

Electronic Supplementary Information

Mono-Functionalized Derivatives and Revised Configurational Assignment of Amide Naphthotubes

Huan Yao,[‡] Xiaoping Wang,[‡] Mo Xie, Yu-Mei Wang, Mao Quan, Liu-Pan Yang, and

Wei Jiang*

Shenzhen Grubbs Institute and Department of Chemistry, Southern University of Science and Technology, Shenzhen, 518055, China.

*E-mail: jiangw@sustech.edu.cn

[‡] These authors contributed equally

Table of Contents

1. Characterization Data	S2
2. Assignment Data of the Configurational Isomers of 2	S19
3. ITC Titration Data of 2a and 2b and Between 1b and G4	S22
4. Supporting Data for the New Assignments of 1a and 1b	S25
5. Supporting Data for the Consistent Assignments 1a and 1b	S28
6. ¹ H NMR Spectra of 1a ” and 1b ”	S34
7. X-Ray Crystallography	S35
8. Computational Data	S37
9. References	S50

1. Characterization Data

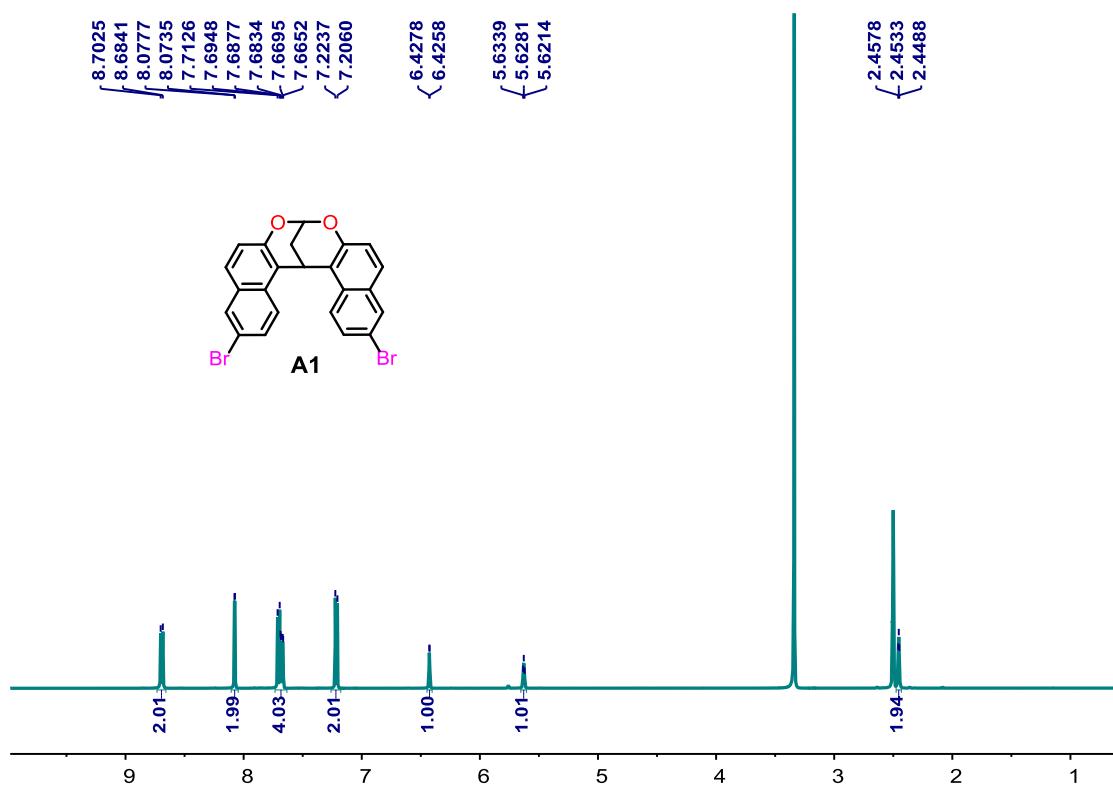


Fig. S1 ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$, 25 °C) of A1

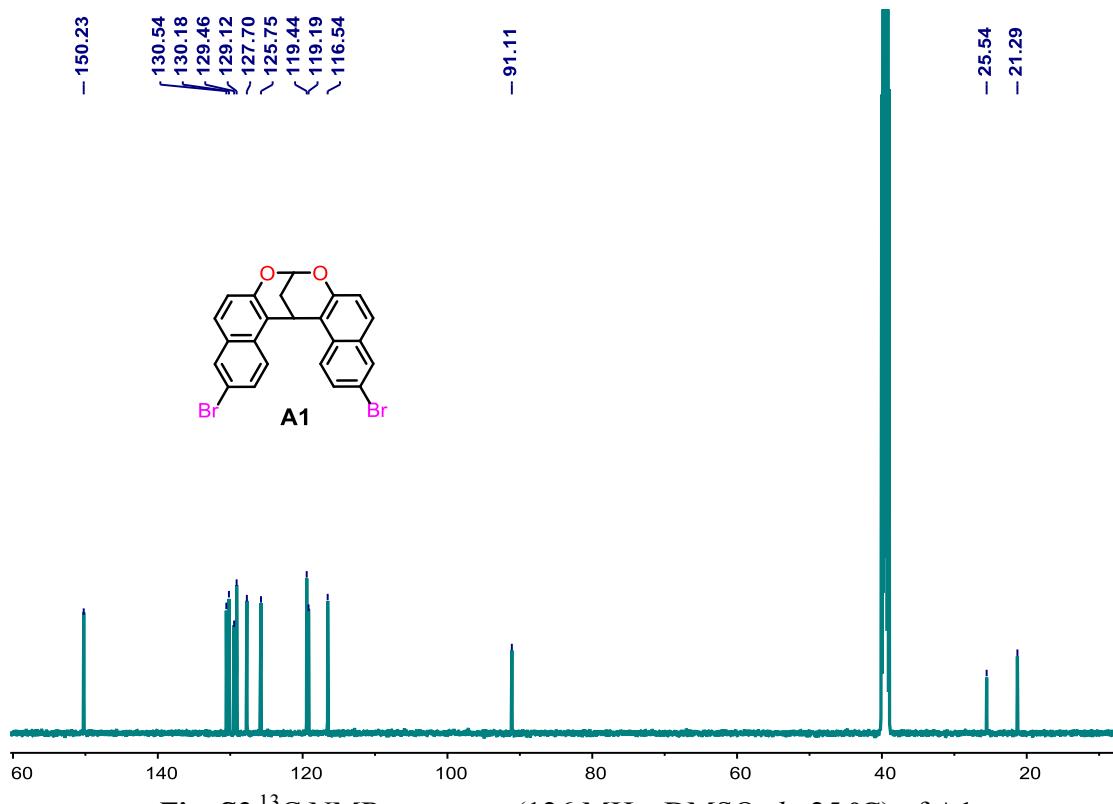


Fig. S2 ^{13}C NMR spectrum (126 MHz, $\text{DMSO}-d_6$, 25 °C) of A1

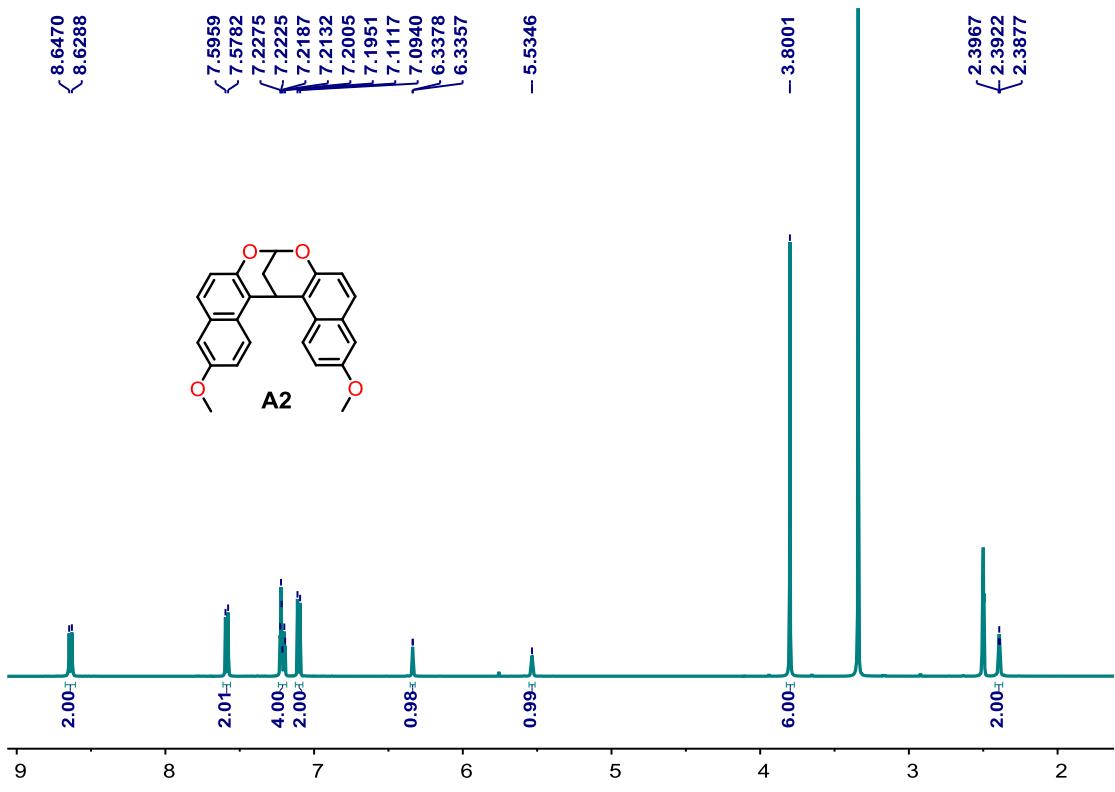


Fig. S3 ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$, 25 °C) of **A2**

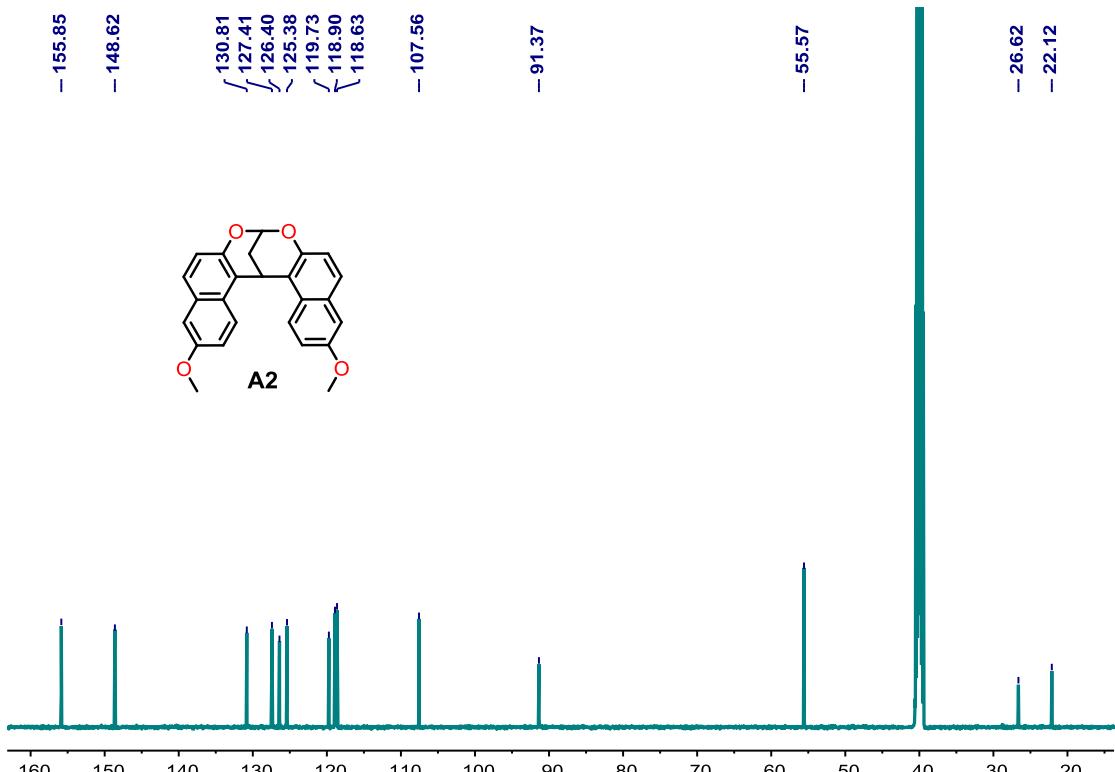


Fig. S4 ^{13}C NMR spectrum (126 MHz, $\text{DMSO}-d_6$, 25 °C) of **A2**

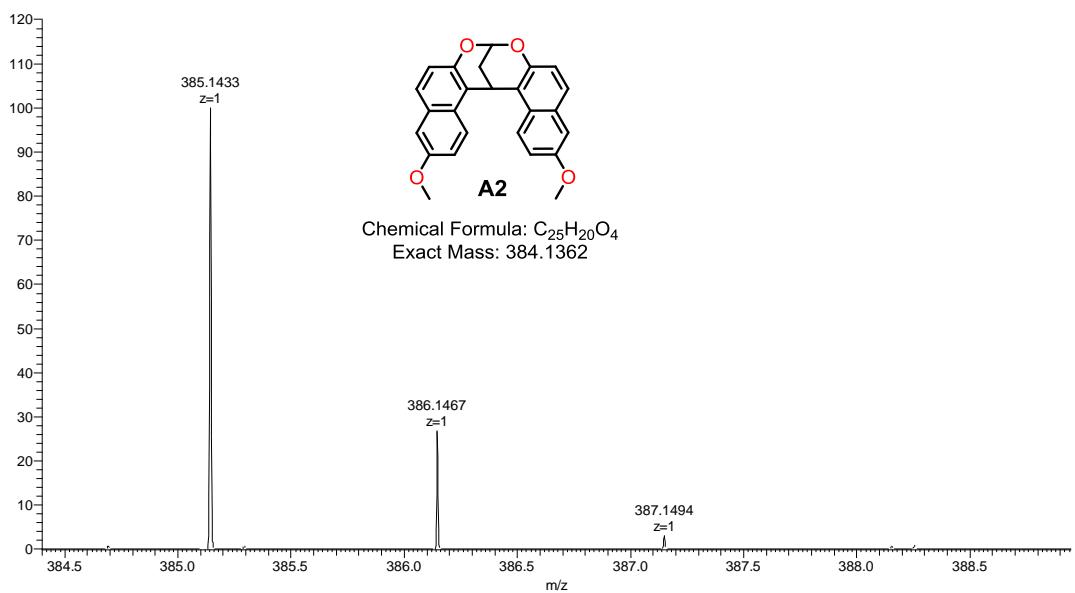


Fig. S5 ESI mass spectrum of A2

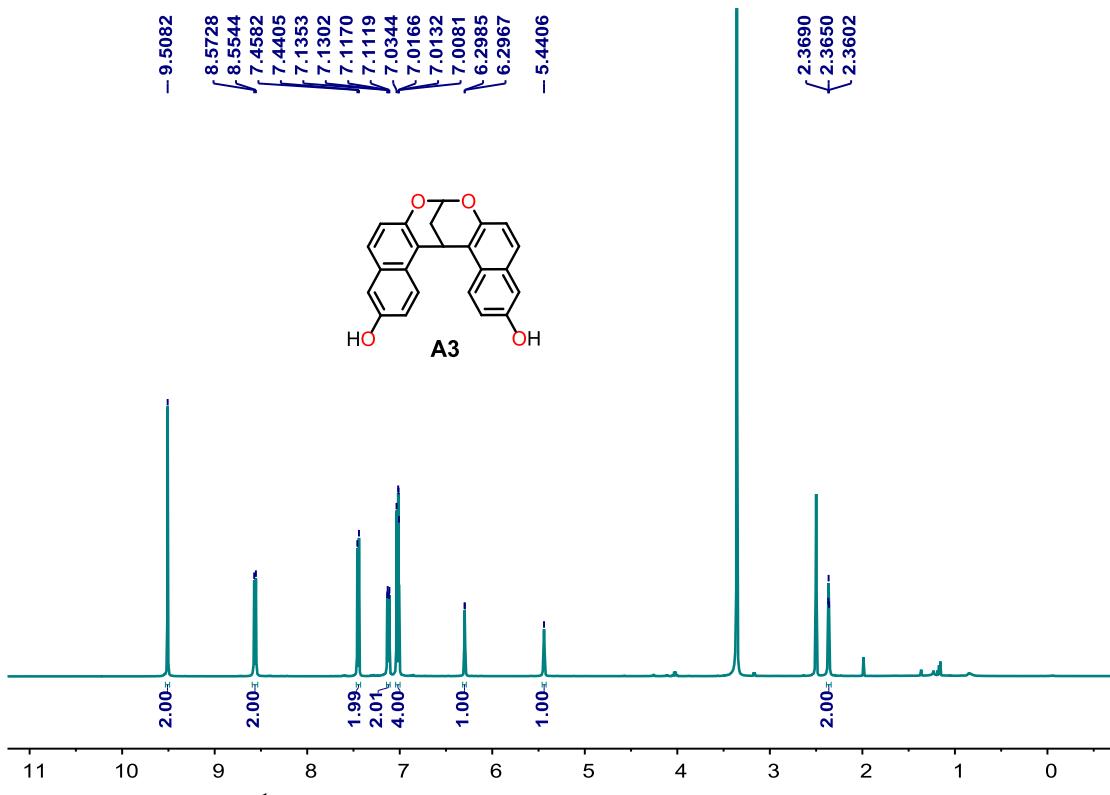


Fig. S6 ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$, 25 °C) of A3

