pharmaceutics

MDPI

Supplementary Materials: Quantitative Structure–Activity Relationship of Enhancers of Licochalcone A and Glabridin Release and Permeation Enhancement from Carbomer Hydrogel

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Methods S1 The HPLC methods of LicA and Gla

The HPLC method of LicA was showed as follows: The samples were analyzed by HPLC (Agilent 1260, USA)equipped with C18 column and DAD detector. The mobile phase consisted of combinations of A (methanol), B (acetonitrile) and C (0.1% phosphate in water, *v*/*v*) at a flow rate of 1.0 mL/min with an elution as follows: 0–13 min, 20% A and 45% B. The detection wavelength was set at 300 nm with a retention time of 8.36 min. The calibration curve was linear over the range 0.01–100 μg/mL (r^2 = 0.9992). The injection volume was 20 μL. For Gla, the detection wavelength was set at 230 nm with a retention time of 12.44 min, and the calibration curve was linear over the range 0.01–100 μg/mL (r^2 = 0.9995)

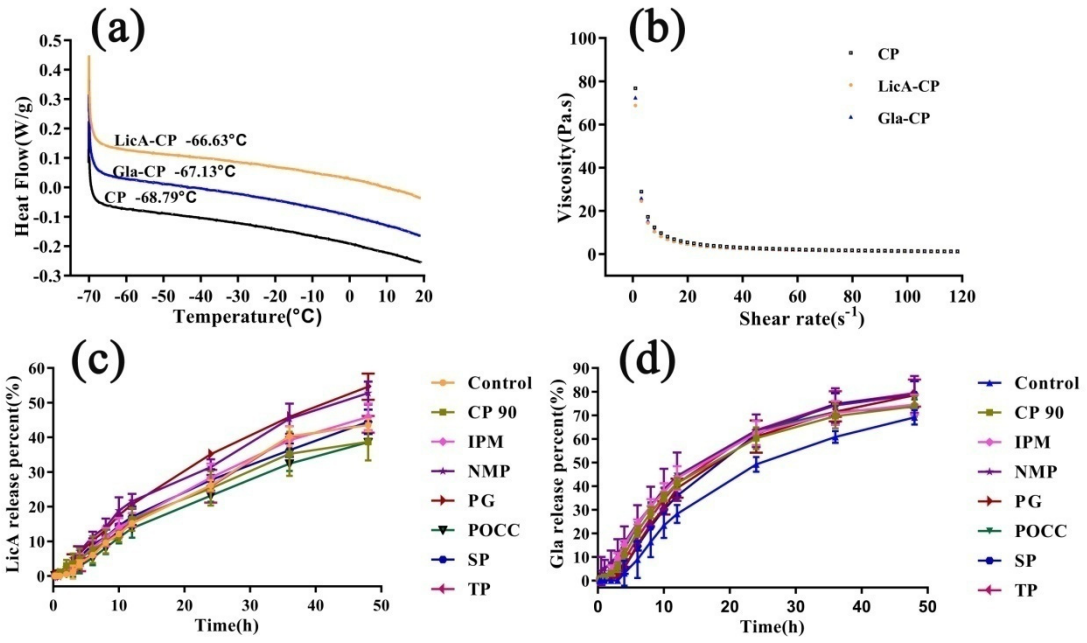

Figure S1. (**a**) DSC curves of different hydrogels; (**b**) Flow characterization of the hydrogels (n = 3); (**c**) In vitro drug release profiles of LicA-CP hydrogel when enhancers were added (n = 3); (**d**) In vitro drug release profiles of LicA-CP hydrogel when enhancers were added (n = 3).

