Electronic Supplementary Material (ESI) for RSC Advances

Fluorimetric anion sensing by bisquinolinium pyridine-2,6-dicarboxamide receptors in water

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Electronic Supplementary Information

Table S1. Crystallographic data for compounds, **2-6**

Crystal data[a]	**2**[b]	**3**[b]	**4**[b]	**5**[c]	**6**[c]
Formula	$C_{29}H_{29}F_6N_5O_{11}S_2$	$C_{29}H_{25}F_6N_5O_9S_2$	$C_{18}H_{15}F_3N_2O_4$ S	$C_{17}H_{15}IN_2O$	$C_{18}H_{15}F_3N_2O_4S$
MW (g mol^{-1})	801.71	765.66	412.38	390.21	412.38
Space group	*P-1*	*P 2$_1$/c*	*P 2$_1$/c*	*P-1*	*P 2$_1$/c*
a (Å)	8.9610(8)	17.2140(5)	8.4540(3)	8.2858(12)	9.3966(18)
b (Å)	11.921(1)	13.4000(3)	15.135048(5)	8.3312(12)	15.386(3)
c (Å)	16.3160(17)	14.3990(4)	14.5480(5)	11.5680(17)	12.114(2)
α (°)	83.883(8)	90	90	86.458(2)	90
β (°)	81.552(8)	103.862(3)	104.356(3)	77.472(2)	91.451(3)
γ (°)	87.348(7)	90	90	81.506(2)	90
V (Å^3)	1773.3(3)	3224.65(15)	1803.31(11)	770.62(19)	1750.8(6)
Z	2	4	4	2	4
μ (mm^{-1})	2.307	2.376	2.141	2.078	0.254
ρ_{calcd} (g cm^{-3})	1.554	1.577	1.519	1.682	1.564
R[b, c]	0.053	0.056	0.049	0.030	0.063
R_w [d, e]	0.134	0.172	0.150	0.072	0.152

[a] T = 130 K for **2**, 293-298 K for **3**-**6**. [b] $F_o > 4\sigma(F_o)$. [c] $R = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. [d] all data. [e] $R_w = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{½}$.
[b] $\lambda_{MoK\alpha}$ = 1.5418 Å
[c] $\lambda_{MoK\alpha}$ = 0.7103 Å

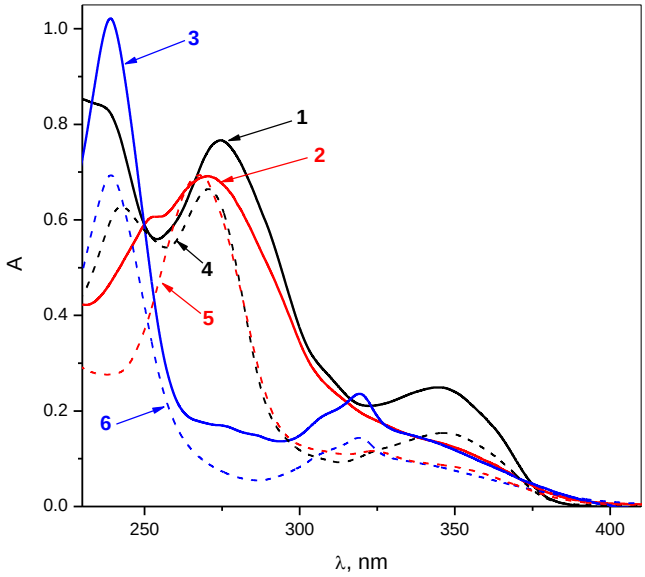

Figure 1S. Absorption spectra of 20 μM **1** – **3** (solid lines) and **4** – **6** (dashed lines) at pH 6.5.

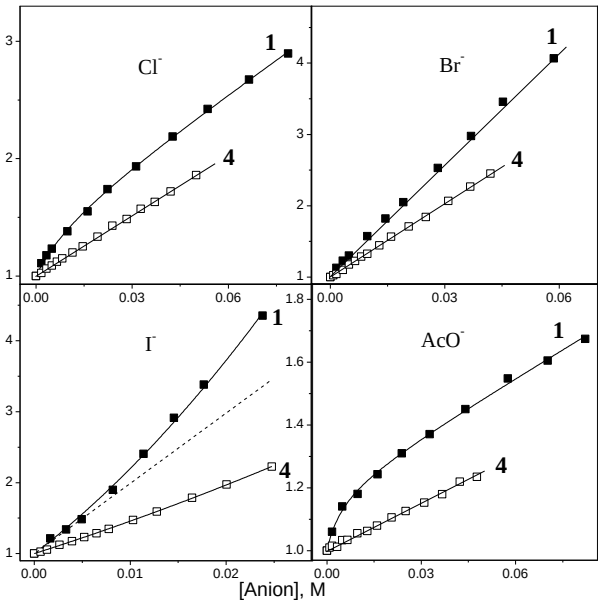

Figure 2S. Stern-Volmer plots for **1** (solid symbols) and **4** (open symbols) at pH 6.5 (excitation at 350 nm).

