Supporting Information

A facile, metal-free, oxidative coupling of new 6-(hetero)aryl-[1,2,5]oxadiazolo[3,4-*b*]pyrazines with pyrroles, indoles and carbazoles.

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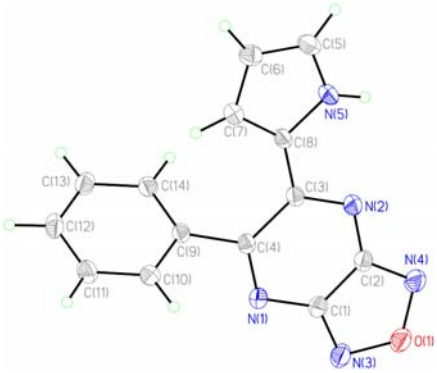


Figure S1. X-ray structure of **9a**.

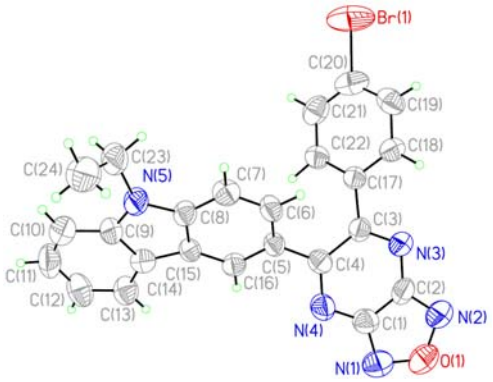


Figure S2. X-ray structure of **21c**.

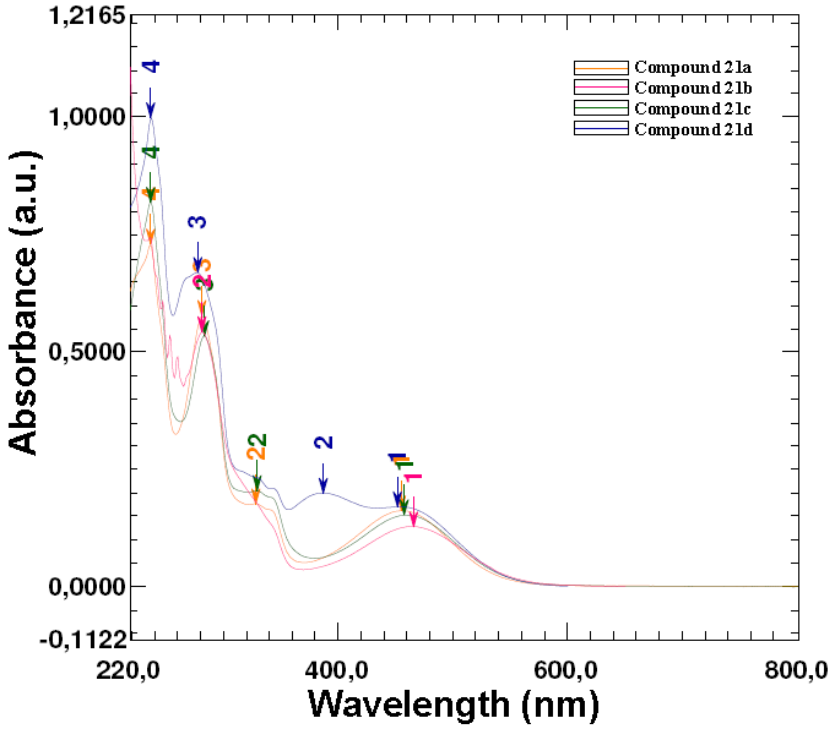


Figure S3. UV–vis absorption spectra of **21a-d**.

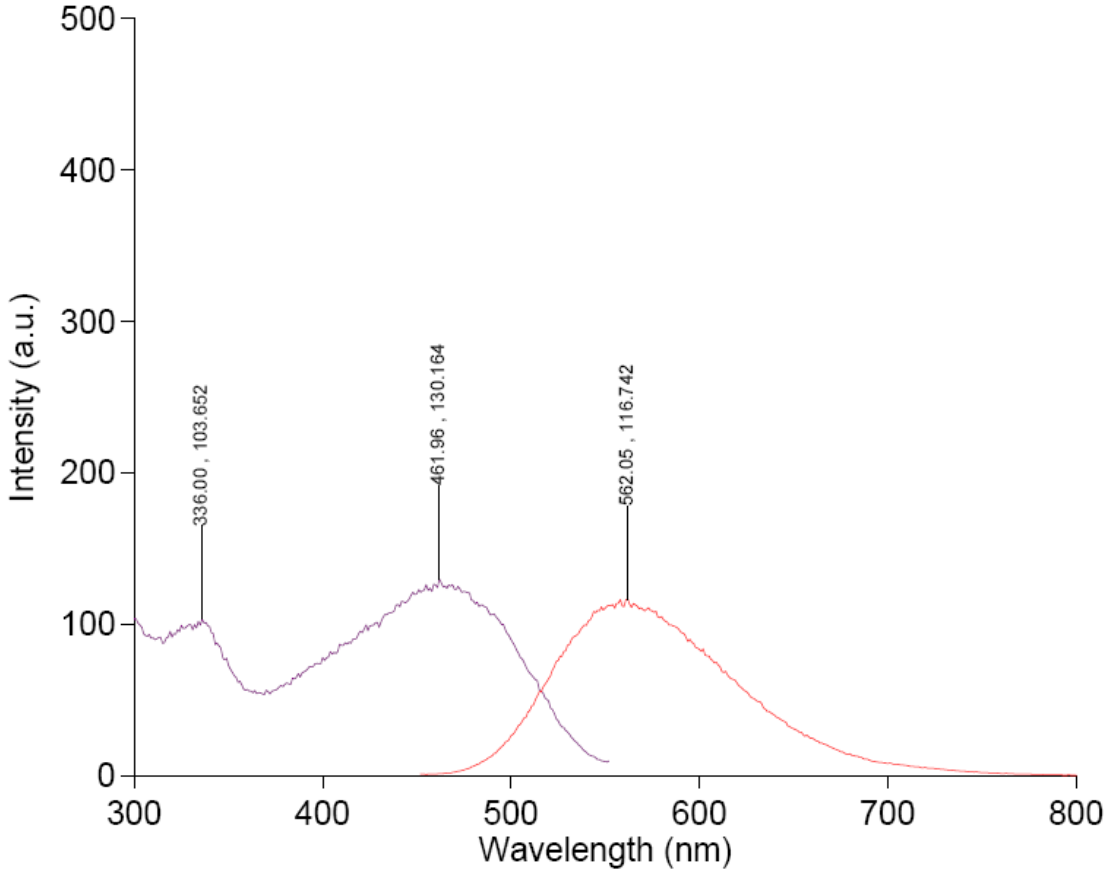


Figure S4. Excitation (*left*) and emission (*right*) spectra of compound **20a** in PMMA film.

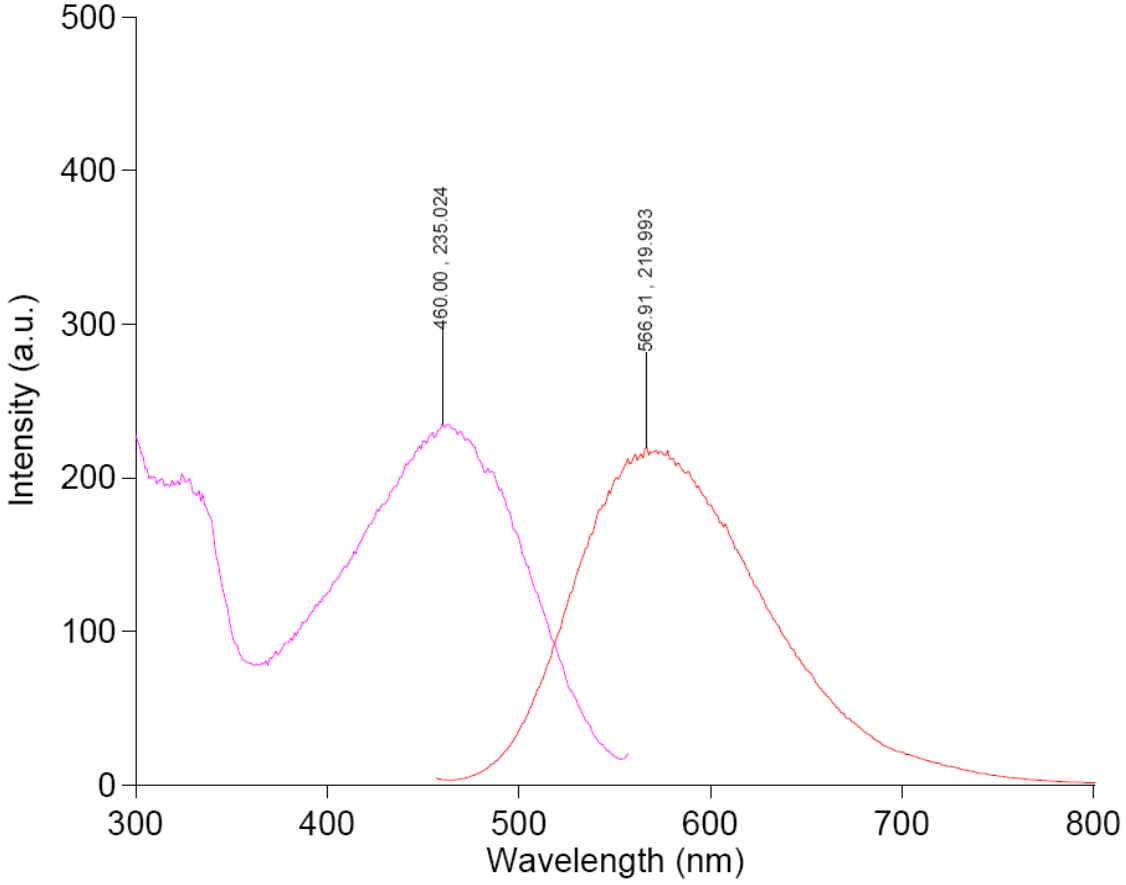


Figure S5. Excitation (*left*) and emission (*right*) spectra of compound **20b** in PMMA film.

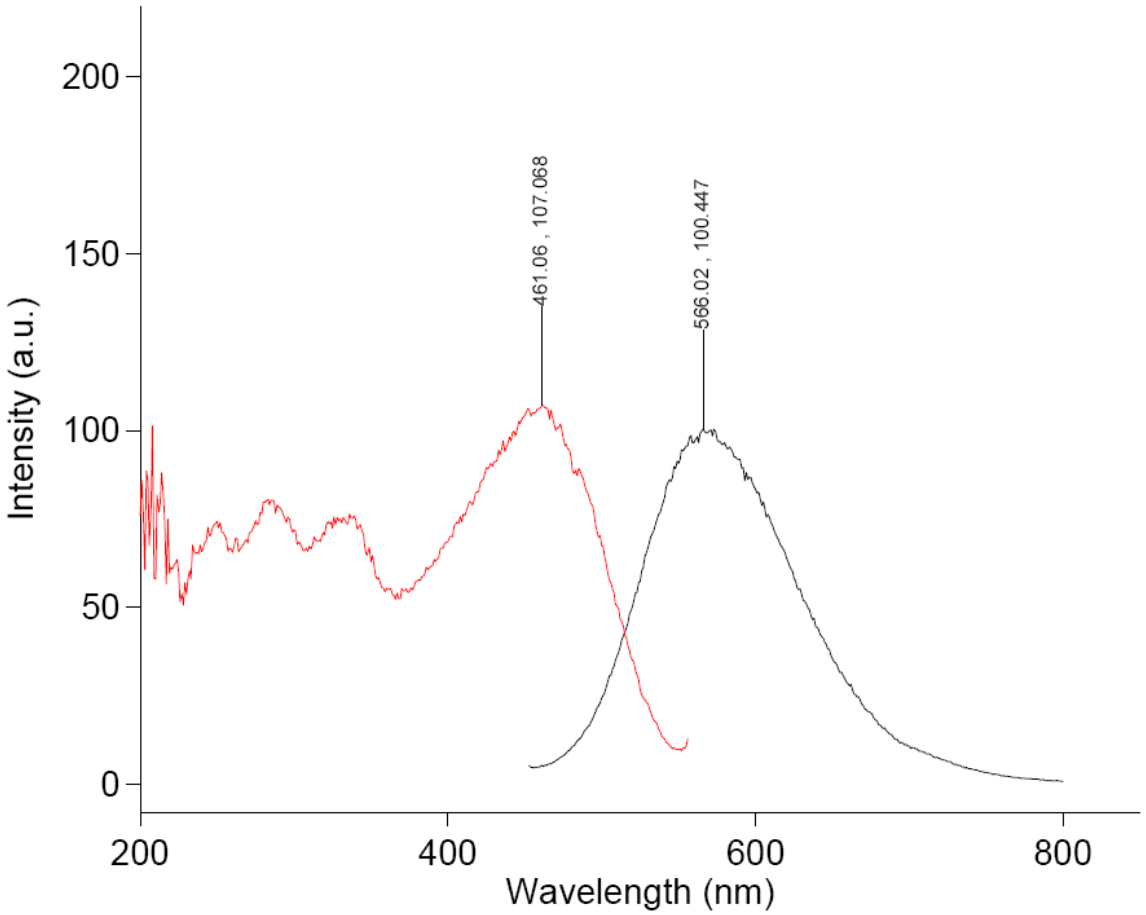


Figure S6. Excitation (*left*) and emission (*right*) spectra of compound **20c** in PMMA film.

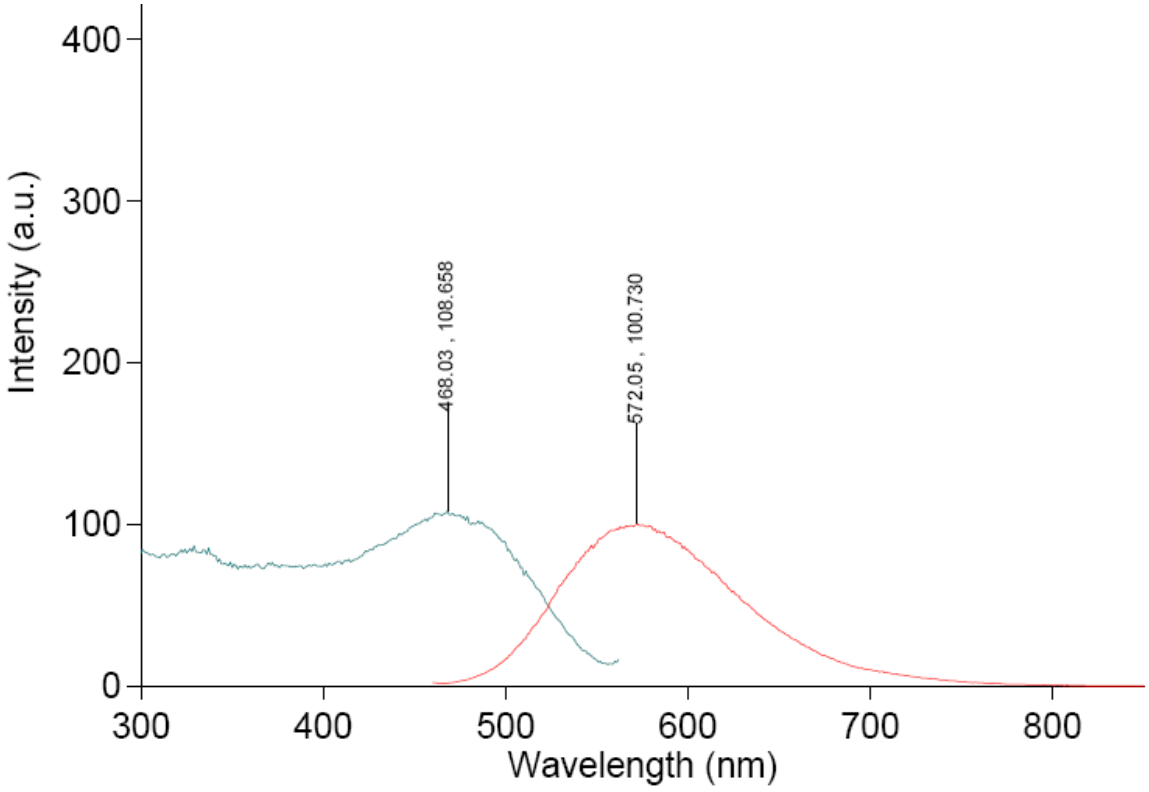


Figure S7. Excitation (*left*) and emission (*right*) spectra of compound **20d** in PMMA film.

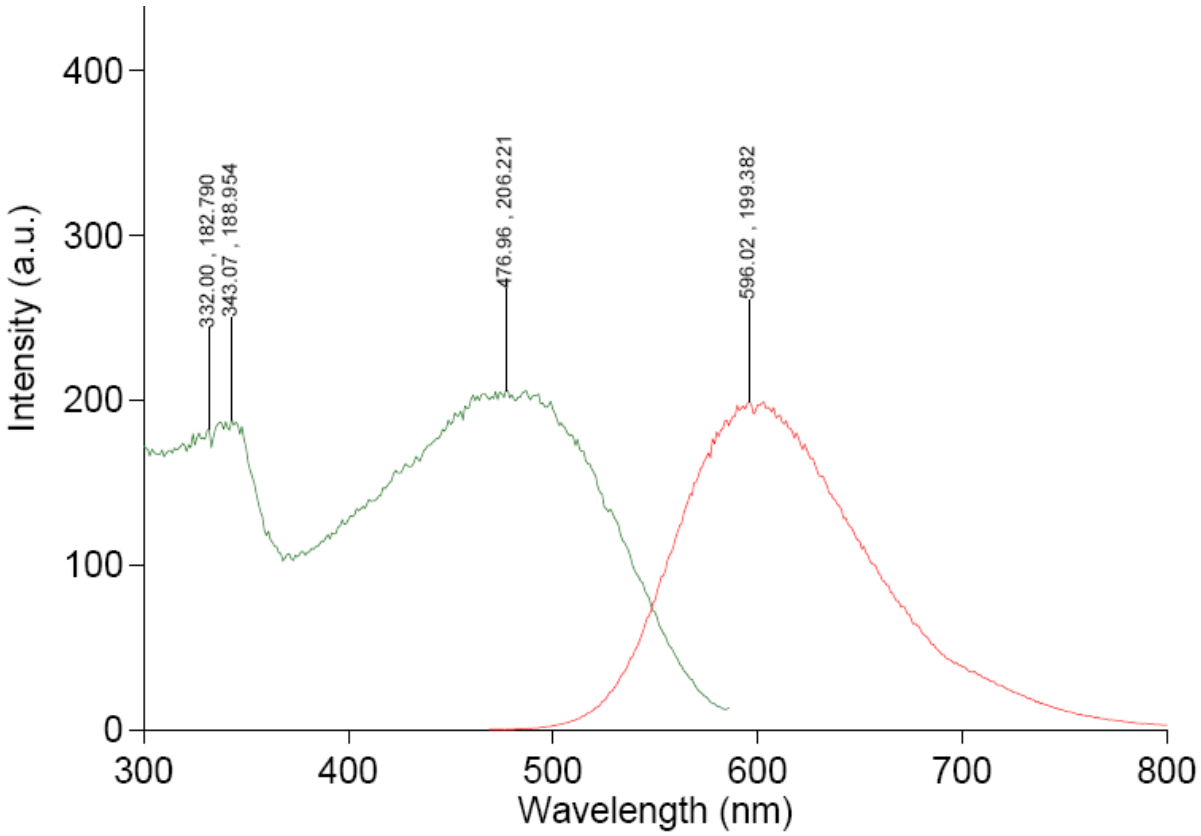


Figure S8. Excitation (*left*) and emission (*right*) spectra of compound **21a** in PMMA film.

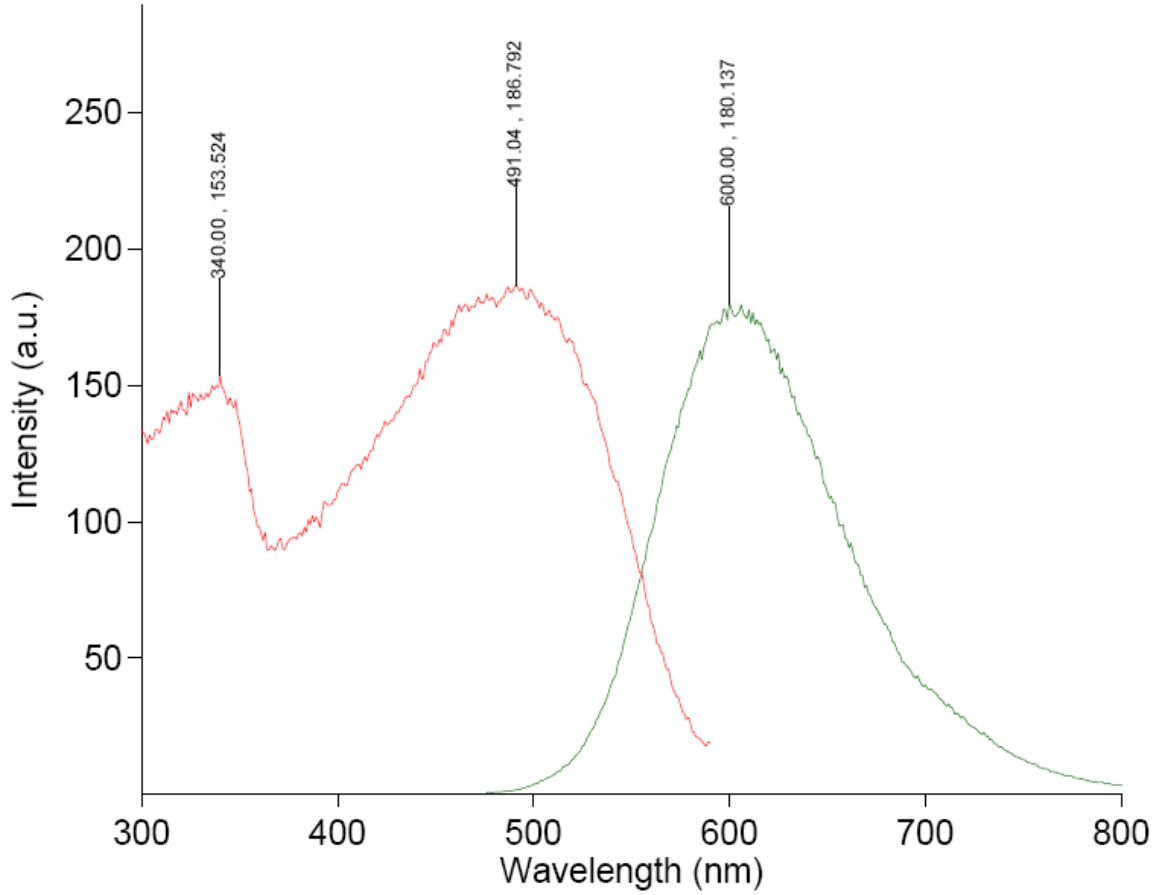


Figure S9. Excitation (*left*) and emission (*right*) spectra of compound **21b** in PMMA film.

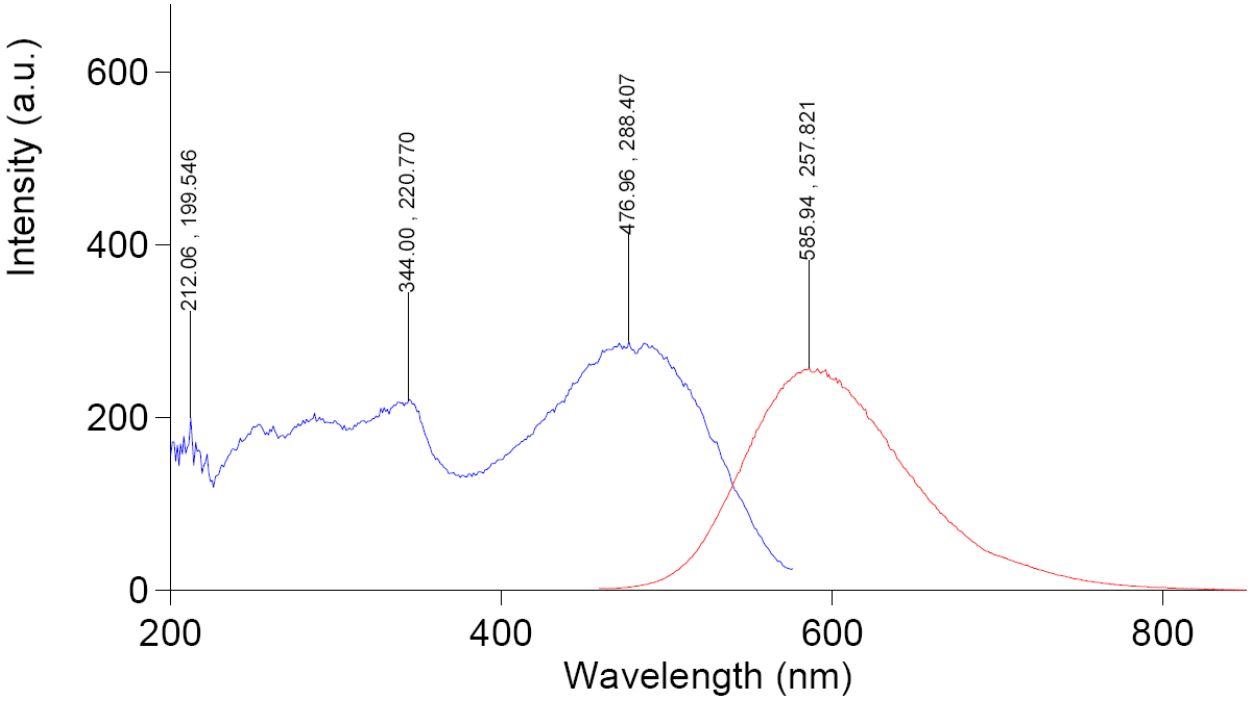


Figure S10. Excitation (*left*) and emission (*right*) spectra of compound **21c** in PMMA film.

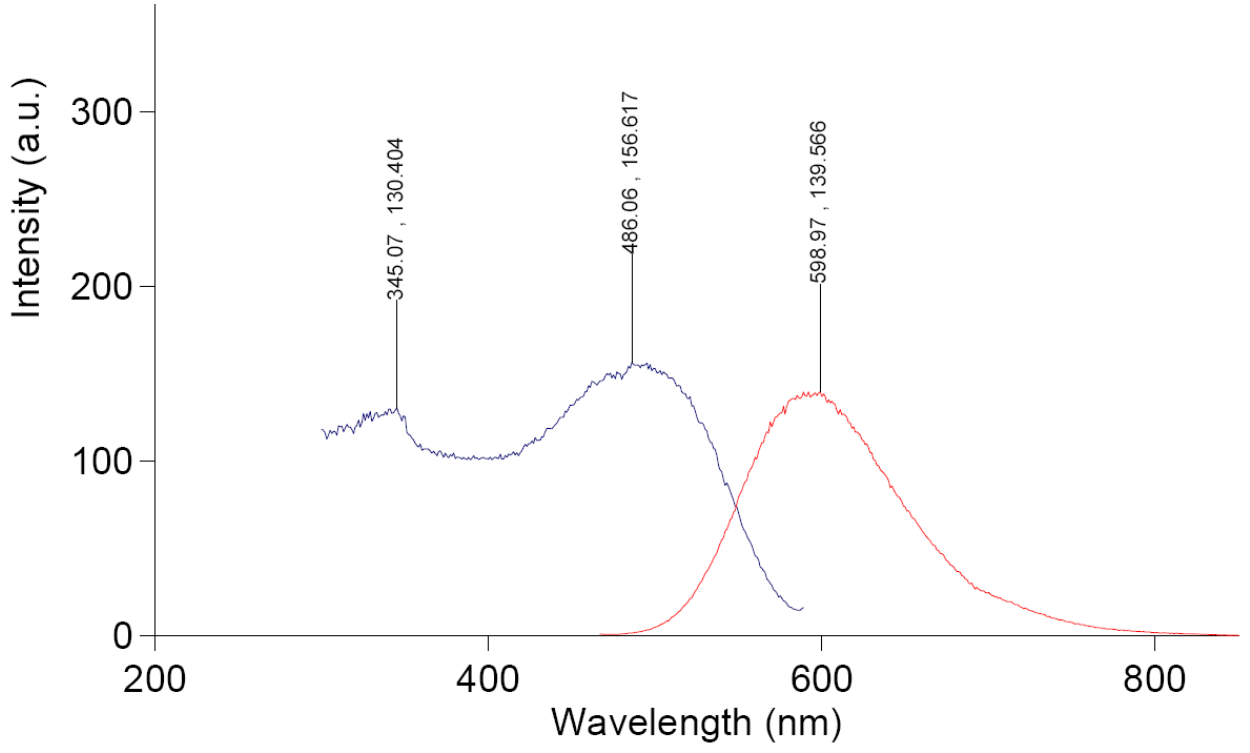


Figure S11. Excitation (*left*) and emission (*right*) spectra of compound **21d** in PMMA film.

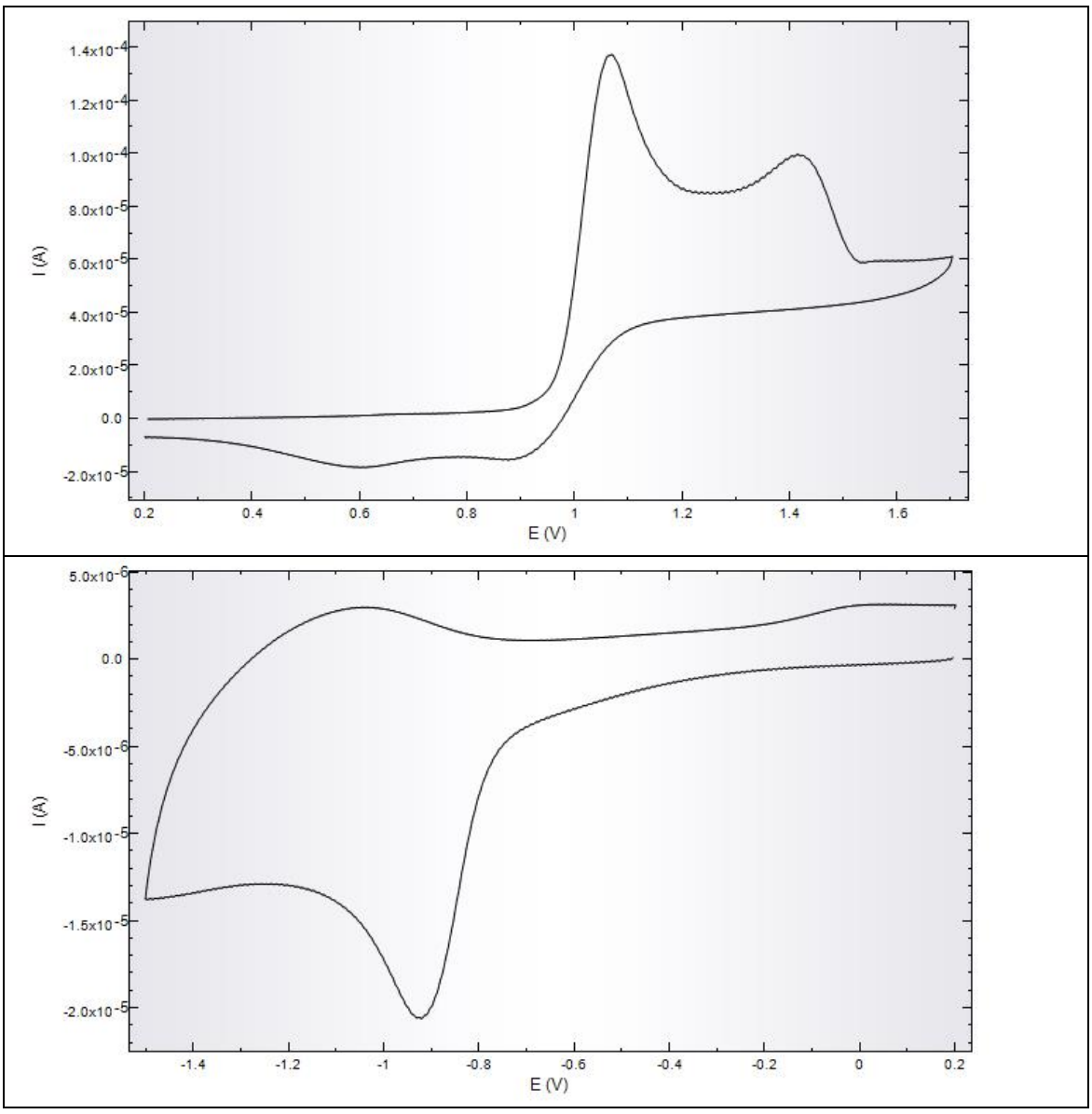


Figure S12. Cyclic voltammograms of **20a** measured in anhydrous CH_3CN with 0.1 M LiClO4 at 100 mV/s ($Ag/AgNO_3$ reference electrode).

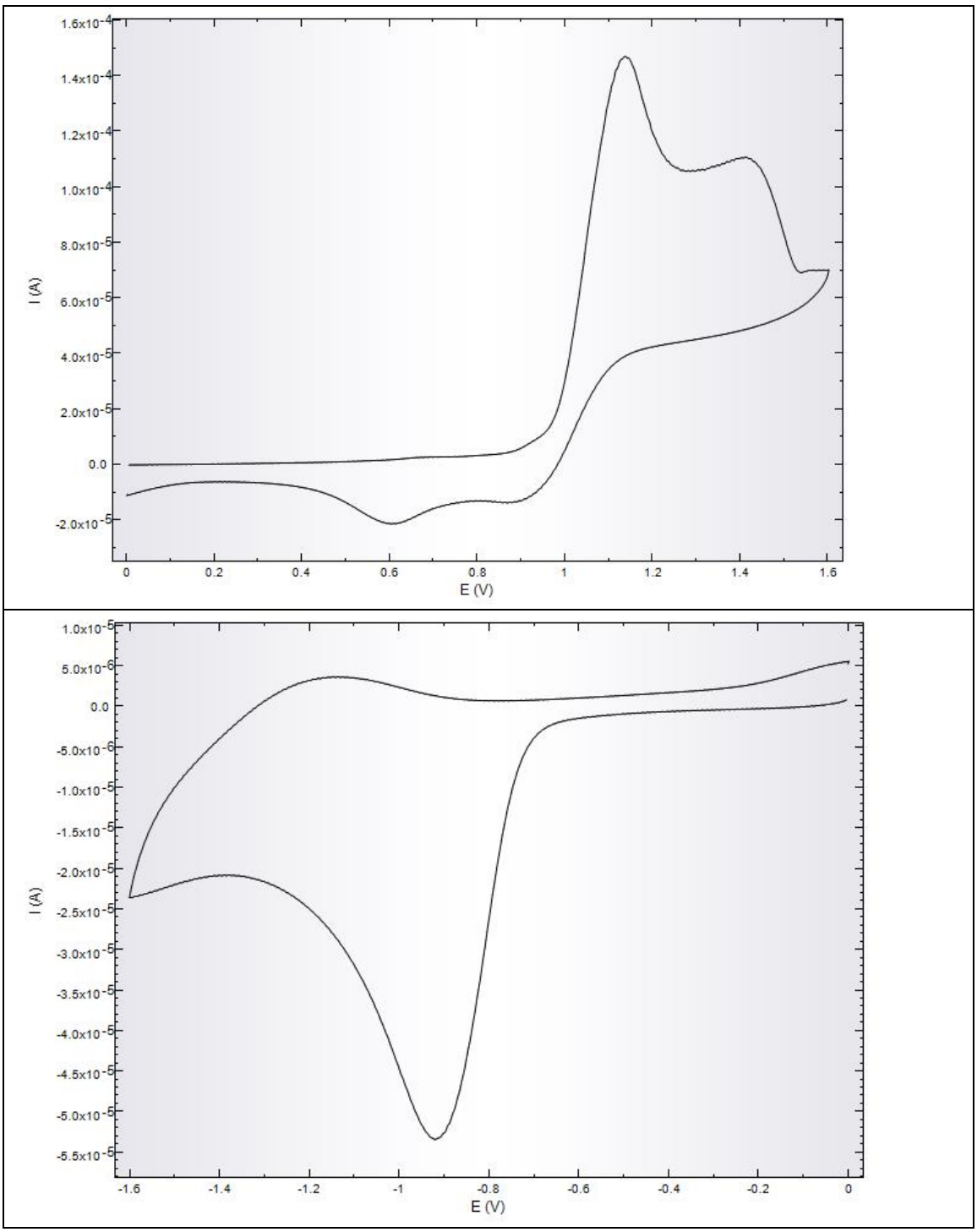


Figure S13. Cyclic voltammograms of **20b** measured in anhydrous CH_3CN with 0.1 M LiClO4 at 100 mV/s ($Ag/AgNO_3$ reference electrode).

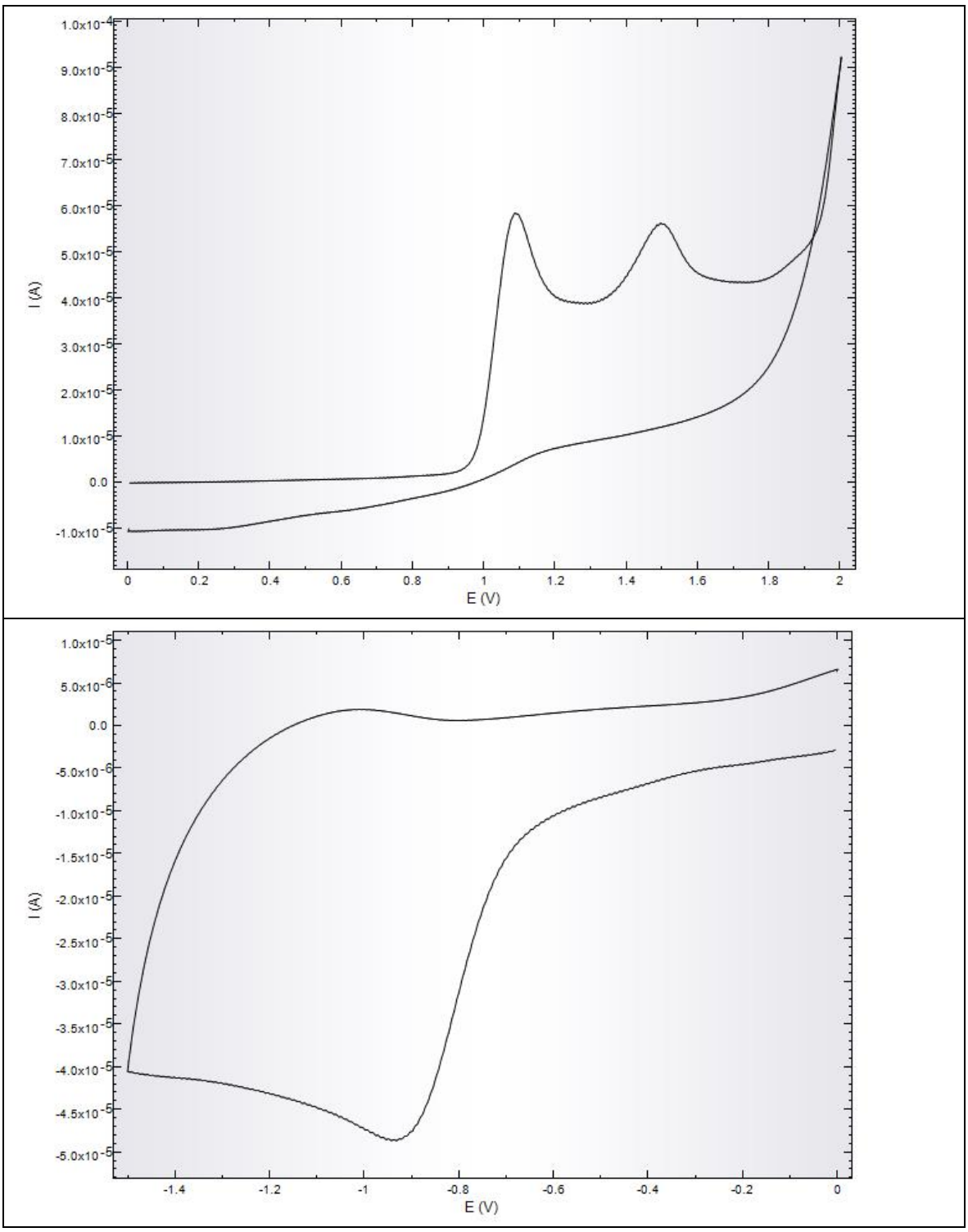


Figure S14. Cyclic voltammograms of **20c** measured in anhydrous CH_3CN with 0.1 M LiClO4 at 100 mV/s ($Ag/AgNO_3$ reference electrode).

