**ELECTRONIC SUPPLEMENTARY INFORMATION**

# Photoresponsive Macrocycles for Selective Binding and Release of Sulfate

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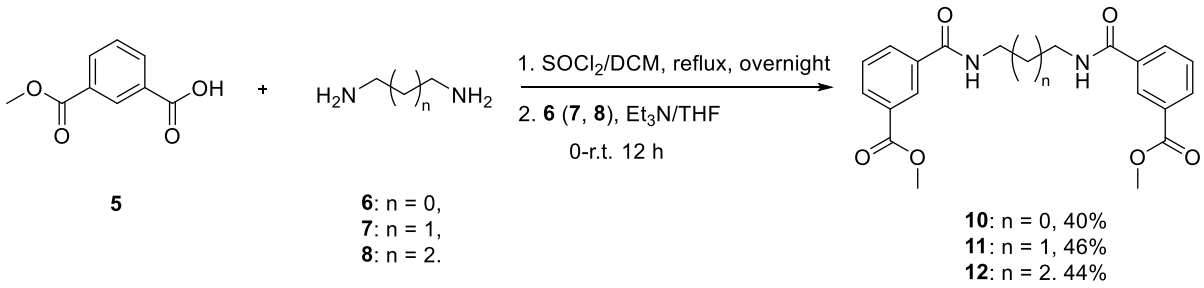
**Contents**

## 1. General experimental

All solvents and chemicals used were purchased from Sigma–Aldrich, TCI, Energy–Chemical, or Acros and used without further purification. TLC analyses were carried out using Sorbent Technologies silica gel (200 mesh) sheets. $^{1}H$ and $^{13}C$ NMR spectra were recorded on Bruker AVANCE 400 spectrometers and the spectroscopic solvents were purchased from Cambridge Isotope Laboratories or Sigma–Aldrich. Either residual solvent peak or tetramethylsilane (TMS) was used as an internal reference. The chemical shifts are expressed in δ (ppm). High–resolution mass spectra (HRMS) were recorded on a Bruker Apex–Q IV FTMS mass spectrometer using ESI (electrospray ionization). X–ray crystallographic analyses were carried out on a Brucker D8 Venture diffractometer using a $\mu$–focused Cu Kα radiation source (λ = 1.5418 Å). All theoretical calculations were carried out with the Gaussian 09 suite[1] of programs using the X3LYP density functional.[2] Structural optimization was performed using a 6–31G* basis set while single–point energy was calculated with a 6–31+g* basis set. Complexation energies were corrected for basis set superposition error (BSSE) using the counterpoise correction method.[3, 4]

## 2. Synthesis



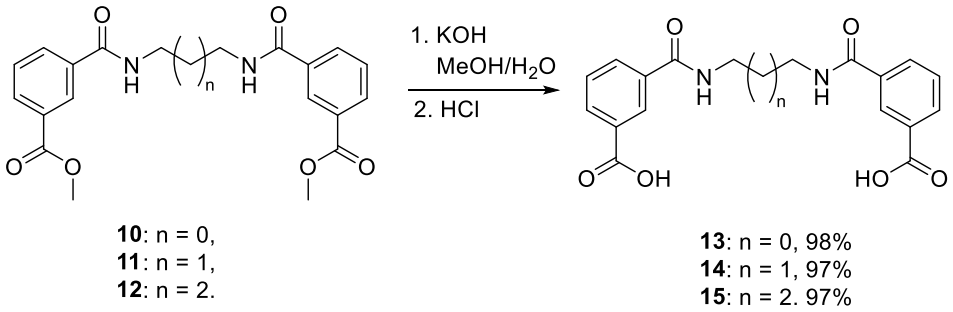

**Scheme S1**. Synthesis of **9**–**11**.

**General synthetic method for 10–12:** To a mixture of mono methyl isophthalate (5.00 g, 27.75 mmol) and $SOCl_2$ (6.60g, 55.48 mmol) in dichloromethane (40 mL) one drop of DMF was added. The resulting solution was refluxed overnight under $N_2$ atmosphere. After the volatiles were removed under reduced pressure, the residue was dissolved in dry THF (100 mL) and added slowly at 0 °C to a solution of **6** (**7** or **8)** (13.49 mmol) and triethylamine (5.50 g, 54.35 mmol) in dry THF (150 mL) under $N_2$ atmosphere. Then the resulting mixture was stirred at room temperature for further 12 h. After the solvent was removed under reduced pressure, the residue was suspended in massive water, stirred vigorous overnight and filtered. The filter cake was washed with massive water and small amount of methanol consecutively, then dried under oven at 60 °C overnight to give the pure product as white solid without further purification.

**10**: 40%. $^{1}H$ NMR (400 MHz, $CDCl_3$) δ 8.45 (s, 2H, ArH), 8.18 (d, $J$ = 7.6 Hz, 2H, ArH), 8.07 (d, $J$ = 8.0 Hz, 2H, ArH), 7.56 (d, $J$ = 7.6 Hz, 2H, ArH), 3.95 (s, 6H, $CH_3$), 3.77 (brs, 4H, $CH_2$) ppm. $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 168.0, 166.4, 134.4, 132.8, 131.8, 130.8, 129.1, 128.1, 52.5, 41.3 ppm. HRMS (ESI) m/z 383.1249 $[M - H]^-$ calcd for $C_{20}H_{19}N_2O_6^-$, found 383.1244.

**11**: 46%. $^{1}$H NMR (400 MHz, DMSO–$d_6$) δ 8.75 (t, $J$ = 5.6 Hz, 2H, amide–H), 8.44 (t, $J$ = 1.6 Hz, 2H, ArH), 8.12 (dd, $J$ = 8.0, 1.6 Hz, 4H, ArH), 7.64 (t, $J$ = 8.0 Hz, 2H, ArH), 3.89 (s, 6H, OMe), 3.36–3.34 (m， 4H, $CH_2$), 1.85 – 1.79 (m, 2H, $CH_2$) ppm. $^{13}$C NMR (100 MHz, DMSO–$d_6$) δ 165.8, 165.2, 135.0, 131.8, 131.6, 129.8, 128.9, 127.8, 52.3, 37.3, 29.0 ppm. HRMS (ESI) m/z 397.1405 [M – H]$^-$ calcd for $C_{21}H_{21}N_2O_6^-$, found 397.1399.

**12**: 44%. $^{1}$H NMR (400 MHz, DMSO–$d_6$) δ 8.72 (t, $J$ = 5.6 Hz, 2H, amide–H), 8.44 (t, $J$ = 1.6 Hz, ArH), 8.12 (t, $J$ = 8.0 Hz, 4H, ArH), 7.63 (t, $J$ = 8.0 Hz, 4H, ArH), 3.88 (s, 6H, $CH_3$), 3.34–3.30 (m, 8H, $CH_2$) ppm. $^{13}$C NMR (100 MHz, DMSO–$d_6$) δ165.8, 165.1, 135.1, 131.9, 131.5, 129.8, 128.9, 127.9, 52.3, 39 (hidden in DMSO), 26.6 ppm. HRMS (ESI) m/z 411.1562 [M – H]$^-$ calcd for $C_{22}H_{23}N_2O_6^-$, found 411.1557.




**Scheme S2.** Synthesis of **13**–**15**.

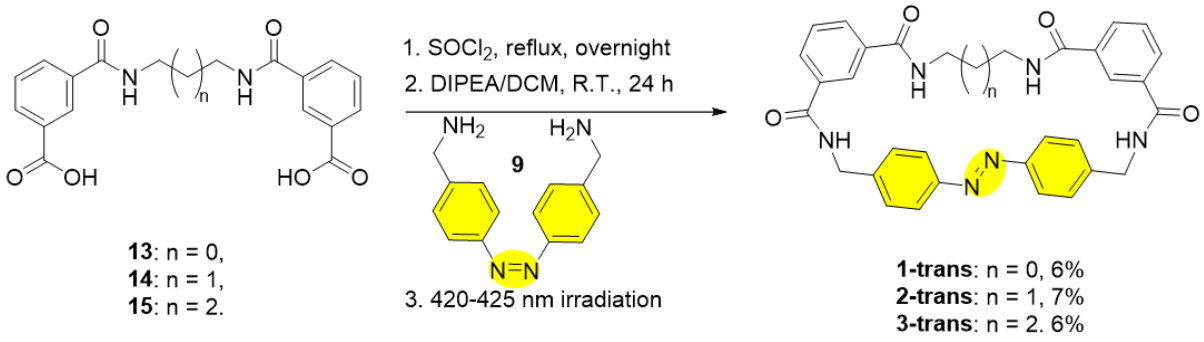
**General synthetic method for 13–15: 10** (**11** or **12**) (5.00 g) was suspended in a solution of MeOH (100 mL) and aqueous KOH (1 M, 100 mL), stirred at 20 °C for 31 h (14 h or 92 h). After acidification (pH < 3) with aqueous HCl (1 M), the suspension was filtered, washed with HCl (1 M) and dried under oven at 60 °C overnight to obtain the product as white solid without further purification.

**13**: 98%. $^{1}$H NMR (400 MHz, DMSO–$d_6$) δ 13.17 (brs, 2H, COOH), 8.82 (t, $J$ = 5.2 Hz, 2H, amide–NH), 8.45 (t, $J$ = 1.6 Hz, 2H, ArH), 8.10 – 8.06 (m, 4H, ArH), 7.61 (t, $J$ = 7.6 Hz, 2H, ArH), 3.48–3.47 (m, 4H, $CH_2$) ppm. $^{13}$C NMR (100 MHz, DMSO–$d_6$) δ 166.9, 165.7, 134.9, 131.8, 131.6, 130.9, 128.7, 128.1, 39.1 ppm. HRMS (ESI) m/z 355.0936 [M – H]$^-$ calcd for $C_{18}H_{15}N_2O_6^-$, found 355.0931.

**14**: 97%. $^{1}$H NMR (400 MHz, DMSO–$d_6$) δ 13.18 (s, 2H, COOH), 8.72 (t, J = 5.6 Hz, 2H, amide–NH), 8.44 (t, J = 1.6 Hz, ArH), 8.09–8.06 (m, 4H, ArH), 7.61 (t, J = 7.6 Hz, 2H, ArH), 3.37 (q, J = 6.4 Hz, 4H, $CH_2$), 1.85–1.78 (m, 2H, CH2) ppm. 13C NMR (100 MHz, DMSO–$d_6$) δ 166.9, 165.4, 134.9, 131.8, 131.5, 130.9, 128.7, 128.0, 37.3, 29.1 ppm. HRMS (ESI) m/z 369.1092 [M – H]$^-$ calcd for $C_{19}H_{17}N_2O_6^-$, found 369.1087.

**15**: 97%. $^{1}$H NMR (400 MHz, $D_2O$) δ 8.14 (t, $J$ = 2.0 Hz, 2H, ArH), 8.00 (d, $J$ = 8.0 Hz, 2H, ArH), 7.79 (d, $J$ = 8.0 Hz, 2H, ArH), 7.51 (t, $J$ = 7.6 Hz, 2H, ArH), 3.46 – 3.38 (m, 4H, $CH_2$), 1.70 (p, $J$ = 3.1 Hz, 4H, $CH_2$)

ppm. $^{13}$C NMR (100 MHz, DMSO–$d_6$) δ 166.9, 165.3, 135.0, 131.7, 131.5, 130.9, 128.7, 128.0, 39 (hidden in DMSO), 26.6 ppm. HRMS (ESI) m/z 383.1249 $[M - H]^-$ calcd for $C_{20}H_{19}N_2O_6^-$, found 383.1244.




**Scheme S3.** Synthesis of **1**–***trans***, **2**–***trans***, and **3**–***trans***.

**General synthetic method for 1–3: 13** (**14** or **15**) (2.44 mmol) was suspended in 20 mL of $SOCl_2$ and refluxed overnight. After the volatiles were removed *in vacuo*, the off–white solid residues were dissolved in dichloromethane (150 mL). The resulting solution and **9** (586 mg, 2.44 mmol) in dry dichloromethane (150 mL) were added dropwise in parallel into a solution of DIPEA (1.58 g, 12.25 mmol) in dry dichloromethane (200 mL). The reaction was then stirred at room teperature for 24 h under $N_2$ atmosphere. Subsequently, the reaction mixture was diluted with dichloromethane (500 mL) and washed with 1 M of HCl (3 × 500 mL), water (500 mL), 1 M of NaOH (3 × 500 mL), water (500 mL), and 100 mL brine consecutively. The combined organic solution was exposed to 420–425 nm light irradiation under $N_2$ atmosphere and stired until the photostationary state (PSS) was achieved. Then the resulting solution was concentrated *in vacuo* to give the corresponding mixture of *trans* and *cis* isomers. After the resulting solid was suspended in methanol (80 mL) and ultrasounded for 1 h, filtered, and washed with methanol. The corresponding pure ***trans*** compounds were obtained as orange solid without further purification.

Notably, **1**-***cis***, **2**-***cis***, and **3**-***cis*** were successfully obtained from **1**–***trans***, **2**-***trans***, and **3**-***trans***, respetively, by 365–370 nm light irradiation.

**1–trans**: $^1$H NMR (400 MHz, DMSO–$d_6$) δ 9.00 (t, $J$ = 6.0 Hz, 2H, amide–H), 8.51 (s, 2H, amide–H), 7.85–7.76 (m, 10H, ArH), 7.56 (d, $J$ = 8.4 Hz, 4H, ArH), 7.48 (t, $J$ = 8.0 Hz, 2H, ArH), 4.40 (d, $J$ = 6.0 Hz, 4H, $CH_2$), 3.3 (4H, $CH_2$, hidden in DHO) ppm. $^{13}$C NMR (100 MHz, DMSO–$d_6$) δ 166.5, 166.1, 151.5, 143.6, 135.1, 135.0, 130.0, 129.9, 128.9, 128.3, 126.2, 122.8, 43.4, 39.0 (hidden in DMSO) ppm.

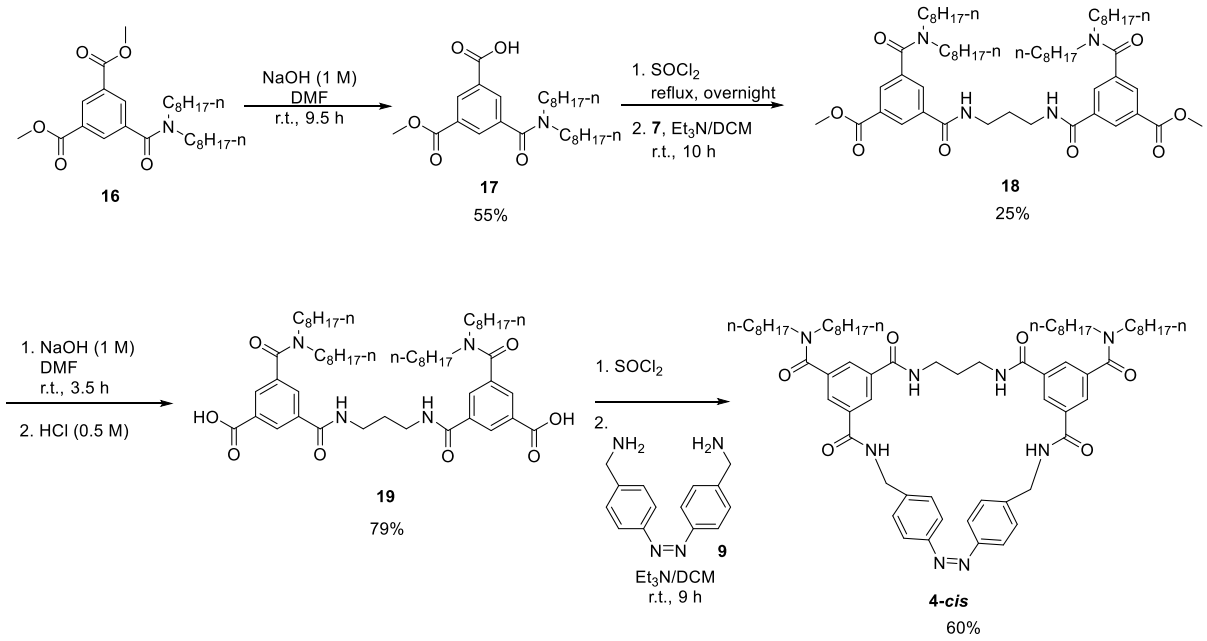
**1–cis**: $^1$H NMR (400 MHz, DMSO–$d_6$) δ 9.17 (t, $J$ = 6.0 Hz, 2H, amide–H), 8.55 (brs, 2H, amide–H), 8.27 (s, 2H, ArH), 8.05 (d, $J$ = 7.6 Hz, 2H, ArH), 7.96 (d, $J$ = 7.6 Hz, 2H, ArH), 7.56 (t, $J$ = 7.6 Hz, 2H, ArH), 7.25 (d, $J$ = 8.4 Hz, 4H, ArH), 6.86 (d, $J$ = 8.4 Hz, 4H, ArH), 4.46 (d, $J$ = 6.0 Hz, 4H, ArH), 3.50–3.48 (m, 4H) ppm. $^3$C NMR (100 MHz, DMSO–$d_6$) δ 166.2, 165.5, 152.2, 138.6, 135.1, 133.7, 130.4, 129.6, 128.5, 127.8, 126.1, 120.0, 42.1, 39.0 (hidden in DMSO) ppm. HRMS (ESI) m/z 559.2099 $[M - H]^-$ calcd for $C_{32}H_{27}N_6O_4^-$, found 559.2088, 898.4543 $[M + TBA + SO_4]^-$ calcd for **1**, found 898.4533.

**2–*trans***: $^{1}$H NMR (400 MHz, DMSO–$d_6$) δ 9.05 (t, $J$ = 6.4 Hz, 2H, amide–H), 8.44 (t, $J$ = 5.6 Hz, 2H, amide–H), 7.87–7.78 (m, 8H, ArH), 7.72 (t, $J$ = 1.6 Hz, 2H, ArH), 7.57 (d, $J$ = 8.0 Hz, 4H, ArH), 7.51 (t, $J$ = 7.6 Hz, 2H, ArH), 4.42 (d, $J$ = 6.0 Hz, 4H, $CH_2$), 3.17–3.12 (m, 4H, $CH_2$), 1.67–1.59 (m, 2H, $CH_2$) ppm. $^{13}$C NMR (100 MHz, DMSO–$d_6$) δ 166.95, 165.49, 151.17, 143.70, 135.90, 134.74, 129.79, 129.65, 128.92, 128.33, 125.70, 122.70, 43.32, 37.46, 29.13 ppm.

**2–*cis***: $^{1}$H NMR (400 MHz, DMSO–$d_6$) δ 9.17 (t, $J$ = 6.0 Hz, 2H, amide–H), 8.50 (t, $J$ = 5.6 Hz, 2H, amide–H), 8.28 (s, 2H, ArH), 8.04 (d, $J$ = 7.6 Hz, 2H, ArH), 7.96 (d, $J$ = 7.6 Hz, 2H, ArH), 7.58 (t, J = 7.6 Hz, 2H, ArH), 7.25 (d, $J$ = 8.0 Hz, 4H, ArH), 6.88 (d, $J$ = 8.0 Hz, 4H, ArH), 4.54 (d, $J$ = 6.0 Hz, 4H, $CH_2$), 3.3 (4H, $CH_2$, hidden in DHO), 1.79 – 1.76 (m, 2H, $CH_2$). $^{13}$C NMR (100 MHz, DMSO–$d_6$) δ 166.1, 165.8, 152.2, 138.5, 135.1, 134.0, 130.0, 129.9, 128.6, 127.4, 125.8, 120.0, 42.0, 36.3, 29.0. HRMS (ESI) m/z 573.2256 $[M - H]^-$ calcd for $C_{33}H_{29}N_6O_4^-$, found 573.2244.

**3–*trans***: $^{1}$H NMR (400 MHz, DMSO–$d_6$) δ 9.12 (t, $J$ = 6.0 Hz, 2H, amide–H), 8.49 (t, $J$ = 5.2 Hz, amide–H), 7.91 – 7.84 (m, 6H, ArH), 7.81 (d, $J$ = 8.4 Hz, 4H, ArH), 7.58 (d, $J$ = 8.4 Hz, 4H, ArH), 7.51 (t, $J$ = 8.0 Hz, 2H, ArH), 4.42 (d, $J$ = 6.0 Hz, 4H, $CH_2$), 3.17 – 3.16 (m, 4H, $CH_2$), 1.43 (brs, 4H, CH2) ppm. $^{13}$C NMR (100 MHz, DMSO–$d_6$) δ 166.5, 165.5, 151.1, 143.7, 135.3, 134.8, 130.1, 129.7, 128.9, 128.3, 125.7, 122.6, 43.3, 39 (hidden in DMSO), 27.1 ppm.

**3–*cis***: $^{1}$H NMR (400 MHz, DMSO–$d_6$) δ 9.15 (t, $J$ = 6.0 Hz, 2H, amide–H), 8.50 (t, $J$ = 5.6 Hz, 2H, amide–H), 8.30 (s, 2H, ArH), 8.03 (d, $J$ = 7.6 Hz, 2H, ArH), 7.96 (d, $J$ = 7.6 Hz, 2H, ArH), 7.56 (t, $J$ = 7.6 Hz, 2H, ArH), 7.23 (d, $J$ = 8.4 Hz, 4H, ArH), 6.85 (d, $J$ = 8.4 Hz, 4H, ArH), 4.48 (d, $J$ = 6.0 Hz, 4H, $CH_2$), 3.3 (4H, $CH_2$, hidden in DHO), 1.56 (brs, 4H, $CH_2$) ppm. $^{13}$C NMR (100 MHz, DMSO–$d_6$) δ 165.7, 165.6, 152.2, 138.6, 134.9, 133.9, 130.0, 129.8, 128.5, 127.4, 126.0, 120.0, 41.9, 39 (hidden in DMSO), 26.8 ppm. HRMS (ESI) m/z 587.2412 $[M - H]^-$ calcd for $C_{34}H_{31}N_6O_4^-$, found 587.2400, 685.2086 $[M + H + SO_4]^-$ calcd for **3**, found 685.2070, and 1273.4571 $[2M + H + SO_4]^-$ calcd for **3**, found 1273.4544.




**Scheme S4.** Synthesis of **4–cis**.

Compound **16** was prepared according to the literature.[5]

Synthesis of compound **17**

To a solution of **16** (2.631 g, 5.70 mmol) in DMF (220 mL), 5.1 mL (5.10 mmol) of NaOH aquous solution (1M) was added at the rate of 0.013 mL/min by using an injection pump. After the mixture was stirred for futher 3 h, the solvent was removed under reduced pressure. The resulting resudue was redissoved in 200 mL of ethyl acetate and washed with 100 mL of aquous solution of HCl (0.5 M), then 100 mL of brine. The organic phase was separated and dried over anhydrous $Na_2SO_4$ for 1.5 hour. After the solvent was removed under reduced pressure, the residue was purified by column chromatography over silica gel (eluent: EA/DCM (15/100 - 35/100, v/v) to give 1.402 g (3.13 mmol, 55% yield) of **17** as colorless oil. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.75 (s, 1H, ArH), 8.28 (s, 1H, ArH), 8.26 (s, 1H, ArH), 3.96 (s, 3H, $OCH_3$), 3.44 (t, $J$ = 7.6 Hz, 2H, $NCH_2$), 3.10 (t, $J$ = 7.6 Hz, 2H, $NCH_2$), 1.68 (s, 2H, $CH_2$), 1.52 (s, 2H , $CH_2$), 1.36 – 1.11 (m, 20H, $CH_2$), 0.89 – 0.82 (m, 6H, $CH_3$). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 169.9, 167.8, 165.3, 137.2, 132.0, 131.9, 131.6, 131.0, 130.8, 52.3, 49.3, 45.3, 31.7, 31.5, 29.2, 29.1, 28.8, 28.8, 28.5, 27.3, 26.9, 26.3, 22.5, 22.4, 13.9, 13.9 ppm. HRMS (ESI) m/z 446.2912 $[M - H]^-$ calcd for **17**, found 446.2907.

Synthesis of compound **18**

**17** (5.162 g, 11.53 mmol) was dissolved in 20 mL of $SOCl_2$ and refluxed overnight. After the volatiles were removed in *vacuo*, the residue was dissolved in dichloromethane (50 mL), to which a solution of $Et_3N$ (4.165g, 41.16 mmol) and **6** (427 mg, 5.76 mmol) in dichloromethane (30 mL) was added at 0 °C in 2h. The reaction mixture was stirred at RT for further 10 h. The solution was then concentrated in *vacuo* and the resulting resudue was dissolved in 200 mL of ethyl acetate, followed by consecutive wash with 0.5 M of HCl (3 × 200 mL), water (200 mL), saturated $NaHCO_3$ (3 × 200 mL), water (500 mL), and brine (100 mL). After the organic phase was separated and dried over anhydrous $Na_2SO_4$, the solvent was removed in *vacuo*. The residue was then subject to column chromatography over silica gel (eluent: EA/DCM (33/100 - 67/100, v/v) to give 2.660 g (2.85 mmol, 25% yield) of **18** as light yellow oil. $^1$H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 2H, ArH), 8.06 (s, 2H, ArH), 8.04 (s, 2H,

ArH), 7.90 (t, $J$ = 6.3 Hz, 2H, CONH), 3.90 (s, 6H, $OCH_3$), 3.49 – 3.42 (m, 8H, $NCH_2$), 3.13 (t, $J$ = 7.7 Hz, 4H, $NCH_2$), 1.84 – 1.78 (m, 2H, $CH_2$), 1.67 - 1.57 (m, 4H, $CH_2$), 1.48 (t, $J$ = 7.4 Hz, 4H, $CH_2$), 1.28 (d, $J$ = 23.5 Hz, 22H, $CH_2$), 1.10 (d, $J$ = 15.6 Hz, 18H, $CH_2$), 0.89 – 0.76 (m, 12H, $CH_3$) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) δ 169.9, 166.3, 165.7, 137.8, 135.4, 130.8, 130.1, 129.8, 128.8, 52.6, 49.4, 45.3, 36.7, 31.9, 31.7, 29.7, 29.4, 29.3, 29.1, 28.7, 27.6, 27.2, 26.6, 22.7, 22.6, 14.1, 14.1 ppm. HRMS (ESI) m/z 931.6529 $[M - H]^-$ calcd for **18**, found 931.6521, 967.6296 $[M + Cl]^-$ calcd for **18**, found 967.6283.

Synthesis of compound **19**

To a solution of **18** (2.660 g, 2.85 mmol) in DMF (100 mL), 5.7 mL (5.70 mmol) of NaOH aquous solution (1M) was added. The mixture was stirred at ambient temperature for 3.5 h. After removal of solvent in *vacuo*, the resulting resudue was dissolved in 100 mL of ethyl acetate and washed with 50 mL of HCl (0.5 M) and brine (100 mL), respecitvely. The organic phase was separated and dried over anhydrous $Na_2SO_4$. After the solvent was removed under reduced pressure, 2.05 g (2.26 mmol, 79% yield) of pure **19** was obtained as light yellow oil without futher purification. $^1$H NMR (400 MHz, $CDCl_3$) δ 10.66 (brs, 2H, COOH), 8.51 (s, 2H, ArH), 8.33 (brs, 2H, NH), 8.15 (s, 2H, ArH), 8.09 (s, 2H, ArH), 3.45 (brs, 8H, $NCH_2$), 3.14 (brs, 4H, $NCH_2$), 1.87 (s, 2H, $CH_2$), 1.62 (brs, 4H, $CH_2$), 1.47 (brs, 4H, $CH_2$), 1.34 – 1.24 (m, 22H, $CH_2$), 1.17 – 1.06 (m, 18H, $CH_2$), 0.84 (t, $J$ = 7.2 Hz, 6H, $CH_3$), 0.76 (t, $J$ = 7.1 Hz, 6H, $CH_3$) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) δ 170.6, 167.7, 166.6, 136.9, 135.1, 131.0, 130.5 (2C), 129.5, 49.5, 45.5, 37.6, 31.9, 31.7, 29.4, 29.3, 29.0, 28.6, 27.5, 27.2, 26.5, 22.7, 22.6, 14.1, 14.1 ppm. HRMS (ESI) m/z 903.6216 $[M - H]^-$ calcd for **19**, found 903.6212.

Synthesis of compound **4-*cis***

**19** (954 mg, 1.05 mmol) was dissolved in 20 mL of $SOCl_2$ and the mixture was refluxed overnight. After the volatiles were removed *in vacuo*, the oil residue was dissolved in dry dichloromethane (100 mL). The resulting solution and the readily formed **9-*cis*** (253 mg, 1.05 mmol) in dry dichloromethane (100 mL) were added dropwise in parallel into a solution of $Et_3N$ (531 mg, 5.25 mmol) in dry dichloromethane (300 mL) at 20°C over 6 h. The reaction mixture was then stirred for further 3 h at room teperature under $N_2$ atmosphere. Subsequently, the reaction mixture was washed with 1 M of HCl (3 × 200 mL), water (300 mL), saturated $NaHCO_3$ aqueous solution (3 × 200 mL), water (300 mL), and 100 mL of brine, consecutively. After the organic phase was separated, dried over anhydrous $Na_2SO_4$, the solvent was removed to give 699 mg (0.63 mmol, 60% yield) of crude product **19** as orange solid. Pure **19** could be obtained by preparative thin layer chromatography (DCM:MeOH:$Et_3N$ = 50 :1:1). $^1$H NMR (400 MHz, $CDCl_3$) δ 8.33 (s, 2H, ArH), 8.01 (s, 2H, ArH), 7.99 (s, 2H, ArH), 7.69 (brs, 4H, amide-NH), 7.18 (d, $J$ = 8.0 Hz, 4H, Azo-ArH), 6.79 (d, $J$ = 8.0 Hz, Azo-ArH), 4.57 (d, $J$ = 5.6 Hz, 4H, $NCH_2$), 3.48 – 3.41 (m, 8H, $NCH_2$), 3.20 – 3.17 (m, 4H, $NCH_2$), 1.70 – 1.62 (m, 6H, $CH_2$, hidden in HDO), 1.50 (brs, 4H, $CH_2$), 1.35 – 1.67 (m, 40H, $CH_2$), 0.89 – 0.82 (m, 12H, $CH_3$). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 170.5, 166.4, 166.0, 152.8, 137.8, 135.2, 134.8, 128.9, 128.5, 127.5, 126.6, 126.0, 120.7, 49.5, 46.4, 45.3, 43.1, 36.2, 31.9, 31.8, 29.5, 29.4, 29.2, 28.8, 27.6, 27.2, 26.7, 22.7, 22.7, 14.2, 14.2, 8.7. HRMS (ESI) m/z 1109.7526 $[M + H]^+$ calcd for **4-*cis***, found 1109.7504.

## 3. Stability of 1–*trans*, 2-*trans*, and 3-*trans*

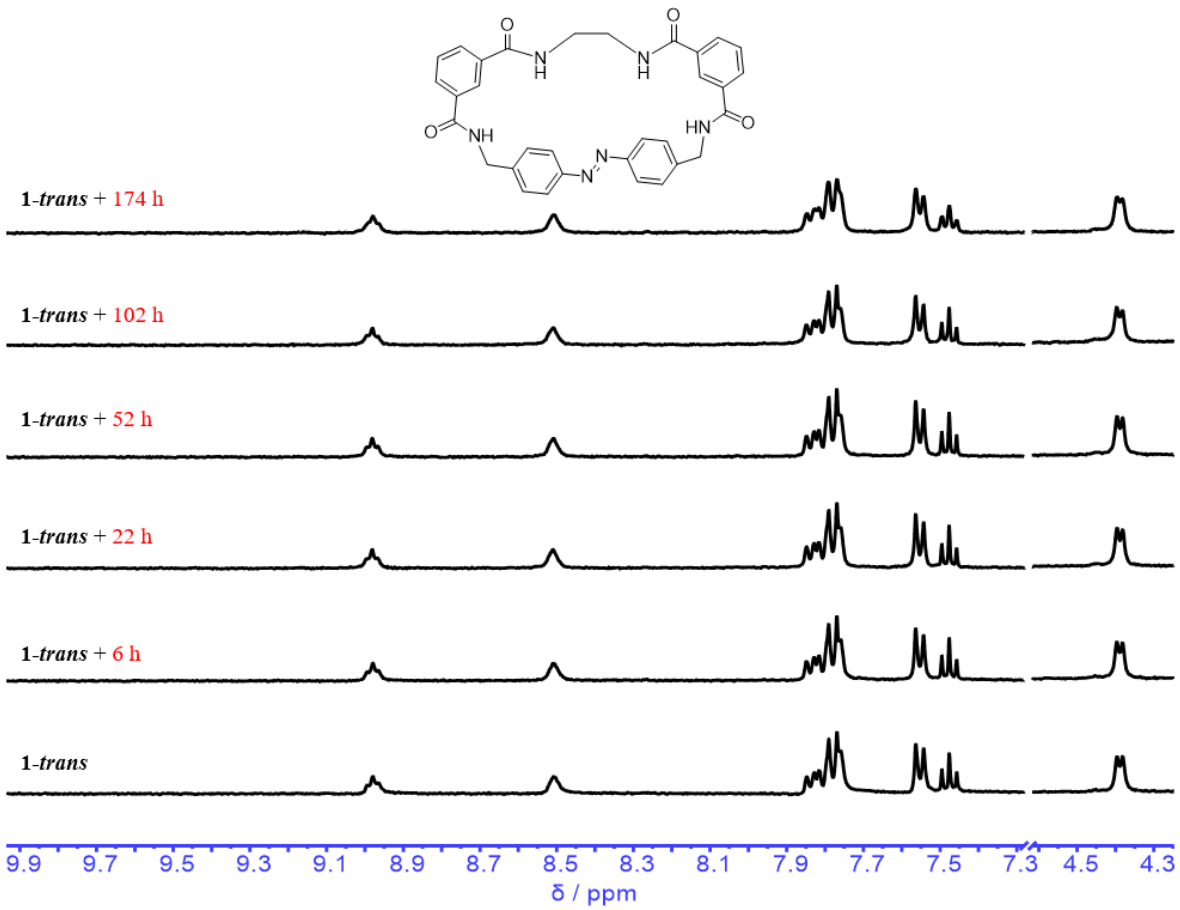



**Fig. S1.** Partial $^{1}$H NMR spectra of **1**–***trans*** (1.0 mM in DMSO–$d_6$) recorded under dark conditions at room temperature after letting stand for 6 h, 22 h, 52 h, 102 h, and 174 h, respectively.

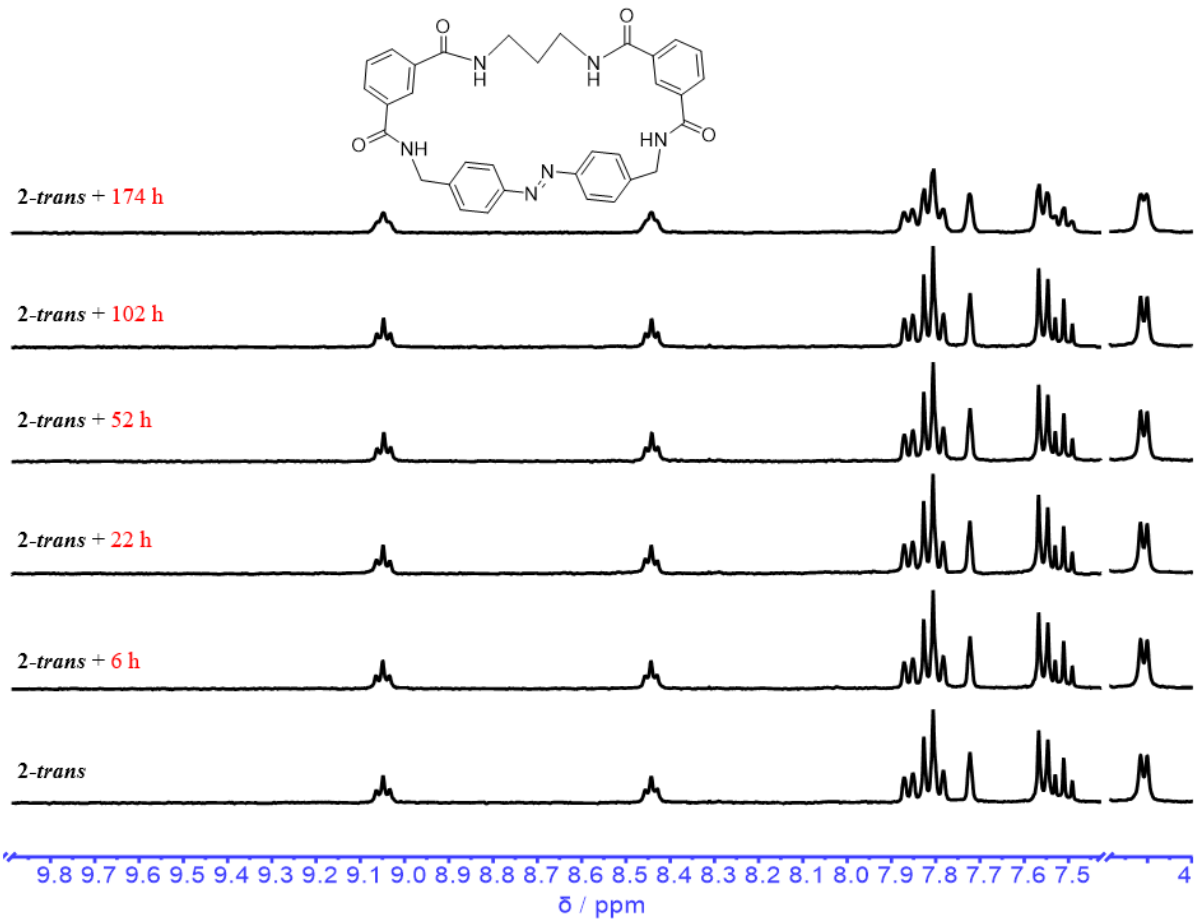



**Fig. S2.** Partial $^{1}$H NMR spectra of **2**–***trans*** (1.0 mM in DMSO–$d_6$) recorded under dark conditions at room temperature after letting stand for 6 h, 22 h, 52 h, 102 h, and 174 h, respectively.

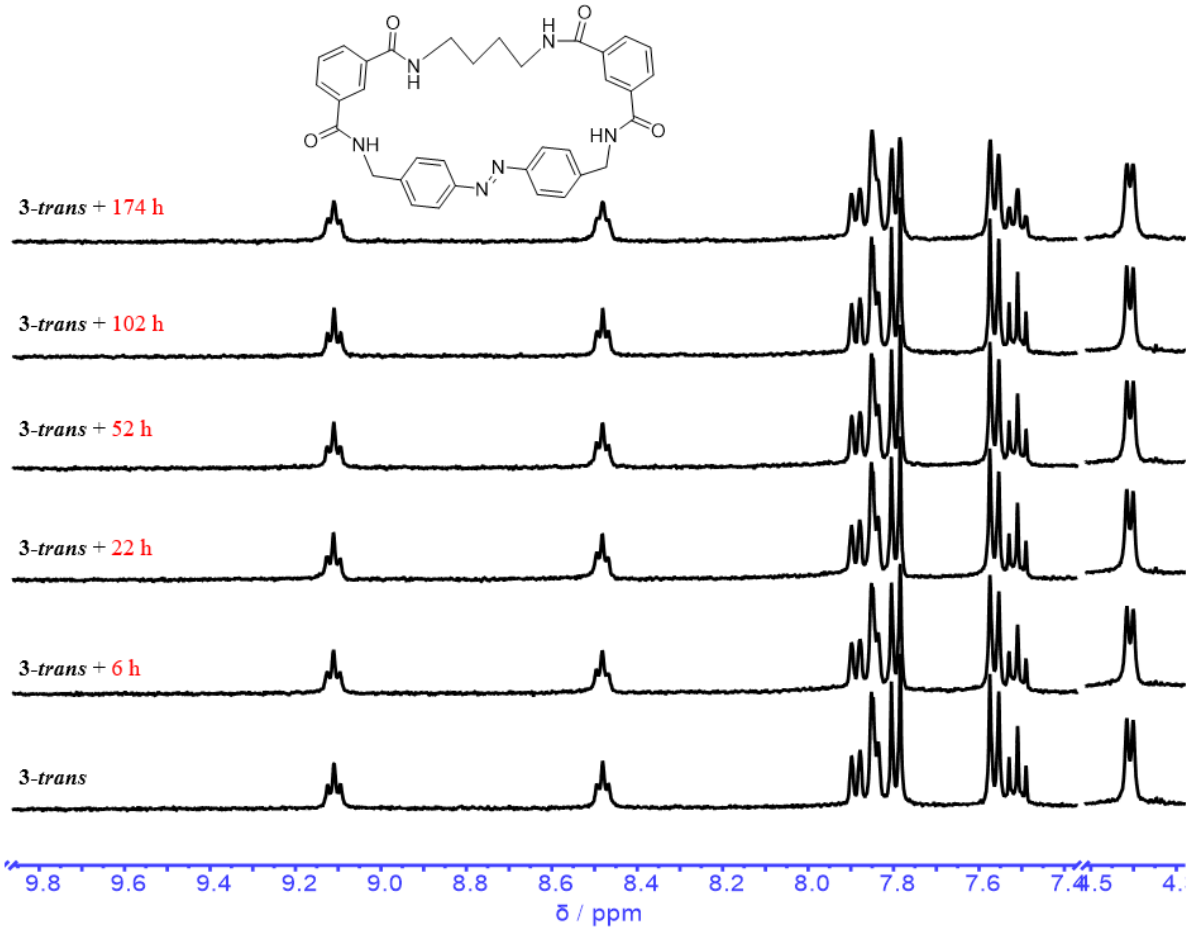



**Fig. S3.** Partial $^{1}$H NMR spectra of **3–*trans*** (1.0 mM in DMSO–$d_6$) recorded under dark conditions at room temperature after letting stand for 6 h, 22 h, 52 h, 102 h, and 174 h, respectively.

