Supporting Information

Steric group enforced aromatic cyclic trimer conformer in tripodal molecules

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Table S1. Crystallographic data for **1**, **3** and **5**.

	1	**3**	**5**
CCDC	1419799	1051126	1051212
formula	$C_{48}H_{42}N_6O_3$	$C_{48}H_{42}N_6S_3$	$C_{51}H_{45}N_9$
M_r	750.87	799.05	783.96
crystal system	Triclinic	Triclinic	Triclinic
space group	P-1	P-1	P-1
a (Å)	11.134(3)	9.8655(16)	11.0412(8)
b (Å)	14.065(3)	11.631(2)	14.3405(14)
c (Å)	16.0333(3)	19.330(4)	16.4975(18)
α (deg)	65.252(13)	89.169(8)	108.993(9)
β (deg)	69.867(14)	83.089(8)	107.036(8)
Γ (deg)	79.935(17)	73.788(6)	99.777(7)
V (Å^3)	2139.5(9)	2113.9(7)	2257.7(4)
Z	2	2	2
T (K)	120(2)	150(2)	296(2)
λ (Å)	0.71075	0.71075	1.54184
D_{calc} (g cm^{-3})	1.166	1.255	1.153
μ(Mo Kα) (mm^{-1})/μ(Cu Kα)	0.074	0.217	0.547
F (000)	792	840	828
θ range (deg)	2.475-25.023	2.772-25.005	3.054-72.060
Data/restraints/parameters	7463/182/561	7327/49/514	8621/0/544
R_1 [$I > 2\sigma(I)$]	0.0778	0.0628	0.0653
wR_2 (all data)	0.2137	0.1604	0.1835
GooF	1.112	1.011	0.878

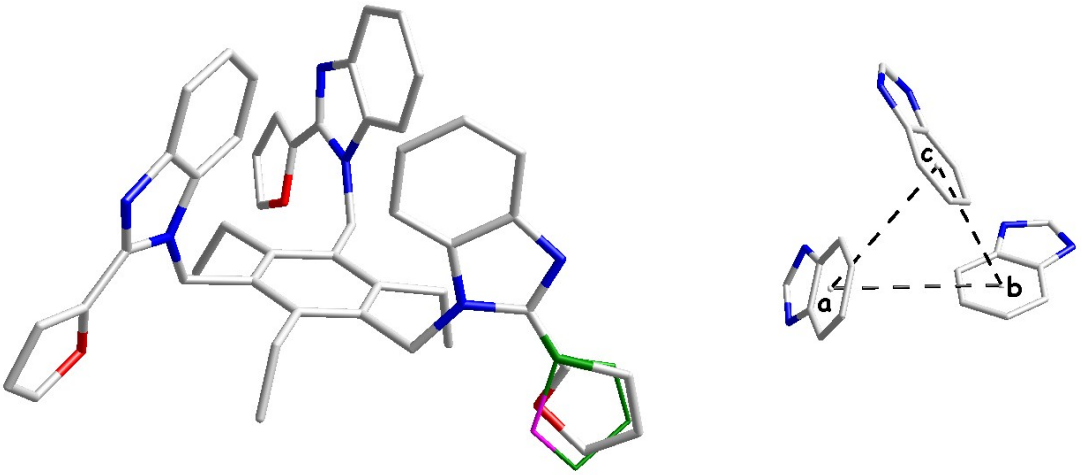

Fig. S1 Molecular structure of **1** (top-left, H atoms are removed). Cyclic aromatic trimer motif in **1** (top-right, a/b/c = COM of benzene, other units are omitted). C = gray, green, turquoise; N = blue; O = red, pink.