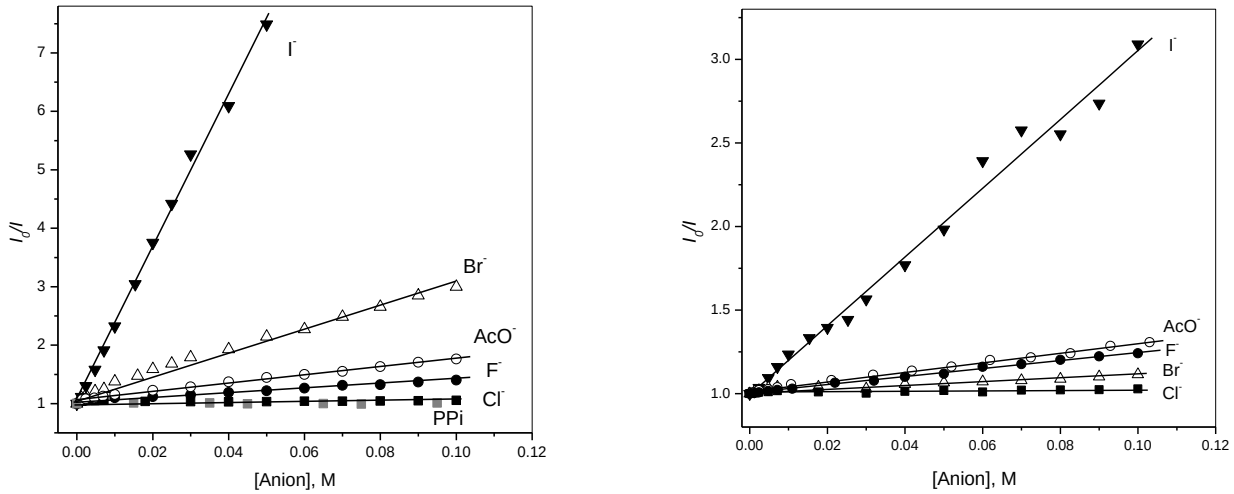

Figure 3S. (a) Quenching of **3** (excitation at 350 nm, emission at 516 nm) and (b) quenching of **6** (excitation at 350 nm, emission at 531 nm) by anions at pH 6.5.

Table 2S. Stern-Volmer constants for quenching of **3** and **6**.

Anion	**K_{SV}, M^{-1}**	
	3	**6**
F	3.6	2.45
Cl	0	0
Br	18	0.93
I	132	20.6
AcO	7.4	3.0
PPi	0	0

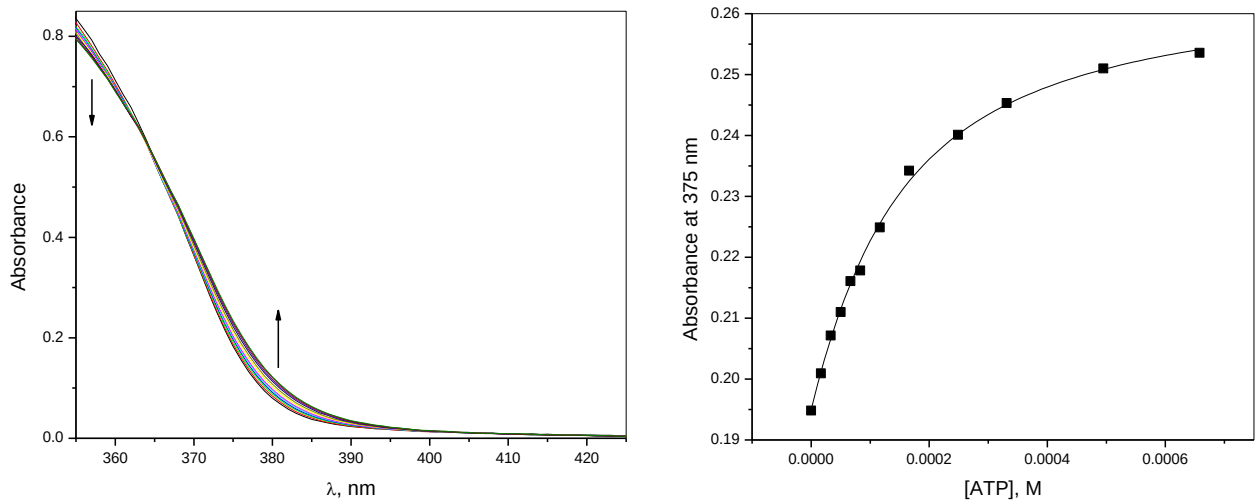

Figure 4S. (a) The course of spectrophotometric titration of 0.06 mM **1** by ATP at pH 6.5; arrows show the direction of spectral changes on addition of increased amounts of ATP. An isosbestic point is observed at 364 nm. (b) Fitting the absorbance at 375 nm to 1:1 binding isotherm.

