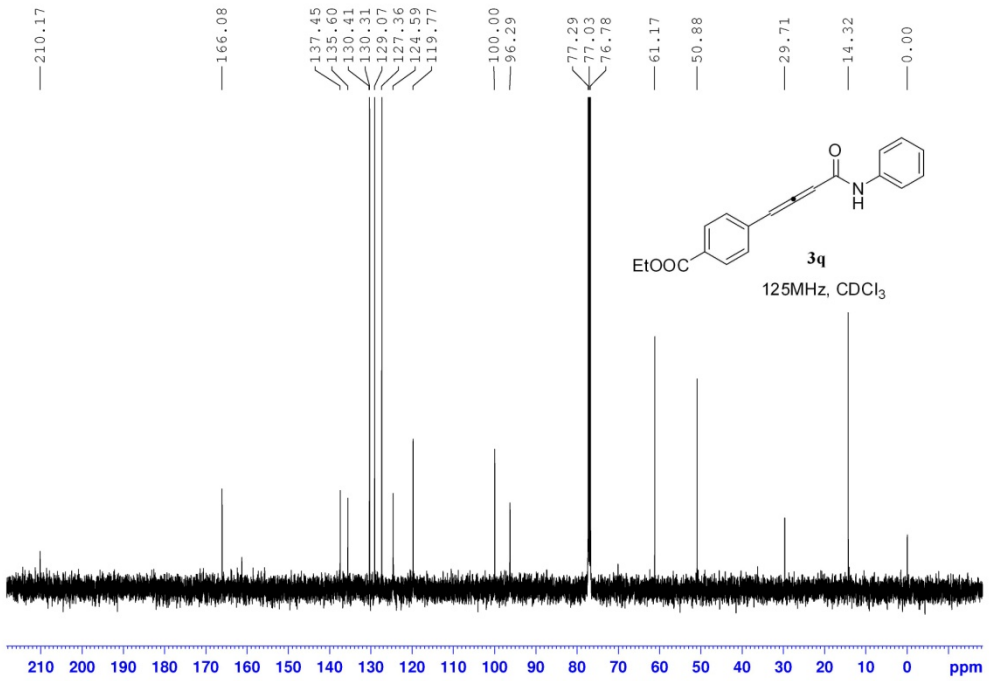
NMR spectra of compounds 3p



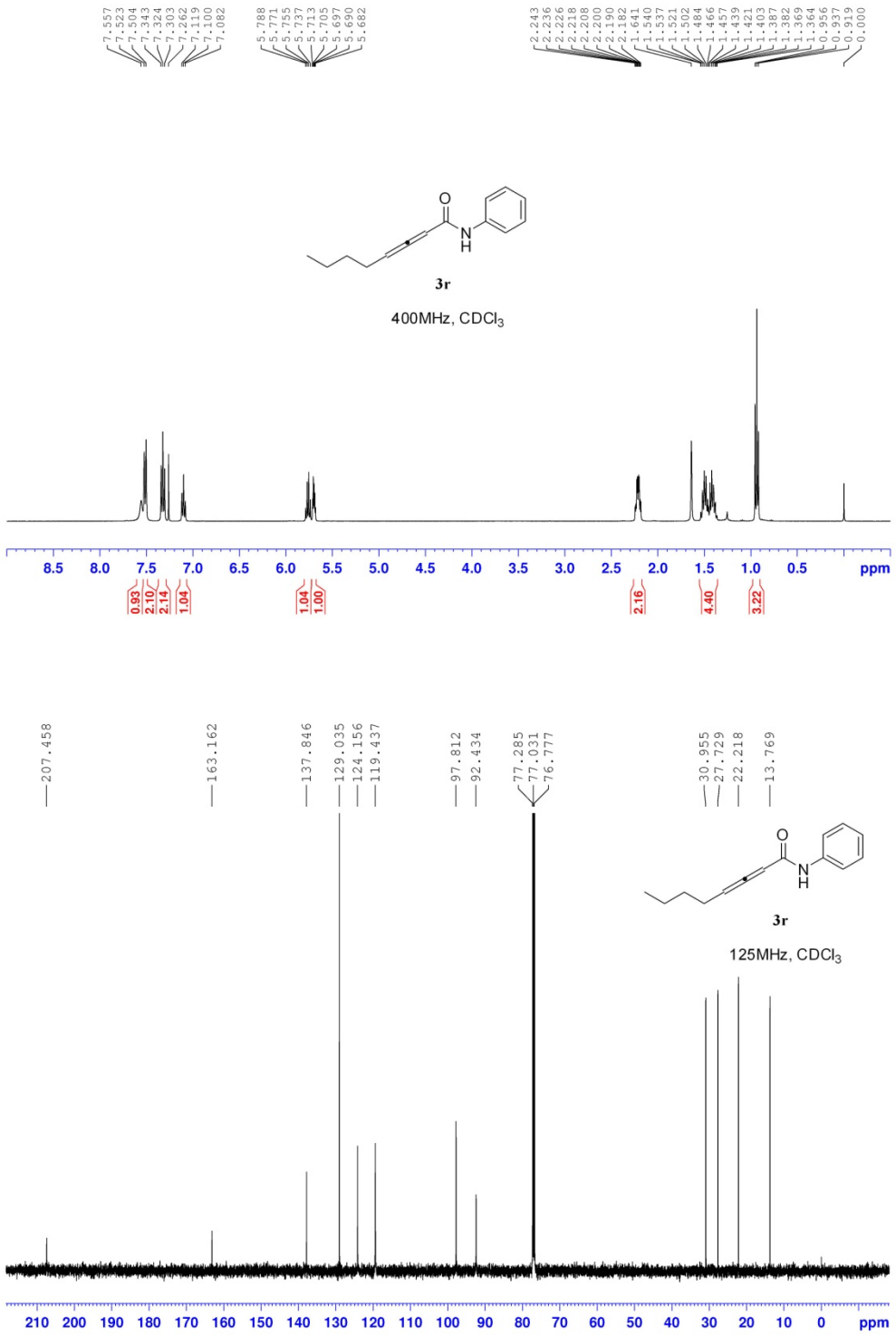


NMR spectra of compounds 3q

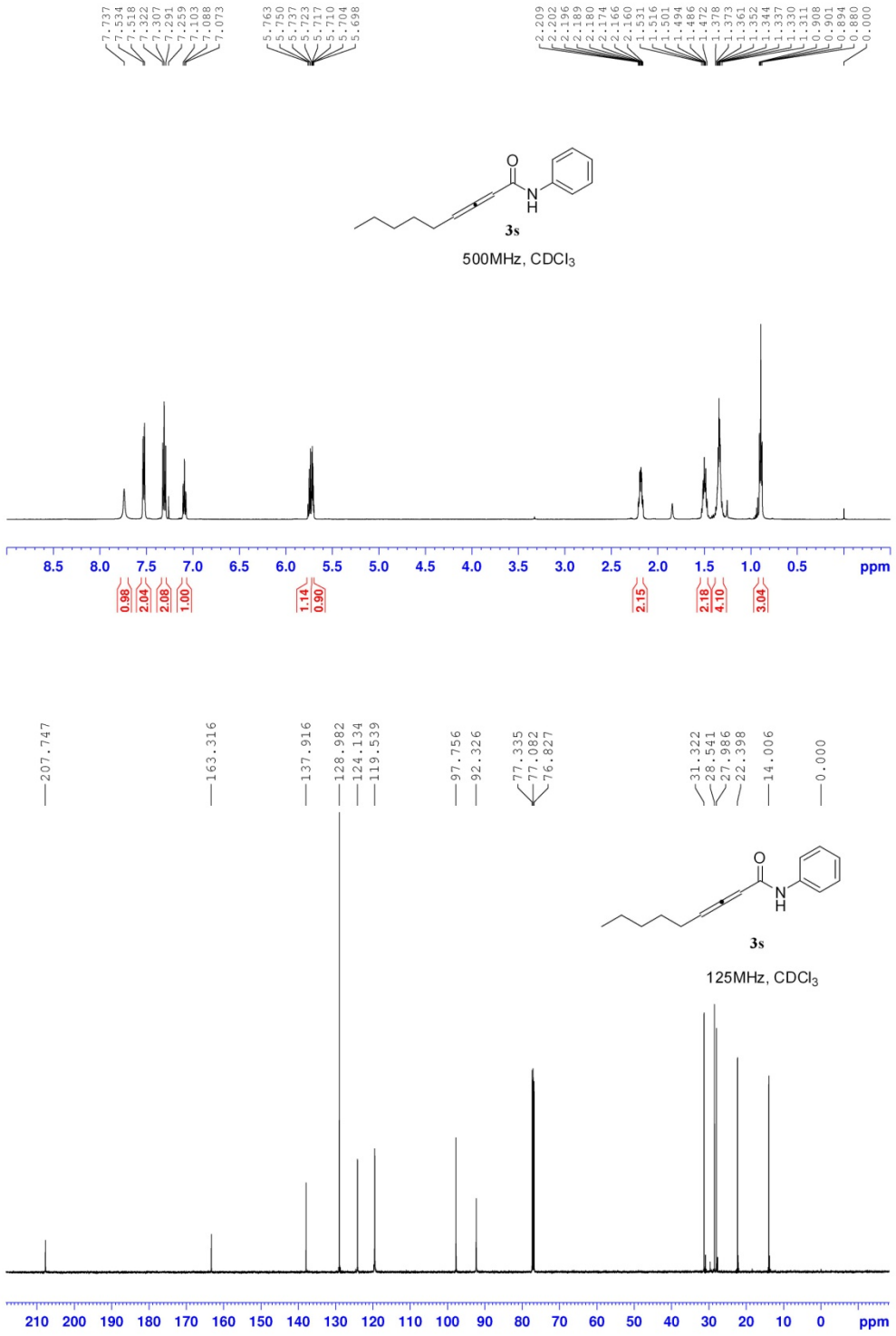




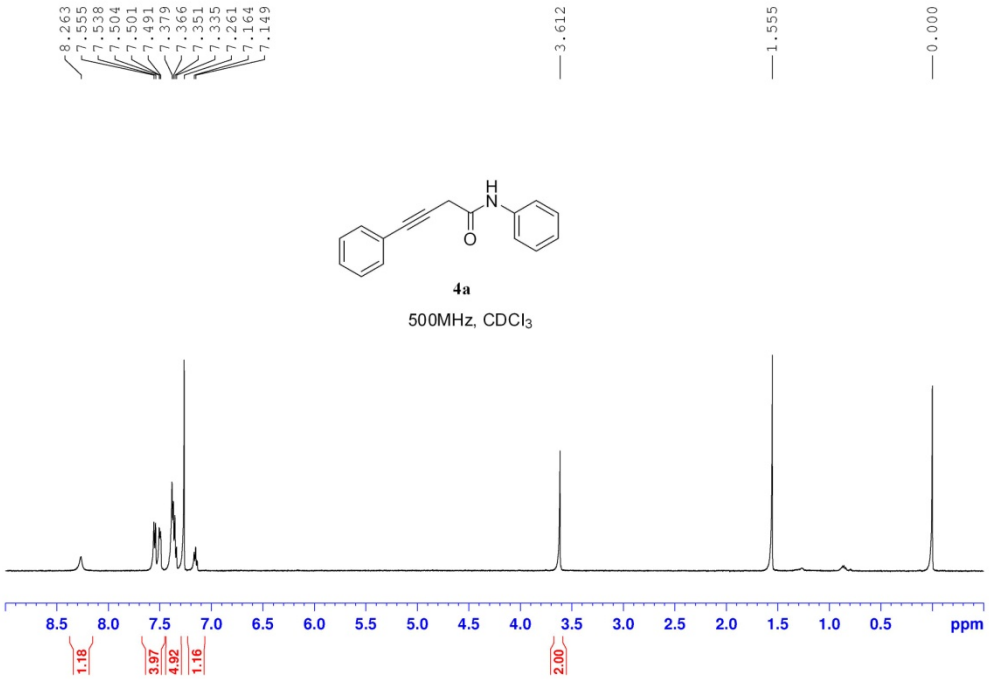
