

Supplementary Information

Electrochemical study of fast blue BB. A green strategy for sulfination of fast blue BB

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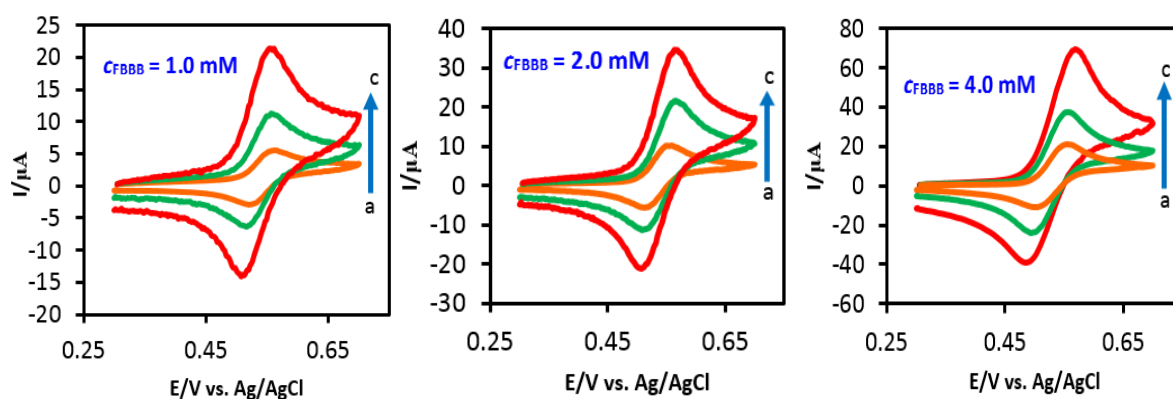
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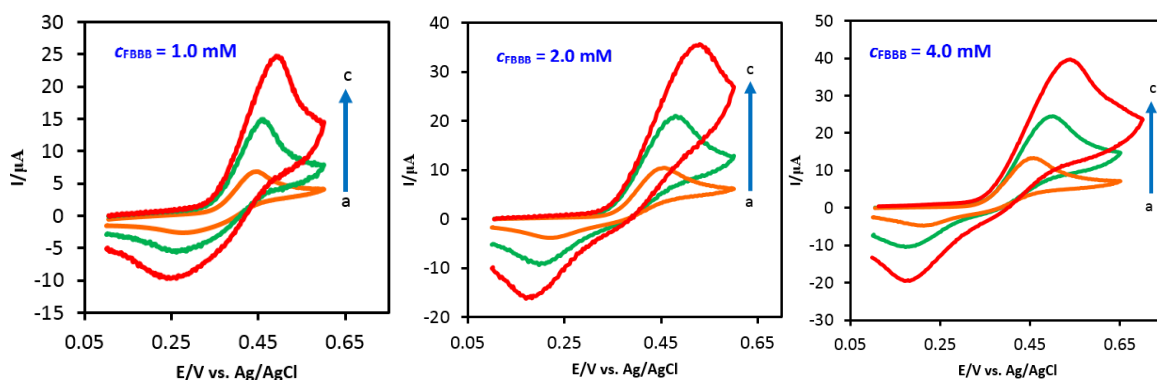
Table 1: ΔE obtained from cyclic voltammogram of 1 mM **FBBB**, in water (different pH values/ethanol mixture) (70/30, v/v). Scan rate: 10 mV/s. Temperature = 25 ± 1 °C.

pH	1.0	1.6	2.4	3.3	4.1	5.0	6.0	6.9	7.8	9.7	10.9
$\Delta E/V$	0.037	0.039	0.056	0.074	0.115	0.177	0.267	0.272	0.314	0.364	0.375

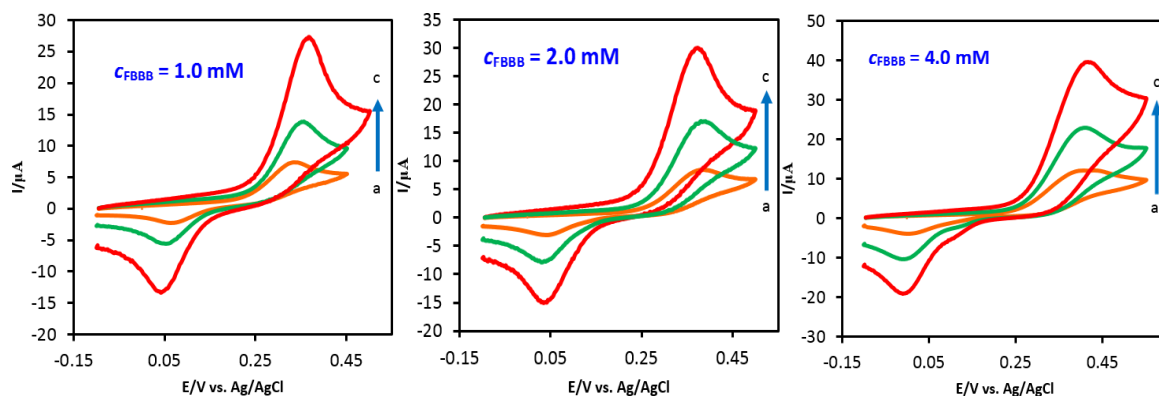
Effect of scan rate on cyclic voltammogram of **FBBB** in various pH values



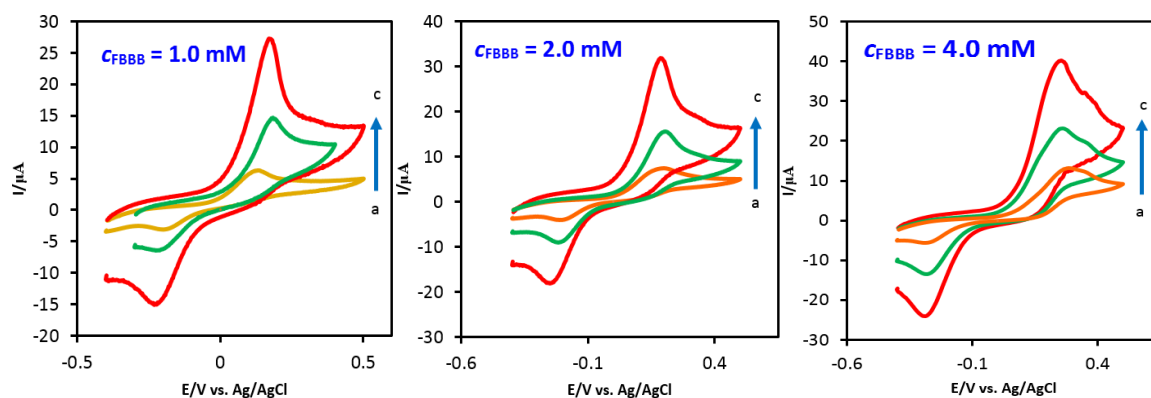
Cyclic voltammograms of different amounts of **FBBB** (1.0, 2.0 and 4.0 mM) in various scan rates at glassy carbon electrode, in water (perchloric acid, 0.1 M)/ethanol mixture (70/30, v/v). Scan rate: (a) 25 mV/s, (b) 100 mV/s and (c) 300 mV/s. Temperature = 25 ± 1 °C.



Cyclic voltammograms of different amounts of **FBBB** (1.0, 2.0 and 4.0 mM) in various scan rates at glassy carbon electrode, in acetate buffer ($c = 0.2$ M, $\text{pH} = 4.0$) /ethanol mixture (70/30, v/v). Scan rate: (a) 25 mV/s, (b) 100 mV/s and (c) 300 mV/s. Temperature = 25 ± 1 °C.

