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SUPPLEMENTARY MATERIAL

Multicomponent crystals of anti-Tuberculosis drugs: A mini-review

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Table S1 Co-crystal formers, CCDC ref codes, common synthons and physical properties addressed for multicomponent crystals of isoniazid.

Co-crystal former	CCDC ref code	Physical property addressed
4-cyanobenzoic acid	ACUDAG[1,a,b,d]	-
p-aminobenzoic acid	ACUDEK[1,a,c]	-
p-aminobenzoic acid	ACUDEK01[1,a,c,f]	-
4-nitrobenzoic acid	ACUDIO[1,a,b,d]	-
Nicotinamide Succinic acid	BICQAH[2,a,f]	Solubility and dissolution rate
Nicotinamide Fumaric acid	BICQEL[2,a,f]	Solubility and dissolution rate
4-hydroxybenzoic acid	BICQUB[2,a,b]	Solubility and dissolution rate
4-hydroxybenzoic acid	BICQUB01[2,a,f]	Solubility and dissolution rate
2,2'-dithiodibenzoic acid	BIZMAZ[3,a,c,e]	-
18-crown-6	BIZMUU[4]	-
2,3-dihydroxybenzoic acid	BOMBOW[5,a,b]	-
3,5-dihydroxybenzoic acid	BOMBUC[5,f]	-
3-hydroxybenzoic acid	BOMCAJ[5,a]	-
DL Tartaric acid	BOPHOG[6]	-
4-hydroxy-3,5-dimethoxybenzoic acid	COSKUT[7,e]	Solubility and dissolution rate.
6-chloro-3,4-dihydro-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide	DADLUS[8,e]	Solubility and dissolution rate
3-,4-hydroxybenzoic acid	EJOYEJ[9,a,b]	Solubility and stability
Malonic acid	FADGEY[10,a]	-
Succinic acid	FADGIC[10,a,b,d]	-
Succinic acid	FADGIC01[11,c,d,e]	-
Succinic acid	FADGIC02[12,a,d]	Solubility, stability and dissolution rate
Succinic acid	FADGIC03[*,a,b,d]	-
Glutaric acid	FADGOI[10,a,c]	-
Adipic acid	FADGUO[10,a,b,f]	-
Adipic acid	FADGUO01[13,a]	-
Adipic acid	FADGUO02[*,a,b,f]	Solubility
Pimelic acid	FADHAV[10,a,c]	-
4-hydroxybenzoic acid	FADHEZ[10,a,c]	-
4-hydroxybenzoic acid	FADHEZ01[10]	-
2,4-hydroxyybenzoic acid	FADHID[10,a,c,f]	-
Ferulic acid	FOSFIE[14,d]	Stability
Resorcinol	FOSFOK[14,c]	Stability
Vanillic acid	FOSFUQ[14,d]	Stability