NMR spectra of compounds 3r

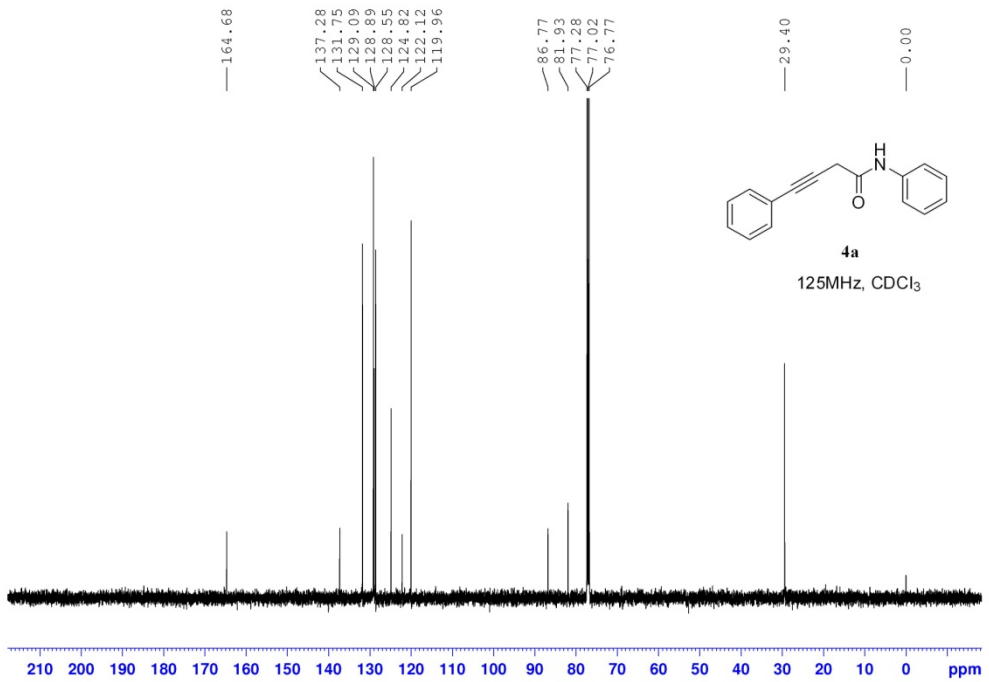


NMR spectra of compounds 3s

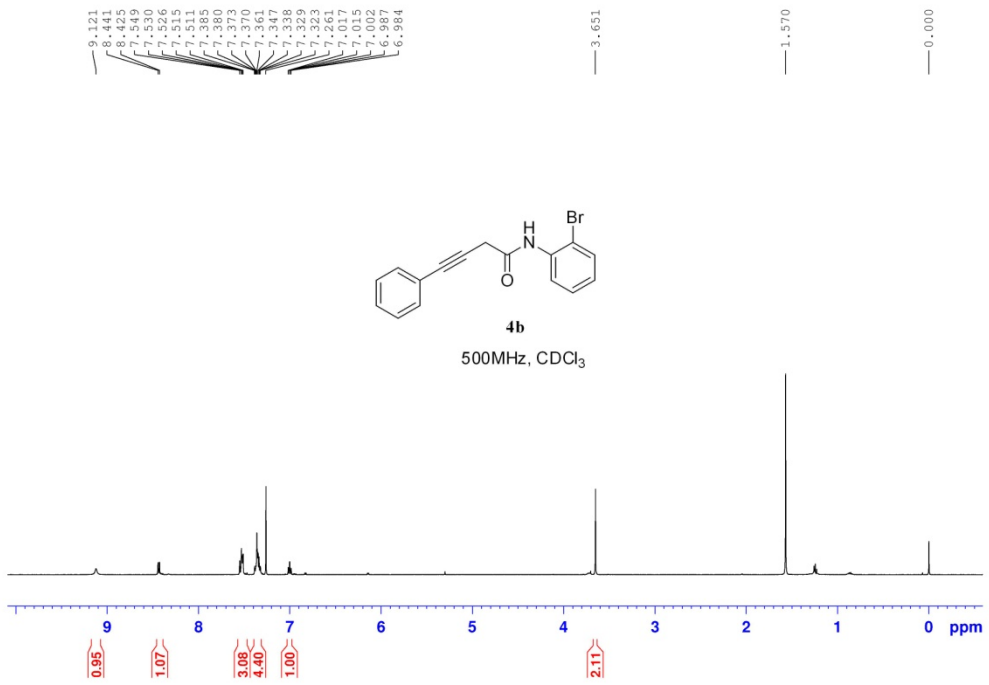


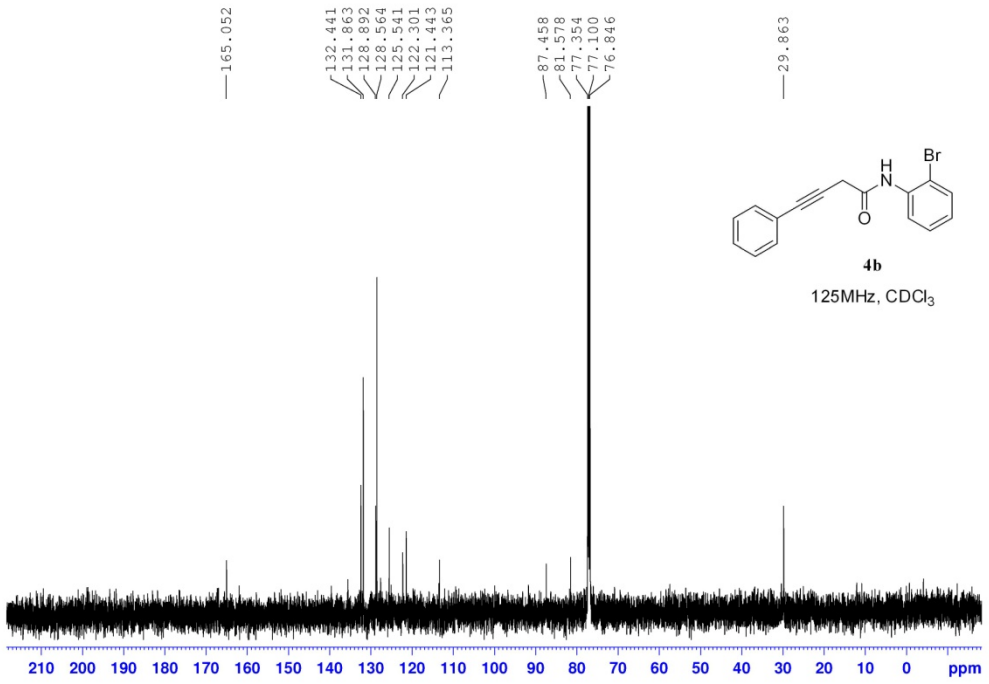
