

Supporting information:

Spectral, Electrochemical and Theoretical studies on the Charge Transfer Complexes of azacyclonol with novel substituted 1,4-benzoquinones possessing tunable electron acceptor property

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Table 1S. Effect of concentration of the donor and the acceptors on the rate of the interaction at 298 K.

| [D] (10 ⁻⁴ M) | [A] (10 ⁻⁵ M) | k ₁ (10 ⁻⁴), s ⁻¹ | | | | | k ₂ s ⁻¹ mol ⁻¹ dm ³ | | | | |
|-----------------------------|-----------------------------|---|---------------------|---------------------|---------------------|---------------------|--|---------------------|---------------------|---------------------|---------------------|
| | | AZA-CHL | AZA-MQ ₁ | AZA-MQ ₂ | AZA-MQ ₃ | AZA-MQ ₄ | AZA-CHL | AZA-MQ ₁ | AZA-MQ ₂ | AZA-MQ ₃ | AZA-MQ ₄ |
| 4 | 5 | 16.2 | 14.6 | 12.2 | 10.6 | 8.1 | 4.1 | 3.6 | 3.1 | 2.6 | 2.0 |
| 6 | 5 | 24.1 | 21.2 | 17.9 | 15.9 | 12.3 | 4.0 | 3.5 | 3.0 | 2.7 | 2.1 |
| 8 | 5 | 31.8 | 28.7 | 23.5 | 20.7 | 15.7 | 4.0 | 3.6 | 3.0 | 2.6 | 2.0 |
| 10 | 5 | 38.5 | 35.8 | 29.8 | 26.5 | 20.2 | 3.9 | 3.6 | 3.0 | 2.6 | 2.0 |
| 10 | 5 | 37.6 | 35.9 | 29.1 | 26.3 | 20.5 | | | | | |
| 10 | 4 | 38.2 | 34.8 | 29.4 | 26.4 | 20.7 | | | | | |
| 10 | 3 | 38.6 | 35.2 | 29.6 | 26.9 | 20.4 | | | | | |
| 10 | 2 | 38.1 | 35.7 | 29.2 | 26.8 | 19.9 | | | | | |

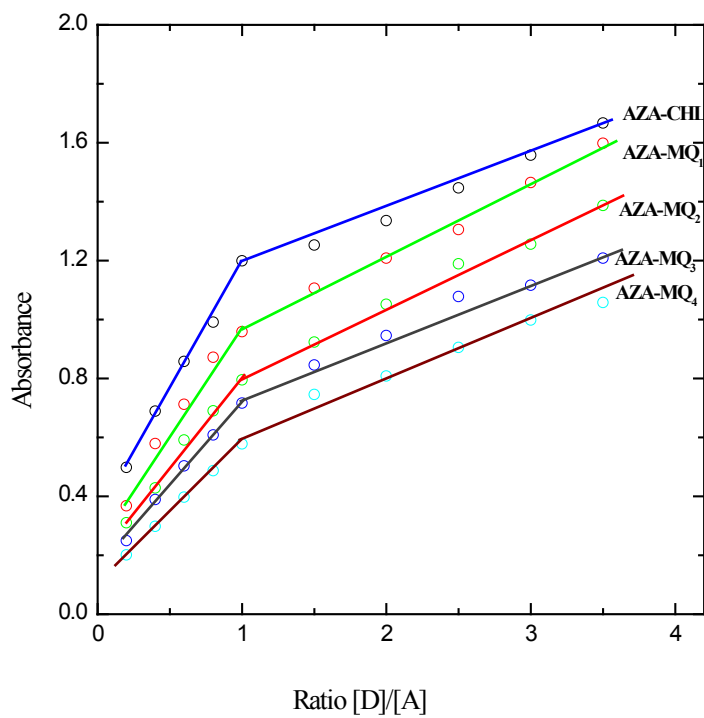


Fig. 1S. Photometric titration plots for AZA-CHL, AZA-MQ₁, AZA-MQ₂, AZA-MQ₃ and AZA-MQ₄ in 1,2-dichloroethane at 298 K.

