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Electronic Supplementary Information

Radical-mediated nitrile translocation as the key step in the stereoselective transformation of 2-(4-chloro-2-cyanobutyl)aziridines to methyl *cis*-(1-arylmethyl-4-phenylpiperidin-2-yl)acetates

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Compound 3a

Table 1. Crystal data and structure refinement for compound **3a**.

Identification code	Compound3a	
Empirical formula	C20 H22 N2	
Formula weight	290.40	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 5.7575(3) Å	α= 74.944(1)°.
	b = 10.4335(5) Å	β= 84.193(1)°.
	c = 14.3548(7) Å	γ = 77.533(1)°.
Volume	812.14(7) $Å^3$	
Z	2	
Density (calculated)	1.188 Mg/m^3	
Absorption coefficient	0.070 mm^{-1}	
F(000)	312	
Crystal size	0.5 x 0.20 x 0.10 mm^3	
Theta range for data collection	2.06 to 28.77°.	
Index ranges	-7<=h<=7, -14<=k<=14, -19<=l<=19	
Reflections collected	12358	
Independent reflections	4224 [R(int) = 0.0260]	
Completeness to theta = 28.77°	99.8 %	
Absorption correction	Multiscan	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4224 / 0 / 199	
Goodness-of-fit on F^2	1.050	
Final R indices [I>2sigma(I)]	R1 = 0.0458, wR2 = 0.1246	
R indices (all data)	R1 = 0.0516, wR2 = 0.1293	
Largest diff. peak and hole	0.373 and -0.171 $e.Å^{-3}$	

Table 2. Bond lengths [Å] and angles [°] for COMPOUND3A.

N(1)-C(1)	1.4643(13)
N(1)-C(5)	1.4694(14)
N(1)-C(8)	1.4763(13)
C(1)-C(2)	1.5378(14)
C(1)-C(6)	1.5425(15)
C(1)-H(1A)	1.0000
N(2)-C(7)	1.1448(16)
C(2)-C(3)	1.5279(15)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(15)	1.5184(14)
C(3)-C(4)	1.5353(15)
C(3)-H(3A)	1.0000
C(4)-C(5)	1.5177(14)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.4708(16)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(8)-C(9)	1.5159(15)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(14)	1.3902(16)
C(9)-C(10)	1.4013(16)
C(10)-C(11)	1.3885(16)
C(10)-H(10A)	0.9500
C(11)-C(12)	1.3921(18)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.3862(18)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.3983(17)
C(13)-H(13A)	0.9500

C(14)-H(14A)	0.9500
C(15)-C(16)	1.3985(15)
C(15)-C(20)	1.3999(15)
C(16)-C(17)	1.3910(15)
C(16)-H(16A)	0.9500
C(17)-C(18)	1.3877(16)
C(17)-H(17A)	0.9500
C(18)-C(19)	1.3872(16)
C(18)-H(18A)	0.9500
C(19)-C(20)	1.3923(15)
C(19)-H(19A)	0.9500
C(20)-H(20A)	0.9500

C(1)-N(1)-C(5)	110.53(8)
C(1)-N(1)-C(8)	113.60(8)
C(5)-N(1)-C(8)	108.97(8)
N(1)-C(1)-C(2)	109.69(8)
N(1)-C(1)-C(6)	111.85(9)
C(2)-C(1)-C(6)	108.22(9)
N(1)-C(1)-H(1A)	109.0
C(2)-C(1)-H(1A)	109.0
C(6)-C(1)-H(1A)	109.0
C(3)-C(2)-C(1)	113.87(9)
C(3)-C(2)-H(2A)	108.8
C(1)-C(2)-H(2A)	108.8
C(3)-C(2)-H(2B)	108.8
C(1)-C(2)-H(2B)	108.8
H(2A)-C(2)-H(2B)	107.7
C(15)-C(3)-C(2)	113.96(9)
C(15)-C(3)-C(4)	111.35(8)
C(2)-C(3)-C(4)	108.33(8)
C(15)-C(3)-H(3A)	107.7
C(2)-C(3)-H(3A)	107.7
C(4)-C(3)-H(3A)	107.7
C(5)-C(4)-C(3)	110.35(8)
C(5)-C(4)-H(4A)	109.6

