Electronic Supplementary Information

The Exploration of Kemp's Tri Acid(KTA) as a Core for the Synthesis of 3- Fold Symmetric 2_3-Cyclophane, 2_2-Cyclophane and Novel Linker Directed Designs

Santhosh Reddy Naini,[a] Subramania Ranganathan,*[a] Jhillu Singh Yadav,*[a] K. V. S. Ramakrishna,*[b] G. Gayatri[c], G. Narahari Sastry*[c], K. Basu Roy[d], N. Shamala*[d]

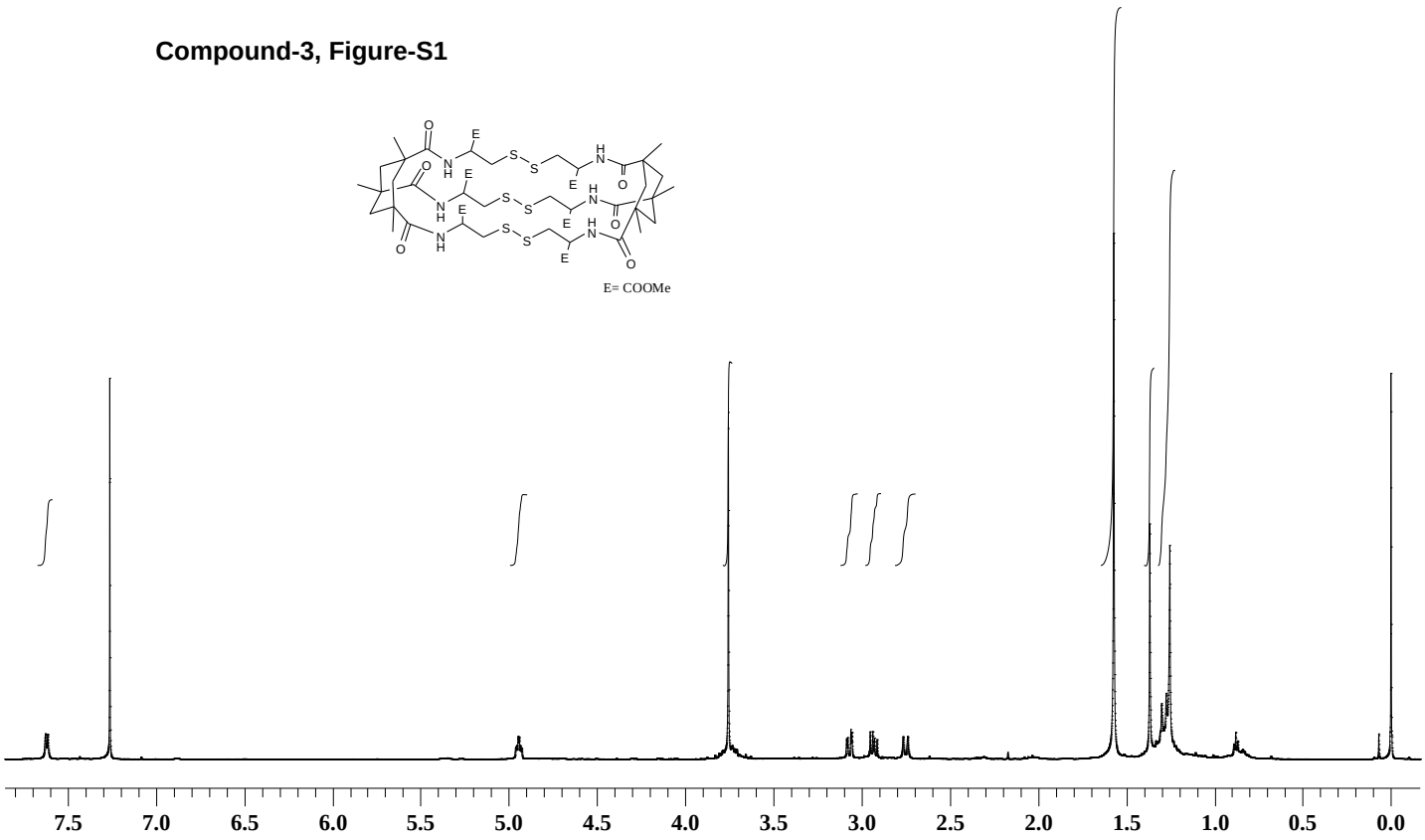


