Crystal Structures of Large-Volumecommercial Pharmaceuticals

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As part of a continuing project, the room-temperature crystal structures of eight commercial pharmaceutical APIs have been solved and refined using synchrotron X-ray powder diffraction data (11-BM at APS) and optimized using density functional techniques. Danofloxacin mesylate (C19H21FN3O3) (CH3O3S) crystallizes in space group P1 with a = 6.77467, b = 12.4975, c = 12.8277 Å, α = 84.8277, β = 87.7524, γ = 74.9923°, V = 1044.67 Å3, and Z = 2. Meglumine diatrizoate (C7H17NO5) (C11H8I3N2O4) crystallizes in space group P21 (#4) with a = 10.74697(4), b = 6.49364(2), c = 18.52774(7) Å, β = 90.2263(3), V = 1292.985(5) Å3, and Z = 2. Encorafenib C22H27ClFN7O4S crystallizes in space group P21 (#4) with a = 16.17355(25), b = 9.52338(11), c = 17.12368(19) Å, β = 89.9928(22), V = 2637.49(4) Å3, and Z = 4. Omadacycline dihydrate C29H40N4O7(H2O)2 crystallizes in space group R3 (#146) with a = 24.34435(8), c = 14.55213(5) Å, V = 7468.849(29) Å3, and Z = 9. Nicarbazin (C12H10N4O5) (C6H8N2O) crystallizes in space group P-1 (#2) with a = 6.90659(8), b = 12.0794(4), c = 13.5040(7) Å, α = 115.5709(11), β = 102.3658(6), γ = 91.9270(4)°, V = 982.466(5) Å3, and Z = 2. Oxfendazole C15H13N3O3S crystallizes in space group P21/c (#14) with a = 18.87326(26), b = 10.40333(5), c = 7.25089(5) Å, β = 91.4688(10)° V = 1423.206(10) Å3, and Z = 4. Butenafine hydrochloride C23H28NCl crystallizes in space group P21 (#4) with a = 13.94807(5), b = 9.10722(2), c = 16.46676(6) Å, β = 93.9663(5)°, V = 2086.733(8) Å3, and Z = 4. Besifloxacin hydrochloride C19H22ClFN3O3Cl crystallizes in space group P1 (#1) with a = 5.36596(8), b = 10.3234(4), c = 17.9673(14) Å, α = 98.122(5), β = 92.9395(9), γ = 96.1135(3)°, V = 977.483(13) Å3, and Z = 2. All of structure solutions presented "interesting" features. Other new structures may be presented as they become available.