Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Regioselective Opening of Unsymmetrical Cyclic Anhydrides: Synthesis of *N*-Glycosylated Isoasparagine and Isoglutamine Conjugates

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[†] Deceased on 9th February, 2013

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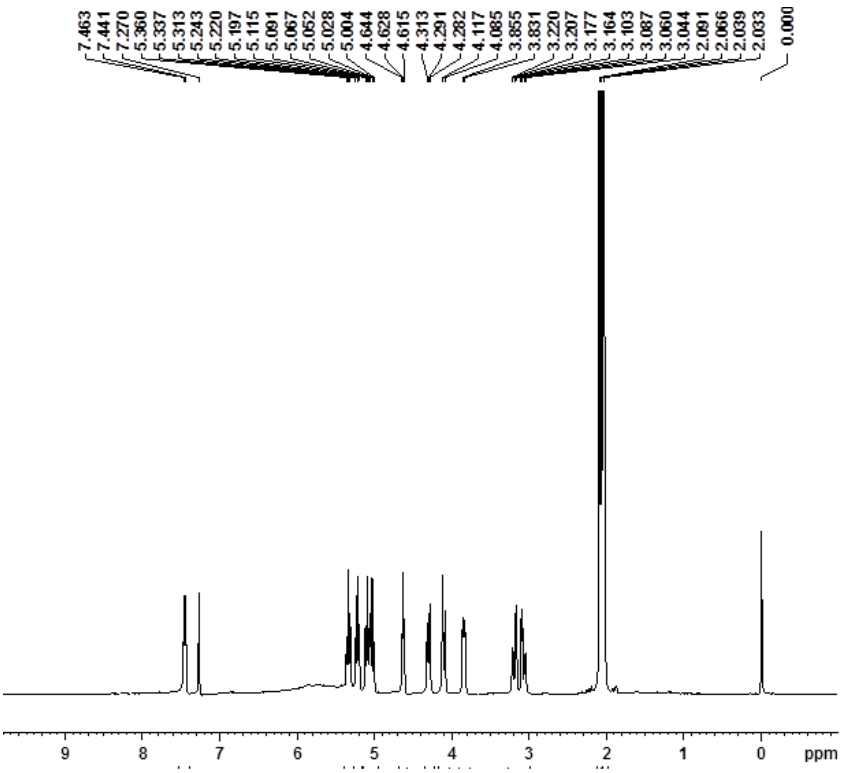