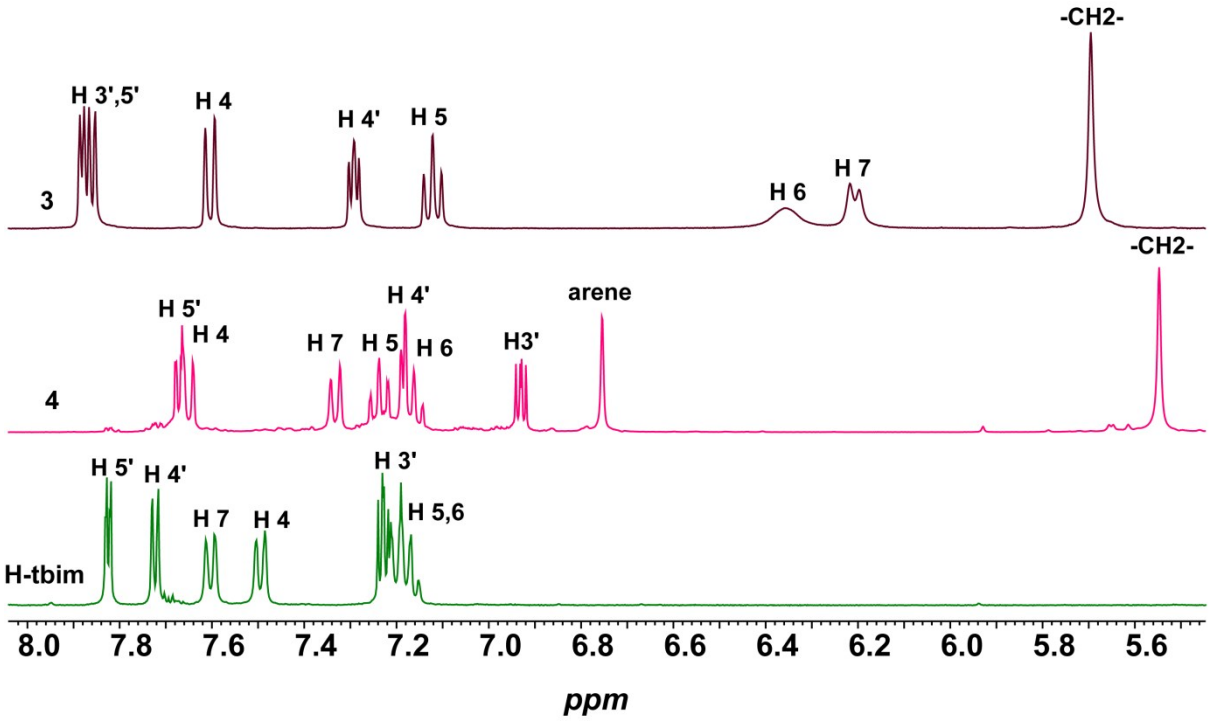

Fig. S2 Partial ^{1}H NMR spectra of H-tbim, **4** and **3** in d_6-DMSO.