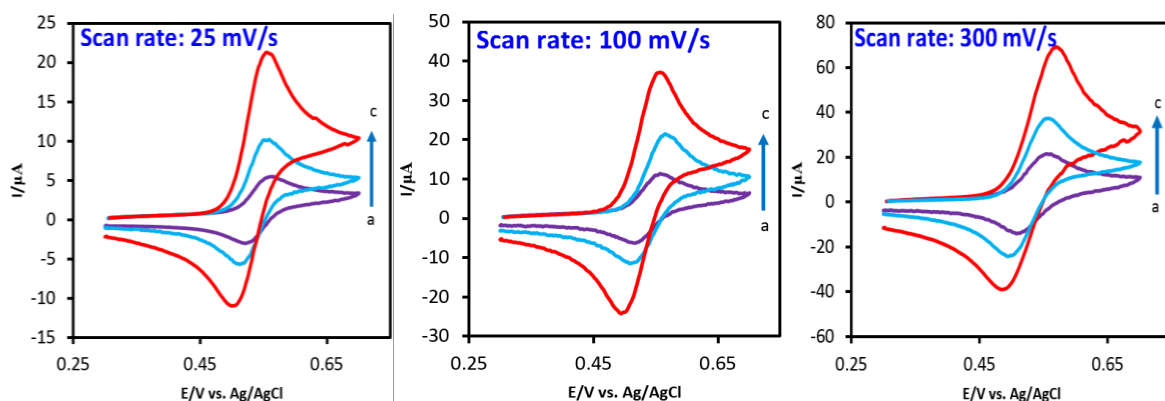


Cyclic voltammograms of different amounts of **FBBB** (1.0, 2.0 and 4.0 mM) in various scan rates at glassy carbon electrode, in water (phosphate buffer, $c = 0.2$ M, $\text{pH} = 7.0$)/ethanol mixture (70/30, v/v). Scan rate: (a) 25 mV/s, (b) 100 mV/s and (c) 300 mV/s. Temperature = 25 ± 1 °C.

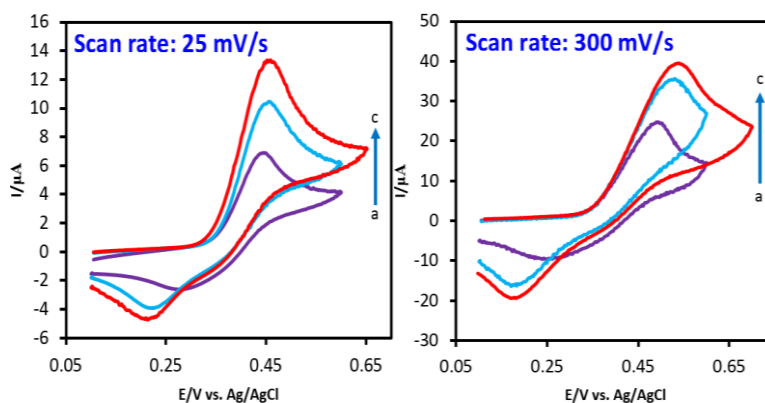


Cyclic voltammograms of different amounts of **FBBB** (1.0, 2.0 and 4.0 mM) in various scan rates at glassy carbon electrode, in water (carbonate buffer, $c=0.2$, $\text{pH}=11$)/ethanol mixture (70/30, v/v). Scan rate: (a) 25 mV/s, (b) 100 mV/s and (c) 300 mV/s. Temperature = 25 ± 1 °C.

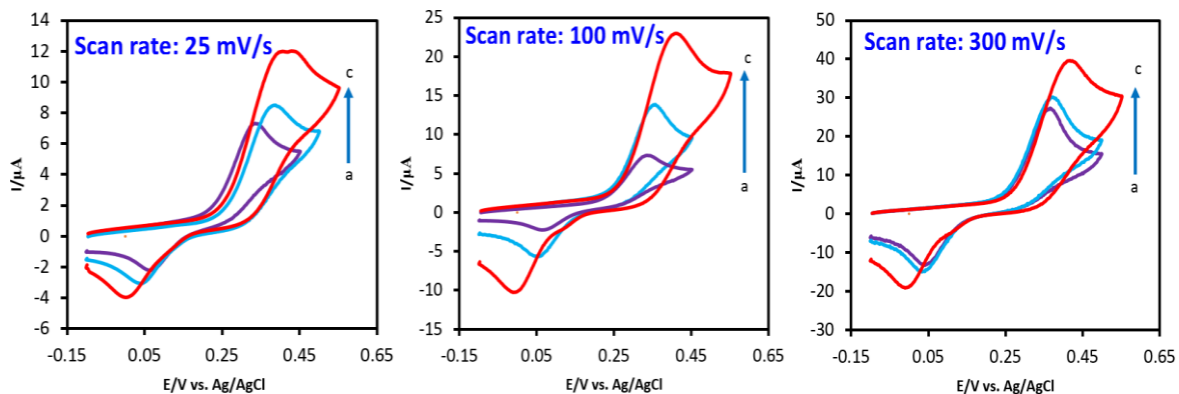
Effect of **FBBB** concentration on cyclic voltammograms in various pH values



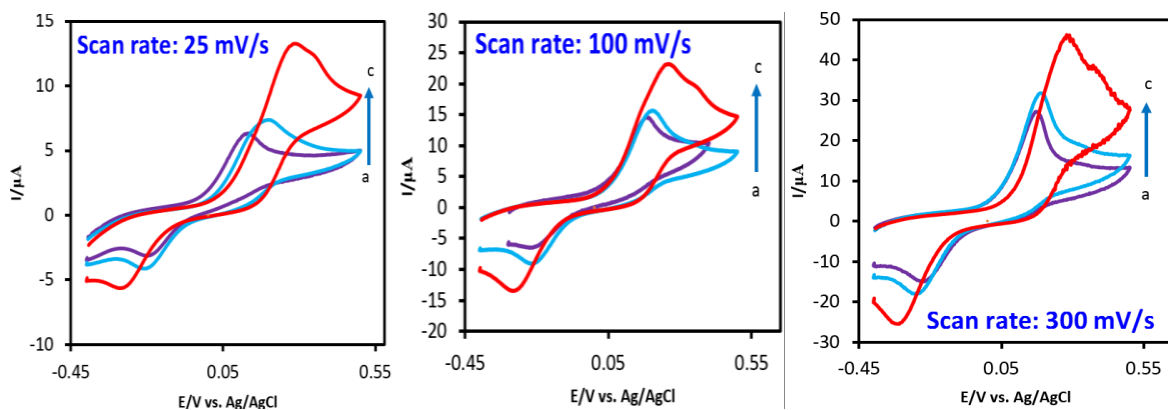
Cyclic voltammograms of **FBBB** in various concentrations at glassy carbon electrode, in water (perchloric acid, 0.1 M)/ethanol mixture (70/30, v/v). **FBBB** concentration: (a) 1 mM, (b) 2 mM and (c) 3 mM. Temperature = 25 ± 1 °C.



Cyclic voltammograms of **FBBB** in various concentrations at glassy carbon electrode, in acetate buffer ($c = 0.2$ M, pH = 4.0)/ethanol mixture (70/30, v/v). **FBBB** concentration: (a) 1 mM, (b) 2 mM and (c) 3 mM. Temperature = 25 ± 1 °C.



Cyclic voltammograms of **FBBB** in various concentrations at glassy carbon electrode in water (phosphate buffer, $c = 0.2$ M, $\text{pH} = 7.0$)/ethanol mixture (70/30, v/v). **FBBB** concentration: (a) 1 mM, (b) 2 mM and (c) 3 mM. Temperature = 25 ± 1 °C.