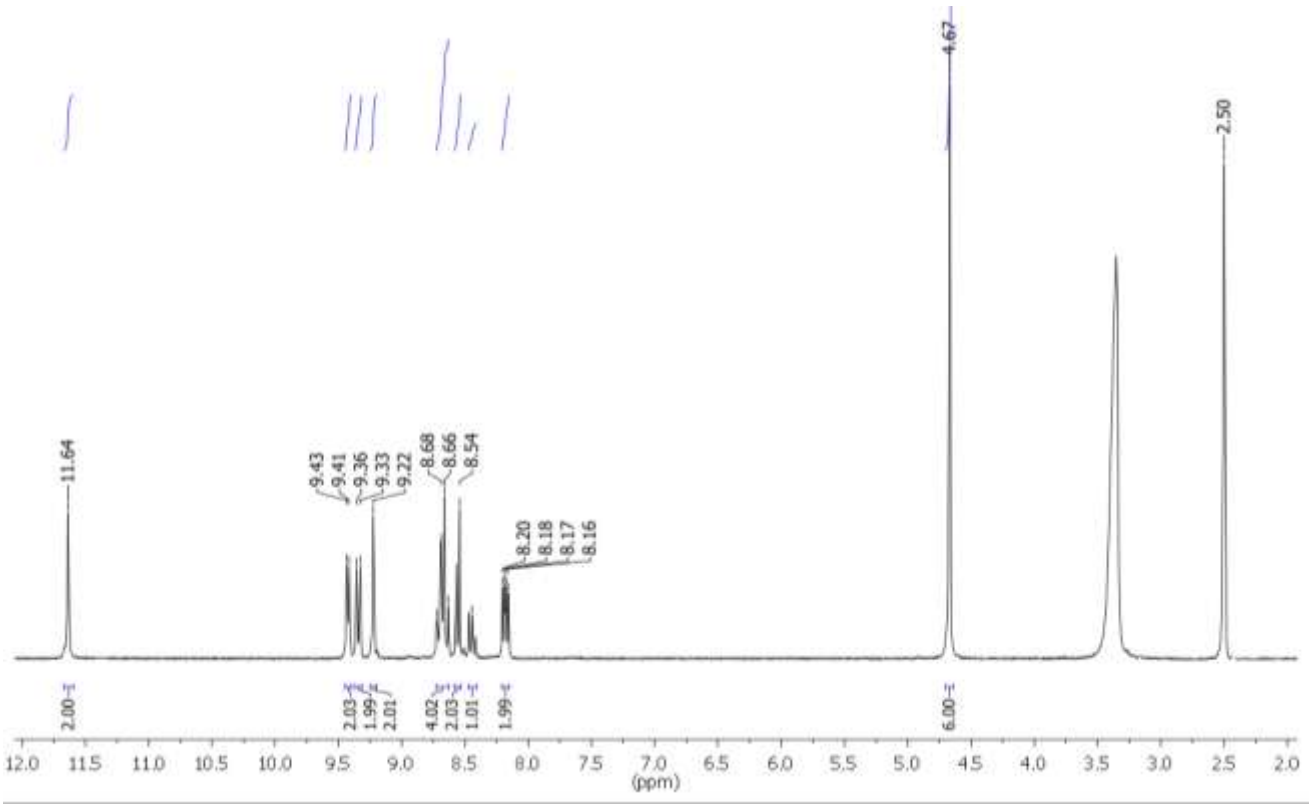

Figure 5S. ^{1}H NMR spectrum of **2** in DMSO-d_6

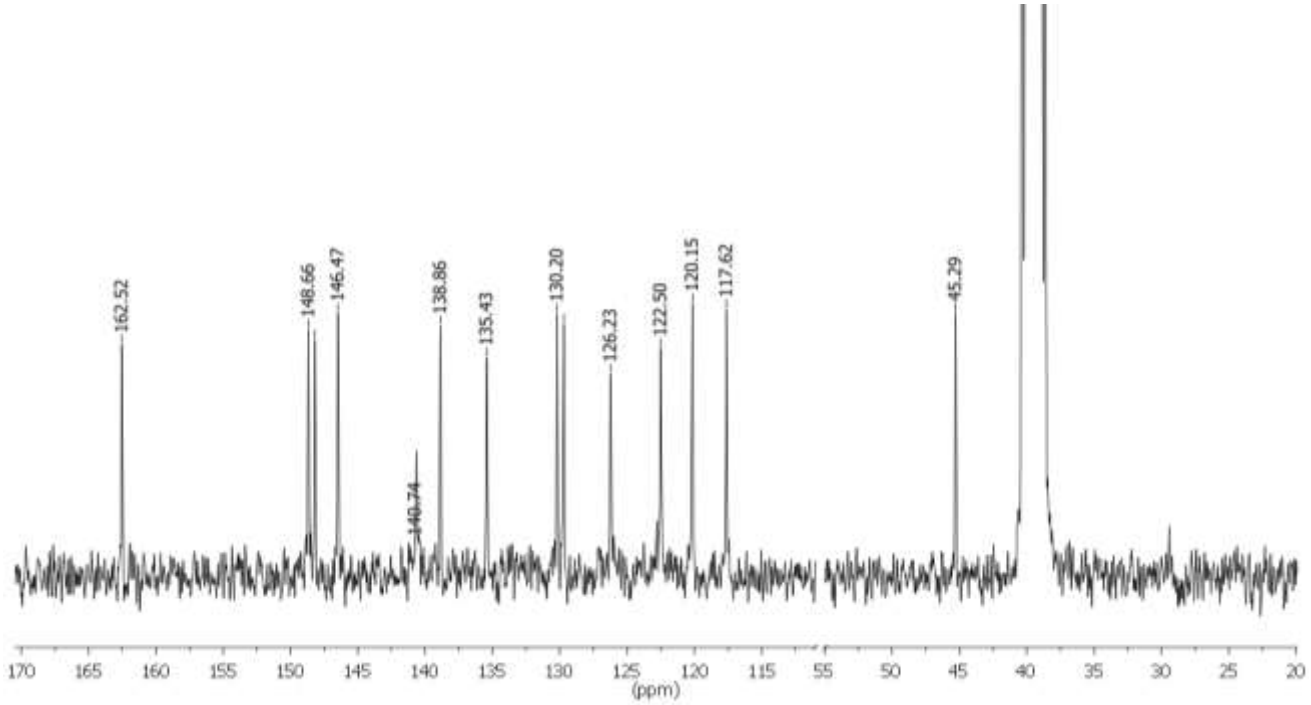

