Electronic Supplementary Material (ESI) for Biomaterials Science.

Exploring LDS 821 dye as a potential NIR probe for two photon imaging of amyloid fibrils

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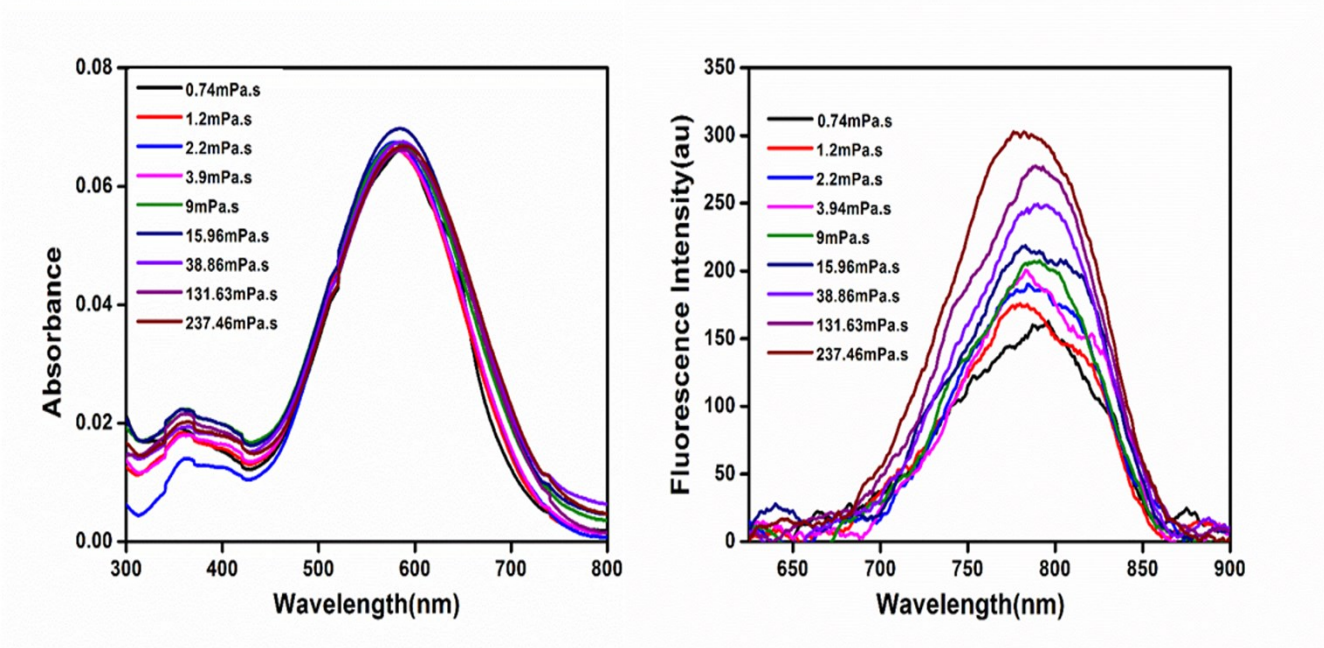

Figure 1: Absorption and emission spectrum of LDS 821 on methanol-glycerol mixtures