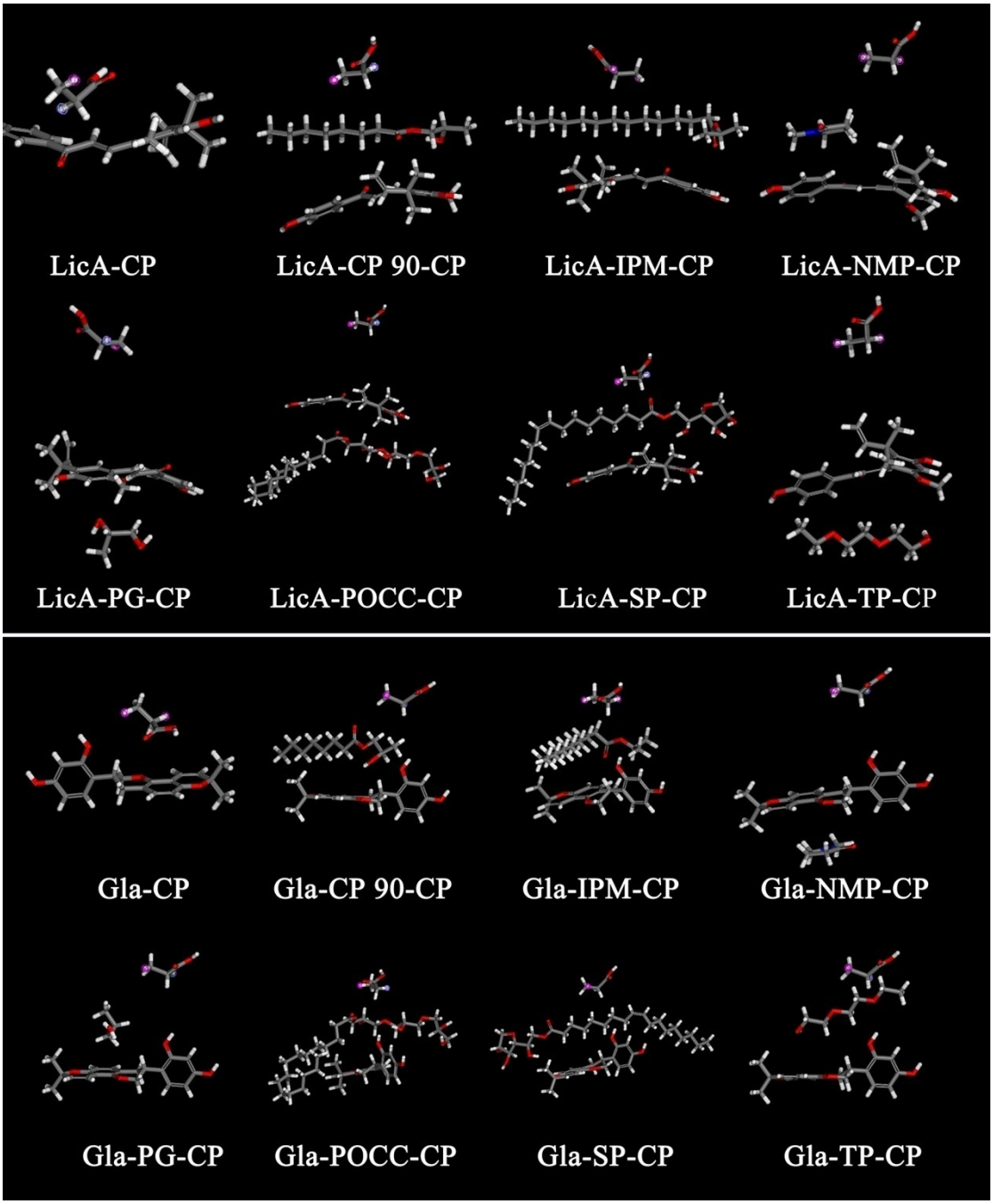

Figure S2. Conformation of LicA-enhancers-CP and Gla-enhancers-CP ternary systems.

