

Supplementary Information

Electrophile-dependent reactivity of lithiated *N*-benzylpyrene-1-carboxamide

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Table S1. X-ray diffraction data for **6**

Compound	6
Empirical formula	C ₂₄ H ₁₇ N ₁ O ₁
Formula weight	335.38
Crystal system	monoclinic
Space group	C 2/c
a/Å	25.8302(6)
b/Å	4.71042(11)
c/Å	27.0073(8)
α/°	90
β/°	93.353(2)
γ/°	90
Volume/Å ³	3280.39(15)
Z / Z'	8 / 1
μ/mm ⁻¹	0.645
Max. transmission	1.000
Min. transmission	0.645
Absorption correction	gaussian
Crystal color	colorless
ρ _{calc} /mg/mm ³	1.358
Crystal habit	needle
F(000)	1408
Crystal size/mm	0.41 0.08 0.03
R _{int}	0.022
R _{sigma}	0.021
Index ranges	
h	-29 : 31
k	-5 : 3
l	-33 : 32
Reflections collected	10475
2Θ range for data collection	73.934 3.278
Temperature/K	120.1(1)
X-ray wavelength/Å	1.54184
Independent reflections	
I > 2 σ(I)	2866
Independent reflections	3253
Largest diff. peak/hole /e Å ⁻³	0.26 ; -0.22
Goodness-of-fit on F ²	1.036
Parameters	238
Data	3253
Restraints	0
R1 all data	0.044
R1 [I >= 2σ (I)]	0.038
wR2 [I >= 2σ (I)]	0.103
wR2 all data	0.108

Z' - indicates the number of crystallographically independent molecules

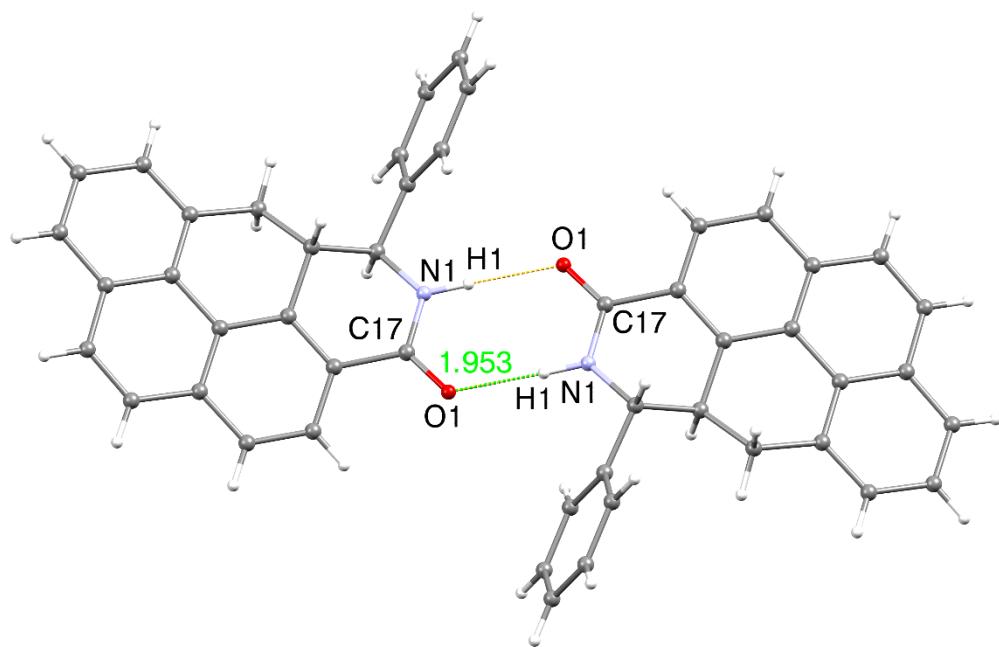


Figure S1. A set of strong N – H ... O hydrogen bonds, connecting two molecules of **6** related by center of inversion. The crystal structure of **6** is composed of the stacks of such H-bonded dimers in [010] direction.

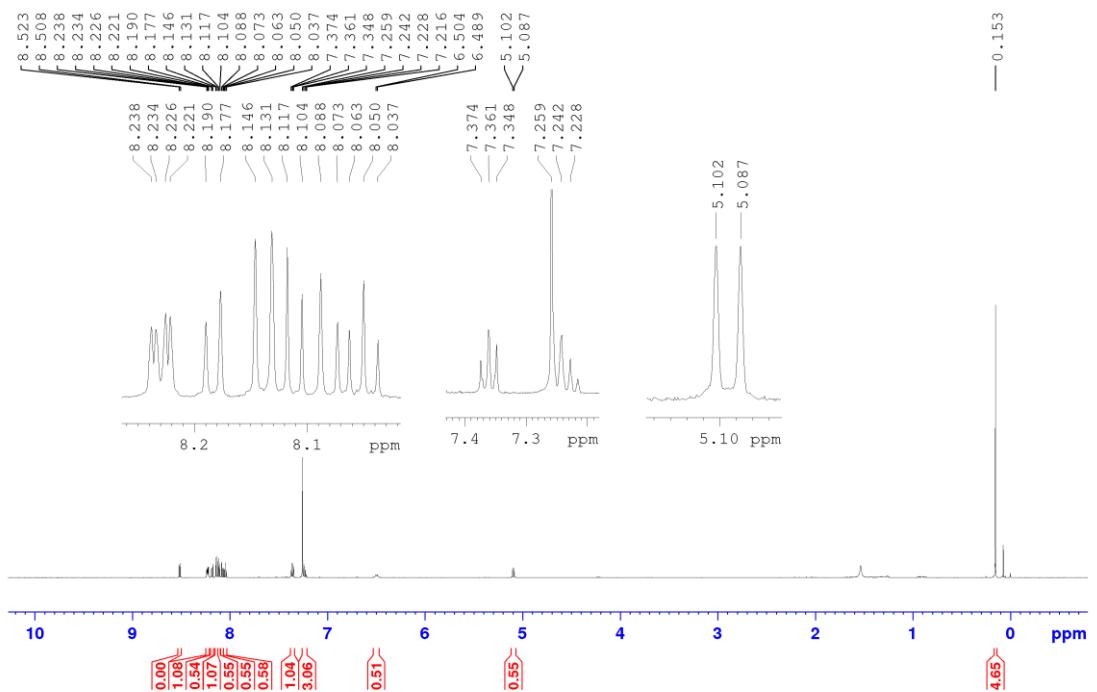


Figure S2. ^1H NMR spectrum of compound **3** (600 MHz, CDCl_3 , room temperature).

