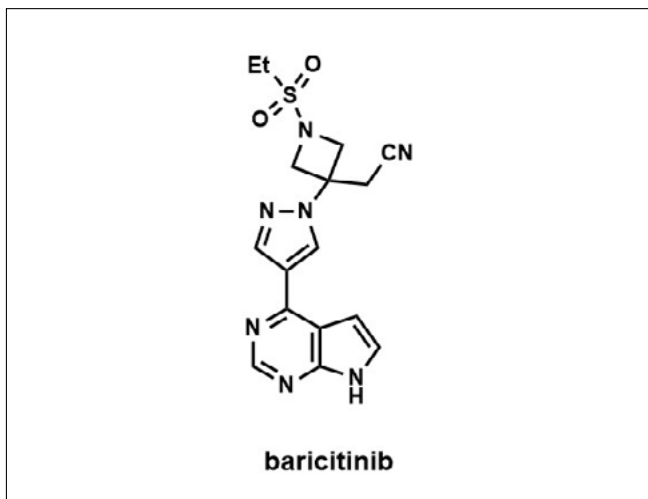


Baricitinib



Related reviews in Science of Synthesis

- Pyrimidines
- Pyrazoles
- Azetidines
- Alkanesulfonamides
- Nitriles
- Hetarylboron Cross-Coupling Reactions (Suzuki–Miyaura)

Synonyms: INCB-28050; LY-3009104

ATC: L04AA37

Use: rheumatoid arthritis, JAK inhibitor

Chemical name: 2-[1-(Ethylsulfonyl)-3-[4-(7H-pyrrolo[2,3-d]pyrimidin-4-yl)-1H-pyrazol-1-yl]azetidin-3-yl]acetonitrile

Formula: C₁₆H₁₇N₇O₂S

MW: 371.42 g/mol

CAS-RN: 1187594-09-7

InChI Key: XUZMWHLSFXCVMG-UHFFFAOYSA-N

InChI: InChI=1S/C16H17N7O2S/c1-2-26(24,25)22-9-16(10-22,4-5-17)23-8-12(7-21-23)14-13-3-6-18-15(13)20-11-19-14/h3,6-8,11H,2,4,9-10H2,1H3,(H,18,19,20)