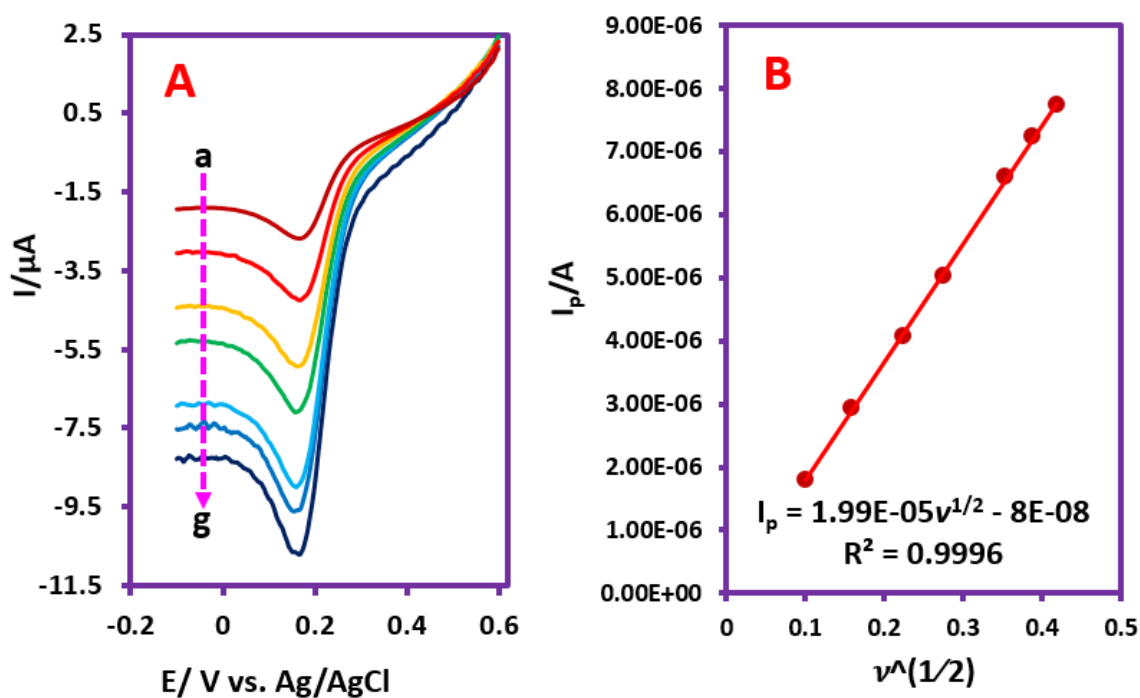
Cyclic voltammograms of **FBBB** in various concentrations at glassy carbon electrode in water (carbonate buffer, $c = 0.2$, $\text{pH} = 11$)/ethanol mixture (70/30, v/v). **FBBB** concentration: (a) 1 mM, (b) 2 mM and (c) 3 mM. Temperature = 25 ± 1 °C.

The diffusion coefficient of **FBBB** was calculated using randles-sevcik equation:

$$i_p = (2.69 \times 10^5) n^{\frac{3}{2}} A D_0^{\frac{1}{2}} C_{ox}^* v^{\frac{1}{2}}$$

$$i_p = k v^{\frac{1}{2}}$$

To reach this goal, the linear sweep voltammograms of a solution containing 32 mg (1 mM) $K_3[Fe(CN)_6]$ in 0.5 M of KCl were recorded at several scan rates and then I_p vs. $v^{\frac{1}{2}}$ was plotted.



A) Linear sweep voltammograms of 1 mM $K_3[Fe(CN)_6]$ in KCl (0.5 M), in various scan rate at glassy carbon electrode. Scan rate from a to g: 10, 25, 50, 75, 125, 150 and 175 mV/s. B) The plot of I vs. $v^{1/2}$. Temperature = 25 ± 1 °C.

The slope (k) of the line is equal to: 1.99×10^{-5}

$$\text{Slope} = (2.69 \times 10^5) n^{\frac{3}{2}} A D_0^{\frac{1}{2}} C_{ox}^* = 1.99 \times 10^{-5}$$

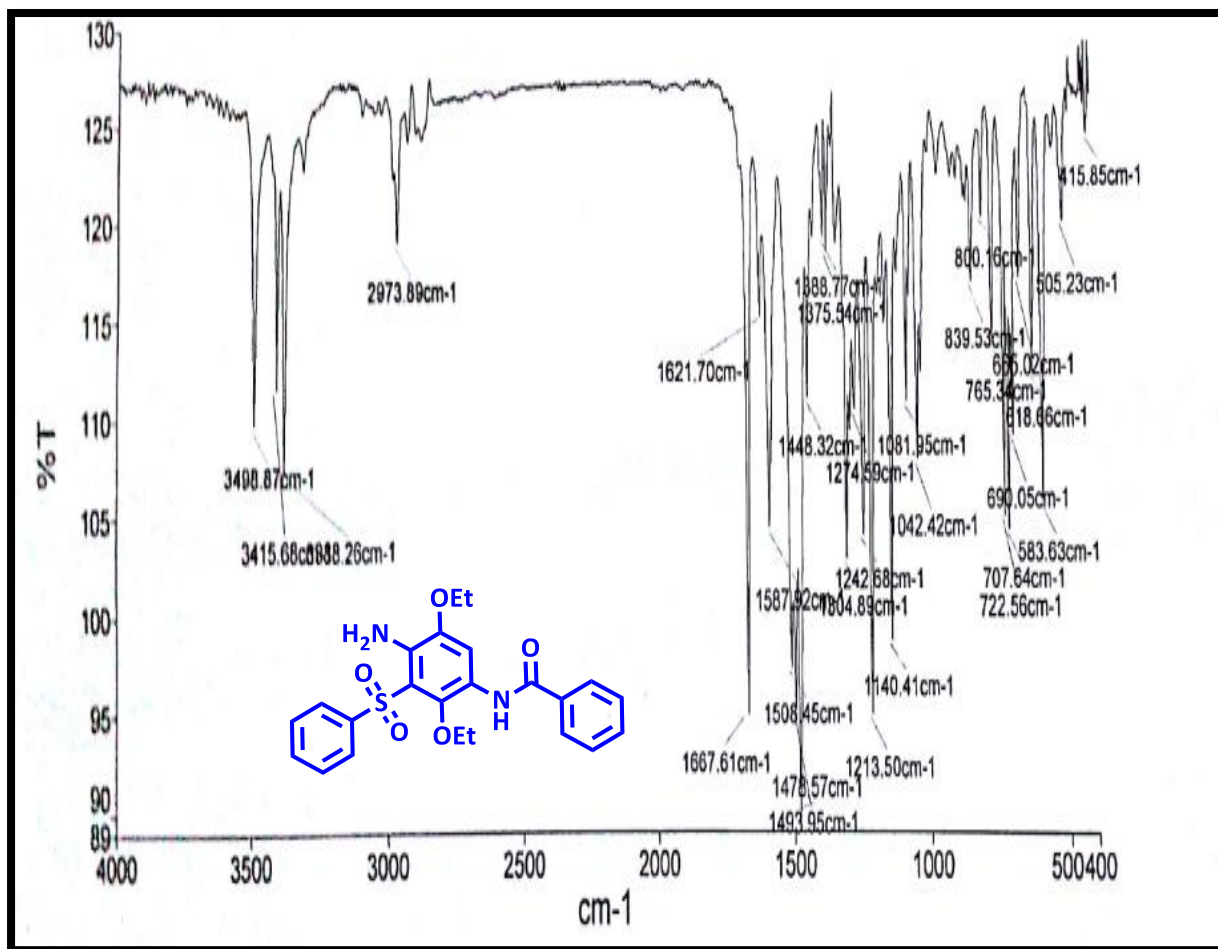
In randles-sevcik equation, D is the diffusion coefficient (7.6×10^{-6}), n is the number of the electron, A is the electroactive surface and C_{ox}^* is the $K_3[Fe(CN)_6]$ concentration.

$$1.99 \times 10^{-5} = (2.69 \times 10^5) (1)^{\frac{3}{2}} A (7.6 \times 10^{-6})^{\frac{1}{2}} (10^{-6})$$