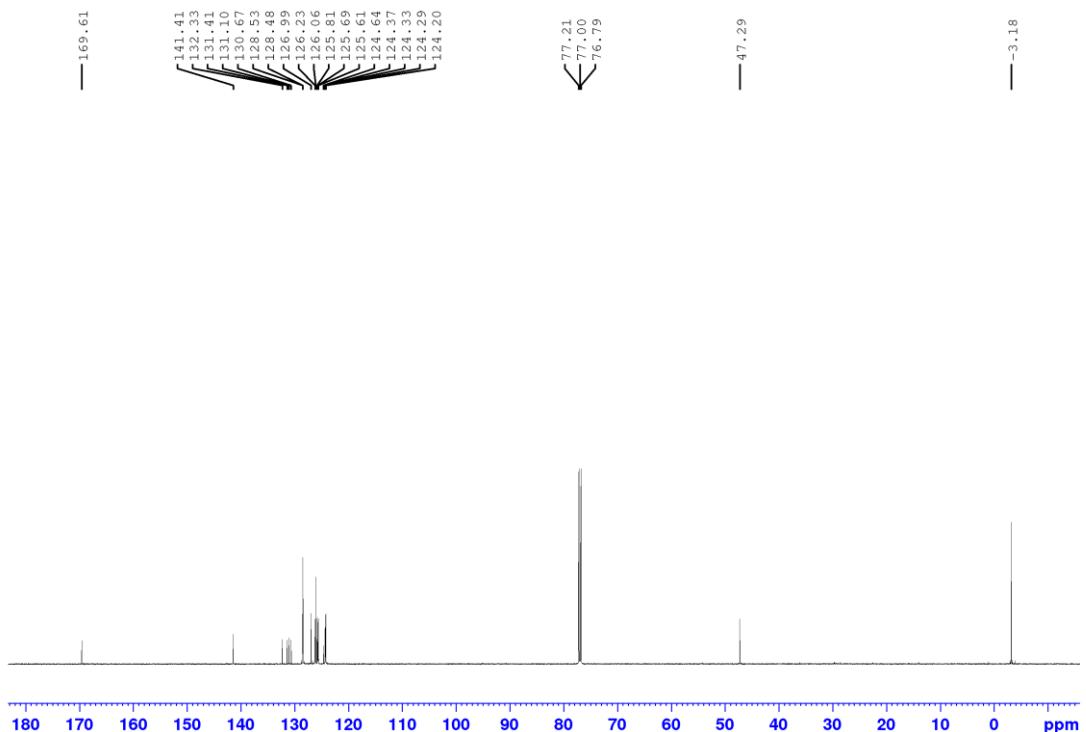
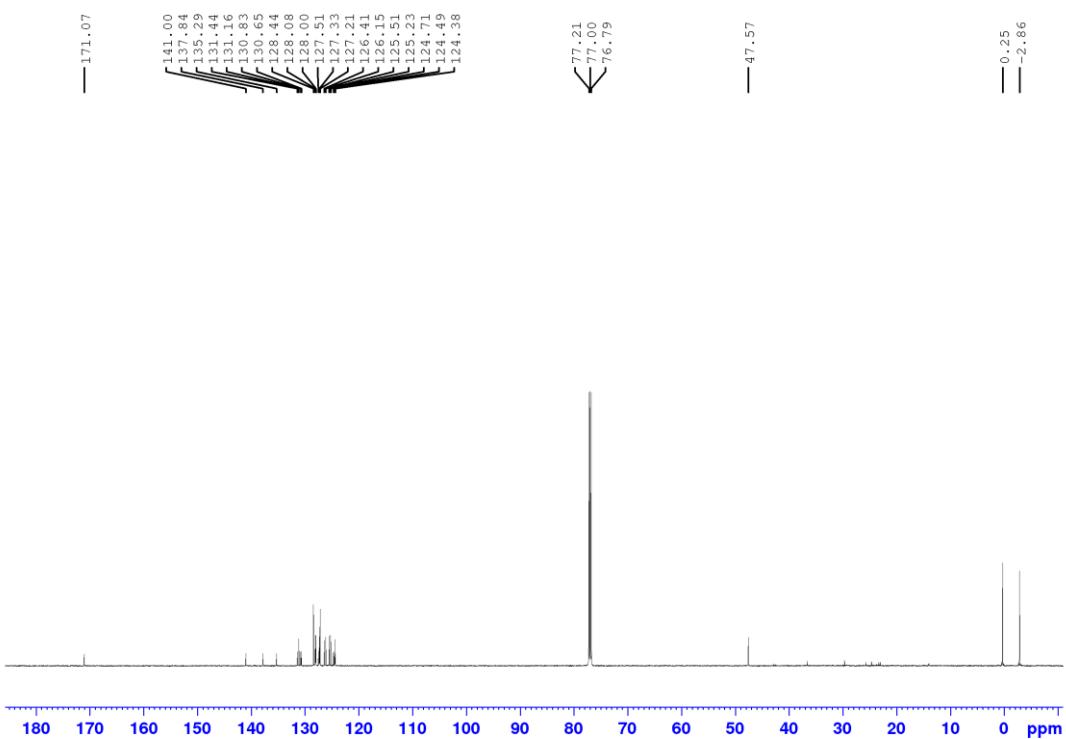
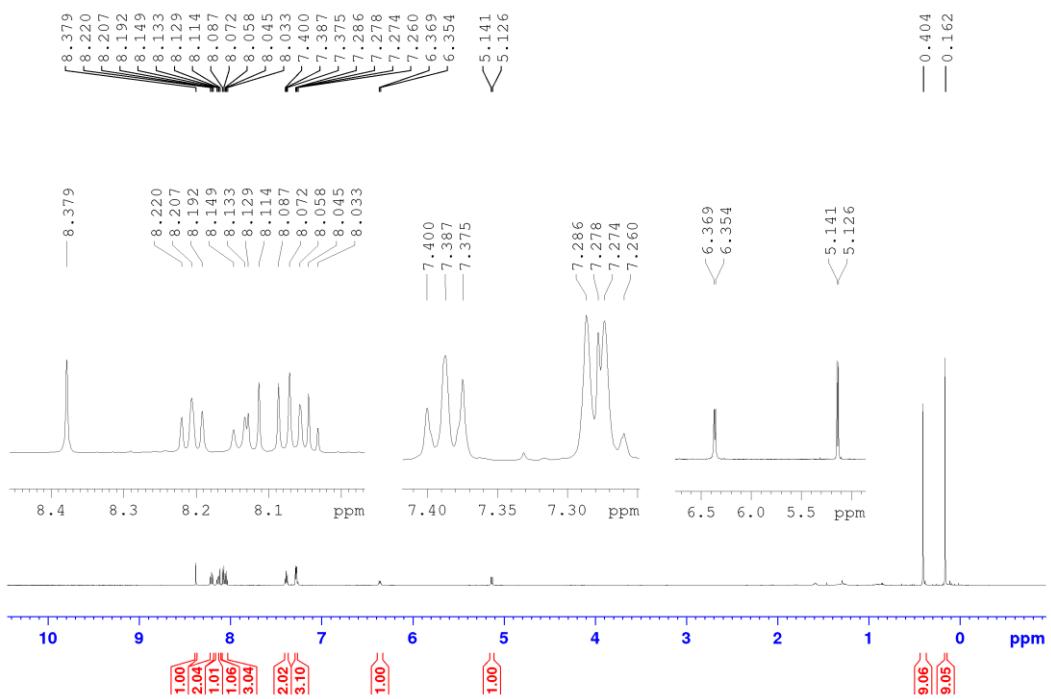