Derivatives

Phosphate

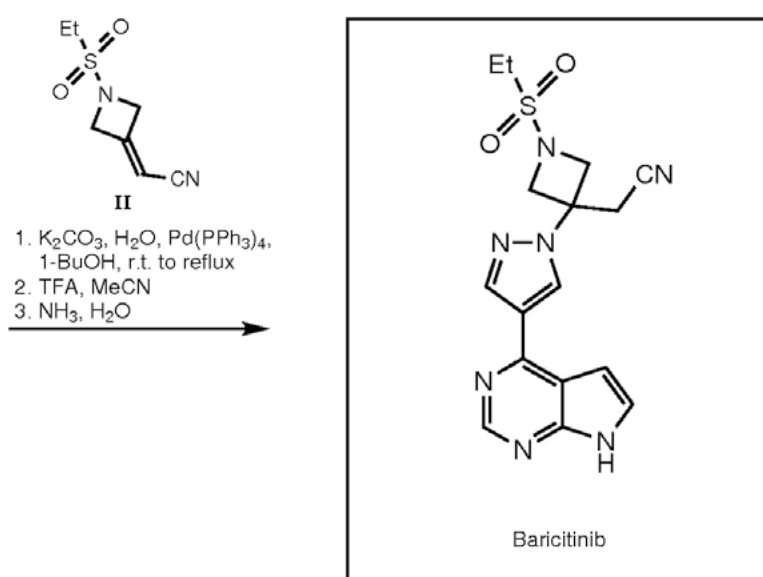
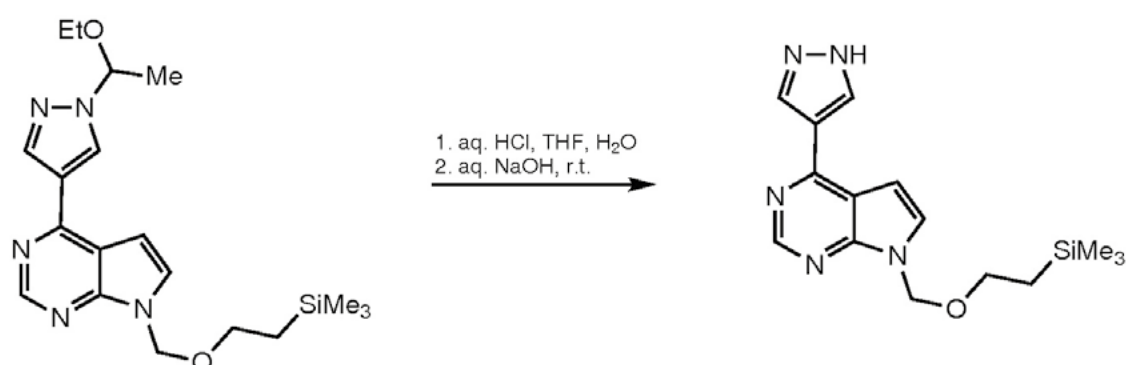
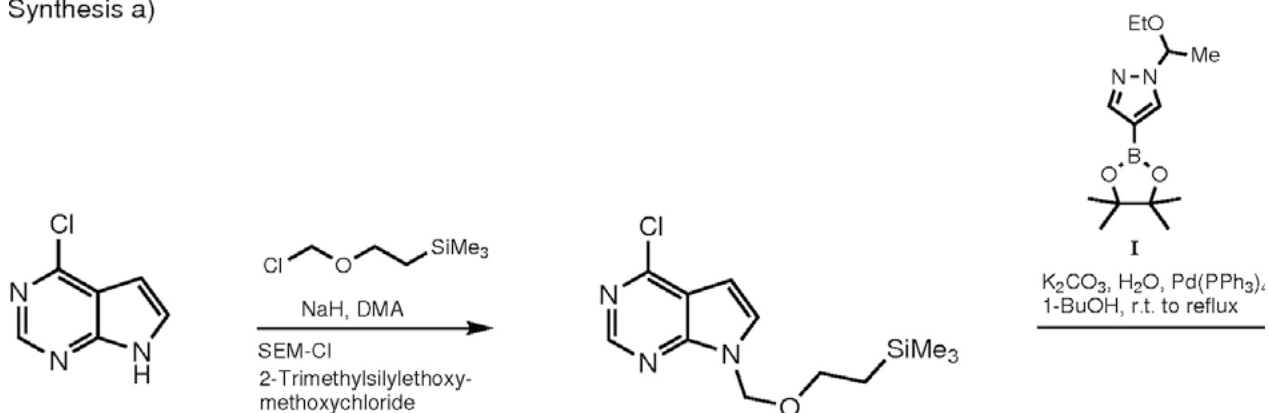
Formula: C₁₉H₁₇N₇O₆PS

MW: 469.41 g/mol

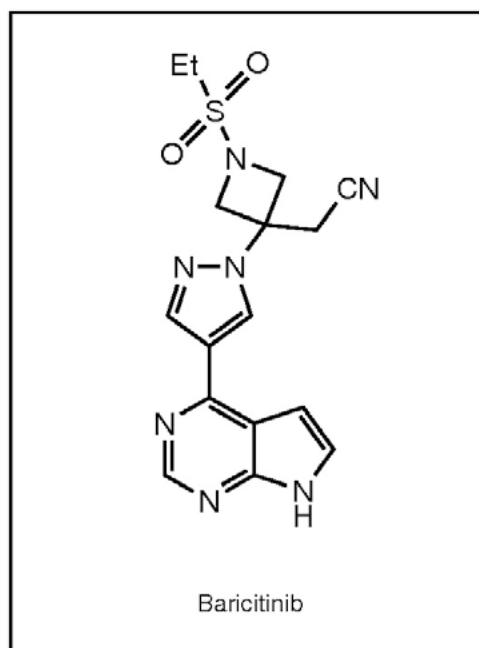
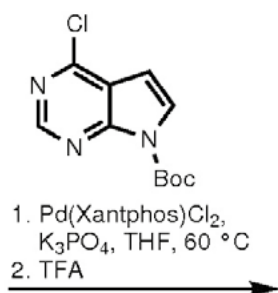
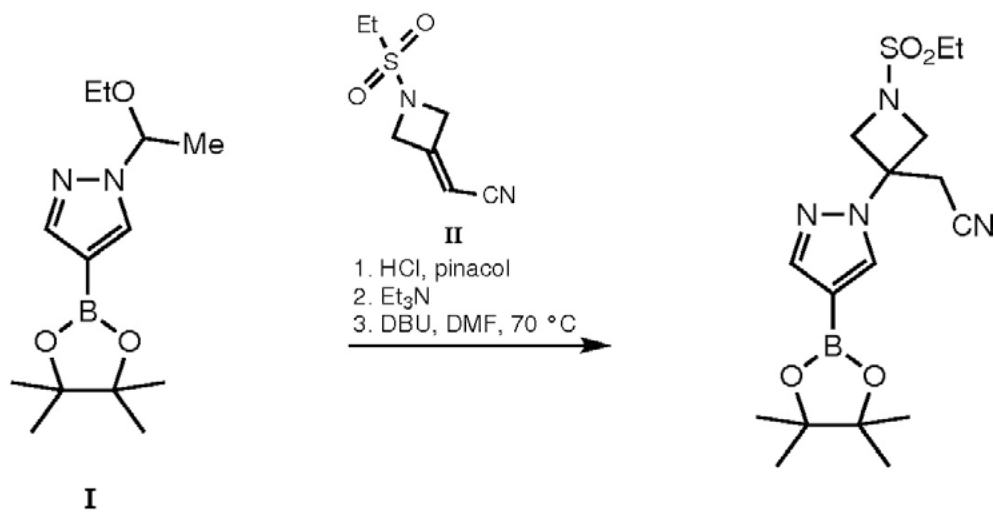
CAS-RN: 1187595-84-1

