Regioselective Synthesis of an Imidazo[4,5-c]pyridine Through Selective Acylation of 3,4-Diaminopyridine. Synthesis of CP-885,316.

Stéphane Caron,* Nga M. Do, Ruth E. McDermott, S. Bahmanyar
Chemical R&D, Pfizer Global R&D, MS-8118D/4002, Groton CT 06340
stephane.caron@pfizer.com

Supporting Information
Computational

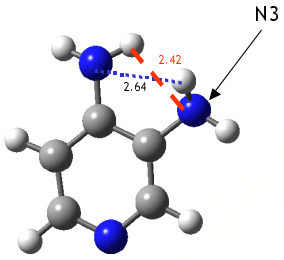
Coordinates for optimized geometry:

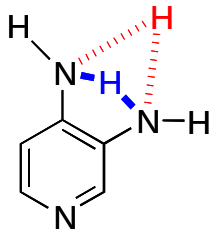
Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.716698	-1.355473	-0.020532
2	6	0.505086	-0.684071	0.000311
3	6	0.485101	0.728805	0.006909
4	6	-0.762381	1.358759	0.029532
5	6	-1.918547	0.578970	0.016068
6	7	-1.915658	-0.757486	-0.022613
7	7	1.699185	1.413331	0.037320
8	1	-0.721352	-2.446916	-0.039700
9	7	1.758636	-1.336877	-0.046016
10	1	-0.829551	2.444157	0.042327
11	1	-2.895714	1.059116	0.029285
12	1	1.633186	2.395778	-0.202065
13	1	2.427637	0.946180	-0.495580
14	1	2.369163	-1.044984	0.715273
15	1	1.666134	-2.348046	-0.024106

Optimized Geometry of 3,4-diaminopyridine

Structural Features: N3 is slightly more pyramidalized than N4





Intramolecular hydrogen bonding between the two N's (distances reported in Å above).

N3 is more pyramidalized than N4
Sum of N3 angles = 333°
Sum of N4 angles = 338°
For reference: sum of angles for ammonia = 327°

The HOMO/LUMO maps are simply the value of the HOMO <orbital|orbital> (or LUMO) displayed on the van der Waals surface

HOMO Maps: N3 has larger HOMO values when compared to N4