Electronic Supplementary Material (ESI) for Photochemical & Photobiological Science

Studies of the Solvatochromic Emission Properties of *N*-Aroylurea Derivatives I: Influence of the Substitution Pattern

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SUPPORTING INFORMATION

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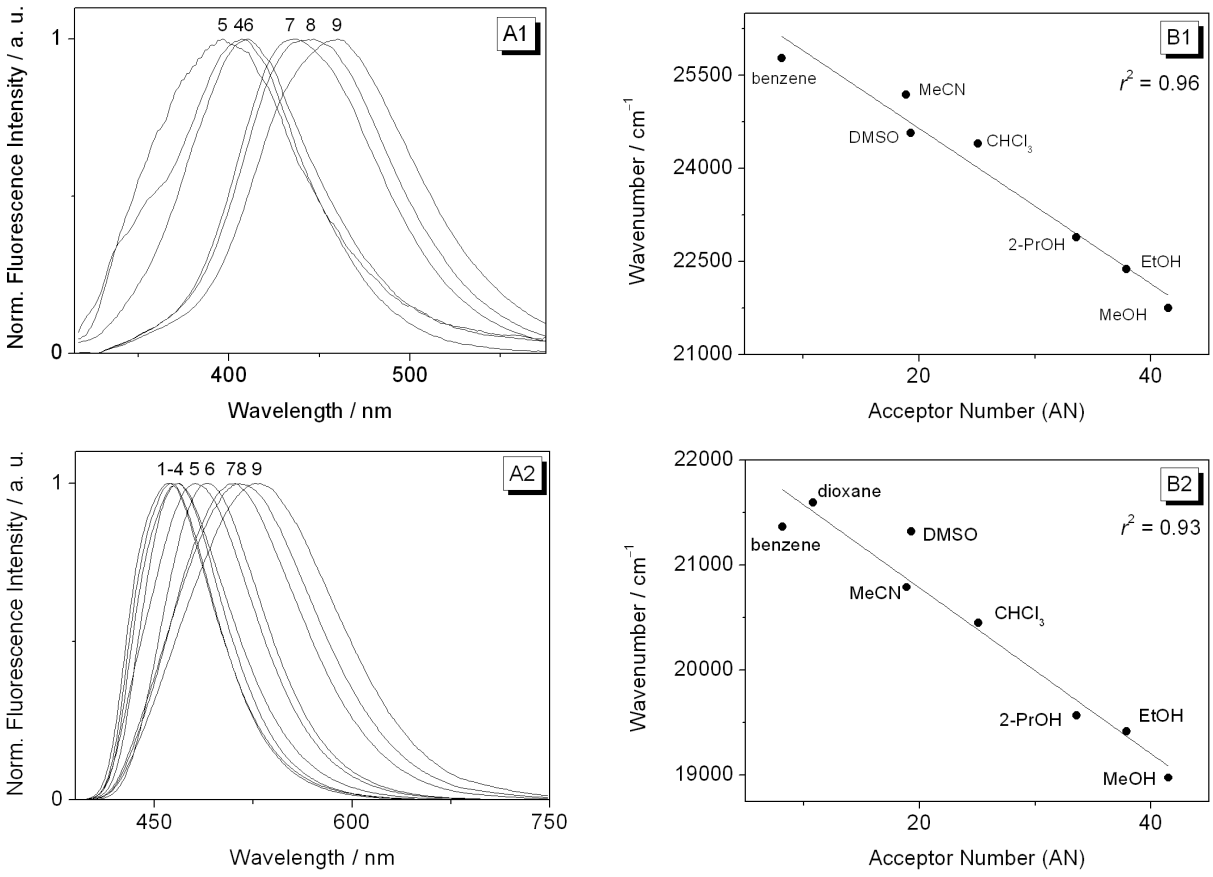

Fig. S1 A: Normalized emission spectra of **2f** (1) and **2j** (2) (**2f**: λ_{ex} = 300 nm, **2j**: λ_{ex} = 380 nm) in selected solvents (1: cyclohexane; 2: 1,4-dioxane; 3: benzene; 4: DMSO; 5: MeCN; 6: $CHCl_3$; 7: 2-PrOH; 8: EtOH; 9: MeOH). B: Correlation of the emission maxima (in cm^{-1}) of **2f** (1) and **2j** (2) with the acceptor number of the solvent.