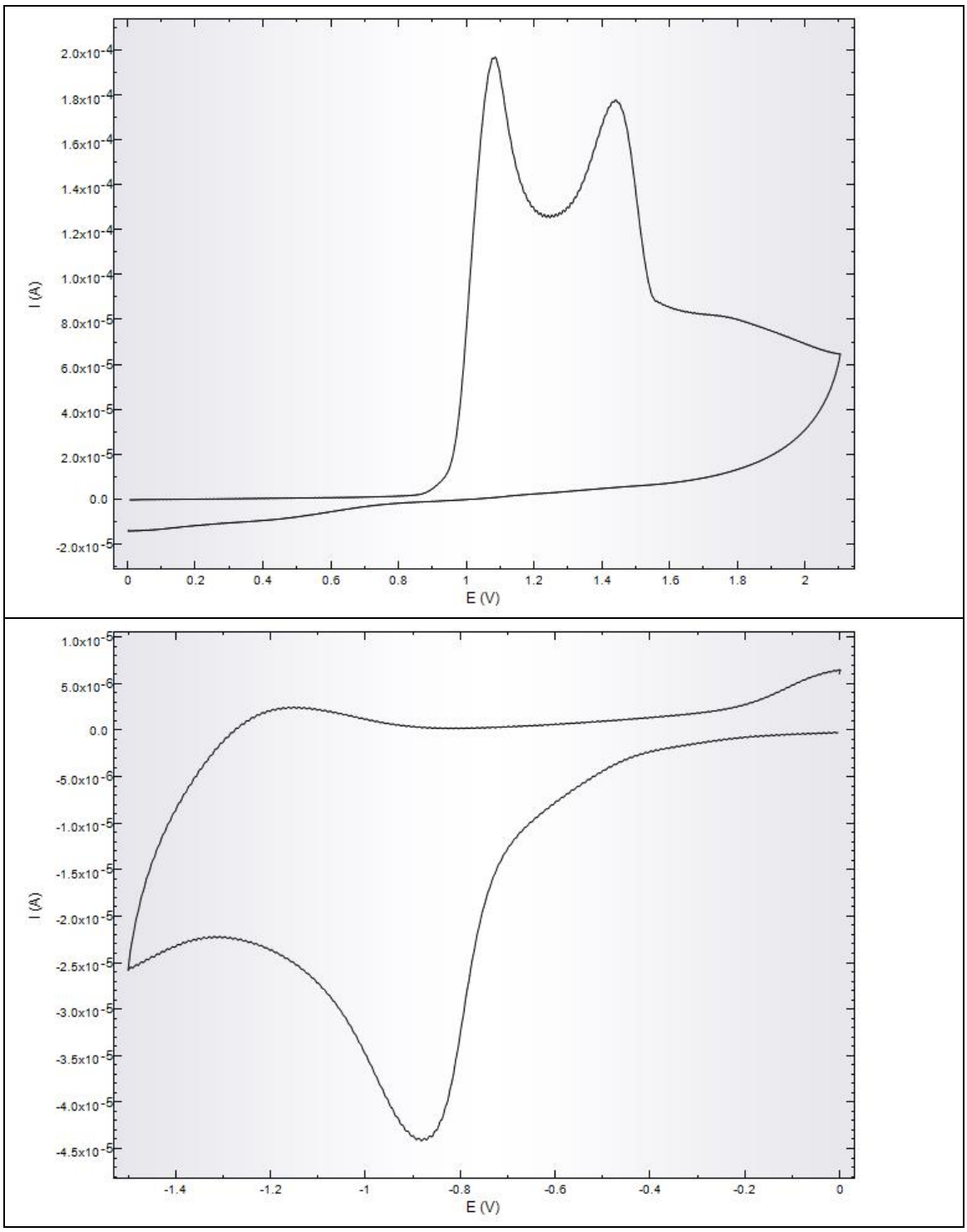


Figure S15. Cyclic voltammograms of **20d** measured in anhydrous CH_3CN with 0.1 M LiClO4 at 100 mV/s ($Ag/AgNO_3$ reference electrode).

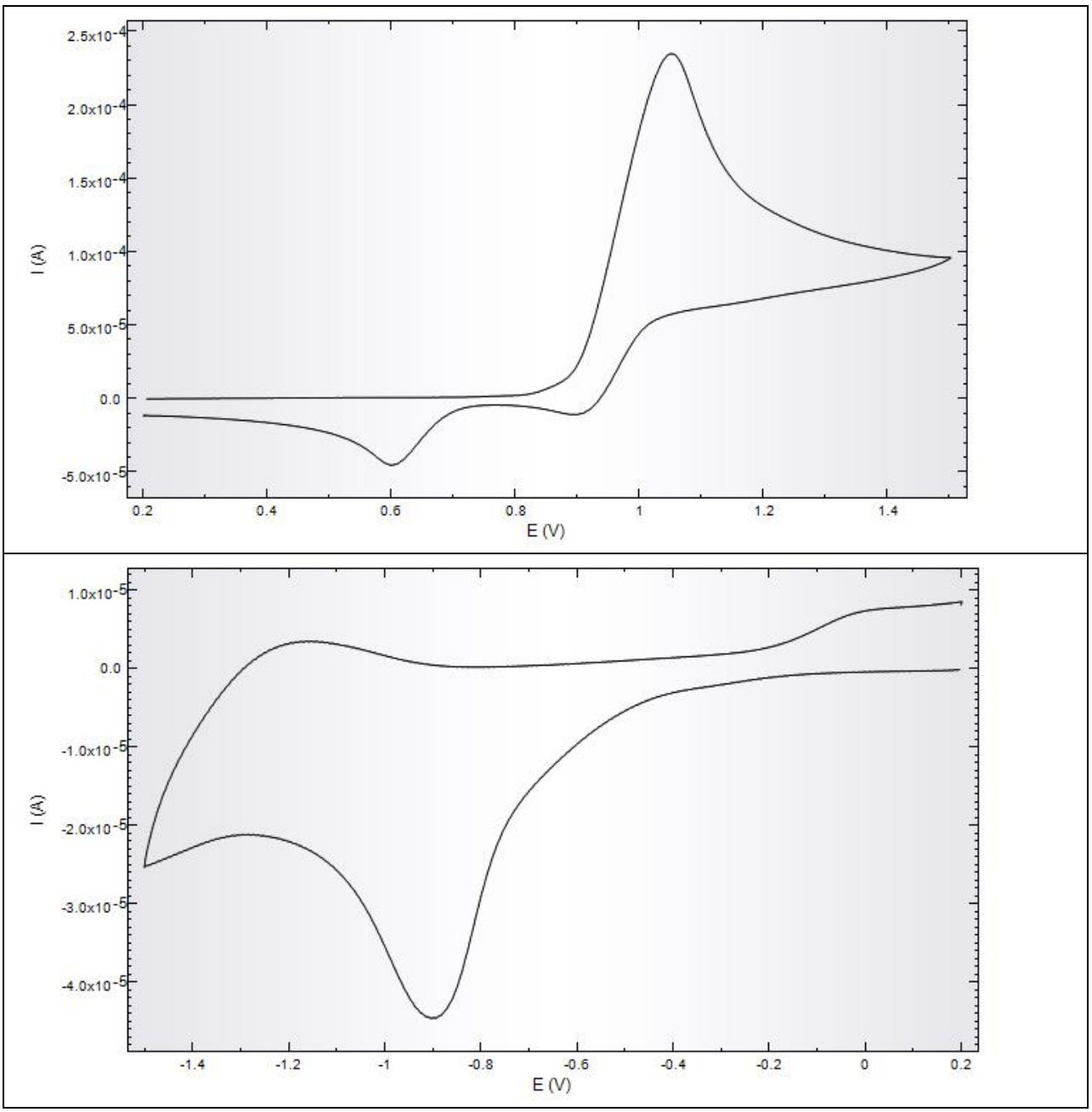


Figure S16. Cyclic voltammograms of **21a** measured in anhydrous CH_3CN with 0.1 M LiClO4 at 100 mV/s ($Ag/AgNO_3$ reference electrode).

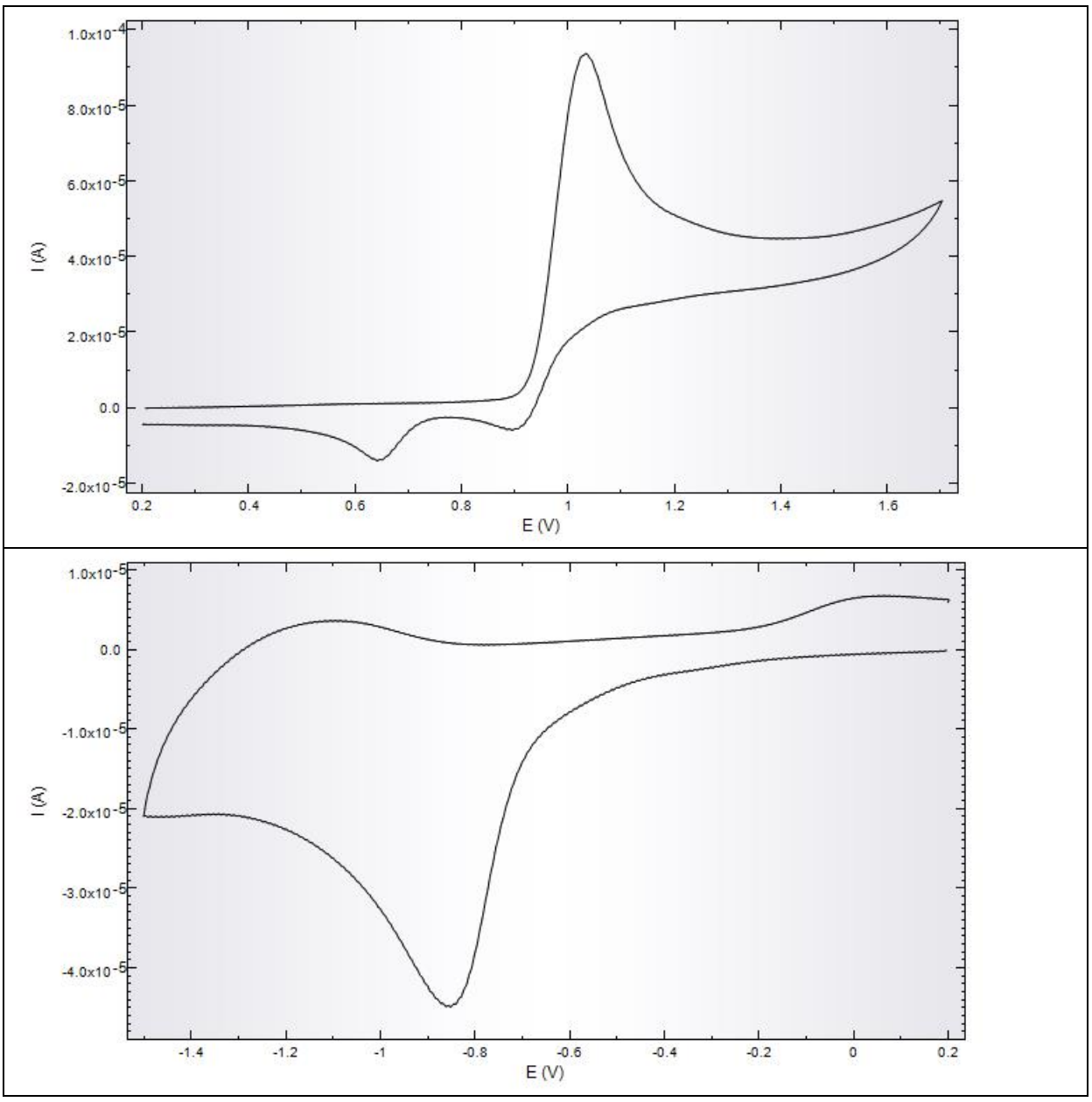


Figure S17. Cyclic voltammograms of **21b** measured in anhydrous CH_3CN with 0.1 M LiClO4 at 100 mV/s ($Ag/AgNO_3$ reference electrode).

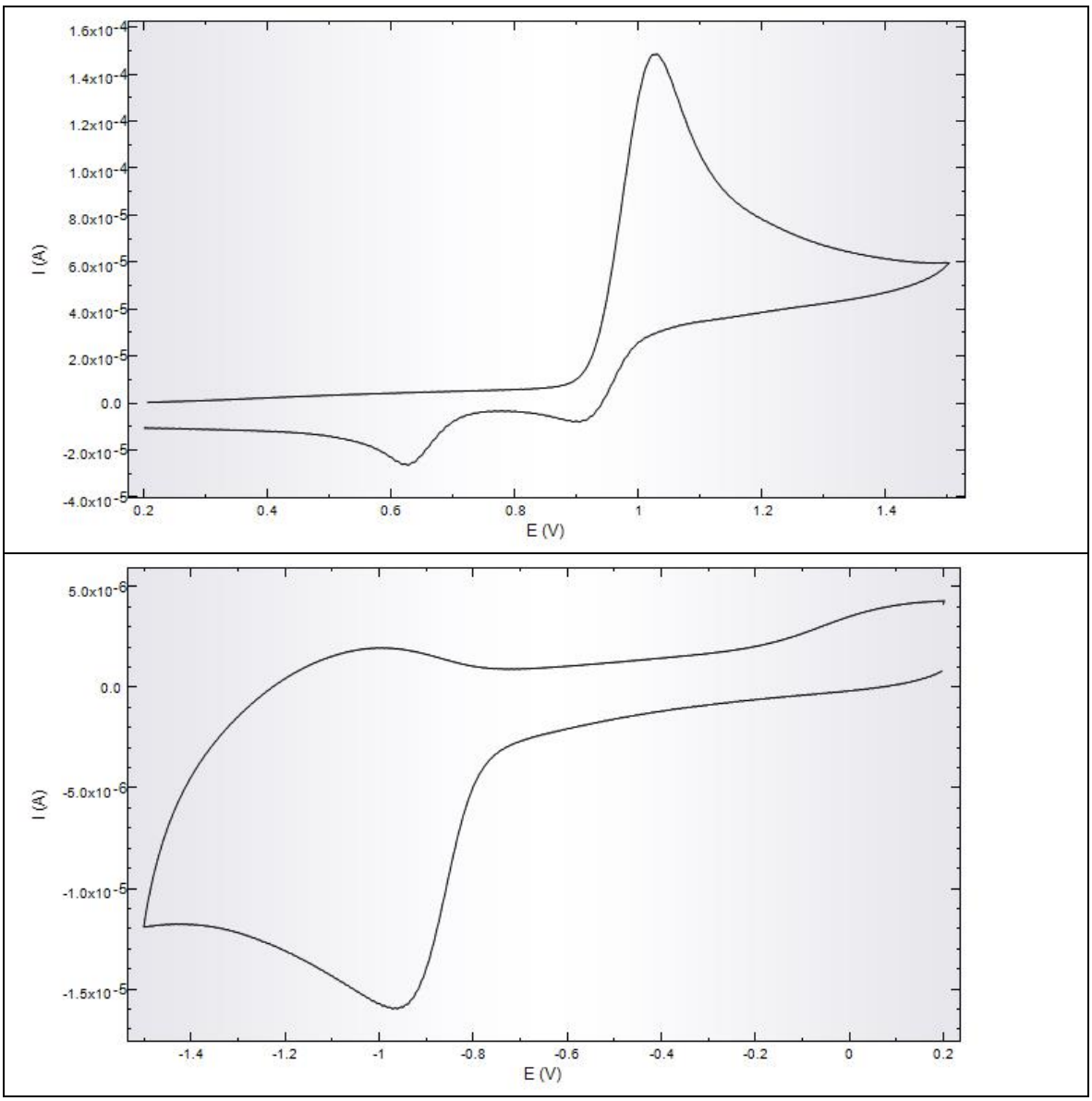


Figure S18. Cyclic voltammograms of **21c** measured in anhydrous CH_3CN with 0.1 M LiClO4 at 100 mV/s ($Ag/AgNO_3$ reference electrode).

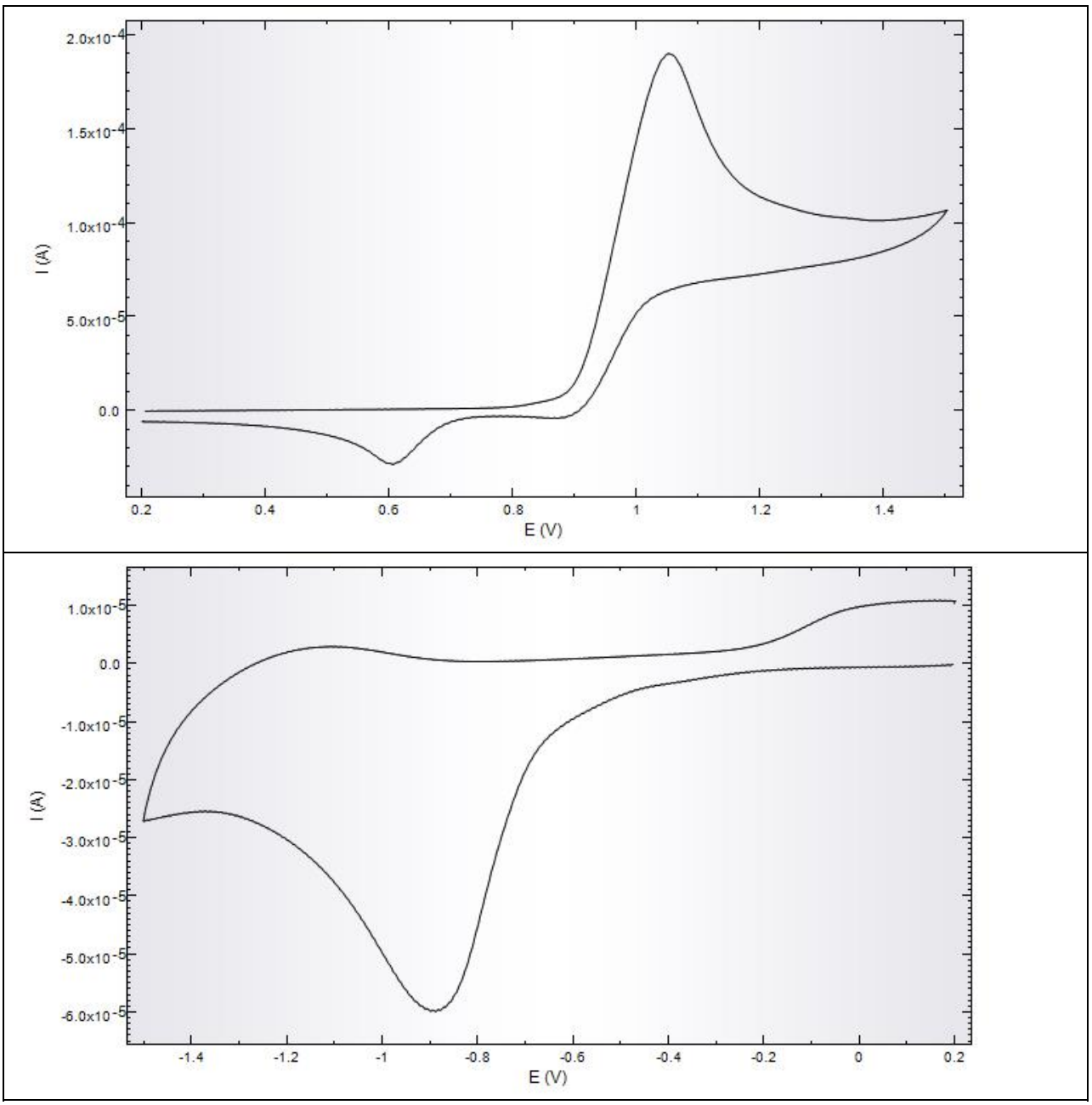
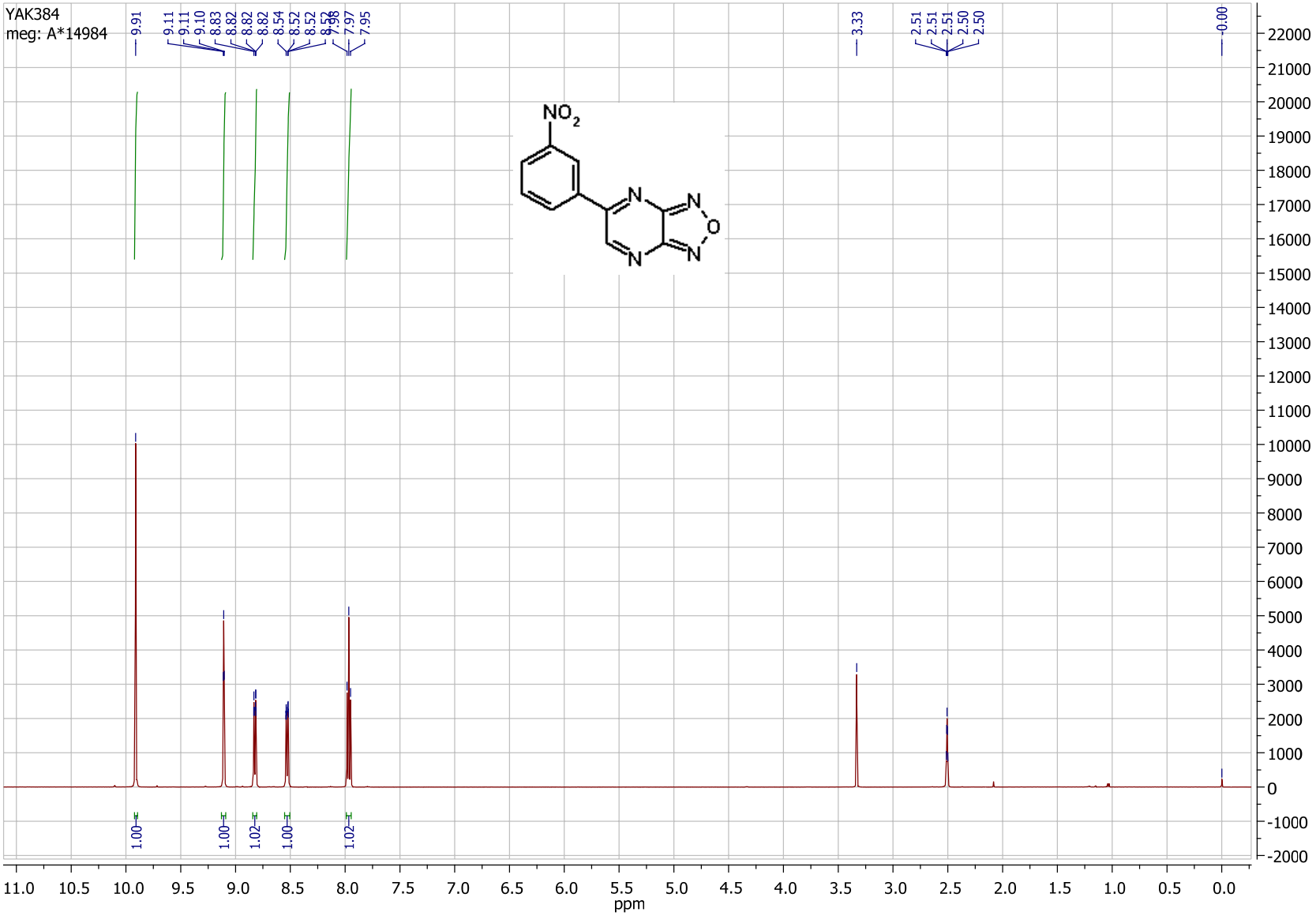


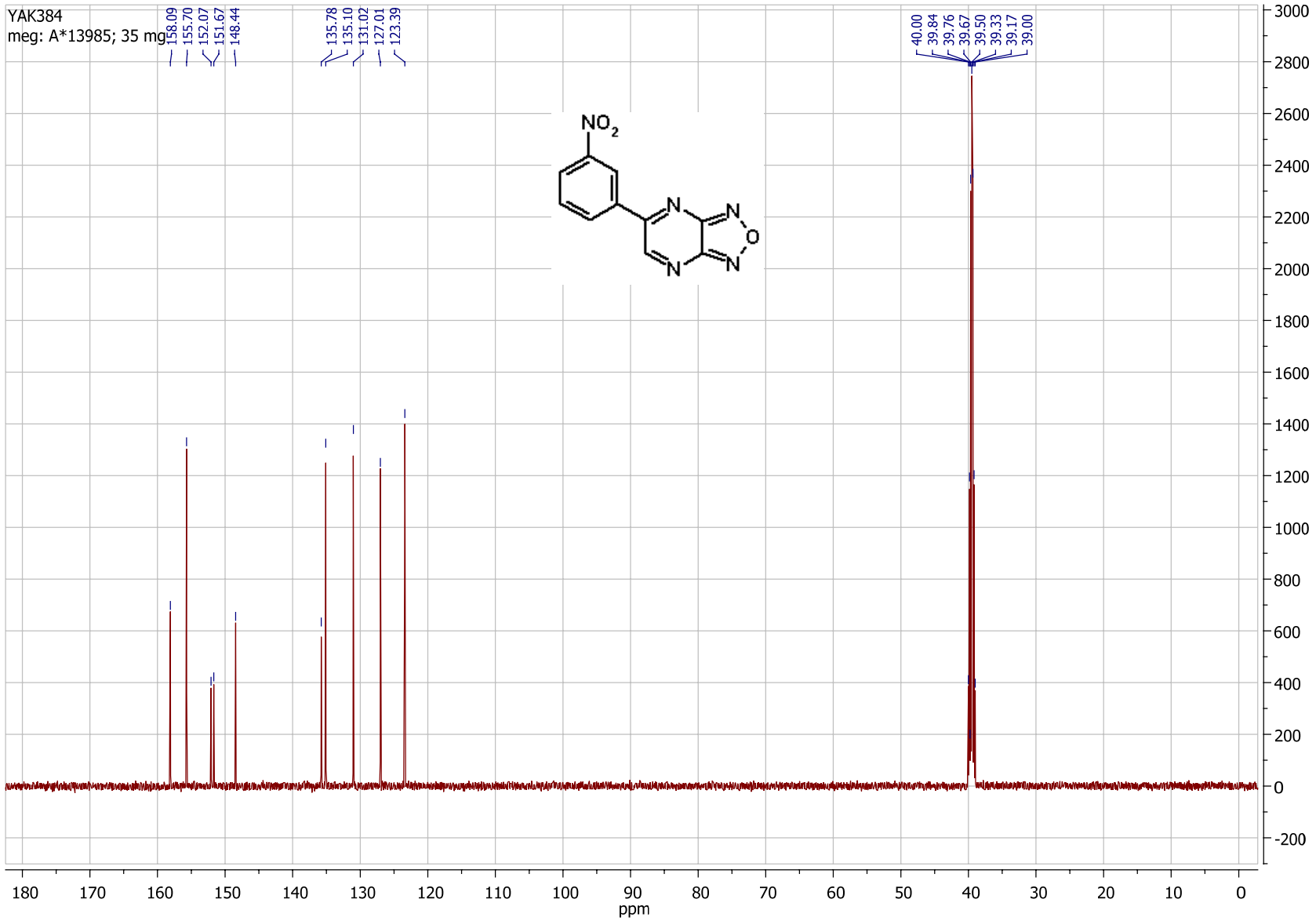
Figure S19. Cyclic voltammograms of **21d** measured in anhydrous CH_3CN with 0.1 M LiClO4 at 100 mV/s ($Ag/AgNO_3$ reference electrode).

Table S1. Crystal data and structure refinement.

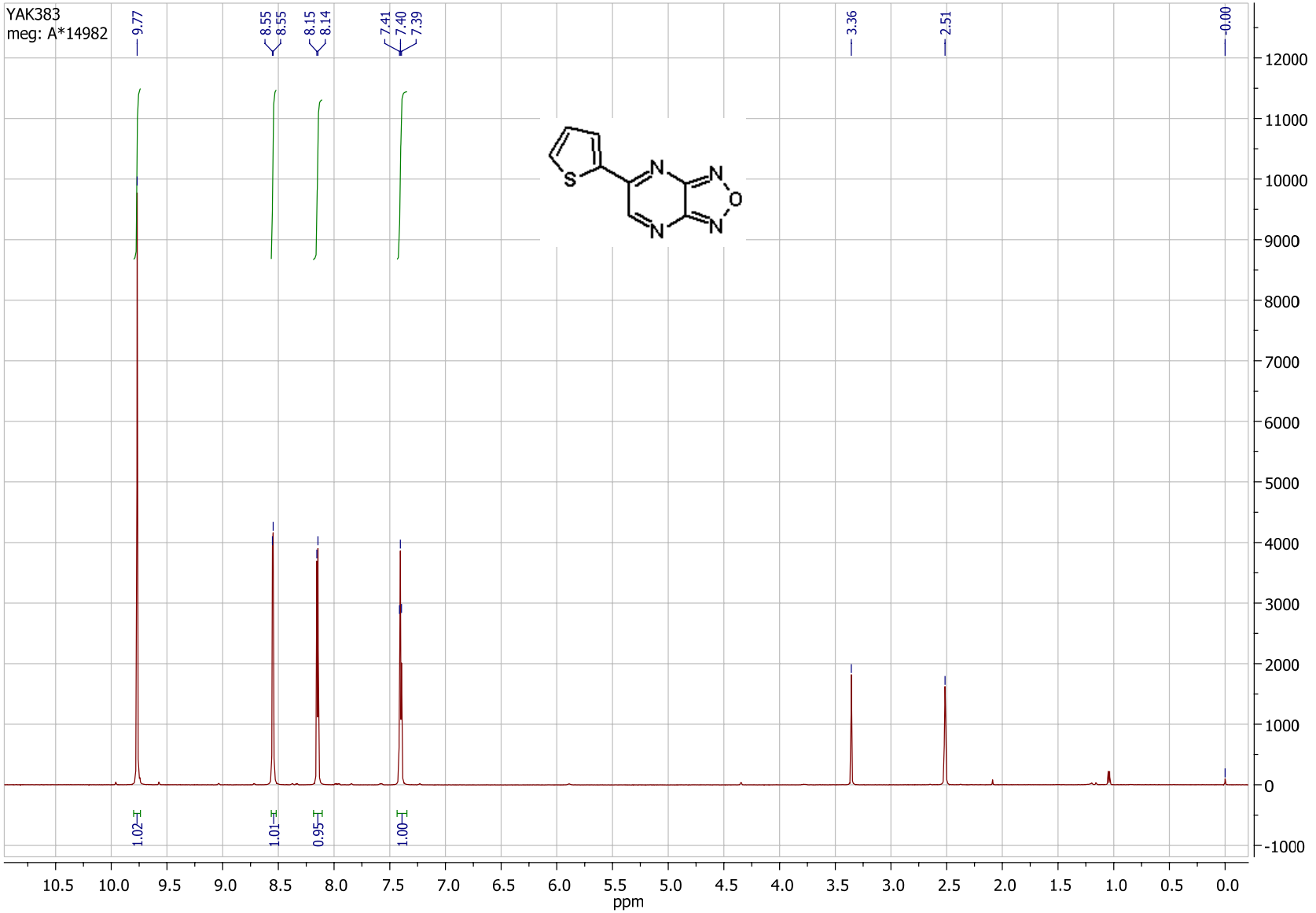
Compound	**7a**	**10d**	**14a**	**21a**	**21c**	**22c**
Empirical formula	$C_{14}H_9N_5O$	$C_{18}H_{11}N_5OS$	$C_{39}H_{30}N_{10}O_3$	$C_{24}H_{17}N_5O$	$C_{24}H_{16}BrN_5O$	$C_{24}H_{15}Br_2N_5O$
Formula weight	263.26	345.38	686.73	391.425	470.33	549.23
Temperature, K	133(2)	295(2)	295(2)	295(2)	295(2)	295(2)
Crystal system	Monoclinic	Monoclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$	P-1	$P2_1/n$	$P2_1/c$	$P2_1/c$
Unit cell dimensions						
a, Å	11.6264(3)	6.1567(10)	10.2841(6)	12.0497(11)	10.3383(17)	10.5892(15)
b, Å	7.7250(2)	18.228(8)	10.7873(8)	10.0517(9)	9.1307(12)	10.0002(7)
c, Å	14.1019(4)	14.204(3)	17.8266(12)	16.4916(16)	22.192(3)	20.990(3)
α, ^{o}	90	90	98.851(6)	90.00	90	90.00
β, ^{o}	109.742(3)	94.210(17)	98.494(5)	90.937(8)	101.397(12)	101.212(11)
γ, ^{o}	90	90	115.283(7)	90.00	90	90.00
Volume (Å^3), Z	1192.10(6), 4	1589.7(8), 4	1715.8(2), 2	1997.2(3), 4	2053.5(5), 4	2180.3(4), 4
μ, mm^{-1}	0.100	0.221	0.089	0.084	2.029	3.745
Θ range for data collection	$3.00 < \Theta < 28.29^o$	$2.66 < \Theta < 28.29$	$2.70 < \Theta < 28.28^o$	$2.90 < \Theta < 28.28^o$	$2.91 < \Theta < 26.39^o$	$2.83 < \Theta < 26.37^o$
Reflections collected	7214	11608	9732	11546	9083	10074
Independent reflections	2919 (R_{int} = 0.0164)	3943 (R_{int}= 0.0346)	8228 (R_{int}= 0.0227)	4696 (R_{int}= 0.0576)	4017 (R_{int}= 0.0397)	4308 (R_{int}= 0.0408)
Completeness (to Θ)	98.4 % (28.29^o)	99.9 % (28.29^o)	96.6 % (28.28^o)	96.5 % (26.00^o)	95.6 % (26.39^o)	96.7 % (26.37^o)
R_1 [I>2σ(I)]	0.0316	0.0436	0.0473	0.0494	0.0385	0.0395
wR_2 [I>2σ(I)]	0.0885	0.0911	0.1201	0.0883	0.0430	0.0460
R_1 (all data)	0.0402	0.1122	0.0968	0.1801	0.1312	0.1248
wR_2 (all data)	0.0915	0.0944	0.1265	0.0978	0.0456	0.0491
GooF	1.000	1.008	1.020	1.006	0.999	1.000
$\Delta\rho_{\bar{e}}$, ēÅ^{-3}	0.326/-0.174	0.501/-0.256	0.284/-0.263	0.218/-0.141	0.350/-0.444	0.659/-0.536



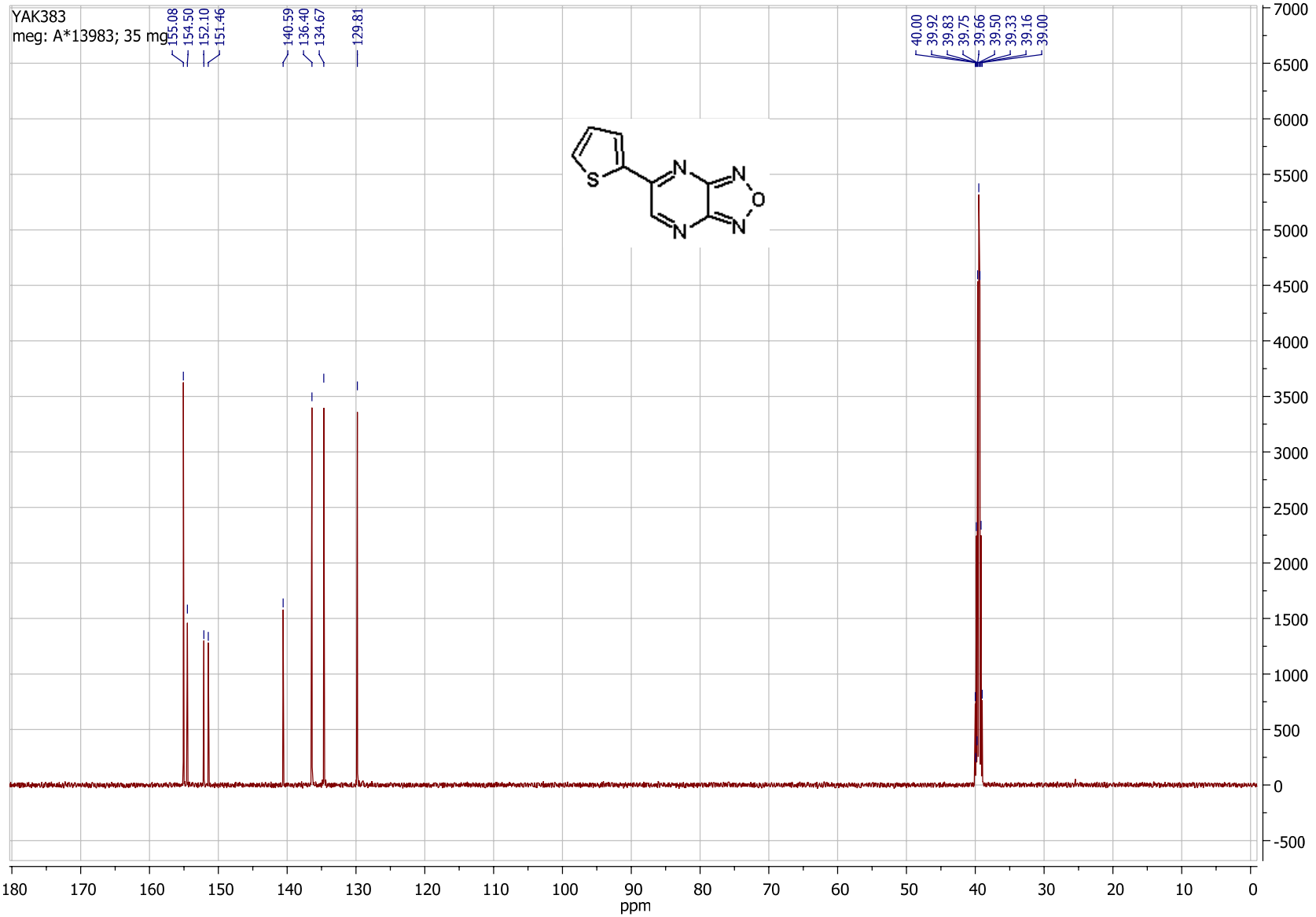
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **1b**.



