

Supporting information for

Synthesis and Electrochemistry of Novel Dumbbell-shaped Bis-pyrazolino[60]fullerene Derivatives Formed Using Microwave Radiation

Mohammad H. BinSabit^{*a}, Hamad M. Al-Matar^{*a}, Alan L. Balch^b, and Mona A. Shalaby^a

^a Chemistry Department, Faculty of Science, University of Kuwait, P.O. Box 5969, Safat 13060, Kuwait

^b Department of Chemistry, University of California at Davis, One Shields Avenue, Davis, California 95616, United States

^a *Corresponding author. Tel.: +965 24987559; fax: +965 24816482.

E-mail address: mohammad.binsabt@ku.edu.kw (M.H.B.), h.almatar@ku.edu.kw (H.M.A.)

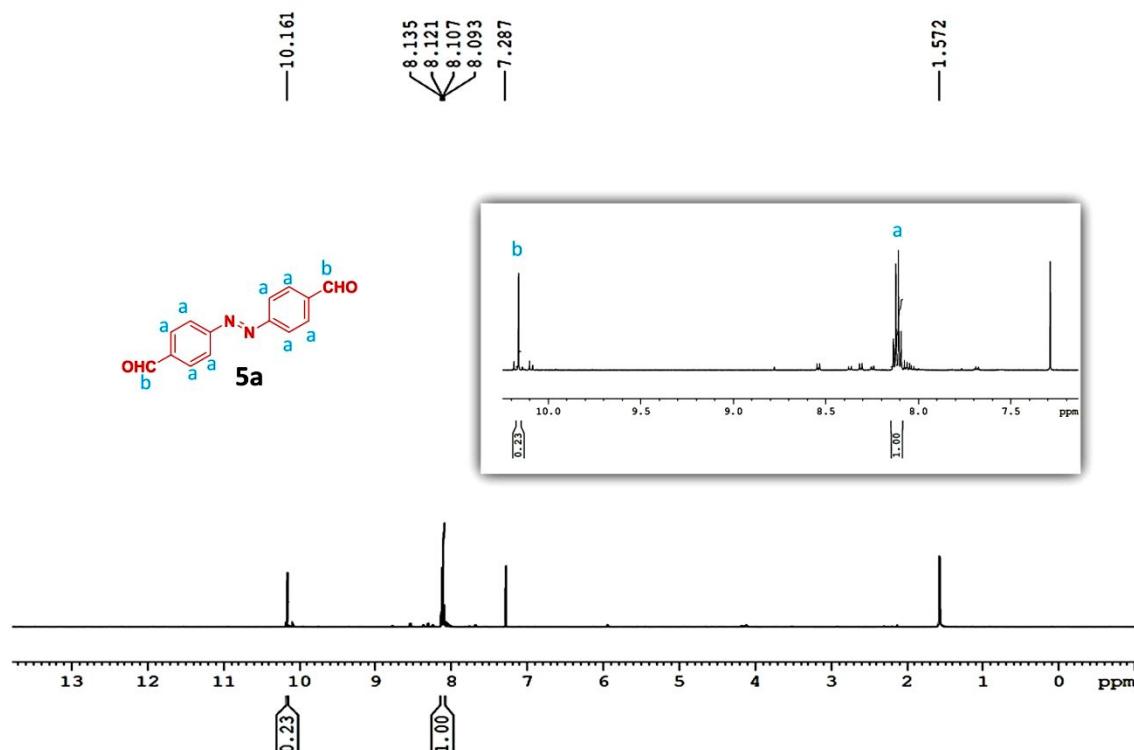


Figure S1. The ¹H NMR spectrum of compound **5a** (600.13 MHz, solvent CDCl₃)

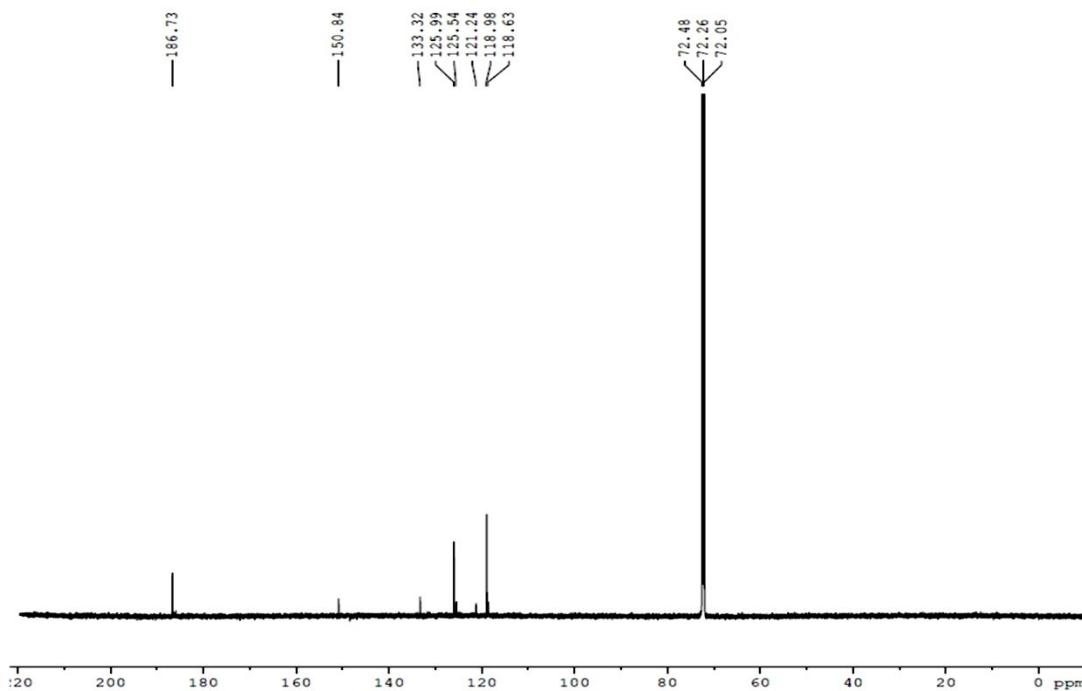
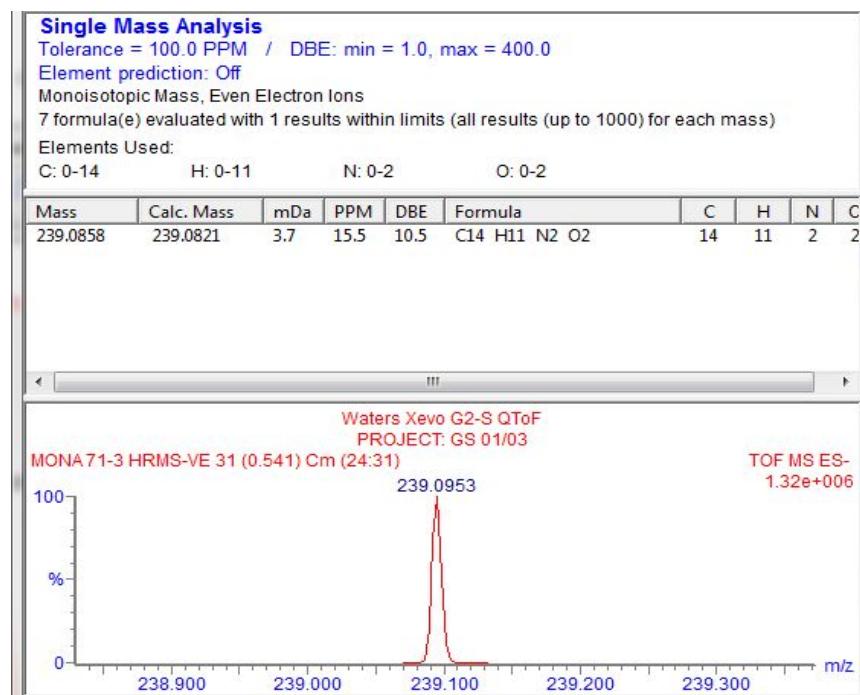


Figure S2. The ^{13}C NMR spectrum of compound **5a** (150 MHz, solvent CDCl_3)



