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**Supporting information for article:**

# Binary and ternary cocrystals of sulfa drug acetazolamide with pyridine carboxamides and cyclic amides

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**Table S1** Hydrogen bond geometry of the crystal structures (neutron normalized) in this paper.

| Ccocrystal | Interaction | H···A /Å | D···A /Å | ∠D–H···A /º | Symmetry code |
|---|---|---|---|---|---|
| ACZ–VLM (1:2) | N3–H3A···O4 | 1.93 | 2.789(2) | 174 | 1+x,1/2-y,-1/2+z |
| | N4–H4A···O5 | 2.03 | 2.881(3) | 170 | 1+x,y,z |
| | N4–H4B···O4 | 2.21 | 2.920(3) | 159 | 1+x,y,z |
| | N5–H5A···O5 | 2.03 | 2.873(2) | 166 | x,-y,1-z |
| | N6–H6C···N1 | 2.15 | 2.999(3) | 167 | -1+x,y,z |
| ACZ–CPR hydrate (1:1:1) | N3–H3A···N2 | 2.13 | 2.937(2) | 176 | -x,1-y,-z |
| | N4–H4D···O4 | 1.9 | 2.810(2) | 176 | 1-x,-y,1-z |
| | N4–H4E···O5 | 1.96 | 2.844(3) | 164 | x,-1+y,z |
| | N5–H5A···O4 | 2.13 | 2.931(3) | 176 | 1-x,1-y,-z |
| | O5–H5B···O2 | 2.26 | 3.020(3) | 155 | -1+x,1+y,z |
| | O5–H5B···O2 | 2.59 | 3.125(3) | 124 | 1-x,1-y,-z |
| | O5–H5C···N1 | 2.41 | 3.123(3) | 167 | 1-x,1-y,-z |
| | C4–H4B···O2 | 2.58 | 3.516(3) | 165 | 1-x,1-y,-z |
| | C10–H10B···O3 | 2.51 | 3.471(3) | 172 | ----[a] |
| ACZ–2HP (1:2) | N3–H3A···O5 | 1.85 | 2.705(3) | 173 | 1-x,1-y,-z |
| | N4–H4A···O4 | 2.01 | 2.834(3) | 172 | 2-x,1-y,1-z |
| | N4–H4B···O1 | 2.09 | 2.967(3) | 172 | 2-x,2-y,-z |
| | N5–H5A···O4 | 1.98 | 2.822(3) | 166 | 2-x,1-y,1-z |
| | N6–H6A···N2 | 2.10 | 2.954(3) | 169 | 1-x,1-y,-z |
| | C6–H6···O3 | 2.51 | 3.143(4) | 126 | 1-x,1-y,1-z |
| | C12–H12···O1 | 2.58 | 3.479(3) | 162 | 1-x,2-y,-z |
| | C13–H13···O2 | 2.58 | 3.471(4) | 160 | 1-x,2-y,-z |
| ACZ–2HP (1:1) | N3–H3A···O4 | 1.86 | 2.744(2) | 177 | 1+x,y,1+z |
| | N4–H4D···N1 | 2.152 | 2.973(2) | 163 | -1+x,y,z |
| | N4–H4E···O3 | 2.056 | 2.893(2) | 167 | 1/2+x,1/2-y,1/2+z |
| | N5–H5A···N2 | 2.21 | 2.966(3) | 171 | -1+x,y,-1+z |
| | C4–H4B···O1 | 2.58 | 3.528(3) | 170 | -x,-y,1-z |
| ACZ–MeHP (1:1) | N4–H4D···N5 | 2.368 | 2.368(4) | 147 | ----[a] |
| | N4–H4E···O12 | 2.133 | 2.966(5) | 178 | x,-y+1,+z-1/2 |
| | N8–H6A···O3 | 2.244 | 3.141(1) | 150 | x,-y+1,+z-1/2 |