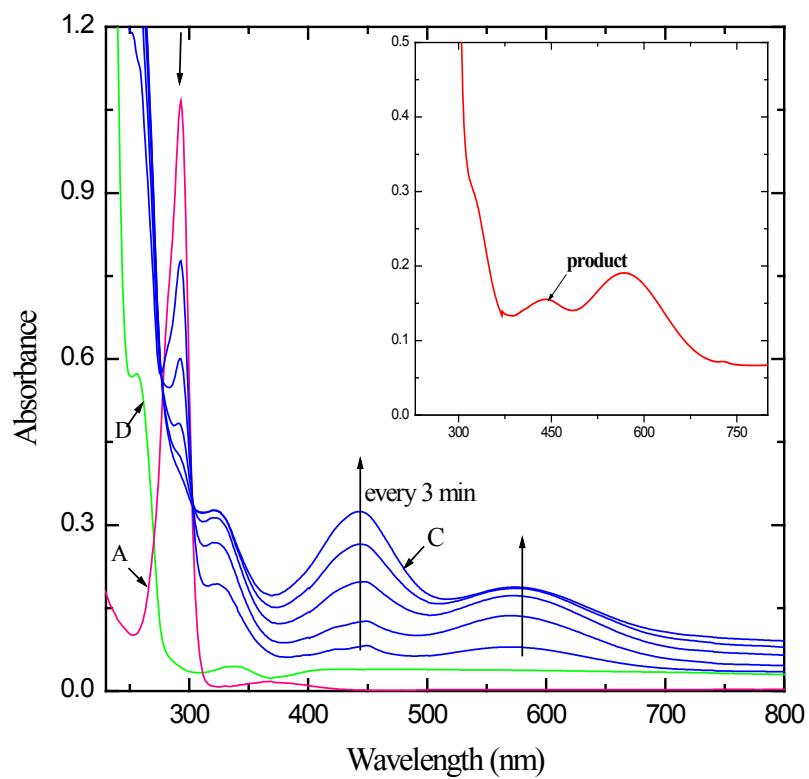


Fig. 2S. Electronic spectra of AZA with CHL in 1,2-dichloroethane at 298 K.