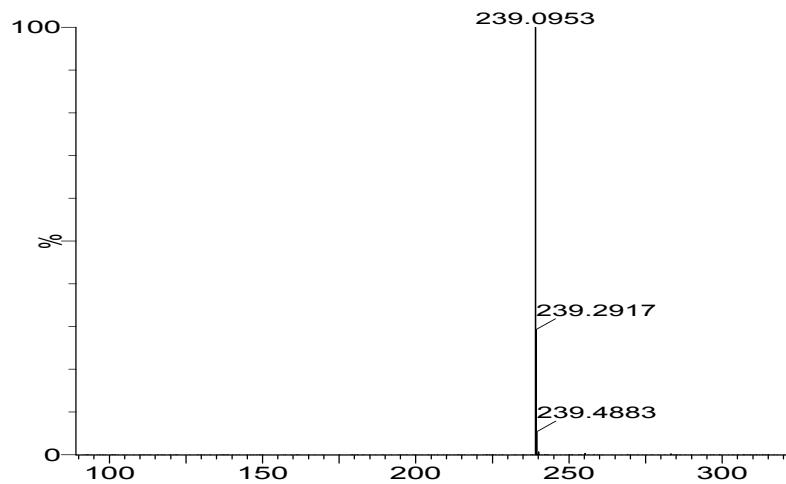


Figure S3. HRMS (ESI-TOF) of compound **5a**

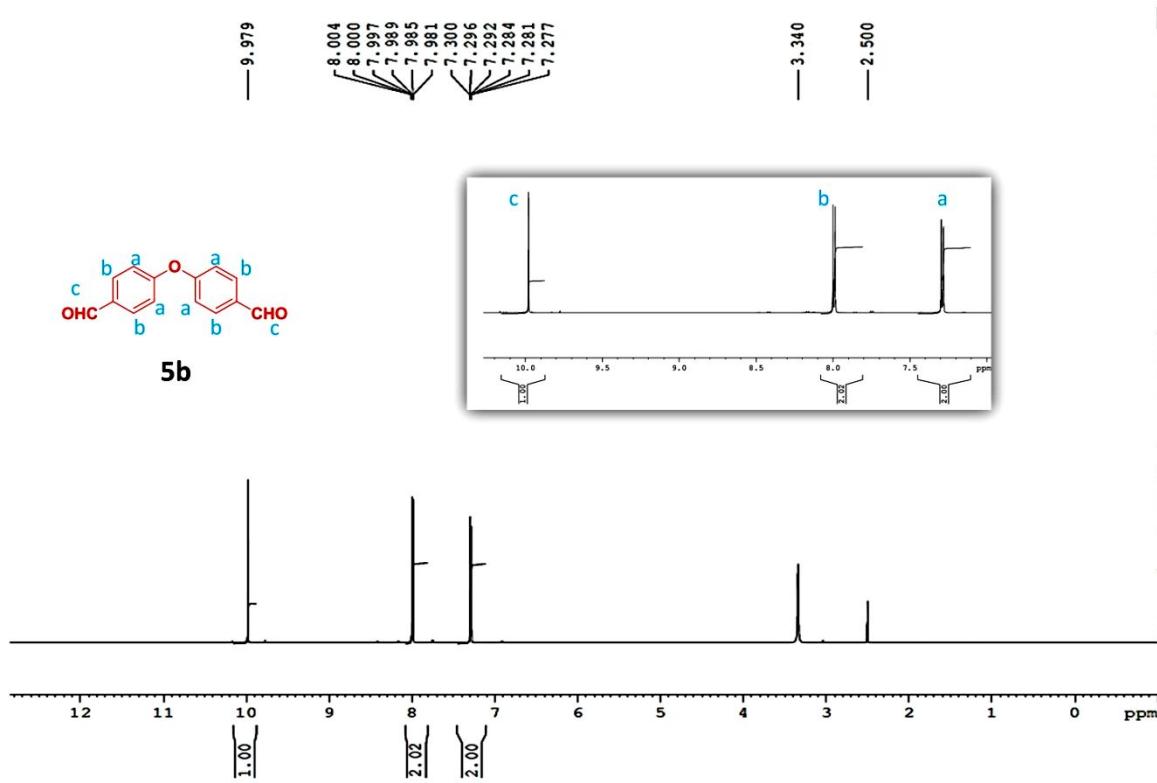


Figure S4. The ^1H NMR spectrum of compound **5b** (600.13 MHz, solvent DMSO)

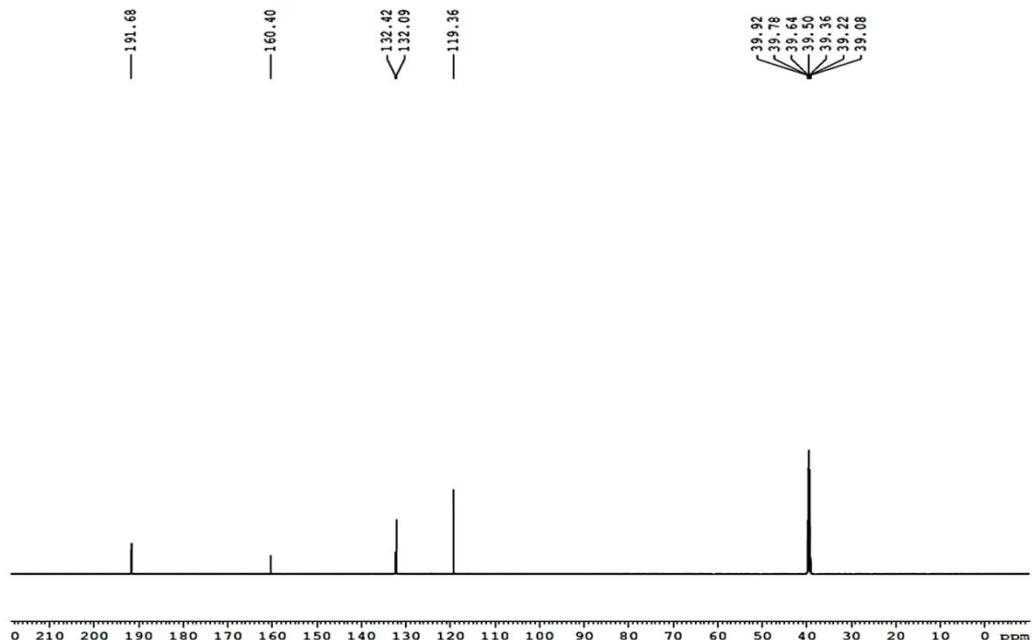


Figure S5. The ^{13}C NMR spectrum of compound **5b** (150 MHz, solvent DMSO)

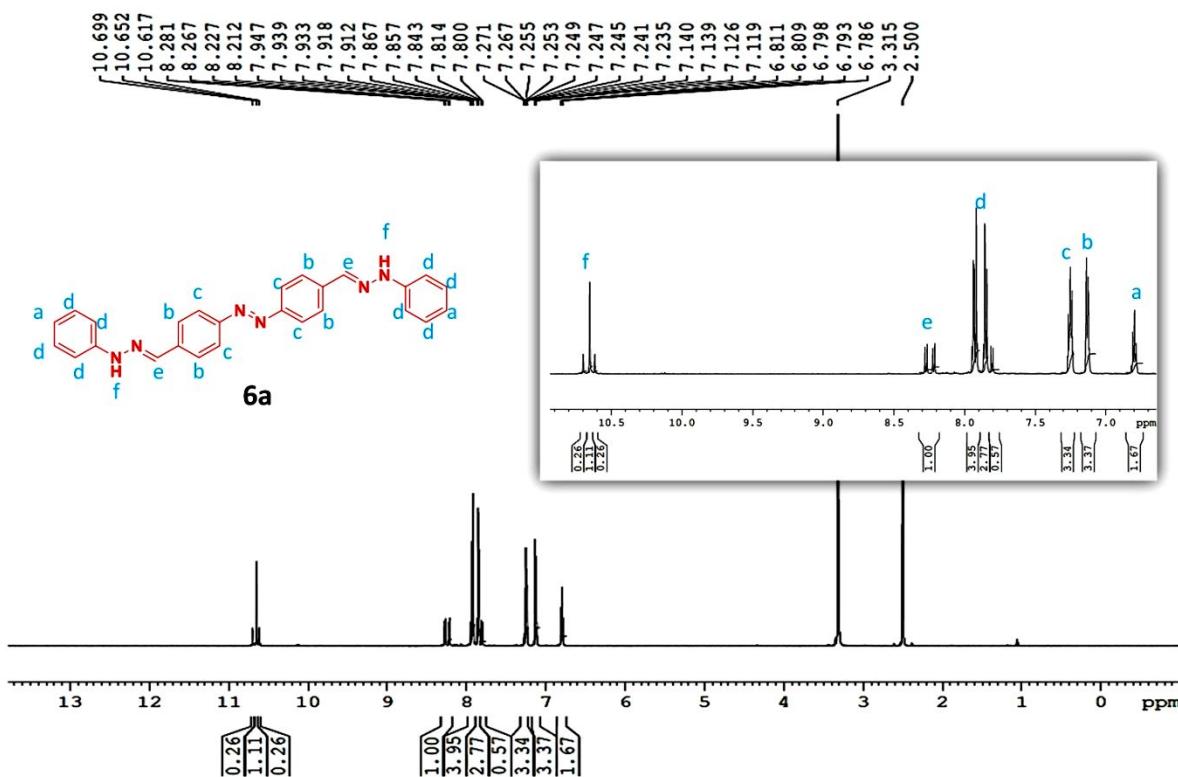


Figure S6. The ^1H NMR spectrum of compound **6a** (600.13 MHz, solvent DMSO)