NMR spectra of compounds 4a



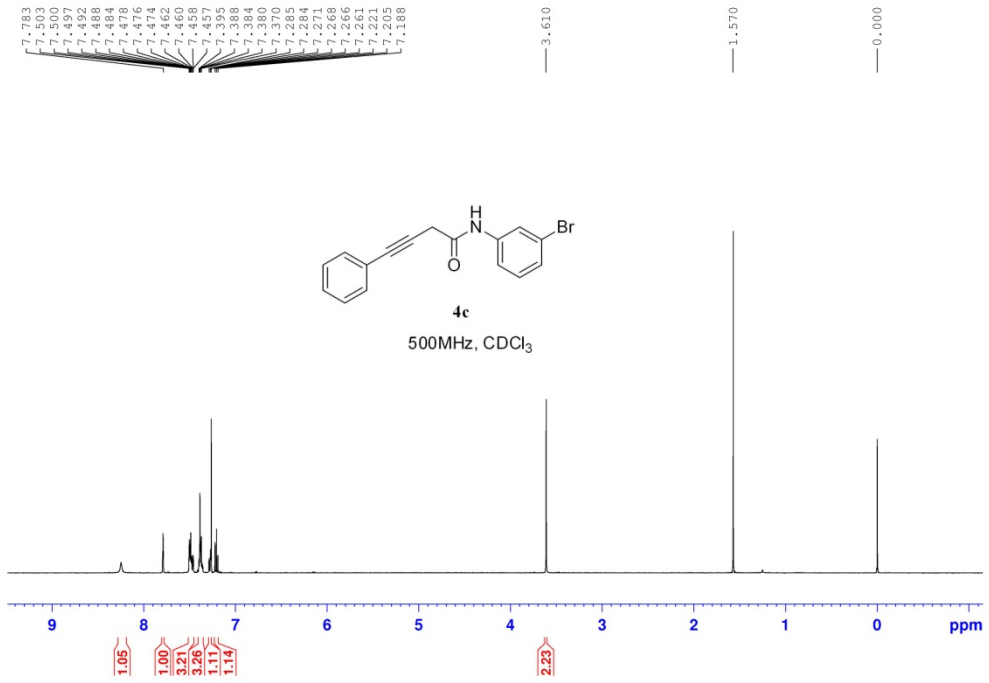


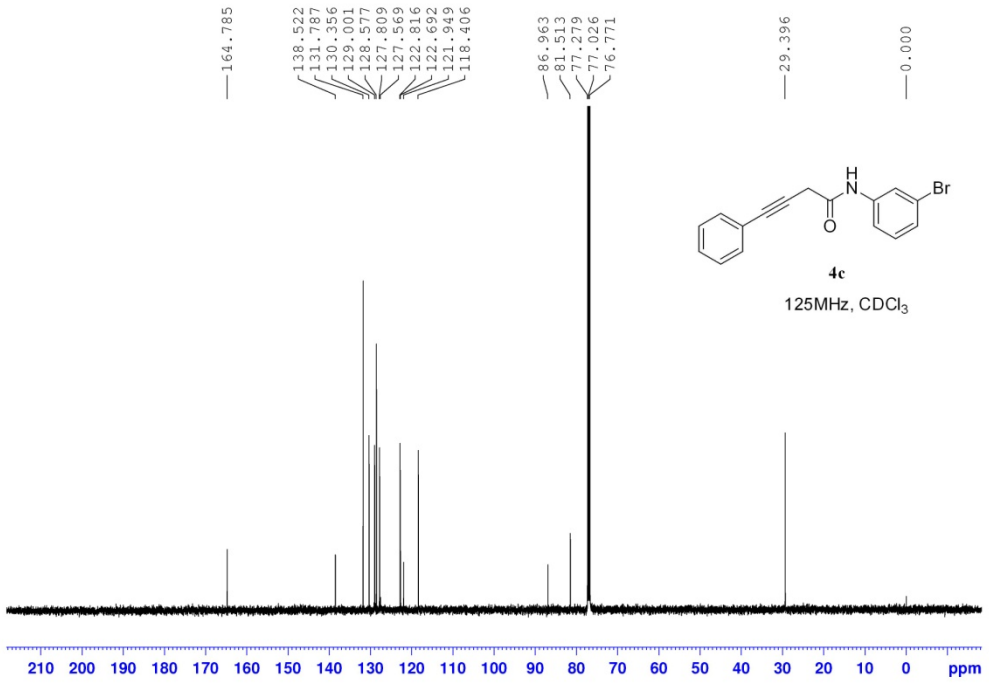
NMR spectra of compounds 4b



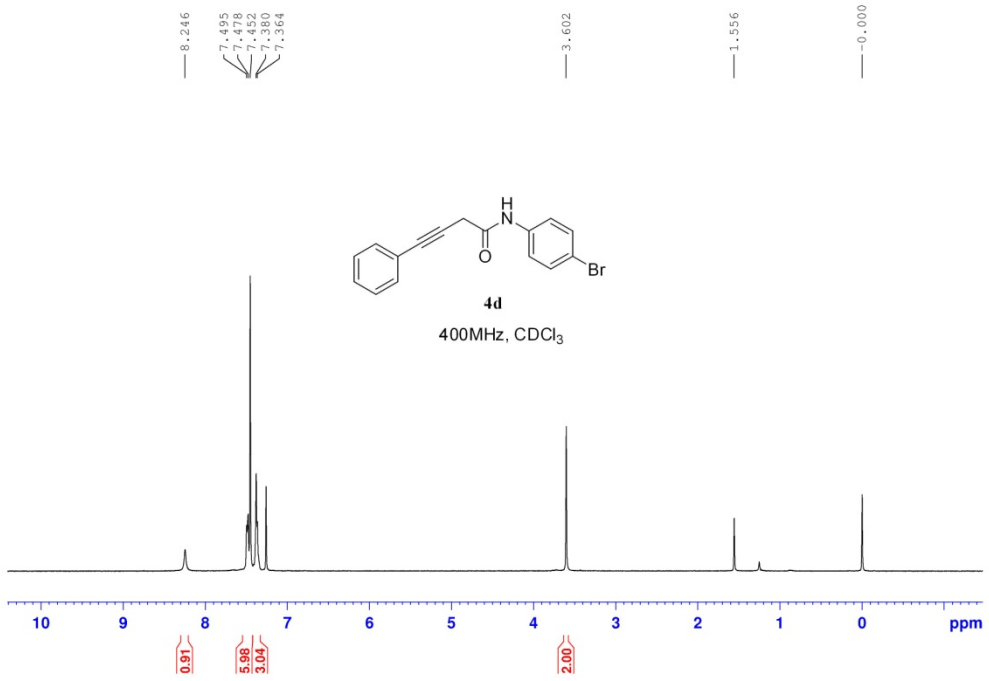


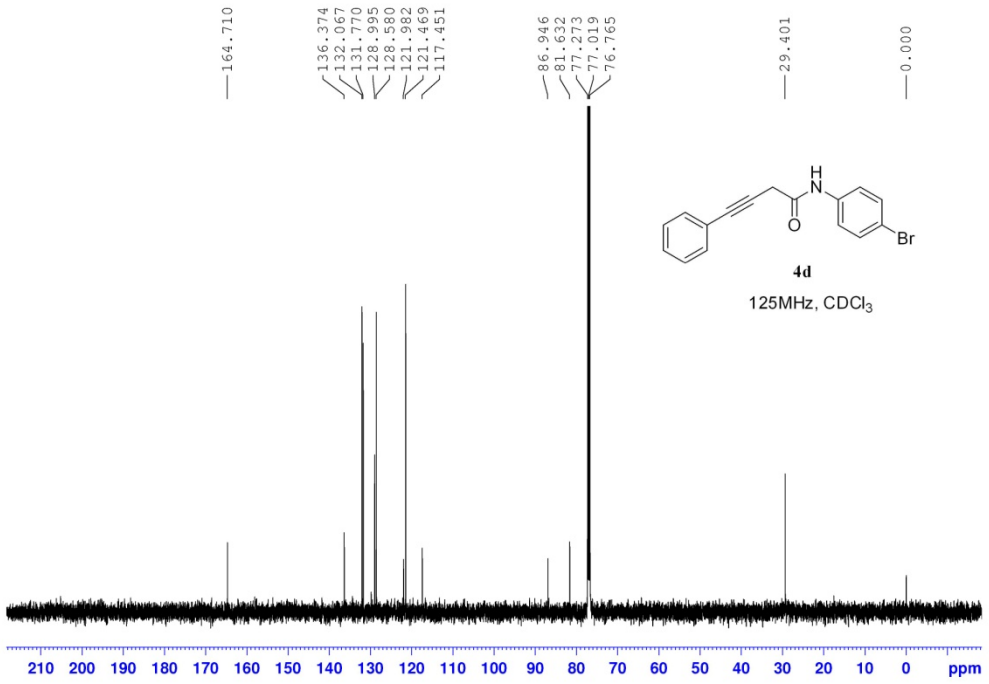