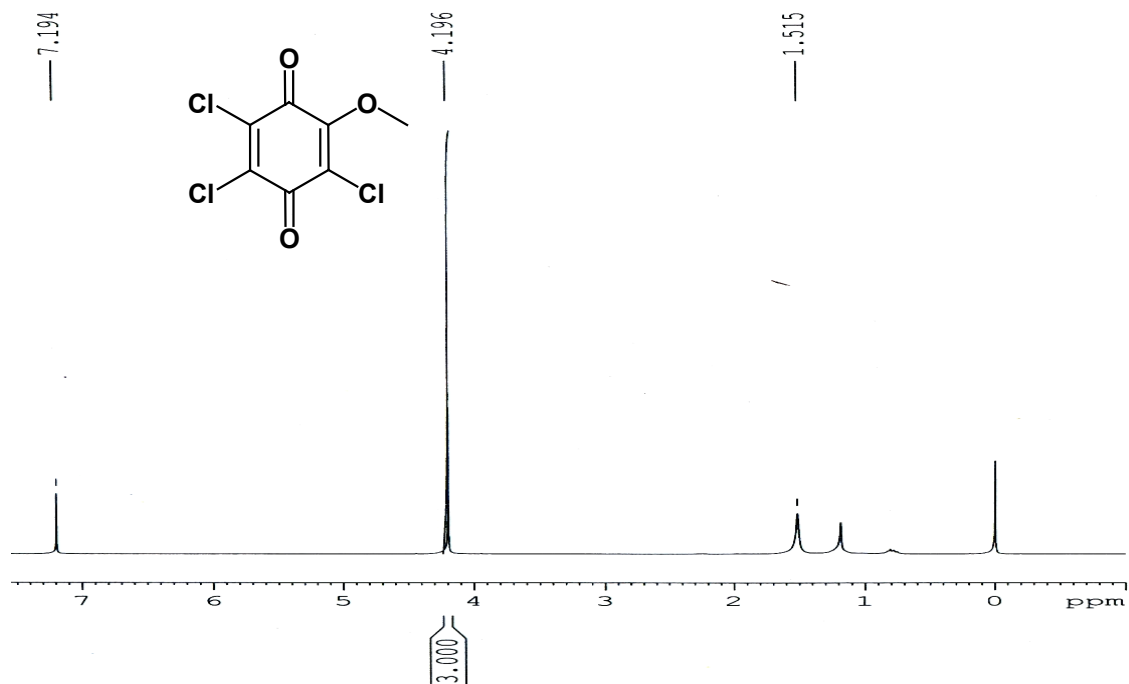


Fig. 3S. ¹H NMR Spectrum of MQ₁

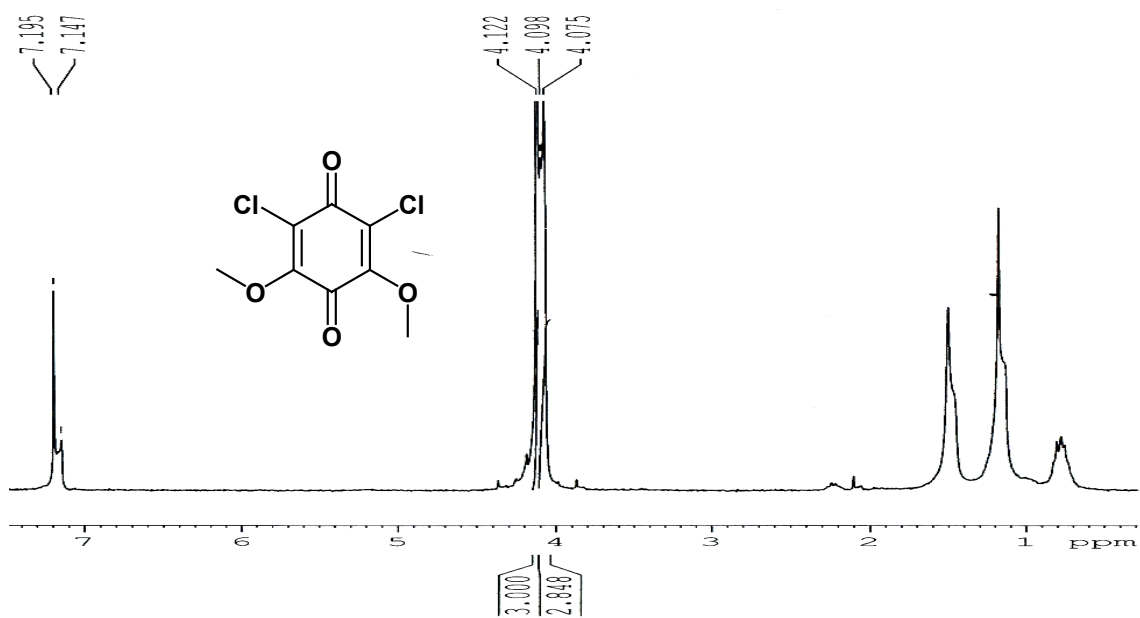


Fig. 4S. ¹H NMR Spectrum of MQ₂

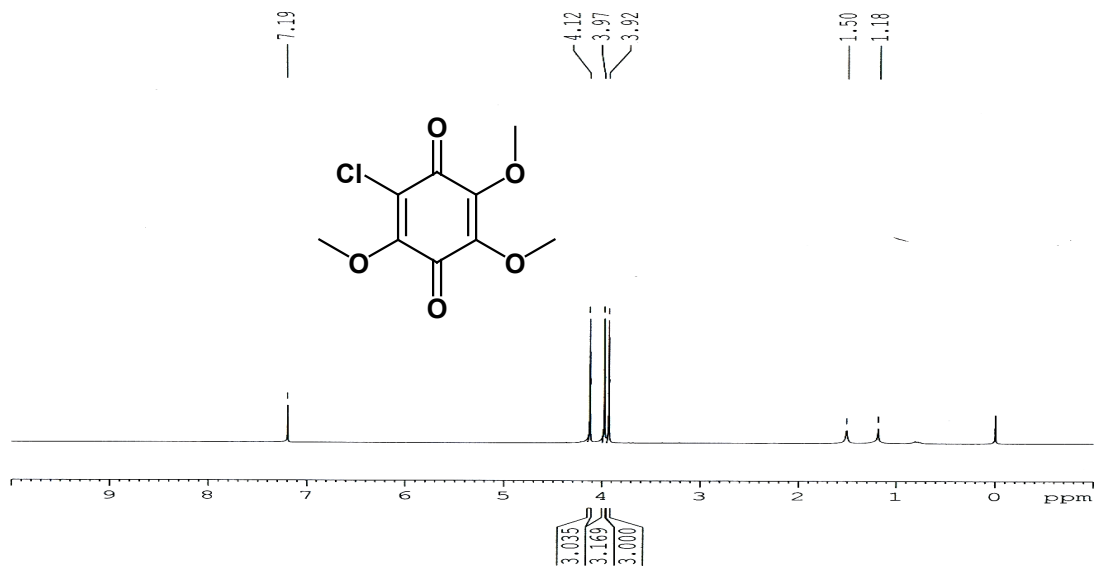


Fig. 5S. ¹H NMR spectrum of MQ₃

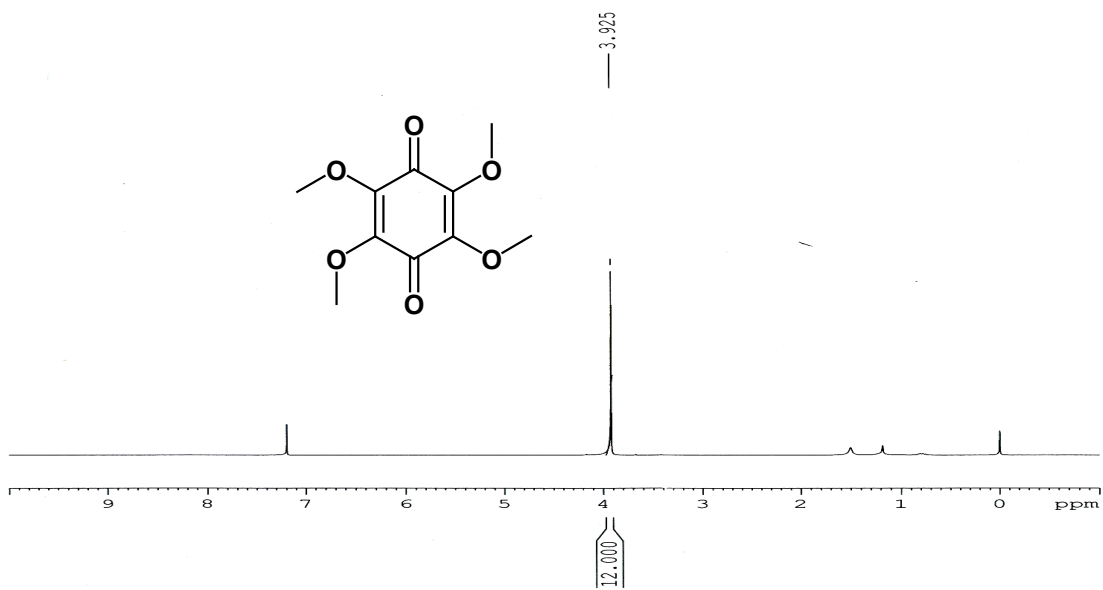


Fig. 6S. ¹H NMR Spectrum of MQ₄