Figure-S1: ^{1}H NMR of compound **3(2_3-Cyclophane)** in $CDCl_3$, 500MHz

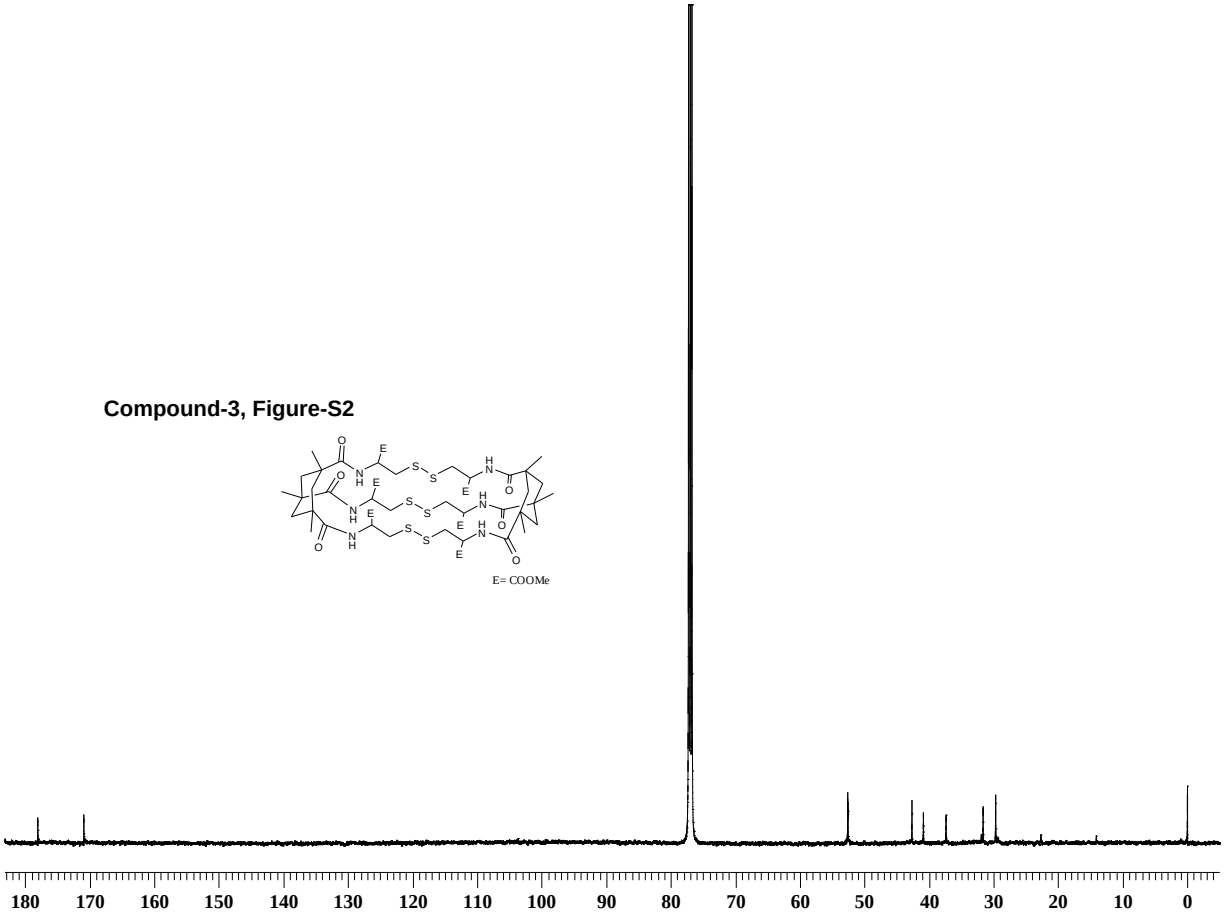


Figure-S2: ^{13}C NMR of compound **3(2_3-Cyclophane)** in $CDCl_3$, 125MHz

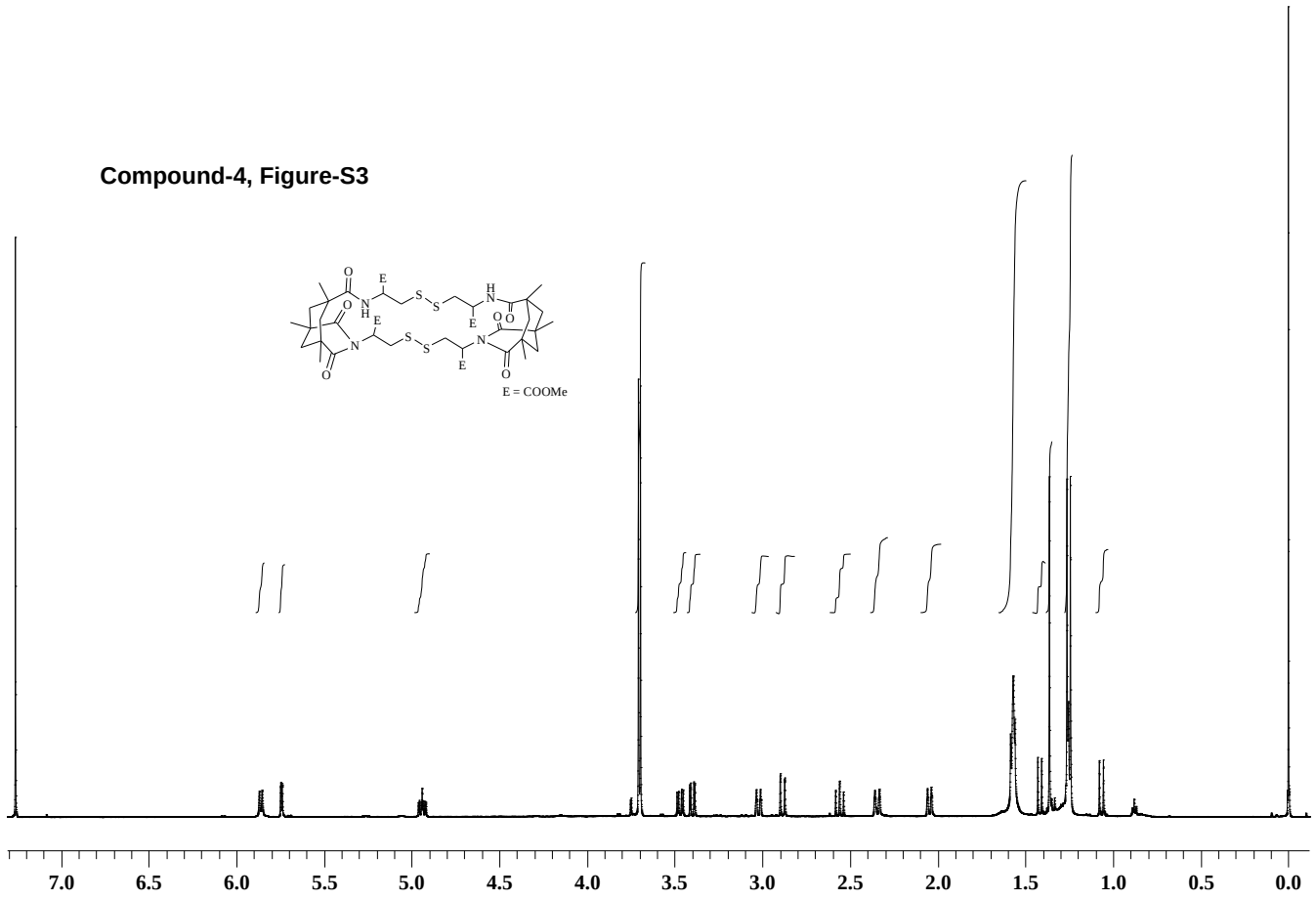