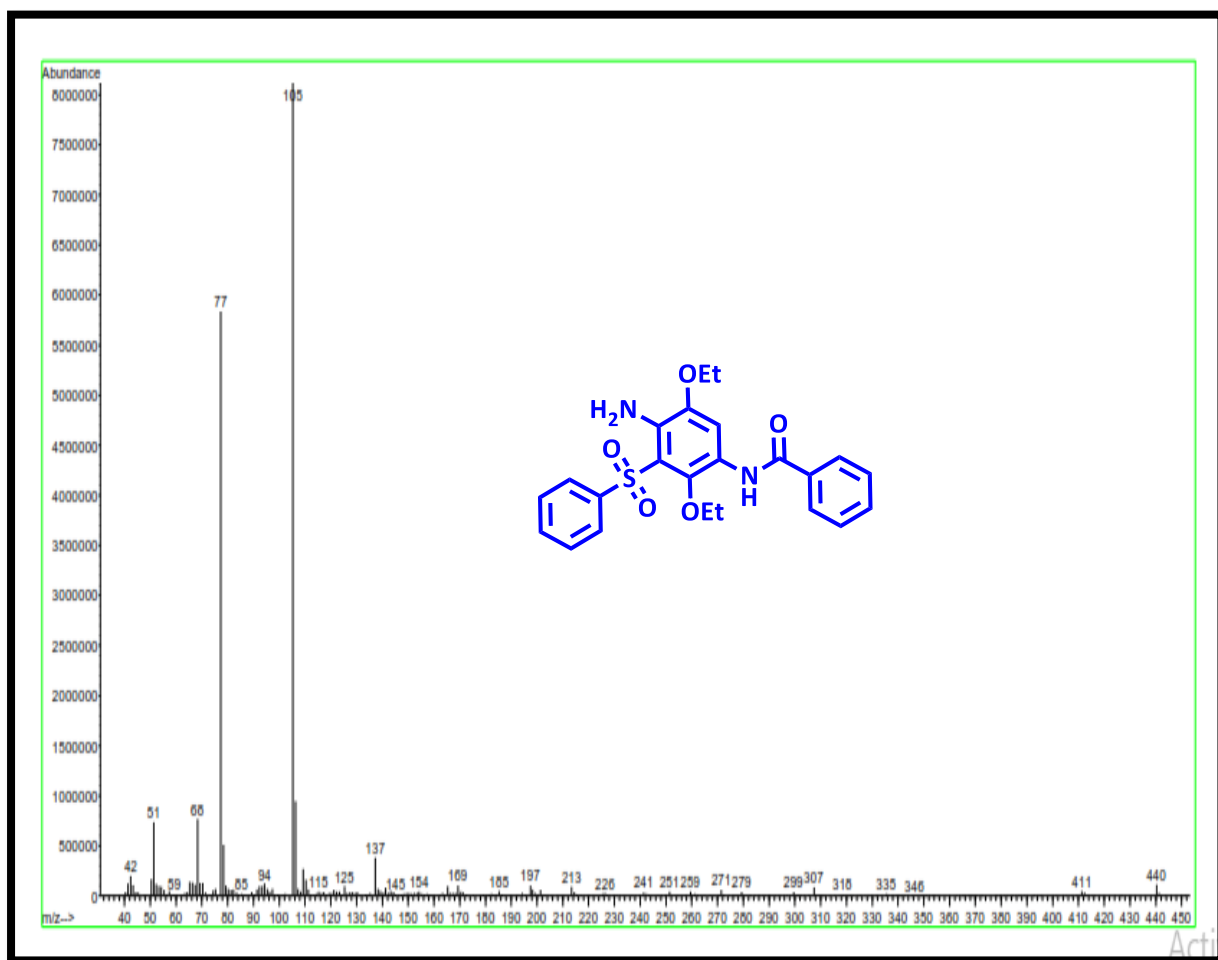
$$A = 0.026 \text{ cm}^2$$

M. J. A. Shiddiky, A. A. J. Torriero, C. Zhao, I. Burgar, G. Kennedy, and A. M. Bond, J. Am. Chem. Soc., 2009, 131, 7976- 7989