Synthesis Path

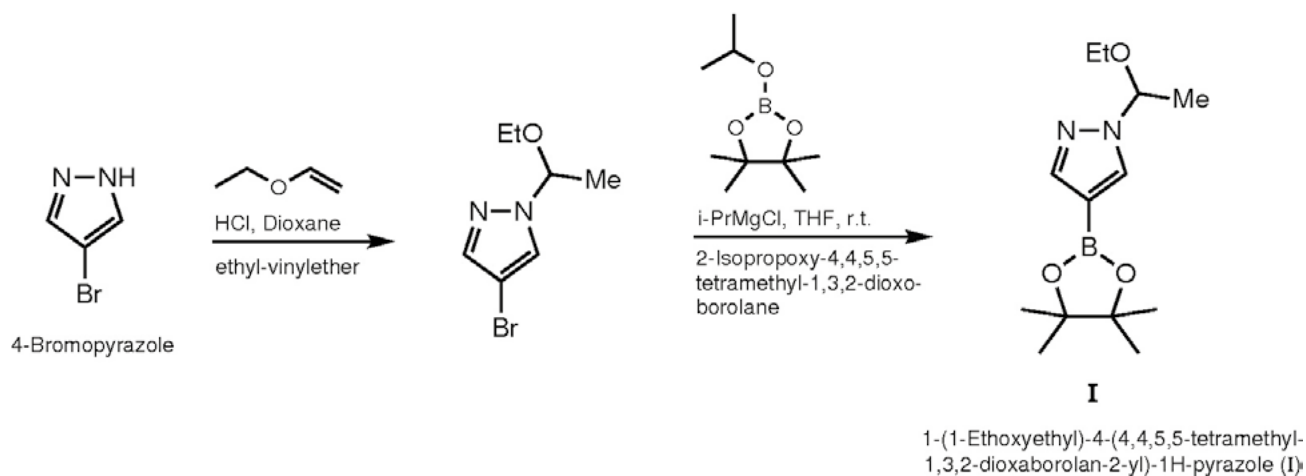
Synthesis a)