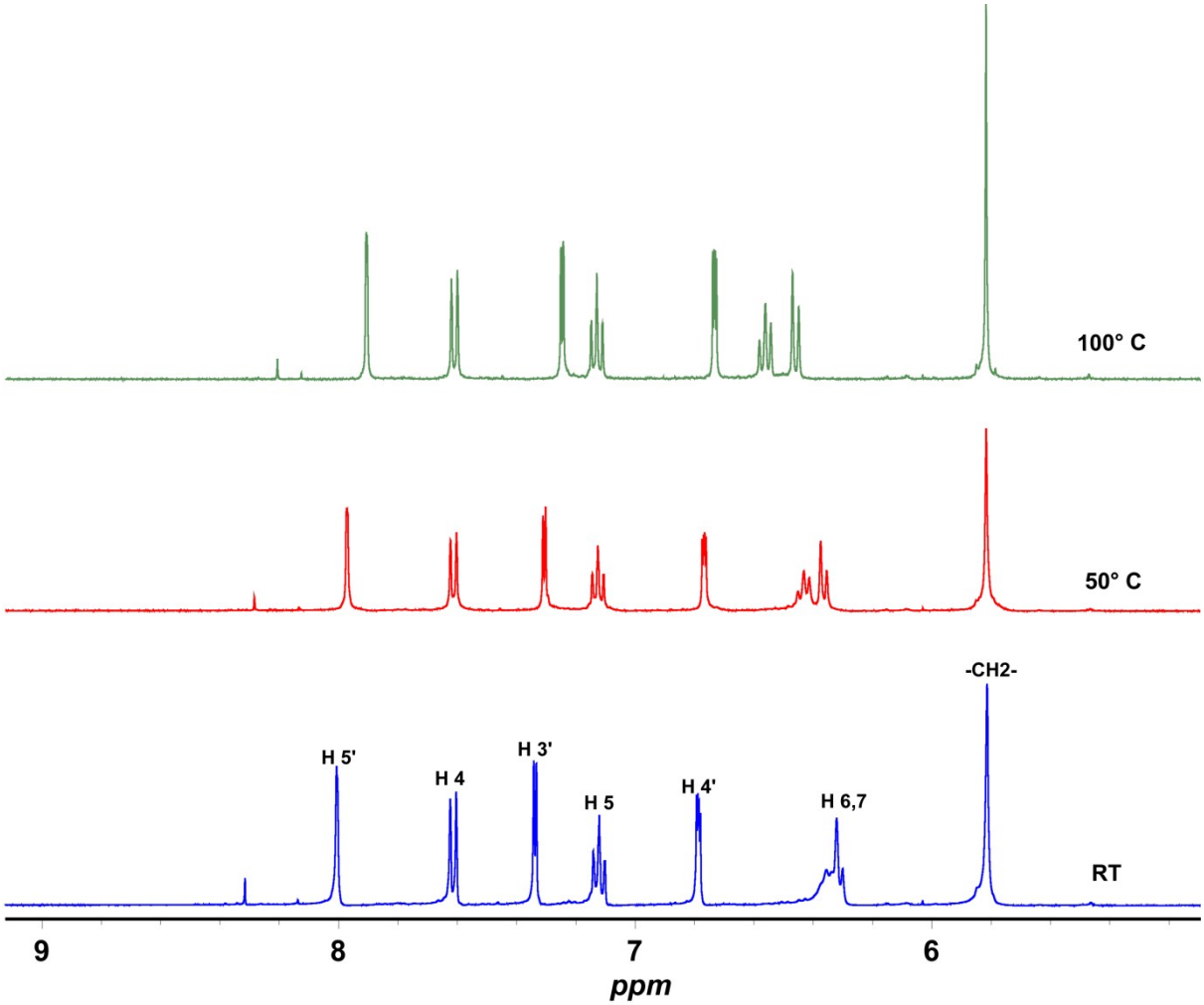

Fig. S3 Partial variable temperature ^{1}H NMR spectra of **1** in d_6-DMSO.

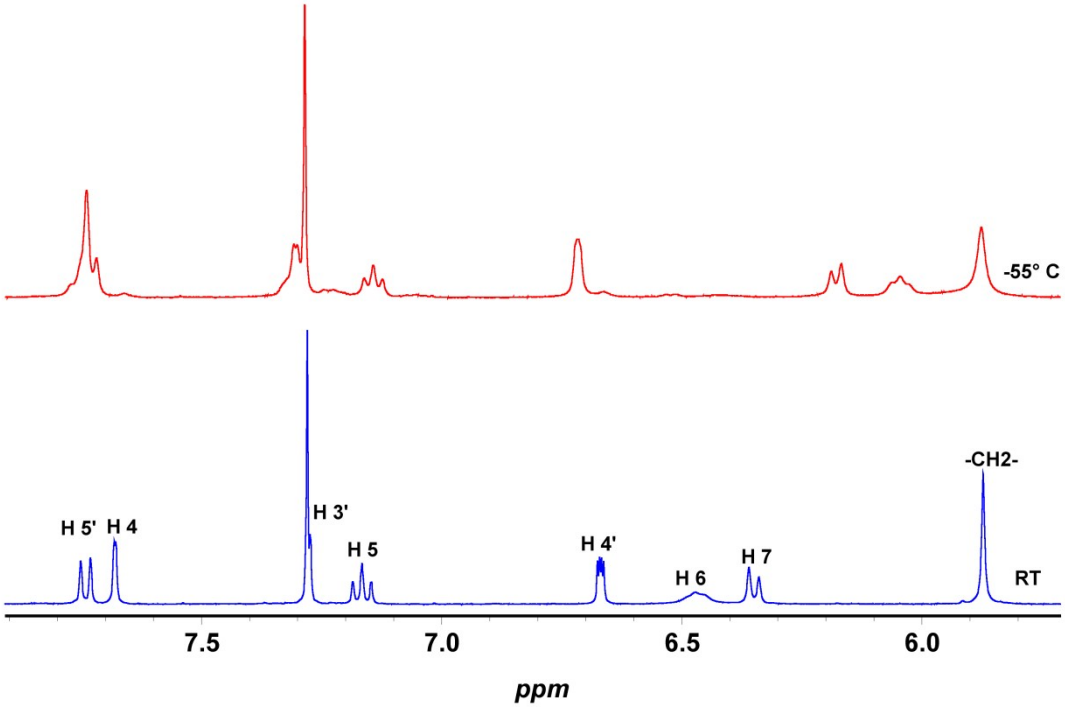

Fig. S4 Partial variable temperature ^{1}H NMR spectra of **1** in $CDCl_3$.