Figure-S3: ^{1}H NMR of compound **4(2_2-Cyclophane)** in $CDCl_3$, 600MHz

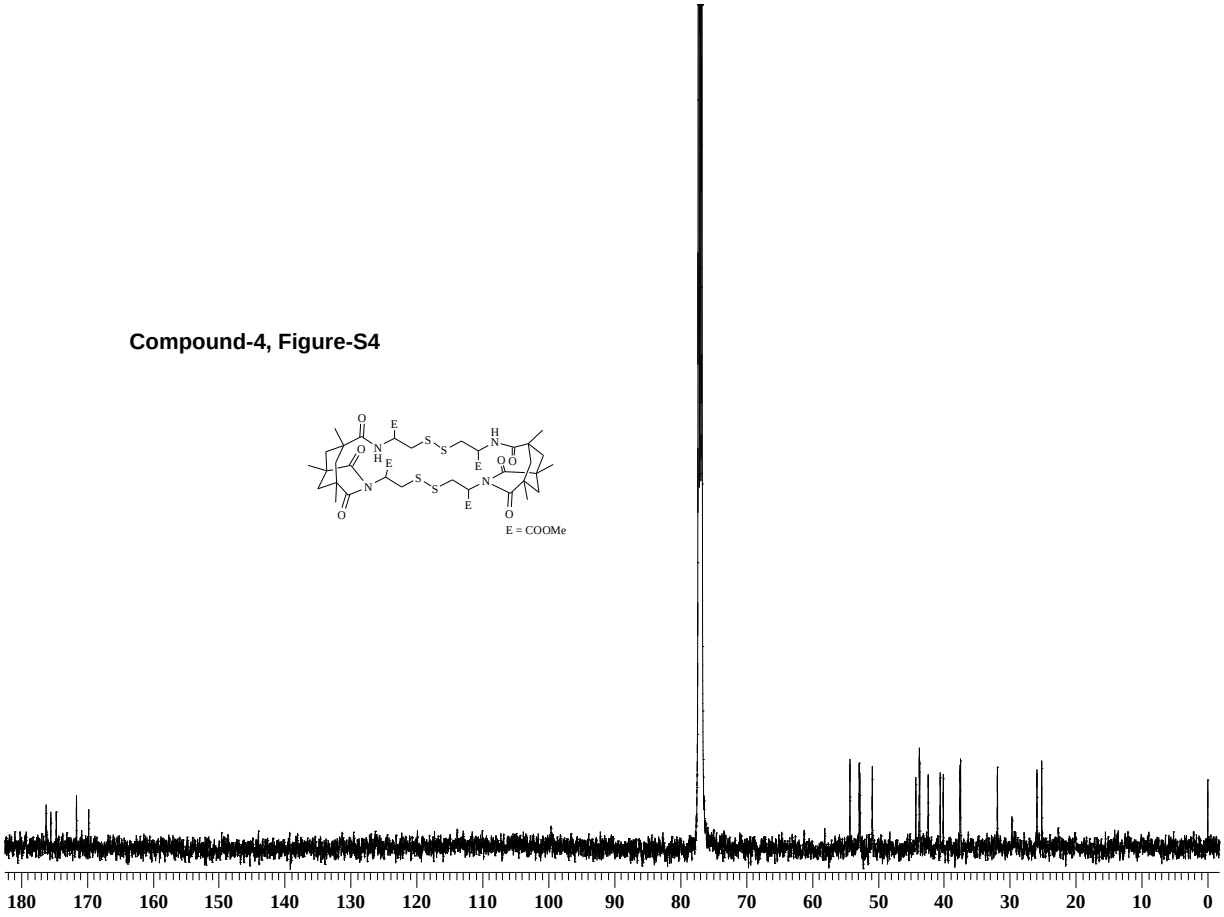


Figure-S4: ^{13}C NMR of compound **4(2_2-Cyclophane)** in $CDCl_3$, 125MHz