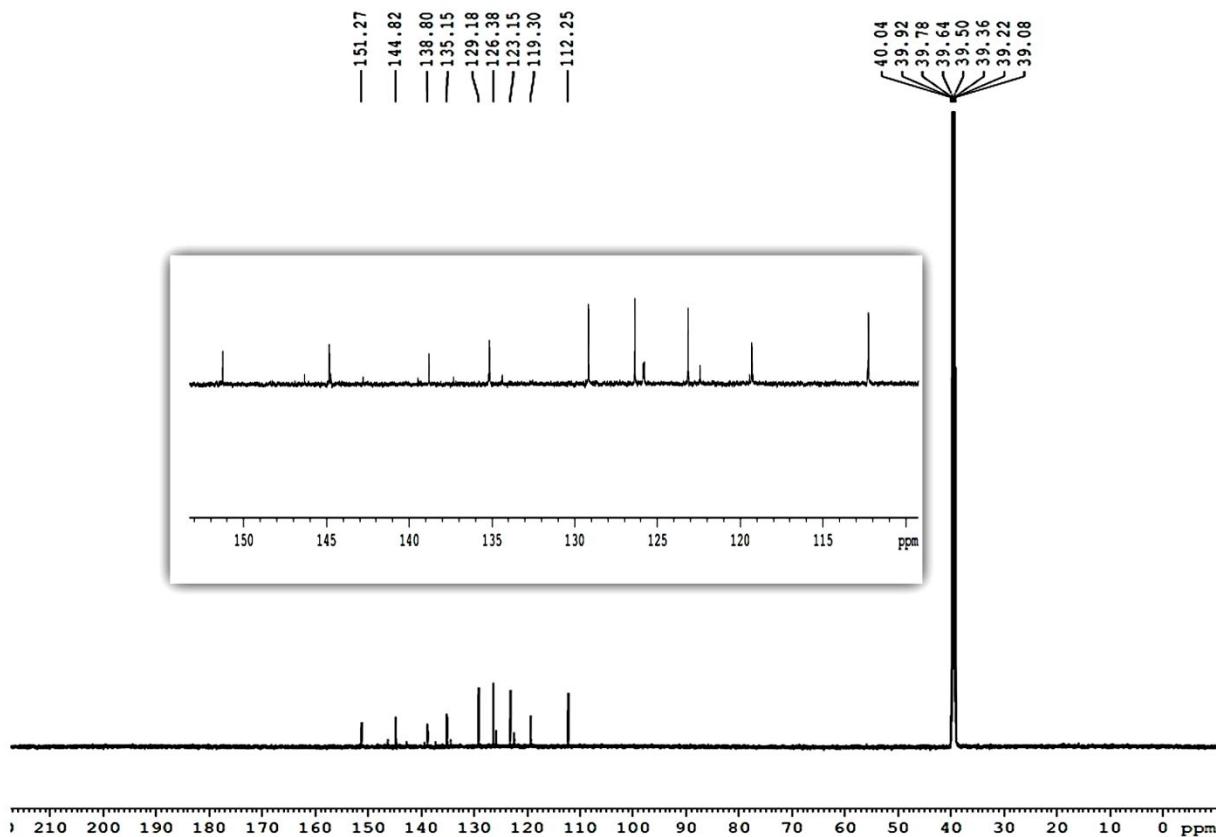
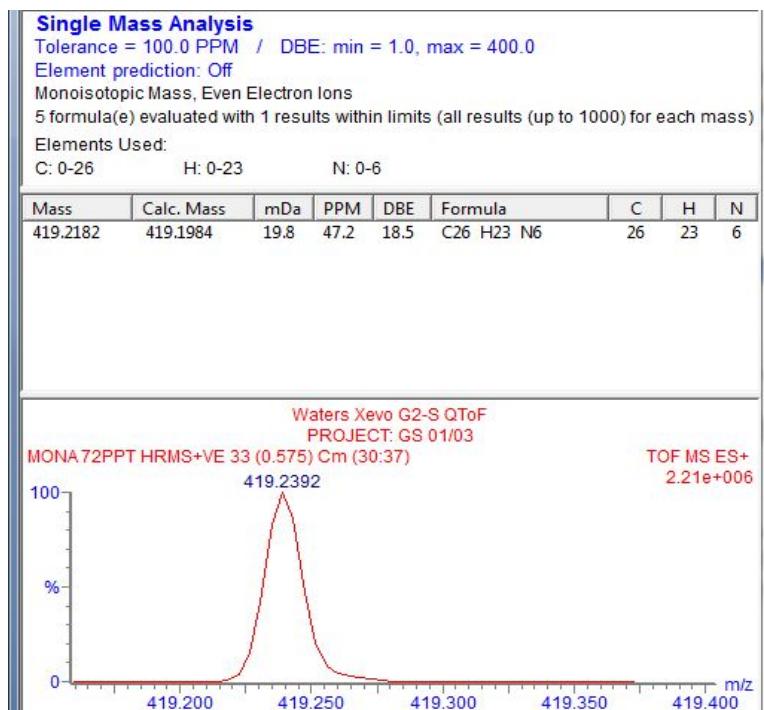


Figure S7. The ^{13}C NMR spectrum of compound **6a** (150 MHz, solvent DMSO)



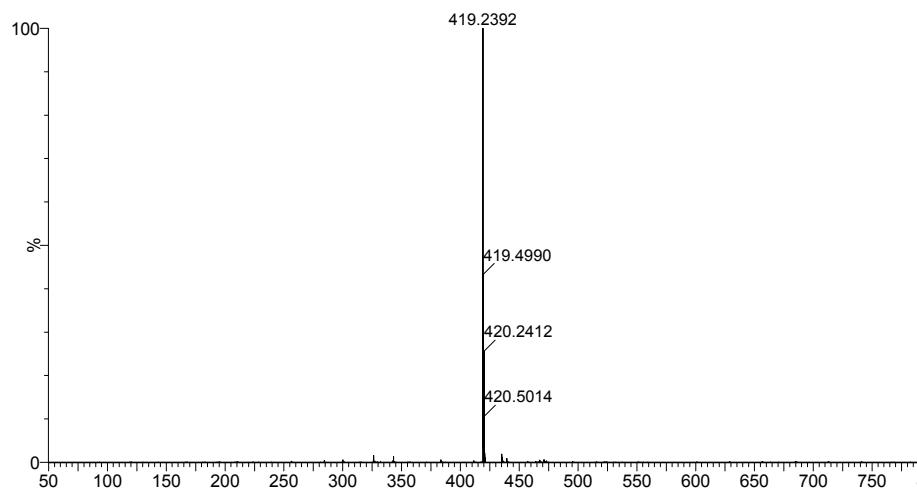
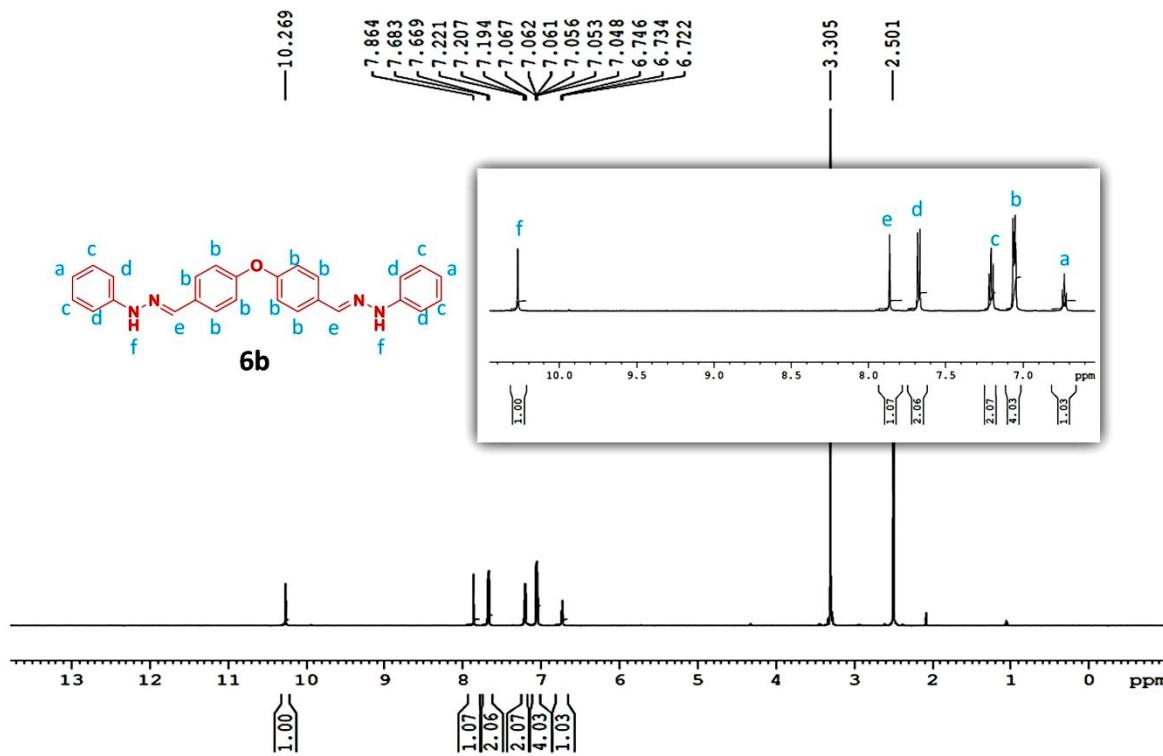