Figure S3. ^{13}C NMR spectrum of compound **3** (150 MHz, CDCl_3 , room temperature).



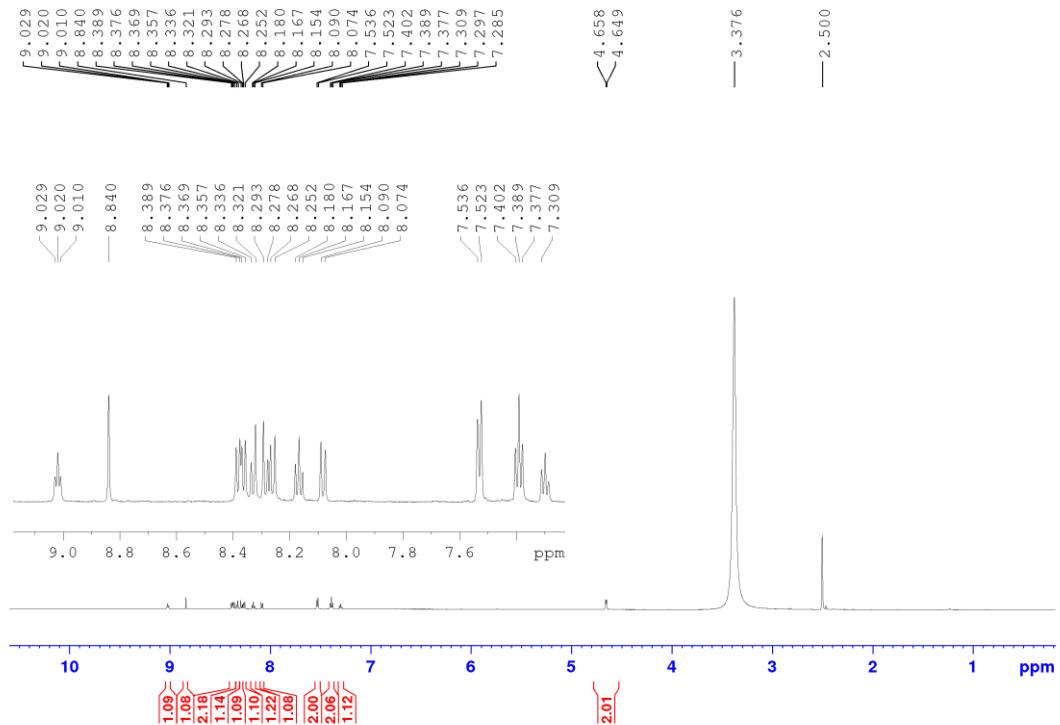


Figure S6. ^1H NMR spectrum of compound **5** (600 MHz, DMSO, room temperature).

