## **Supplementary Materials**

Table of	Contents
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S1 S7

1. X-ray crystallographic data for 2i 2. <sup>1</sup>H and <sup>13</sup>C-NMR spectra

1. X-ray crystallographic data for 2i:



Table S1. Crystal data and structure refinement for 2i (15 January 2009).

Identification code	snow20	
Empirical formula	$C_{22}H_{15}NO_2$	
Formula weight	325.35	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.0621(2)  Å	$\alpha = 87.277(2)$ °.
	b = 9.8863(2)  Å	$\beta = 67.4190(10)$ °.
	c = 10.2723(2)  Å	$\gamma = 79.943(2)^{\circ}$ .
Volume	$836.50(3) \text{ Å}^3$	
Z	2	
Density (calculated)	$1.292 \text{ Mg/m}^3$	
Absorption coefficient	$0.083 \text{ mm}^{-1}$	
F(000)	340	
Crystal size	$0.50 \times 0.40 \times 0.28 \text{ mm}^3$	
Theta range for data collection	2.09 to 27.68 °.	
Index ranges	$-11 \le h \le 11, -12 \le k \le 12, -13 \le l \le 13$	
Reflections collected	17175	
Independent reflections	3858 [R(int) = 0.0446]	
Completeness to theta = $27.68^{\circ}$	98.9%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.817	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data/restraints/parameters	3858/0/226	
Goodness-of-fit on $F^2$	1.001	
Final R indices [I>2sigma(I)]	R1 = 0.0446, $wR2 = 0.1112$	
R indices (all data)	R1 = 0.1025, wR2 = 0.1364	
Largest diff. peak and hole	$0.120 \text{ and } -0.151 \text{ e.} \text{\AA}^{-3}$	

	X	У	Z	U(eq)
O(1)	7689(1)	6326(1)	4917(1)	67(1)
O(2)	5083(1)	7352(1)	5617(1)	79(1)
N(1)	7646(1)	8373(1)	7096(2)	82(1)
C(1)	6982(2)	7965(1)	3431(1)	56(1)
C(2)	8495(2)	7609(1)	2366(2)	69(1)
C(3)	8888(2)	8318(2)	1117(2)	82(1)
C(4)	7799(2)	9380(2)	942(2)	85(1)
C(5)	6303(2)	9754(2)	1990(2)	81(1)
C(6)	5888(2)	9046(1)	3234(2)	68(1)
C(7)	6452(2)	7219(1)	4763(1)	60(1)
C(8)	7314(2)	5561(1)	6168(2)	62(1)
C(9)	6573(2)	4411(1)	6246(2)	74(1)
C(10)	6297(2)	3619(1)	7402(2)	77(1)
C(11)	6737(2)	3926(1)	8513(2)	66(1)
C(12)	6389(2)	3141(1)	9748(2)	81(1)
C(13)	6772(2)	3473(2)	10827(2)	86(1)
C(14)	7535(2)	4611(2)	10727(2)	82(1)
C(15)	7883(2)	5399(1)	9554(2)	69(1)
C(16)	7493(2)	5089(1)	8414(1)	58(1)
C(17)	7786(1)	5919(1)	7195(1)	56(1)
C(18)	8578(2)	7160(1)	7038(1)	56(1)
C(19)	10179(2)	7034(2)	6840(2)	75(1)
C(20)	10869(2)	8189(2)	6681(2)	91(1)
C(21)	9937(2)	9436(2)	6735(2)	90(1)
C(22)	8366(2)	9480(2)	6936(2)	99(1)

**Table S2.** Atomic coordinates (×10<sup>4</sup>) and equivalent isotropic displacement parameters ( $\mathring{A}^2 \times 10^3$ ) for **2i**. U(eq) is defined as one third of the trace of the orthogonalized U<sup>ij</sup> tensor.

 Table S3. Bond lengths [Å] and angles [ ] for 2i.

		1
O(1)-C(7)	1.3563(16)	
O(1)-C(8)	1.4143(16)	
O(2)-C(7)	1.2018(15)	
N(1)-C(18)	1.3301(16)	
N(1)-C(22)	1.3419(19)	
C(1)-C(2)	1.3846(17)	
C(1)-C(6)	1.3885(18)	
C(1)-C(7)	1.4736(18)	
C(2)-C(3)	1.384(2)	
C(2)-H(2A)	0.9300	
C(3)-C(4)	1.366(2)	
C(3)-H(3A)	0.9300	
C(4)-C(5)	1.370(2)	
C(4)-H(4A)	0.9300	
C(5)-C(6)	1.379(2)	
C(5)-H(5A)	0.9300	
C(6)-H(6A)	0.9300	

Table S3. Cont.