Figure S8. HRMS (ESI-TOF) of compound **6a**



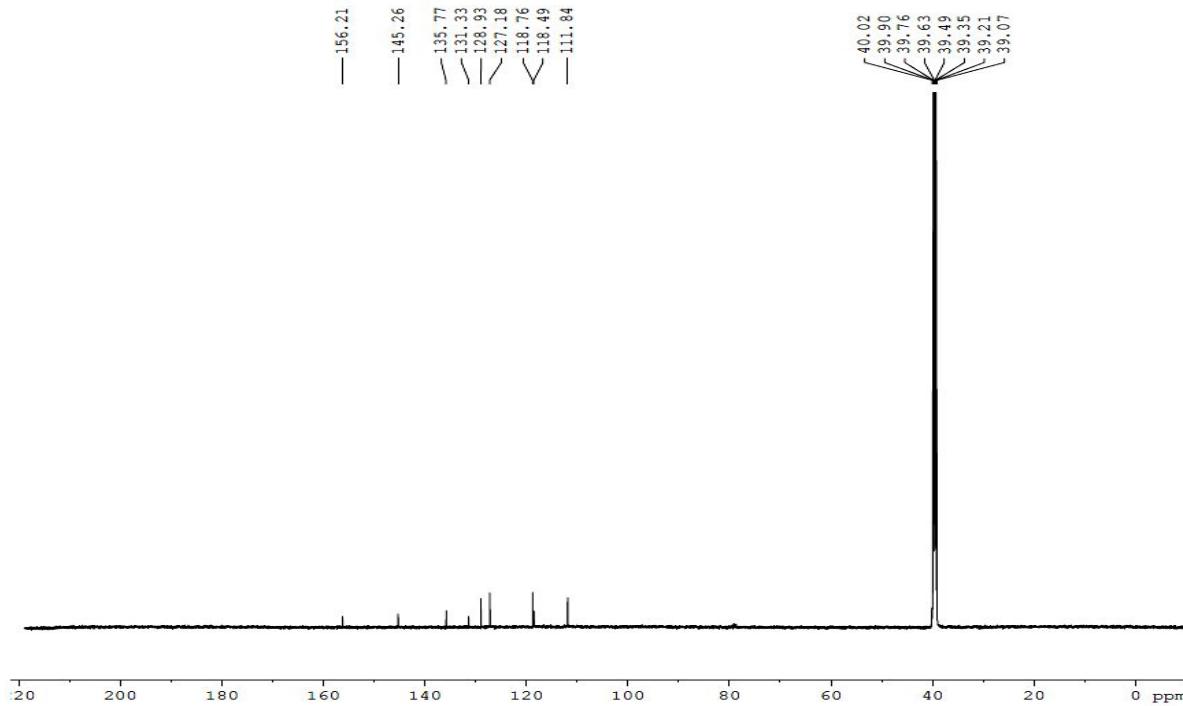
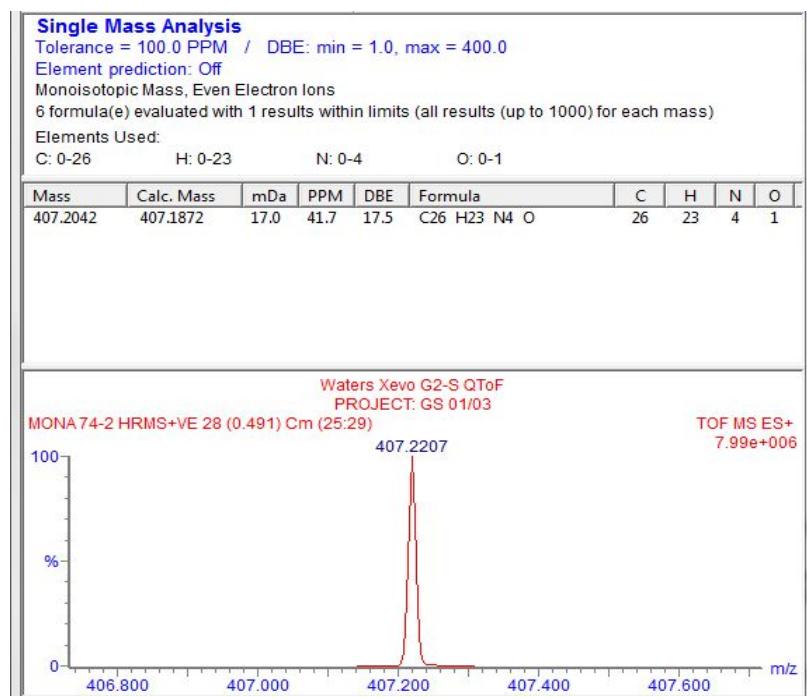


Figure S10. The ^{13}C NMR spectrum of compound **6b** (150 MHz, solvent DMSO)



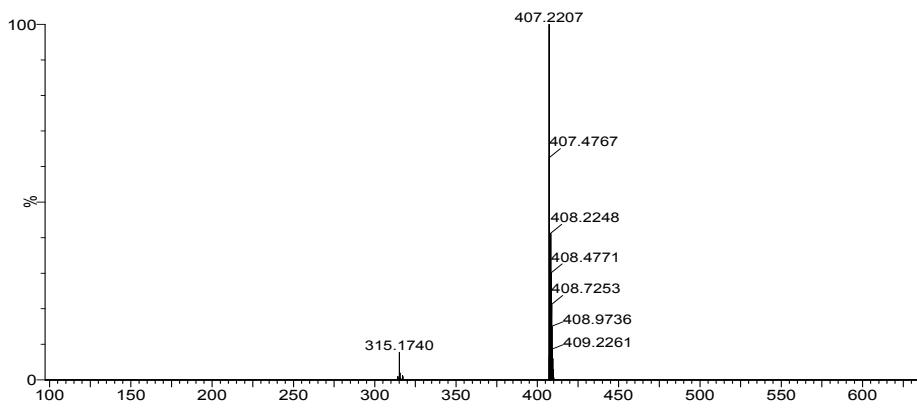


Figure S11. HRMS (ESI-TOF) of compound **6b**

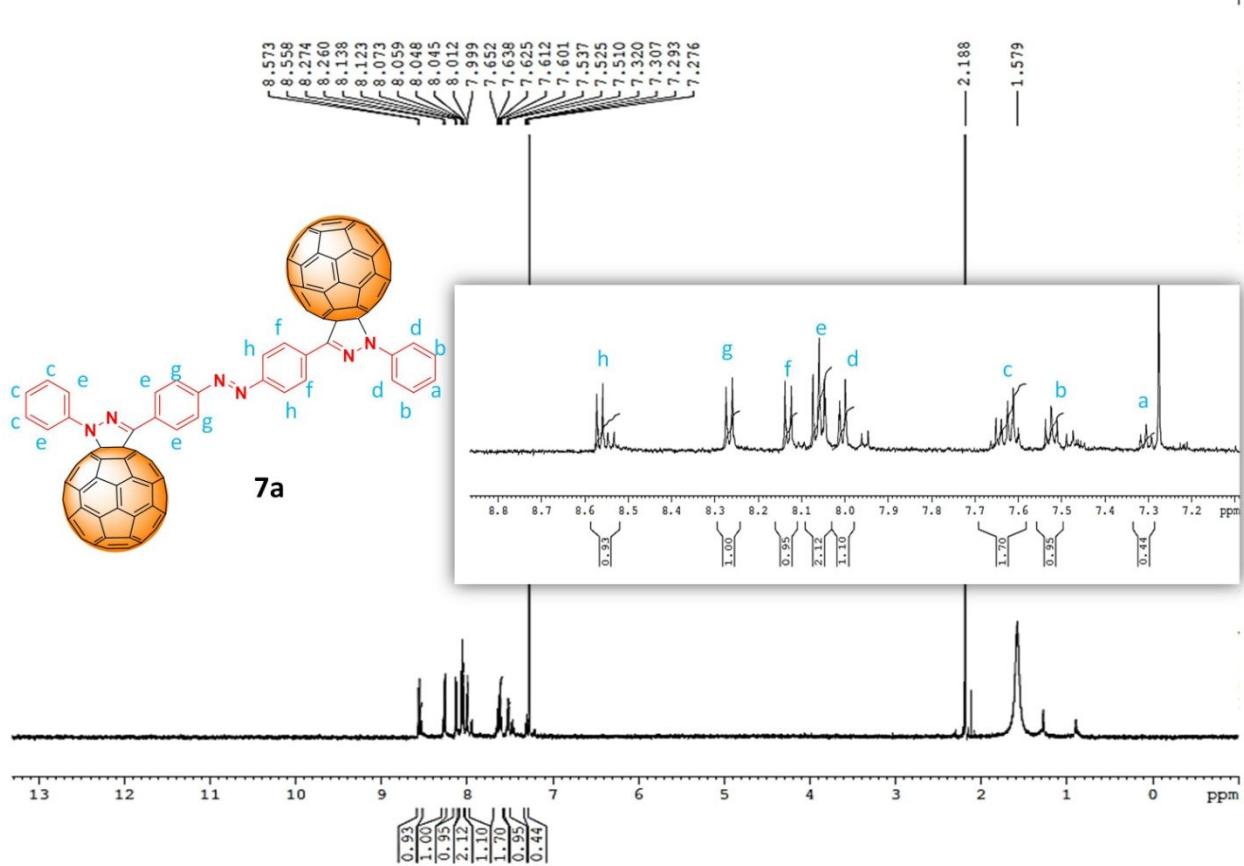


Figure S12. The ^1H NMR spectrum of compound **7a** (600.13 MHz, solvent CDCl_3)