Figure 6S. ^{13}C NMR spectrum of **2** in DMSO-d_6

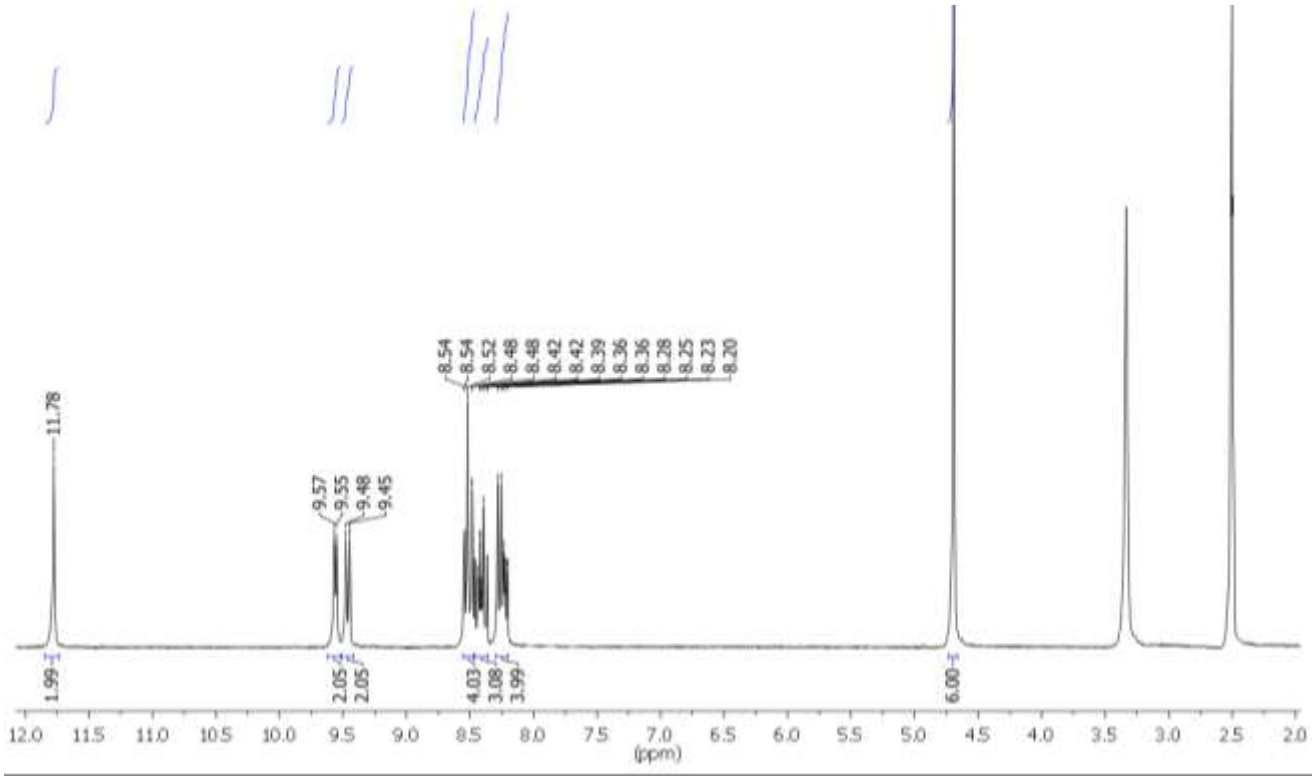

Figure 7S. ^{1}H NMR spectrum of **3** in DMSO-*d*$_6$

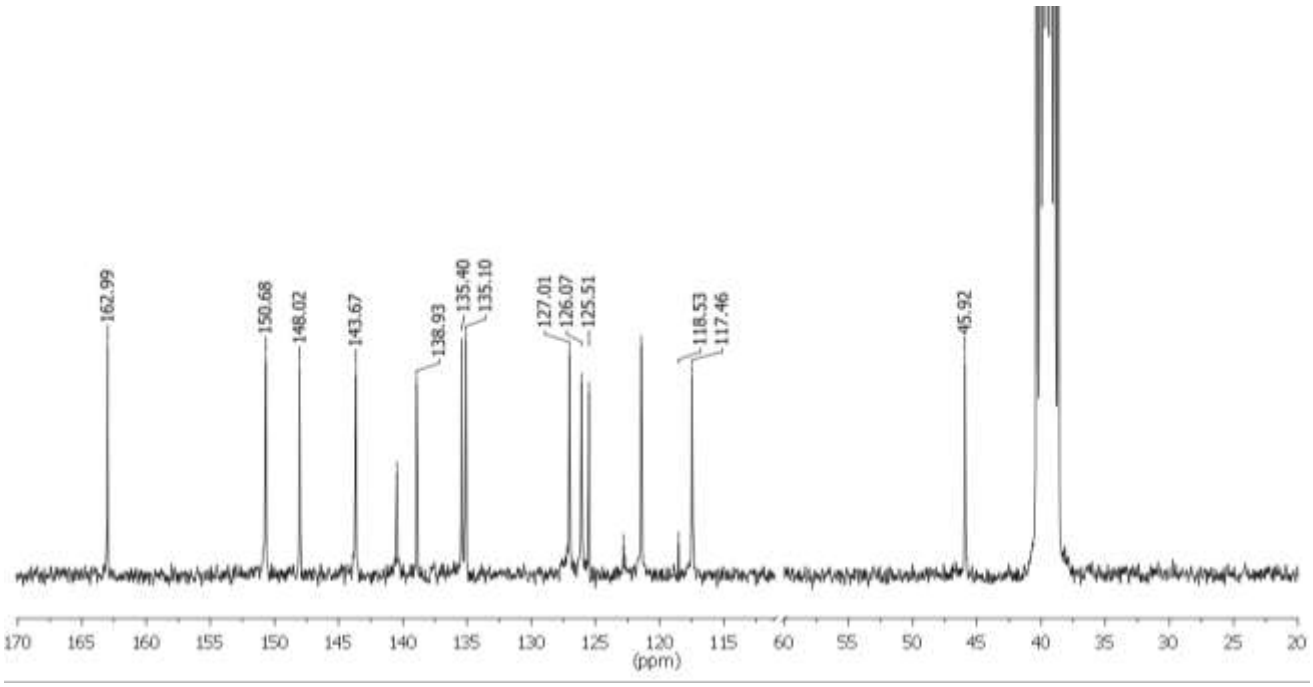

