Supporting Information

Powder Structure Analysis of Vapochromic Quinolone Antibacterial Agent Crystals

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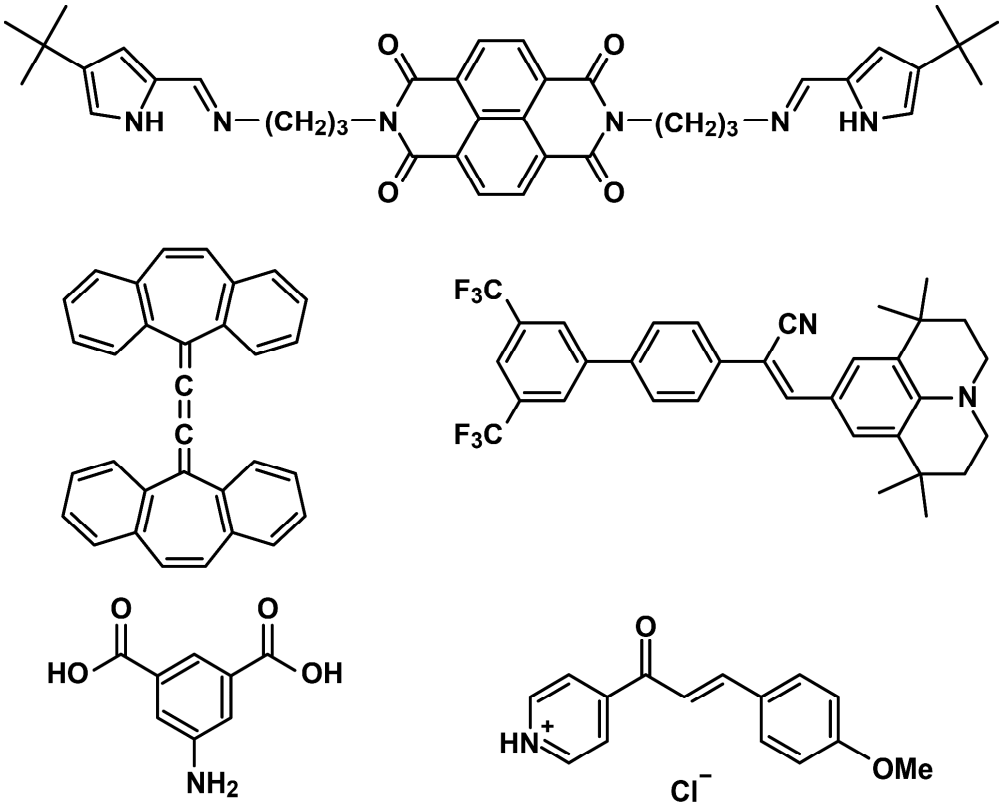

Figure S1. The molecular structures of the vapochromic organic crystals reported previously.

Table S1. The results of phase transformation (dehydration / hydration) of PPA and ENX when exposed to various kinds of solvent vapors identified by PXRD measurements. "No change": No phase transformation, "Wet": The samples became wet because of absorbing the solvent vapors, "Change to X": Phase transformations by solvent vapors.

Solvent Vapors	PPA			ENX	
	Trihydrate phase	Anhydrous A phase	Anhydrous B phase	Trihydrate phase	Anhydrous phase
Water	No change	Change to Trihydrate	Change to Trihydrate	No change	Change to Trihydrate
Methanol	Wet	Wet	Wet	No change	No change
Ethanol	No change	No change	No change	No change	No change
2-Propanol	No change	No change	No change	No change	No change
Acetone	Wet	Wet	Wet	Wet	Wet
1,4-Dioxane	No change	No change	No change	No change	No change
THF	Wet	Wet	Wet	No change	No change
Methyl acetate	No change	No change	No change	No change	No change
Acetonitrile	Change to Anhydrous B phase via A phase	No change	No change	No change	No change
Chloroform	No change	No change	No change	No change	No change
Dichloromethane	No change	No change	No change	No change	No change
hexane	No change	No change	No change	No change	No change
diethyl ether	No change	No change	No change	No change	No change
DMSO	No change	No change	No change	No change	No change

Table S2. The crystallographic data of ENX anhydrous phase, PPA anhydrous A phase and PPA anhydrous B phase

