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Supporting information for article:

An acetonitrile-solvated cocrystal of piroxicam and succinic acid with co-existing zwitterionic and non-ionized piroxicam molecules

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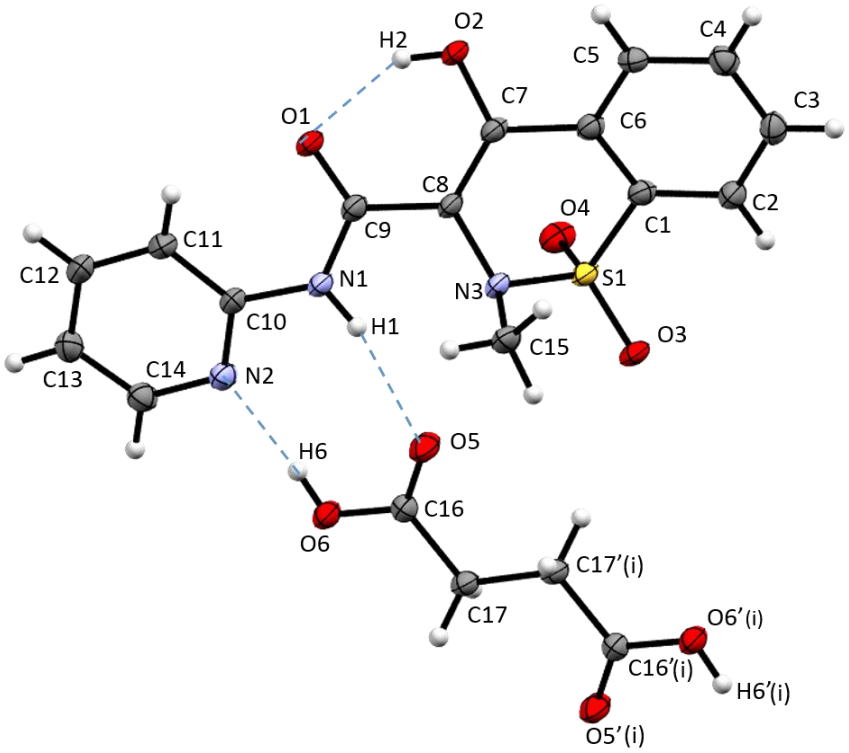

Figure S1 Displacement ellipsoid plot of the crystal structure of the asymmetric unit of PRX-SA at 120 K. All hydrogen atoms are located in calculated positions. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. [Symmetry code: (i) 1-x, -y, -z;]

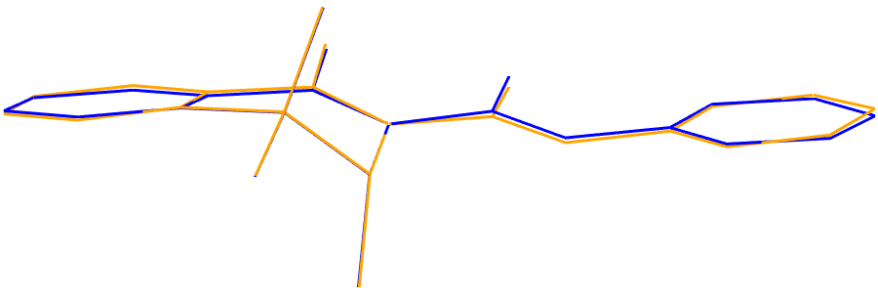

Figure S2 Comparison of the geometry of the neutral PRX molecules: orange denotes PRX from the PRX-SA structure, while blue denotes that from the PRX-SA·ACN structure.