Figure 8S. ^{13}C NMR spectrum of **3** in DMSO-d_6

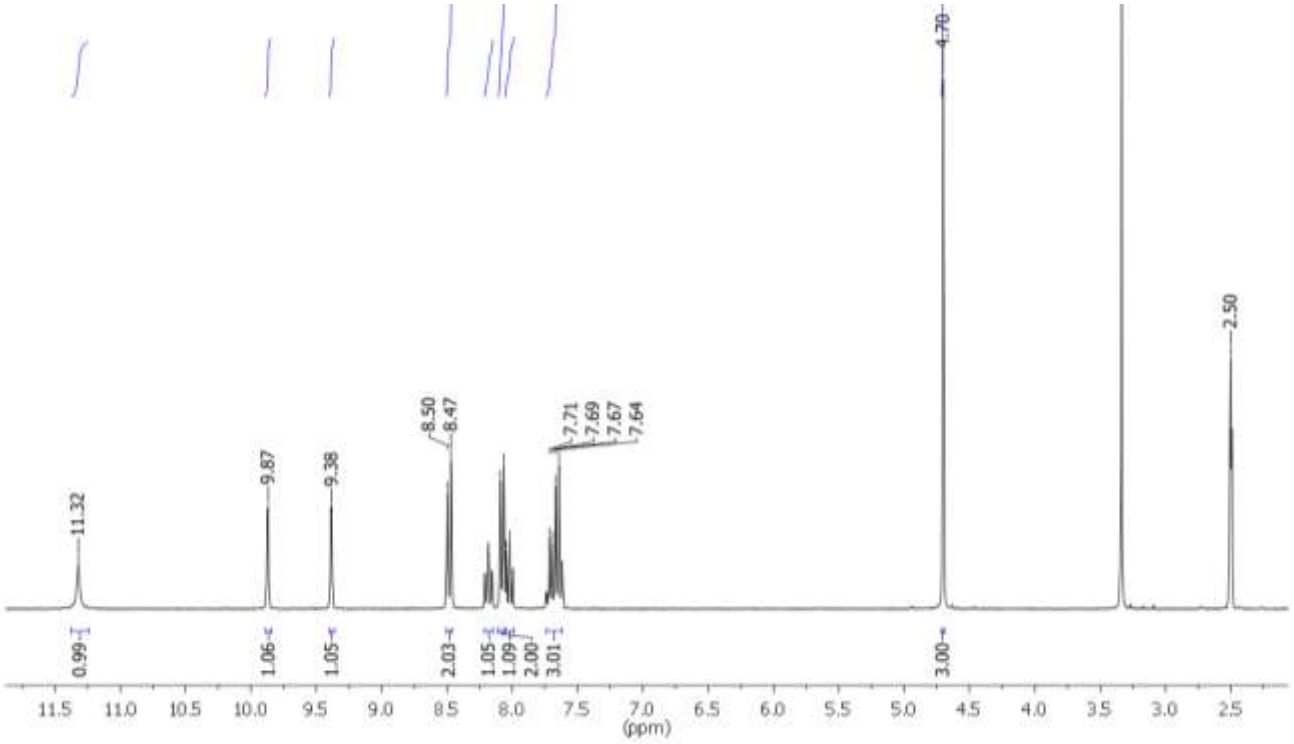

Figure 9S. ^{1}H NMR spectrum of **4** in DMSO-d_6