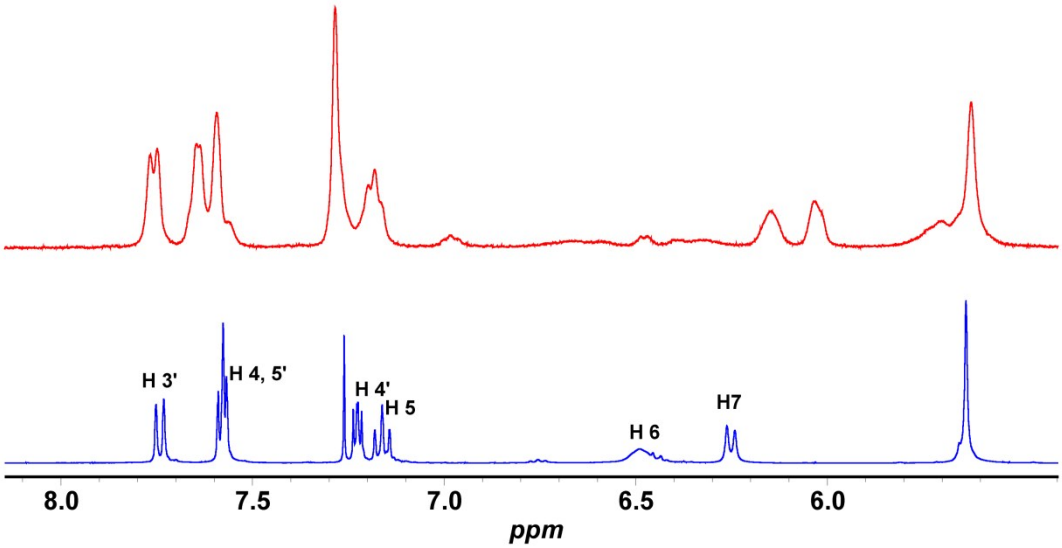

Fig. S5 Partial variable temperature ^{1}H NMR spectra of **3** in $CDCl_3$.

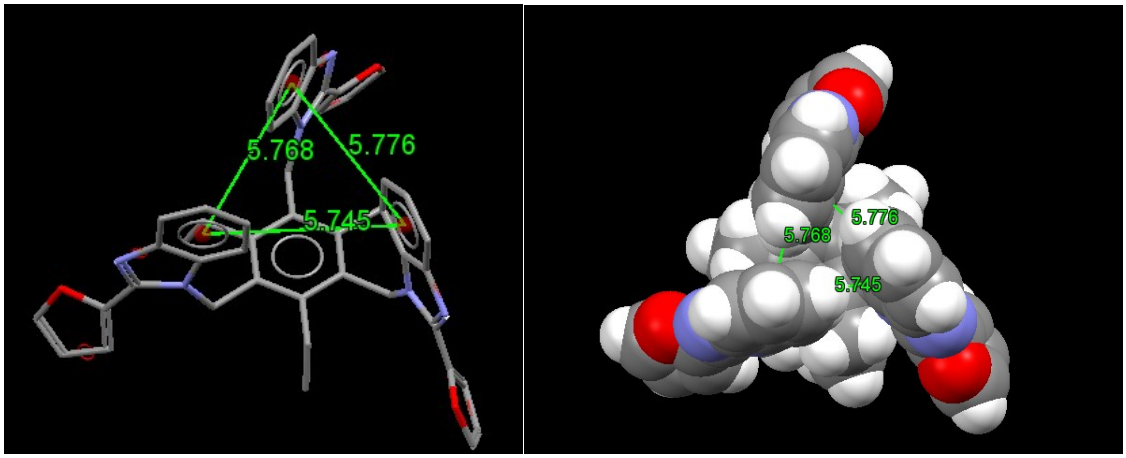

Fig. S6 Two different views of optimized structure of **1** (top-left, H atoms are removed). C = gray; O = red; H = white.