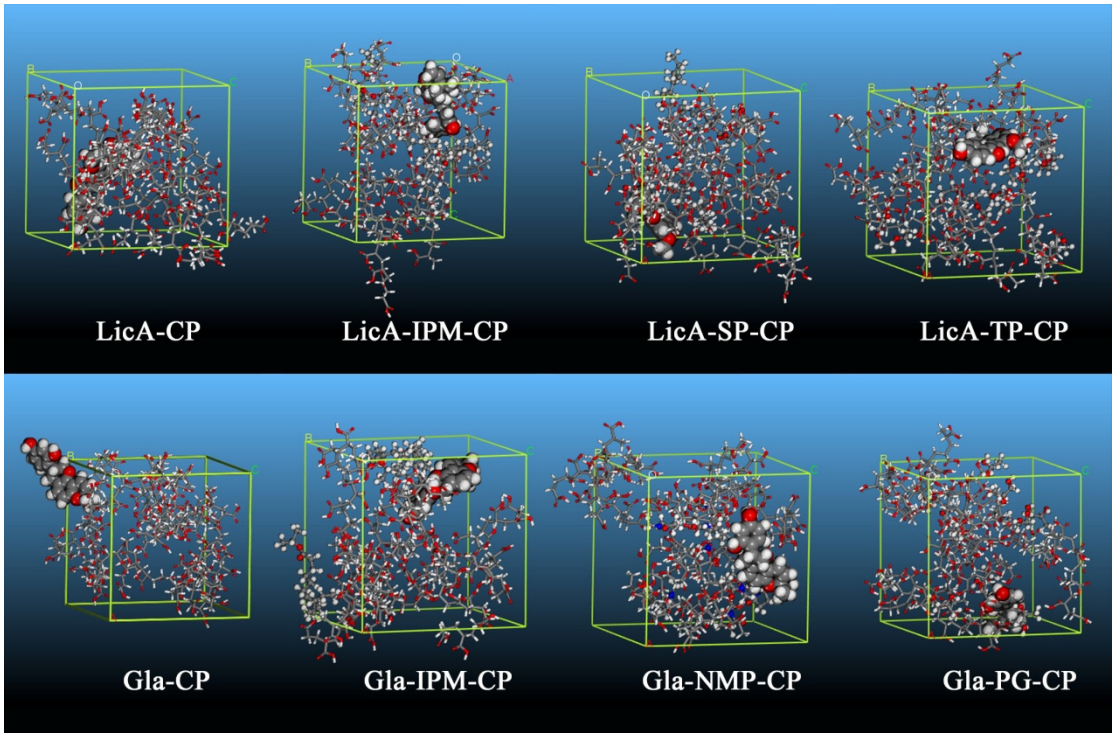

Figure S3. The snapshots of LicA (Gla)-enhancers-CP systems at the end of the MD. (Drug: Ball and stick model; Enhancers: CPK model).