C(3)-C(4)-H(4A)	109.6
C(5)-C(4)-H(4B)	109.6
C(3)-C(4)-H(4B)	109.6
H(4A)-C(4)-H(4B)	108.1
N(1)-C(5)-C(4)	111.76(9)
N(1)-C(5)-H(5A)	109.3
C(4)-C(5)-H(5A)	109.3
N(1)-C(5)-H(5B)	109.3
C(4)-C(5)-H(5B)	109.3
H(5A)-C(5)-H(5B)	107.9
C(7)-C(6)-C(1)	111.62(9)
C(7)-C(6)-H(6A)	109.3
C(1)-C(6)-H(6A)	109.3
C(7)-C(6)-H(6B)	109.3
C(1)-C(6)-H(6B)	109.3
H(6A)-C(6)-H(6B)	108.0
N(2)-C(7)-C(6)	179.06(13)
N(1)-C(8)-C(9)	110.75(8)
N(1)-C(8)-H(8A)	109.5
C(9)-C(8)-H(8A)	109.5
N(1)-C(8)-H(8B)	109.5
C(9)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	108.1
C(14)-C(9)-C(10)	118.55(10)
C(14)-C(9)-C(8)	121.95(10)
C(10)-C(9)-C(8)	119.49(10)
C(11)-C(10)-C(9)	120.59(11)
C(11)-C(10)-H(10A)	119.7
C(9)-C(10)-H(10A)	119.7
C(10)-C(11)-C(12)	120.37(11)
C(10)-C(11)-H(11A)	119.8
C(12)-C(11)-H(11A)	119.8
C(13)-C(12)-C(11)	119.59(11)
C(13)-C(12)-H(12A)	120.2
C(11)-C(12)-H(12A)	120.2
C(12)-C(13)-C(14)	119.99(11)

C(12)-C(13)-H(13A)	120.0
C(14)-C(13)-H(13A)	120.0
C(9)-C(14)-C(13)	120.91(11)
C(9)-C(14)-H(14A)	119.5
C(13)-C(14)-H(14A)	119.5
C(16)-C(15)-C(20)	117.80(10)
C(16)-C(15)-C(3)	119.66(9)
C(20)-C(15)-C(3)	122.44(9)
C(17)-C(16)-C(15)	121.20(10)
C(17)-C(16)-H(16A)	119.4
C(15)-C(16)-H(16A)	119.4
C(18)-C(17)-C(16)	120.26(10)
C(18)-C(17)-H(17A)	119.9
C(16)-C(17)-H(17A)	119.9
C(19)-C(18)-C(17)	119.35(10)
C(19)-C(18)-H(18A)	120.3
C(17)-C(18)-H(18A)	120.3
C(18)-C(19)-C(20)	120.43(10)
C(18)-C(19)-H(19A)	119.8
C(20)-C(19)-H(19A)	119.8
C(19)-C(20)-C(15)	120.95(10)
C(19)-C(20)-H(20A)	119.5
C(15)-C(20)-H(20A)	119.5

Symmetry transformations used to generate equivalent atoms:

Table 3. Torsion angles [°] for COMPOUND3A.

C(5)-N(1)-C(1)-C(2)	57.89(11)
C(8)-N(1)-C(1)-C(2)	-179.26(9)
C(5)-N(1)-C(1)-C(6)	177.98(8)
C(8)-N(1)-C(1)-C(6)	-59.17(12)
N(1)-C(1)-C(2)-C(3)	-55.21(11)
C(6)-C(1)-C(2)-C(3)	-177.48(8)
C(1)-C(2)-C(3)-C(15)	176.83(8)
C(1)-C(2)-C(3)-C(4)	52.29(11)
C(15)-C(3)-C(4)-C(5)	-179.03(9)
C(2)-C(3)-C(4)-C(5)	-52.95(11)
C(1)-N(1)-C(5)-C(4)	-61.91(11)
C(8)-N(1)-C(5)-C(4)	172.58(8)
C(3)-C(4)-C(5)-N(1)	59.38(12)
N(1)-C(1)-C(6)-C(7)	-51.97(12)
C(2)-C(1)-C(6)-C(7)	68.97(11)
C(1)-C(6)-C(7)-N(2)	-68(8)
C(1)-N(1)-C(8)-C(9)	164.39(9)
C(5)-N(1)-C(8)-C(9)	-71.91(11)
N(1)-C(8)-C(9)-C(14)	120.88(11)
N(1)-C(8)-C(9)-C(10)	-60.01(13)
C(14)-C(9)-C(10)-C(11)	0.58(16)
C(8)-C(9)-C(10)-C(11)	-178.55(10)
C(9)-C(10)-C(11)-C(12)	-0.36(17)
C(10)-C(11)-C(12)-C(13)	-0.11(17)
C(11)-C(12)-C(13)-C(14)	0.34(17)
C(10)-C(9)-C(14)-C(13)	-0.35(17)
C(8)-C(9)-C(14)-C(13)	178.76(10)
C(12)-C(13)-C(14)-C(9)	-0.10(17)
C(2)-C(3)-C(15)-C(16)	145.65(10)
C(4)-C(3)-C(15)-C(16)	-91.45(12)
C(2)-C(3)-C(15)-C(20)	-38.24(14)
C(4)-C(3)-C(15)-C(20)	84.66(12)
C(20)-C(15)-C(16)-C(17)	-1.64(16)
C(3)-C(15)-C(16)-C(17)	174.65(10)

C(15)-C(16)-C(17)-C(18)	1.36(17)
C(16)-C(17)-C(18)-C(19)	-0.20(17)
C(17)-C(18)-C(19)-C(20)	-0.62(17)
C(18)-C(19)-C(20)-C(15)	0.31(17)
C(16)-C(15)-C(20)-C(19)	0.80(16)
C(3)-C(15)-C(20)-C(19)	-175.38(10)

Symmetry transformations used to generate equivalent atoms: