SUPPLEMENTARY MATERIAL

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

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

| Co-crystal former          | CCDC ref code | Physical property addressed                  |
|----------------------------|---------------|-----------------------------------------------|
| 4-cyanobenzoic acid        | ACUDAG        | -                                             |
| p-aminobenzoic acid        | ACUDEK        | -                                             |
| p-aminobenzoic acid        | ACUDEK01      | -                                             |
| 4-nitrobenzoic acid        | ACUDIO        | -                                             |
| Nicotinamide               |               | Solubility and dissolution rate               |
| Succinic acid              | BICQAH        | -                                             |
| Nicotinamide               | BICQEL        | Solubility and dissolution rate               |
| Succinic acid              | BICQUB        | Solubility and dissolution rate               |
| 4-hydroxybenzoic acid      | BICQUB01      | Solubility and dissolution rate               |
| 2,2'-dithiodibenzoic acid  | BIZMAZ        | -                                             |
| 18-crown-6                 | BIZMUU        | -                                             |
| 2,3-dihydroxybenzoic acid  | BOMBOW        | -                                             |
| 3,5-dihydroxybenzoic acid  | BOMBUC        | -                                             |
| 3-hydroxybenzoic acid      | BOMCA         | -                                             |
| DL Tartaric acid           | BOPHOG        | -                                             |
| 4-hydroxy-3,5-dimethoxybenzoic acid | COSKUT | Solubility and dissolution rate |
| 6-chloro-3,4-dihydro-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide | DADLUS | Solubility and dissolution rate |
| 3-,4-hydroxybenzoic acid   | EJOYE         | Solubility and stability                      |
| Malonic acid               | FADGEY        | -                                             |
| Succinic acid              | FADGIC        | -                                             |
| Succinic acid              | FADGIC01      | Solubility, stability and dissolution rate    |
| Glutaric acid              | FADGO         | -                                             |
| Adipic acid                | FADGUO        | -                                             |
| Adipic acid                | FADGUO01      | -                                             |
| Adipic acid                | FADGUO02      | Solubility                                   |
| Pimelic acid               | FADHAY        | -                                             |
| 4-hydroxybenzoic acid      | FADHEZ        | -                                             |
| 4-hydroxybenzoic acid      | FADHEZ01      | -                                             |
| 2,4-hydroxybenzoic acid    | FADHID        | -                                             |
| Ferulic acid               | FOSFIE        | Stability                                    |
| Resorcinol                 | FOSFOK        | Stability                                    |
| Vanillic acid              | FOSFUQ        | Stability                                    |
| Chemical Name                        | Designation       | Properties                   |
|-------------------------------------|-------------------|------------------------------|
| Vanillic acid                       | FOSFUQ01          | Stability                    |
| Caffeic acid                        | FOSMIL14          | Stability                    |
| Caffeic acid                        | FOSMIL01          | Stability                    |
| 4-t-butylbenzoic acid               | GIYLUY15          | -                            |
| Salicylic acid                      | LATKUO17          | Stability                    |
| 2-chloro-4-nitrobenzoic acid        | LATLEZ11          | -                            |
| Fumaric acid                        | LATSUW12          | Solubility and dissolution rate |
| Fumaric acid                        | LATTAD12          | Solubility and dissolution rate |
| Fumaric acid                        | LATTAD01          | Stability, solubility and dissolution rate |
| Fumaric acid                        | LATTAD02          | Stability, solubility and dissolution rate |
| 3,4,5-trihydroxybenzoic acid        | LODHIX16          | -                            |
| 3,4,5-trihydroxybenzoic acid        | LODHIX01          | -                            |
| 3,4,5-trihydroxybenzoic acid        | LODHOD16          | -                            |
| 3,4,5-trihydroxybenzoic acid        | LODHOD01          | -                            |
| 3,4,5-trihydroxybenzoic acid        | LODHOD02          | -                            |
| 2,6-dihydroxybenzoic acid           | NAKZEH18          | -                            |
| 2,6-dihydroxybenzoic acid           | NAKZEH01          | -                            |
| Phthalic acid                       | NAKZOR23          | -                            |
| Terephthalic acid                   | ORAWIQ19          | -                            |
| 3-(4-hydroxyphenyl)acrylic acid     | PEHFUF20          | -                            |
| 2,4,6-trinitrophenol                | PEZVAU           | -                            |
| 5-fluorocytosine                    | PINJII21          | Stability and solubility     |
| Oxalic acid                         | QICJIY22          | Solubility                   |
| Maleic acid                         | QICJOE22          | Solubility                   |
| Methane sulfonic acid               | QICJUK22          | Solubility                   |
| Benzoic acid                        | SETRIU23          | Stability and solubility     |