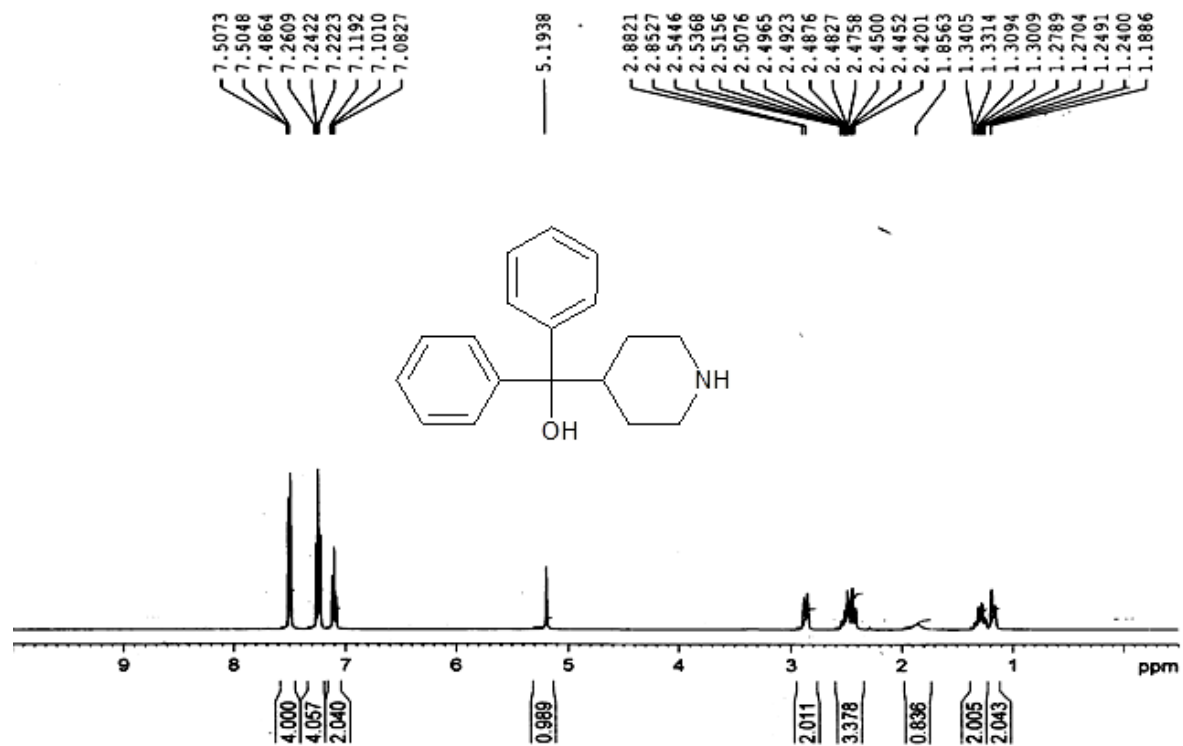


Fig. 7S. ¹H NMR Spectrum of pure AZA

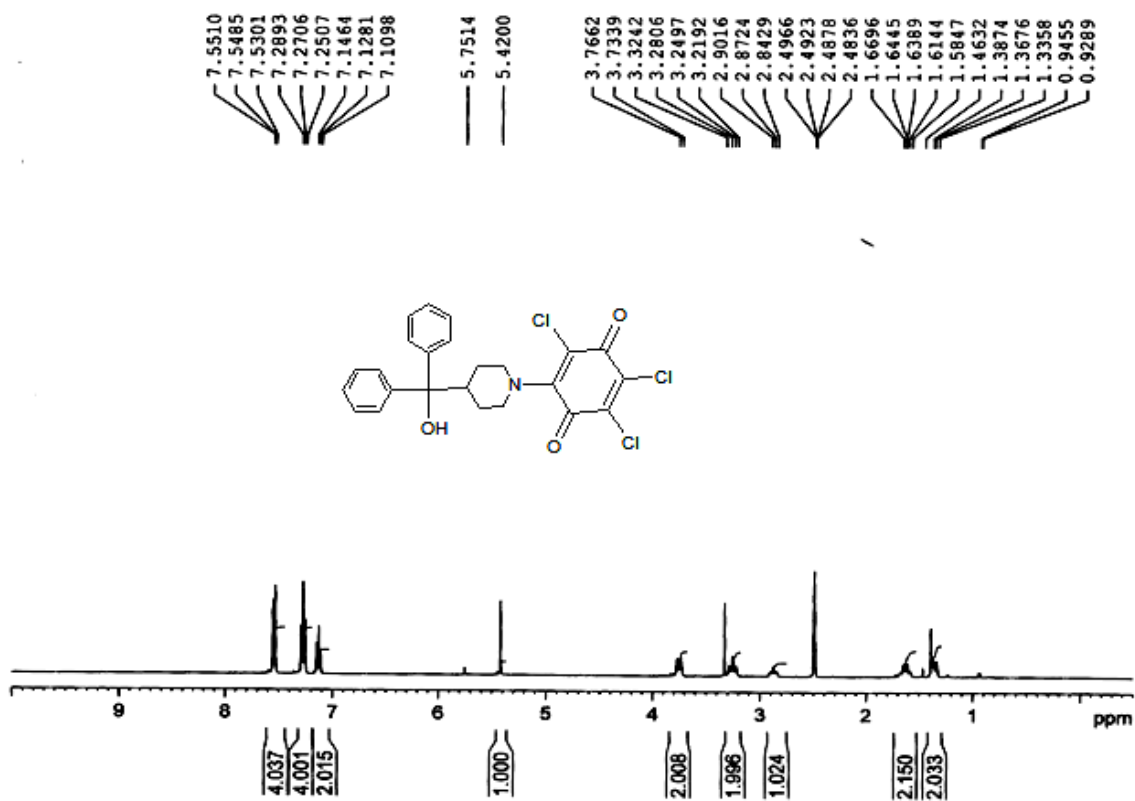


Fig. 8S. ¹H NMR Spectrum of AZA-CHL product



Fig. 9S. ¹H NMR Spectrum of AZA-MQ₁ product

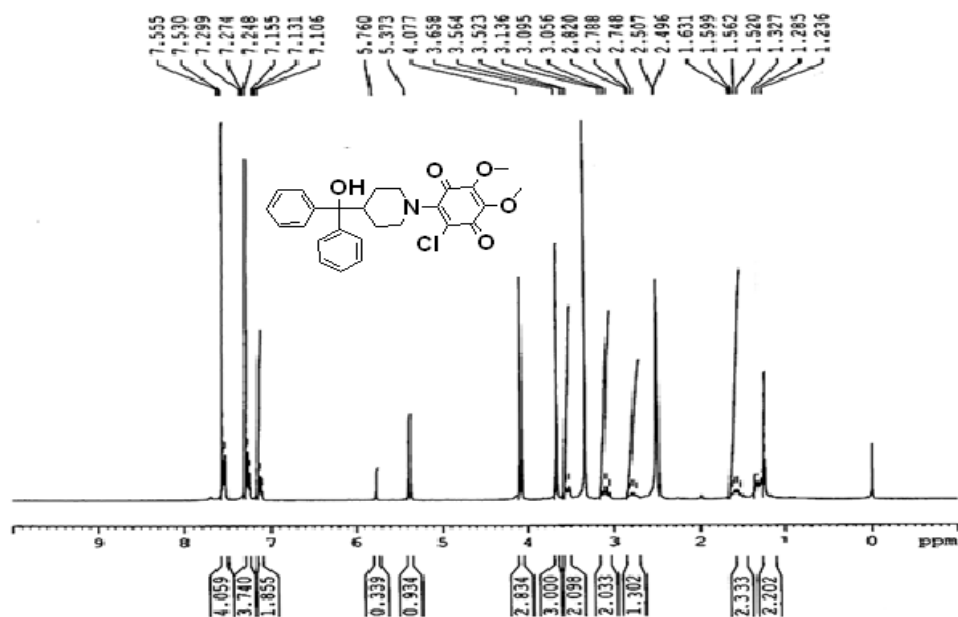