NMR spectra of compounds 4c



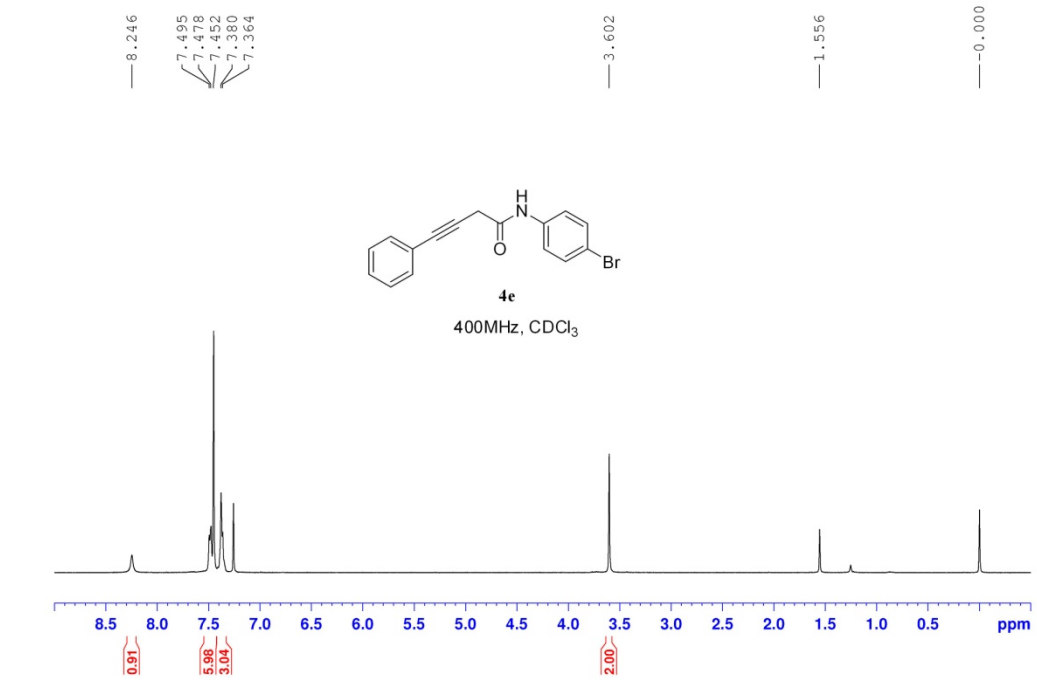


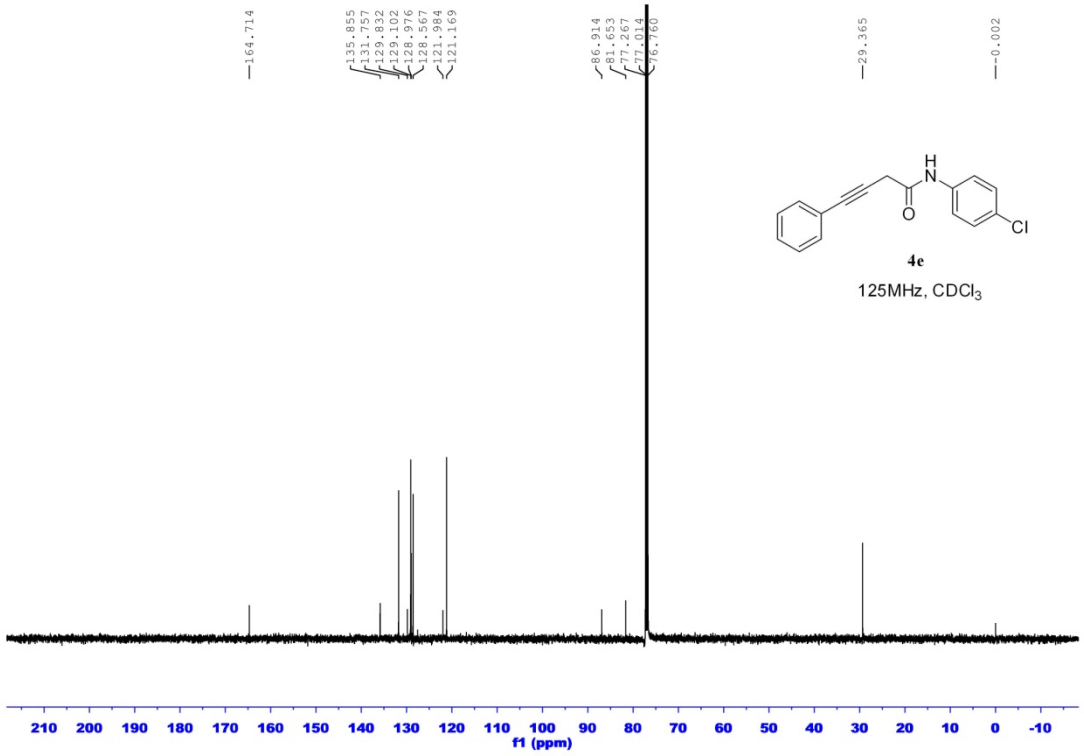
NMR spectra of compounds 4d



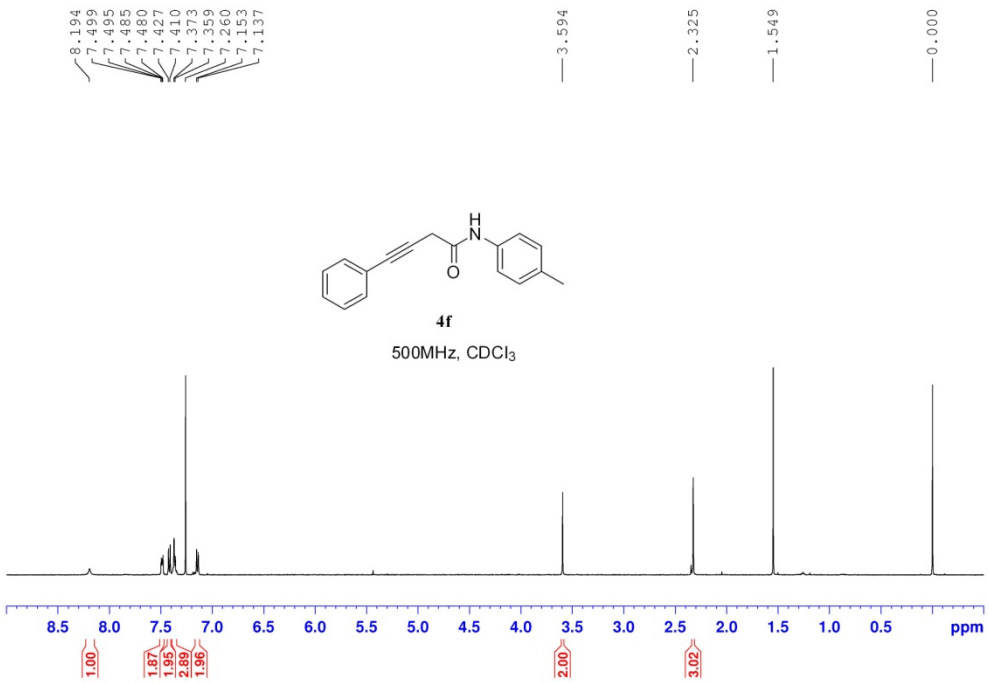


