

Supporting information

On the parallelism between the mechanisms behind chromatography and drug delivery: the role of interactions with stationary phase

Filippo Rossi ^{a,*,1}, Franca Castiglione ^{a,1}, Matteo Salvalaglio ^b, Monica Ferro ^a,
Marta Moioli ^a, Emanuele Mauri ^a, Maurizio Masi ^a and Andrea Mele ^{a,c,*}

a Department of Chemistry, Materials and Chemical Engineering “Giulio Natta”, Politecnico di Milano, via Mancinelli 7, 20131 Milan, Italy;

b Department of Chemical Engineering, University College London, Torrington Place, London WC1E 7JE, United Kingdom;

c CNR-ICRM, via Luigi Mancinelli 7, 20131 Milan, Italy

* corresponding author, email: filippo.rossi@polimi.it, Tel: (+39) 02 23993145, fax: (+39) 02 23993180;

* corresponding author, email: andrea.mele@polimi.it, Tel: (+39) 02 23993006, fax: (+39) 02 23993180;

¹ these authors equally contributed to this work

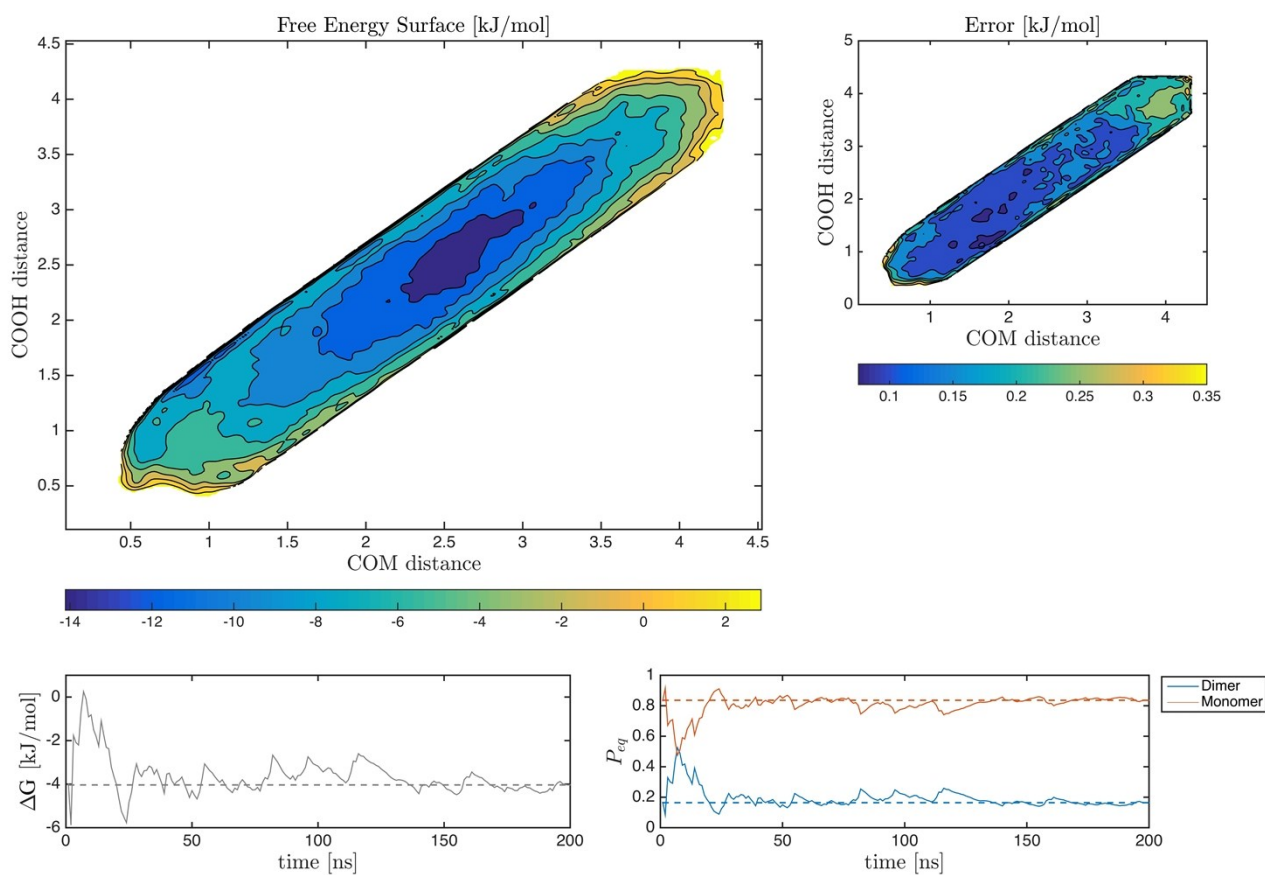


Figure S1. Free energy of dimerization of protonated IP molecules obtained from simulation S2. (*Top left*) Free Energy Surface (FES) as a function of the CVs used to enhance the sampling through WTmetaD. (*Top right*) FES error in the space of CVs evaluated as the standard deviation of the time-independent estimator of the free energy in the CVs space. (*Bottom-left*) Free energy difference between dissociated and dimer-like states as a function of simulation time. (*Bottom-right*) Equilibrium probabilities of undissociated and dissociated states.