Fig. 10S. ¹H NMR Spectrum of AZA-MQ₂ product

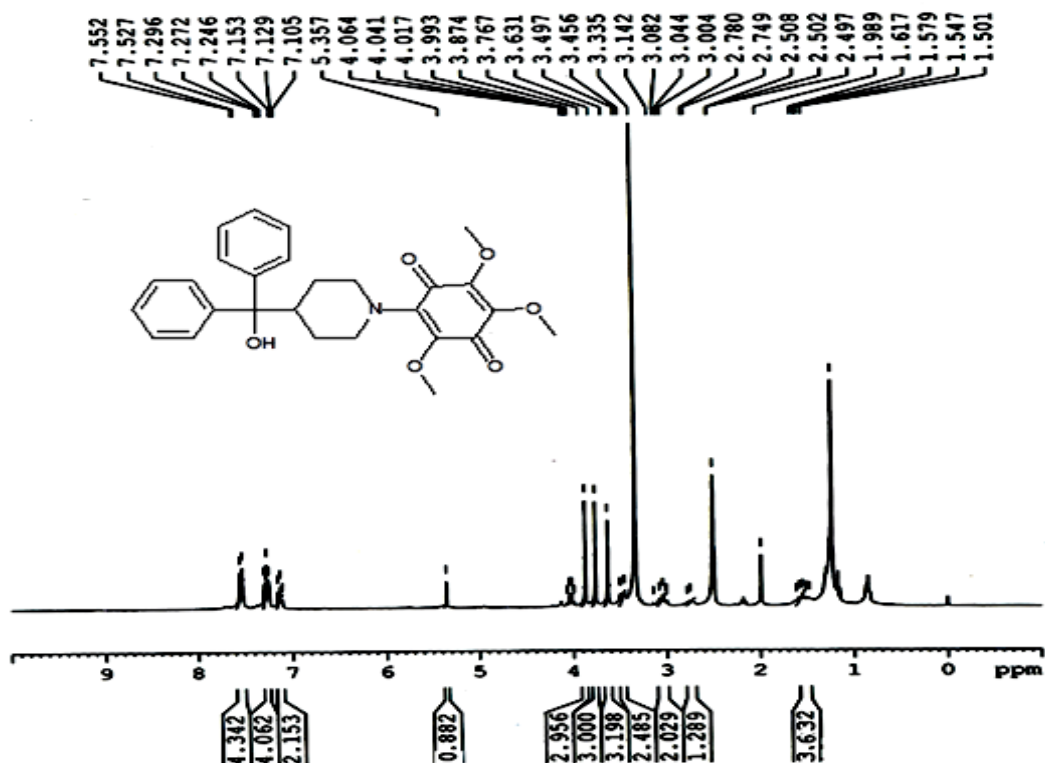


Fig.11S. ¹H NMR Spectrum of AZA-MQ₃ product

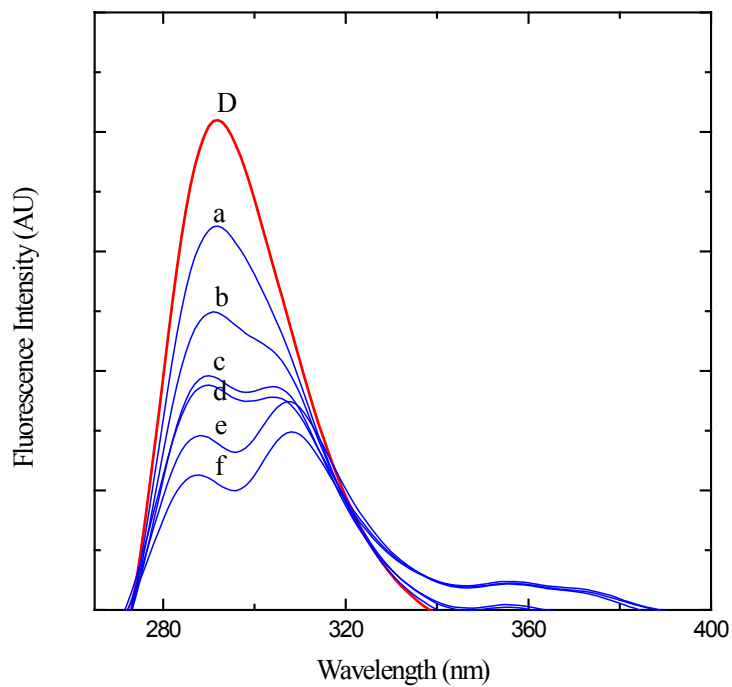


Fig. 12S. Fluorescence spectra for AZA-CHL system in 1,2-dichloroethane at fixed concentrations of $[D] = 8 \times 10^{-4} \text{ M}$ (curve D) and variable concentration of $[A] (\times 10^{-5}) = \{1 \text{ (curve a), } 2 \text{ (curve b), } 3 \text{ (curve c), } 4 \text{ (curve d), } 5 \text{ (curve e), } 6 \text{ (curve f)}\} \text{ M}$ at 298 K

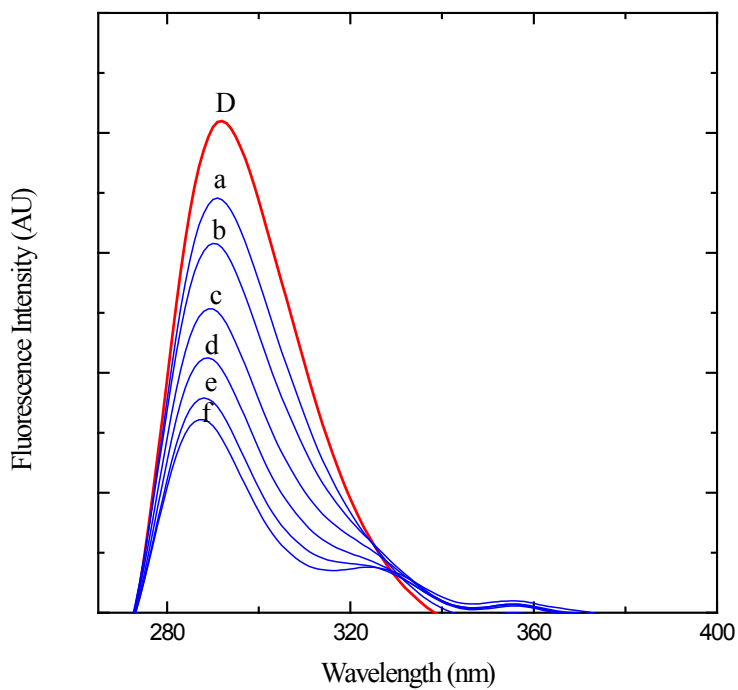


Fig. 13S. Fluorescence spectra for AZA-MQ₂ system in 1,2-dichloroethane at fixed concentrations of $[D] = \{8 \times 10^{-4} \text{ M (curve D)}\}$ and variable concentration of $[A] (\times 10^{-5}) = \{1 \text{ (curve a), 2 (curve b), 3 (curve c), 4 (curve d), 5 (curve e), 6 (curve f)}\} \text{ M}$ at 298 K