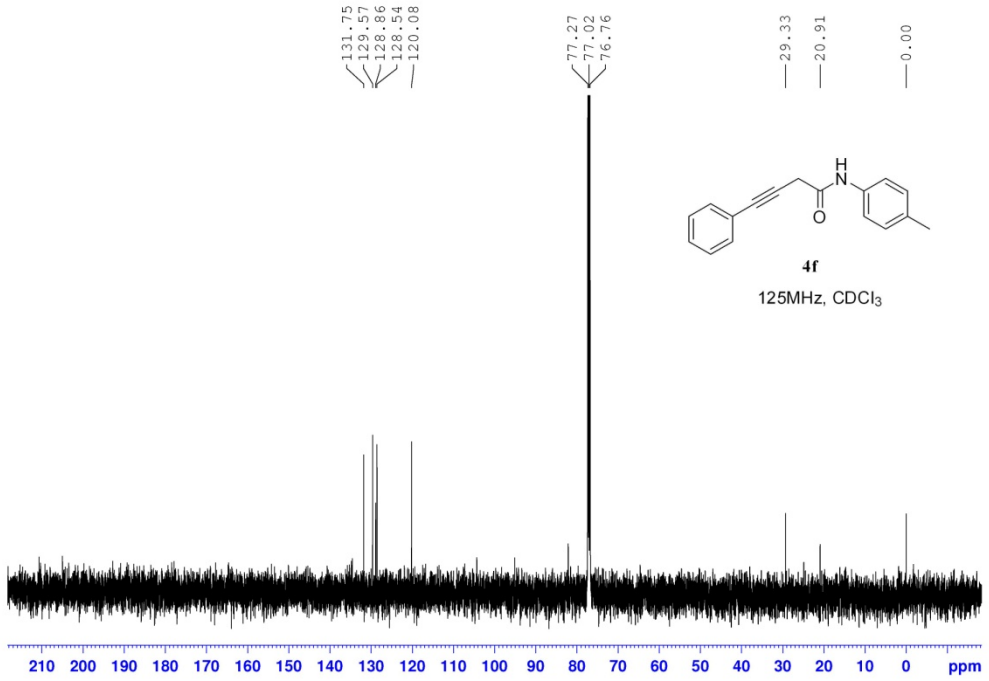
NMR spectra of compounds 4e



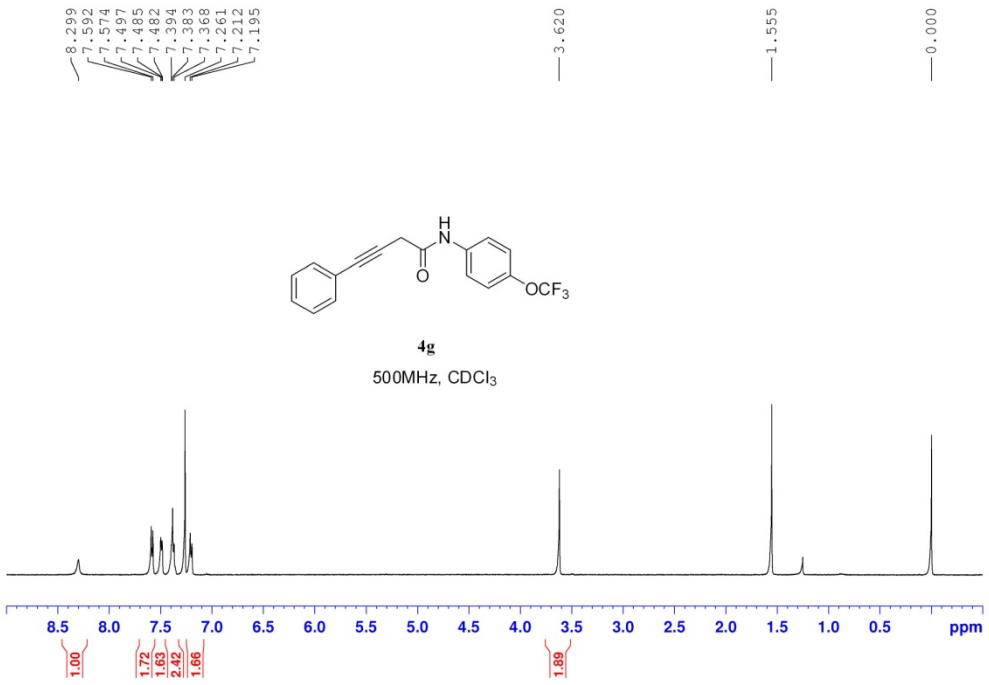


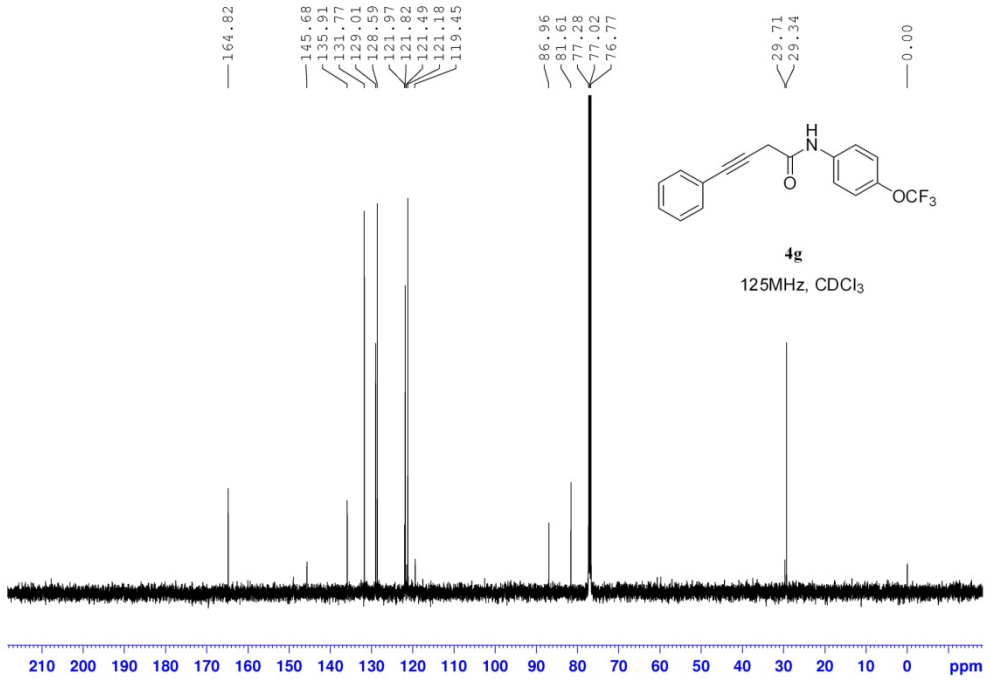
NMR spectra of compounds 4f



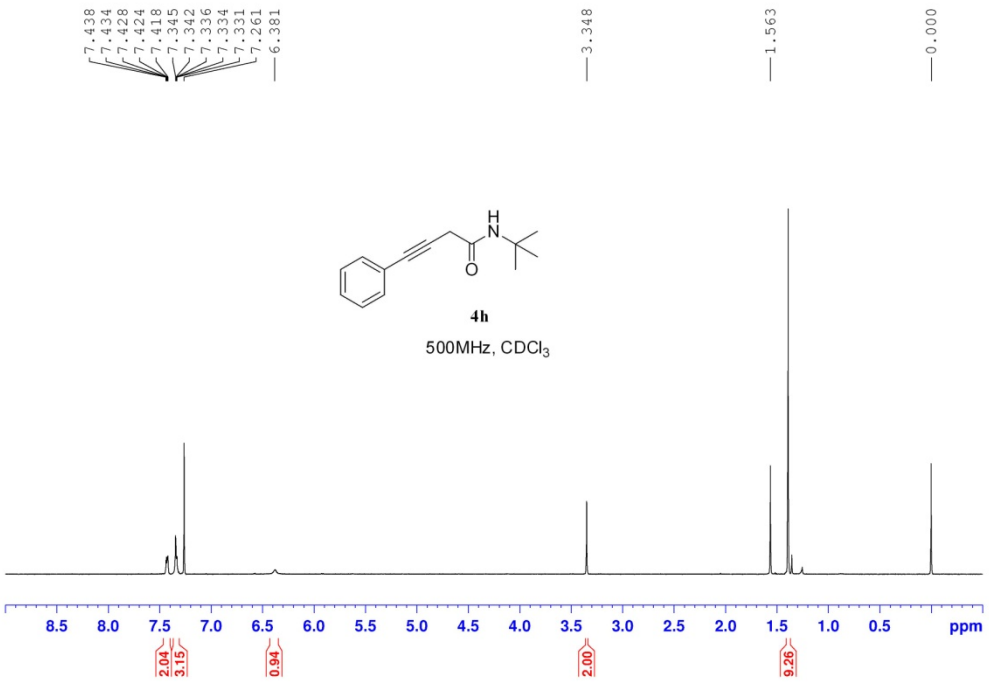