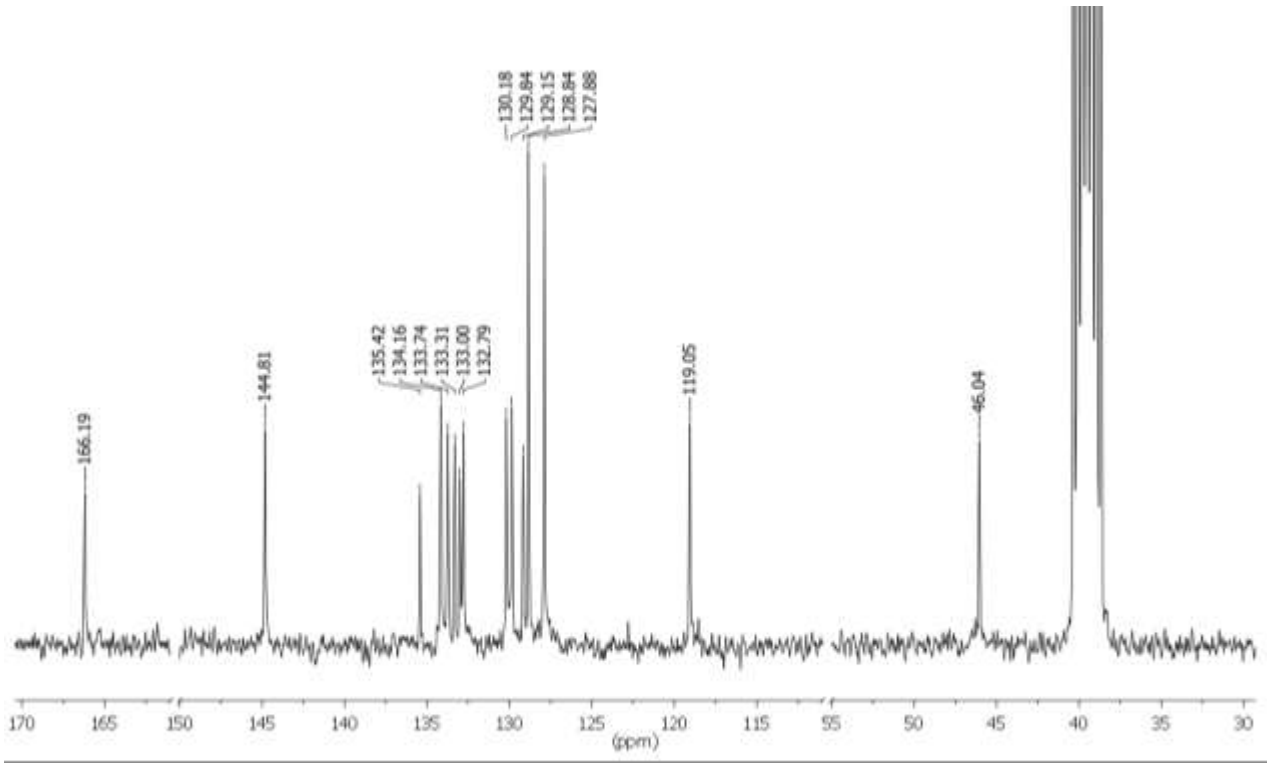

Figure 10S. ^{13}C NMR spectrum of **4** in DMSO-d_6

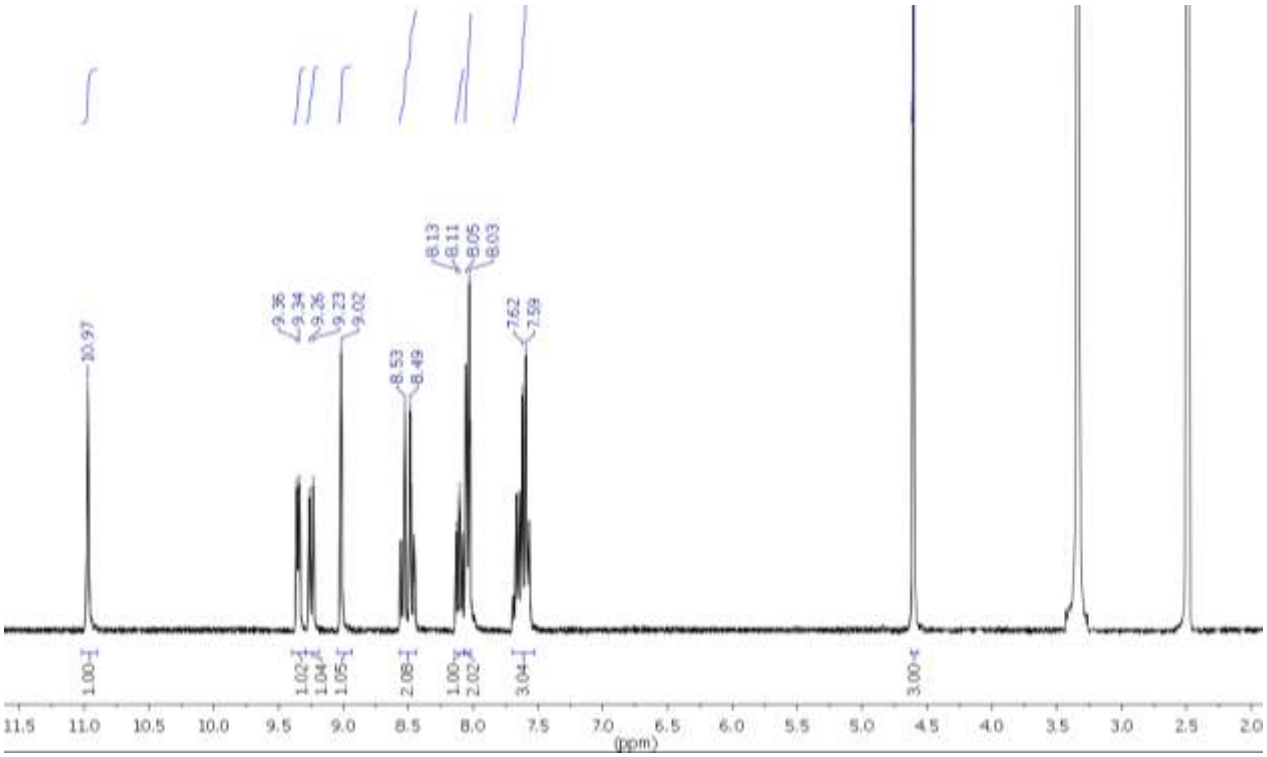