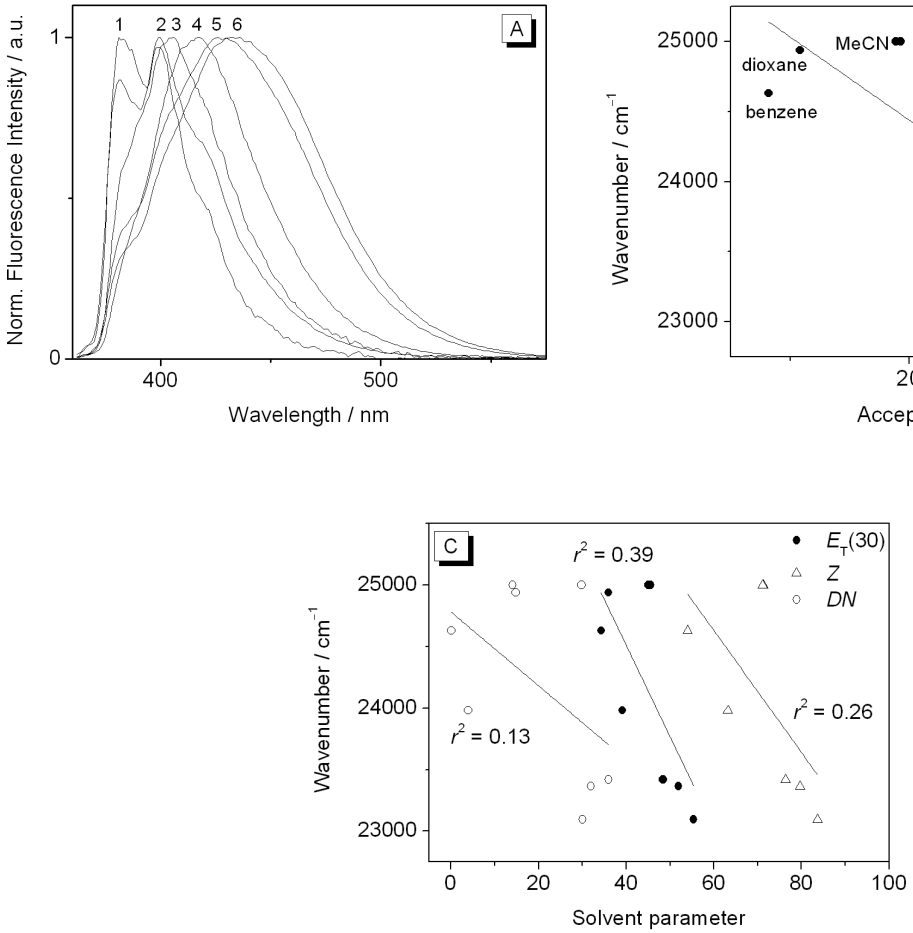

Fig. S2 A: Normalized emission spectra of **2b** (λ_{ex} = 345 nm) in selected solvents (1: cyclohexane; 2: MeCN; 3: benzene; 4: $CHCl_3$; 5: EtOH; 6: MeOH). Correlation of the emission maxima (in cm^{-1}) of **2b** with the acceptor number (B) or the $E_T(30)$, Z and DN-parameters (C) of the solvent.

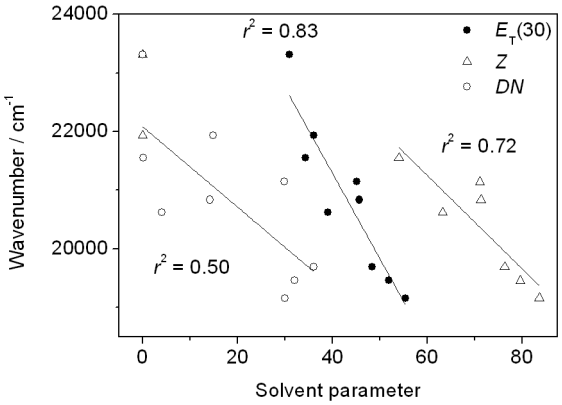

Fig. S3 Correlation of the emission maxima (in cm^{-1}) of **2c** with the $E_T(30)$, Z and DN-parameters of the solvent.

Table S1 Transient Lifetimes of the Aroylurea Derivatives **2d** and **2g** in MeCN[a].

	cond.[b]	τ_i / μs	ΔA_{max}
2d	N_2	12.7	6.3×10^{-2}
2d	Air	0.2	5.8×10^{-2}
2d	O_2	0.04	5.7×10^{-2}
2g	N_2	5.8	7.1×10^{-2}
2g	Air	0.4	6.0×10^{-2}
2g	O_2	0.1	4.7×10^{-2}

[a] **2d**: $c = 10^{-4}$ M, λ_{ex} = 355 nm; **2g**: $c = 8 \times 10^{-5}$ M, λ_{ex} = 266 nm; [b] solutions were saturated for 20 min either with nitrogen or oxygen or equilibrated with air.

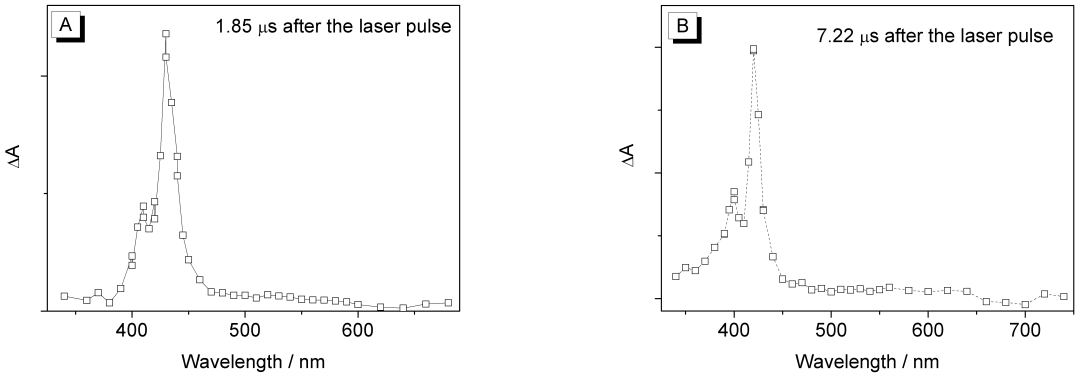

Fig. S4 Transient absorption spectra of **2d** (A: $c = 10^{-4}$ M) and **2g** (B: $c = 8 \times 10^{-5}$ M) in acetonitrile.

X-ray diffraction analysis

Single crystals of **2d** were measured on a SIEMENS SMART 1K CCD diffractometer at approx. 171 K. The structure was determined by direct methods using the program SHELXS.[1] Refinement was performed on F^2 values using the program SHELXL-97. Hydrogen atoms were geometrically positioned and were constrained. The crystal data and the structure refinement details are collected in Table S2.

[1] Sheldrick, G. M. *Acta Cryst.*, 2008, **A64**, 112-122.

Table S2 Crystal data and structure refinement details of compound **2d**.