$\begin{array}{cccccccccccccccccccccccccccccccccccc$
$\begin{array}{c} C(8)-C(9) & 1.4029(19) \\ C(9)-C(10) & 1.356(2) \\ C(9)-H(9A) & 0.9300 \\ C(10)-C(11) & 1.407(2) \\ C(10)-C(11) & 0.9300 \\ C(10)-C(10)-C(10) \\ C(10)-C(10)-C(10)-C(10) \\ C(10)-C(10)-C(10)-C(10)-C(10) \\ C(10)-C$
C(9)-C(10)       1.536(2)         C(9)-H(9A)       0.9300         C(10)-C(11)       1.407(2)
C(9)-H(9A) 0.9300 C(10)-C(11) 1.407(2)
C(10)-C(11) 1.407(2)
C(10)-H(10A) 0.9300
C(11)-C(12) 1.413(2)
C(11)-C(16) 1.4188(18)
C(12)-C(13) 1.351(2)
C(12)-H(12A) 0.9300
C(13)-C(14) 1.401(2)
C(13)-H(13A) 0.9300
C(14)-C(15) 1.365(2)
C(14)-H(14A) 0.9300
C(15)-C(16) 1.406(2)
C(15)-H(15A) 0.9300
C(16)-C(17) 1.4269(18)
C(17)-C(18) 1.4981(17)
C(18)-C(19) 1.3693(18)
C(19)-C(20) 1.370(2)
C(19)-H(19A) 0.9300
C(20)-C(21) 1.358(2)
C(20)-H(20A) 0.9300
C(21)-C(22) 1.351(2)
C(21)-H(21A) 0.9300
C(22)-H(22A) 0.9300
C(7)-O(1)-C(8) 116.89(10)
C(18)-N(1)-C(22) 116.23(13)
C(2)-C(1)-C(6) 119.28(13)
C(2)-C(1)-C(7) 122.78(12)
C(6)-C(1)-C(7) 117.91(11)
C(3)-C(2)-C(1) 119.72(13)
C(3)-C(2)-H(2A) 120.1
C(1)-C(2)-H(2A) 120.1
C(4)-C(3)-C(2) 120.24(14)
C(4)-C(3)-H(3A) 119.9
C(2)-C(3)-H(3A) 119.9
C(3)-C(4)-C(5) 120.73(15)
C(3)-C(4)-H(4A) 119.6
C(5)-C(4)-H(4A) 119.6
C(4)-C(5)-C(6) 119.65(15)
C(4)-C(5)-H(5A) 120.2
C(6)-C(5)-H(5A) 120.2
C(5)-C(6)-C(1) 120.37(13)
C(5)-C(6)-H(6A) 119.8
C(1)-C(6)-H(6A) 119.8
O(2)-C(7)-O(1) 122.85(13)
O(2)-C(7)-C(1) 122.05(13)
O(1)-C(7)-C(1) 112.25(11)

 Table S3. Cont.