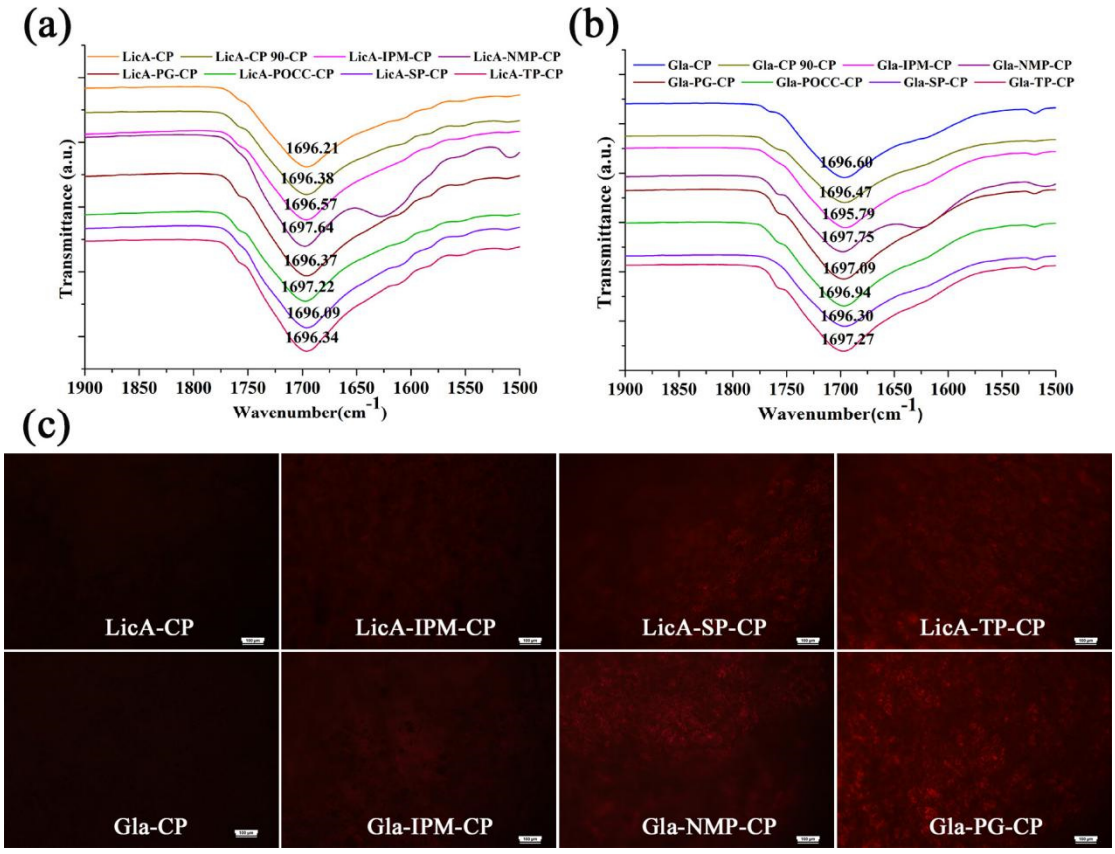

Figure S4. (**a**) FT-IR spectra (C=O group) of LicA-enhancers-CP systems; (**b**) FT-IR spectra (C=O group) of Gla-enhancers-CP systems; (**c**) PLM images of drug-CP films after different enhancers were added.