Figure 11S. ^{1}H NMR spectrum of **5** in DMSO-d_6

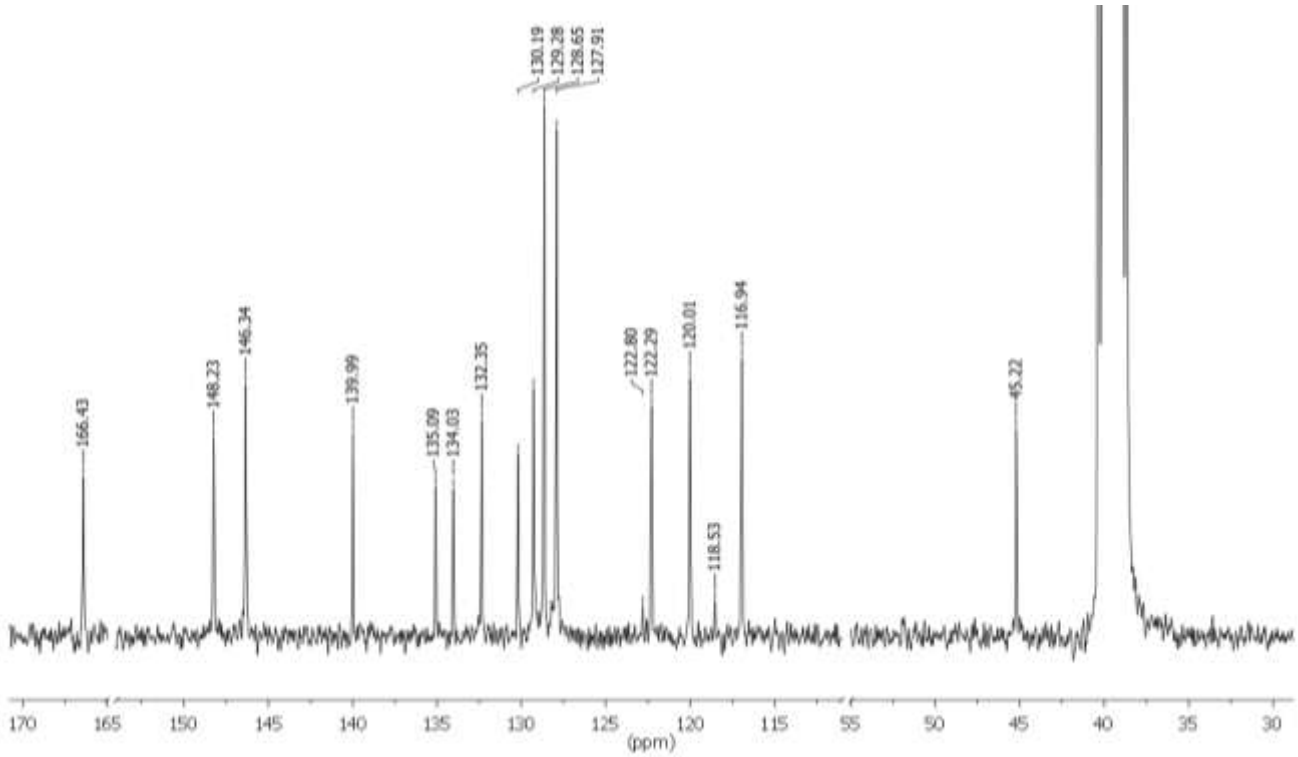

Figure 12S. ^{13}C NMR spectrum of **5** in DMSO-d_6

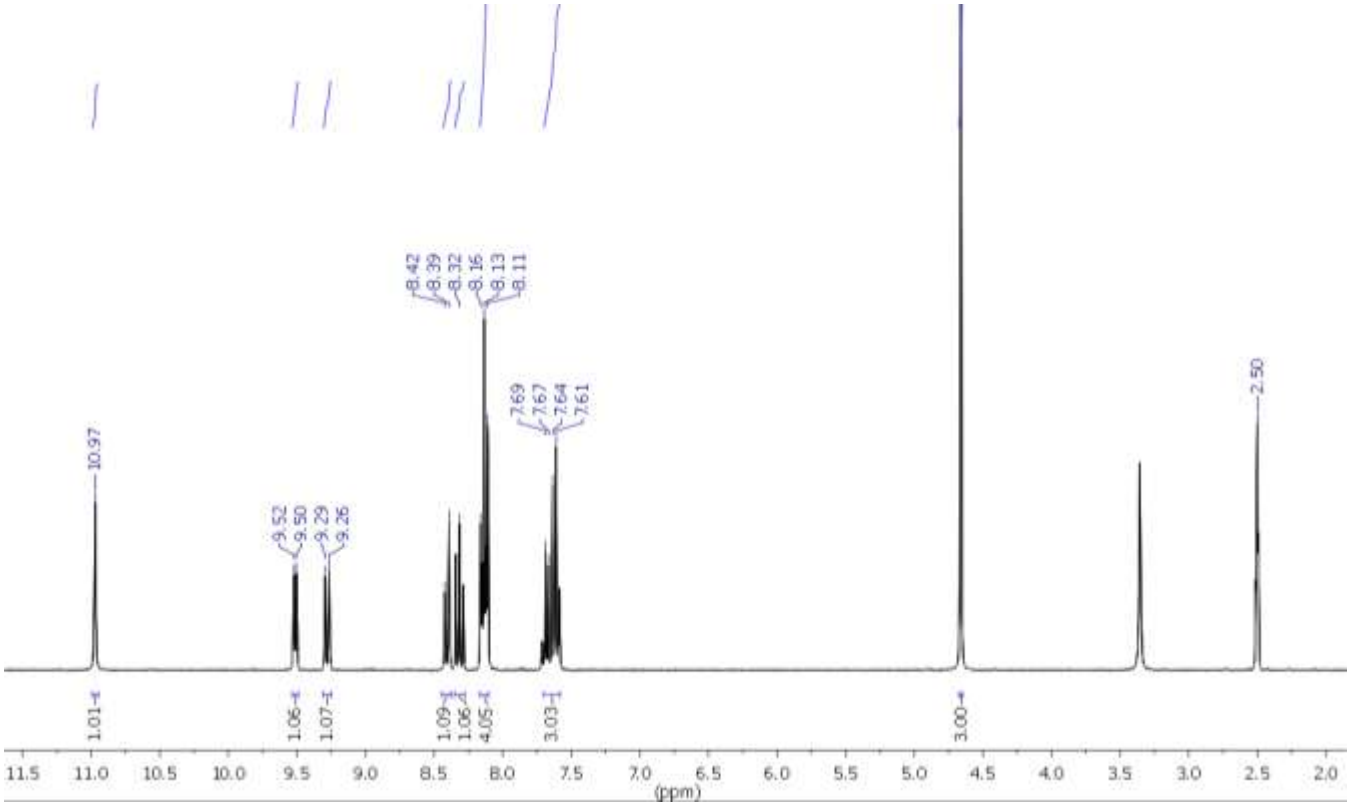

