Chitosan containing azo-based Schiff bases: Thermal, antibacterial and

birefringence properties for bio-optical devices

Nidhi Nigam¹, Santosh Kumar^{1#}, P.K.Dutta^{1*}, S.Pei² and Tamal Ghosh^{1*}

¹Department of Chemistry, Motilal Nehru National Institute of Technology, Allahabad - 211004, India.

²Department of Physics, Jilin University, P. R. China.

^{*} Corresponding authors. e-mail: pkd@mnnit.ac.in (PKD), tamalghosh@mnnit.ac.in (TG), Fax: +91 532 2545341.

[#] Present address: Department of Chemistry, University of Coimbra, Coimbra, Portugal.

Characterization of the synthesized azo dyes:

The synthesized azo dyes (a) HNAB and (b) HMAB were characterized by FTIR, ¹H NMR and ESI-Mass spectroscopy.

a) 2-hydroxy-5-(4-nitrophenylazo)-benzaldehyde (HNAB): IR (KBr Pellet, cm⁻¹): 1343, 1480, 1525, 1583, 1608, 1663, 3104, 3423. ¹H NMR (300 MHz, DMSO-d₆, TMS) δ/ppm:
7.11 (d, 1H, J = 8.7 Hz), 8.03 (d, 2H, J = 8.7 Hz), 8.11 (d, 1H, J = 8.4 Hz), 8.21 (s, 1H), 8.41 (d, 2H, J = 8.4 Hz), 10.34 (s, 1H). ESI-MS (*m*/*z*): 271.09 [M]⁺.

b) 2-hydroxy-5-(4-tolylazo)-benzaldehyde (HMAB): IR (KBr Pellet, cm⁻¹): 1284, 1378, 1482, 1577, 1666, 2919, 3030, 3220, 3424. ¹H NMR (300 MHz, CDCl₃, TMS) δ/ppm: 2.44 (s, 3H), 7.13 (d, 1H, J = 8.4 Hz), 7.33 (d, 2H, J = 7.8 Hz), 7.82 (d, 2H, J = 8.1 Hz), 8.81 (d, 2H, J = 9 Hz), 10.03 (s, 1H), 11.30 (s, 1H). ESI-MS (*m/z*): 240.8 [M]⁺.

FTIR analysis of the derivatives

In CHNAB (Fig S1) and CHMAB (Fig S2), the peculiar Schiff base linkage i.e. (>C=N-) imine bond vibrational frequency comes at 1588 and 1580 cm⁻¹ respectively. This suggests the formation of Schiff base between aryl azo dye and chitosan polymer.



Fig. S1. FTIR spectra of pure chitosan and CHNAB.



Fig. S2. FTIR spectra of pure chitosan and CHMAB.



Fig. S3. FTIR spectra of the azo dyes (a) HNAB and (b) HMAB.



Fig. S4. ¹H NMR spectra (300 MHz) of azo dyes (a) HNAB (DMSO-*d*₆) and (b) HMAB (CDCl₃)



Fig. S5. ESI-Mass spectra of azo dyes (a) HNAB and (b) HMAB