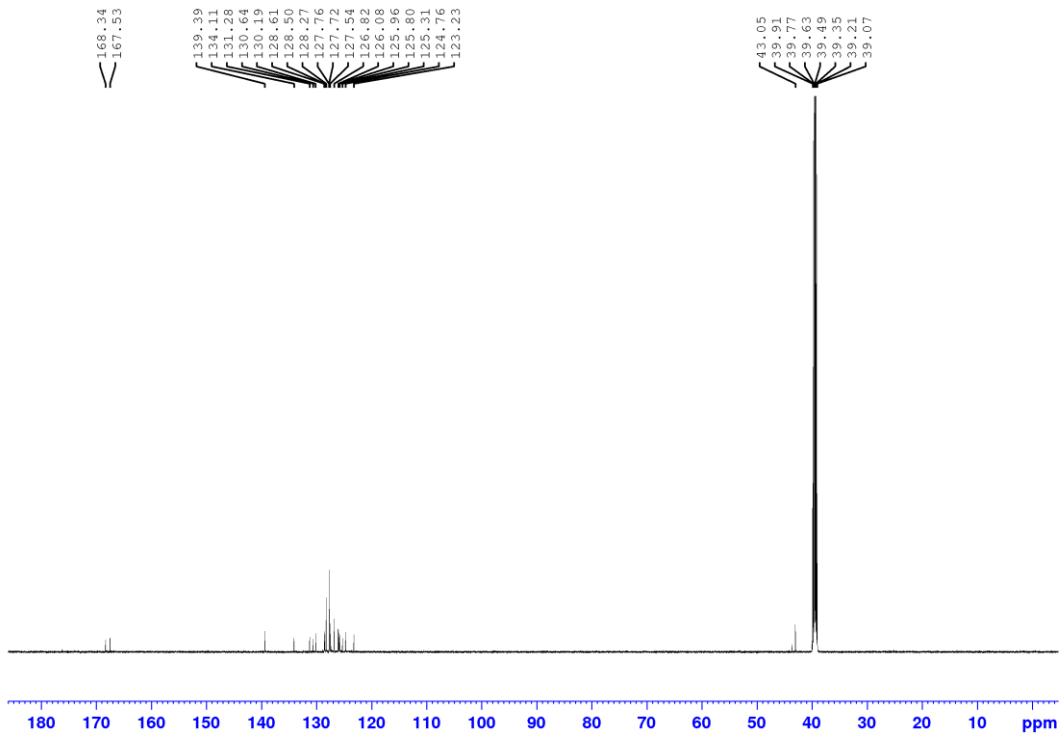


Figure S7. ^{13}C NMR spectrum of compound 5 (150 MHz, DMSO, room temperature).

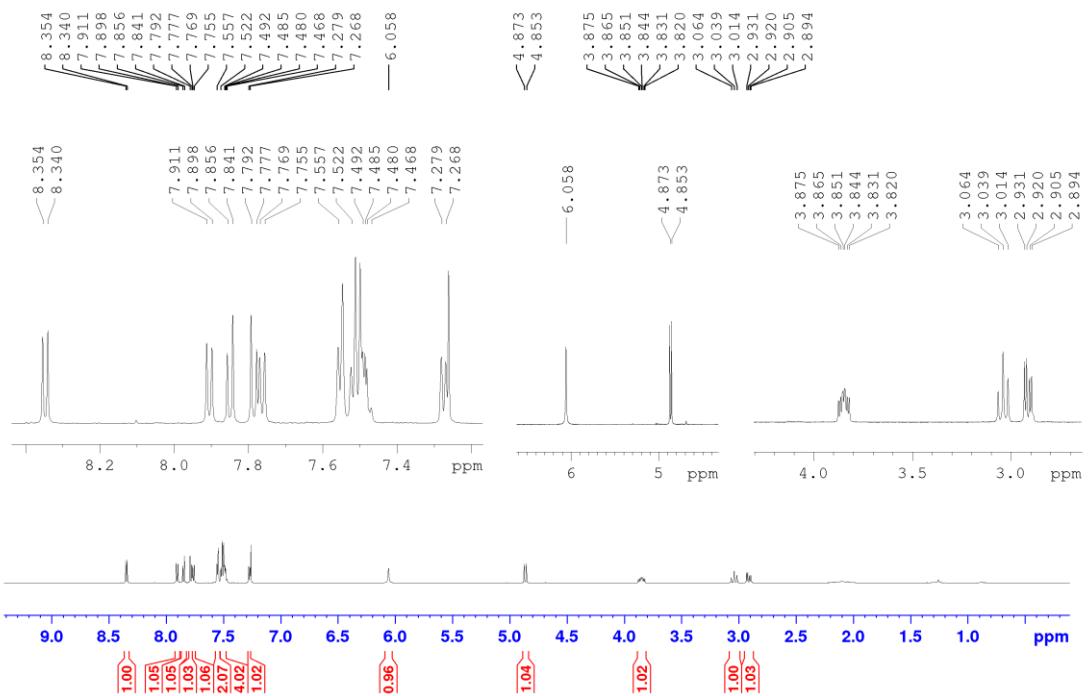


Figure S8. ^1H NMR spectrum of compound **6** (600 MHz, CDCl_3 , room temperature).

