## **Supporting Information**

## Self-assembled Supramolecular Nanomicelles from Bile Acid-Docetaxel Conjugate are Highly Tolerable with Improved Therapeutic

## Efficacy

Vedagopuram Sreekanth,<sup>1,2</sup> Sanjay Pal,<sup>1,3</sup> Sandeep Kumar,<sup>1,2</sup> Varsha Komalla,<sup>1</sup> Poonam Yadav,<sup>1</sup> Radhey Shyam,<sup>4</sup> Sagar Sengupta,<sup>4</sup> and Avinash Bajaj<sup>1,\*</sup>

1. Laboratory of Nanotechnology and Chemical Biology, Regional Centre for Biotechnology, NCR Biotech Science Cluster, 3<sup>rd</sup> Milestone Faridabad-Gurgaon Expressway, Faridabad, Haryana, 121001, India.

- 2. Manipal Academy of Higher Education, Manipal, 576104, India.
- 3. Kalinga Institute of Industrial Technology, Bhubaneswar, Odisha, 751024, India.
- 4. National Institute of Immunology, Aruna Asaf Ali Marg, New Delhi, 110067, India.

Vedagopuram Sreekanth: Current address: Brigham and Women's Hospital, Division of Renal Medicine and Engineering, Boston, MA 02115, USA.

Varsha Komalla: Current address: Graduate School of Health, University of Technology, Sydney, Chippendale, NSW 2008, Australia.

Sandeep Kumar: Current address: Translational Tissue Engineering Center, Wilmer Eye Institute and Department of Biomedical Engineering, Johns Hopkins University School of Medicine, Baltimore, MD 21205, USA.

\*Corresponding Author:

Email: <u>bajaj@rcb.res.in</u>

Ph: +91-124-2848831

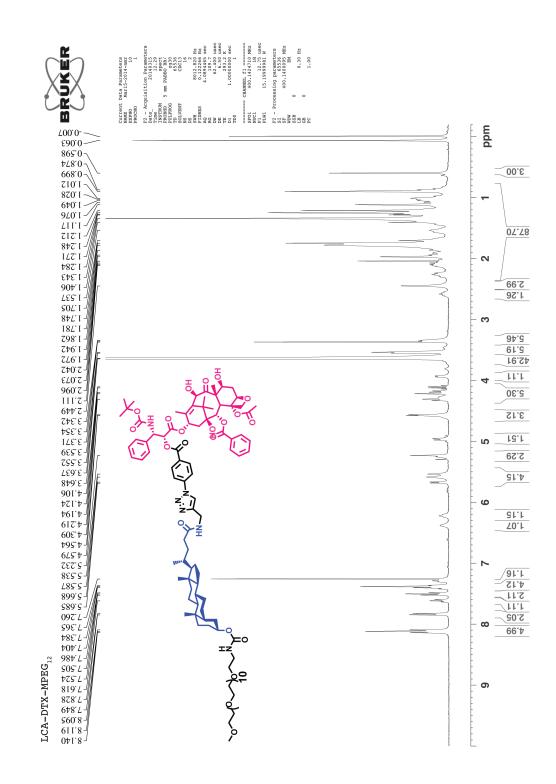


Figure S1. <sup>1</sup>H NMR Spectra of LCA-DTX-PEG.

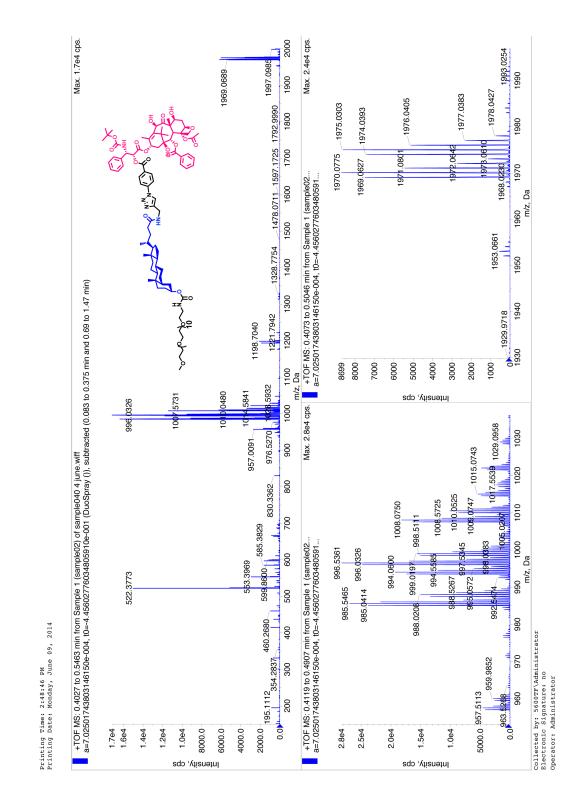


Figure S2. HRMS of LCA-DTX-PEG.

