The Role of Biorelevant Dissolution Media in the Selection of Optimal Salt Forms of Oral Drugs: Maximising the Gastrointestinal Solubility and *In Vitro* Activity of the Antimicrobial Molecule, Clofazimine.

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TABLES:

Solid from	Bond observed and peak position (1/cm)	
	N_C^+-H	C=N_C
CFZ F III	n/a	1626.5
CFZ.Sul	3299.8	1624.3 (br)
CFZ.Pho	3325.2 (br)	1620.9
CFZ.Cit	3323.9 (br)	1616.9
CFZ.Ace	3325.2 (br)	1621.4

Table S1: Summary of the peaks position for the key function groups in various CFZ solid forms from the FTIR spectra

Bond observed								
Solid form	**Chemical shift (ppm)**	**Intermolecular distance** (A)**	**Chemical shift (ppm)**	**Intermolecular distance** (A)**	**Chemical shift (ppm)**	**Intermolecular distance** (A)**	**Chemical shift (ppm)**	**Intermolecular distance** (A)**
CFZ F I*	*49.4*	*1.465*	*149 - 151.4 (m)*	*1.293*	*149 - 151.4 (m)*	*1.311*		
CFZ F II	*48.7*	*1.457*	*149.4 - 151.6 (m)*	*1.298*	*149.4 - 151.6 (m)*	*1.302*		
CFZ F III	*49*	*1.457*	*149.73*	*1.296*	*150.7*	*1.309*		
Citrate	*48.84 - 46.46 (m), 45.47, 44.71*	*1.471*	*143.05, 141.65*	*1.328*	*151.08*	*1.324*		
Phosphate	*48.21, 47.16*	*1.469*	*143.84*	*1.322*	*152.35 - 150.24 (m), 149.70*	*1.351*		
Sulphate	*51.21, 48.23*	*1.462*	*144.26 - 142.46 (m)*	*1.322*	*150.96*	*1.320*		
Solution NMR: CFZ in $CDCl_3$	*49.4*	*n/a*	*150.4*	*n/a*	*151.1*	*n/a*		
CFZ from Gaussian 09 software (cal)	*50.46*	*n/a*	*152.12*	*n/a*	*152.55*	n/a		

taken from FI resolved as DAKXUI01 exhibits disorder in its isopropyl group.

****Calculated using Mercury software from single crystal cif files (average taken for solid Z' numbers greater > 1)***

Table S2: Summary of bond lengths from crystal structures of CFZ solid forms and ^{13}C chemical shifts of the same key functional groups in CPMAS ^{13}C spectra for CFZ solid forms. The chemical shifts of the CFZ carbons from solution NMR and molecular modelling are also shown for comparison

FIGURES:

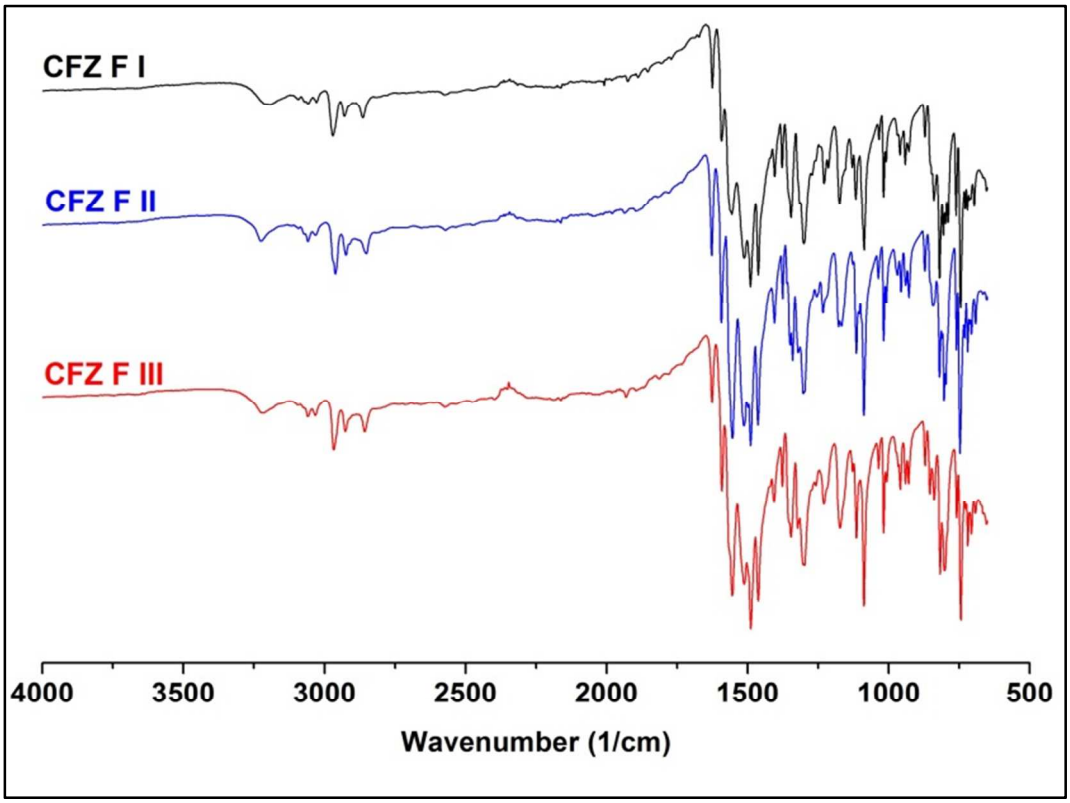

Figure S1: Comparison of the full FTIR spectra for the CFZ polymorphs F I, F II and F III.

