

Supplementary Information

Drug-nutrient cocrystallization-driven strategy towards self-assembly of milrinone and ferulic acid provides an exemplification in perfecting *in vitro/vivo* characteristics of anti-heart failure drugs

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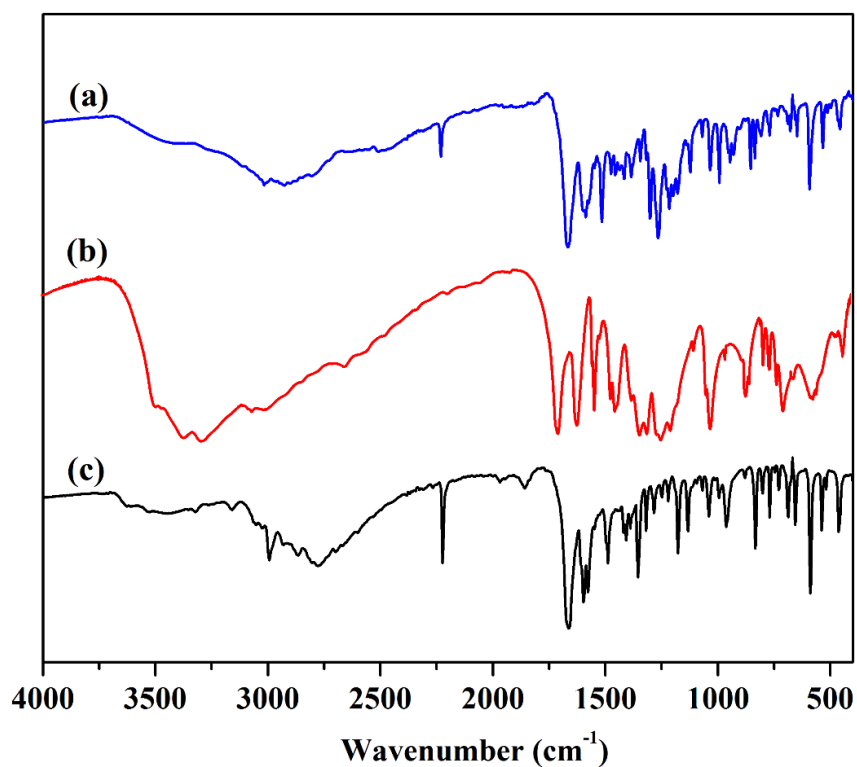


Fig. S1 FT-IR spectra of MLN-FEA cocrystal (a), FEA (b) and MLN (c).