Figure 13S. ^{1}H NMR spectrum of **6** in DMSO-d_6

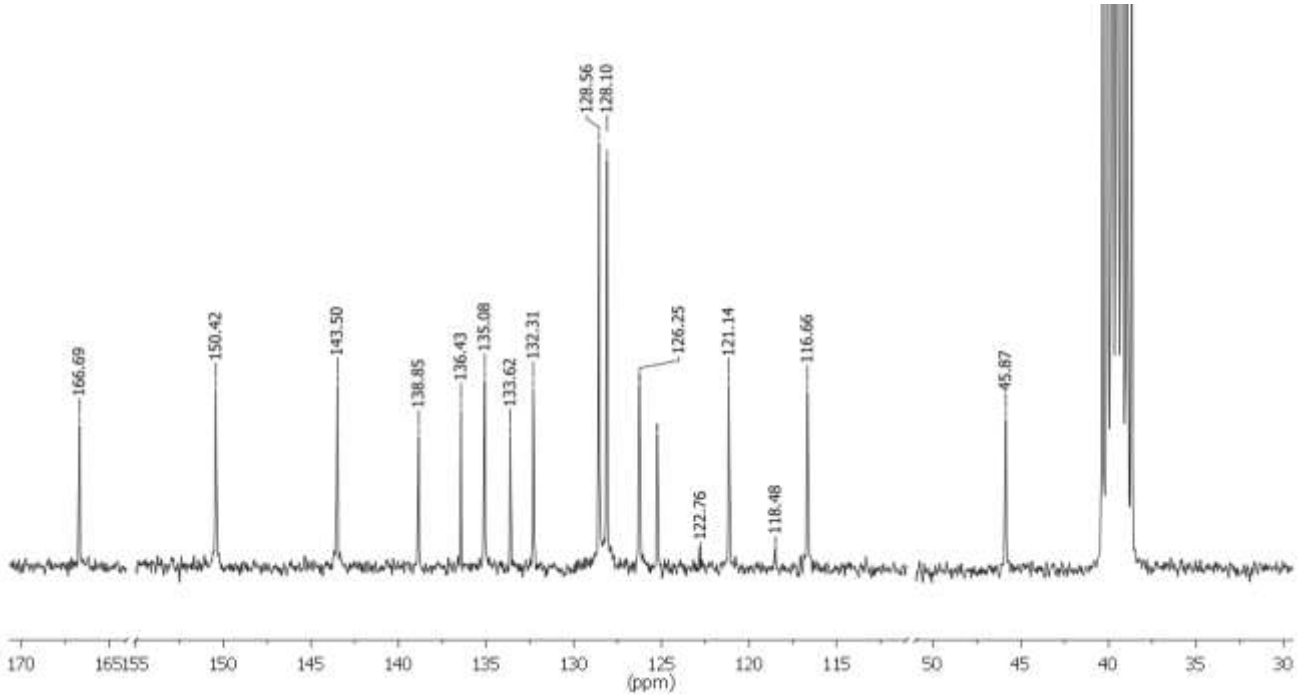

Figure 14S. ^{13}C NMR spectrum of **6** in DMSO-d_6