Parameter		
Molecular formula (formula weight)	$C_{28}H_{32}N_2O_2$ (428.56 g/mol)	
Temperature / K	171 (2)	
Wavelength / Å	0.71073	
Crystal system, space group	Monoclinic, $P2_1/n$	
Unit cell dimensions	a = 10.6241 (8) Å	$\alpha = 90°$
	b = 9.6218 (7) Å	β = 93.646 (2)°
	c = 22.9510 (16) Å	$\gamma = 90°$
Volume / Å^3	2341.4 (3)	
Z	4	
Calculated density /g·cm^{-1}	1.216	
Absorption coefficient / mm^{-1}	0.076	
F (000)	920	
Crystal size / mm	0.55 × 0.14 × 0.12	
Meausured θ range	$1.78 \geq \theta \geq 25.00$	
Limiting indices	$-12 \geq h \geq 12$	
	$-11 \geq k \geq 11$	
	$-27 \geq l \geq 26$	
Reflections collected / unique	19491 / 4056	
R_{int}	0.164	
Data / restraints/ parameters	4056 / 0 / 289	
Goodness of fit on F^2	1.12	
R values [$I \geq 2\sigma$ (I)]	R_1 = 0.109; wR_2 = 0.132	
R values (all data)	R_1 = 0.237; wR_2 = 0.163	
Final Fourier residuals	0.19 and –0.22 eÅ^{-3}	

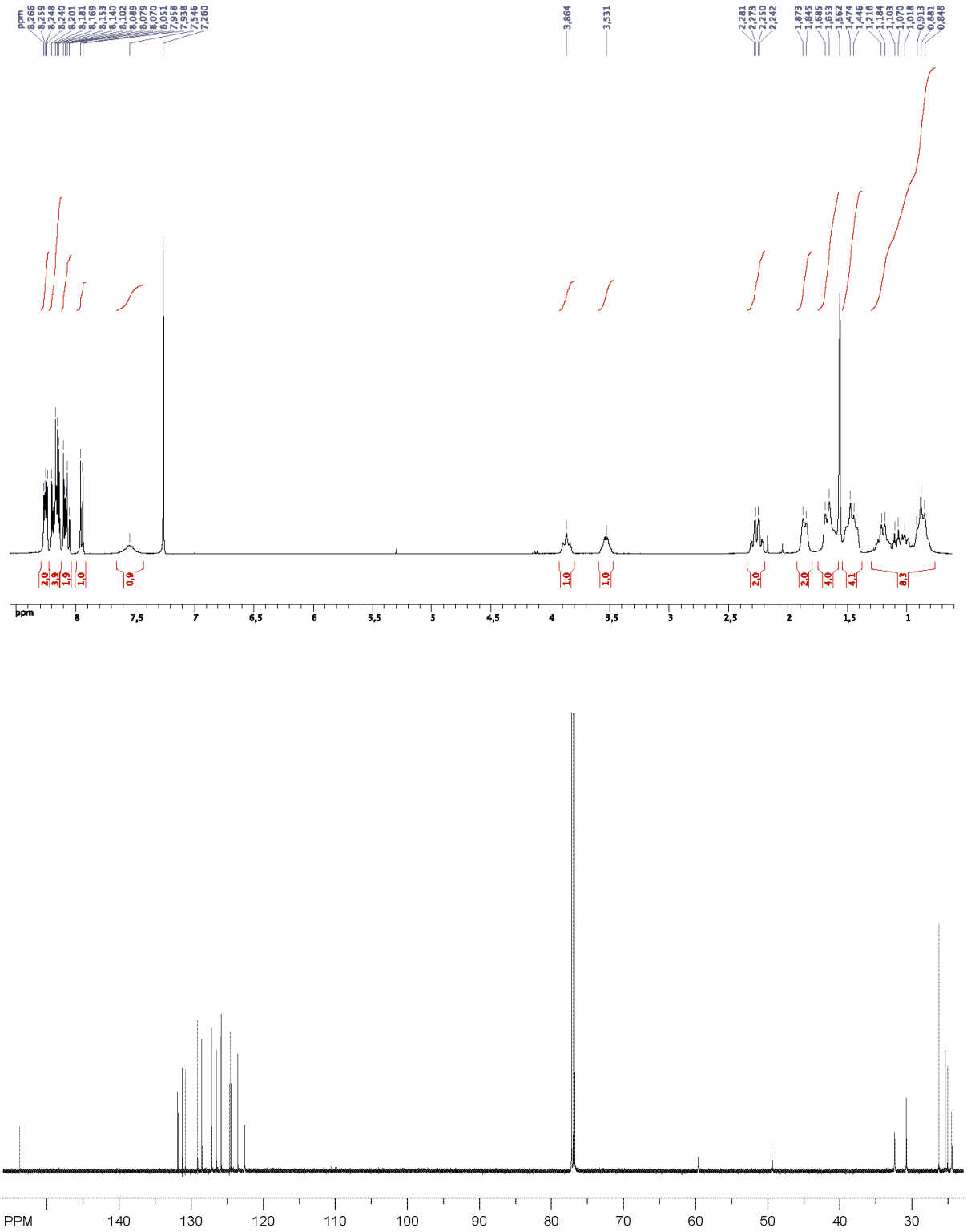

Fig. S5 ^{1}H- and ^{13}C-NMR spectra of **2b** in $CDCl_3$.

