SUPPLEMENTARY MATERIAL TO

A thermodynamic approach for correlating the solubility of drug compounds in supercritical CO2 based on Peng-Robinson and Soave-Redlich-Kwong equations of states coupled with van der Waals mixing rules

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The constants of PR and SRK equations of state are as below:

For SRK equation of state we have *c*1=0 and *c*2=1.

  (S1)

  (S2)

  (S3)

  (S4)

Where, *T*c, *P*c and *ω* are indicative of critical temperature, critical pressure and acentric factor. *T*r and *R* are reduced temperature and universal gas constant. Similarly, for PR equation of state we have *c*1=1-21/2 and *c*2=1+21/2.

  (S5)

  (S6)

  (S7)

  (13)

For a mixture of heavy component and SCF, the EOS parameters a and b are calculated by the following mixing rules:1

vdW1 mixing rule:

  (S8)

  (S9)

  (S10)

vdW2 mixing rule:

  (S11)

  (S12)

  (S13)

  (S14)

Where, *y*i and *y*j are mole fractions of components i and j and *k*ij and *l*ij are the binary interaction parameters and i and j refer to ith and jth compounds in the mixture.

*â*i and  in equation (6) of the manuscript are derivatives related to the attractive and repulsive parameters of EOS which are calculated from following equations:

vdW1 mixing rule:

  (S15)

  (S16)

vdW2 mixing rule:

  (S17)

  (S18)