Supporting Information

Kinetic exploration appended by Spectroscopic and Molecular Docking analysis in search of an optimal condition for effective degradation of Malachite Green

Somnath Dasmandal^a, Harasit Kumar Mandal^a, Suparna Rudra^a, Arjama Kundu^a, Tapas Majumdar^b and Ambikesh Mahapatra^a,*

^aDepartment of Chemistry, Jadavpur University, Kolkata 700 032, India

^bDepartment of Chemistry, University of Kalyani, Kalyani 741235, India

E-mail addresses amahapatra@chemistry.jdvu.ac.in, ambikeshju@gmail.com

^{*}Corresponding author. Tel.: +9133 2457 2770 (office), +9133 2432 4586 (residence); fax: +9133 2414 6223.

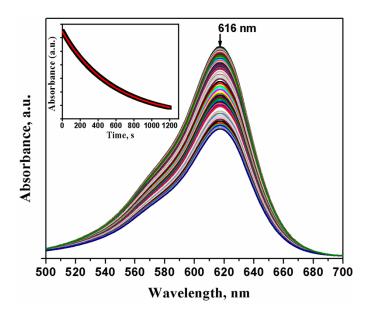


Fig. S1 UV-Vis Spectra of MG and $^{-}$ OH reaction mixture at different time intervals (Inset: Change of absorbance as a function of time at 616 nm) [MG] $_{0}$ =1.25 × 10⁻⁵M, [$^{-}$ OH] $_{0}$ = 1.875 mM, μ = 5.0 mM at 298 K

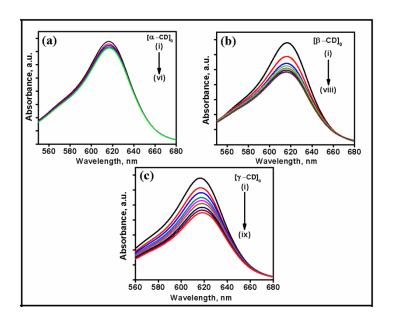


Fig.S2: Spectral change of MG upon addition of CDs. (a): $[\alpha\text{-CD}]_0 = (i)~0.0$ to (vi) 5.0 mM, (b) $[\beta\text{-CD}]_0 = (i)~0.0$ to (viii) 6.0 mM and $[\gamma\text{-CD}]_0 = (i)~0.0$ to (ix) 7.0 mM.

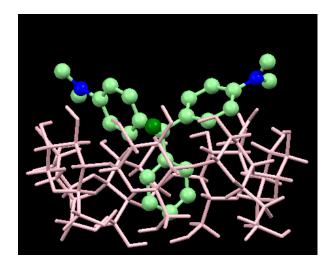


Fig.S3: Molecular modeling of MG- β -CD 1: 1 complex; MG and β -CD have been depicted in the ball stick and capped stick model respectively.