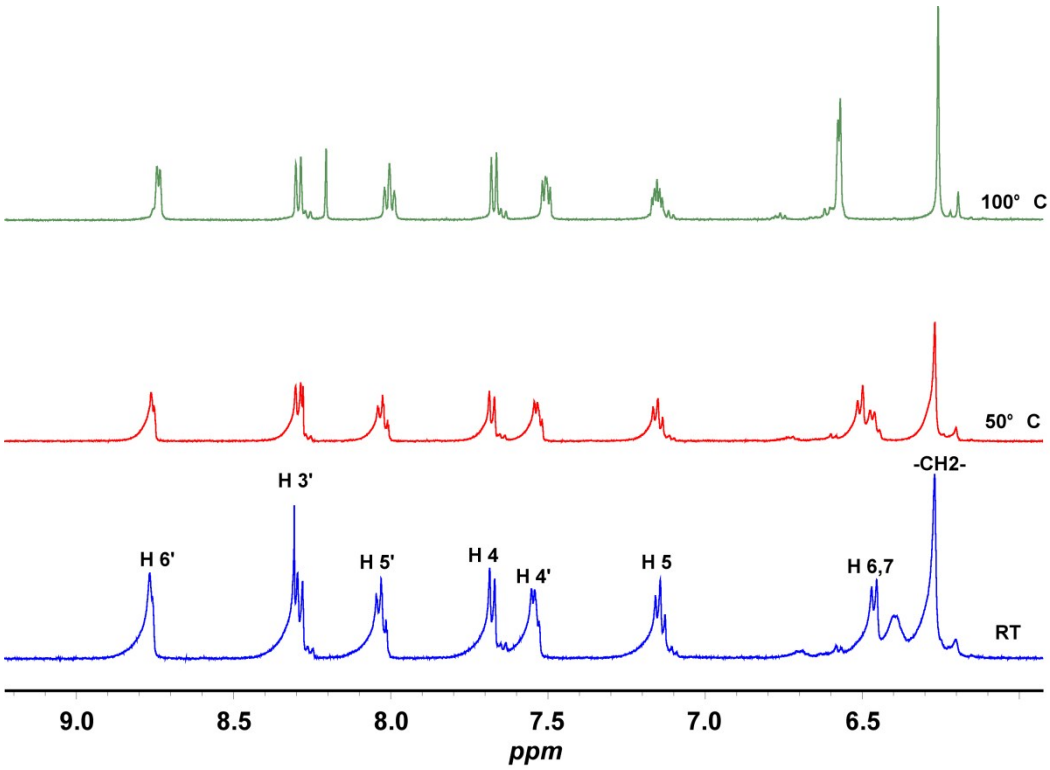

Fig. S7 Partial variable temperature ^{1}H NMR spectra of **5** in d_6-DMSO.