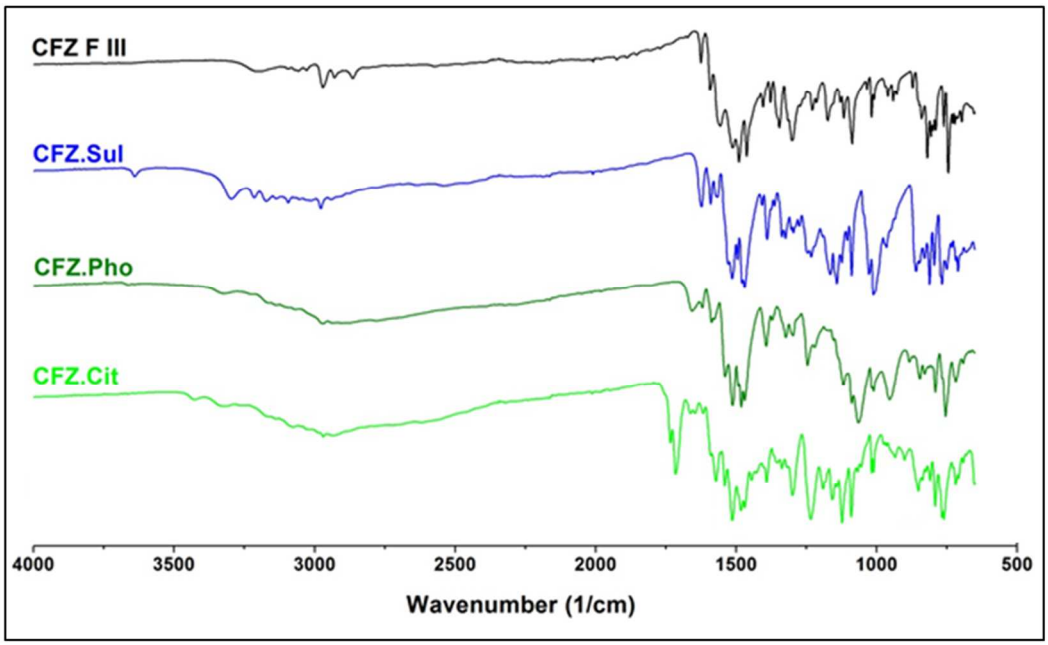

Figure S2: Comparison of the full FTIR spectra of the new CFZ salts with CFZ F III.

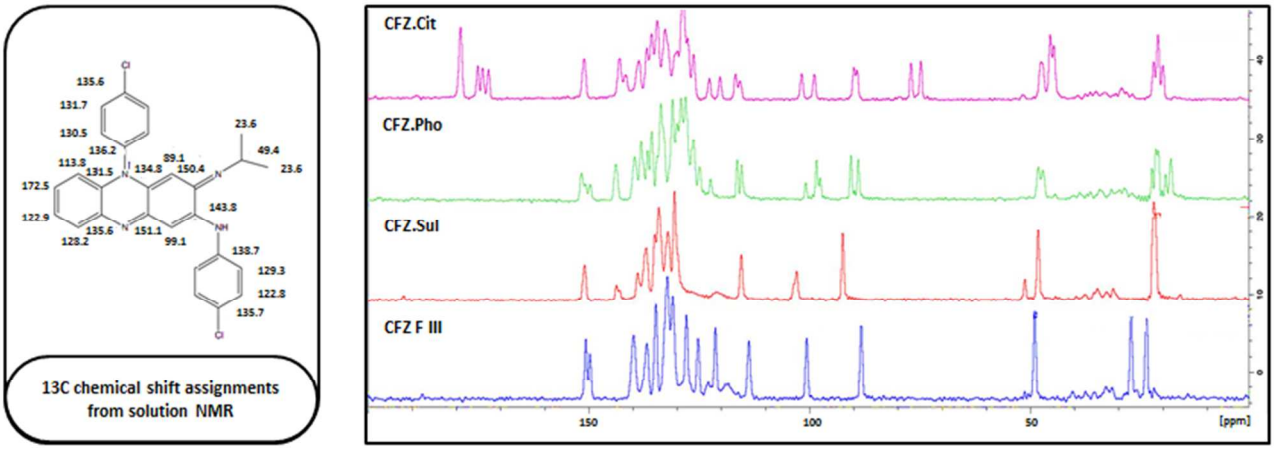

Figure S3: Left; Chemical structure of CFZ with ^{13}C peaks assigned. Right; Comparison of full ^{13}C CPMAS spectra obtained of acetate, citrate, phosphate, sulphate and CFZ F III, peaks corresponding to the secondary ketimine carbon (green) and the isopropyl carbon (blue) are highlighted.