Phase	ENX anhydrous phase	PPA anhydrous A phase	PPA anhydrous B phase
Formula	$C_{15}H_{17}FN_4O_3$	$C_{14}H_{17}N_5O_3$	$C_{14}H_{17}N_5O_3$
Formula weight	320.32	303.32	303.32
Crystal system	triclinic	triclinic	triclinic
Space group	*P* -1	*P* -1	*P* -1
***a* / Å**	7.9273 (4)	7.9145 (5)	4.58119 (15)
***b* / Å**	8.6645 (3)	8.0992 (6)	10.7188 (4)
***c* / Å**	10.2255 (4)	11.9317 (10)	15.4858 (4)
***α* / °**	91.587 (3)	94.067 (5)	72.442 (2)
***β* / °**	94.701 (3)	104.188 (4)	88.809 (3)
***γ* / °**	93.179 (3)	101.593 (5)	81.802 (2)
***V* / Å^3**	698.54 (7)	720.53 (10)	717.39 (5)
Z, Z'	2, 1	2, 1	2, 1
d / Mg m^{-3}	1.523	1.398	1.404
2*θ* range / °	3.00 - 60.00	3.00 - 60.00	3.00 - 60.00
R_{wp}	0.0993	0.0840	0.0870
R_p	0.0713	0.0585	0.0615
R_F^2	0.1027	0.0459	0.0597
goodness-of-fit	2.46	2.73	2.64
CCDC deposit number	1447069	1447070	1447072

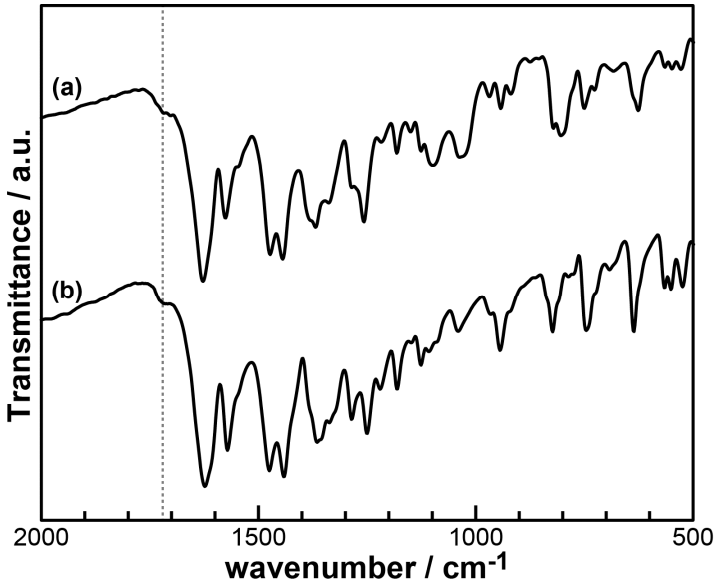

Figure S2. FT-IR spectra of (a) ENX trihydrate and (b) ENX anhydrous phases with no strong peaks around 1700 cm^{-1}, which means there is no stretching vibration of C=O of carboxylic acid.

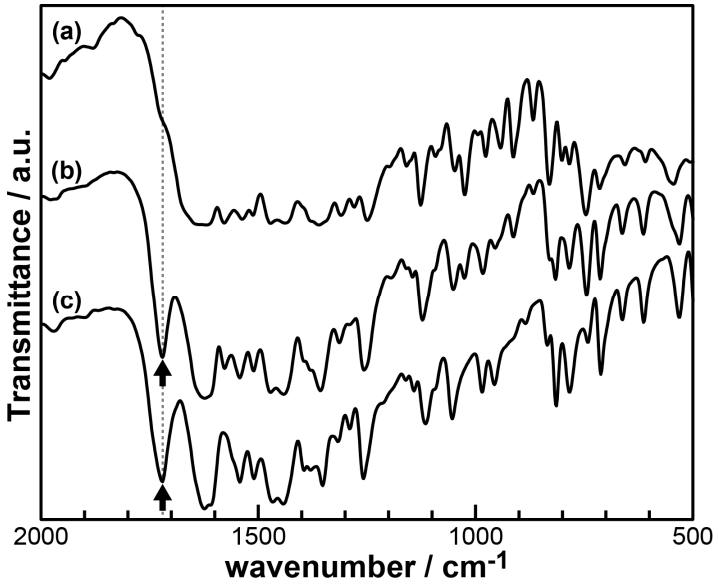

Figure S3. FT-IR spectra of (a) PPA trihydrate, (b) PPA anhydrous A and (b) PPA anhydrous B phases. The strong peaks at 1720 cm^{-1} in (b) and (c) indicated by arrows correspond to the stretching vibration of C=O of carboxylic acid.