Supplementary Material

Morphological transition triggered by mannose conjugation to cyclic hexapeptide

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Dedicated to Prof. Richard R Schmidt on the occasion of his 78th anniversary

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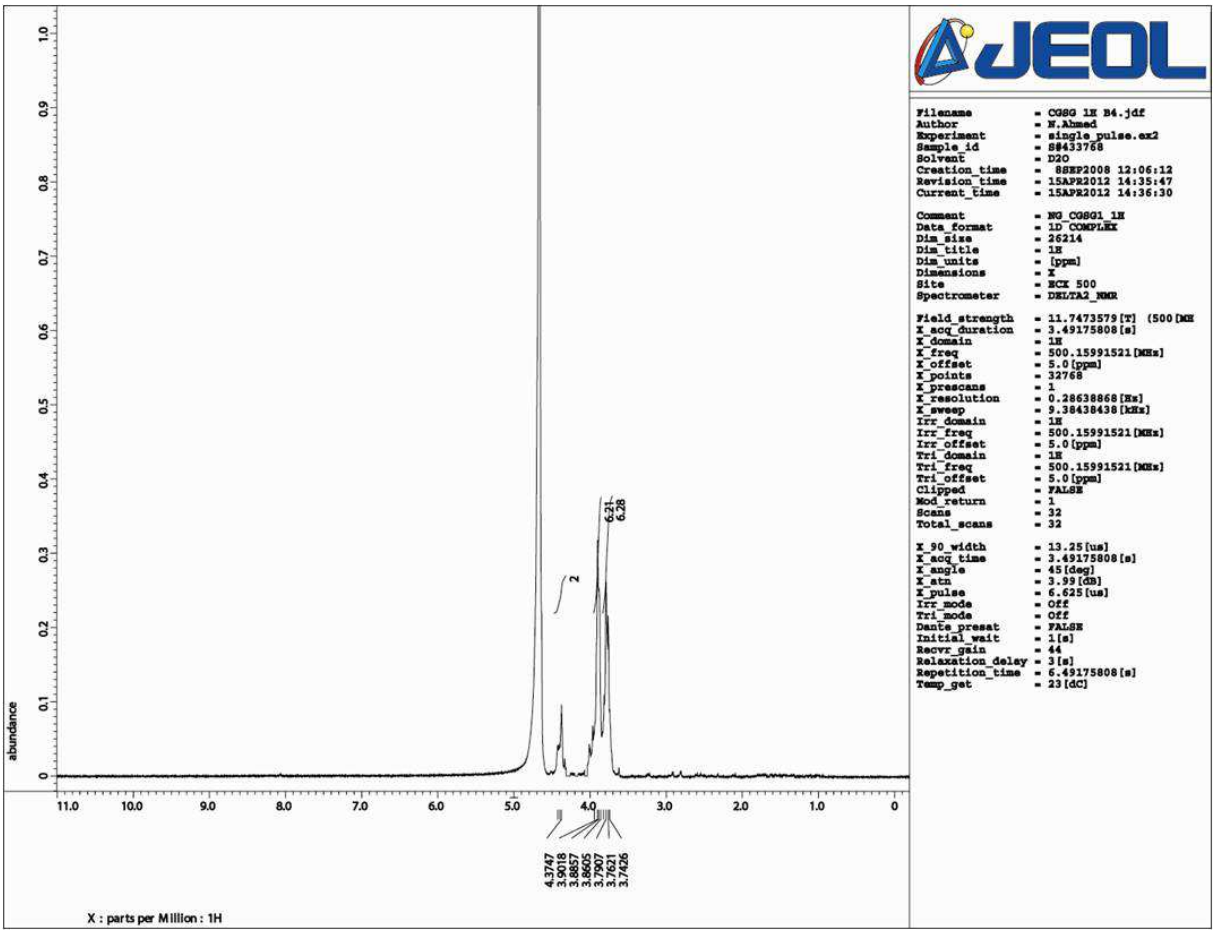
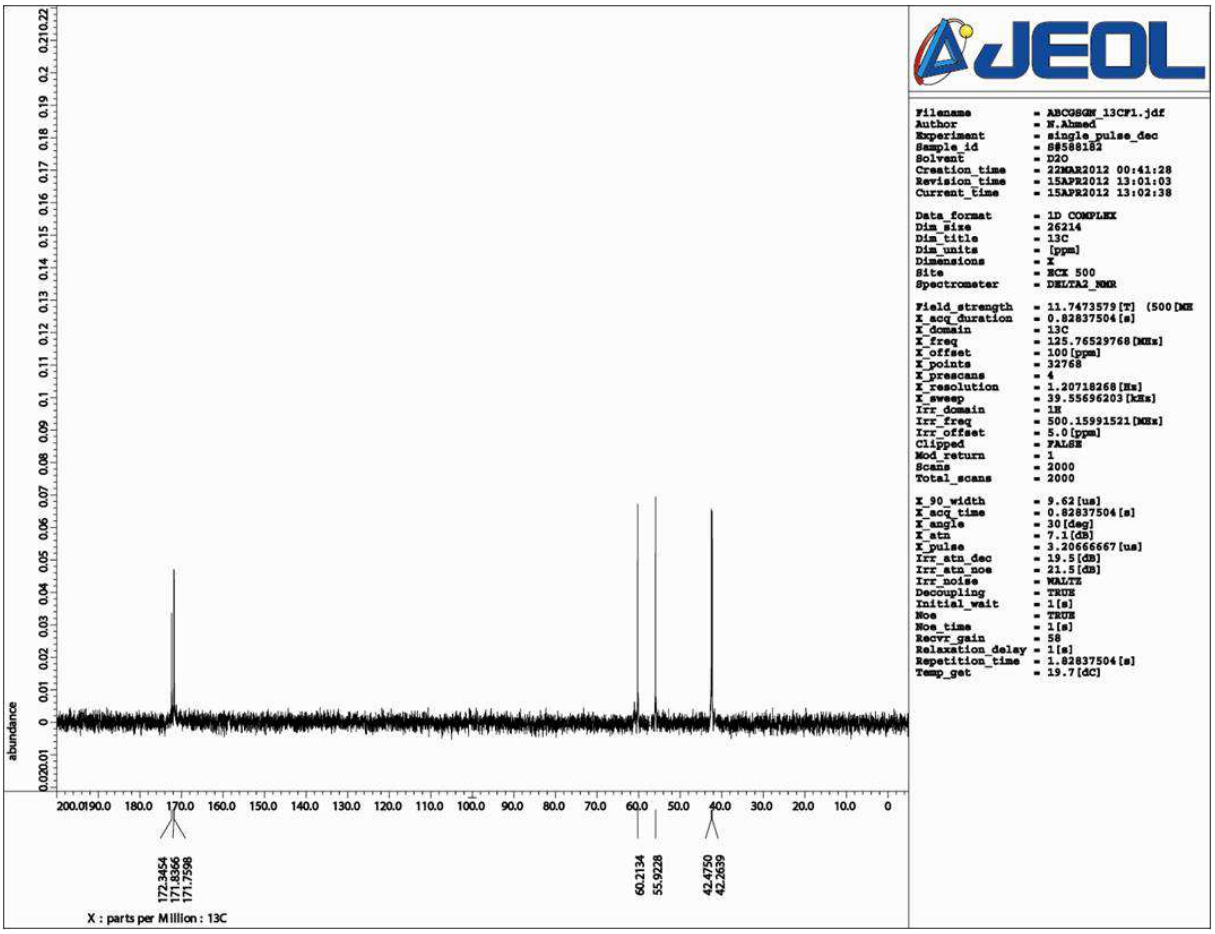
^{1}H NMR spectra of **6:**