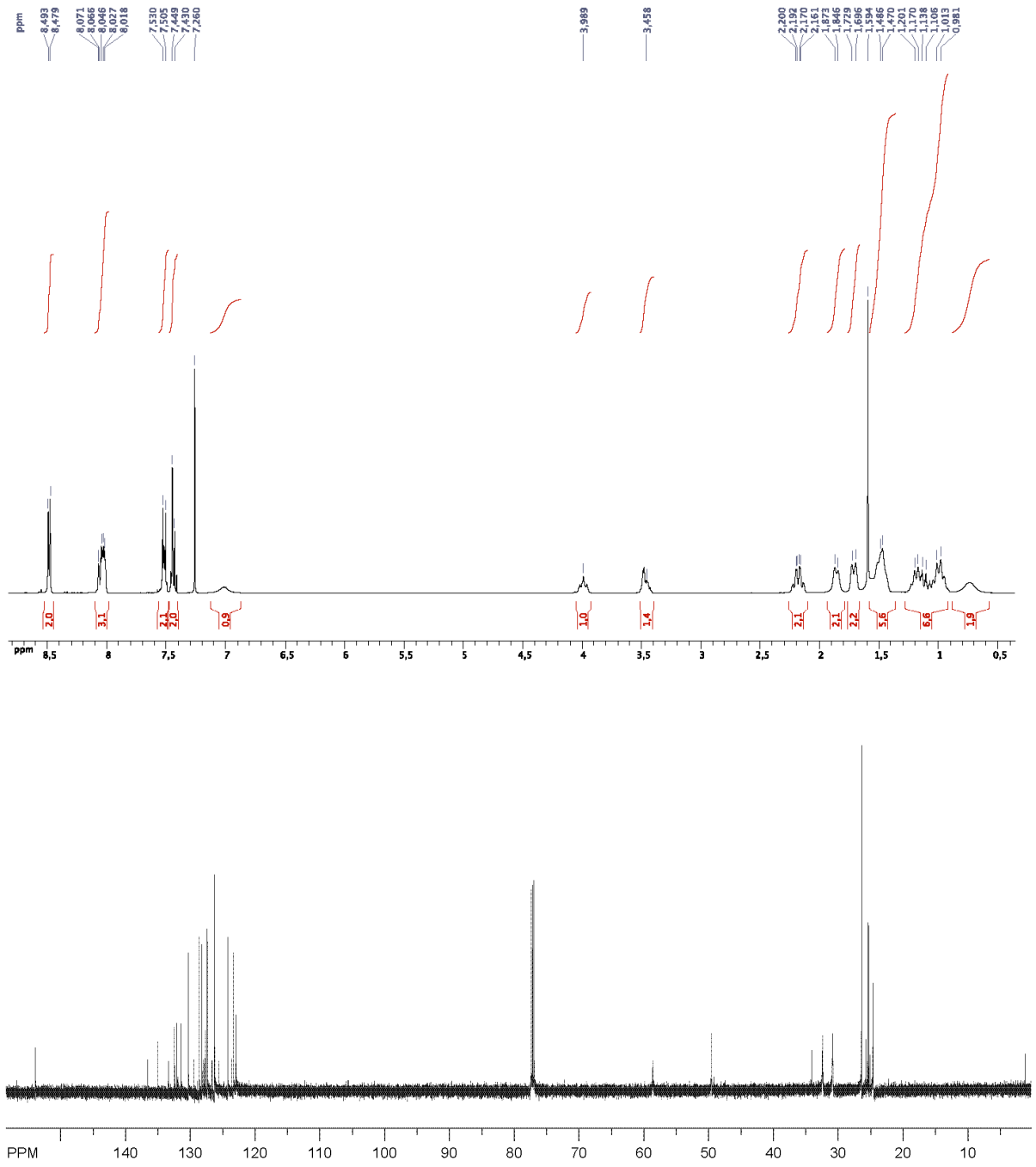

Fig. S6 ^{1}H- and ^{13}C-NMR spectra of **2c** in $CDCl_3$.

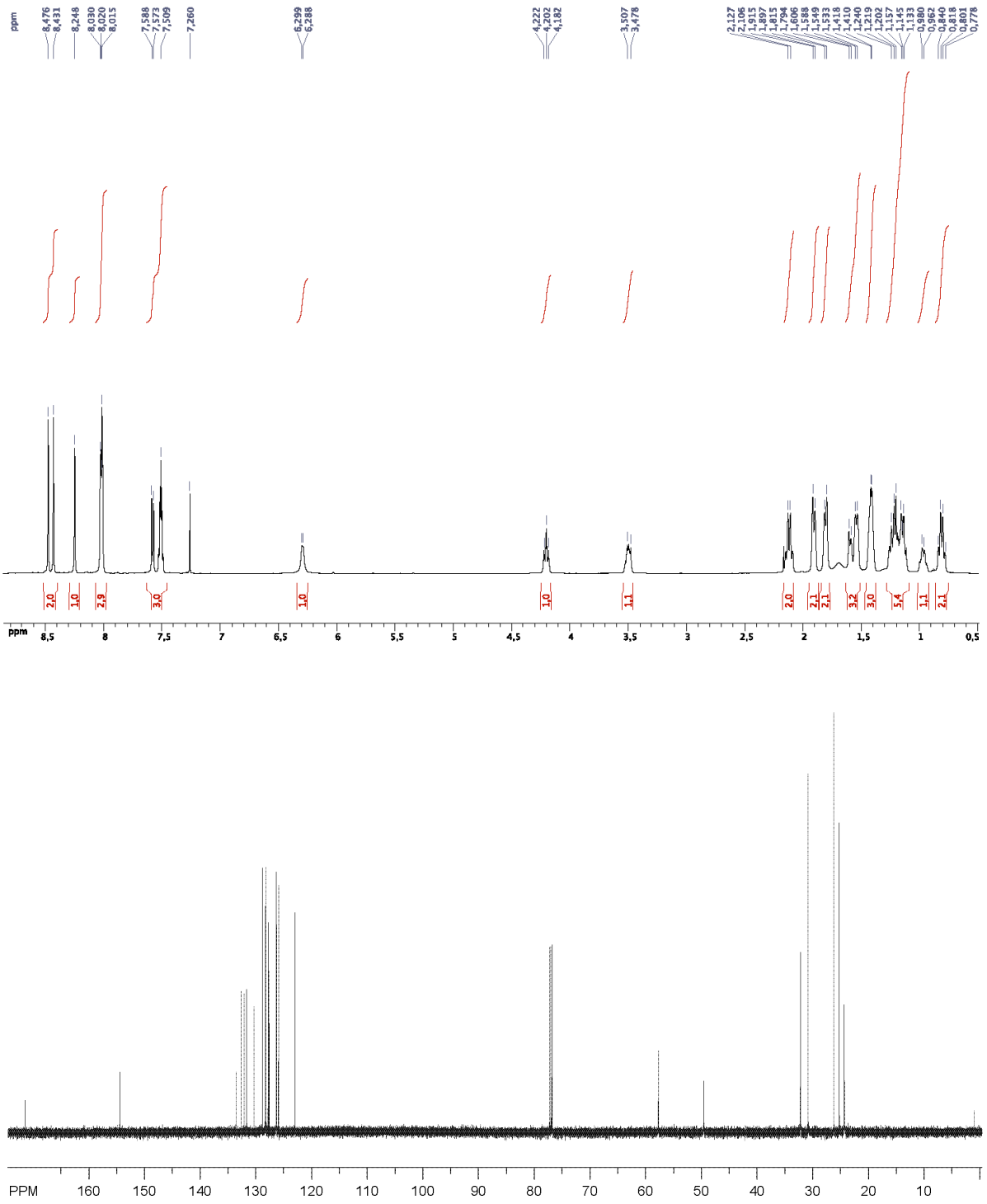

Fig. S7 ^{1}H- and ^{13}C-NMR spectra of **2d** in $CDCl_3$.