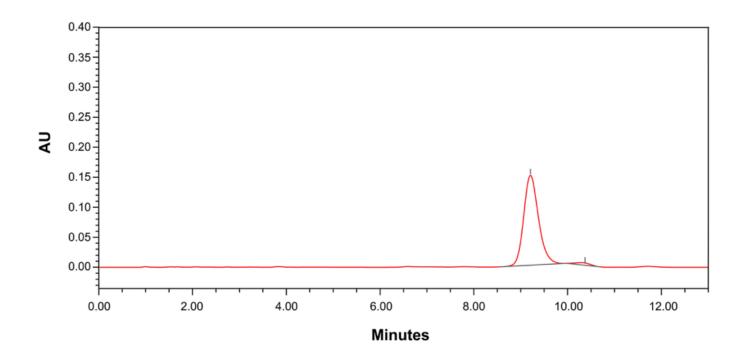
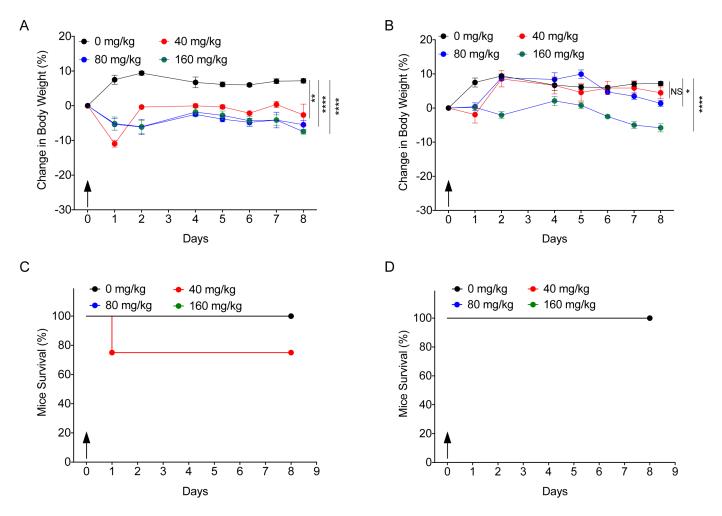
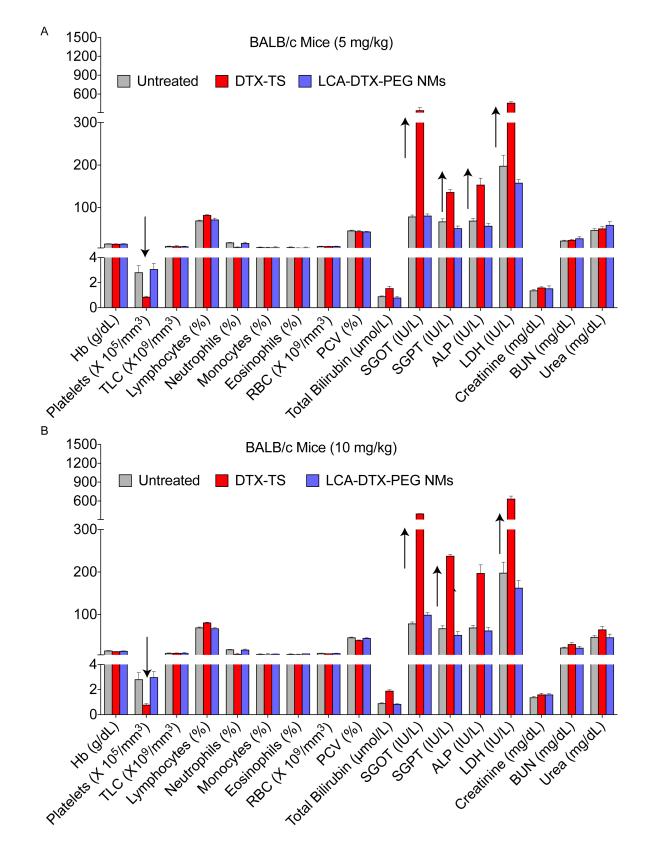