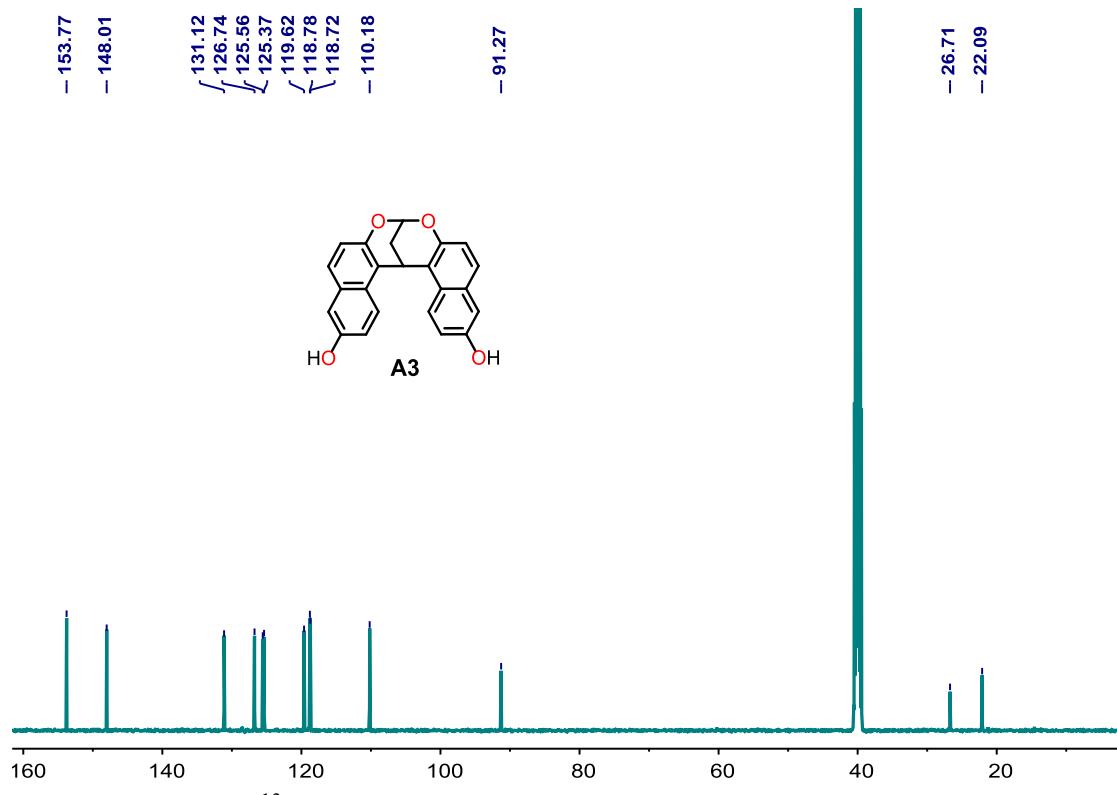


Fig. S7 ^{13}C NMR spectrum (126 MHz, $\text{DMSO}-d_6$, 25 °C) of A3

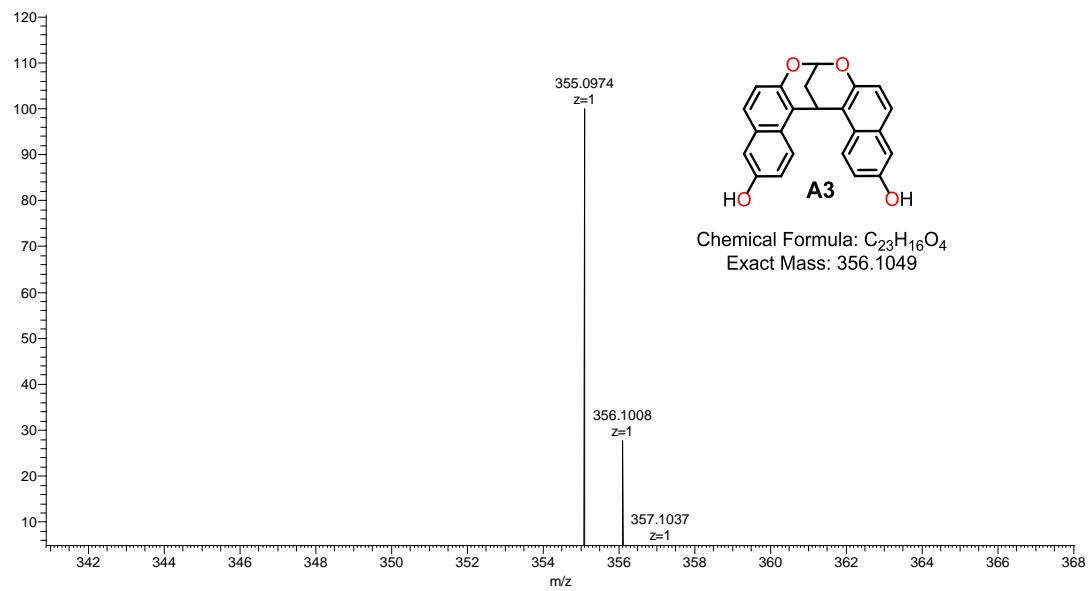


Fig. S8 ESI mass spectrum of A3

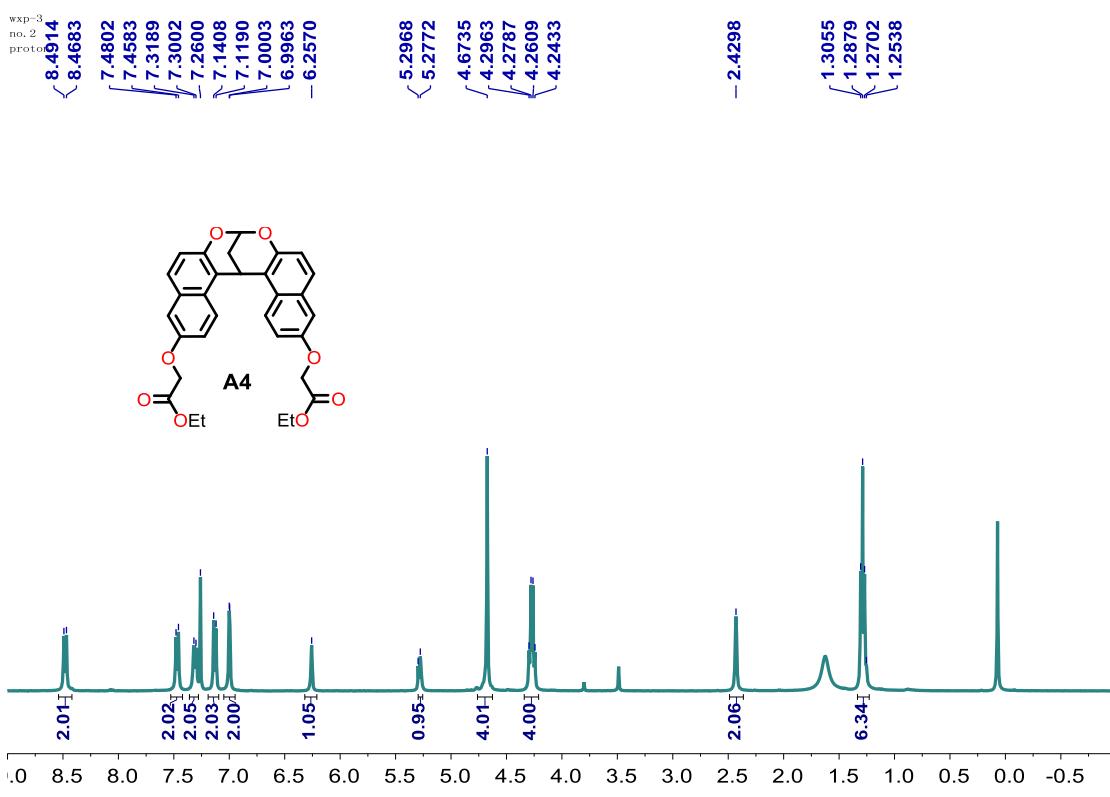


Fig. S9 ^1H NMR spectrum (400 MHz, CDCl_3 , 25 °C) of A4

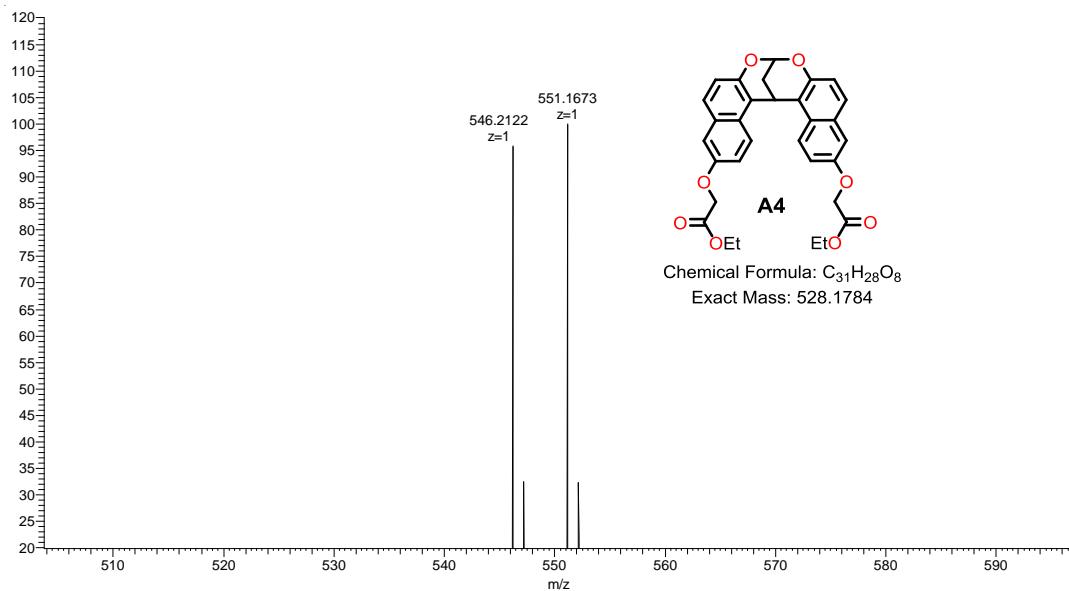


Fig. S10 ESI mass spectrum of A4

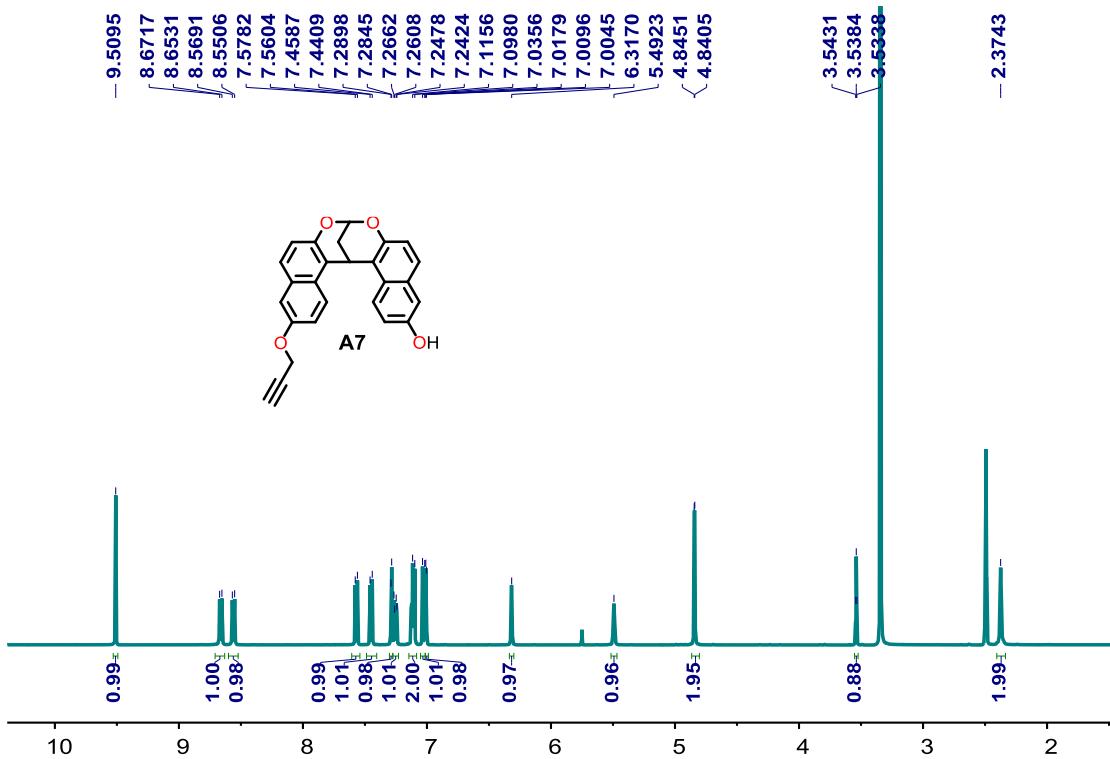


Fig. S11 ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$, 25 °C) of A7

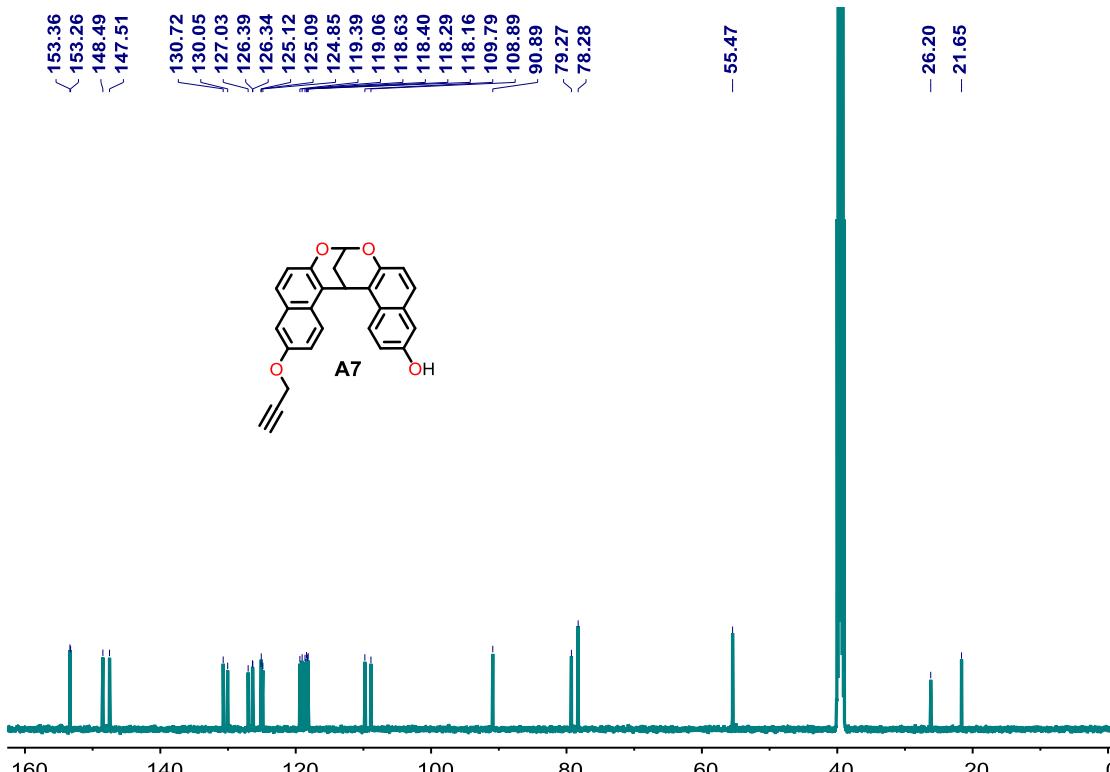


Fig. S12 ^{13}C NMR spectrum (126 MHz, $\text{DMSO}-d_6$, 25 °C) of A7

yh-87-1 #10 RT: 0.09 AV: 1 NL: 7.58E7
T: FTMS - p ESI Full ms [100.0000-1500.0000]

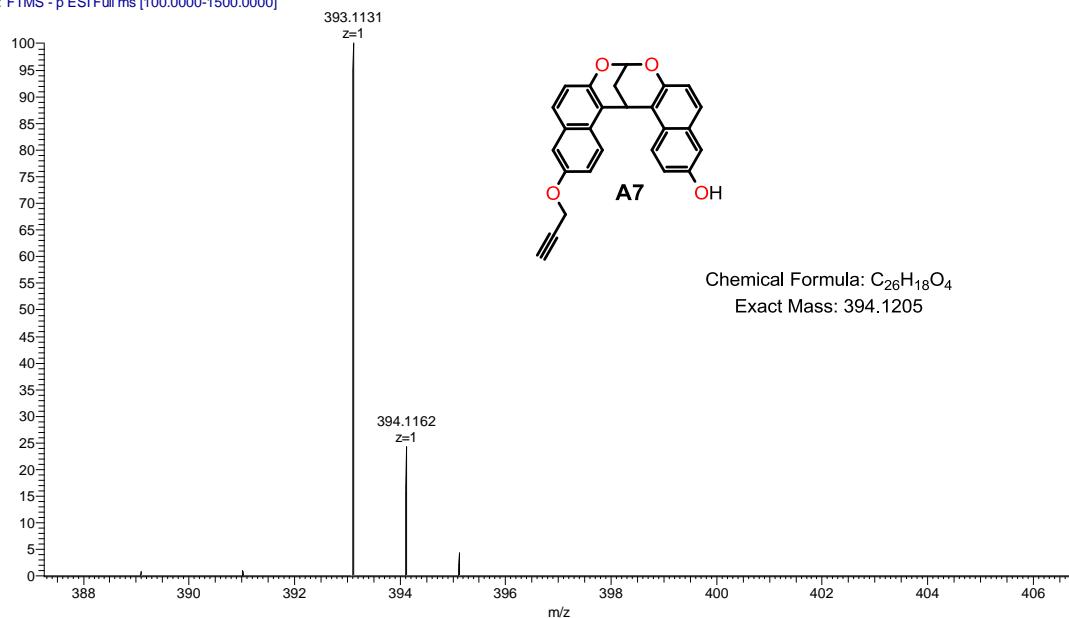


Fig. S13 ESI mass spectrum of A7

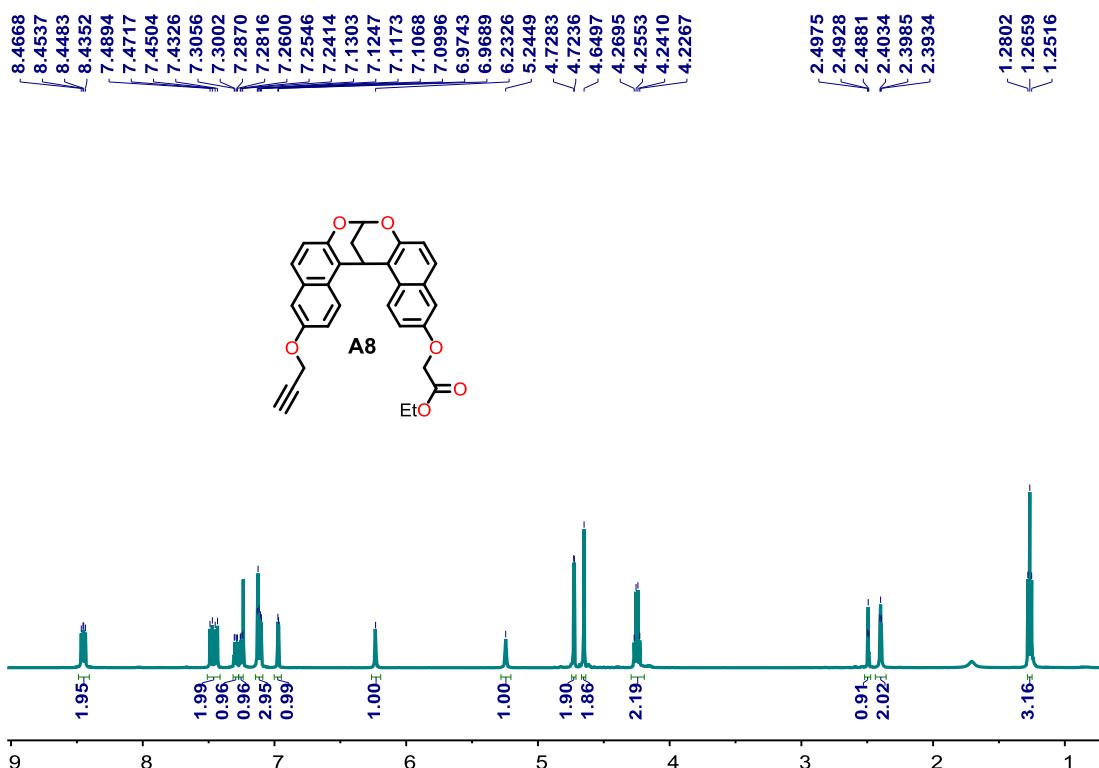


Fig. S14 1H NMR spectrum (500 MHz, $CDCl_3$, 25 °C) of A8

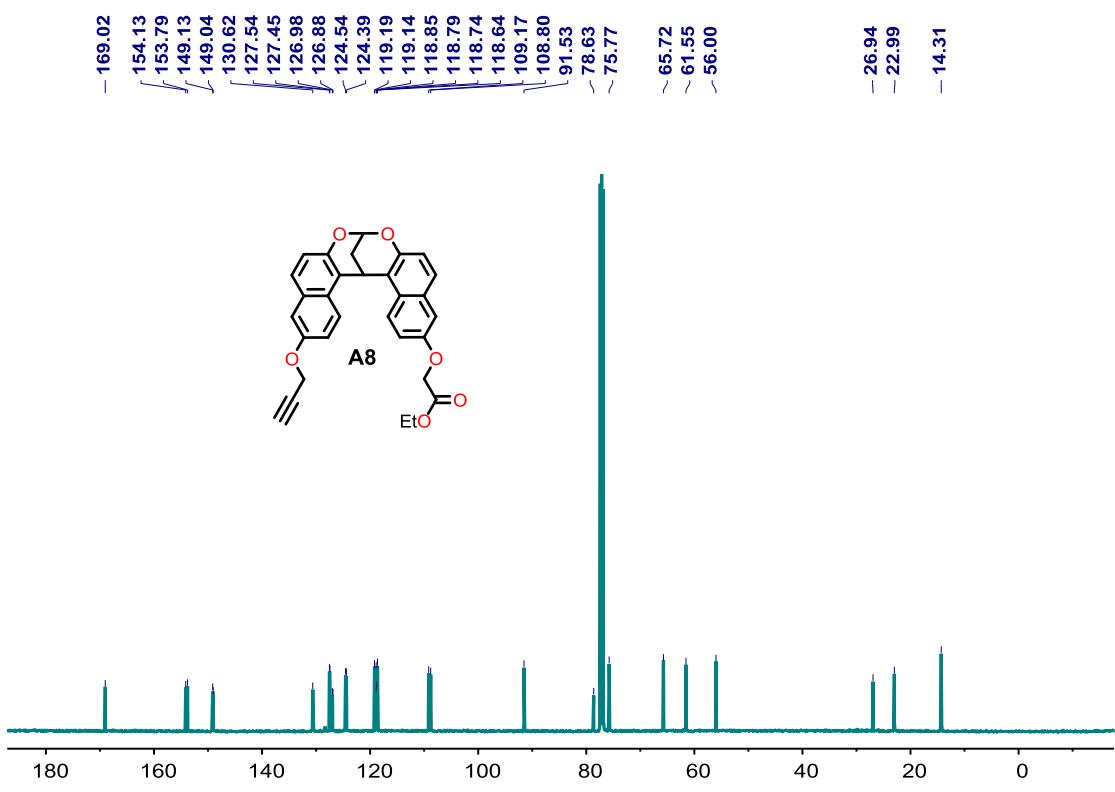


Fig. S15 ^{13}C NMR spectrum (126 MHz, CDCl_3 , 25 °C) of A8

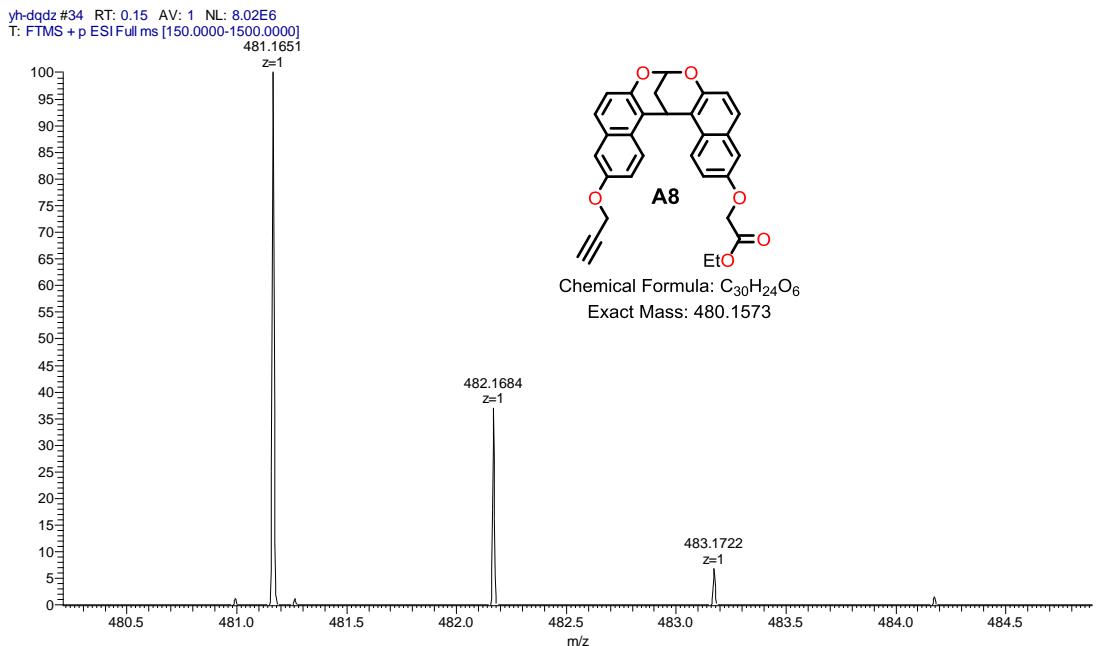


Fig. S16 ESI mass spectrum of A8

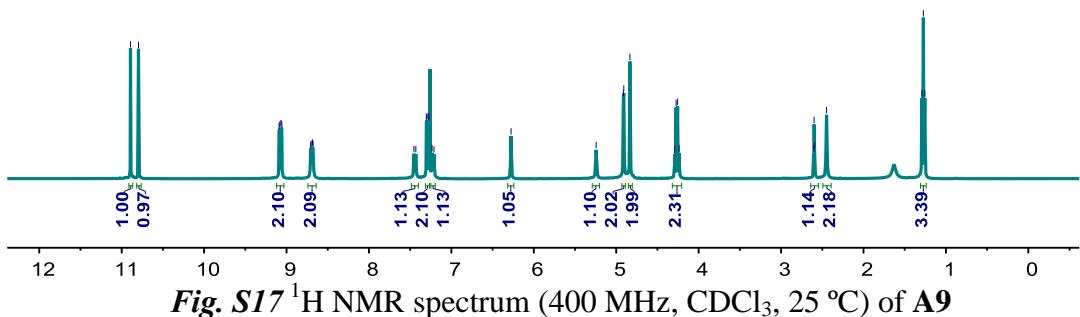
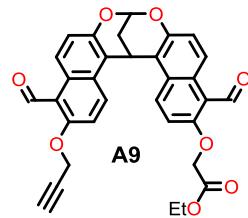
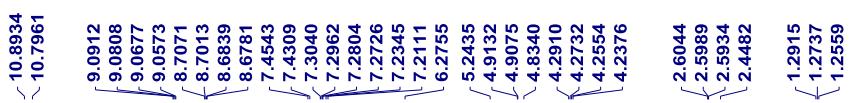


Fig. S17 ^1H NMR spectrum (400 MHz, CDCl_3 , 25 °C) of A9

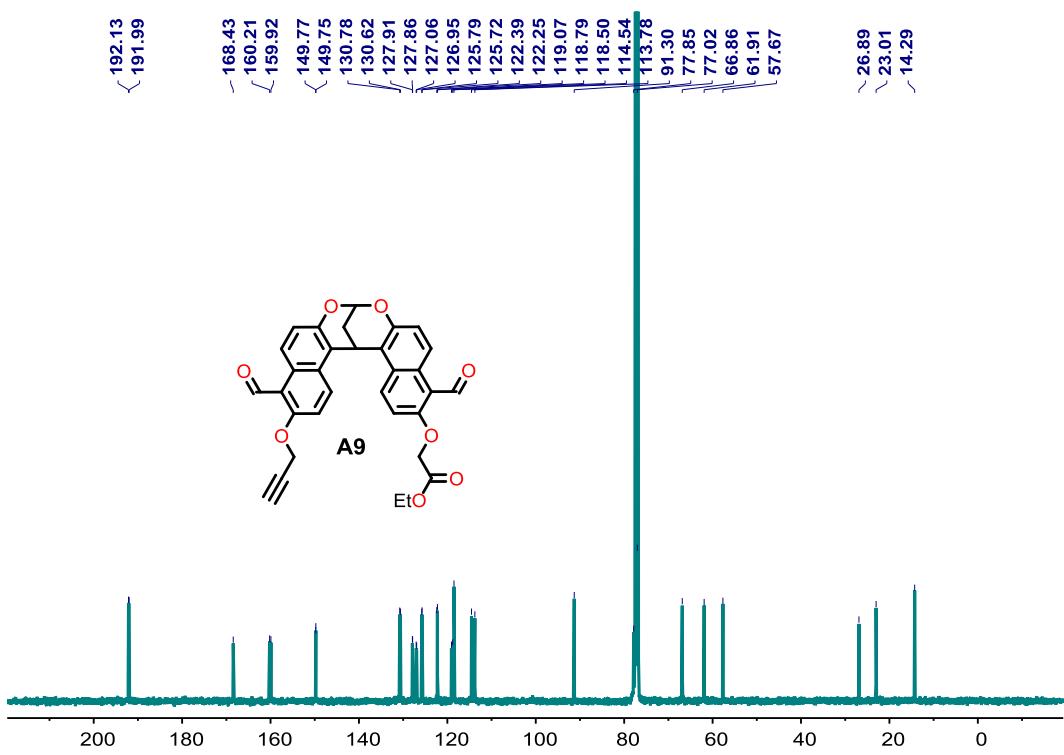
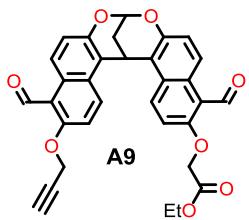


Fig. S18 ^{13}C NMR spectrum (101 MHz, CDCl_3 , 25 °C) of A9

yh-187 #11 RT: 0.10 AV: 1 NL: 3.12E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]