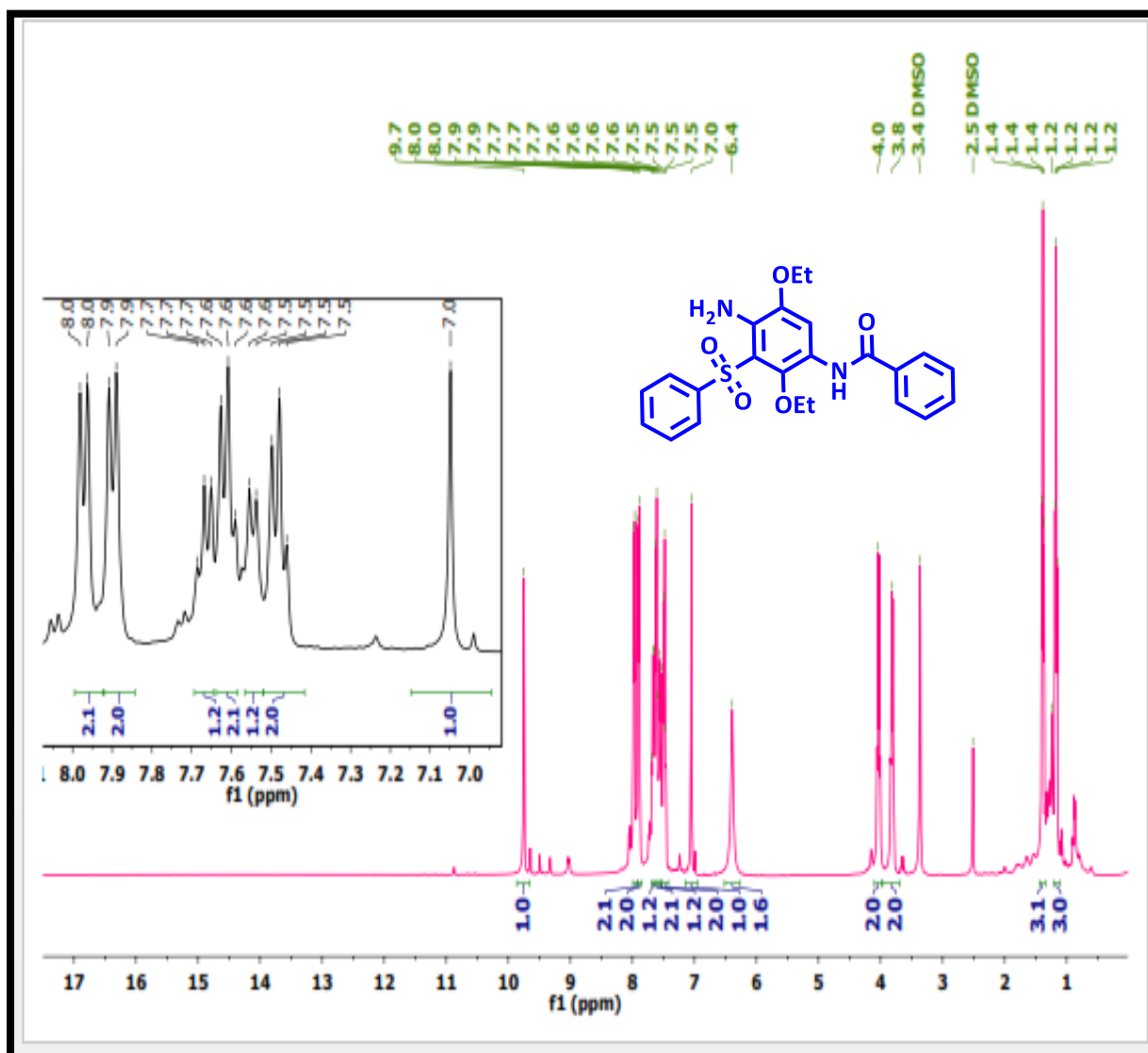
FTIR spectrum of **3a**



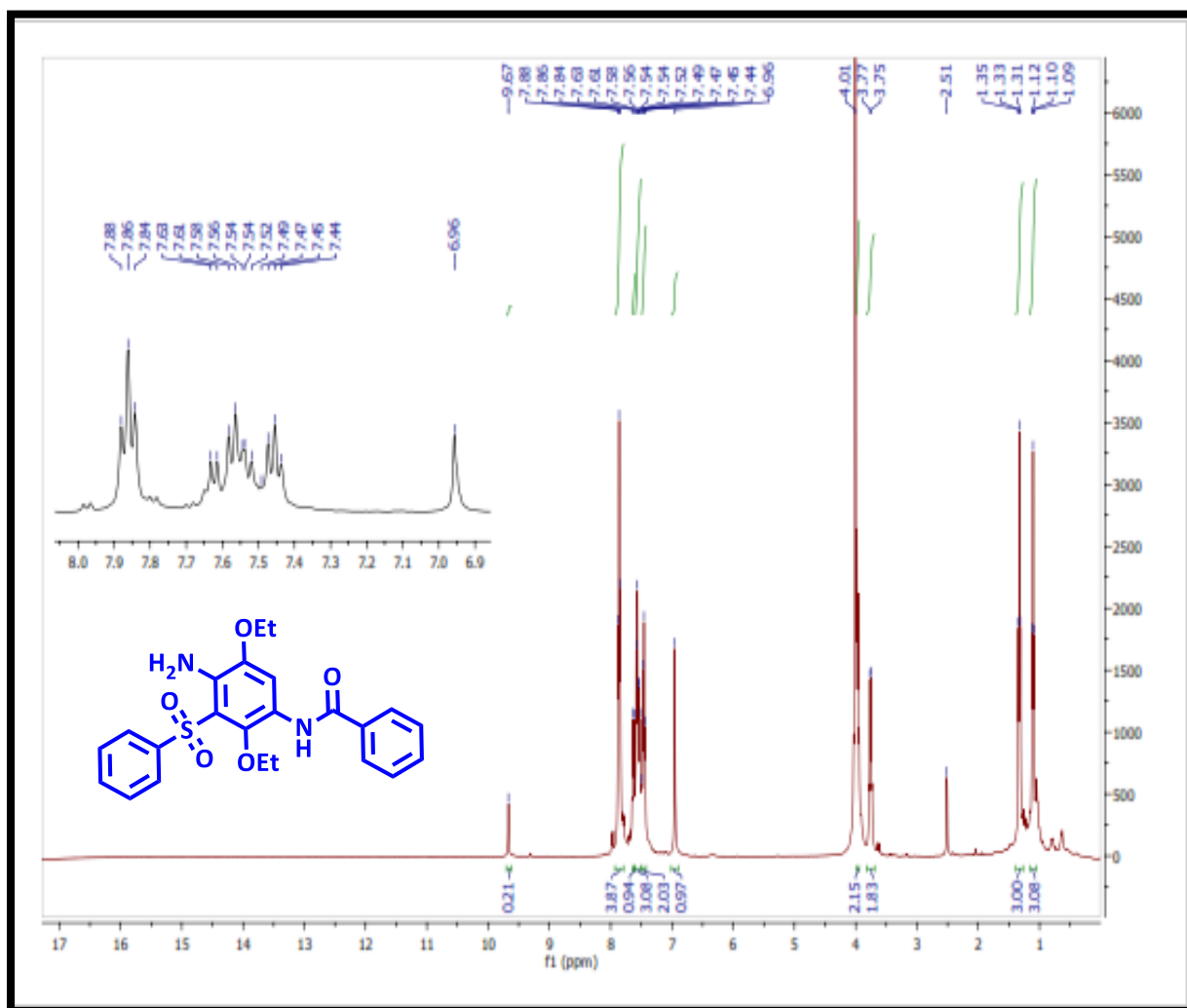
Mass spectrum of **3a**