Table S1 Hydrogen-bond geometry (Å, º)

(A) PRX-SA	*D-H*	*H···A*	*D···A*	*H-D···A*
O2-H2···O1	0.91(4)	1.81(3)	2.626(2)	149(3)
O6-H6···N2	0.94(4)	1.80(4)	2.718(2)	168(3)
N1-H1···O5	0.81(4)	2.19(4)	2.980(3)	167(4)
O2-H2···O1’ (i)	0.91(4)	2.31(3)	2.822(2)	116(3)
N1-H1···N3	0.81(4)	2.32(4)	2.732(3)	113(3)

Symmetry code: (i) 1-x, 1-y, 1-z;

(B) PRX-SA·ACN	*D-H*	*H···A*	*D···A*	*H-D···A*
O2A-H2A···O1A	0.88(3)	1.78(3)	2.5823(17)	152(3)
O6-H6···N1A	0.89(3)	1.81(3)	2.697(2)	176(3)
N2-H2···O2	0.88(2)	1.82(2)	2.6009(19)	147.1(19)
N1-H1···O1	0.85(2)	1.97(2)	2.6322(19)	134.5(18)
N2A-H2AA···O5	0.86(2)	2.08(2)	2.927(2)	168.8(19)
N1-H1··· O1’ (i)	0.85(2)	2.22(2)	2.8690(18)	132.9(18)

Symmetry code: (i) 2-x, 1-y, 1-z

(C) PRX-FA(Childs & Hardcastle, 2007)	*D···A*
N_{2B}···O_{2G}	2.8970(21)
O_{1G}···N_{3B}	2.6441(20)
O_{1B}···O_{4B}	2.5357(20)
N3···O4’ (i)	2.8238(20)
N2···O1	2.5971(20)
N3···O4	2.6109(19)

Symmetry code: (i) 2-x, 1-y, 1-z;

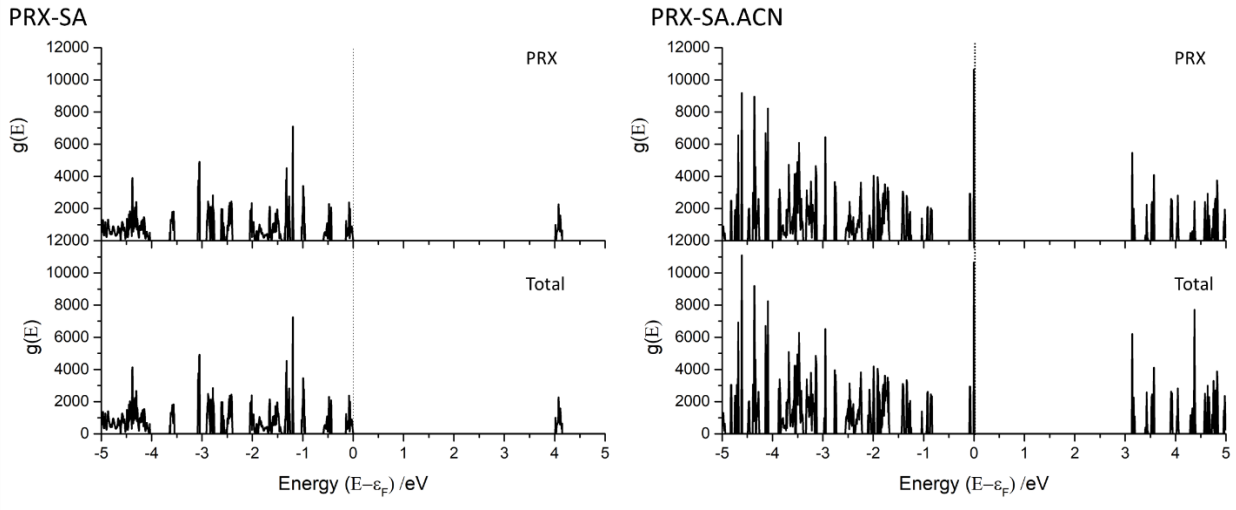

Figure S3 Electronic density of states for (left) PRX-SA, and (right) PRX-SA·ACN. The projected density of states for PRX is given alongside the total density of states in each case. The energy is shown with respect to the Fermi level (ϵ_F) in each case and is indicated by a dotted line.