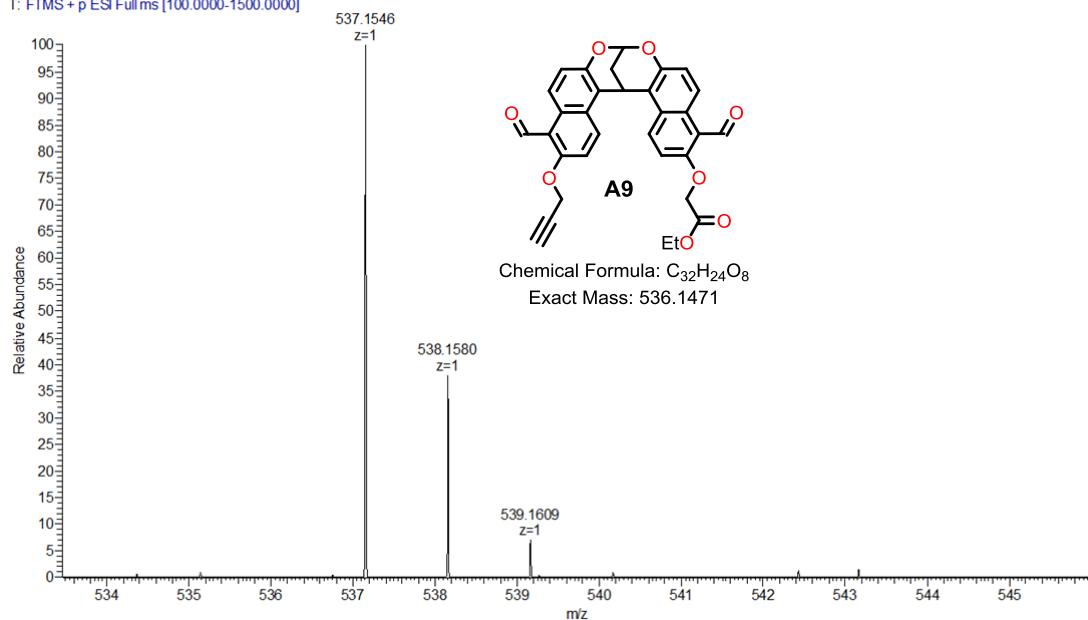


Fig. S19 ESI mass spectrum of **A9**

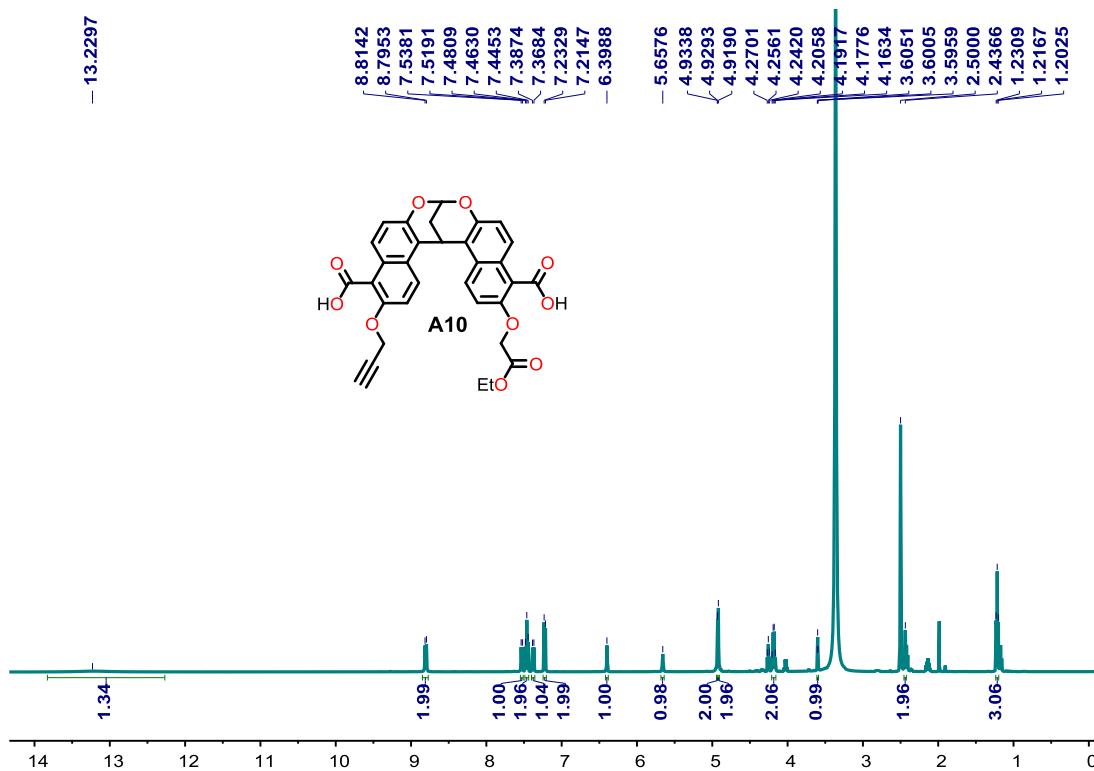


Fig. S20 ¹H NMR spectrum (500 MHz, DMSO-*d*₆, 25 °C) of **A10**

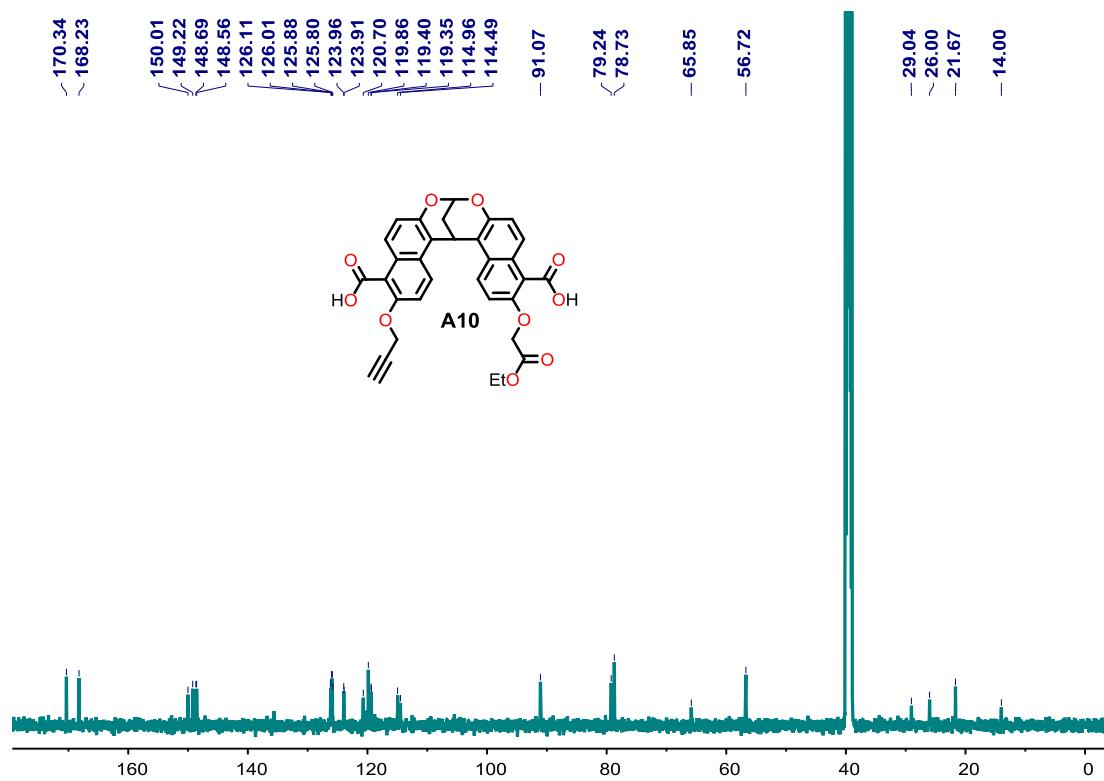


Fig. S21 ^{13}C NMR spectrum (126 MHz, $\text{DMSO}-d_6$, 25 °C) of A10

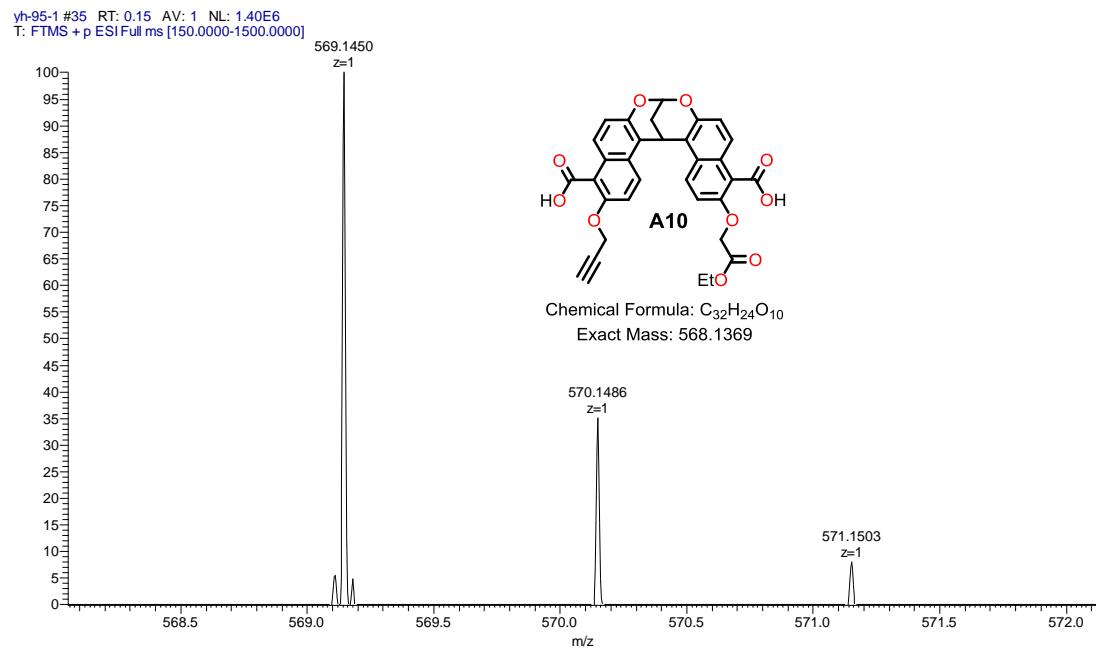


Fig. S22 ESI mass spectrum of A10

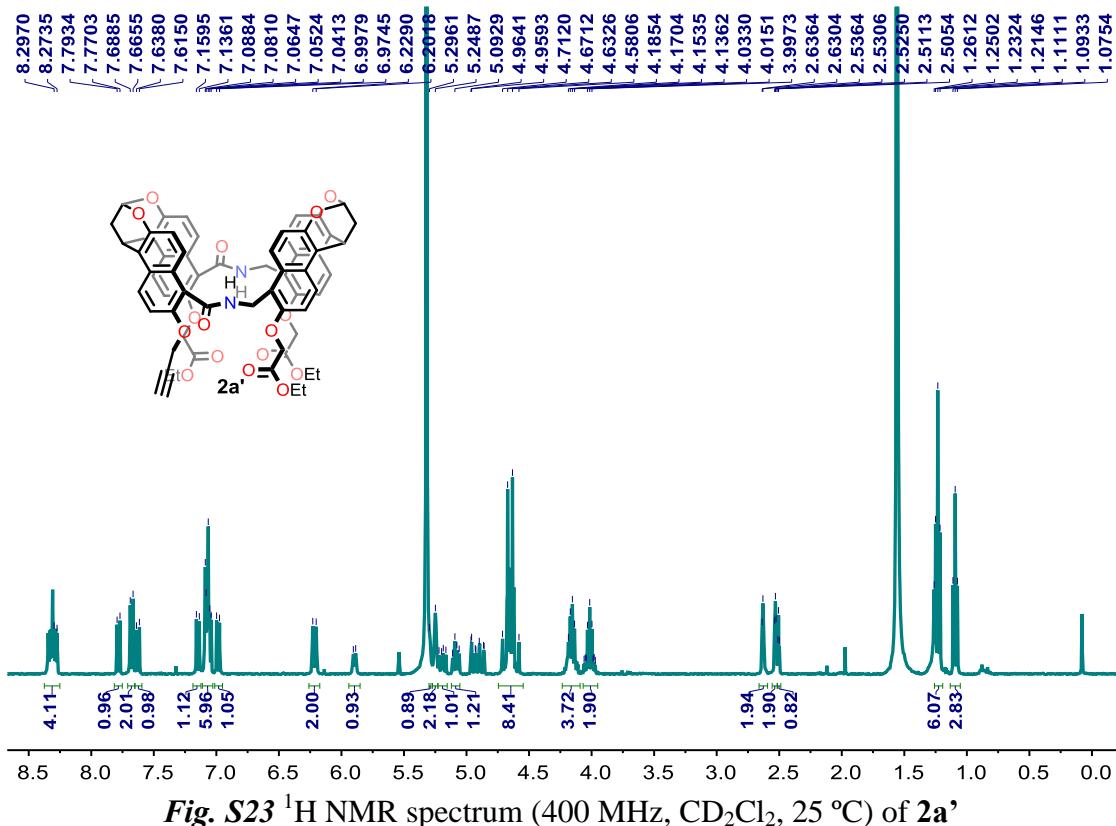


Fig. S23 ^1H NMR spectrum (400 MHz, CD_2Cl_2 , 25 °C) of $\mathbf{2a}'$

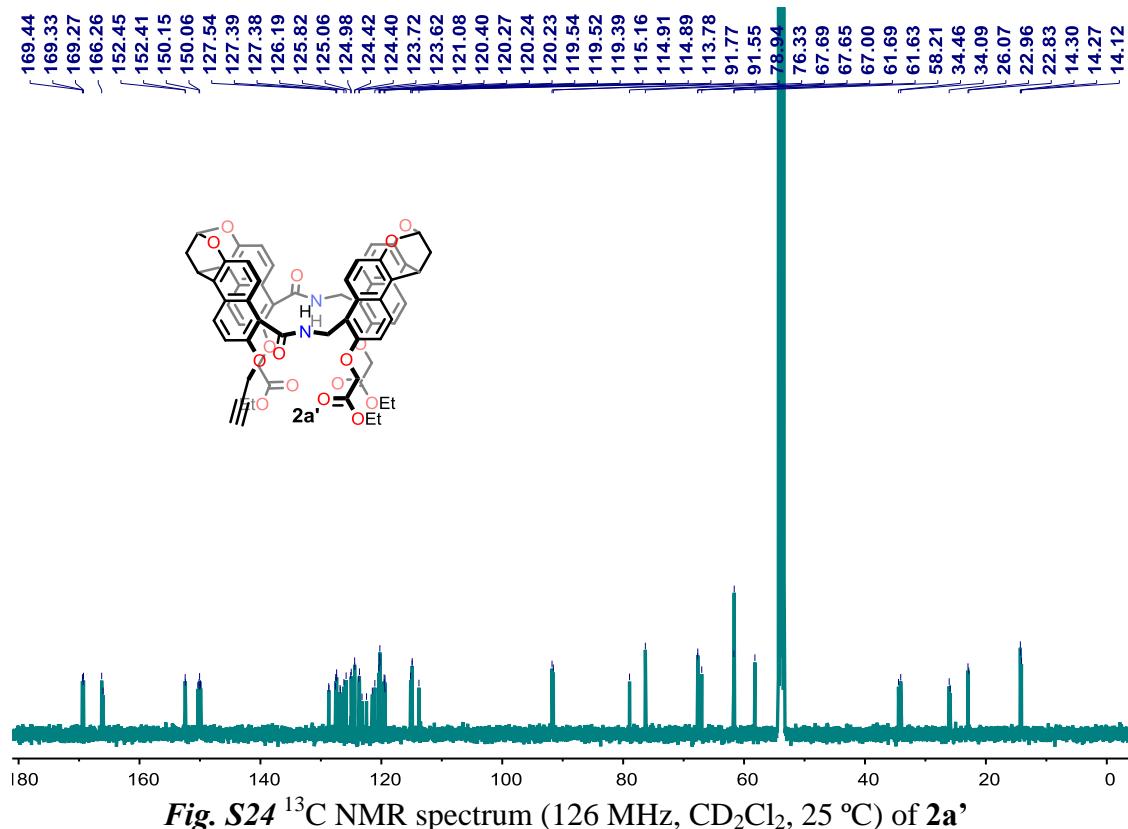


Fig. S24 ^{13}C NMR spectrum (126 MHz, CD_2Cl_2 , 25 °C) of $\mathbf{2a}'$

yh-4a #6-9 RT: 0.06-0.08 AV: 2 NL: 1.65E8
T: FTMS + p ESI Full ms [200.0000-3000.0000]

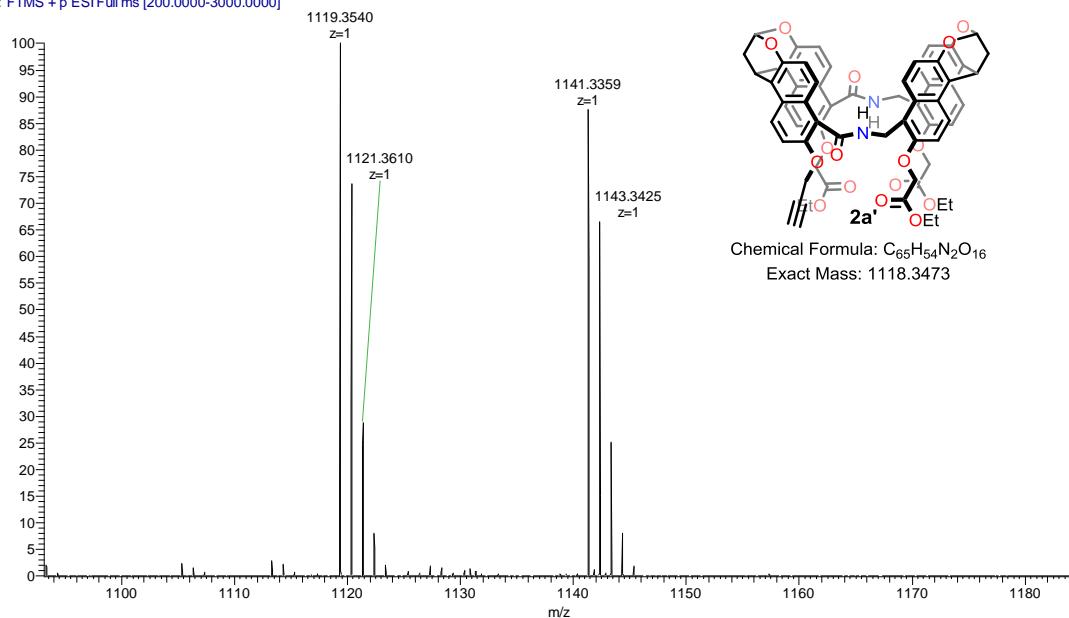


Fig. S25 ESI mass spectrum of $\mathbf{2a}'$

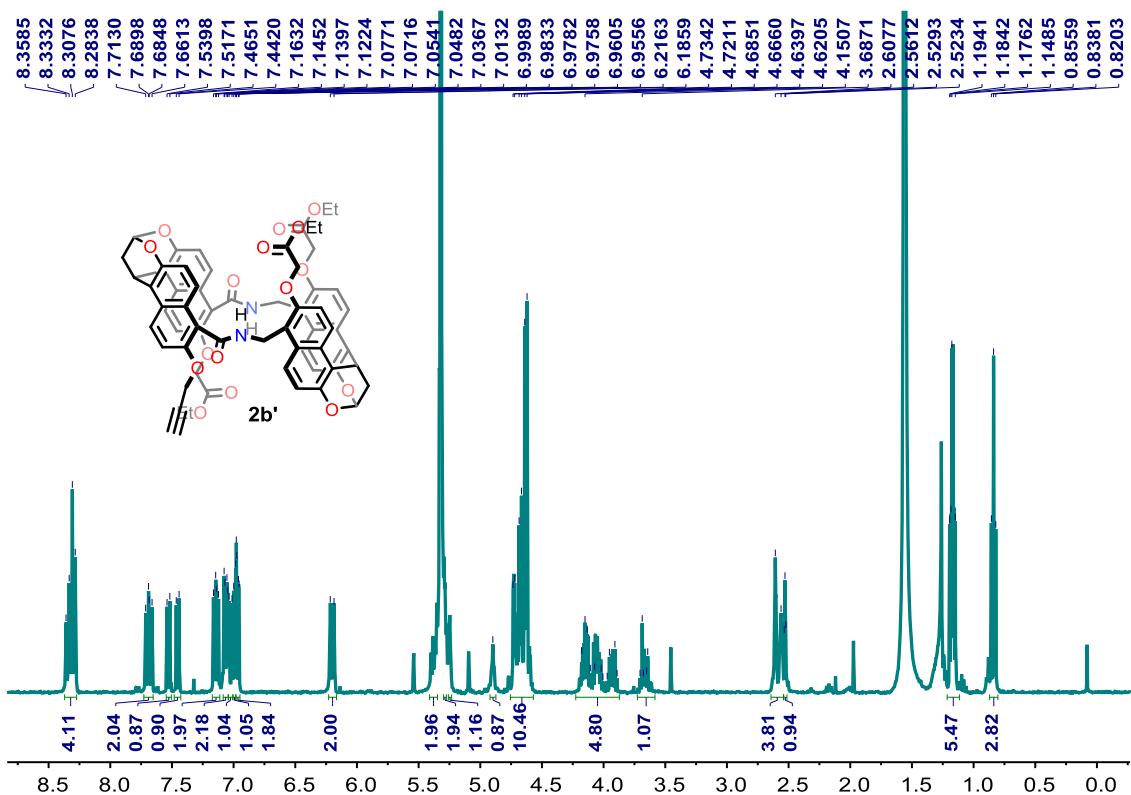


Fig. S26 ^1H NMR spectrum (400 MHz, CD_2Cl_2 , 25 °C) of $\mathbf{2b}'$

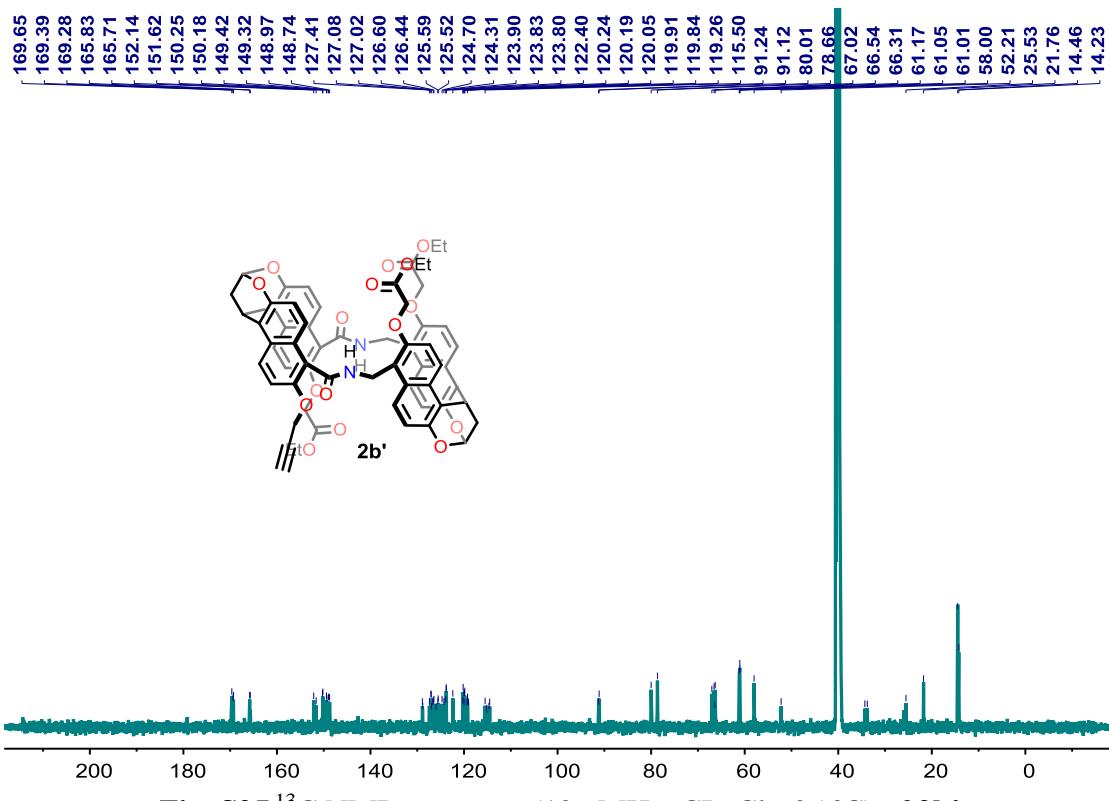


Fig. S27 ^{13}C NMR spectrum (126 MHz, CD_2Cl_2 , 25 °C) of $\mathbf{2b}'$

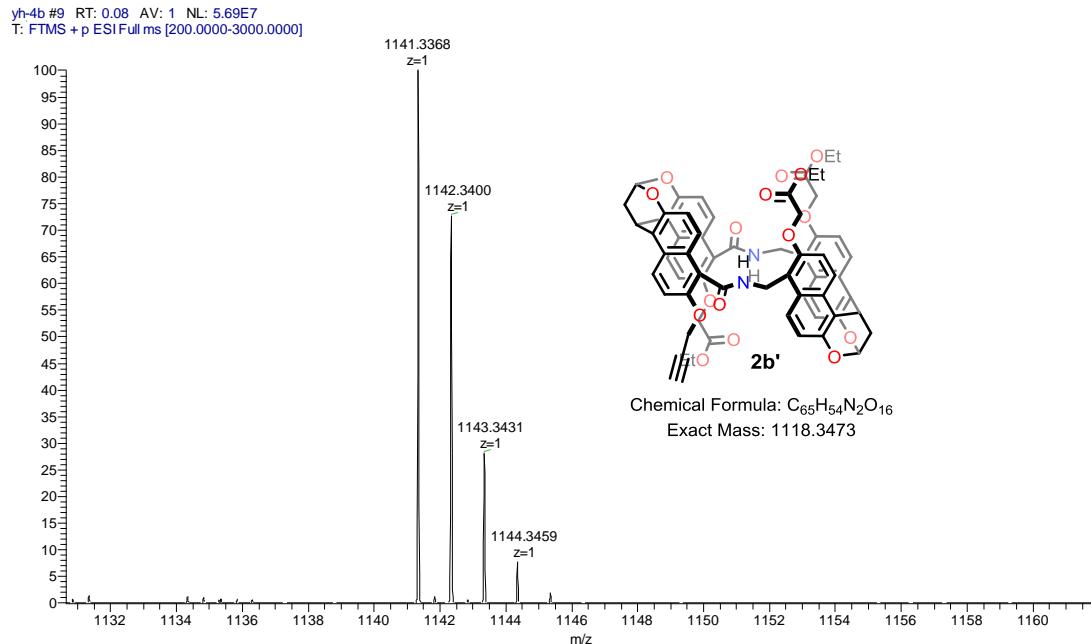


Fig. S28 ESI mass spectrum of $\mathbf{2b}'$

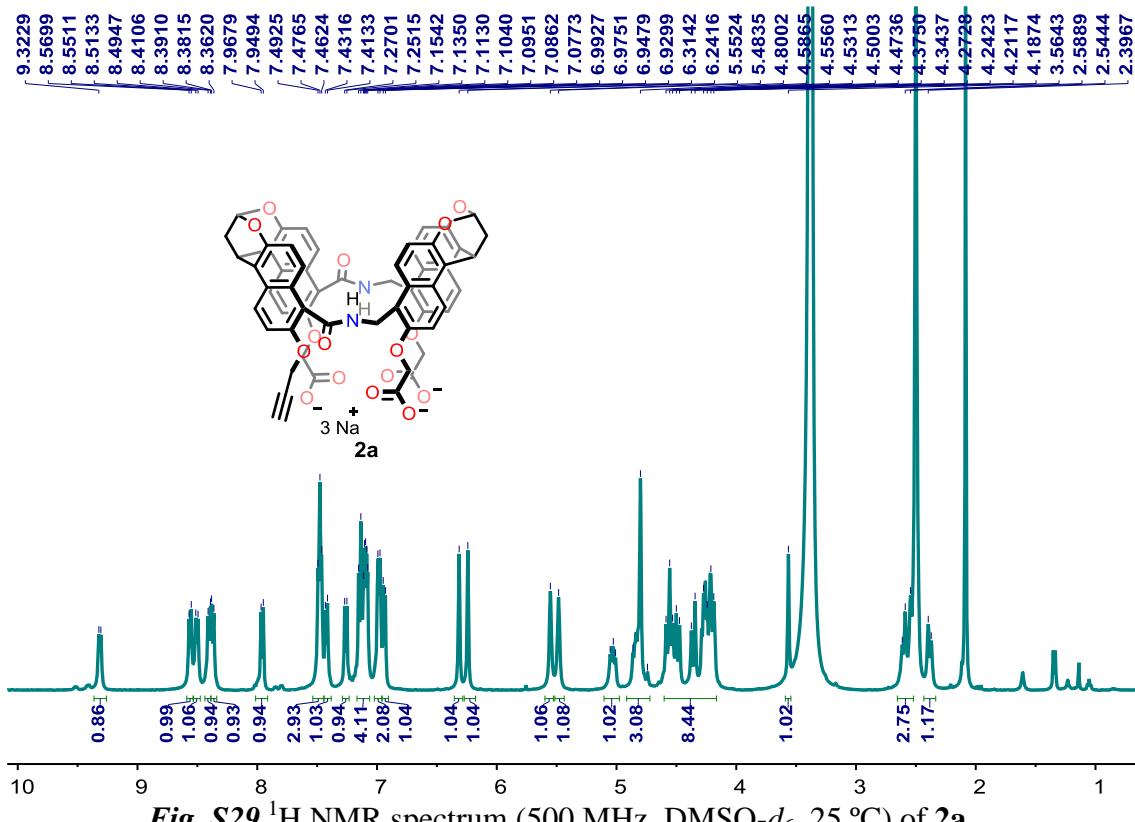


Fig. S29 ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$, 25 °C) of **2a**.