## 4. Photoisomerization of the azomacrocycles

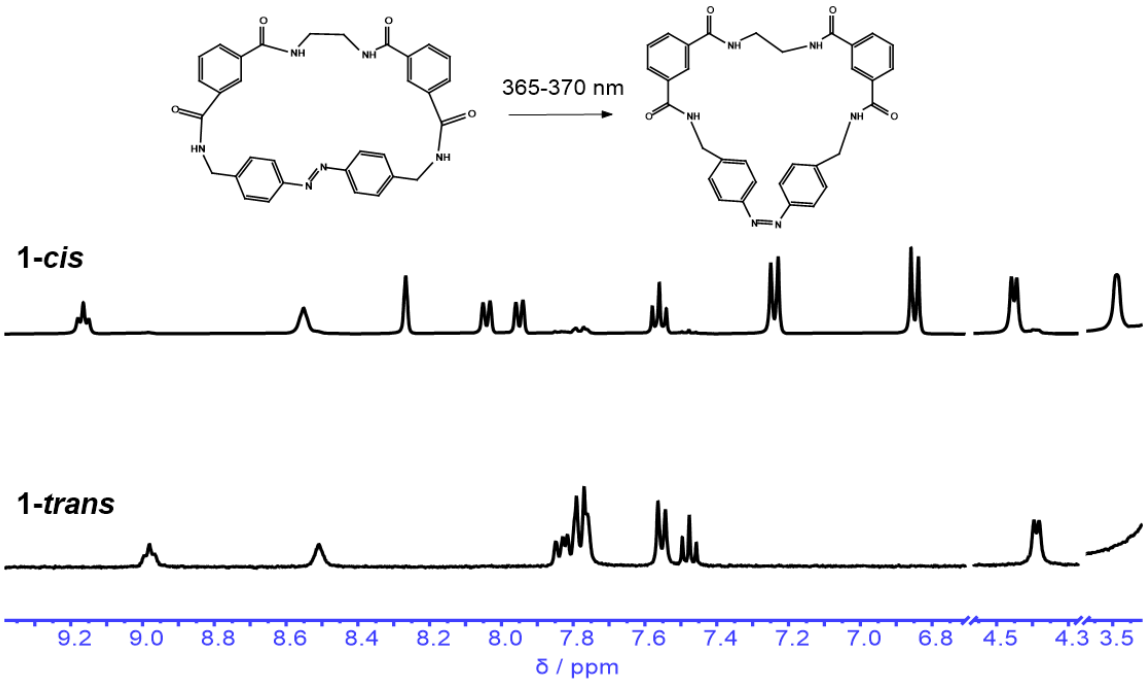



**Fig. S4.** Partial $^{1}$H NMR spectra of **1**–***trans*** (1.0 mM in DMSO–$d_6$) recorded under UV light irradiation of 365–370 nm UV light over 0 min (bottom) and 5 min (top) at room temperature.

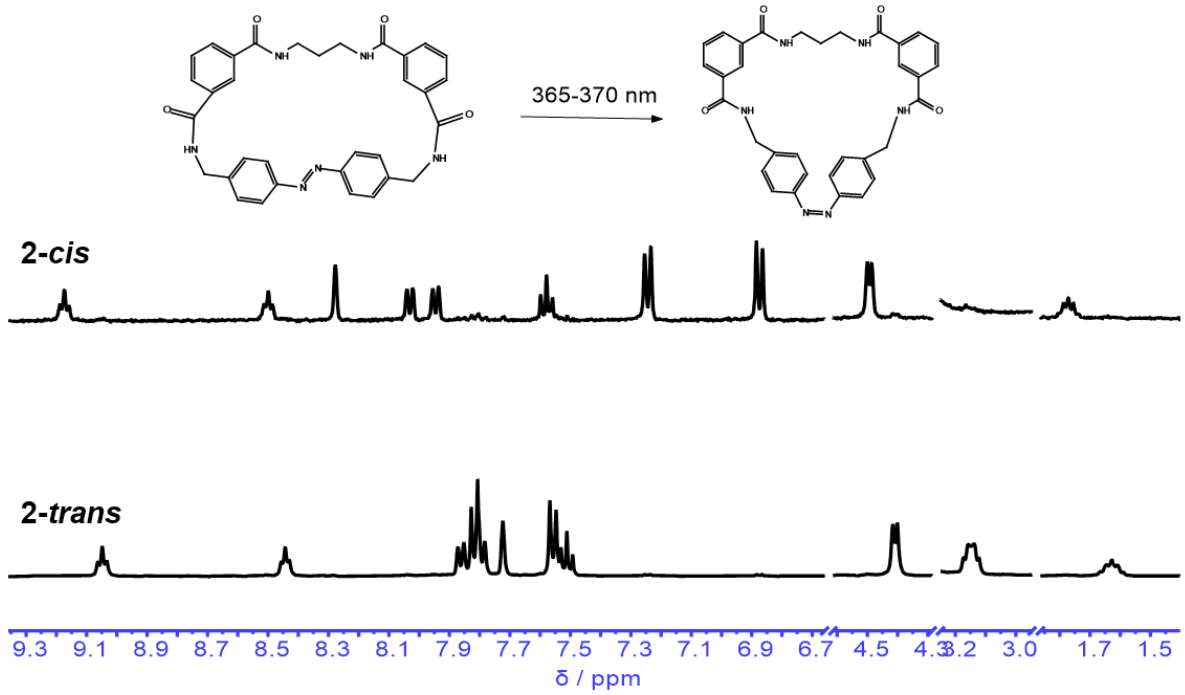



**Fig. S5.** Partial $^{1}$H NMR spectra of **2**–***trans*** (1.0 mM in DMSO–$d_6$) recorded under UV light irradiation of 365–370 nm UV light over 0 min (bottom) and 5 min (top) at room temperature.

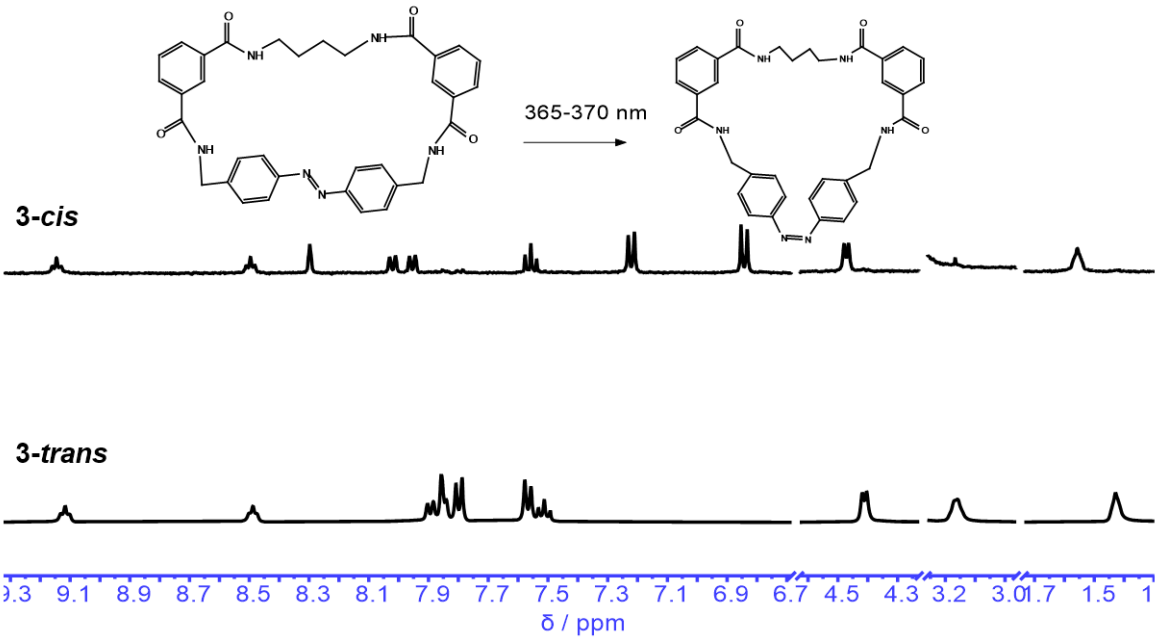



**Fig. S6.** Partial $^{1}$H NMR spectra of **3–*trans*** (1.0 mM in DMSO–$d_6$) recorded under UV light irradiation of 365–370 nm UV light over 0 min (bottom) and 5 min (top) at room temperature.

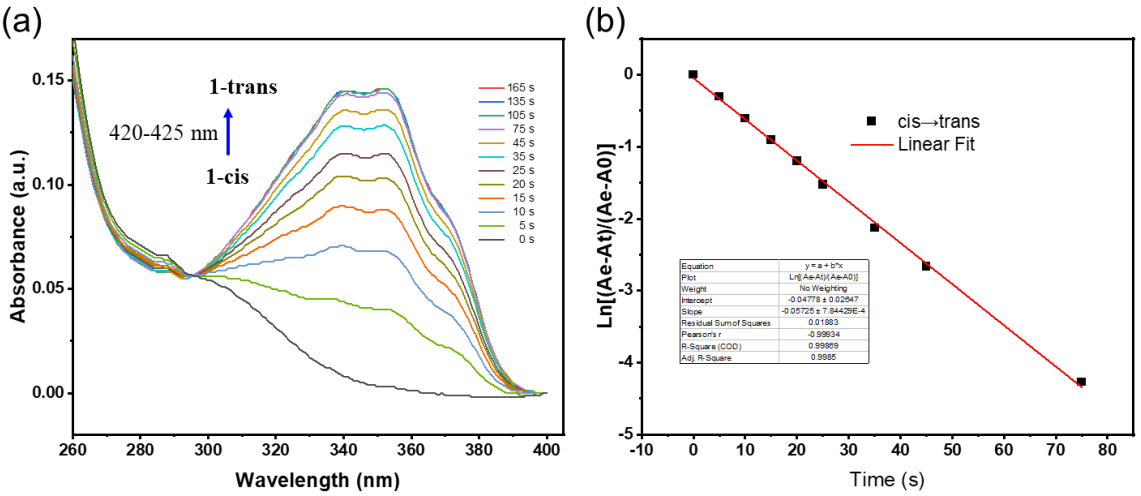



**Fig. S7.** UV–Vis spectra and photoisomerization kinetics of **1-cis** (10 μM) in DMSO under visible light (420-425 nm, 100 W) irradiation. This photo *cis*→*trans* rate constant was calculated to be $k_1 = 0.05725\ s^{-1}$.

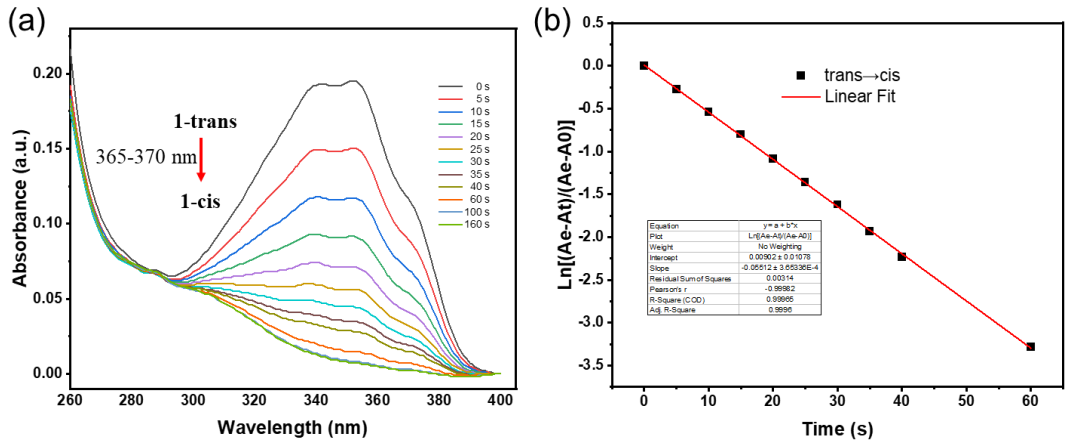



**Fig. S8.** UV–Vis spectra and photoisomerization kinetics of **1-trans** (10 μM) in DMSO under visible light (365-370 nm, 100 W) irradiation. This photo *trans→cis* rate constant was calculated to be $k_1 = 0.05512\ s^{-1}$.

## 5. Calculations, crystal structures and binding studies

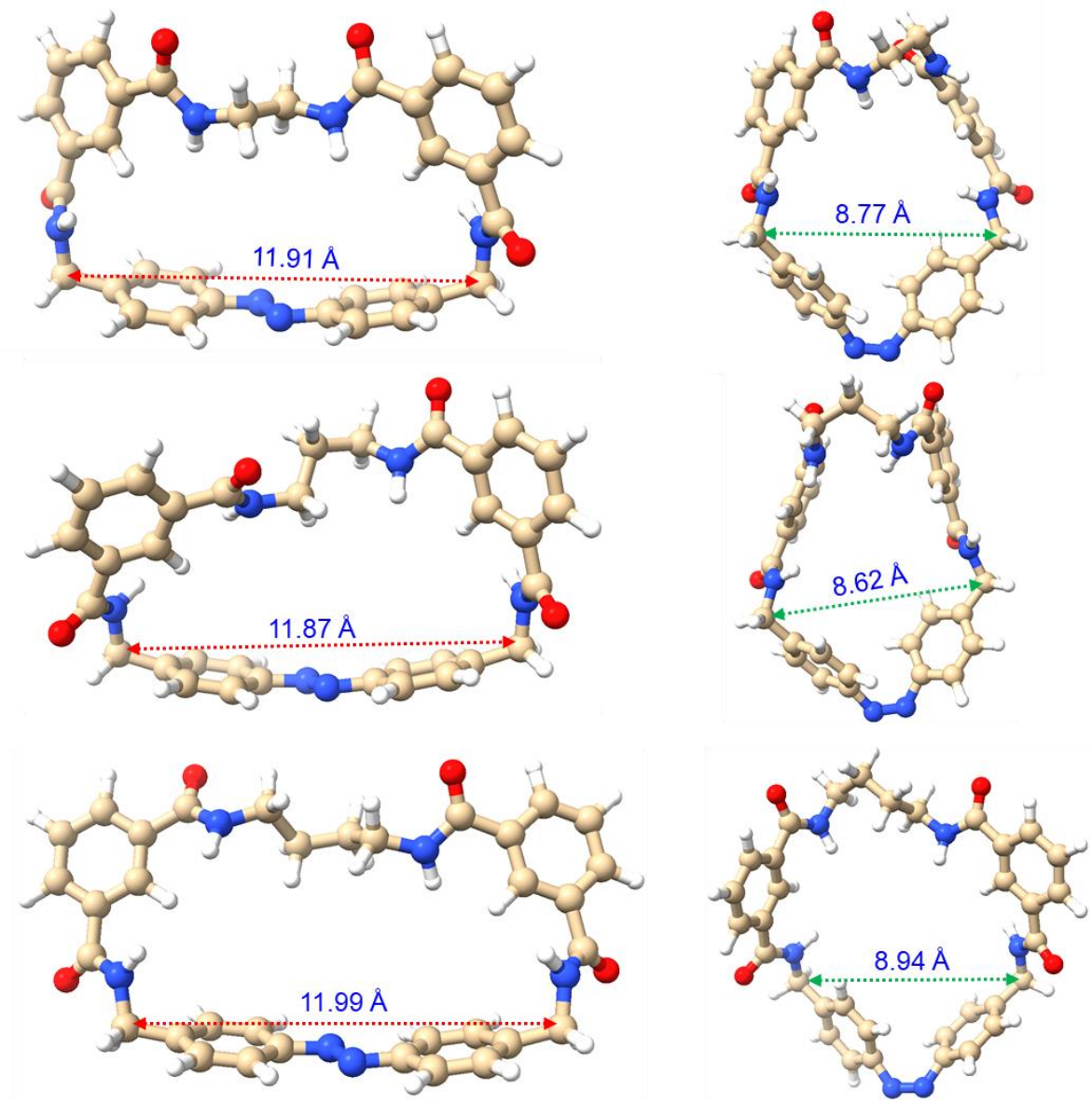



**Fig. S9.** DFT–optimized structures of **1**–***trans***, **2**–***trans***, **3**–***trans***, **1**–***cis***, **2**–***cis***, and **3**–***cis***.

**Table S1.** Relative energies (kJ/mol) of **1**–***trans*** and **1**–***cis***, **2**–***trans*** and **2**–***cis***, **3**–***trans*** and **3**–***cis***.

| | 1 | 2 | 3 |
|---|---|---|---|
| trans | 0 | 0 | 0 |
| cis | 52.51 | 57.76 | 63.01 |

According to Table S1, **1**–***trans***, **2**–***trans*** and **3**–***trans*** are energetically stable than **1**–***cis***, **2**–***cis***, and **3**–***cis***, respectively.

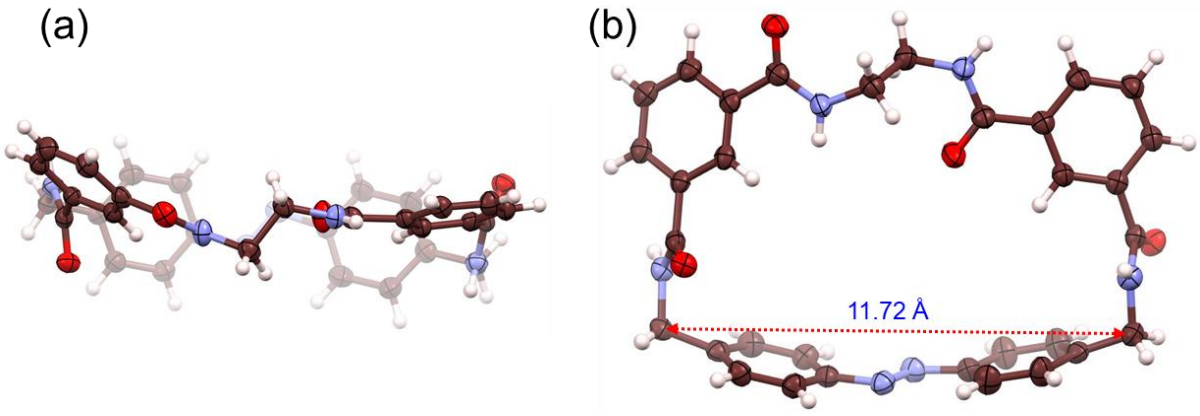



**Fig. S10.** (a) Top view and (b) front view of the single crystal structure of **1**–***trans***. Displacement ellipsoids are scaled to the 50% probability level. Solvent molecules are omitted for clarity

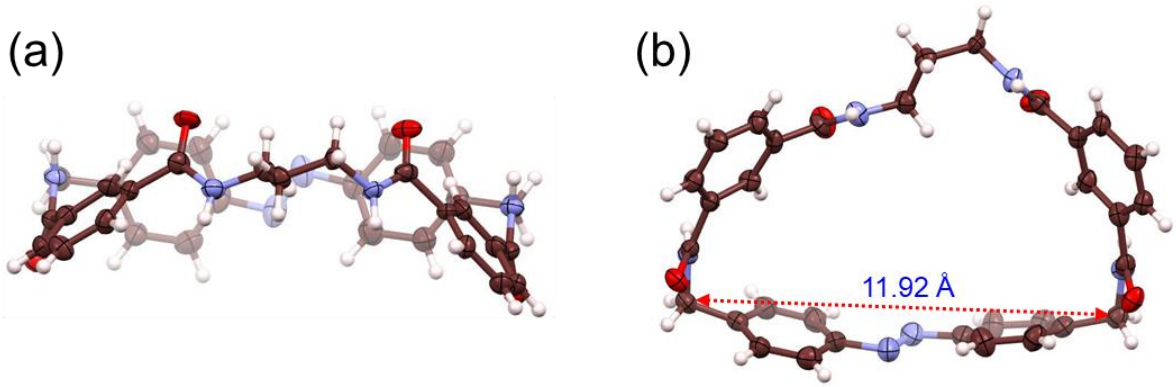



**Fig. S11.** (a) Top view and (b) front view of the single crystal structure of **2**–***trans***. Displacement ellipsoids are scaled to the 50% probability level. Solvent molecules are omitted for clarity

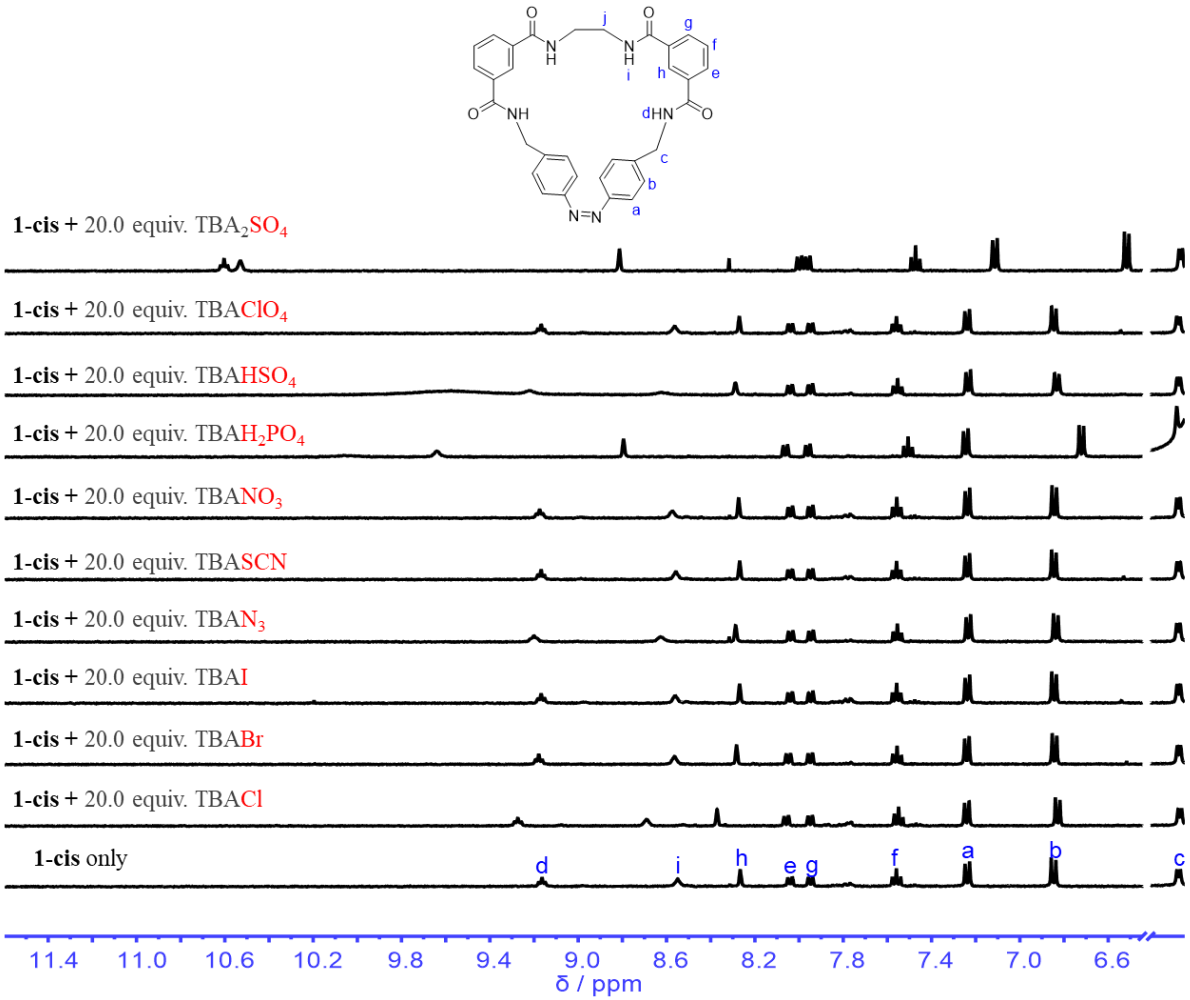



**Fig. S12.** Partial $^{1}$H NMR spectra of a 1.0 mM solution of **1–cis** recorded in the absence and presence of 20.0 equiv. of $Cl^{-}$, $Br^{-}$, $I^{-}$, $N_3^{-}$, $SCN^{-}$, $NO_3^{-}$, $H_2PO_4^{-}$, $HSO_4^{-}$, $ClO_4^{-}$, and $SO_4^{2-}$ (as their TBA salts) in DMSO–$d_6$.

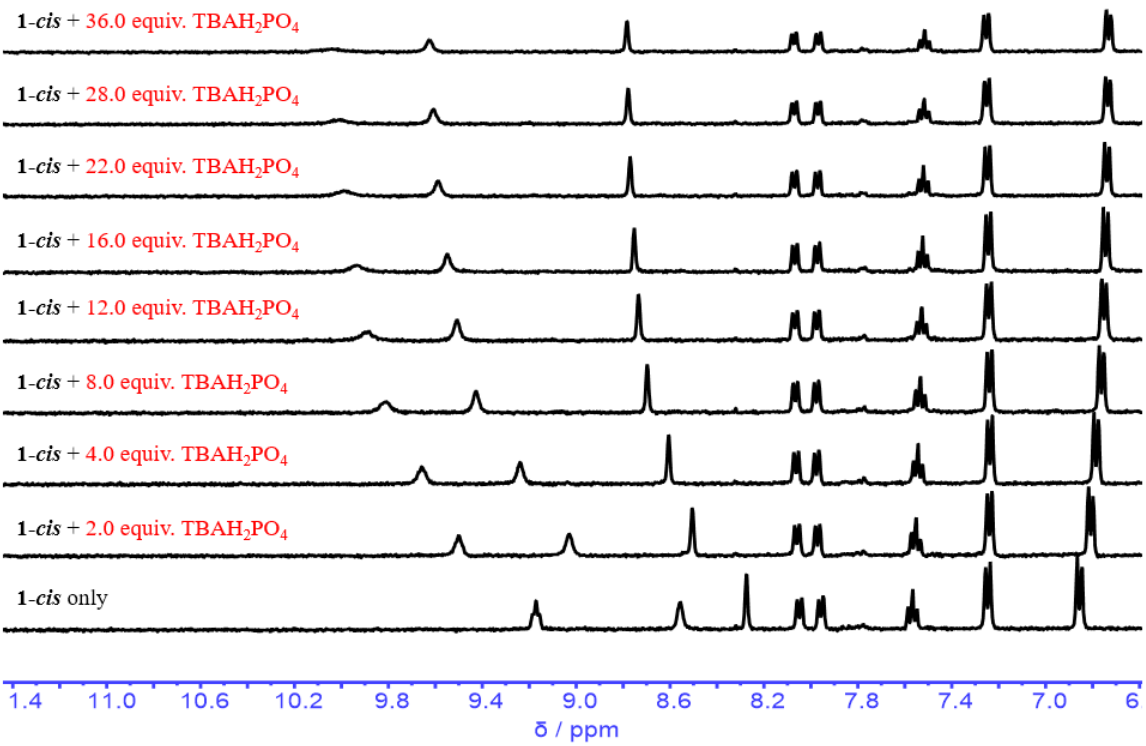



**Fig. 13.** $^{1}$H NMR spectroscopic titration of receptor **1–*cis*** with $TBAH_2PO_4$ in DMSO–$d_6$. The concentration of **1–*cis*** was 1.0 mM.

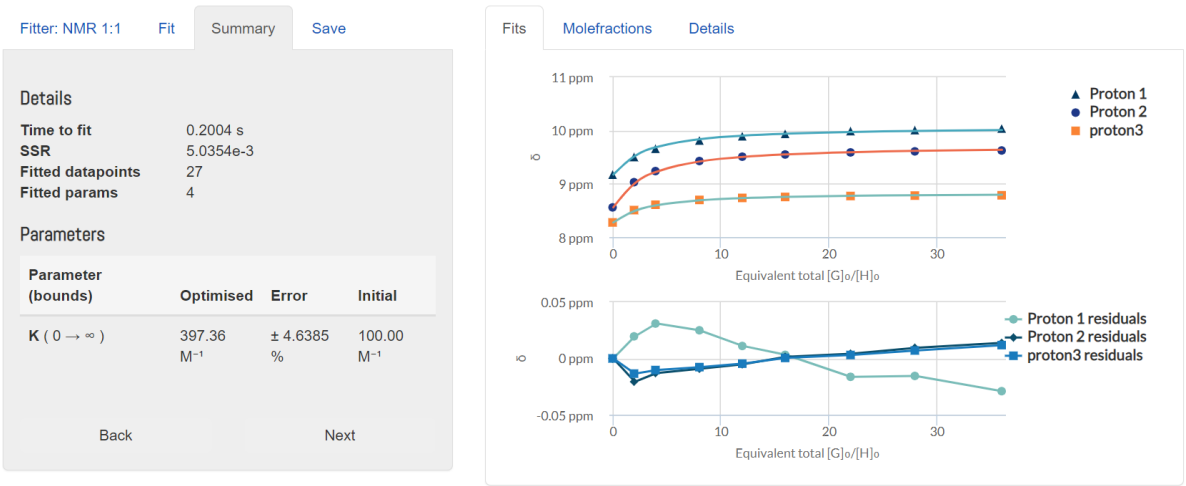



**Fig. S14.** Nonlinear least–square analysis of the $^{1}$H NMR binding data corresponding to the formation of **1–*cis***•$H_2PO_4^-$ complex. The data extracted from Fig. S13 were fitted to a 1:1 binding model to give $K_a$ = (4.0 ± 0.18) ×$10^2$ $M^{-1}$. The residual distribution is shown below the binding isotherm. All solid lines were obtained from non–linear curve–fitting to a 1:1 binding model using the www.supramolecular.org web applet.[6]

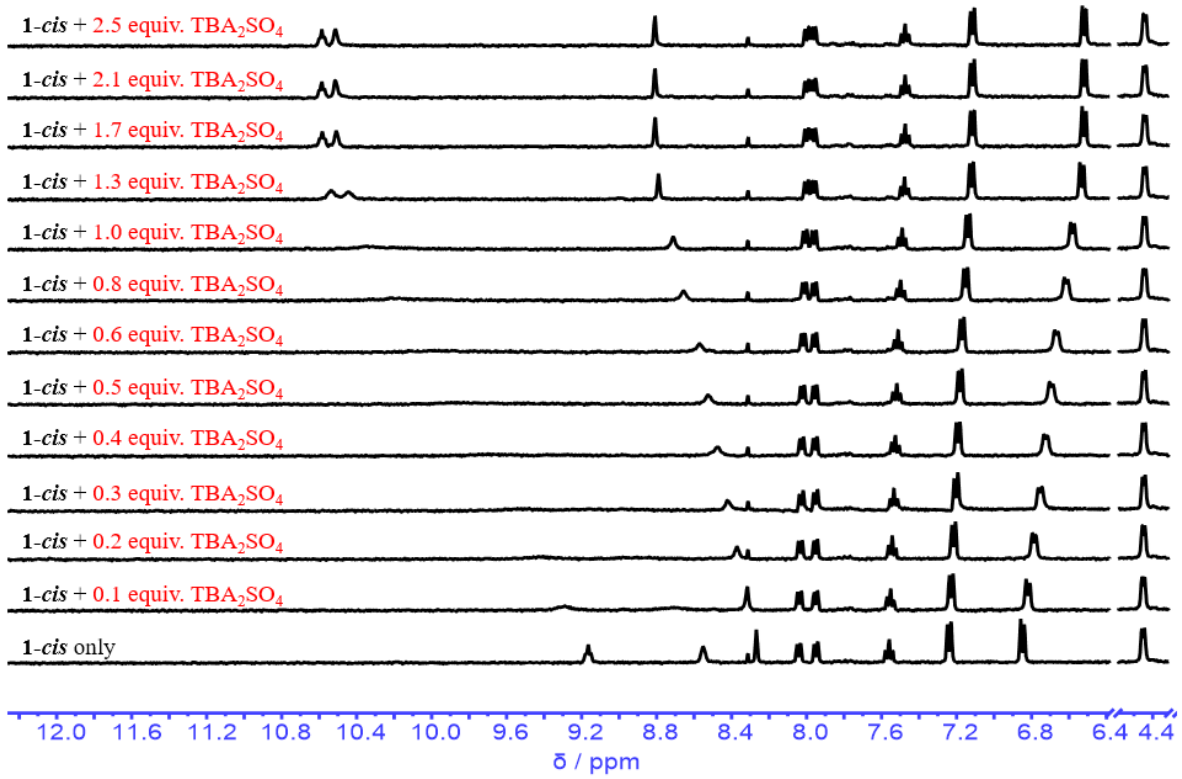



**Fig. S15.** $^1$H NMR spectroscopic titration of receptor **1–*cis*** with $TBA_2SO_4$ in DMSO–$d_6$. The concentration of **1–*cis*** was 1.0 mM.

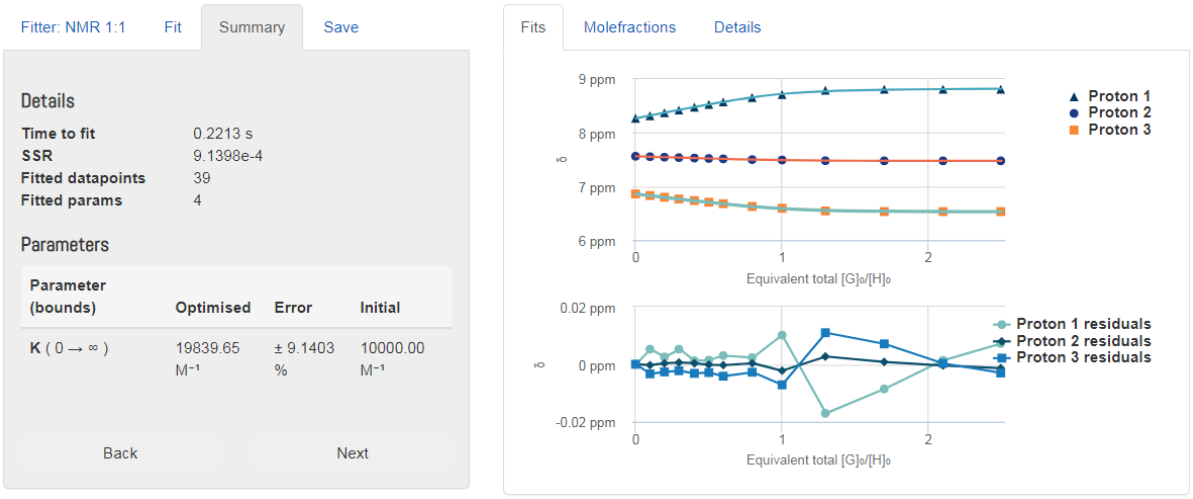



**Fig. S16.** Nonlinear least–square analysis of the $^1$H NMR binding data corresponding to the formation of **1–*cis***•$SO_4^{2-}$ complex. The data extracted from Fig. S15 were fitted to a 1:1 binding model to give $K_a = (2.0 \pm 0.18) \times 10^4$ $M^{-1}$. The residual distribution is shown below the binding isotherm. All solid lines were obtained from non–linear curve–fitting to a 1:1 binding model using the www.supramolecular.org web applet.[6]

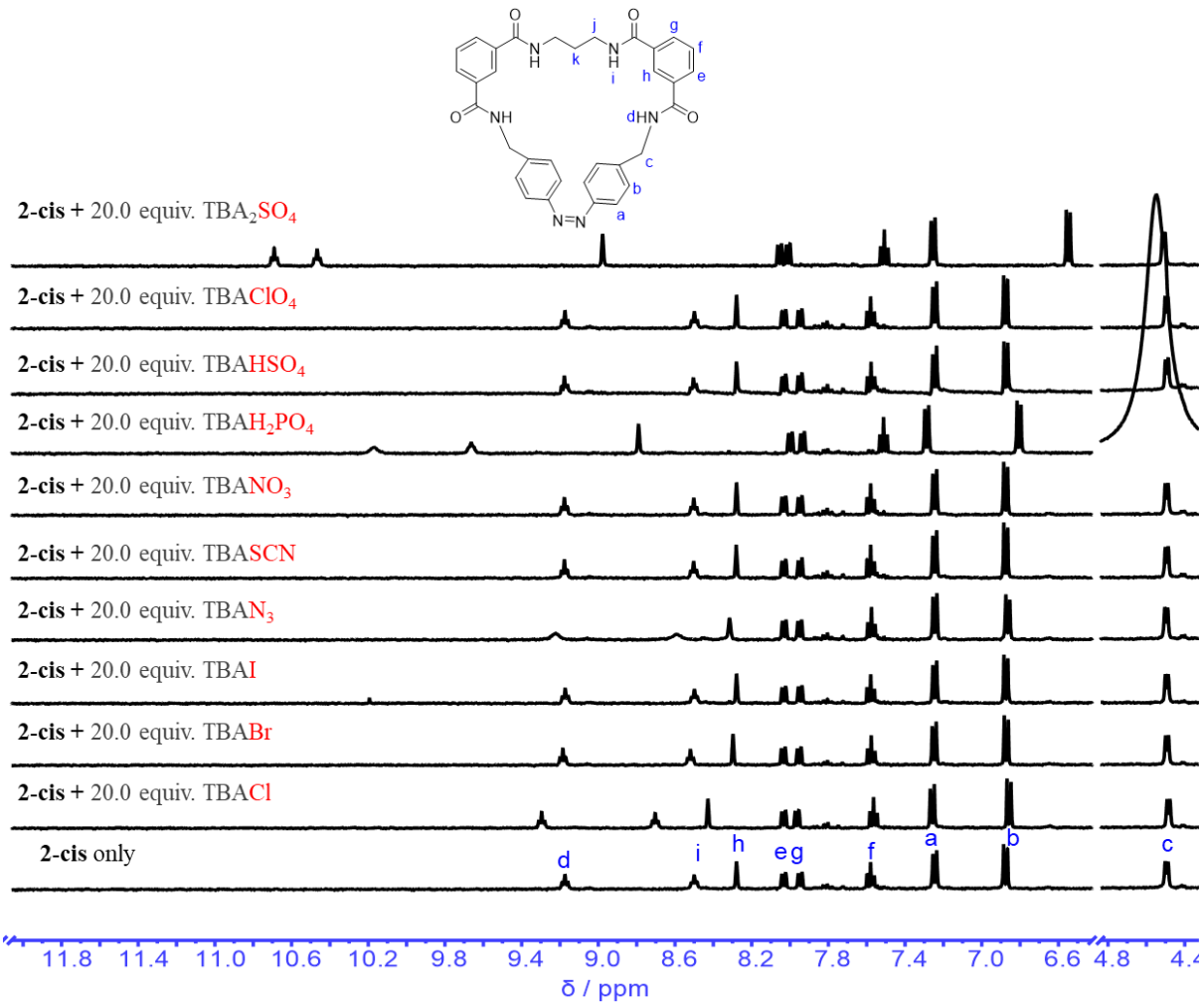



**Fig. S17.** Partial $^{1}$H NMR spectra of a 1.0 mM solution of **2–*cis*** recorded in the absence and presence of 20 equiv. of $Cl^{-}$, $Br^{-}$, $I^{-}$, $N_3^{-}$, $SCN^{-}$, $NO_3^{-}$, $H_2PO_4^{-}$, $HSO_4^{-}$, $ClO_4^{-}$, and $SO_4^{2-}$ (as their TBA salts) in DMSO–$d_6$.

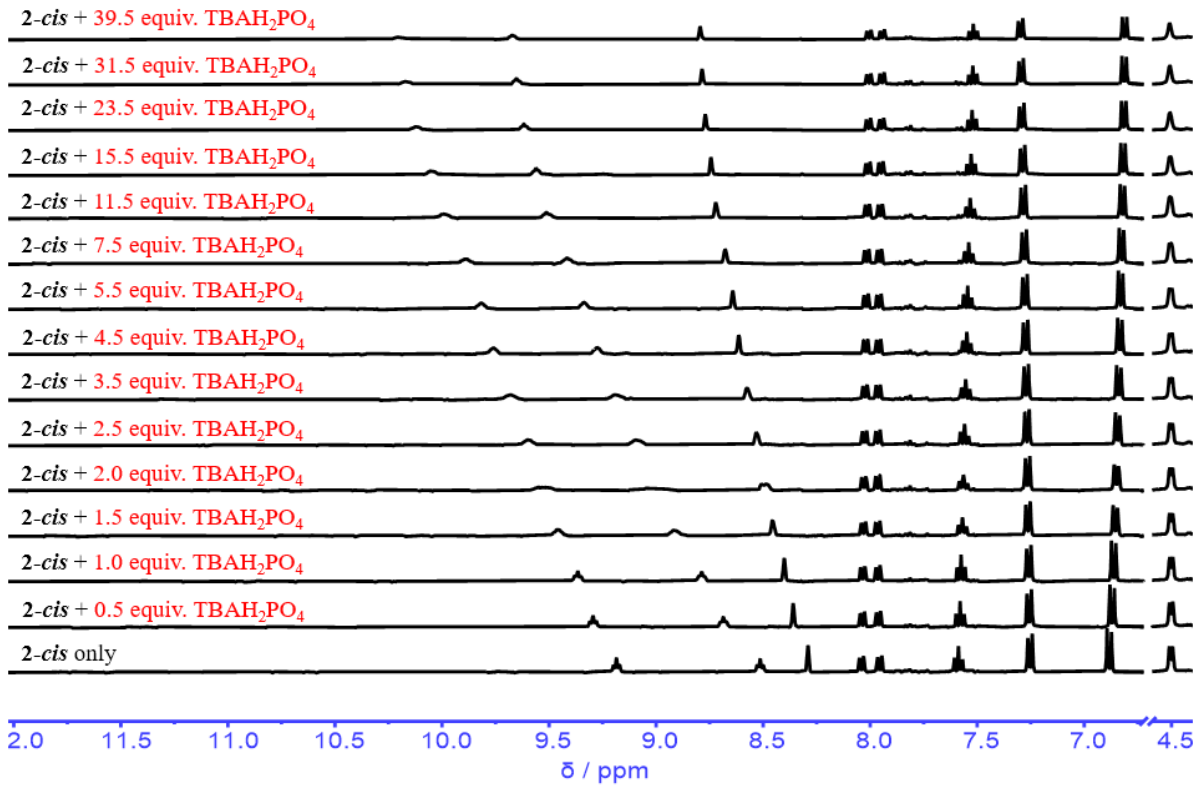



**Fig. S18.** $^1$H NMR spectroscopic titration of receptor **2–*cis*** with $TBAH_2PO_4$ in DMSO–$d_6$. The concentration of **2–*cis*** was 1.0 mM.