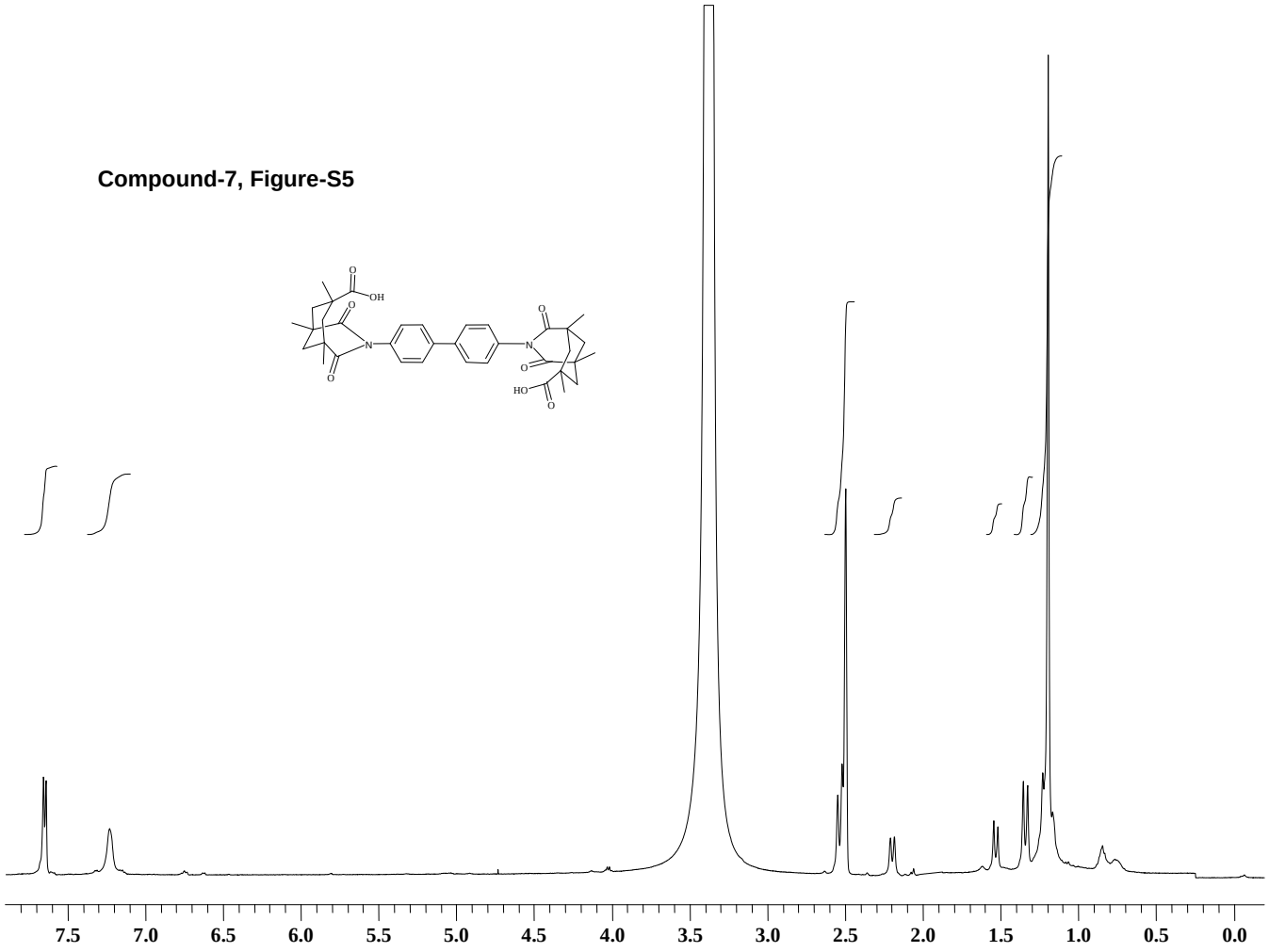


Figure-S5: ^{1}H NMR of compound **7(Kemp-Benzidine)**in DMSO-d_6, 500MHz

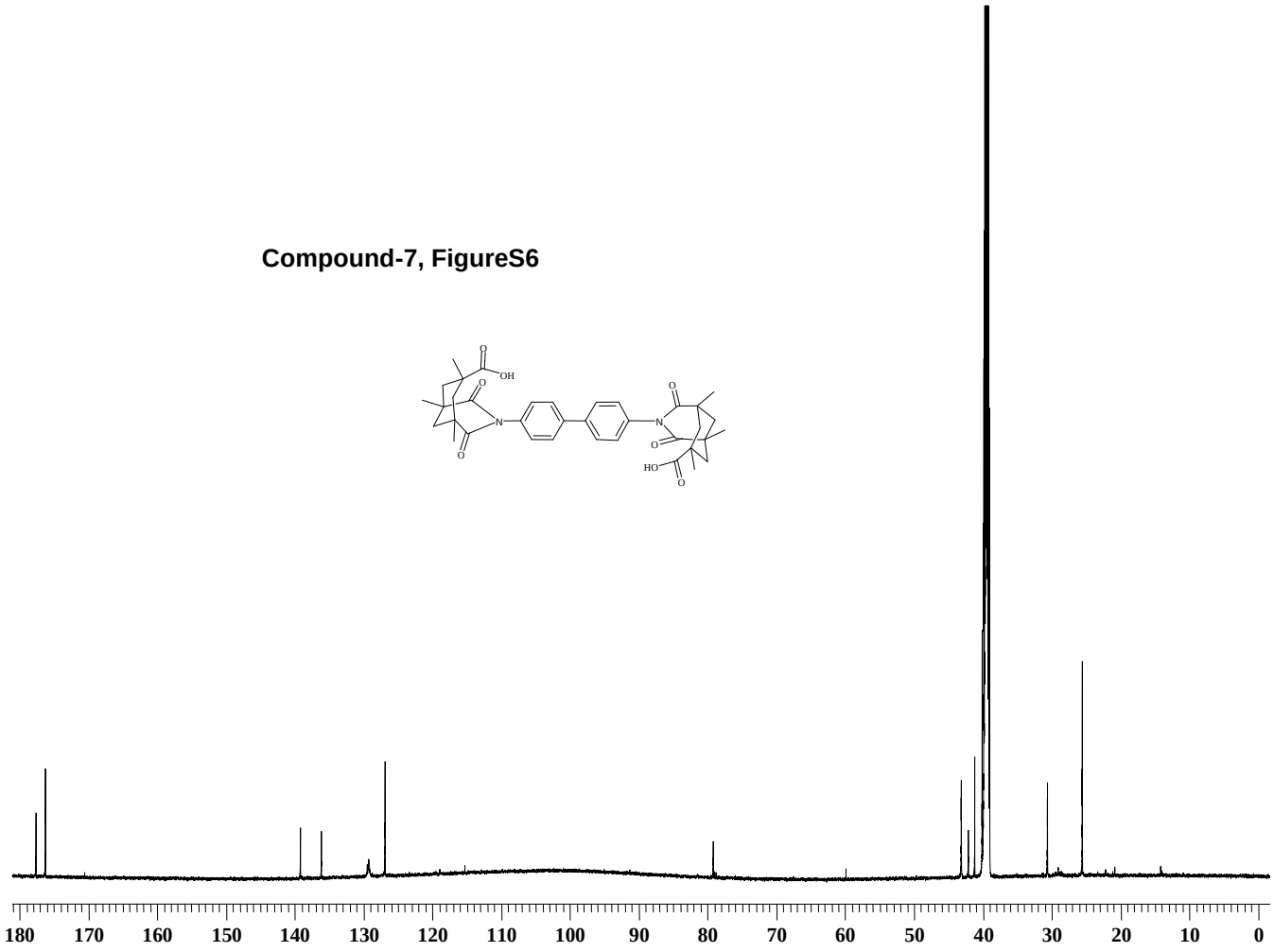


Figure-S6: ^{13}C NMR of compound **7(Kemp-Benzidine)**in DMSO-d_6,125MHz