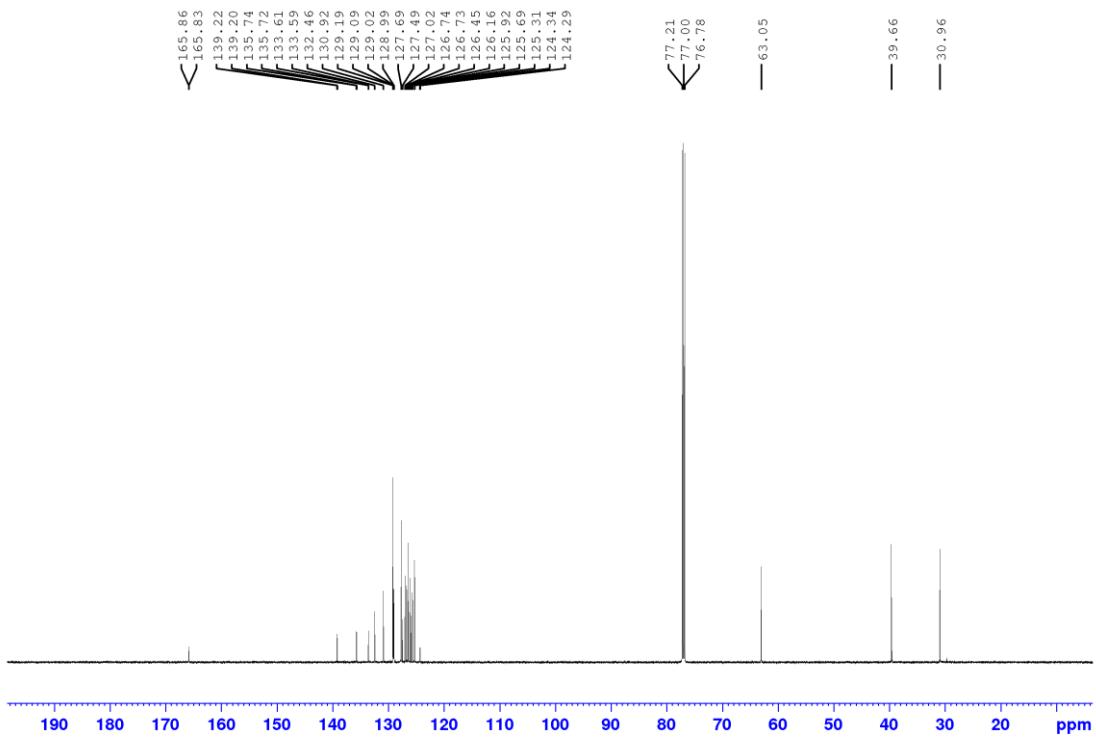


Figure S9. ^{13}C NMR spectrum of compound **6** (150 MHz, CDCl_3 , room temperature).

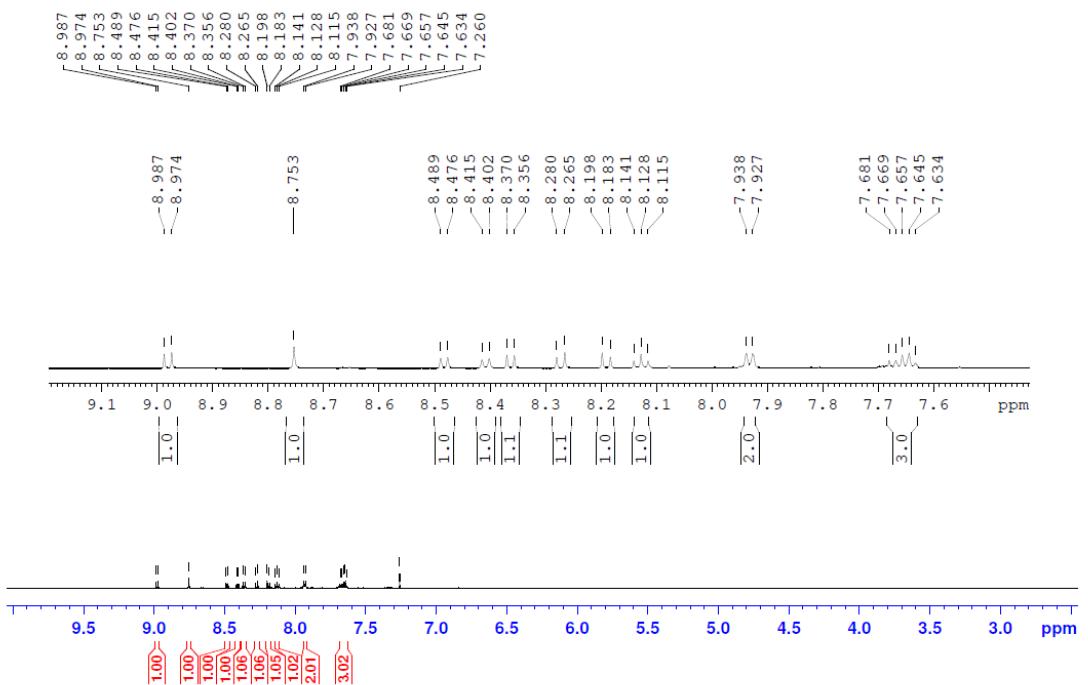


Figure S10. ^1H NMR spectrum of compound **7** (600 MHz, CDCl_3 , room temperature).

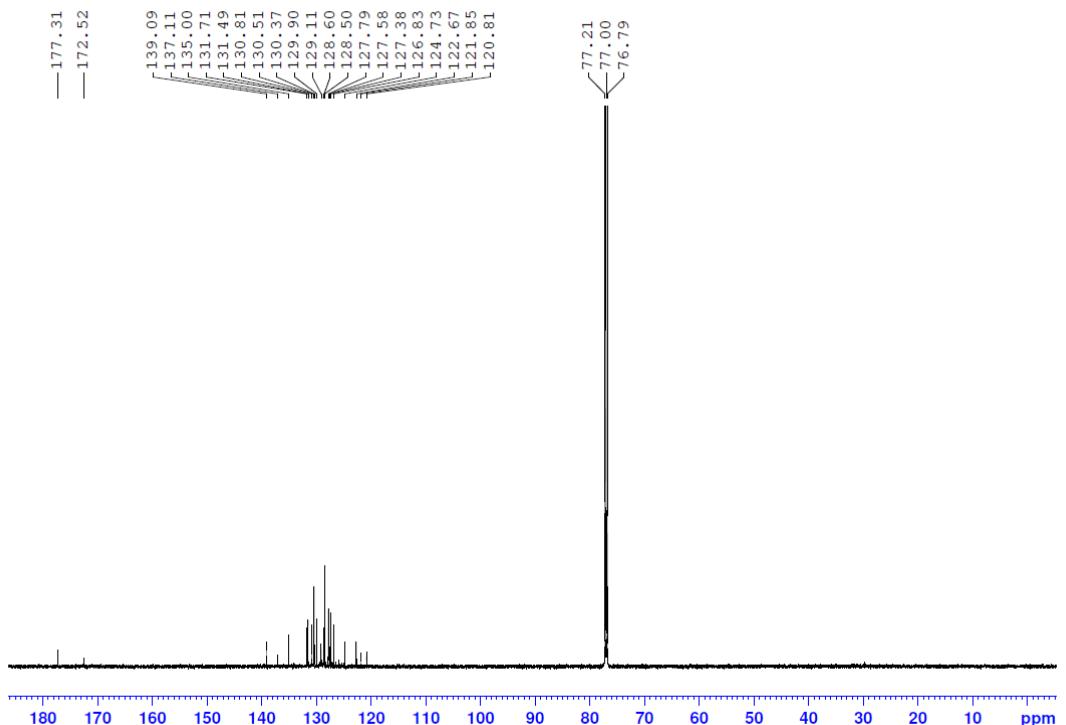


Figure S11. ^{13}C NMR spectrum of compound **7** (150 MHz, CDCl_3 , room temperature).