C(17)-C(8)-C(9)	123.21(13)
C(17)-C(8)-O(1)	118.59(11)
C(9)-C(8)-O(1)	118.04(13)
C(10)-C(9)-C(8)	118.72(15)
C(10)-C(9)-H(9A)	120.6
C(8)-C(9)-H(9A)	120.6
C(9)-C(10)-C(11)	121.51(13)
C(9)-C(10)-H(10A)	119.2
C(11)-C(10)-H(10A)	119.2
C(10)-C(11)-C(12)	121.82(13)
C(10)-C(11)-C(16)	119.05(13)
C(12)-C(11)-C(16)	119.08(15)
C(13)-C(12)-C(11)	121.24(15)
C(13)-C(12)-H(12A)	119.4
C(11)-C(12)-H(12A)	119.4
C(12)-C(13)-C(14)	119.87(15)
C(12)-C(13)-H(13A)	120.1
C(14)-C(13)-H(13A)	120.1
C(15)-C(14)-C(13)	120.57(16)
C(15)-C(14)-H(14A)	119.7
C(13)-C(14)-H(14A)	119.7
C(14)-C(15)-C(16)	121.14(14)
C(14)-C(15)-H(15A)	119.4
C(16)-C(15)-H(15A)	119.4
C(15)-C(16)-C(11)	118.09(13)
C(15)-C(16)-C(17)	122.54(12)
C(11)-C(16)-C(17)	119.34(13)
C(8)-C(17)-C(16)	118.17(12)
C(8)-C(17)-C(18)	120.28(12)
C(16)-C(17)-C(18)	121.55(12)
N(1)-C(18)-C(19)	122.43(12)
N(1)-C(18)-C(17)	116.50(11)
C(19)-C(18)-C(17)	121.08(12)
C(18)-C(19)-H(19A)	120.2
C(20)-C(19)-H(19A)	120.2
C(21)-C(20)-C(19)	118.81(15)
C(21)-C(20)-H(20A)	120.6
C(19)-C(20)-H(20A)	120.6
C(22)-C(21)-C(20)	118.28(15)
C(22)-C(21)-H(21A)	120.9
C(20)-C(21)-H(21A)	120.9
N(1)-C(22)-C(21)	124.68(15)
N(1)-C(22)-H(22A)	117.7
C(21)-C(22)-H(22A)	117.7

Symmetry transformations used to generate equivalent atoms.

proven	•••••••••••••••••••••••••••••••••••••••	-ponone mile				" ° ° ].
	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
O(1)	60(1)	73(1)	68(1)	0(1)	-27(1)	-7(1)
O(2)	56(1)	95(1)	81(1)	8(1)	-22(1)	-9(1)
N(1)	74(1)	56(1)	125(1)	2(1)	-49(1)	-9(1)
C(1)	54(1)	57(1)	62(1)	-6(1)	-25(1)	-14(1)
C(2)	62(1)	65(1)	80(1)	-5(1)	-25(1)	-10(1)
C(3)	75(1)	86(1)	74(1)	-5(1)	-12(1)	-19(1)
C(4)	93(1)	79(1)	78(1)	13(1)	-26(1)	-24(1)
C(5)	83(1)	70(1)	92(1)	12(1)	-36(1)	-12(1)
C(6)	63(1)	66(1)	76(1)	-5(1)	-26(1)	-9(1)
C(7)	54(1)	63(1)	69(1)	-9(1)	-30(1)	-9(1)
C(8)	58(1)	60(1)	69(1)	0(1)	-27(1)	-6(1)
C(9)	75(1)	66(1)	90(1)	-12(1)	-38(1)	-13(1)
C(10)	77(1)	52(1)	109(1)	-1(1)	-40(1)	-15(1)
C(11)	58(1)	49(1)	88(1)	4(1)	-28(1)	-4(1)
C(12)	71(1)	55(1)	110(1)	19(1)	-32(1)	-8(1)
C(13)	78(1)	76(1)	95(1)	26(1)	-31(1)	-3(1)
C(14)	79(1)	87(1)	83(1)	15(1)	-38(1)	-4(1)
C(15)	65(1)	67(1)	77(1)	9(1)	-32(1)	-9(1)
C(16)	48(1)	51(1)	73(1)	2(1)	-24(1)	-1(1)
C(17)	48(1)	51(1)	68(1)	-1(1)	-24(1)	-3(1)
C(18)	53(1)	57(1)	61(1)	2(1)	-25(1)	-11(1)
C(19)	54(1)	80(1)	91(1)	6(1)	-29(1)	-13(1)
C(20)	69(1)	117(1)	95(1)	6(1)	-32(1)	-41(1)
C(21)	109(1)	88(1)	93(1)	12(1)	-45(1)	-53(1)
C(22)	110(1)	59(1)	144(2)	8(1)	-64(1)	-20(1)

**Table S4.** Anisotropic displacement parameters  $(\text{\AA}^2 \times 10^3)$  for **2i**. The anisotropic displacement factor exponent takes the form:  $-2\pi^2[h^2a^{*2}U^{11} + ... + 2h k a^* b^* U^{12}]$ .