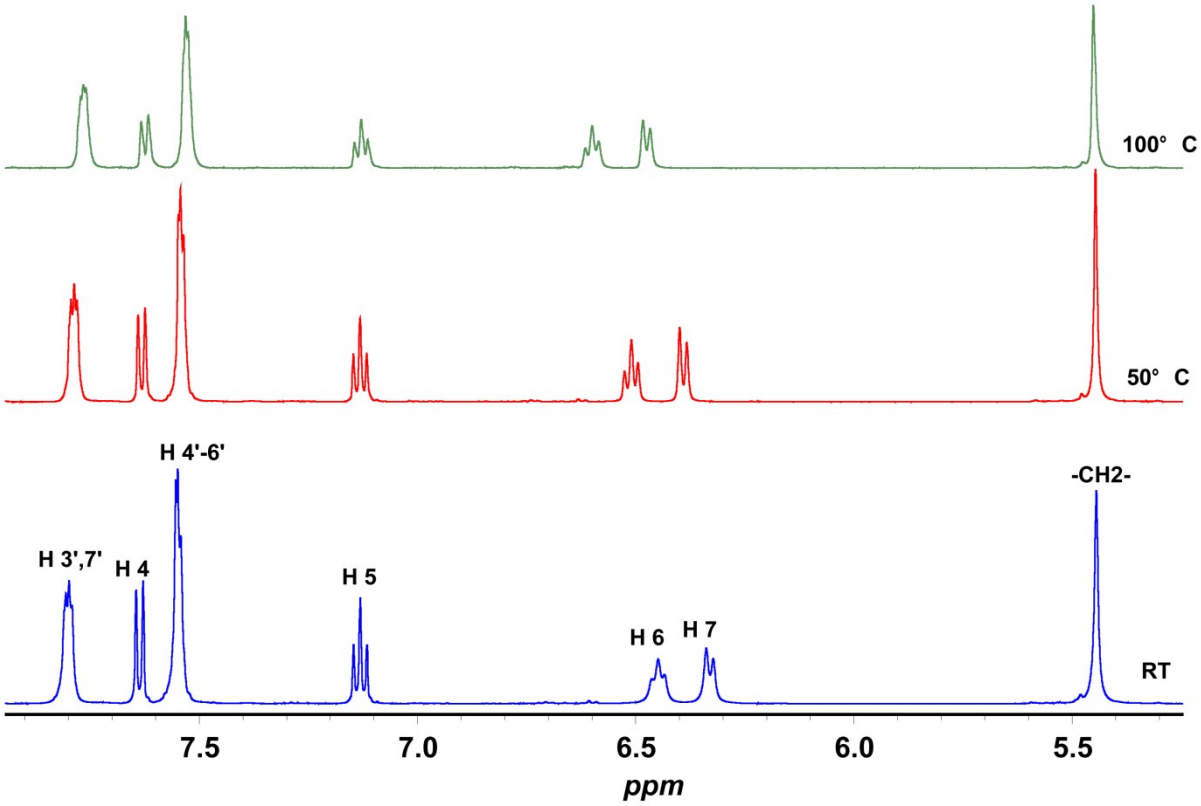

Fig. S8 Partial variable temperature ^{1}H NMR spectra of **6** in d_6-DMSO.

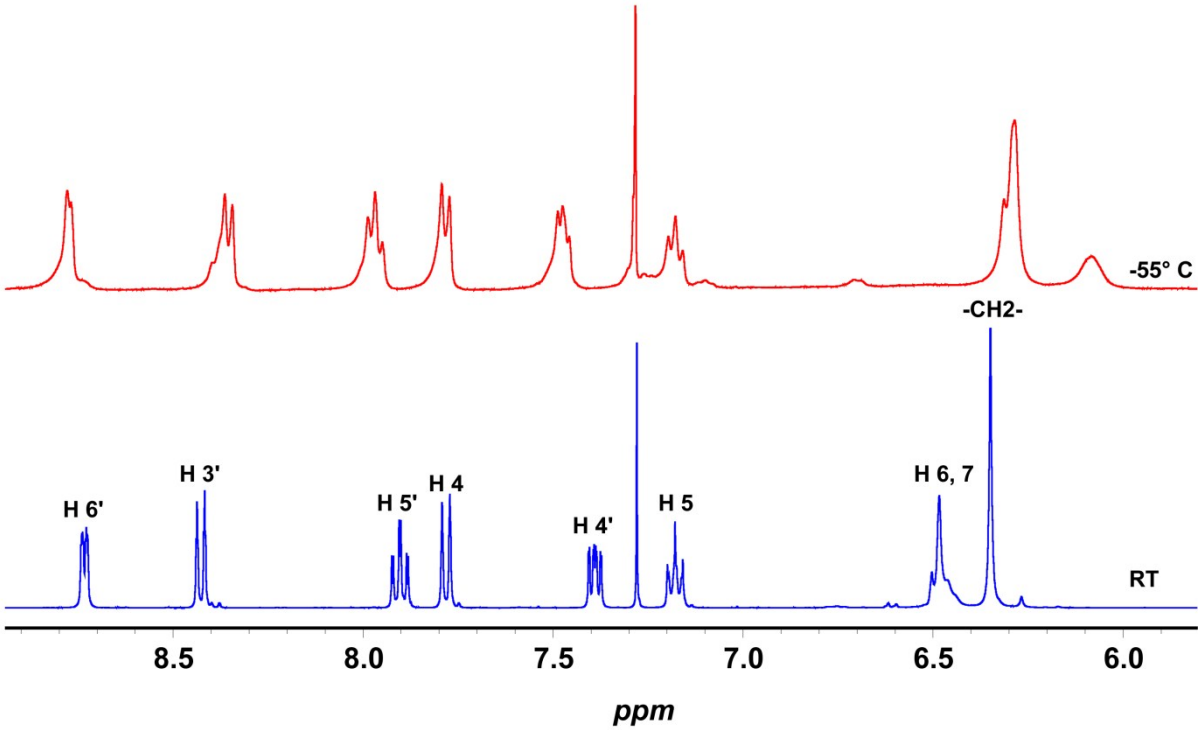

Fig. S9 Partial variable temperature ^{1}H NMR spectra of **5** in $CDCl_3$.