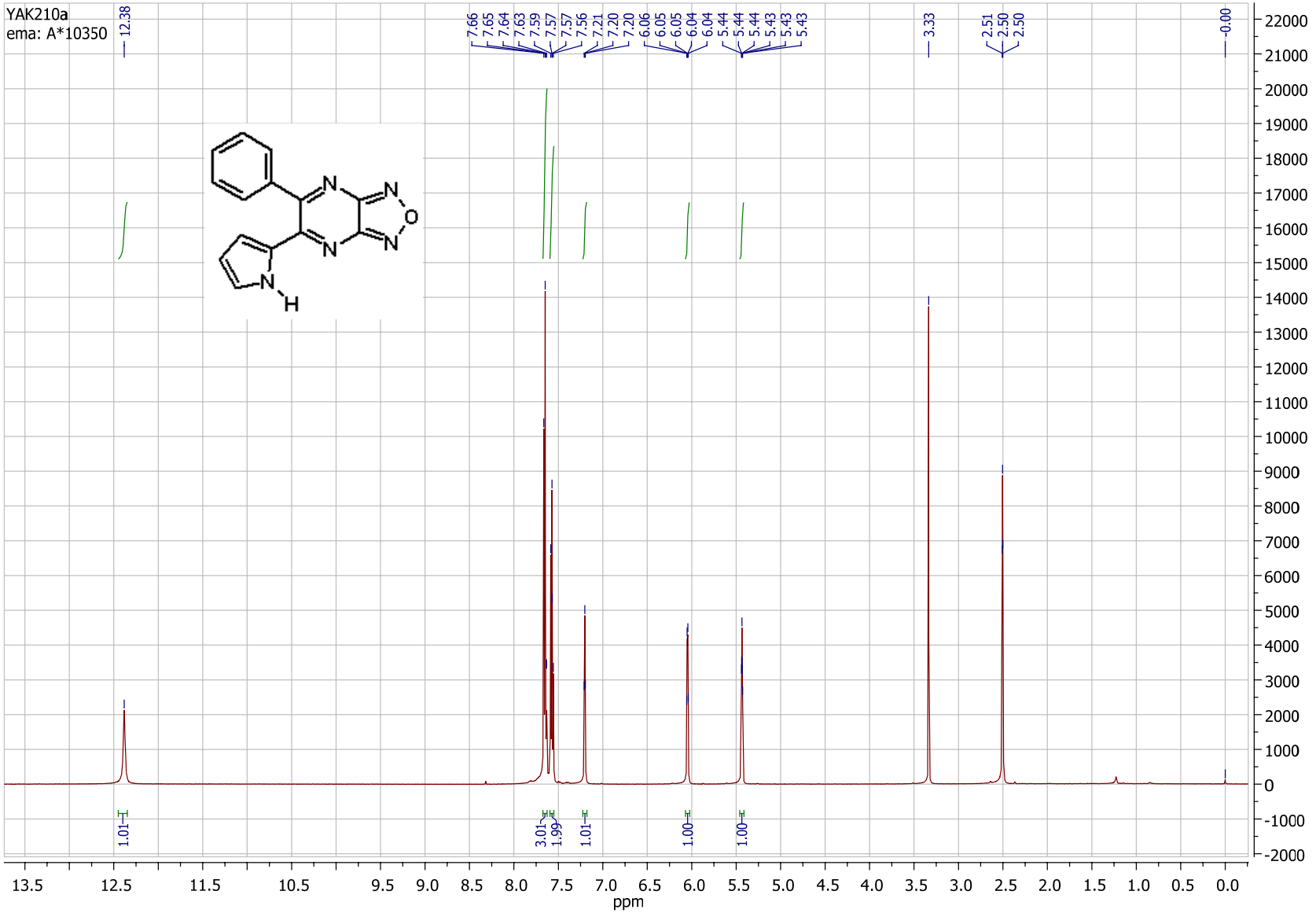
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **1b**.



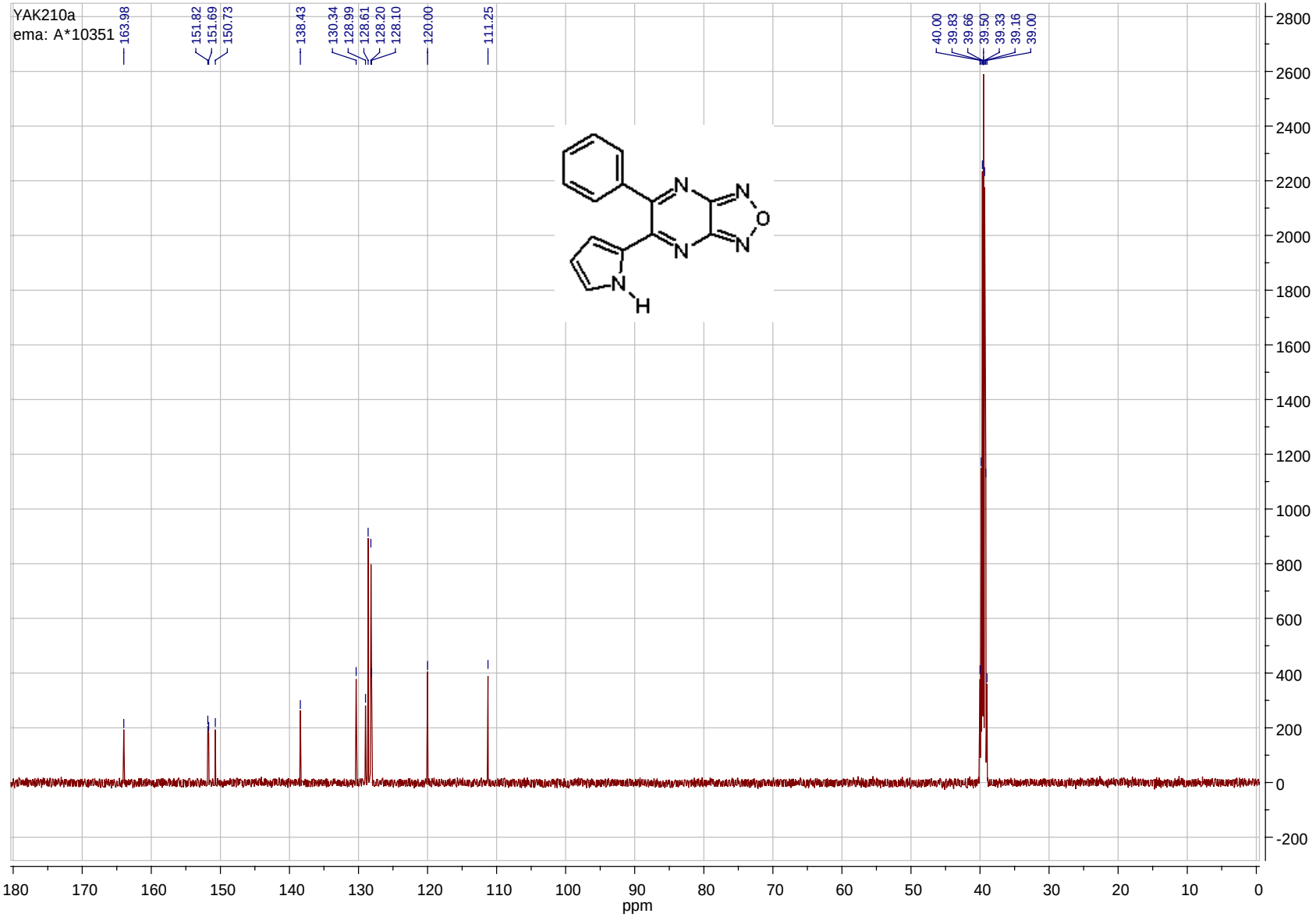
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **1d**.



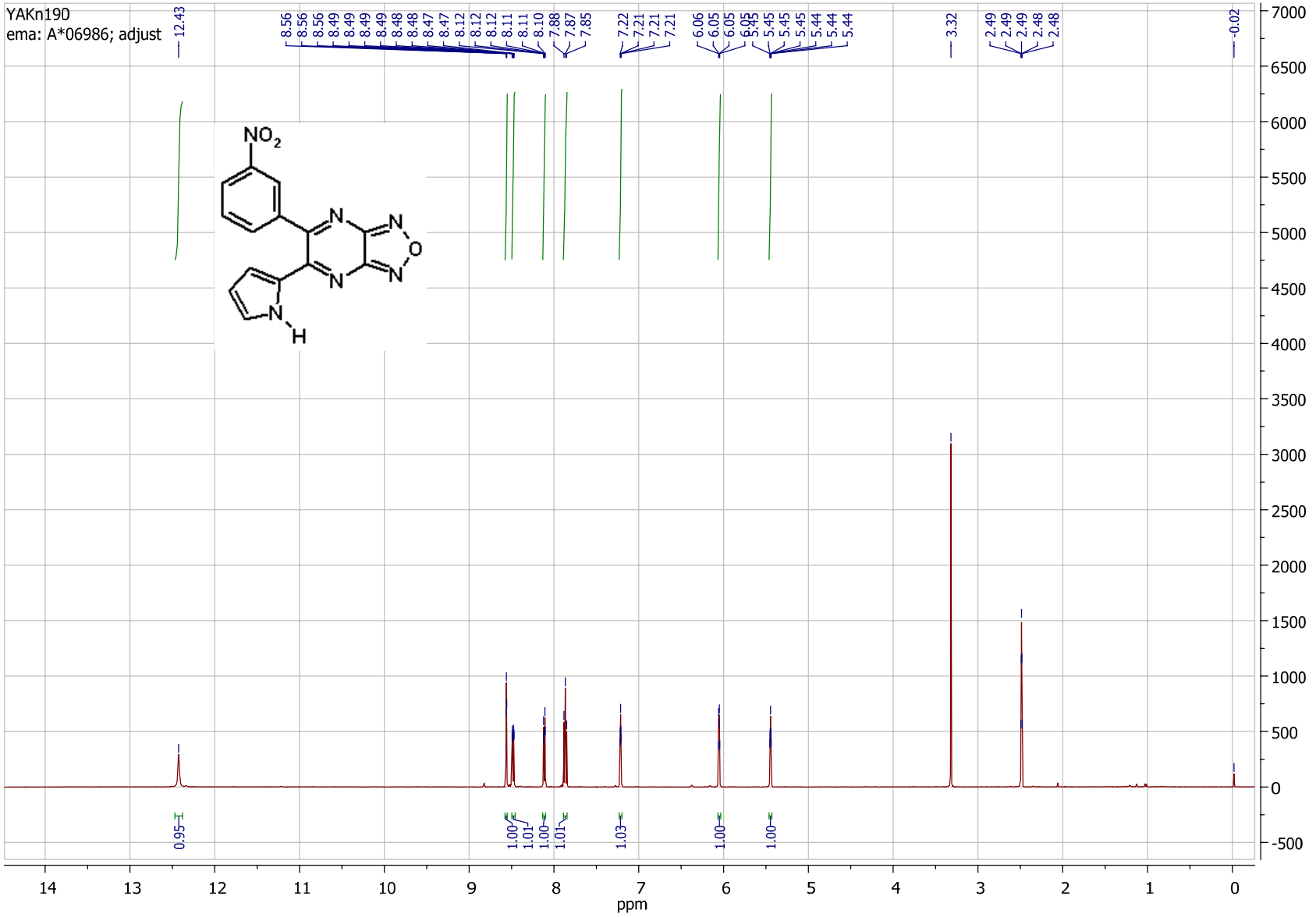
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **1d**.



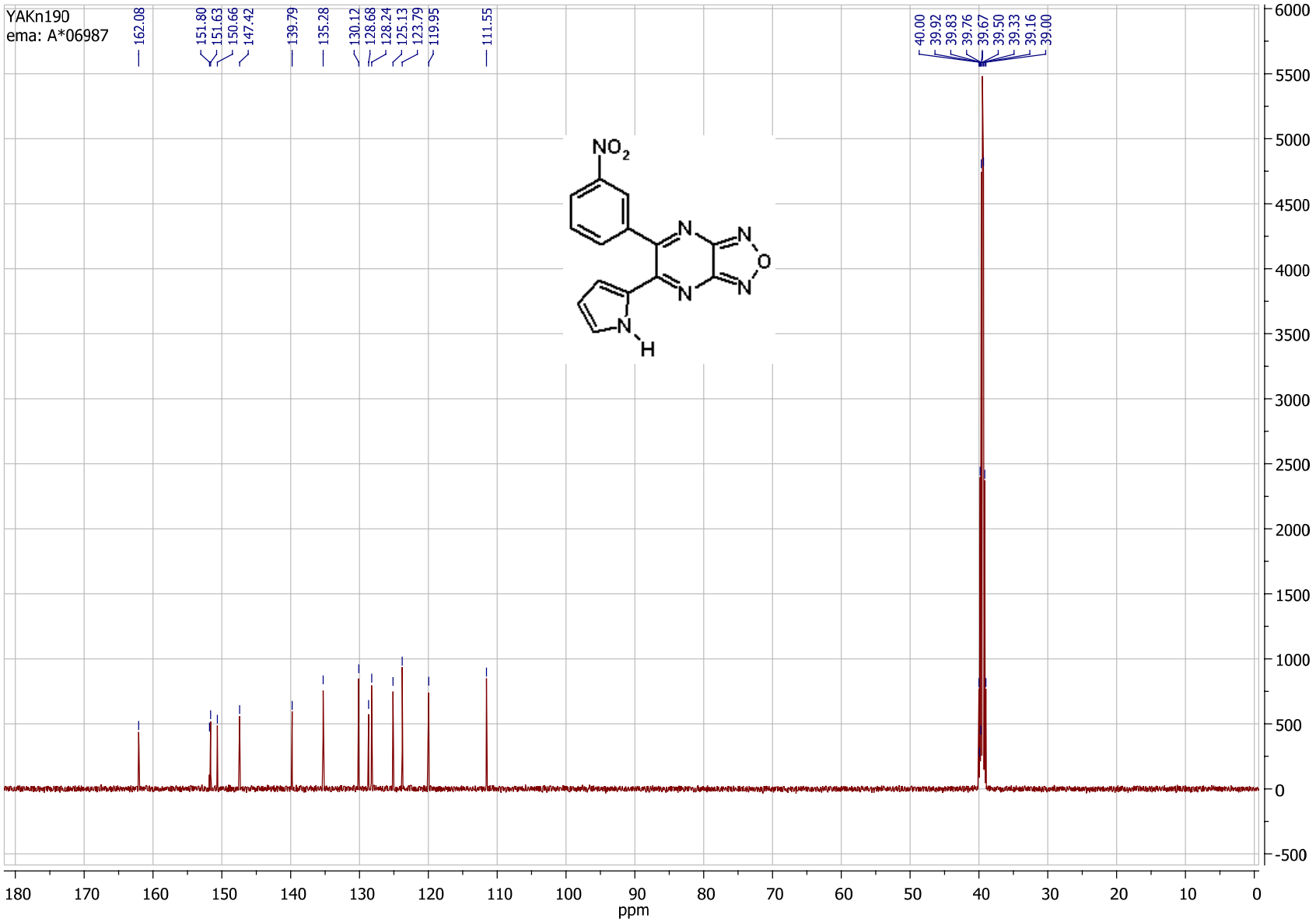
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **9a**.



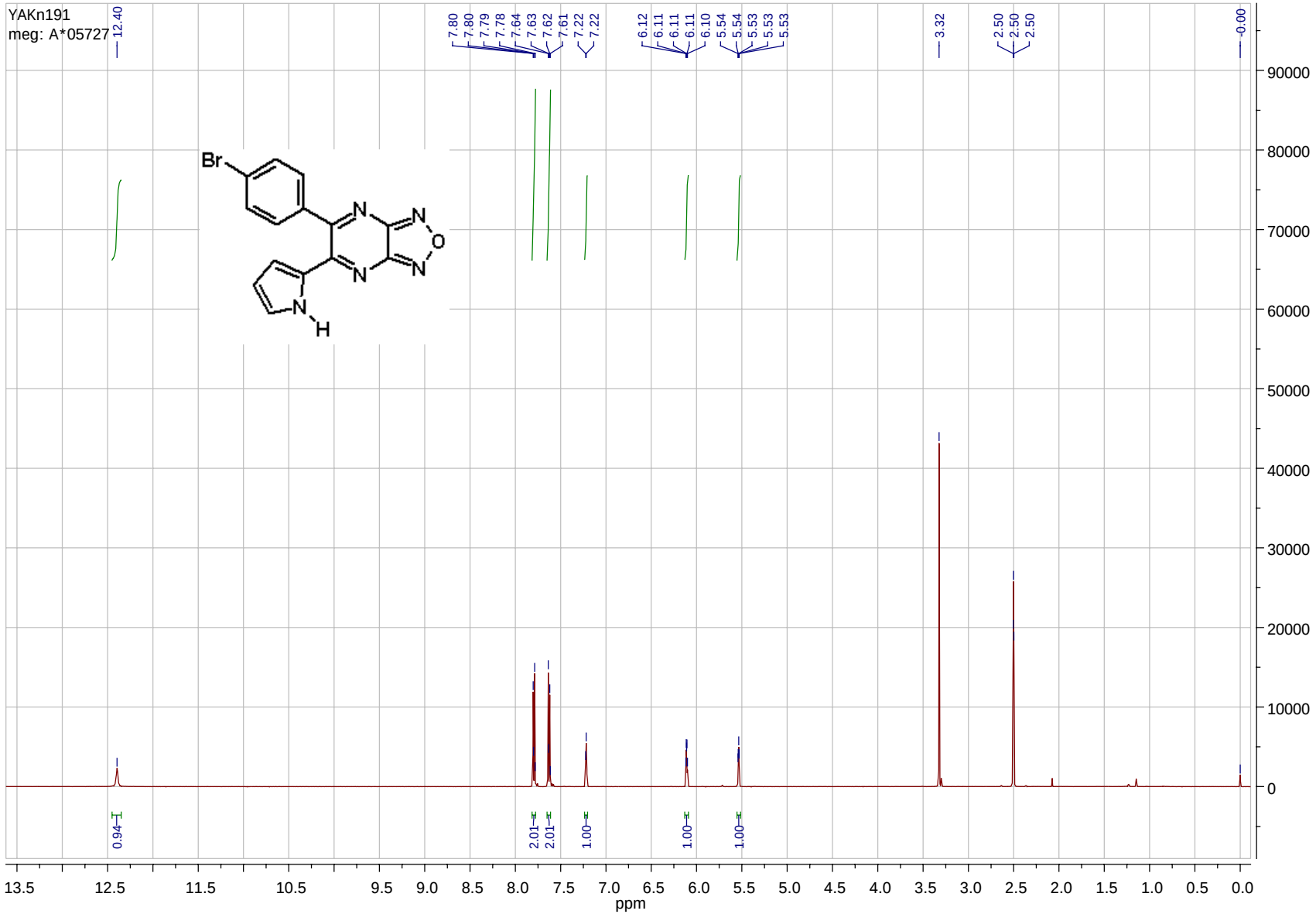
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **9a**.



^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **9b**.



^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **9b**.



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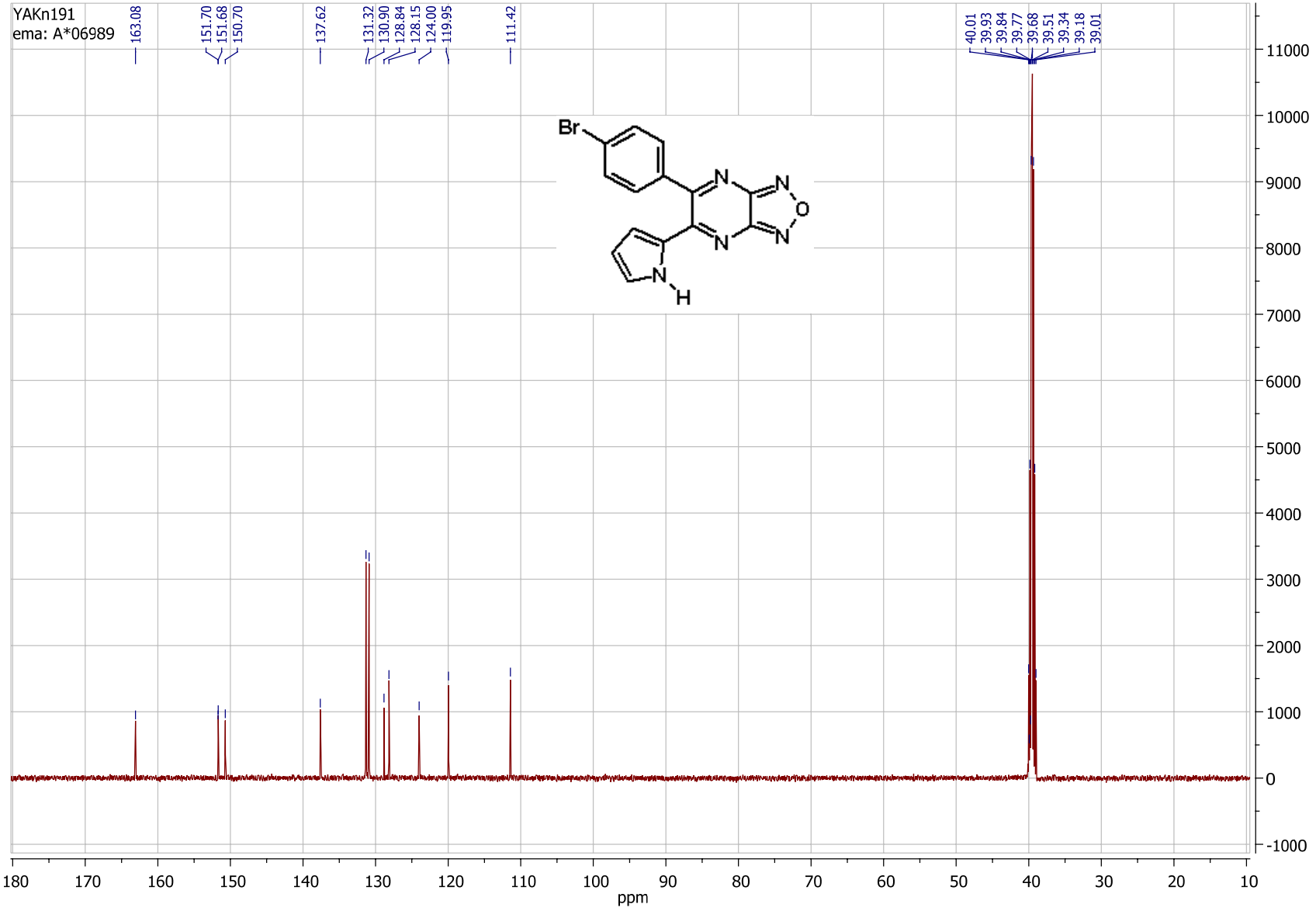
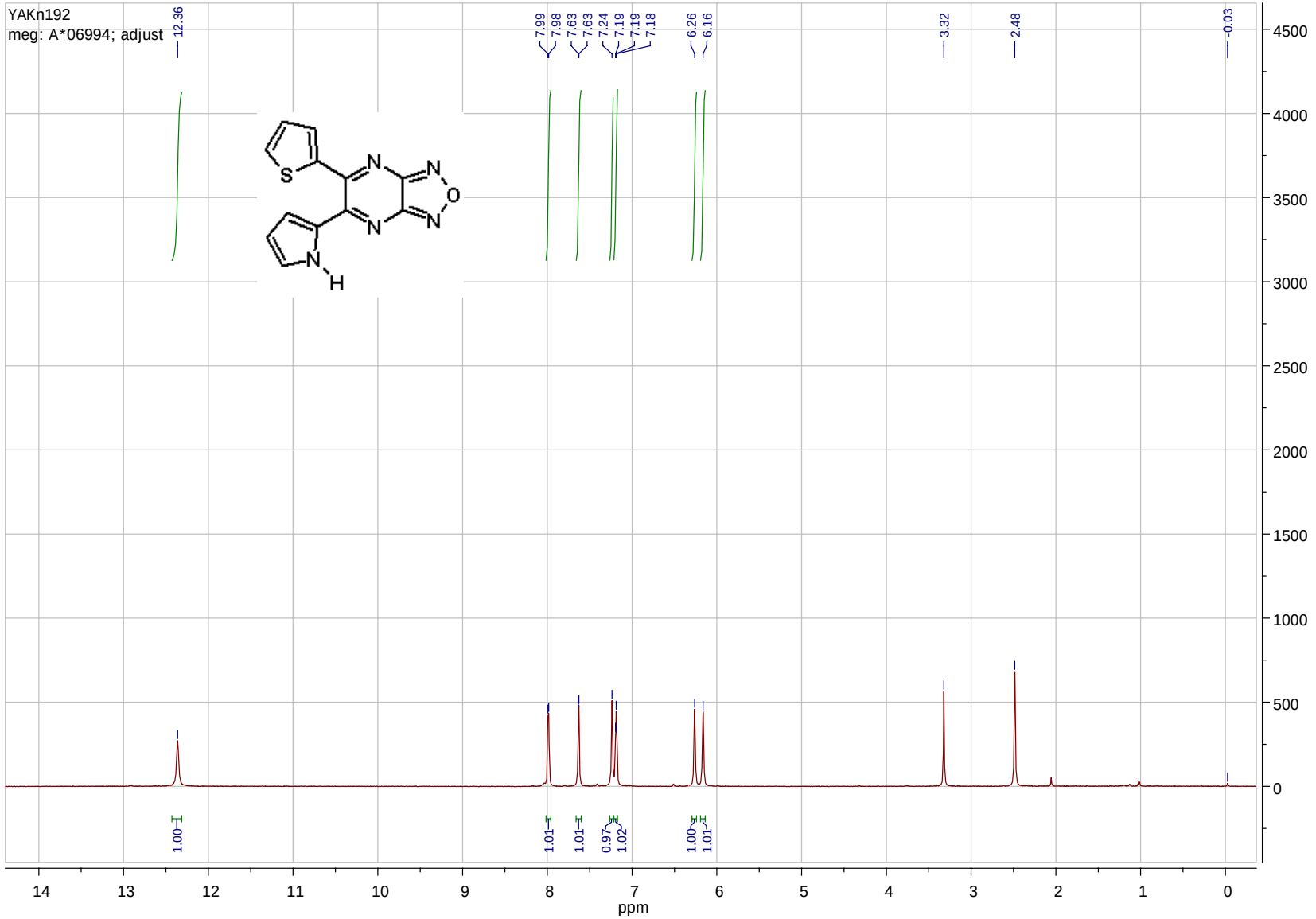
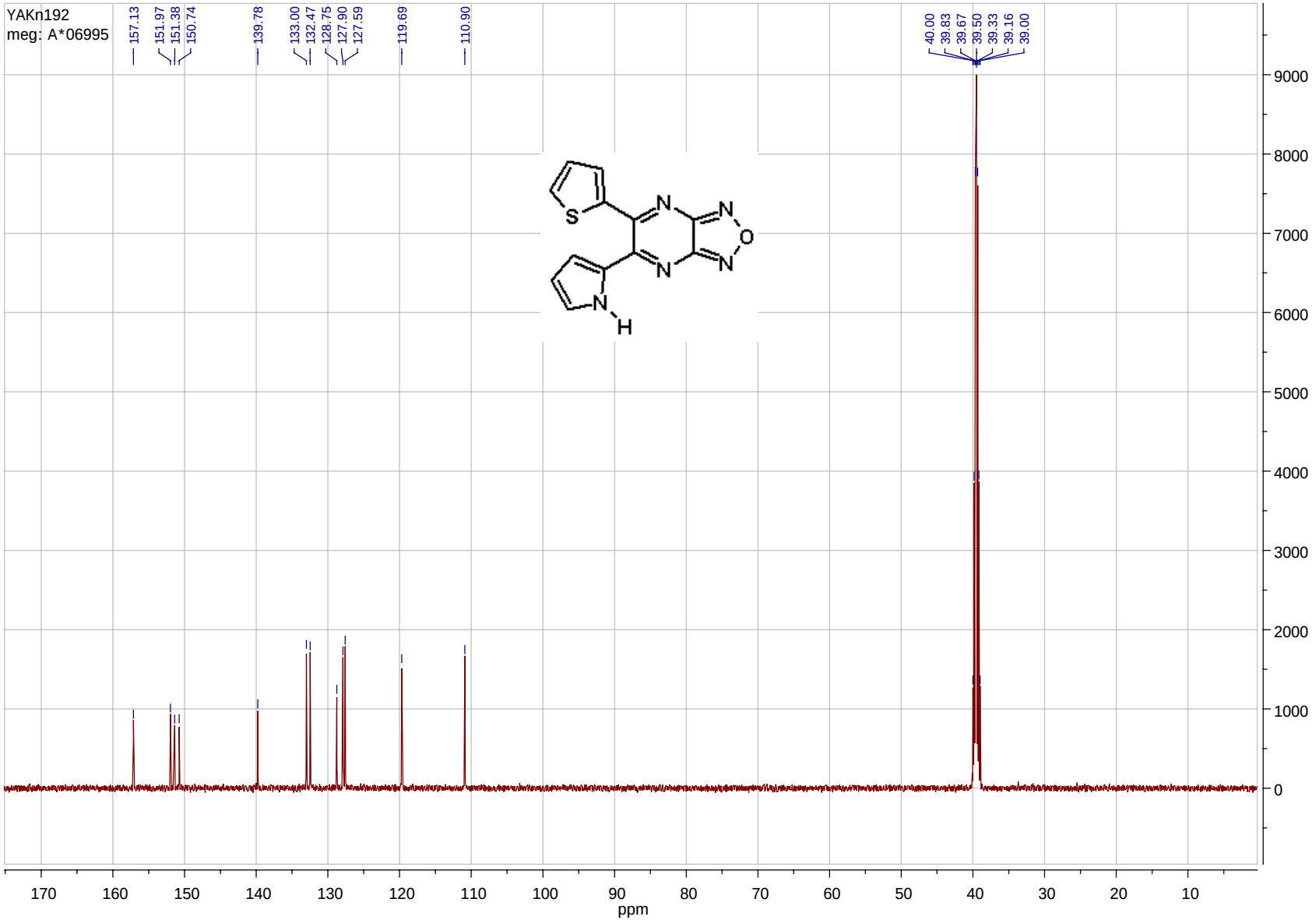


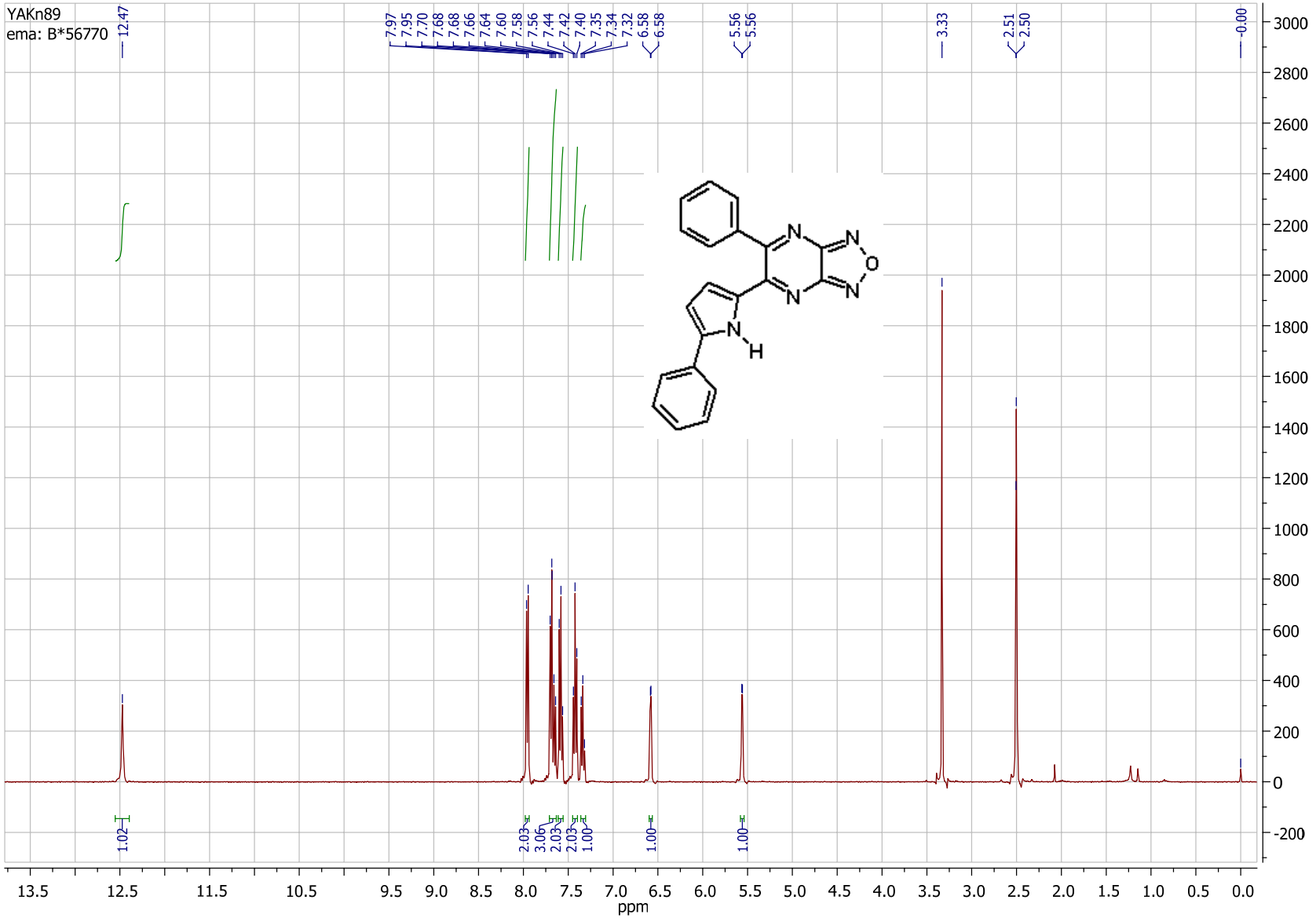
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **9c**.



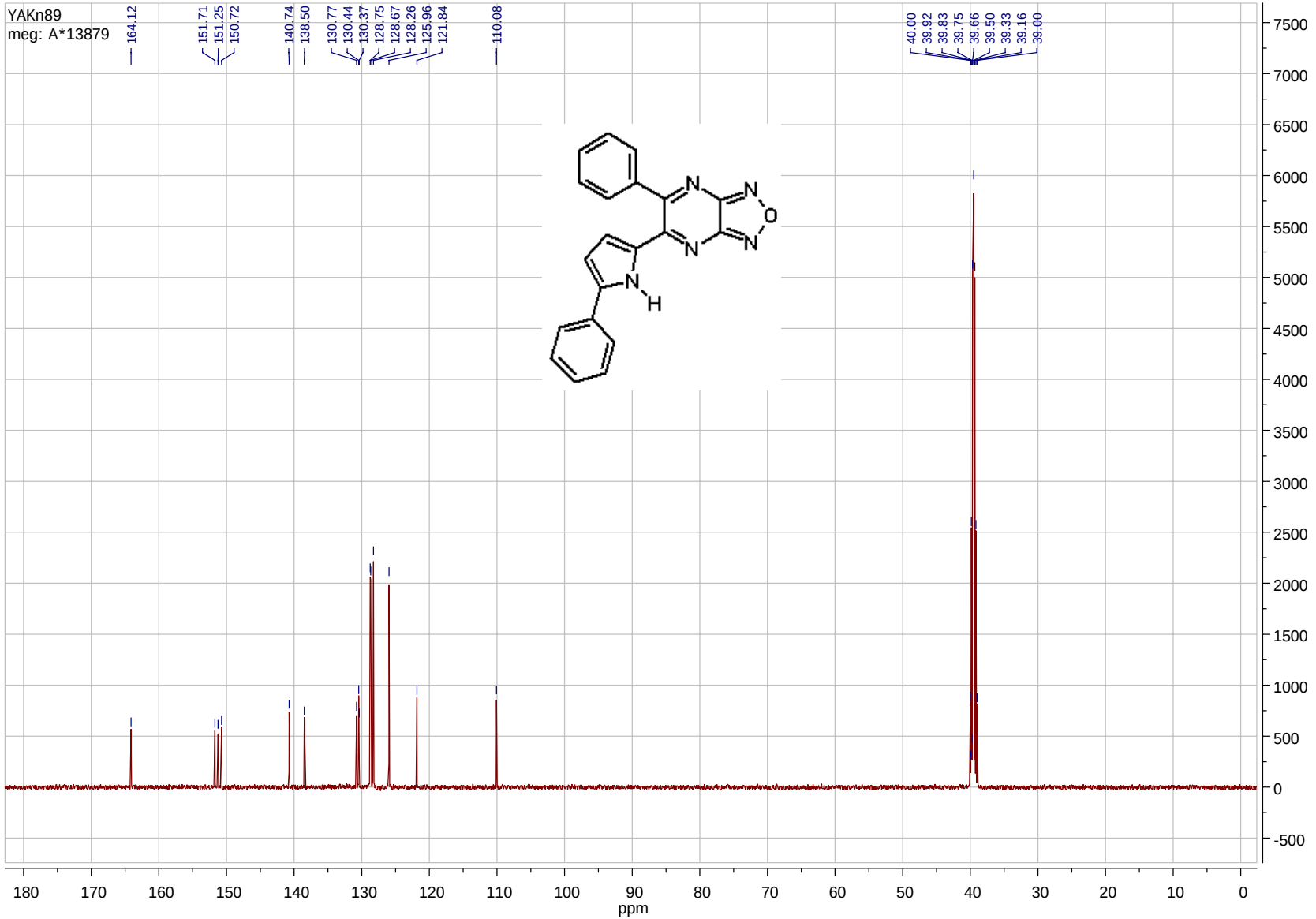
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **9d**.



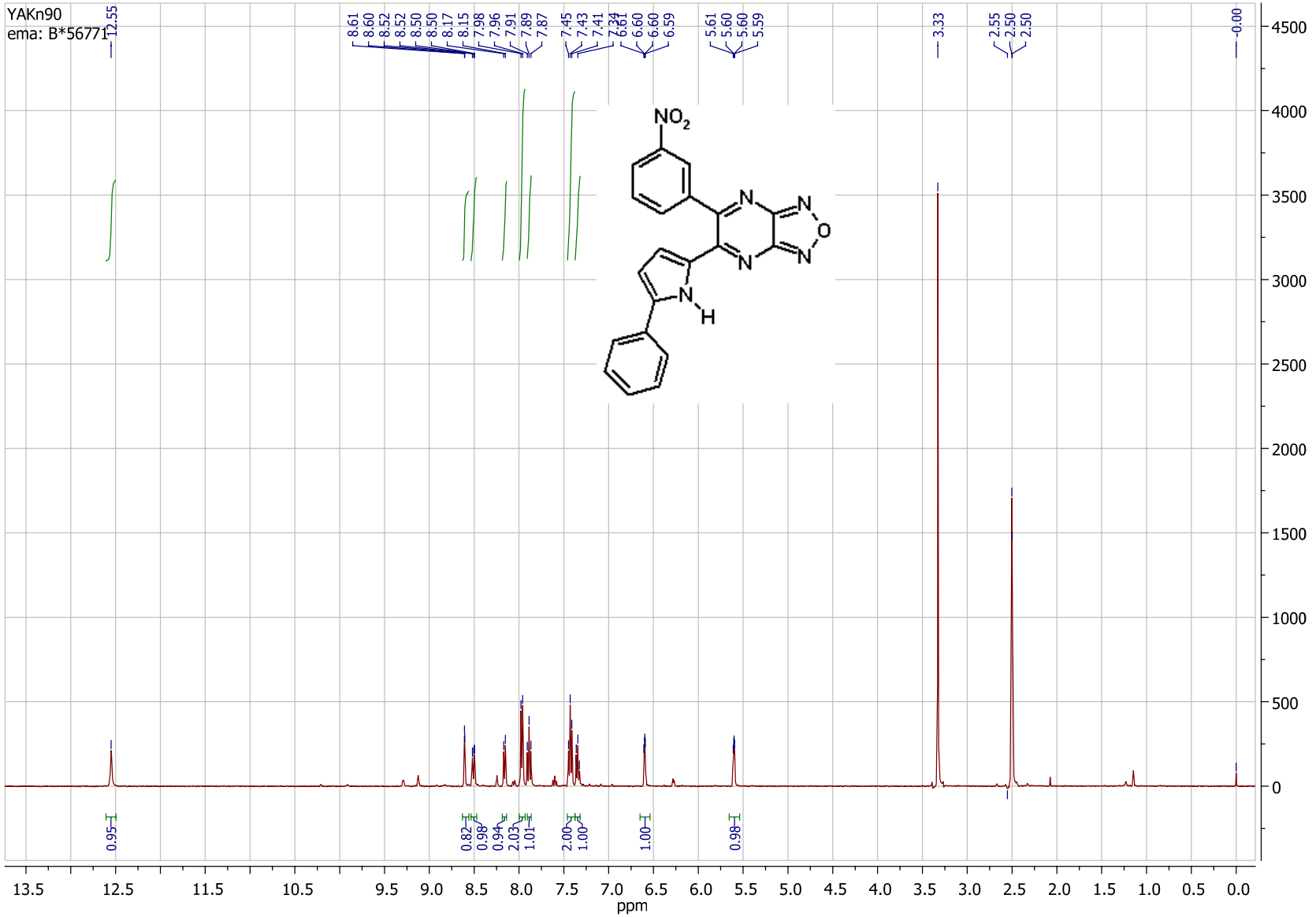
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **9d**.