Vanillic acid	FOSFUQ01[14,a,c]	Stability
Caffeic acid	FOSMIL[14,a]	Stability
Caffeic acid	FOSMIL01[14,a,b]	Stability
4-t-butylbenzoic acid	GIYLUY[15,a,d]	-
Salicylic acid	LATKUO[11,a,f]	-
2-chloro-4-nitrobenzoic acid	LATLEZ[11,a,d,e]	-
Fumaric acid	LATSUW[12]	Solubility and dissolution rate
Fumaric acid	LATTAD[12,a]	Solubility and dissolution rate
Fumaric acid	LATTAD01[2,a,b]	Stability, solubility and dissolution rate
Fumaric acid	LATTAD02[2,a]	Stability, solubility and dissolution rate
3,4,5-trihydroxybenzoic acid	LODHIX[16]	-
3,4,5-trihydroxybenzoic acid	LODHIX01[16]	-
3,4,5-trihydroxybenzoic acid	LODHOD[16,a,b]	-
3,4,5-trihydroxybenzoic acid	LODHOD01[16,a]	-
3,4,5-trihydroxybenzoic acid	LODHOD02[5,a,b]	-
3,4,5-trihydroxybenzoic acid	LODHOD03[17,a,b]	-
2,6-dihydroxybenzoic acid	NAKZEH[18]	-
2,6-dihydroxybenzoic acid	NAKZEH01[17]	-
Phthalic acid	NAKZOR[18,d]	-
Terephthalic acid	ORAWIO[19,a,b,f]	-
3-(4-hydroxyphenyl)acrylic acid	PEHFUF[20]	-
2,4,6-trinitrophenol	PEZVAU[*]	
5-fluorocytosine	PINJII[21,f]	Stability and solubility
Oxalic acid	QICJIY[22]	Solubility
Oxalic acid	QICJIY01[*]	-
Maleic acid	QICJOE[22]	Solubility
Methane sulfonic acid	QICJUK[22]	Solubility
Benzoic acid	SETRIU[23,a,b,f]	Stability and solubility
Sebacic acid	SETROA[23,a,b,d]	Stability and solubility
Suberic acid	SETRUG[23,a,b,d]	Stability and solubility
Cinnamic acid	SETSAN[23,a,b]	Stability and solubility
Cinnamic acid	SESTAN01[23,a,b]	Stability and solubility
Cinnamic acid	SESTAN02[23,a,b,f]	Stability and solubility
5,7-dihydroxy-2-(4-hydroxyphenyl)-2,3dihydro-4H-1-benzopyran-4-one	UDUJIP[*,c]	
4-aminosalicylic acid	URUDER[24,a,f]	-
4-aminosalicylic acid	URUDER01[24,a,f]	-
4-aminosalicylic acid	URUDER02[24,a,f]	-
4-aminosalicylic acid	URUDER03[24,a,f]	-
4-aminosalicyclic acid	URUDER04[24,a,f]	-
4-aminosalicylic acid	URUDER05[24,a,b,f]	-
4-aminosalicylic acid	URUDER06[24,a,f]	-
4-aminosalycylic acid	URUDER07[24,a,b,f]	-
4-aminosalycylic acid	URUDER08[24,a,b,f]	-
4-aminosalycylic acid	URUDER09[24,a,b,f]	-
4-aminosalicylic acid	URUDER10[24,a,b,f]	-
But-2-ynoic acid	VAXROD[25]	-
But-2-ynoic acid	VAXRUJ[25]	-
Benzene-1,2,4,5-tetracarboxylic acid	VEGHOH[26]	-
Naphthalene-1,5-disulfonic acid	VEGHUN[26]	-
Resveratrol	VOPQEZ[27]	Solubility
Tartaric acid	WETZAZ*	-
Tartaric acid	WETZAZ01[*]	-
D-tartaric acid	WETZAZ02[6]	-
D-tartaric acid	WETZAZ03[6]	-
Benzene 1,3,5 triol	WIWNAU[17,e]	-
Fumaric acid Pyrazinamide	YEVBAF[28,a]	Solubility, dissolution and mem-brane permeability
3-carboxy-4-hydroxybenzenesulfonic acid	YIFXOB[29]	-
3,4-dihydroxycinnamic acid	FOSMIL02[30,a]	
3,4-dihydroxycinnamic acid	FOSMIL03[30,a]	
4-hydroxycinnamic acid	PEHFUF01[30]	
2-hydroxycinnamic acid	PUMFOV[30,a,b]	
2,4-dihydroxycinnamic acid	PUMGAI[30]	

3-hydroxycinnamic acid	PUMGOW[30]	
cinnamic acid	SETSAN03[30,a,b]	

a = synthon type I, b = synthon type II, c = synthon type III, d = synthon type IV, e = synthon type V, F = synthon type VI.

Table S2 Co-crystal co-formers, CCDC ref codes, common synthons and physical properties addressed for multicomponent crystals of pyrazinamide.