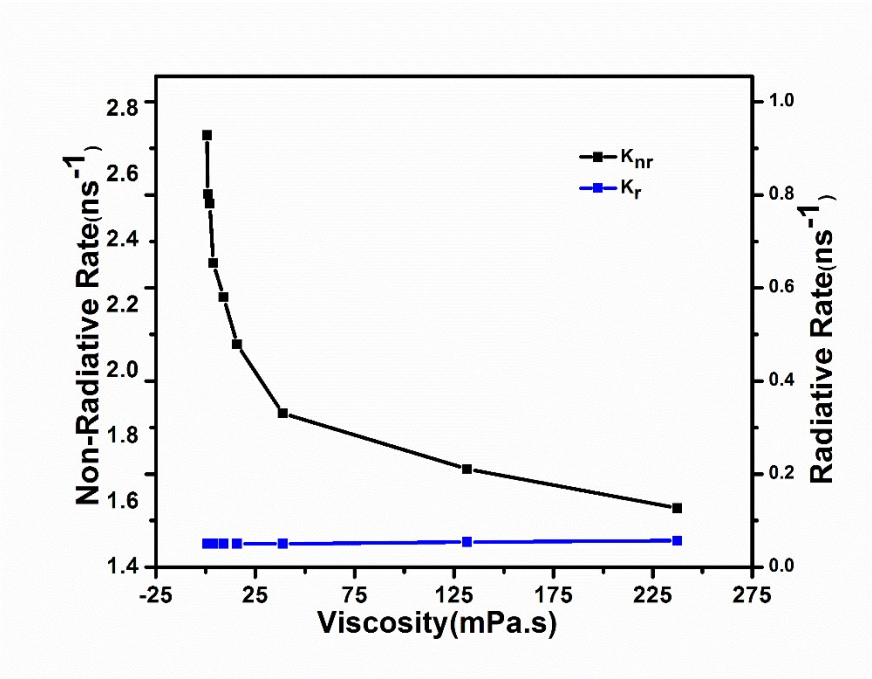

Figure 2: Radiative and non-radiative rates of LDS 821 as function of viscosity of the media

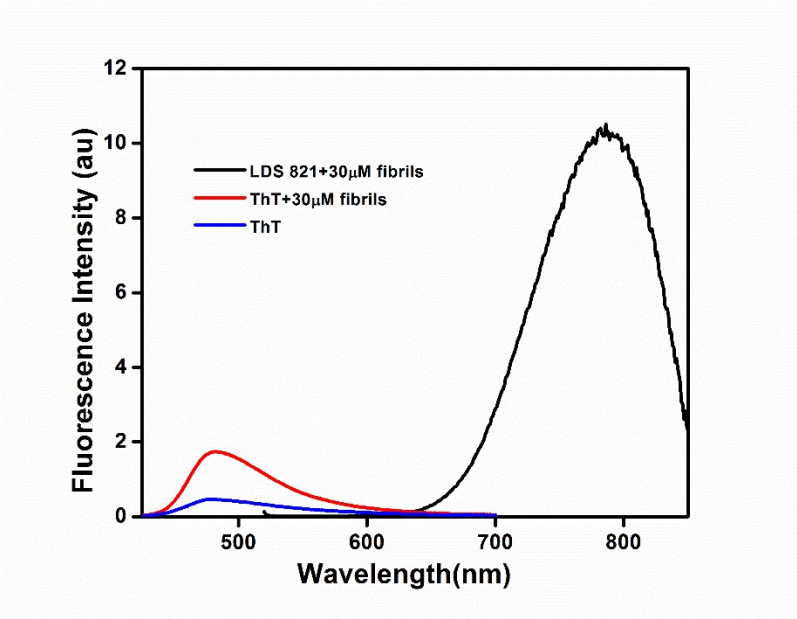

Figure 3: Fluorescence spectrum of ThT and LDS 821 in 25μM of lysozyme fibrils. The concentration of ThT and LDS 821 is 20μM

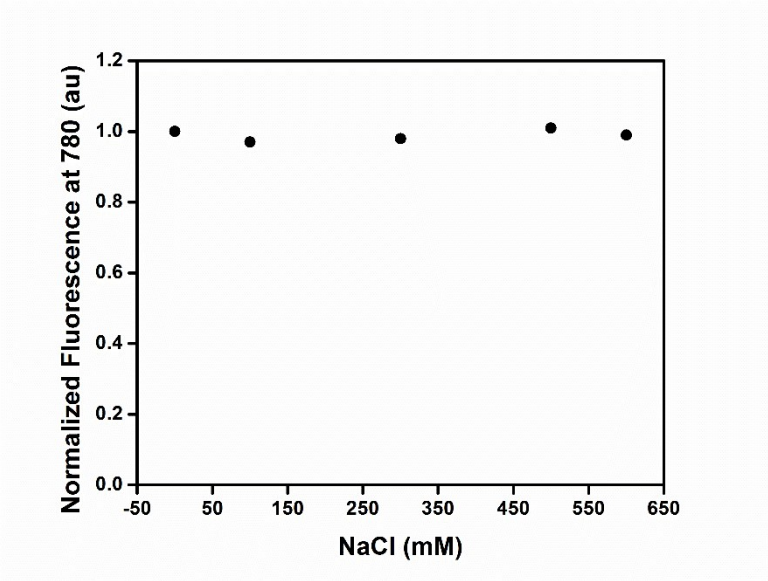

Figure 4: Normalized fluorescence spectrum of LDS 821 lysozyme fibrils (25µM) with various concentration of NaCl