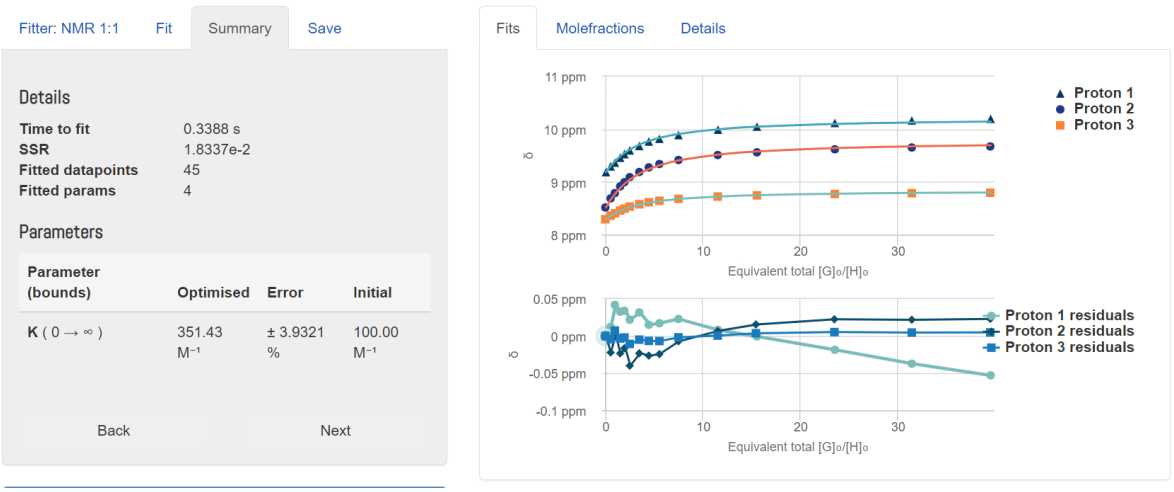



**Fig. S19.** Nonlinear least–square analysis of the $^1$H NMR binding data corresponding to the formation of **2–*cis*•**$H_2PO_4^-$ complex. The data extracted from Fig. S18 were fitted to a 1:1 binding model to give $K_a$ = (3.5 ± 0.14) ×$10^2$ $M^{-1}$. The residual distribution is shown below the binding isotherm. All solid lines were obtained from non–linear curve–fitting to a 1:1 binding model using the www.supramolecular.org web applet.[6]

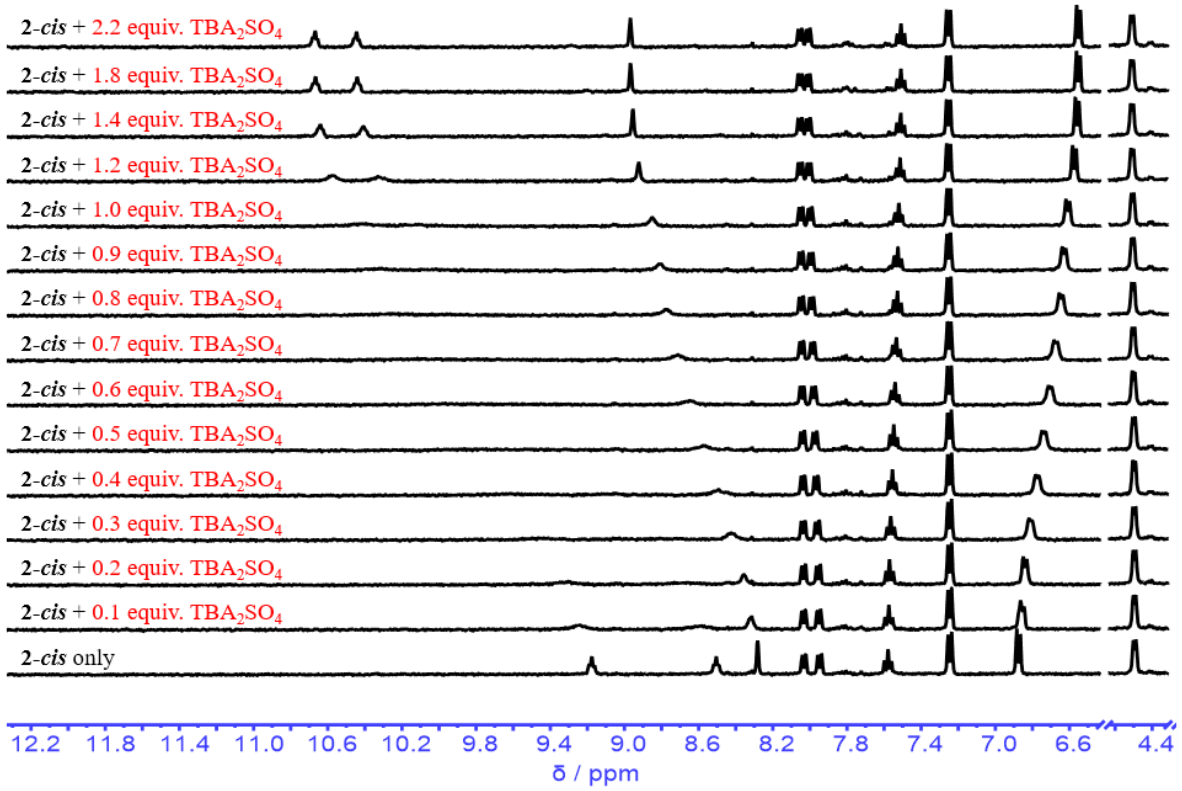



**Fig. S20.** $^1$H NMR spectroscopic titration of receptor **2–*cis*** with $TBA_2SO_4$ in DMSO–$d_6$. The concentration of **2–*cis*** was 1.0 mM.

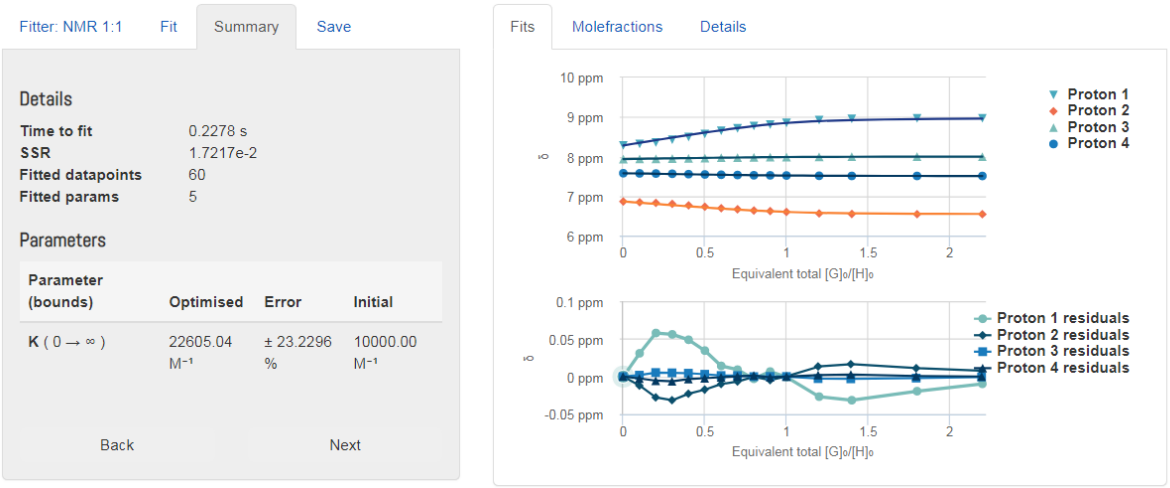



**Fig. S21.** Nonlinear least–square analysis of the $^1$H NMR binding data corresponding to the formation of **2–*cis*•**$SO_4^{2-}$ complex. The data extracted from Fig. S20 were fitted to a 1:1 binding model to give $K_a = (2.3 \pm 0.5) \times 10^4$ $M^{-1}$. The residual distribution is shown below the binding isotherm. All solid lines were obtained from non–linear curve–fitting to a 1:1 binding model using the www.supramolecular.org web applet.[6]

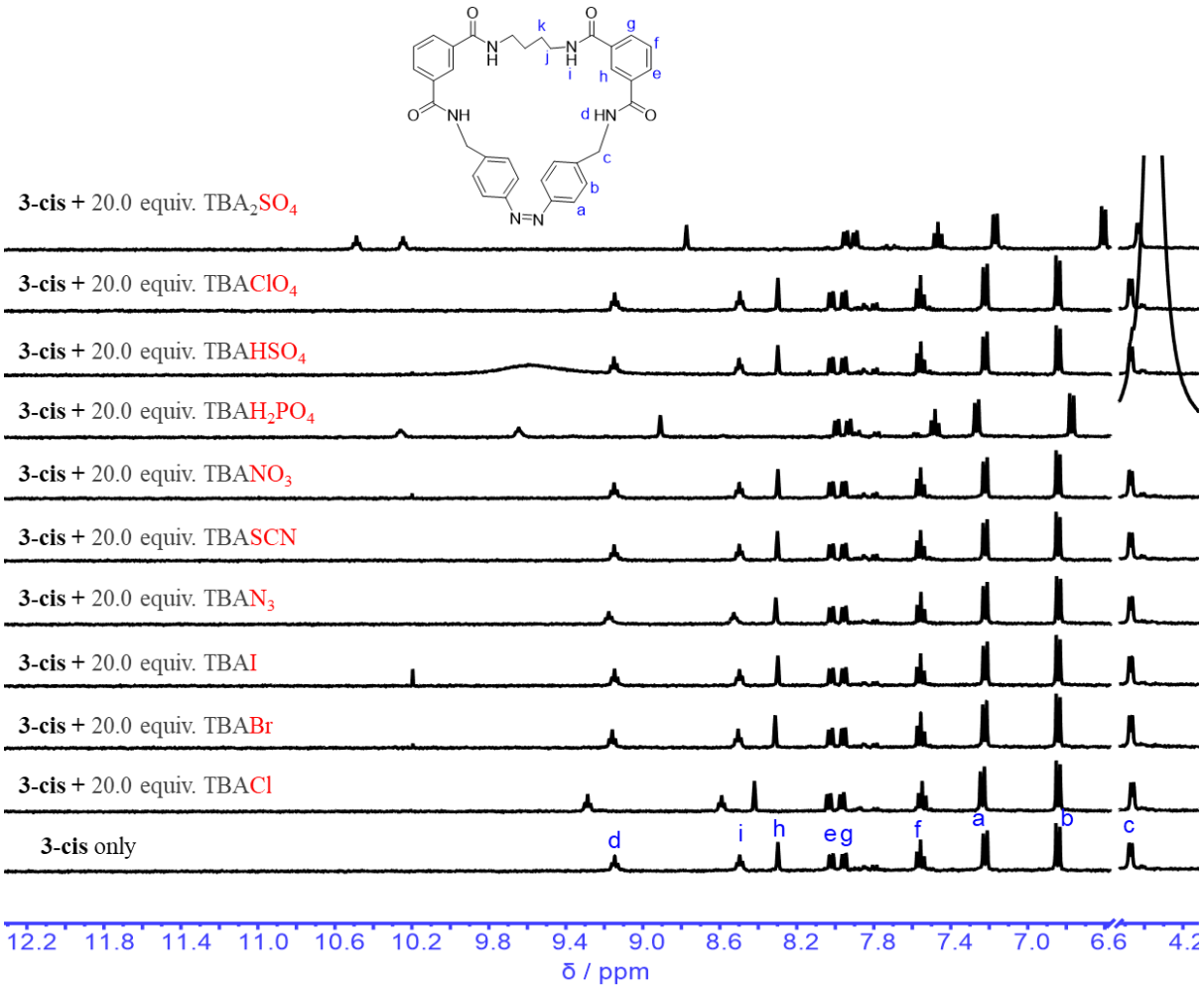



**Fig. S22.** Partial $^{1}$H NMR spectra of a 1.0 mM solution of **3–*cis*** recorded in the absence and presence of 20 equiv. of $Cl^{-}$, $Br^{-}$, $I^{-}$, $N_3^{-}$, $SCN^{-}$, $NO_3^{-}$, $H_2PO_4^{-}$, $HSO_4^{-}$, $ClO_4^{-}$, and $SO_4^{2-}$ (as their TBA salts) in DMSO–$d_6$.

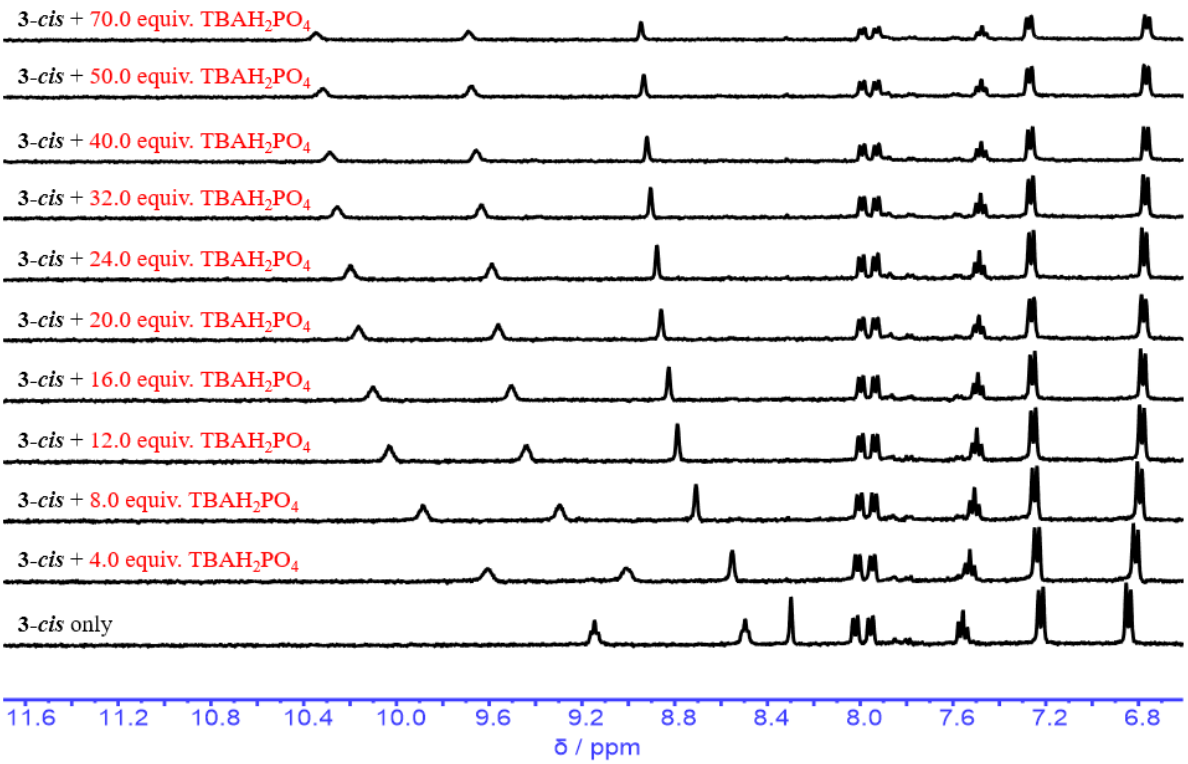



**Fig. S23.** $^1$H NMR spectroscopic titration of receptor **3–*cis*** with $TBAH_2PO_4$ in DMSO–$d_6$. The concentration of **3–*cis*** was 1.0 mM.

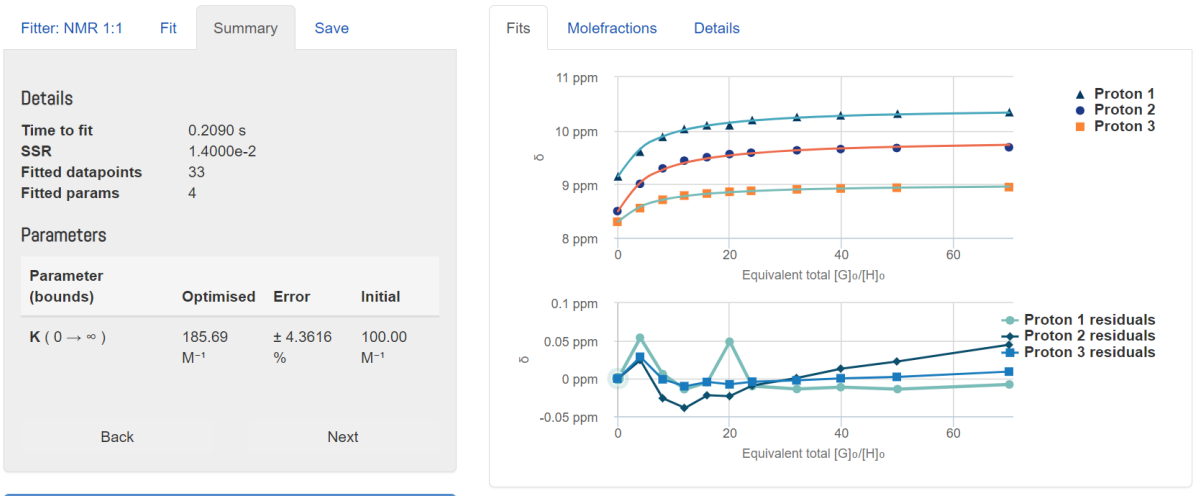



**Fig. S24.** Nonlinear least–square analysis of the $^1$H NMR binding data corresponding to the formation of **3–*cis*•**$H_2PO_4^-$ complex. The data extracted from Fig. S23 were fitted to a 1:1 binding model to give $K_a$ = (1.8 ± 0.08) ×$10^2$ $M^{-1}$. The residual distribution is shown below the binding isotherm. All solid lines were obtained from non–linear curve–fitting to a 1:1 binding model using the www.supramolecular.org web applet.[6]

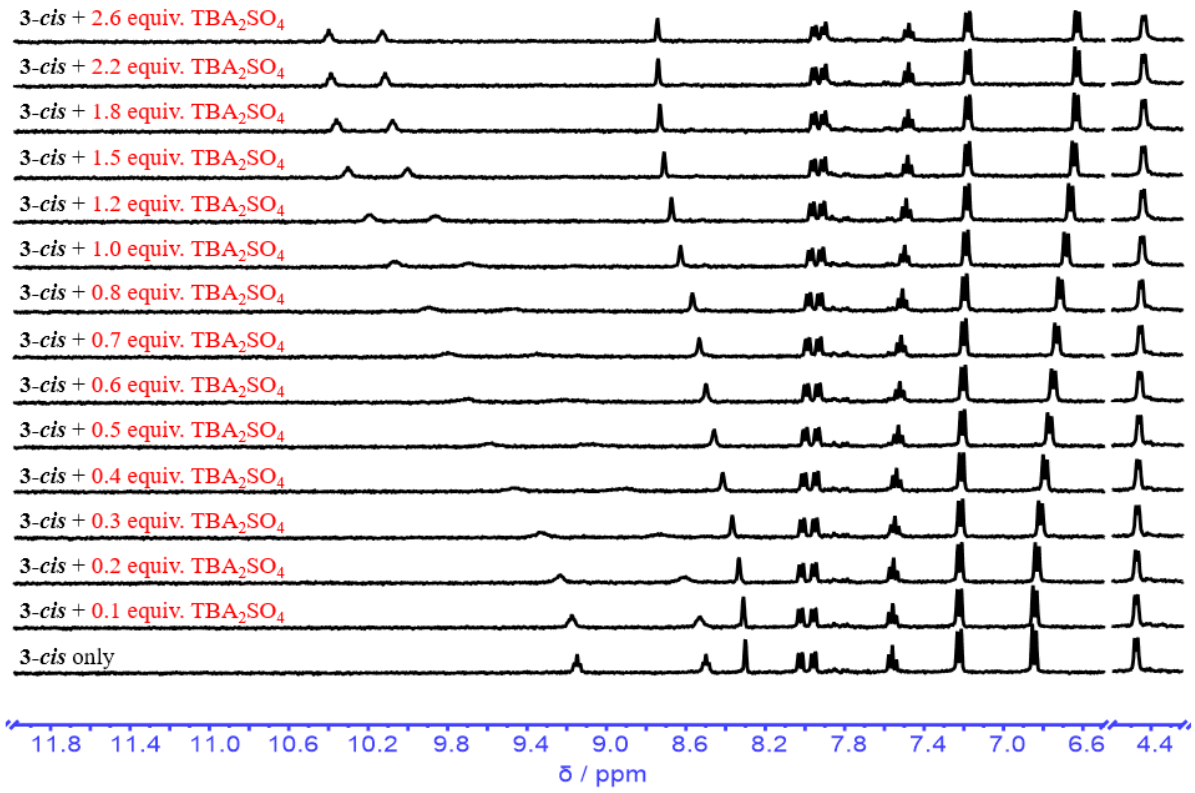



**Fig. S25.** $^{1}$H NMR spectroscopic titration of receptor **3–*cis*** with $TBA_2SO_4$ in DMSO–$d_6$. The concentration of **3–*cis*** was 1.0 mM.

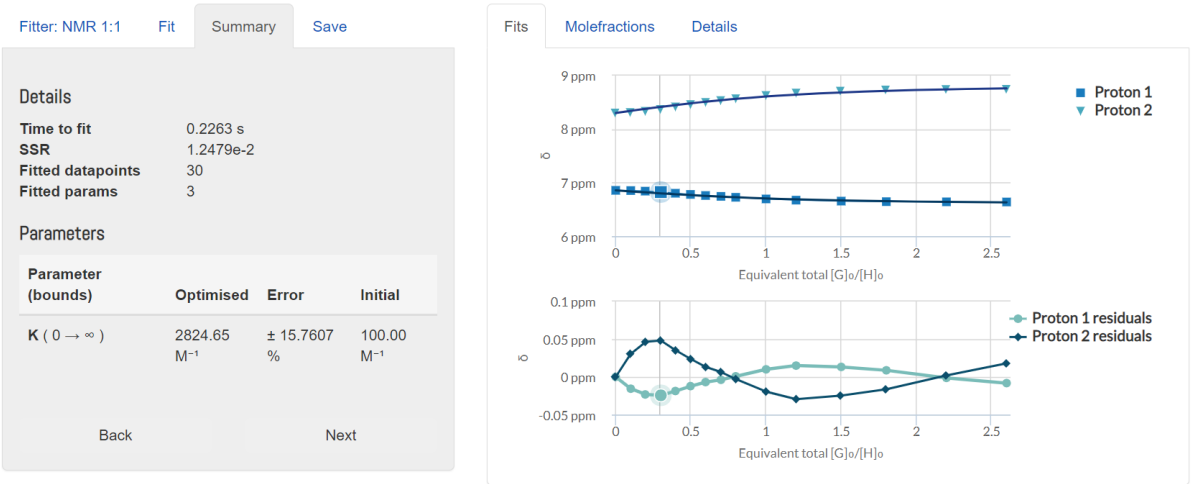



**Fig. S26.** Nonlinear least–square analysis of the $^{1}$H NMR binding data corresponding to the formation of **3–cis**•$SO_4^{2-}$ complex. The data extracted from Fig. S25 were fitted to a 1:1 binding model to give $K_a$ = (2.8 ± 0.44) ×$10^3$ $M^{-1}$. The residual distribution is shown below the binding isotherm. All solid lines were obtained from non–linear curve–fitting to a 1:1 binding model using the www.supramolecular.org web applet.[6]

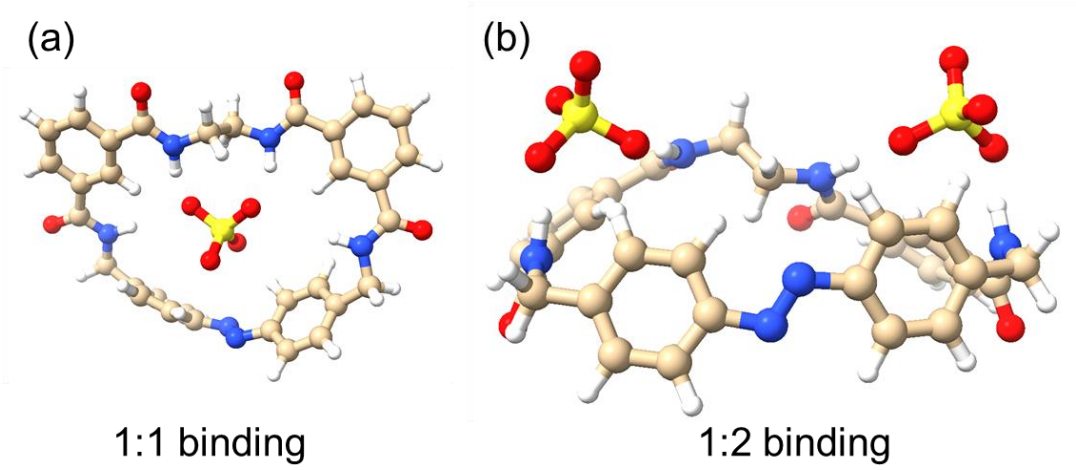



**Fig. S27.** DFT–optimized structures of (a) $SO_4^{2-}$ ⊂ **1**–***trans***, and (b) $2SO_4^{2-}$ ⊂ **1**–***trans***.

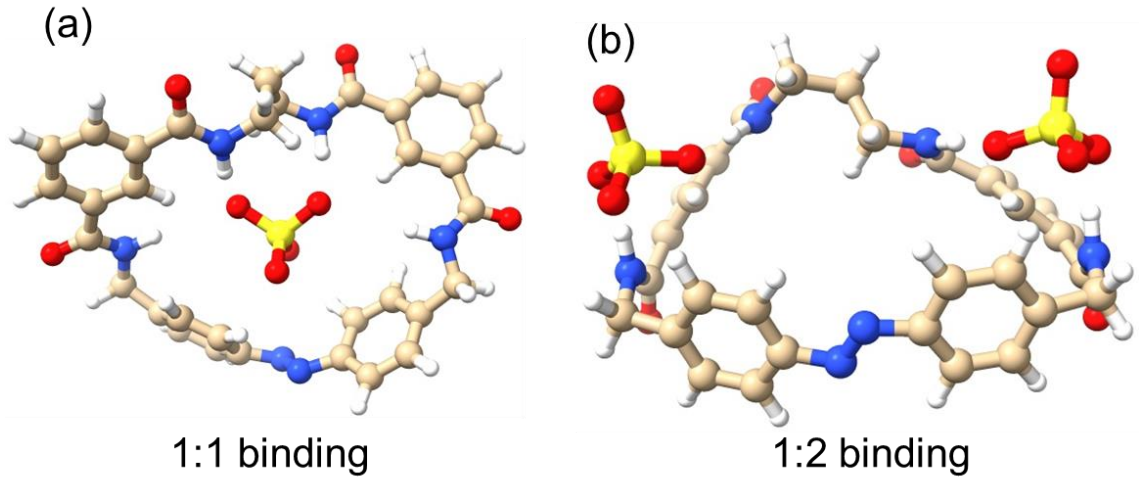



**Fig. S28.** DFT–optimized structures of (a) $SO_4^{2-}$ ⊂ **2**–***trans***, and (b) $2SO_4^{2-}$ ⊂ **2**–***trans***.

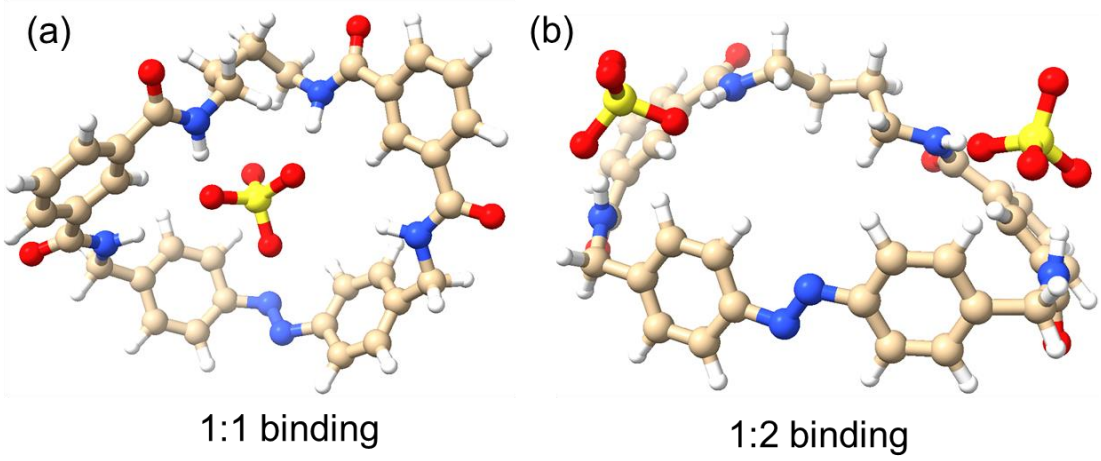



**Fig. S29.** DFT–optimized structures of (a) $SO_4^{2-}$ ⊂ **3**–***trans***, and (b) $2SO_4^{2-}$ ⊂ **3**–***trans***.

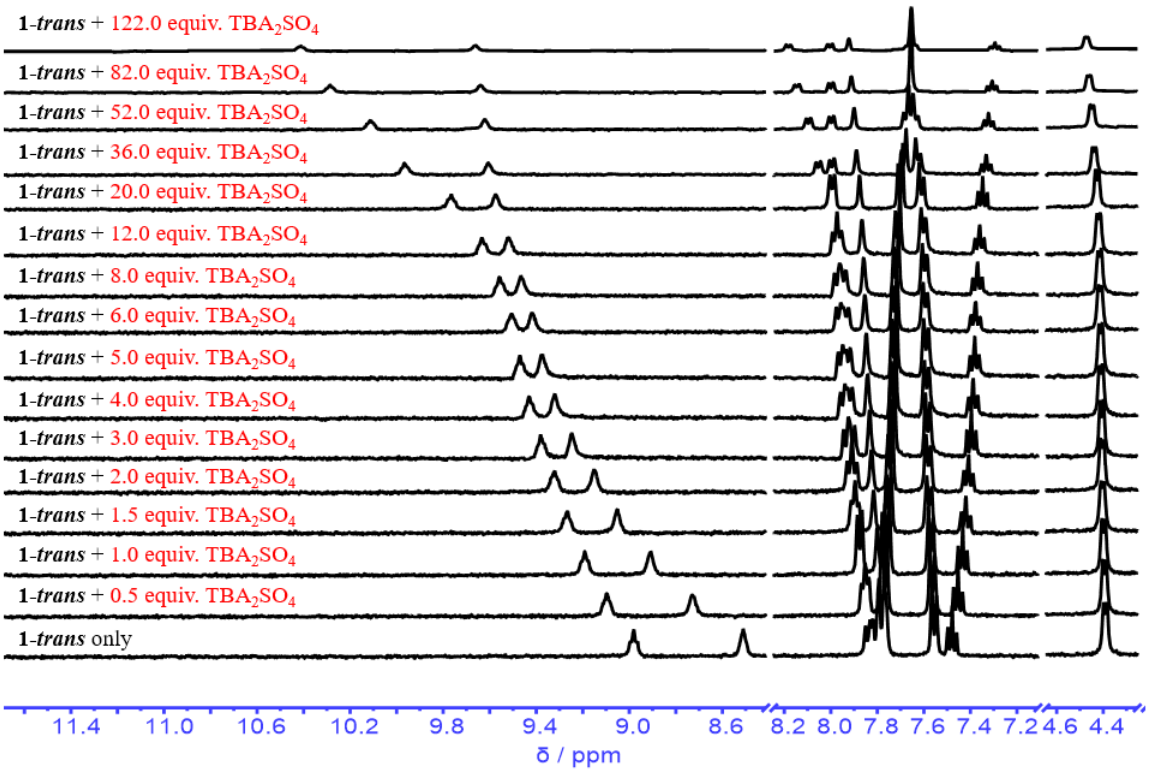



**Fig. S30.** $^{1}$H NMR spectroscopic titration of receptor **1–*trans*** with $TBA_2SO_4$ in DMSO–$d_6$. The concentration of **1–*trans*** was 1.0 mM.

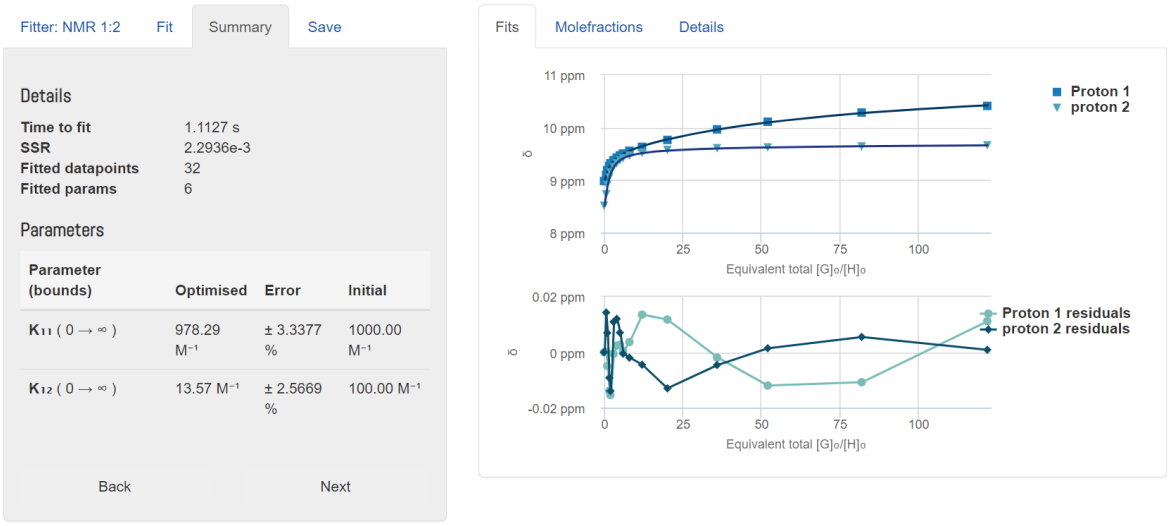



**Fig. S31.** Nonlinear least–square analysis of the $^{1}$H NMR binding data corresponding to the formation of **1–*trans*•** $2SO_4^{2-}$ complex. The data extracted from Fig. S30 were fitted to a 1:2 binding model to give $K_{a1}$ = (9.8 ± 0.33) ×10$^2$ M$^{-1}$, $K_{a2}$ = (1.4 ± 0.03) ×10 M$^{-1}$. The residual distribution is shown below the binding isotherm. All solid lines were obtained from non–linear curve–fitting to a 1:2 binding model using the www.supramolecular.org web applet.[6]

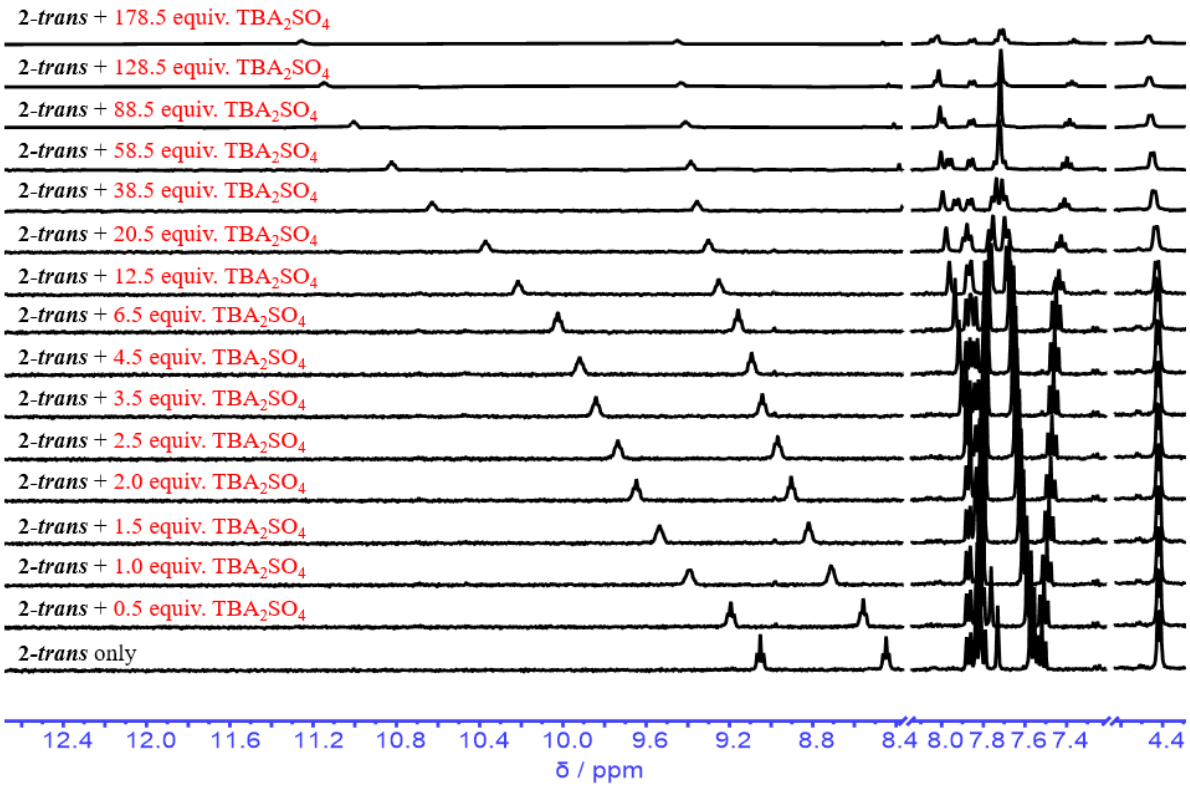



**Fig. S32.** $^{1}$H NMR spectroscopic titration of receptor **2–*trans*** with $TBA_2SO_4$ in DMSO–$d_6$. The concentration of **2–*trans*** was 1.0 mM.

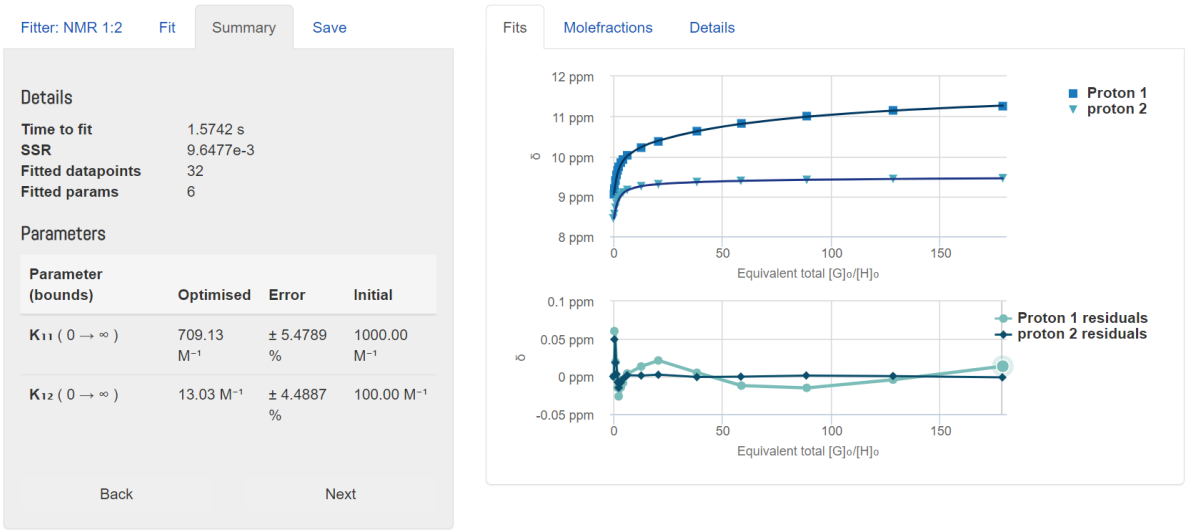



**Fig. S33.** Nonlinear least–square analysis of the $^{1}$H NMR binding data corresponding to the formation of **2–*trans*•** $2SO_4^{2-}$ complex. The data extracted from Fig. S32 were fitted to a 1:2 binding model to give $K_{a1}$ = $(7.1 \pm 0.4) \times 10^2$ M$^{-1}$, $K_{a2} = (1.3 \pm 0.1) \times 10$ M$^{-1}$. The residual distribution is shown below the binding isotherm. All solid lines were obtained from non–linear curve–fitting to a 1:2 binding model using the www.supramolecular.org web applet.[6]

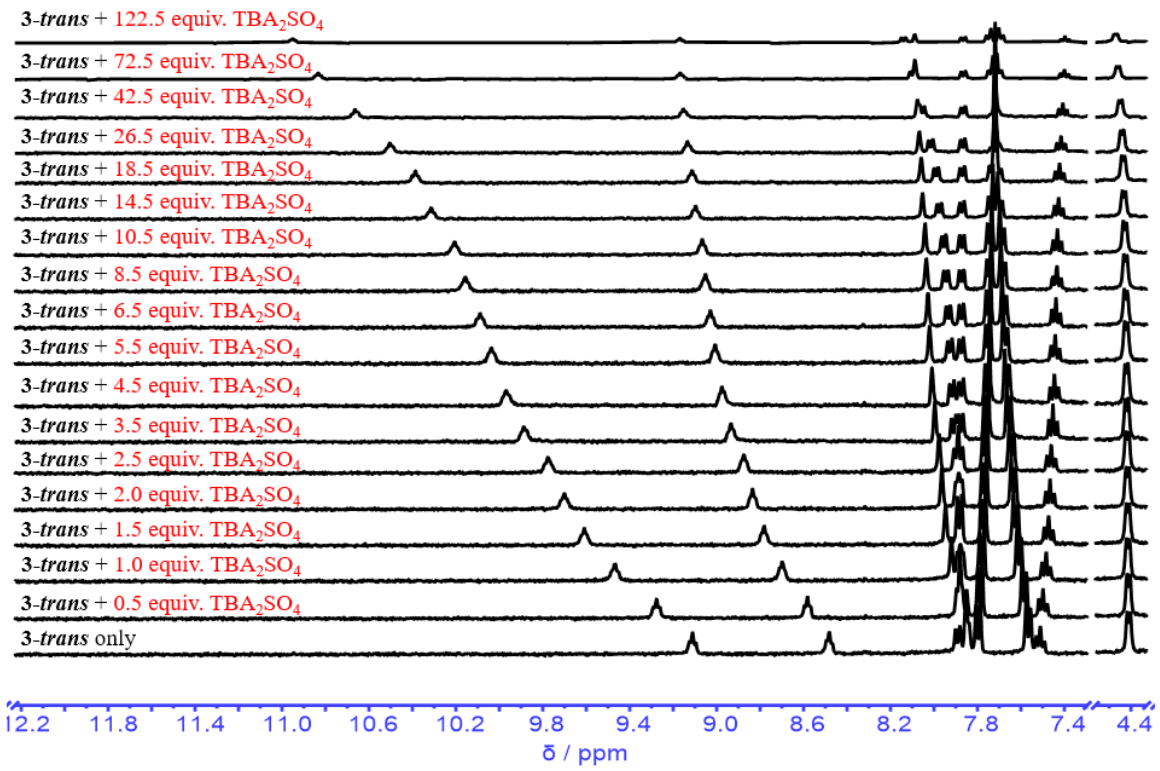



**Fig. S34.** $^1$H NMR spectroscopic titration of receptor **3–*trans*** with $TBA_2SO_4$ in DMSO–$d_6$. The concentration of **3–trans** was 1.0 mM.

