

Simple, powerful retrosynthesis tool

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Conditions	Yield	Reference
Stage #1: 4-(4-N-methylpiperazine-1-yl)methyl benzoic acid dihydrochloride With N-ethyl-N,N-diisopropylamine In dichloromethane at 10 - 20°C; for 0.5h; Stage #2: With tetrabutyl ammonium fluoride; 1,1'-carbonyldiimidazole In dichloromethane at 20°C; for 3h; Stage #3: C ₂₂ H ₃₁ N ₅ Si ₂ In dichloromethane at 0 - 20°C; for 3h; Solvent; Reagent/catalyst;	91.3%	Anhui Haikang Pharmaceutical Co., Ltd.; Zhang Xiaoshun CN108752314, 2018, A Location in patent: Paragraph 0015; 0016; 0028; 0033; 0036; 0037 Full Text Details Abstract
1; 2 Synthesis of Compound (I) In the second step, 4-[(4-methyl-1-piperazine)methyl]benzoic acid dihydrochloride 33.1 g (107.8 mmol, 1.1 eq) and 100 g of tetrahydrofuran were placed in a reaction flask at a temperature of 10-20 °C. After adding 21.8 g (215.6 mmol, 2.2 eq) of triethylamine under stirring for 30 minutes, 0.26 g (0.98 mmol, 1% eq) of tetrabutylammonium fluoride was added, and N,N'-carbonyldiimidazole 17.5 g was added in portions. (107.8 mmol, 1.1 eq) was stirred at room temperature for 3 hours, and 41.3 g of the compound (IV) (98.1 mmol, 1.0 eq) obtained in the above step was added dropwise to a solution of 60 g of tetrahydrofuran at 0-10 °C, and the mixture was stirred at room temperature for 2 hours. The TLC controlled raw material was completely reacted, the solvent was distilled off under reduced pressure, 150 g of a 10% aqueous hydrochloric acid solution was added, stirred for 2 hours, extracted with dichloromethane (90 gx2), and the aqueous layer was adjusted to adjust the pH with 10% sodium hydroxide. 8-9, filtration, solid recrystallized from isopropanol to give a white solid imatinib 43.8 g, yield 90.6%,	91.3%	Anhui Haikang Pharmaceutical Co., Ltd.; Zhang Xiaoshun CN108774210, 2018, A Location in patent: Paragraph 0028; 0031; 0032; 0033



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"Seamless way to navigate from a compound to retrosynthesis straight away"

"You can easily make an informed decision on what route you want to take to the lab"