Drug-drug co-crystals. Temperature-dependent proton mobility in the molecular complex of isoniazid with 4-aminosalicylic acid

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Electronic Supplementary Information

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Fig. S1 Thermal ellipsoid diagram of co-crystal **1**

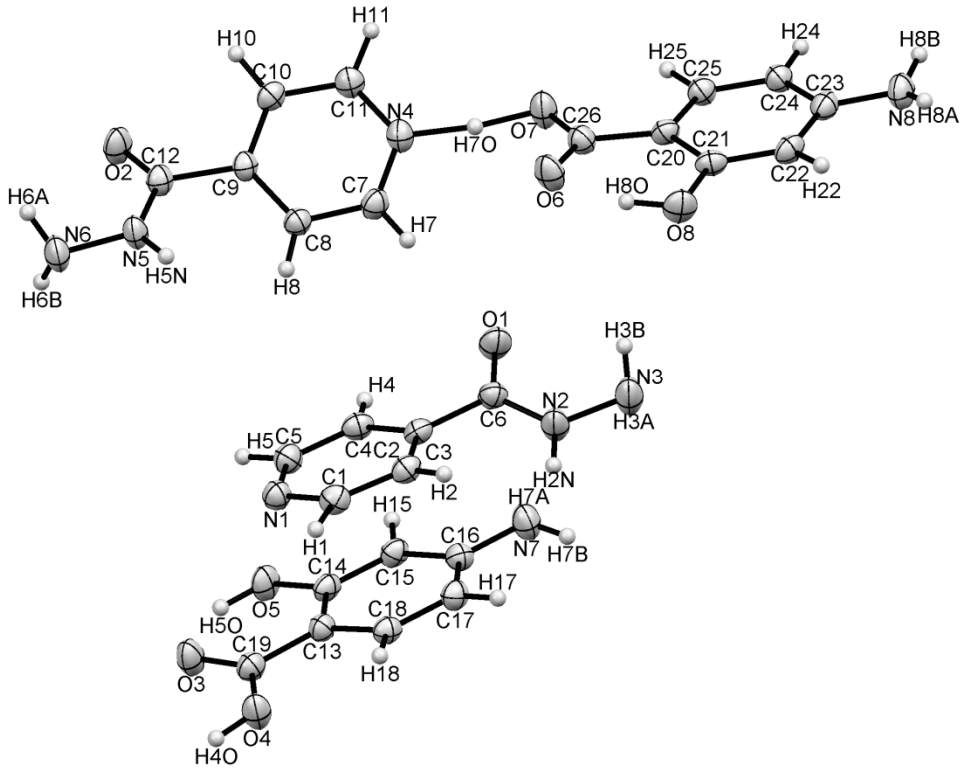

Fig. S2 Thermal ellipsoid diagram of crystal **2**

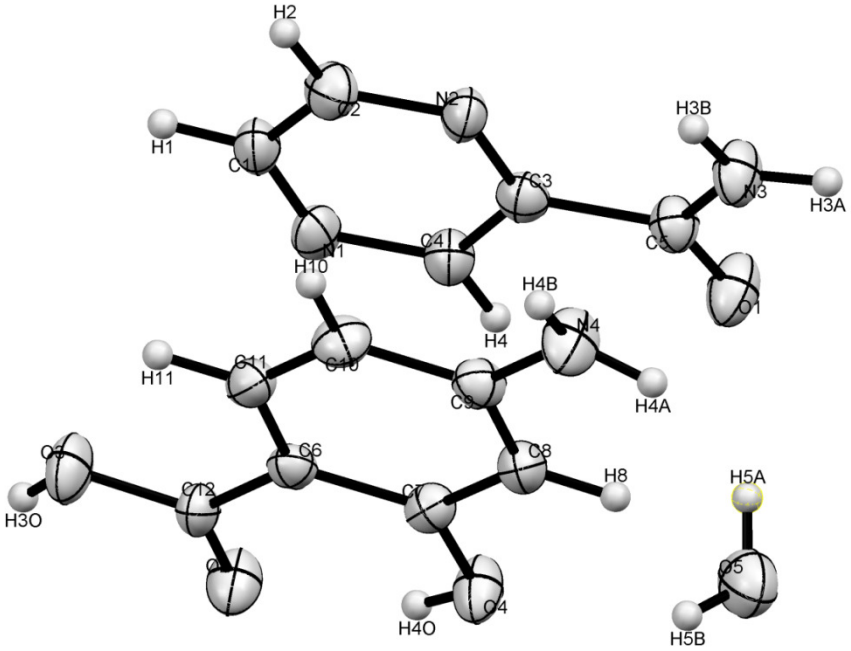

Table S1. Crystallographic information of co-crystals 1 at different temperatures

	100 K	120 K	140 K	160 K	180 K	200 K	220 K	240 K	260 K	280 K
Formula	$C_{26}H_{28}N_8O_8$	$C_{26}H_{28}N_8O_8$	$C_{26}H_{28}N_8O_8$	$C_{26}H_{28}N_8O_8$	$C_{26}H_{28}N_8O_8$	$C_{26}H_{28}N_8O_8$	$C_{13}H_{14}N_4O_4$	$C_{13}H_{14}N_4O_4$	$C_{13}H_{14}N_4O_4$	$C_{13}H_{14}N_4O_4$
Molecularweight	580.56	580.56	580.56	580.56	580.56	580.56	290.28	290.28	290.28	290.28
Crystal system	Orthorhombic									
Space group	$Pna2_1$									
a (Å)	21.837(2)	21.845(2)	21.859(2)	21.879(9)	21.889(2)	21.893(10)	21.893(2)	21.926(10)	21.969(2)	21.942(2)
b (Å)	16.5073(14)	16.5081(13)	16.5084(14)	16.520(7)	16.5223(14)	16.515(7)	16.5073(18)	16.514(8)	16.485(2)	16.515(2)
c (Å)	7.2252(6)	7.2355(6)	7.2459(6)	7.263(3)	7.2750(6)	7.283(3)	7.2990(7)	7.310(3)	7.3209(9)	7.3435(8)