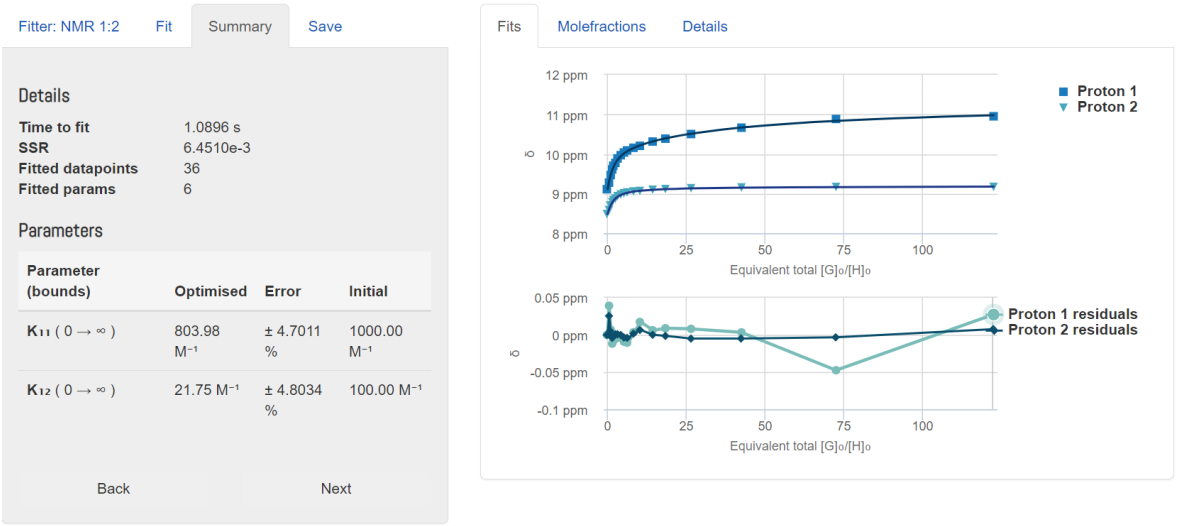



**Fig. S35.** Nonlinear least–square analysis of the $^1$H NMR binding data corresponding to the formation of **3–*trans***•$2SO_4^{2-}$ complex. The data extracted from Fig. 34 were fitted to a 1:1 binding model to give $K_{a1}$ = (8.0 ± 0.4) ×$10^2$ $M^{-1}$, $K_{a2}$ = (2.2 ± 0.1) ×10 $M^{-1}$. The residual distribution is shown below the binding isotherm. All solid lines were obtained from non–linear curve–fitting to a 1:1 binding model using the www.supramolecular.org web applet.[6]

## 6. Light-controlled binding-and-release studies

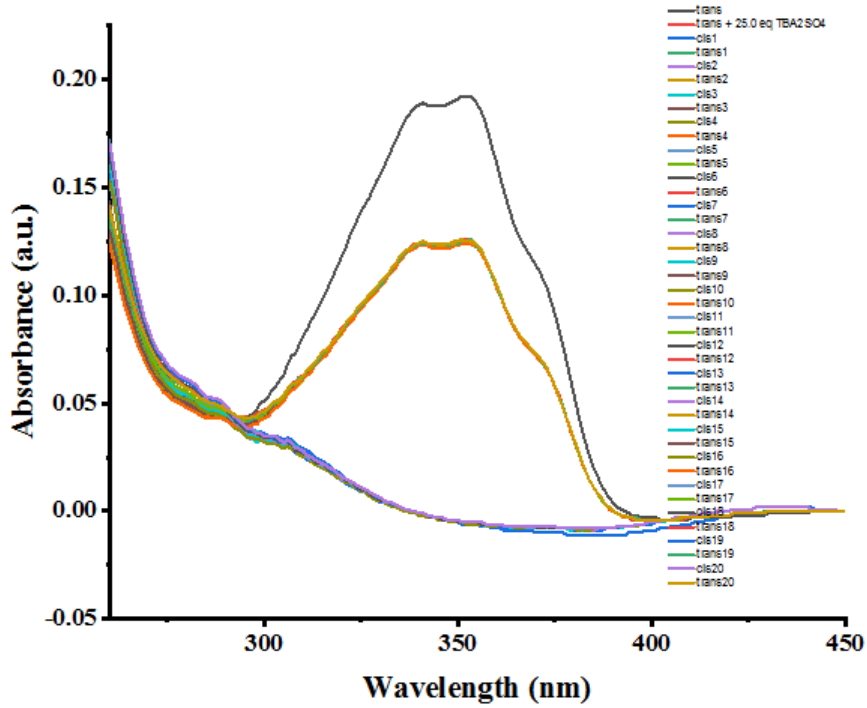



**Fig. S36.** Reversible photo–switch between **1**–***trans*** and **1**–***cis*** (10.0 μM) in the presence of 25.0 equiv of $TBA_2SO_4$ in DMSO monitored by UV–vis spectroscopy.

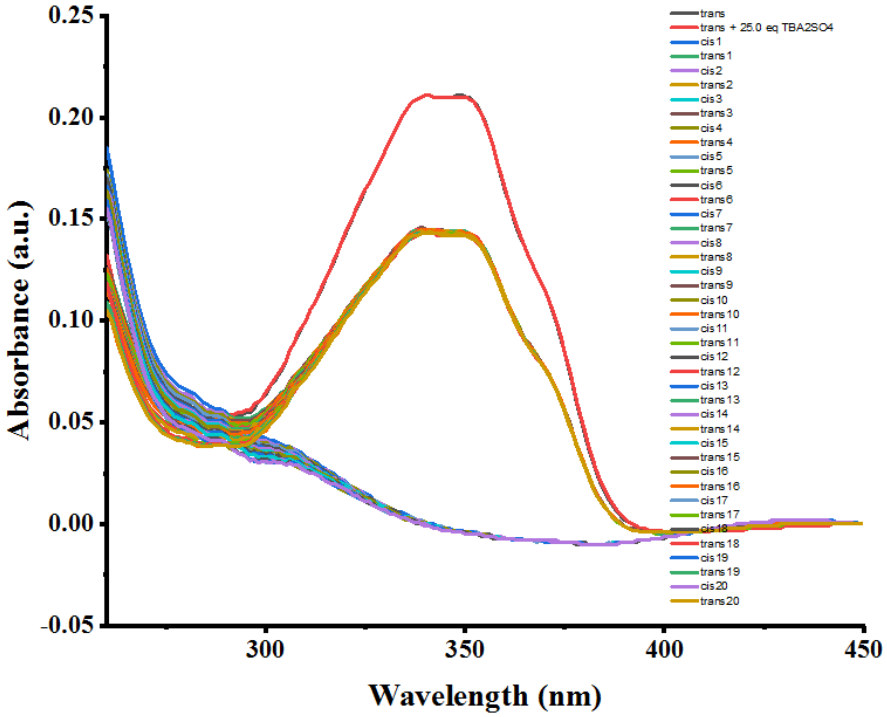



**Fig. S37.** Reversible photo–switch between **2**–***trans*** and **2**–***cis*** (10.0 μM) in the presence of 25.0 equiv of $TBA_2SO_4$ in DMSO monitored by UV–vis spectroscopy.

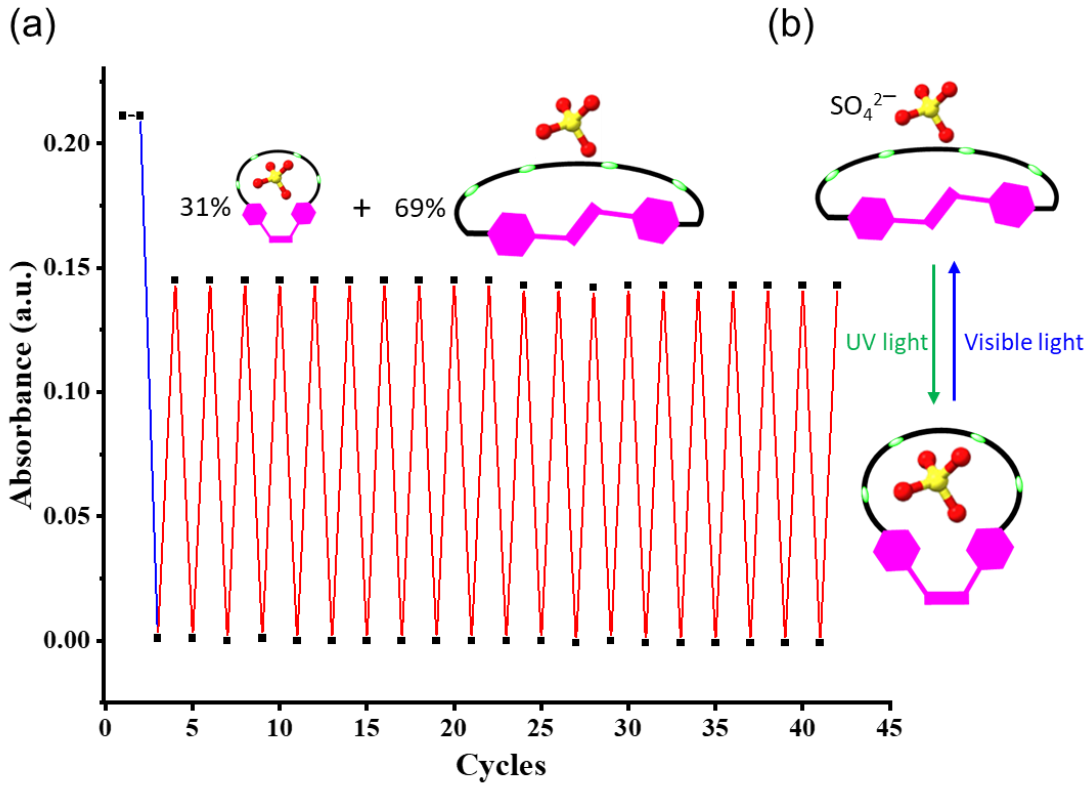



**Fig. 38.** (a) Switching cycles of **2**–***trans*** (10.0 μM in DMSO) in the presence of 25.0 equiv of $TBA_2SO_4$ upon alternating irradiation using 365–370 (ca. 5 min; 100 W) and 420–425 (ca. 5 min; 100 W) nm light sources. The absorbance change at 340 nm was monitored during the switching cycles. (b) Cartoon illustration of the switchable binding and release of sulfate anions.

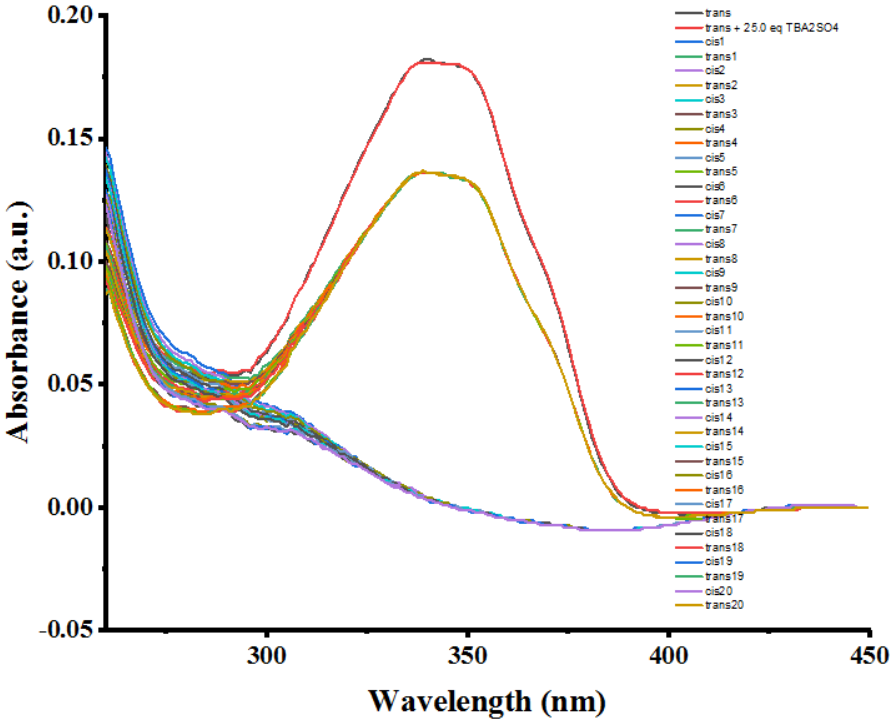



**Fig. S39.** Reversible photo–switch between **3–*trans*** and **3–*cis*** (10.0 μM) in the presence of 25.0 equiv of $TBA_2SO_4$ in DMSO monitored by UV–vis spectroscopy.

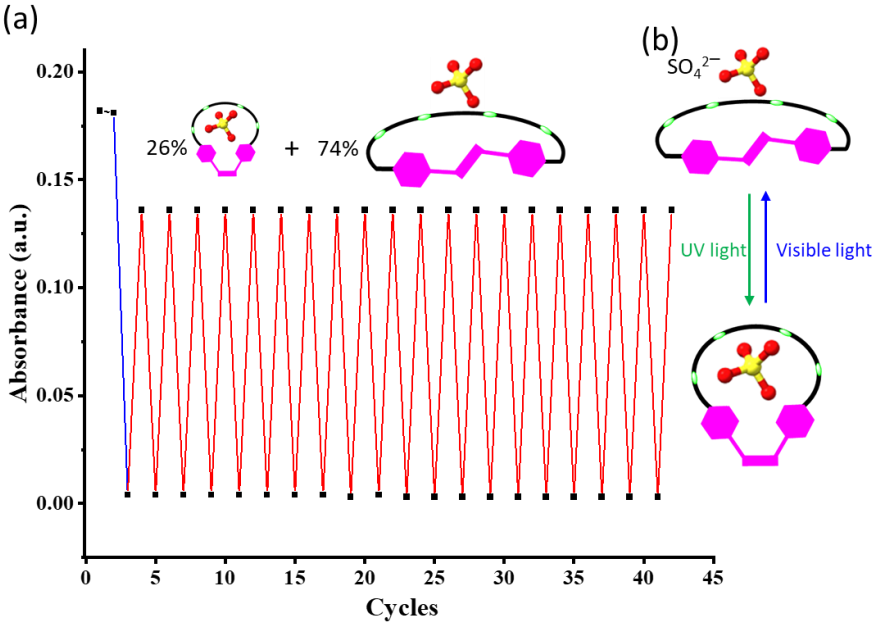



**Fig. S40.** (a) Switching cycles of **3–*trans*** (10.0 μM in DMSO) in the presence of 25.0 equiv of $TBA_2SO_4$ upon alternating irradiation using 365–370 (ca. 5 min; 100 W) and 420–425 (ca. 5 min; 100 W) nm light sources. The absorbance change at 340 nm was monitored during the switching cycles. (b) Cartoon illustration of the switchable binding and release of sulfate anions.

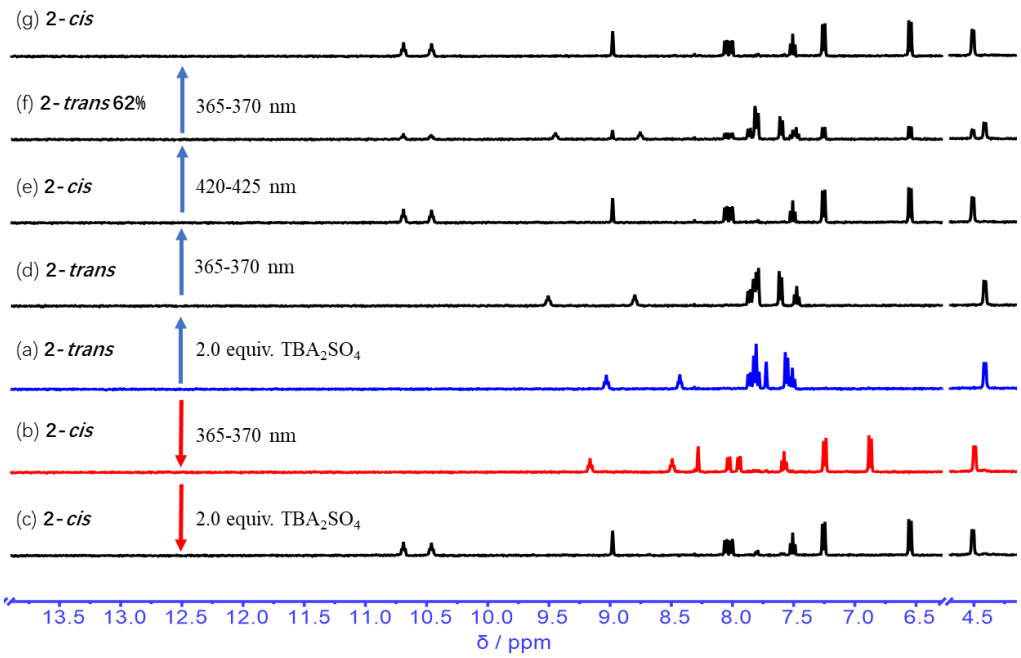



**Fig. S41.** Partial $^1$H NMR spectra (DMSO–$d_6$) of (a) **2**–***trans*** (1.0 mM) before and (b) after photoirradiation (365–370 nm) and (c) followed by the addition of 2.0 equiv of $TBA_2SO_4$; (d) **2**–***trans*** after the addition of 2.0 equiv of $TBA_2SO_4$, (e) followed by photoirradiation (365–370 nm); (f) after exposure of the solution in (e) to photoirradiation (420–425 nm), (g) further followed by photoirradiation (365–370 nm).

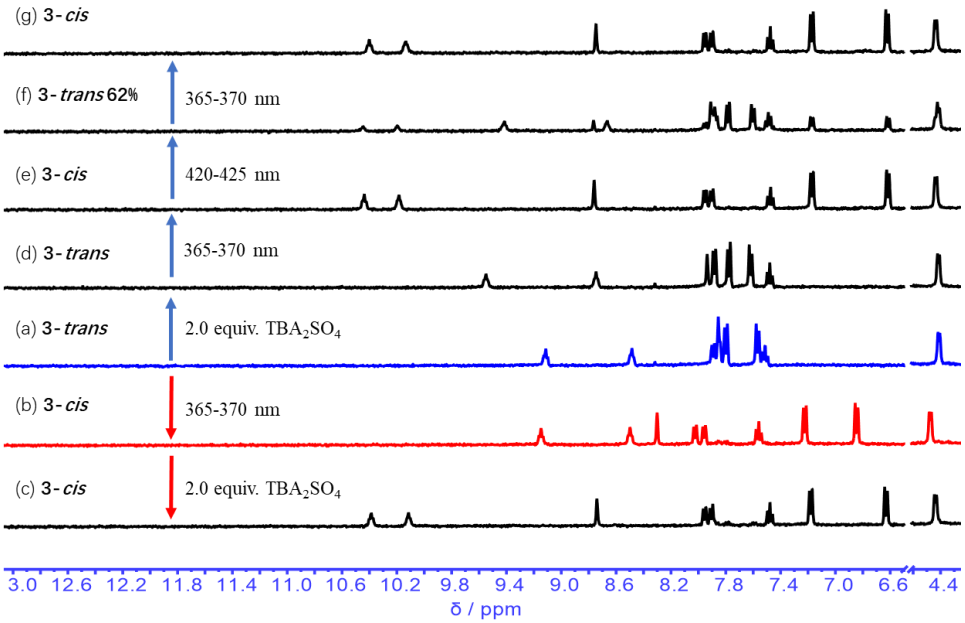



**Fig. S42.** Partial $^1$H NMR spectra (DMSO–$d_6$) of (a) **3**–***trans*** (1.0 mM) before and (b) after photoirradiation (365–370 nm) and (c) followed by the addition of 2.0 equiv of $TBA_2SO_4$; (d) **3**–***trans*** after the addition of 2.0 equiv of $TBA_2SO_4$, (e) followed by photoirradiation (365–370 nm); (f) after exposure of the solution in (e) to photoirradiation (420–425 nm), (g) further followed by photoirradiation (365–370 nm).

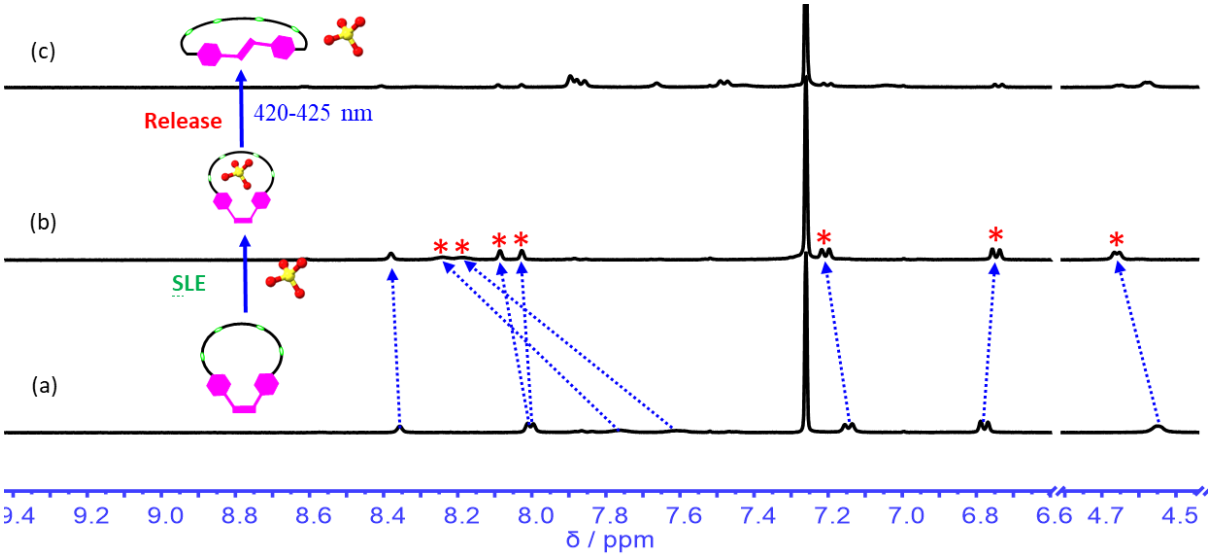



**Fig. S43.** Partial $^{1}$H NMR spectra of **4–*cis*** (2.0 mM) in $CDCl_3$ (a) before and (b) after contact (or SLE: solid-liquid extraction) of excess solid $TMA_2SO_4$, (c) followed by photoirradiation (420–425 nm).

## 7. X–ray experimental details

### X–ray experimental for 1–*trans*

Single crystals of complex **1–*trans*** were obtained as orange needle via the slow evaporation of a DCM–MeOH solution of receptor **1–*trans*** in a brown vial. A suitable crystal was selected and the data were collected on a Bruker D8 VENTURE PHOTON 100 CMOS system equipped with a mirror monochromator and a Cu–Kα INCOATEC IμS micro focus source (λ = 1.54178 Å). The crystal was kept at 173 K during data collection. Using Olex2,[7] the structure was solved with the ShelXT[8] structure solution program using Direct Methods and refined with the ShelXL[9] refinement package using Least Squares minimization. Tables of positional and thermal parameters, bond lengths and angles, torsion angles and figures are in the CIF file. CCDC deposition number: 2112716.

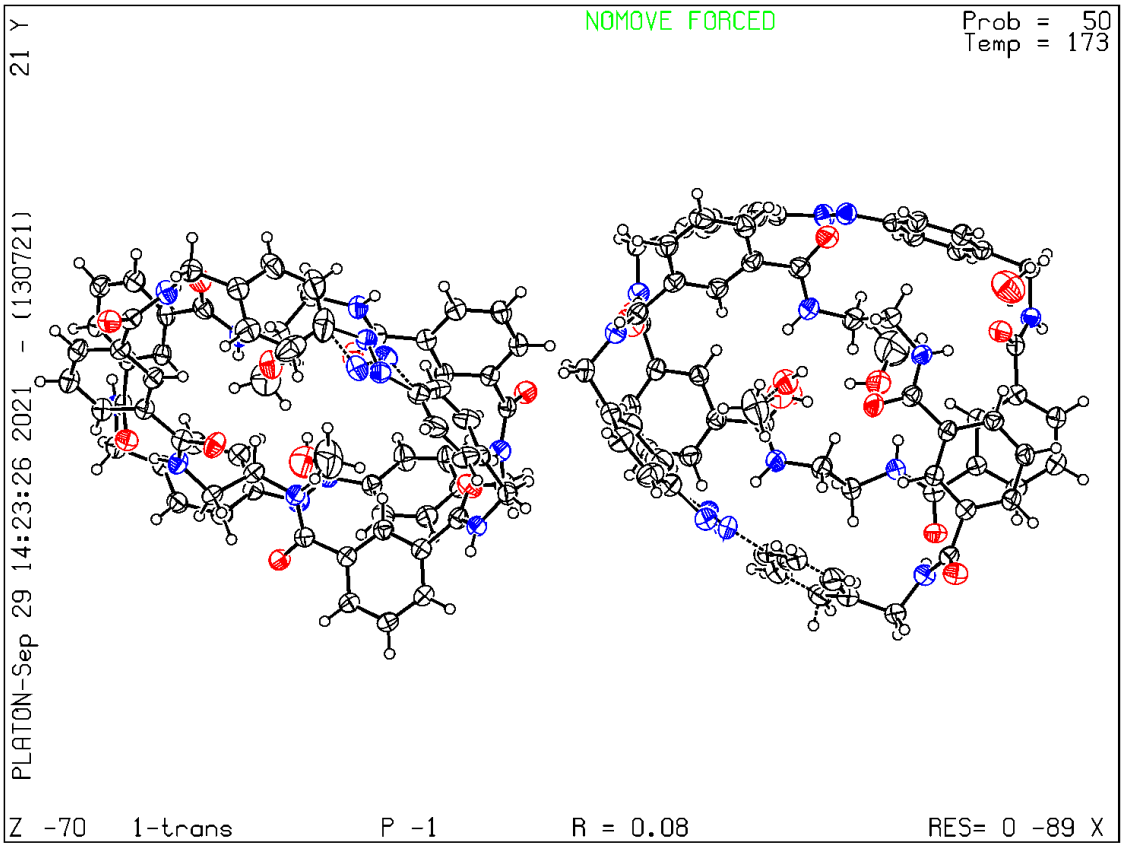



**Figure S44.** View of **1–*trans***. Displacement ellipsoids are scaled to the 50% probability level

**Table S2 Crystal data and structure refinement for 1–trans.**

| | |
|---|---|
| Identification code | **1–*trans*** |
| Empirical formula | $C_{132}H_{129}N_{24}O_{21}$ |
| Formula weight | 2387.95 |
| Temperature/K | 173.0 |
| Crystal system | triclinic |
| Space group | P–1 |
| a/Å | 11.0498(17) |
| b/Å | 19.163(3) |
| c/Å | 29.251(4) |
| α/° | 99.650(10) |
| β/° | 90.341(8) |
| γ/° | 90.270(7) |
| Volume/Å$^3$ | 6106.1(15) |
| Z | 2 |
| $\rho_{calc}$g/cm$^3$ | 1.299 |
| μ/mm$^{-1}$ | 0.737 |
| F(000) | 2515.0 |
| Crystal size/mm$^3$ | 0.074 × 0.066 × 0.035 |
| Radiation | CuKα (λ = 1.54178 Å) |
| 2Θ range for data collection/° | 3.064 to 133.682 |
| Index ranges | $-13 \leq h \leq 13$, $-22 \leq k \leq 22$, $-34 \leq l \leq 34$ |
| Reflections collected | 72233 |
| Independent reflections | 21062 [$R_{int}$ = 0.0963, $R_{sigma}$ = 0.0845] |
| Data/restraints/parameters | 21062/81/1685 |
| Goodness–of–fit on F$^2$ | 1.039 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0764, $wR_2$ = 0.1956 |
| Final R indexes [all data] | $R_1$ = 0.1091, $wR_2$ = 0.2170 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.77/–0.67 |

**X–ray experimental for 2–trans**

Single crystals of complex **2–trans** were obtained as orange plates via the slow evaporation of a DMF solution of receptor **2–*trans*** in a brown vial. A suitable crystal was selected and the data were collected on a Bruker D8 VENTURE PHOTON 100 CMOS system equipped with a mirror monochromator and a Cu–Kα INCOATEC IμS micro focus source (λ = 1.54178 Å). The crystal was kept at 173 K during data collection. Using Olex2,[7] the structure was solved with the ShelXT[8] structure solution program using Direct Methods and refined with the ShelXL[9] refinement package using Least Squares minimization. Tables of positional and thermal parameters, bond lengths and angles, torsion angles and figures are in the CIF file. CCDC deposition number: 2112715.

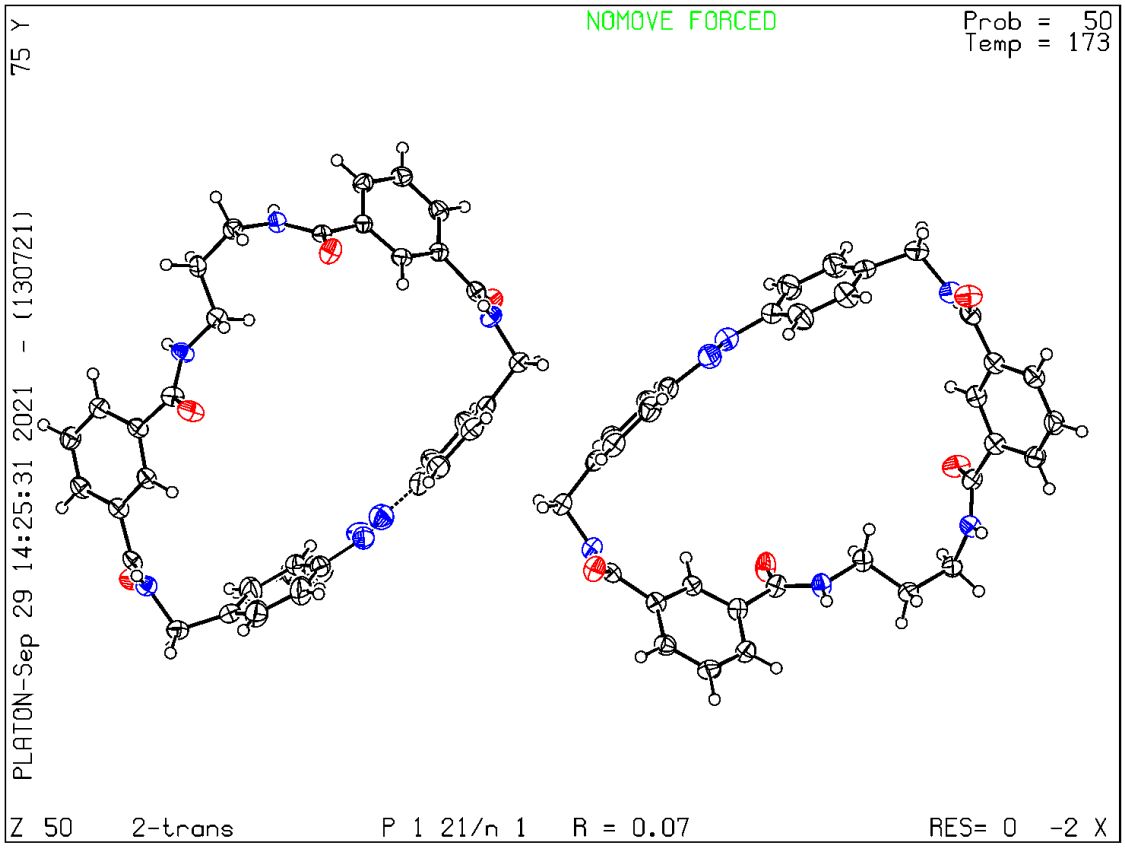



**Figure S45.** View of **2–*trans***. Displacement ellipsoids are scaled to the 50% probability level.

**Table S3 Crystal data and structure refinement for 2–trans.**

| | |
|---|---|
| Identification code | **2–*trans*** |
| Empirical formula | $C_{66}H_{60}N_{12}O_8$ |
| Formula weight | 1149.26 |
| Temperature/K | 173.00 |
| Crystal system | monoclinic |
| Space group | $P2_1/n$ |
| a/Å | 9.3970(2) |
| b/Å | 15.8981(4) |
| c/Å | 50.4387(15) |
| α/° | 90 |
| β/° | 92.499(2) |
| γ/° | 90 |
| Volume/Å$^3$ | 7528.1(3) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.014 |
| μ/mm$^{-1}$ | 0.557 |
| F(000) | 2416.0 |
| Crystal size/mm$^3$ | 0.087 × 0.069 × 0.032 |
| Radiation | CuKα (λ = 1.54178 Å) |
| 2Θ range for data collection/° | 3.506 to 134.266 |
| Index ranges | $-11 \leq h \leq 8$, $-18 \leq k \leq 18$, $-60 \leq l \leq 60$ |
| Reflections collected | 52172 |
| Independent reflections | 13304 [$R_{int}$ = 0.0730, $R_{sigma}$ = 0.0551] |
| Data/restraints/parameters | 13304/34/816 |
| Goodness–of–fit on F$^2$ | 1.090 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0728, $wR_2$ = 0.2194 |
| Final R indexes [all data] | $R_1$ = 0.0881, $wR_2$ = 0.2302 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.93/–0.33 |