^{13}C NMR spectra of **6:**



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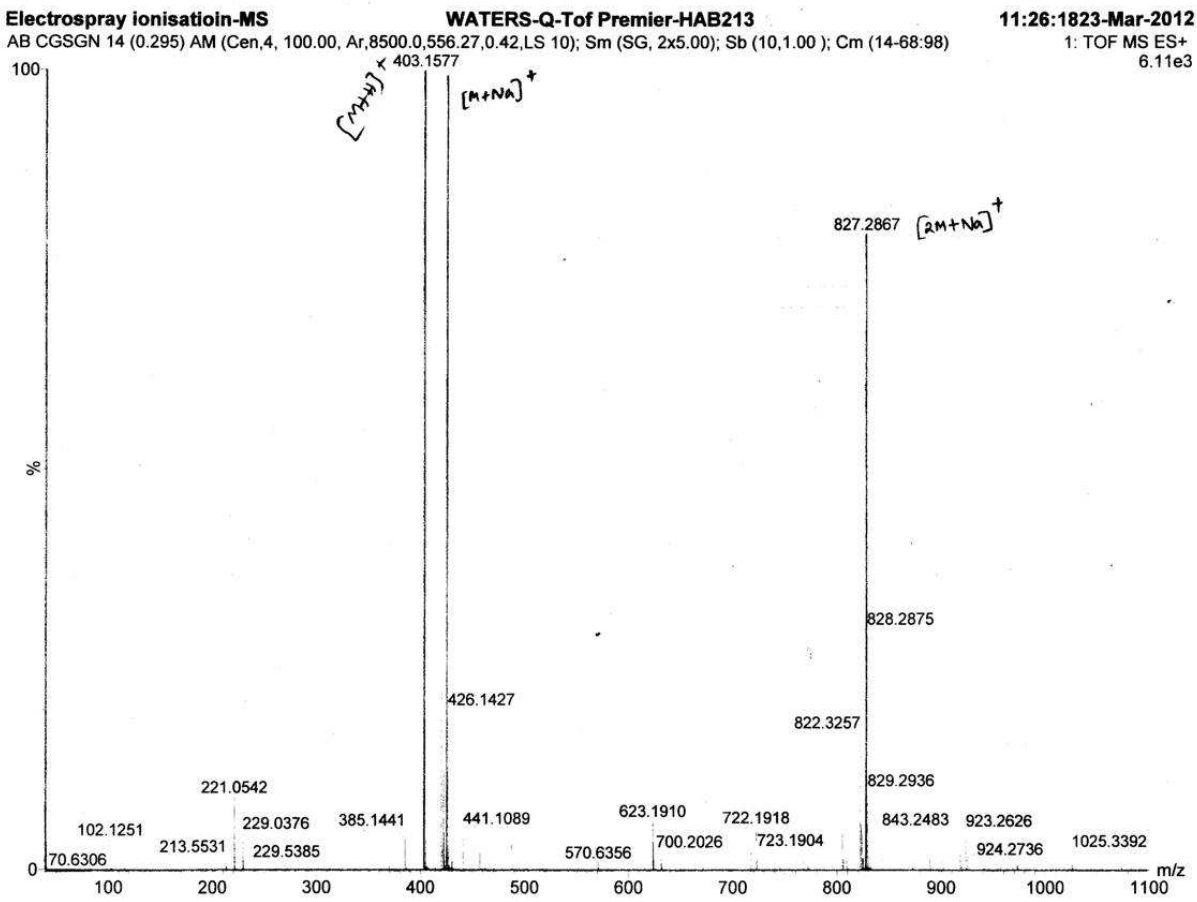

