# Supporting information

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## 1. Materials and methods

Unless otherwise noted, all chemicals and starting materials were obtained commercially from ABCR and Sigma-Aldrich and used without further purification. Pd(dba)$_2$ was synthesized according to a known method[1] and used without recrystallization. *N$^1$,N$^{1\prime}$*-(ethane-1,2-diyl)diethane-1,2-diamine ($N_4C_6$) and *N$^1$-(*2-aminoethyl*)-N$^2$-(*2-(2-aminoethylamino)ethyl)ethane-1,2-diamine ($N_5C_8$) were prepared by treatment of the corresponding commercially available hydrochlorides with a 2.5 M solution of KOH in methanol. 1,2-Bis(3-bromophenyl)ethane-1,2-dione (**1**) was synthesized in two steps according to previously reported procedure[2] from 3-bromobenzaldehyde. Dioxane was distilled successively over NaOH and sodium under argon, $CH_2Cl_2$ was distilled over $CaH_2$, MeOH was used freshly distilled. Preparative column chromatography was carried out using Silica gel 60 (40–63 µm) from Merck.

The $^1$H and $^{13}$C NMR spectra were recorded using a Bruker Avance-400 spectrometer in chloroform-*d1*, methanol-*d4* or DMSO-*d6.* The residual proton signals of solvents was used as internal standards. MALDI-TOF mass-spectra of macrocycles $N_2C_nO_xQ$ and $N_yC_nQ$ were registered on a Bruker Daltonics Autoflex II mass-spectrometer in positive ion mode with a dithranol matrix and polyethyleneglycols as internal standards. Mass spectroscopy studies of complexes were recorded on a MicrOTOFQ II (Bruker) apparatus equipped with an electrospray ionization (ESI) source. FT-IR spectra were registered on a Nicolet iS 5 with iD3 ATR accessory (ZnSe). Melting points were determined using Electrothermal IA 9200 apparatus. The nanoparticle size was measured using Zetasizer Nano-ZS analyzer. UV–vis spectra were recorded with a Hitachi U-2900 apparatus (Tokyo, Japan) in a quartz cuvette (Hellma, $l$ = 1 cm). Photoluminescence (PL) spectra were registered with Horiba Jobin Yvon Fluoromax-4 apparatus in a quartz cuvette (Hellma, $l$ = 1 cm), all the spectra were corrected. Fluorescence quantum yields were determined in dry toluene at 293 K by a relative method using quinine sulfate ($\Phi_{em}$ = 0.53 in 0.05 M $H_2SO_4$) and fluorescein ($\Phi_{em}$ = 92% in 0.1 M NaOH) as standards.[3] The following equation was used to determine the relative fluorescence quantum yield:

$$\Phi_x = \Phi_{st} \times ((F_x \times A_{st} \times \eta_x^2)/(F_{st} \times A_x \times \eta_{st}^2))$$

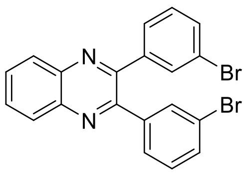
where $A$ is the absorbance (in the range of 0.01–0.1 A.U.), $F$ is the area under the emission curve, $\eta$ is the refractive index of the solvents (at 293 K) used in measurements, and the subscripts st and x represent standard and studied compound, respectively. The following refractive index values are used: 1.494 for toluene and 1.333 for aqueous solutions.

DFT computations were performed using the Firefly quantum chemistry package,[4] which is partially based on the GAMESS (US)[5] source code. The B3LYP functional with the 6-31G(d,p) basis set for all elements was used. Full optimization of geometry was achieved, and the minima were confirmed by computation of vibration frequencies.

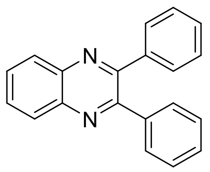
Additional information on the methods is provided in the respective sections.