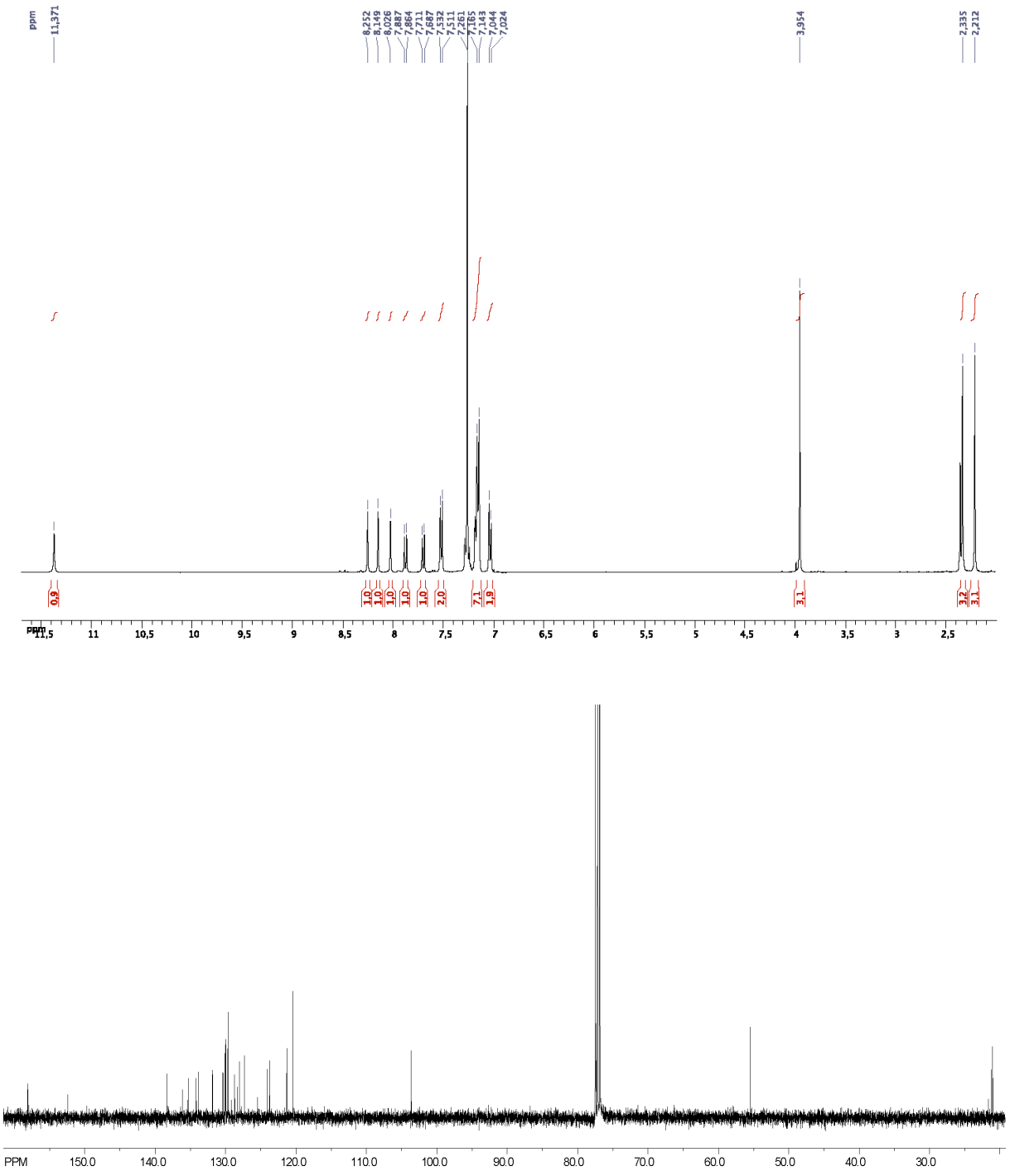

Fig. S8 ^{1}H- and ^{13}C-NMR spectra of **2e** in $CDCl_3$.