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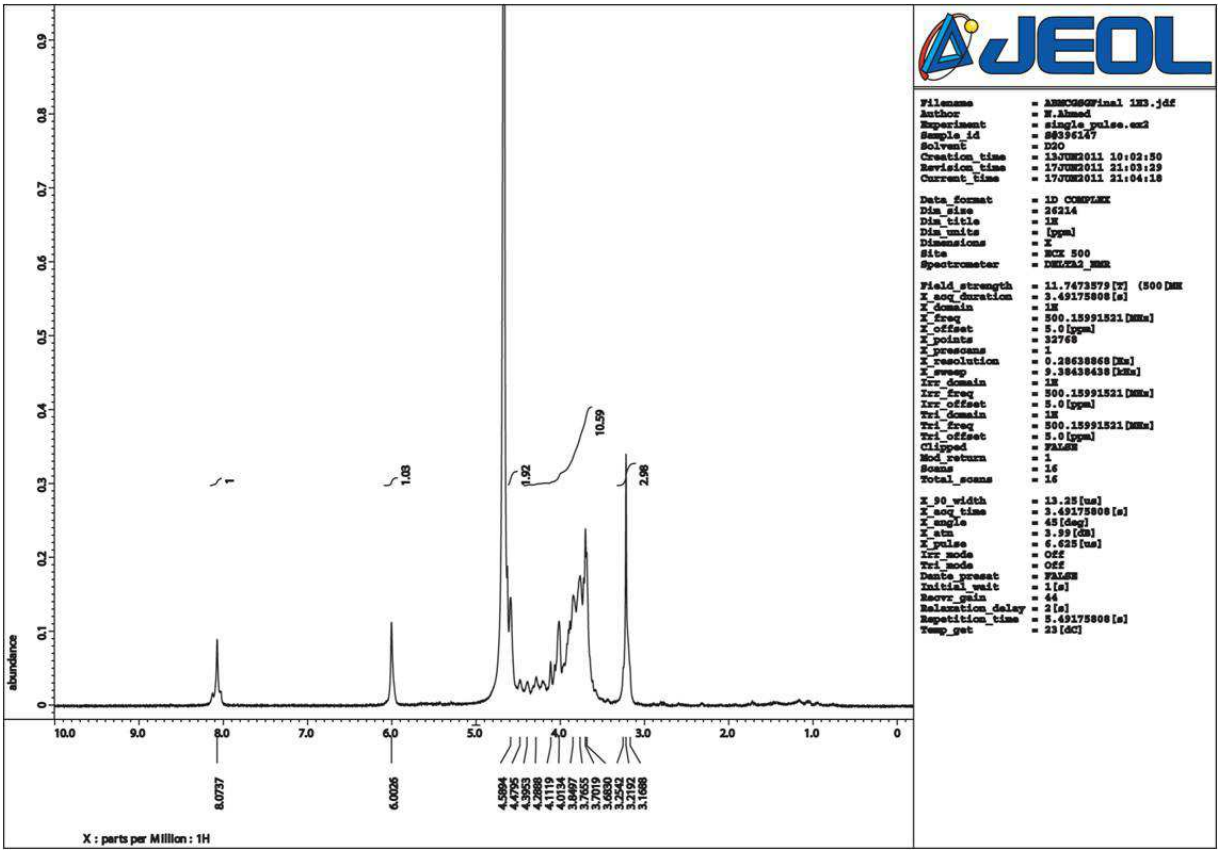
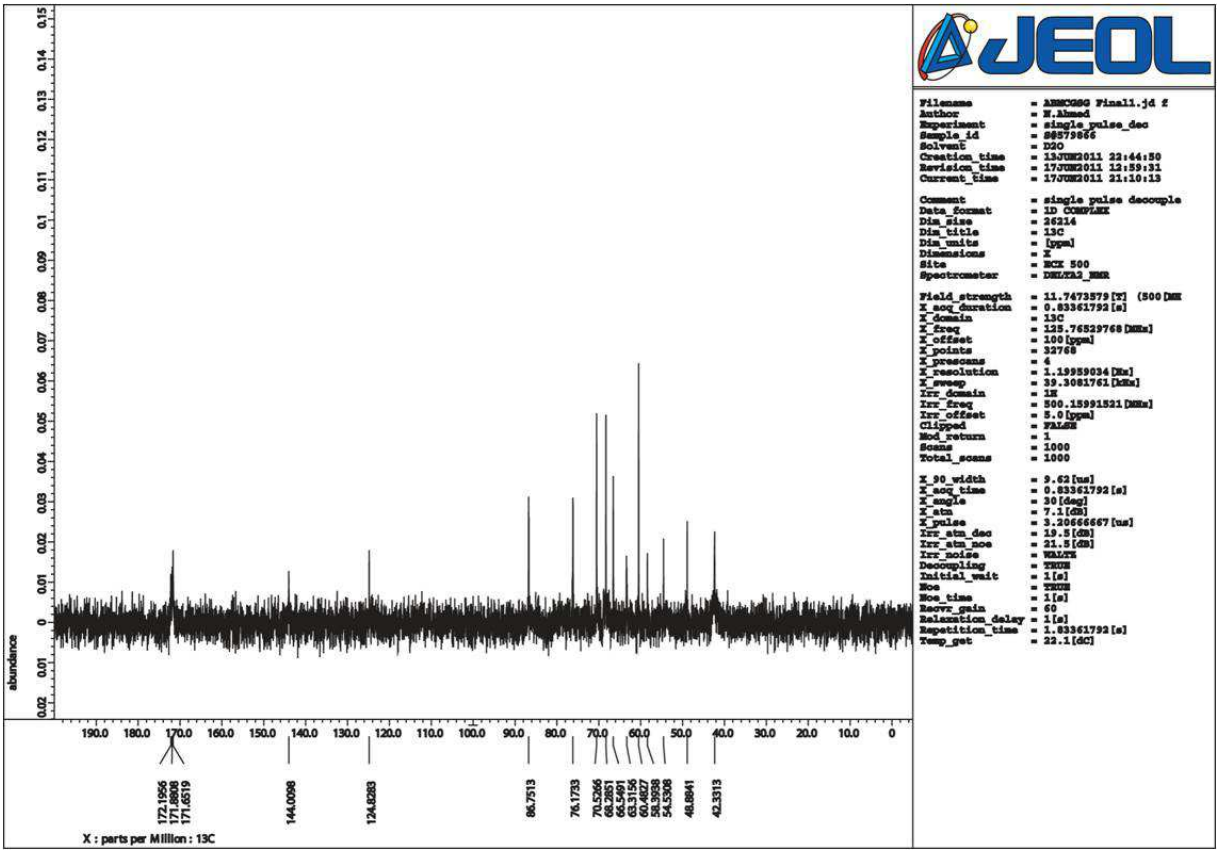