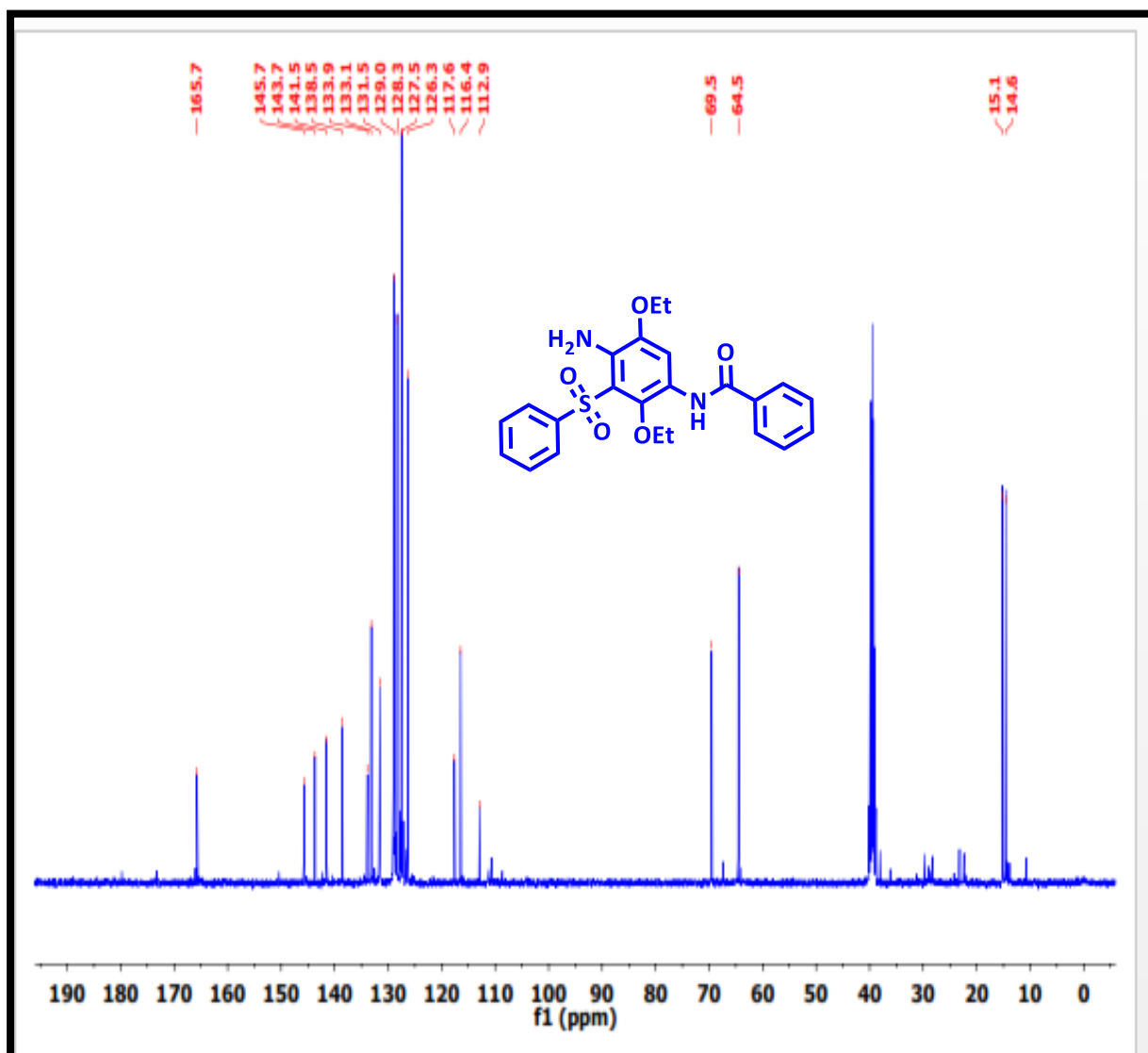
¹H NMR spectrum of **3a**



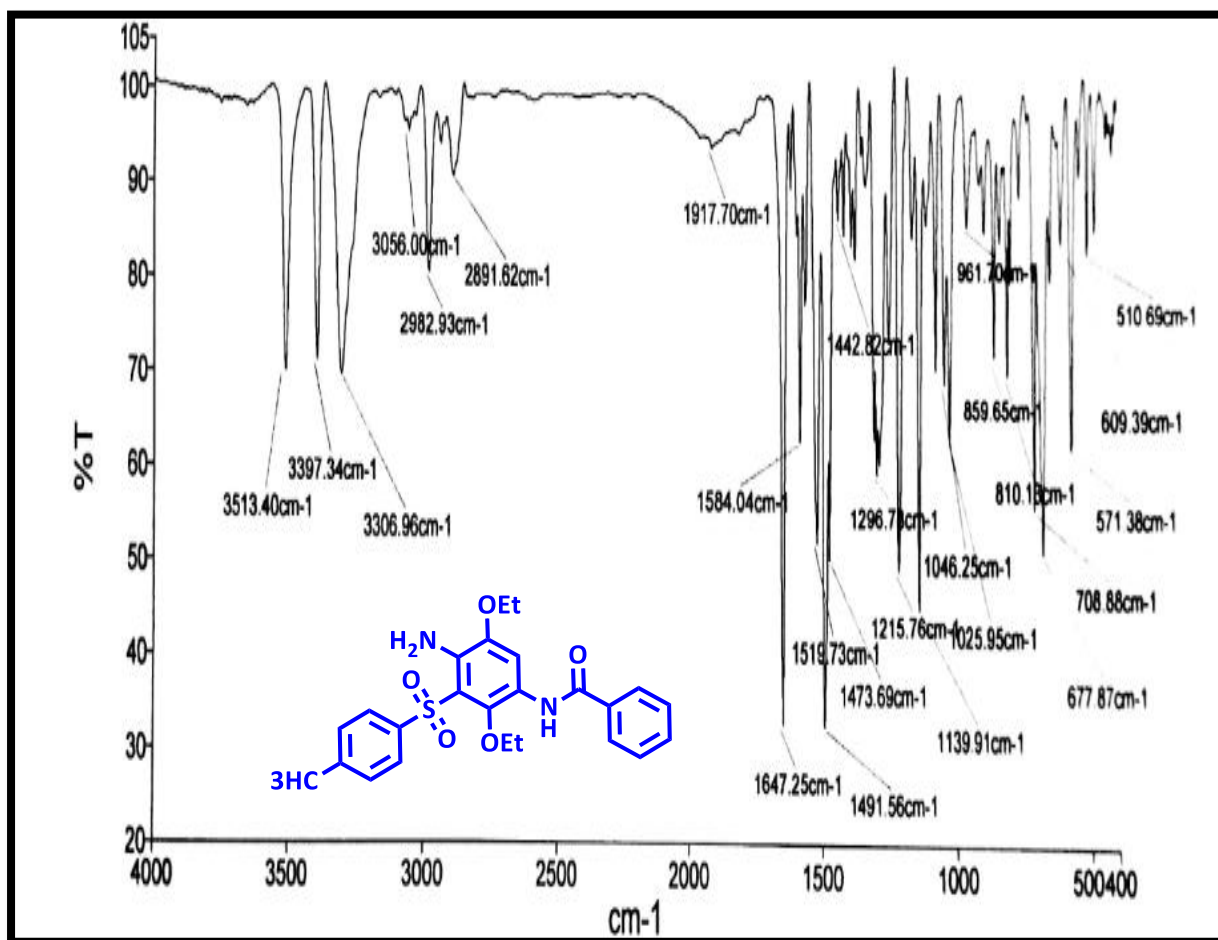
^1H NMR spectrum of **3a** (with D_2O)