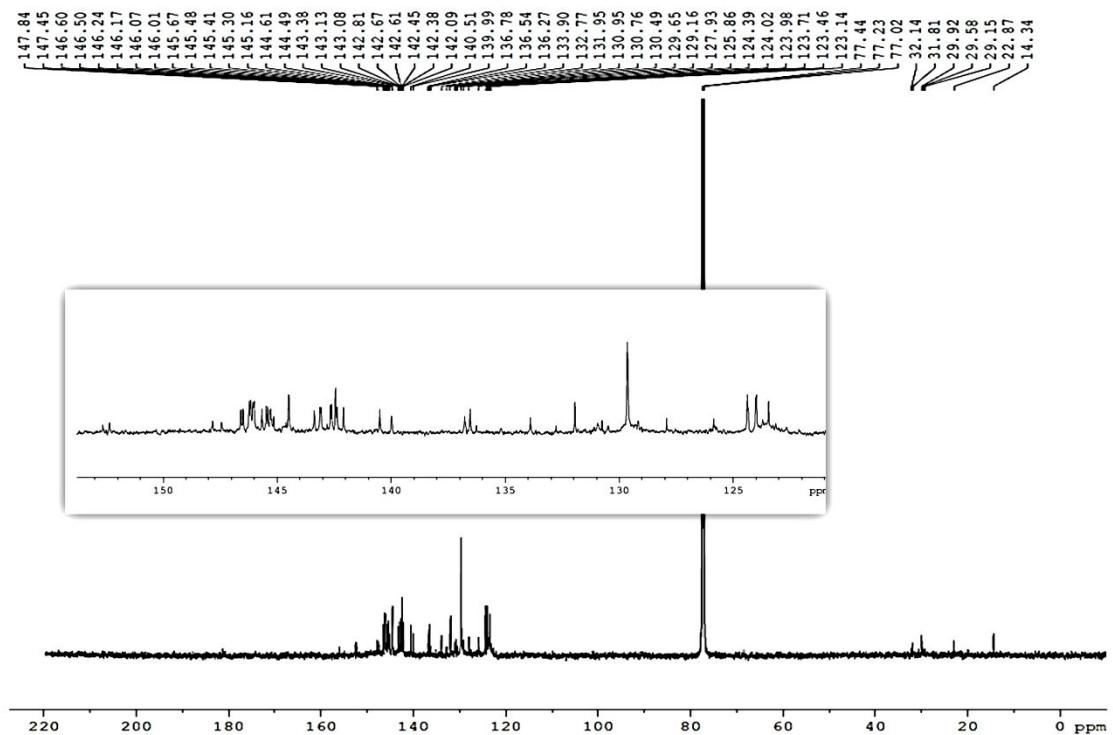


Figure S13. The ^{13}C NMR spectrum of compound **7a** (150 MHz, solvent CDCl_3)

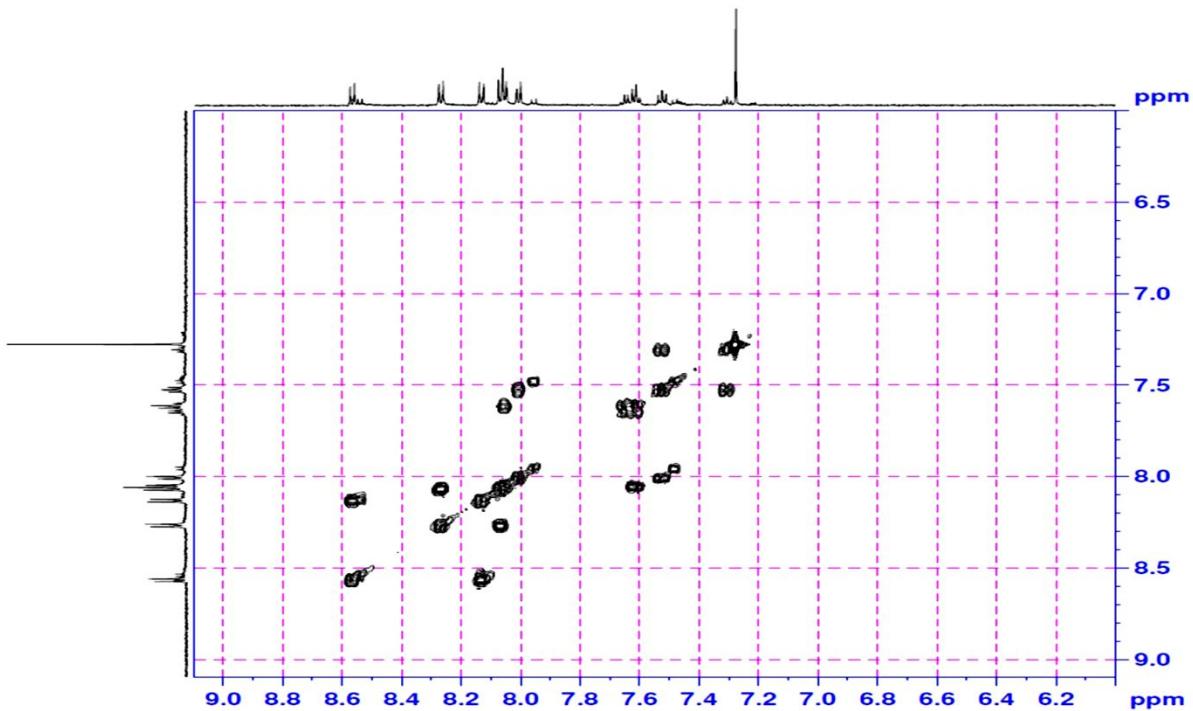


Figure S14. H-H COSY NMR spectrum of compound **7a** (600.13 MHz, solvent CDCl_3)

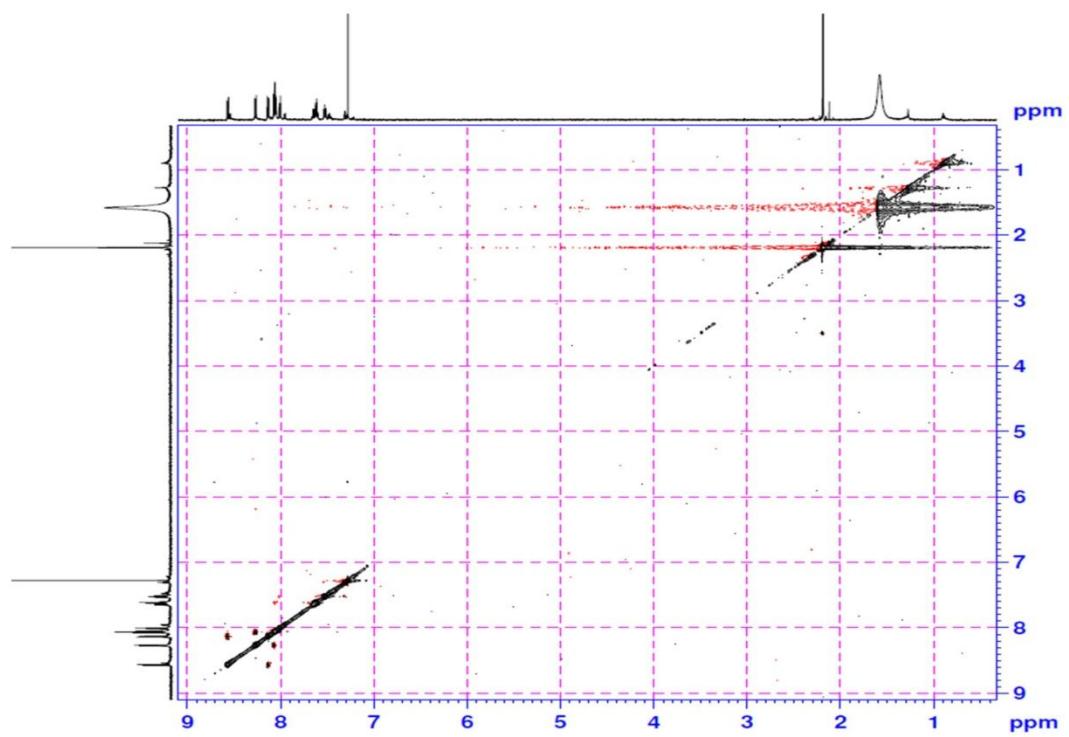


Figure S15. H-H NOESY of compound **7a** (600.13 MHz, solvent CDCl_3)

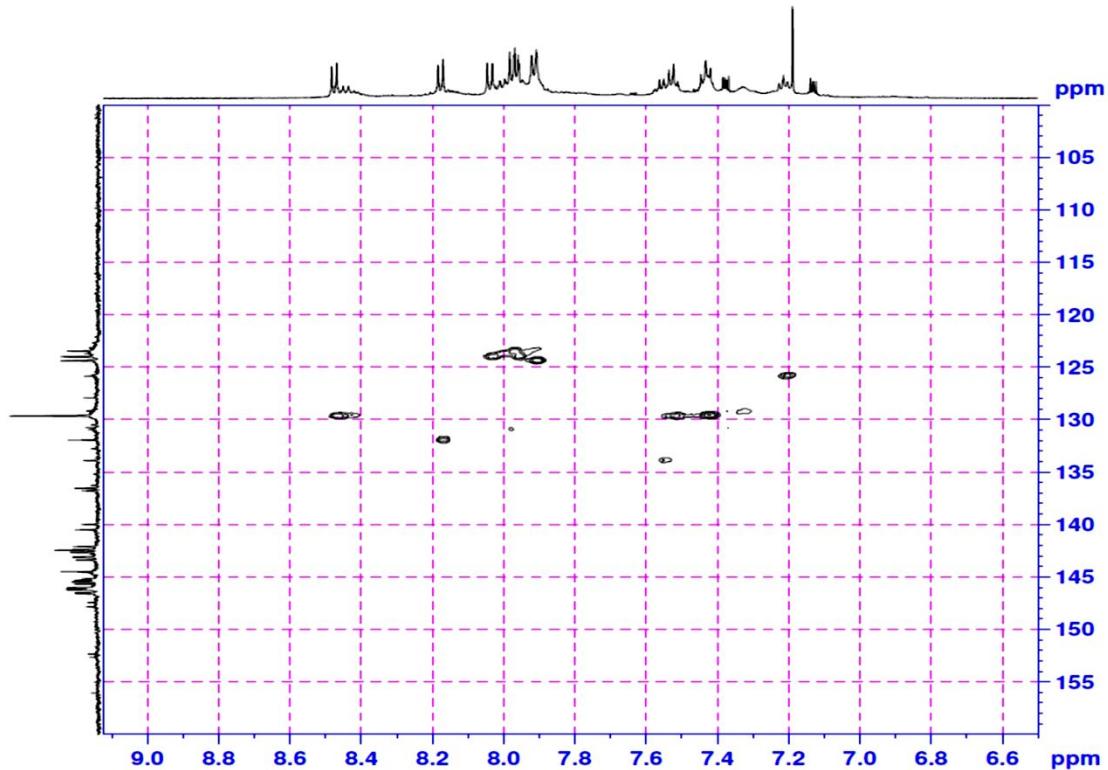


Figure S16. The HSQC spectrum of compound **7a** (600.13 MHz for ^1H and ^{13}C , solvent CDCl_3)