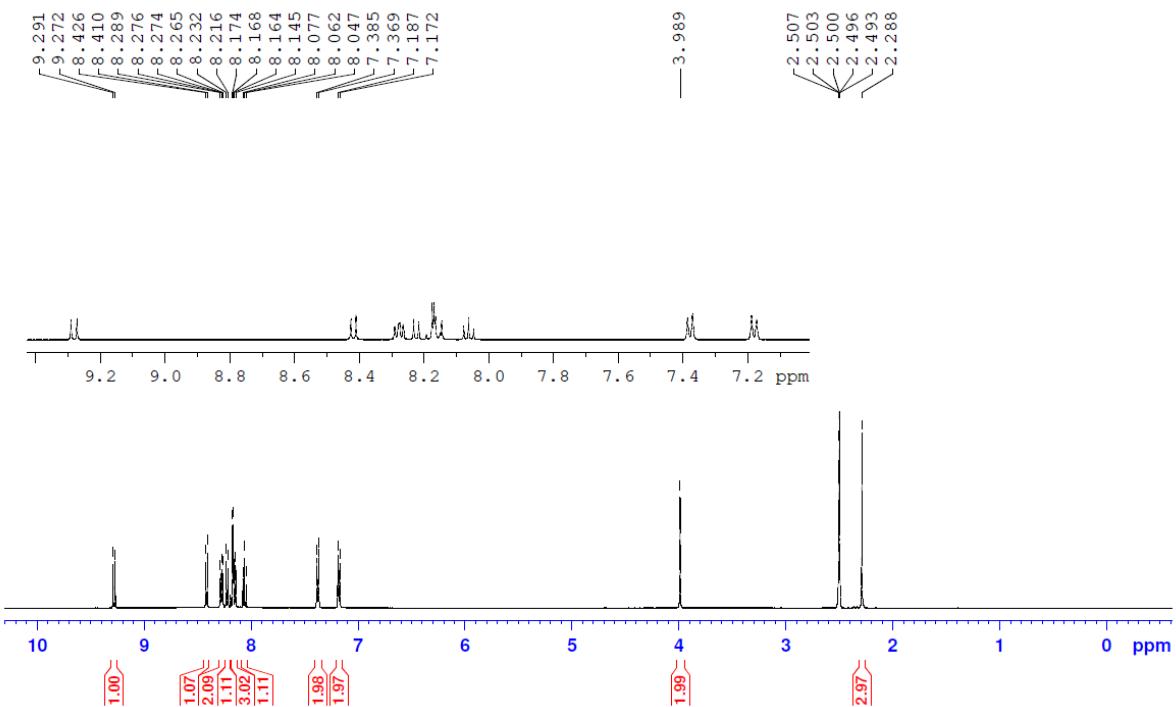


Figure S12. ^1H NMR spectrum of compound **8a** (500 MHz, DMSO, room temperature).

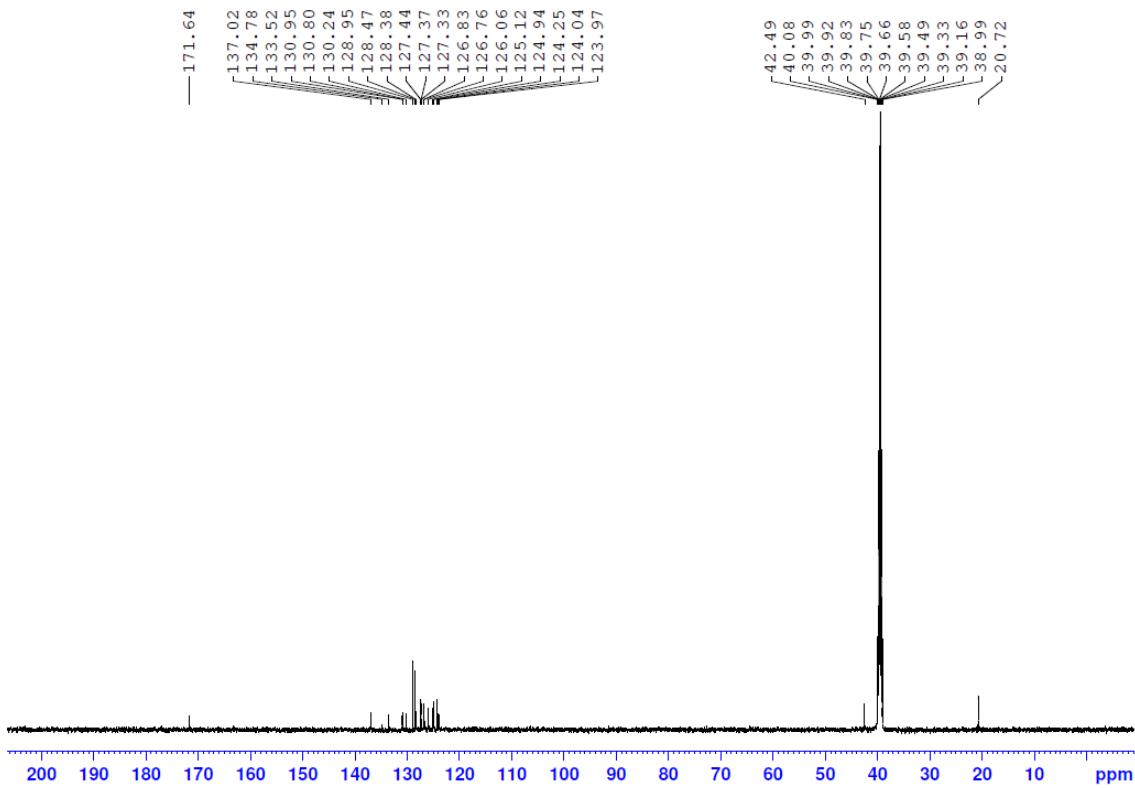


Figure S13. ^{13}C NMR spectrum of compound **8a** (125 MHz, DMSO, room temperature).