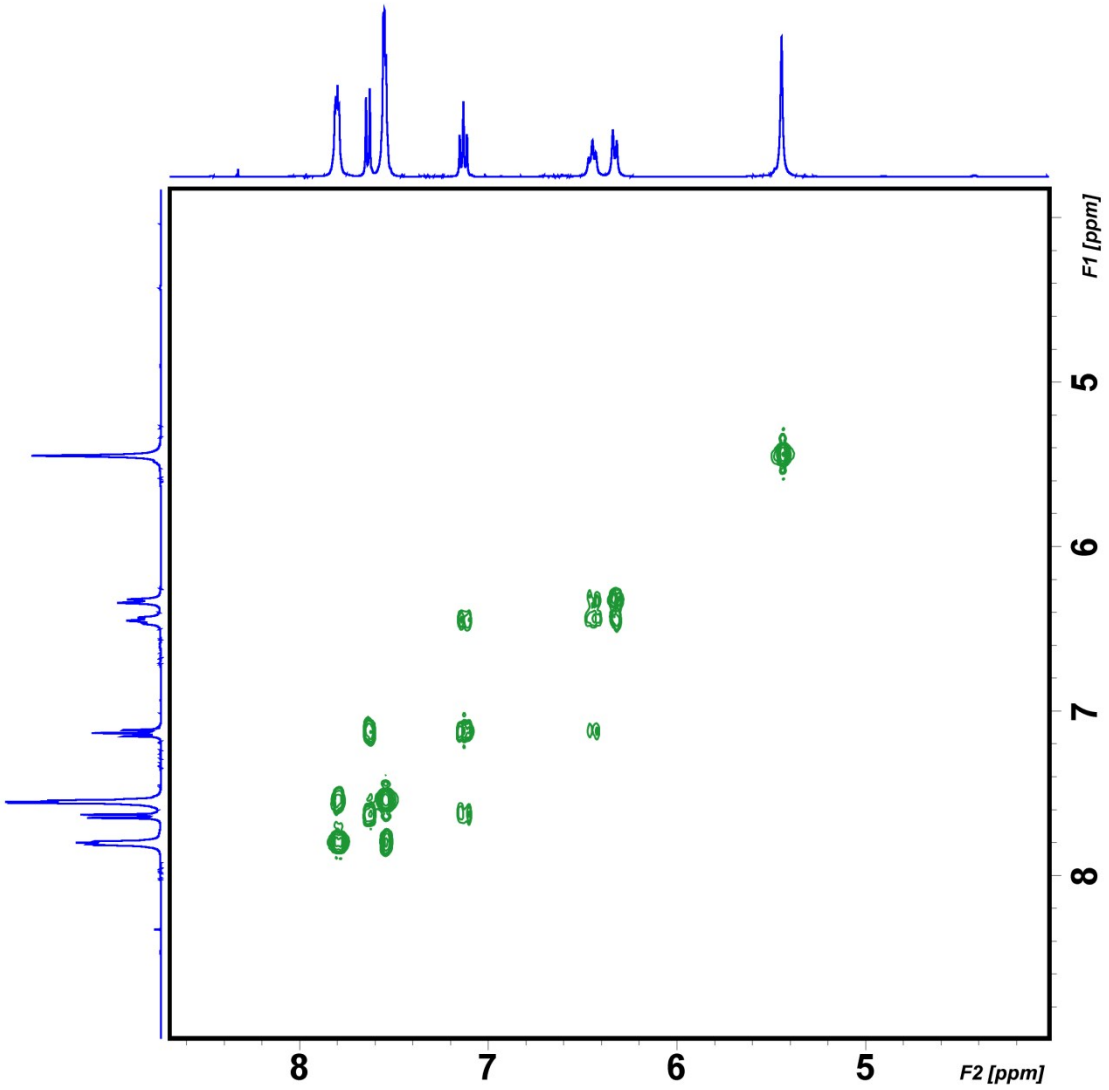

Fig. S10 Partial ^{1}H-^{1}H COSY NMR spectrum of **6** in d_6-DMSO.