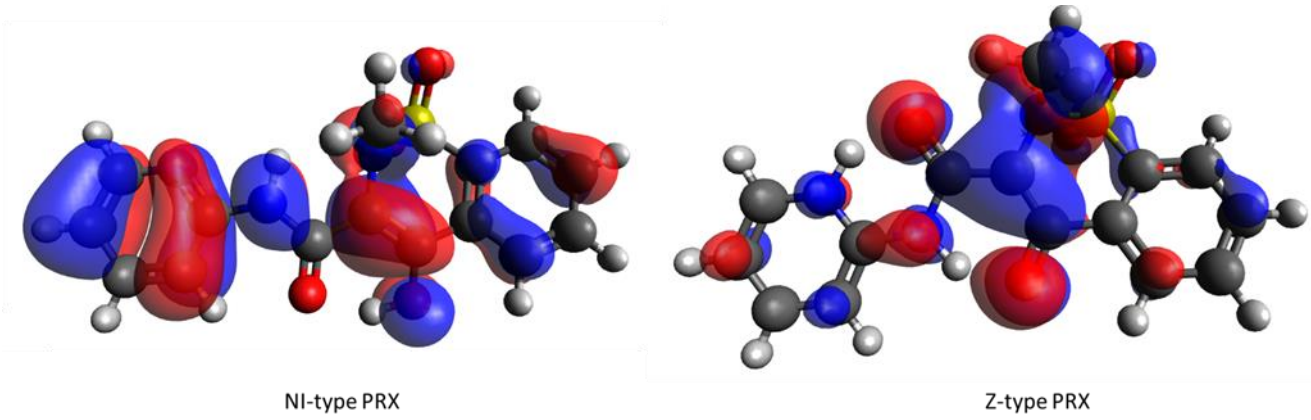

Figure S4 Highest occupied molecular orbitals for the (left) NI-type and (right) Z-type PRX molecules. Absolute energy of NI-HOMO is -0.2307 Ha and that for Z-HOMO is -0.1954 Ha. This corresponds to a difference in energy of 0.0353 Ha = 0.9606 eV

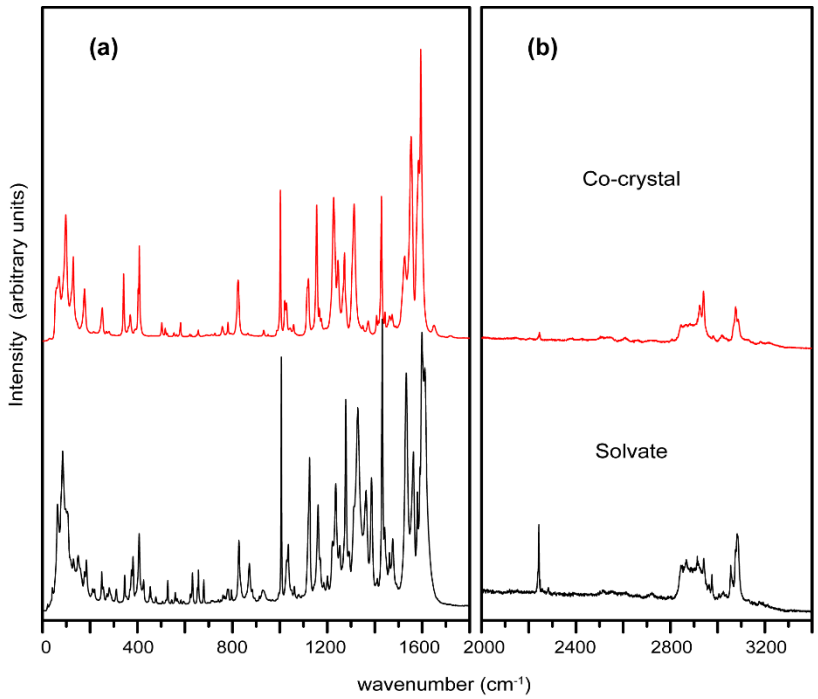

Figure S5 Raman spectral comparison of PRX-SA (red) and PRX-SA·ACN (black). The arbitrary unit of (a) is 20 times the unit of (b).