## 2. Synthesis

**2,3-Bis(3-bromophenyl)quinoxaline (3).**[6] A 50 mL round-bottomed flask with a magnetic stirrer and a reflux condenser was charged with bis(3-bromophenyl)glyoxal (3.56 g, 9.67 mmol), 1,2-diaminobenzene (1.046 g, 9.67 mmol) and isopropanol (21 mL). The reaction mixture was stirred for 4 h at 80°C. The resulting precipitate was collected on glass filter, washed with isopropanol (3 × 5 mL) and dried under reduced pressure. Yield 4.15 g (98%), beige powder. M. p. 178–181°C. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 7.16 (t, $J$ = 7.9 Hz, 2H, H5 (Ph)), 7.29 (d, $J$ = 7.8 Hz, 2H, H6 (Ph)), 7.52 (d, $J$ = 7.9 Hz, 2H, H4 (Ph)), 7.77–7.83 (m, 2H, H6, H7, Q), 7.83 (s, 2H, H2 (Ph)) 8.12–8.19 (m, 2H, H5, H8(Q)). $^{13}$C NMR (400 MHz, $CDCl_3$): $\delta$ = 122.6 (2C, CBr (Ph)), 128.5 (2C, CH (Ph)), 129.2 (2C, C5, C8 (Q)), 129.6 (2C, C6, C7 (Q)), 130.5 (2C, CH(Ph)), 132.0 (2C, CH(Ph)), 132.7 (2C, CH(Ph)), 140.5 (2C, C4a, C8a, Q), 141.2 (2C, $C_{ipso}$(Ph)), 151.4 (2C, C2, C3, Q); IR (neat): $\nu_{max}$ ($cm^{-1}$) 661 (m), 669 (m), 685 (s), 698 (s), 723 (w), 736 (m), 759 (vs), 795 (s), 814 (m), 875 (m), 884 (w), 996 (m), 1058 (m), 1074 (m), 1142 (w), 1175 (w), 1212 (m), 1232 (w), 1267 (m), 1276 (m), 1295 (w), 1330 (m), 1340 (m), 1393 (w), 1406 (w), 1418 (m), 1457 (w), 1473 (m), 1507 (w), 1540 (m), 1559 (m), 3060 (w). HRMS (MALDI-TOF): $m/z$ $[M+H]^+$ calcd. for $C_{20}H_{13}Br_2N_2$: 438.9446; found: 438.9512.

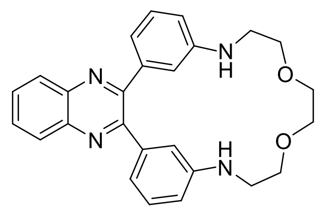



**2,3-Diphenylquinoxaline ($H_2Q$)**[6] was prepared according the same procedure from 1,2-diaminobenzene (100 mg, 0.93 mmol) and benzyl ( 195 mg, 0.93 mmol) in isopropanol (1.9 mL). Yield 137 mg (52%), beige powder. M. p. 124–125 °C (lit. 124–125 °C) $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 7.30–7.40 (m, 6H, H3, H4, H5 (Ph)), 7.50–7.55 (m, 4H, H2, H6 (Ph)), 7.74–7.80 (m, 2H, H6, H7 (Q)), 8.17–8.23 (m, 2H, H5, H8 (Q)).

