Title:	Structural Landscape of Pure Enrofloxacin and Its Novel Salts: Enhanced Solubility for Better Pharmaceutical Applicability
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Abstract:	The crystal structures of anhydrous enrofloxacin (EFC) (1), enrofloxacin hexahydrate (EFC·6H2O) (2), enrofloxacin maleate (EFC-M) (3), enrofloxacin hemifumarate (EFC-F) (4), enrofloxacin hemisuccinate (EFC-S) (5), enrofloxacin hemioxalate (EFC-O) (6), enrofloxacin acetate (EFC-A) (7) and ammonium salt of enrofloxacin (Am-EFC) (8) have been determined by using single crystal X-ray diffraction (SCXRD). The crystals of 1 were grown from a dilute solution of EFC in dilute ammonium hydroxide. The crystals of 2 were grown from a solution of EFC with nicotinic acid. Solvent drop grinding experiments on enrofloxacin with various dicarboxylic acids resulted in four new salts (3–6). When a solution of EFC in glacial acetic acid evaporated to dryness over a period of time, crystals of 7 were grown. Crystals of 8 were found to grow when EFC was dissolved in liquid ammonia and solution was slowly evaporated at room temperature (RT). All these products (1–8) were characterized by 1H and 13C NMR spectroscopy, Fourier transform infrared (FTIR) spectroscopy, differential scanning calorimetry (DSC) and powder X-ray diffraction (PXRD). Single crystal X-ray diffraction study has indicated that the products 3–6 had a cation of enrofloxacin and an anion of the acid in common. Four of these eight products have been found to contain water of crystallization. Three of these salts were found to have one neutral acid molecule. The proton transfer and hydrate stoichiometry were confirmed from single crystal X-ray diffraction. Solubility of 1 and 3–6 was determined in water (pH = 6.8) using UV–vis spectroscopy at RT. The alteration between the neutral, zwitterionic, anionic and cationic forms EFC has led to very interesting structures of these salt/cocrystals and also the pure forms (1 and 2).
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