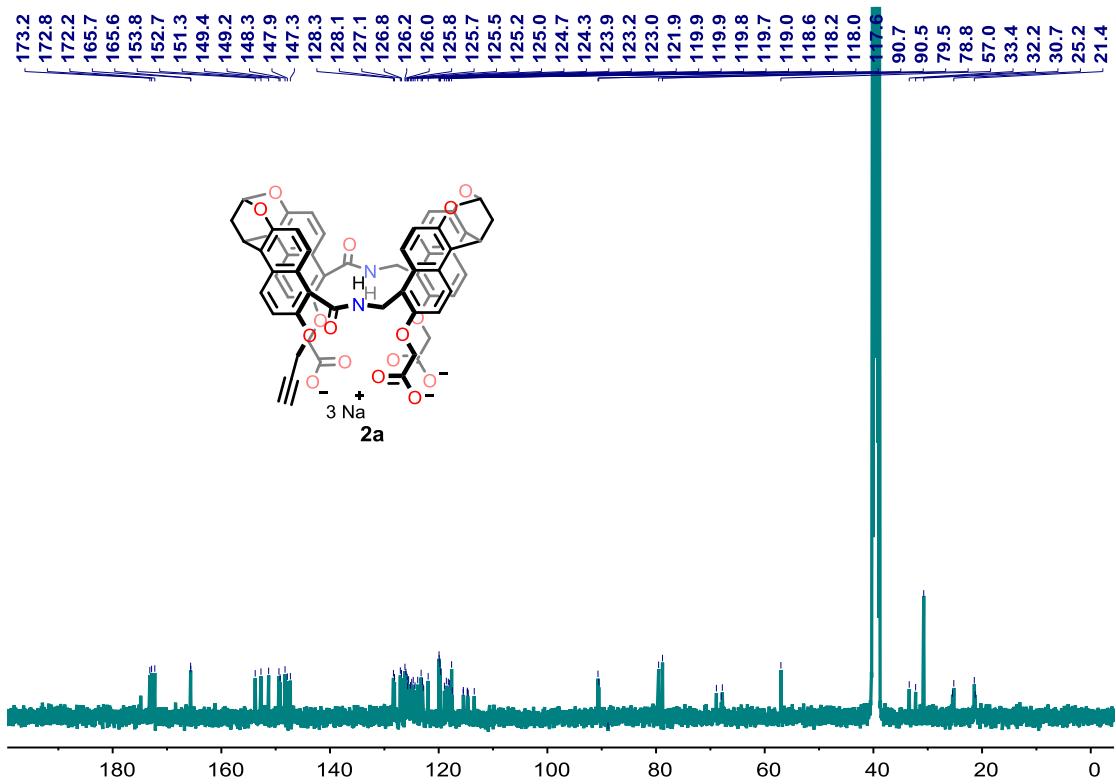


Fig. S30 ^{13}C NMR spectrum (101 MHz, $\text{DMSO}-d_6$, 25 °C) of **2a**.

v4-4ana #10 RT: 0.09 AV: 1 NL: 4.29E8
T: FTMS - p ESI Full ms [100.0000-1500.0000]

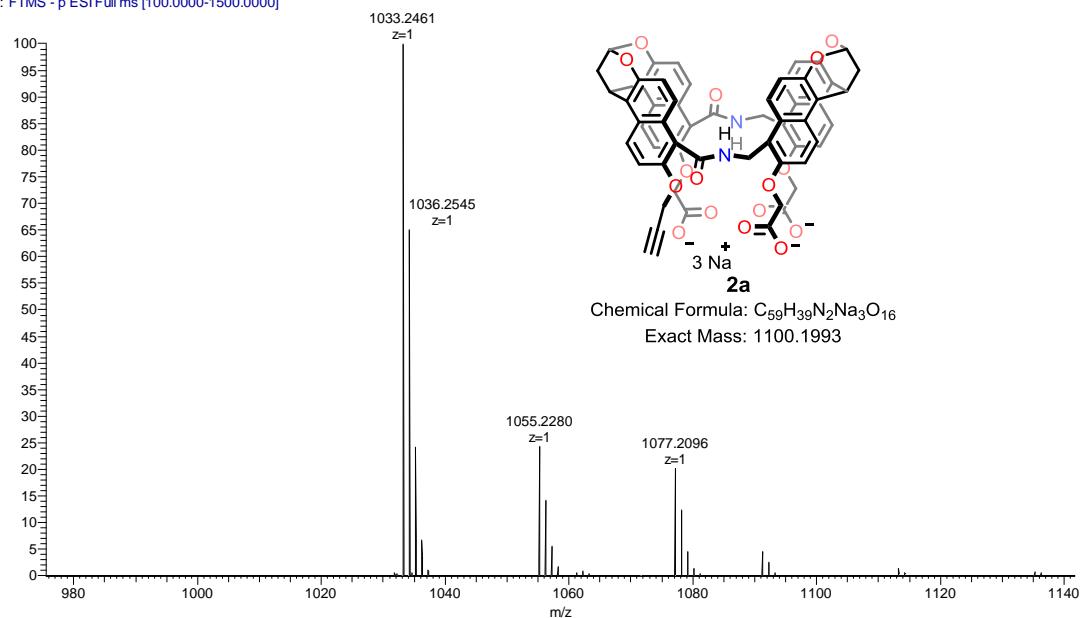


Fig. S31 ESI mass spectrum of **2a**

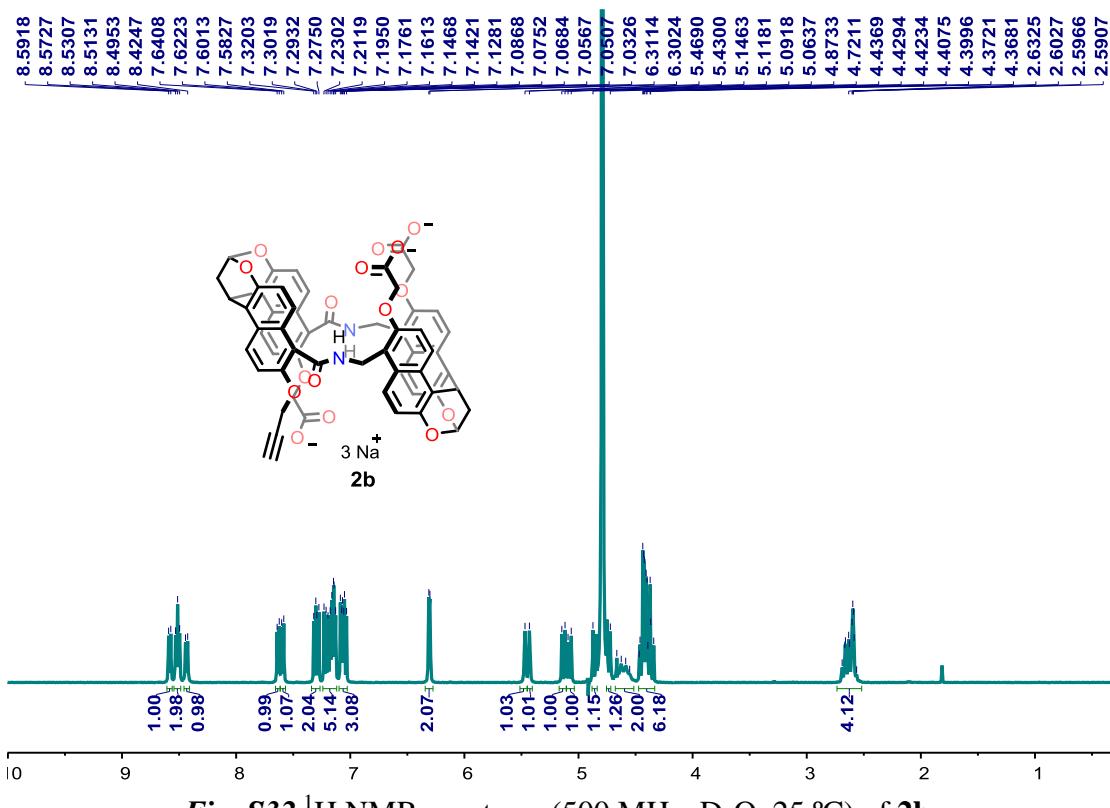


Fig. S32 ^1H NMR spectrum (500 MHz, D_2O , 25 °C) of **2b**.

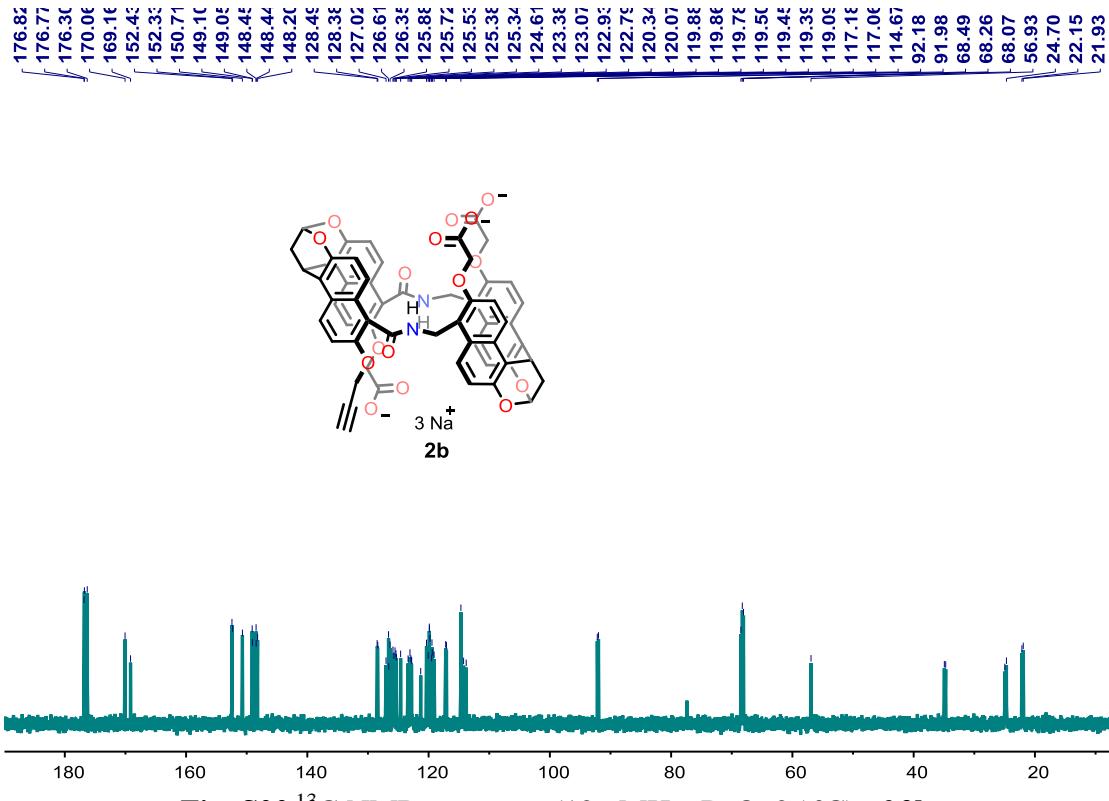


Fig. S33 ^{13}C NMR spectrum (126 MHz, D_2O , 25 °C) of **2b**.

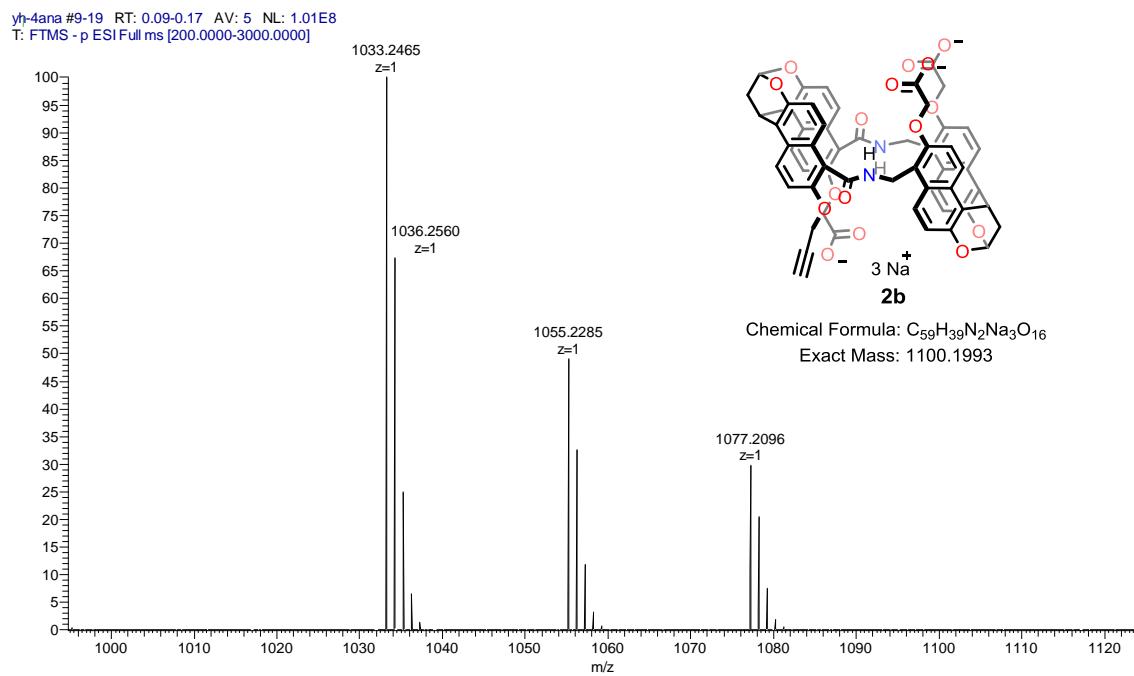


Fig. S34 ESI mass spectrum of **2b**.

2. Assignment Data of the Configurational Isomers of 2

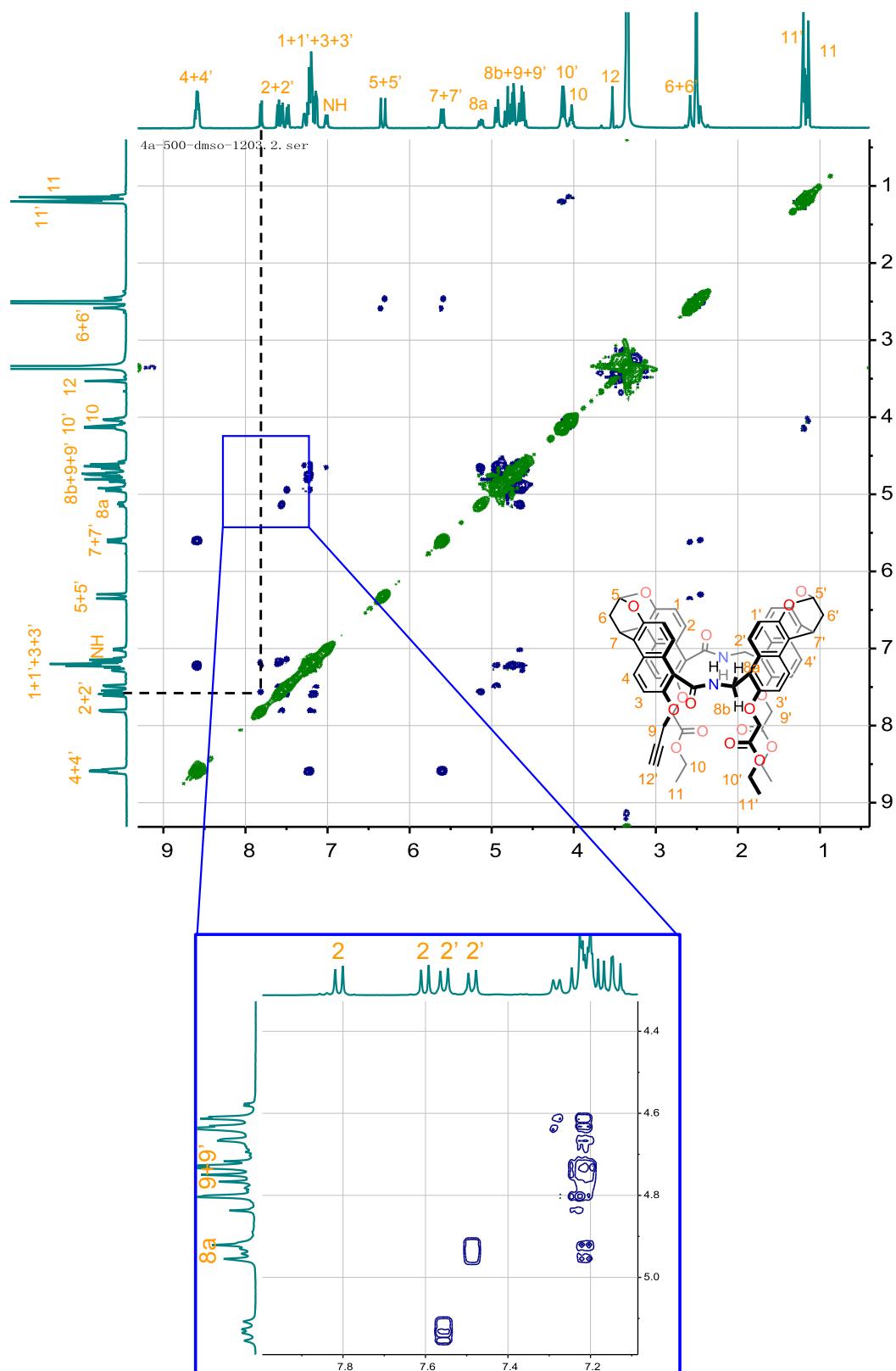


Fig. S35 ^1H , ^1H -ROESY NMR spectrum (500 MHz, DMSO- d_6 , 25 °C) of $\mathbf{2a}'$

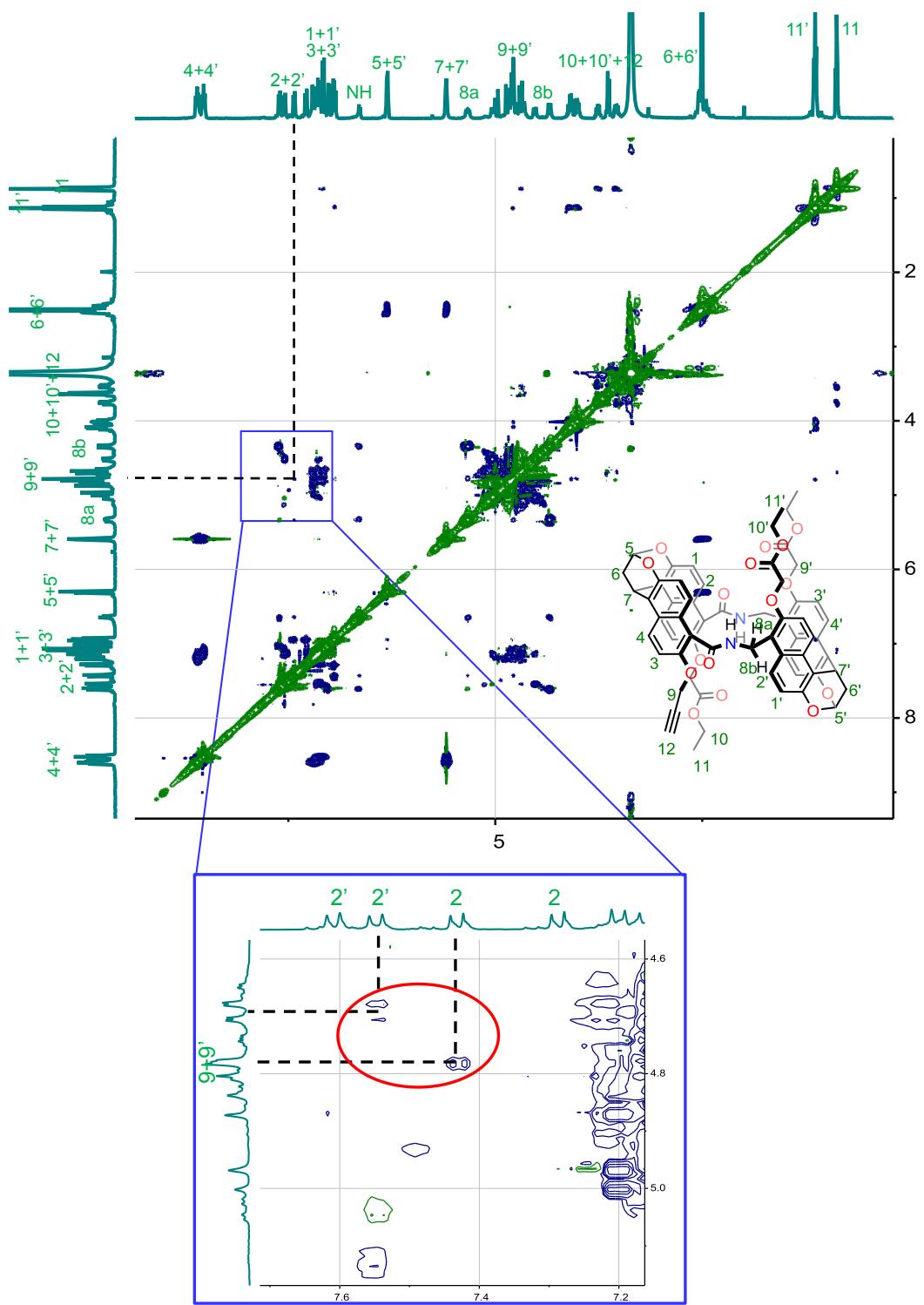


Fig. S36 ^1H , ^1H -ROESY NMR spectrum (500 MHz, $\text{DMSO}-d_6$, 25 °C) of **2b'**

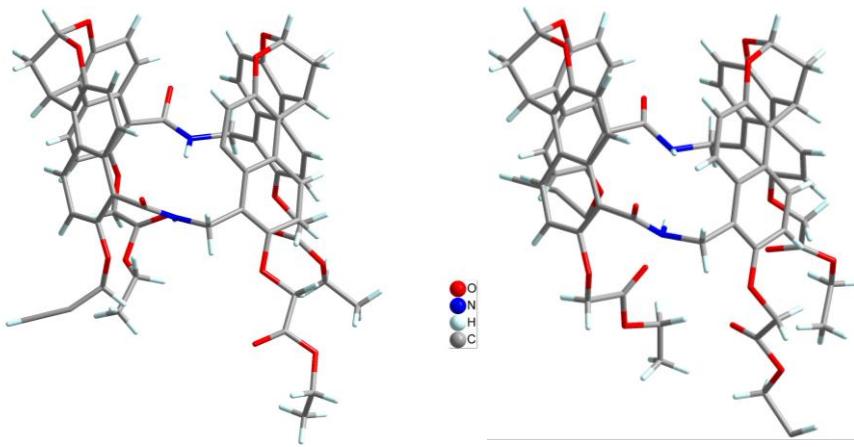


Fig. S37 A pair of enantiomers are both detected in **2a'** crystal structures

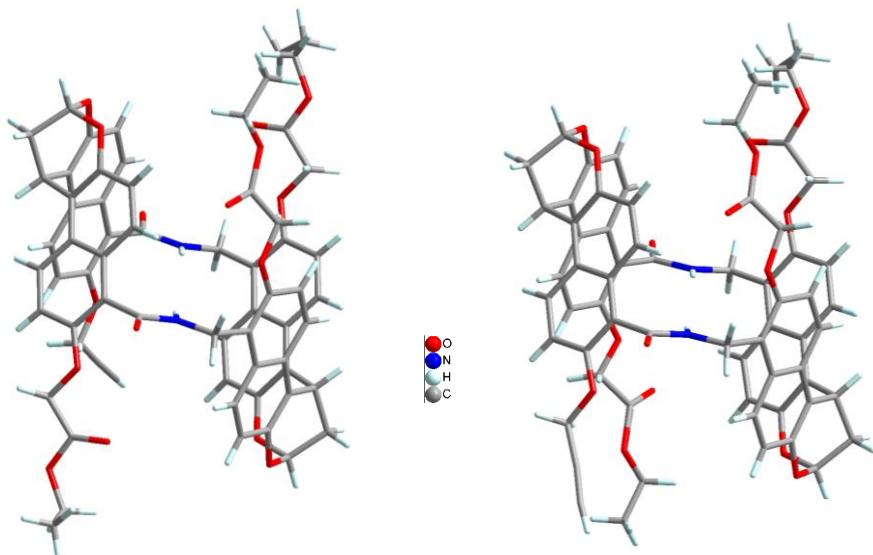


Fig. S38 A pair of enantiomers are both detected in **2b'** crystal structures

3. ITC Titration Data of **2a** and **2b** and Between **1b** and **G4**

All of these ITC titration experiments have been repeated three times, and the average values and standard deviations are given. Errors are smaller than $\pm 20\%$.

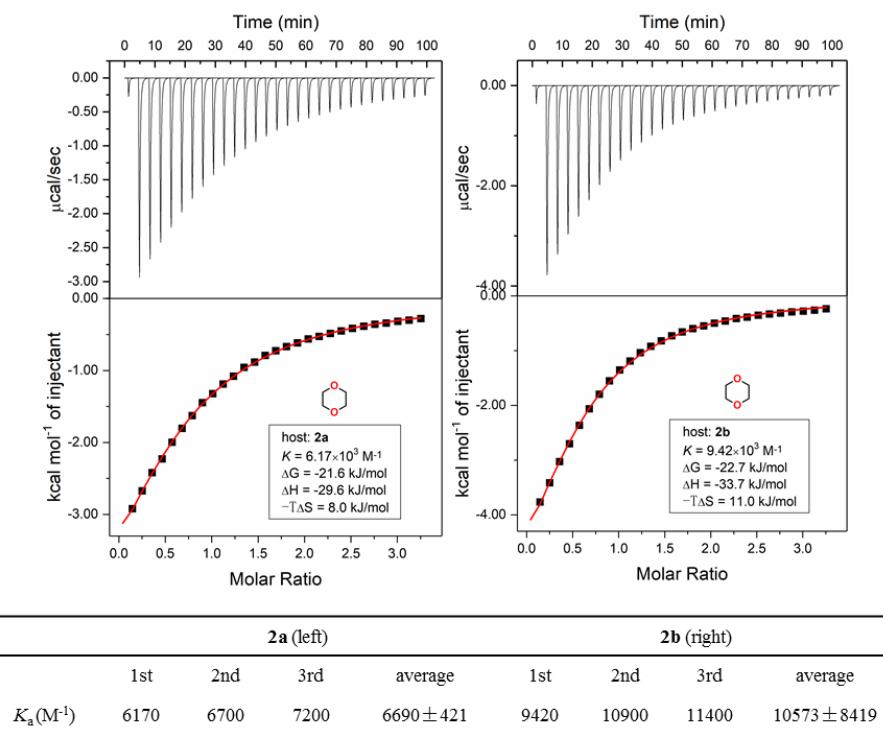


Fig. S39 Titration plots (heat rate versus time and heat versus guest/host ratio) obtained from ITC experiments of **2a** and **2b** with **G1** in H_2O (298 K).

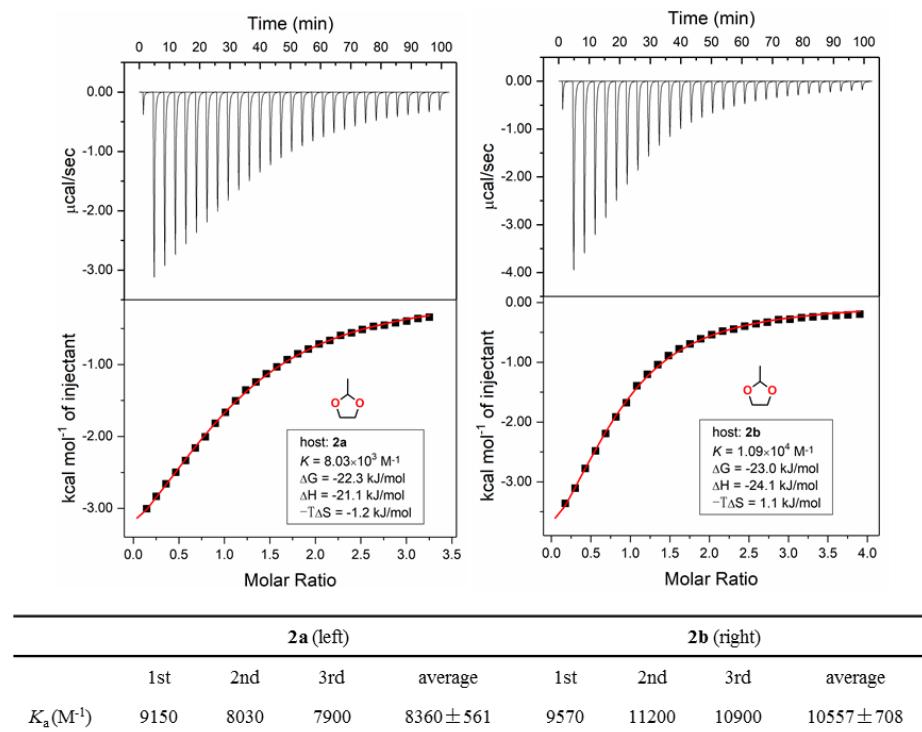


Fig. S40 Titration plots (heat rate versus time and heat versus guest/host ratio)

obtained from ITC experiments of **2a** and **2b** with **G2** in H₂O (298 K).

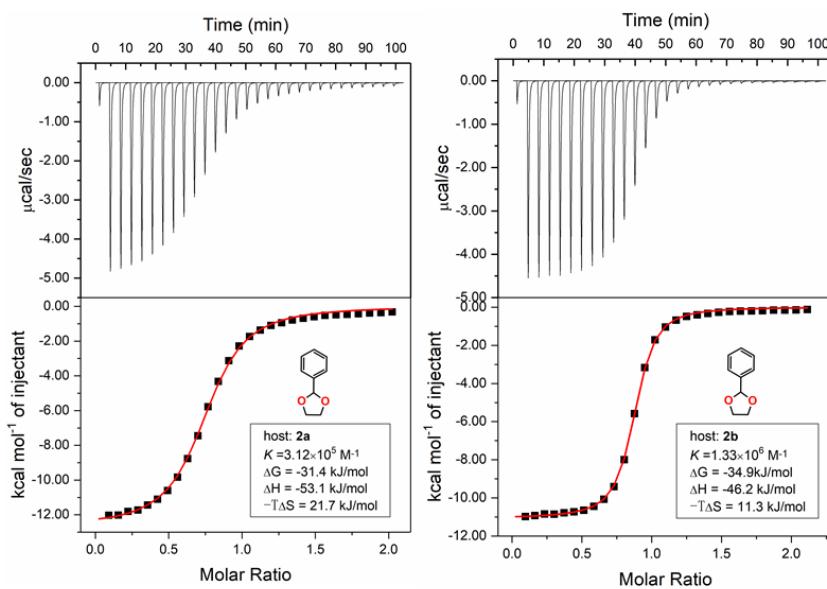


Fig. S41 Titration plots (heat rate versus time and heat versus guest/host ratio) obtained from ITC experiments of **2a** and **2b** with **G3** in H₂O (298 K).