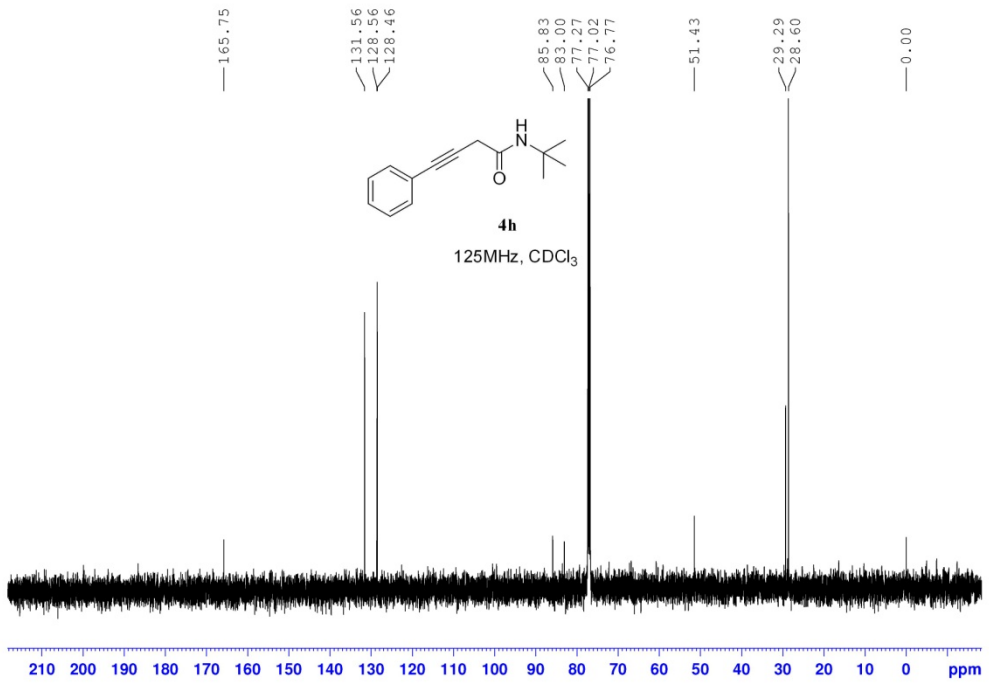
NMR spectra of compounds 4g



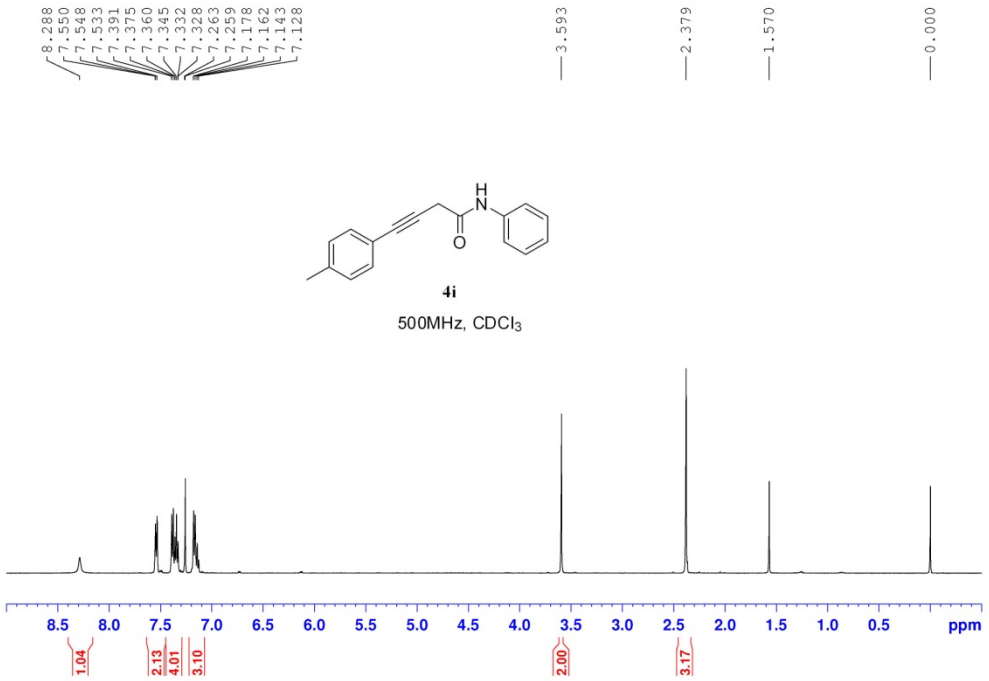


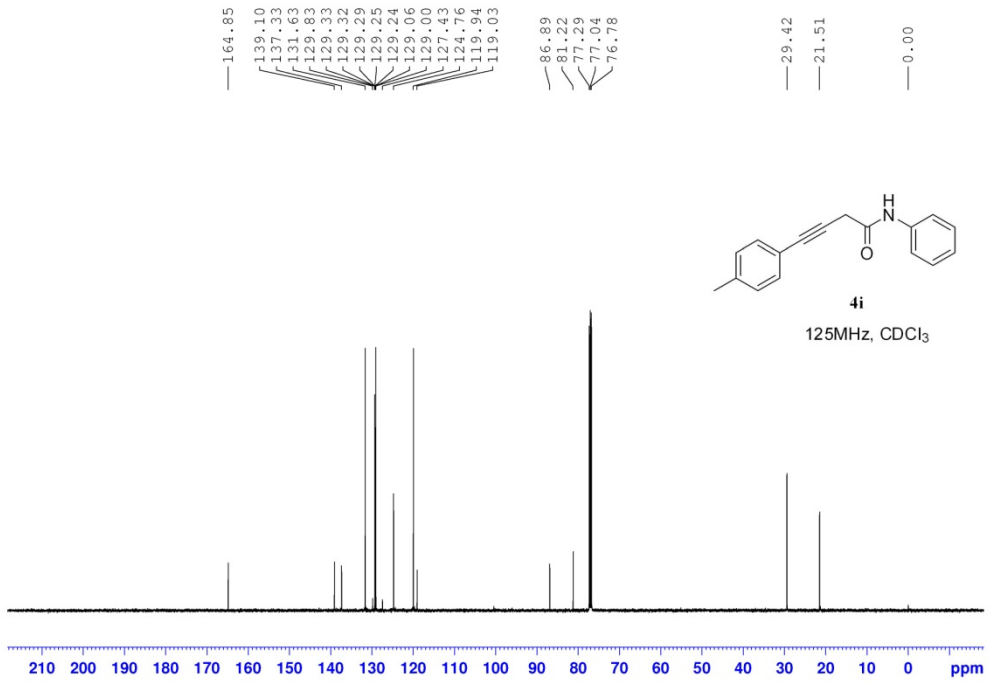
NMR spectra of compounds 4h



