

Supporting information

Solubility Data, Solubility Parameters and Thermodynamic Behavior of an Antiviral Drug Emtricitabine in Different Pure Solvents: Molecular Understanding of Solubility and Dissolution

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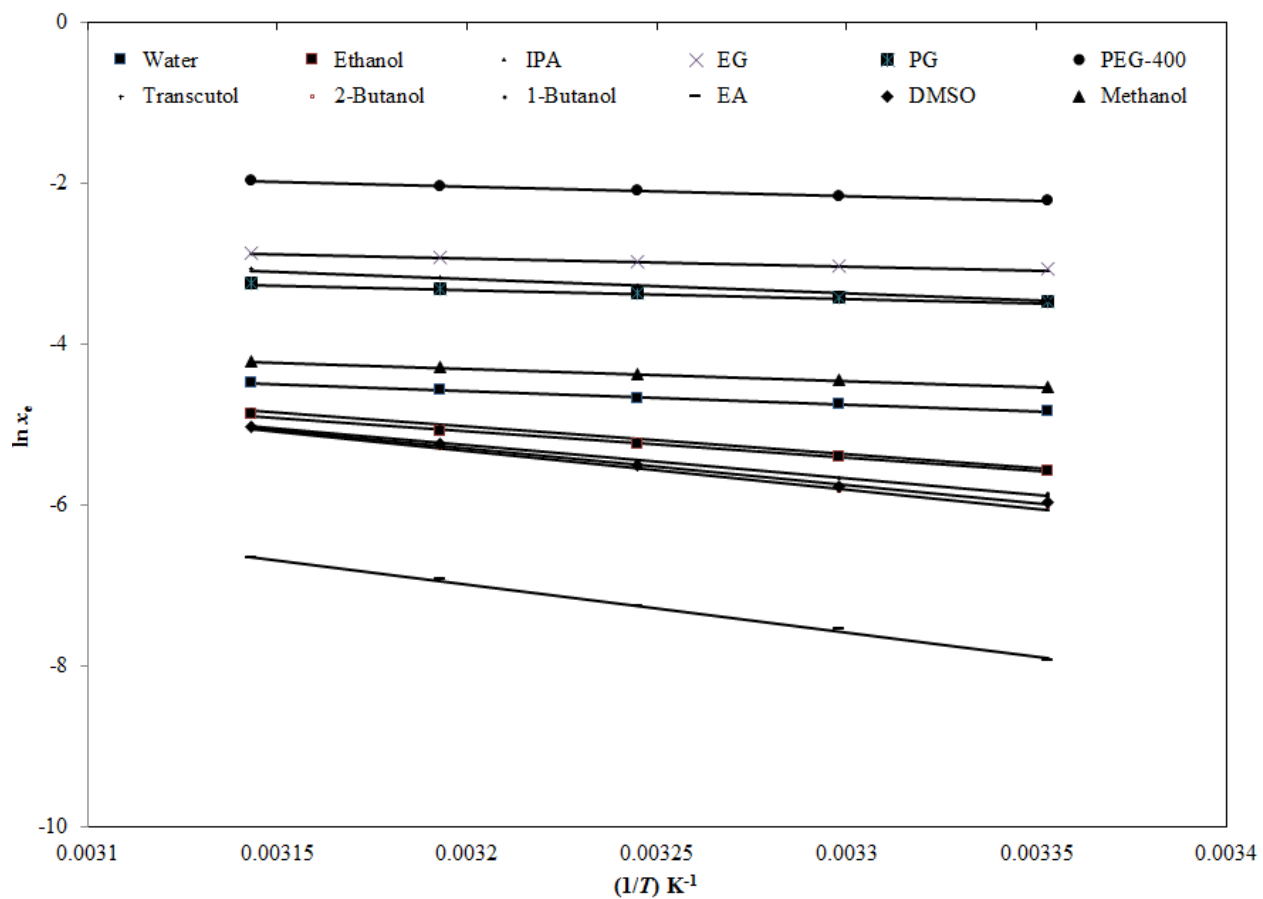


Figure S1. Correlation of experimental natural logarithmic solubilities ($\ln x_e$) of emtricitabine (ECT) with “van’t Hoff model” in various pure solvents (*PS*) as a function of $1/T$; symbols represent the experimental $\ln x_e$ values of ECT and the solid lines represent the $\ln x^{\text{van't}}$ values calculated by “van’t Hoff model”.