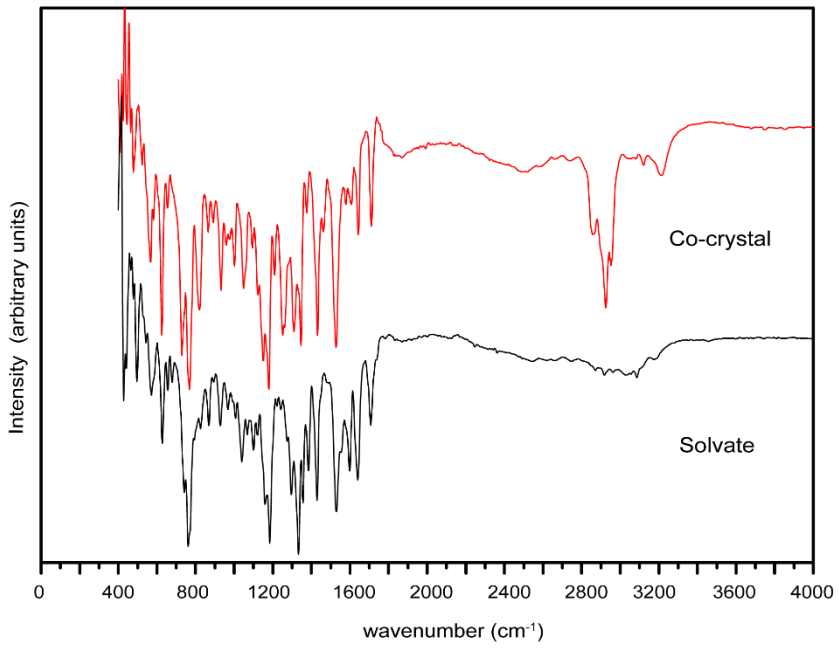

Figure S6 FT-IR spectral comparison of PRX-SA (red) and PRX-SA·ACN (black)

Table S2 Attributions of IR and Raman vibrations of acetonitrile (Neelakantan, 1964)

Attributions	IR (cm^{-1})	Raman (cm^{-1})
δ C-C≡N	379	380
	674	-
ν C-C	917	920
ρ CH_3	1047	1044
δ CH_3	1376	1378
	1443	1449
	-	1558
	2204	2197
ν C≡N	2254	2248
ν_s C-H	2944	2942
ν_{as} C-H	3002	2999

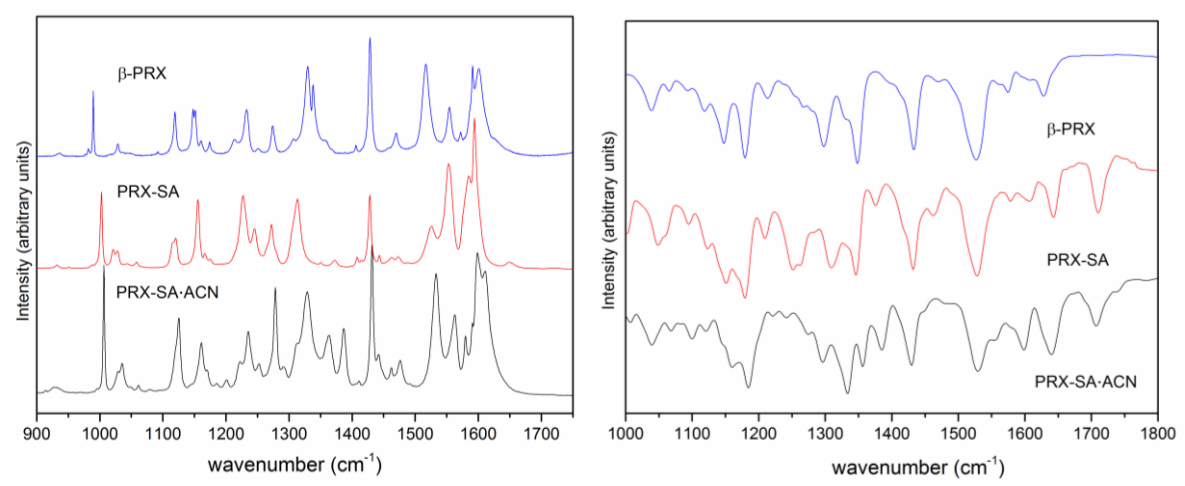

Figure S7 Comparisons of spectra of β-PRX (blue), PRX-SA (red), and PRX-SA·ACN (black): Raman spectra (left) and FT-IR spectra (right)