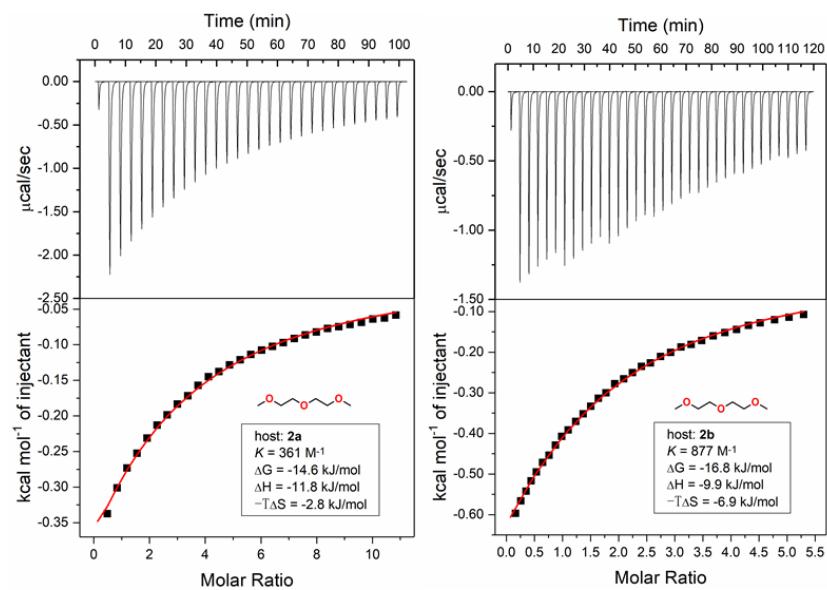


Fig. S42 Titration plots (heat rate versus time and heat versus guest/host ratio) obtained from ITC experiments of **2a** and **2b** with **G4** in H₂O (298 K).

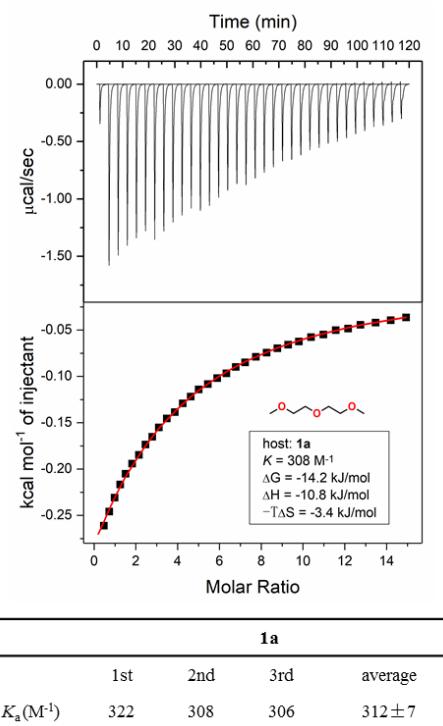


Fig. S43 Titration plots (heat rate versus time and heat versus guest/host ratio) obtained from ITC experiments of **1a** with **G4** in H₂O (298 K).

4. Supporting Data for the New Assignments of **1a** and **1b**

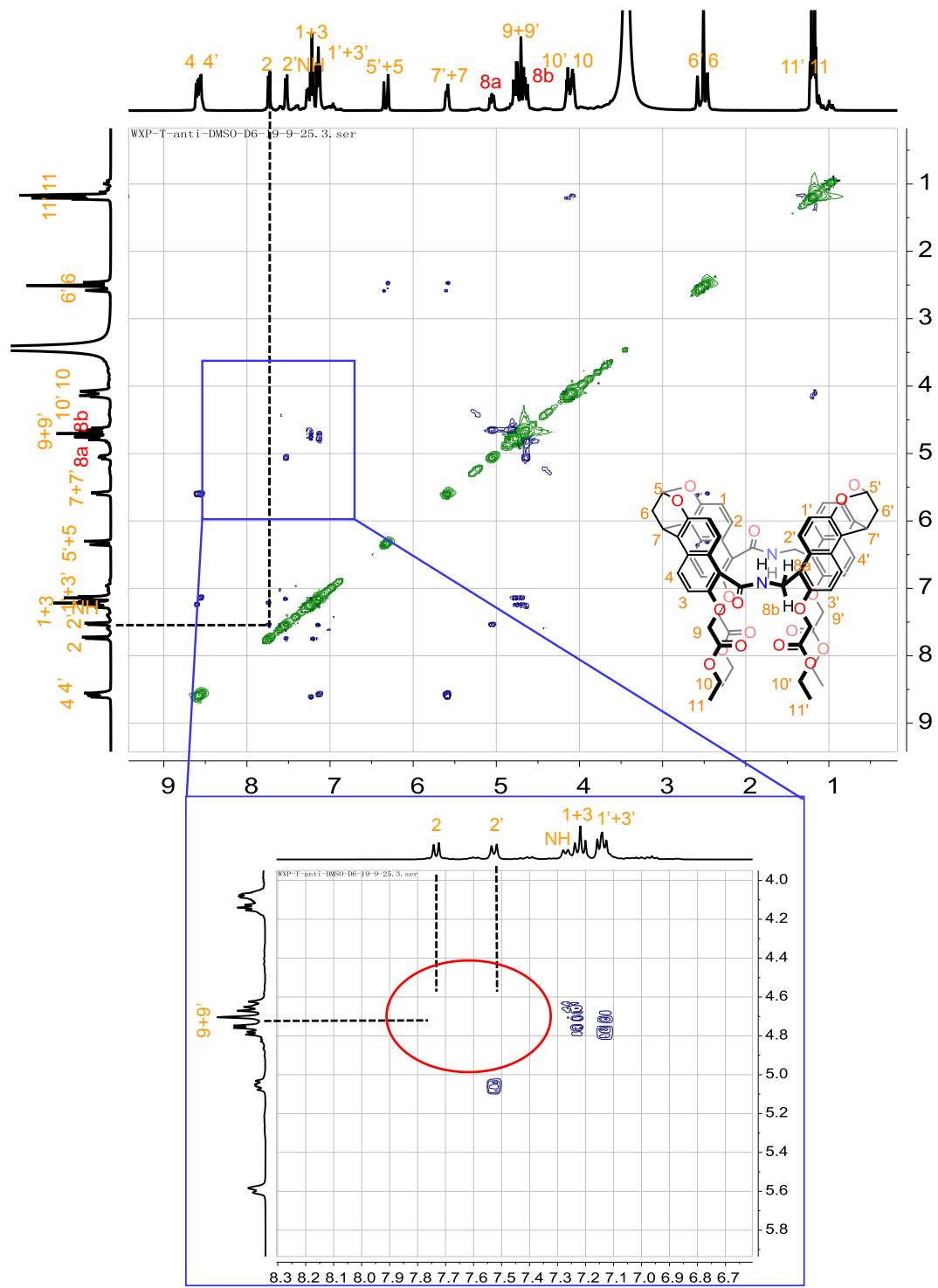


Fig. S44 ¹H-¹H-ROESY NMR spectrum (500 MHz, DMSO-*d*₆, 25 °C) of **1a''**

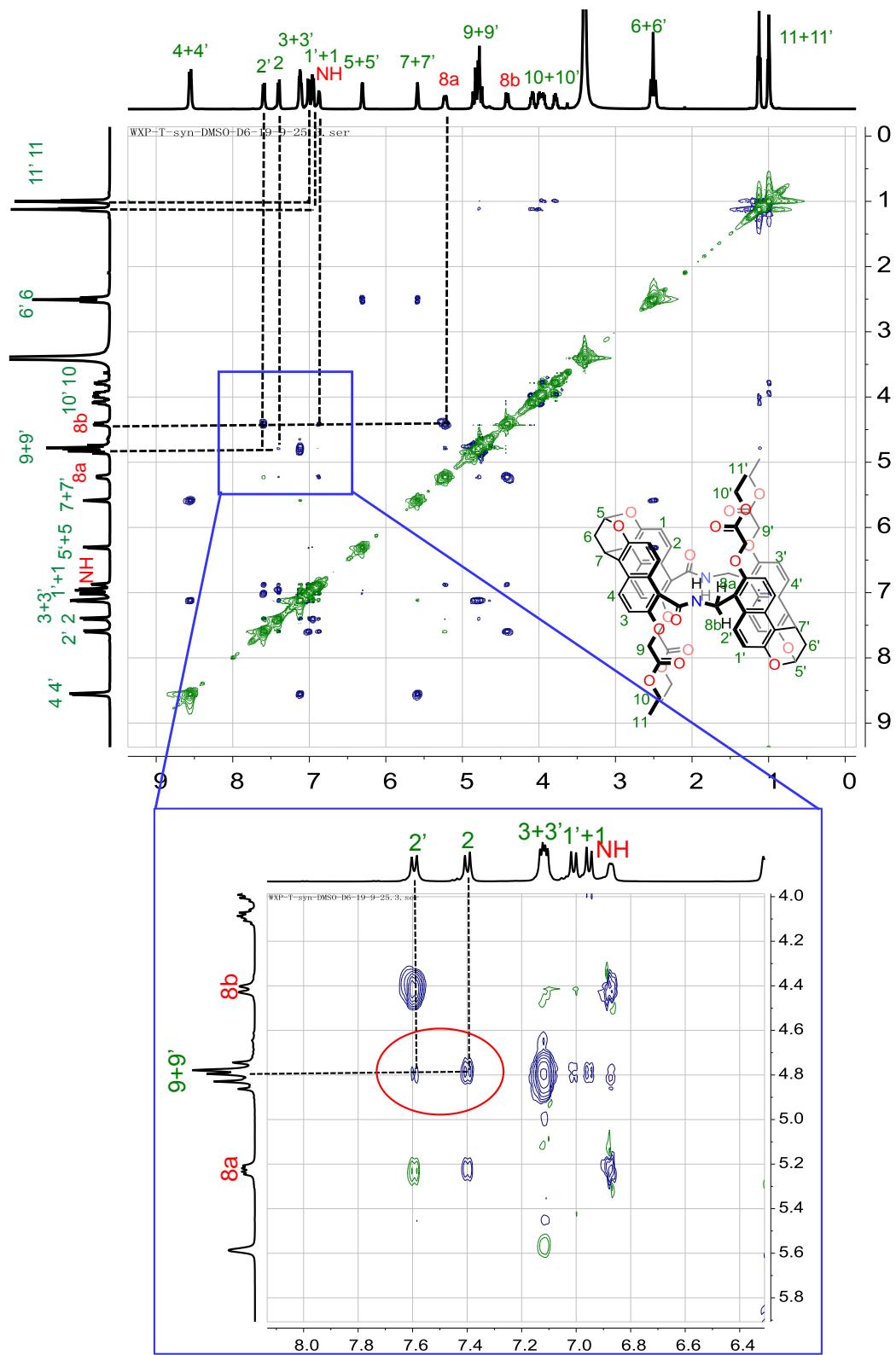


Fig. S45 ^1H , ^1H -ROESY NMR spectrum (500 MHz, $\text{DMSO}-d_6$, 25 °C) of $\mathbf{1b}''$.

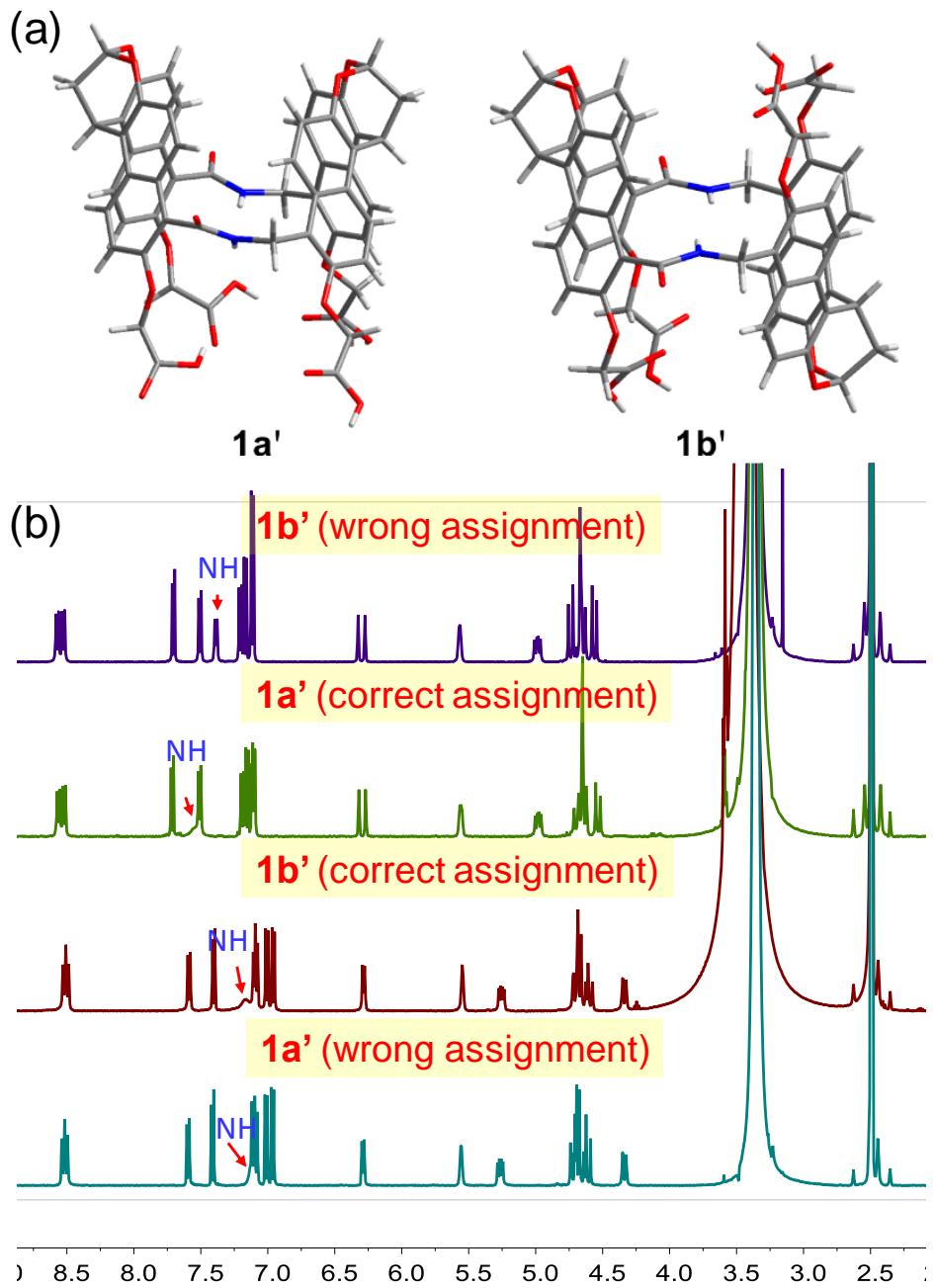


Fig. S46 (a) X-ray single crystal structures of **1a'** and **1b'**. (b) Comparison between the ^1H NMR spectra (500 MHz, $\text{DMSO}-d_6$, 25 °C) of **1a'** and **1b'** (correct assignments, the samples were collected from the crystals for X-ray crystallography) and the ^1H NMR spectra of the samples previously assigned to **1a'** and **1b'** by us in 2016.¹ The crystal structures and ^1H NMR spectra show that our earlier assignments are wrong. The two samples originally thought to be **1a** and **1b** should be **1b** and **1a**, respectively.

5. Supporting Data for the Consistent Assignments of **1a** and **1b**

In the following six publications,^{2,3,4,5,6,7} we followed the assignments made in our first related publication.¹ In order to confirm our assignments are consistent, we selected typical guests (having very different binding affinities to the two configurational isomers, enabling the differentiation of the two isomers from binding constants) from each of the previously publications and one from the Glass's publication (Scheme 1), and re-determined the binding constants. The used titrations methods and the fitting equations are all consistent with the earlier publications. The results show our assignments in the seven related publications^{1,2,3,4,5,6,7} are consistent.

Scheme S1. Chemical structures of the selected typical guests.

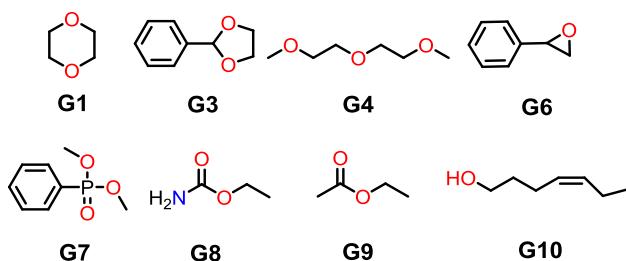


Table S1. Previously reported (in blue) and newly determined (in red) binding constants K_a (M^{-1}) of **1a** and **1b** with guests **G1**, **G3** and **G6** in water at 25 °C as determined by ITC titrations.

	G1 ¹	G3 ²	G6 ⁴
1a ^a	3.0×10^3	4.6×10^5	1.3×10^4
1a ^b	4.0×10^3	4.5×10^5	1.5×10^4
1b ^a	1.0×10^4	1.4×10^6	4.1×10^4
1b ^b	1.3×10^4	1.5×10^6	3.9×10^4

^a the data was retrieved from earlier publications;^{1,2,4} ^b the data were newly determined in the present research.

Table S2. Previously reported (in blue) and newly determined (in red) binding constants K_a (M^{-1}) of **1a** and **1b** with guests **G4**, **G7** and **G8** in water at 25 °C as determined by NMR titrations.

	G4 ³	G7 ⁷	G8 ⁶
1a ^a	406	3800	1210
1a ^b	340	3300	1180
1b ^a	3090	15000	1750
1b ^b	2940	14600	1640

^a the data was retrieved from earlier publications;^{3,6,7} ^b the data were newly determined in the present research.

Table S3. Previously reported (in blue) and newly determined (in red) binding constants K_a (M^{-1}) of **1a** and **1b** with guests **G9** and **G10** in water at 25 °C as determined by fluorescence titrations.

Guests	1a ^a		1b ^a		1a ^b		1b ^b	
	K_a (M^{-1})	I_{sat}/I_o						
G9 ⁵	2300	4.6	3600	3.7	2220	4.5	3220	3.0
G10 ⁸	1200	1.3	5200	0.58	2260	1.4	4920	0.53

^a the data was retrieved from earlier publications;^{5,8} ^b the data were newly determined in the present research.

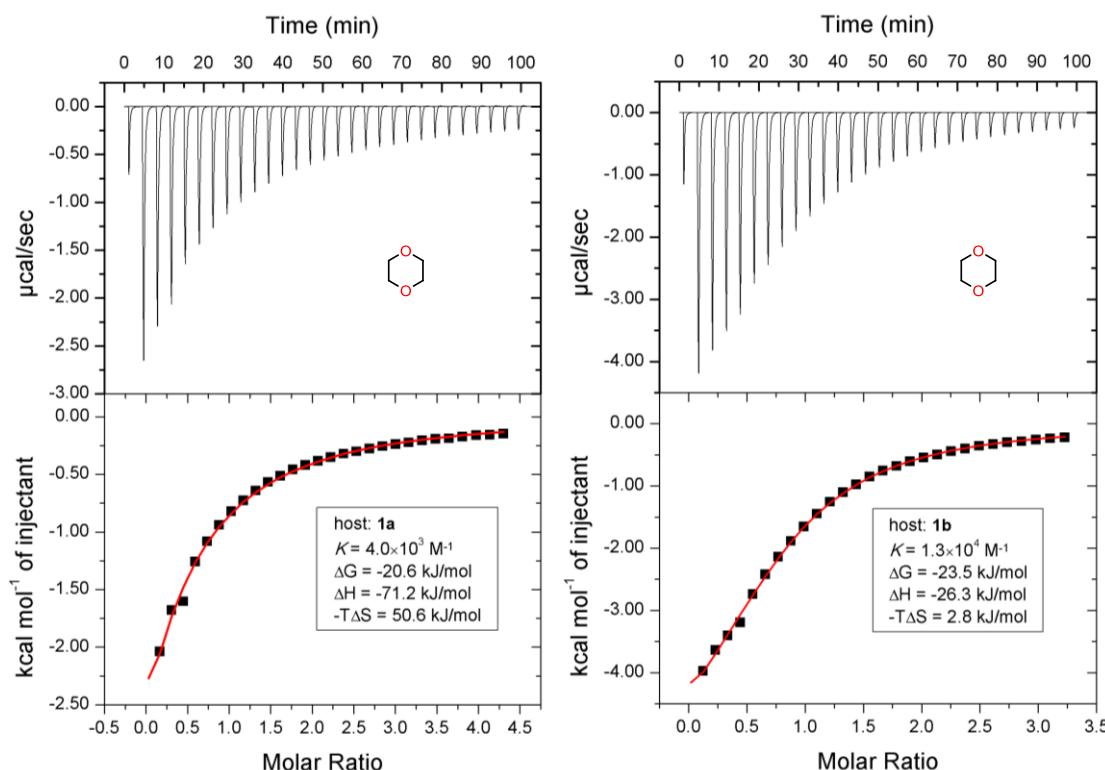


Fig. S47 Titration plots (heat rate versus time and heat versus guest/host ratio) obtained from ITC experiments of **1a** and **1b** with **G1** in H_2O (298 K).

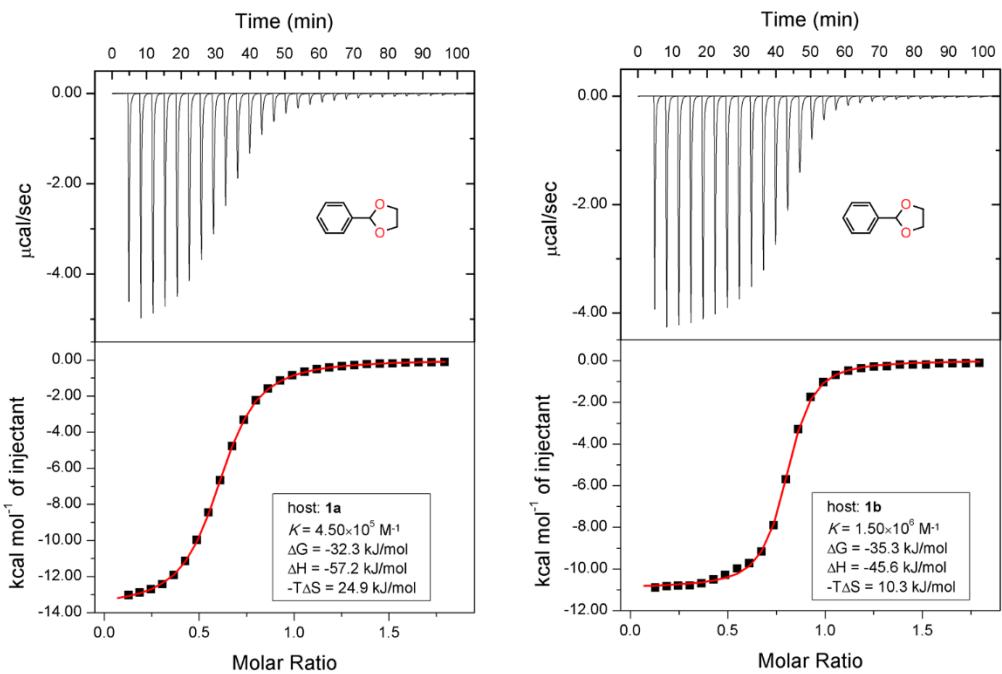


Fig. S48 Titration plots (heat rate versus time and heat versus guest/host ratio) obtained from ITC experiments of **1a** and **1b** with **G3** in H₂O (298 K).

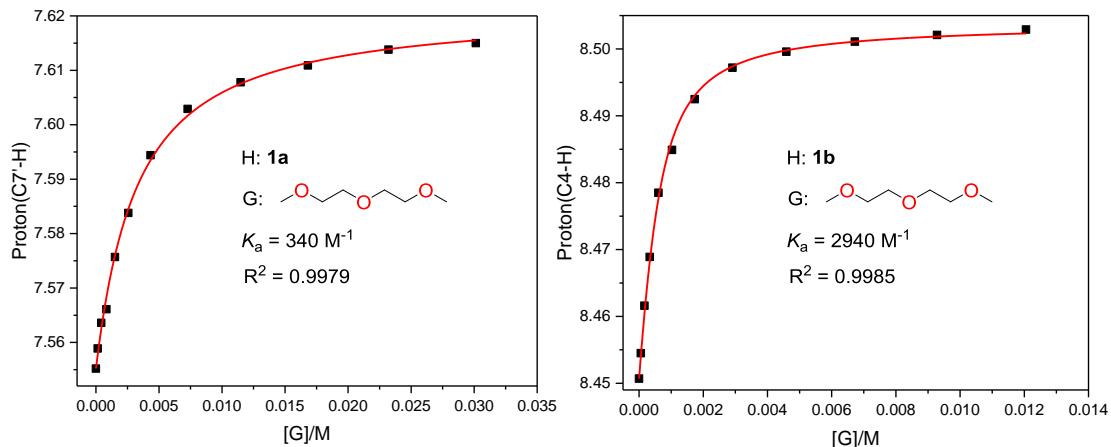


Fig. S49 Non-linear curve-fitting for the complexation of **1a** and **1b** with **G4** in D₂O at 298 K based on ¹H NMR titrations.

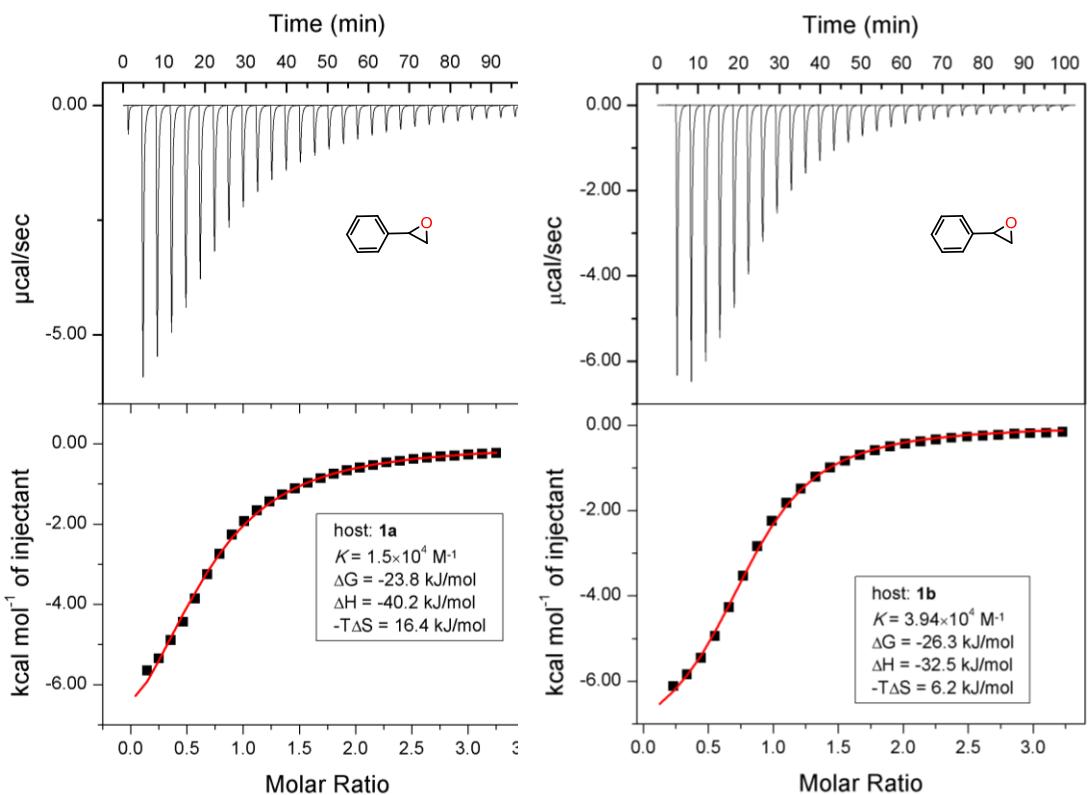


Fig. S50 Titration plots (heat rate versus time and heat versus guest/host ratio) obtained from ITC experiments of **1a** and **1b** with **G6** in H_2O (298 K).

