Molecular Interactions between APIs and Enteric Polymeric Excipients in Solid Dispersion: Insights from Molecular Simulations and Experiments

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Table S1. Solubilities, melting points, and degradation temperatures of the API and polymers.

Drug	**MW (Da)**	**Solubility**	**Melting point/Tg (°C)**	**Degradation temp (°C)**
Diclofenac Sodium	318.13	Soluble in water	285	285
Naproxen	230.25	Practically insoluble at pH below 4	155	196
Dimethyl fumarate	144.12	Soluble in water	102	Not reported
Omeprazole	345.4	Very slightly soluble in water	156	156
HPMC-P 55	35000	Soluble above pH 5.5	143	199
HPMC-AS (LF)	16000	Soluble above pH 5.5	122	204
Eudragit L100-55	135000	Soluble above pH 5.5	120	170

Table S2. Number of Hydrogen-bonds between polymer excipients and APIs.

Polymer excipients	**Drug APIs**			
	Naproxen	**Diclofenac sodium**	**Dimethyl fumarate**	**Omeprazole**
HPMC(P)	0.73	1.37	0.36	1.29
HPMC(AS)	0.86	1.84	0.62	1.50
Eudragit L100	1.07	1.61	0.93	1.78

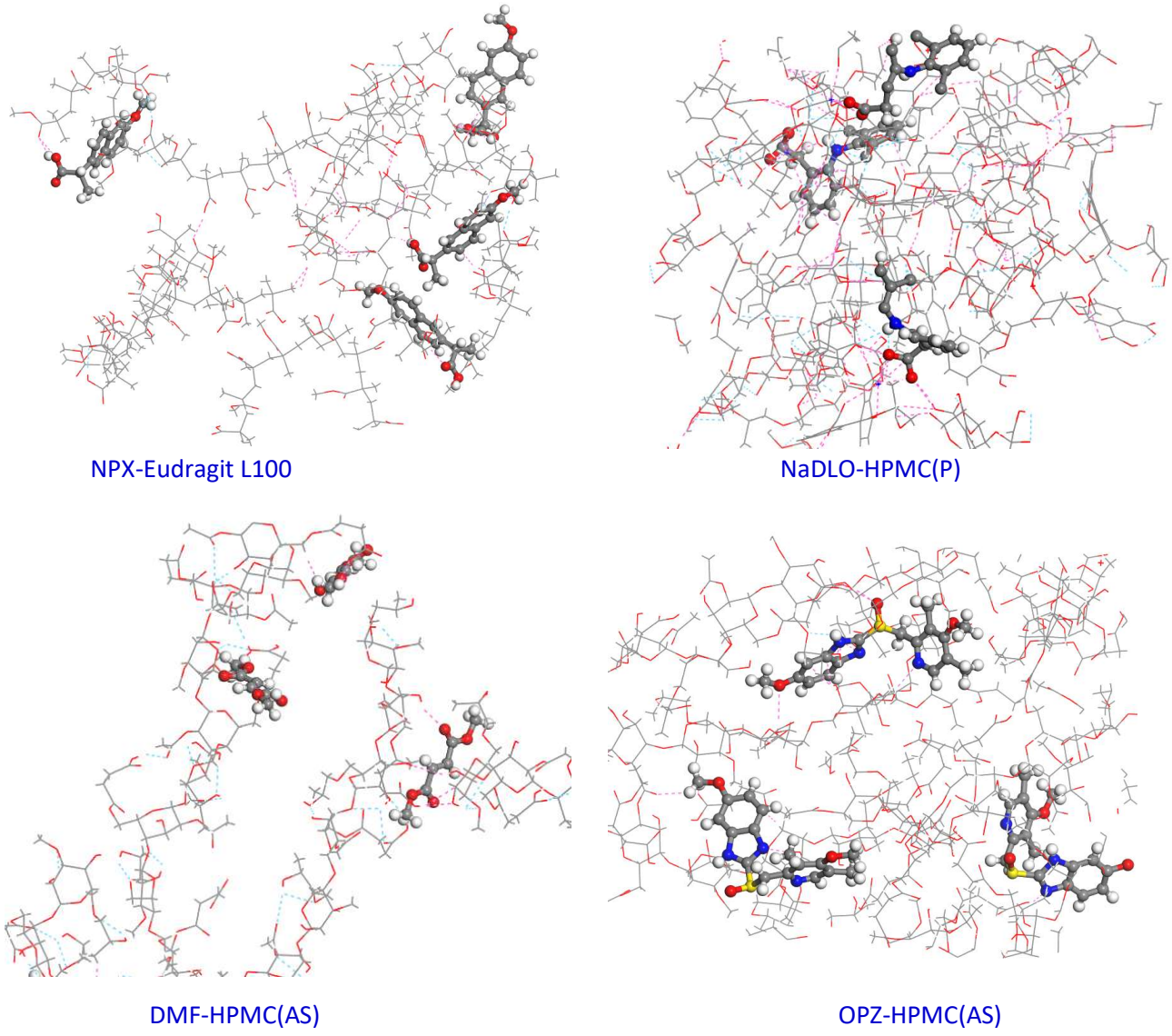
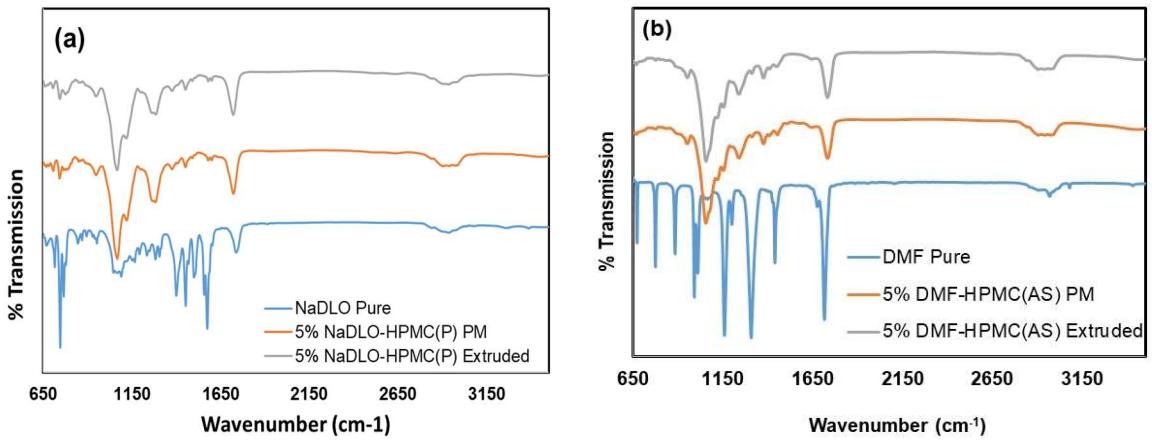