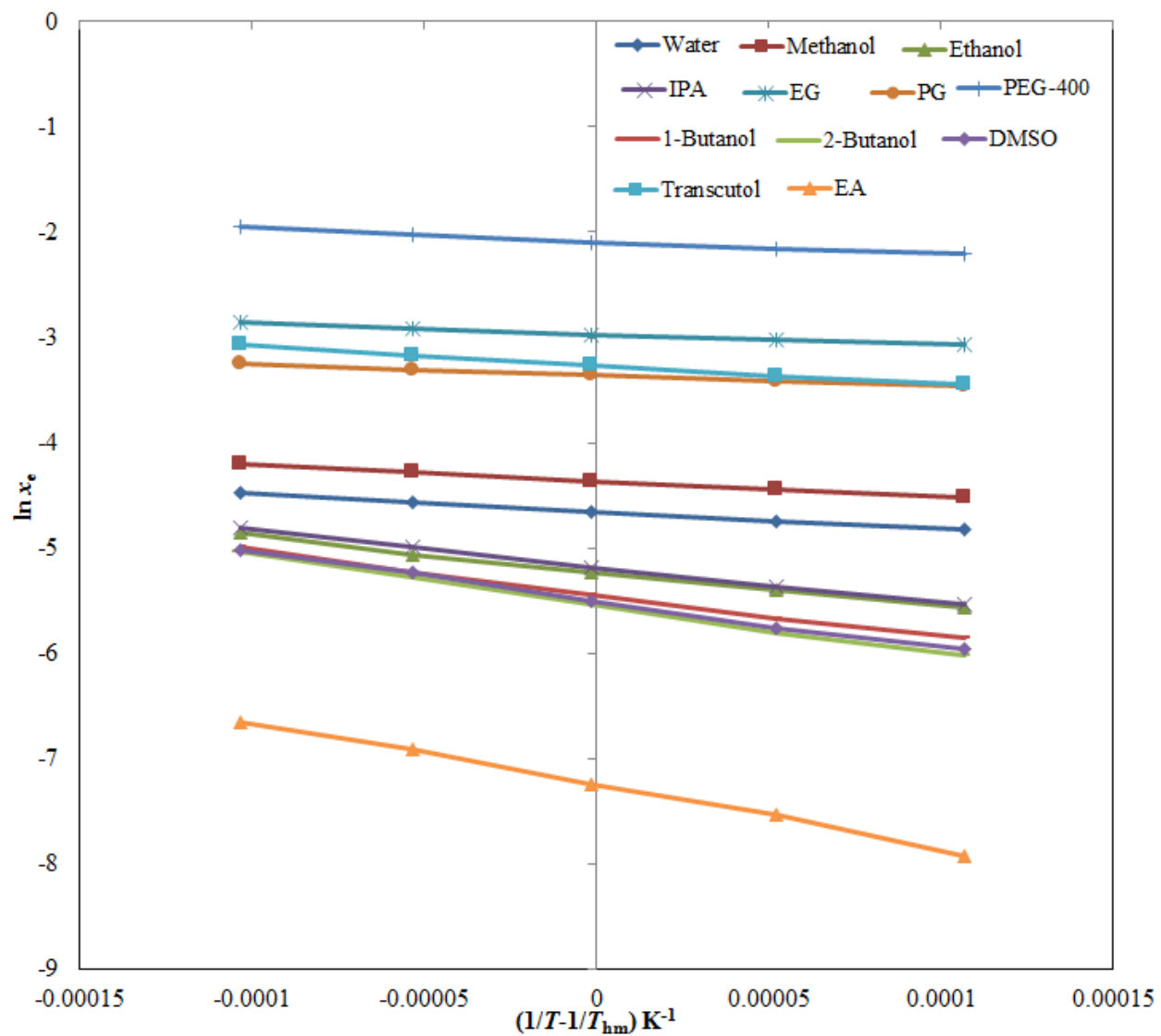


Figure S2. van't Hoff plots for ECT plotted between $\ln x_e$ and $1/T - 1/T_{hm}$ for ECT in various PS.

Table S1: List of materials and their properties.

Material	Molecular formula	Molar mass (g mol ⁻¹)	CAS Registry no.	Purification method	Mass fraction purity	Analysis method	Source
ECT	C ₈ H ₁₀ FN ₃ O ₃ S	247.24	143491-57-0	None	>0.98	HPLC	Sigma Aldrich
Methanol	CH ₃ OH	32.04	67-56-1	None	>0.99	GC	Sigma Aldrich
Ethanol	C ₂ H ₅ OH	46.07	64-17-5	None	>0.99	GC	Sigma Aldrich
EG	C ₂ H ₆ O ₂	62.07	107-21-1	None	>0.99	GC	Fluka Chemica
Transcutol	C ₆ H ₁₄ O ₃	134.17	111-90-0	None	>0.99	GC	Gattefosse
PG	C ₃ H ₈ O ₂	76.09	57-55-6	None	>0.99	GC	Fluka Chemica
PEG-400	H(OCH ₂ CH ₂) _n OH	400	25322-68-3	None	>0.99	HPLC	Fluka Chemica
IPA	C ₃ H ₈ O	60.10	67-63-0	None	>0.99	GC	Sigma Aldrich
1-Butanol	C ₄ H ₁₀ O	74.12	71-36-3	None	>0.99	GC	Sigma Aldrich
2-Butanol	C ₄ H ₁₀ O	74.12	78-92-2	None	>0.99	GC	Sigma Aldrich
DMSO	C ₂ H ₆ OS	78.13	67-68-5	None	>0.99	GC	Fluka Chemica
EA	C ₄ H ₈ O ₂	88.11	141-78-6	None	>0.99	GC	Fluka Chemica
Water	H ₂ O	18.07	7732-18-5	None	-	-	Milli-Q

Both the analysis method and purity were provided by supplier of each material.