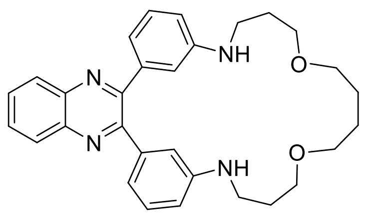



**General procedure for palladium-catalyzed macrocyclization of 2,3-bis(3-bromophenyl)quinoxaline and polyamines.** A two-neck flask, equipped with a magnetic stirrer and a reflux condenser, was charged with 2,3-bis(3-bromophenyl)quinoxaline (132 mg, 0.3 mmol), $Pd(dba)_2$ (14 mg, 8 mol%) and PhPF-*t*Bu (15 mg, 9 mol%). The flask was filled with argon and absolute dioxane (15 mL) was added into the flask in a flow of dry argon. After stirring for 2–3 min, amine (0.3 mmol) and sodium *tert*-butoxide (0.9 mmol) were added and the reaction mixture was refluxed for 24 h under argon atmosphere. Upon completion of the reaction, the precipitate was separated by filtration, washed with dichloromethane, the combined filtrates were concentrated under reduced pressure, the residue was chromatographed on silica gel using gradual elution with $CH_2Cl_2$ and $CH_2Cl_2$–MeOH (50 : 1–5 : 1 v/v) mixtures. For *pa*-$N_4C_9Q$ and $N_5C_8Q$, eluents $CH_2Cl_2$–MeOH–$NH_3$(aq.) (100 : 20 : 1–100 : 20 : 3 v/v/v) were additionally used.

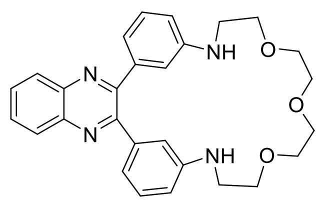
**12,13,15,16,19,20-Hexahydro-11*H*,18*H*-10,6:25,21-dimetheno[1,4,7,20]dioxadiazacyclodo-cosino[13,14-*b*]quinoxaline ($N_2C_6O_2Q$)** was synthesized according to the general procedure from 2,3-bis(3-bromophenyl)quinoxaline (132 mg, 0.3 mmol) and 2,2'-(ethane-1,2-diylbis(oxy))bis(ethan-1-amine) ($N_2C_6O_2$) (44 mg, 0.3 mmol) in dioxane (15 mL), in the presence Pd(dba)$_2$ (14 mg, 8 mol%), PhPF-*t*Bu (15 mg, 9 mol%) and *t*BuONa (86 mg, 0.9 mmol). The product was eluted with $CH_2Cl_2$–MeOH (50 : 1 v/v) mixture. Yield 69 mg (54%), yellow glassy substance. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 3.13 (t, $J$ = 5.5 Hz, 4H, $CH_2N$), 3.42 (t, $J$ = 5.5 Hz, 4 H, $CH_2O$), 3.55 (s, 4 H, $CH_2O$), 3.90 (br. s, 2H, NH), 6.61 (d, $J$ = 8.1 Hz, 2H, H4 (Ph)), 6.64 (s, 2H, H2 (Ph)), 7.03 (d, $J$ = 7.6 Hz, 2H, H6 (Ph)), 7.17 (t, $J$ = 7.8 Hz, 2H, H5 (Ph)), 7.69–7.74 (m, 2H, H6, H7 (Q)), 8.12–8.16 (m, 2H, H5, H8 (Q)). $^{13}$C NMR (400 MHz, $CDCl_3$): $\delta$ = 43.5 (2C, $CH_2N$), 68.7 (2C, $CH_2O$), 70.5 (2C, $CH_2O$), 114.0 (2C), 114.4 (2C), 118.6 (2C), 129.0 (2C), 129.2 (2C), 129.6 (2C), 140.0 (2C), 141.0 (2C), 147.4 (2C), 153.8 (2C); IR (neat): $\nu_{max}$ (cm$^{-1}$) 3376 (w), 3050 (w), 2924 (w), 2858 (w), 1728 (w), 1603 (m), 1585 (m), 1512 (w), 1473 (w), 1430 (w), 1393 (w), 1345 (m), 1264 (m), 1203 (w), 1167 (w), 1125 (m), 1060 (m), 1031 (w), 991 (m), 928 (w), 858 (m), 815 (w), 782 (m), 762 (m), 730 (s), 700 (s), 612 (m); HRMS (MALDI-TOF): $m/z$ [M+H]$^+$ calcd. for $C_{26}H_{27}N_4O_2$: 427.2185; found: 427.2218.




