

W0037

Taxol - Single Crystal Structures and Solid State Behavior of Six Forms. John DiMarco, Jack Gougoutas, Solid State Chemistry, Bristol-Myers Squibb Pharmaceutical Research Institute, Route 206 & Province Line Rd., Princeton, NJ 08543.

Taxol is a potent anti-cancer natural product discovered by the National Institutes of Health (NIH). Bristol-Myers Squibb Pharmaceutical Research Institute undertook the challenging research and development necessary to bring this drug to market. We have solved the structures and characterized the solid state behavior of five crystal forms, including the neat (solvent-free) crystal form A – the registered form of commerce. Our studies revealed a remarkably invariant hydrogen bonded “dimer” ($Z'=2$) in all forms of Taxol. Most of the forms have been shown to be topotactic solid state precursors of form A and/or the tri-hydrate form B. The solid state molecular conformations are compared to the proposed bound conformation in Tubulin.