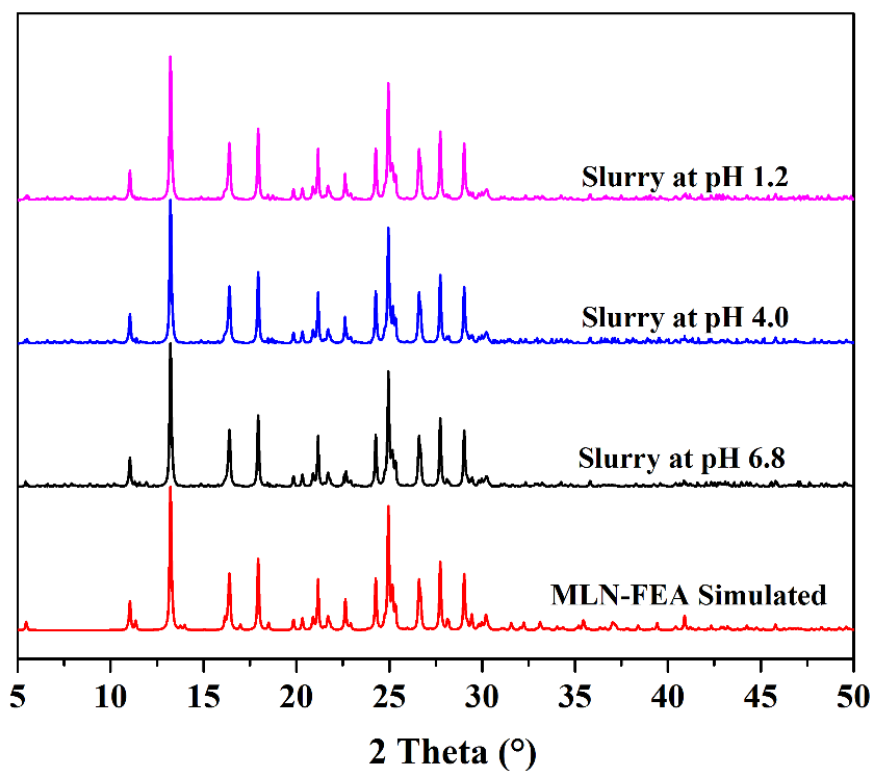


Fig. S2 PXRD comparison of simulated pattern and experimental pattern for remaining solids after the powder dissolution measurements.

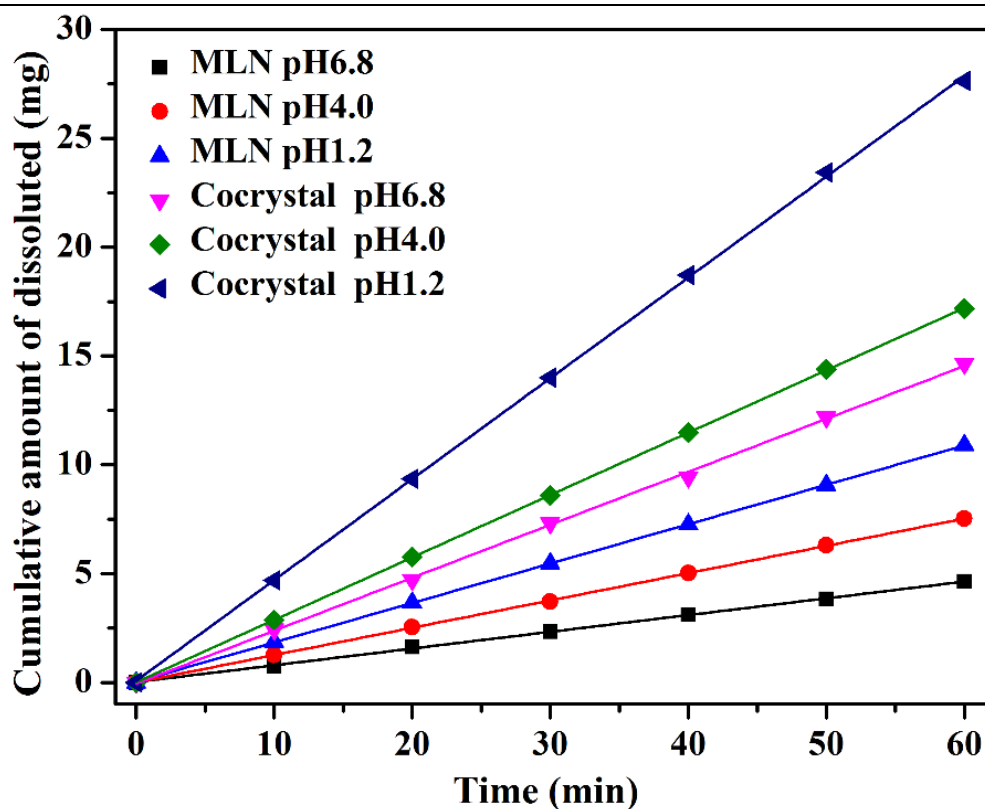


Fig. S3. IDR profiles of MLN and MLN-Fea cocrystal at pH 1.2, 4.0, and 6.8 buffers.

Table S1 Some parameters related to molecular electrostatic potentials.

| Samples | Global average positive electrostatic potential (kJ/mol) | Global average negative electrostatic potential (kJ/mol) | Molecular polarity index (kJ/mol) | Polar surface area percentage (%) |
|-----------|----------------------------------------------------------|----------------------------------------------------------|-----------------------------------|-----------------------------------|
| MLN | 60.85 | -75.06 | 65.23 | 70.99% |
| Cocrystal | 70.60 | -80.29 | 75.34 | 73.68% |