## 8. HRMS Spectra and NMR Spectra

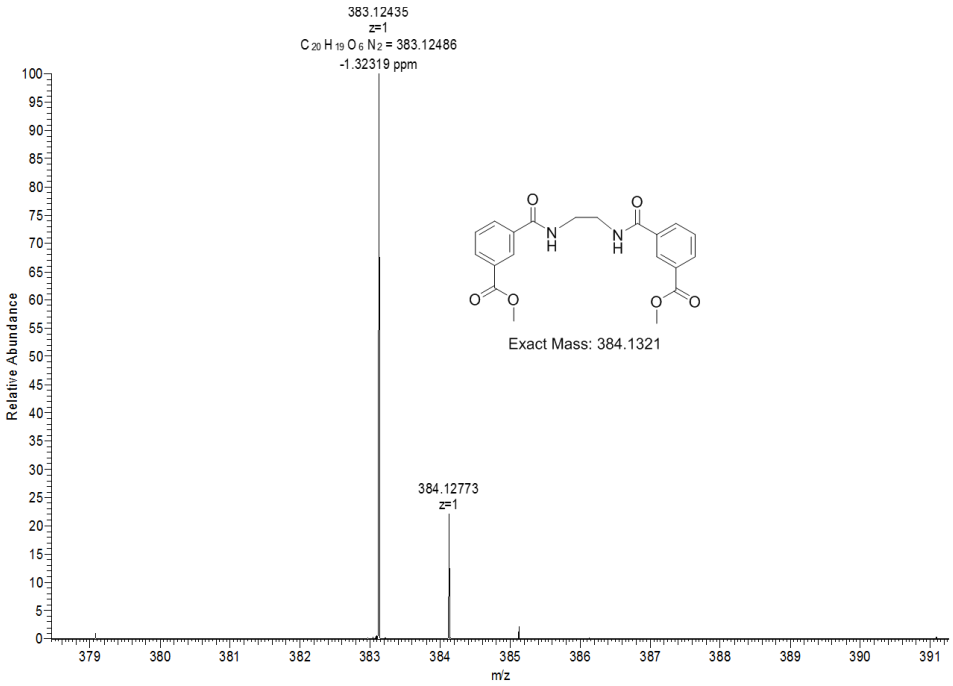



**Fig. S46**. HRMS spectrum of compound **10**.

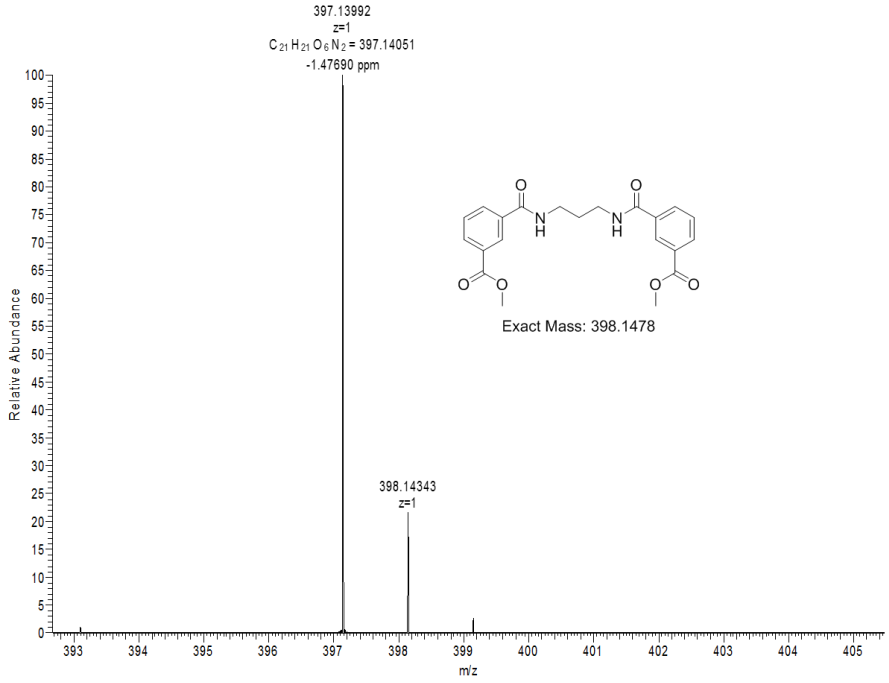



**Fig. S47**. HRMS spectrum of compound **11**.

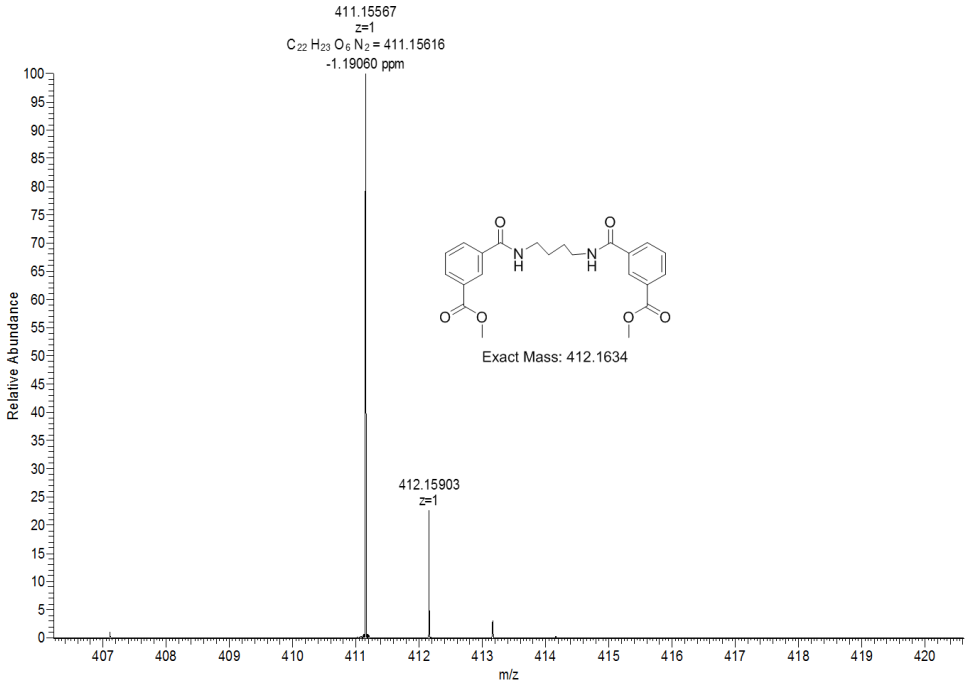



**Fig. S48**. HRMS spectrum of compound **12**.

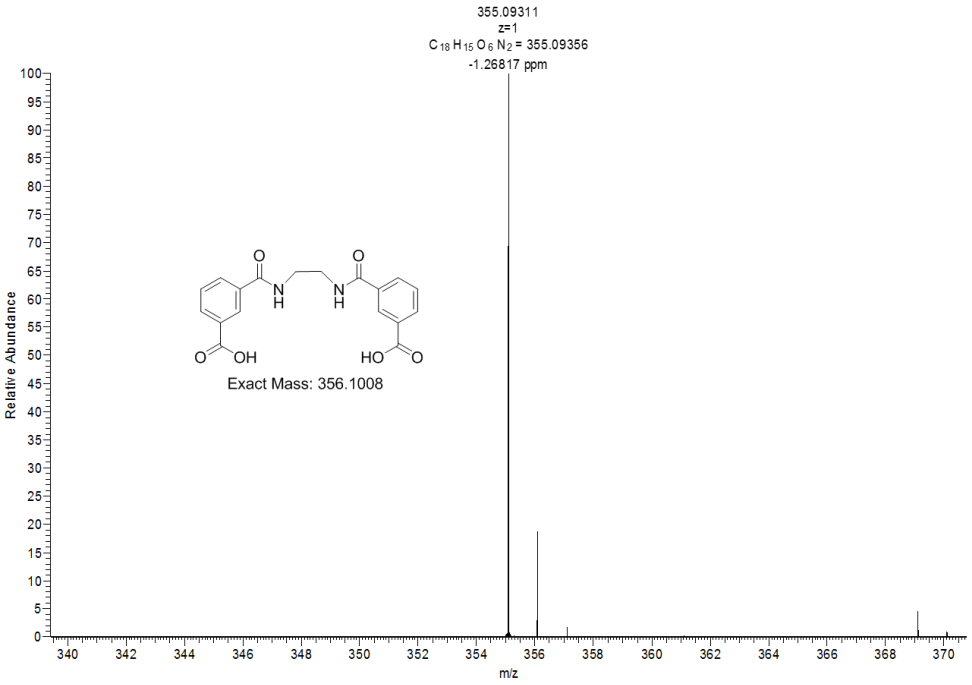



**Fig. S49**. HRMS spectrum of compound **13**.

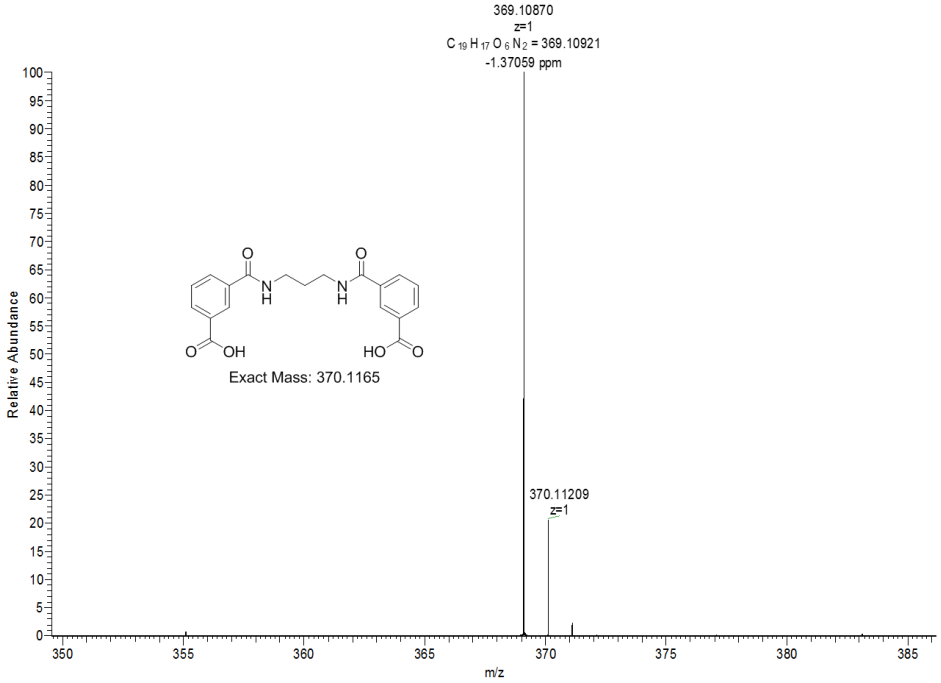



**Fig. S50**. HRMS spectrum of compound **14**.

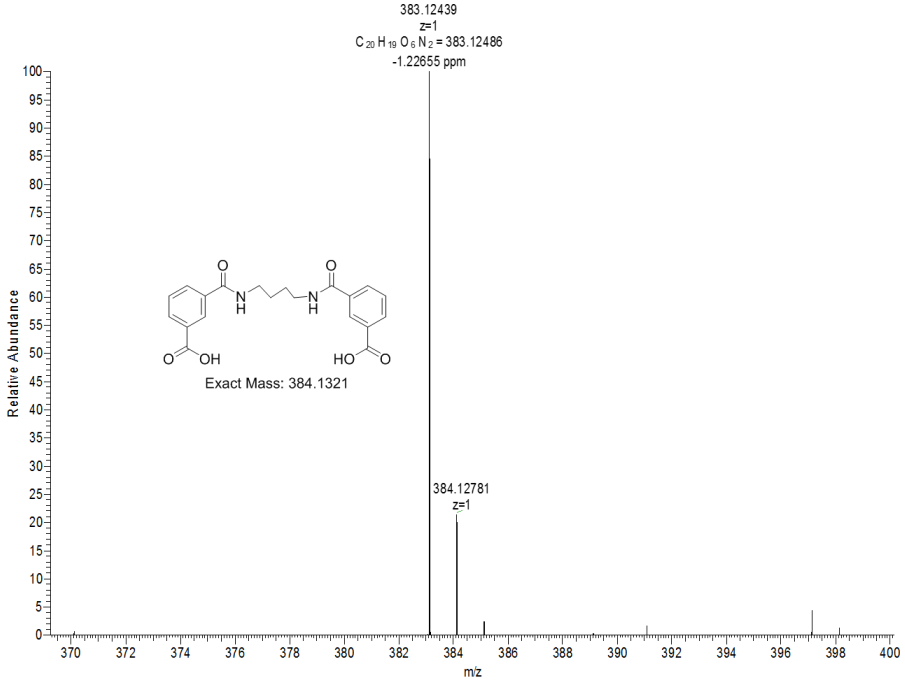



**Fig. S51**. HRMS spectrum of compound **15**.

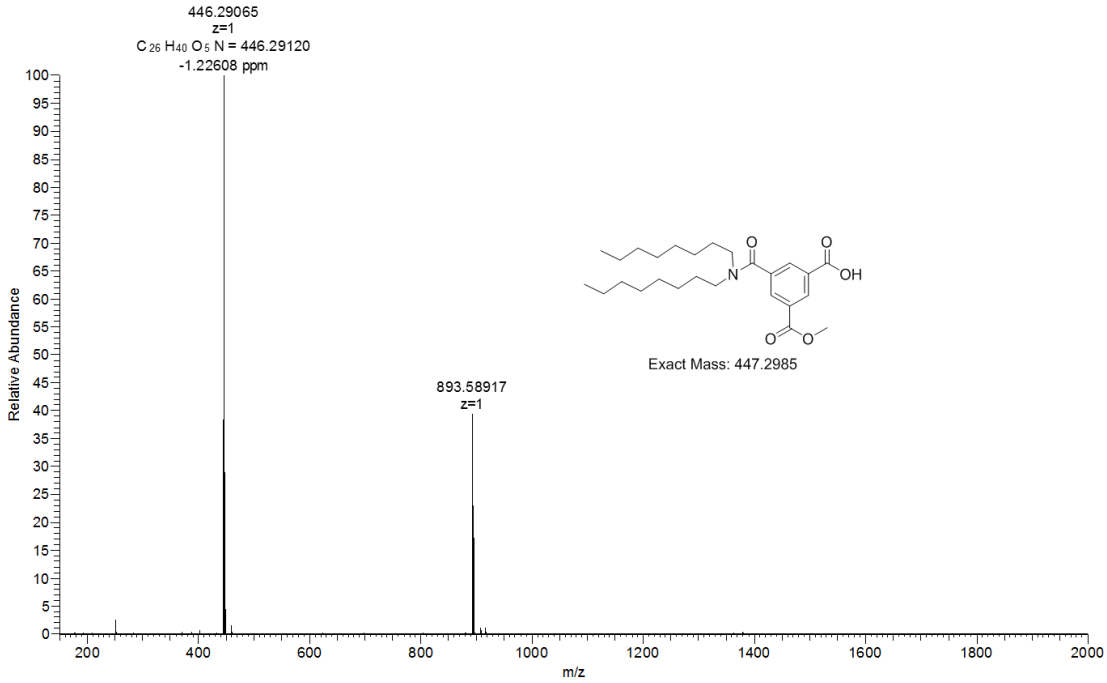



**Fig. S52**. HRMS spectrum of compound **17**.

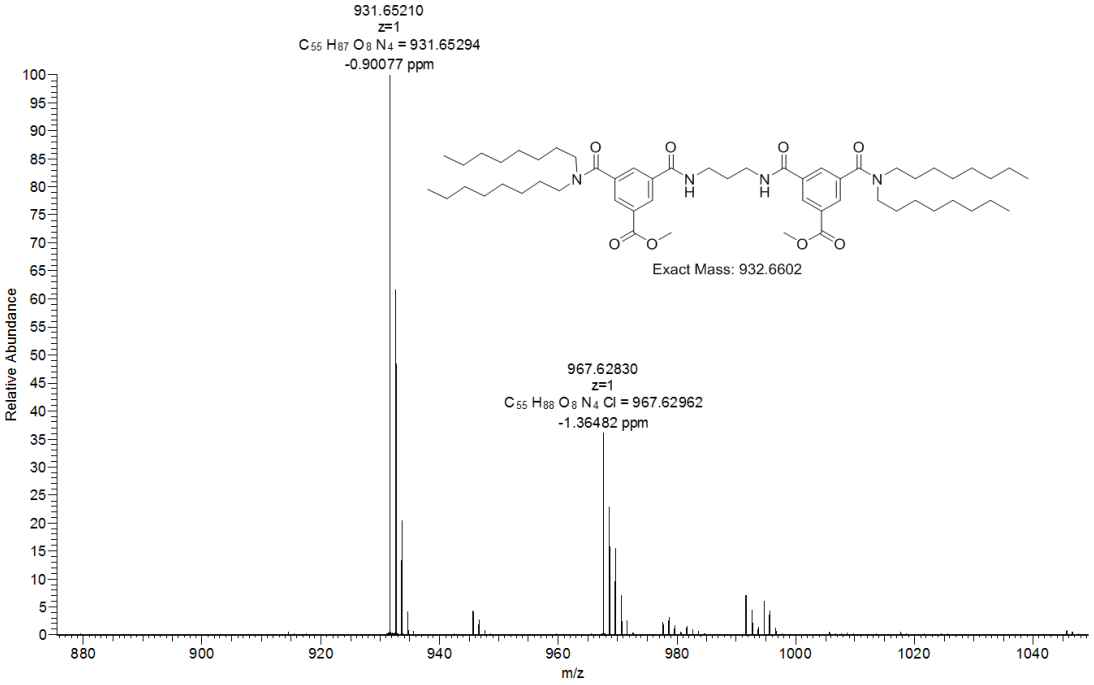



**Fig. S53**. HRMS spectrum of compound **18**.

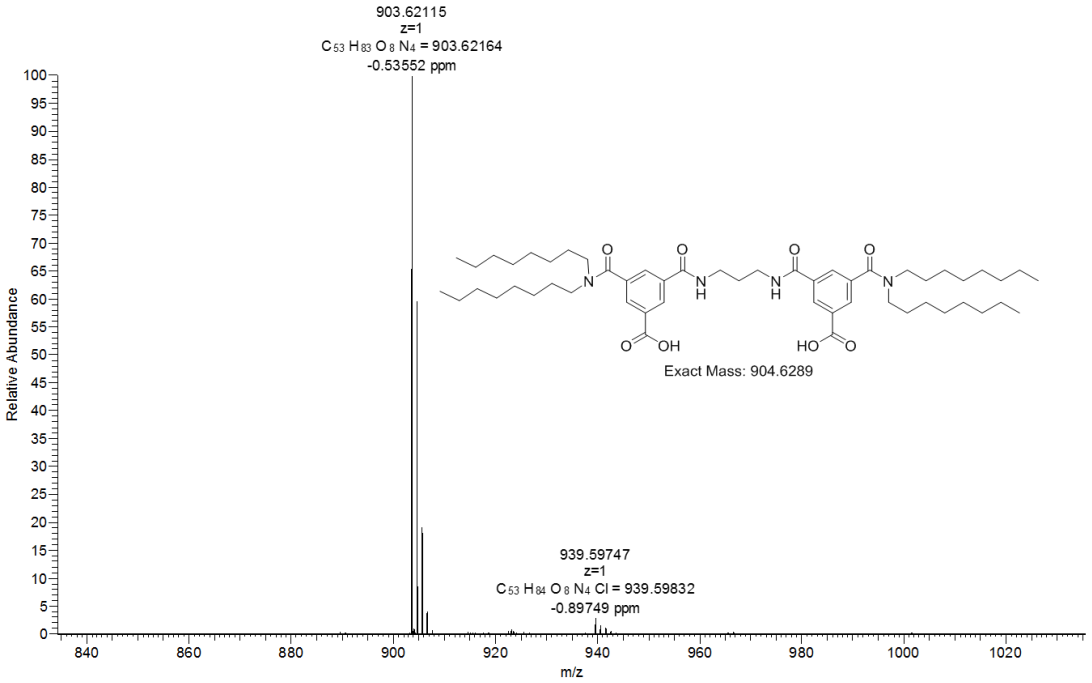



**Fig. S54**. HRMS spectrum of compound **19**.

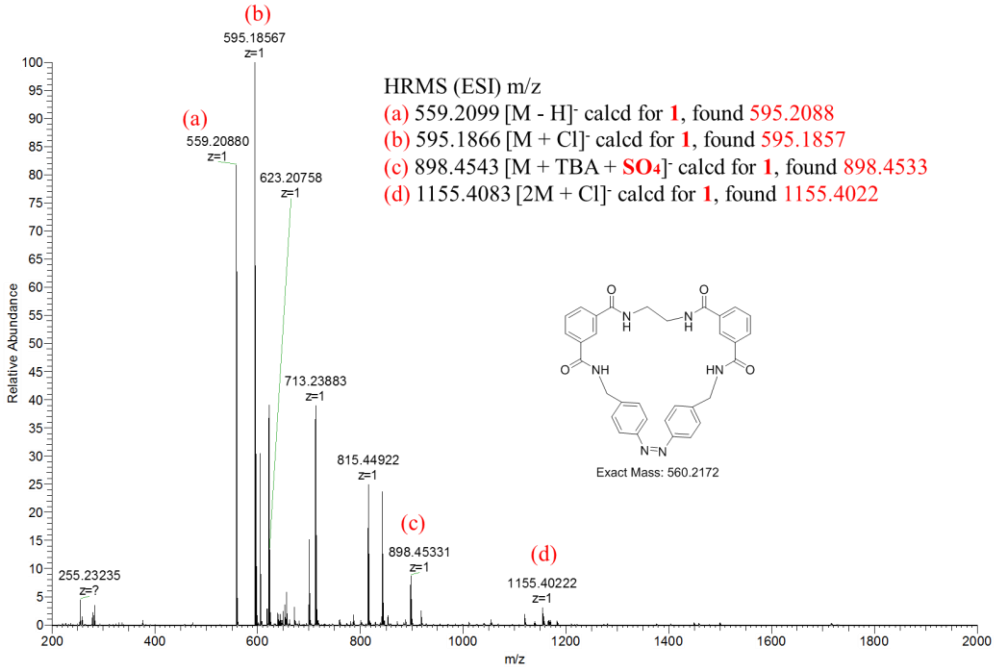



**Fig. S55**. HRMS spectrum of compound **1**.

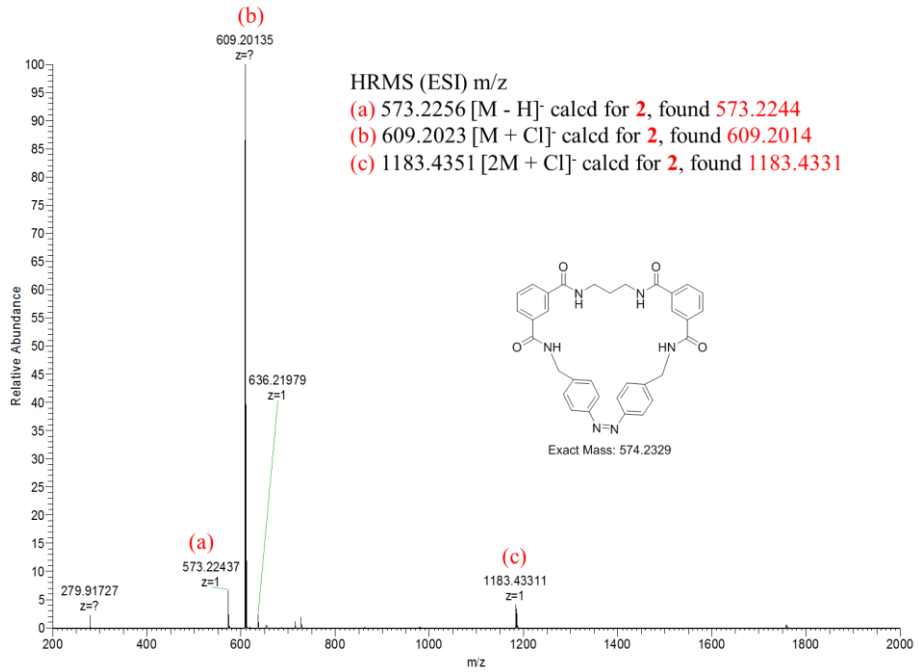



**Fig. S56**. HRMS spectrum of compound **2**.

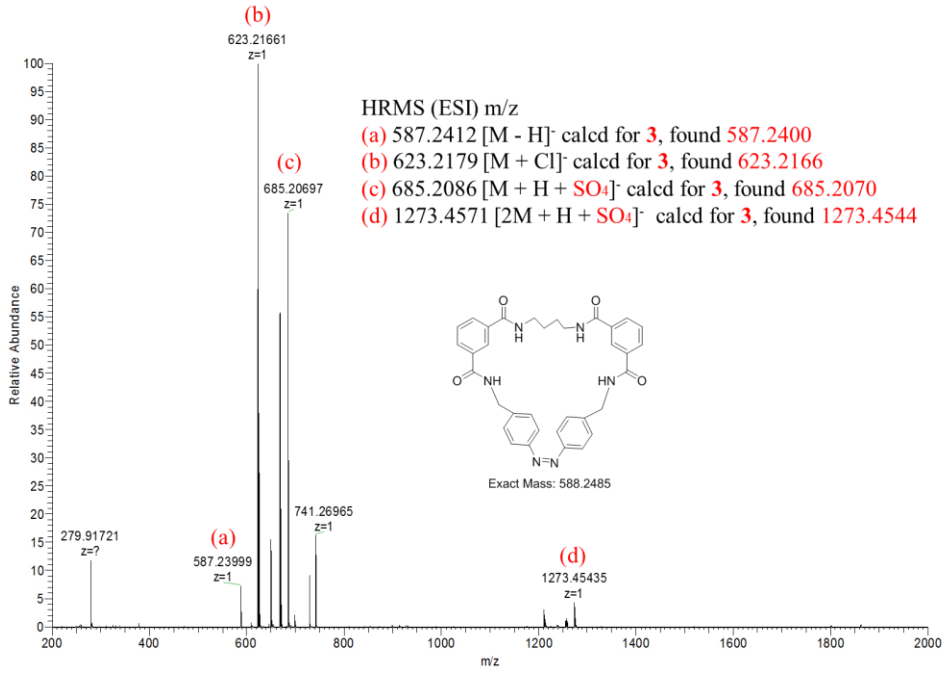



**Fig. S57**. HRMS spectrum of compound **3**.

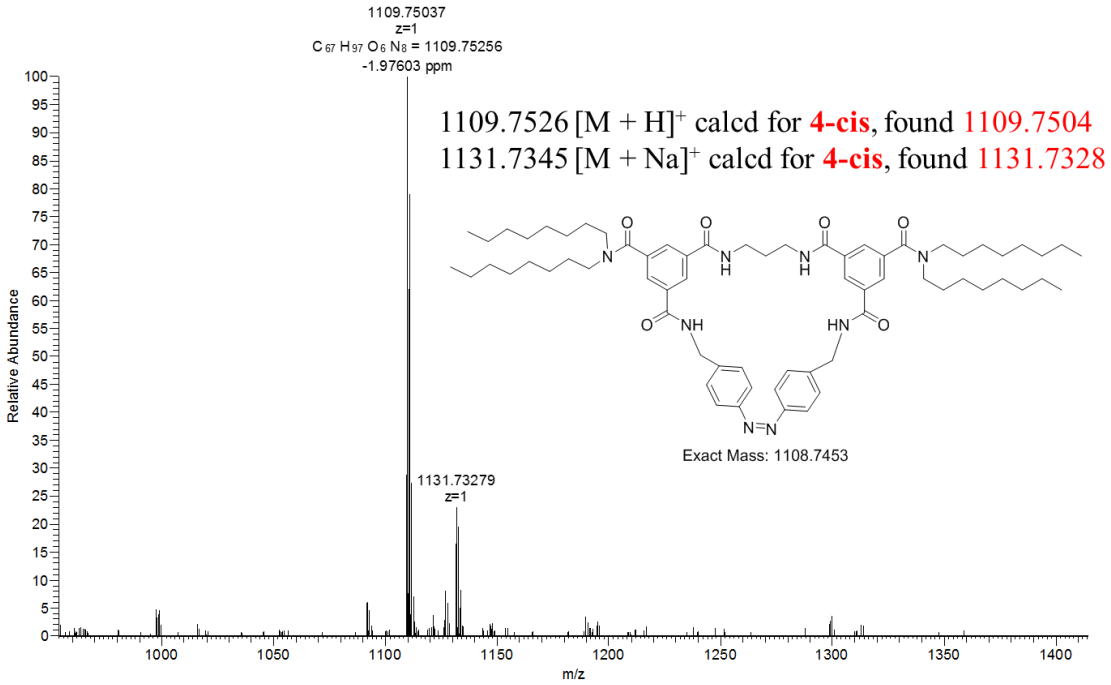



**Fig. S58**. HRMS spectrum of compound **4**.

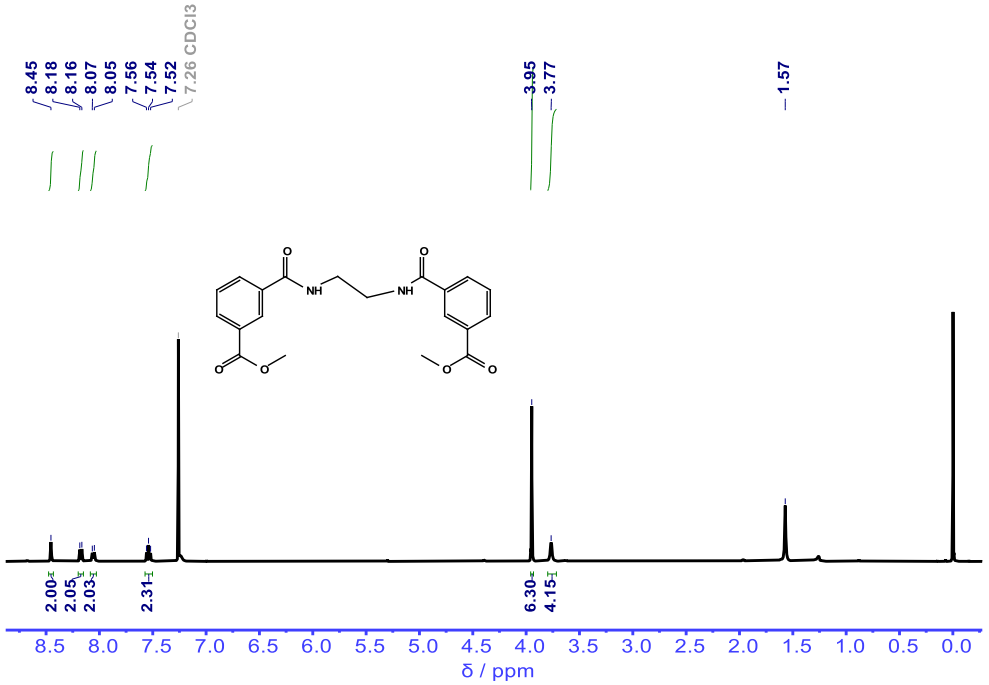



**Fig. S59.** $^{1}$H NMR spectrum of **10** recorded in $CDCl_3$ at 298 K.

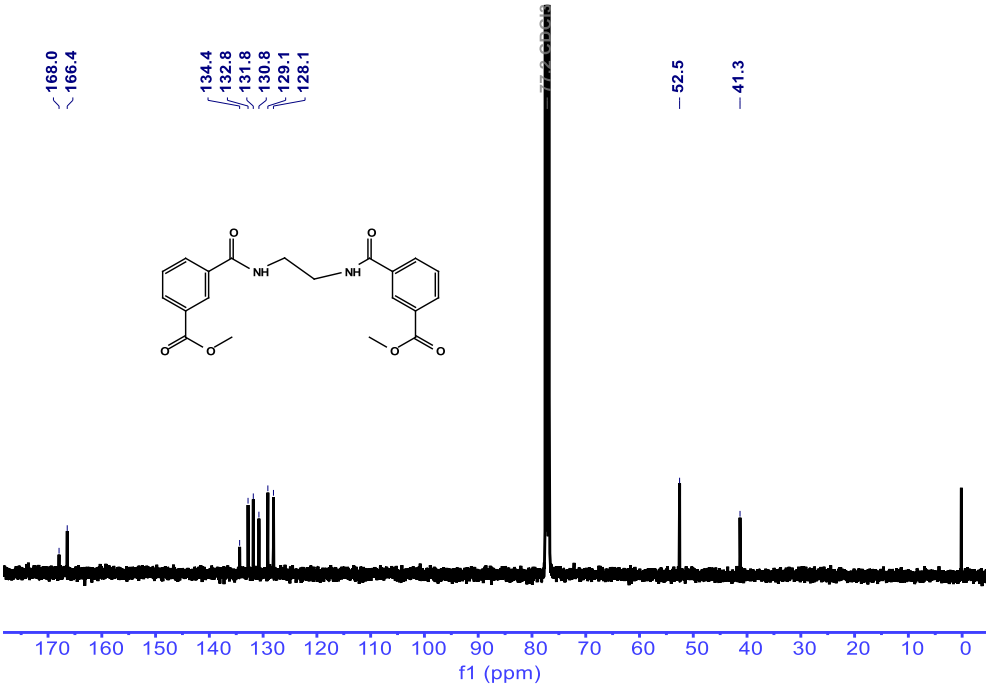



**Fig. S60.** $^{13}C$ NMR spectrum of **10** recorded in $CDCl_3$ at 298 K.

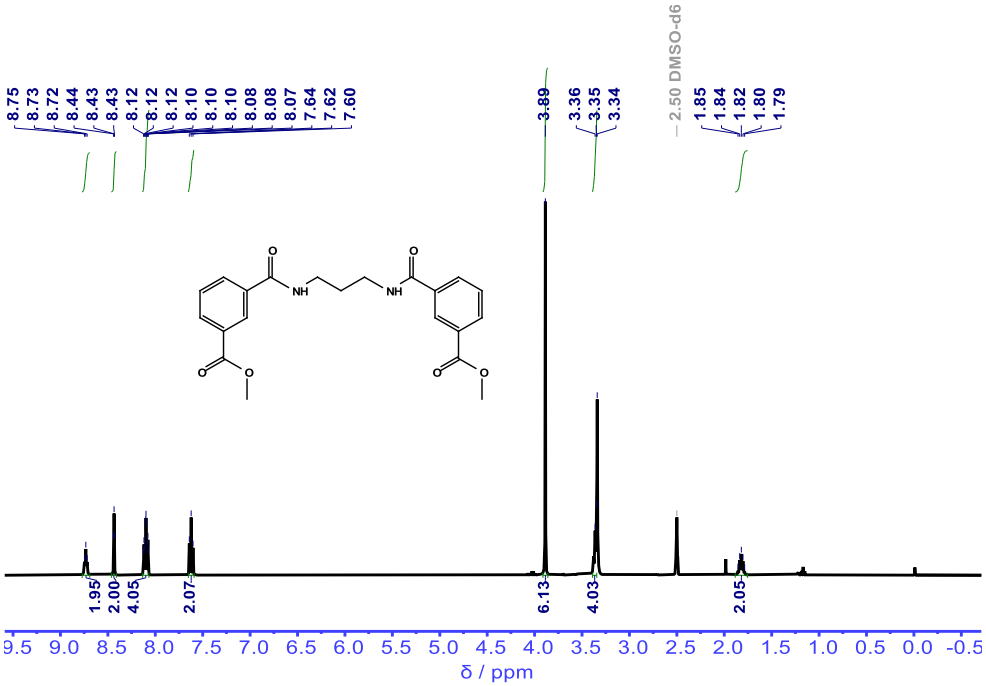



**Fig. S61.** $^{1}H$ NMR spectrum of **11** recorded in DMSO–$d_6$ at 298 K.

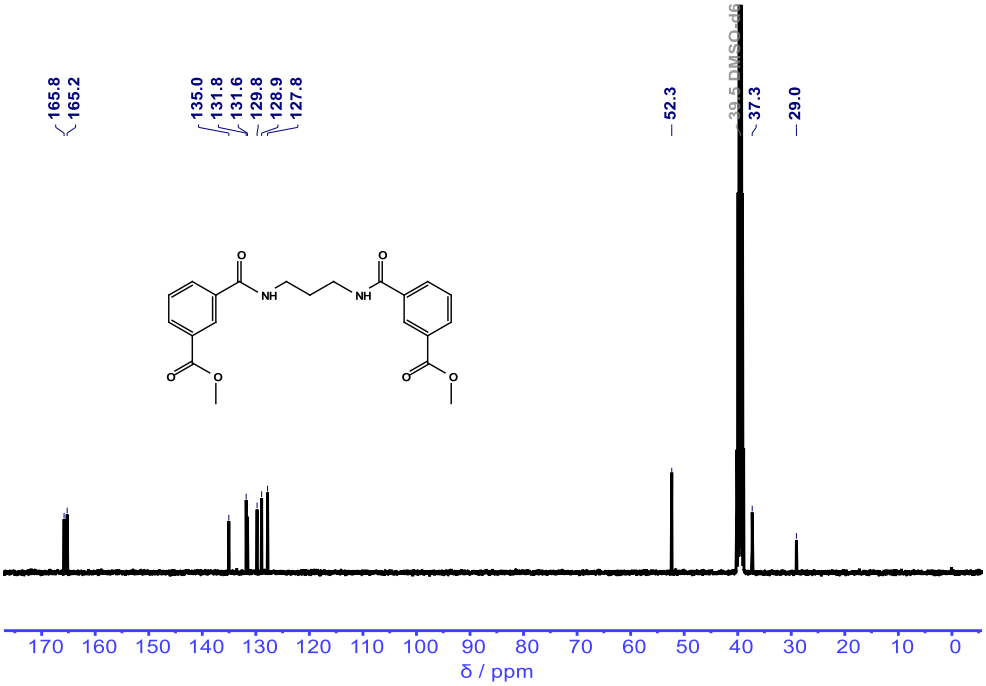



**Fig. S62.** $^{13}$C NMR spectrum of **11** recorded in DMSO–$d_6$ at 298 K.

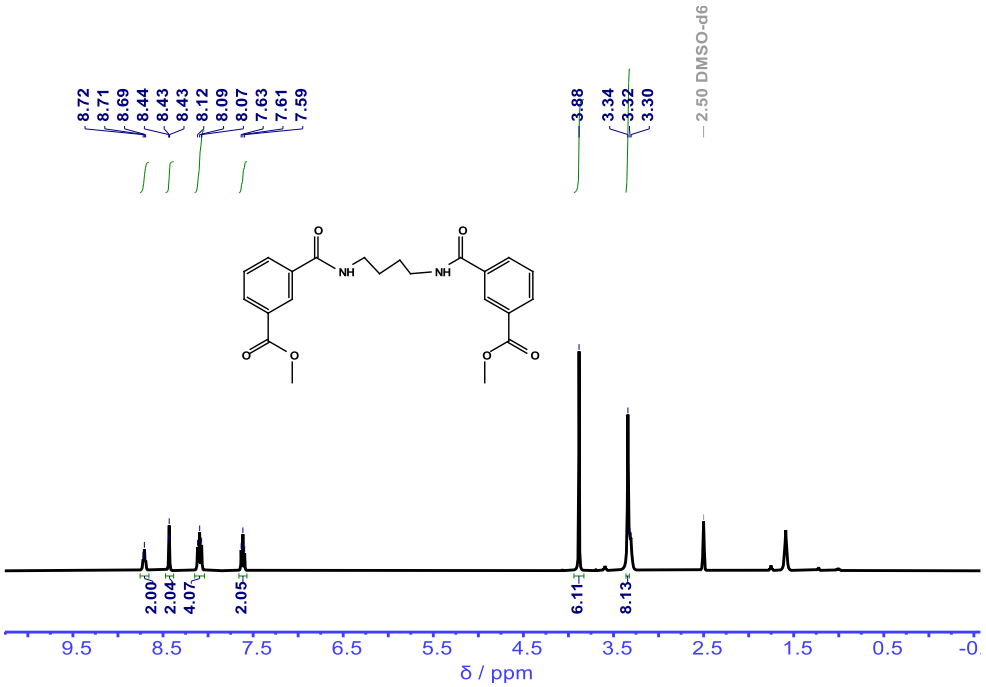



**Fig. S63.** $^{1}$H NMR spectrum of **12** recorded in DMSO–$d_6$ at 298 K.

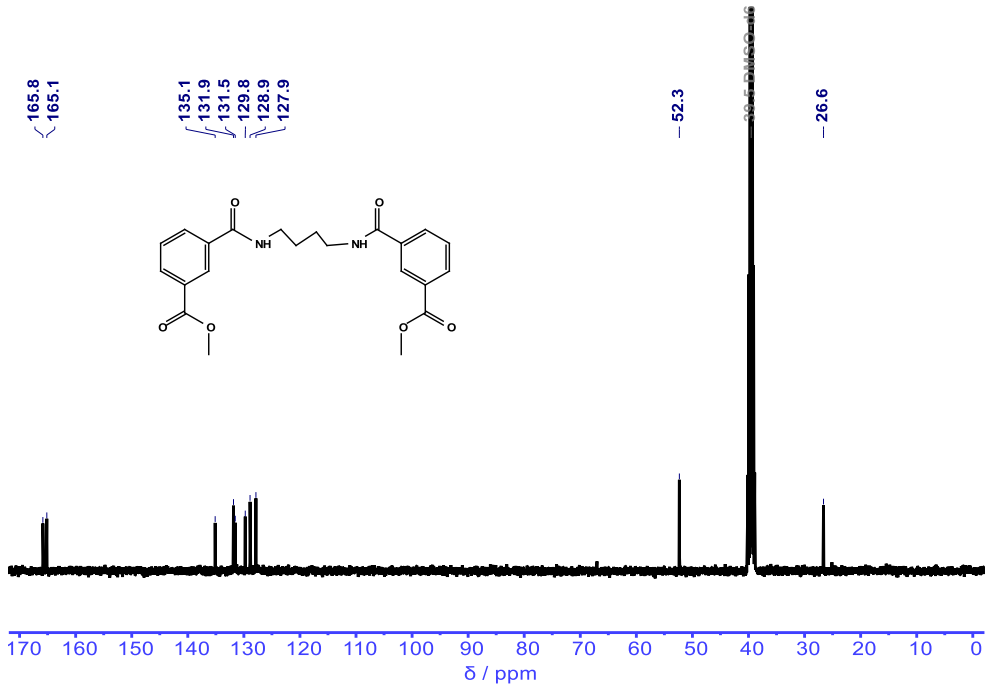



**Fig. S64.** $^{13}$C NMR spectrum of **12** recorded in DMSO–$d_6$ at 298 K.

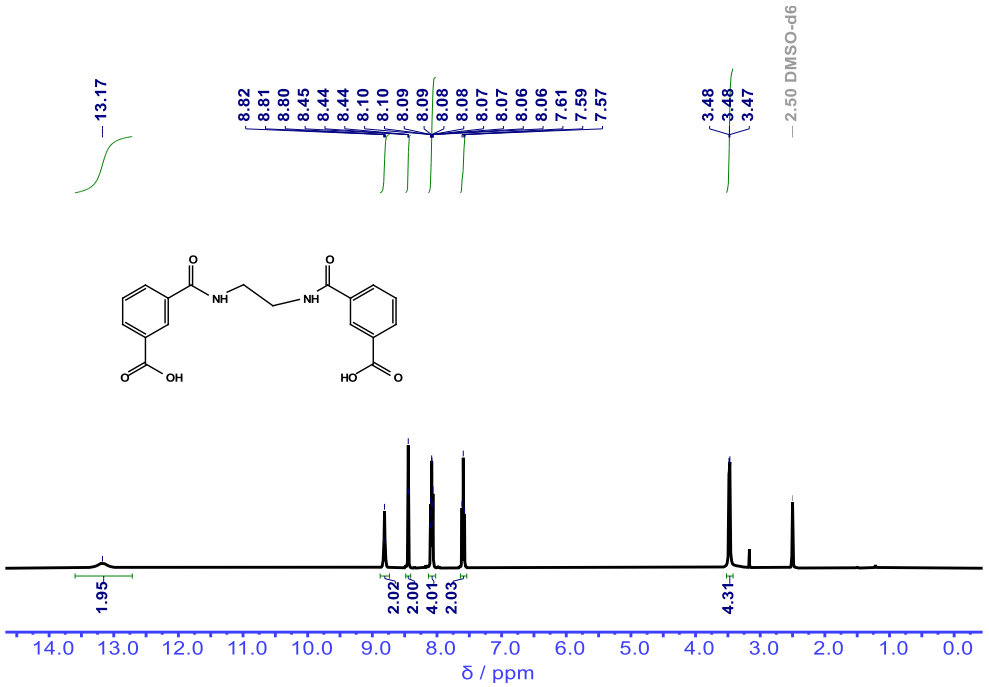



**Fig. S65.** $^{1}$H NMR spectrum of **13** recorded in DMSO–$d_6$ at 298 K.

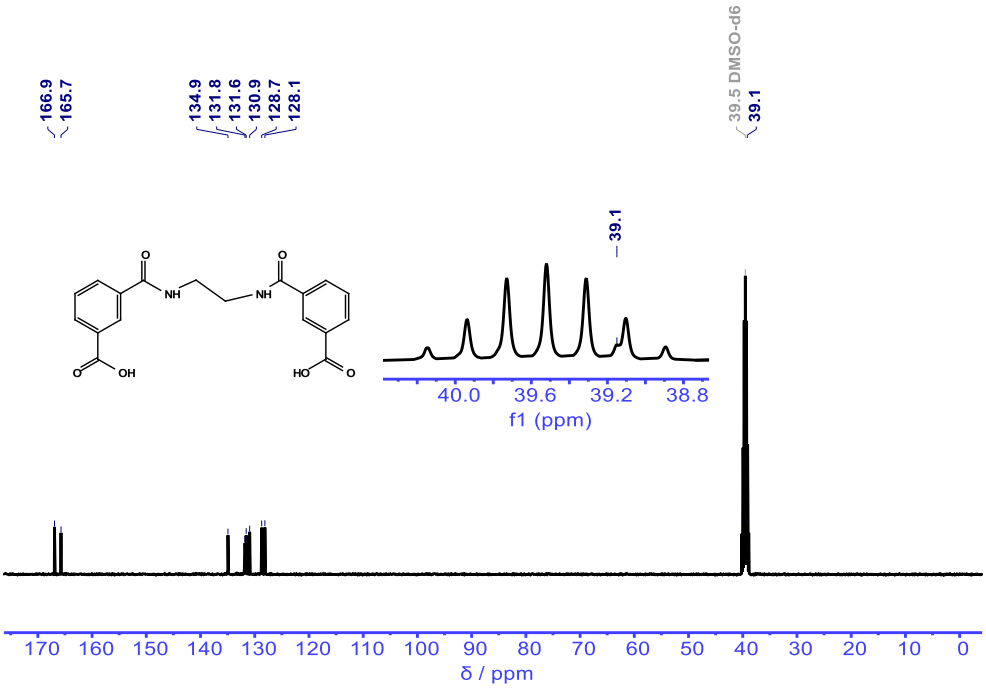



**Fig. S66.** $^{13}$C NMR spectrum of **13** recorded in DMSO–$d_6$ at 298 K.

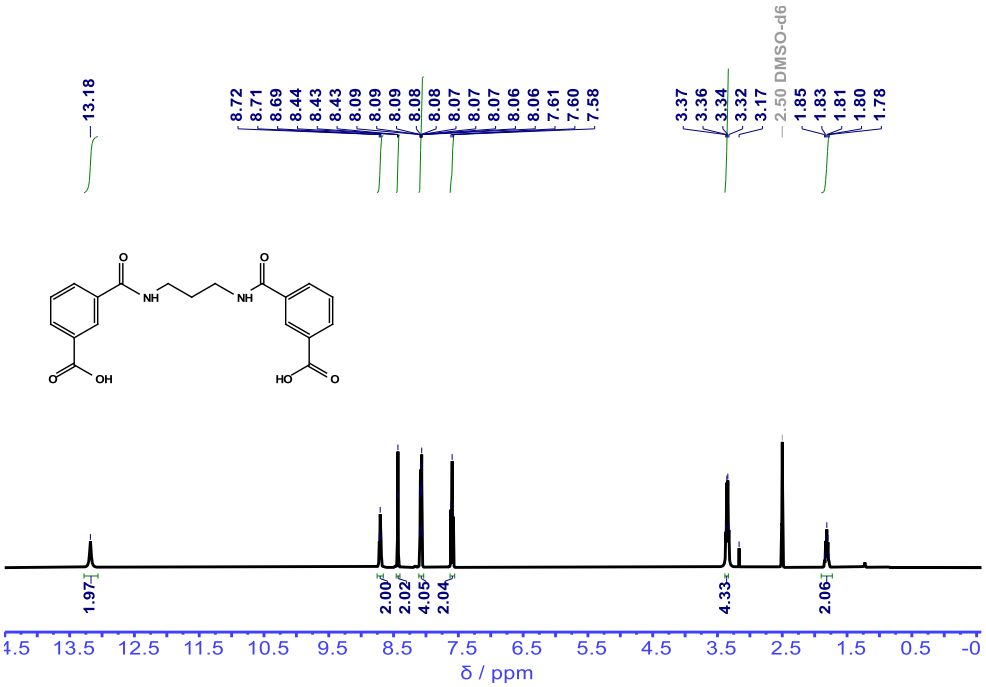



**Fig. S67.** $^{1}$H NMR spectrum of **14** recorded in DMSO–$d_6$ at 298 K.

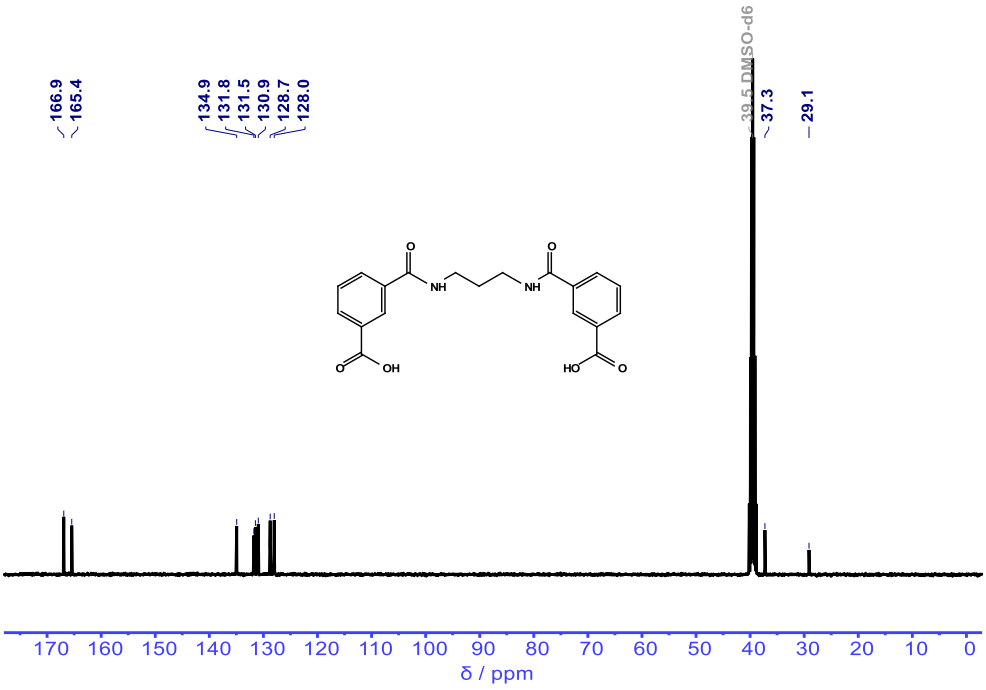



**Fig. S68.** $^{13}$C NMR spectrum of **14** recorded in DMSO–$d_6$ at 298 K.

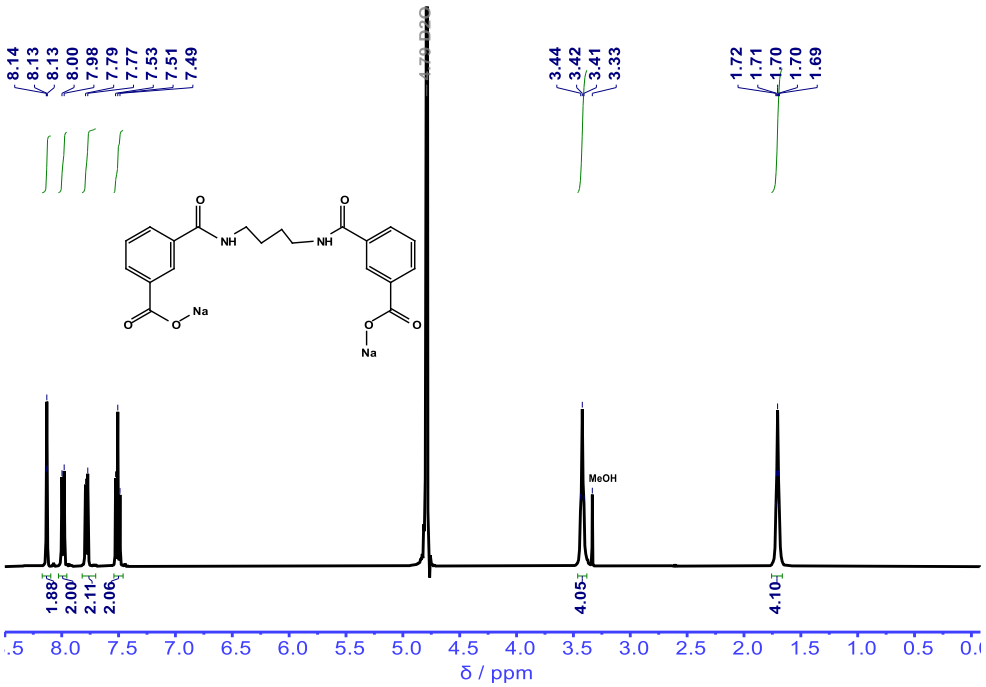



**Fig. S69.** $^{1}$H NMR spectrum of **15** recorded in $D_2O$ at 298 K.

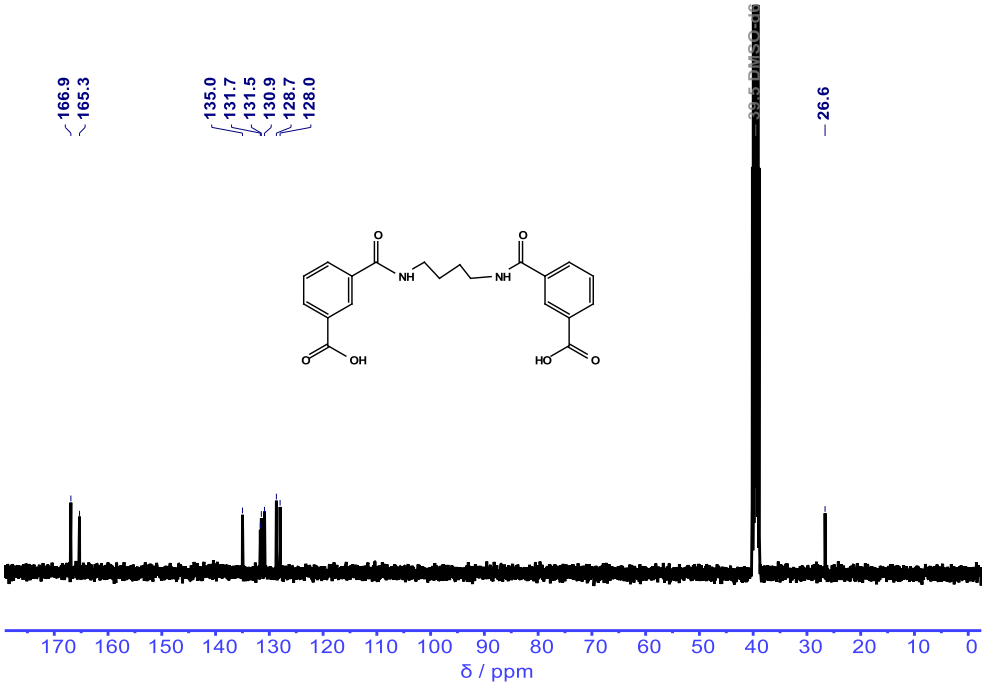



**Fig. S70.** $^{13}$C NMR spectrum of **15** recorded in DMSO–$d_6$ at 298 K.

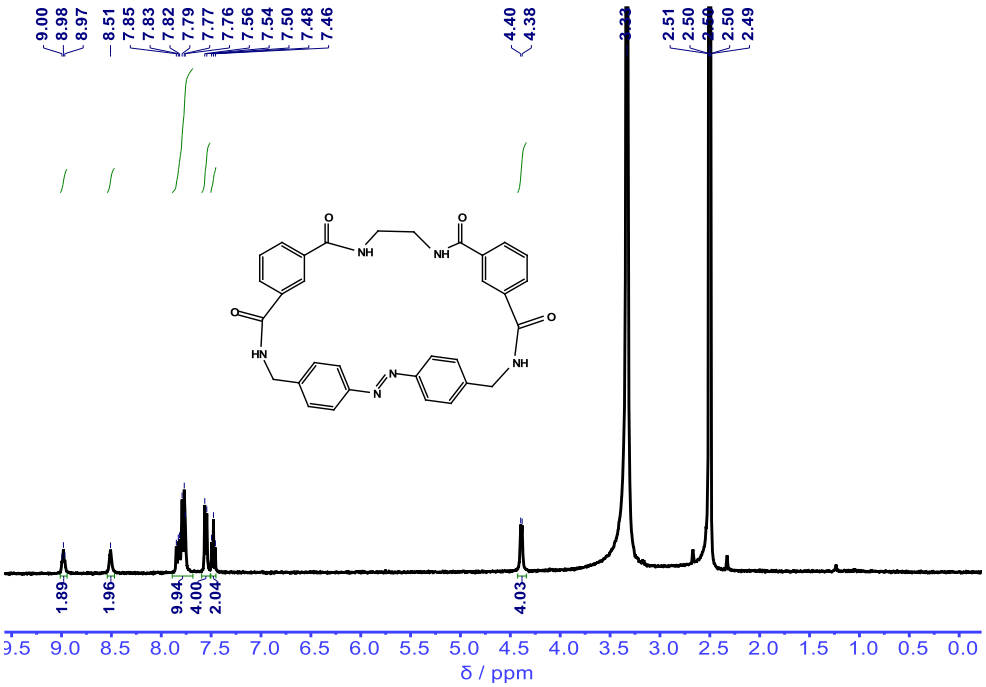



**Fig. S71.** $^{1}$H NMR spectrum of **1–trans** recorded in DMSO–$d_6$ at 298 K.

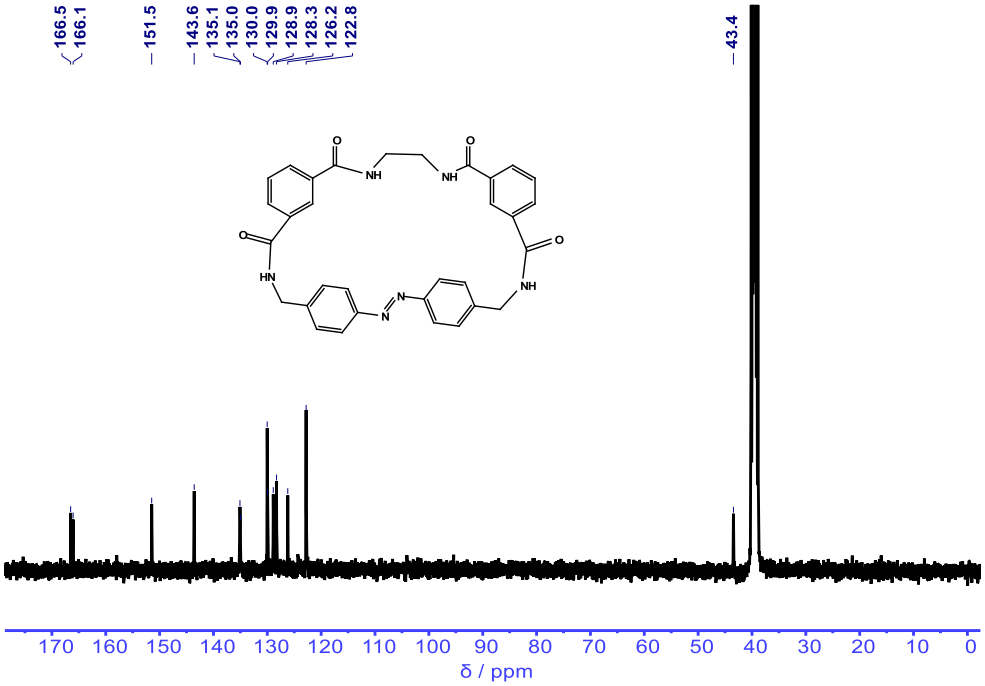