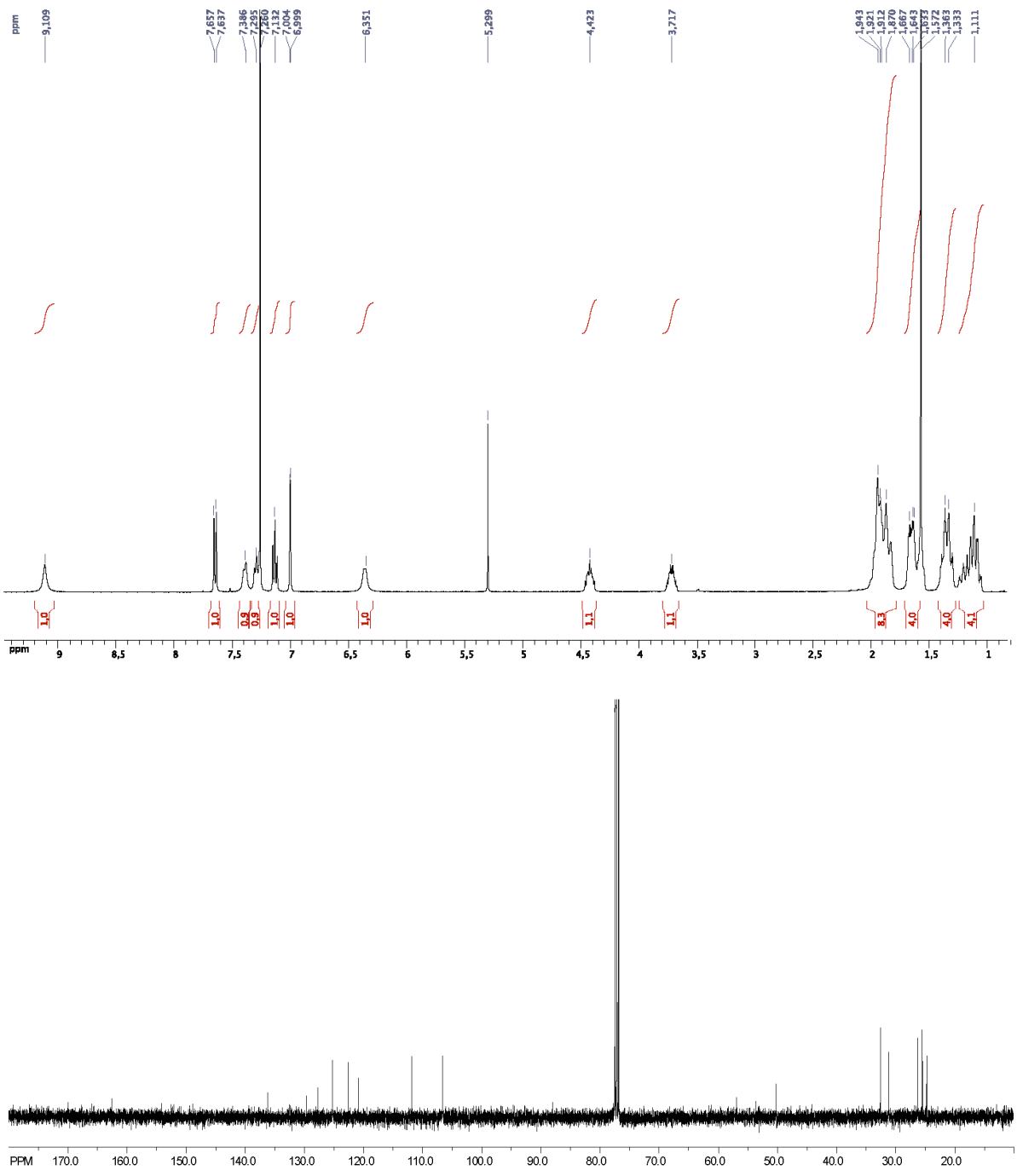

Fig. S9 ^{1}H- and ^{13}C-NMR spectra of **2f** in $CDCl_3$.

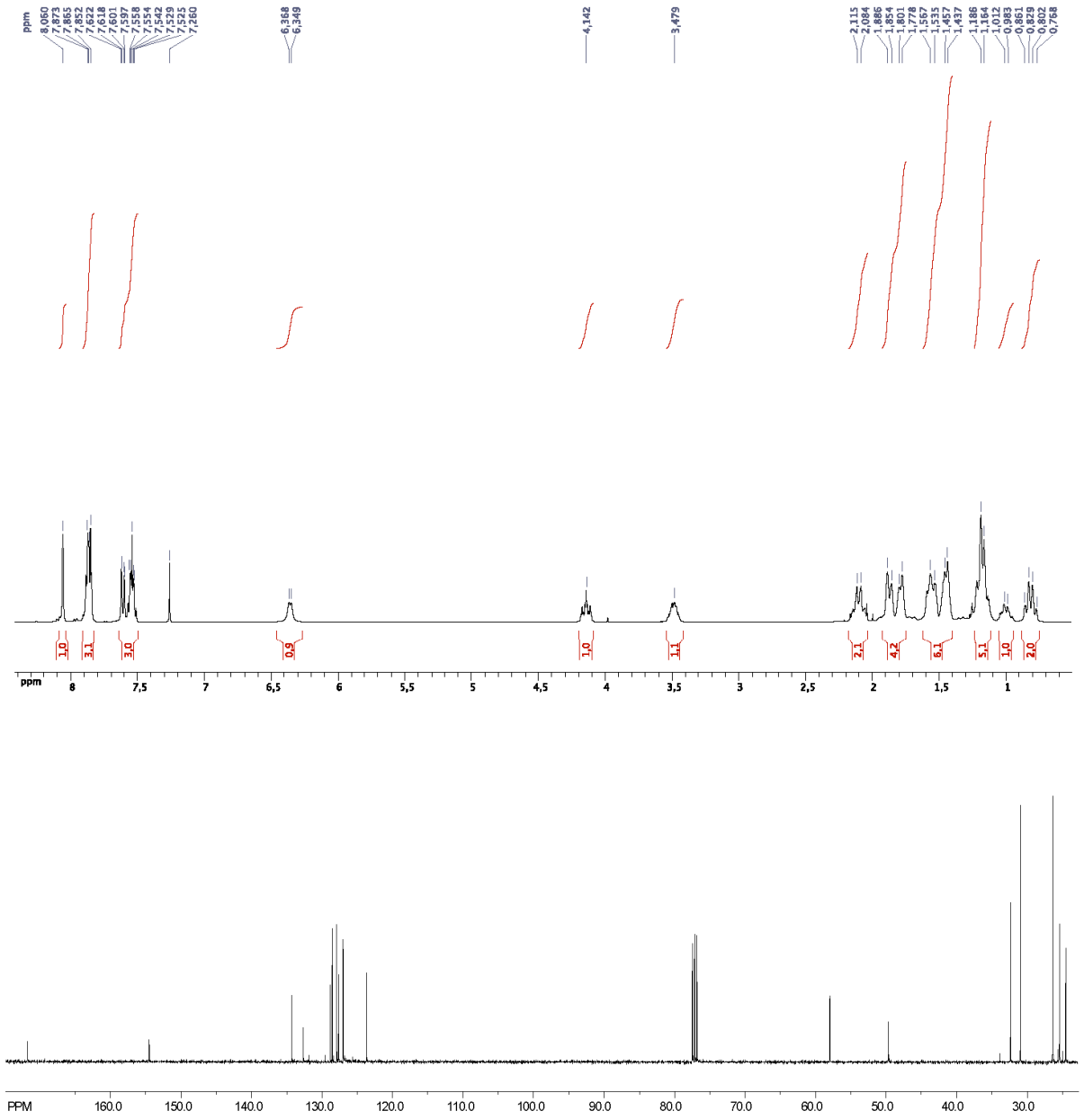

Fig. S10 ^{1}H- and ^{13}C-NMR spectra of **2g** in $CDCl_3$.