Figure S1 ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3**

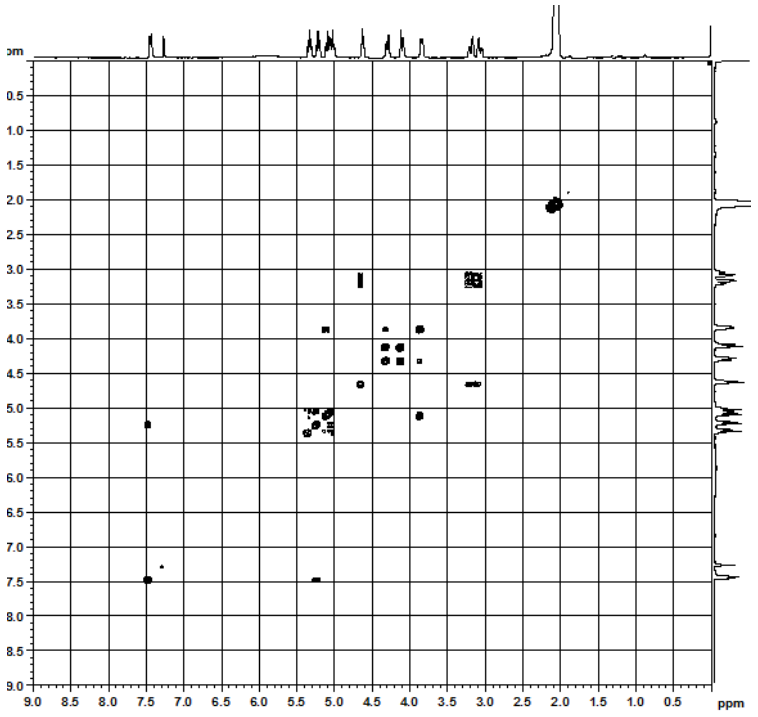

Figure S2 ^{1}H-^{1}H COSY NMR spectrum of **3**

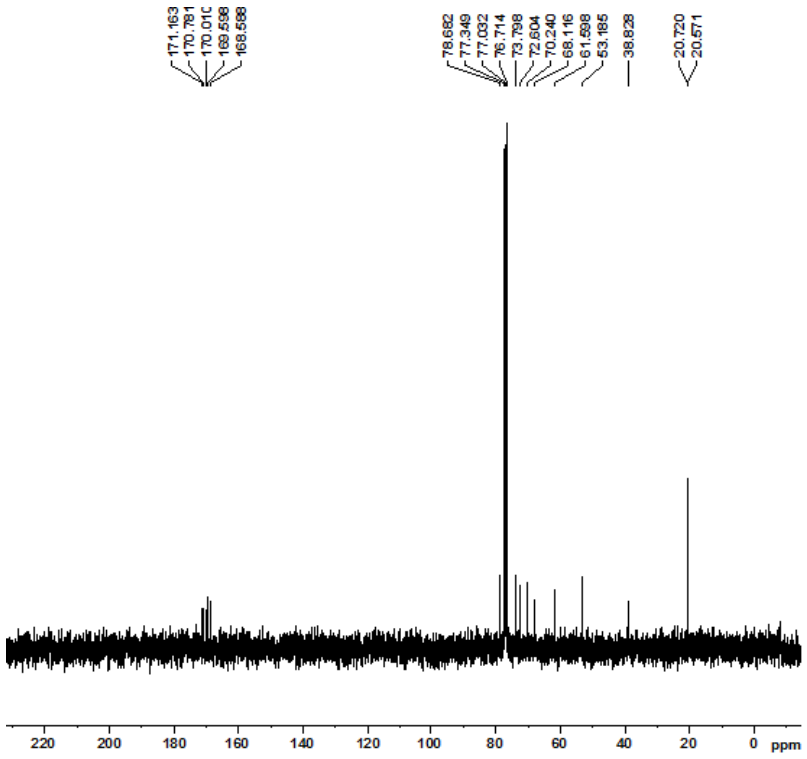

Figure S3 ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **3**

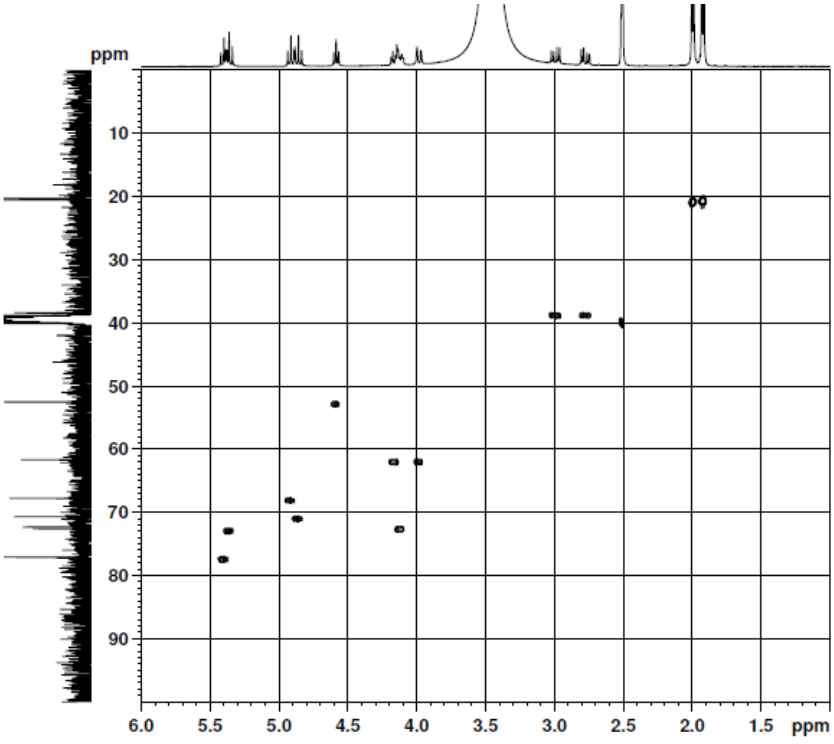

Figure S4 HSQC (DMSO-d6) spectrum of **3**

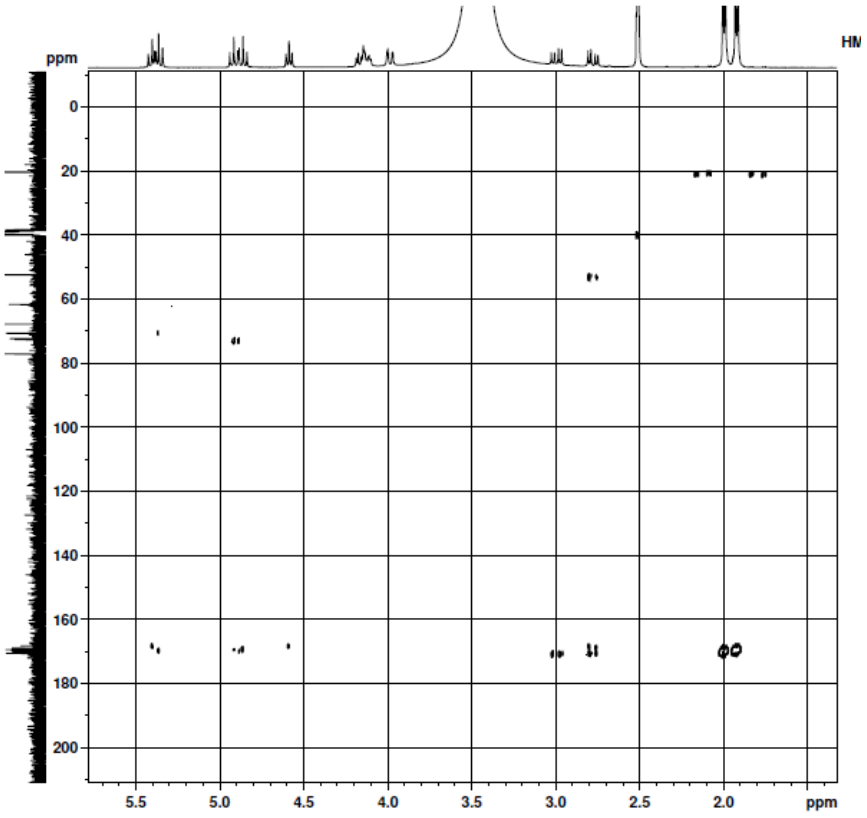

Figure S5 HMBC (DMSO-d6) spectrum of **3**