**Table S5.** Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters (Å<sup>2</sup> × 10<sup>3</sup>) for **2i**.

	X	У	Z	U(eq)	
H(2A)	9244	6895	2489	83	
H(3A)	9898	8071	395	99	
H(4A)	8076	9855	101	101	
H(5A)	5570	10481	1864	98	
H(6A)	4871	9294	3945	82	
H(9A)	6277	4195	5518	89	
H(10A)	5805	2855	7462	93	
H(12A)	5888	2381	9820	97	
H(13A)	6529	2947	11634	104	
H(14A)	7807	4833	11467	99	
H(15A)	8386	6153	9507	82	
H(19A)	10793	6170	6813	90	
H(20A)	11957	8120	6539	109	
H(21A)	10369	10240	6637	109	
H(22A)	7739	10338	6966	119	

Table S6. Torsion angles [ °] for 2i.

C(6)-C(1)-C(2)-C(3)	-0.9(2)
C(7)-C(1)-C(2)-C(3)	177.30(13)
C(1)-C(2)-C(3)-C(4)	1.0(2)
C(2)-C(3)-C(4)-C(5)	-0.4(3)
C(3)-C(4)-C(5)-C(6)	-0.3(3)
C(4)-C(5)-C(6)-C(1)	0.4(2)
C(2)-C(1)-C(6)-C(5)	0.2(2)
C(7)-C(1)-C(6)-C(5)	-178.08(13)
C(8)-O(1)-C(7)-O(2)	-1.70(19)
C(8)-O(1)-C(7)-C(1)	179.57(10)
C(2)-C(1)-C(7)-O(2)	-168.00(13)
C(6)-C(1)-C(7)-O(2)	10 2(2)
C(2)-C(1)-C(7)-O(1)	10.69(18)
C(6)-C(1)-C(7)-O(1)	-171.09(11)
C(7) - O(1) - C(8) - C(17)	$-105\ 10(13)$
C(7) - O(1) - C(8) - C(9)	79 31(14)
C(17)-C(8)-C(9)-C(10)	0.6(2)
O(1) C(8) C(9) C(10)	176.01(12)
C(8) C(9) C(10) C(11)	-0.1(2)
C(0) - C(10) - C(11) - C(12)	177 21(13)
C(9)- $C(10)$ - $C(11)$ - $C(12)$	-0.3(2)
C(10) - C(11) - C(12) - C(13)	-177.85(13)
C(16) - C(11) - C(12) - C(13)	-0.4(2)
C(10)-C(11)-C(12)-C(13) C(11)-C(12)-C(13)-C(14)	-0.3(2)
C(11)- $C(12)$ - $C(13)$ - $C(14)C(12)$ $C(13)$ $C(14)$	0.5(2)
C(12) - C(13) - C(14) - C(15) C(13) - C(14) - C(15) - C(16)	-0.2(2)
C(14) - C(15) - C(16) C(14) - C(15) - C(11)	-0.45(19)
C(14) - C(15) - C(16) - C(17)	177.66(12)
C(14) - C(15) - C(16) - C(17)	177.00(12) 178.30(12)
C(10)-C(11)-C(10)-C(15)	0.74(18)
C(12) - C(11) - C(10) - C(13)	0.12(18)
C(10)-C(11)-C(10)-C(17)	-177 43(11)
C(12)- $C(11)$ - $C(10)$ - $C(17)$	-0.77(19)
O(1)-C(8)-C(17)-C(16)	-17612(10)
C(0) C(8) C(17) C(18)	170.12(10) 170.75(12)
O(1)-C(8)-C(17)-C(18)	A A 0(17)
C(15)-C(16)-C(17)-C(18)	-17771(11)
C(11)-C(16)-C(17)-C(8)	0.38(17)
C(11)-C(10)-C(17)-C(0) C(15) C(16) C(17) C(18)	1.77(18)
C(11)-C(16)-C(17)-C(18)	179 85(11)
C(11)-C(10)-C(17)-C(10) C(22) N(1) C(18) C(10)	0.6(2)
C(22) - N(1) - C(18) - C(17)	-179 15(14)
C(22)- $N(1)$ - $C(18)$ - $N(1)$	68 44(16)
C(16) - C(17) - C(18) - N(1)	-11102(14)
C(10)-C(17)-C(18)-N(1) C(2)-C(17)-C(18)-C(10)	-111.02(14)
C(16) - C(17) - C(18) - C(19)	-111.33(13)
N(1) C(18) C(10) C(19)	-0.6(2)
N(1)-C(18)-C(19)-C(20)	-0.0(2)
C(17) - C(10) - C(17) - C(20) C(18) C(10) C(20) C(21)	1/7.13(14) 0 5(2)
C(10) - C(19) - C(20) - C(21) C(10) - C(20) - C(21) - C(22)	-0.4(3)
C(17)-C(20)-C(21)-C(22) C(18) N(1) C(22) C(21)	-0.4(3)
$C(10)^{-1}(1)^{-}C(22)^{-}C(21)$ $C(20)^{-}C(21)^{-}C(22)^{-}N(1)^{-}$	0.3(3)
(20) - ((21) - ((22) - N(1))	0.4(3)