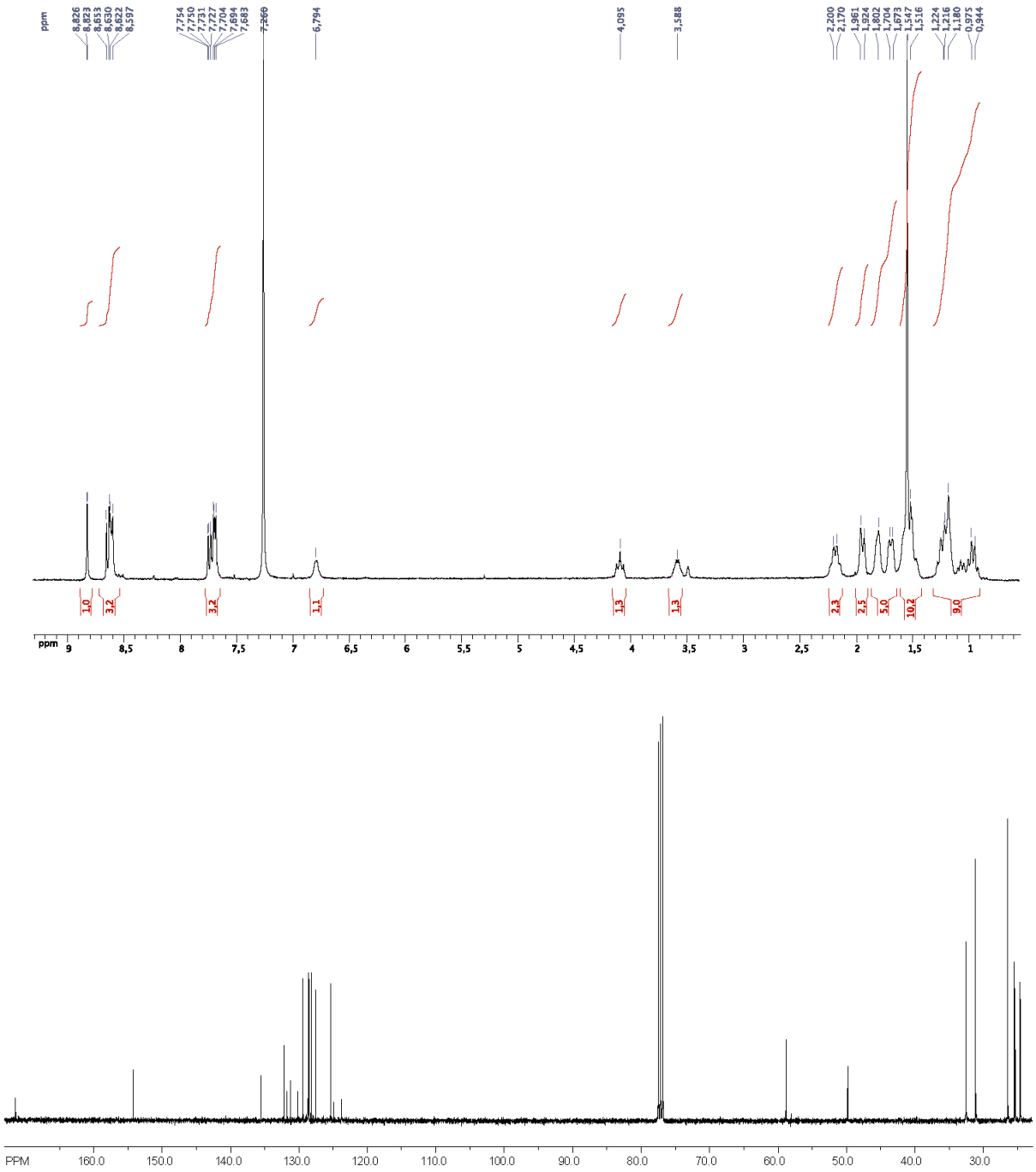

Fig. S11 ^{1}H- and ^{13}C-NMR spectra of **2h** in $CDCl_3$.