^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **10a**.



^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **10a**.



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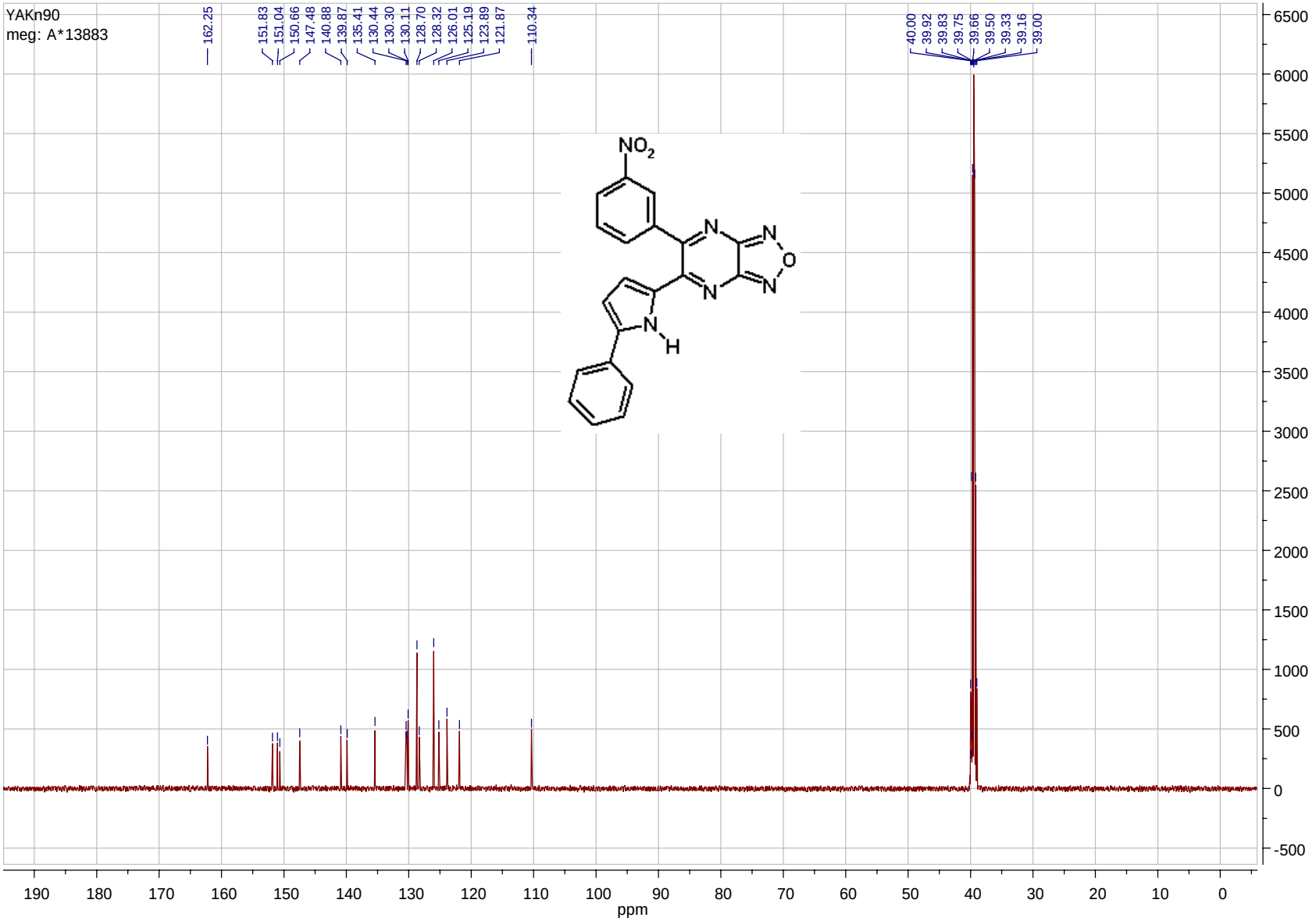
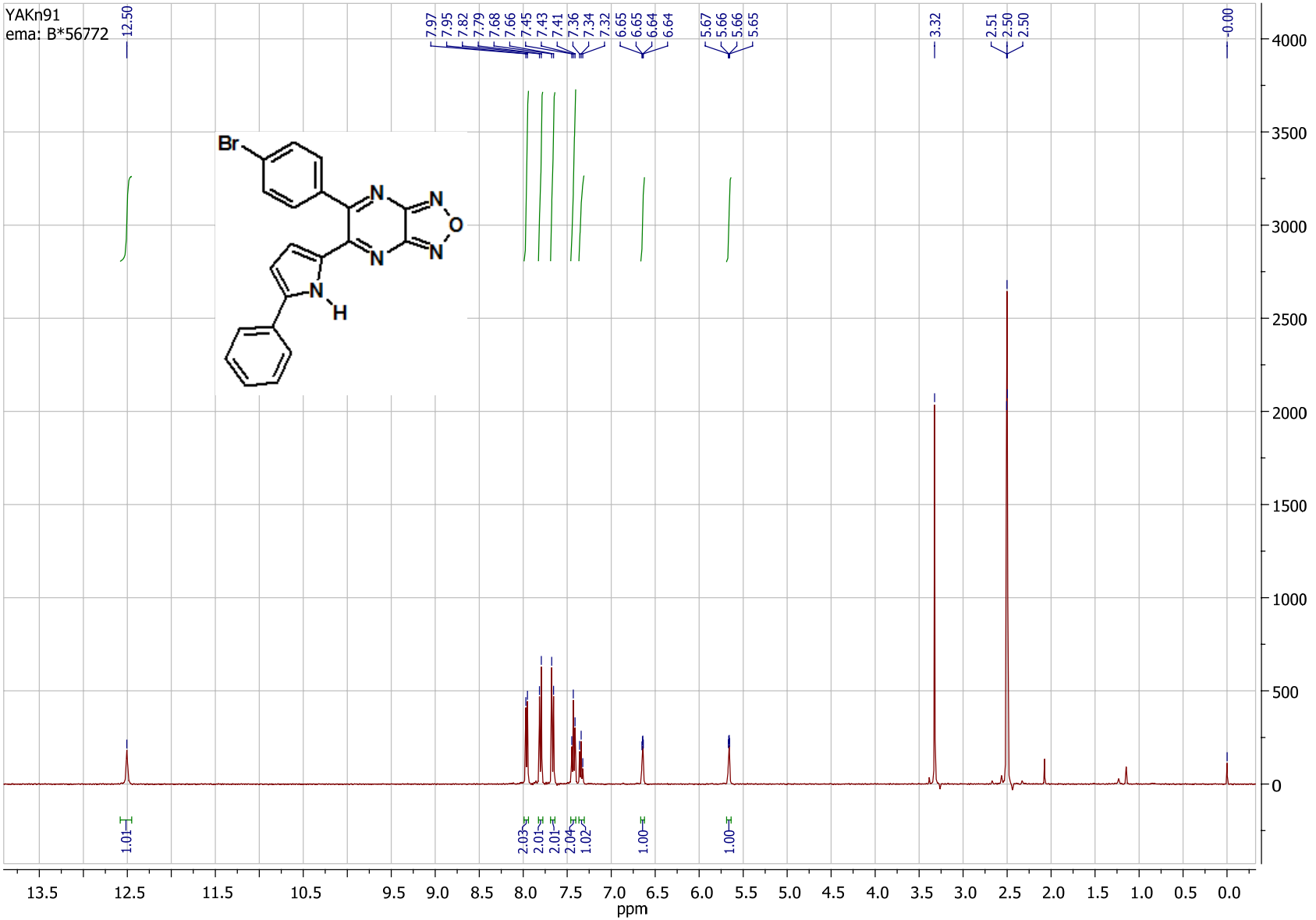


^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **10b**.



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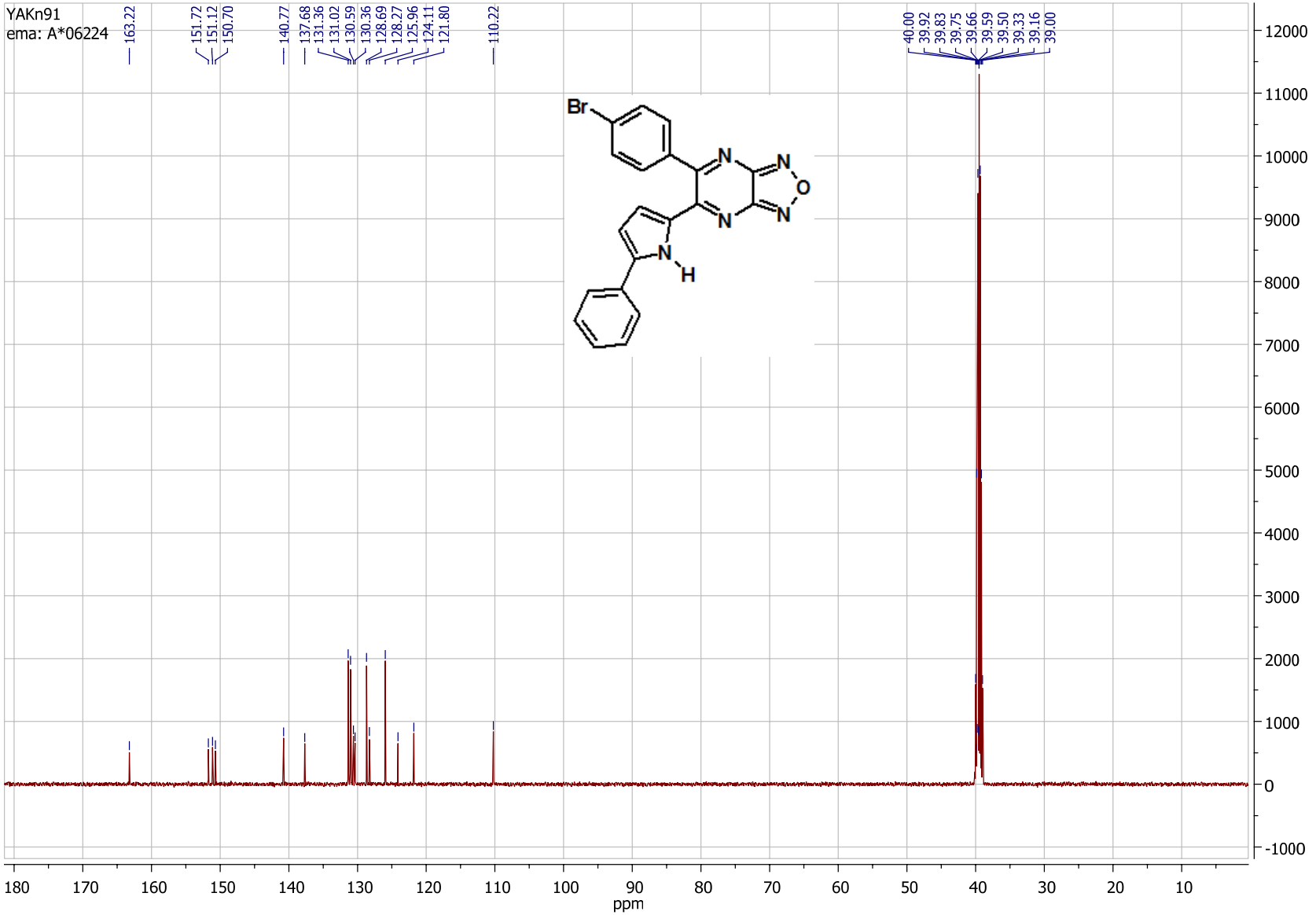

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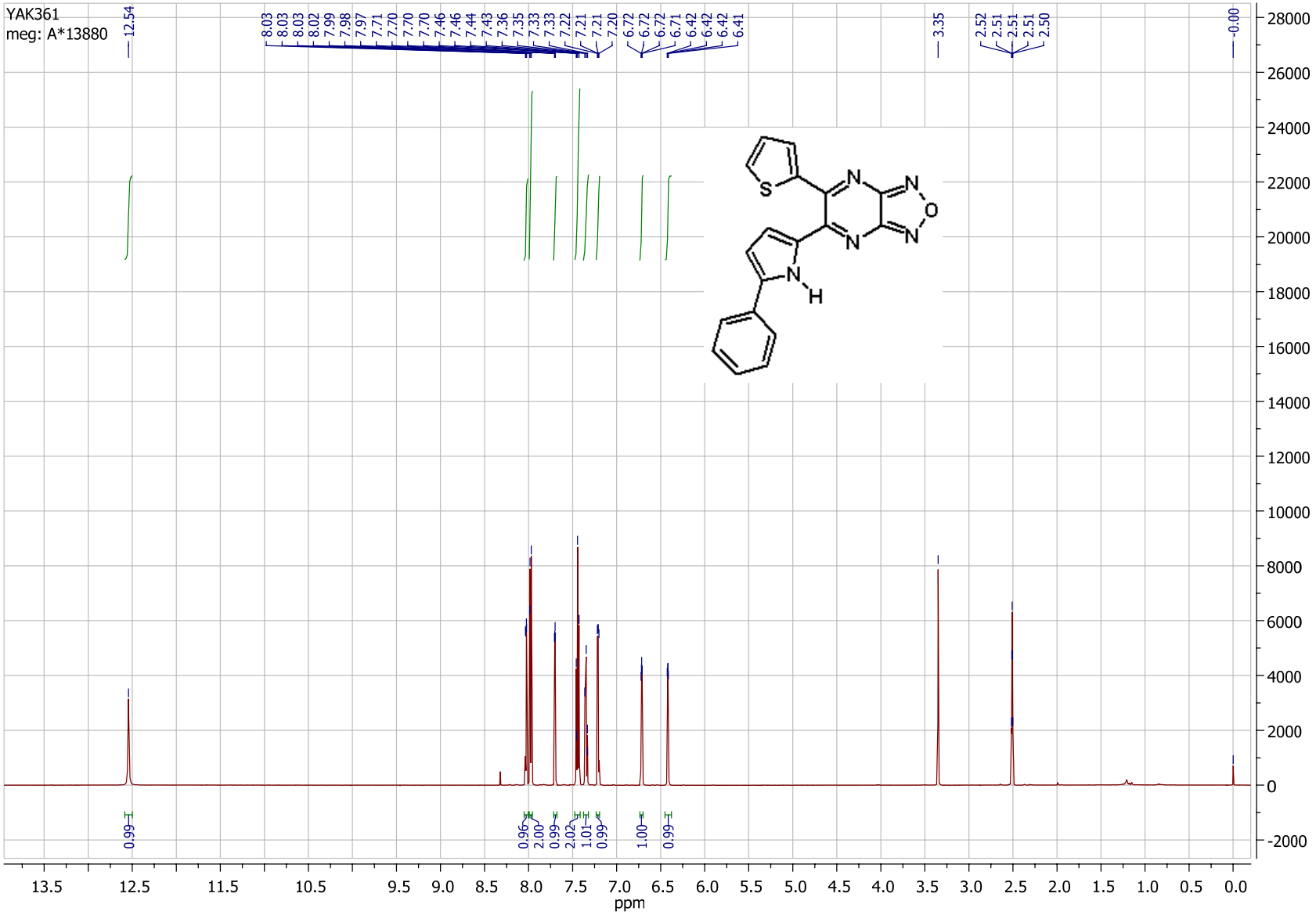
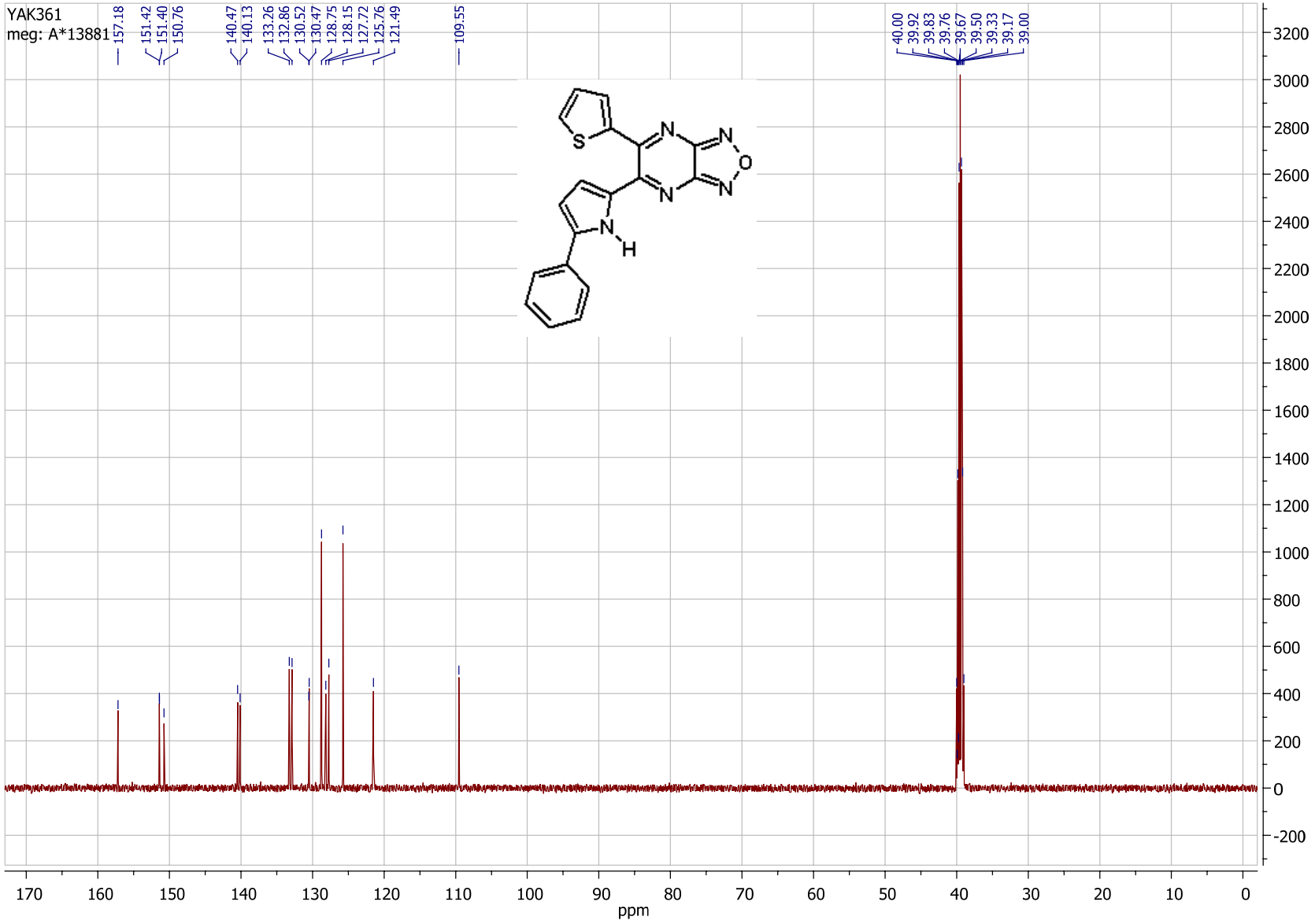
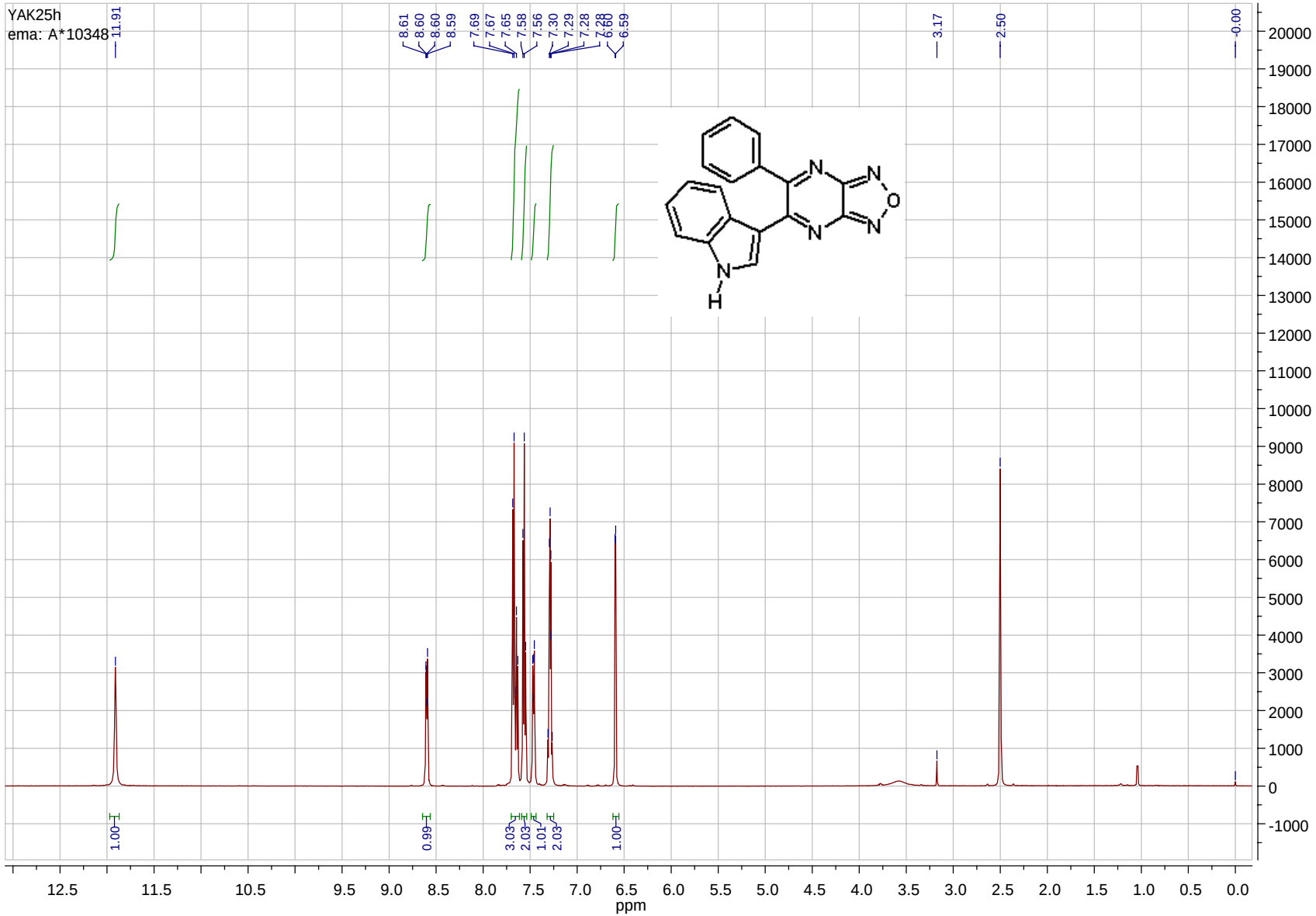


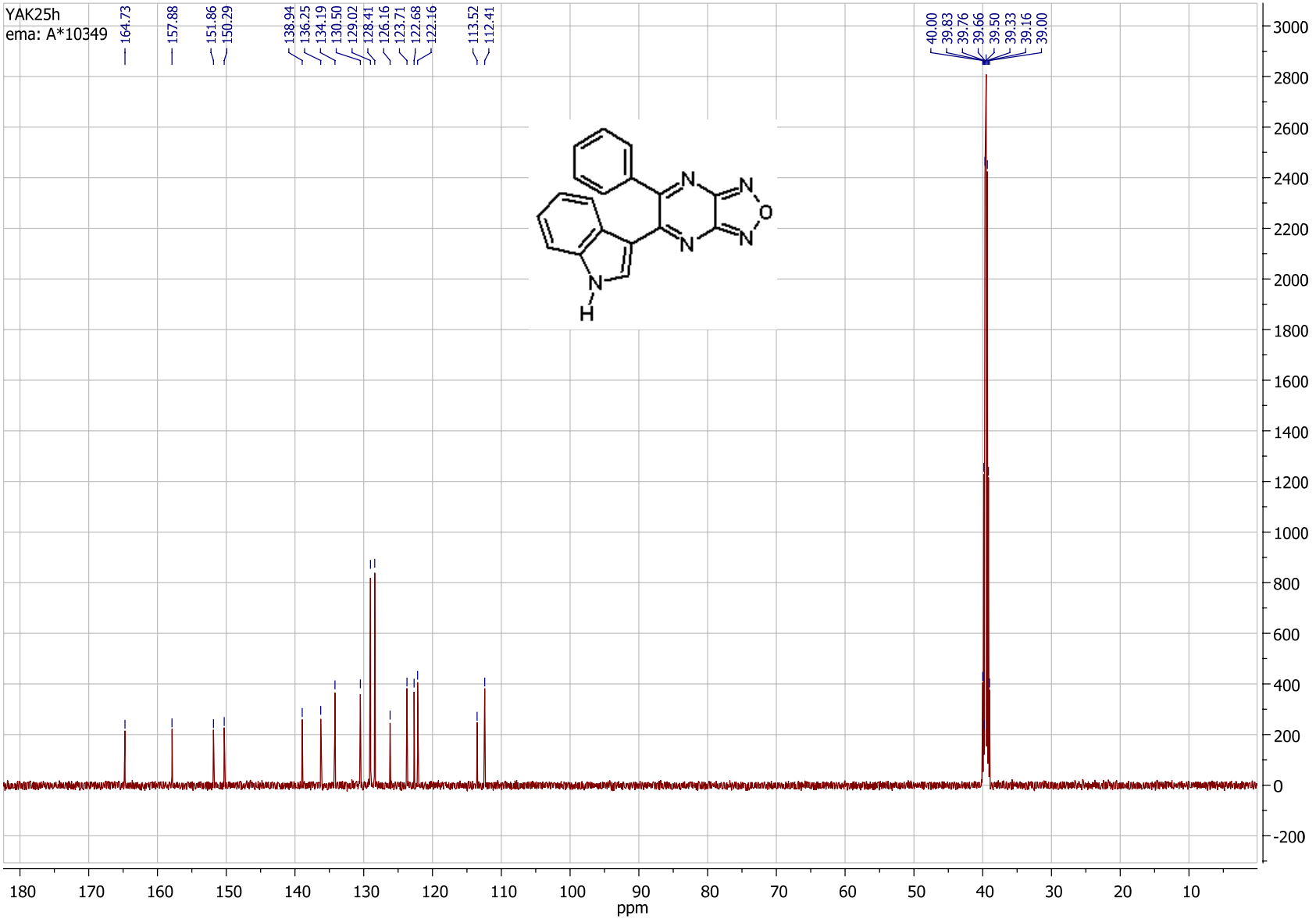
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **10d**.



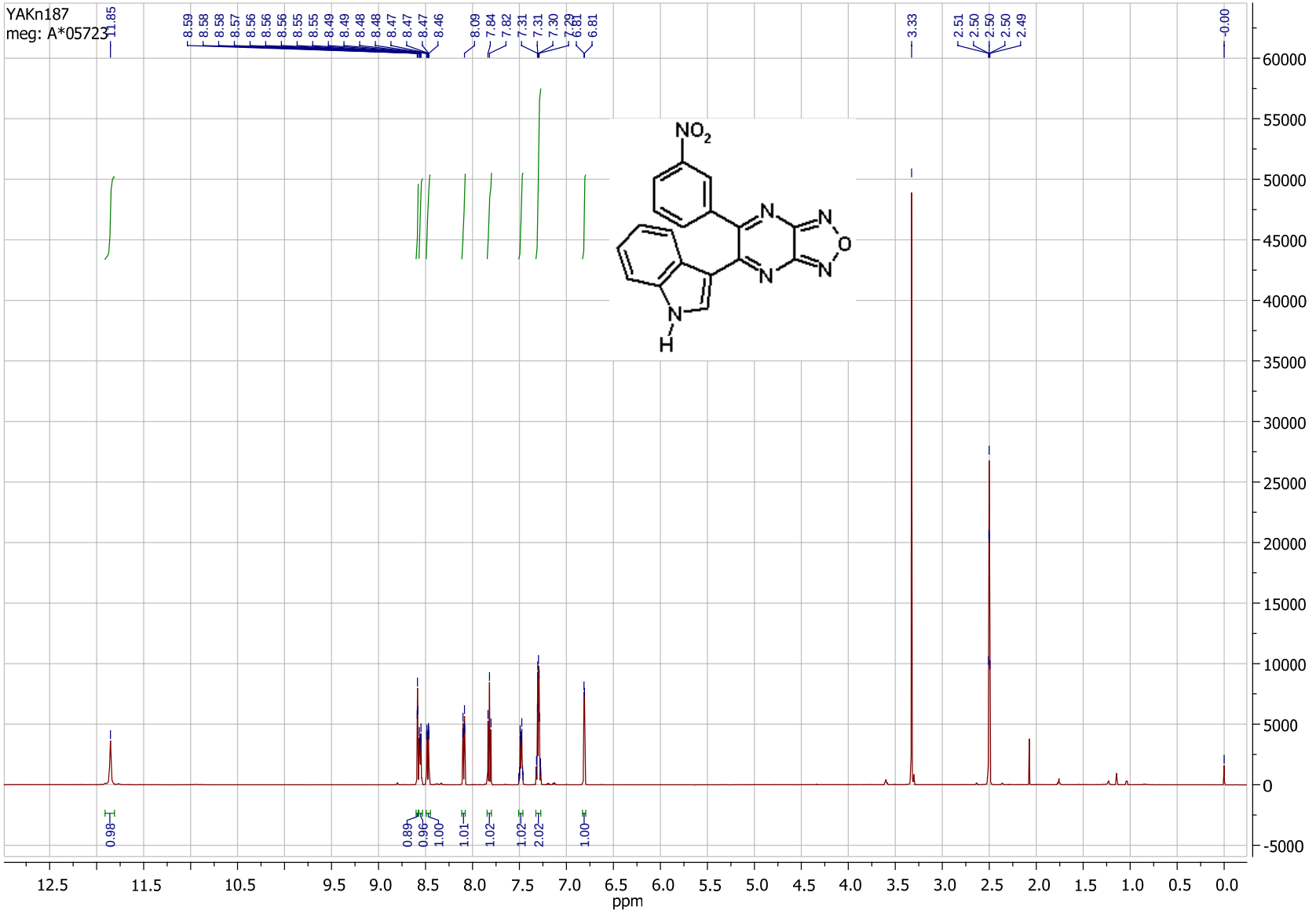
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **10d**.



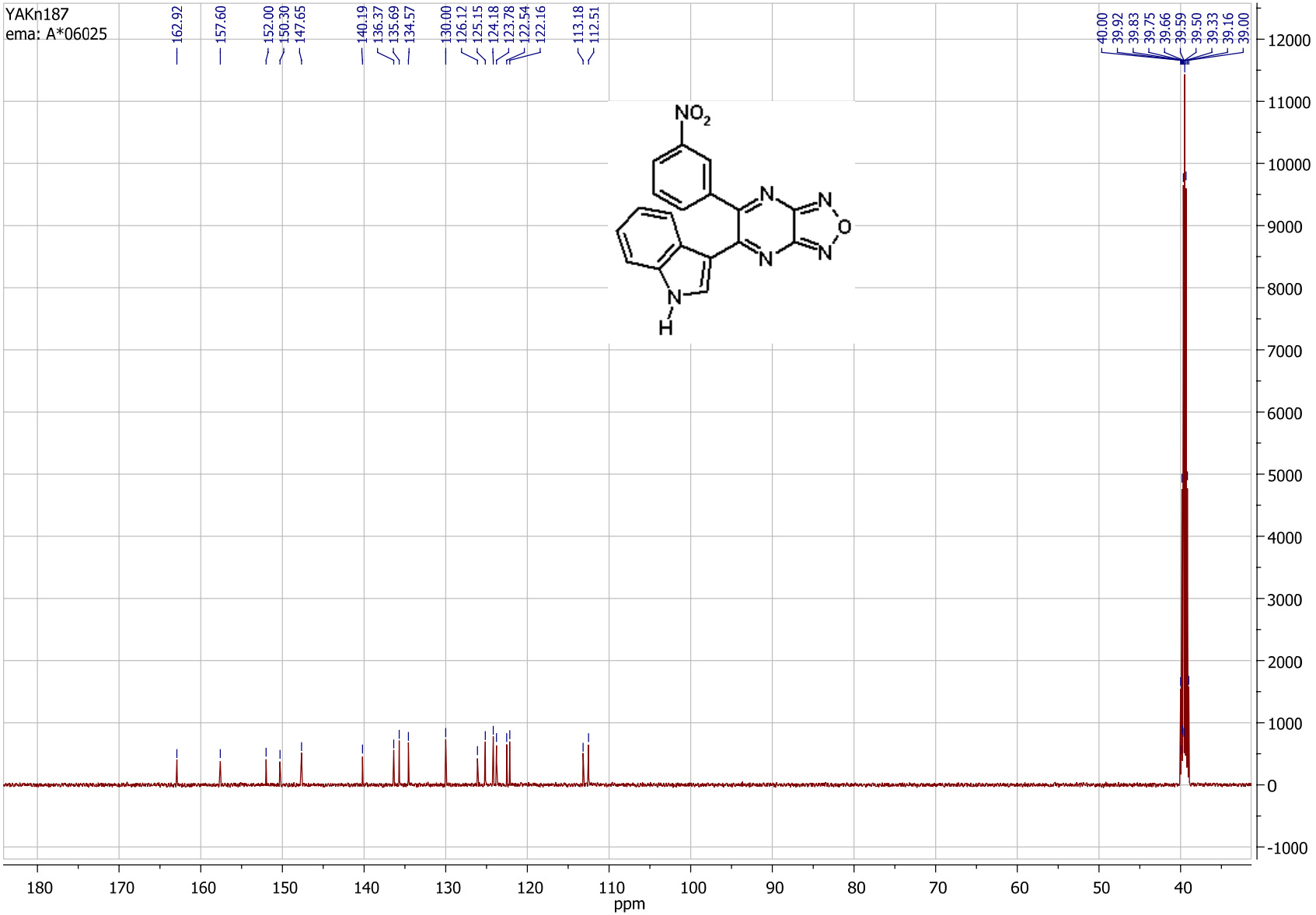
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **14a**.



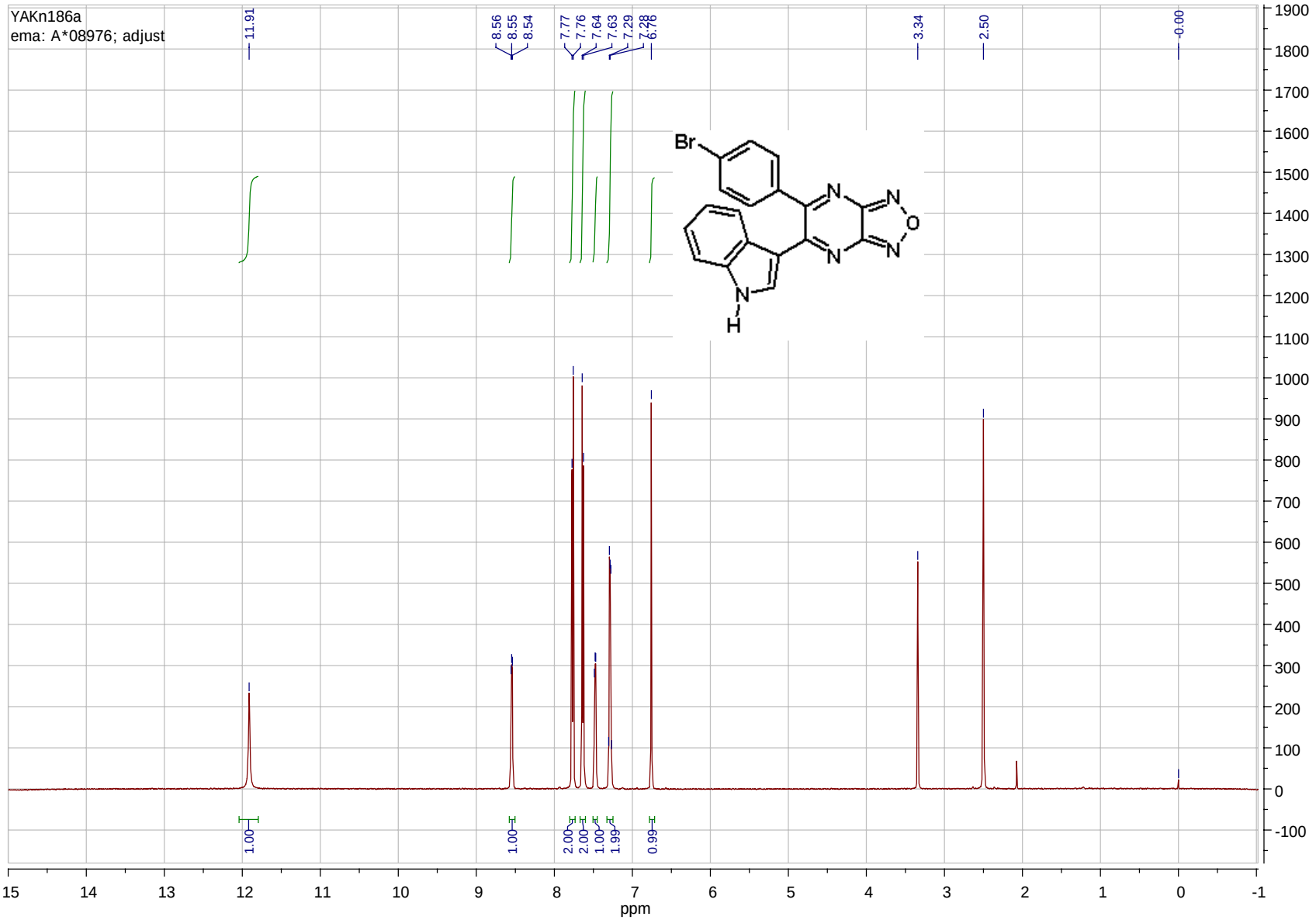
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **14a**.



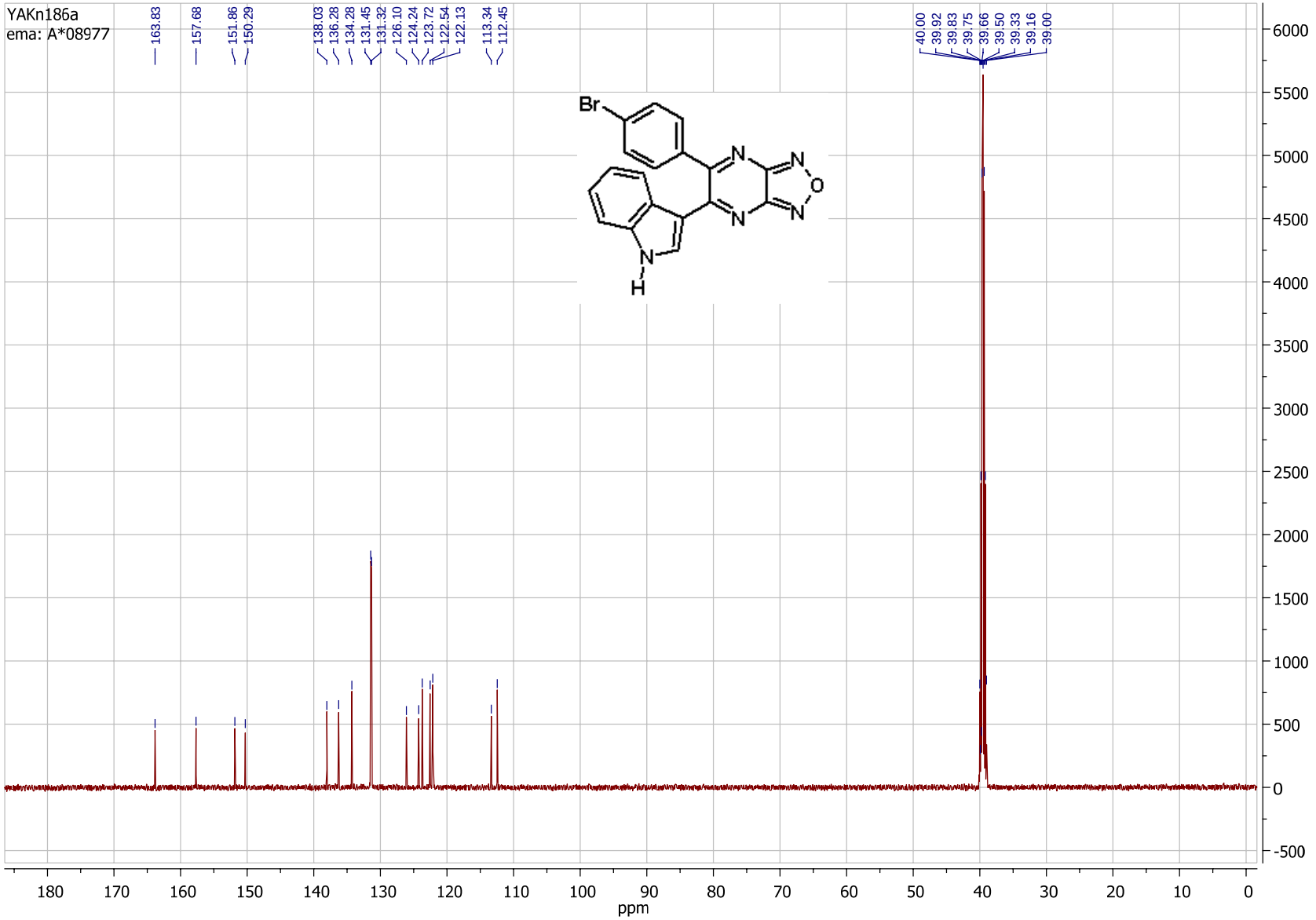
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **14b**.



