

# Effect of *para* sulfonato calix[4]resorcinarene (PSC[4]R) on the solubility, bioavailability of a poorly water soluble drug lamotrigine (LMN) and their computational investigation

Manishkumar B. Patel,<sup>a</sup> Nikunj N. Valand,<sup>a</sup> Nishith R. Modi,<sup>a</sup> Kuldeep V. Joshi,<sup>a</sup> Uma Harikrishnan,<sup>a</sup> Sivakumar Prasanth Kumar,<sup>b</sup> Yogesh T. Jasrai,<sup>b</sup> Shobhana K. Menon\*<sup>a</sup>

<sup>a</sup>Department of Chemistry, University School of Sciences, Gujarat University, Navrangpura, Ahmedabad-380009, Gujarat, India.

<sup>b</sup>Department of Bioinformatics, Applied Botany Centre (ABC), University School of Sciences, Gujarat University, Navrangpura, Ahmedabad-380009, Gujarat, India.

**Corresponding Author:** \* Tel: +91 79 26302286; fax: +91 79 26308545

E-mail address: [shobhanamenon07@gmail.com](mailto:shobhanamenon07@gmail.com)

## SUPPLEMENTARY FILES

**Figure-S<sub>1</sub>:** The MD trajectory of PSC[4]R-LMN inclusion complex over 10 ns in AVI format.

**Figure-S<sub>2</sub>:** Docked pose of PSC[4]R-LMN inclusion complex in PDB format.

**Figure-S<sub>3</sub>:** The equilibrated structure of PSC[4]R-LMN inclusion complex from MD studies in PDB format.