Fig. S1. Part of the final snapshots from MD simulations corresponding to the best API-polymer pairs.



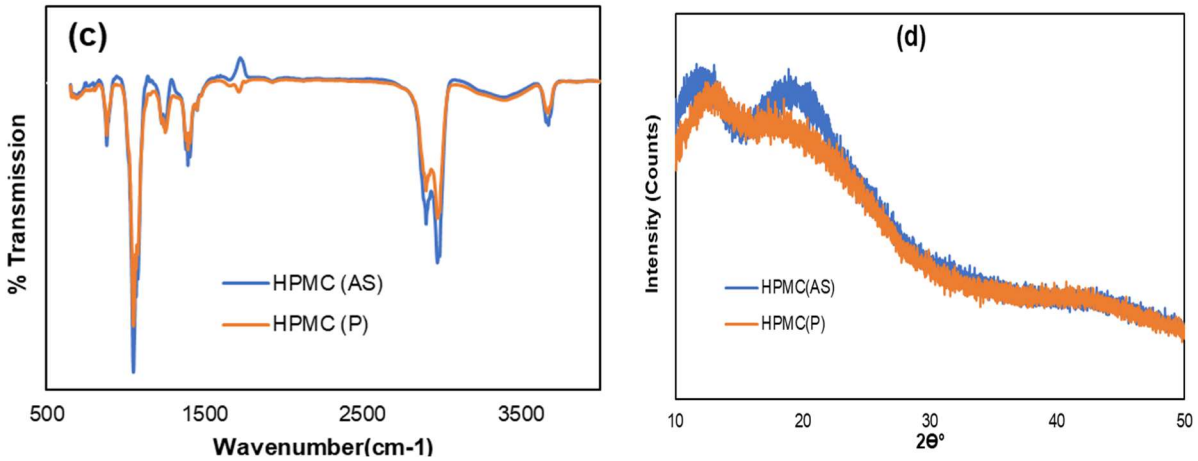


Fig. S2. FTIR spectra of at 5% w/w API loading in (a) NaDLO–HPMC(P) physical mixture and extruded, (b) DMF– HPMC(AS) physical mixture and extruded, (c) FTIR and (d) PXRD of pure polymers.

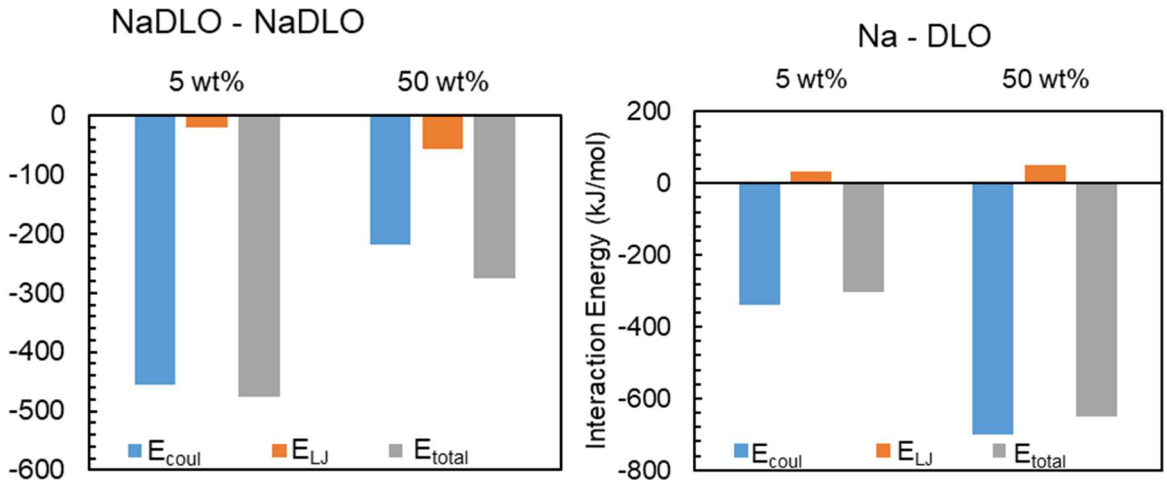


Fig. S3. Interaction energies between: NaDLO and NaDLO, and Na^+ and DLO at 5 and 50 wt% NaDLO.

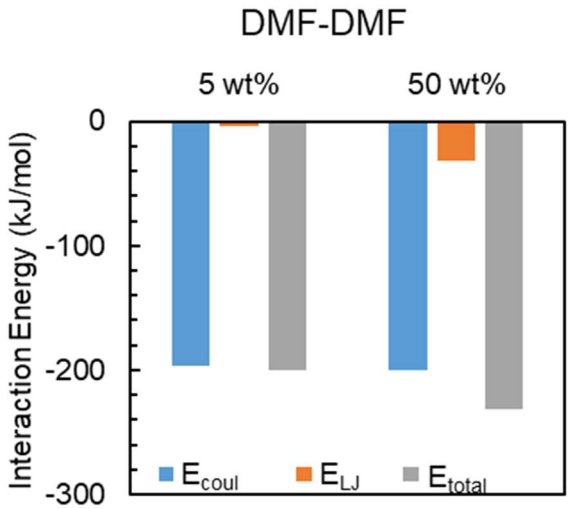


Fig. S4. Interaction energies between DMF and DMF at 5 and 50 wt% DMF.