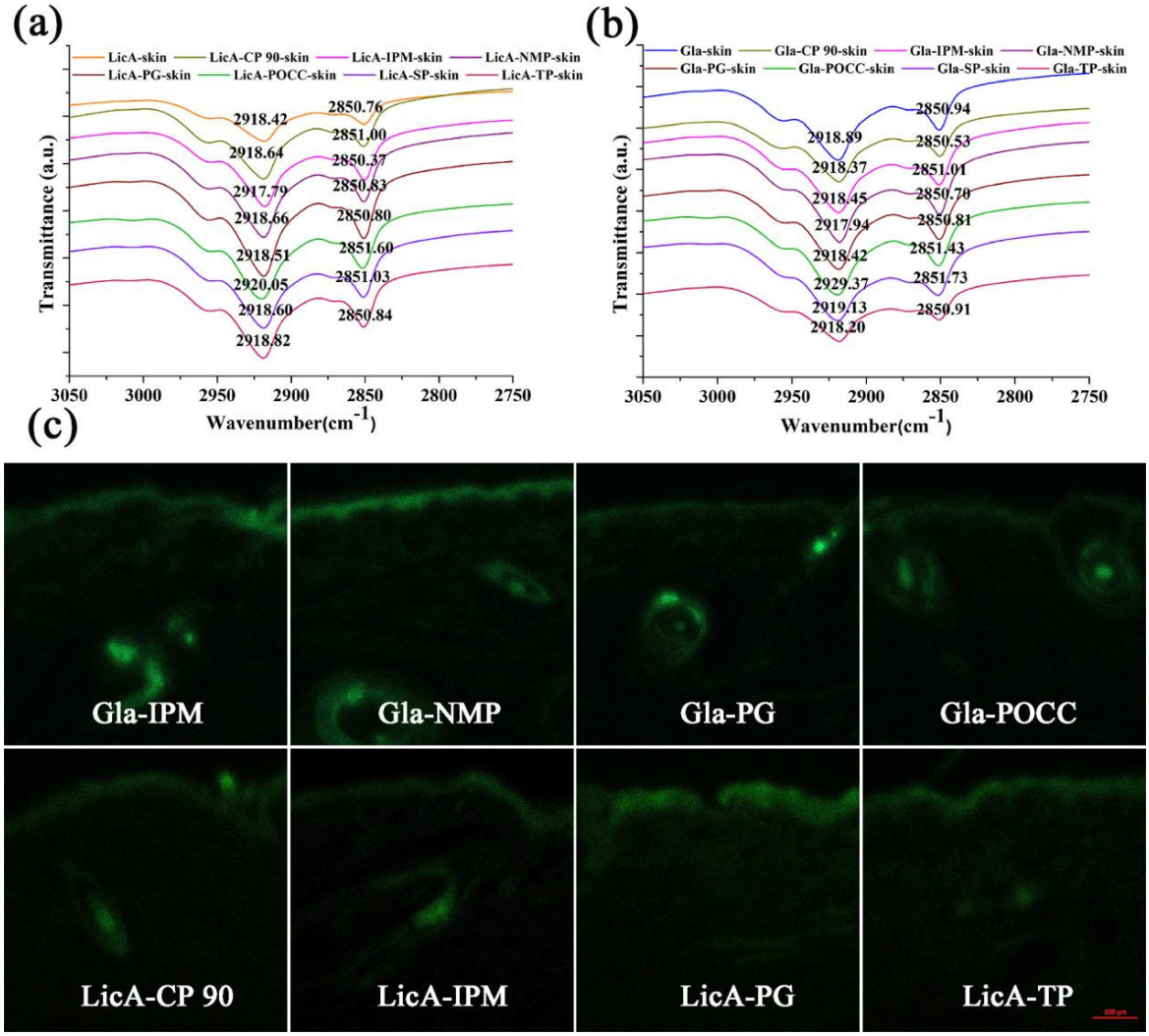

Figure S5. (**a**) FT-IR spectra (CH_2-group) of LicA-enhancers-skin systems; (**b**) FT-IR spectra (CH_2-group) of Gla-enhancers-skin systems; (**c**) CLSM images of penetration depth and fluorescence intensity LicA and C6 in porcine skin treated by enhancers (bar = 100 μm).