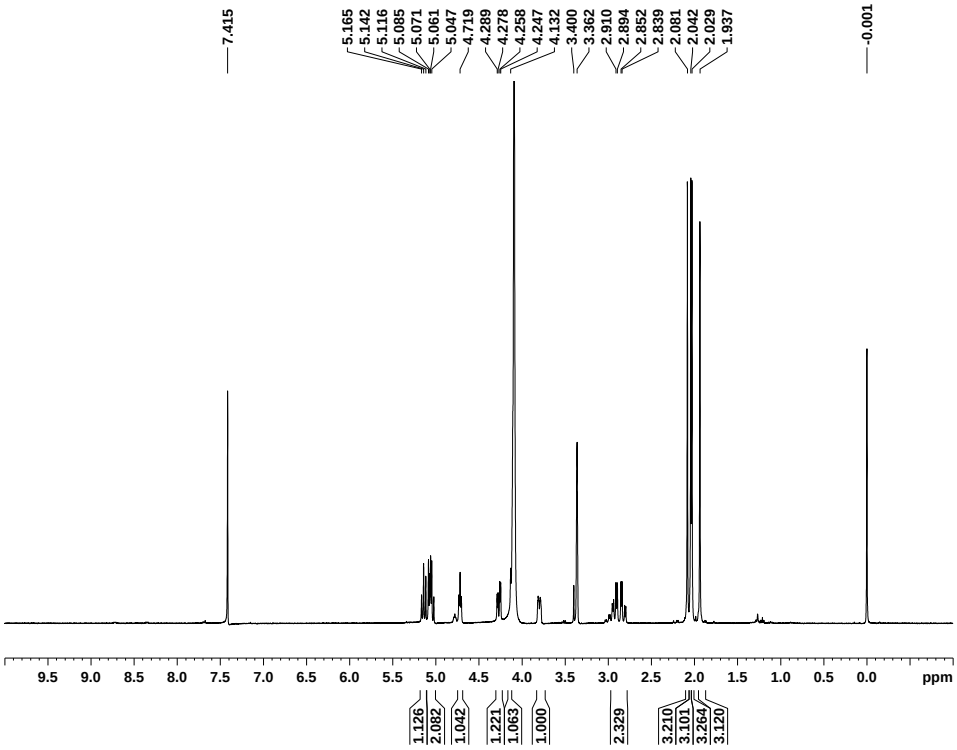

Figure S6 ^{1}H NMR (400 MHz, MeOD + $CDCl_3$) spectrum of **7**

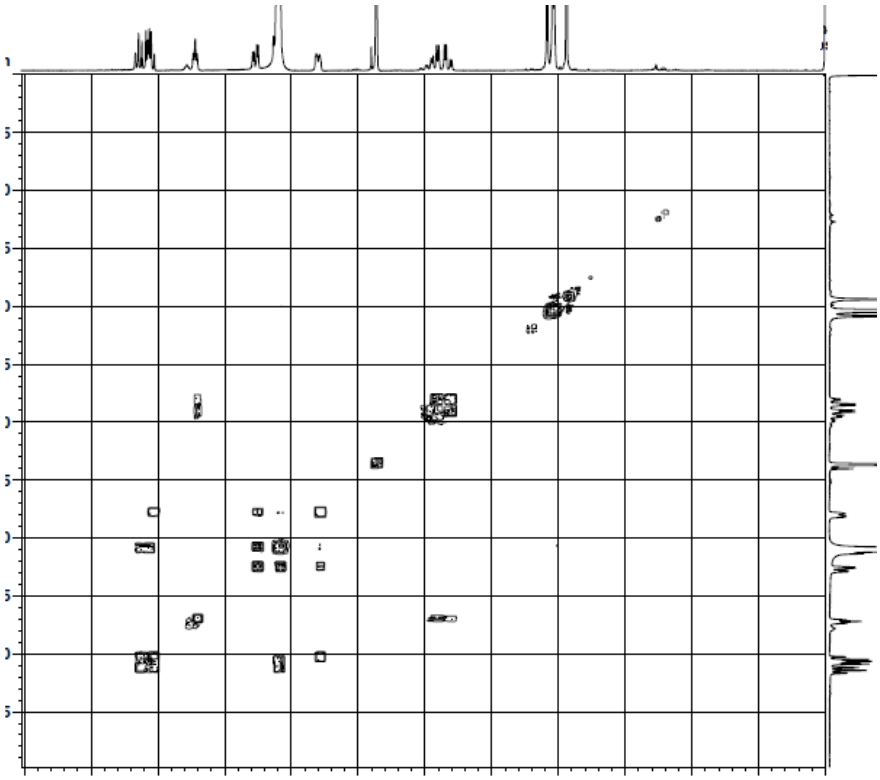

Figure S7 ^{1}H-^{1}H COSY NMR spectrum of **7**

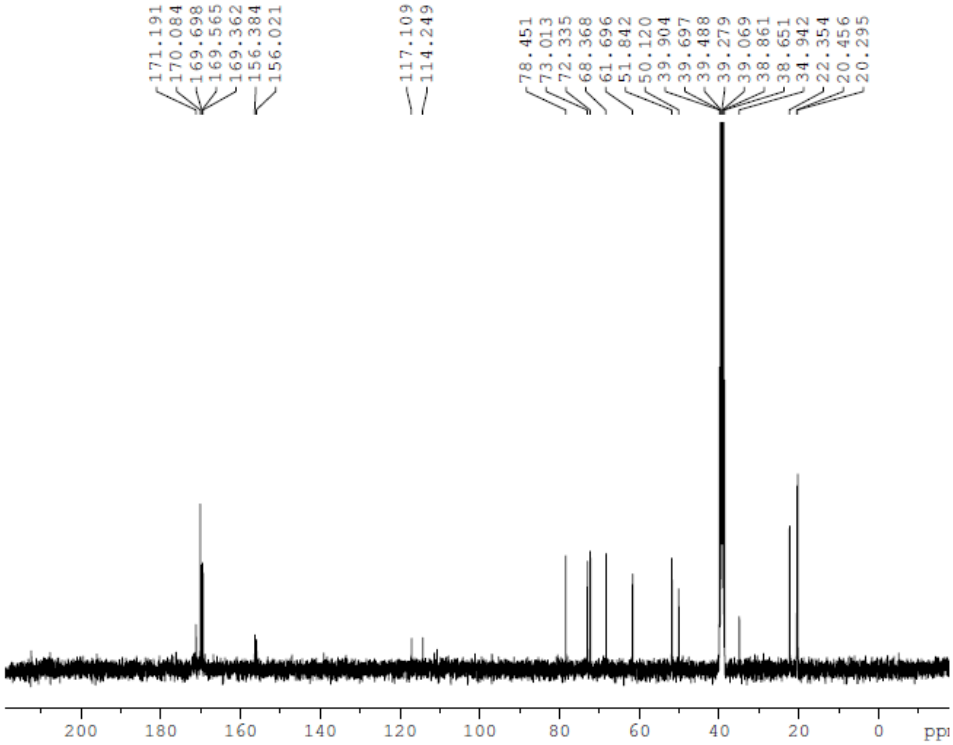

Figure S8 ^{13}C NMR (100 MHz, DMSO-d6) spectrum of **7**

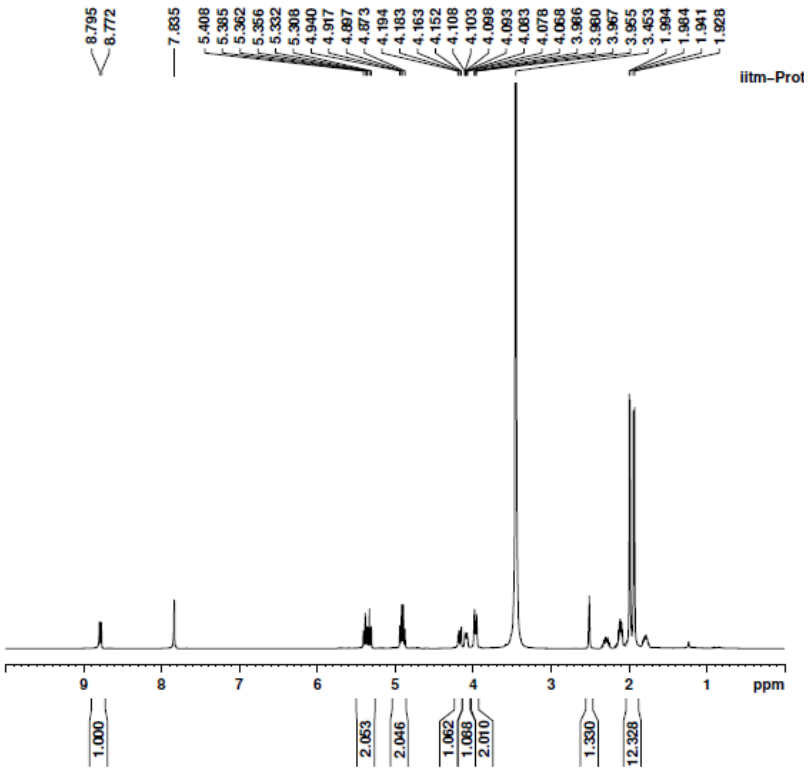

Figure S9 ^{1}H NMR (400 MHz, DMSO-d6) spectrum of **10**