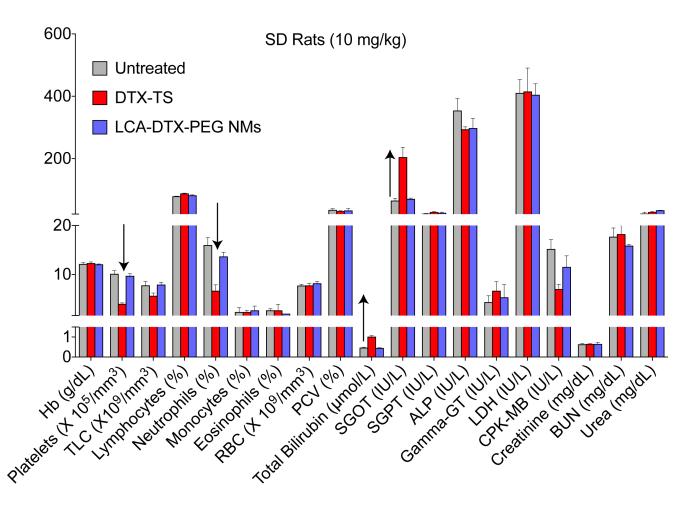
Figure S3. HPLC profile of LCA-DTX-PEG.



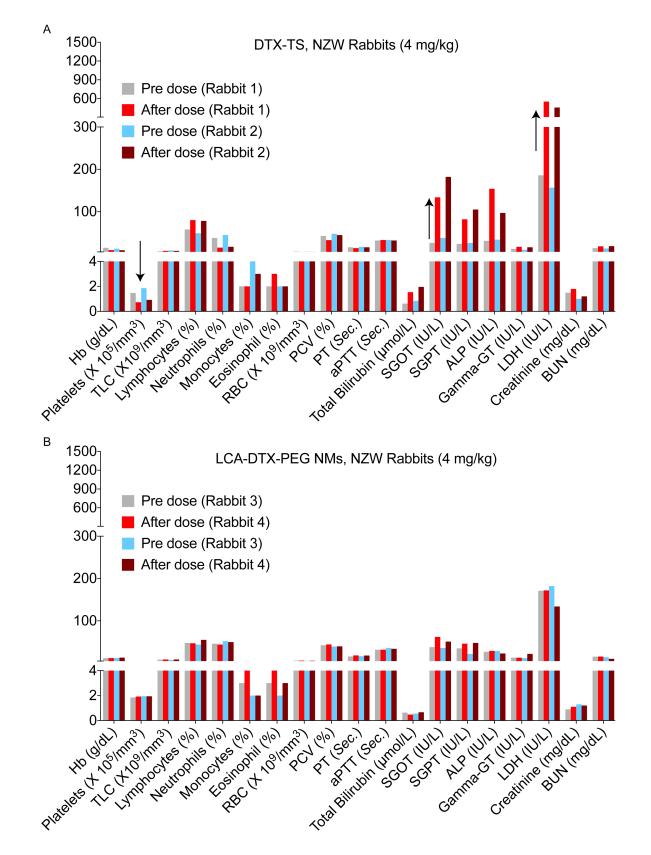
**Figure S4. Maximum tolerated dose estimation upon single dose.** (A-D) Percentage change in body weight (A, B) and survival (C, D) of BALB/c mice upon single dose administration of 40, 80 or 160 mg/kg (DTX equivalent) of DTX-TS (A, C) and LCA-DTX-PEG NMs (B, D).



**Figure S5. Toxicological studies in BALB/c mice.** Changes in critical hematological and serological biomarkers of BALB/c mice after five doses of 5 (A) or 10 (B) mg/kg of DTX-TS and LCA-DTX-PEG NMs. Critical changes in the levels are indicated by upward/ downward arrow.



**Figure S6. Toxicological studies in SD rats** Changes in critical hematological and serological biomarkers of SD rats after 24 h of single dose administration of 10 mg/kg of DTX-TS and LCA-DTX-PEG NMs. Critical changes in the levels are indicated by upward/ downward arrow.



**Figure S7. Toxicological studies in rabbits.** Changes in critical hematological and serological biomarkers of each rabbit after 24 h of single dose administration of 4 mg/kg of DTX-TS (A) and LCA-DTX-PEG NMs (B). Critical changes in the levels are indicated by upward/ downward arrow.