| | | | | | |
|---|---|---|---|---|---|
| | N8–H6B···O5 | 1.861 | 2.939(1) | 175 | x,-y+1,+z-1/2 |
| | N7–H41···O10 | 1.816 | 2.674(2) | 175 | x,-y+1,+z-1/2 |
| | N8–H6B···O7 | 2.257 | 2.995(3) | 157 | x,+y,+z-1 |
| | N11–H11A···O12 | 1.881 | 2.740(2) | 178 | x-1,+y,+z |
| | N12–H12E···O9 | 2.708 | 2.965(1) | 103 | x,-y,+z+1/2 |
| | N12–H12E···O4 | 2.311 | 2.986(2) | 156 | x,+y,+z+1 |
| | N13–H13A···N6 | 2.143 | 2.995(2) | 170 | x,-y+1,+z+1/2 |
| | N3–H53A···O11 | 1.964 | 2.771(2) | 170 | x+1,+y,+z |
| ACZ–OMeHP hydrate (1:1:1) | N3–H3A···O5 | 2.00 | 2.795(3) | 174 | 2-x,-y,-z |
| | N4–H4D···O6 | 2.05 | 2.844(3) | 168 | 1-x,-y,1-z |
| | N4–H4E···O4 | 2.23 | 3.047(3) | 150 | ---- |
| | N5–H5A···N2 | 2.03 | 2.959(3) | 176 | 2-x,-y,-z |
| | O6–H6A···O5 | 1.95 | 2.846(3) | 167 | ---- |
| | O6–H6B···N1 | 2.34 | 3.006(4) | 149 | -1+x,y,z |
| | C4–H4A···O2 | 2.49 | 3.404(4) | 160 | x,y,-1+z |
| | C7–H7···O1 | 2.50 | 3.426(3) | 177 | 1-x,1-y,-z |
| ACZ–NAM (1:1) | N3–H3A···N2 | 2.02 | 2.873(5) | 175 | -x,-y,1-z |
| | N4–H4D···N5 | 2.13 | 2.915(6) | 165 | x,-1+y,z |
| | N4–H4E···O4 | 2.11 | 2.893(5) | 165 | 2-x,1-y,-z |
| | N6–H6A···O4 | 2.06 | 2.916(5) | 174 | 3-x,1-y,-z |
| | N6–H6B···O2 | 2.31 | 3.089(5) | 151 | ---- |
| | C6–H6···O4 | 2.48 | 2.805(6) | 101 | Intramolecular |
| | C7vH7···O3 | 2.55 | 3.438(6) | 160 | -1+x,1+y,z |
| | C8–H8···O1 | 2.55 | 3.469(7) | 168 | ---- |
| ACZ–NAM–2HP (1:1:1) | N3–H3A···N5 | 2.05 | 2.904(3) | 176 | 1-x,1-y,1-z |
| | N4–H4D···O5 | 1.89 | 2.810(3) | 168 | 2-x,-y,1-z |
| | N4–H4E···O4 | 2.14 | 2.954(3) | 173 | 2-x,1-y,-z |
| | N6–H6B···O1 | 1.98 | 2.840(3) | 174 | ----- |
| | N7–H7A···O1 | 1.93 | 2.785(3) | 174 | 1+x,-1+y,z |
| | C7–H7···N1 | 2.61 | 3.238(4) | 126 | ------ |
| | C8–H8···N2 | 2.62 | 3.446(4) | 149 | ------ |
| | C9–H9···N2 | 2.61 | 3.400(4) | 143 | 1-x,1-y,1-z |
| | C15–H15···O5 | 2.52 | 3.359(4) | 151 | 1-x,-y,1-z |

**Table S2** REFCODEs of sulfonamide−amide, sulfonamide−pyridine and sulfonamide−acid supramolecular synthons in the CSD.

| Sulfonamide−amide (25) | | | | |
|---|---|---|---|---|
| DATFEL | DATFIP | EGENIP | LIQQEJ | LIQQIN |
| LIQQIN01 | LIQQIN02 | LOFLID | NUMGUZ | NUMHAG |
| NUMHEK | NUMHIO | NUMHOU | NUMHUA | NUMJAI |
| NUMJEM | NUMJIQ | NUMJOW | NUMJUC | NUMKAJ |
| NUMKEN | PIRYAS | SANAPY | XAVTEV | YASGOQ02[a] |
| YASGOQ04[a] | | | | |
| Sulfonamide−pyridine (4) | | | | |
| EGEPAJ | POVGAK | POVGEO | POVGIS | |
| Sulfonamide−acid (3) | | | | |
| ACIFAT | BOKHAM | LOFLAV | | |

[a] The same Refcode is repeated twice.