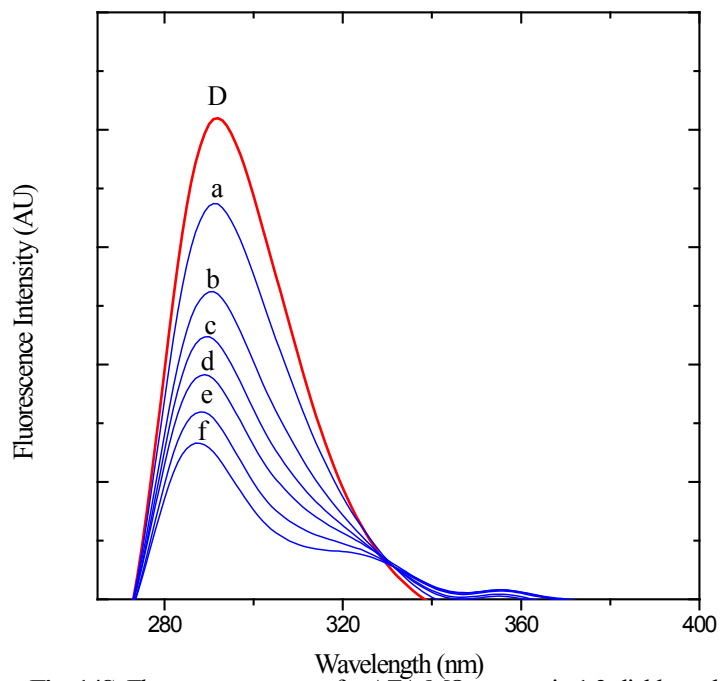


Fig. 14S. Fluorescence spectra for AZA-MQ₃ system in 1,2-dichloroethane at fixed concentrations of [D] = 8×10^{-4} M (curve D) and variable concentration of [A] ($\times 10^{-5}$) = {1 (curve a), 2 (curve b), 3 (curve c), 4 (curve d), 5 (curve e), 6 (curve f)} M at 298 K

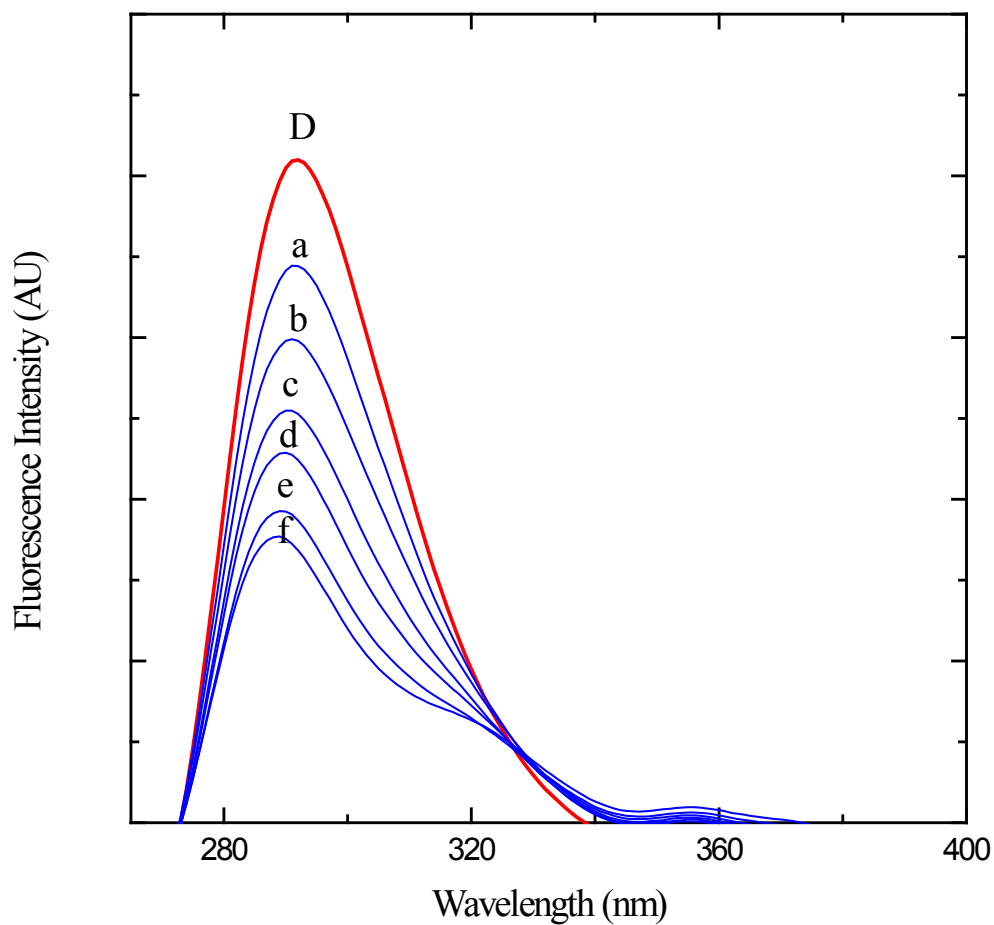


Fig. 15S. Fluorescence spectra for AZA-MQ₄ in 1,2-dichloroethane at fixed concentrations of $[D]=\{8\times 10^{-4}\text{M (curve D)}\}$ and variable concentration of $[A](\times 10^{-5})=\{1 \text{ (curve a), } 2 \text{ (curve b), } 3 \text{ (curve c), } 4 \text{ (curve d), } 5 \text{ (curve e), } 6 \text{ (curve f)}\}\text{M}$ at 298 K