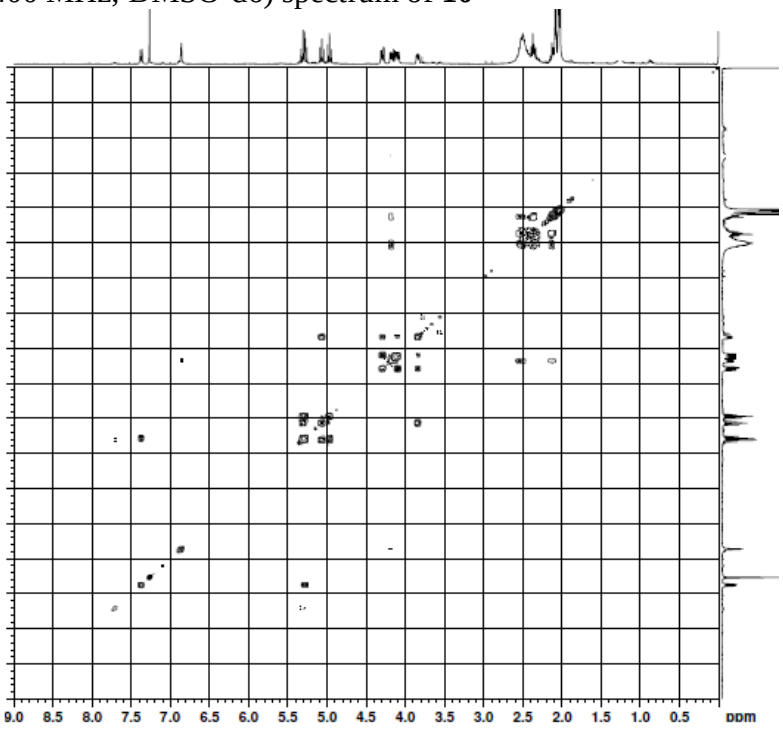

Figure S10 ^{1}H-^{1}H COSY NMR spectrum of **10**

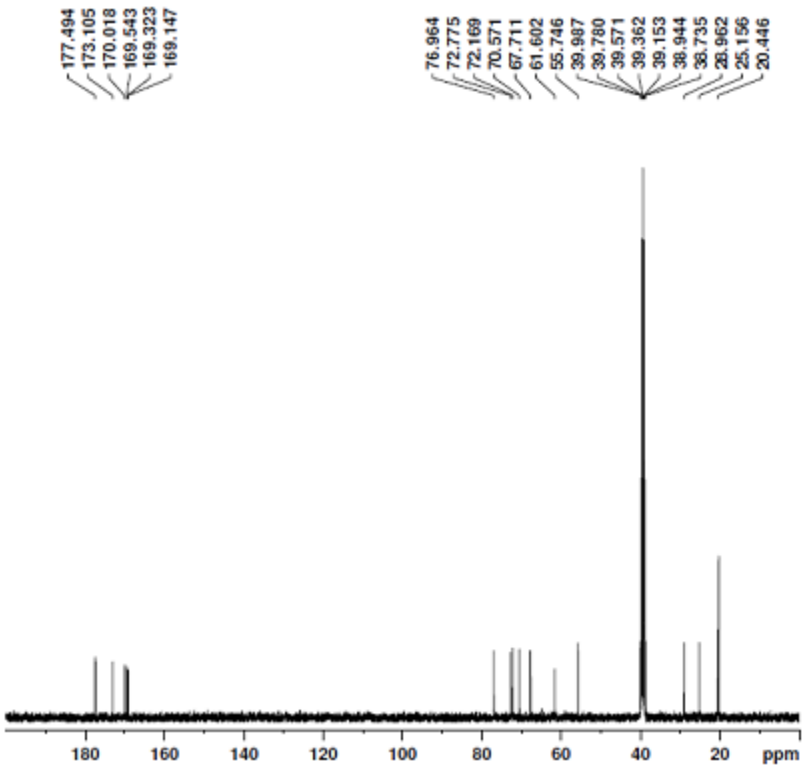

Figure S11 ^{13}C NMR (100 MHz, DMSO-d6) spectrum of **10**

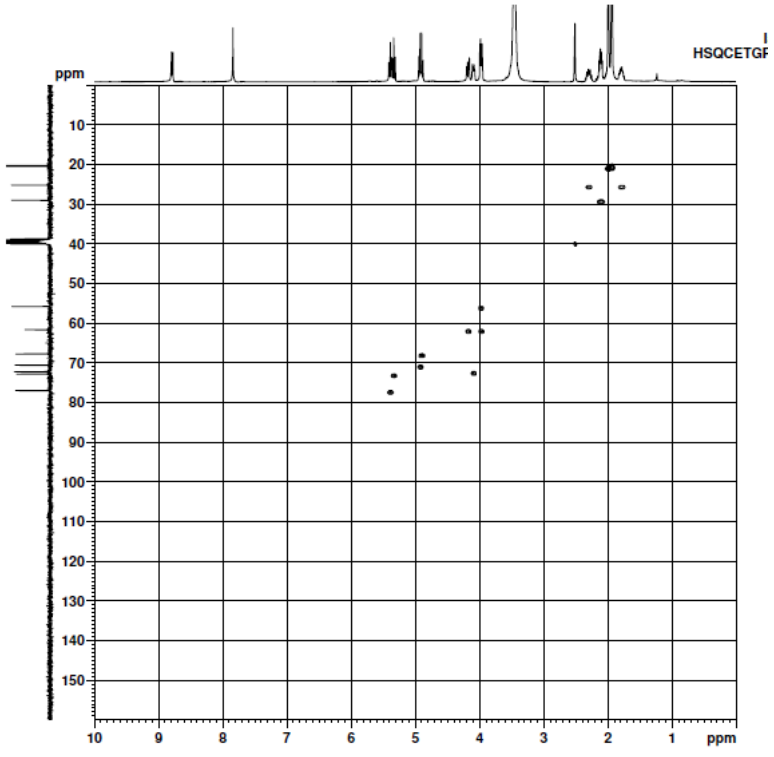

Figure S12 HSQC (DMSO-d6) spectrum of **10**

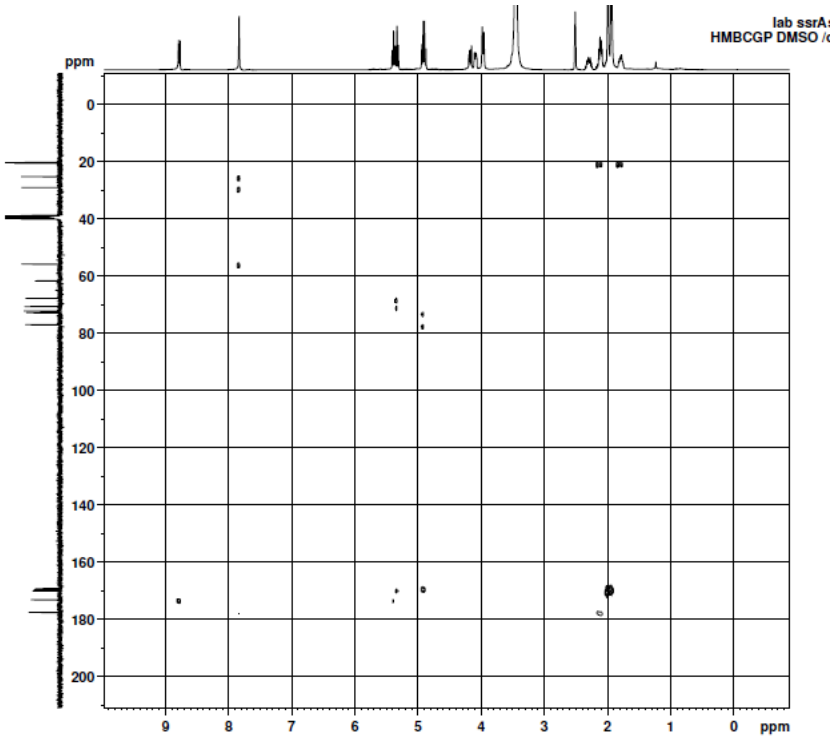

Figure S13 HMBC (DMSO-d6) spectrum of **10**

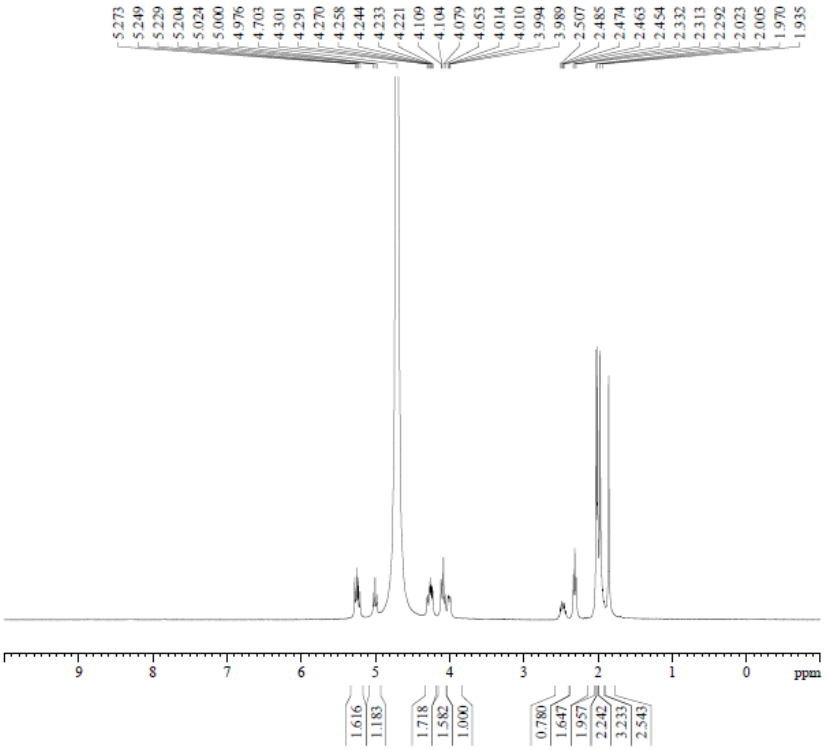