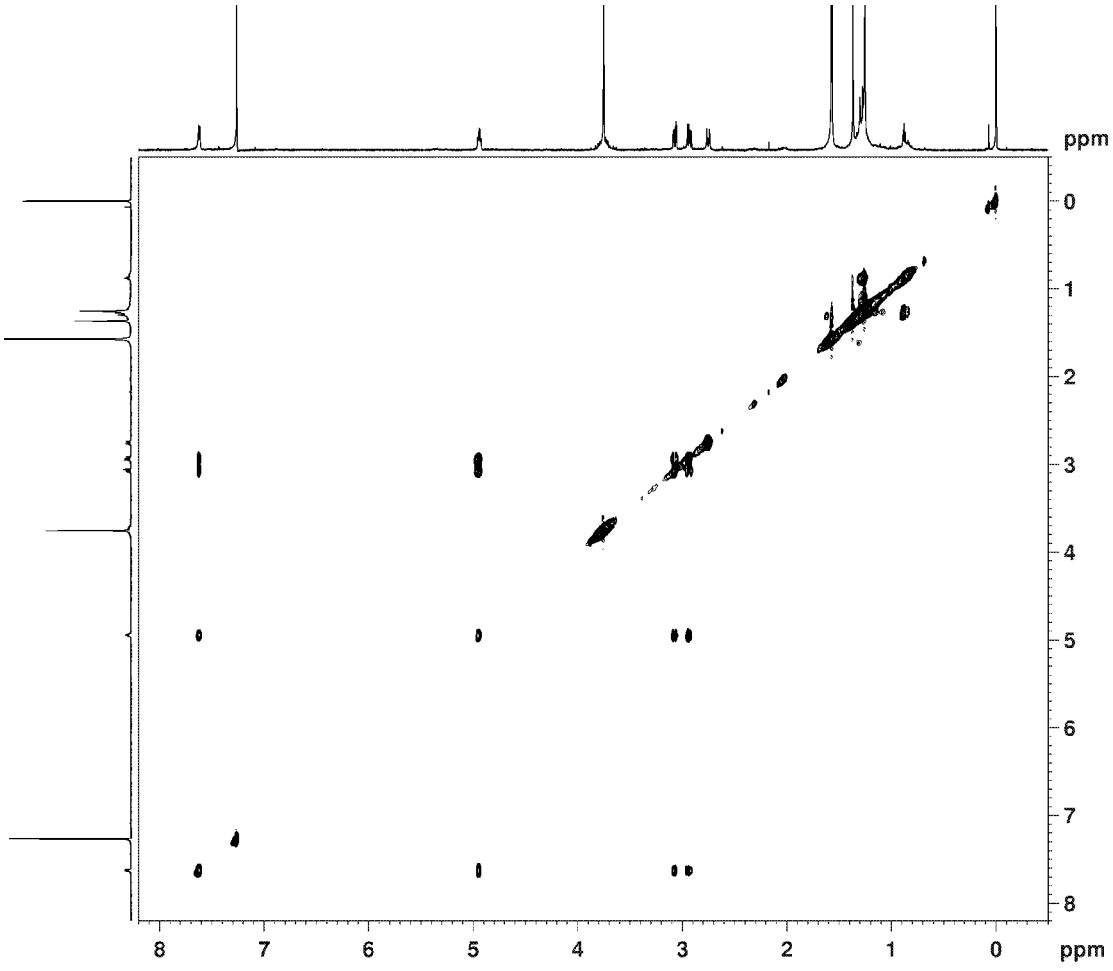


Figure-S7: The TOCSY spectrum of 2_3 cyclophane(**3**)

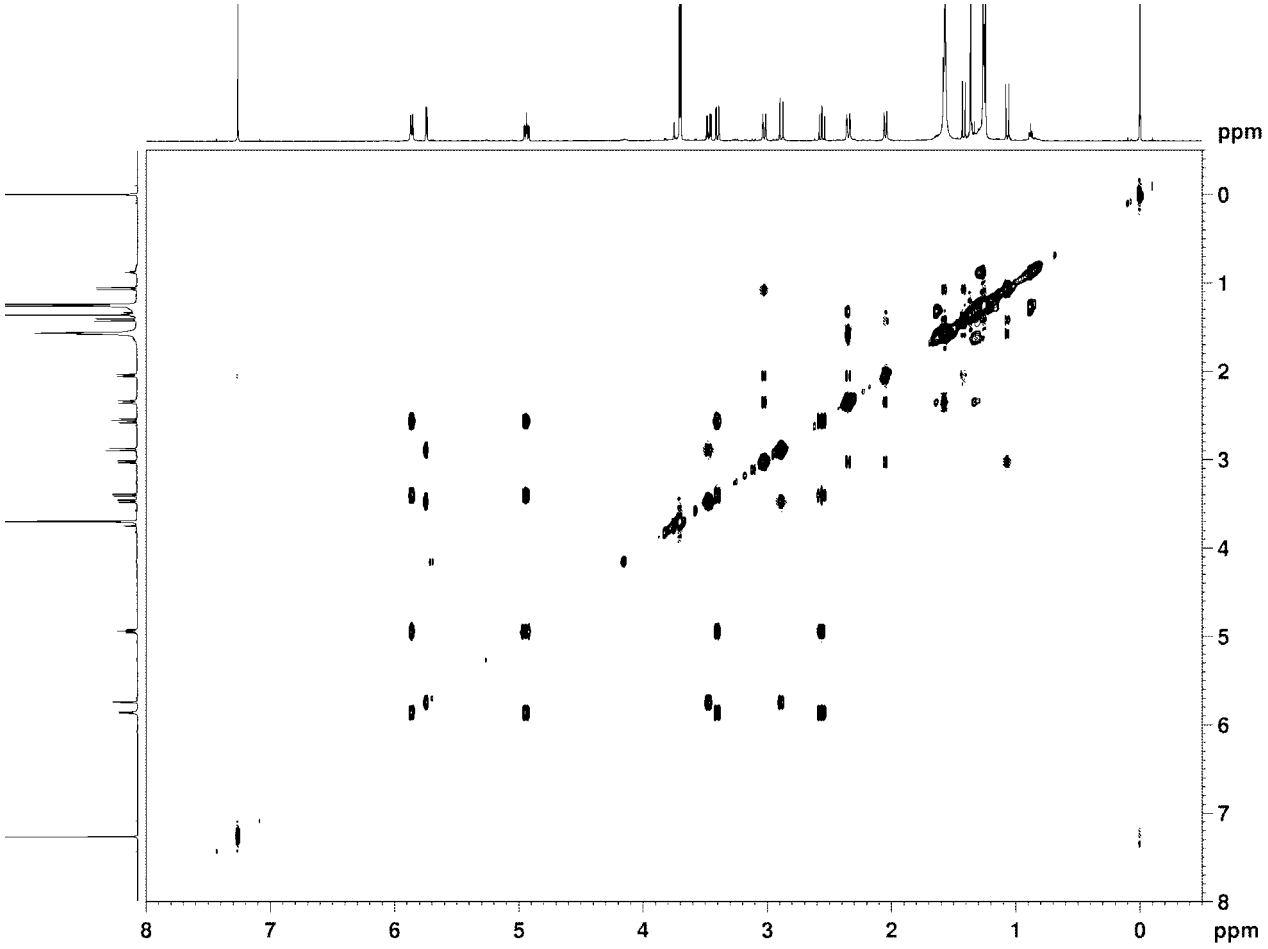
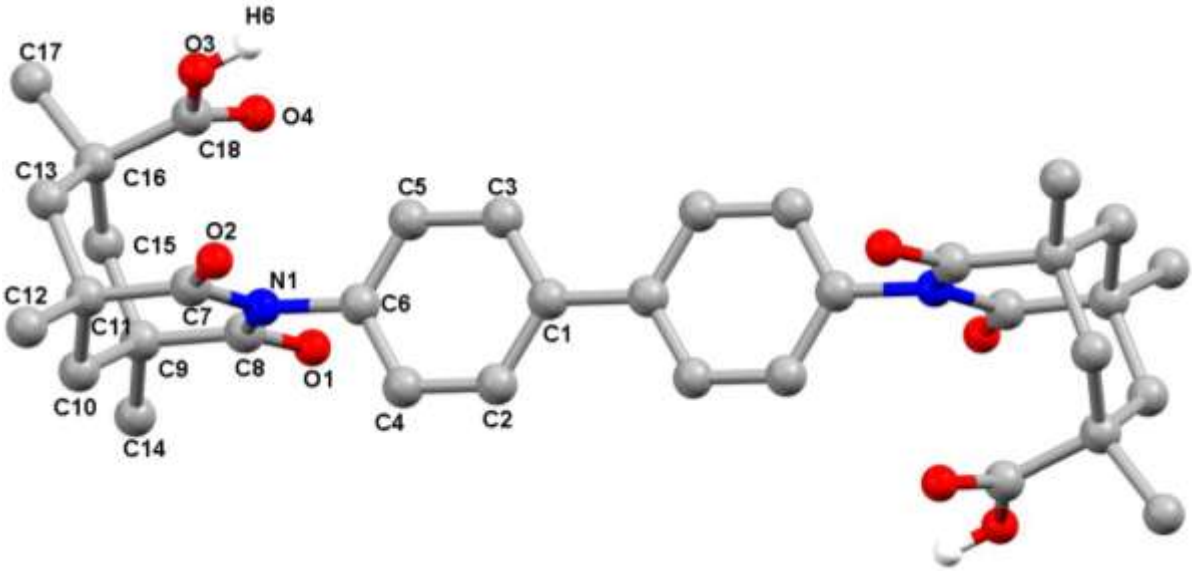