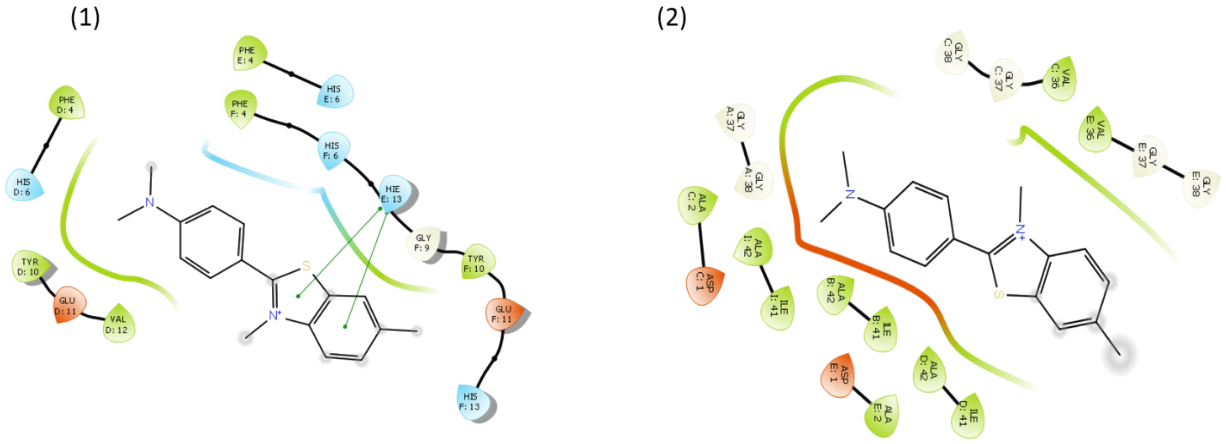

Figure 5: 2D interaction diagrams of ThT on amyloid fibrils ((1) for PDB: 5OQV and (2) for 2NAO)

ADME properties of LDS 821 dye were predicted using QikProp. The octanol /water partition coefficient QPlogPo/w is used to express the lipophilicity of the compound. The gut-blood barrier were predicted using Caco-2 cell permeability (QPPCaco, in nm/sec). QPlogBB predicted brain/blood partition coefficient. QPPMDCK predicted apparent MDCK cell permeability in nm/s, MDCK cells are considered to be a good mimic for the blood brain barrier. QPlogKp is used to predict the skin permeability. Table 1gives predicted ADME properties of LDS 821 dye.

	QPlogPo/w	QPPCaco	QPlogBB	QPPMDCK	QPlogKp
Acceptable range	(-2.0 to 6.5)	<25 poor >500 great	(-3 to 1.2)	<25 poor >500 great	(-8.0 to -0.1)
	7.625	2467.048	0.604	2026.967	-1.71