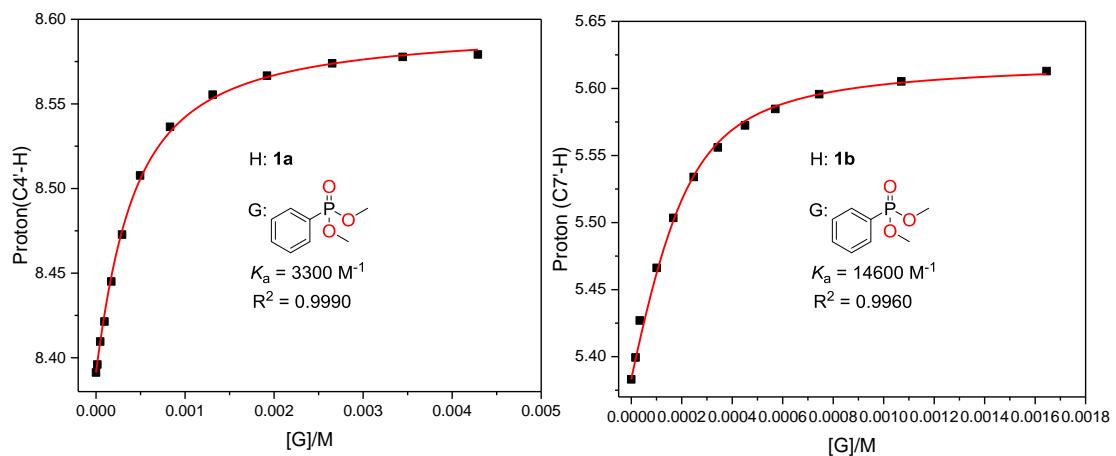


Fig. S51 Non-linear curve-fitting for the complexation of **1a** and **1b** with **G7** in D_2O at 298 K based on ^1H NMR titrations.

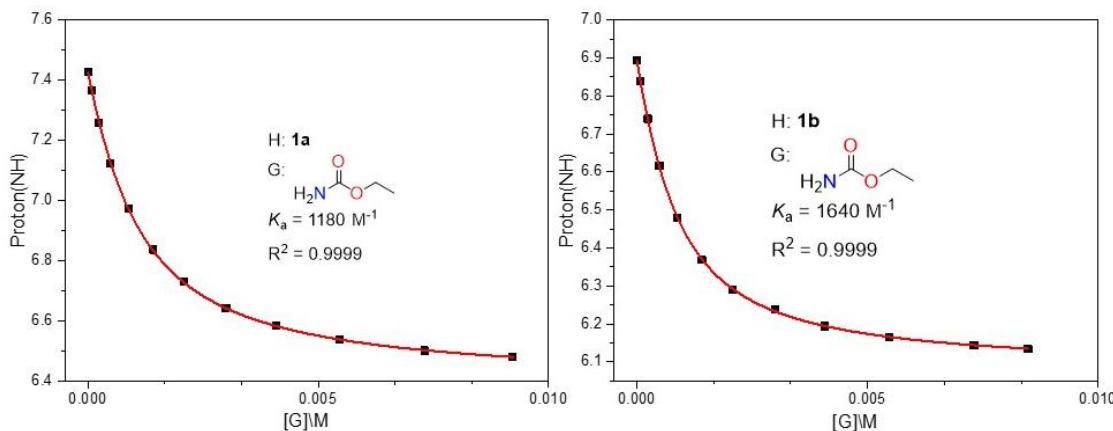


Fig. S52 Non-linear curve-fitting for the complexation of **1a** and **1b** with **G8** in D₂O at 298 K based on ¹H NMR titrations.

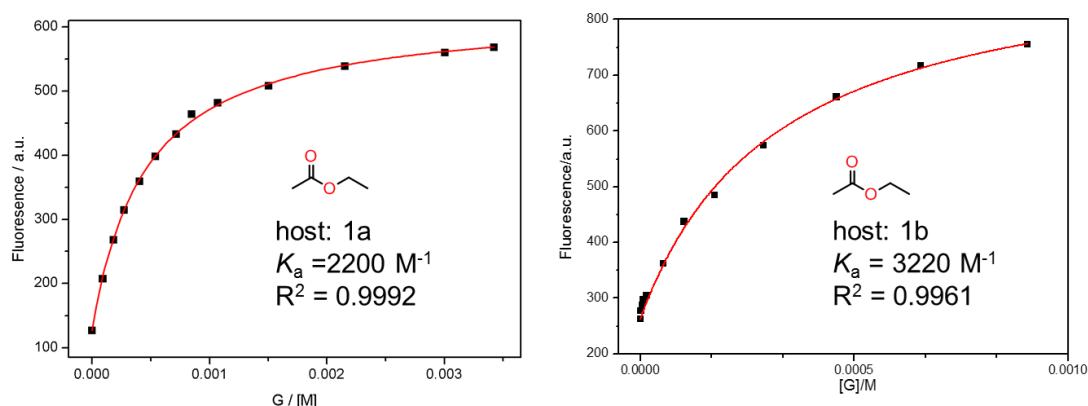


Fig. S53 Fluorescence titration of compound **1a** and **1b** with **G9** in water ($[G] = 100$ mM; $[1a] = 3.33 \times 10^{-6}$ M; $\lambda_{ex} = 330$ nm; $[G] = 5$ mM; $[1b] = 1 \times 10^{-5}$ M; $\lambda_{ex} = 330$ nm). Non-linear fitting of the titration data at $\lambda_{em} = 403$ nm according to a single-site binding isotherm.

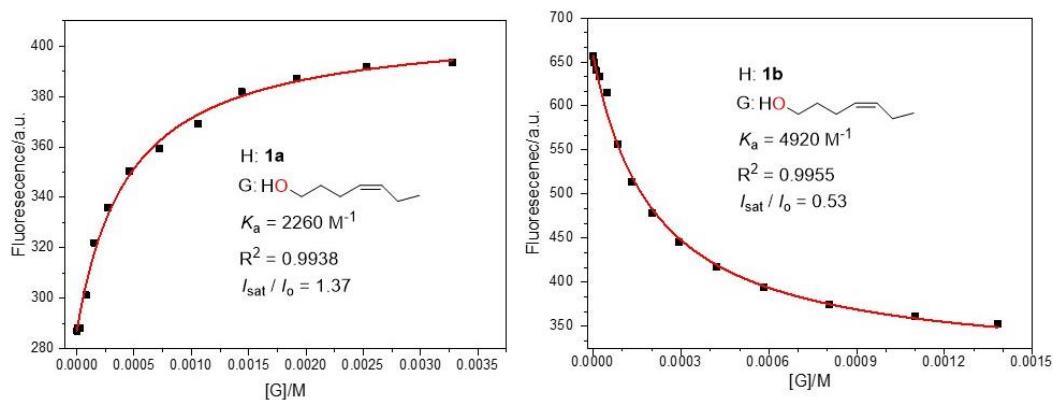


Fig. S54 Fluorescence titration of compound **1a** and **1b** with **G10** in buffer (20 mM HEPES; pH = 8.4 ($[G]$ = 5 mM; $[1b]$ = 1×10^{-5} M; λ_{ex} = 365 nm). Non-linear fitting of the titration data at λ_{em} = 396 nm according to a single-site binding isotherm.

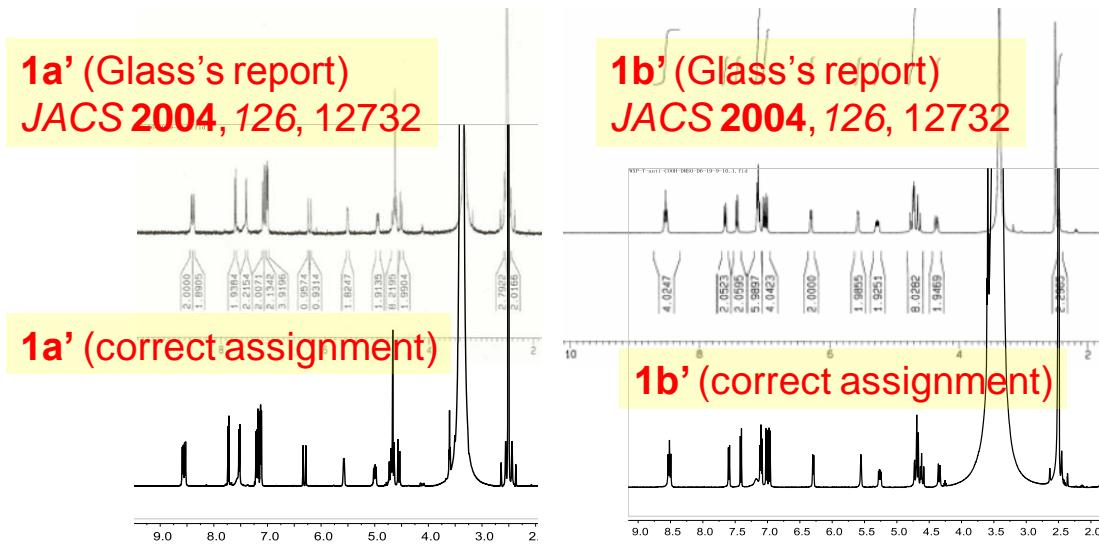
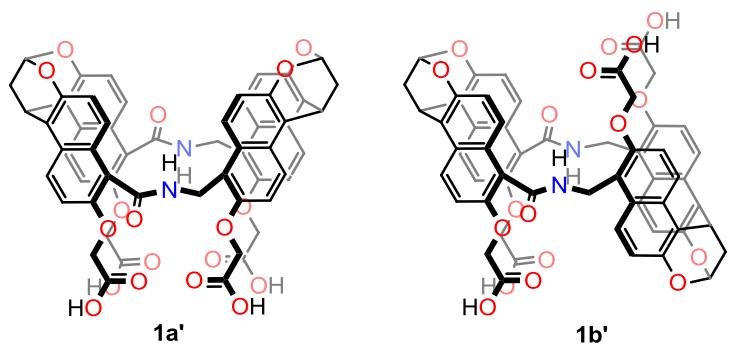


Fig. S55 Comparison between ^1H NMR spectra ($\text{DMSO}-d_6$) of **1a'** and **1b'** (correct assignments based on X-ray Crystallography in **Fig. S46**) and ^1H NMR spectra of **1a'** and **1b'** reported by Glass and coworkers in 2004.⁸ This clearly indicates that Glass's assignments of the structures **1a'** and **1b'** are correct.

6. ^1H NMR Spectra of **1a''** and **1b''**

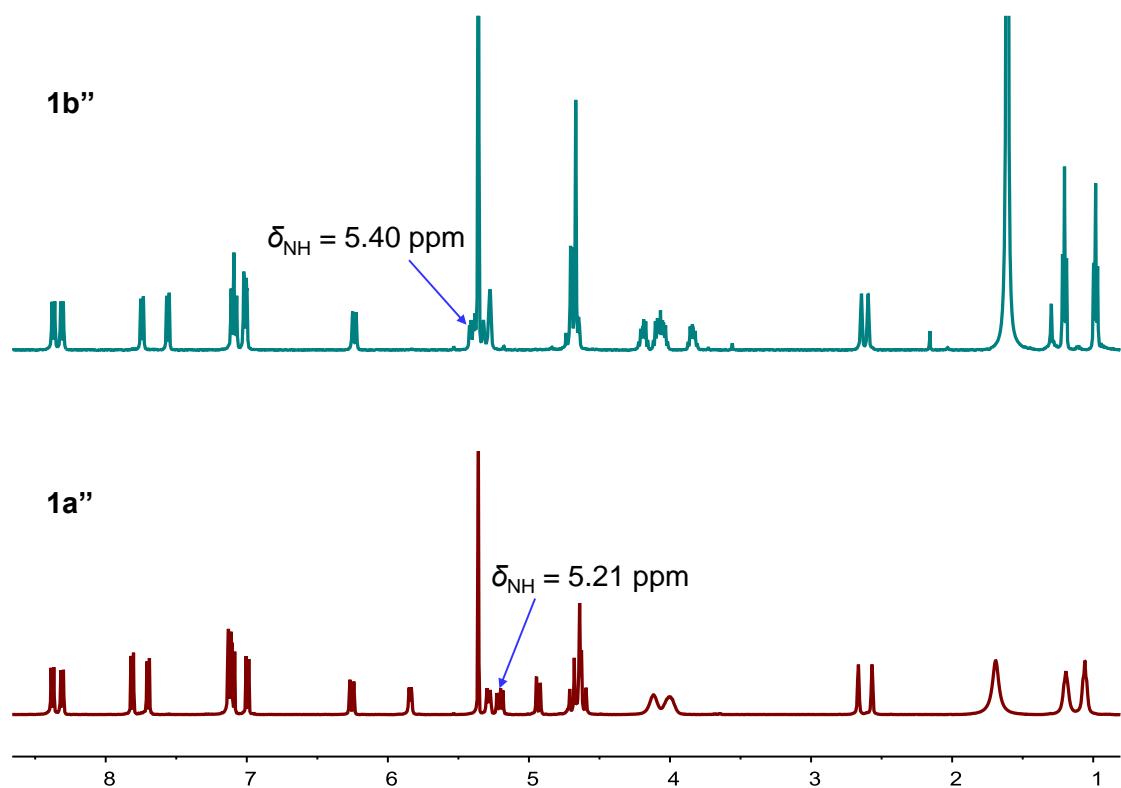


Fig. S56 ^1H NMR spectra (500 MHz, CD_2Cl_2 , 25 °C) of **1a''** and **1b''**

7. X-Ray Crystallography

Single crystals of **1a'** and **1b'** were obtained by slow evaporation of 3:1:1 THF-MeCN-C₂H₅OH solution and 4:1 THF-H₂O solution, respectively. Single crystals of **2a'** and **2b'** were obtained by slow evaporation of 4:1 DCM-MeOH solution. The reflections were collected on a Bruker D8 VENTURE with Cu K α radiation ($\lambda = 1.54178 \text{ \AA}$) at 100(1) K. The structures were solved by intrinsic phasing methods (SHELXT⁹) and refined by full-matrix least squares on F² using SHELXL¹⁰ in the OLEX2 program package.¹¹ All non-hydrogen atoms were refined with anisotropic thermal parameters and the hydrogen atoms were fixed at calculated positions and refined by a riding mode. SQUEEZE routine implemented on PLATON was used to remove electron densities corresponding to disordered solvent molecules in the crystal data.

Crystal data for THF@**1a'**•2C₂H₅OH•CH₃CN: CCDC: 1956259. C₆₈H₆₅N₃O₂₁, $M = 1260.23 \text{ g/mol}$, monoclinic, space group *P*2₁/n (no. 14), $a = 18.6966(10) \text{ \AA}$, $b = 19.0196(10) \text{ \AA}$, $c = 18.8502(10) \text{ \AA}$, $\beta = 111.438(3)$, $V = 6239.4(6) \text{ \AA}^3$, $Z = 4$, $T = 100.03 \text{ K}$, $\mu(\text{CuK}\alpha) = 0.837 \text{ mm}^{-1}$, $D_{\text{calc}} = 1.342 \text{ g/cm}^3$, 76181 reflections measured ($5.698^\circ \leq 2\theta \leq 119.496^\circ$), 9043 unique ($R_{\text{int}} = 0.0597$, $R_{\text{sigma}} = 0.0298$) which were used in all calculations. The final R_1 was 0.0715 ($I > 2\sigma(I)$) and wR_2 was 0.2028 (all data).

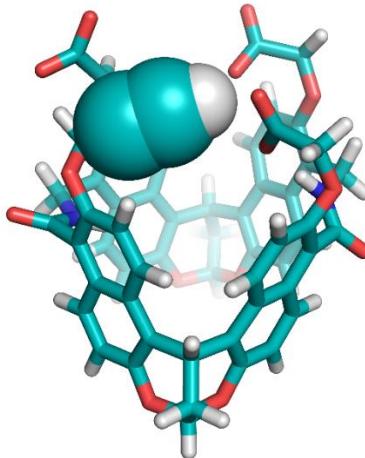
Crystal data for THF@**1b'**•2H₂O•2THF: CCDC: 1956258. C₇₀H₇₀N₂O₂₃, $M = 1307.28 \text{ g/mol}$, triclinic, space group P-1 (no. 2), $a = 13.2399(5) \text{ \AA}$, $b = 15.4494(6) \text{ \AA}$, $c = 15.6625(6) \text{ \AA}$, $\alpha = 80.635(2)$, $\beta = 85.048(2)$, $\gamma = 74.885(2)$, $V = 3048.4(2) \text{ \AA}^3$, $Z = 2$, $T = 99.98 \text{ K}$, $\mu(\text{CuK}\alpha) = 0.897 \text{ mm}^{-1}$, $D_{\text{calc}} = 1.424 \text{ g/cm}^3$, 39128 reflections measured ($5.724^\circ \leq 2\theta \leq 118.458^\circ$), 8755 unique ($R_{\text{int}} = 0.0333$, $R_{\text{sigma}} = 0.0270$) which were used in all calculations. The final R_1 was 0.0591 ($I > 2\sigma(I)$) and wR_2 was 0.1787 (all data).

Crystal Data for **2a'**•0.5 CH₂Cl₂: CCDC: 1966659. C_{65.5}H_{55.5}ClN₂O₁₆ ($M = 1162.07 \text{ g/mol}$): monoclinic, space group P2₁ (no. 4), $a = 15.4706(3) \text{ \AA}$, $b = 42.3400(9) \text{ \AA}$, $c =$

$19.1101(4)$ Å, $\beta = 105.1060(10)^\circ$, $V = 12085.1(4)$ Å³, $Z = 8$, $T = 100.0$ K, $\mu(\text{CuK}\alpha) = 1.150$ mm⁻¹, $D_{\text{calc}} = 1.277$ g/cm³, 84603 reflections measured ($4.174^\circ \leq 2\Theta \leq 117.872^\circ$), 32548 unique ($R_{\text{int}} = 0.0587$, $R_{\text{sigma}} = 0.0730$) which were used in all calculations. The final R_1 was 0.1065 ($I > 2\sigma(I)$) and wR_2 was 0.3249 (all data).

Crystal Data for **2b'**: CCDC:1966658. C_{65.5}H₅₂N₂O_{16.5}, $M = 1131.10$ g/mol, triclinic, space group P-1 (no. 2), $a = 9.7417(4)$ Å, $b = 11.8403(5)$ Å, $c = 11.9923(5)$ Å, $\alpha = 96.716(3)^\circ$, $\beta = 99.839(3)^\circ$, $\gamma = 94.798(3)^\circ$, $V = 1345.94(10)$ Å³, $Z = 1$, $T = 100.01$ K, $\mu(\text{CuK}\alpha) = 0.846$ mm⁻¹, $D_{\text{calc}} = 1.400$ g/cm³, 9001 reflections measured ($7.55^\circ \leq 2\Theta \leq 118.082^\circ$), 3832 unique ($R_{\text{int}} = 0.0297$, $R_{\text{sigma}} = 0.0354$) which were used in all calculations. The final R_1 was 0.0848 ($I > 2\sigma(I)$) and wR_2 was 0.2558 (all data).

8. Computational Data



Optimized geometry of **2a**

There is no imaginary frequency after optimization and frequency analysis.

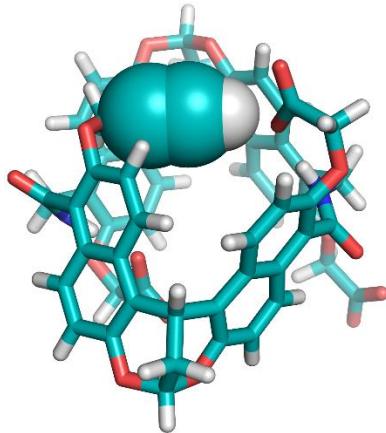
ZPVE Corrected Energy (a.u.) = -3583.296405.

Free Energy (298 K, a.u.) = -3583.388933.

Enthalpies (298 K, a.u.) = -3583.236779.

O	6.28514300	41.39479000	18.20111700	C	9.63826100	32.81142100	17.78532400
O	6.98044300	41.83126900	16.04874200	C	8.63671600	34.05816900	19.68823500
O	10.01023200	38.85408300	10.93754500	C	9.71485700	37.49687700	20.30595000
O	14.29636500	39.97684300	14.33206900	C	10.46128500	34.28902000	12.12471000
N	11.48693900	38.40319500	12.61626300	H	11.14091100	33.45252600	12.00747500
H	11.91395400	37.65199600	13.17888600	C	8.86345600	38.53181600	19.81754800
O	4.64070000	35.81048900	13.25041400	C	12.10148900	39.71879200	12.66085900
O	12.16088700	35.87217100	11.41221900	H	11.60457900	40.33535300	11.90814400
O	11.83950500	36.55318400	20.56730600	H	13.15348800	39.63518200	12.37950000
O	10.71832300	32.48583700	18.56583600	C	13.24279700	36.56678500	20.32925000
O	4.08459500	34.61511200	15.13182800	H	13.70153900	37.43034300	20.82781700
O	15.15883400	35.27008900	20.64024000	H	13.44021800	36.65222800	19.25336000
C	10.64016700	41.31236500	15.86457000	C	11.64557900	38.76972900	19.58460400
O	13.22664000	34.42844900	21.44823500	H	12.71695200	38.87085300	19.46282800
C	9.41977400	39.69249900	19.20110800	C	5.22680700	34.29514100	15.81506900
C	8.24697600	41.51166600	15.62744600	C	7.42342200	33.76057200	17.46152500
O	8.69253200	33.38300600	20.70968400	C	8.58873300	32.69192200	15.61383400
C	13.92643600	35.28409300	20.86407600	H	8.62972400	32.35219500	14.58867600
N	8.71093200	35.40979100	19.68135800	C	4.13124100	34.58146900	13.72258900
H	8.73772500	35.86780200	18.78085700	H	3.08927400	34.55912600	13.40741700
O	16.44896800	39.45875300	17.18119600	C	9.17236300	34.06111900	12.52515400
C	7.68339400	37.47026400	12.26620800	H	8.86641900	33.03627100	12.69342300
H	7.98790700	38.46665500	11.97138000	O	14.50937700	38.43476400	16.63916300
C	6.77851000	42.39075100	17.33496400	C	8.03144000	43.01717700	17.91030100
H	5.95668000	43.09669600	17.22340300	H	8.33979800	43.87560200	17.30809700
C	8.33881800	41.07385100	14.28870700	H	7.81303700	43.36195900	18.92459200
H	7.43093700	41.02367200	13.69559100	C	7.45150200	33.40232400	16.08094800
C	5.97812000	35.92434200	12.97267000	C	12.00067800	40.35033200	14.03265100
C	10.51367400	38.07098600	11.75391500	C	6.36644900	33.59598300	13.71010400
C	8.64775600	36.42422900	12.27827600	H	6.96366900	32.73633200	13.40657600
C	11.85445000	41.56914300	16.55163200	O	12.72637700	36.33174400	14.06613300
H	11.84453300	42.11965400	17.48585500	C	15.46897200	40.05440400	15.13403300
C	8.22567500	35.11176400	12.64901300	H	15.71423500	41.10078600	15.35514500
C	8.55321100	33.49378200	18.29057800	H	16.26286900	39.66538300	14.49031600
C	6.37611100	37.21574500	12.56448900	C	12.42593700	33.97093900	17.74950900
H	5.62433800	37.99703600	12.52075100	C	5.16537800	34.58624400	17.19660200

C	9.35932400	41.59078200	16.43350100	H	4.25322100	35.02137200	17.59081700
C	10.83011800	39.77566700	19.13816900	C	11.61549900	33.55332400	18.89627000
H	11.29802200	40.64405900	18.70256300	H	12.24792300	33.18333400	19.70456600
C	9.10524400	41.92839600	17.89441100	H	11.07771200	34.41736800	19.29854500
H	10.00300100	42.30618100	18.38496800	C	6.24723300	34.35747600	17.99351400
C	6.34657800	33.74028200	15.23216900	H	6.20103300	34.61621100	19.04596300
C	10.73775800	40.77723200	14.54615200	C	9.13204000	36.20838200	20.82981500
C	13.13527600	40.47798300	14.81710800	H	9.88456500	35.64394000	21.38381800
C	7.44406000	38.42509100	19.88777400	H	8.28914600	36.38372300	21.50614900
H	6.98293000	37.55417900	20.34010900	C	4.92946100	33.39347400	13.22835100
C	13.06162200	41.16615000	16.05407900	H	4.49340900	32.47856600	13.63809900
H	13.96046100	41.36639000	16.62384100	H	4.88396000	33.34429300	12.13738100
C	9.54446500	40.68270200	13.77422400	C	9.64080400	32.39281000	16.43851700
H	9.58377300	40.31033100	12.75574700	H	10.50220200	31.84630100	16.06998200
C	6.87890400	34.88801600	13.08130800	C	15.45565000	39.22809500	16.45264500
C	6.64294500	39.39629800	19.36269800	O	14.31214300	34.73803200	14.05724300
H	5.56147000	39.31493900	19.39997800	C	13.08422300	34.31655800	16.79750800
C	8.57020500	40.70382900	18.64081800	H	13.64217600	34.61421200	15.91543000
C	10.90051900	35.60491900	11.85334600	C	13.24675700	35.17998300	12.01135100
C	10.01484400	36.65871900	11.93822600	H	14.13327700	35.53249000	11.47781200
C	7.20764000	40.52395300	18.72393800	H	13.17840200	34.09917100	11.84555900
C	11.09033600	37.60121300	20.15542000	C	13.43331800	35.45118100	13.52016600



Optimized geometry of **2b**

There is no imaginary frequency after optimization and frequency analysis.

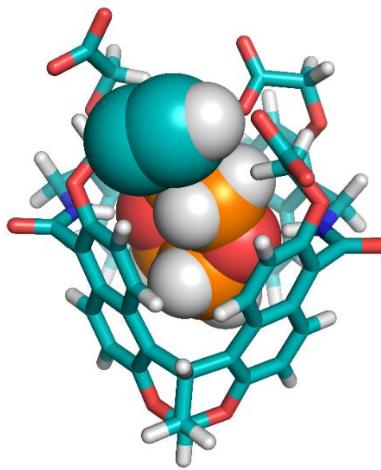
ZPVE Corrected Energy (a.u.) = -3583.302139.

Free Energy (298 K, a.u.) = -3583.392928.