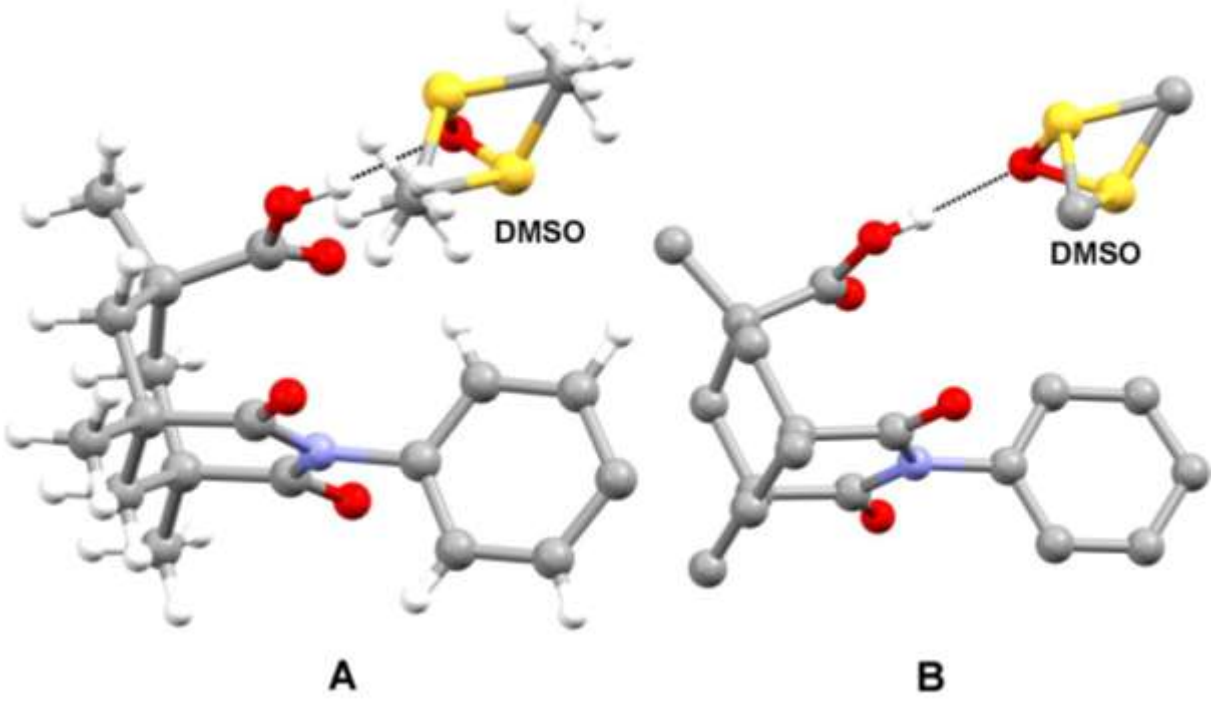
Figure-S8: The TOCSY spectrum of 2_2 cyclophane(**4**)