Symmetry transformations used to generate equivalent atoms.

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## 2. <sup>1</sup>H and <sup>13</sup>C-NMR Spectra:













<sup>1</sup>H-NMR of **2e** Current Data Parameters NAME H1.0NP13 EXPNO 55 PROCNO 1 87518 F2 - Acq Date\_\_ Time INSTRUM PROBHD FULPROS TO SOLVENT NS SWH FIDRES AQ RG DW DE TE D1 NUC1 P1 PL1 SF01 f1 = 1H 10.00 usec -5.00 dB 328009 MHz F2 -SI SF WDW SSB LB GB PC 400.13 MHz 094 EM 0 0.00 Hz 1.00 1D NHI CX F1P F1 F2P F2 PPMCM HZCM 9 279 ppm 9 279 ppm 3712 96 Hz -0 000 ppm -0.00 Hz 0.46397 ppm/cm 85.64786 Hz/cm 2.9886 1.9914 2.1536 2.0743 1.0000 Integrai ppm 6

























<sup>13</sup>C-NMR of **2k** 



<sup>1</sup>H-NMR of **2**l





<sup>1</sup>H-NMR of **2m** 



<sup>&</sup>lt;sup>13</sup>C-NMR of **2m** 



<sup>1</sup>H-NMR of **2n** 





S20

EL f1 =

ameters

eters 19.50



<sup>&</sup>lt;sup>13</sup>C-NMR of **20** 



<sup>1</sup>H-NMR of **2p** 











<sup>1</sup>H-NMR of **2r** Current Data Parameters NAME H1.GNP13 EXPNO 2 PROCND 1 PROCNO F2 - Acquisition Data\_\_\_\_\_ Time 2 Time 2 Time 2 State PHORMO 5 mm PHORMO 5 mm PHORMO 5 mm PHORMO 5 mm SGLVFNT NS SGLVFNT NS SGLVFNT NS SGLVFNT NS SGLVFNT SGLVFNT DS SGLVFNT SGLVFNT DS SGLVFNT DS SGLVFNT DS SGLVFNT SGLVFNT DS SGLVFNT DS SGLVFNT SGLVFNT DS SGLVFNT SGL NUC1 P1 PL1 SF01 f1 1H 10.00 usec -5.00 dB 328009 MHz F2 -SI SF WDW SSB LB GB PC 400.13 MHZ 094 EN 0 0.00 1.00 1D NH CX F1P F1 F2 PPMCM HZCM 20.00 cm 8.869 ppm 3548.72 Hz -0.000 ppm -0.00 Hz 0.44345 ppm/cm 177.43596 Hz/cm Integral 1.0000 9819 1756 2.1556 3.0255 1.2555 1.2555 1.2555 1.1656 1.1988 ppm 6 3

<sup>13</sup>C-NMR of **2r** 



<sup>1</sup>H-NMR of **2s** 



<sup>&</sup>lt;sup>13</sup>C-NMR of **2s** 







<sup>1</sup>H-NMR of  $2\mathbf{u}$ 





<sup>&</sup>lt;sup>13</sup>C-NMR of **2u** 



it id

<sup>1</sup>H-NMR of 2v



=2 - Pr SI SF WDW SSB \_B S8 S8 S8

10 NMR plot CX F1P F1 F2P F2 PNCM

HTCH

no parameters

sing parameters 65536 100.6127073 MHz EM 0 0.30 Hz 0 .1.00

aneters 19.50 cm 178.000 ppm 17909 06 Hz 0.000 ppm 0.00 Hz 9.12820 ppm/cm 916.41333 H7/cm <sup>1</sup>H-NMR of **2**w