Table 1: Predicted ADME properties of LDS 821

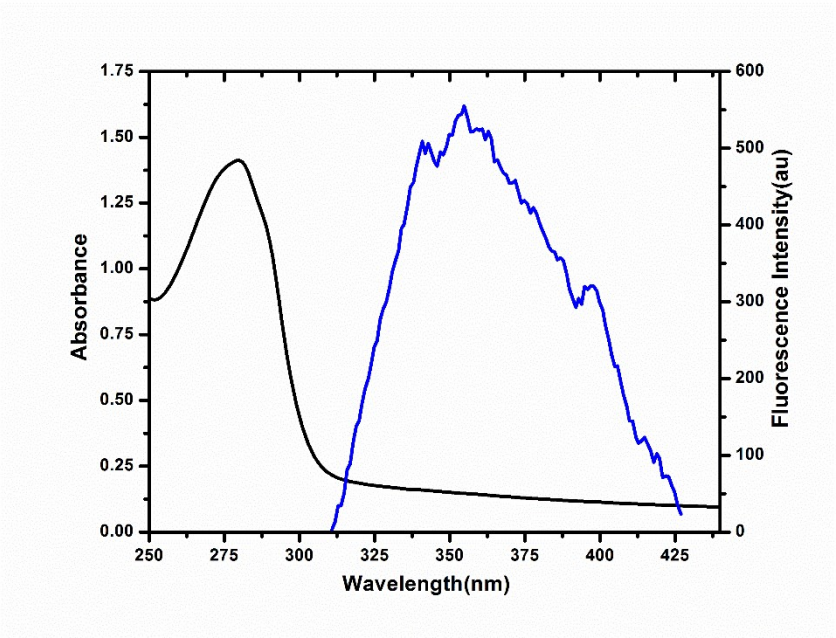

Figure 6: Absorption and emission spectrum of 14μM of lysozyme fibrils

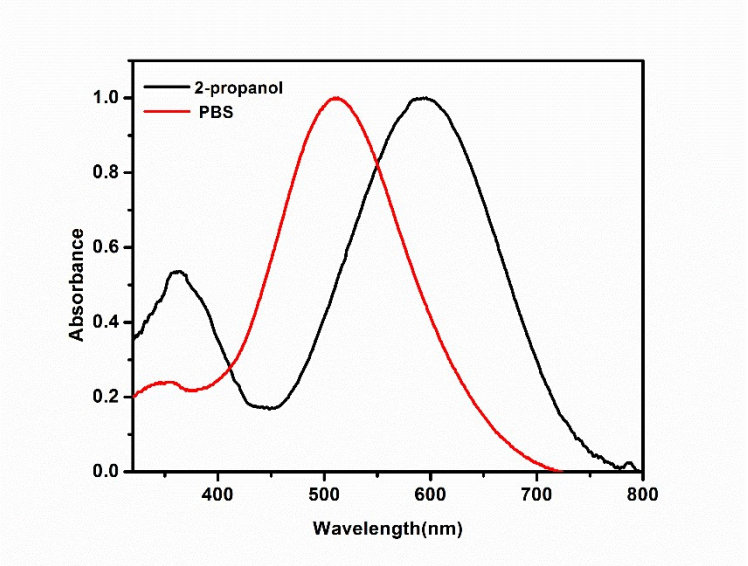

Figure 7: Absorption LDS 821on 2-propanol and on PBS buffer

Z scan technique is used to measure the nonlinear optical properties of LDS 821 on lysozyme amyloid fibrils. Figure 8 shows the experimental setup of Z-scan. First and second harmonic (1064, 532nm) from an Nd: YAG laser with a repetition rate of 10Hz and pulse duration of 10 ns is used as the light source. Nonlinear optical properties of the sample is measured by moving the sample along the beam axis of a focused laser beam. Calculated beam waist radius ω_0 are 0.085mm and

0.042mm for 1064 and 532nm laser input. The estimated Rayleigh length is 21.32mm and 10.4mm for 1064nm and 532nm input source which is greater than the sample cuvette (1mm). Two identical pyroelectric detectors are used to measure the transmitted beam, reference beam and sample cuvette their ratio. Open Z-scan is used to determine the nonlinear absorption of the sample. In open Z-scan as the sample approaches the focus of the laser beam transmittance valley is observed indicating the presence of a reverse saturable absorption or two photon absorption in the sample. The nonlinear absorption, were calculated from the experimental data which were fitted using equation 1.

$$T(z) = \sum_{m=0}^{\infty} \frac{\left[\frac{-\beta I_0 L_{eff}}{1+\frac{z^2}{Z_0^2}}\right]^m}{(m+1)^{3/2}} \qquad (1)$$

Where β is the two photon absorption coefficient, I_0 is the laser intensity at the focal point, $L_{eff} = \frac{1-e^{-\propto L}}{\propto}$, is the effective interaction length, L is the sample length and α is the linear absorption coefficient.