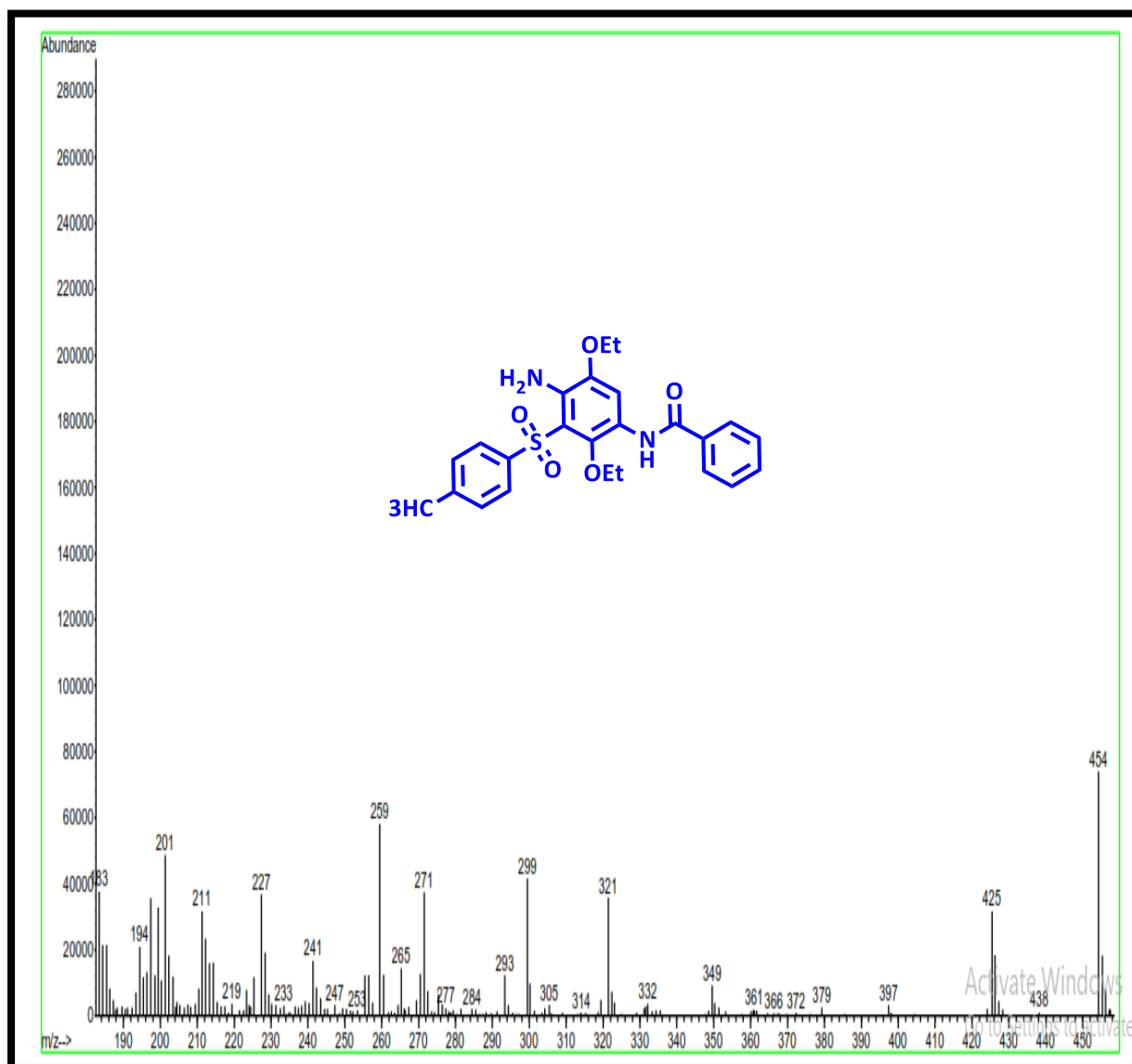
¹³C NMR spectrum of **3a**



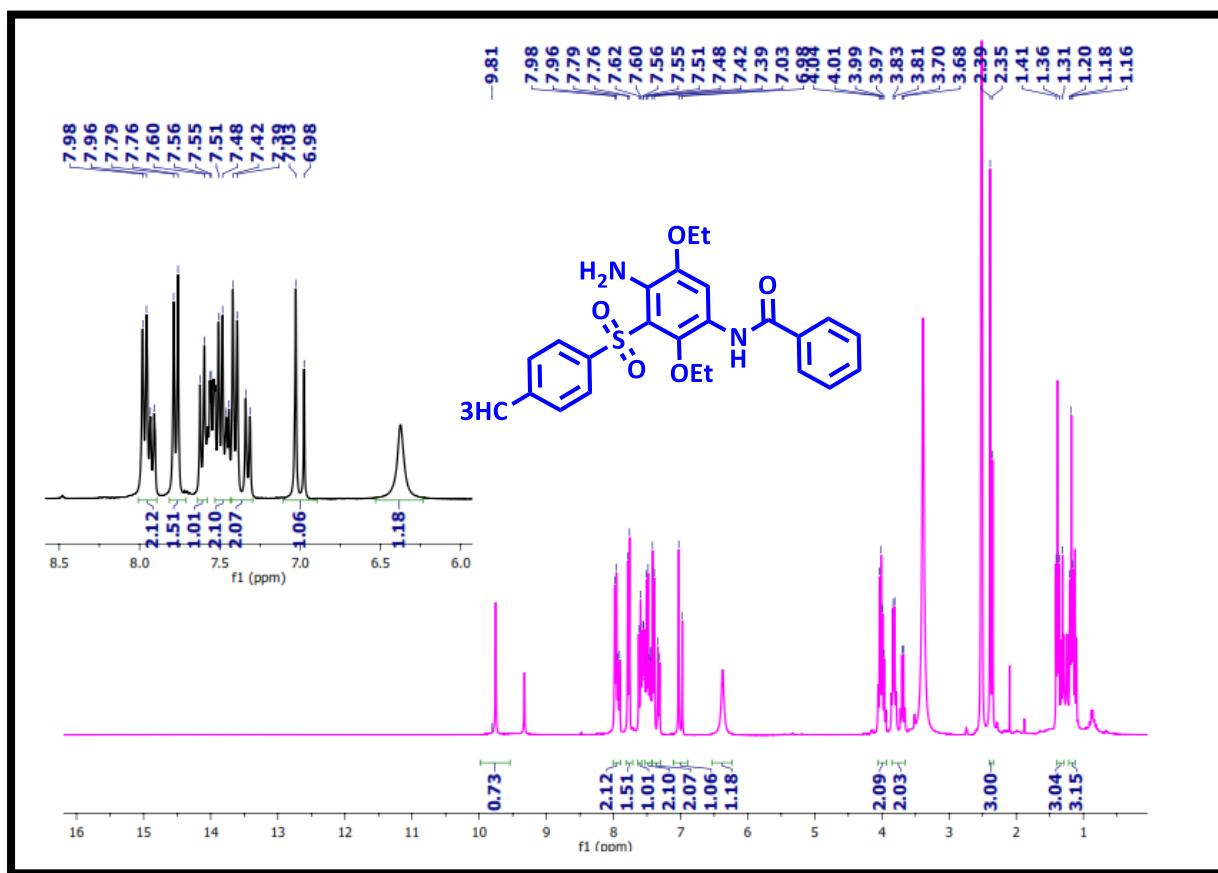
FTIR spectrum of **3b**



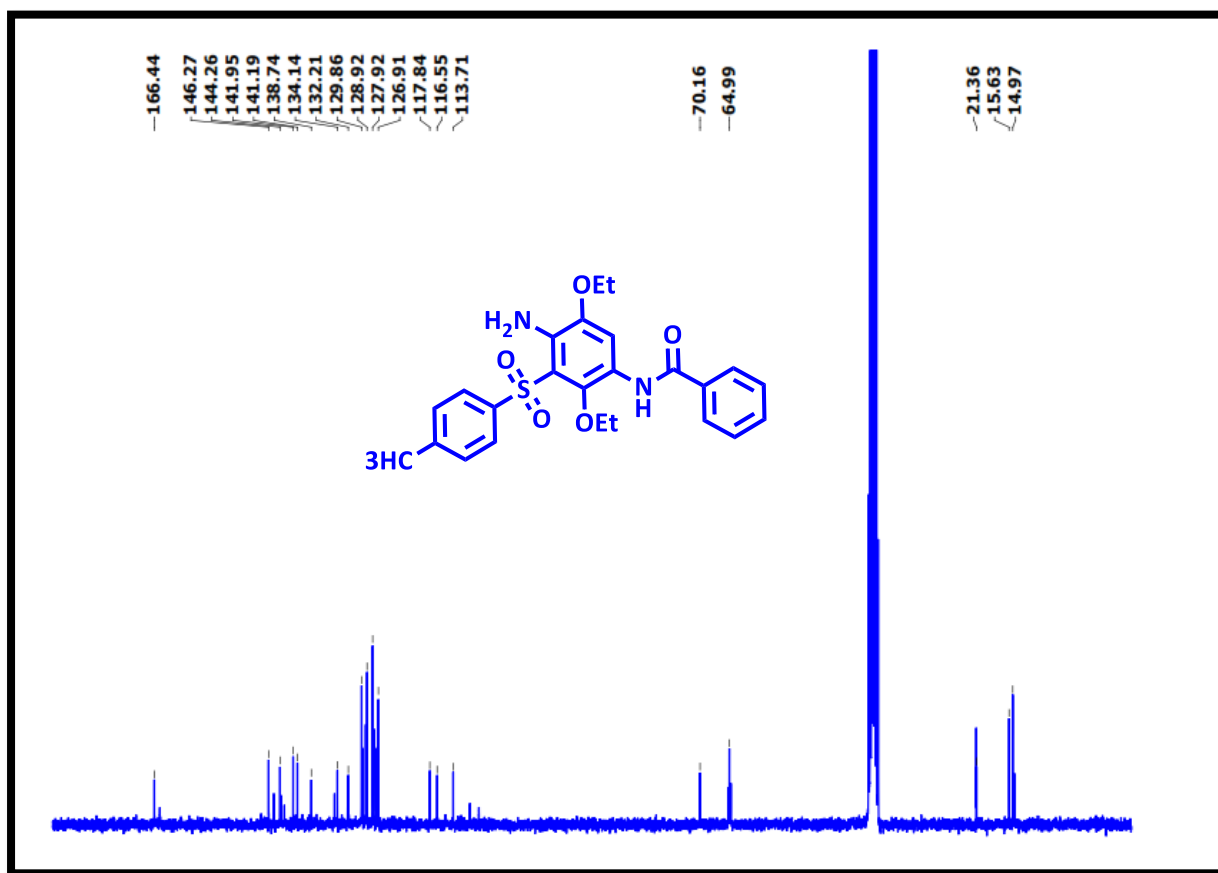
Mass spectrum of **3b**



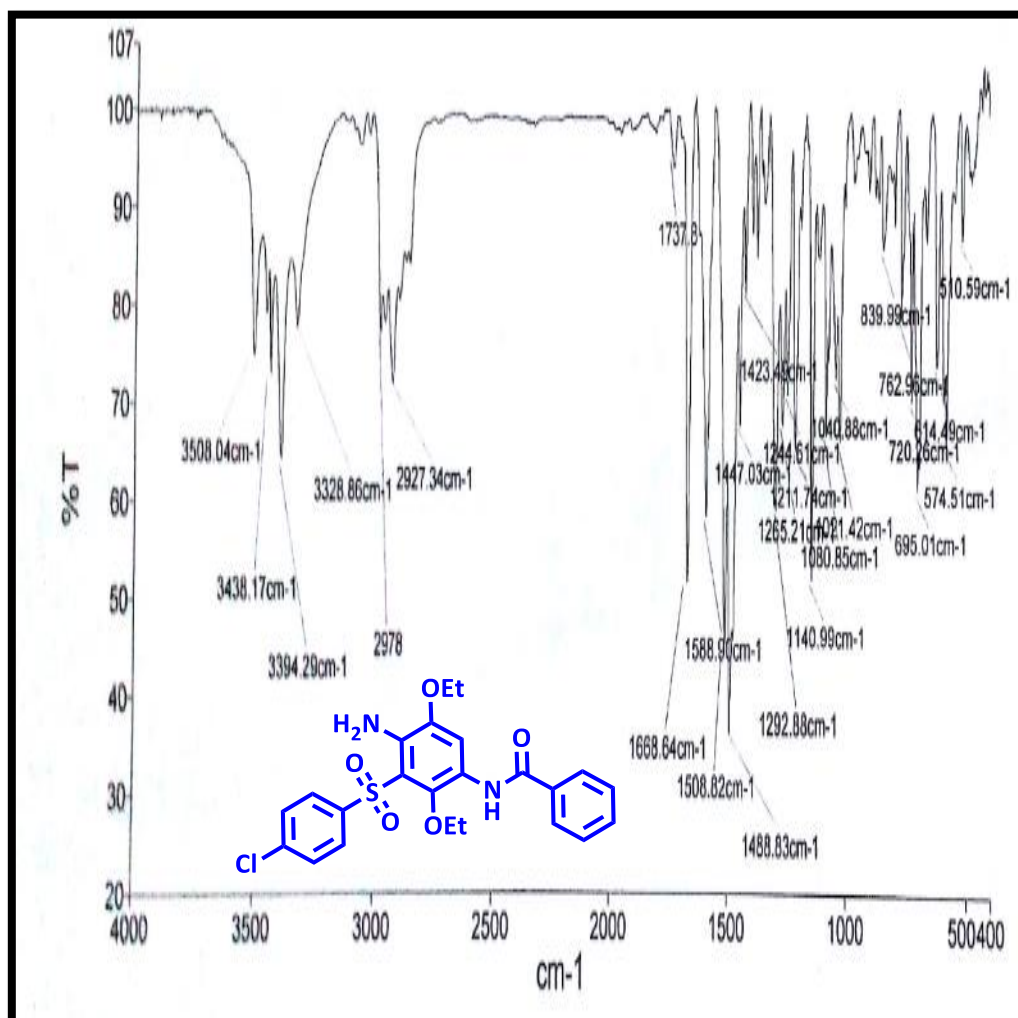