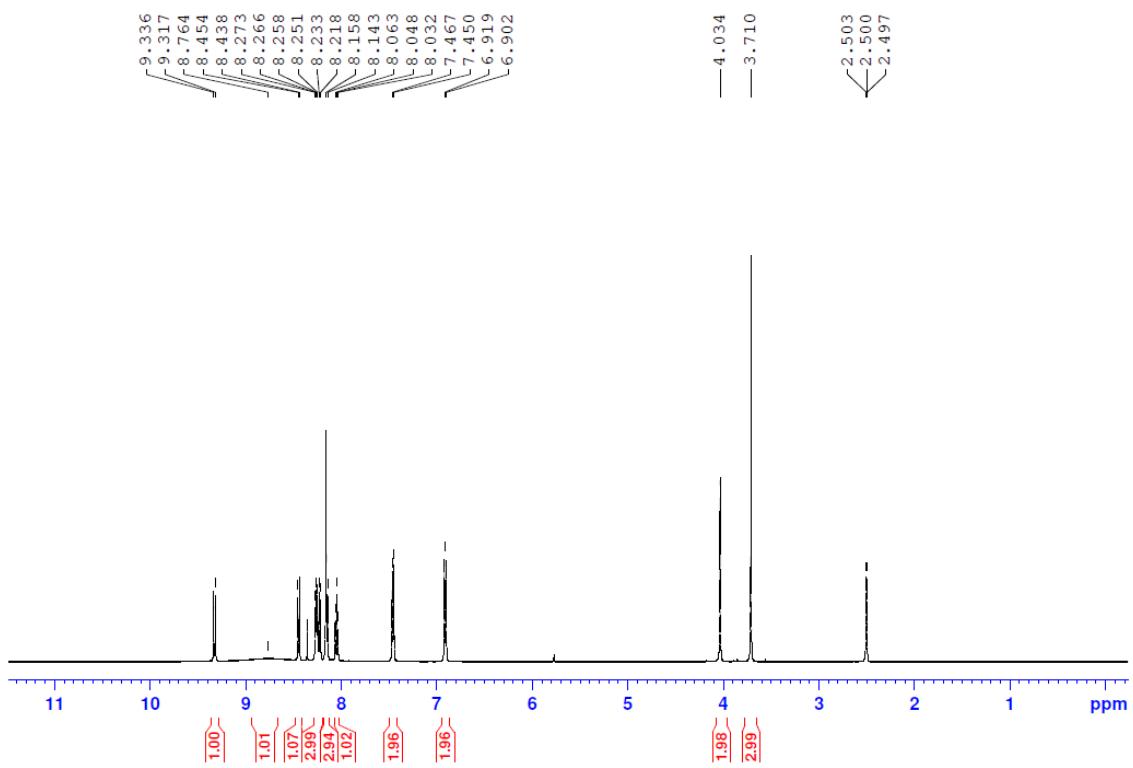


Figure S14. ^1H NMR spectrum of compound **8b** (500 MHz, DMSO, room temperature).

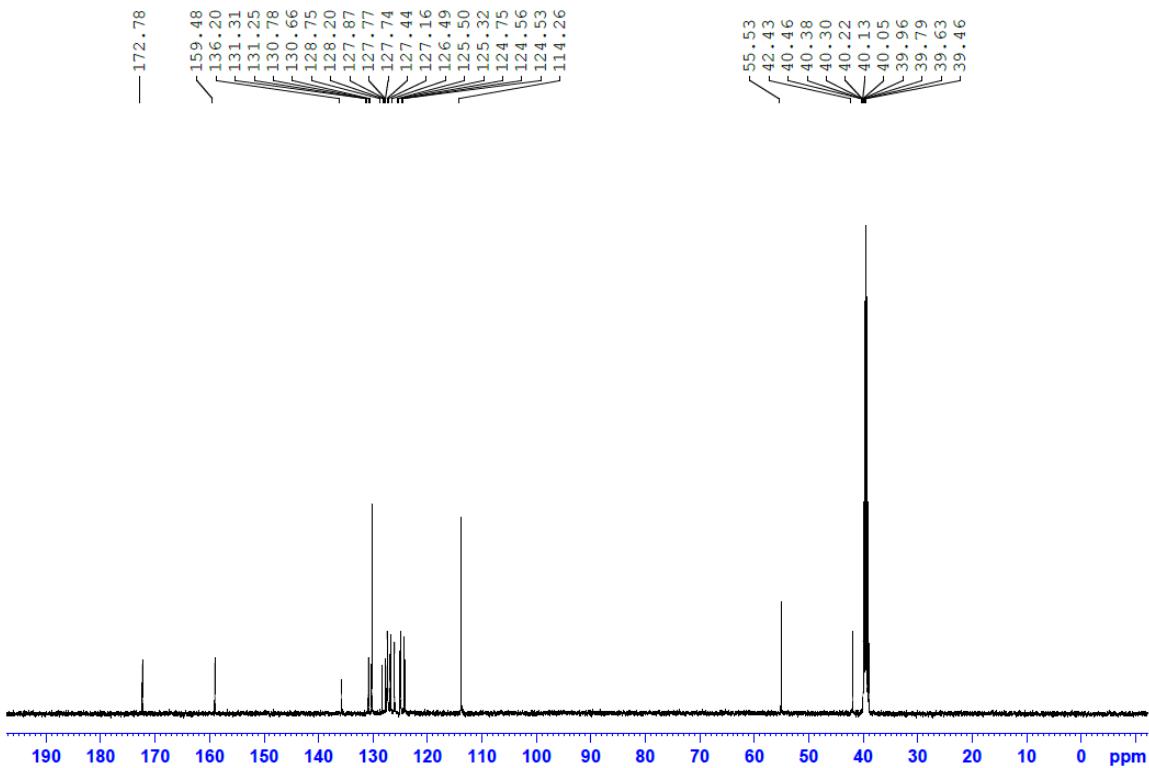


Figure S15. ^{13}C NMR spectrum of compound **8b** (125 MHz, DMSO, room temperature).