Enthalpies (298 K, a.u.) = -3583.242930.

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O	7.18347200	42.28968600	15.92308400	C	8.80295100	36.03740800	12.28880300
O	10.57732400	33.37726200	20.49665900	C	10.53987900	37.57077300	11.39092500
O	13.86381400	39.01608300	13.79586200	C	9.85904800	37.26376700	20.39127700
N	11.44828100	38.12755600	12.21302700	C	8.01044300	32.06045200	16.77015800
H	11.80670700	37.59022900	13.02135600	H	7.00906300	31.72461600	16.52568500
O	13.83391800	31.90047300	14.92589600	C	9.05307900	38.19695100	19.67228100
O	7.30328300	32.84783600	18.96108900	C	11.77979900	39.54666100	12.19073500
O	11.89382400	36.67901100	21.39495200	H	11.05325800	40.05094600	11.55446100
O	7.87102300	37.04496600	12.18503600	H	12.76628800	39.70185500	11.74517700
O	13.90925600	32.19489900	12.64875200	C	13.24189000	36.97149100	21.72968200
O	15.11517500	36.03506200	22.76448800	H	13.29162500	37.87387000	22.35409400
C	10.59609900	40.87740000	15.63547800	H	13.82455900	37.16239400	20.81911700
O	13.21708200	34.81407600	22.80823400	C	11.68565700	38.86144700	20.34330700
C	9.60111200	39.43924900	19.22403100	H	12.68913100	39.14729100	20.63337000
C	8.36676100	41.77806900	15.45551900	C	12.88326200	33.07747600	12.43034000
O	10.04839200	38.13414700	10.41191700	C	11.02893000	35.12338800	11.99035200
C	13.90746300	35.80908000	22.50966000	C	9.28119100	33.79907700	13.04649000

N	9.18017200	34.99414700	19.68290800	H	8.93417800	32.88984700	13.51570300
H	8.44107800	35.16545700	18.98919500	C	13.69312500	31.25190200	13.67194800
O	14.25012000	35.86574200	15.48978300	H	14.52922100	30.55801900	13.59806600
C	11.98906600	33.02817500	17.81658900	C	9.02503800	31.86570600	15.87171500
H	12.20611100	33.44068800	18.79452500	H	8.79230500	31.36223600	14.93967000
C	6.98358000	42.22100400	17.31448400	O	12.45418400	36.73127700	14.44210000
H	6.11665200	42.85220700	17.50543400	C	8.22934900	42.67378800	18.04656800
C	8.41791300	41.63426000	14.05124500	H	8.51907100	43.65431600	17.65903200
H	7.55446200	41.94415300	13.47144200	H	8.03468800	42.76497600	19.11798900
C	12.73087000	32.19305100	15.68487800	C	10.63689300	33.92163700	12.64934900
C	9.81136300	33.80462000	19.62940700	C	11.76644300	40.03226100	13.62521500
C	10.63599400	32.77922700	17.45293900	C	11.29586100	31.66803000	13.76880100
C	11.73136000	40.48933500	16.38796200	H	10.30569700	31.27448000	13.53706600
H	11.74921700	40.64771300	17.45550100	O	6.96459000	35.33629300	17.90144500
C	10.36563800	32.23575500	16.16124900	C	14.53149300	37.96077200	14.47548500
C	10.10315300	36.20040800	11.86058900	H	15.03775900	38.32141600	15.37824800
C	13.01106300	32.69842100	16.97228600	H	15.30888800	37.63311900	13.78011000
H	14.04776000	32.84535100	17.25600300	C	7.68205500	37.62558900	14.51057200
C	9.42996500	41.43238800	16.26047400	C	13.24995700	34.21720100	11.67787000
C	10.92399100	39.74548900	19.62557400	H	14.26737000	34.28373700	11.30693400
H	11.34887200	40.71890800	19.40852000	C	7.99947100	38.08709000	13.15677000
C	9.29778600	41.61123000	17.77601800	H	7.30814400	38.86995000	12.83607600
H	10.24571300	41.94782600	18.19713100	H	9.01035300	38.50750300	13.13725200
C	11.60292100	32.89387100	12.90511600	C	12.35361600	35.22459300	11.48374900
C	10.64095000	40.67609600	14.22023300	H	12.65702900	36.11834100	10.94968300
C	12.82604400	39.63798200	14.42011200	C	9.31563300	35.90957000	20.80620800
C	7.67900600	37.93856000	19.40282500	H	10.00068200	35.44603200	21.51406700
H	7.23126300	36.99645400	19.69086500	H	8.34464400	36.02204200	21.30284500
C	12.81986200	39.89684400	15.80643400	C	12.34365400	30.58821600	13.49291300
H	13.66286900	39.60655600	16.42336700	H	12.28145400	30.20453700	12.47103300
C	9.51925900	41.09812200	13.45153100	H	12.22980600	29.75276300	14.18815000
H	9.51816600	40.98027100	12.37402800	C	8.38704900	34.81913300	12.86133400
C	11.43879400	32.03333600	15.23789500	H	7.35464700	34.72395400	13.17954400
C	6.89926200	38.85761600	18.76100500	C	13.64800100	36.74039200	14.83628100
H	5.84649500	38.66970800	18.57684400	O	4.82942700	34.89062200	17.34512200
C	8.80353700	40.33655100	18.44399900	C	7.44158100	37.17402700	15.60459600
C	8.26918900	32.68038200	18.01475700	H	7.21060100	36.69989700	16.55389000
C	9.55403600	33.05580400	18.34312000	C	6.00388500	33.23012700	18.53576600
C	7.46562800	40.05959800	18.28544800	H	5.40565300	33.25626600	19.45069100
O	6.58687900	40.90335900	17.65653900	H	5.55422500	32.47867000	17.87732500



Optimized geometry of the **G1@2a**

There is no imaginary frequency after optimization and frequency analysis.

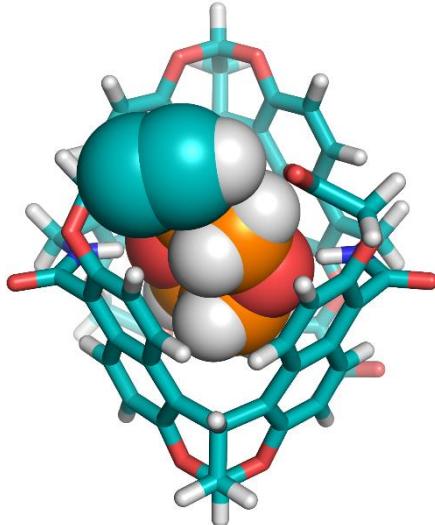
ZPVE Corrected Energy (a.u.) = -3890.783801.

Free Energy (298 K, a.u.) = -3890.883414.

Enthalpies (298 K, a.u.) = -3890.717430.

O	6.34241400	41.32053900	18.65877100	H	10.91904500	40.51368400	11.95334100
O	6.81973500	41.96492400	16.50122900	H	12.51615200	39.80411500	12.15377300
O	11.29714800	38.15787400	10.27830600	C	13.50841200	36.64799200	20.29190700
O	13.81847500	39.71722000	14.07584300	H	13.99079900	37.43863800	20.88076900
N	10.93872000	38.48690300	12.50023100	H	13.65380600	36.88679300	19.22902800
H	10.54441500	38.08013300	13.34946000	C	11.83165700	38.89055600	19.89821600
O	4.89353500	35.80963800	12.68353000	H	12.89909800	39.06320900	19.83237400
O	12.56262100	35.60254400	11.72807700	C	5.50445100	34.60079200	15.49042600
O	12.12302300	36.57738200	20.59708500	C	7.62214700	33.96690000	17.20347700
O	10.88104100	32.71370500	18.38368800	C	8.71179200	32.69359300	15.43913000
O	4.40305800	34.97746400	14.77218200	H	8.70747100	32.24791100	14.45565700
O	15.45447800	35.35663500	20.37578400	C	4.36474700	34.70723600	13.38523200
C	10.40722500	41.18967100	16.01162900	H	3.30622500	34.68865400	13.13118500
O	13.54625800	34.35391500	21.04282800	C	9.41017400	33.87289400	12.41520400
C	9.56405100	39.71196500	19.53533200	H	9.06557000	32.87206300	12.63795900
C	8.02474700	41.56342000	15.98524200	O	13.84535800	37.60560300	15.88421800
O	8.54317900	33.41586100	20.44466900	C	8.05416800	42.99135700	18.33045000
C	14.22505700	35.31093000	20.60641600	H	8.30506100	43.87201000	17.73322600
N	9.11772200	35.44384200	19.59131600	H	7.93819400	43.29771000	19.37345500
H	9.29220400	35.97930400	18.73850300	C	7.62560300	33.50962000	15.85040700
O	15.60446700	38.53981700	16.94306900	C	11.54692400	40.28739400	14.00387700
C	8.02011600	37.22963700	11.59122300	C	6.54101600	33.60113700	13.46577300
H	8.36759300	38.17522300	11.18635300	H	7.09126300	32.68987500	13.23143700
C	6.74841600	42.39675000	17.84561200	O	13.75831800	33.09548000	11.48518900
H	5.91959500	43.10240500	17.87622200	C	14.98029200	39.45404200	14.85517400
C	7.96584100	41.12891300	14.64261600	H	15.40660200	40.38619300	15.24345000
H	7.00169800	41.12159500	14.14463000	H	15.69674400	39.03631700	14.14150000
C	6.24086100	35.84061100	12.42755400	C	12.69159500	33.72344900	17.14929600
C	10.90533900	37.75480700	11.37324800	C	5.47711400	35.02248800	16.83980200
C	8.95081000	36.18253100	11.82381100	H	4.62282800	35.59725700	17.18150100
C	11.68465700	41.27036600	16.61855500	C	11.87444600	33.74899300	18.36683700
H	11.79573900	41.74015500	17.58566200	H	12.49139900	33.60111900	19.25840200
C	8.47364300	34.93750100	12.32362800	H	11.39211700	34.72700500	18.48176200
C	8.72561400	33.67301400	18.05263900	C	6.52017700	34.73355600	17.66964100
C	6.69167000	37.05018700	11.85320300	H	6.50987500	35.09380000	18.69338200
H	5.96451800	37.83264400	11.66255500	C	9.44459000	36.10103900	20.85139200
C	9.20486800	41.56021500	16.69547000	H	10.20961500	35.52153000	21.37287100
C	10.96863700	39.88370300	19.51931600	H	8.56527500	36.13893600	21.50207600
H	11.39152400	40.82505600	19.20421800	C	5.08269100	33.41882000	13.04403900
C	9.11753200	41.90249300	18.18053400	H	4.61353800	32.58876300	13.57868700
H	10.06667000	42.28613700	18.55552300	H	5.00081200	33.23329200	11.96995900
C	6.55871200	33.88169500	14.96817400	C	9.77474000	32.43474600	16.26432400
C	10.35925400	40.72581300	14.66215200	H	10.60808300	31.82716900	15.92914900
C	12.73944900	40.23974200	14.70433100	C	14.77395900	38.43376800	16.01200900
C	7.65610300	38.33398900	20.19092900	O	14.78916500	33.35084900	13.47377600
H	7.23893900	37.42783400	20.61485800	C	13.36731600	33.68615500	16.14794600
C	12.80991800	40.79077500	16.00711500	H	13.96254300	33.64334100	15.23949800
H	13.75579500	40.83431900	16.53358200	C	13.39313900	35.09872500	12.77485700
C	9.09574900	40.69752900	14.00760900	H	12.82479900	35.06337300	13.71198500
H	9.01637800	40.31683200	12.99520100	H	14.18889000	35.83825400	12.90628100
C	7.10038600	34.79765700	12.69960100	C	14.03178400	33.71334600	12.53284600
C	6.80476500	39.29708200	19.73173800	C	10.88721300	36.49979400	15.47290600
H	5.72836700	39.17708600	19.79948200	C	10.94411000	37.23240200	16.79490200
C	8.66504800	40.68337000	18.98531500	C	8.66217700	37.76368900	16.61903400
C	11.23077500	35.34499100	11.84208500	C	8.59522000	37.05104100	15.28073100
C	10.34691400	36.37507800	11.62468100	H	11.66579100	36.77275000	17.47250800
C	7.31177700	40.46128100	19.11357400	H	10.68838100	35.42822600	15.62865700
C	11.32912800	37.64313500	20.33538600	H	11.83239800	36.63171500	14.94466000
C	9.79653600	32.95591300	17.57368400	H	7.72198100	37.66389900	17.16783100
C	8.77293500	34.15122600	19.48678900	H	8.88273700	38.83002000	16.47498100
C	9.96514100	37.47225400	20.50357500	H	8.26876900	36.01301300	15.42307400
C	10.74444800	34.05902900	12.17645200	H	7.90654500	37.55078200	14.59495000
H	11.44715600	33.23469400	12.22447100	H	11.23772600	38.27753700	16.63428300
C	9.06624800	38.50294600	20.10431200	O	9.86834900	37.05996700	14.65607500

C	11.50658400	39.82167500	12.56977600	O	9.67204100	37.17867600	17.42610100
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Optimized geometry of the **G1@2b**

There is no imaginary frequency after optimization and frequency analysis.

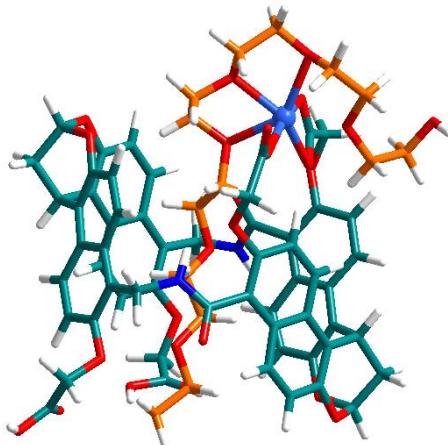
ZPVE Corrected Energy (a.u.) = -3890.785032.

Free Energy (298 K, a.u.) = -3890.883594.

Enthalpies (298 K, a.u.) = -3890.718986.

O	6.74246100	41.15037800	18.54086800	H	10.92752400	40.28724700	11.67386900
O	7.19575300	42.02026600	16.46313500	H	12.50557200	39.52379600	11.82691500
O	8.72210200	33.12794700	20.90402900	C	13.57079900	35.95403300	19.87138200
O	13.98009700	39.63662400	13.59749200	H	14.34728700	36.62169900	20.26817100
N	10.90390600	38.35307900	12.49931400	H	13.46813700	36.16524700	18.79919900
H	10.72142000	38.05352200	13.46052000	C	12.12368000	38.42551500	19.63717700
O	13.63728200	31.63394400	16.02898700	H	13.20048800	38.54025800	19.57928800
O	6.49805900	33.22707000	18.54440000	C	13.05380800	33.40282400	13.57366100
O	12.33254700	36.18015800	20.53312500	C	11.19316100	35.21972300	12.55626700
O	8.00643400	36.61419400	11.31273000	C	9.39238300	33.61704600	12.88242800
O	14.07784000	32.60113800	13.99532200	H	9.03299300	32.64248200	13.18112000
O	15.07051500	34.22306100	19.38556700	C	13.76208900	31.38950500	14.64911500
C	10.71650900	41.08804500	15.79069300	H	14.65338100	30.77284200	14.54456800
O	13.37599200	33.73483500	20.79344800	C	8.73381800	32.04907100	15.86849900
C	9.89804200	39.34593500	19.25740500	H	8.65906800	31.63707600	14.87013000
C	8.35858700	41.58725400	15.87864200	O	14.57871400	37.65370300	15.45958400
O	10.96748400	37.70349100	10.31995900	C	8.52949000	42.76772800	18.35348100
C	14.03664100	34.48619900	20.04512300	H	8.81048000	43.69226700	17.84251300
N	9.22814800	34.98240700	19.68677000	H	8.45604800	42.96833300	19.42566400
H	9.45165400	35.31671300	18.74811200	C	10.76699200	33.94350900	13.03236500
O	16.51784800	38.68962200	15.96598100	C	11.72622100	40.25025200	13.69347300
C	11.27139500	32.73441300	18.50838100	C	11.36700300	31.72263300	14.29076800
H	11.32656400	33.08744200	19.53281600	H	10.45537800	31.29490000	13.87319000
C	7.18272500	42.29543700	17.84681100	O	5.59670600	35.20139200	16.82119500
H	6.39243400	43.03182500	17.98563100	C	15.27300300	39.57625600	14.18448400
C	8.23582400	41.28596300	14.50568200	H	15.58667700	40.56867500	14.52942800
H	7.26381400	41.39799800	14.03644800	H	15.93412200	39.29493000	13.35943100
C	12.40441900	31.97199900	16.53126500	C	6.67558200	37.02897700	13.28609800
C	8.89582900	33.68410500	19.82025500	C	13.48085900	34.66370100	13.10115700
C	10.02571800	32.64901900	17.82763900	H	14.53834200	34.89982700	13.15087100
C	12.02257900	41.08441900	16.34214400	C	7.44490500	37.60369700	12.17951500
H	12.18912200	41.47289800	17.33850400	H	6.81041500	38.21837500	11.53665900
C	10.00609700	32.21410100	16.47204600	H	8.24091700	38.24450000	12.58169700
C	10.24610300	36.12665000	11.99841300	C	12.57051600	35.56234300	12.63129500
C	12.42826700	32.36513900	17.88767400	H	12.90571200	36.54162600	12.30612000
H	13.38038500	32.42601700	18.40511800	C	9.62264200	35.81727500	20.81124800

C	9.55546500	41.44963800	16.54658700	H	10.37281900	35.29194900	21.40686200
C	11.31059300	39.44905300	19.22635100	H	8.76511100	36.00243700	21.46662900
H	11.77742200	40.35475500	18.87039200	C	12.52201600	30.74646600	14.06296900
C	9.53052500	41.64843800	18.05948700	H	12.68291500	30.55880000	12.99803500
H	10.50901900	41.94449400	18.43810600	H	12.33660600	29.79205100	14.56251200
C	11.72293200	33.03966600	13.60104600	C	8.49751500	34.49881000	12.33532200
C	10.59522900	40.72728600	14.41735900	H	7.45111200	34.23711600	12.22394500
C	12.95893800	40.16221200	14.31471400	C	15.45399600	38.53631000	15.32328200
C	7.92941600	38.02631800	19.87471200	O	4.10818600	33.75320400	15.94178500
H	7.47907200	37.11525800	20.25112200	C	6.09970200	36.53601700	14.22677800
C	13.11049100	40.64309000	15.63834000	H	5.67376500	36.07642800	15.11919900
H	14.08333100	40.64545200	16.11508800	C	5.23082200	33.10263400	17.91590200
C	9.31659600	40.83407500	13.80414700	H	4.50601900	33.28635500	18.71467800
H	9.18793200	40.57291100	12.75989000	H	5.07550300	32.07943900	17.55592400
C	11.24047800	31.94776400	15.79454000	C	4.96587500	34.11506100	16.77396100
C	7.12024400	39.03805400	19.45008900	C	11.12898100	35.76530200	16.40944300
H	6.03952500	38.95717600	19.50346900	C	11.43599100	37.21571200	16.08415800
C	9.03748200	40.38339300	18.76469100	C	9.13791800	37.63956100	15.81930600
C	7.59918400	32.86217900	17.84292800	C	8.83089000	36.18449800	16.11782500
C	8.81411800	33.00181100	18.47776100	H	11.46414400	37.80659900	17.01093300
C	7.67685900	40.21642400	18.90501600	H	12.39280000	37.32932200	15.56776900
C	11.56742000	37.22582400	20.13745700	H	11.18291700	35.14991900	15.49977900
C	8.92494000	35.76925800	11.89542000	H	11.82793100	35.36315900	17.14786400
C	10.72794600	37.47028600	11.50326200	H	9.10967500	38.23398000	16.74477400
C	10.19608100	37.10528700	20.27495800	H	8.42471000	38.05664100	15.10580000
C	7.56524300	32.34885800	16.52355500	H	7.86988500	36.05541200	16.62239900
H	6.62083700	32.21229500	16.00939200	H	8.81035000	35.61220100	15.17794800
C	9.34571800	38.15205100	19.81446400	O	9.83137900	35.65308800	16.97612300
C	11.54106400	39.65298700	12.32265700	O	10.42555800	37.74170200	15.23164000



Coordinate of the optimized geometry of the intrachain coordinated complex

There is no imaginary frequency after optimization and frequency analysis.

ZPVE Corrected Energy (a.u.) = -5019.480051.

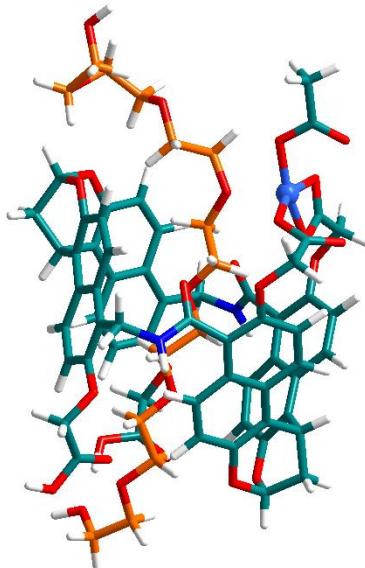
Free Energy (298 K, a.u.) = -5019.598323.

Enthalpies (298 K, a.u.) = -5019.392640.

H	-1.355267	4.517115	4.209379	H	2.020945	2.186036	-4.945709
C	-0.418465	4.089287	3.876347	C	1.072697	0.281215	5.492765
H	-0.538028	2.375295	5.110667	H	0.361958	0.892884	6.048806
C	0.058994	2.919541	4.398298	H	1.821817	-0.100311	6.188676
C	1.469198	4.28441	2.338139	H	-4.119805	-3.290014	2.27088
C	1.285313	2.358807	3.932473	H	4.655046	0.945405	2.591979
C	0.270374	4.756552	2.836155	H	6.428231	0.928428	-4.815299
C	2.014084	3.082543	2.916428	H	4.932049	-1.859494	4.897739

C	1.785024	1.108714	4.42337	H	-5.368843	-1.704811	3.24221
H	3.848995	3.073612	1.770547	H	-2.598896	-0.524022	-4.622215
C	2.972809	0.605281	3.905776	C	1.411863	-0.796411	-4.026881
C	3.725057	1.344677	2.97137	C	-0.675238	-0.77367	4.091426
C	3.255676	2.547162	2.49837	O	2.348189	-1.266821	-4.719851
C	2.164885	5.055012	1.193147	O	-1.190697	0.354996	3.913088
C	0.078791	4.330885	-1.907687	C	-4.592541	-0.35071	1.762159
H	0.457423	3.096945	-3.590377	C	7.478527	1.399511	-3.00646
C	0.845326	3.471703	-2.652453	C	5.138614	-1.510538	2.779923
C	1.80219	4.483932	-0.185376	O	4.712981	-2.586064	2.324823
C	2.155723	3.110463	-2.228249	O	8.654018	1.785902	-3.562358
C	0.549016	4.812971	-0.666011	O	7.476702	0.992503	-1.844068
C	2.6673	3.695253	-1.012553	O	-5.406956	0.612529	1.408281
C	2.963654	2.203417	-2.990281	O	-3.807458	-0.887837	0.922554
H	4.494448	3.977903	0.132811	O	5.914225	-0.647434	2.120846
C	4.259306	1.954033	-2.578785	C	-3.556333	3.619432	-0.851967
C	4.807357	2.621338	-1.460182	H	-3.656507	4.70759	-0.923484
H	5.833787	2.424774	-1.191147	H	-3.043396	3.226237	-1.7338
C	4.037036	3.466578	-0.702507	C	-2.835056	3.231377	0.426096
O	-0.381872	5.906363	2.366153	H	-3.402214	3.599181	1.284743
O	-0.350339	5.625473	0.02743	H	-1.832262	3.664135	0.446249
C	0.137473	6.456019	1.139185	O	-2.824956	1.763277	0.547432
H	-0.348094	7.4224	1.027482	C	-1.611112	1.084102	0.024892
C	1.656596	6.516647	1.195096	H	-1.379976	1.411729	-0.988722
H	2.053568	7.057943	0.333341	H	-1.903145	0.039428	0.002121
H	1.942451	7.037308	2.112714	C	-0.452889	1.219158	1.012948
H	3.244053	5.055875	1.347046	H	-0.84666	1.137785	2.025416
H	-0.89883	4.65112	-2.242562	H	0.101867	2.156515	0.901209
O	5.045565	1.017017	-3.298638	O	0.432277	0.05758	0.856046
O	3.375031	-0.662701	4.356477	C	1.538954	0.24311	-0.076523
C	6.263651	1.533097	-3.918268	H	2.177757	1.081682	0.220706
H	6.150171	2.583078	-4.213815	H	1.208454	0.403135	-1.107289
C	4.801266	-1.02876	4.204308	O	-4.893155	3.005137	-0.740444
H	5.447687	-0.192969	4.472255	C	-5.821809	3.400539	-1.82606
H	3.007683	-3.949191	2.575957	H	-5.849099	4.492223	-1.906498
C	1.938969	-3.969389	2.412956	H	-5.489133	2.941633	-2.760962
H	1.648685	-2.215489	3.533596	C	-7.170533	2.864548	-1.378169
C	1.150697	-2.985345	2.963976	H	-7.945162	3.077943	-2.122912
C	0.072848	-4.80255	1.118819	H	-7.445972	3.309793	-0.420267
C	-0.263027	-2.96539	2.761945	O	-7.071164	1.415767	-1.129539
C	1.393131	-4.899031	1.506489	C	-7.297739	0.593786	-2.342575
C	-0.803154	-3.937426	1.840418	H	-6.51412	0.798303	-3.076254
C	-1.160028	-2.005382	3.367999	H	-8.29249	0.800161	-2.754302
H	-2.643416	-4.833082	1.11324	C	-7.216617	-0.837795	-1.860855
C	-2.531074	-2.11317	3.142551	H	-7.280001	-1.517865	-2.71889
C	-3.050561	-3.175548	2.367853	H	-8.000551	-1.086868	-1.14893
C	-2.216886	-4.038271	1.712679	O	-5.894813	-0.989672	-1.211399
C	-0.299091	-5.599267	-0.130914	C	-5.439507	-2.385694	-1.099974
C	2.328622	-4.83852	-2.836986	H	-4.403372	-2.312994	-0.7781
H	2.513782	-3.119088	-4.100713	H	-5.50712	-2.86524	-2.084999
C	1.936179	-3.632273	-3.349192	C	-3.665505	0.784561	-3.267064
C	0.407812	-4.928527	-1.33502	O	-4.619033	1.235419	-3.948403
C	0.754481	-2.98896	-2.87446	O	-3.621212	0.606705	-1.977027
C	1.603198	-5.452577	-1.793014	C	2.327625	-1.059497	0.015663
C	-0.063018	-3.698754	-1.91835	H	1.715749	-1.886291	-0.365316
C	0.391214	-1.652138	-3.288951	H	2.568159	-1.267649	1.06366
H	-1.954925	-3.631078	-0.855988	O	3.536275	-0.871929	-0.779887
C	-0.832303	-1.143167	-2.865993	C	4.356575	-2.086263	-0.819428
C	-1.691949	-1.893239	-2.038374	H	4.458789	-2.522265	0.178686
H	-2.619677	-1.425764	-1.742001	H	3.91964	-2.829999	-1.498982
C	-1.30702	-3.118283	-1.551669	C	5.714124	-1.657326	-1.341663
O	2.274198	-5.8516	0.981351	H	6.298748	-2.531059	-1.647018
O	2.214502	-6.59248	-1.253623	C	-6.229315	-3.165842	-0.052617
C	1.7734	-6.900886	0.096294	H	-5.759256	-4.151945	0.073484
H	2.299303	-7.813123	0.367216	H	-6.16931	-2.629907	0.895742
C	0.255671	-7.024149	0.087297	O	-7.659432	-3.27198	-0.344208
H	-0.017658	-7.700844	-0.726372	H	-7.761674	-3.866356	-1.136546

H	-0.113195	-7.42649	1.033587	N	1.308485	0.545228	-3.799957
H	-1.376217	-5.642915	-0.292078	H	0.445545	0.88514	-3.373994
H	3.231367	-5.3298	-3.177232	N	0.379913	-0.910507	4.944116
O	-1.201353	0.181274	-3.189029	H	0.722191	-1.827005	5.207152
O	-3.370175	-1.204718	3.774212	H	5.56382	-0.979483	-2.184964
C	-2.39262	0.381937	-4.042214	O	6.453907	-0.919986	-0.294496
H	-2.140118	1.19222	-4.728508	H	6.869768	-0.11103	-0.722117
C	-4.67409	-0.854826	3.204325	H	8.572299	2.123132	-4.495591
H	-5.054853	-0.063348	3.847678	H	6.132403	-0.861512	1.060462
C	2.387263	1.472899	-4.198594	Cu	-4.786637	0.805249	-0.463911
H	3.16577	0.856634	-4.644655				



Coordinate of the optimized geometry of the interchain coordinated complex

There is no imaginary frequency after optimization and frequency analysis.