^{13}C NMR spectra of **15:**



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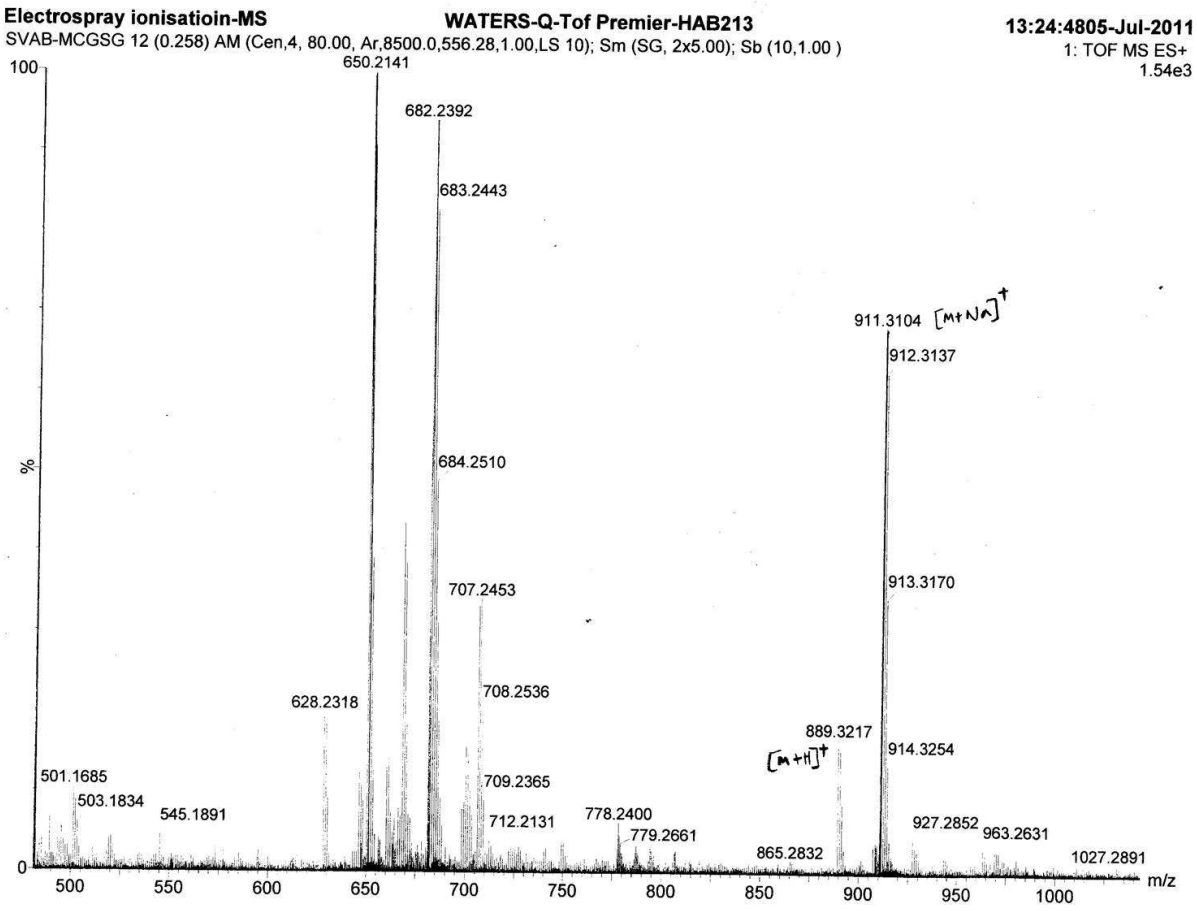

Crystal structure refinement details for 6: Single Crystal of **6** was coated with light hydrocarbon oil and mounted in the 100 K dinitrogen stream of a Bruker SMART APEX CCD diffractometer equipped with CRYO Industries low-temperature apparatus and intensity data were collected using graphite-monochromated Mo KR radiation. The data integration and reduction were processed with the SAINT software.[1] An absorption correction was applied.[2] Structures were solved by the direct method using SHELXS-97 and refined on *F*2 by a full-matrix least-squares technique using the SHELXL-97 program package.[2] Non-hydrogen atoms were refined anisotropically. In the refinement, hydrogens were treated as riding atoms using the SHELXL default parameters. Crystal structure refinement parameters are given in Table S1 whereas H-bonding parameters are provided in Table S2. CCDC contains the supplementary crystallographic data for this paper with a deposition number of CCDC 878652 for **6**. Copies of this information can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK. [Fax: +44-1223/336-033; E-mail: deposit@ccdc.cam.ac.uk].

Table S1. Crystal structure refinement parameters for Cyclo(Gly-L-Ser-Gly)$_2$ (**6**)