Crystal data and structure refinement parameters for Kemp-benzidine (7)

Empirical formula	$C_{18}H_{20}NO_4 + C_2H_6OS$
Crystal habit	Rectangular
Crystal size (mm)	(0.56 × 0.45 × 0.13)
Crystallizing solvent	DMSO
Space group	$P2_1/c$
a (Å)	7.585(2)
b (Å)	18.384(3)
c (Å)	14.401(3)
β(˚)	102.535(8)
Volume ($Å^{3)}$	1960.1(6)
Z	2
Molecules/asymmetric unit	1/2
Co-crystallized solvent	C_2H_6OS (DMSO)
Molecular weight	644.71 + 156.27
Calculated density (g/cm^3)	1.330
F (000)	836
Radiation	MoK_α (0.71073Å)
Temperature (K)	200 (2)
2θ max. (˚)	61.36
Measured reflections	23014
R_{int}	0.0366
Unique reflections	6011
Observed reflection [$\lvert F \rvert > 4\sigma(F)$]	4682
Final R (%)/*w*R2 (%)	5.34 / 16.43
Goodness-of-fit on F^2 (S)	0.961
$\Delta\rho_{max}$ ($e.Å^{-3}$)/ $\Delta\rho_{min}$($e.Å^{-3}$)	0.53 / -0.37
No. of restraints/parameters	0/301
Data-to-parameter ratio	15.55: 1



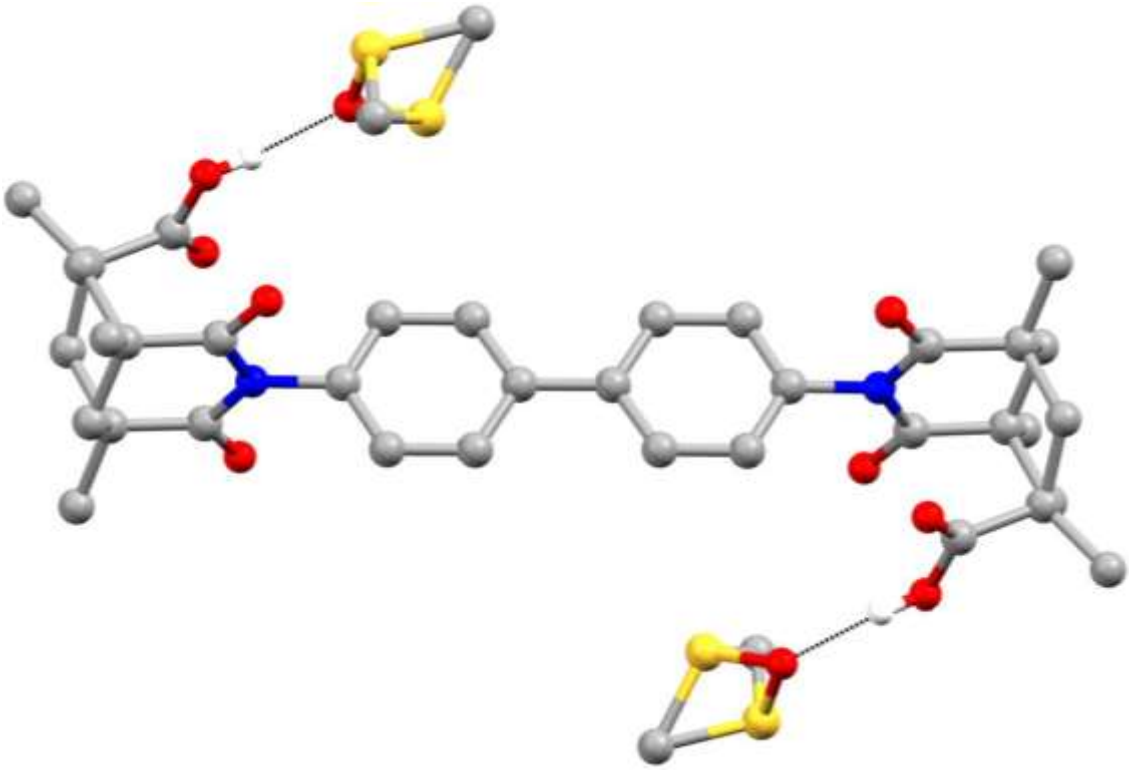
Crystal structure of Kemp-benzidine(**7**)



Crystallographic asymmetric unit of Kemp-benzidine(**7**).

A: With hydrogen atoms.

B: Without hydrogen atoms.



Crystal structure of Kemp-benzidine(**7**) with co-crystallized solvent (DMSO) molecules