Co-crystal former	**CCDC ref code**	**Physical property addressed**
3,5-dihydroxybenzoic acid	ACOPOA[31,j]	Solubility
3-(4-hydroxy-3-methoxyphenyl)prop-2-enoic acid	ACOPUG[31,i,j]	Solubility
p-toluene sulfonic acid	ACOQAN[31,]	Solubility
4-nitrobenzamide	ASAYIC[32,i]	-
2-Aminobenzoic acid	EBONUG[33,i,j,k]	-
6-chloro-3,4-dihydro-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide	EGENIP[34,k]	Solubility and dissolution
Hydrochlorothiazide	EGENIP01[8,k]	Solubility and dissolution rate
Hydrochlorothiazide	EGENIP02[35,k]	Solubility
benzene-1,2,3-triol	HEDRAL[36]	Solubility and dissolution rate
Temozolomide	KIJSED[37,]	-
Hexanedioic acid	KOVSAR[38,g,h,j]	Solubility and dissolution rate
Decanedioic acid	KOVSEV[38,g,h,i]	Solubility and dissolution rate.
prop-1-ene-1,2,3-tricarboxylic acid	KOVSIZ[38]	Solubility and dissolution rate
2-hydroxypropane-1,2,3-tricarboxylate	KOVSOF[38,g]	Solubility and dissolution rate
fumaric acid	LATTIL[12,g,h,i]	Solubility and dissolution rate
succinic acid	LATTOR[12,g,h,i]	Solubility and dissolution rate
succinic acid	LATTOR01[39,g,h,i]	Solubility and dissolution rate
4-nitrobenzoic acid	MUDVUE[40,g,i,j]	Solubility
2,4-dihydroxybenzoic acid	NEFFEM[41,j]	-
2,4-dihydroxybenzoic acid	NEFFEM01[31,j]	Solubility
2,6-dihydroxybenzoic acid	NEFGEN[41]	-
2,6-dihydroxybenzoic acid	NEFGEN01[31,g]	Solubility
2,3-dihydroxybenzoic acid	NEFGIR[41]	-
β-Cyclodextrin	NUFVEQ[42]	-
3,4-dihydroxybenzoic acid	NUSMIZ[43]	-
4-hydroxybenzoic acid	NUVFIV[43,i]	-
4-hydroxybenzoic acid	NUVFIV01[44,i]	-
3-hydroxybenzoic acid	NUVFOB[43]	-
3,4-dihydroxycyclobut-3-ene-1,2-dione	PAQNOM[45,g,h]	-
theophylline	RACFIN[46,i]	-
theophylline	RACFIN01[46,i,g]	-
4-Hydroxy-3-methoxybenzoic acid	REBXED[47,i,j]	Solubility
3,4,5-Trihydroxybenzoic acid	REBXIH[47,i]	Solubility
1-Hydroxy-2-naphthoic acid	REBXON[47,g,h,i]	Solubility
1H-Indole-2-carboxylic acid	REBXUT[47]	Solubility
Hydrochloric acid	SAGBEJ[48]	-
glutaric acid	SIHQOR[39,g,h]	Solubility and dissolution rate
malonic acid	SIHRAE[39,g]	Solubility and dissolution rate
malonic acid	SIHRAE01[49,k]	-
Sinapic acid	TIHSAH[44,i]	-
4-aminosalicylic acid	URUGIY[24,g,h,i]	-
oxalic acid	UZODUK[50,g,h,i]	-
2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-4H-1-benzopyran-4-one	VIHJII[51,i]	Solubility and dissolution
Glutaric acid	VOLROG[52,g,h,i]	-
4-aminobenzoic acid	VUTNAB[53,k]	-
1,4-dibromo-2,3,5,6-tetrafluorobenzene	WEDXOV[54,i]	-
1,2,4,5-tetrafluoro-3,6-diiodobenzene	WEDXUB[54,i]	-
2,5-dyhydroxybenzoic acid	XAQQOW[55]	-
(E)-2-cyano-3-(3,4-dihydroxy-5-nitrophenyl)-N,N-diethylprop-2-enamide	XIPPAQ[56]	Solubility, dissolution rate and stability

4-carbohydrazide bis(but-2-enedioic acid)	YEVBAF[28,g,h]	Solubility, dissolution and mem-brane permeability

g = synthon type VII, h = synthon type VIII, i = synthon type IX, j = synthon type X, k = synthon type XI

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