α (°)	90	90	90	90	90	90	90	90	90	90
β (°)	90	90	90	90	90	90	90	90	90	90
γ (°)	90	90	90	90	90	90	90	90	90	90
Volume ($Å^3$)	2604.5(4)	2609.3(4)	2614.7(4)	2625.2(19)	2631.1(4)	2633(2)	2637.8(5)	2647(2)	2651.3(5)	2661.1(5)
Z	4	4	4	4	4	4	8	8	8	8
ρ_{calc} (g/cm^3	1.481	1.478	1.475	1.469	1.466	1.465	1.462	1.457	1.454	1.449
F(000)	1216	1216	1216	1216	1216	1216	1216	1216	1216	1216
μ (MoK_α) (mm^{-1})	0.113	0.112	0.112	0.112	0.111	0.111	0.111	0.111	0.111	0.110
Crystal size (mm)	0.40 x 0.30 x 0.15									
Temp. (K)	100(2)	120(2)	140(2)	160(2)	180(2)	200(2)	220(2)	240(2)	260(2)	280(2)
θ Range for data collection (°)	1.5 - 27.5	1.5 - 27.5	1.5 - 27.5	1.5 - 27.4	1.5 - 27.5	1.5 - 27.5	1.5 - 27.5	1.5 - 27.5	1.5 - 27.5	1.5 - 27.5
R_1	0.0358	0.0359	0.0384	0.0386	0.0391	0.0415	0.0408	0.0440	0.0439	0.0471
wR_2	0.1101	0.0948	0.1144	0.1169	0.1172	0.1243	0.1238	0.1305	0.1305	0.1393
Goodness-of-fit	1.14	1.09	1.14	1.17	1.14	1.16	1.16	1.16	1.16	1.18
Reflns collected	27056	26990	27058	21255	27155	27060	27057	27304	27415	27333
Unique reflns	3226	3233	3240	3245	3254	3253	3269	3277	3286	3298
observed reflns	3097	3098	3116	3040	3056	3065	3017	3060	2989	2992
CCDC no.	800230	800231	800232	800233	800234	800235	800236	800237	800238	800239