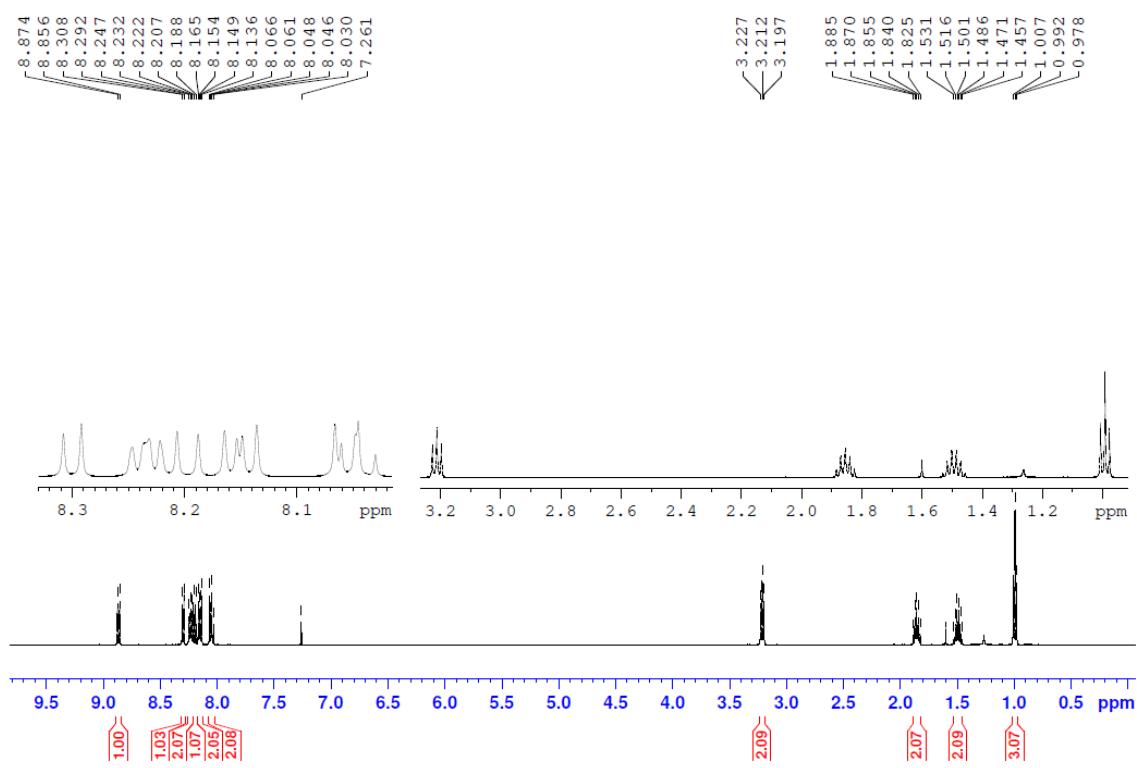


Figure S16. ¹H NMR spectrum of compound 9 (500 MHz, CDCl₃, room temperature).

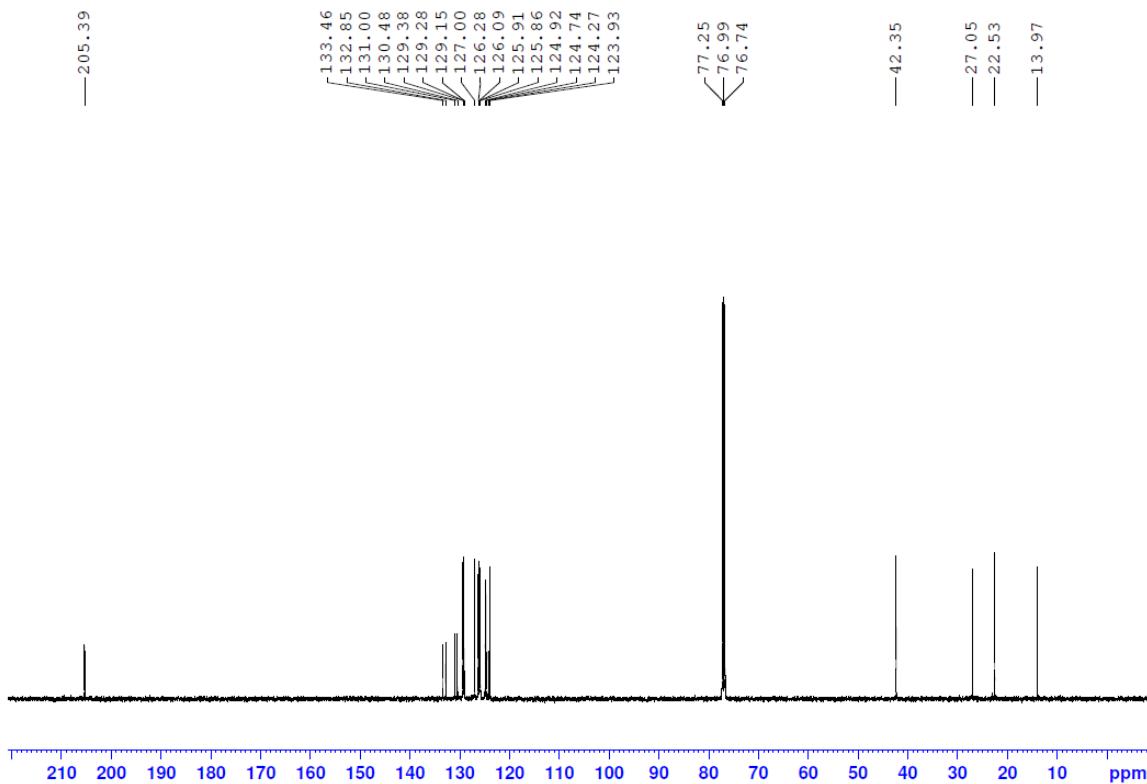


Figure S17. ¹³C NMR spectrum of compound 9 (125 MHz, CDCl₃, room temperature).