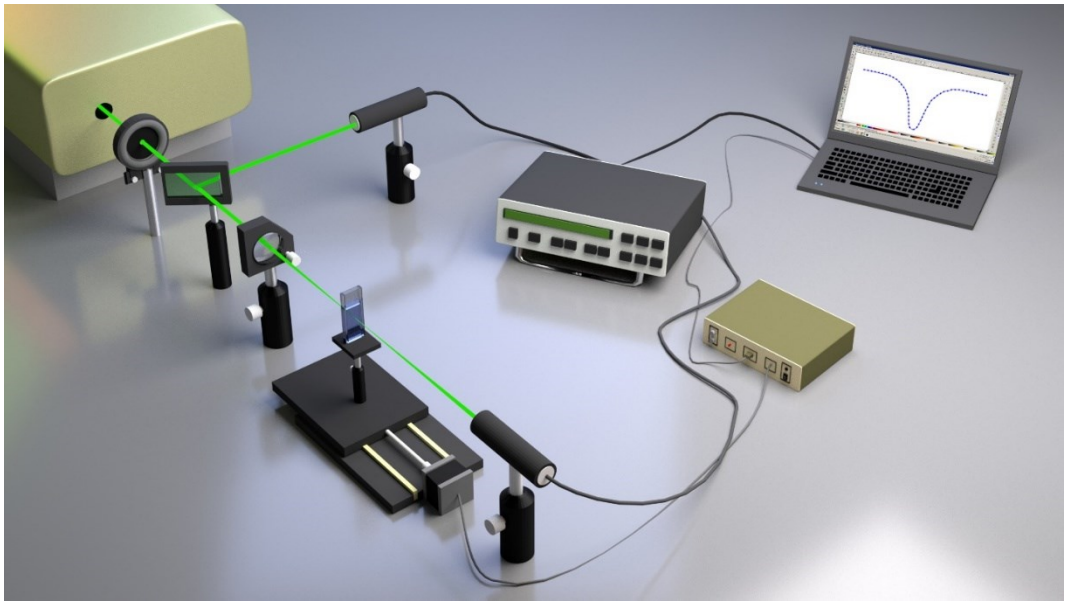

Figure 8: Open aperture Z-scan setup

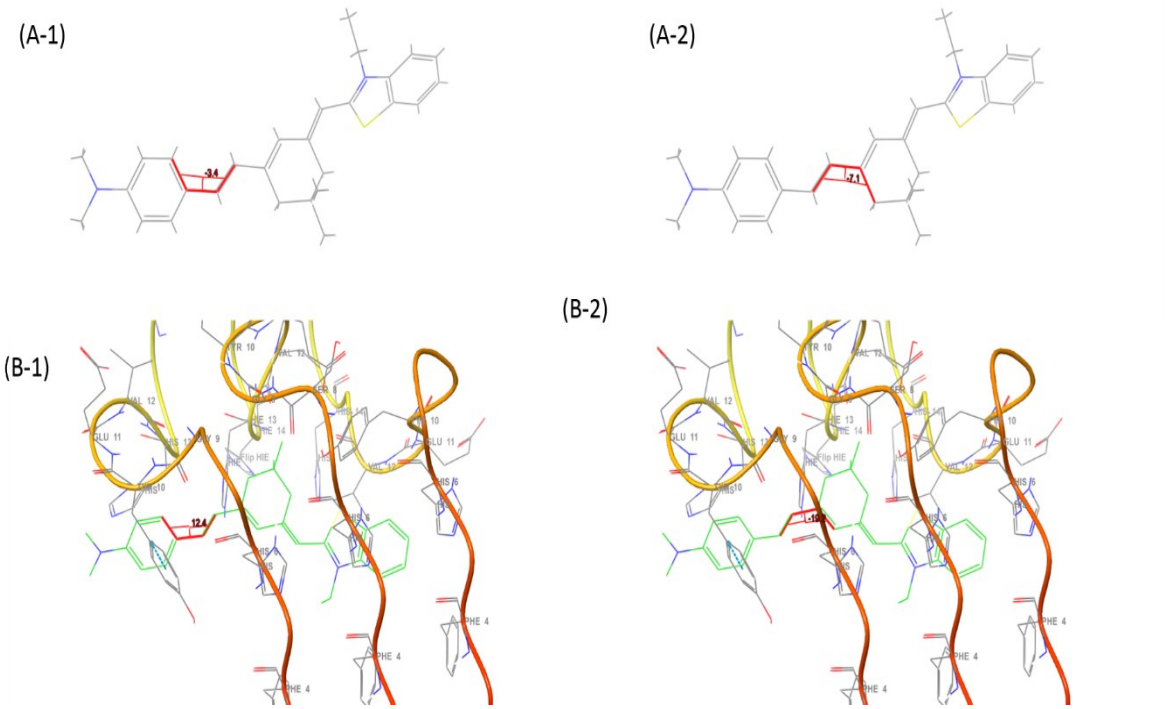

Figure 9: A-1 and B-1 shows the dihedral angle between benzene and double bond of LDS 821and LDS 821 amyloid fibril complex. A-2 and B-2dihedral angle between ethylene and cyclohexene ring of LDS 821and LDS 821 amyloid fibril complex