Supporting Information

OPTIMIZED SYNTHESIS AND SOLID STATE INVESTIGATIONS ON THE DRUG CANDIDATE ENCENICLINE HYDROCHLORIDE

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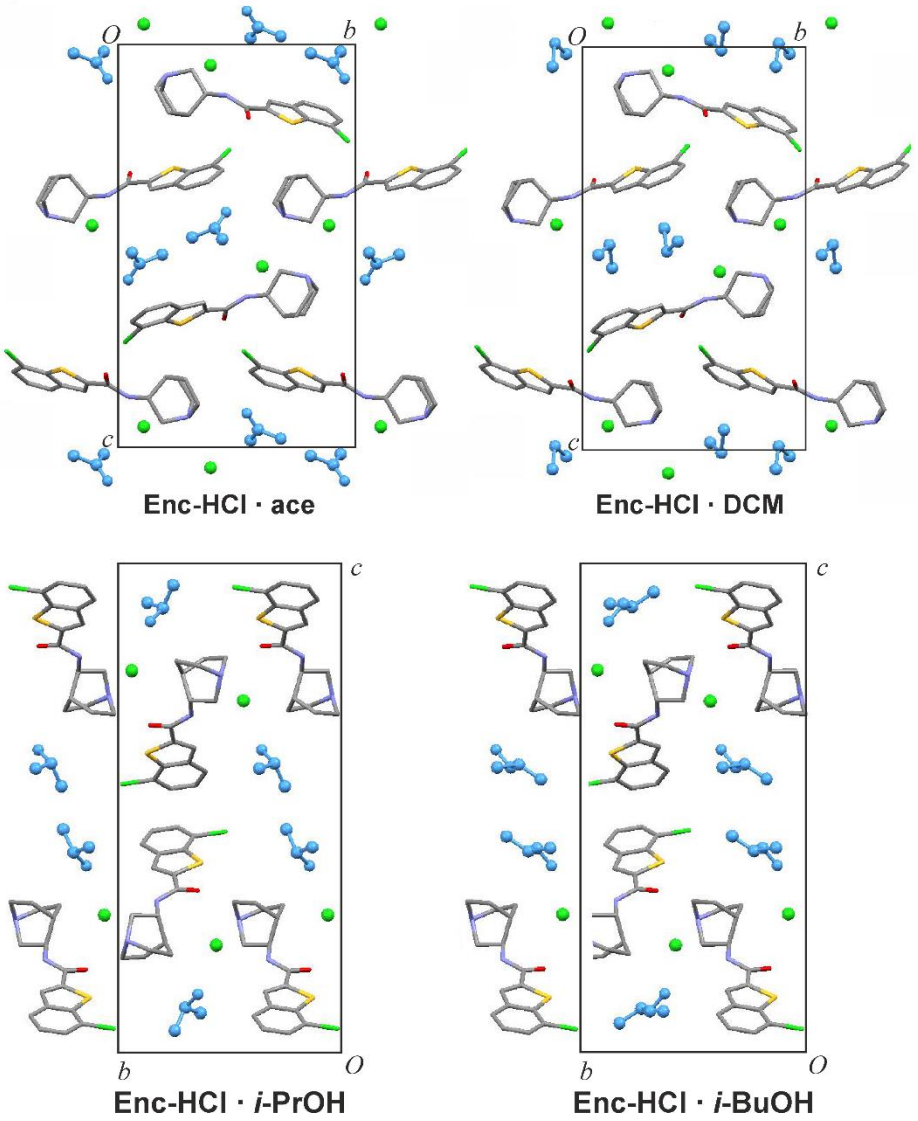

Figure S1. Molecular packing in two sets of isostructural Enc-HCl solvates. Solvent molecules (colored blue) and Cl^- anions are drawn in balls-and-sticks-style. H atoms are omitted for clarity.

Table S1. Geometry of N16–H16···Cl^-···H13–N13 interactions in various forms of Enc-HCl. Data for **A**, **Enc-HCl · *i*-PrOH**, **Enc-HCl · *i*-PrOH**, **Enc-HCl · ace** and **Enc-HCl · DCM** were obtained from this work. Data for **I_D** – **III_D** were obtained from Bobrovs et al., *Cryst. Growth Des.*, 2018, **18**, 2100.

Form	**H16···Cl** / Å	**H13···Cl** / Å	**∠ (N16 H16 Cl)** / °	**∠ (N13 H13 Cl)** / °	**H-bonded structure**
A	2.15(3)	2.46(3)	169(7)	165(5)	Chain (2_1)
Enc-HCl · *i*-PrOH	2.56(4)	2.46(3)	134(4)	162(3)	Chain (*t*) [a]
Enc-HCl · *i*-BuOH	2.58(4)	2.459(17)	154(7)	169(4)	Chain (*t*) [b]
Enc-HCl · ace	2.216(17)	2.50(2)	168(4)	163(5)	Chain (2_1)
Enc-HCl · DCM	2.161(18)	2.50(3)	172(7)	159(5)	Chain (2_1)
I_D	2.14	2.81	170	152	Tetramer
II_D	2.09	2.89	165	156	Chain (2_1)
III_D (A)	2.07	2.86	172	142	Chain (2_1)
III_D (B)	1.97	2.73	170	151	Chain (2_1)

[a]Additional intermolecular interactions in **Enc-HCl · i-PrOH** (H-bonded layer). *Cation/cation*: N16–H16···O11; H16···O11 = 2.23(4) Å; **∠ (**N16 H16 O11**) =** 128(4)°. *Solvent/anion*: O–H···Cl^-; H···Cl = 2.27(3) Å; **∠ (**O H Cl**) =** 170(7)°.
[b]Additional intermolecular interactions in **Enc-HCl · *i*-BuOH** (H-bonded layer). *Cation/cation*: N16–H16···O11; H16···O11 = 2.18(4) Å; **∠ (**N16 H16 O11**) =** 130(4)°. *Solvent/anion*: O–H···Cl^-; H···Cl = 2.35(4) Å; **∠ (**O H Cl**) =** 154(7)°.