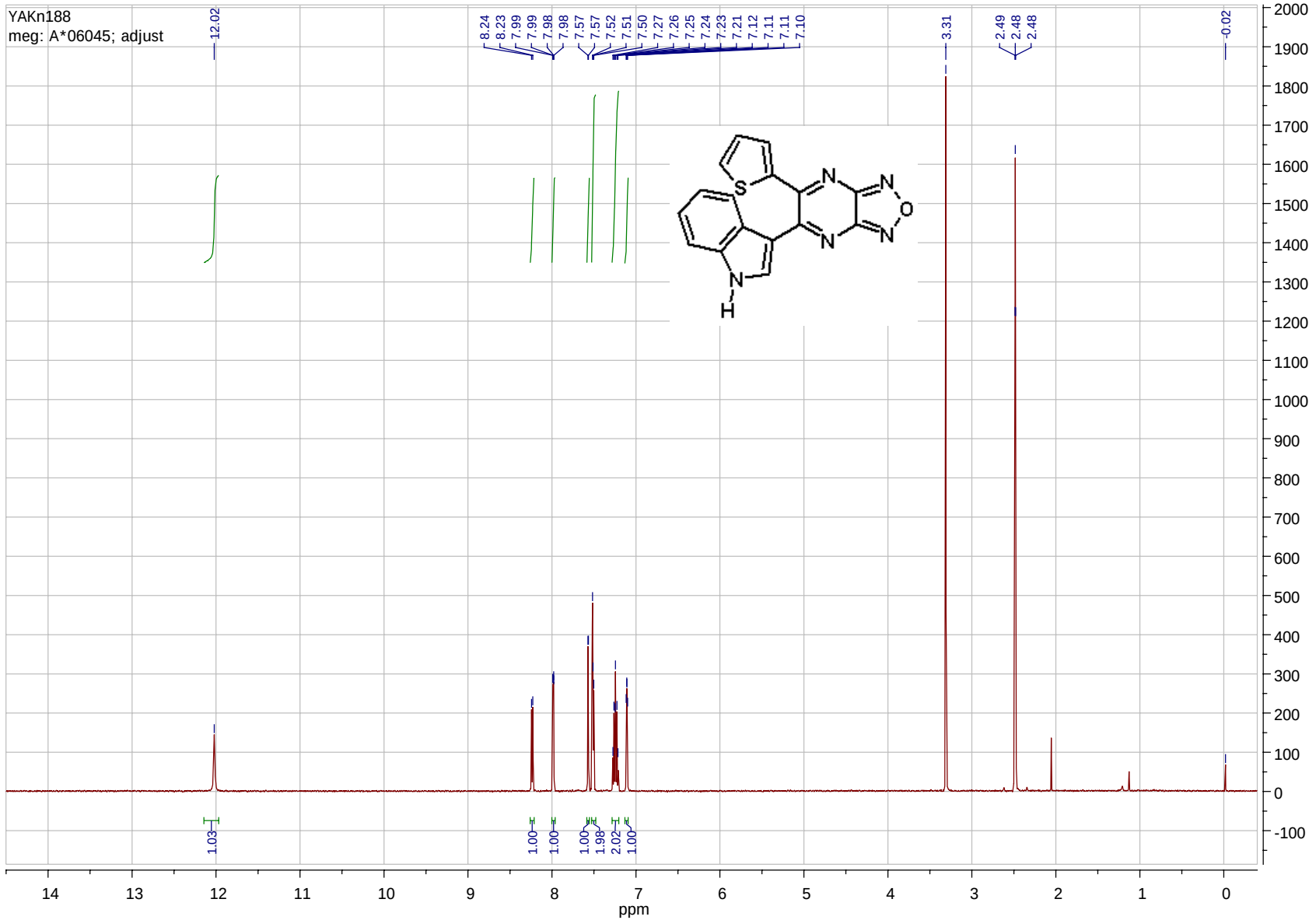
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **14b**.



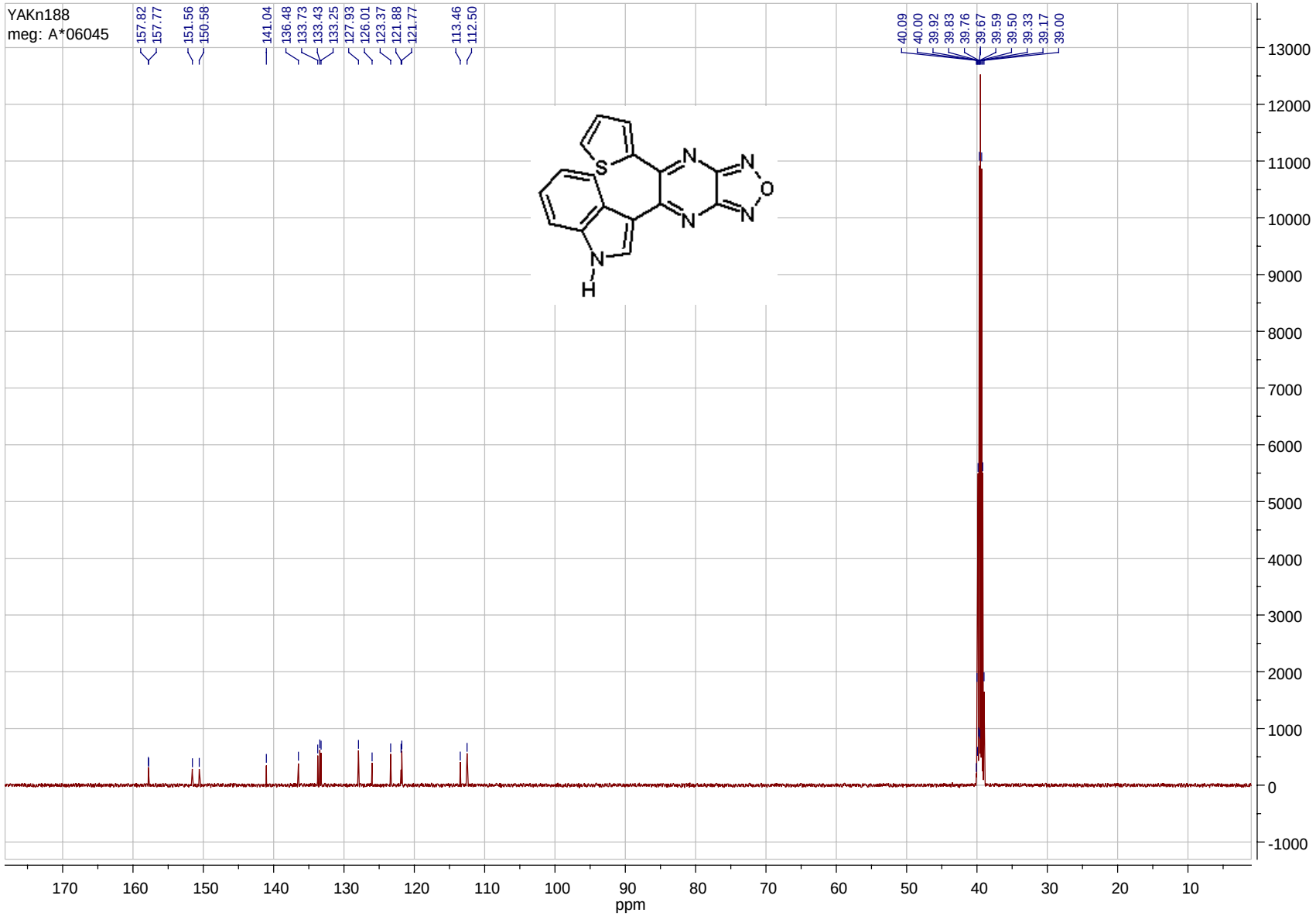
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **14c**.



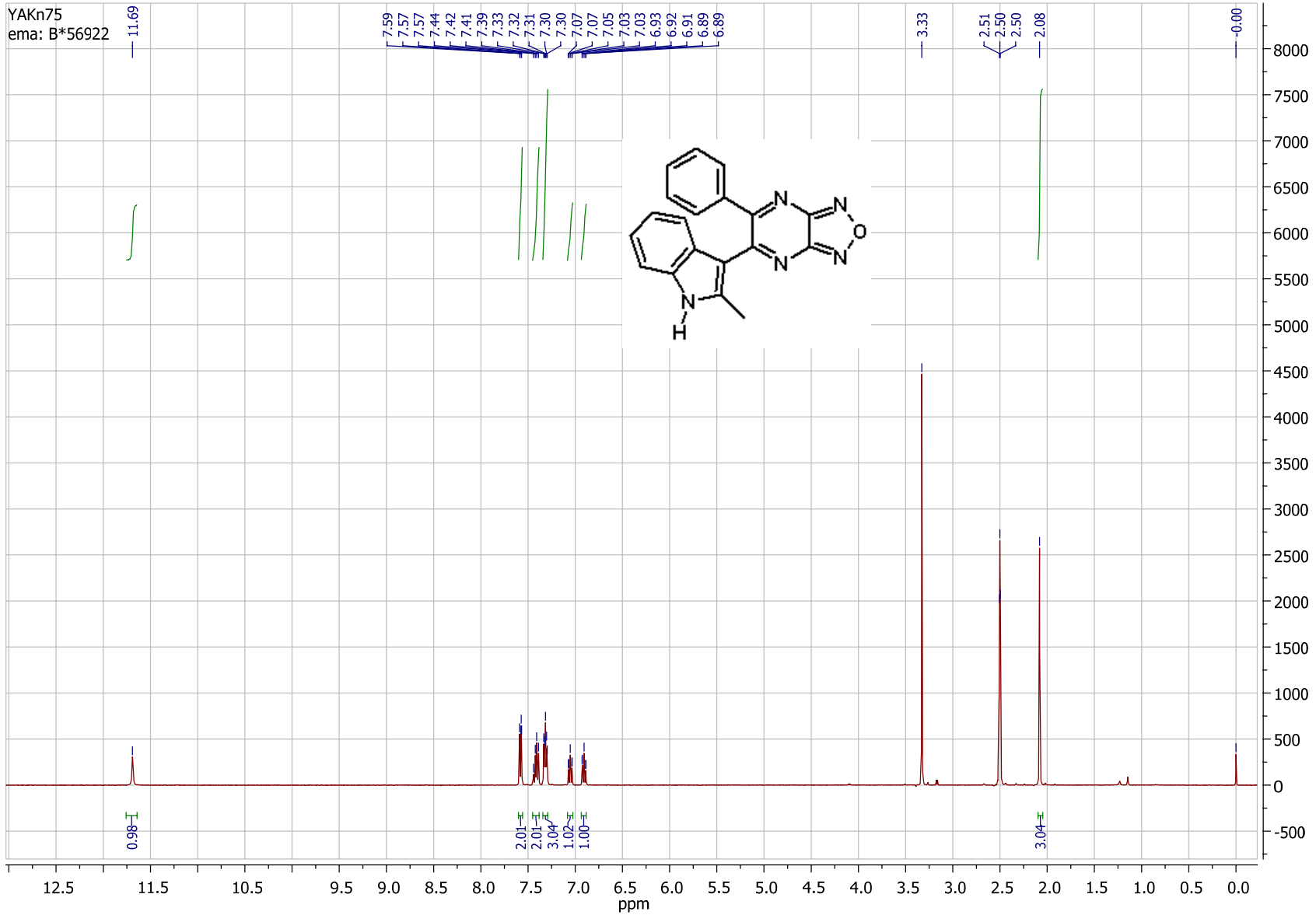
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **14c**.



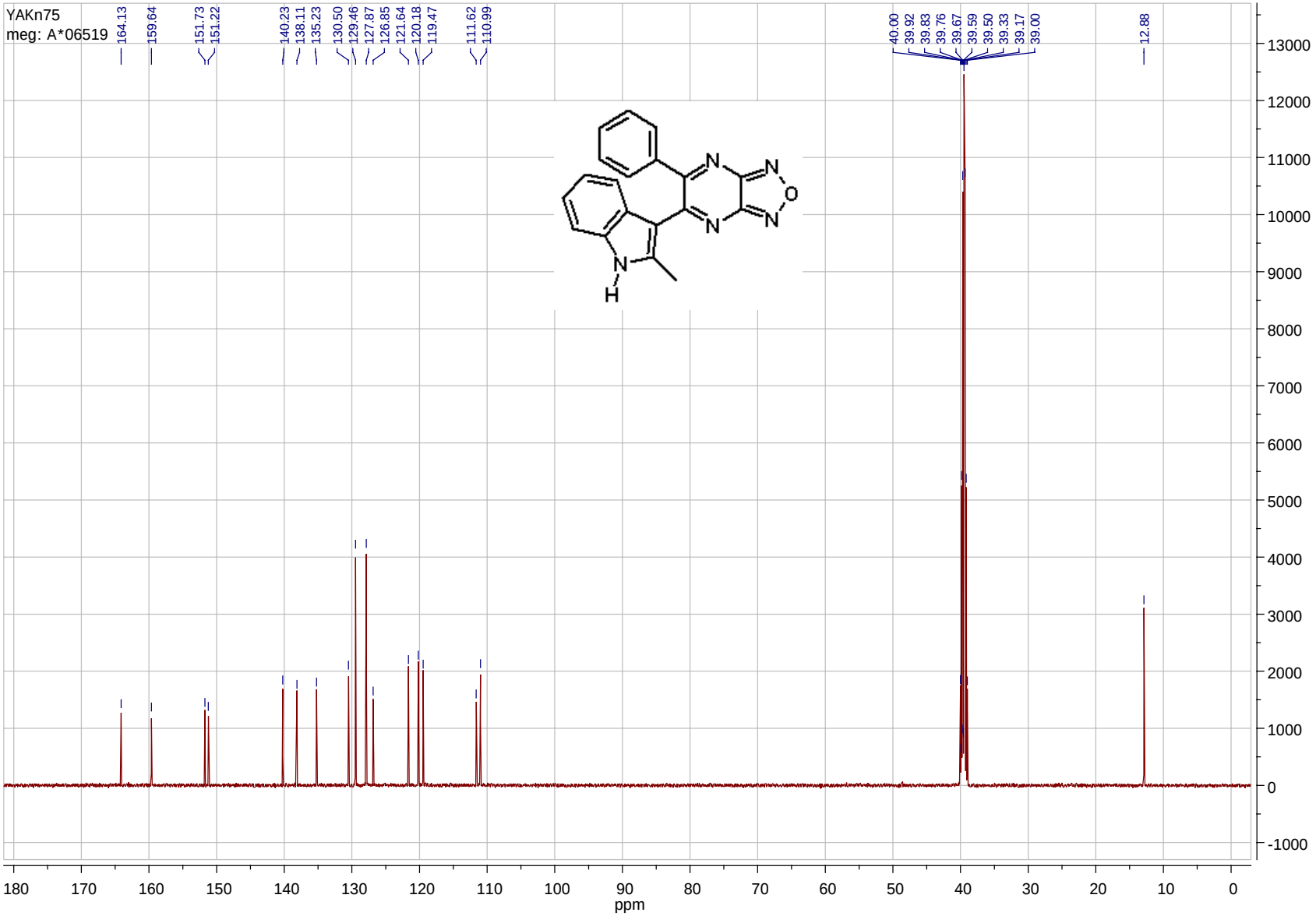
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **14d**.



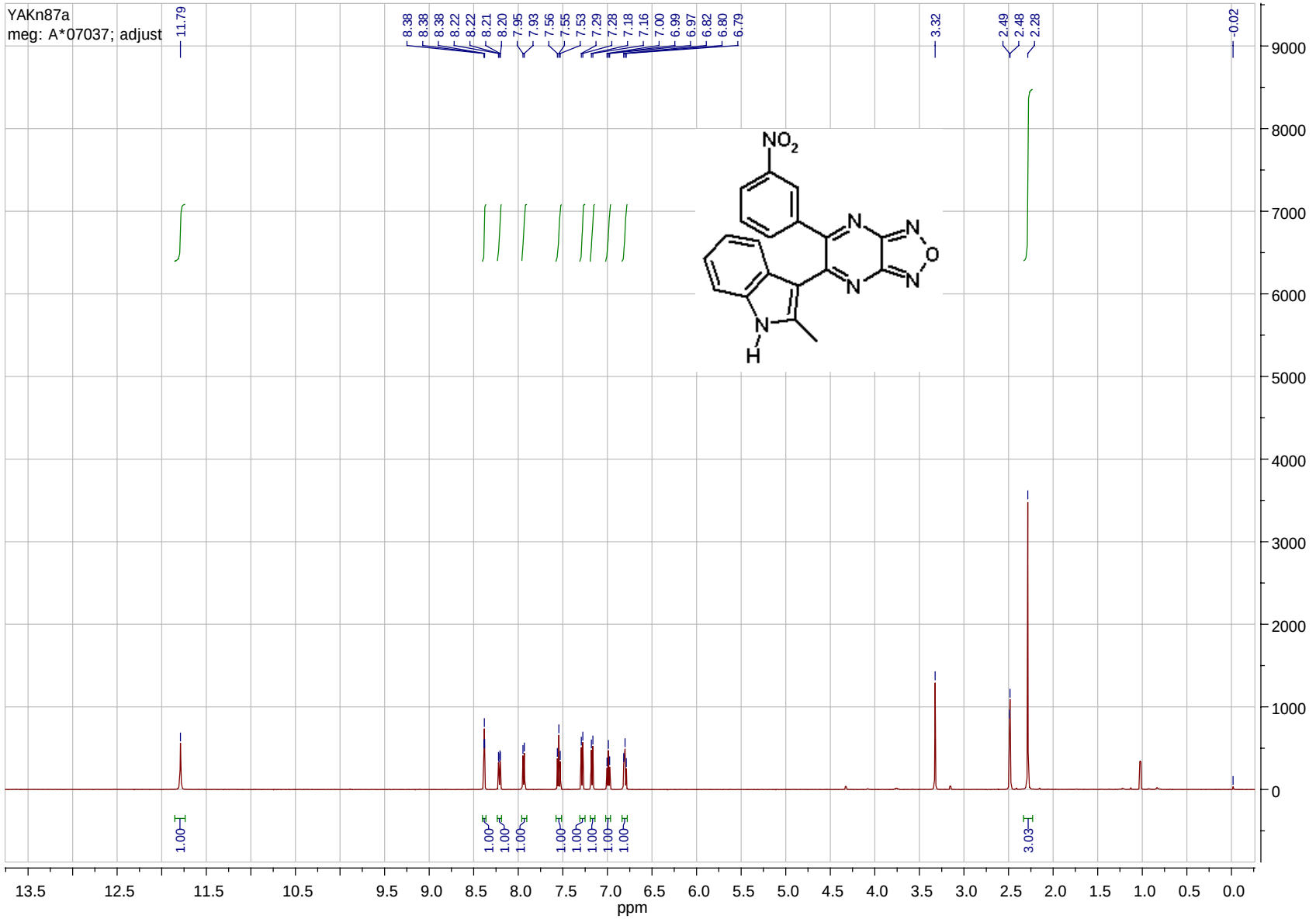
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **14d**.



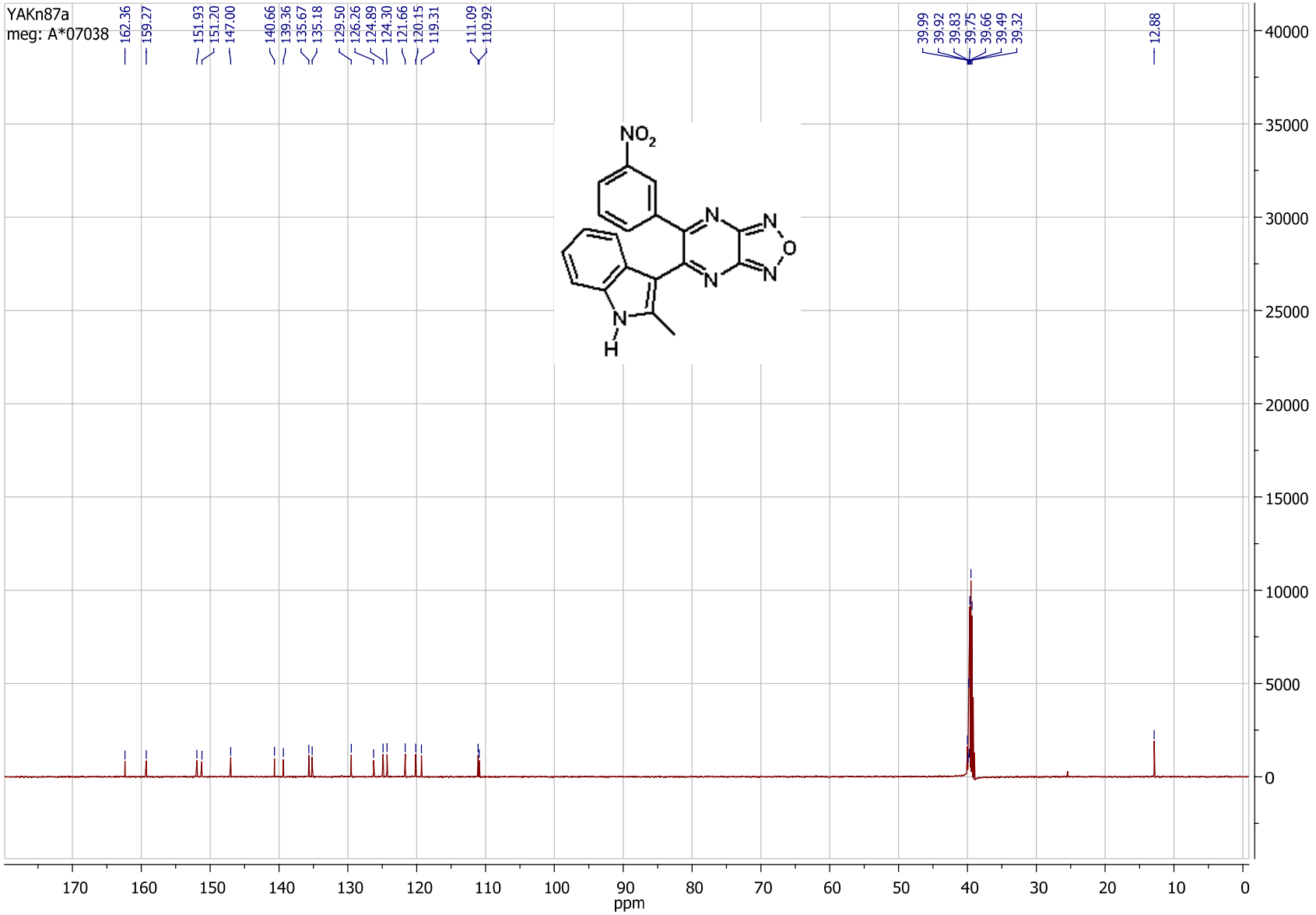
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **15a**.



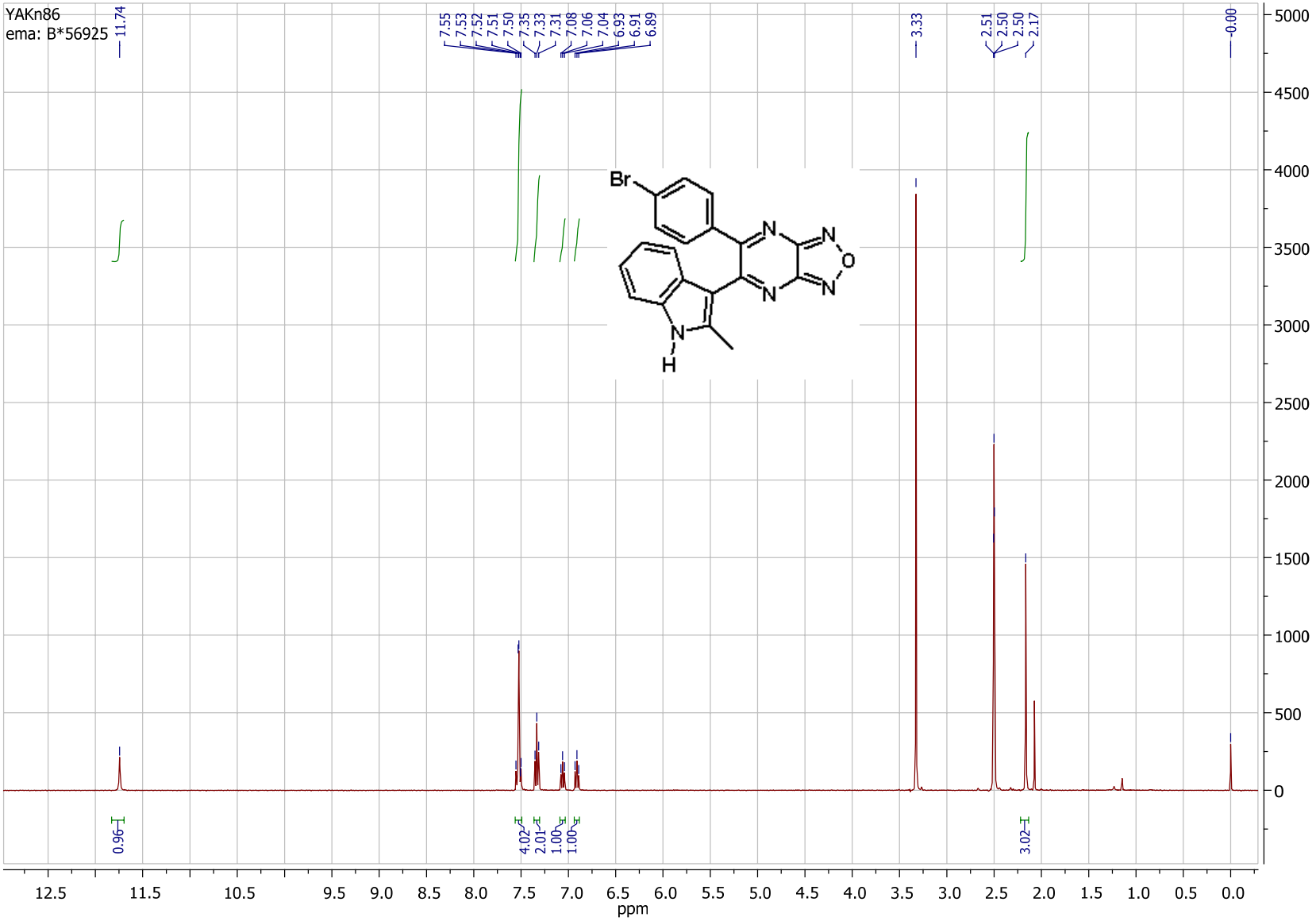
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **15a**.



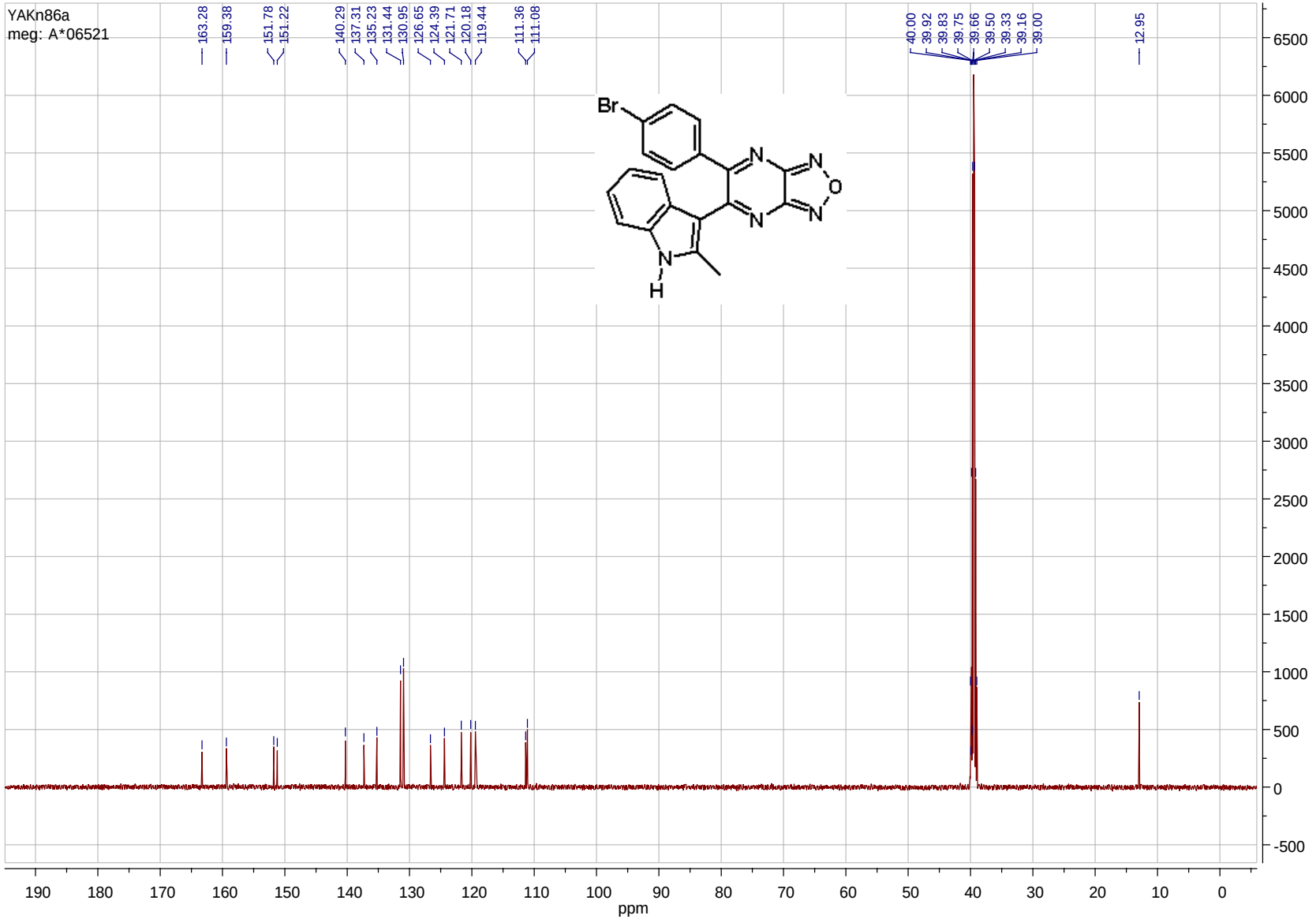
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **15b**.



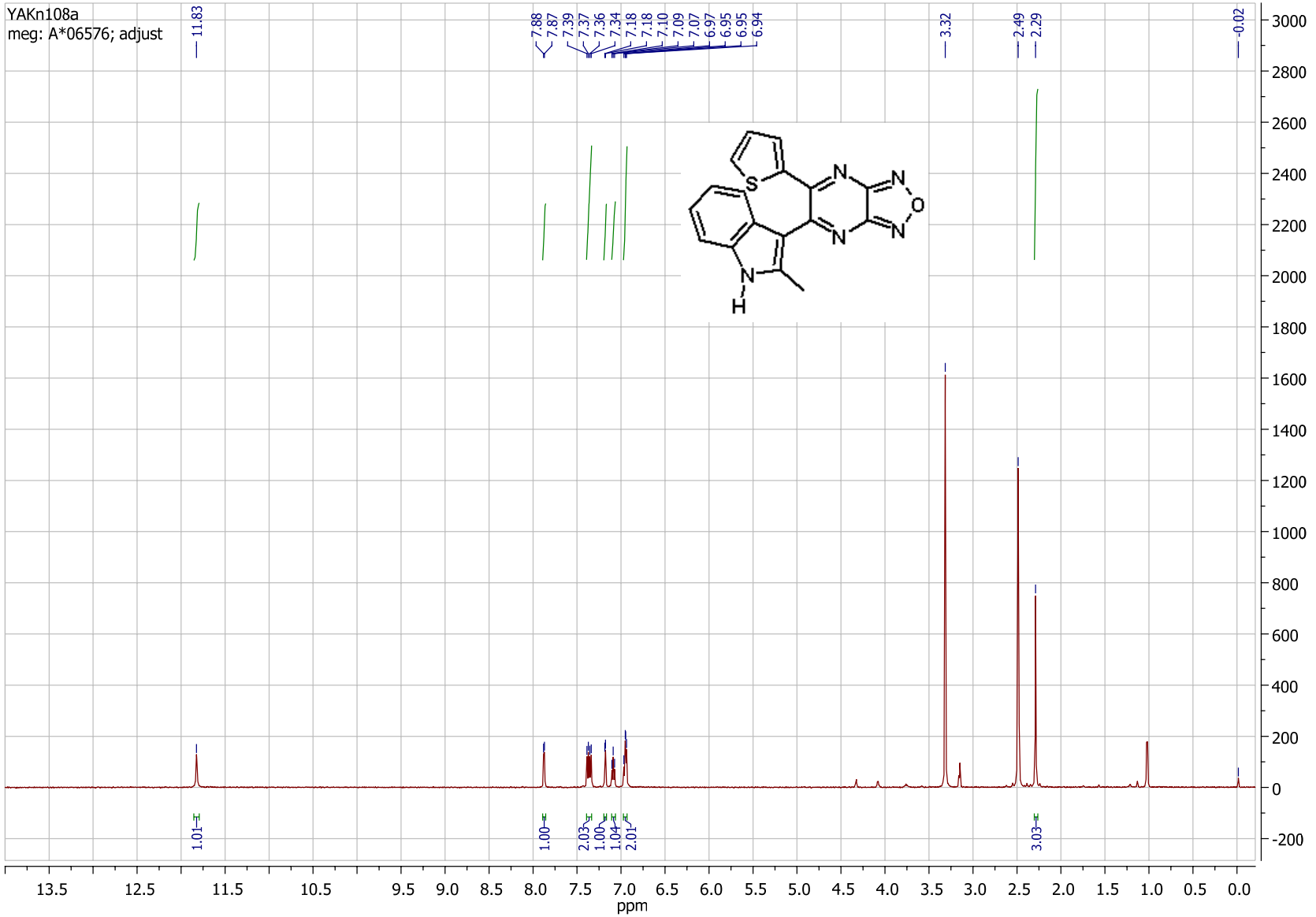
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **15b**.



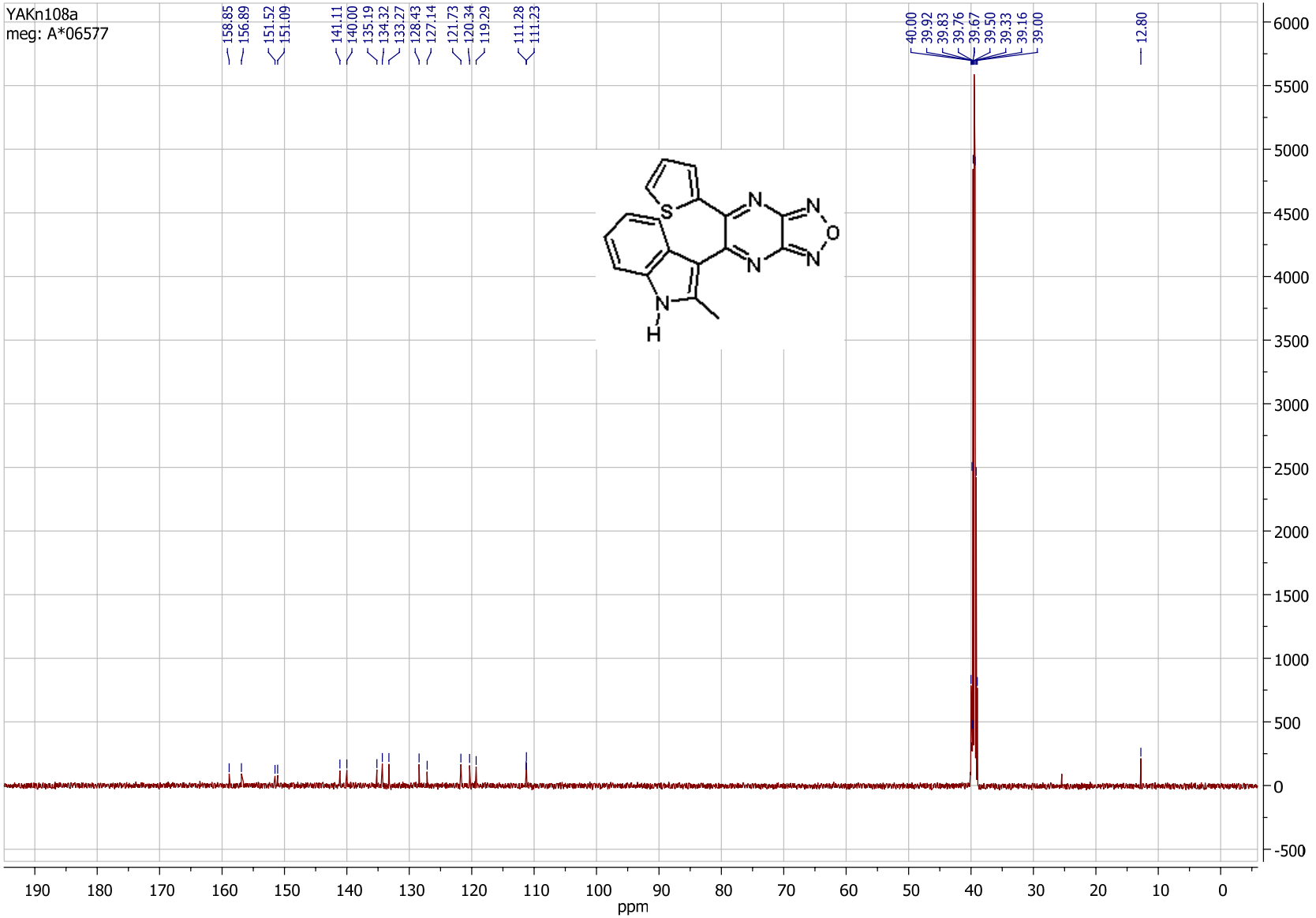
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **15c**.