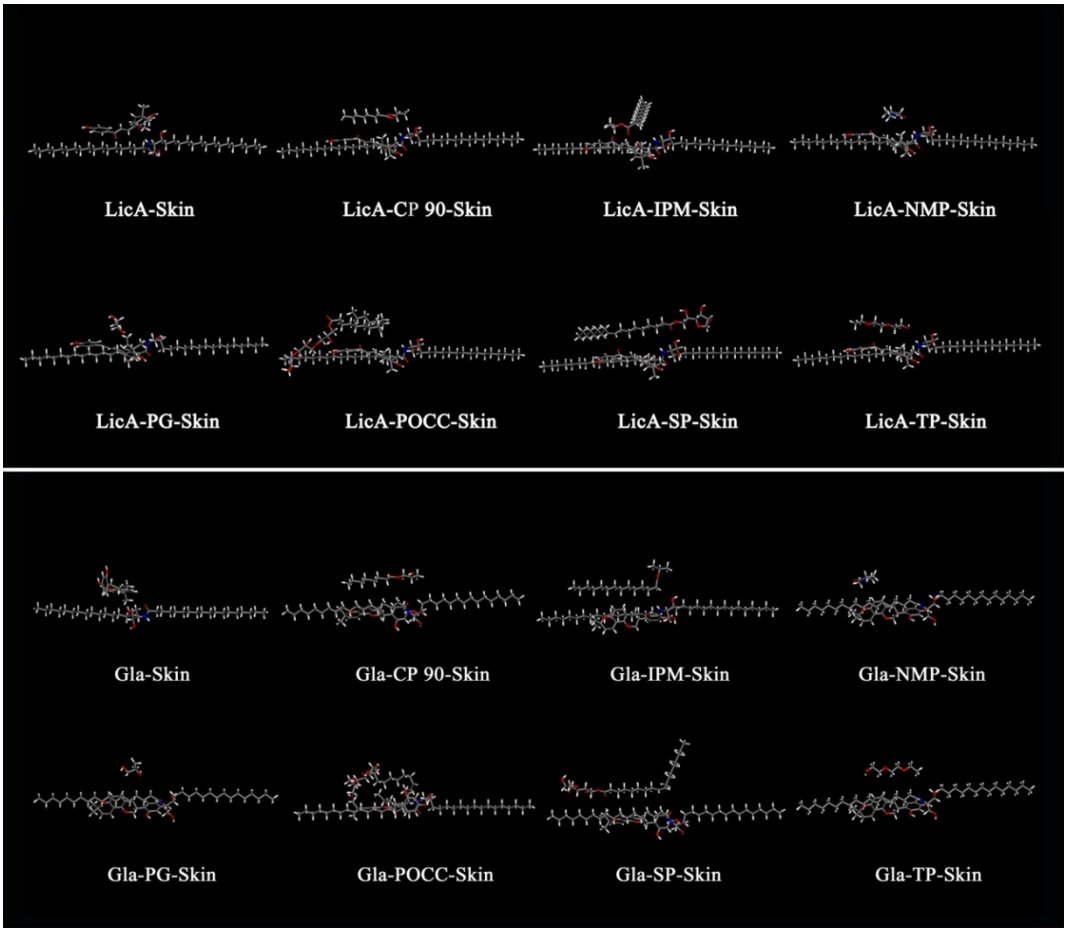

Figure S6. Conformations of LicA-enhancers-skin and Gla-enhancers-skin ternary systems.

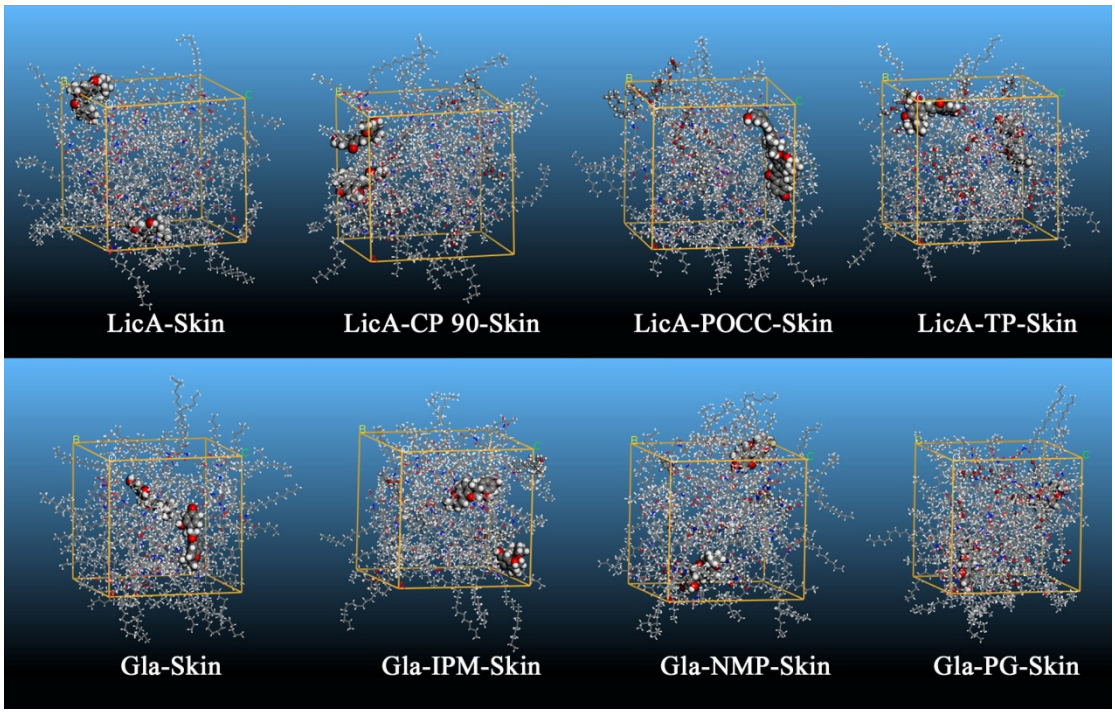

Figure S7. The snapshots of LicA (Gla)-enhancers-skin systems at the end of the MD. (Drug: Ball and stick model; Enhancers: CPK model).