Crystal Structures of Large-Volume Commercial 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 Å, b = 12.4975 Å, c = 12.8277 Å, α = 84.8277, β = 74.9923°, γ = 1044.67 Å³, and Z = 2. Meglumine diatrizoate (C₇H₁₇NO₅) (C₁₁H₈I₃N₂O₄) crystallizes in space group P₂₁ (no.4) with a = 10.74697(4) Å, b = 6.49364(2) Å, c = 18.5277(7) Å, β = 90.2263(3), V = 1292.985(5) Å³, and Z = 2. Encorafenib C₂₂H₂₇ClFN₇O₄S crystallizes in space group P₂₁ (no.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 (no.146) with a = 24.34435(8) Å, b = 7468.849(29) Å, c = 7.52338(11), γ = 17.12368(19) Å, α = 115.5709(11), β = 102.3658(6), γ = 91.9270(4), V = 982.466(5) Å³, and Z = 2. Nicarbazin (C₁₂H₁₀N₄O₅) (C₆H₈N₂O) crystallizes in space group P-1 (no.2) with a = 6.90659(8) Å, b = 12.0794(4) Å, 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 (no.14) with a = 18.87326(26) Å, b = 10.40333(5) Å, c = 7.25089(5) Å, β = 91.4688(10)°, γ = 1423.206(10) Å, and Z = 4. Butenafine hydrochloride C₂₃H₂₈NCl crystallizes in space group P₂₁ (no.4) with a = 13.94807(5) Å, b = 9.10722(2), c = 16.46676(6) Å, β = 93.9663(5), V = 2086.733(8) Å³, and Z = 4. Besifloxacin hydrochloride C₁₉H₂₂ClF₃N₃OCl crystallizes in space group P1 (#1) with a = 5.36596(8) Å, 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.