Supporting Information

Experimental Section

Preparation of the complex of baccatin III with imidazole (4).

To a stirred solution of 250 mg (0.426 mmole) of baccatin III in 6 mL of CH_2Cl_2 at room temperature was added a solution of 32 mg (0.469 mmole) of imidazole in 1 ml of CH_2Cl_2. The resulting solution was stirred at room temperature for 30 minutes and then the precipitated crystalline complex of baccatin III and imidazole was collected by filtration and dried to give 247 mg (89%) of the complex. A crystal suitable for x-ray crystallographic analysis was obtained by recrystallization from acetonitrile.

Recovery of baccatin III from 4 (3).

To 200 mg (0.305 mmole) of **4** was added, at room temperature with stirring, 6 mL of CD_2Cl_2 and 2 mL of D_2O. The resulting solution was stirred 30 minutes at room temperature. At 5-, 15-, and 30-minute intervals, samples were withdrawn from the solution for NMR analysis. The NMR analysis of the sample taken at 5 minutes showed that the complex was completely broken. After 30 minutes, the organic CD_2Cl_2 layer was separated, the water layer was washed once with 5 ml portion of CH_2Cl_2 and separated. The separated 5 mL portion of CD_2Cl_2 was combined with the layer of CH_2Cl_2, dried and then concentrated to give 178 mg (99%) of baccatin III.

Preparation of the complex of baccatin III with imidazole from a cell culture extract containing baccatin III in admixture with other taxanes (4).

A whole broth mixture approximately (400L) derived from plant tissue culture, obtained by U.S. Patent No. 5,407,816, containing 200 mcg/ml of baccatin III was extracted with a solution containing 7% acetic acid and 93% of a mixture of 15% isopropanol in butyl acetate. The resulting organic solution was washed with water and concentrated under vaccum to approx. 70 L and diluted with 10% heptane. The solution was passed trhrough a column containing 40L of alumina packed using 20% butanol in butyl acetate and equilibrated with butyl acetate. The column was eluted successively with 100L of butyl acetate and 150 L of 2.5% butanol in butyl acetate. A portion of the desired fractions containing baccatin III were combined and concentrated to afford a butyl acetate solution of baccatin III assaying at approximately 18 mg/ml.

A 4.5 mL aliquot of the n-butyl acetate solution was concentrated to 2 ml. With stirring at room temperature, 11 mg (0.16 mmole) of imidazole were added. After stirring for five minutes, a precipitate was observed. An additional 11 mg (0.16 mmole) of imidazole was added to the mixture and the mixture was stirred for twenty-five minutes. The mixture was cooled to 0^oC and stirred for one hour. The precipitated solid was collected on a filter and dried to yield 60 mg (67%) of **4**.

Baccatin III-isopropanol complex (5).

Baccatin III (100 mg, 0.17 mmol) was dissolved in dichloromethane (4 mL). 2-propanol was added (130 uL), and the resulting solution was allowed to stir for 1 h. Hexane was added to the cloud point and crystallization began. Work-up afforded 85mg (77%) of

complex **5**. A crystal suitable for x-ray crystallographic analysis was obtained by recrystallization from dichloromethane-2-propanol.

Preparation of Complex of Baccatin III with 2-propanol from a Cell Culture. Extract Containing Baccatin III in Admixture with Other Taxanes (5)

A 10 mL aliquot of a cell culture extract obtained as described above in n-butyl acetate containing 18 mg/ml baccatin III was concentrated to dryness. The residue was dissolved in 3 mL of 2-propanol at 50^0C. After stirring the solution at room temperature for one hour, a precipitate was observed. The mixture was stirred at room temperature overnight. The precipitated solid was collected on a filter and dried to yield 156 mg (87%) of **5**.