| Suberic acid                        | SETROA23          | Stability and solubility     |
| Cinnamic acid                       | SETRUC23          | Stability and solubility     |
| Cinnamic acid                       | SETSAN23          | Stability and solubility     |
| Cinnamic acid                       | SESTAN02          | Stability and solubility     |
| 5,7-dihydroxy-2-(4-hydroxyphenyl)-2,3dihydro-4H-1-benzopyran-4-one | UDUJIP17,c | Stability and solubility |
| 4-aminosalicylic acid               | URUDER24          | -                            |
| 4-aminosalicylic acid               | URUDER01          | -                            |
| 4-aminosalicylic acid               | URUDER02          | -                            |
| 4-aminosalicylic acid               | URUDER03          | -                            |
| 4-aminosalicylic acid               | URUDER04          | -                            |
| 4-aminosalicylic acid               | URUDER05          | -                            |
| 4-aminosalicylic acid               | URUDER06          | -                            |
| 4-aminosalicylic acid               | URUDER07          | -                            |
| 4-aminosalicylic acid               | URUDER08          | -                            |
| 4-aminosalicylic acid               | URUDER10          | -                            |
| But-2-ynoic acid                    | VAXROD25          | -                            |
| But-2-ynoic acid                    | VAXRUJ25          | -                            |
| Benzeno-1,2,4,5-tetra-carboxylic acid | VEGHOH26        | -                            |
| Naphthalene-1,5-disulfonic acid      | VEGHUN26          | -                            |
| Resveratrol                         | VOPQEZ27          | Solubility                   |
| Tartaric acid                       | WETZAZ           | -                            |
| Tartaric acid                       | WETZAZ01          | -                            |
| D-tartaric acid                     | WETZAZ02          | -                            |
| D-tartaric acid                     | WETZAZ03          | -                            |
| Benzene 1,3,5 triol                 | WIWNAU17          | -                            |
| Fumaric acid                        | YEVBAP28          | Solubility, dissolution and membrane permeability |
| Pyrazinamide                        |                   | Solubility, dissolution and membrane permeability |
| 3-carboxy-4-hydroxybenzenesulfonic acid | YIFXOB29       | -                            |
| 3,4-dihydroxycinnamic acid          | FOSMIL02          | -                            |
| 3,4-dihydroxycinnamic acid          | FOSMIL03          | -                            |
| 4-hydroxycinnamic acid              | PEHFUF01          | -                            |
| 2-hydroxycinnamic acid              | PUMFOY30          | -                            |
| 2,4-dihydroxycinnamic acid          | PUMGAI30          | -                            |
| Co-crystal former | CCDC ref code | Physical property addressed |
|-------------------|--------------|-----------------------------|
| 3,5-dihydroxybenzoic acid | ACOPOA31,j | Solubility |
| 3-(4-hydroxy-3-methoxyphenyl)prop-2-enoid acid | ACOPUG31,j | Solubility |
| p-toluene sulfonic acid | ACOAN31 | Solubility |
| 4-nitrobenzamide | ASAYIC32,j | - |
| 2-Aminobenzoic acid | EBOUG33,j,k | - |
| 6-chloro-3,4-dihydro-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide | EGENIP34,k | Solubility and dissolution |
| Hydrochlorothiazide | EGENIP01,8,k | Solubility and dissolution rate |
| Hydrochlorothiazide | EGENIP02,33,k | Solubility |
| benzene-1,2,3-triol | HEDRAL38 | Solubility and dissolution rate |
| Hexanedioic acid | KOVSAR38,9,h,j | Solubility and dissolution rate |
| Decanedioic acid | KOVSAR38,9,g,h,i | Solubility and dissolution rate |
| 2-hydroxypropane-1,2,3-tricarboxylic acid | KOVSIZ38,9 | Solubility and dissolution rate |
| succinic acid | LATTIL1,2,g,h,i | Solubility and dissolution rate |
| succinic acid | LATTOR2,3,g,h,i | Solubility and dissolution rate |
| 4-nitrobenzoic acid | MUVDUE0,9,g,i | Solubility |
| 2,4-dihydroxybenzoic acid | NEFFEM41,j | - |
| 2,4-dihydroxybenzoic acid | NEFFEM0131,j | Solubility |
| 2,6-dihydroxybenzoic acid | NEFGEN41 | - |
| 2,6-dihydroxybenzoic acid | NEFGEN0131,g | Solubility |
| β-Cyclodextrin | NUFVEQ42 | - |
| 3,4-dihydroxybenzoic acid | NUSMIZ42 | - |
| 4-hydroxybenzoic acid | NUVFIV43,9 | - |
| 4-hydroxybenzoic acid | NUVFIV01,44,9 | - |
| 3-hydroxybenzoic acid | NUFQOB44 | - |
| 3,4-dihydroxycyclobut-3-ene-1,2-dione | PAQORM45,9,g,h | - |
| theophylline | RACFIN46,9 | - |
| theophylline | RACFIN0146,1,g | - |
| 4-Hydroxy-3-methoxybenzoic acid | REBXED47,9 | Solubility |
| 3,4,5-Trihydroxybenzoic acid | REBXH47,9 | Solubility |
| 1-Hydroxy-2-naphthoic acid | REBXO47,9,g,h,i | Solubility |
| 1H-Indole-2-carboxylic acid | REBXUT47 | Solubility |
| Hydrochloric acid | SAGBEJ48 | - |
| glutaric acid | SIHQOR38,9,g,h | Solubility and dissolution rate |
| malonic acid | SIHRAE38,9 | Solubility and dissolution rate |
| malonic acid | SIHRAE0149,9 | - |
| Sinapic acid | TIIHSAH44,9 | - |
| 4-aminosalicylic acid | URUGIY24,g,h,i | - |
| oxalic acid | UZODUK0,9,g,h,i | - |
| 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-4H-1-benzenopyran-4-one | VIHHI31,9 | Solubility and dissolution |
| Glutaric acid | VOLROG42,9,g,h,i | - |
| 4-aminobenzoic acid | VUTNAB35,k | - |
| 1,4-dibromo-2,3,5,6-tetrafluorobenzene | WEDX0V34,9 | - |
| 1,2,4,5-tetrafluoro-3,6-diodobenzene | WEDXUB34,9 | - |
| 2,5-dihydroxybenzoic acid | XAQQOW55 | - |
| (E)-2-cyano-3-(3,4-dihydroxy-5-nitrophenyl)-N,N-diethylprop-2-enamide | XIPPAQ56 | Solubility, dissolution rate and stability |
4-carboxyhydrazide bis(but-2-enedioic acid) YEVBAF

Solubility, dissolution and membrane 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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