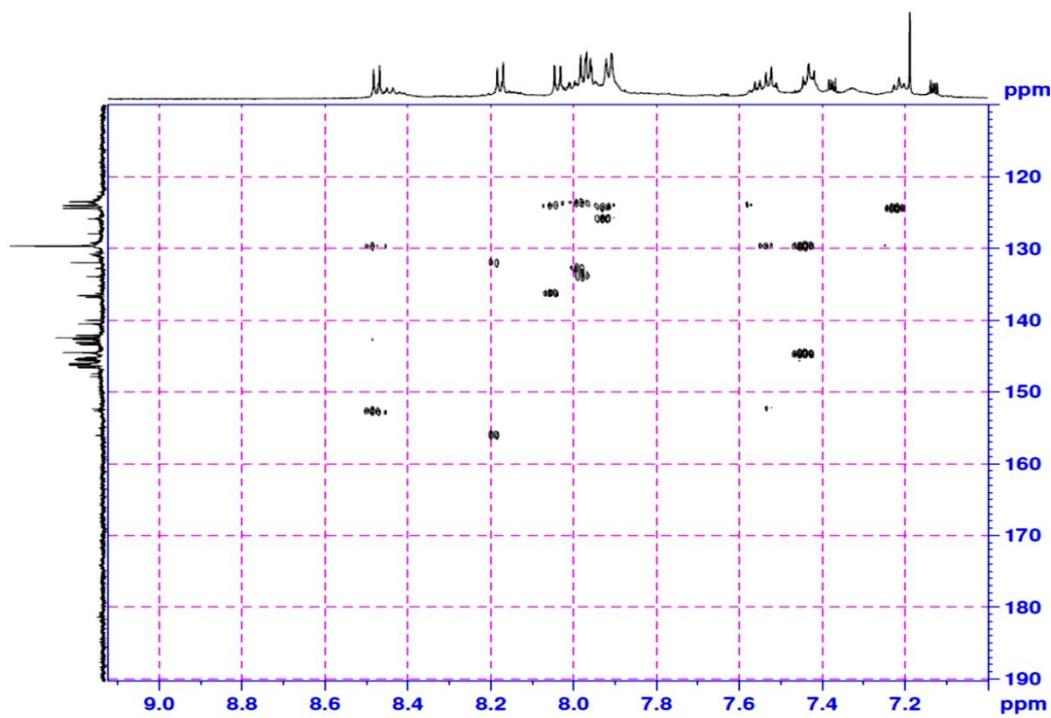


Figure S17. The HMBC spectrum of compound **7a** (600.13 MHz for ^1H and ^{13}C , solvent CDCl_3)

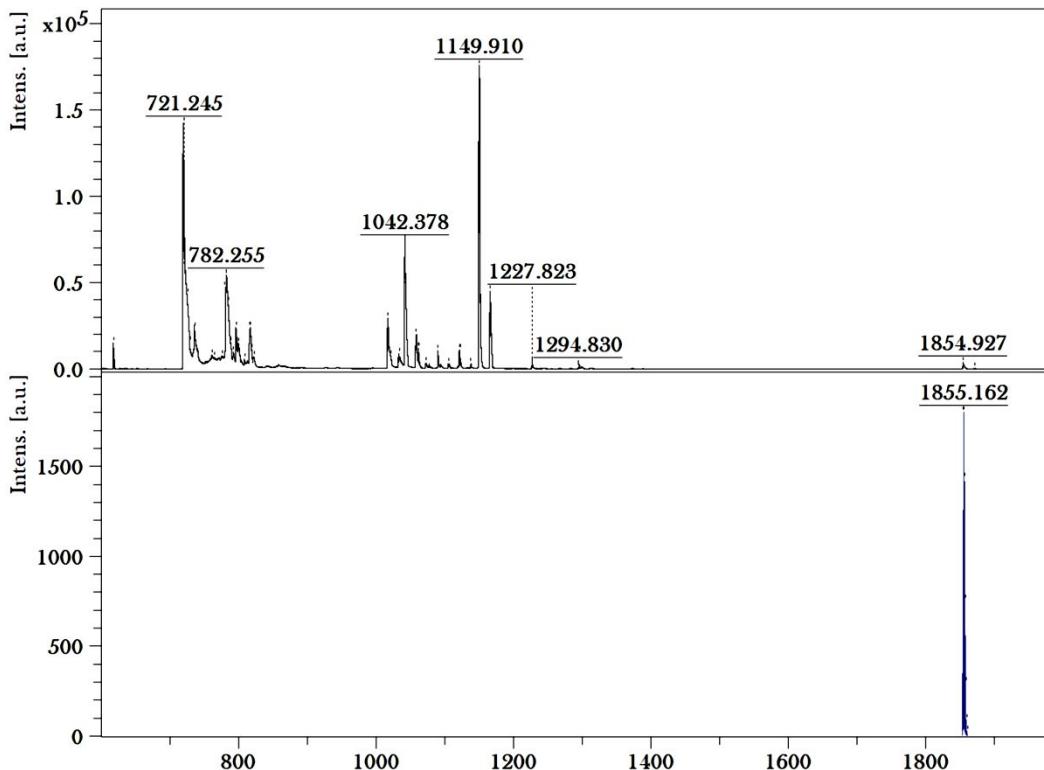
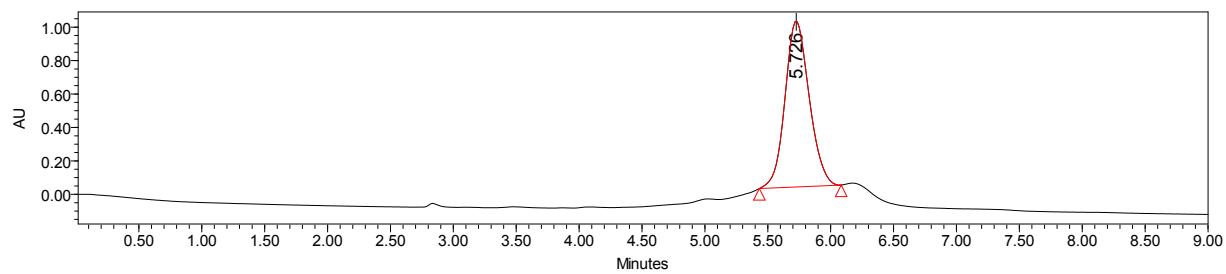