¹H NMR spectrum of **3b**



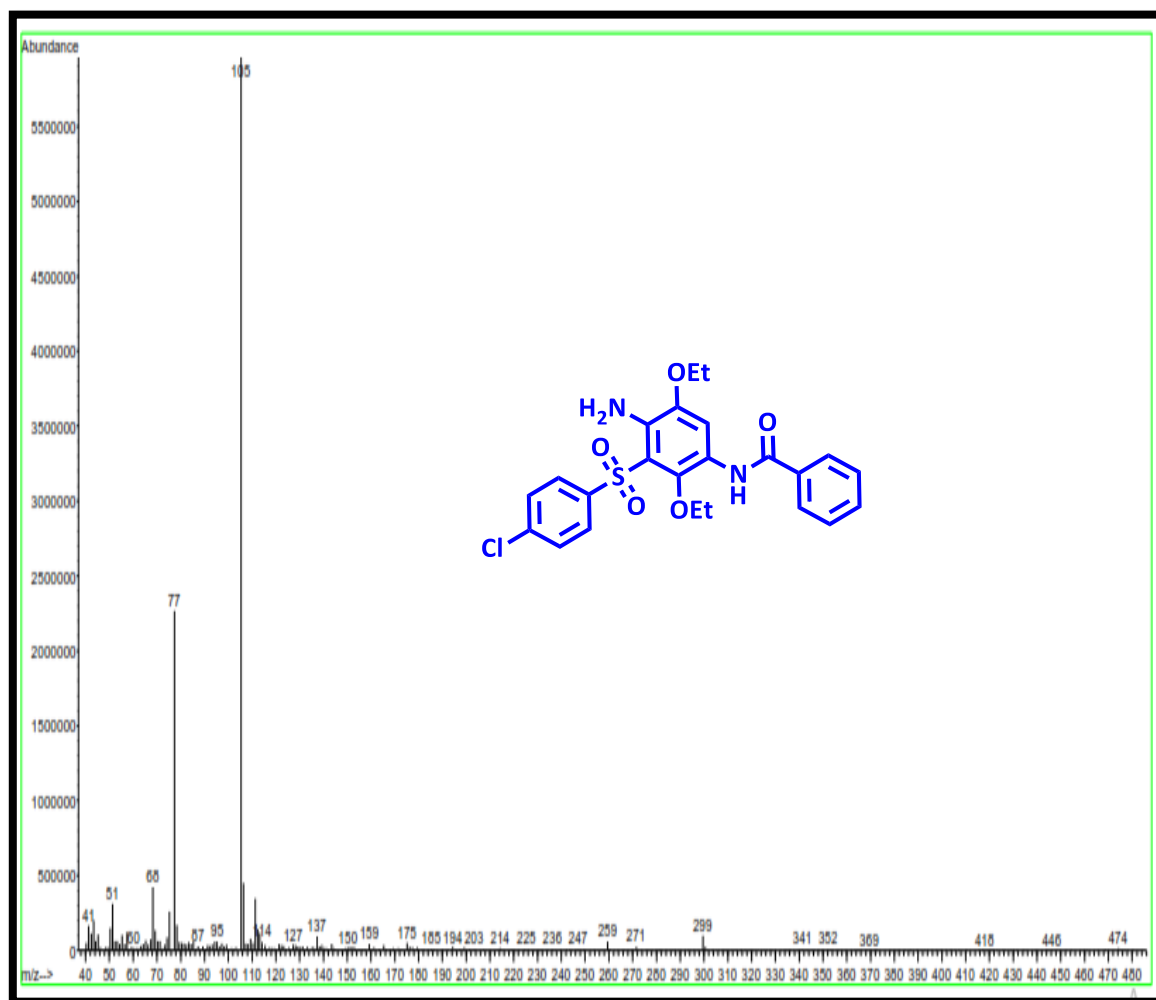
^{13}C NMR spectrum of **3b**



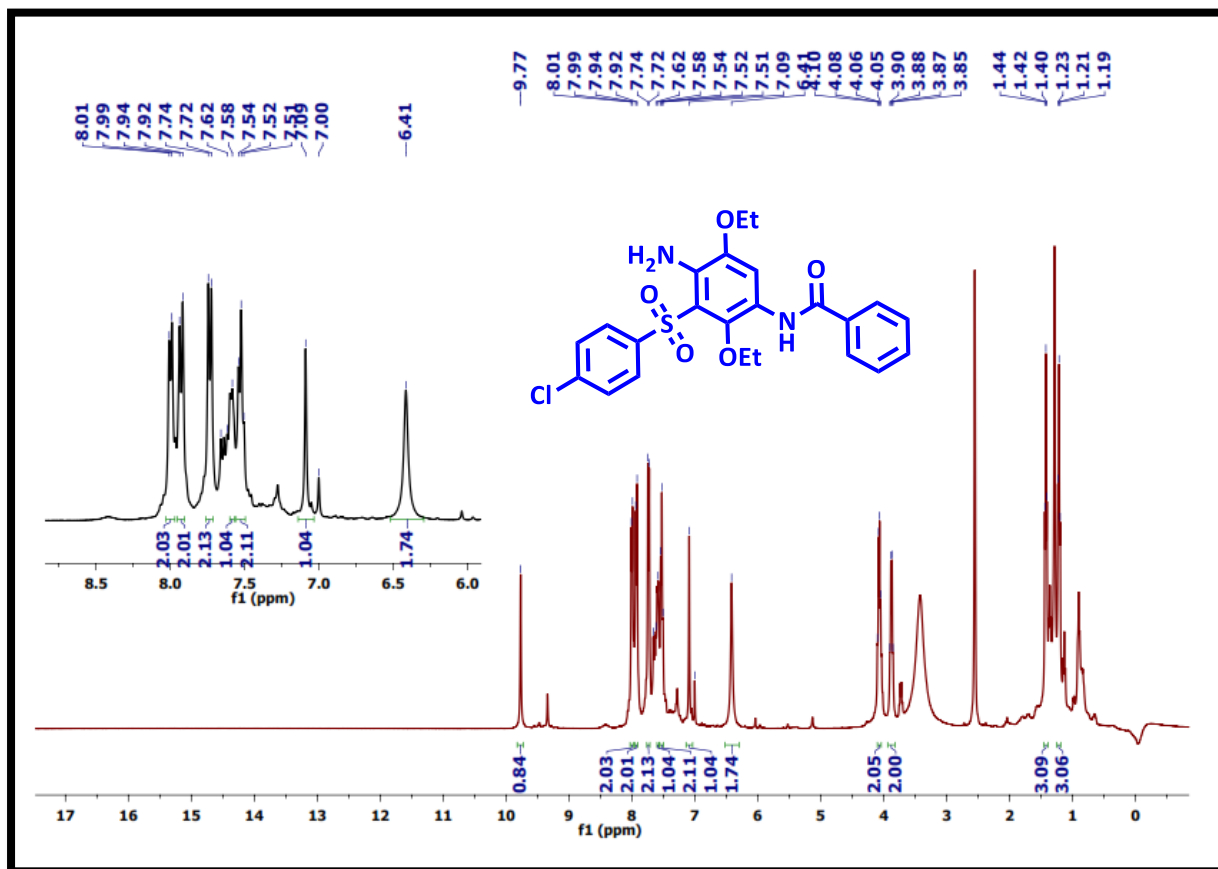
FTIR spectrum of **3c**



Mass spectrum of **3c**



¹H NMR spectrum of **3c**



¹³C NMR spectrum of **3c**