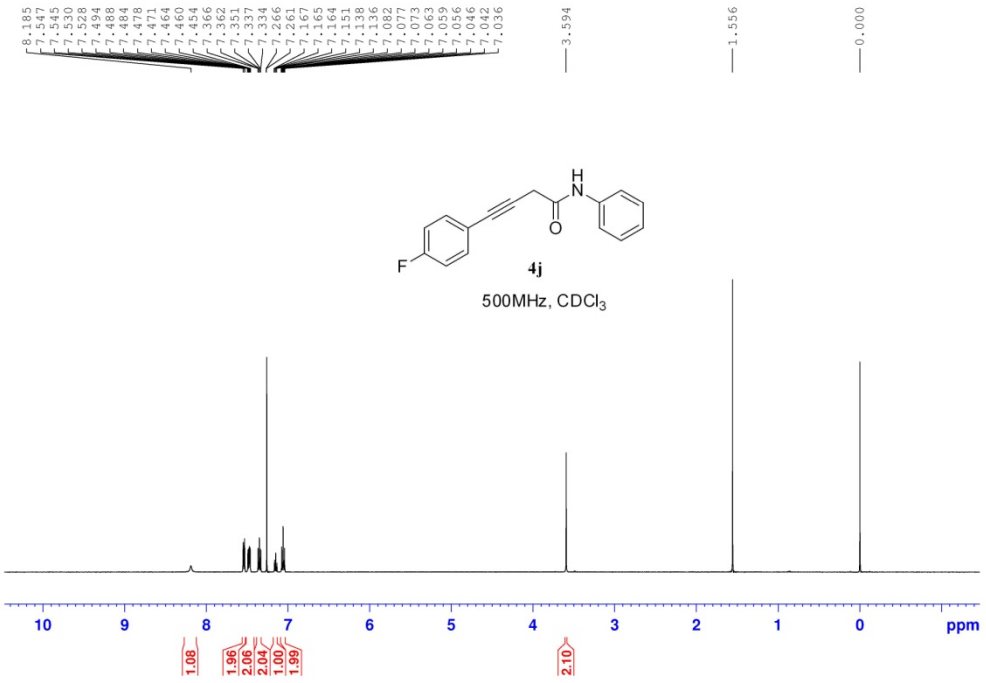


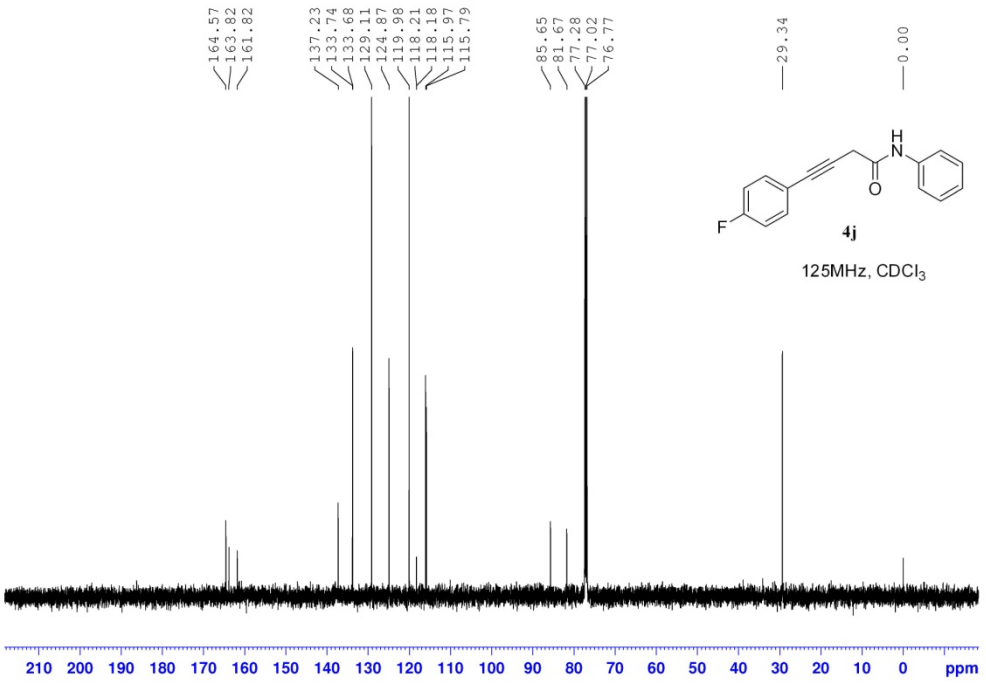
NMR spectra of compounds 4i



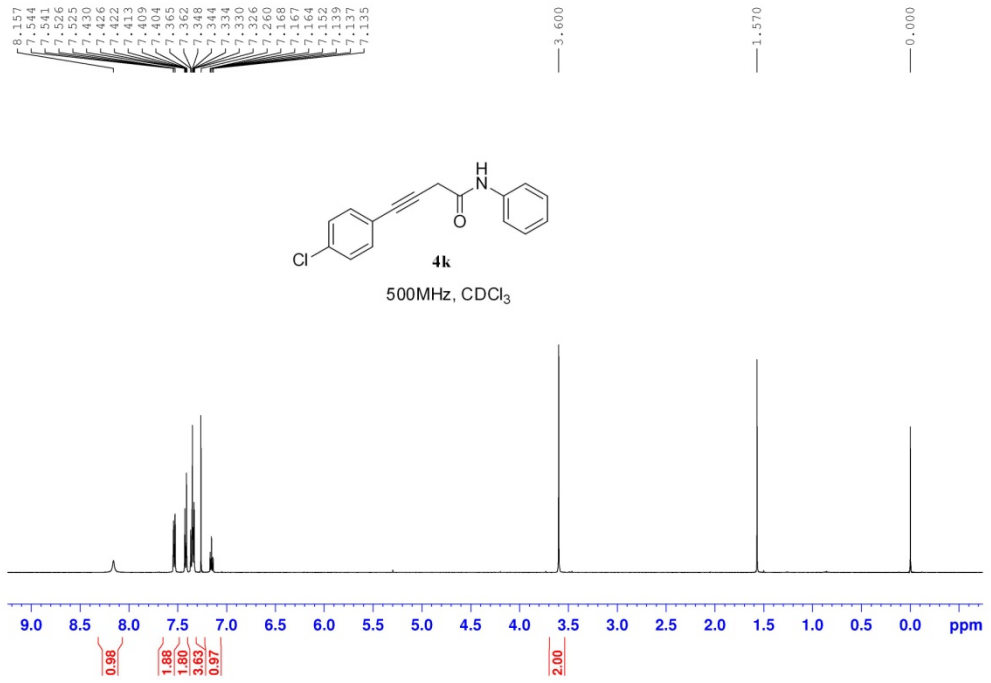


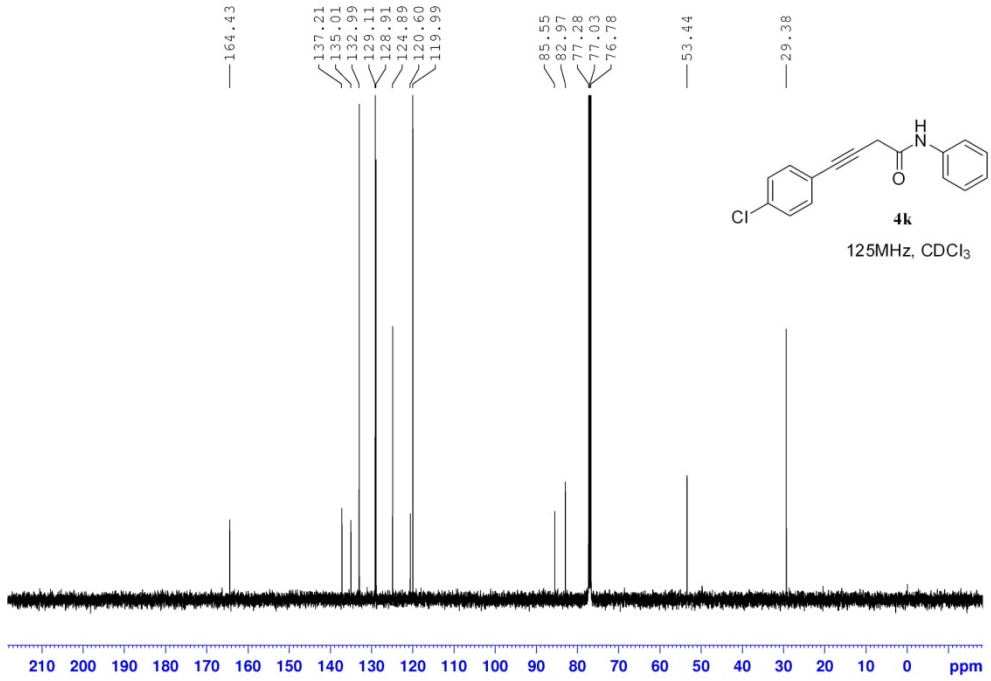
NMR spectra of compounds 4j