Figure S18. MALDI-TOF spectrum of compound **7a**



	Retention Time	Area	% Area	Height	% Height
1	5.726	13239872	100.00	991897	100.00

Figure S19. HPLC chromatogram of compound **7a**

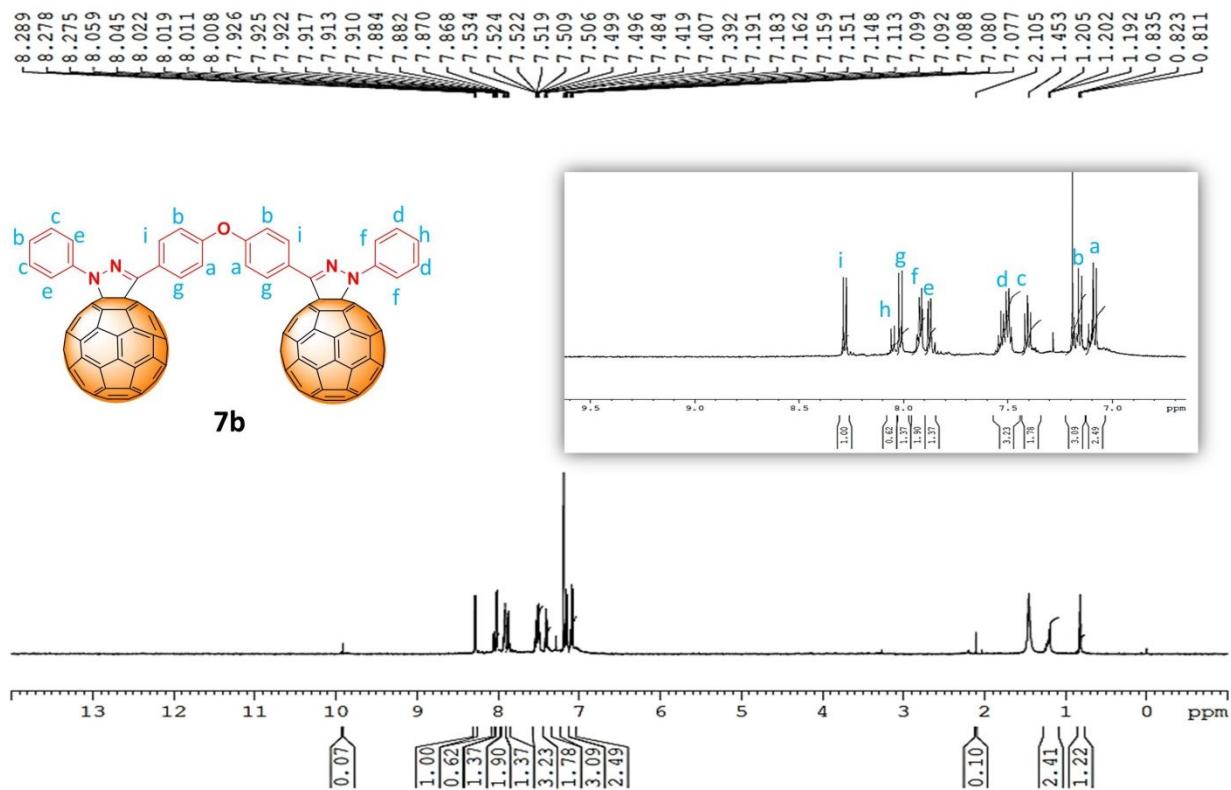


Figure S20. The ^1H NMR spectrum of compound **7b** (600.13 MHz, solvent CDCl_3)

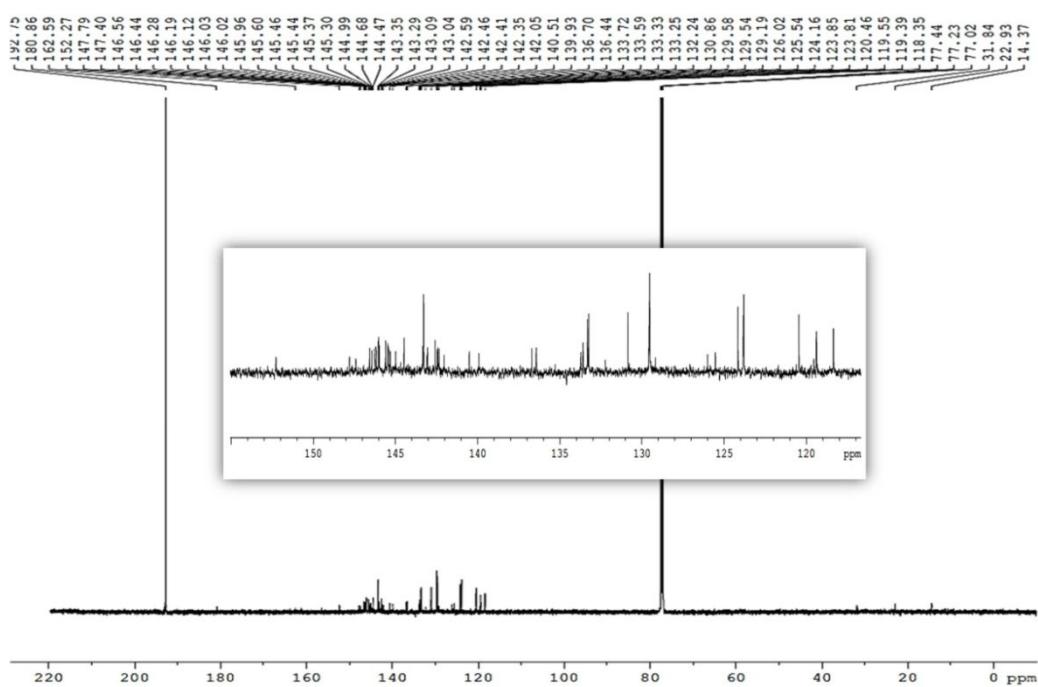


Figure S21. The ^{13}C NMR spectrum of compound **7b** (150 MHz, solvent CS_2 : CDCl_3 = 3:1)

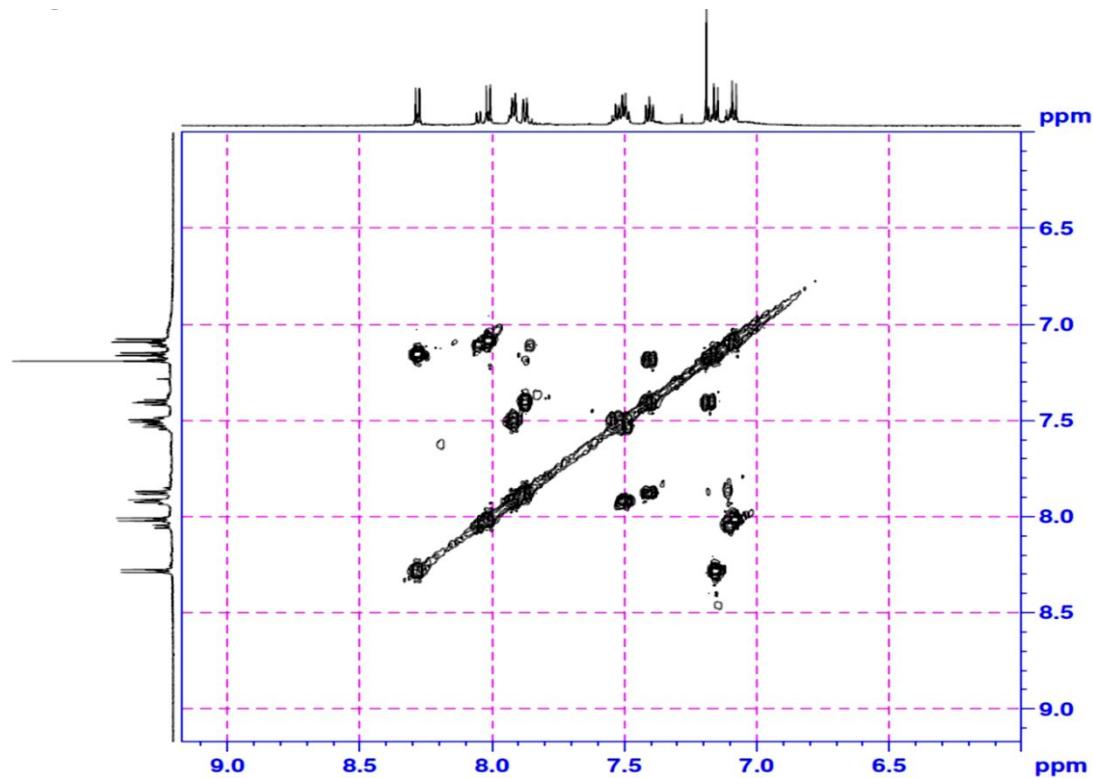


Figure S22. H-H COSY NMR spectrum of compound **7b** (600.13 MHz, solvent CS_2 : CDCl_3 = 3:1)

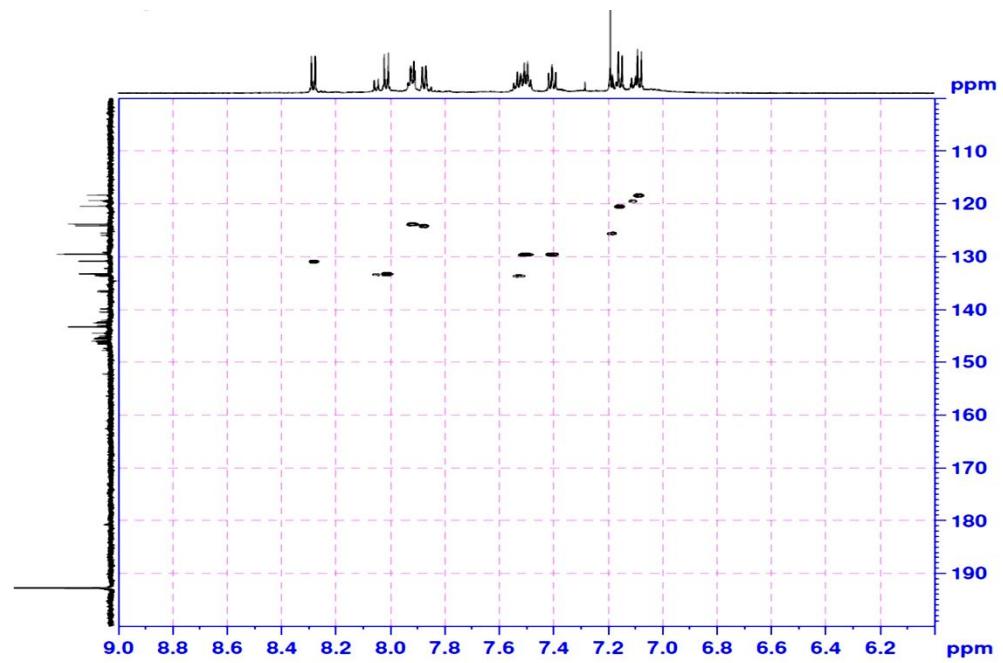


Figure S23. The HSQC spectrum of compound **7b** (600.13 MHz for ¹H and ¹³C, solvent CS₂: CDCl₃ = 3:1)