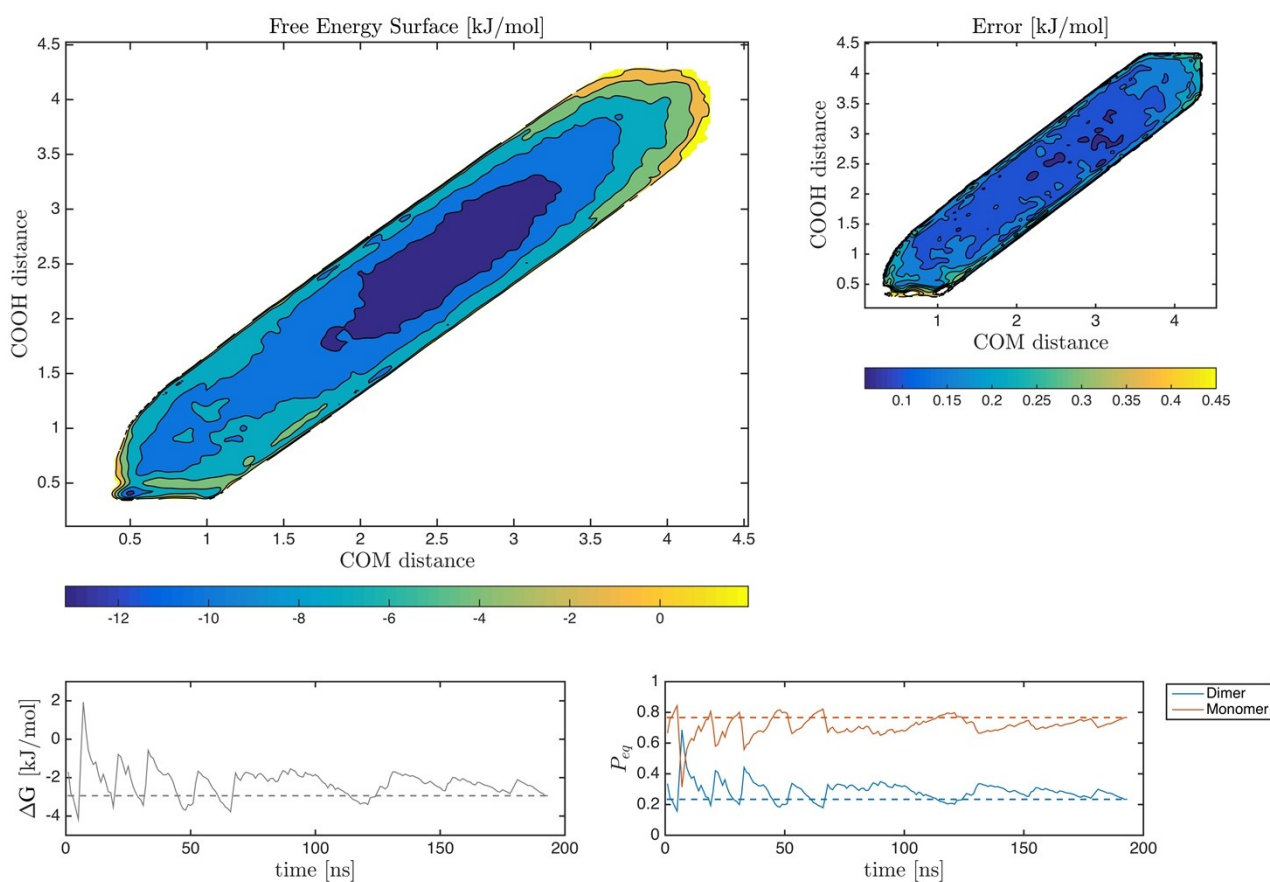


Figure S2. Free energy of dimerization of protonated IP molecules obtained from simulation S3. (*Top left*) Free Energy Surface (FES) as a function of the CVs used to enhance the sampling through WTmetaD. (*Top right*) FES error in the space of CVs evaluated as the standard deviation of the time-independent estimator of the free energy in the CVs space. (*Bottom-left*) Free energy difference between dissociated and dimer-like states as a function of simulation time. (*Bottom-right*) Equilibrium probabilities of undissociated and dissociated states.