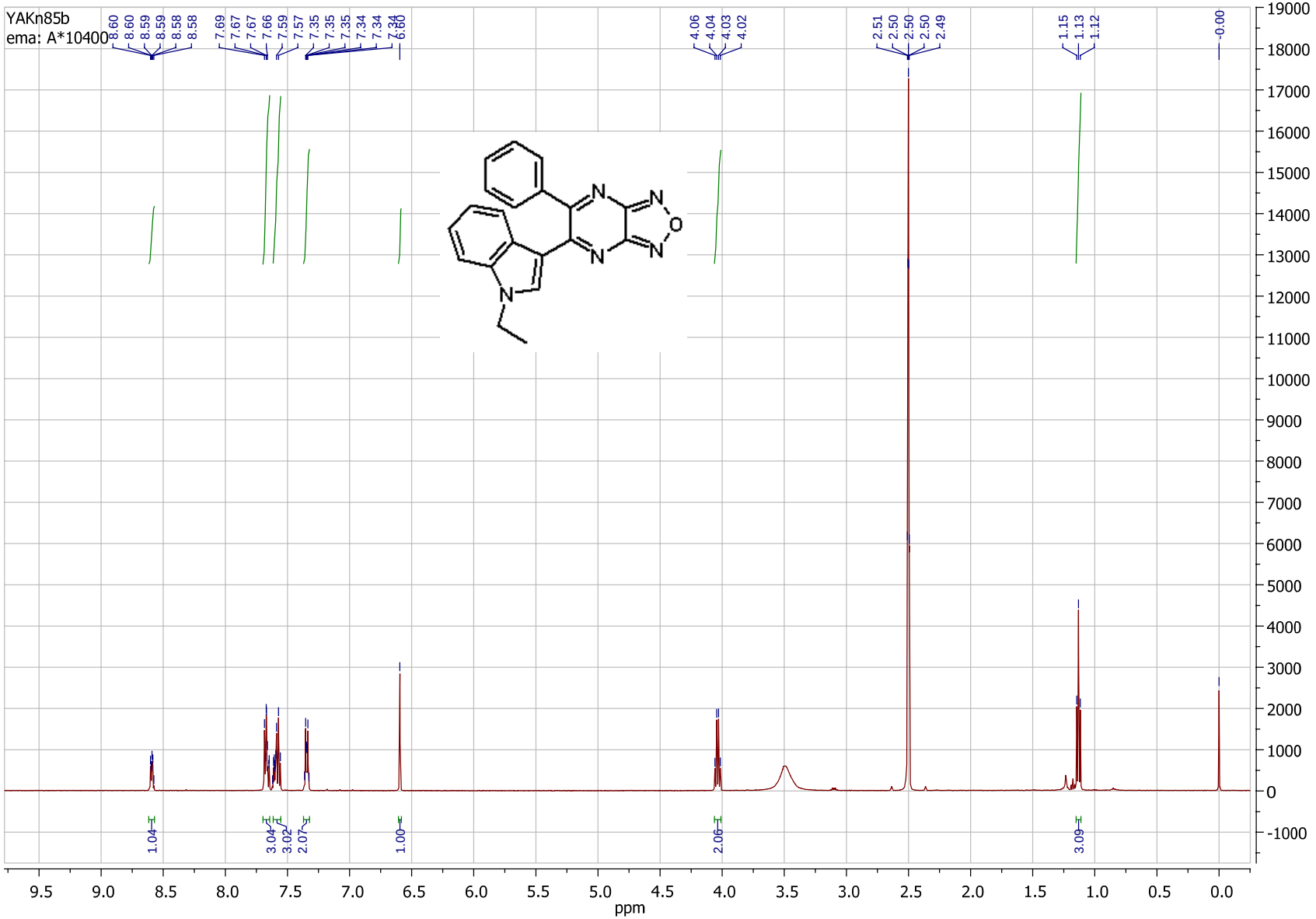
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **15c**.



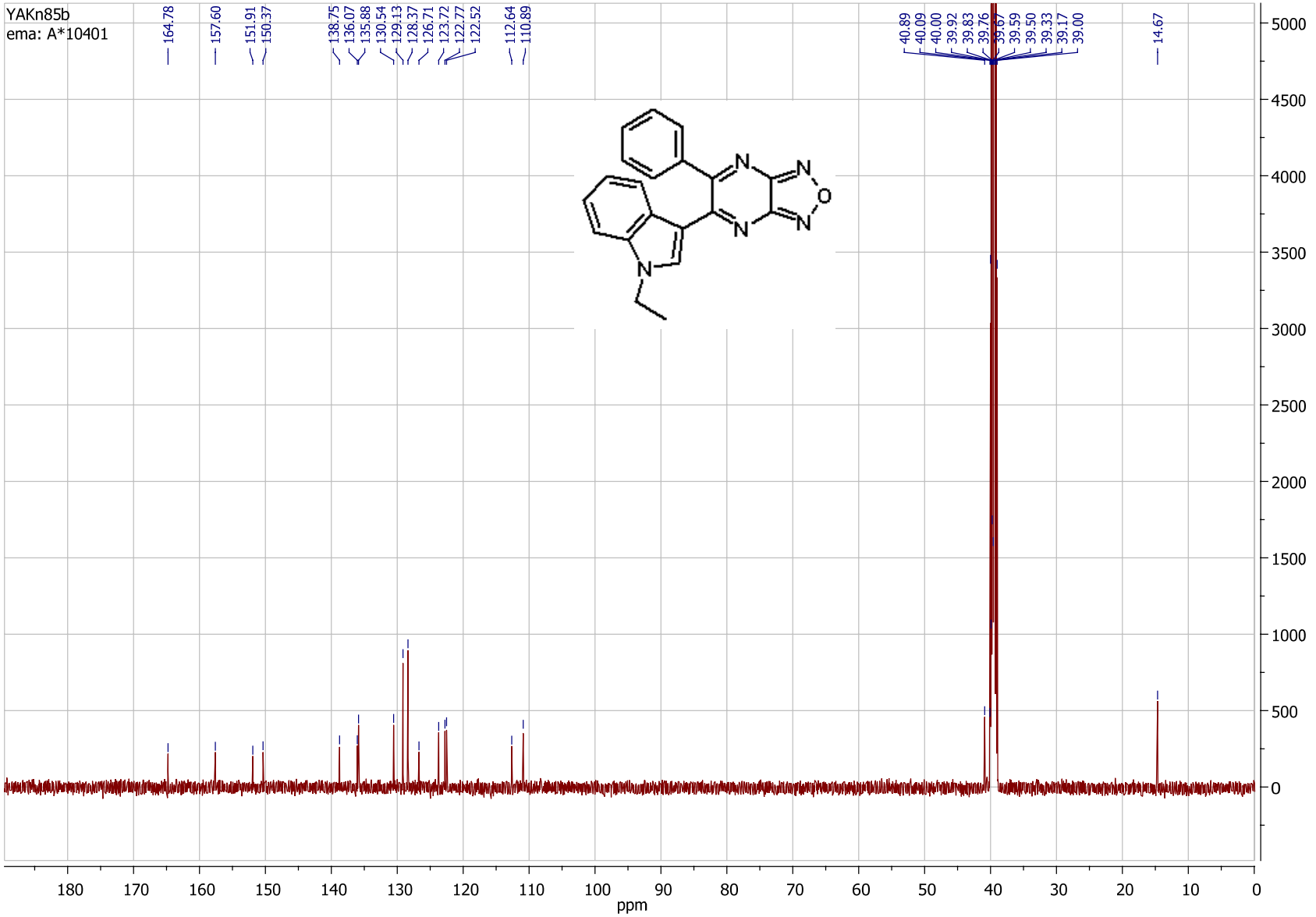
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **15d**.



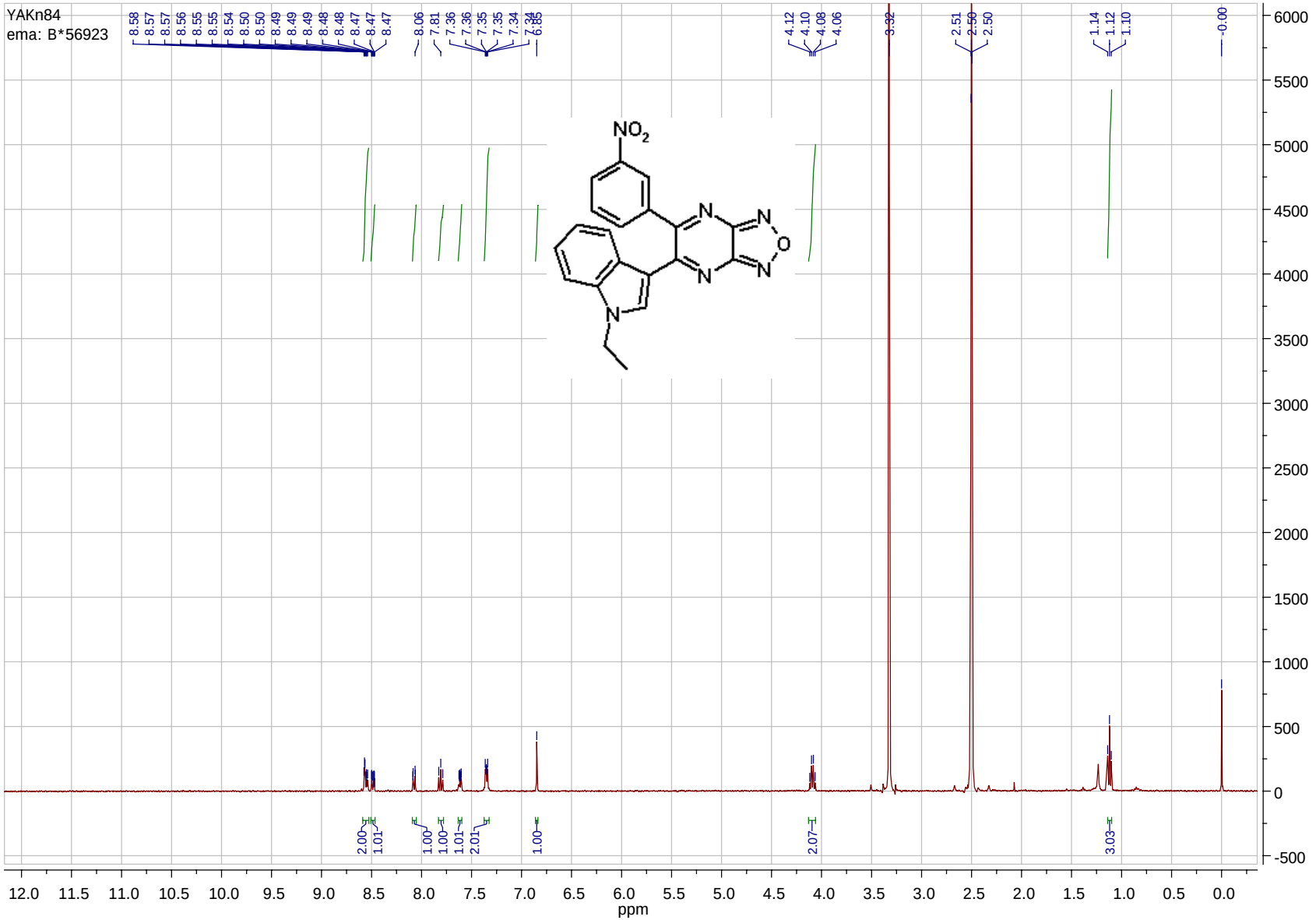
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **15d**.



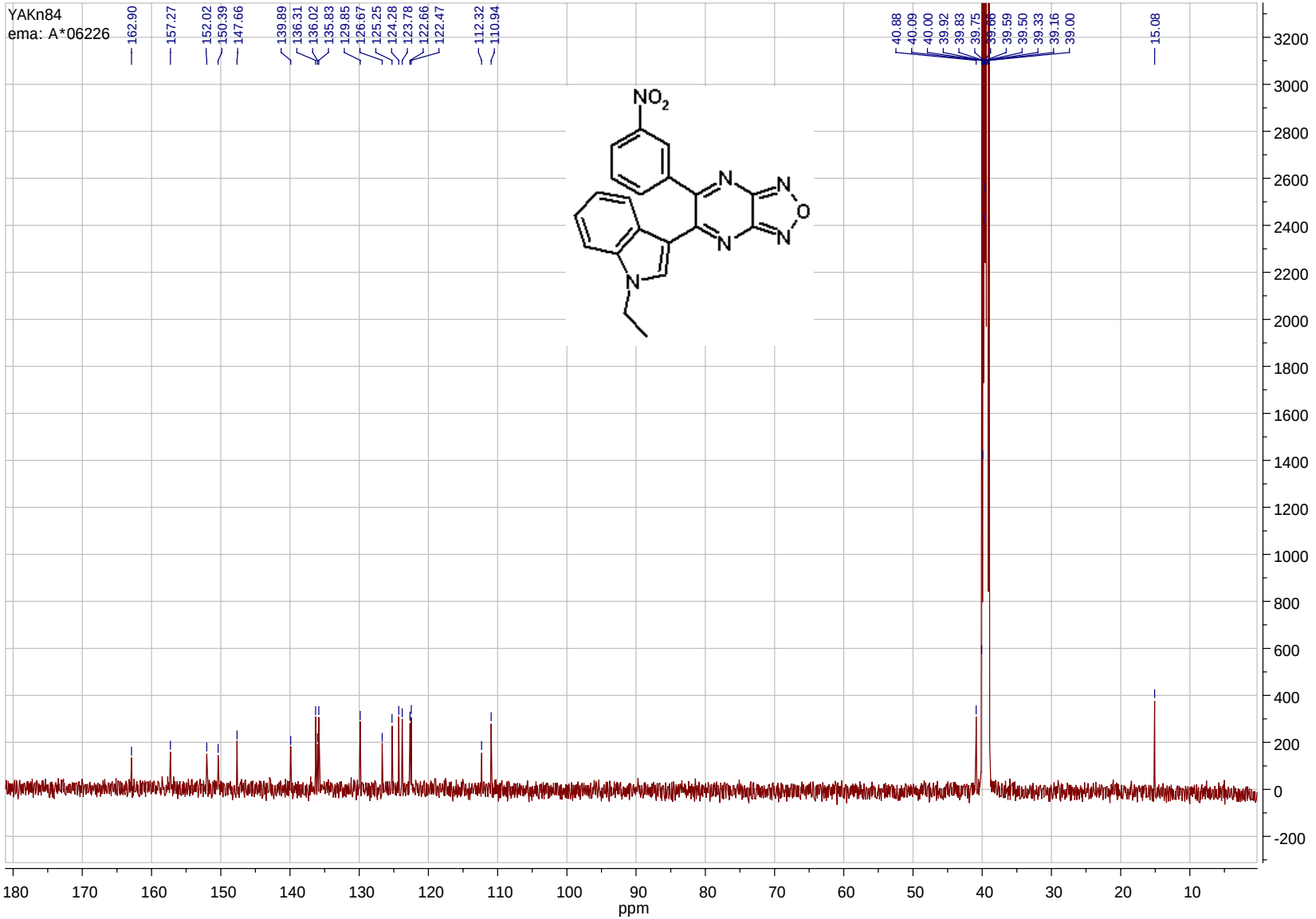
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **16a**.



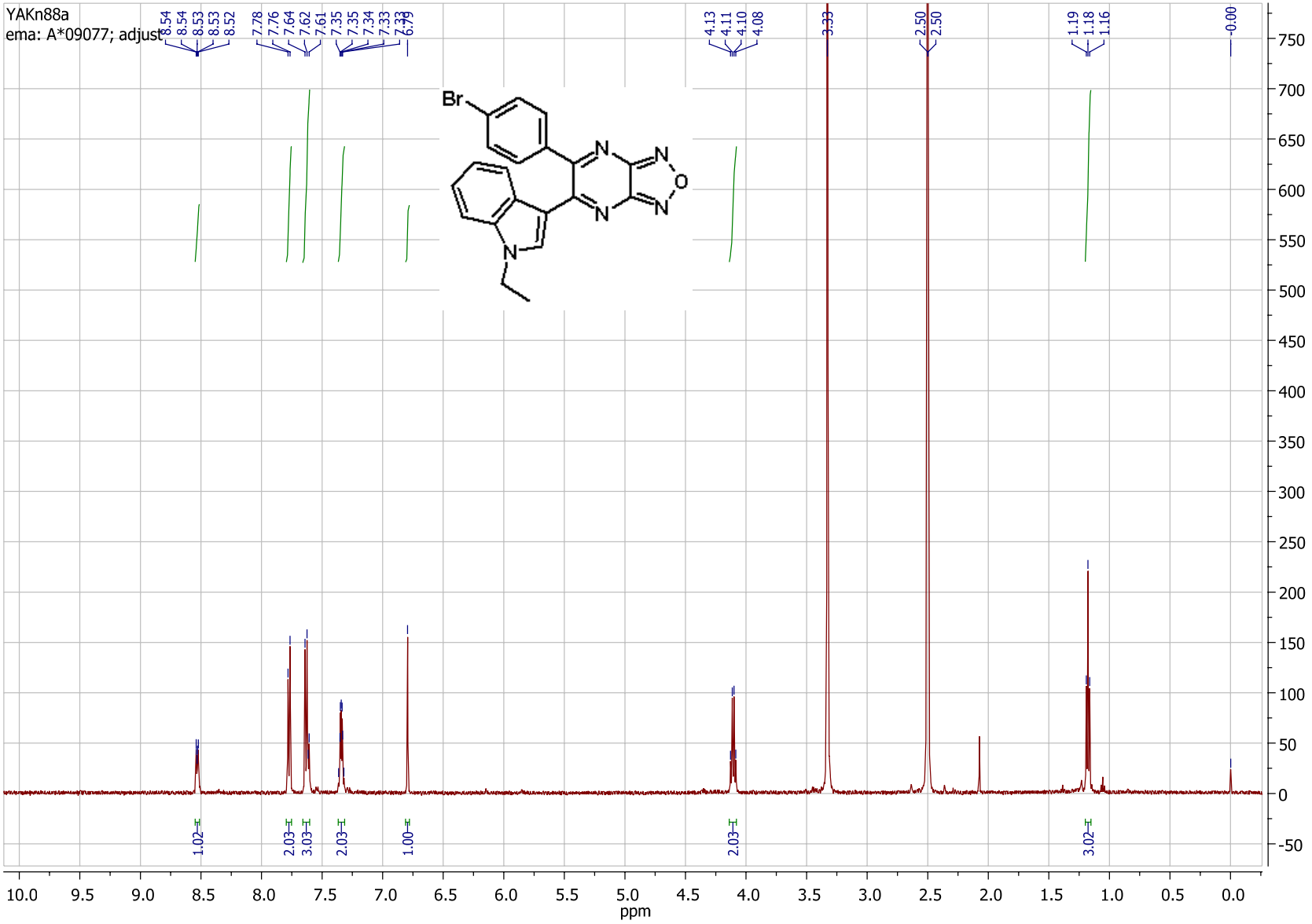
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **16a**.



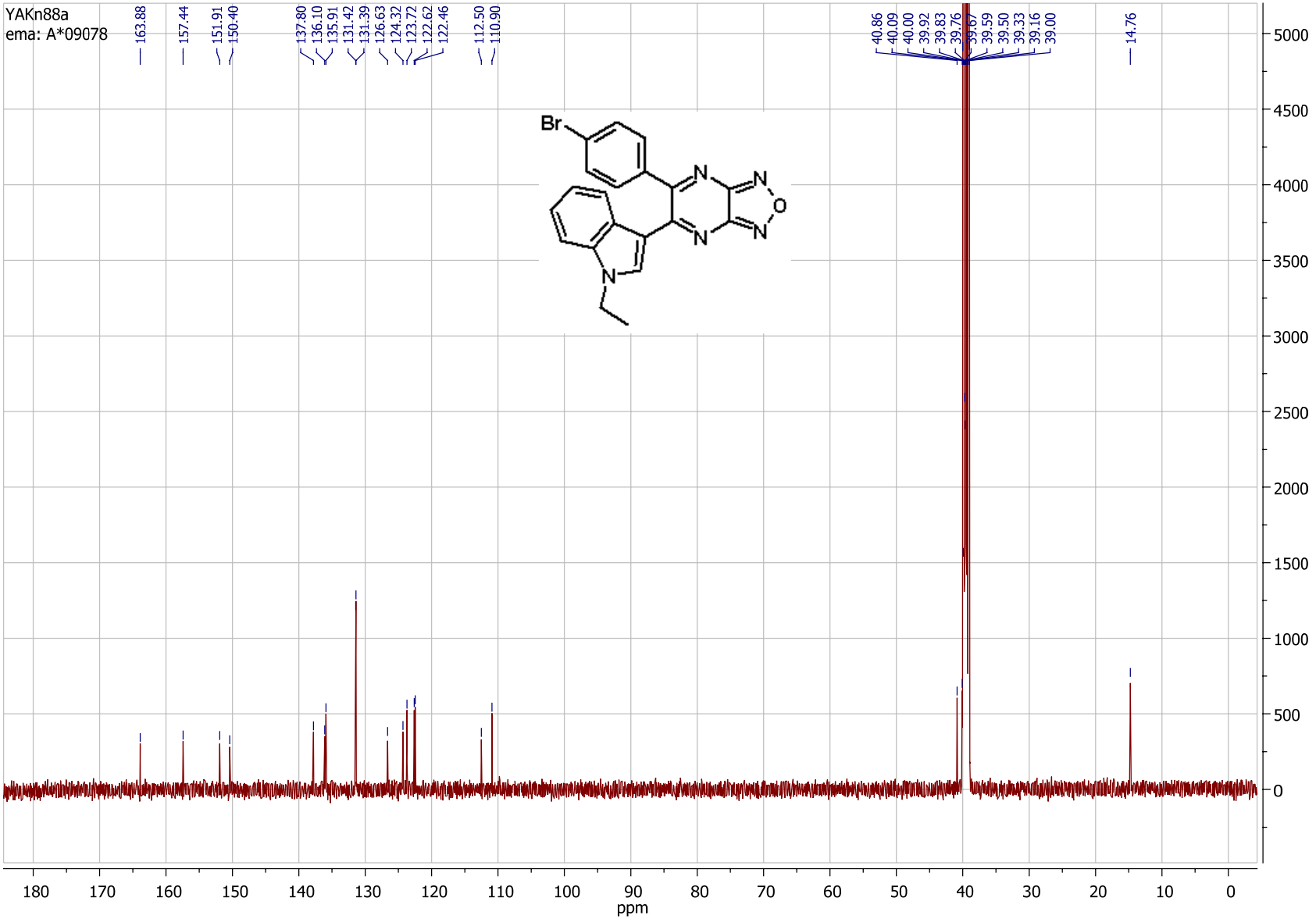
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **16b**.



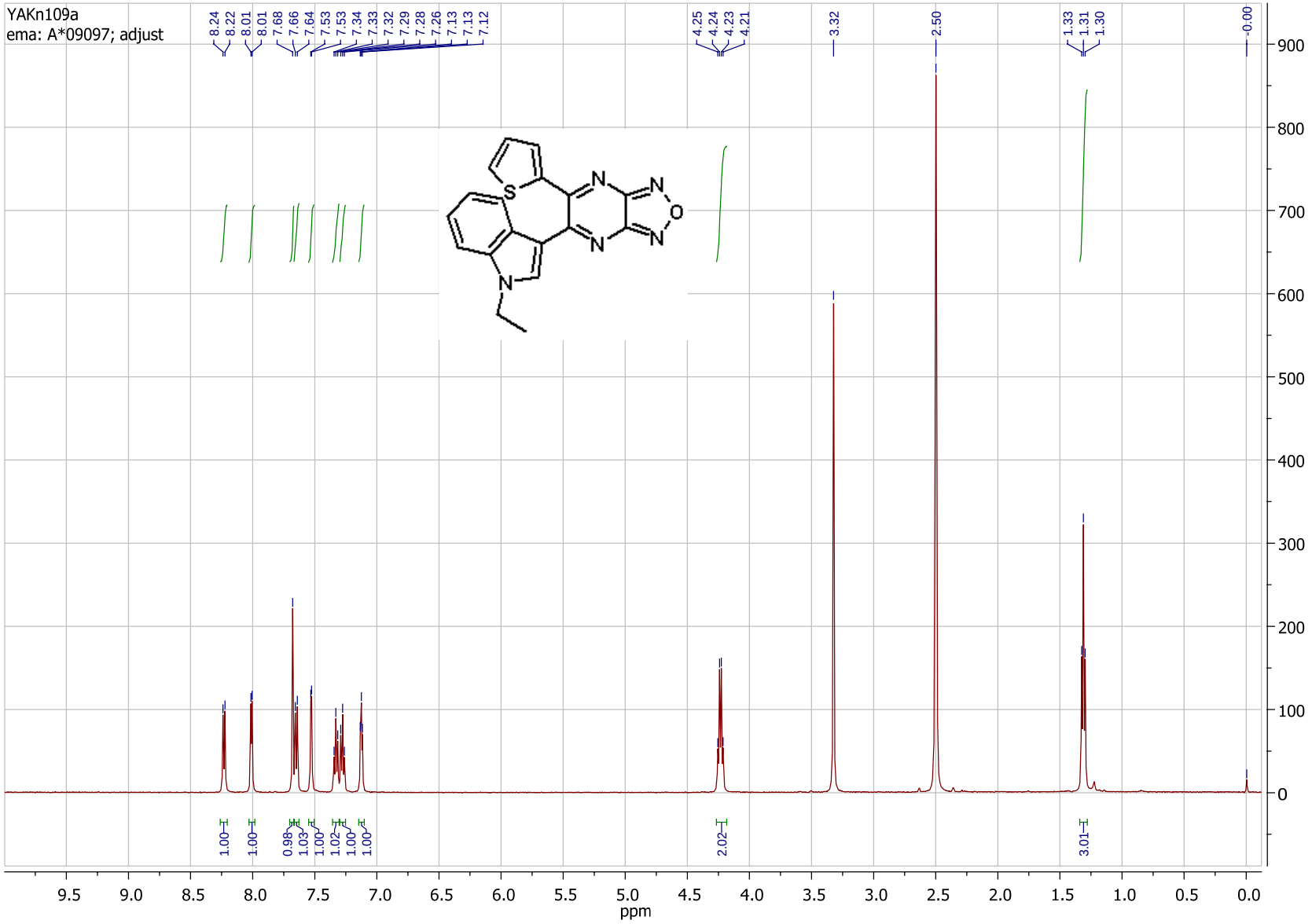
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **16b**.



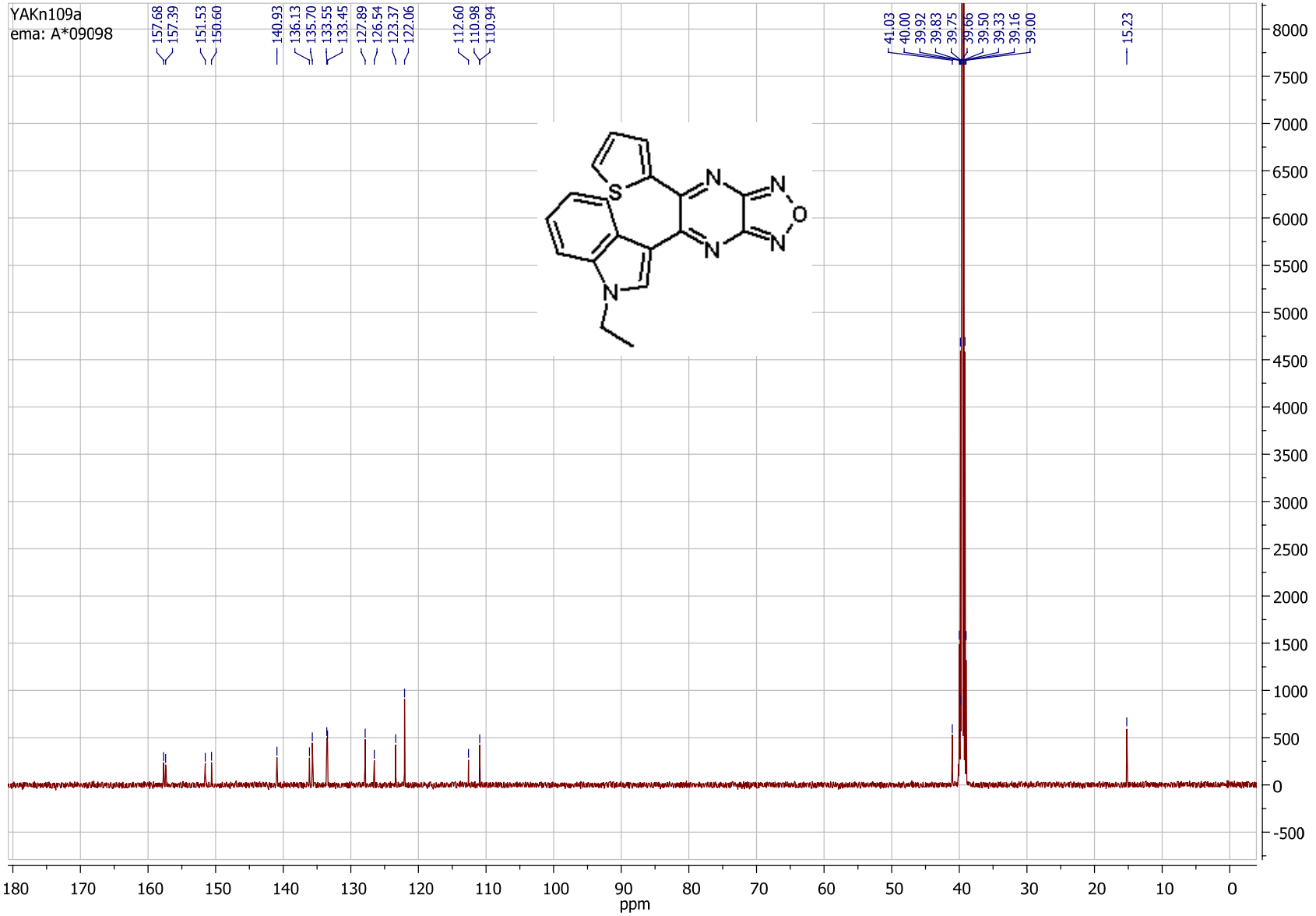
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **16c**.



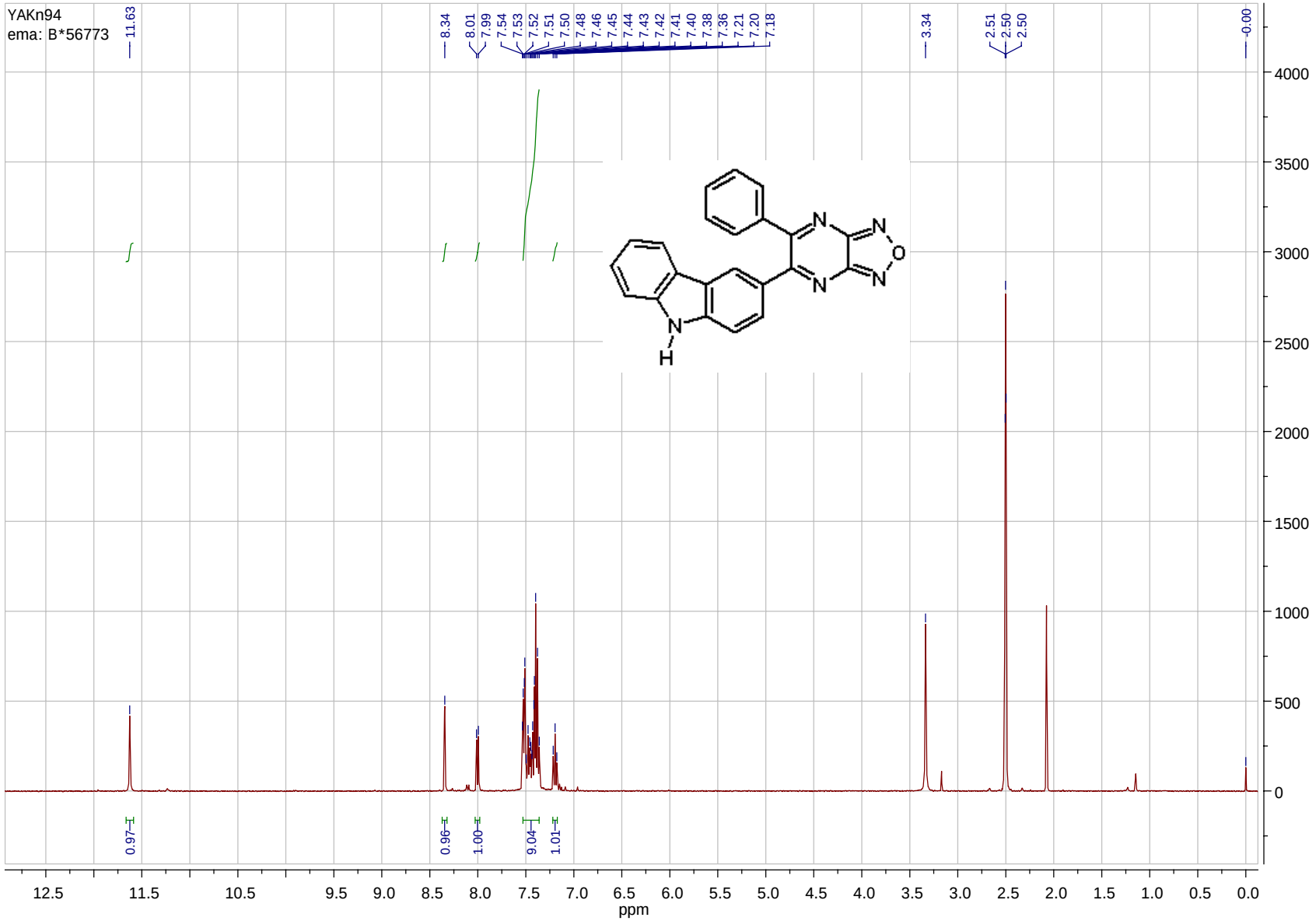
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **16c**.



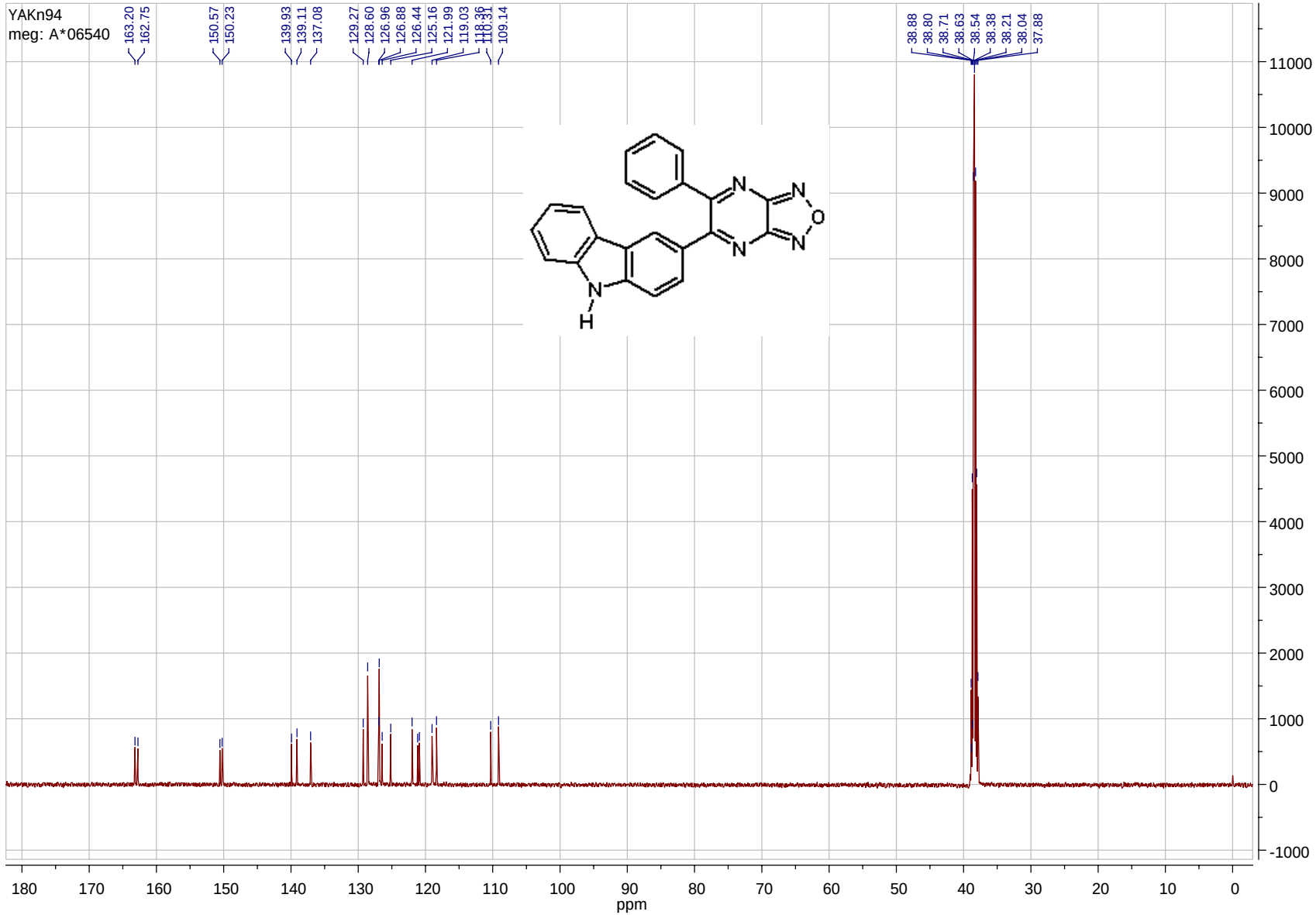
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **16d**.



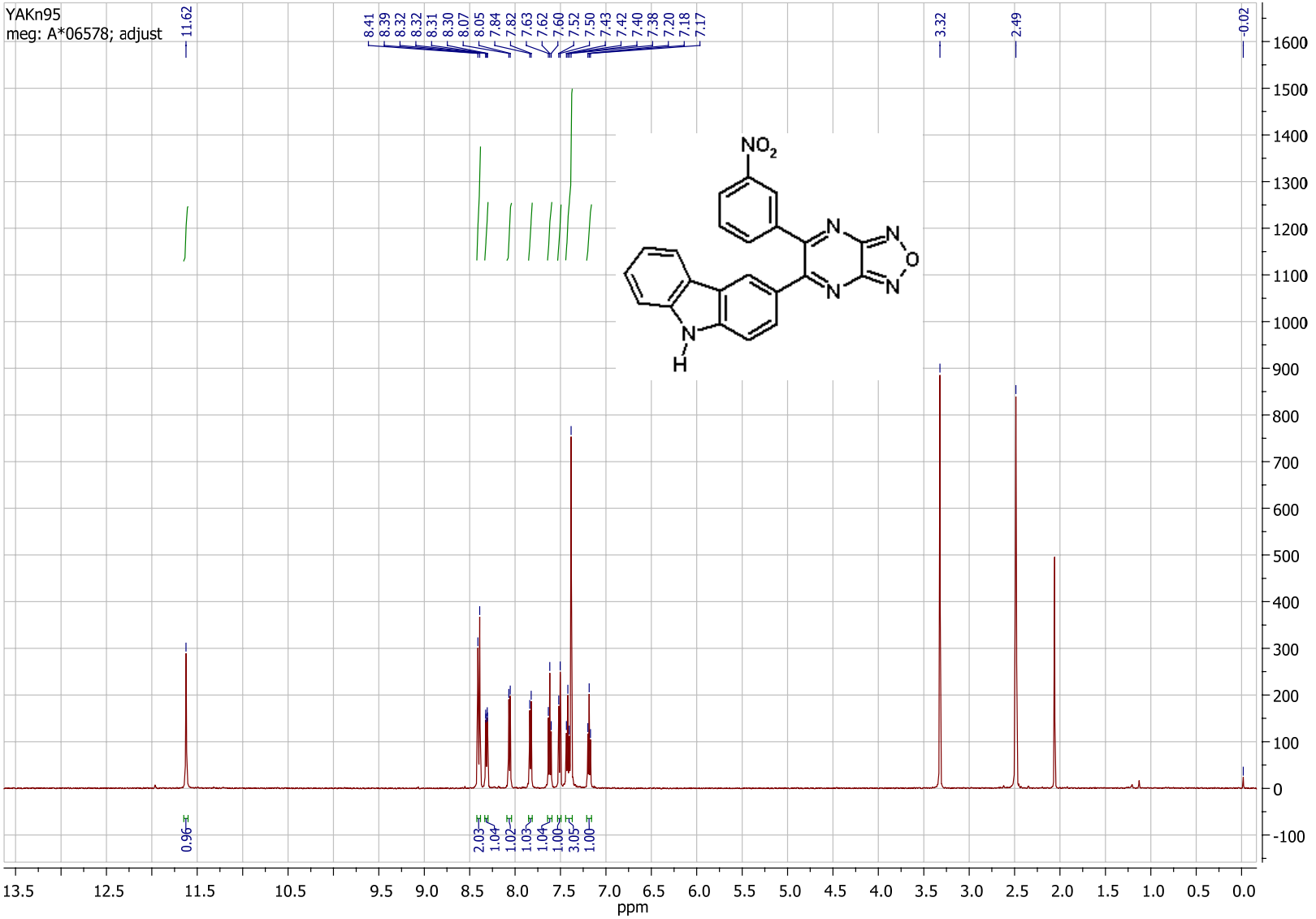
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **16d**.