Figure S14 ^{1}H NMR (400 MHz, D_2O) spectrum of **11**

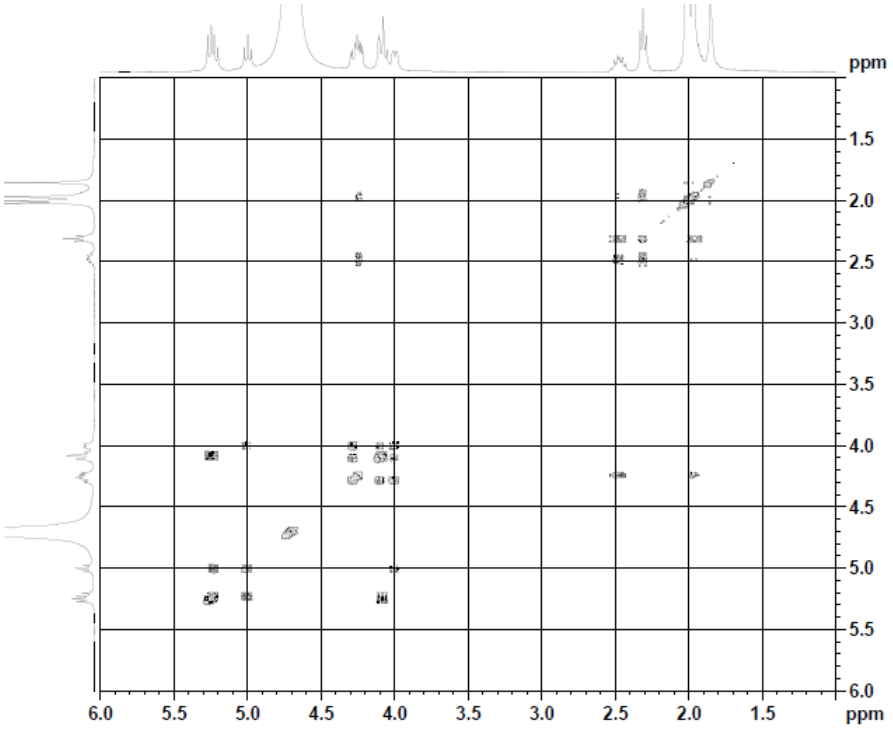

Figure S15 ^{1}H-^{1}H COSY NMR spectrum of **11**

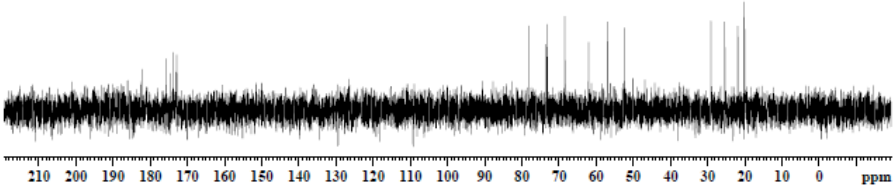

Figure S16 ^{13}C NMR (100 MHz, D_2O) spectrum of **11**

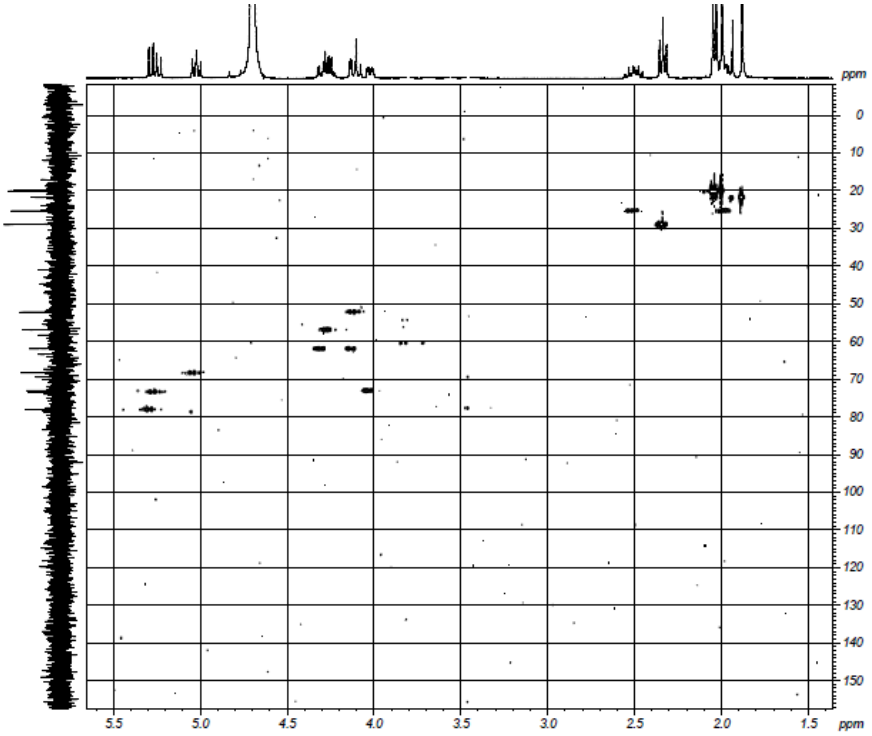

Figure S17 HSQC (D_2O) spectrum of **11**

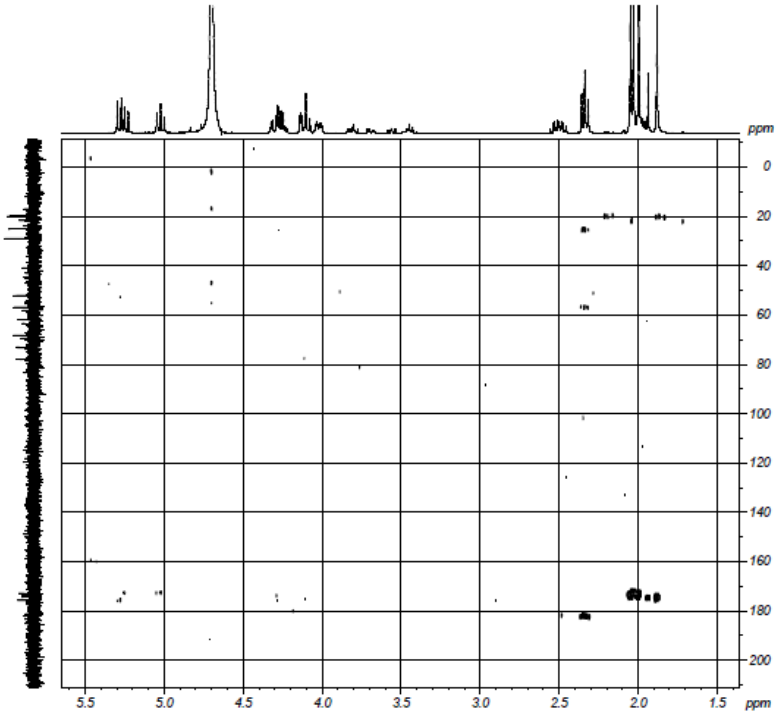

Figure S18 HMBC (D_2O) spectrum of **11**