**Fig. S72.** $^{13}$C NMR spectrum of **1–trans** recorded in DMSO–$d_6$ at 298 K.

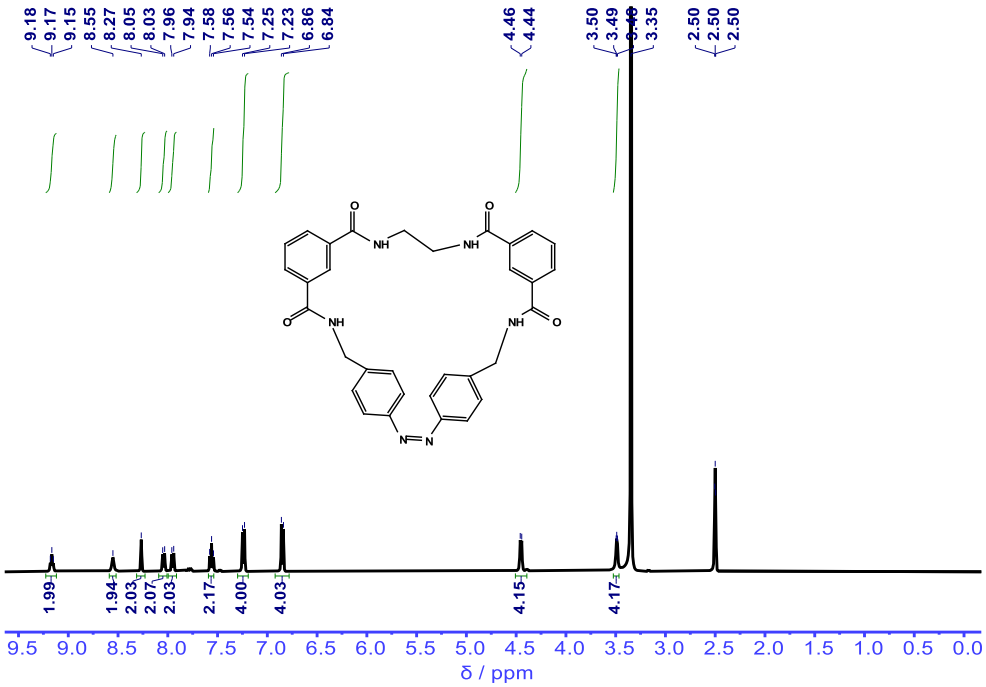



**Fig. S73.** $^{1}$H NMR spectrum of **1–cis** recorded in DMSO–$d_6$ at 298 K.

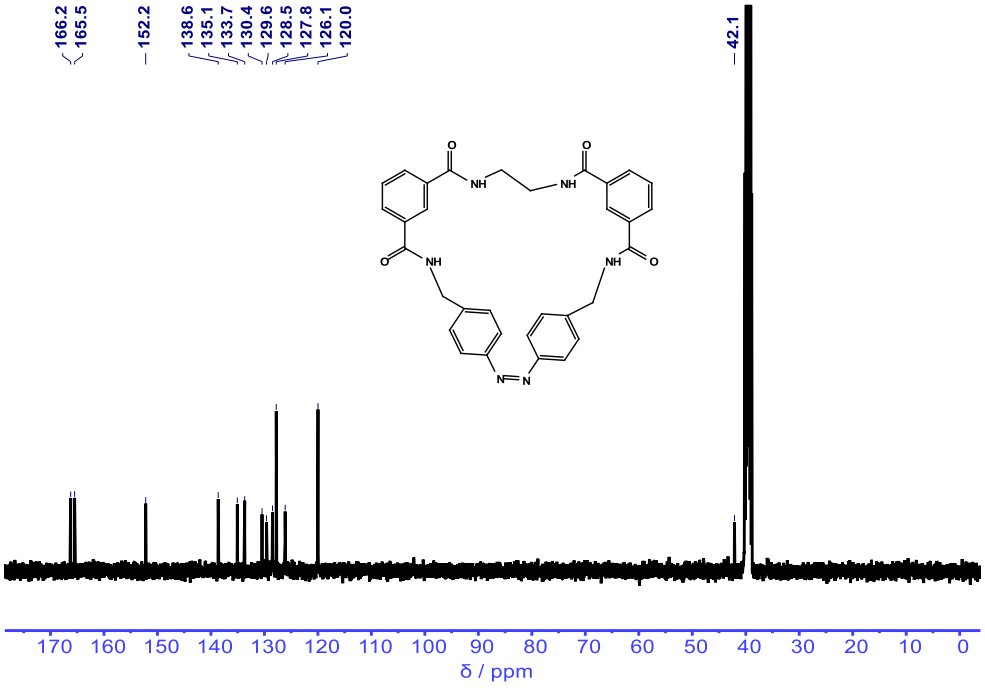



**Fig. S74.** $^{13}$C NMR spectrum of **1–cis** recorded in DMSO–$d_6$ at 298 K.

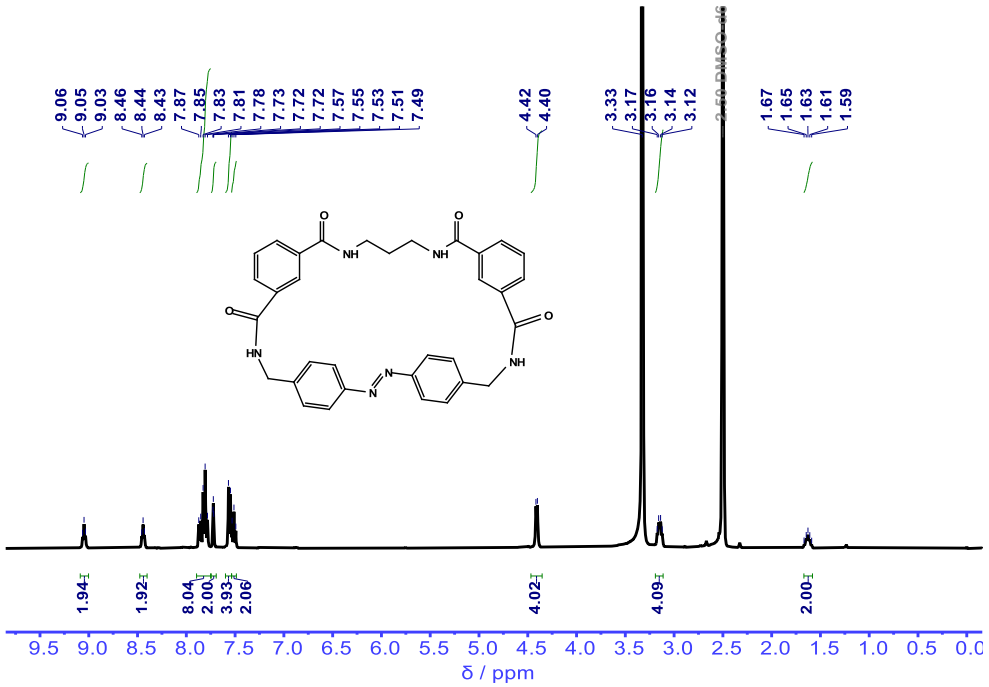



**Fig. S75.** $^{1}$H NMR spectrum of **2–trans** recorded in DMSO–$d_6$ at 298 K.

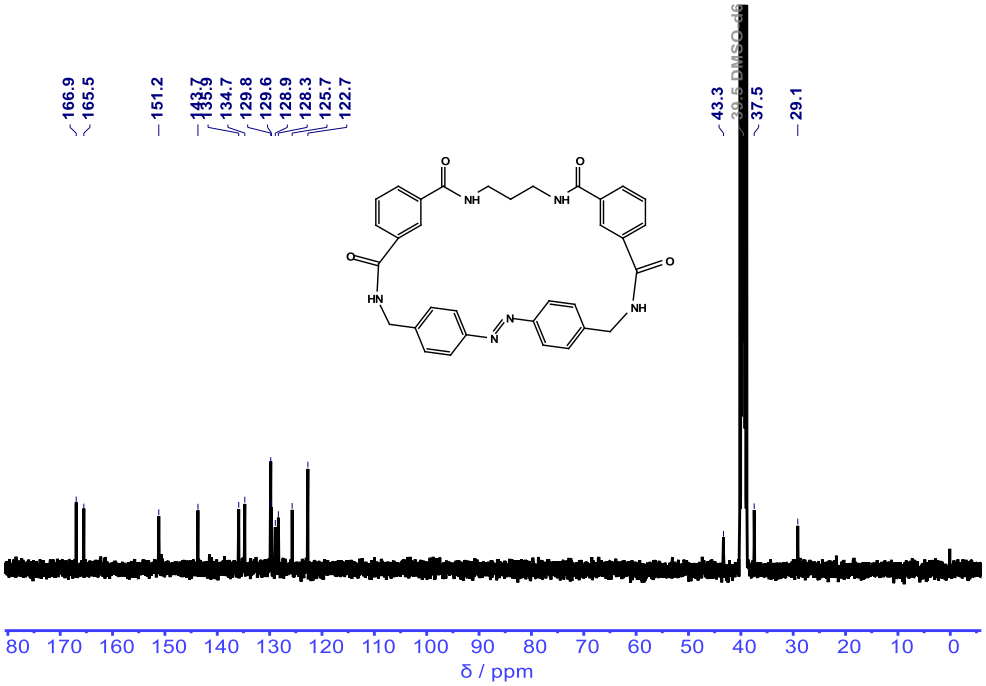



**Fig. S76.** $^{13}$C NMR spectrum of **2–trans** recorded in DMSO–$d_6$ at 298 K.

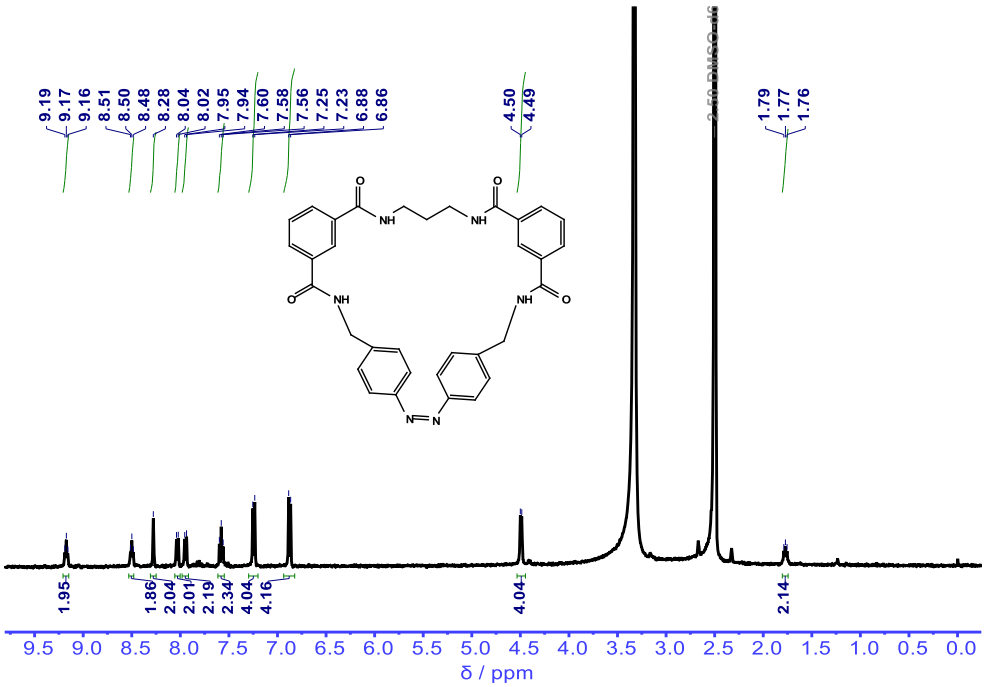



**Fig. S77.** $^{1}$H NMR spectrum of **2–cis** recorded in DMSO–$d_6$ at 298 K.

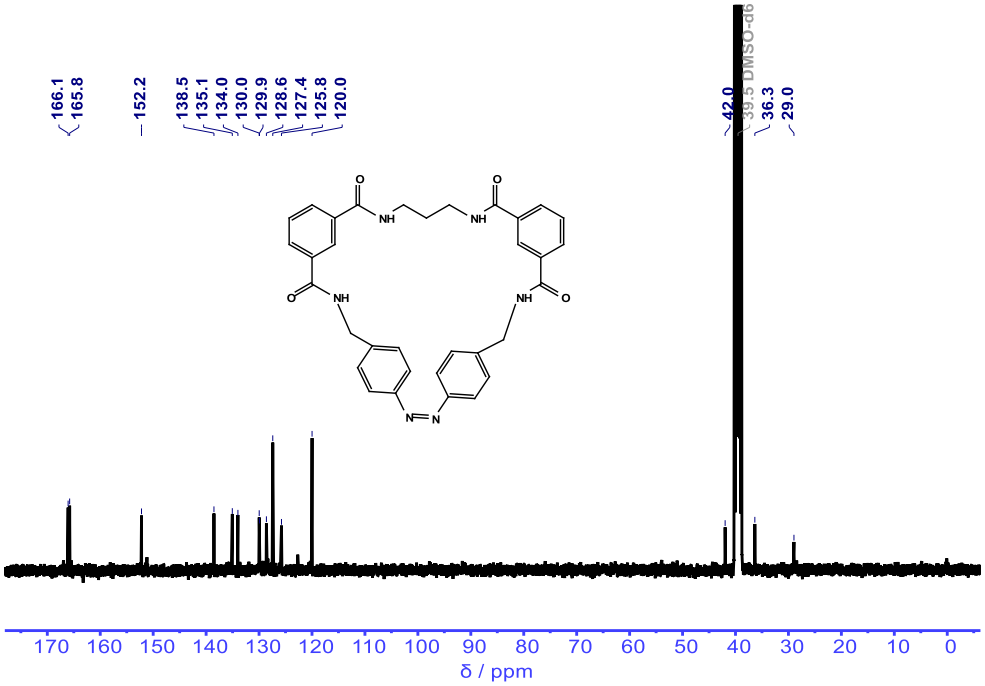



**Fig. S78.** $^{13}$C NMR spectrum of **2–cis** recorded in DMSO–$d_6$ at 298 K.

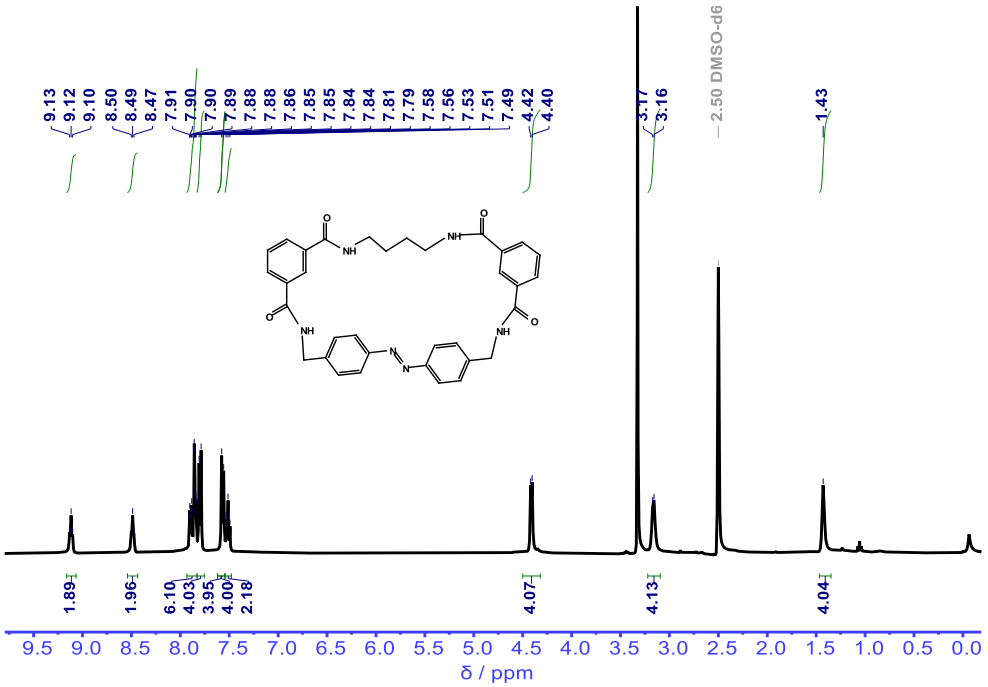



**Fig. S79.** $^{1}$H NMR spectrum of **3–trans** recorded in DMSO–$d_6$ at 298 K.

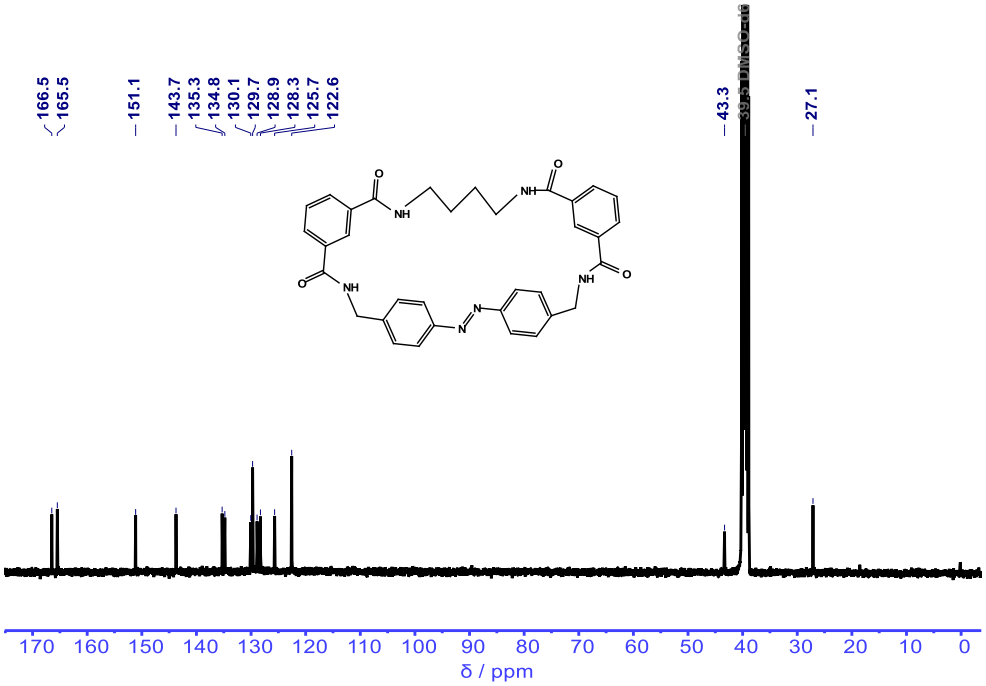



**Fig. S80.** $^{13}$C NMR spectrum of **3–trans** recorded in DMSO–$d_6$ at 298 K.

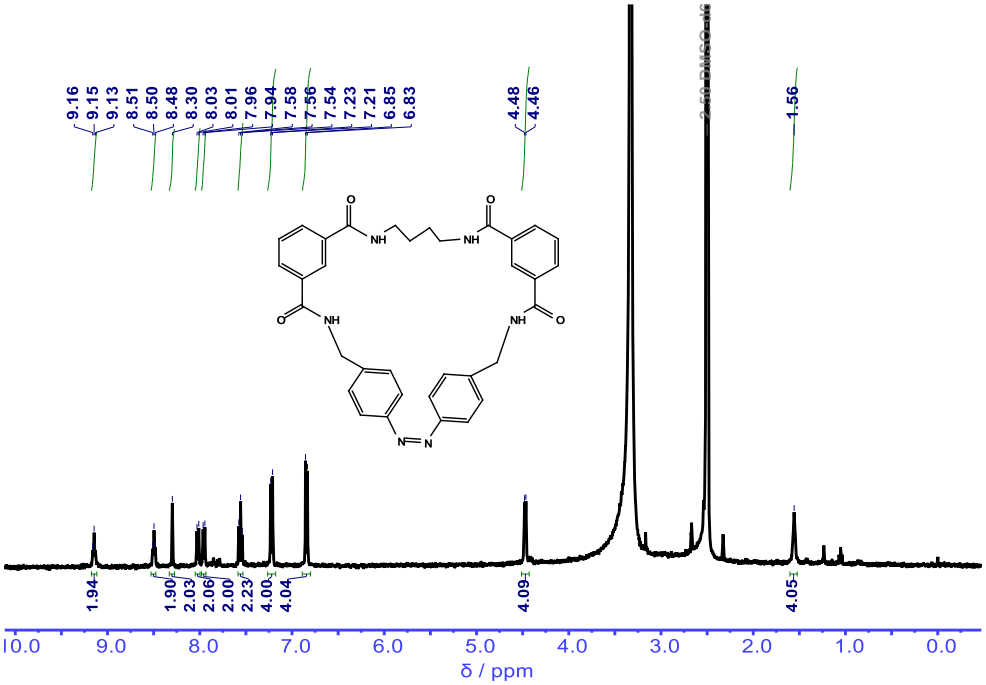



**Fig. S81.** $^{1}$H NMR spectrum of **3–cis** recorded in DMSO–$d_6$ at 298 K.

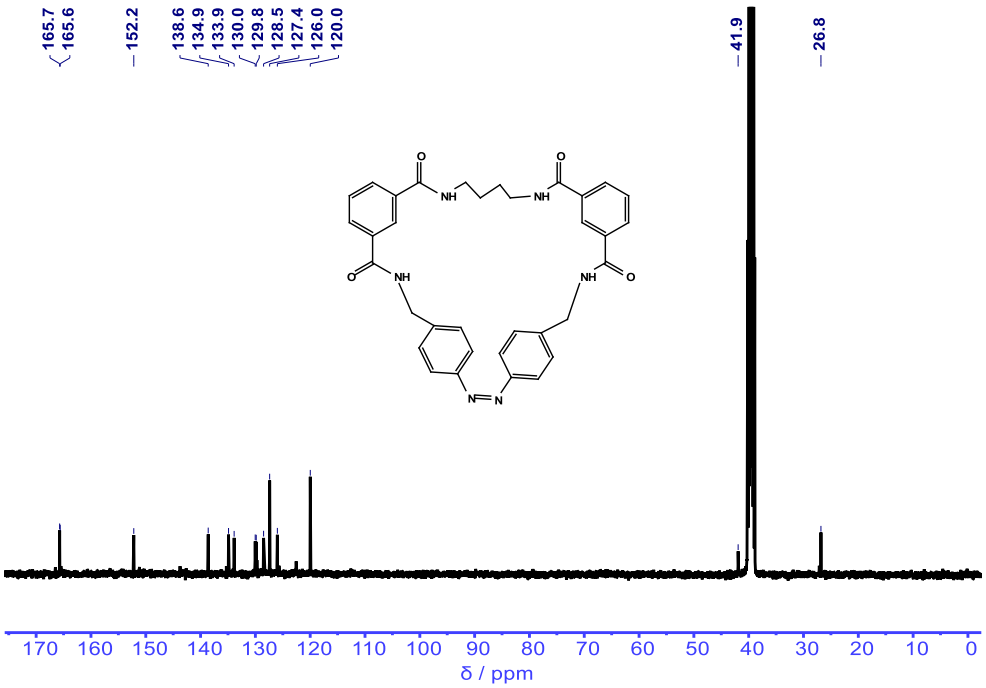



**Fig. S82.** $^{13}$C NMR spectrum of **3–cis** recorded in DMSO–$d_6$ at 298 K.

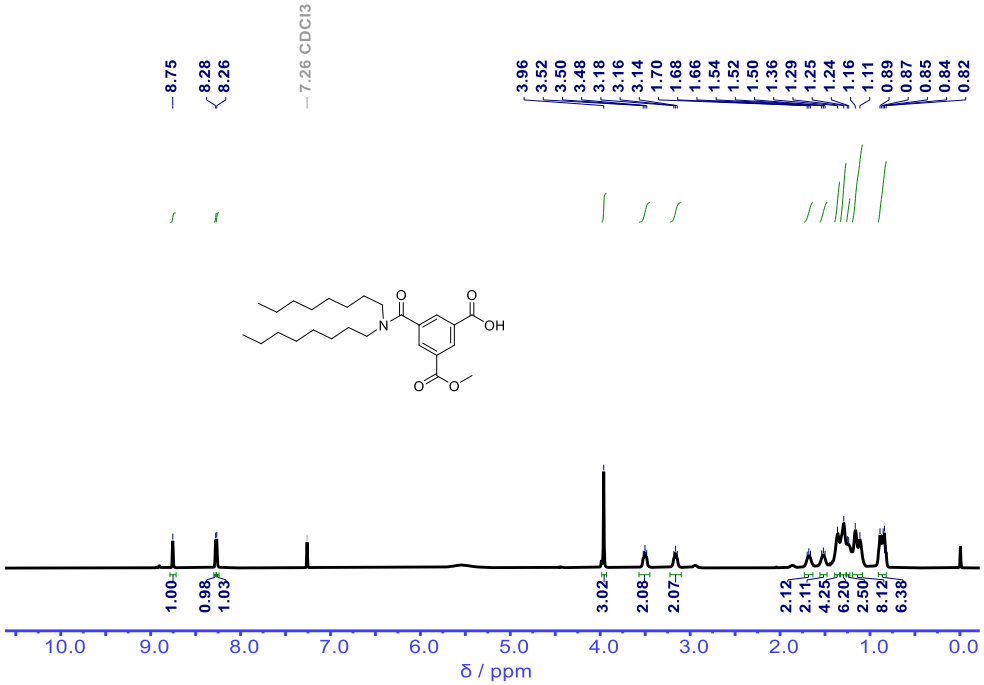



**Fig. S83.** $^{1}$H NMR spectrum of **17** recorded in $CDCl_3$ at 298 K.

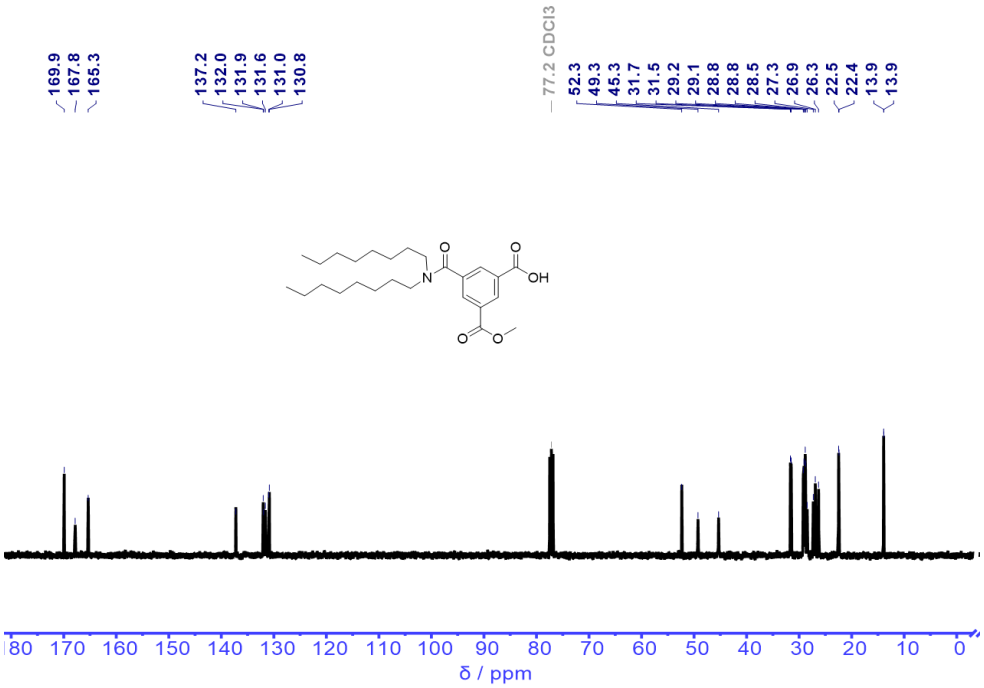



**Fig. S84.** $^{13}$C NMR spectrum of **17** recorded in $CDCl_3$ at 298 K.

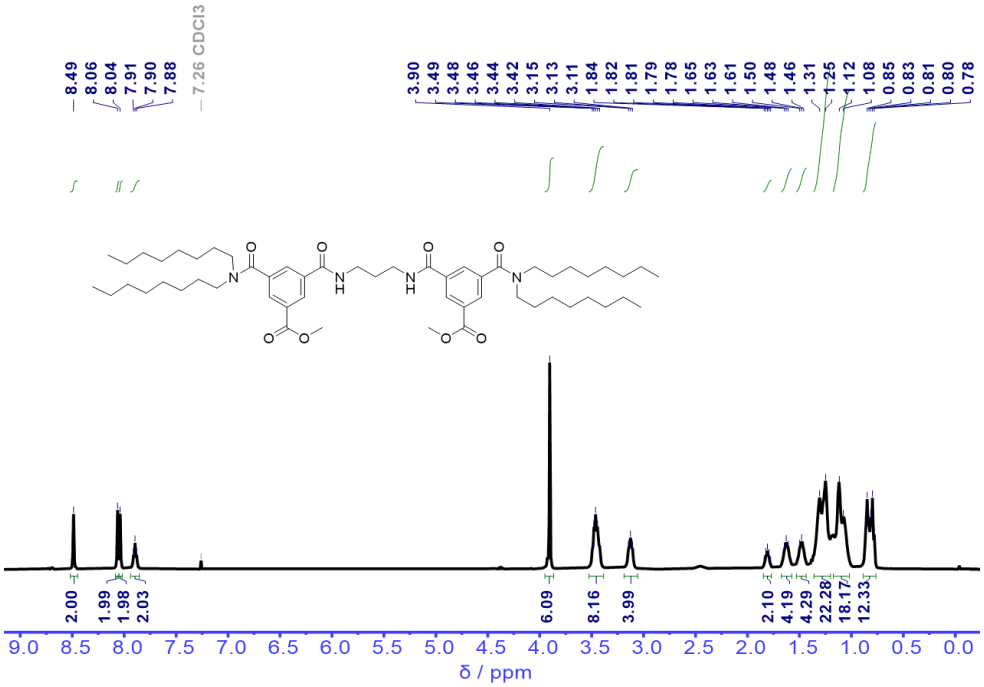



**Fig. S85.** $^{1}$H NMR spectrum of **18** recorded in $CDCl_3$ at 298 K.

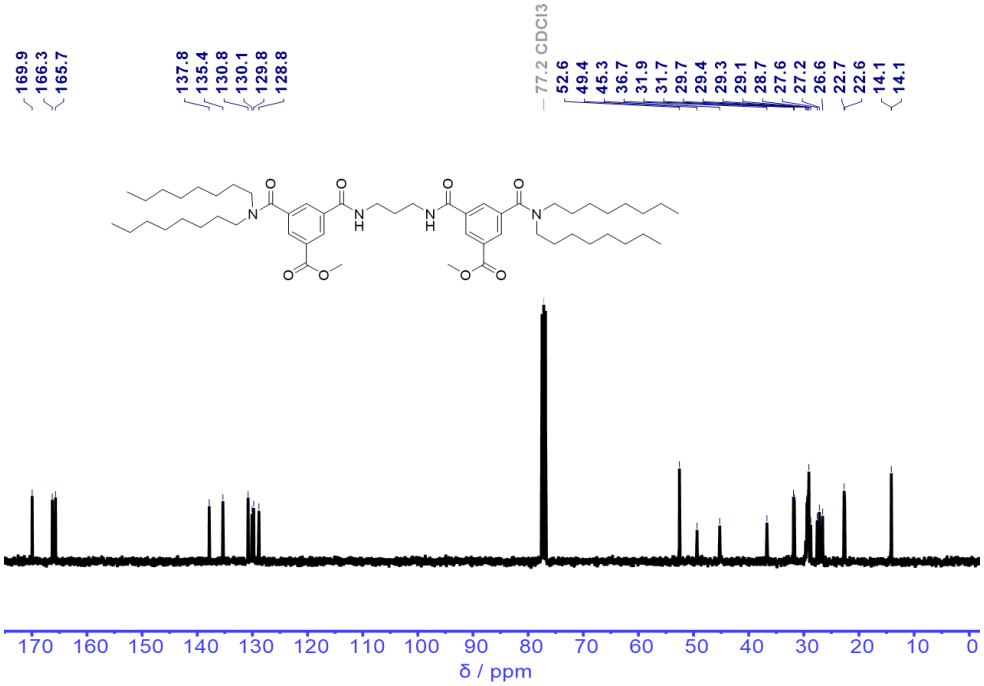



**Fig. S86.** $^{13}C$ NMR spectrum of **18** recorded in $CDCl_3$ at 298 K.

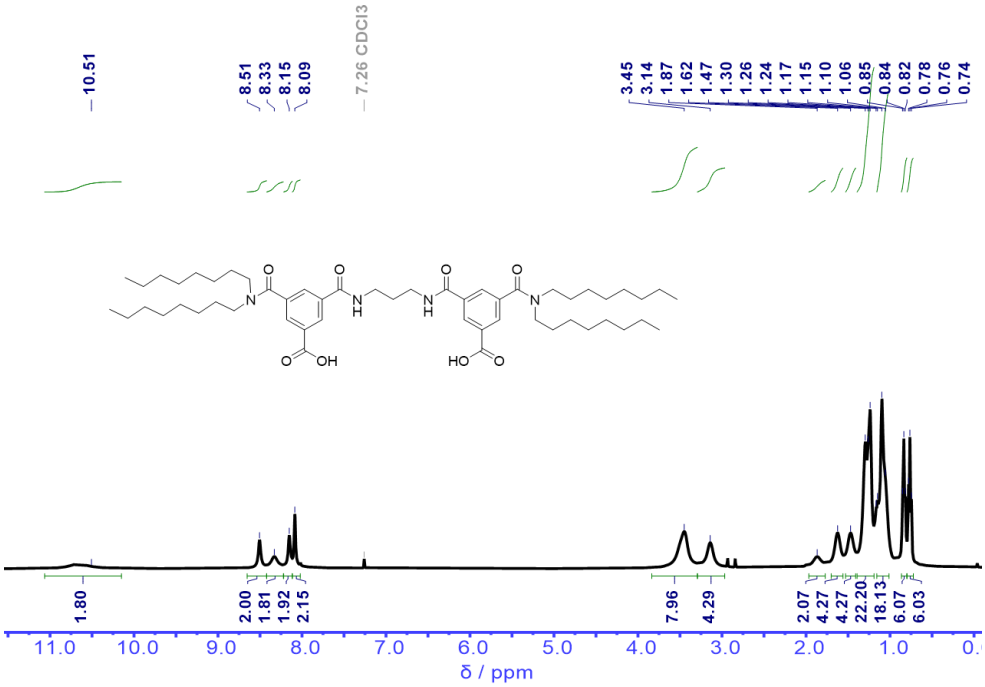



**Fig. S87.** $^{1}H$ NMR spectrum of **19** recorded in $CDCl_3$ at 298 K.

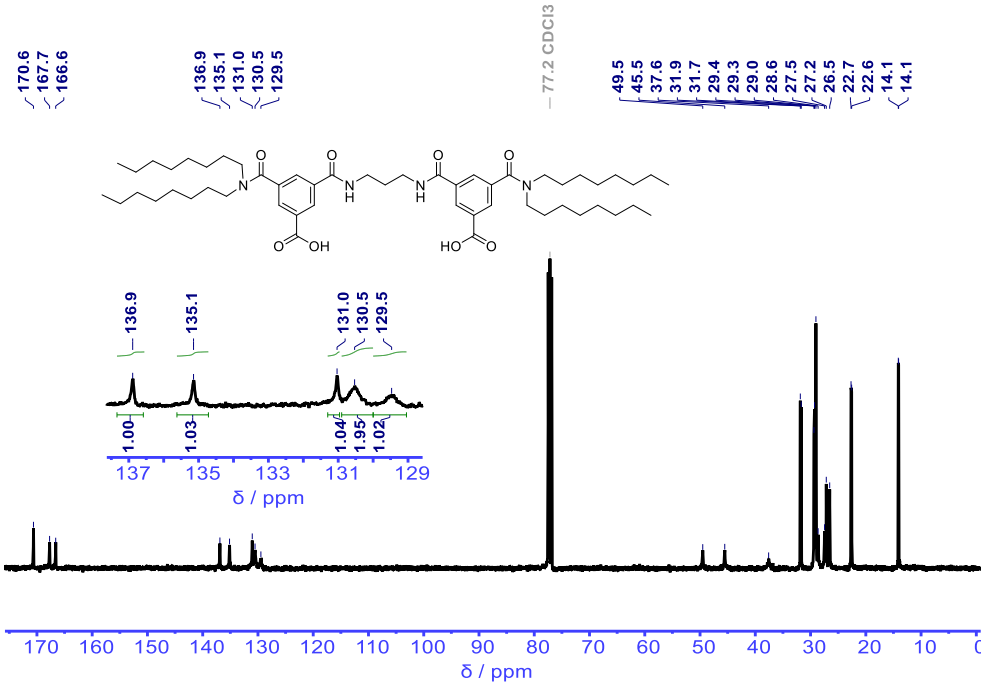



**Fig. S88.** $^{13}C$ NMR spectrum of **19** recorded in $CDCl_3$ at 298 K.

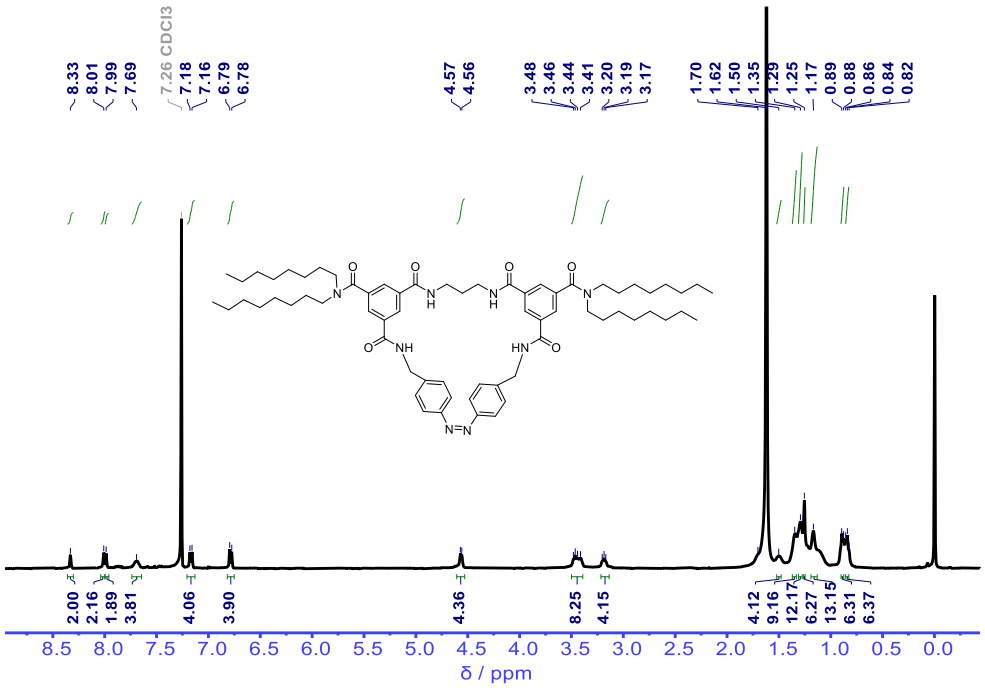



**Fig. S89.** $^{1}H$ NMR spectrum of **4-*cis*** recorded in $CDCl_3$ at 298 K.

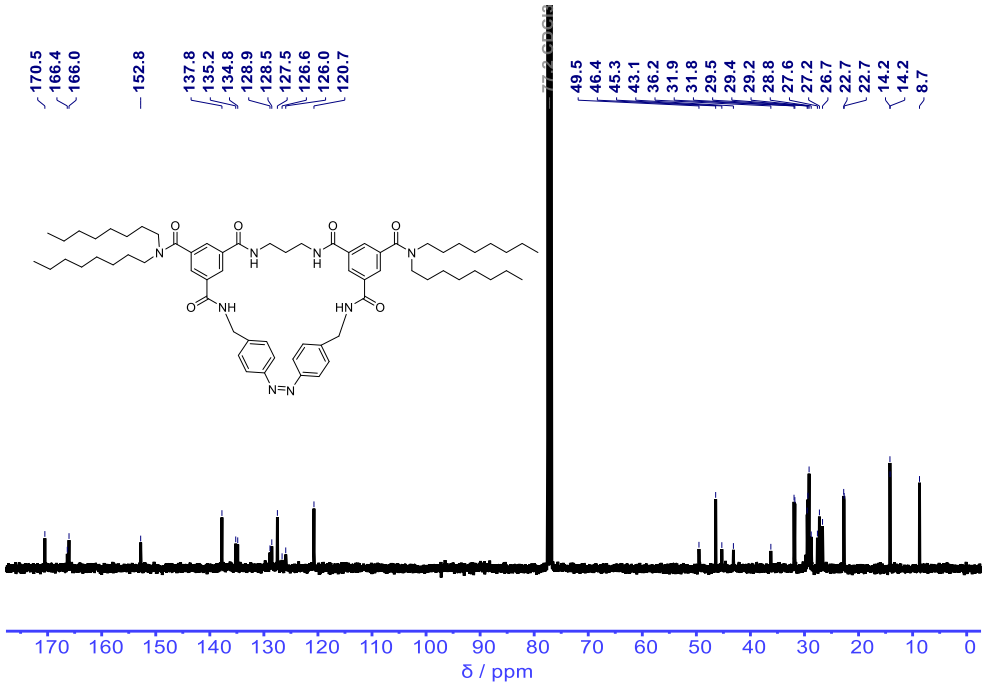



**Fig. S90.** $^{13}$C NMR spectrum of **4-*cis*** recorded in $CDCl_3$ at 298 K.

## 9. Geometrical coordinates of the optimized structure s

### 1–*cis*

**Cartesian coordinates:**

| Symbol | X | Y | Z |
|---|---|---|---|
| C | –4.78104600 | 1.31634600 | 2.16087000 |
| C | –4.11556800 | 0.11812000 | 2.85277900 |
| N | –3.53294300 | –0.82986900 | 1.91582700 |
| C | –4.34943200 | –1.71065500 | 1.24134100 |
| C | –3.68333200 | –2.53217000 | 0.17663200 |
| O | –5.53641200 | –1.84082800 | 1.51386100 |
| C | –4.47180700 | –2.99668700 | –0.88204800 |
| C | –3.89836300 | –3.75624800 | –1.89900900 |
| C | –2.54522800 | –4.08462500 | –1.85104600 |
| C | –1.75403600 | –3.66581400 | –0.77498200 |