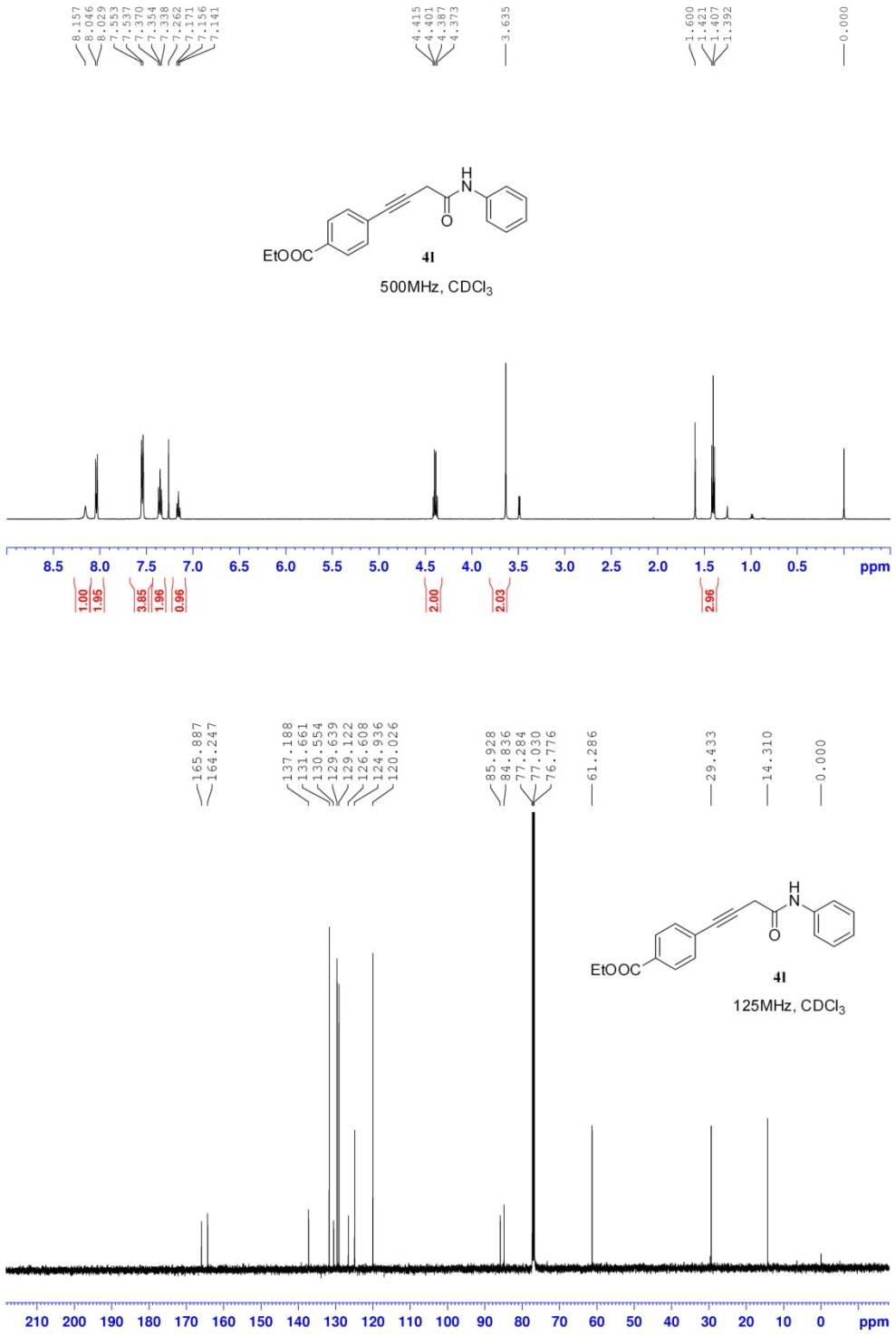


NMR spectra of compounds 4k

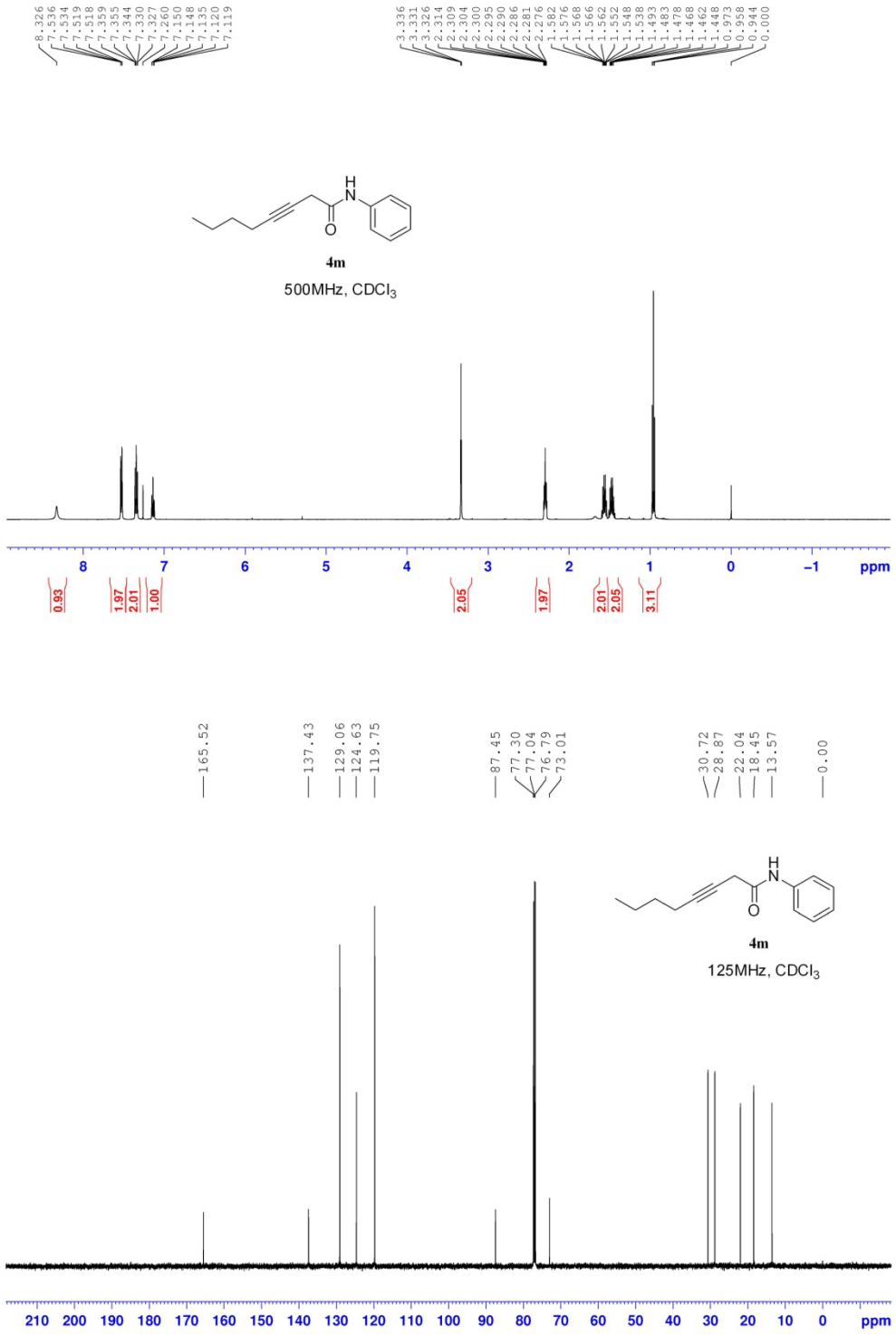




NMR spectra of compounds 4l



NMR spectra of compounds 4m



NMR spectra of compounds 4n