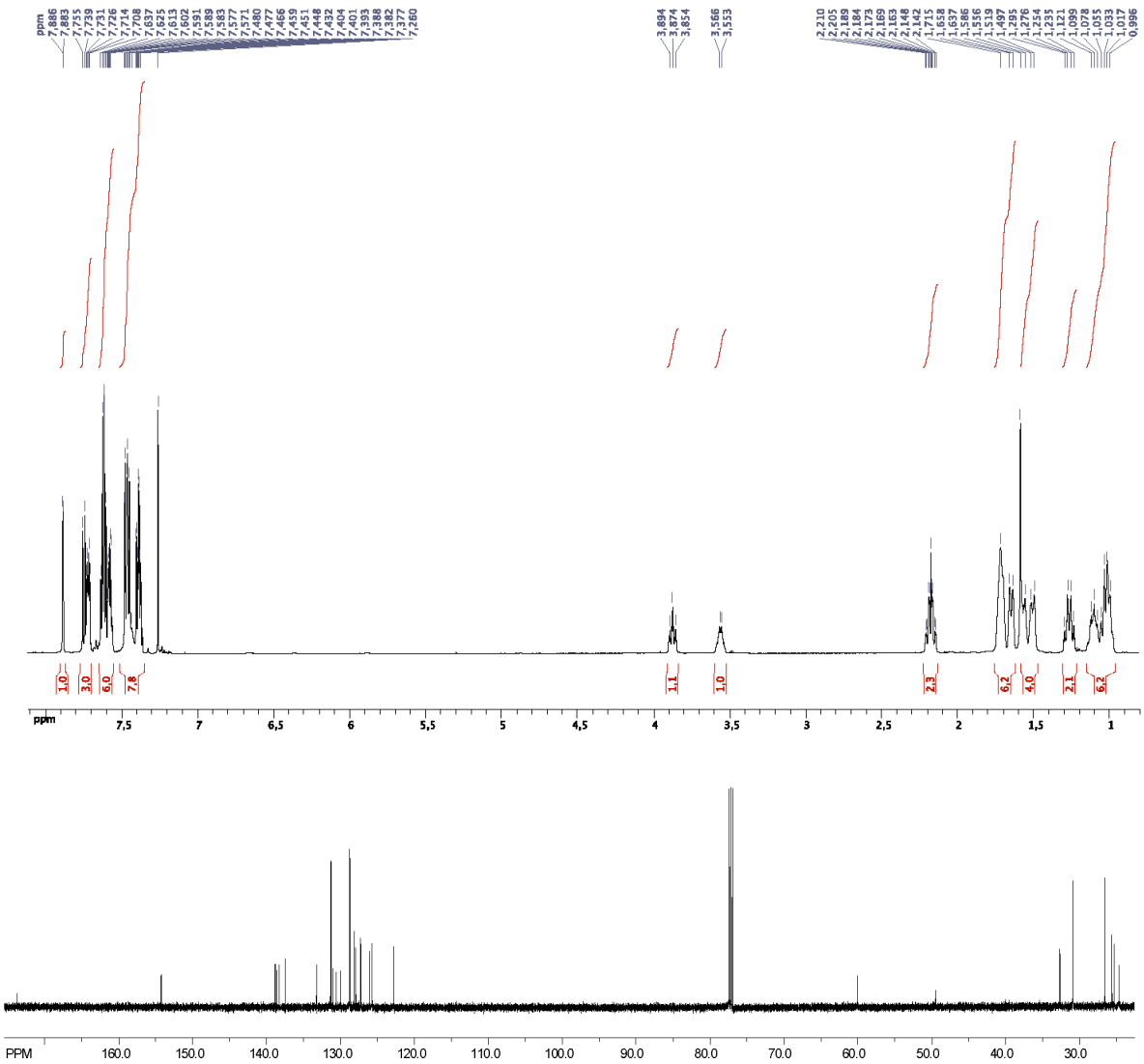

Fig. S12 ^{1}H- and ^{13}C-NMR spectra of **2i** in $CDCl_3$.

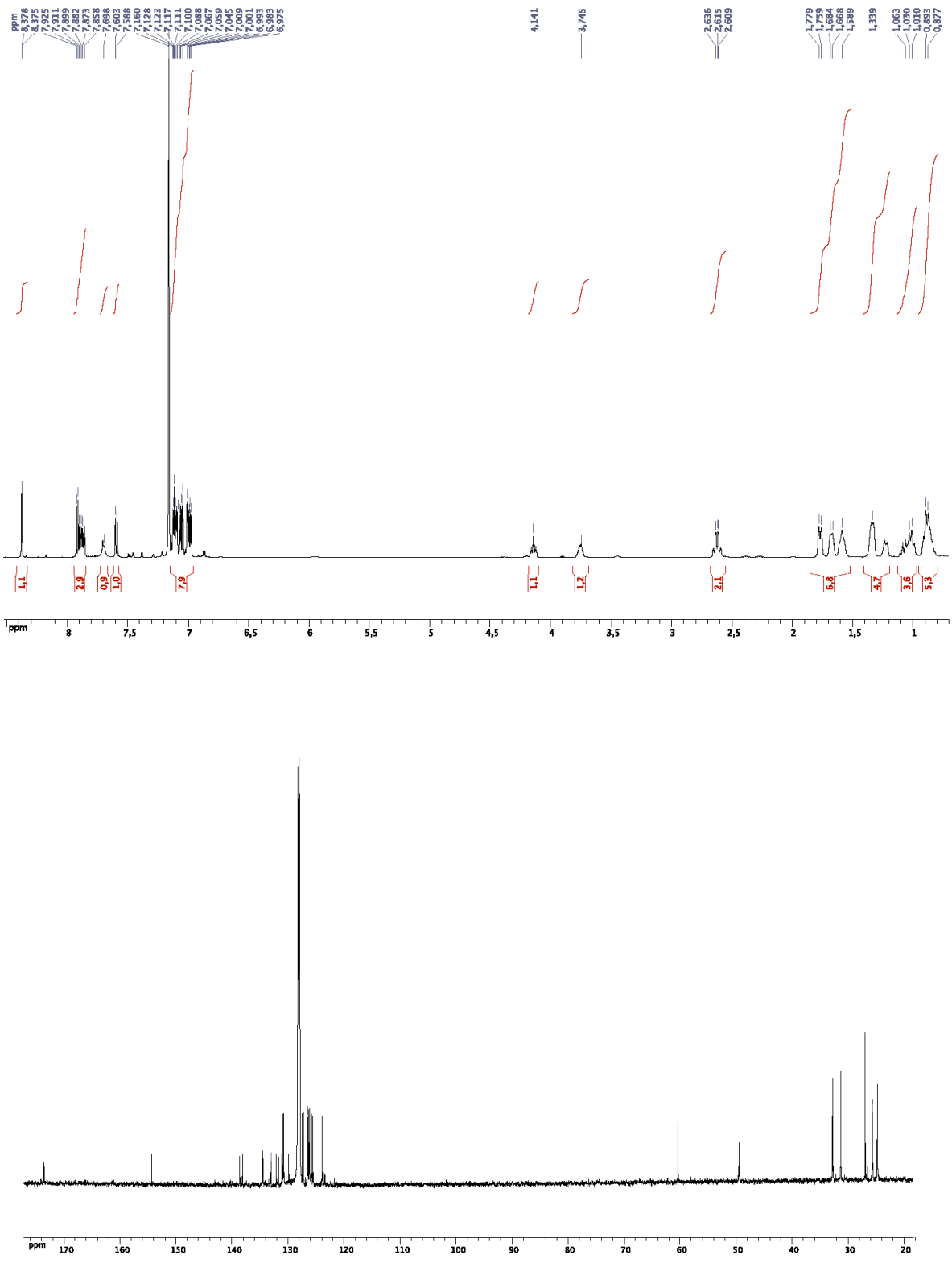

Fig. S13 ^{1}H- and ^{13}C-NMR spectra of **2j** in C_6D_6.