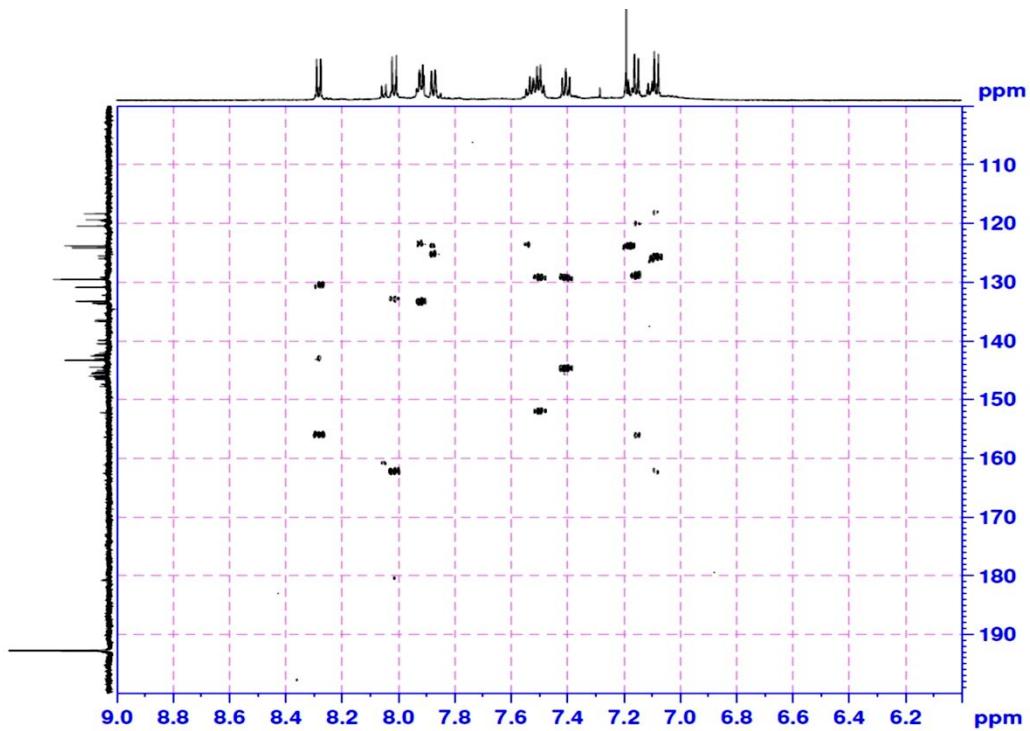


Figure S24. The HMBC spectrum of compound **7b** (600.13 MHz for ¹H and ¹³C, solvent CS₂: CDCl₃ = 3:1)

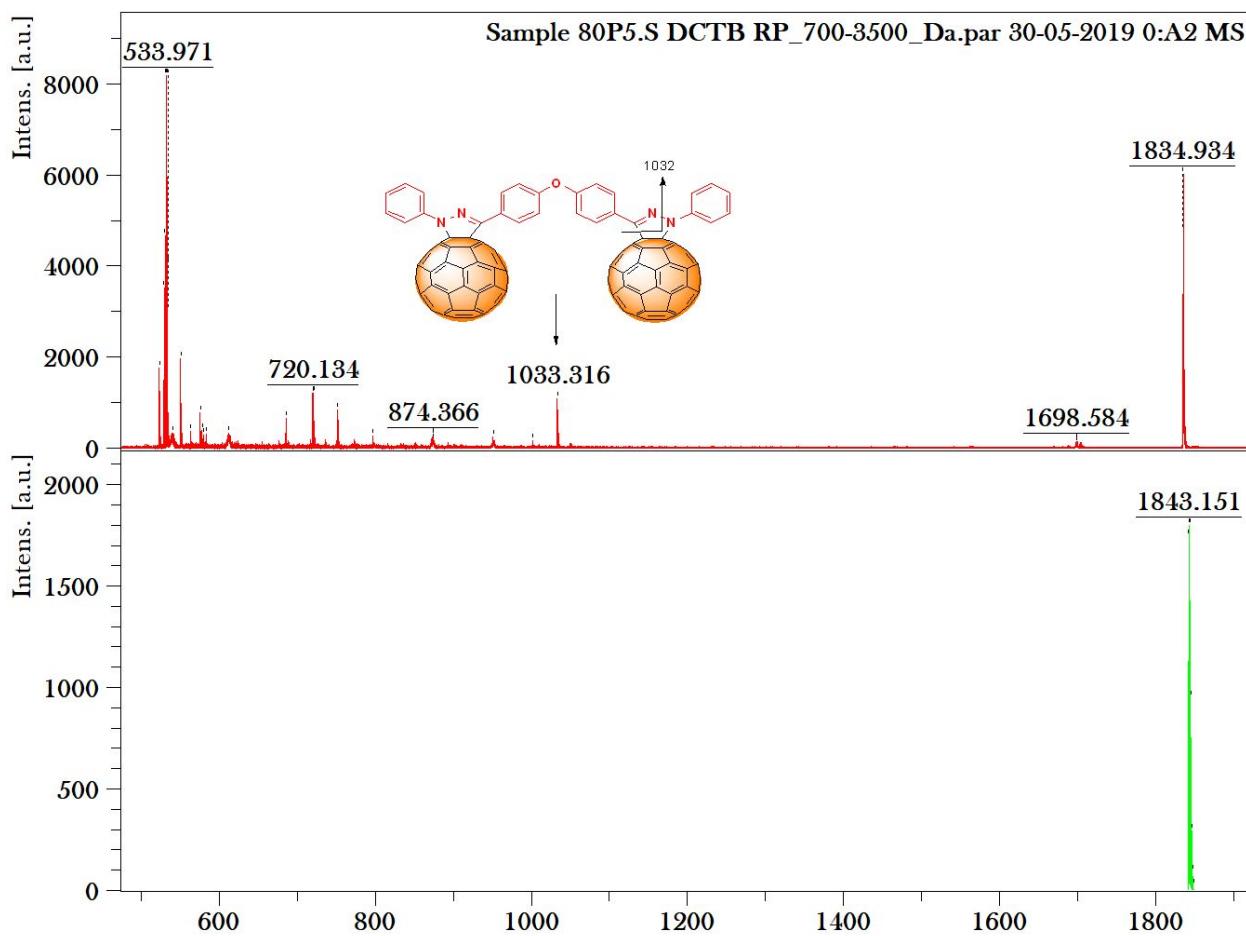
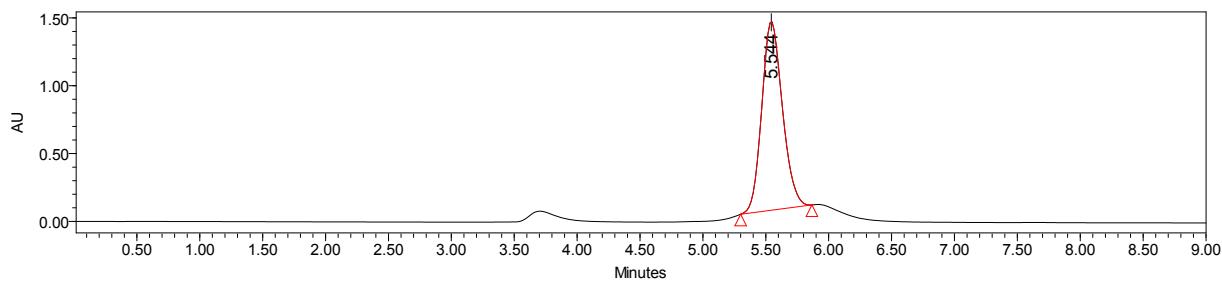


Figure S25. MALDI-TOF spectrum of compound **7b**.



	Retention Time	Area	% Area	Height	% Height
1	5.544	15863478	100.00	1390968	100.00

Figure S26. HPLC chromatogram of compound **7b**

Table S1. Experimental details and crystal data for the compound **6b**

Crystal sample	6b
Chemical formula	C ₂₆ H ₂₂ N ₄ O
M _r	406.49
Crystal system, space group	Triclinic, <i>P</i>
Temperature (K)	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	5.6471 (7), 9.3471 (12), 20.515 (2)
β (°)	86.434 (6), 89.453 (6), 83.523 (6)
<i>V</i> (Å ³)	1073.9 (2)
<i>Z</i>	2
Radiation type	Mo <i>Kα</i>
μ (mm ⁻¹)	0.08
Crystal size (mm)	0.20 × 0.20 × 0.07
Diffractometer	Rigaku R-AXIS RAPID
Absorption correction	Multi-scan <i>ABSCOR</i> (Rigaku, 1995)
<i>T</i> _{min} , <i>T</i> _{max}	0.313, 0.994
No. of measured, independent & observed [<i>I</i> > 2σ(<i>I</i>)] reflections	7387, 3718, 1544
<i>R</i> _{int}	0.057
(sin θ/λ) _{max} (Å ⁻¹)	0.595
<i>R</i> [F ² > 2σ(F ²)], wR(F ²), <i>S</i>	0.048, 0.101, 0.86
No. of reflections	3718
No. of parameters	280
H-atom treatment	Constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.17, -0.14