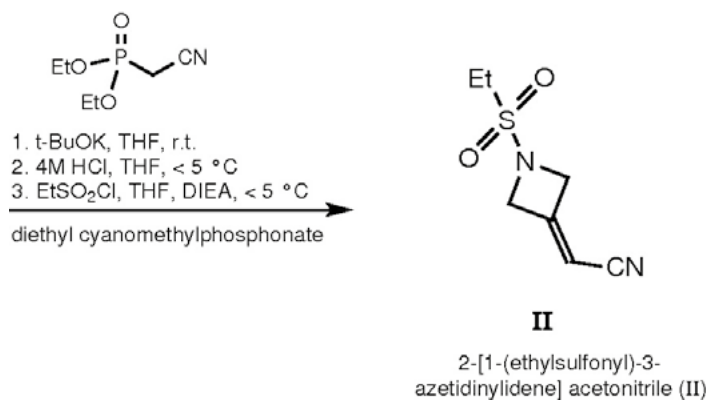
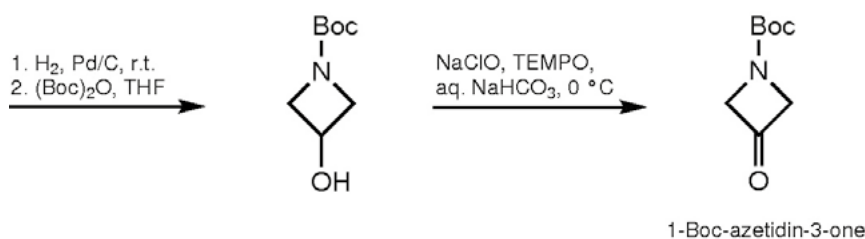
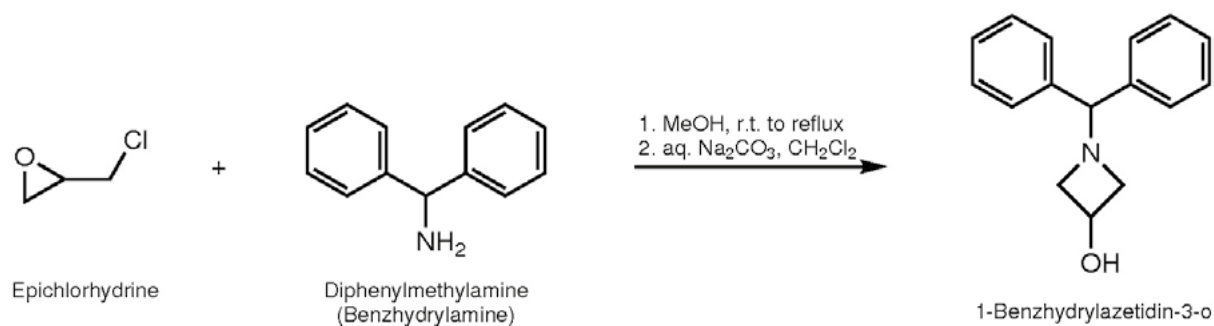
Synthesis b)



Preparation of 1-(1-Ethoxyethyl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-pyrazole (I)



Preparation of 2-[1-(ethylsulfonyl)-3-azetidinylidene] acetonitrile (II)



Substances Referenced in Synthesis Path

CAS-RN	Formula	Chemical Name
76513-69-4	C ₆ H ₁₅ ClOSi	2-Trimethylsilylethoxy-methoxychloride
2075-45-8	C ₃ H ₃ BrN ₂	4-Bromopyrazole
109-92-2	C ₄ H ₈ O	ethyl-vinylether
61676-62-8	C ₉ H ₁₉ BO ₃	2-Isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxo-borolane
1029716-44-6	C ₃ H ₂₃ N ₂ O ₃	1-(1-Ethoxyethyl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-pyrazole
106-89-8	C ₃ H ₅ ClO	Epichlorhydrine
91-00-9	C ₁₃ H ₁₃ N	Diphenylmethylamine
18621-17-5	C ₁₆ H ₁₃ NO	1-Benzhydrylazetid-3-ol
2537-48-6	C ₆ H ₁₂ NO ₃ P	diethyl cyanomethylphosphonate
1187595-85-2	C ₇ H ₁₀ N ₂ O ₂ S	2-[1-(ethylsulfonyl)-3-azetidinylidene] acetonitrile
398489-26-4	C ₈ H ₁₃ NO ₃	1-Boc-azetid-3-one

Trade Names

Country	Trade Name	Vendor
USA	Olumiant	Eli Lilly, 2016
EU	Olumiant	Eli Lilly, 2016

Formulations

f.c. tablet 2 mg, 4 mg (as phosphate)

References

- Jiaojiao, X. et al., *Journal of Chem. Research*, (2016) **40** (4), 205.
a WO 2009 114512 (Incyte; 17.09.2009; US-prior. 11.03.2008).
 US 8 158 616 (Incyte; 17.04.2012; US-prior. 11.03.2008).
b WO 2016 205487 (Eli Lilly & Co.; 22.12.2016; US-prior. 19.06.2015).

Preparation of I

Qiyang, L. et al., *Organic Letters*, (2009) **11**(9), 1999-2002.