Identification Code	Cyclo(Gly-L-Ser-Gly)$_2$ (**6**)
Empirical formula	C_{14} H_{26} N_6 O_{10}
Formula weight	438.41
Crystal system	Monoclinic
Space group	P 21/n
a/Å	9.023(5)
b/Å	7.071(4)
c/Å	15.137(3)
α/°	90
β/°	97.652(5)
γ/°	90
Volume/ Å^3	957.2(8)
Z	2
Dx /Mg m^{-3}	1.521
F(000)	464
μ/ mm^{-1}	0.130
θ range for data collection/ °	2.49 to 28.30
Limiting indices	-11<=h<=11, -9<=k<=7, -18<=l<=19
Reflections collected	5835
Unique reflections	2304
R(int)	0.0455
Completeness to θ	28.30, 96.6
T_{max} / T_{min}	0.974 / 0.971
Data / restraints / parameters	2304 / 3 / 144
Goodness-of-fit on F^2	1.144
*R*1 and *R*2 [$I>2\sigma(I)$]	0.0619, 0.1489
*R*1 and *R*2 (all data)	0.0980, 0.2131
Largest diff. peak and hole/e.A^{-3}	0.474 and -0.474
CCDC No.	878652

Table S2. Table for H-bonding in crystal structure for **6**

D—H···A[a]	D-H	H···A	D···A	D—H···A	Symmetry
Cyclo(Gly-L-Ser-Gly)$_2$ (**6**)					
O1W—H1W1···O3	0.84(4)	1.91(3)	2.744(4)	172(5)	-1/2+x,3/2-y,-1/2+z
O1W—H2W1···O2	0.84(3)	1.98(3)	2.816(4)	174(3)	
N3—H3···N9	0.88	2.35	2.760(4)	109	
N3—H3···O1W	0.88	2.06	2.841(4)	148	1/2-x,-1/2+y,1/2-z
O4—H4A···N3	0.84	2.51	2.837(4)	104	
O4—H4A···O1	0.84	1.92	2.732(4)	162	3/2-x,-1/2+y,1/2-z
N6—H6···O3	0.88	2.40	3.135(4)	141	
N6—H6···N3	0.88	2.38	2.737(4)	104	
N9—H9···O4	0.88	1.95	2.825(4)	170	3/2-x,-1/2+y,1/2-z
C4—H4···O1	1.00	2.42	2.837(4)	104	

Table S3. Table for bond lengths and bond angles for **6**

	Bond length (Å)		Bond angle (°)
O(4)-C(10)	1.431(4)	C(8)-N(9)-C(1)	120.3(3)
O(3)-C(8)	1.226(4)	C(2)-N(3)-C(4)	124.2(3)
O(2)-C(5)	1.239(4)	C(5)-N(6)-C(7)	122.6(3)
O(1)-C(2)	1.234(4)	O(2)-C(5)-N(6)	122.8(3)
N(9)-C(8)	1.350(4)	O(2)-C(5)-C(4)	121.2(3)
N(9)-C(1)	1.444(4)	N(6)-C(5)-C(4)	115.9(3)
N(3)-C(2)	1.334(4)	O(3)-C(8)-N(9)	122.1(3)
N(3)-C(4)	1.451(4)	O(3)-C(8)-C(7)	123.5(3)
N(6)-C(5)	1.331(4)	N(9)-C(8)-C(7)	114.4(3)
N(6)-C(7)	1.447(4)	N(3)-C(4)-C(10)	110.5(3)
C(5)-C(4)	1.536(4)	N(3)-C(4)-C(5)	110.2(2)
C(8)-C(7)	1.526(5)	C(10)-C(4)-C(5)	111.8(3)
C(4)-C(10)	1.521(4)	O(1)-C(2)-N(3)	123.5(3)
C(2)-C(1)	1.519(4)	O(1)-C(2)-C(1)	119.4(3)
C(1)-N(9)	1.444(4)	N(3)-C(2)-C(1)	117.1(3)
		N(6)-C(7)-C(8)	112.2(3)
		N(9)-C(1)-C(2)	115.5(3)
		O(4)-C(10)-C(4)	111.1(3)

References

1. *SAINT+*, 6.02 ed.; Bruker AXS, Madison, WI, 1999.
2. G. M. Sheldrick, *SADABS 2.0*; University of Göttingen: Göttingen, Germany, 2000.
3. G. M. Sheldrick, *SHELXL-97*: *Program for Crystal Structure Refinement*; University of Göttingen: Göttingen, Germany, 1997.