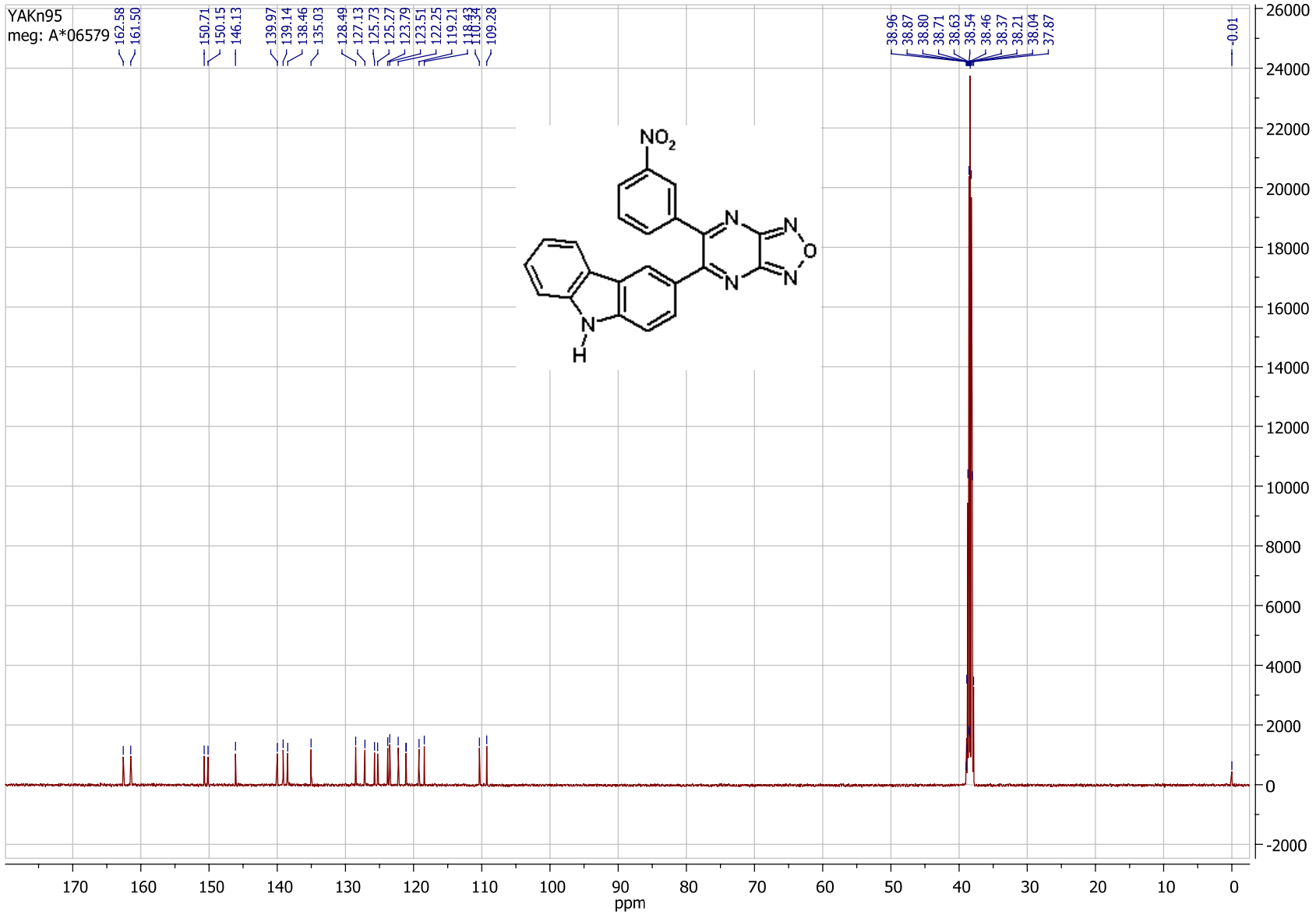
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **20a**.



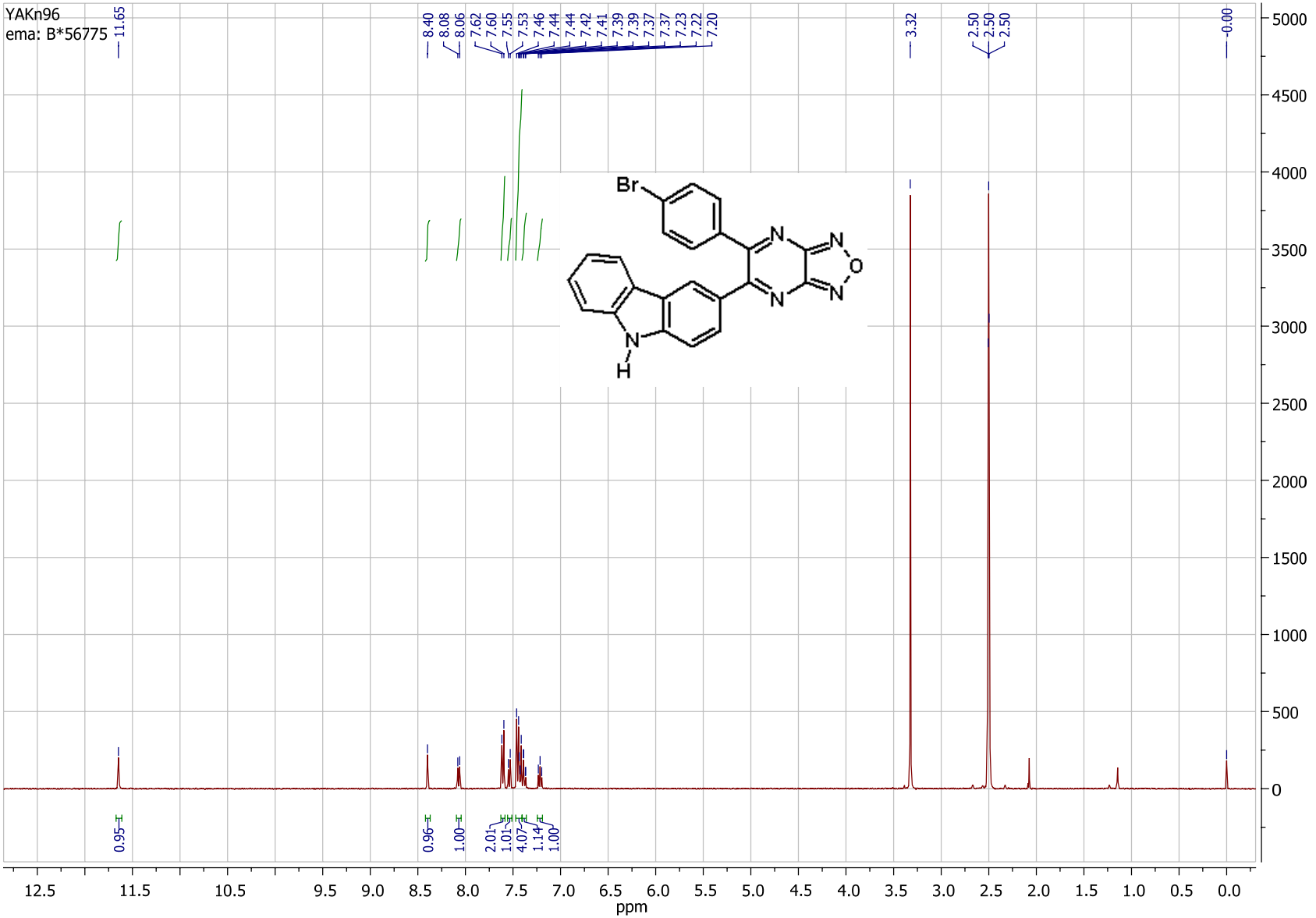
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **20a**.



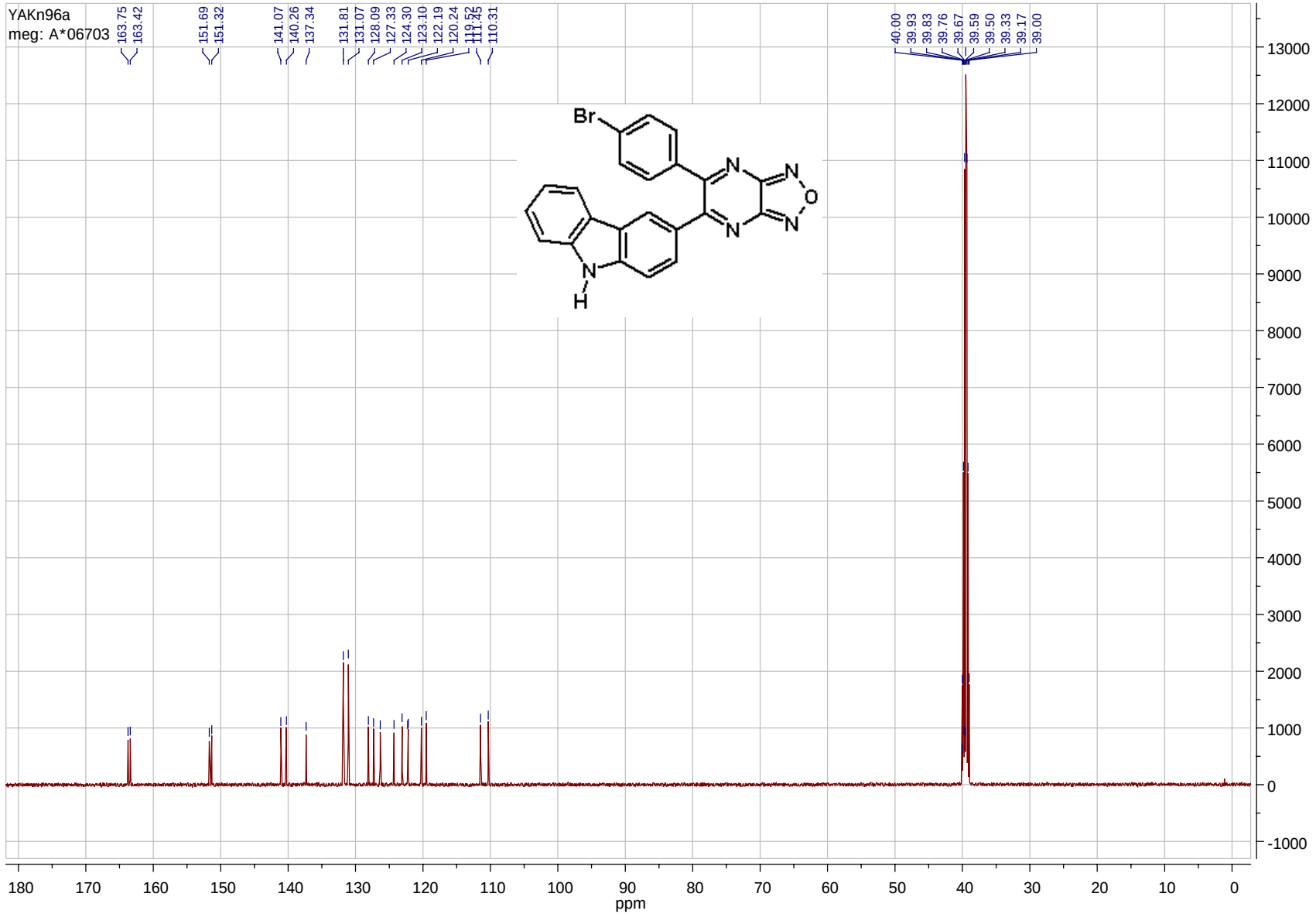
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **20b**.



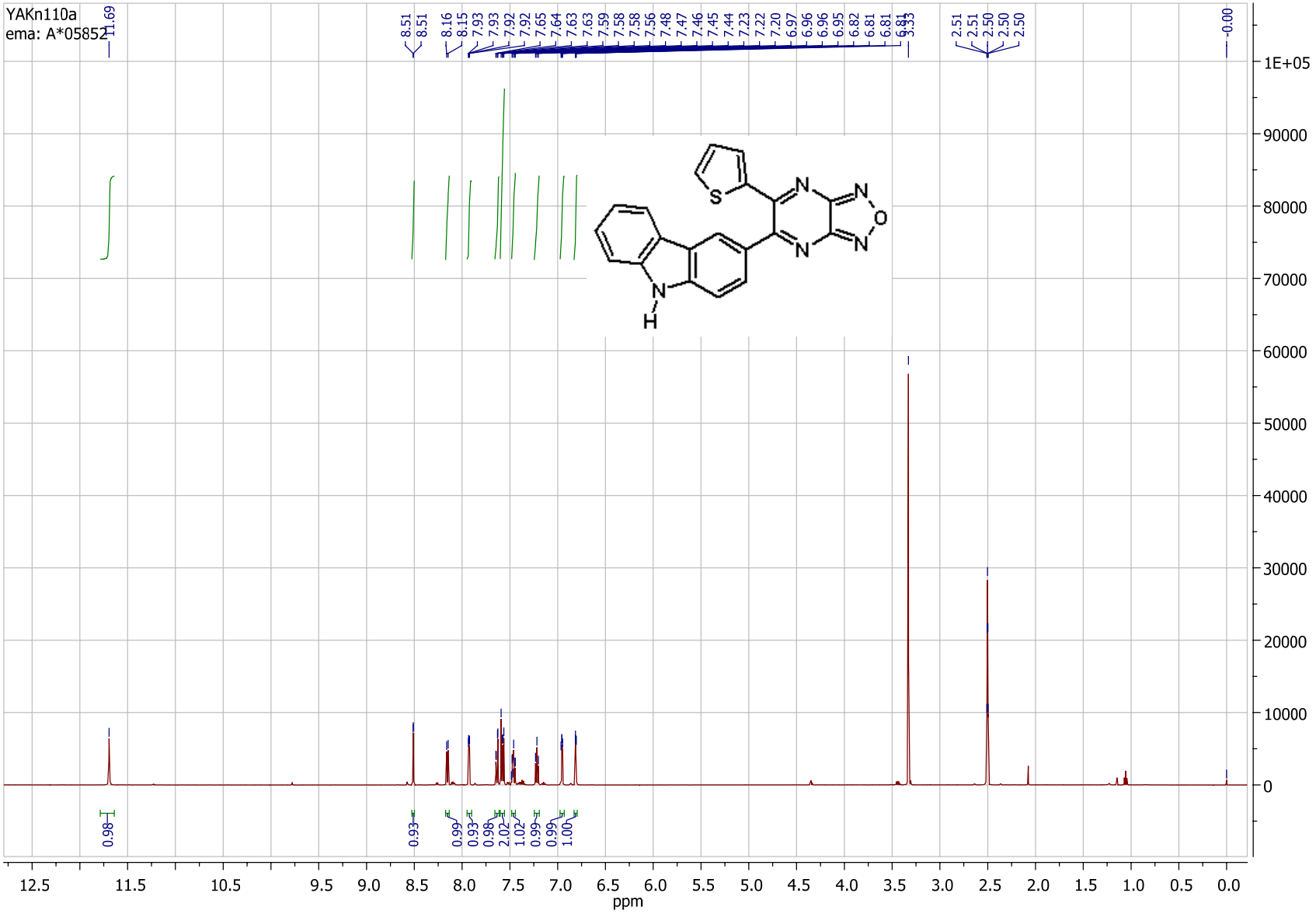
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **20b**.



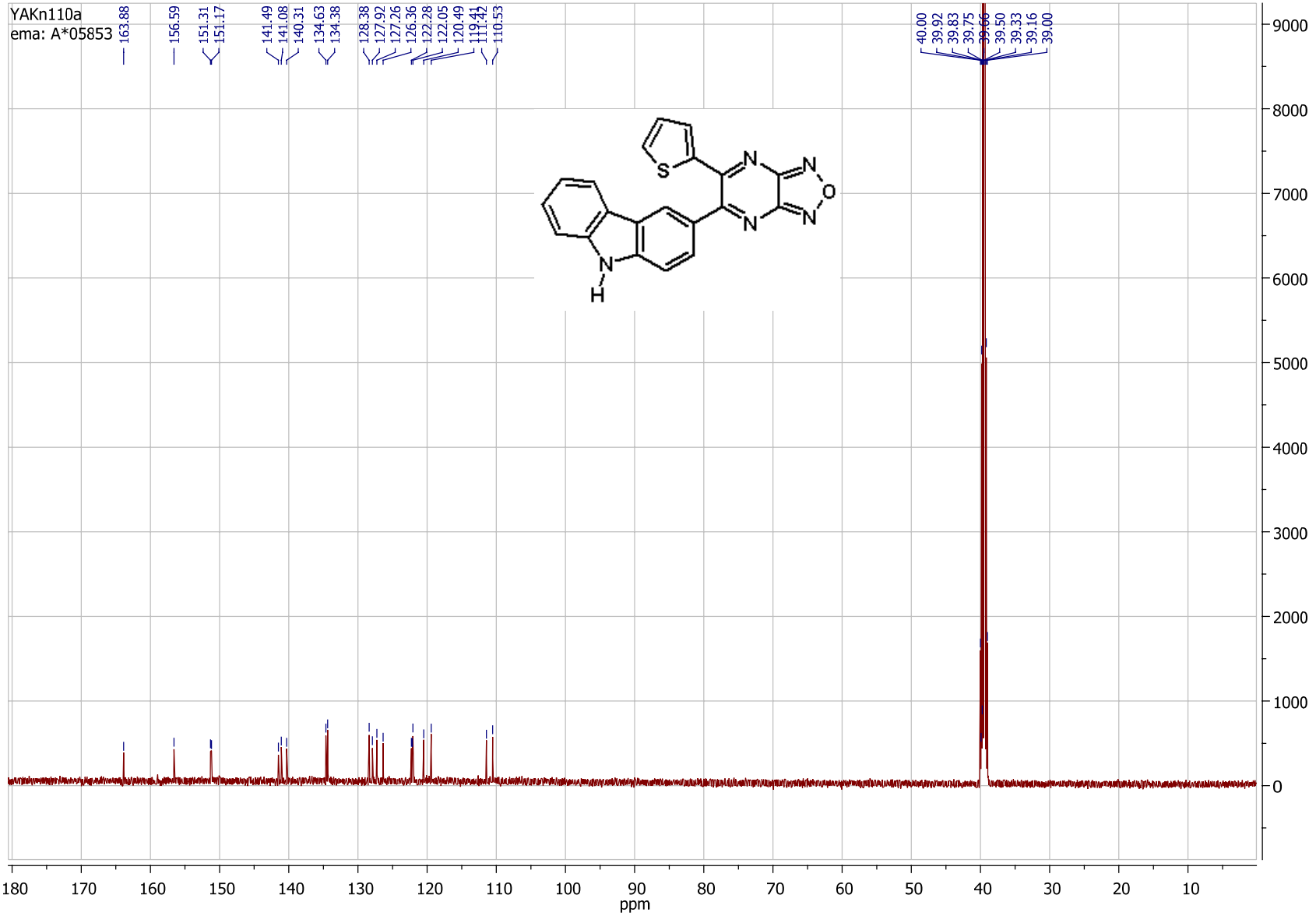
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **20c**.



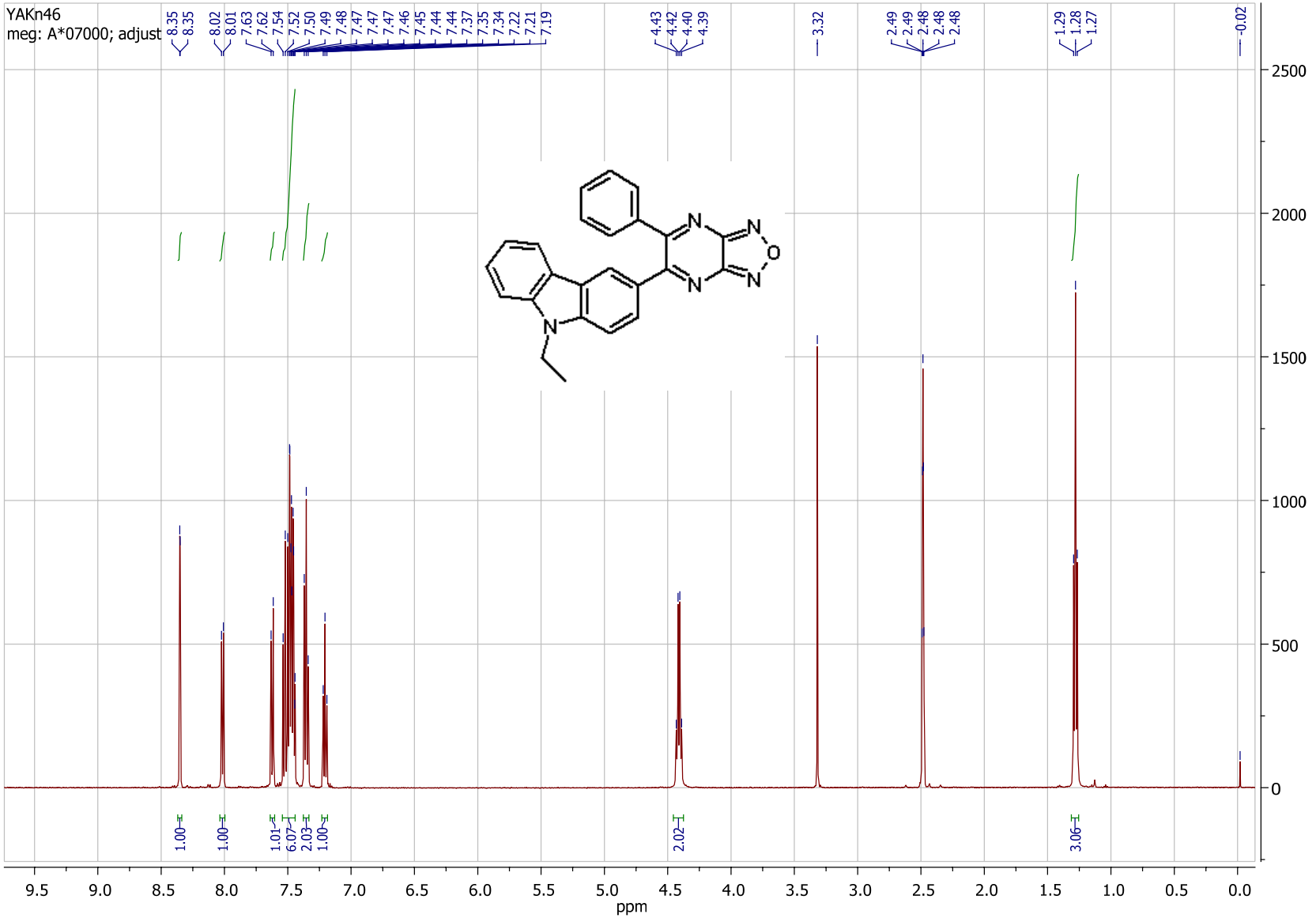
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **20c**.



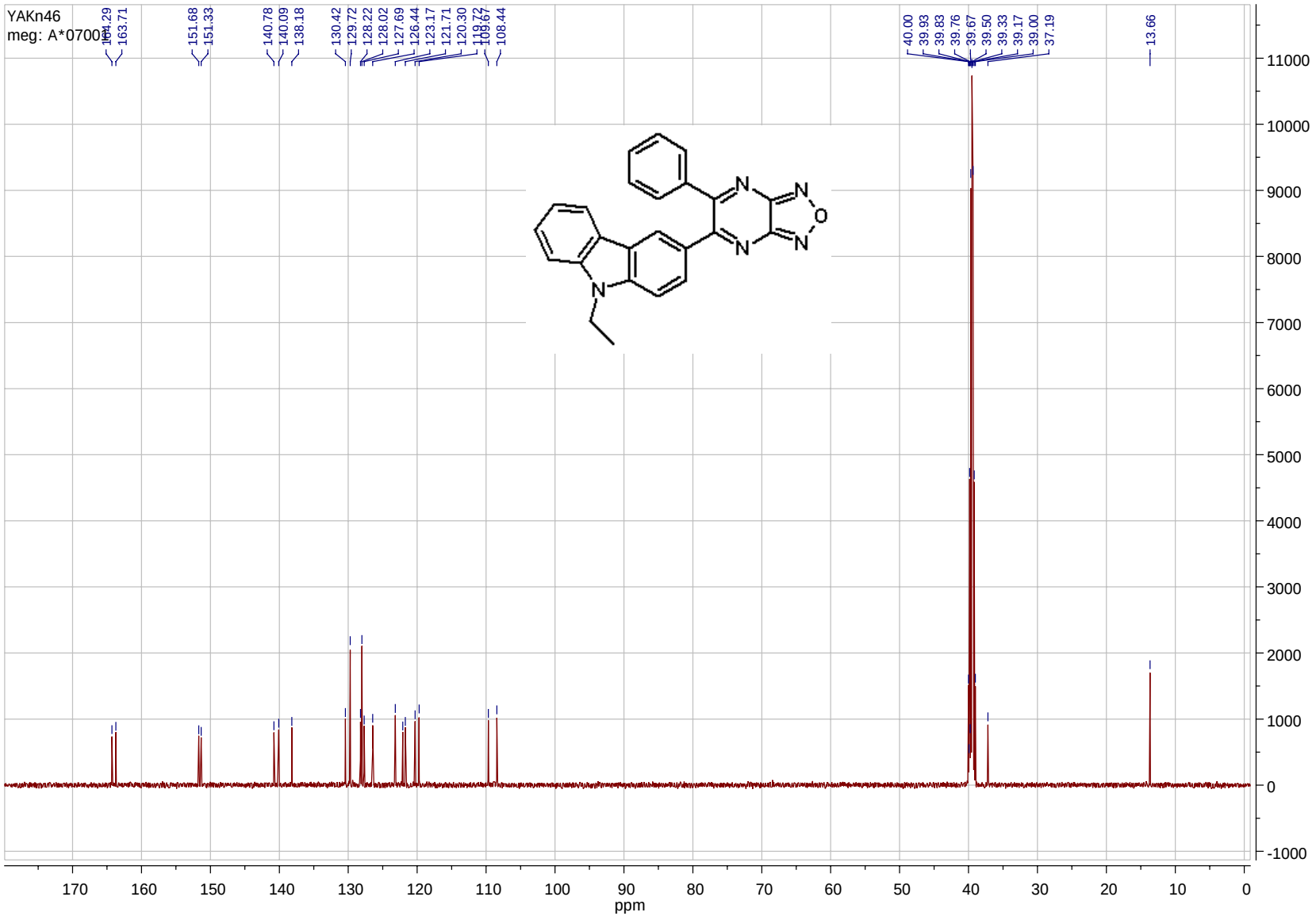
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **20d**.



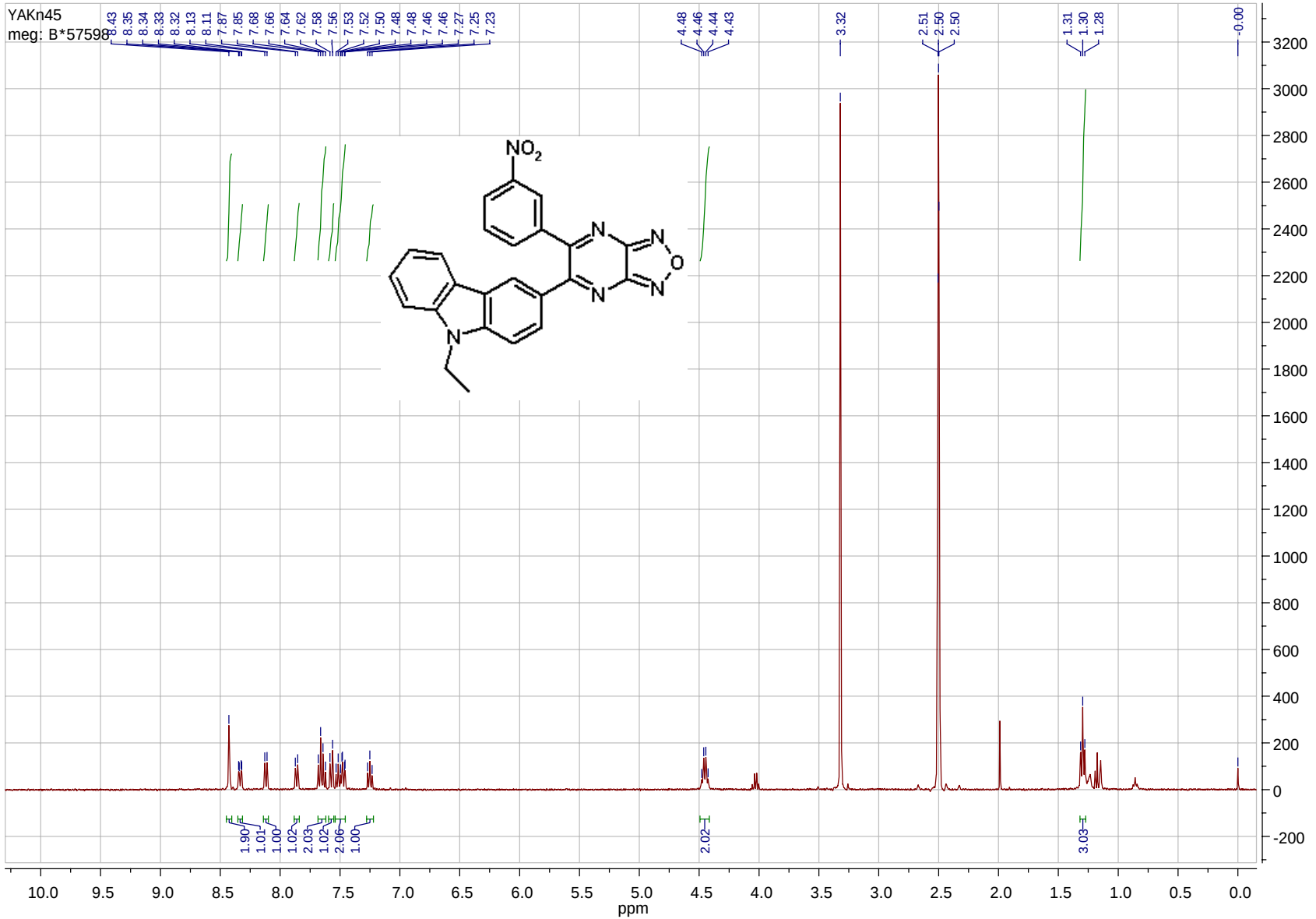
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **20d**.



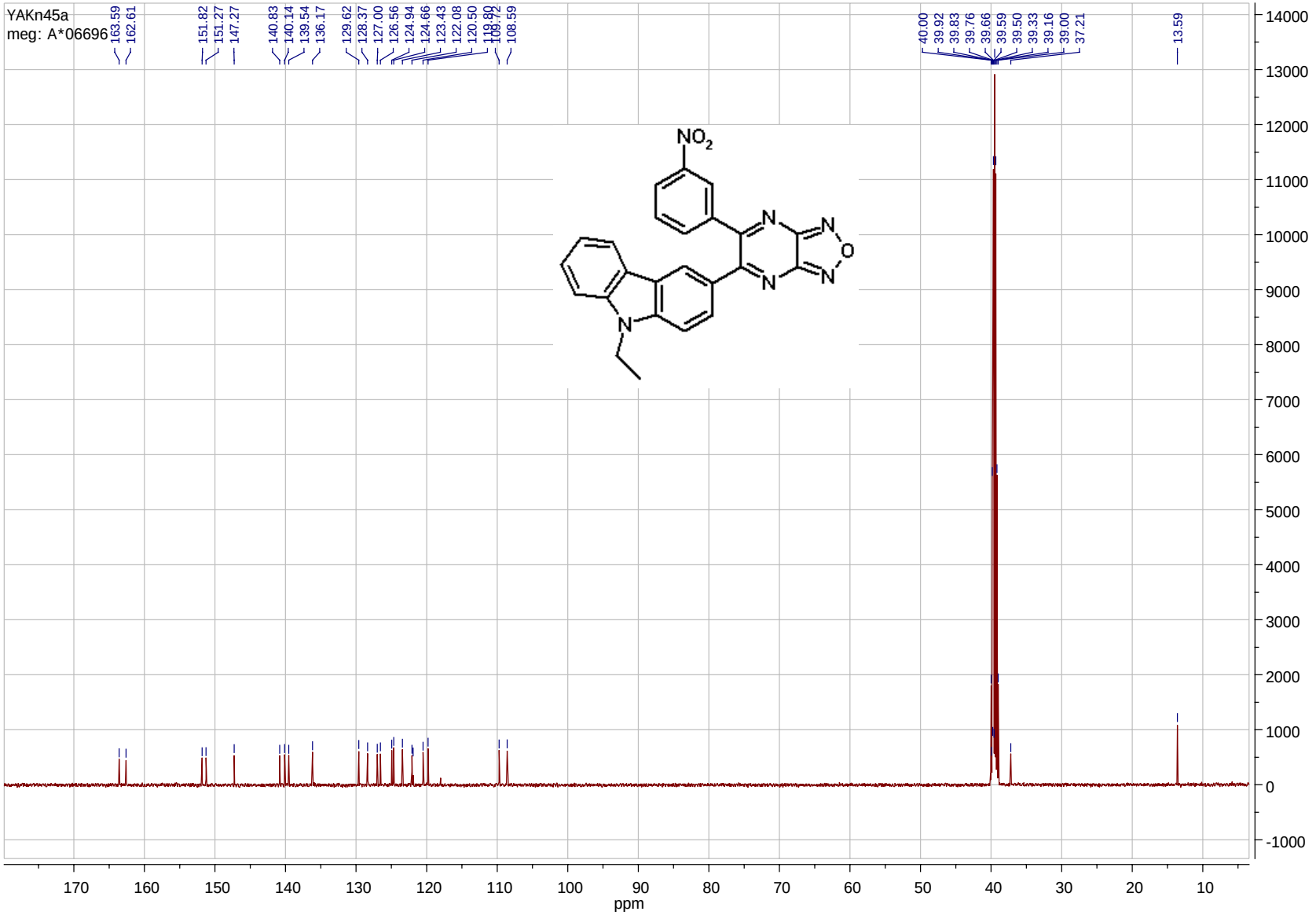
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **21a**.



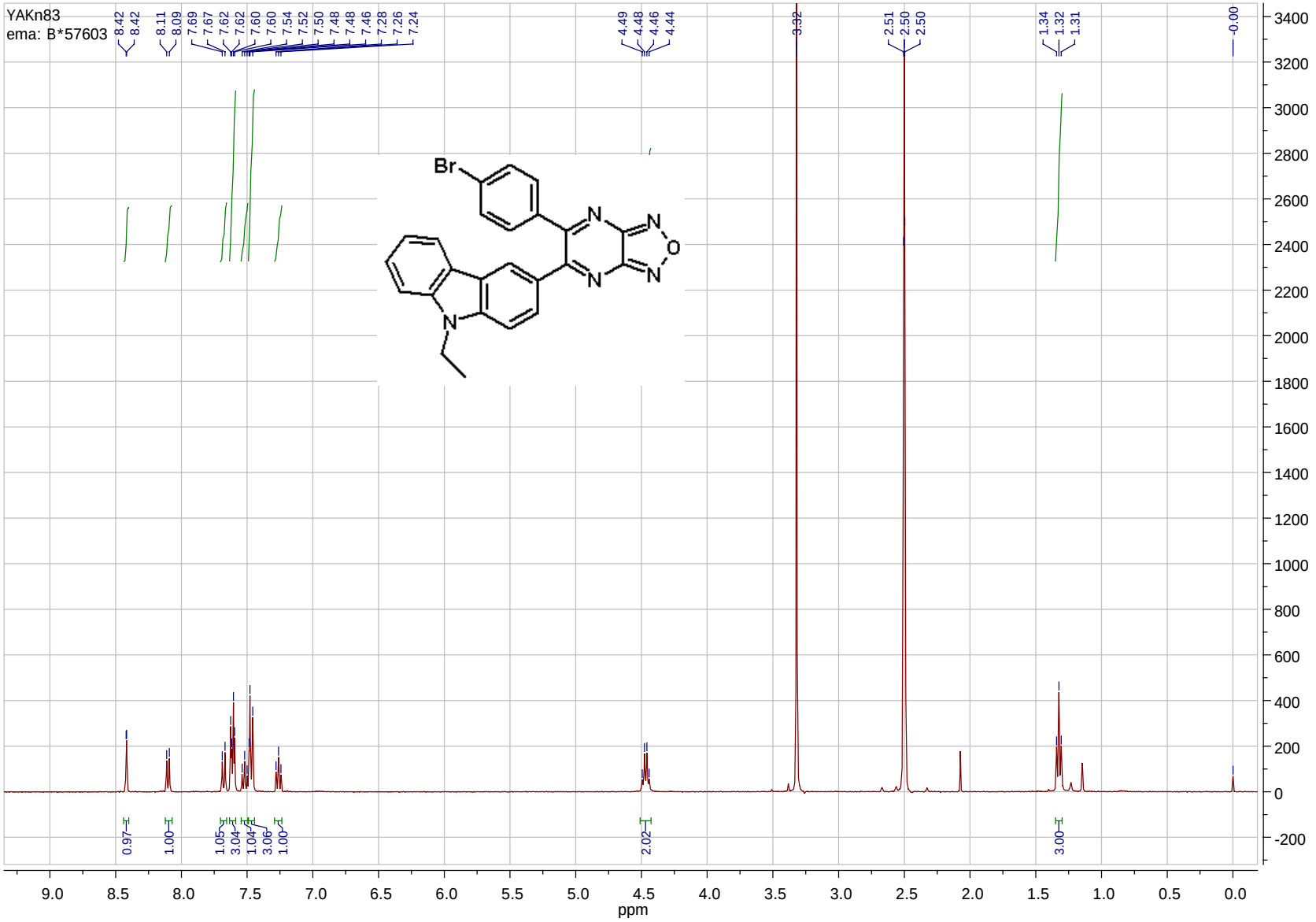
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **21a**.