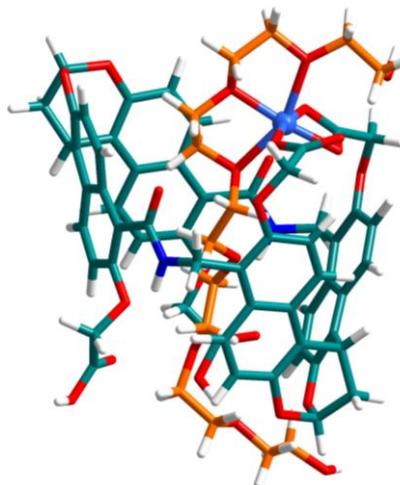
ZPVE Corrected Energy (a.u.) = -5246.714114.

Free Energy (298 K, a.u.) = -5246.850798.

Enthalpies (298 K, a.u.) = -5246.617596.

H	3.650008	4.010124	-2.1606	H	-0.2118	1.592551	-5.85703
C	2.565767	3.968576	-2.14407	H	2.076443	-4.83274	-2.10105
H	2.398679	2.422545	-3.58766	H	-3.44761	3.047579	-2.75837
C	1.867339	3.109004	-2.94663	H	-5.1314	1.123528	5.564704
C	0.529129	4.619974	-0.94796	H	-3.69548	1.505569	-6.25175
C	0.444086	3.055637	-2.89755	H	3.563264	-4.54213	-3.73518
C	1.887408	4.745366	-1.17424	H	2.865509	-4.29914	4.057015
C	-0.23734	3.835174	-1.88443	C	-0.20769	-0.70093	4.097503
C	-0.31048	2.272612	-3.82505	C	0.887757	-0.62264	-3.64278
H	-2.20663	4.412385	-1.17491	O	0.742355	0.049839	3.771162
C	-1.69321	2.288455	-3.7603	O	1.841452	0.002479	-3.11936
C	-2.36854	3.069499	-2.80306	C	4.364121	-3.7876	-1.88654
C	-1.65721	3.818724	-1.89072	C	-6.0514	1.974031	3.815184
C	-0.06227	5.347971	0.279449	C	-4.78465	1.42789	-4.41364
C	1.716427	3.901915	3.353411	O	-4.71175	0.864212	-3.32491
H	1.146697	2.338074	4.665792	O	-7.22002	2.305141	4.44685
C	0.831753	3.00283	3.878274	O	-6.03475	1.867366	2.594757
C	0.154457	4.543325	1.583933	O	5.041271	-4.82087	-1.62891
C	-0.49378	2.9039	3.365364	O	4.124473	-2.84779	-1.00701
C	1.37098	4.684648	2.227003	O	-5.94858	1.71806	-5.06003
C	-0.83834	3.697676	2.202932	C	1.672132	0.825656	-0.00911
C	-1.48398	2.078289	3.996711	H	1.868725	0.62806	-1.0649
H	-2.49421	4.252953	0.91253	H	1.407461	1.879678	0.124267

C	-2.76774	2.062606	3.482676	C	0.521355	-0.0489	0.482224
C	-3.12487	2.861158	2.37725	H	0.477486	0.006256	1.573254
H	-4.14714	2.820671	2.031914	H	0.704092	-1.09442	0.192622
C	-2.18545	3.648947	1.752921	O	-0.6988	0.468867	-0.14261
O	2.720815	5.628972	-0.4714	C	-1.85535	-0.37983	0.135716
O	2.366512	5.589657	1.850731	H	-1.94973	-0.59059	1.202368
C	2.160888	6.366287	0.6459	H	-1.78426	-1.333	-0.39332
H	2.794451	7.24266	0.756687	C	-3.09773	0.372452	-0.33067
C	0.689987	6.69026	0.428378	H	-3.02199	0.645471	-1.38628
H	0.316398	7.25362	1.287354	H	-3.21027	1.28421	0.267732
H	0.583276	7.295625	-0.47525	O	-4.21834	-0.54906	-0.11474
H	-1.12118	5.555496	0.131591	C	-5.51447	0.121728	-0.26748
H	2.713321	4.021041	3.757108	H	-5.54383	0.706752	-1.19098
O	-3.7093	1.195403	4.088808	H	-5.72502	0.764962	0.593828
O	-2.35588	1.468682	-4.69304	O	2.831487	0.493089	0.837618
C	-4.85961	1.805689	4.754607	C	4.024315	0.085147	0.092974
H	-4.60418	2.782139	5.184698	H	4.655701	-0.42124	0.826277
C	-3.62223	1.92667	-5.24695	H	3.786388	-0.62956	-0.69967
H	-3.66882	3.019015	-5.31753	C	4.716259	1.317745	-0.48181
H	-4.10728	-1.35005	-2.95915	H	4.899505	2.049775	0.310507
C	-3.25037	-1.95511	-2.70322	H	4.07368	1.790762	-1.23021
H	-1.91322	-0.6395	-3.6426	O	5.973877	0.864603	-1.09334
C	-1.99468	-1.55883	-3.08485	C	6.400538	1.6762	-2.22968
C	-2.35593	-3.78412	-1.38174	H	5.585511	1.778954	-2.96095
C	-0.84361	-2.33427	-2.74666	H	7.224254	1.122029	-2.69036
C	-3.43478	-3.06479	-1.85256	C	6.885902	3.068053	-1.84497
C	-1.0565	-3.50607	-1.92549	H	7.405227	3.526351	-2.70011
C	0.494777	-2.0021	-3.16508	H	7.560356	3.035554	-0.98901
H	-0.10751	-5.31097	-1.19232	O	5.693848	3.862827	-1.4925
C	1.534114	-2.90196	-2.92403	C	5.988383	5.102471	-0.76552
C	1.283049	-4.11327	-2.24316	H	5.026145	5.616	-0.72733
C	0.040682	-4.3814	-1.72385	H	6.728055	5.711263	-1.30261
C	-2.61348	-4.75354	-0.21412	C	4.02577	-3.06857	2.695229
C	-3.95192	-2.32984	2.409206	O	3.945876	-4.0123	1.778694
H	-2.93056	-1.02543	3.697581	O	4.782673	-2.06615	2.565751
C	-2.83211	-1.88833	3.058631	C	-6.56084	-0.98611	-0.35459
C	-2.67158	-3.90602	1.075211	H	-6.50539	-1.63591	0.525937
C	-1.56207	-2.5014	2.828092	H	-6.36374	-1.61069	-1.23164
C	-3.87644	-3.32601	1.413664	O	-7.85005	-0.29958	-0.44731
C	-1.50826	-3.56746	1.850336	C	-8.95781	-1.23778	-0.56092
C	-0.34868	-2.06515	3.469587	H	-8.85351	-1.87178	-1.4532
H	-0.20266	-5.05013	0.965365	H	-9.01403	-1.88993	0.323485
C	0.835503	-2.77493	3.247423	C	-10.2423	-0.4309	-0.6788
C	0.860058	-3.86645	2.354779	H	-11.0961	-1.10317	-0.51199
H	1.799819	-4.35803	2.14383	C	6.475971	4.86521	0.660041
C	-0.27044	-4.23096	1.66497	H	6.367637	5.800886	1.227687
O	-4.76594	-3.3557	-1.53129	H	5.834616	4.102644	1.11923
O	-5.09798	-3.63062	0.798267	O	7.881716	4.441825	0.603495
C	-5.03137	-4.31991	-0.4775	H	8.140676	4.136212	1.514359
H	-6.04199	-4.67556	-0.66046	N	-1.16909	-0.22922	4.937247
C	-3.9834	-5.4251	-0.43897	H	-1.88433	-0.83139	5.326984
H	-4.22376	-6.1108	0.377671	N	0.151988	-0.04297	-4.62936
H	-3.99214	-5.97212	-1.3852	H	-0.57903	-0.55031	-5.11351
H	-1.84559	-5.52291	-0.14967	H	-10.2407	0.331086	0.112347
H	-4.91266	-1.86624	2.58484	O	-10.2589	0.156962	-2.01701
O	1.969451	-2.37208	3.939965	H	-11.0802	0.713983	-2.08557
O	2.785369	-2.58518	-3.42761	H	-7.13727	2.364094	5.43649
C	3.151473	-3.25164	3.9487	H	-6.73321	1.409264	-4.52529
H	3.717272	-2.91714	4.818315	Cu	5.301042	-3.38951	0.478053
C	3.848718	-3.57383	-3.313	H	9.568099	-4.32817	1.133273
H	4.664788	-3.15884	-3.91167	C	9.210426	-3.39635	0.692296
C	-1.21063	1.223067	5.24008	H	9.642388	-3.24792	-0.29922
H	-2.02473	1.364557	5.951498	H	9.524162	-2.56304	1.333693
H	-0.27993	1.521873	5.719952	C	7.710324	-3.41092	0.602884
C	0.310436	1.403136	-4.91862	O	6.98656	-4.11675	1.41905
H	1.367665	1.621663	-5.0515	O	7.078051	-2.69243	-0.27694



Coordinate of the optimized geometry of the intrachain coordinated complex

There is no imaginary frequency after optimization and frequency analysis.

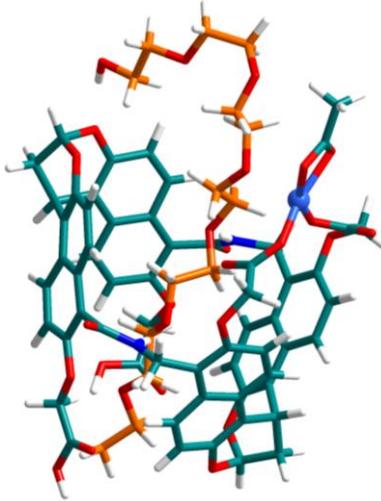
ZPVE Corrected Energy (a.u.) = -5019.477012.

Free Energy (298 K, a.u.) = -5019.595937.

Enthalpies (298 K, a.u.) = -5019.389171.

H	-5.391761	-0.718012	-1.550489	H	0.322454	-0.768515	6.036369
C	-4.598353	-1.442287	-1.455366	C	-1.396184	-1.39847	-4.341655
H	-3.643446	-0.813307	-3.212177	H	-2.295687	-1.542483	-4.948396
C	-3.583913	-1.48185	-2.370909	H	-0.51236	-1.622878	-4.934941
C	-3.489128	-3.103488	-0.050089	H	-1.961459	4.715601	-2.432152
C	-2.479125	-2.353211	-2.20194	H	0.392847	-4.917986	-1.813756
C	-4.554922	-2.262785	-0.310129	H	4.414925	-3.337367	3.94084
C	-2.454407	-3.212413	-1.044019	H	2.544875	-3.715998	-4.524858
C	-1.406638	-2.35727	-3.145443	H	-3.474207	3.242743	-1.91779
H	-1.39344	-4.904271	-0.192671	H	-1.228897	4.194988	4.865559
C	-0.367776	-3.263663	-2.983876	C	1.69267	1.256756	3.882976
C	-0.400765	-4.195647	-1.918579	C	-0.100257	0.672035	-4.020941
C	-1.404252	-4.165341	-0.979663	O	2.847191	0.752585	3.841191
C	-3.478246	-3.833209	1.30515	O	0.918787	0.062696	-4.439684
C	-3.389923	-1.162533	4.05823	C	-4.7836	2.061774	-3.01516
H	-1.766506	-0.35993	5.158731	C	3.603219	-3.650467	1.954395
C	-2.067094	-1.065178	4.395952	C	2.613406	-3.178788	-2.449478
C	-2.930077	-2.914454	2.417695	O	3.339916	-2.119163	-2.584731
C	-1.096214	-1.917897	3.793934	O	3.545663	-2.461975	1.401353
C	-3.816975	-2.071081	3.061707	O	3.767324	-4.754053	1.390535
C	-1.552994	-2.893125	2.831145	O	-4.773052	0.922454	-3.487961
C	0.287344	-1.835511	4.141367	O	-5.839055	2.648816	-2.417778
H	-0.906232	-4.630097	1.708173	O	2.383983	-3.606662	-1.241765
C	1.180975	-2.764521	3.6216	C	0.031516	0.345899	0.950526
C	0.717649	-3.789991	2.762974	H	-0.441065	0.298118	1.938679
H	1.406646	-4.533382	2.386663	H	0.346098	1.382377	0.778876
C	-0.598479	-3.83589	2.368567	C	1.22897	-0.591623	0.947943
O	-5.681179	-2.132777	0.525914	H	0.891706	-1.624574	0.882894
O	-5.196971	-2.043163	2.826499	H	1.825663	-0.46934	1.851498
C	-5.715785	-2.886985	1.769706	O	2.08681	-0.400645	-0.253071
H	-6.770678	-3.016226	1.997818	C	2.938166	0.80816	-0.186386
C	-4.939243	-4.190852	1.660045	H	2.418484	1.630283	0.310523
H	-4.99062	-4.71734	2.616633	H	3.144682	1.084377	-1.219718
H	-5.383611	-4.814602	0.88049	C	4.229556	0.499362	0.552774
H	-2.89584	-4.752753	1.248331	H	4.03634	0.172635	1.57844
H	-4.143294	-0.545742	4.53031	H	4.888521	1.370406	0.551943
O	2.511951	-2.645786	3.998634	O	4.881987	-0.59585	-0.211673

O	0.650562	-3.251121	-3.940688	C	6.135158	-1.073551	0.419097
C	3.462352	-3.634922	3.495097	H	5.879451	-1.531729	1.377645
H	3.20533	-4.645792	3.82289	H	6.817687	-0.2298	0.553924
C	1.952163	-3.868572	-3.625756	O	-0.881266	-0.086313	-0.102156
H	1.862248	-4.932624	-3.410589	C	-1.8594	0.930093	-0.469775
H	4.63008	2.306857	-3.647395	H	-2.25328	0.617287	-1.433942
C	3.694686	2.70266	-3.271797	H	-1.382026	1.912386	-0.57708
H	2.452089	1.222346	-4.19567	C	-3.044696	1.039966	0.501629
C	2.497133	2.112426	-3.591702	H	-2.784553	1.566636	1.426067
C	2.590857	4.365178	-1.893376	H	-3.413524	0.035639	0.729349
C	1.256916	2.669982	-3.152223	O	-4.038021	1.82106	-0.261129
C	3.748575	3.813136	-2.401466	C	-5.227654	2.218694	0.498651
C	1.32877	3.874612	-2.36108	H	-5.615293	3.090392	-0.031668
C	-0.034903	2.092243	-3.479374	H	-4.955774	2.509493	1.516957
H	0.157505	5.560553	-1.656316	C	-6.307444	1.138845	0.526303
C	-1.178296	2.846656	-3.195864	H	-7.136843	1.473959	1.160581
C	-1.076785	4.114377	-2.575987	H	-5.934246	0.176096	0.882806
C	0.127184	4.591415	-2.134388	O	-6.80914	0.953423	-0.860004
C	2.754996	5.435113	-0.805388	C	-7.886679	-0.038025	-1.005997
C	4.734191	3.705131	1.981734	H	-8.771873	0.275172	-0.442504
H	4.044649	2.39386	3.514298	H	-7.531686	-1.004557	-0.64102
C	3.773103	3.06269	2.716633	C	-3.104688	3.707542	3.915106
C	3.066415	4.709803	0.518762	O	-3.351218	3.54128	2.724291
C	2.388549	3.239991	2.420615	O	-4.016684	4.315904	4.723102
C	4.388491	4.475245	0.84861	H	-3.727806	4.402115	5.67166
C	2.044623	4.172895	1.375147	C	6.729191	-2.101593	-0.529546
C	1.34705	2.551537	3.153725	H	7.604248	-2.561352	-0.054657
H	0.385657	5.257794	0.488547	H	7.027575	-1.637375	-1.475915
C	0.043025	3.010702	2.995809	O	5.682078	-3.103141	-0.764994
C	-0.284996	4.00579	2.053961	C	6.199099	-4.394896	-1.244646
H	-1.327096	4.269148	1.945151	H	6.818359	-4.244984	-2.139348
C	0.678328	4.53668	1.235088	H	6.820021	-4.841453	-0.457814
O	5.032012	4.280714	-2.105005	C	5.020134	-5.316142	-1.547563
O	5.478622	4.952342	0.115738	H	5.379275	-6.354374	-1.542747
C	5.185804	5.43078	-1.224822	C	-8.188517	-0.115624	-2.502708
H	6.094399	5.93166	-1.548565	H	-8.636338	0.831101	-2.834534
C	3.953281	6.322495	-1.202994	H	-7.244664	-0.253304	-3.047832
H	4.115569	7.120715	-0.474299	O	-9.103326	-1.244628	-2.631488
H	3.788413	6.761657	-2.189785	H	-9.368796	-1.308895	-3.587109
H	1.866742	6.058063	-0.710572	H	-6.405359	1.943768	-1.873288
H	5.785695	3.598265	2.215505	N	0.66328	0.619334	4.497925
O	-1.028195	2.416905	3.715539	H	-0.258042	1.055248	4.43013
O	-2.437764	2.345011	-3.523833	N	-1.308393	0.037593	-3.979887
C	-1.804167	3.302561	4.596293	H	-2.144019	0.584539	-3.770194
H	-2.017169	2.727488	5.500677	Cu	3.587297	-2.16349	-0.507372
C	-3.61777	3.027787	-2.977729	H	4.279554	-5.173267	-0.760505
H	-3.848282	3.936407	-3.540023	O	4.347808	-5.004468	-2.812928
C	0.822365	-0.7391	5.062989	H	4.998528	-5.148358	-3.551563
H	1.889642	-0.902648	5.194449				



Coordinate of the optimized geometry of the interchain coordinated complex

There is no imaginary frequency after optimization and frequency analysis.

ZPVE Corrected Energy (a.u.) = -5246.818826.

Free Energy (298 K, a.u.) = -5246.947510.

Enthalpies (298 K, a.u.) = -5246.724952.

H	3.622131	3.661789	-2.69248	H	-3.536325	3.696354	-2.362115
C	2.564976	3.710161	-2.467319	H	-5.680579	3.125831	3.237045
H	1.994092	2.172885	-3.826273	H	-4.420225	1.877782	-5.505531
C	1.660802	2.899297	-3.097918	H	2.69989	-5.37207	-3.508665
C	0.814547	4.724993	-1.092164	H	1.907487	-4.629428	3.65017
C	0.268012	3.01345	-2.817589	C	-1.618227	-1.376729	4.514617
C	2.14	4.600995	-1.454669	C	0.551591	-1.237544	-4.373547
C	-0.163312	3.995596	-1.854085	C	3.466697	-4.445053	-1.710208
C	-0.697554	2.231514	-3.518828	C	-6.216985	1.076648	3.515485
H	-1.920404	4.989921	-1.064646	C	-5.32138	1.989516	-3.556853
C	-2.049744	2.507814	-3.368078	O	-5.859809	0.869539	-3.54258
C	-2.47487	3.521265	-2.480818	O	-7.50693	1.41351	3.161428
C	-1.559246	4.225797	-1.734753	O	-5.9287	0.061225	4.134195
C	0.463563	5.554389	0.159117	O	3.884848	-5.516319	-1.221996
C	1.883792	3.39888	2.974703	O	3.381117	-3.294686	-1.080863
H	0.900805	2.013243	4.277523	O	-5.582584	2.982543	-2.699462
C	0.798197	2.724617	3.468735	C	3.439076	-0.032906	0.173157
C	0.492577	4.621232	1.379942	H	3.682481	1.023947	0.319096
C	-0.508553	2.996014	2.967268	H	2.789541	-0.405637	0.963731
C	1.731279	4.322696	1.912512	C	2.775256	-0.290332	-1.188869
C	-0.668726	4.018841	1.965642	H	2.783325	-1.362962	-1.39409
C	-1.642627	2.259164	3.413563	H	3.286464	0.249779	-1.990512
H	-2.167053	5.235205	0.972587	O	1.39378	0.250189	-1.19848
C	-2.915307	2.622744	3.004113	C	0.382782	-0.54872	-0.452581
C	-3.085863	3.731219	2.142605	H	0.845401	-1.430297	-0.006868
H	-4.078252	4.06153	1.869768	H	-0.39118	-0.845311	-1.163818
C	-1.995832	4.393488	1.627251	C	-0.210687	0.347861	0.644554
O	3.170651	5.33754	-0.84564	H	-0.135125	1.395357	0.337785
O	2.927996	4.896871	1.462813	H	0.318131	0.191374	1.585364
C	2.87941	5.939346	0.454006	O	-1.614357	-0.016432	0.92572
H	3.745511	6.566702	0.641647	C	-2.600241	0.706659	0.097972
C	1.535806	6.642974	0.388391	H	-2.426543	0.523829	-0.966999
H	1.342011	7.174675	1.323114	H	-2.55449	1.780653	0.297928
H	1.557738	7.358398	-0.437323	O	4.663701	-0.860843	0.302652
H	-0.508912	6.032767	0.049344	C	5.94668	-0.264673	-0.13913
H	2.880943	3.232259	3.360478	H	6.402186	-0.972266	-0.83374
O	-3.977435	1.86738	3.486163	H	5.77909	0.70392	-0.615121
O	-2.954338	1.718147	-4.078769	C	6.842966	-0.117819	1.106112
C	-5.307304	2.139135	2.94692	H	6.612524	-0.944752	1.777039

H	-5.310888	2.032131	1.850918	H	6.663792	0.845619	1.58573
C	-4.212536	2.343585	-4.54284	O	8.279832	-0.285046	0.813223
H	-4.107209	3.423845	-4.640384	C	8.841946	0.6667	-0.148558
H	-4.359818	-0.772023	-3.460825	H	8.328259	0.611119	-1.115501
C	-3.634079	-1.503451	-3.126879	H	9.879369	0.347867	-0.27776
H	-2.039362	-0.662898	-4.225731	C	8.810039	2.115605	0.321047
C	-2.325495	-1.441485	-3.534912	H	9.474164	2.712056	-0.320945
C	-3.180628	-3.443967	-1.7142	H	9.159729	2.188788	1.358573
C	-1.373682	-2.408243	-3.089757	O	7.428194	2.579015	0.189421
C	-4.053775	-2.498846	-2.21394	C	7.300837	4.035317	0.192056
C	-1.831235	-3.45668	-2.205446	H	7.963465	4.486281	-0.558727
C	-0.004111	-2.365881	-3.506072	H	7.537428	4.465421	1.173397
H	-1.241847	-5.347324	-1.318731	C	2.350301	-2.865383	2.460571
C	0.859991	-3.384582	-3.116242	O	3.354568	-3.50491	1.921367
C	0.385936	-4.46474	-2.336476	O	1.791272	-1.819736	2.061678
C	-0.913835	-4.493606	-1.892783	C	-3.953291	0.148091	0.535993
C	-3.753424	-4.424016	-0.676217	H	-3.979894	0.108319	1.626275
C	-5.157579	-2.393736	2.270024	H	-4.091858	-0.858809	0.142821
H	-4.165595	-1.512438	3.910312	O	-5.019066	1.052536	0.056974
C	-4.066804	-2.181012	3.067877	C	-6.214242	0.334088	-0.448218
C	-3.854906	-3.744073	0.703257	H	-6.106415	0.165008	-1.519787
C	-2.817027	-2.786138	2.754528	H	-6.350337	-0.629642	0.050357
C	-5.035973	-3.121852	1.064315	C	-7.430357	1.203148	-0.184638
C	-2.744964	-3.661397	1.613757	H	-8.322329	0.684653	-0.554244
C	-1.653366	-2.538544	3.543386	C	5.857539	4.306745	-0.206576
H	-1.472748	-5.129413	0.652739	H	5.649887	3.686841	-1.089325
C	-0.500945	-3.276436	3.322251	H	5.166183	4.004558	0.587799
C	-0.472618	-4.242271	2.288988	O	5.753846	5.735319	-0.504316
H	0.409361	-4.847896	2.13273	H	4.885295	5.811512	-0.991942
C	-1.54595	-4.401782	1.444453	N	-1.718593	-0.108483	3.742479
O	-5.410238	-2.437536	-1.86228	H	-1.838368	-0.146128	2.714666
O	-6.192649	-3.100251	0.26369	N	0.39199	0.099617	-3.753165
C	-6.011538	-3.533285	-1.111401	H	0.756004	0.246731	-2.789394
H	-7.019706	-3.649443	-1.501843	H	-7.539095	1.406436	0.882941
C	-5.173336	-4.802292	-1.155226	O	-7.247757	2.476386	-0.912137
H	-5.631631	-5.542359	-0.494029	H	-8.04244	3.058069	-0.823011
H	-5.138644	-5.198451	-2.172916	H	-8.144069	0.710389	3.471997
H	-3.148771	-5.328736	-0.612798	H	-6.289885	2.726323	-1.929304
H	-6.107648	-1.935253	2.50621	Cu	4.545386	-3.122416	0.464024
O	0.572768	-3.053355	4.177551	H	8.874954	-3.869284	-0.32606
O	2.178565	-3.309035	-3.556881	C	8.470471	-3.427585	0.585911
C	1.88175	-3.54288	3.764574	H	8.77993	-2.374012	0.655495
H	2.554889	-3.260938	4.578409	H	8.822133	-3.964899	1.468895
C	3.084923	-4.395142	-3.203644	C	6.971921	-3.40444	0.544567
H	3.991916	-4.180275	-3.776221	O	6.325421	-3.355223	-0.583699
C	-1.466689	1.075626	4.345934	O	6.267749	-3.322823	1.634773
O	-1.079497	1.177909	5.534383	H	1.606092	-1.444744	-4.558711
C	-0.328479	1.057284	-4.401418	H	0.028634	-1.175279	-5.332731
O	-0.765611	0.908113	-5.565898	H	-2.43677	-1.426529	5.242564
H	1.049205	-5.276214	-2.071036	H	-0.676709	-1.392412	5.064731

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