| | | | |
|---|---|---|---|
| C | –2.32762600 | –2.87323400 | 0.22607800 |
| C | –0.31806100 | –4.10886300 | –0.75843500 |
| O | 0.25910700 | –4.47531400 | –1.77838600 |
| C | 3.39842700 | 2.92135300 | 0.75468900 |
| C | 3.20379900 | 2.05879700 | –0.32973100 |
| C | 4.10559900 | 1.03412200 | –0.60446200 |
| C | 5.24747900 | 0.87801100 | 0.19048100 |
| C | 5.47741800 | 1.76564400 | 1.24878600 |
| C | 4.54105900 | 2.74870200 | 1.54755600 |
| N | 6.30913300 | –0.01691100 | –0.16498300 |
| N | 6.13648500 | –1.22330200 | –0.43092400 |
| C | 4.91130400 | –1.92749200 | –0.18615100 |
| C | 4.29896500 | –1.93748400 | 1.07464600 |
| C | 3.24920500 | –2.81688600 | 1.32206900 |
| C | 2.77015700 | –3.67309500 | 0.32372900 |
| C | 3.37585300 | –3.63817800 | –0.93867000 |
| C | 4.45951600 | –2.80048400 | –1.18290500 |
| C | 2.44499700 | 4.06339000 | 1.05516100 |
| C | 1.65103000 | –4.65527000 | 0.61369900 |
| N | 0.30458200 | –4.10181400 | 0.46050600 |
| H | –5.56796700 | 0.95525000 | 1.49616200 |
| H | –5.23336300 | 1.97203800 | 2.91410900 |
| H | –4.86707900 | –0.41616600 | 3.43868400 |
| H | –3.32488300 | 0.45554300 | 3.53274100 |
| H | –2.69996400 | –0.52545500 | 1.43018500 |
| H | –5.52601400 | –2.74191400 | –0.89191500 |
| H | –4.50849700 | –4.09663500 | –2.73030300 |
| H | –2.07851600 | –4.67535000 | –2.63194100 |

| | | | |
|---|---|---|---|
| H | –1.72285700 | –2.51793300 | 1.05564500 |
| H | 2.33881900 | 2.18964000 | –0.97321500 |
| H | 3.94028900 | 0.37444100 | –1.44953300 |
| H | 6.38717000 | 1.66522000 | 1.83292300 |
| H | 4.71344600 | 3.41217800 | 2.39188600 |
| H | 4.67075600 | –1.29035800 | 1.86201700 |
| H | 2.80493800 | –2.84635500 | 2.31482000 |
| H | 2.99849000 | –4.28644700 | –1.72322200 |
| H | 4.96845000 | –2.81333200 | –2.14195500 |
| H | 2.43903400 | 4.26017600 | 2.13534500 |
| H | 2.77503800 | 4.98436700 | 0.56309700 |
| H | 1.73350600 | –5.01566700 | 1.64374400 |
| H | 1.73857500 | –5.51674700 | –0.05492100 |
| H | –0.26132200 | –4.00017200 | 1.28909600 |
| N | 1.08938700 | 3.83692200 | 0.58298300 |
| C | 0.51589100 | 4.63772900 | –0.37330400 |
| C | –0.82595200 | 4.19556100 | –0.88779600 |
| O | 1.06068500 | 5.64944700 | –0.79956700 |
| C | –1.20567000 | 4.65398100 | –2.15479900 |
| C | –2.41099900 | 4.24308900 | –2.71926700 |
| C | –3.25605600 | 3.38688500 | –2.01787600 |
| C | –2.91535200 | 2.96221500 | –0.72835200 |
| C | –1.69526900 | 3.36350800 | –0.17309600 |
| C | –3.87610500 | 2.04792100 | –0.02161600 |
| O | –4.62819900 | 1.30756200 | –0.64367500 |
| N | –3.84385700 | 2.08834200 | 1.35190100 |
| H | 0.68494100 | 2.92730300 | 0.75312700 |
| H | –0.53296900 | 5.32214400 | –2.68141800 |

| | | | |
|---|---|---|---|
| H | –2.68948200 | 4.58695000 | –3.71086800 |
| H | –4.18925800 | 3.03724600 | –2.44620800 |
| H | –1.42206200 | 3.01989500 | 0.82105600 |
| H | –3.37497100 | 2.87049300 | 1.78599400 |

**2–*cis***

**Cartesian coordinates:**

| Symbol | X | Y | Z |
|---|---|---|---|
| C | 4.57084600 | 0.03825700 | –3.00659800 |
| C | 4.50942200 | –2.47802100 | –2.37521200 |
| N | 3.42979100 | –2.35702300 | –1.39037900 |
| C | 3.68995100 | –2.42084600 | –0.04492900 |
| C | 2.50414500 | –2.55378600 | 0.87135500 |
| O | 4.83323700 | –2.34295000 | 0.39075400 |
| C | 2.68045700 | –2.17165700 | 2.20705300 |
| C | 1.63669700 | –2.30084400 | 3.12010100 |
| C | 0.40940600 | –2.81935000 | 2.71329500 |
| C | 0.21376700 | –3.20176900 | 1.38161000 |
| C | 1.26870100 | –3.07499400 | 0.47065400 |
| C | –1.12913700 | –3.75953200 | 1.00171400 |
| O | –1.88138700 | –4.25809400 | 1.83149900 |
| C | –2.65385600 | 3.56249000 | –0.34496600 |
| C | –2.92380300 | 2.53105600 | 0.56564500 |
| C | –4.08695400 | 1.77659200 | 0.46256700 |
| C | –5.02473600 | 2.06546700 | –0.54152400 |
| C | –4.77956400 | 3.11615700 | –1.43121300 |
| C | –3.58728000 | 3.83110200 | –1.35162000 |

| | | | |
|---|---|---|---|
| N | –6.33798100 | 1.48875700 | –0.56991900 |
| N | –6.56239400 | 0.26715100 | –0.45228100 |
| C | –5.53446100 | –0.73051800 | –0.50841800 |
| C | –4.70752700 | –0.85761500 | –1.63149400 |
| C | –3.85069000 | –1.94911700 | –1.73259600 |
| C | –3.77358200 | –2.90605700 | –0.71370900 |
| C | –4.60711900 | –2.76748500 | 0.40391800 |
| C | –5.50810600 | –1.71056100 | 0.49023000 |
| C | –1.43155800 | 4.44448500 | –0.17699600 |
| C | –2.78272200 | –4.04826900 | –0.80717800 |
| N | –1.44423400 | –3.68753000 | –0.33390900 |
| H | 5.26370400 | 0.76090600 | –3.44155200 |
| H | 3.82415200 | –0.21077200 | –3.77135600 |
| H | 5.16910300 | –3.29787000 | –2.06954400 |
| H | 4.03723300 | –2.76393200 | –3.32206600 |
| H | 2.48616900 | –2.51795500 | –1.70687200 |
| H | 3.64923400 | –1.78724800 | 2.50703700 |
| H | 1.78209600 | –2.00142000 | 4.15359200 |
| H | –0.41143900 | –2.94407900 | 3.41133000 |
| H | 1.13678100 | –3.45882900 | –0.53762600 |
| H | –2.22543100 | 2.34309500 | 1.37537600 |
| H | –4.29033400 | 0.99280900 | 1.18383900 |
| H | –5.53124200 | 3.36253200 | –2.17497500 |
| H | –3.40023700 | 4.63616800 | –2.05860700 |
| H | –4.75938900 | –0.12002100 | –2.42563500 |
| H | –3.23313400 | –2.05808700 | –2.62233600 |
| H | –4.54815300 | –3.49962600 | 1.20346900 |
| H | –6.18755600 | –1.62507700 | 1.33285000 |

| | | | |
|---|---|---|---|
| H | –1.36990700 | 5.15039000 | –1.01123300 |
| H | –1.53406500 | 5.02477900 | 0.74630800 |
| H | –2.68611200 | –4.38763700 | –1.84415000 |
| H | –3.10902600 | –4.89462600 | –0.20120400 |
| H | –0.95293200 | –2.99200600 | –0.87852900 |
| N | –0.15060400 | 3.74254800 | –0.08642500 |
| C | 0.42811900 | 3.49721500 | 1.13013300 |
| C | 1.86254500 | 3.04779000 | 1.12231200 |
| O | –0.18438200 | 3.66473300 | 2.18205400 |
| C | 2.59458700 | 3.26660900 | 2.29570400 |
| C | 3.95228800 | 2.96001500 | 2.34725200 |
| C | 4.58940800 | 2.42217600 | 1.23227000 |
| C | 3.85939200 | 2.14666500 | 0.07013000 |
| C | 2.49738300 | 2.46316500 | 0.01918900 |
| C | 4.60526800 | 1.57282200 | –1.10109100 |
| O | 5.77677500 | 1.86332200 | –1.31560500 |
| N | 3.88812900 | 0.73456000 | –1.91928200 |
| H | 0.43820500 | 3.74054800 | –0.90589100 |
| H | 2.07890400 | 3.69462200 | 3.14835800 |
| H | 4.51652800 | 3.15116200 | 3.25521100 |
| H | 5.65171300 | 2.20260100 | 1.23989300 |
| H | 1.94322300 | 2.25711100 | –0.89281600 |
| H | 3.09047100 | 0.26885700 | –1.50819900 |
| C | 5.35162600 | –1.21281600 | –2.57427900 |
| H | 5.90649500 | –0.99126900 | –1.65917300 |
| H | 6.09457200 | –1.44341600 | –3.34959700 |

**3–*cis***

**Cartesian coordinates:**

| Symbol | X | Y | Z |
|---|---|---|---|
| C | 3.84178400 | 3.89722900 | 1.69474700 |
| C | 0.68282900 | 4.25077100 | 1.38006400 |
| N | –0.62579000 | 3.88992500 | 0.84766700 |
| C | –1.52141600 | 4.85883200 | 0.46856100 |
| C | –2.79895800 | 4.37054300 | –0.15493300 |
| O | –1.30887300 | 6.05352700 | 0.64476500 |
| C | –3.51161300 | 5.26795600 | –0.95858900 |
| C | –4.69652800 | 4.86994300 | –1.57274200 |
| C | –5.19259700 | 3.58422500 | –1.37019400 |
| C | –4.51526700 | 2.68872100 | –0.53400400 |
| C | –3.31170200 | 3.08632300 | 0.05877500 |
| C | –5.13583000 | 1.33378100 | –0.33257200 |
| O | –5.96447400 | 0.88667200 | –1.12226900 |
| C | 1.68149200 | –4.26375400 | 0.87992100 |
| C | 0.96443300 | –3.59117400 | –0.11150100 |
| C | –0.24916700 | –4.08852500 | –0.58577900 |
| C | –0.74890800 | –5.29715000 | –0.08932900 |
| C | –0.01591900 | –6.00110600 | 0.87588200 |
| C | 1.16449500 | –5.46900400 | 1.37680200 |
| N | –1.86050200 | –5.97581000 | –0.68685600 |
| N | –2.96931200 | –5.44833600 | –0.90467100 |
| C | –3.37813600 | –4.17688600 | –0.38448900 |
| C | –3.25588900 | –3.83344100 | 0.96789500 |
| C | –3.88948800 | –2.68870600 | 1.44700400 |
| C | –4.62908700 | –1.85975300 | 0.59742300 |

| | | | |
|---|---|---|---|
| C | –4.73354200 | –2.20501700 | –0.75867100 |
| C | –4.13986100 | –3.36615500 | –1.23793100 |
| C | 3.01355600 | –3.76691600 | 1.42359200 |
| C | –5.35513300 | –0.64082600 | 1.13396600 |
| N | –4.74164000 | 0.63877700 | 0.77555900 |
| H | 4.81239500 | 4.30424300 | 1.98842300 |
| H | 3.28781800 | 3.67225200 | 2.61242700 |
| H | 0.54054000 | 5.15867800 | 1.97123800 |
| H | 0.99427900 | 3.45299500 | 2.06529300 |
| H | –0.72009400 | 2.97771000 | 0.42332900 |
| H | –3.11449200 | 6.26886900 | –1.08910800 |
| H | –5.23672500 | 5.56432300 | –2.20928100 |
| H | –6.11015500 | 3.25047600 | –1.84235100 |
| H | –2.76607500 | 2.39697000 | 0.69688500 |
| H | 1.36412400 | –2.67527700 | –0.53637200 |
| H | –0.78978900 | –3.55892100 | –1.36332900 |
| H | –0.38445100 | –6.96339800 | 1.21798500 |
| H | 1.71566500 | –6.01592200 | 2.13866900 |
| H | –2.70167000 | –4.47556600 | 1.64382200 |
| H | –3.81950600 | –2.44818100 | 2.50574400 |
| H | –5.31303100 | –1.56979300 | –1.42178200 |
| H | –4.26842800 | –3.67192600 | –2.27182100 |
| H | 2.93584100 | –3.62628900 | 2.50974100 |
| H | 3.78197100 | –4.52482800 | 1.24880200 |
| H | –5.40650100 | –0.68882400 | 2.22605100 |
| H | –6.37795100 | –0.62019200 | 0.74718600 |
| H | –4.16744500 | 1.09907300 | 1.46472700 |
| N | 3.52225200 | –2.54443400 | 0.83242000 |

| | | | |
|---|---|---|---|
| C | 4.48393500 | –2.56963300 | –0.14781900 |
| C | 4.91573400 | –1.23988200 | –0.70166400 |
| O | 4.97482600 | –3.61709300 | –0.55089500 |
| C | 5.56147900 | –1.25135500 | –1.94410600 |
| C | 6.02683600 | –0.06575500 | –2.50675800 |
| C | 5.86270500 | 1.14057200 | –1.83067500 |
| C | 5.21591700 | 1.17211600 | –0.58991300 |
| C | 4.75126900 | –0.02343600 | –0.02832900 |
| C | 5.09726200 | 2.50795900 | 0.09087300 |
| O | 5.85934500 | 3.43296200 | –0.17023500 |
| N | 4.09641700 | 2.62876200 | 1.01829100 |
| H | 3.03613300 | –1.68045900 | 1.01833100 |
| H | 5.69970000 | –2.20552500 | –2.44068300 |
| H | 6.52822600 | –0.08366100 | –3.46979500 |
| H | 6.23878800 | 2.07310000 | –2.23751800 |
| H | 4.33220800 | –0.01189200 | 0.97463400 |
| H | 3.36977000 | 1.92907000 | 1.02536200 |
| C | 3.10432700 | 4.93644400 | 0.83327300 |
| H | 2.98581000 | 5.84878700 | 1.43371000 |
| H | 3.75724800 | 5.19551900 | –0.00636900 |
| C | 1.73683400 | 4.49789500 | 0.29190600 |
| H | 1.85294200 | 3.59223100 | –0.32074400 |
| H | 1.35119500 | 5.27660800 | –0.37511700 |

**1–*trans***

**Cartesian coordinates:**

| Symbol | X | Y | Z |
|---|---|---|---|
| C | 0.43096100 | –2.43432100 | 0.63986900 |

| | | | |
|---|---|---|---|
| C | –0.43149900 | –2.43502100 | –0.63868900 |
| N | –1.83815600 | –2.21518100 | –0.35654300 |
| C | –2.78482800 | –3.20690500 | –0.41631100 |
| C | –4.18405200 | –2.77854000 | –0.06260900 |
| O | –2.52300700 | –4.35984500 | –0.73502200 |
| C | –5.06992900 | –3.75158800 | 0.41235700 |
| C | –6.35957300 | –3.39530100 | 0.80525000 |
| C | –6.78211900 | –2.07021600 | 0.71612900 |
| C | –5.92728400 | –1.09774900 | 0.18622700 |
| C | –4.63092700 | –1.45924000 | –0.19552800 |
| C | –6.37990300 | 0.33489200 | 0.13947500 |
| O | –7.07635100 | 0.82094700 | 1.02370700 |
| C | 4.47479400 | 2.95995500 | 0.57972700 |
| C | 4.04819100 | 2.95264700 | –0.75508900 |
| C | 2.71064400 | 3.17268300 | –1.06600400 |
| C | 1.77270900 | 3.38815800 | –0.04703500 |
| C | 2.20097000 | 3.45359200 | 1.28838300 |
| C | 3.54081100 | 3.24387400 | 1.58877500 |
| N | 0.42208900 | 3.45108200 | –0.46834100 |
| N | –0.42091600 | 3.45098200 | 0.46856000 |
| C | –1.77156200 | 3.38825400 | 0.04724800 |
| C | –2.19984200 | 3.45406900 | –1.28814100 |
| C | –3.53971200 | 3.24457700 | –1.58856500 |
| C | –4.47371600 | 2.96051400 | –0.57957300 |
| C | –4.04706800 | 2.95276900 | 0.75522100 |
| C | –2.70949300 | 3.17258200 | 1.06617900 |
| C | 5.88088600 | 2.51446600 | 0.92982400 |
| C | –5.87989700 | 2.51538900 | –0.92974300 |

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|---|---|---|---|
| N | –5.94540400 | 1.05309600 | –0.94590400 |
| H | 0.34790200 | –3.39088300 | 1.15843200 |
| H | –0.34843400 | –3.39214000 | –1.15622800 |
| H | –0.07820400 | –1.64734400 | –1.31819700 |
| H | –2.09202300 | –1.34409900 | 0.08709700 |
| H | –4.72264200 | –4.77725300 | 0.47826800 |
| H | –7.03433700 | –4.15286300 | 1.19263800 |
| H | –7.77115100 | –1.77186900 | 1.04828100 |
| H | –3.96109700 | –0.69903200 | –0.58782800 |
| H | 4.76559200 | 2.74097900 | –1.54321700 |
| H | 2.35837800 | 3.14651400 | –2.09247000 |
| H | 1.46944500 | 3.63866800 | 2.06663600 |
| H | 3.86907500 | 3.27701800 | 2.62557500 |
| H | –1.46831000 | 3.63925300 | –2.06636200 |
| H | –3.86798900 | 3.27799500 | –2.62535200 |
| H | –4.76447200 | 2.74099800 | 1.54332400 |
| H | –2.35720900 | 3.14608700 | 2.09263000 |
| H | 6.61022100 | 2.84496400 | 0.18791200 |
| H | 6.18414200 | 2.89900200 | 1.90899000 |
| H | –6.18315100 | 2.90034700 | –1.90875100 |
| H | –6.60913600 | 2.84580800 | –0.18769700 |
| H | –5.35121000 | 0.57958900 | –1.61224400 |
| N | 5.94611800 | 1.05214100 | 0.94561000 |
| C | 6.37961200 | 0.33405100 | –0.14018300 |
| C | 5.92687900 | –1.09857700 | –0.18662900 |
| O | 7.07515100 | 0.82017900 | –1.02511100 |
| C | 6.78132200 | –2.07126100 | –0.71671700 |
| C | 6.35839500 | –3.39624500 | –0.80569500 |

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|---|---|---|---|
| C | 5.06873400 | –3.75216800 | –0.41253900 |
| C | 4.18324300 | –2.77887500 | 0.06265200 |
| C | 4.63052100 | –1.45970000 | 0.19546900 |
| C | 2.78394100 | –3.20683600 | 0.41653900 |
| O | 2.52173400 | –4.35979700 | 0.73485900 |
| N | 1.83764700 | –2.21468600 | 0.35762000 |
| H | 5.35278700 | 0.57855600 | 1.61266700 |
| H | 7.77035300 | –1.77322400 | –1.04915700 |
| H | 7.03288400 | –4.15399200 | –1.19319800 |
| H | 4.72111700 | –4.77772200 | –0.47844400 |
| H | 3.96106600 | –0.69930400 | 0.58804400 |
| H | 2.09158500 | –1.34361500 | –0.08600400 |
| H | 0.07769500 | –1.64590900 | 1.31852700 |

**2–*trans***

**Cartesian coordinates:**

| Symbol | X | Y | Z |
|---|---|---|---|
| C | –0.26402600 | –1.94152000 | 1.12890400 |
| C | 1.70731300 | –2.82069600 | 2.50218000 |
| N | 2.72048500 | –2.36484000 | 1.56052600 |
| C | 3.86988000 | –3.06595300 | 1.30881000 |
| C | 4.83501800 | –2.41470100 | 0.35423200 |
| O | 4.11580200 | –4.15072000 | 1.82447700 |
| C | 5.71404800 | –3.24383300 | –0.35118200 |
| C | 6.61145100 | –2.69858400 | –1.26754500 |
| C | 6.65446100 | –1.32151200 | –1.47435800 |
| C | 5.82096200 | –0.47423400 | –0.73577700 |

| | | | |
|---|---|---|---|
| C | 4.90895600 | –1.02959900 | 0.16877900 |
| C | 5.88456200 | 1.00276400 | –1.00719800 |
| O | 6.16080300 | 1.43966200 | –2.12039700 |
| C | –5.10271000 | 2.50529100 | 0.60387500 |
| C | –4.48534600 | 2.99698200 | 1.75722300 |
| C | –3.15760100 | 3.42295100 | 1.72281000 |
| C | –2.42704100 | 3.35293400 | 0.53242900 |
| C | –3.06249800 | 2.92708900 | –0.64851900 |
| C | –4.38294300 | 2.51096400 | –0.60596800 |
| N | –1.04275800 | 3.63743900 | 0.64158500 |
| N | –0.38897000 | 3.42718900 | –0.41514800 |
| C | 1.01414000 | 3.55534600 | –0.29138800 |
| C | 1.69014600 | 3.92682300 | 0.88155300 |
| C | 3.07834700 | 3.87990500 | 0.91493000 |
| C | 3.81692500 | 3.46466900 | –0.20400900 |
| C | 3.13594100 | 3.14546100 | –1.38666400 |
| C | 1.74759600 | 3.19353800 | –1.43001200 |
| C | –6.44780900 | 1.80952800 | 0.66645600 |
| C | 5.31366500 | 3.24035500 | –0.11295700 |
| N | 5.61811700 | 1.81993400 | 0.05966100 |
| H | 0.28365600 | –1.76329300 | 0.19775400 |
| H | 2.12163200 | –3.71048800 | 2.97972300 |
| H | 1.57552400 | –2.05368800 | 3.27971600 |
| H | 2.52292000 | –1.55312200 | 0.99491800 |
| H | 5.66887200 | –4.31276000 | –0.17230600 |
| H | 7.27572000 | –3.35053200 | –1.82698200 |
| H | 7.32924500 | –0.88125100 | –2.20088700 |
| H | 4.24426600 | –0.37625600 | 0.72759900 |

| | | | |
|---|---|---|---|
| H | –5.03439700 | 3.01658200 | 2.69570300 |
| H | –2.65282400 | 3.77041600 | 2.61888500 |
| H | –2.49082400 | 2.89552600 | –1.56864300 |
| H | –4.86512900 | 2.14779600 | –1.51030700 |
| H | 1.11269100 | 4.21601800 | 1.75233600 |
| H | 3.60195500 | 4.14989200 | 1.82973500 |
| H | 3.70193900 | 2.82820600 | –2.25782000 |
| H | 1.20140300 | 2.92224000 | –2.32791000 |
| H | –6.97716400 | 2.05836100 | 1.59233900 |
| H | –7.09251800 | 2.06882400 | –0.17650900 |
| H | 5.74276100 | 3.79740000 | 0.72600400 |
| H | 5.82005200 | 3.55149900 | –1.02877000 |
| H | 5.37349100 | 1.39435600 | 0.94205600 |
| N | –6.23555000 | 0.36210500 | 0.58635400 |
| C | –6.46965700 | –0.34642200 | –0.56731500 |
| C | –5.67232700 | –1.61300800 | –0.71804400 |
| O | –7.25206600 | 0.03027600 | –1.43149600 |
| C | –6.23399400 | –2.69884400 | –1.39828700 |
| C | –5.46884800 | –3.83590900 | –1.65187900 |
| C | –4.13010300 | –3.88488700 | –1.26515300 |
| C | –3.55212100 | –2.80409100 | –0.59082400 |
| C | –4.33280800 | –1.67528900 | –0.31634400 |
| C | –2.08230500 | –2.85992900 | –0.27477900 |
| O | –1.30053400 | –3.52981200 | –0.94145900 |
| N | –1.66940900 | –2.08980900 | 0.77797700 |
| H | –5.55128900 | –0.01786800 | 1.22556000 |
| H | –7.26203600 | –2.62721600 | –1.73822500 |
| H | –5.91070100 | –4.67873100 | –2.17506600 |

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|---|---|---|---|
| H | –3.50872800 | –4.74374700 | –1.49623800 |
| H | –3.86607600 | –0.79822100 | 0.12396000 |
| H | –2.36273300 | –1.72213200 | 1.41145800 |
| C | 0.34747600 | –3.14191100 | 1.86753200 |
| H | 0.43549300 | –3.98057200 | 1.17048000 |
| H | –0.33135800 | –3.45236900 | 2.67263800 |
| H | –0.18378800 | –1.03632100 | 1.74404200 |

**3–*trans***

**Cartesian coordinates:**

| Symbol | X | Y | Z |
|---|---|---|---|
| C | 1.10374500 | –2.47421000 | –0.60730600 |
| C | –1.98103500 | –3.26525900 | –0.54562900 |
| N | –3.33052600 | –2.73001000 | –0.65775100 |
| C | –4.42658100 | –3.32944000 | –0.09935100 |
| C | –5.68347700 | –2.49931100 | –0.07597500 |
| O | –4.40187200 | –4.46738100 | 0.35649600 |
| C | –6.91307700 | –3.16424900 | –0.01220900 |
| C | –8.10000500 | –2.43955700 | 0.08129000 |
| C | –8.07273200 | –1.04690500 | 0.13337900 |
| C | –6.85230400 | –0.36676200 | 0.06699100 |
| C | –5.66477600 | –1.10094500 | –0.03266300 |
| C | –6.85437000 | 1.13212100 | 0.19226500 |
| O | –7.71610600 | 1.73380000 | 0.82263600 |
| C | 5.03237000 | 3.01323000 | –0.15596000 |
| C | 4.46853300 | 3.72015600 | –1.22093300 |
| C | 3.10289300 | 4.00184200 | –1.24110900 |
| C | 2.28004200 | 3.57374200 | –0.19481800 |

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|---|---|---|---|
| C | 2.84786300 | 2.90739100 | 0.90700200 |
| C | 4.20572100 | 2.63338000 | 0.91823700 |
| N | 0.89291100 | 3.79925100 | –0.37240400 |
| N | 0.16546900 | 3.31648400 | 0.53620100 |
| C | –1.22779900 | 3.43426500 | 0.31469600 |
| C | –1.81771000 | 4.01569700 | –0.81787700 |
| C | –3.19841400 | 3.96890600 | –0.97355200 |
| C | –4.01633100 | 3.35122300 | –0.01609600 |
| C | –3.42043600 | 2.80910000 | 1.13116600 |
| C | –2.04161900 | 2.85107100 | 1.29642700 |
| C | 6.47212000 | 2.54246500 | –0.19940100 |
| C | –5.50288100 | 3.17951900 | –0.25159000 |
| N | –5.81264700 | 1.76638800 | –0.43027700 |
| H | 0.70577900 | –1.52374900 | –0.98845200 |
| H | –2.07951500 | –4.33127200 | –0.32813700 |
| H | –1.48452700 | –3.16600400 | –1.51806900 |
| H | –3.43707800 | –1.81060200 | –1.05877100 |
| H | –6.91345800 | –4.24907500 | –0.01848800 |
| H | –9.05002300 | –2.96341100 | 0.13039100 |
| H | –8.98448700 | –0.46873000 | 0.24131500 |
| H | –4.71418800 | –0.57628400 | 0.01277000 |
| H | 5.09597000 | 4.03122000 | –2.05249800 |
| H | 2.64660800 | 4.52378700 | –2.07627400 |
| H | 2.20230800 | 2.59939200 | 1.72147200 |
| H | 4.64273500 | 2.09933900 | 1.75871100 |
| H | –1.18003900 | 4.46775100 | –1.56893700 |
| H | –3.65291200 | 4.40019800 | –1.86245400 |
| H | –4.04326500 | 2.33389600 | 1.88432500 |

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|---|---|---|---|
| H | –1.56389700 | 2.41828600 | 2.16980400 |
| H | 7.02536200 | 3.06637200 | –0.98764800 |
| H | 6.99448600 | 2.71204700 | 0.74592700 |
| H | –5.82031000 | 3.76359100 | –1.12493000 |
| H | –6.10017700 | 3.51672100 | 0.60045100 |
| H | –5.20868000 | 1.23072800 | –1.03557300 |
| N | 6.50434000 | 1.10054000 | –0.42537800 |
| C | 7.03150200 | 0.20815800 | 0.47119900 |
| C | 6.60018000 | –1.21842300 | 0.27038800 |
| O | 7.77848900 | 0.53991900 | 1.38427000 |
| C | 7.48935600 | –2.25487500 | 0.57366300 |
| C | 7.09122700 | –3.58182600 | 0.41837400 |
| C | 5.79487600 | –3.88560300 | 0.00323100 |
| C | 4.87736100 | –2.85943400 | –0.24554500 |
| C | 5.29725700 | –1.52985100 | –0.13175300 |
| C | 3.47174500 | –3.23252200 | –0.63457000 |
| O | 3.20957800 | –4.29929600 | –1.17855700 |
| N | 2.52192200 | –2.28880800 | –0.34379300 |
| H | 5.93365900 | 0.74076700 | –1.17697700 |
| H | 8.48539000 | –2.00362700 | 0.92347100 |
| H | 7.79178200 | –4.38409600 | 0.63037000 |
| H | 5.46813500 | –4.91266600 | –0.12138000 |
| H | 4.60026000 | –0.72511400 | –0.34728100 |
| H | 2.77555500 | –1.54726600 | 0.29337700 |
| H | 1.03133300 | –3.21369100 | –1.40719600 |
| C | –1.18666800 | –2.55069000 | 0.55874800 |
| H | –1.27677700 | –1.46399100 | 0.40895000 |
| H | –1.66829300 | –2.76990500 | 1.51893500 |

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|---|---|---|---|
| C | 0.30334500 | –2.90994200 | 0.63481600 |
| H | 0.72586200 | –2.40718700 | 1.51480700 |
| H | 0.44188600 | –3.98544700 | 0.79980800 |

**1–*cis*•$SO_4^{2-}$** complex

**Cartesian coordinates:**

| Symbol | X | Y | Z |
|---|---|---|---|
| C | –5.19324900 | 0.54874400 | 0.41702400 |
| C | –4.76383700 | –0.69144500 | 1.20270600 |
| N | –3.90317200 | –1.60397300 | 0.47318600 |
| C | –4.29541300 | –2.85394000 | 0.14928800 |
| C | –3.20632800 | –3.74946400 | –0.39225600 |
| O | –5.44730700 | –3.29249700 | 0.29028100 |
| C | –3.56953000 | –4.77741300 | –1.26777000 |
| C | –2.60604800 | –5.66027300 | –1.75296500 |
| C | –1.28123700 | –5.54209100 | –1.33886700 |
| C | –0.90647600 | –4.53361700 | –0.44211000 |
| C | –1.87345300 | –3.63370900 | 0.02339500 |
| C | 0.52708000 | –4.52874000 | 0.02293900 |
| O | 1.27879400 | –5.47543400 | –0.27046700 |
| C | 3.26537700 | 2.86875900 | 0.42773100 |
| C | 2.94645200 | 1.87675600 | –0.50929400 |
| C | 3.95013700 | 1.14818500 | –1.13458600 |
| C | 5.29639200 | 1.39368900 | –0.83681800 |
| C | 5.62858700 | 2.46734400 | –0.00482600 |
| C | 4.61540000 | 3.17937500 | 0.63726500 |

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|---|---|---|---|
| N | 6.36929600 | 0.61490700 | –1.39197900 |
| N | 6.35575600 | –0.64111100 | –1.34986300 |
| C | 5.35262600 | –1.36494200 | –0.61247900 |
| C | 5.07128000 | –1.09696900 | 0.73196100 |
| C | 4.08074800 | –1.81987000 | 1.38684500 |
| C | 3.35204400 | –2.81623500 | 0.72977400 |
| C | 3.69476900 | –3.12983700 | –0.59315900 |
| C | 4.70324800 | –2.42865700 | –1.25044100 |
| C | 2.19577900 | 3.51908700 | 1.29493600 |
| C | 2.22928400 | –3.54103200 | 1.45073700 |
| N | 0.93729800 | –3.49190800 | 0.78887600 |
| H | –5.57944300 | 0.25368500 | –0.56649900 |
| H | –6.03058000 | 1.03151900 | 0.94259100 |
| H | –5.66015900 | –1.25324900 | 1.47772300 |
| H | –4.23973100 | –0.37631900 | 2.11278500 |
| H | –2.96158600 | –1.26199400 | 0.19308900 |
| H | –4.61524800 | –4.86975900 | –1.54529500 |
| H | –2.89032500 | –6.45001100 | –2.44585100 |
| H | –0.51446700 | –6.23061600 | –1.67845700 |
| H | –1.60068200 | –2.85424800 | 0.72591400 |
| H | 1.90996500 | 1.60481000 | –0.67699700 |
| H | 3.68287000 | 0.34542100 | –1.81300700 |
| H | 6.67645100 | 2.69339100 | 0.17587300 |
| H | 4.87926700 | 3.97702200 | 1.32983400 |
| H | 5.58899300 | –0.29249000 | 1.24319400 |
| H | 3.83365300 | –1.57190800 | 2.41612500 |
| H | 3.15434600 | –3.92545500 | –1.09752900 |
| H | 4.96200200 | –2.65986100 | –2.28041100 |

| | | | |
|---|---|---|---|
| H | 2.15311000 | 2.95447200 | 2.23692700 |
| H | 2.47636700 | 4.54978300 | 1.52679400 |
| H | 2.10265600 | –3.09376000 | 2.44220800 |
| H | 2.49241000 | –4.59768800 | 1.57064800 |
| H | 0.37185900 | –2.64011400 | 0.98012700 |
| N | 0.86015900 | 3.54373600 | 0.73730100 |
| C | 0.32652300 | 4.69971300 | 0.28254000 |
| C | –1.07663200 | 4.64625300 | –0.27619800 |
| O | 0.93941800 | 5.77808600 | 0.30319700 |
| C | –1.45134500 | 5.74450600 | –1.06057400 |
| C | –2.72256000 | 5.81080600 | –1.62021000 |
| C | –3.63400700 | 4.78618400 | –1.38699900 |
| C | –3.28652200 | 3.68303800 | –0.59670200 |
| C | –1.99862100 | 3.61264400 | –0.04018000 |
| C | –4.38669400 | 2.65613000 | –0.41191100 |
| O | –5.51563900 | 2.88733800 | –0.87717100 |
| N | –4.11724100 | 1.51754100 | 0.25445500 |
| H | 0.39287200 | 2.62055200 | 0.66254900 |
| H | –0.72077500 | 6.53309100 | –1.20563100 |
| H | –3.00486600 | 6.66321200 | –2.23540400 |
| H | –4.63772600 | 4.80700300 | –1.79726900 |
| H | –1.72919300 | 2.76998000 | 0.59359700 |
| H | –3.19384200 | 1.29107100 | 0.66770600 |
| O | 0.34727600 | 0.88087700 | 0.56889300 |
| S | –0.80259100 | –0.03608900 | 0.92683900 |
| O | –0.30017400 | –1.19641100 | 1.76508300 |
| O | –1.83870600 | 0.75825400 | 1.70867800 |
| O | –1.44791900 | –0.57175400 | –0.33116500 |

**2–*cis*•$SO_4^{2-}$** complex

**Cartesian coordinates:**

| Symbol | X | Y | Z |
|---|---|---|---|
| C | –5.09039100 | –1.24754500 | –1.76738200 |
| C | –4.93689700 | 1.35179100 | –1.57657400 |
| N | –3.96995400 | 1.79631700 | –0.58972500 |
| C | –4.19545900 | 2.92048900 | 0.12649700 |
| C | –3.00063900 | 3.51152700 | 0.83241300 |
| O | –5.28651900 | 3.50950900 | 0.17768900 |
| C | –3.22488800 | 4.28863600 | 1.97301900 |
| C | –2.16975000 | 4.96541900 | 2.58214100 |
| C | –0.89498400 | 4.91147600 | 2.02363100 |
| C | –0.65795500 | 4.15074800 | 0.87195600 |
| C | –1.71091000 | 3.43238400 | 0.29151600 |
| C | 0.71524800 | 4.24029300 | 0.26136100 |
| O | 1.48751500 | 5.15372100 | 0.60593400 |
| C | 3.37913900 | –2.93699400 | –0.42844600 |
| C | 3.13503200 | –1.81730000 | 0.37750800 |
| C | 4.18978400 | –1.05384100 | 0.86227000 |
| C | 5.51383800 | –1.38489900 | 0.54071400 |
| C | 5.76893900 | –2.56276500 | –0.17042000 |
| C | 4.70660500 | –3.31614200 | –0.66552800 |
| N | 6.65861000 | –0.61748800 | 0.94705700 |
| N | 6.69320900 | 0.63539600 | 0.85423600 |
| C | 5.63688500 | 1.37392500 | 0.21439400 |