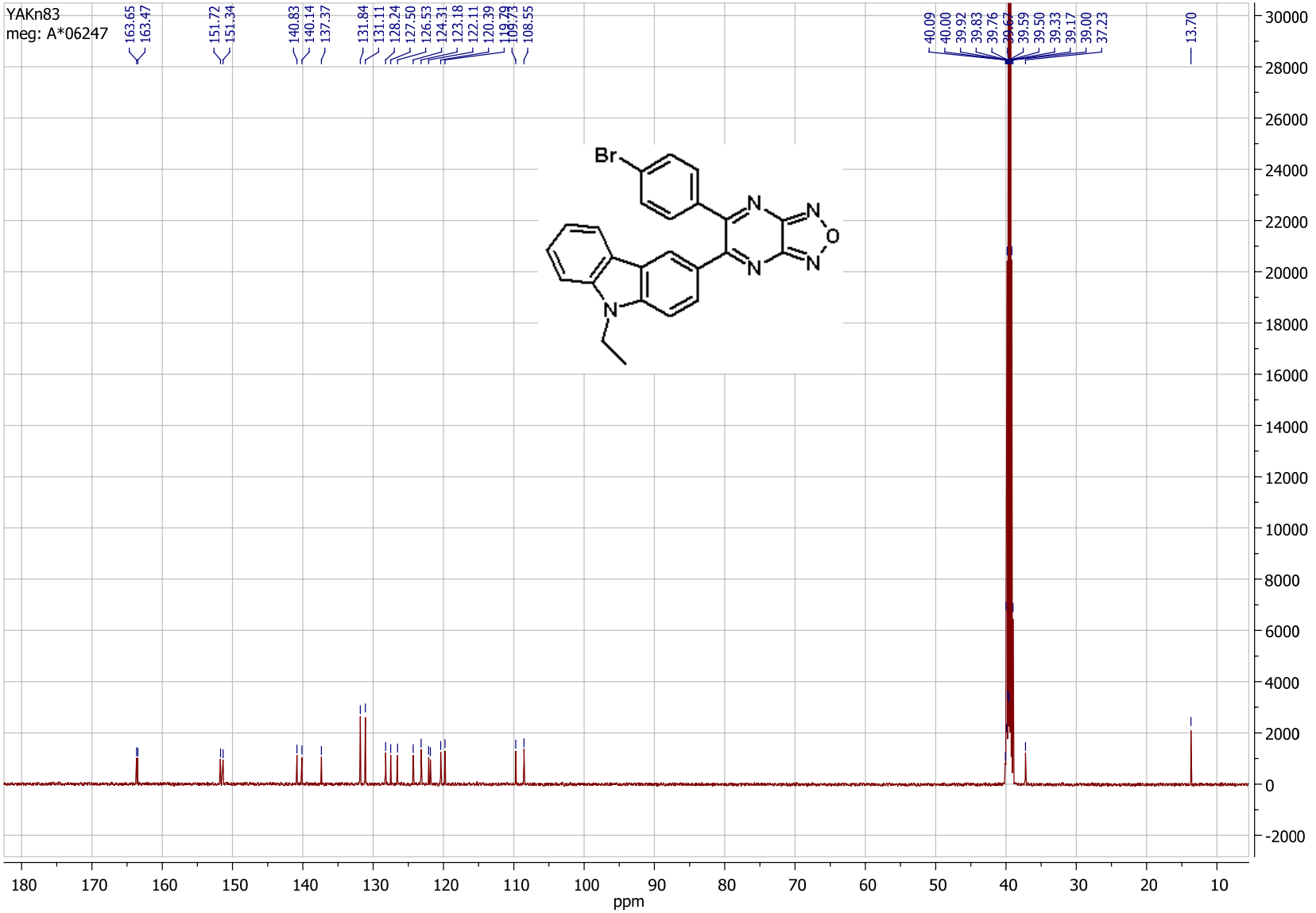
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **21b**.



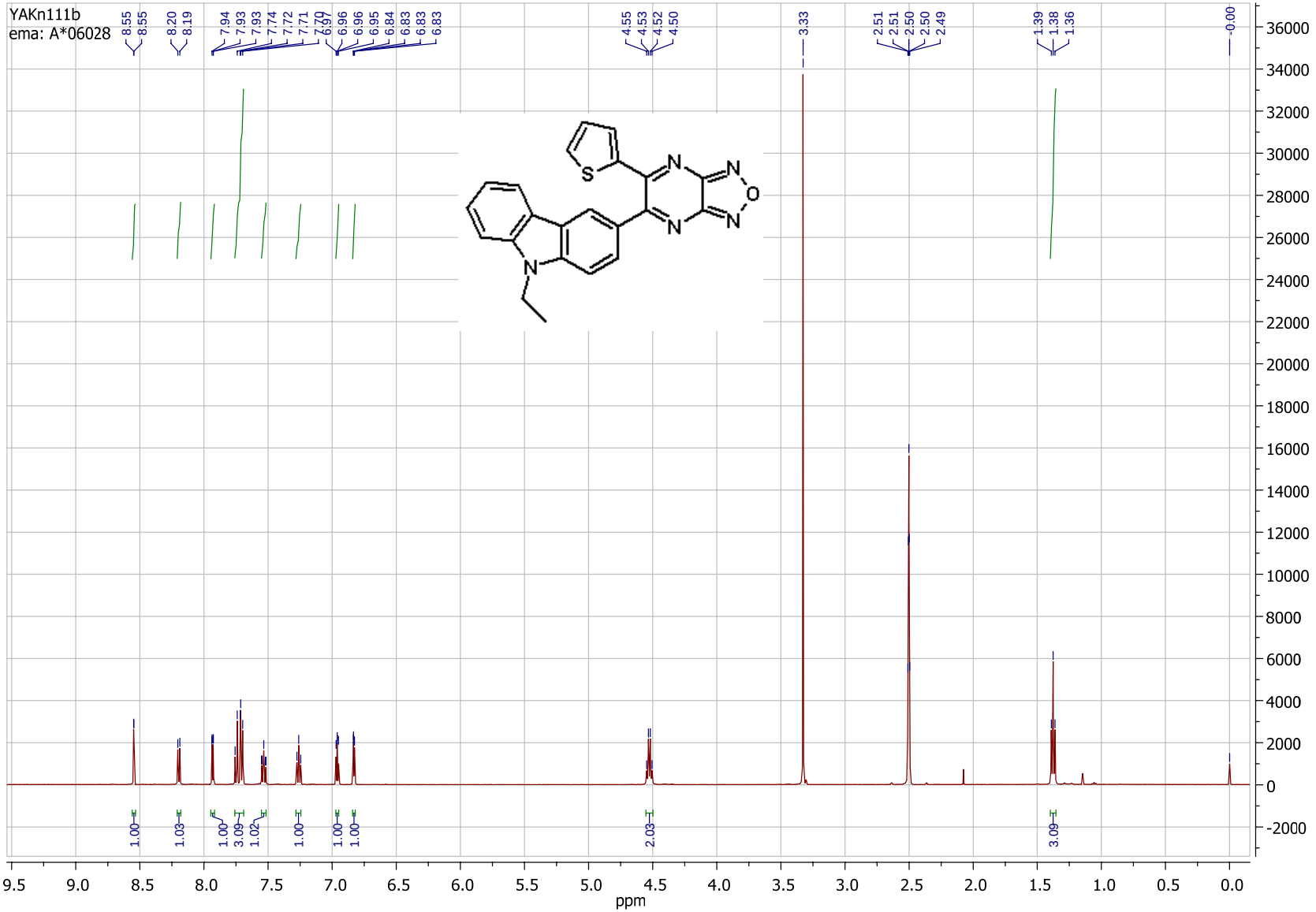
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **21b**.



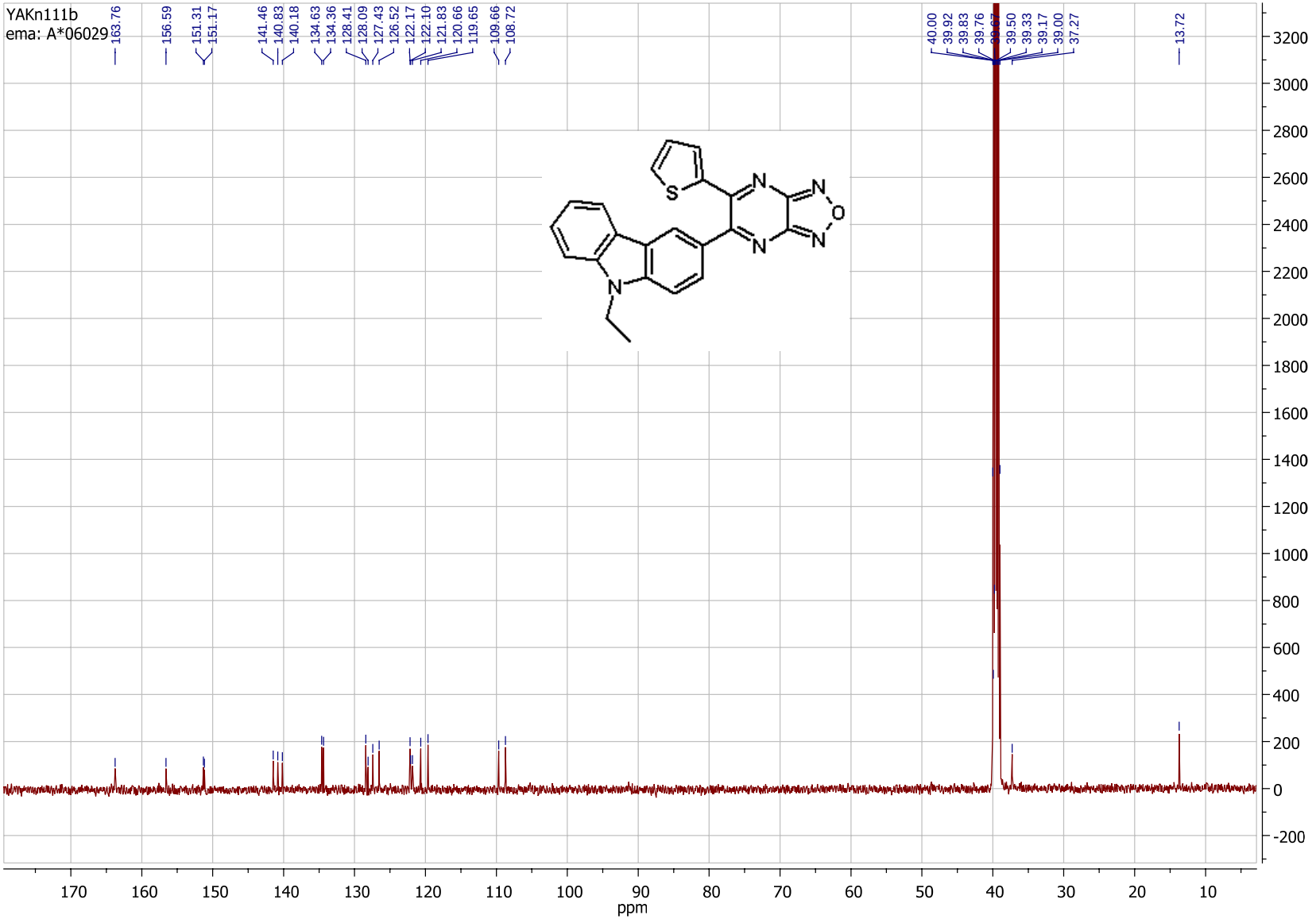
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **21c**.



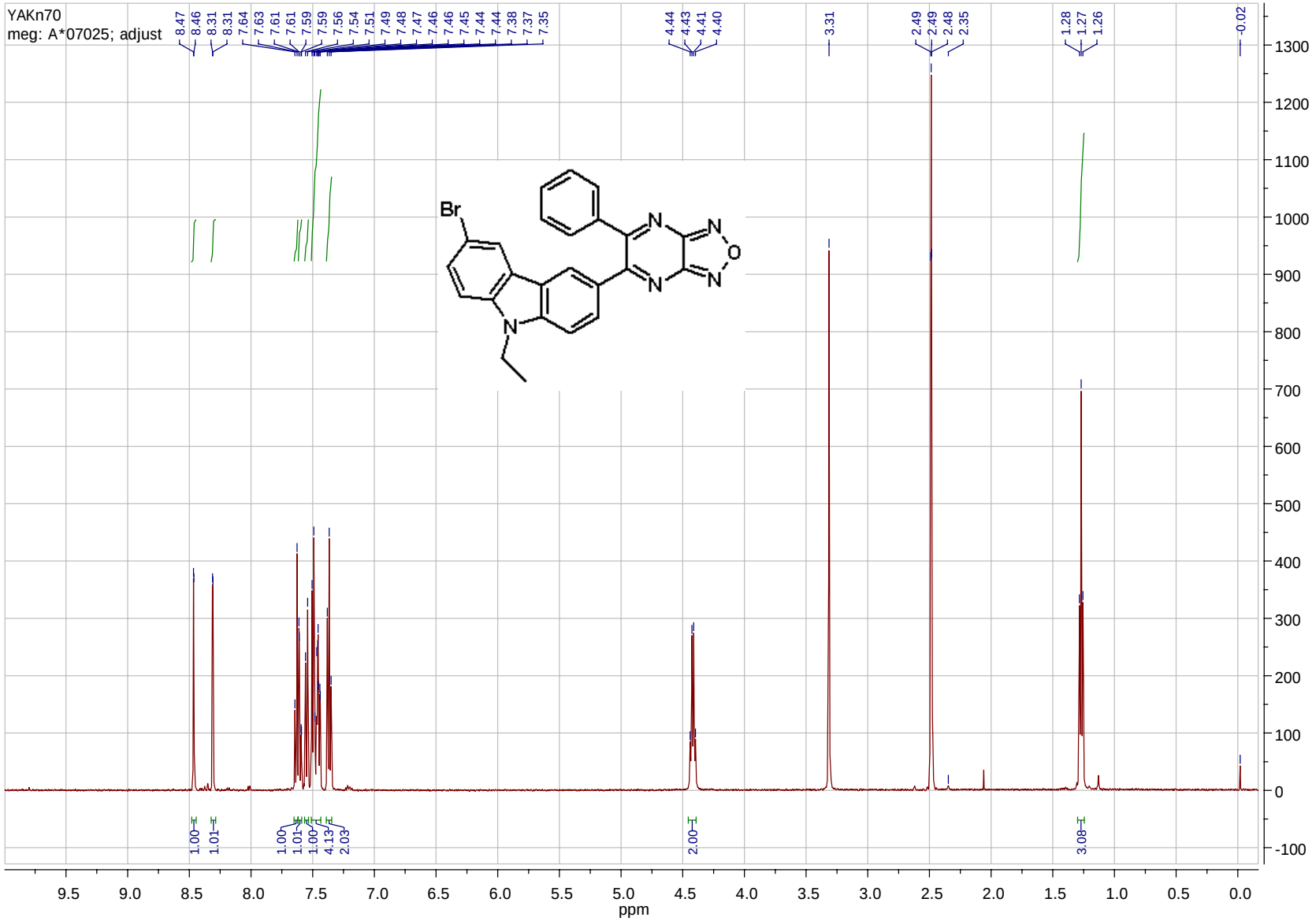
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **21c**.



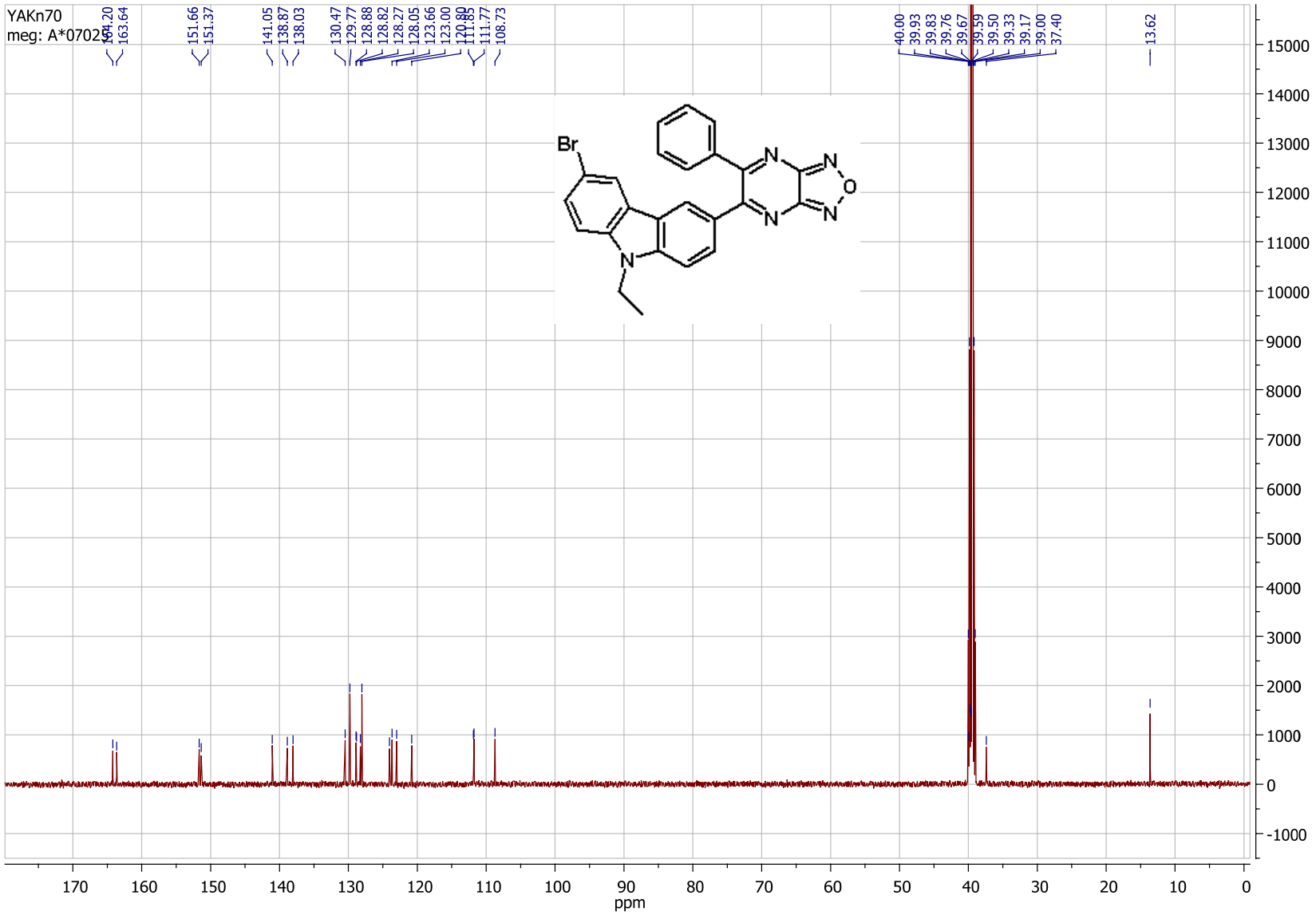
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **21d**.



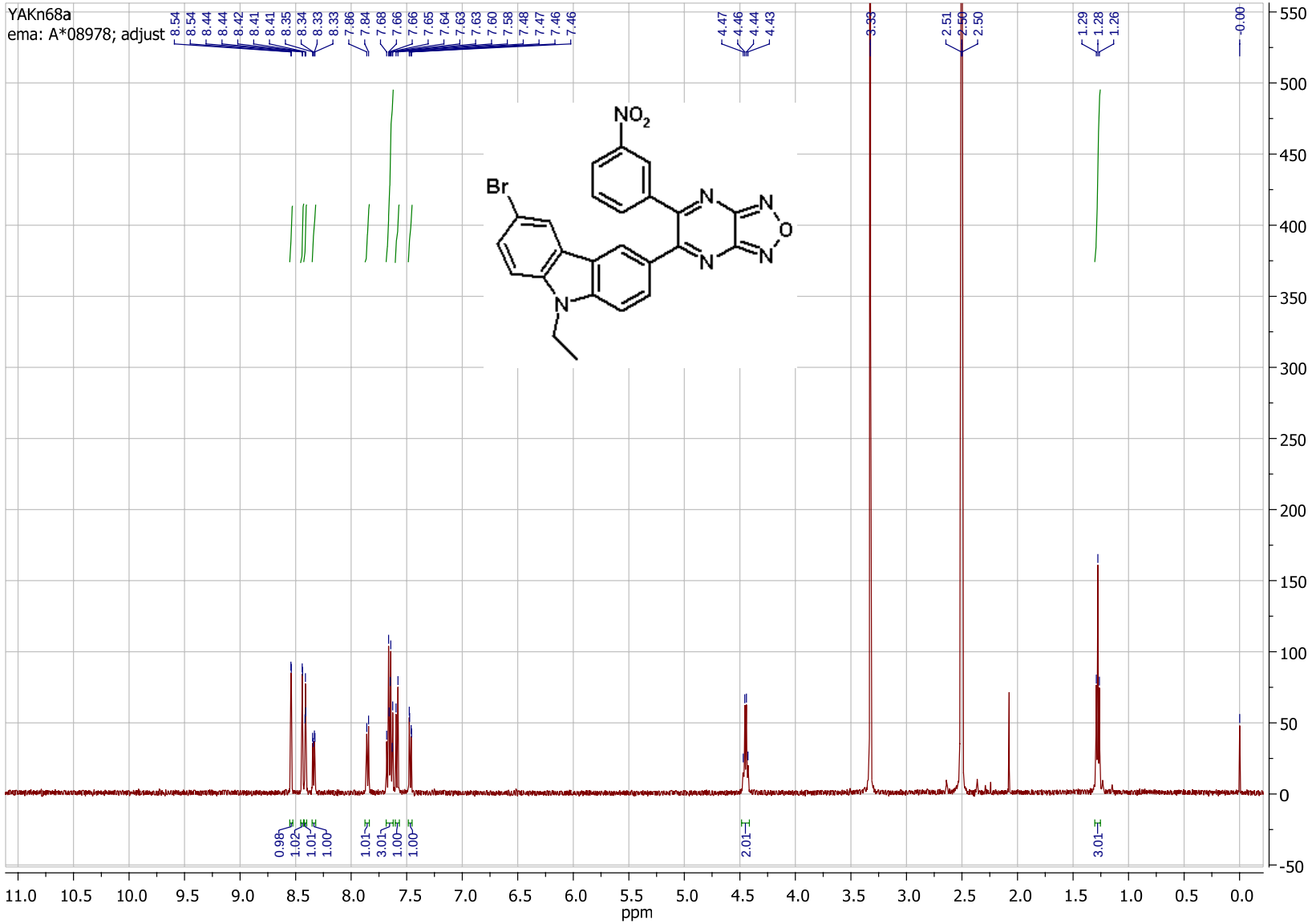
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **21d**.



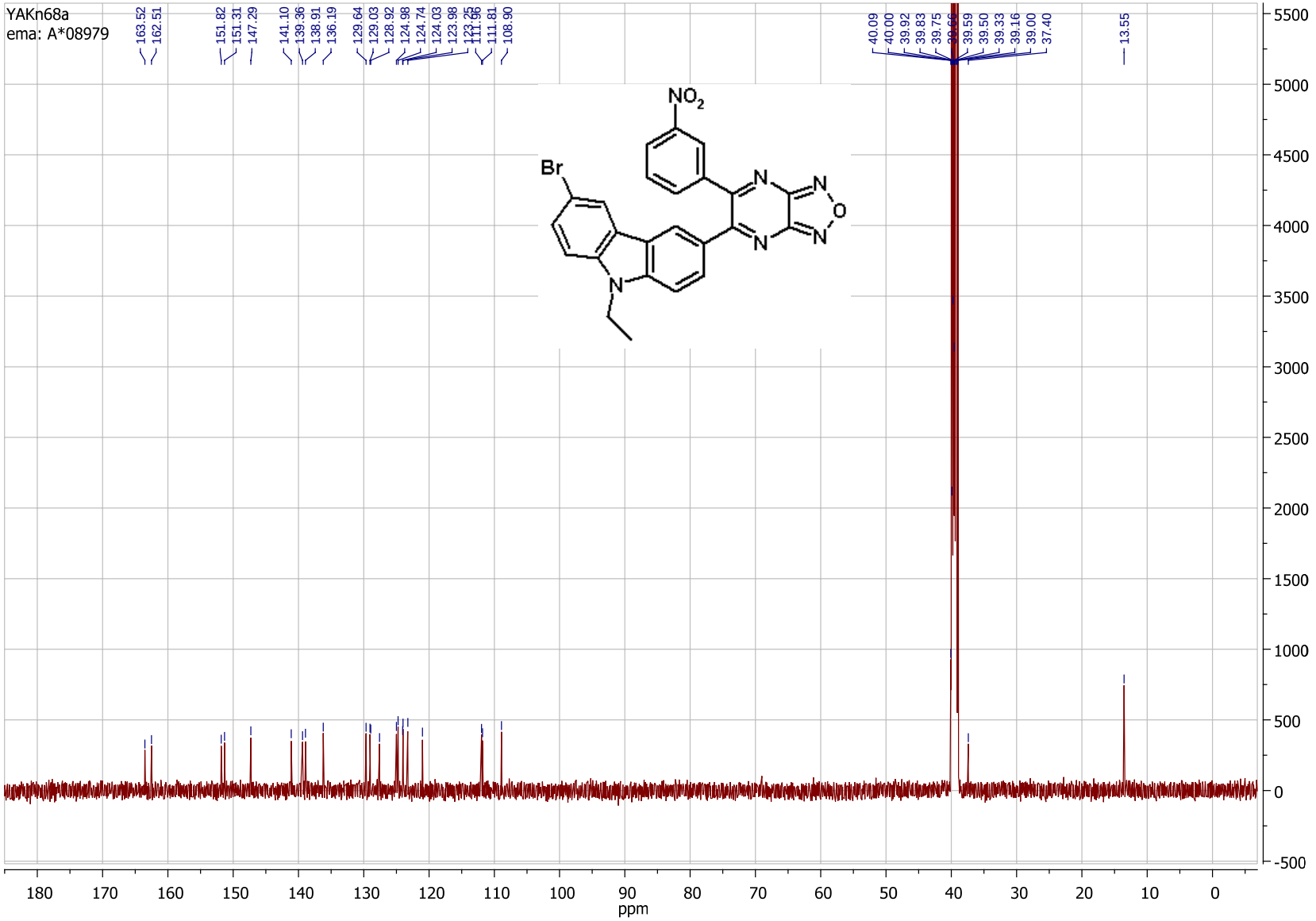
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **22a**.



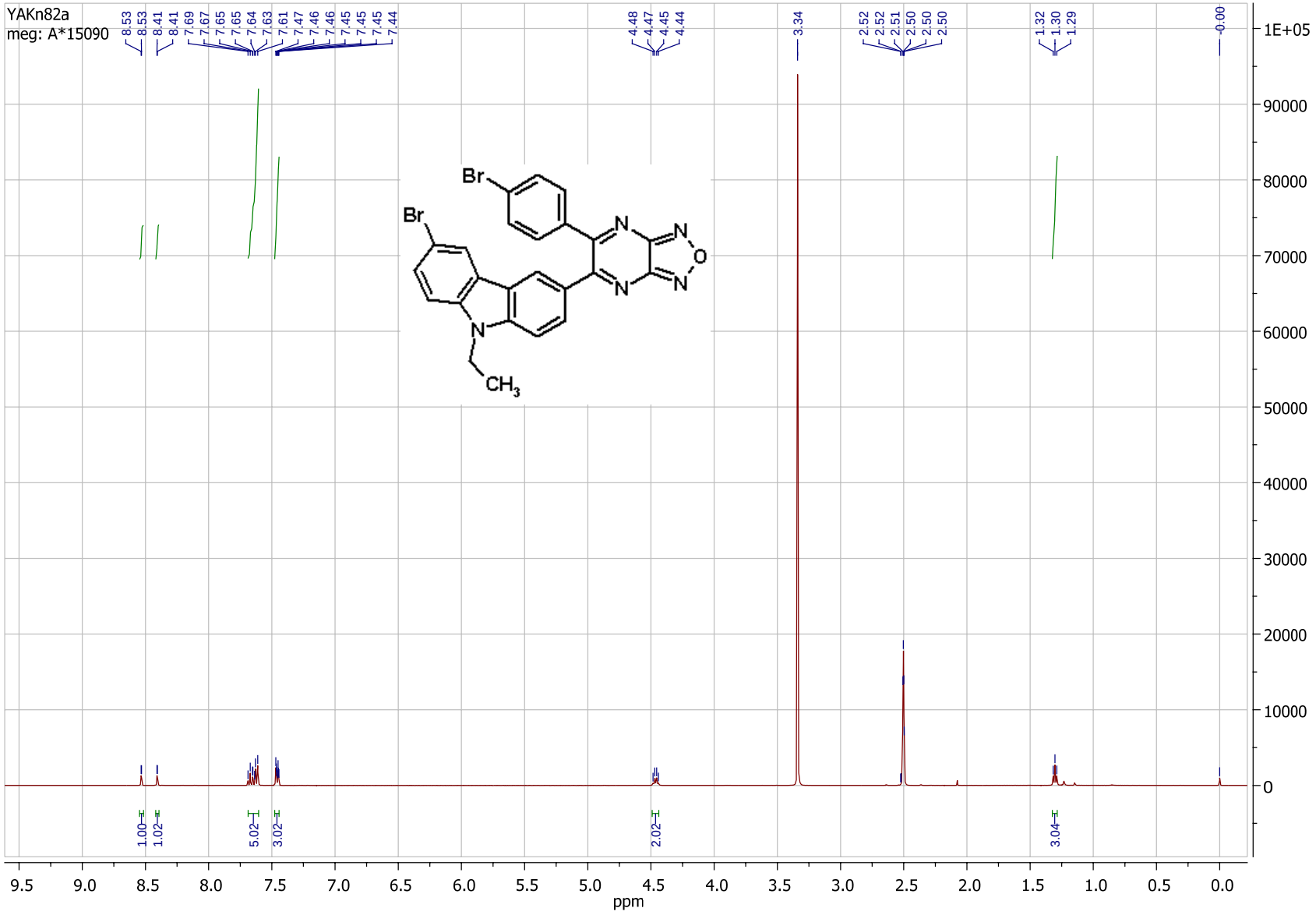
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **22a**.



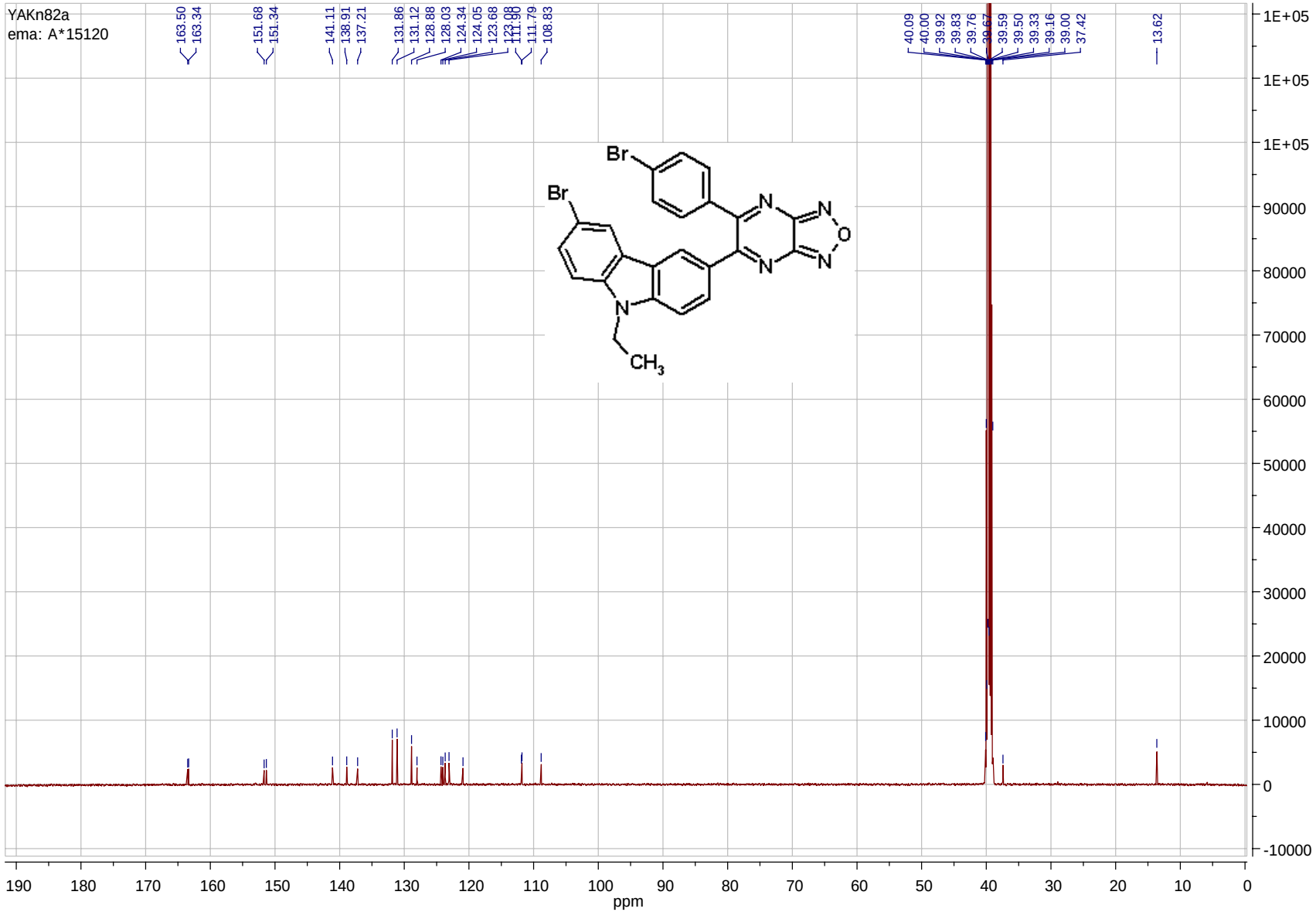
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **22b**.



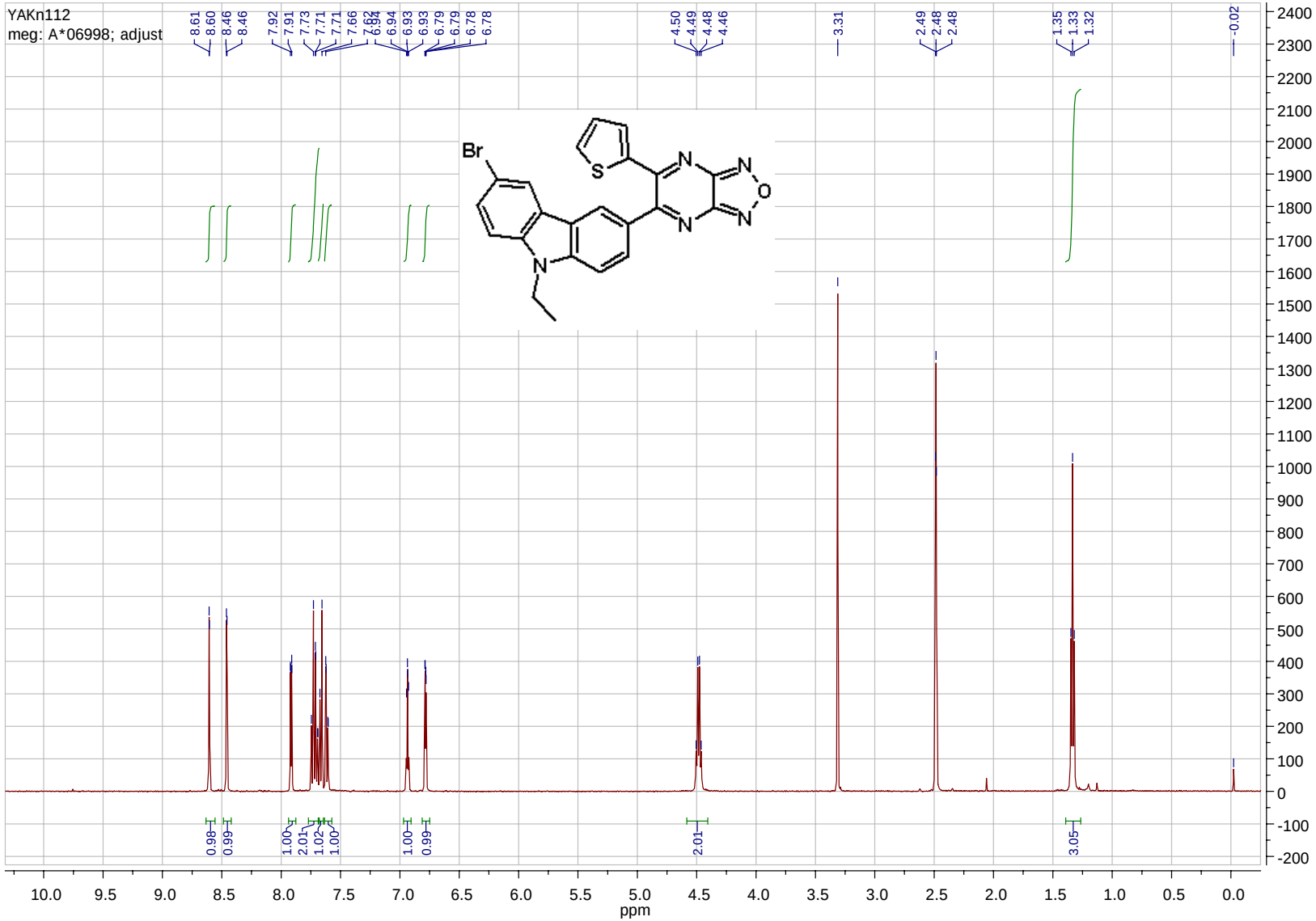
^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **22b**.



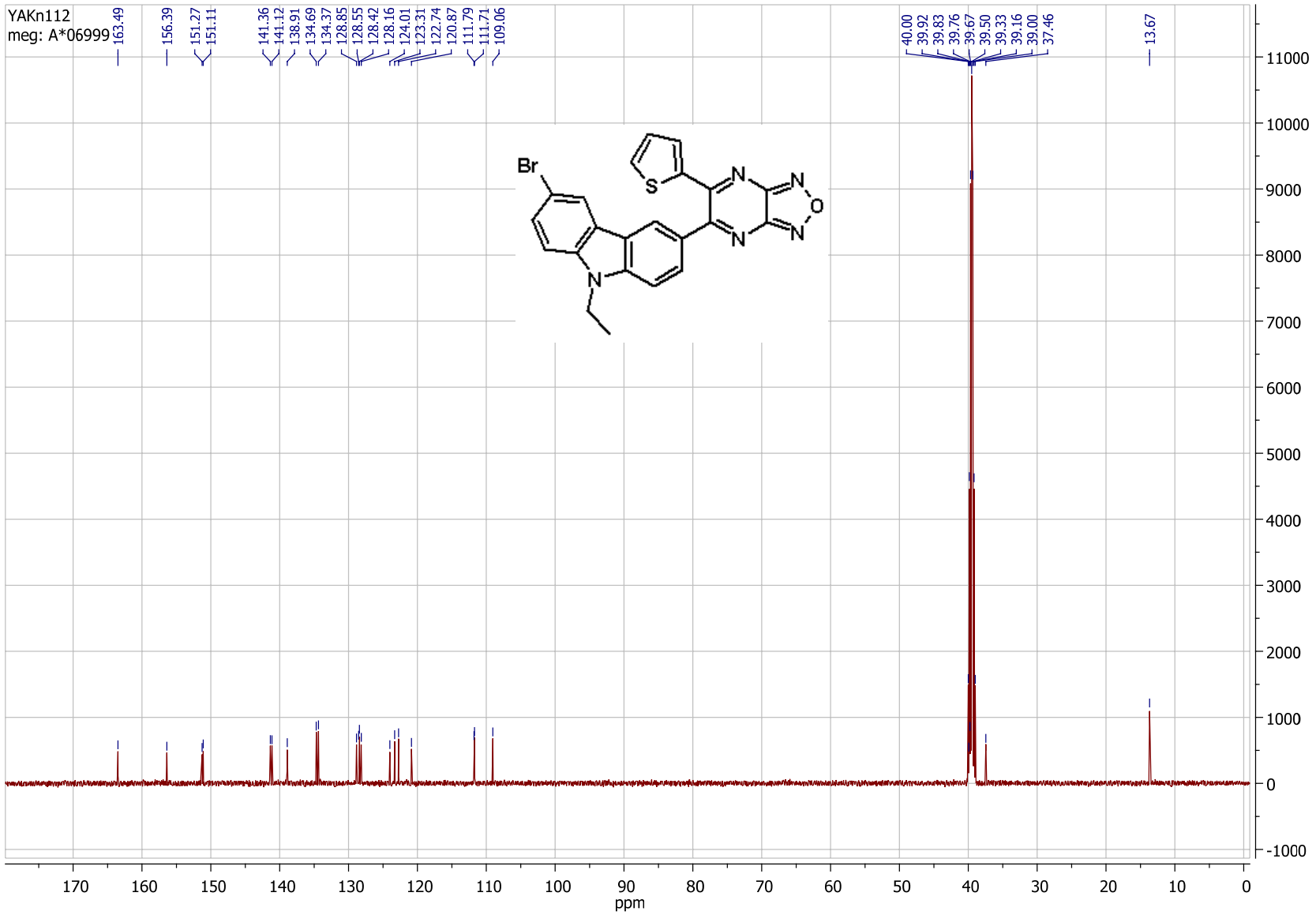
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **22c**.



^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **22c**.



^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **22d**.



^{13}C NMR (126 MHz, DMSO-d_6) spectrum of **22d**.