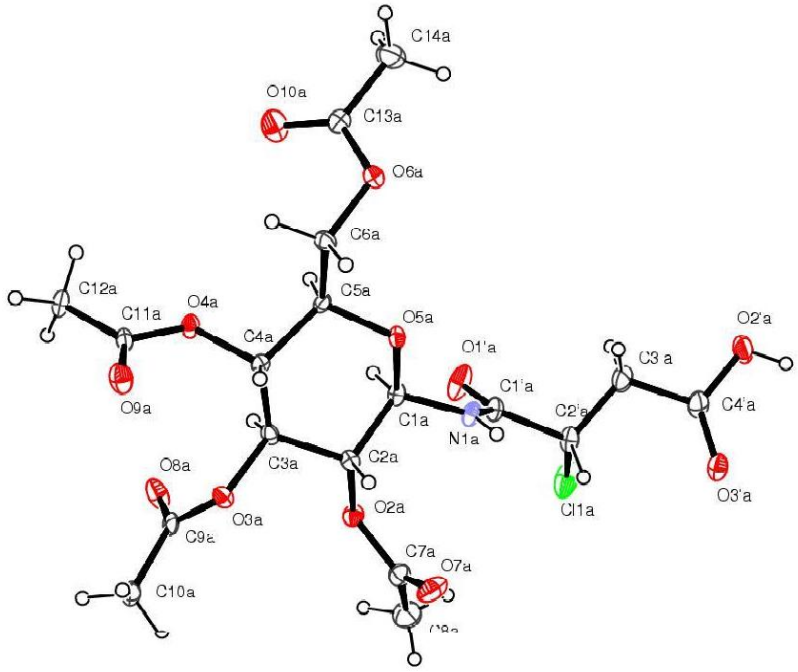

Figure S9 ORTEP diagram of the compound **3**

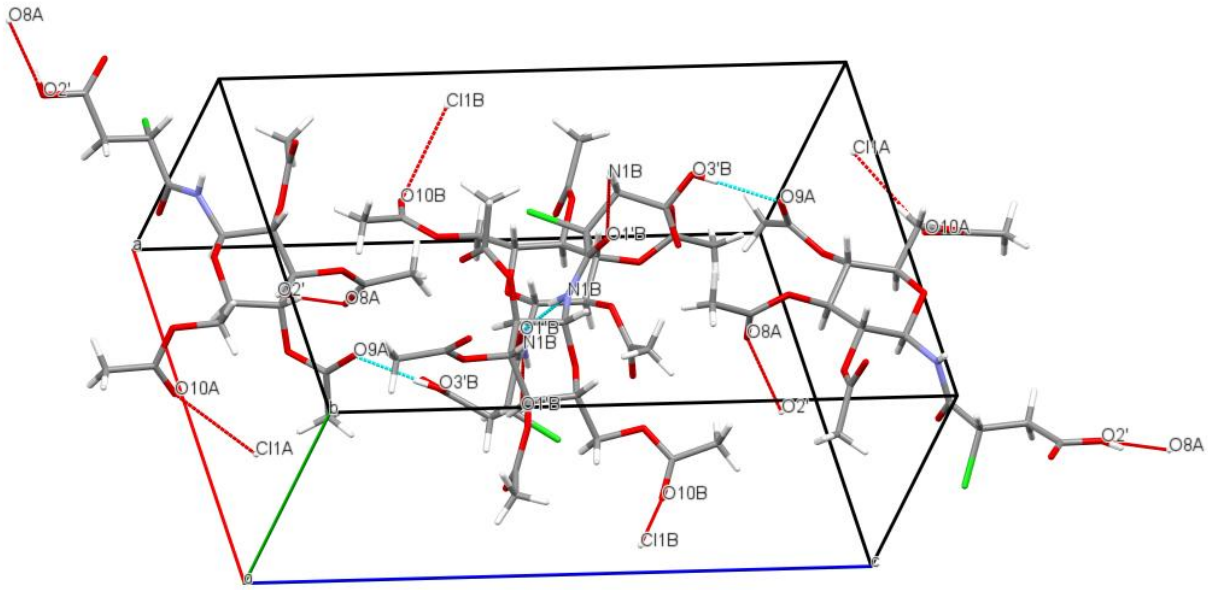

Figure S10 Unit cell packing diagram of compound **3** with H-bonding

Table S1 Data collection and refinement parameters for the compound **3**

Parameters	
Empirical formula	$C_{18}H_{24}ClNO_{12}$
Formula weight	481.83
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system space group	Monoclinic, ***P2$_1$***
Unit cell dimensions	a = 11.9031(9)Å alpha = 90 deg. b = 9.4411(5)Å beta = 94.702 (2) deg. c = 19.8615(15)Å gamma = 90 deg.
Volume	2224.5(3) Å^3
Z	4
Calculated density	1.439 Mg/m^3
Absorption coefficient	0.235 mm^{-1}
F (000)	1008
Crystal size	0.25 x 0.20 x 0.15 mm
Theta range for data collection	1.03 to 26.99 deg.
Limiting indices	-14<=h<=12, -9<=k<=11, -24<=l<=23
Reflections collected / unique	11342 / 6448 [R(int) = 0.0447]
Completeness to theta = 25.00	91.3%
Absorption correction	None
Max. and min. transmission	0.9655 and 0.9435
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6448 / 1 / 596
Goodness-of-fit on F^2	0.877
Final R indices [I>2sigma(I)]	R1 = 0.0539, wR2 = 0.1283
R indices (all data)	R1 = 0.0846, wR2 = 0.1495
Absolute structure parameter	0.04(10)
Largest difference peak and hole	0.564 and -0.364 e. Å $^{-3}$