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|---|---|---|---|
| C | 5.20613200 | 1.09471500 | –1.08681100 |
| C | 4.13964300 | 1.80613600 | –1.62682400 |
| C | 3.48433400 | 2.80071000 | –0.89349400 |
| C | 3.98376200 | 3.13329000 | 0.37479700 |
| C | 5.06701900 | 2.44368900 | 0.91360700 |
| C | 2.24462700 | –3.68305500 | –1.11630600 |
| C | 2.26019200 | 3.49676700 | –1.46367700 |
| N | 1.04358200 | 3.33228900 | –0.68380600 |
| H | –5.87492400 | –2.00929100 | –1.82732800 |
| H | –4.68103700 | –1.08952800 | –2.77300200 |
| H | –5.64401600 | 2.17782500 | –1.68807600 |
| H | –4.40934200 | 1.22143700 | –2.53232200 |
| H | –3.08970800 | 1.25822700 | –0.44549200 |
| H | –4.23952700 | 4.36429900 | 2.35200700 |
| H | –2.34629600 | 5.55672900 | 3.47858300 |
| H | –0.06568000 | 5.47007800 | 2.44513800 |
| H | –1.54008200 | 2.83595200 | –0.59784000 |
| H | 2.11467800 | –1.49224100 | 0.55565800 |
| H | 3.97643200 | –0.16957800 | 1.45126600 |
| H | 6.80017400 | –2.84625600 | –0.36454900 |
| H | 4.91103500 | –4.20731100 | –1.25677900 |
| H | 5.66298900 | 0.28388400 | –1.64492600 |
| H | 3.77302300 | 1.54639800 | –2.61676600 |
| H | 3.49398800 | 3.92551200 | 0.93282500 |
| H | 5.44195700 | 2.68191900 | 1.90562700 |
| H | 2.18420400 | –3.31684500 | –2.15064500 |
| H | 2.47319000 | –4.75232300 | –1.14744900 |
| H | 2.05393800 | 3.09455200 | –2.46038700 |

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|---|---|---|---|
| H | 2.45598300 | 4.57172800 | –1.54861300 |
| H | 0.45728500 | 2.50825200 | –0.93511100 |
| N | 0.93753400 | –3.52606400 | –0.52043600 |
| C | 0.45467800 | –4.46929700 | 0.32300700 |
| C | –0.92714400 | –4.23052900 | 0.87323500 |
| O | 1.07950700 | –5.49598200 | 0.62532400 |
| C | –1.26538100 | –4.91185000 | 2.04820800 |
| C | –2.54153200 | –4.78700900 | 2.58982300 |
| C | –3.49860500 | –4.01269800 | 1.93913800 |
| C | –3.18241000 | –3.33451800 | 0.75624900 |
| C | –1.88584100 | –3.43241800 | 0.23347200 |
| C | –4.32094800 | –2.62370600 | 0.06389200 |
| O | –5.48992500 | –2.86406100 | 0.40883600 |
| N | –4.02036500 | –1.79524000 | –0.95728600 |
| H | 0.50255900 | –2.58343700 | –0.60714100 |
| H | –0.51041100 | –5.54170200 | 2.50759800 |
| H | –2.79626700 | –5.30787300 | 3.51081300 |
| H | –4.51459900 | –3.93010900 | 2.31037700 |
| H | –1.63399500 | –2.91284300 | –0.68623700 |
| H | –3.05815900 | –1.49510500 | –1.19877200 |
| C | –5.72460600 | 0.06300600 | –1.26680300 |
| H | –5.93036700 | –0.01303300 | –0.19450900 |
| H | –6.70041700 | 0.15120000 | –1.76989900 |
| O | 0.37448200 | –0.86451600 | –0.66663700 |
| S | –0.80872400 | –0.04557600 | –1.14523300 |
| O | –0.30983800 | 1.20733200 | –1.84369800 |
| O | –1.64059700 | –0.88141100 | –2.10183100 |
| O | –1.67342900 | 0.34661100 | 0.03261700 |

**3–*cis*•$SO_4^{2-}$ complex**

**Cartesian coordinates:**

| Symbol | X | Y | Z |
|---|---|---|---|
| C | –5.50093500 | –0.38934400 | –1.30596000 |
| C | –4.44934600 | 2.55307600 | –0.56632200 |
| N | –3.19150100 | 3.10460500 | –0.09993500 |
| C | –3.05909900 | 4.39534800 | 0.25718500 |
| C | –1.65824400 | 4.84007000 | 0.60232600 |
| O | –3.99008200 | 5.21628900 | 0.28909000 |
| C | –1.52699900 | 5.98398200 | 1.39621100 |
| C | –0.26567000 | 6.49297200 | 1.69608800 |
| C | 0.86977200 | 5.88520500 | 1.16837300 |
| C | 0.75453500 | 4.74913100 | 0.35630400 |
| C | –0.51304500 | 4.21575700 | 0.08909600 |
| C | 2.02984800 | 4.23279900 | –0.25466100 |
| O | 3.06988700 | 4.90979000 | –0.16806900 |
| C | 2.76489000 | –3.47443800 | –0.39159500 |
| C | 2.72737100 | –2.40362200 | 0.51216800 |
| C | 3.89353700 | –1.95750300 | 1.12075700 |
| C | 5.12112100 | –2.56950100 | 0.83273300 |
| C | 5.14628400 | –3.72149200 | 0.04242900 |
| C | 3.97495600 | –4.15193000 | –0.58130300 |
| N | 6.37608300 | –2.07572700 | 1.33479700 |
| N | 6.69839400 | –0.86910900 | 1.19293800 |
| C | 5.88516800 | 0.03119600 | 0.41524600 |

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|---|---|---|---|
| C | 5.52170300 | –0.24256200 | –0.90779300 |
| C | 4.66865600 | 0.62493800 | –1.58057000 |
| C | 4.16395000 | 1.77416500 | –0.96333000 |
| C | 4.61943900 | 2.09104400 | 0.32414000 |
| C | 5.49078700 | 1.23915400 | 0.99929600 |
| C | 1.55282000 | –3.81988600 | –1.24174300 |
| C | 3.16093900 | 2.65047200 | –1.69462700 |
| N | 2.00035100 | 3.05290100 | –0.91610500 |
| H | –6.32731800 | –0.96725200 | –1.73495100 |
| H | –5.00024400 | 0.14683500 | –2.11712300 |
| H | –5.15205000 | 3.38224500 | –0.68662300 |
| H | –4.27314600 | 2.10887600 | –1.55417200 |
| H | –2.43818000 | 2.40487600 | 0.05785200 |
| H | –2.43454500 | 6.46237600 | 1.75063200 |
| H | –0.16812800 | 7.37556700 | 2.32532600 |
| H | 1.86372200 | 6.28090300 | 1.34757300 |
| H | –0.61276000 | 3.33081500 | –0.53392600 |
| H | 1.79634400 | –1.86339500 | 0.66562800 |
| H | 3.85965600 | –1.09072700 | 1.77154900 |
| H | 6.09338600 | –4.22729100 | –0.12746800 |
| H | 4.00617800 | –5.01546600 | –1.24317500 |
| H | 5.84959400 | –1.16273500 | –1.37958900 |
| H | 4.34426800 | 0.37533400 | –2.58819900 |
| H | 4.27587900 | 3.00868700 | 0.78971900 |
| H | 5.82058500 | 1.46784100 | 2.00931300 |
| H | 1.58153900 | –3.18267900 | –2.13603000 |
| H | 1.61582700 | –4.86271300 | –1.56362100 |
| H | 2.79456300 | 2.11045600 | –2.57298800 |

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|---|---|---|---|
| H | 3.65919400 | 3.56720500 | –2.03076700 |
| H | 1.17743600 | 2.42021200 | –0.95417900 |
| N | 0.25997900 | –3.62933100 | –0.61738300 |
| C | –0.37500200 | –4.69102600 | –0.06783900 |
| C | –1.77098800 | –4.46807600 | 0.45343600 |
| O | 0.12419800 | –5.82477100 | –0.02181800 |
| C | –2.26265100 | –5.42911800 | 1.34497000 |
| C | –3.57368100 | –5.35688500 | 1.80525400 |
| C | –4.41344700 | –4.34705600 | 1.34447600 |
| C | –3.94194100 | –3.38165000 | 0.44655700 |
| C | –2.60808100 | –3.43146300 | 0.01669300 |
| C | –4.96474800 | –2.39046300 | –0.05595900 |
| O | –6.17075600 | –2.59673700 | 0.16022400 |
| N | –4.52947900 | –1.32187400 | –0.75549600 |
| H | –0.05973100 | –2.64800700 | –0.49445300 |
| H | –1.59701700 | –6.23217800 | 1.64367900 |
| H | –3.94769500 | –6.09969600 | 2.50713300 |
| H | –5.45380200 | –4.28707300 | 1.64566800 |
| H | –2.22984700 | –2.67838900 | –0.67030100 |
| H | –3.52912600 | –1.08047200 | –0.88599200 |
| C | –6.07173800 | 0.59554300 | –0.26786200 |
| H | –6.83800200 | 1.21441300 | –0.76265500 |
| H | –6.58785300 | 0.00289400 | 0.49503400 |
| C | –5.00848500 | 1.48669000 | 0.38586300 |
| H | –4.17768200 | 0.86183000 | 0.73003900 |
| H | –5.42296600 | 1.98429400 | 1.27297100 |
| O | 0.02432400 | –0.89401400 | –0.15293700 |
| S | –0.87955200 | 0.20321500 | –0.67546700 |

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|---|---|---|---|
| O | –0.07467500 | 1.19461400 | –1.49423500 |
| O | –1.96079800 | –0.43273300 | –1.53066300 |
| O | –1.52235800 | 0.94225400 | 0.47836100 |

**1–*trans*•$SO_4^{2-}$** complex

**Cartesian coordinates:**

| Symbol | X | Y | Z |
|---|---|---|---|
| C | –0.26570800 | 3.35263700 | 0.72756500 |
| C | 0.28664200 | 3.34437300 | –0.72255800 |
| N | 1.66134200 | 2.87506400 | –0.75598000 |
| C | 2.70803400 | 3.70659400 | –0.85555000 |
| C | 4.09680100 | 3.10563400 | –0.71135500 |
| O | 2.60958200 | 4.92710900 | –1.06212200 |
| C | 5.15824500 | 3.97908700 | –0.97639200 |
| C | 6.47846000 | 3.55502300 | –0.86243400 |
| C | 6.75287700 | 2.25008300 | –0.47021900 |
| C | 5.70828100 | 1.36140900 | –0.18362200 |
| C | 4.37553500 | 1.78977600 | –0.31155500 |
| C | 6.13698700 | –0.02523100 | 0.22153100 |
| O | 7.30038000 | –0.40515500 | 0.04736800 |
| C | –4.14944600 | –3.11556400 | –0.79272000 |
| C | –3.60287800 | –3.88293300 | –1.82895100 |
| C | –2.34849500 | –4.46503400 | –1.68519900 |
| C | –1.62733000 | –4.28782700 | –0.49730000 |
| C | –2.20720800 | –3.59307400 | 0.57733800 |
| C | –3.46291500 | –3.02937500 | 0.42456000 |
| N | –0.24433700 | –4.54665400 | –0.53340600 |
| N | 0.31827800 | –4.56128300 | 0.59796800 |

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|---|---|---|---|
| C | 1.68838500 | –4.23611600 | 0.54760000 |
| C | 2.15144300 | –3.34177700 | –0.43228300 |
| C | 3.41094700 | –2.78046700 | –0.29881000 |
| C | 4.21768300 | –3.06062600 | 0.81055200 |
| C | 3.76964900 | –3.99510000 | 1.75373200 |
| C | 2.51259000 | –4.57957800 | 1.62761100 |
| C | –5.36654500 | –2.25139300 | –1.01228800 |
| C | 5.47288000 | –2.24929100 | 1.03437300 |
| N | 5.20629900 | –0.83297700 | 0.79292900 |
| H | –0.21620200 | 4.34674700 | 1.17574700 |
| H | 0.23686900 | 4.33425400 | –1.17984500 |
| H | –0.31262700 | 2.63600900 | –1.30009400 |
| H | 1.69809900 | 1.86221900 | –0.53013000 |
| H | 4.90096400 | 4.99163600 | –1.26757300 |
| H | 7.29384400 | 4.24253700 | –1.07791200 |
| H | 7.76900400 | 1.88193400 | –0.37912800 |
| H | 3.54730700 | 1.10966600 | –0.11866900 |
| H | –4.12638400 | –3.94928600 | –2.78082100 |
| H | –1.86661500 | –4.97293900 | –2.51589200 |
| H | –1.59860100 | –3.36428000 | 1.44033900 |
| H | –3.86346000 | –2.40540100 | 1.21888800 |
| H | 1.45223200 | –2.95694400 | –1.16900400 |
| H | 3.72613600 | –2.02709800 | –1.01528400 |
| H | 4.38252300 | –4.21218100 | 2.62714400 |
| H | 2.12454500 | –5.24275400 | 2.39629200 |
| H | –5.71134600 | –2.33591800 | –2.05295700 |
| H | –6.21361300 | –2.54238900 | –0.38008100 |
| H | 6.28914600 | –2.52885100 | 0.35822400 |

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|---|---|---|---|
| H | 5.84640200 | –2.40351100 | 2.05697400 |
| H | 4.24977100 | –0.51880800 | 0.90570200 |
| N | –5.05702200 | –0.86063300 | –0.68563200 |
| C | –6.03758000 | –0.02322300 | –0.26107900 |
| C | –5.64581400 | 1.36249900 | 0.17961600 |
| O | –7.22191800 | –0.38318100 | –0.23823000 |
| C | –6.70708000 | 2.24064700 | 0.43694400 |
| C | –6.45523900 | 3.54393600 | 0.85115100 |
| C | –5.14212300 | 3.97902200 | 1.00875400 |
| C | –4.06802300 | 3.11646500 | 0.76291100 |
| C | –4.32315700 | 1.80020800 | 0.34968700 |
| C | –2.68348100 | 3.71487700 | 0.93695900 |
| O | –2.58192500 | 4.91714500 | 1.23249400 |
| N | –1.64131500 | 2.89108200 | 0.75018200 |
| H | –4.08039700 | –0.57796800 | –0.70631800 |
| H | –7.71661700 | 1.86673800 | 0.30428400 |
| H | –7.28291600 | 4.22267800 | 1.04794400 |
| H | –4.90304300 | 4.99067800 | 1.31897100 |
| H | –3.48581300 | 1.12617200 | 0.17546200 |
| H | –1.71087000 | 1.89198700 | 0.45487600 |
| H | 0.33110800 | 2.64680000 | 1.31096100 |
| S | –0.16983100 | –0.50111000 | –0.07019400 |
| O | –0.37285000 | –1.36323200 | 1.13888700 |
| O | 0.06121400 | –1.31367600 | –1.31110100 |
| O | –1.42031200 | 0.37979300 | –0.29612500 |
| O | 1.03340500 | 0.42118100 | 0.18272500 |

**2–*trans*•$SO_4^{2-}$** complex

**Cartesian coordinates:**

| Symbol | X | Y | Z |
|---|---|---|---|
| C | 0.29374900 | 3.44325700 | –1.24621500 |
| C | –0.25812100 | 3.43044600 | 1.25590700 |
| N | –1.55843100 | 2.77611000 | 1.16875200 |
| C | –2.66787400 | 3.46354000 | 1.48334100 |
| C | –4.01528900 | 2.82592100 | 1.19976200 |
| O | –2.64620600 | 4.60408700 | 1.97928500 |
| C | –5.12753600 | 3.54621400 | 1.65154300 |
| C | –6.41957300 | 3.09185900 | 1.40654200 |
| C | –6.61241300 | 1.91562900 | 0.69182200 |
| C | –5.51387300 | 1.18232700 | 0.22311500 |
| C | –4.20925300 | 1.63328300 | 0.48657400 |
| C | –5.85699000 | –0.07630900 | –0.52873100 |
| O | –7.02318700 | –0.48786900 | –0.56619100 |
| C | 3.92223600 | –3.02566300 | 1.31842800 |
| C | 3.39417100 | –3.95994800 | 2.22138100 |
| C | 2.21719800 | –4.63958500 | 1.92866200 |
| C | 1.55171300 | –4.39176600 | 0.71886200 |
| C | 2.11720300 | –3.51570400 | –0.22145500 |
| C | 3.29996100 | –2.86062600 | 0.07733200 |
| N | 0.19159300 | –4.73681400 | 0.60566700 |
| N | –0.24023100 | –4.73534900 | –0.58320900 |
| C | –1.60039700 | –4.39306700 | –0.70182300 |
| C | –2.18625600 | –3.54259000 | 0.24974000 |
| C | –3.36164500 | –2.87810500 | –0.05725000 |
| C | –3.95640700 | –3.00965800 | –1.31609000 |

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|---|---|---|---|
| C | –3.41301300 | –3.92422600 | –2.22950800 |
| C | –2.24336000 | –4.61259500 | –1.92909500 |
| C | 5.05264100 | –2.10199300 | 1.71679800 |
| C | –5.06962600 | –2.06727500 | –1.71785400 |
| N | –4.85098400 | –0.73568600 | –1.16463800 |
| H | 0.28807600 | 4.08134600 | –2.13473600 |
| H | –0.24653500 | 4.05785800 | 2.15193200 |
| H | 0.49007800 | 2.63834200 | 1.35109000 |
| H | –1.54017700 | 1.83561100 | 0.71330000 |
| H | –4.93339300 | 4.46970900 | 2.18611200 |
| H | –7.27616000 | 3.65806000 | 1.76705800 |
| H | –7.60399300 | 1.53118400 | 0.47948100 |
| H | –3.33671500 | 1.06832300 | 0.15847400 |
| H | 3.86569200 | –4.09142400 | 3.19401000 |
| H | 1.75009900 | –5.29016300 | 2.66332300 |
| H | 1.53030700 | –3.20573000 | –1.07745300 |
| H | 3.66808500 | –2.11139500 | –0.61571600 |
| H | –1.61786900 | –3.26277300 | 1.12722300 |
| H | –3.74561200 | –2.14539900 | 0.64509000 |
| H | –3.86366800 | –4.02979900 | –3.21499000 |
| H | –1.75986900 | –5.24342000 | –2.67020000 |
| H | 5.13006400 | –2.06480800 | 2.81297900 |
| H | 6.02726900 | –2.43408900 | 1.34236400 |
| H | –6.05194400 | –2.38555200 | –1.35172700 |
| H | –5.13835100 | –2.02319200 | –2.81428400 |
| H | –3.88885800 | –0.41772100 | –1.08556700 |
| N | 4.85208300 | –0.76405200 | 1.17249700 |
| C | 5.86170300 | –0.11920100 | 0.52725800 |

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|---|---|---|---|
| C | 5.52955900 | 1.14547000 | –0.21949300 |
| O | 7.02202400 | –0.54742600 | 0.55370600 |
| C | 6.63460100 | 1.87067400 | –0.68547700 |
| C | 6.45236800 | 3.05169300 | –1.39502800 |
| C | 5.16449100 | 3.51889100 | –1.63767400 |
| C | 4.04570100 | 2.80656800 | –1.18944000 |
| C | 4.22895800 | 1.60908300 | –0.48147400 |
| C | 2.70425100 | 3.45858600 | –1.46919100 |
| O | 2.69375600 | 4.60511300 | –1.95156100 |
| N | 1.58839800 | 2.77695200 | –1.16554400 |
| H | 3.89462900 | –0.43180100 | 1.09950100 |
| H | 7.62270100 | 1.47620500 | –0.47527900 |
| H | 7.31400500 | 3.61165800 | –1.75321800 |
| H | 4.97872300 | 4.44681900 | –2.16751100 |
| H | 3.35121000 | 1.04997000 | –0.15722900 |
| H | 1.55974300 | 1.83051200 | –0.72271300 |
| C | 0.02092600 | 4.28823900 | 0.00987700 |
| H | –0.84200000 | 4.94557500 | –0.15748300 |
| H | 0.88876200 | 4.93704800 | 0.18496600 |
| H | –0.46132100 | 2.65893700 | –1.35163600 |
| S | –0.00397700 | –0.43809800 | –0.02806200 |
| O | 0.27313000 | –1.24608900 | –1.25669200 |
| O | –0.27729800 | –1.28911000 | 1.17154800 |
| O | 1.20748300 | 0.47758400 | 0.27373100 |
| O | –1.21784300 | 0.48387500 | –0.29879100 |

**3–*trans*•$SO_4^{2-}$** complex

**Cartesian coordinates:**

| Symbol | X | Y | Z |
|---|---|---|---|
| C | 0.11398900 | –3.55078600 | –0.35075000 |
| C | –1.53536900 | –2.43380000 | –3.07260900 |
| N | –2.38757600 | –2.08152200 | –1.94350800 |
| C | –3.52163800 | –2.76576000 | –1.72204300 |
| C | –4.39242500 | –2.33776700 | –0.55818900 |
| O | –3.90775300 | –3.70720500 | –2.43672700 |
| C | –5.38282100 | –3.24554900 | –0.16543600 |
| C | –6.29886400 | –2.91455500 | 0.82927800 |
| C | –6.26040500 | –1.65207900 | 1.41117300 |
| C | –5.27786100 | –0.72853600 | 1.03173200 |
| C | –4.32559300 | –1.08281700 | 0.06260500 |
| C | –5.39797600 | 0.64428400 | 1.63317300 |
| O | –6.45570900 | 1.02029400 | 2.15268500 |
| C | 4.38233900 | 2.54962300 | –1.20273000 |
| C | 3.35924100 | 2.13828600 | –2.06120000 |
| C | 2.18368000 | 2.87152700 | –2.16488100 |
| C | 2.02310900 | 4.02558600 | –1.39041600 |
| C | 3.08386800 | 4.51448000 | –0.61622400 |
| C | 4.25743900 | 3.77537500 | –0.53072200 |
| N | 0.66674400 | 4.40854800 | –1.26536700 |
| N | 0.37827800 | 4.87210200 | –0.12991600 |
| C | –0.99307700 | 4.72219000 | 0.19562200 |
| C | –1.88466400 | 3.98883300 | –0.60486000 |
| C | –3.05840100 | 3.50427300 | –0.05749100 |
| C | –3.34885100 | 3.68826100 | 1.30253900 |
| C | –2.51410200 | 4.51147600 | 2.06410600 |
| C | –1.34929500 | 5.03877400 | 1.51100200 |

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|---|---|---|---|
| C | 5.48650000 | 1.58378600 | –0.85596800 |
| C | –4.44719100 | 2.87443300 | 1.94261400 |
| N | –4.32478800 | 1.47263700 | 1.54881600 |
| H | –0.09256400 | –4.58419600 | –0.05823700 |
| H | –2.18316600 | –2.61696400 | –3.93770600 |
| H | –0.90529200 | –1.55842600 | –3.25719500 |
| H | –1.97590600 | –1.39095800 | –1.27252300 |
| H | –5.41891300 | –4.19853200 | –0.68226500 |
| H | –7.05843000 | –3.63201400 | 1.13293600 |
| H | –6.99361600 | –1.34179500 | 2.14813500 |
| H | –3.54267900 | –0.39030900 | –0.23579500 |
| H | 3.41654600 | 1.17367100 | –2.55813400 |
| H | 1.32712300 | 2.45289100 | –2.68155600 |
| H | 2.93439100 | 5.40342900 | –0.01179400 |
| H | 5.05931300 | 4.10600300 | 0.12700400 |
| H | –1.57440300 | 3.70199400 | –1.60030500 |
| H | –3.69879200 | 2.86160900 | –0.65564000 |
| H | –2.72979800 | 4.66605900 | 3.11953600 |
| H | –0.63560200 | 5.58357300 | 2.12267300 |
| H | 5.97164400 | 1.18407400 | –1.75942100 |
| H | 6.27228100 | 2.06053200 | –0.26132700 |
| H | –5.45051700 | 3.20077300 | 1.64139800 |
| H | –4.40730600 | 2.97763900 | 3.03622400 |
| H | –3.41988000 | 1.13575700 | 1.23340400 |
| N | 4.92811200 | 0.47645000 | –0.07700200 |
| C | 5.74079800 | –0.32110100 | 0.66175900 |
| C | 5.10077500 | –1.49241500 | 1.35395400 |
| O | 6.95789700 | –0.11257800 | 0.74695300 |

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|---|---|---|---|
| C | 5.83294700 | –2.12785600 | 2.36405800 |
| C | 5.32408000 | –3.26606200 | 2.98562900 |
| C | 4.09855400 | –3.79447500 | 2.58153400 |
| C | 3.35315600 | –3.16678600 | 1.57890200 |
| C | 3.85626500 | –2.00925400 | 0.97398400 |
| C | 2.09031400 | –3.84399800 | 1.09068500 |
| O | 1.95364400 | –5.06644600 | 1.26045700 |
| N | 1.20998100 | –3.04700800 | 0.46318800 |
| H | 3.91406400 | 0.37199400 | –0.05225700 |
| H | 6.80411400 | –1.72079800 | 2.62703600 |
| H | 5.89518400 | –3.75583000 | 3.77207100 |
| H | 3.70318500 | –4.71043800 | 3.00953400 |
| H | 3.27969500 | –1.53985800 | 0.18345500 |
| H | 1.32894400 | –2.01482800 | 0.39533300 |
| C | 0.49689100 | –3.45606000 | –1.84127000 |
| H | 1.29421000 | –4.19070300 | –2.02622200 |
| H | –0.75812900 | –2.93120800 | –0.13948800 |
| C | –0.65142600 | –3.67377000 | –2.84054600 |
| H | –1.28786300 | –4.51820300 | –2.54542600 |
| H | –0.21678700 | –3.94095700 | –3.81621000 |
| H | 0.92789500 | –2.46255700 | –2.01367000 |
| S | 0.15923800 | 0.33928700 | –0.67983100 |
| O | 0.08386900 | 1.76439700 | –0.23202100 |
| O | 0.23235300 | 0.22894400 | –2.18395300 |
| O | 1.40879000 | –0.32562800 | –0.07243300 |
| O | –1.08383200 | –0.41740800 | –0.17419200 |

**1**–***trans***•$2SO_4^{2-}$ complex

**Cartesian coordinates:**

| Symbol | X | Y | Z |
|---|---|---|---|
| C | 0.10135100 | 1.59307800 | 0.52154700 |
| C | –0.85015300 | 2.67877500 | 1.08679700 |
| N | –2.24232500 | 2.34678200 | 0.78384000 |
| C | –3.01888000 | 3.21007400 | 0.08827400 |
| C | –4.30150400 | 2.67073700 | –0.52776400 |
| O | –2.70325300 | 4.38686700 | –0.15374500 |
| C | –5.11121900 | 3.59557500 | –1.19622600 |
| C | –6.20884100 | 3.17313200 | –1.94705000 |
| C | –6.48757300 | 1.81373600 | –2.06850400 |
| C | –5.70666500 | 0.87497000 | –1.38487500 |
| C | –4.62941800 | 1.30939300 | –0.59816300 |
| C | –5.95445500 | –0.59256000 | –1.64133200 |
| O | –6.39603600 | –0.96801100 | –2.74556400 |
| C | 4.94166900 | –2.62977600 | –0.16138700 |
| C | 4.19606100 | –2.48289100 | 1.01543300 |
| C | 2.86054900 | –2.86911300 | 1.03243800 |
| C | 2.24246100 | –3.40687200 | –0.10590700 |
| C | 3.00593100 | –3.61434400 | –1.27020100 |
| C | 4.34156300 | –3.22464600 | –1.28796900 |
| N | 0.84397900 | –3.53849300 | 0.01373100 |
| N | 0.19640800 | –3.90653500 | –1.00668700 |
| C | –1.21021200 | –3.74727400 | –0.84674000 |
| C | –1.78372900 | –2.95827500 | 0.16746200 |
| C | –3.14647000 | –2.70598800 | 0.18730200 |
| C | –3.98238100 | –3.23141900 | –0.81454900 |
| C | –3.41720000 | –4.04010600 | –1.80796400 |

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|---|---|---|---|
| C | –2.04290700 | –4.29279600 | –1.83210700 |
| C | 6.30624200 | –1.95635100 | –0.25061400 |
| C | –5.45859900 | –2.84536200 | –0.82232200 |
| N | –5.62808400 | –1.41765000 | –0.62866100 |
| H | –0.29935400 | 1.30512300 | –0.45634400 |
| H | –0.63522900 | 3.63367400 | 0.60793900 |
| H | –0.70531600 | 2.78393200 | 2.16983200 |
| H | –2.65678600 | 1.48644700 | 1.21165600 |
| H | –4.82785000 | 4.64181800 | –1.13868500 |
| H | –6.82690000 | 3.90628300 | –2.46692100 |
| H | –7.29209200 | 1.45185400 | –2.70378200 |
| H | –4.02779700 | 0.58581900 | –0.05512800 |
| H | 4.61982900 | –1.96351700 | 1.88307900 |
| H | 2.24602300 | –2.67182200 | 1.90492300 |
| H | 2.51848100 | –4.01079400 | –2.15592700 |
| H | 4.91795700 | –3.30878800 | –2.20802700 |
| H | –1.14144100 | –2.49631600 | 0.90746300 |
| H | –3.54791200 | –2.03972600 | 0.95016600 |
| H | –4.05159700 | –4.43855800 | –2.59992100 |
| H | –1.58959300 | –4.87743000 | –2.63021100 |
| H | 6.84641500 | –2.08190700 | 0.69381300 |
| H | 6.90210600 | –2.37023600 | –1.07188100 |
| H | –5.97535500 | –3.36290200 | –0.00204500 |
| H | –5.92945400 | –3.13121900 | –1.76865600 |
| N | 6.12102600 | –0.52953500 | –0.46761500 |
| C | 6.02530000 | –0.01541800 | –1.70663800 |
| C | 5.27901400 | 1.29501400 | –1.79584700 |
| O | 6.44592900 | –0.56678700 | –2.74331300 |

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|---|---|---|---|
| C | 5.62065800 | 2.21559700 | –2.78914200 |
| C | 4.82884900 | 3.34563100 | –2.99768900 |
| C | 3.64737200 | 3.50845700 | –2.27667800 |
| C | 3.27561400 | 2.58060300 | –1.29391200 |
| C | 4.12643800 | 1.50231200 | –1.01904100 |
| C | 1.85149200 | 2.67050100 | –0.77347500 |
| O | 1.02638000 | 3.29685100 | –1.45539200 |
| N | 1.50745500 | 1.97473100 | 0.33592100 |
| H | 6.49362300 | 2.01523600 | –3.40595500 |
| H | 5.10580800 | 4.07407100 | –3.76041500 |
| H | 2.95897800 | 4.31987600 | –2.49221200 |
| H | 3.87166000 | 0.80214000 | –0.22740200 |
| H | 2.23115100 | 1.53916900 | 0.93597100 |
| H | 0.08931500 | 0.71005100 | 1.16621000 |
| H | –5.50199600 | –1.09031900 | 0.38533900 |
| H | 5.92727100 | 0.09269700 | 0.39305200 |
| S | 4.83384000 | 0.72483900 | 2.65179000 |
| O | 5.22477100 | –0.62014000 | 3.23251100 |
| O | 4.78725400 | 1.78332800 | 3.70266200 |
| O | 5.88499500 | 1.10577400 | 1.58879600 |
| O | 3.49034100 | 0.57838000 | 1.93662900 |
| S | –4.60221400 | –0.06625900 | 2.69770200 |
| O | –3.26753500 | –0.01592600 | 1.92659100 |
| O | –5.46437600 | –1.12951400 | 1.97483900 |
| O | –4.38191300 | –0.50538700 | 4.10901300 |
| O | –5.27872500 | 1.26789000 | 2.60566700 |

**2–*trans*•$2SO_4^{2-}$** complex

**Cartesian coordinates:**

| Symbol | X | Y | Z |
|---|---|---|---|
| C | 0.54578700 | 1.93051200 | 0.98030800 |
| C | –1.58292700 | 2.94052500 | 2.05817000 |
| N | –2.58643400 | 2.45863100 | 1.11181900 |
| C | –3.13025300 | 3.30264600 | 0.20579700 |
| C | –4.10719200 | 2.71175100 | –0.79411100 |
| O | –2.82242000 | 4.50339100 | 0.12337300 |
| C | –4.57350200 | 3.56547600 | –1.80151700 |
| C | –5.38924700 | 3.07990700 | –2.82295300 |
| C | –5.73549100 | 1.72944000 | –2.85658500 |
| C | –5.30779900 | 0.87083900 | –1.83974500 |
| C | –4.49937000 | 1.36626600 | –0.80504900 |
| C | –5.61789100 | –0.60455500 | –1.94389900 |
| O | –5.74026000 | –1.14864100 | –3.05822600 |
| C | 4.80623400 | –2.78532300 | –0.10113900 |
| C | 4.07033500 | –2.56976900 | 1.07203500 |
| C | 2.71937600 | –2.89986300 | 1.10431700 |
| C | 2.07059700 | –3.43044800 | –0.02019100 |
| C | 2.81766200 | –3.69118500 | –1.18355100 |
| C | 4.17169300 | –3.37107600 | –1.21321900 |
| N | 0.66829500 | –3.52860100 | 0.11560700 |
| N | 0.00714700 | –3.81325400 | –0.92229500 |
| C | –1.39955900 | –3.67678000 | –0.74849500 |
| C | –2.00878200 | –3.19830400 | 0.42664300 |
| C | –3.37070900 | –2.93636100 | 0.46437100 |
| C | –4.16358800 | –3.14470700 | –0.68084800 |

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|---|---|---|---|
| C | –3.56617600 | –3.65632400 | –1.83910700 |
| C | –2.19629700 | –3.92375100 | –1.87410700 |
| C | 6.21723400 | –2.21573600 | –0.20110300 |
| C | –5.61839900 | –2.69203500 | –0.66201300 |
| N | –5.71007600 | –1.24366200 | –0.76429800 |
| H | –0.05104000 | 1.47974200 | 0.17860800 |
| H | –1.93483500 | 3.88049900 | 2.50652400 |
| H | –1.53604300 | 2.18683000 | 2.85132400 |
| H | –3.07865600 | 1.58191000 | 1.38616300 |
| H | –4.25184500 | 4.60182300 | –1.76838100 |
| H | –5.73282800 | 3.75166300 | –3.61016900 |
| H | –6.32342200 | 1.31239500 | –3.67043300 |
| H | –4.16677100 | 0.69405300 | –0.01863300 |
| H | 4.53579000 | –2.05616200 | 1.91979300 |
| H | 2.11805400 | –2.67240300 | 1.97906800 |
| H | 2.30818700 | –4.08452400 | –2.05805800 |
| H | 4.74091500 | –3.50660000 | –2.13108600 |
| H | –1.38426000 | –2.98045600 | 1.28495700 |
| H | –3.83303300 | –2.51560600 | 1.36210400 |
| H | –4.17028100 | –3.78474100 | –2.73495300 |
| H | –1.71019300 | –4.27280400 | –2.78254500 |
| H | 6.71950800 | –2.30072000 | 0.76703200 |
| H | 6.79979000 | –2.73608800 | –0.97048900 |
| H | –6.07102900 | –2.95890500 | 0.29750900 |
| H | –6.17630500 | –3.15878500 | –1.48366300 |
| H | –5.82151700 | –0.69852600 | 0.14748000 |
| N | 6.14751100 | –0.79735500 | –0.52241700 |
| C | 6.00773000 | –0.36857400 | –1.78968800 |

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|---|---|---|---|
| C | 5.34782600 | 0.98217900 | –1.93428500 |
| O | 6.31695600 | –1.02571600 | –2.80301600 |
| C | 5.65282700 | 1.78993900 | –3.03254500 |
| C | 4.91734100 | 2.95142600 | –3.27182000 |
| C | 3.82523800 | 3.26279300 | –2.46299200 |
| C | 3.49212800 | 2.45139600 | –1.37049600 |
| C | 4.28879500 | 1.33632600 | –1.08264500 |
| C | 2.15543400 | 2.70985500 | –0.69772200 |
| O | 1.31104900 | 3.38205100 | –1.31062500 |
| N | 1.91805500 | 2.12217300 | 0.49423400 |
| H | 6.06245900 | –0.10752900 | 0.29507800 |
| H | 6.44869300 | 1.47581200 | –3.70370400 |
| H | 5.16481400 | 3.58931700 | –4.12084700 |
| H | 3.17565900 | 4.10436200 | –2.68394200 |
| H | 4.05902000 | 0.71596900 | –0.22068600 |
| H | 2.67548800 | 1.64889900 | 1.02333000 |
| C | –0.17601700 | 3.19570400 | 1.47101600 |
| H | –0.25346800 | 3.90573500 | 0.64466000 |
| H | 0.43057200 | 3.66703800 | 2.25839800 |
| H | 0.61815200 | 1.19848400 | 1.79094000 |
| S | 5.20239800 | 0.62713300 | 2.60266300 |
| O | 5.55210200 | –0.76234500 | 3.10103900 |
| O | 5.32163800 | 1.64467800 | 3.68942500 |
| O | 6.16872900 | 0.97901600 | 1.45666900 |
| O | 3.78873500 | 0.59458100 | 2.01819400 |
| S | –5.18569500 | –0.28454700 | 2.58434700 |
| O | –3.79394600 | 0.11464900 | 2.08067200 |
| O | –5.22193200 | –1.79052100 | 2.74413300 |

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|---|---|---|---|
| O | –5.52147800 | 0.41595100 | 3.86029800 |
| O | –6.19898800 | 0.10531600 | 1.49392900 |

**3–*trans*•**$2SO_4^{2-}$ complex

**Cartesian coordinates:**

| Symbol | X | Y | Z |
|---|---|---|---|
| C | –1.19705000 | –2.27632800 | 0.39311500 |
| C | 2.02978700 | –2.91954100 | 1.27844300 |
| N | 3.30648700 | –2.42257000 | 0.77213400 |
| C | 4.14944000 | –3.19619800 | 0.05978500 |
| C | 5.28132700 | –2.48175800 | –0.65857700 |
| O | 3.99269000 | –4.41790900 | –0.12091200 |
| C | 6.17034400 | –3.26248100 | –1.40331700 |
| C | 7.13117400 | –2.66204500 | –2.21985700 |
| C | 7.19216800 | –1.27367800 | –2.32405700 |
| C | 6.32644900 | –0.47634700 | –1.56617600 |
| C | 5.38639300 | –1.08576900 | –0.72614200 |
| C | 6.32640000 | 1.01903400 | –1.78008700 |
| O | 6.66525900 | 1.49451900 | –2.88090400 |
| C | –4.95421700 | 2.80117100 | 0.33067500 |
| C | –4.14248200 | 2.31369800 | 1.36504100 |
| C | –2.77157800 | 2.54655000 | 1.32845900 |
| C | –2.17976000 | 3.26240200 | 0.27674600 |
| C | –2.99708400 | 3.78437900 | –0.74267800 |
| C | –4.36844800 | 3.54892800 | –0.70815400 |
| N | –0.76903300 | 3.29532300 | 0.31765000 |
| N | –0.17212100 | 3.87832200 | –0.63043700 |
| C | 1.24314800 | 3.72135900 | –0.58132900 |

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|---|---|---|---|
| C | 1.91196500 | 2.84917600 | 0.29711800 |
| C | 3.28709000 | 2.67648600 | 0.22154700 |
| C | 4.03918500 | 3.37131100 | –0.74420800 |
| C | 3.37548500 | 4.25150000 | –1.60744100 |
| C | 1.99164700 | 4.42514600 | –1.53312100 |
| C | –6.41943400 | 2.37942200 | 0.28108700 |
| C | 5.54555400 | 3.14466500 | –0.84277200 |
| N | 5.89891500 | 1.74385000 | –0.72770800 |
| H | –0.71450900 | –1.67221400 | –0.38703100 |
| H | 2.18640100 | –3.71464700 | 2.02428000 |
| H | 1.57518600 | –2.07132300 | 1.80017800 |
| H | 3.62768100 | –1.50445500 | 1.17184600 |
| H | 6.06172800 | –4.34150700 | –1.34762800 |
| H | 7.81458900 | –3.28259400 | –2.80047300 |
| H | 7.88806800 | –0.78347200 | –3.00004800 |
| H | 4.71479300 | –0.46891100 | –0.13743200 |
| H | –4.58125100 | 1.69143100 | 2.15109500 |
| H | –2.12028000 | 2.12527900 | 2.08799800 |
| H | –2.53356800 | 4.32245100 | –1.56404200 |
| H | –4.99885300 | 3.89578100 | –1.52503000 |
| H | 1.33604600 | 2.28194200 | 1.01860300 |
| H | 3.76257100 | 1.96084500 | 0.89353300 |
| H | 3.94432800 | 4.78406200 | –2.36970600 |
| H | 1.46472200 | 5.07983000 | –2.22405000 |
| H | –6.83109900 | 2.36362000 | 1.29442200 |
| H | –7.00230100 | 3.06261600 | –0.34783900 |
| H | 6.04188500 | 3.68596500 | –0.02480500 |
| H | 5.92893200 | 3.52666900 | –1.79467600 |

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|---|---|---|---|
| N | –6.52935900 | 1.02511400 | –0.24103200 |
| C | –6.53423600 | 0.77105400 | –1.56195100 |
| C | –6.04508500 | –0.60788500 | –1.93868800 |
| O | –6.83640600 | 1.59292800 | –2.44817500 |
| C | –6.50942300 | –1.22292200 | –3.10337400 |
| C | –5.92276200 | –2.40841500 | –3.55046400 |
| C | –4.81787400 | –2.93424800 | –2.88225800 |
| C | –4.32782400 | –2.31770200 | –1.72344000 |
| C | –4.97773000 | –1.18089800 | –1.22949800 |
| C | –2.97451700 | –2.76179600 | –1.20560000 |
| O | –2.21453800 | –3.35783200 | –1.98837800 |
| N | –2.61728500 | –2.39943000 | 0.04623500 |
| H | –7.30918300 | –0.74265100 | –3.66207400 |
| H | –6.29544400 | –2.89530000 | –4.45196900 |
| H | –4.27991100 | –3.79537900 | –3.26762900 |
| H | –4.62047500 | –0.71107400 | –0.31782800 |
| H | –3.29829000 | –1.95522600 | 0.69728100 |
| H | –1.16437900 | –1.69752800 | 1.31989600 |
| C | –0.40017700 | –3.59695000 | 0.52003200 |
| H | –0.52825000 | –4.02433100 | 1.52556600 |
| H | –0.84069900 | –4.30201700 | –0.18919000 |
| C | 1.09777600 | –3.44846800 | 0.16661800 |
| H | 1.18162500 | –2.77566700 | –0.69686100 |
| H | 1.49755600 | –4.41184500 | –0.16351100 |
| H | 5.89969500 | 1.37110300 | 0.27526400 |
| H | –6.47206700 | 0.21497800 | 0.45713000 |
| S | –5.55464900 | –0.93791500 | 2.54859400 |
| O | –5.73582300 | 0.40161700 | 3.23358200 |

| | | | |
|---|---|---|---|
| O | –5.71003900 | –2.07453500 | 3.50363400 |
| O | –6.60795900 | –1.04881400 | 1.43211900 |
| O | –4.17557700 | –0.95562600 | 1.88040200 |
| S | 5.28155800 | 0.19961500 | 2.60934800 |
| O | 5.05474400 | 0.60018300 | 4.02997700 |
| O | 6.00881400 | 1.34149100 | 1.86997900 |
| O | 6.07050800 | –1.06823200 | 2.48277800 |
| O | 3.93046300 | 0.02158400 | 1.87551200 |

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