**11,12,13,14,16,17,18,19,21,22,23,24-Dodecahydro-10.6:29.25-dimetheno[1.22.5.18]dioxa-diazacyclohexacosino[11.12-*b*]quinoxaline ($N_2C_{10}O_2Q$)** was synthesized according to the general procedure from 2,3-bis(3-bromophenyl)quinoxaline (132 mg, 0.3 mmol) and 3,3'-(butane-1,4-diylbis(oxy))bis(propan-1-amine) ($N_2C_{10}O_2$) (66 mg, 0.3 mmol) in dioxane (15 mL), in the presence Pd(dba)$_2$ (14 mg, 8 mol%), PhPF-*t*Bu (15 mg, 9 mol%) and *t*BuONa (86 mg, 0.9 mmol). The product was eluted with $CH_2Cl_2$–MeOH (50 : 1 v/v) mixture. Yield 72 mg (50%), yellow glassy solid. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 1.62–1.76 (m, 8H, $CH_2$), 3.05 (t, $J$ = 6.3 Hz, 4H, $CH_2N$), 3.39–3.45 (m, 8H, $CH_2O$), 3.99 (br. s, 2H, NH), 6.58 (dd, $J$ = 7.7, 1.9 Hz, 2H, H4 (Ph)), 6.66 (t, $J$ = 1.9 Hz, 2H, H2 (Ph)), 6.95 (d, $J$ = 7.9 Hz, 2H, H6 (Ph)), 7.15 (t, $J$ = 7.9 Hz, 2H, H5 (Ph)), 7.69–7.74 (m, 2H, H6, H7 (Q)), 8.13–8.17 (m, 2H, H5, H8 (Q)). $^{13}$C NMR (400 MHz, $CDCl_3$): $\delta$ = 25.7 (2C, $CH_2$), 28.8 (2C, $CH_2$), 42.1 (2C, $CH_2N$), 69.1 (2C, $CH_2O$), 70.3 (2C, $CH_2O$), 113.7 (2C), 113.9 (2C), 118.5 (2C), 128.9 (2C), 129.0 (2C), 129.5 (2C), 139.9 (2C), 141.0 (2C), 148.0 (2C), 154.1 (2C); IR (neat): $\nu_{max}$ (cm$^{-1}$) 3387 (w), 3048 (w), 2937 (w), 2920 (w), 2858 (m), 2803 (w), 1603 (vs), 1584 (s), 1559 (w), 1540 (w), 1510 (m), 1473 (m), 1430 (m), 1392 (w), 1344 (s), 1264 (s), 1202 (m), 1167 (w), 1109 (s), 1062 (m), 1020 (m), 990 (m), 930 (w), 914 (w), 893 (w), 857 (m), 782 (m), 763 (m), 734 V (s), 703 (s), 669 (w), 616 (w); HRMS (MALDI-TOF): $m/z$ [M+H]$^+$ calcd. for $C_{30}H_{35}N_4O_2$: 483.2755; found: 483.2751.

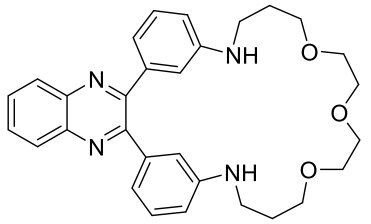


**12,13,15,16,18,19,22,23–Octahydro-11*H*,21*H*-10.6:28.24-dimetheno[1,4,7,10,23]trioxadiaza-cycloheptacosino[16,17-*b*]quinoxaline ($N_2C_8O_3Q$)**



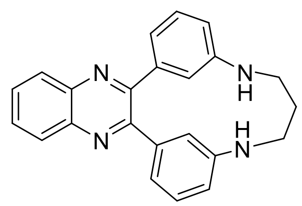
was synthesized according to the general procedure from 2,3-bis(3-bromophenyl)quinoxaline (132 mg, 0.3 mmol) and 2,2'-((oxybis(ethane-2,1-diyl))bis(oxy))bis(ethan-1-amine) ($N_2C_8O_3$) (58 mg, 0.3 mmol) in dioxane (15 mL), in the presence Pd(dba)$_2$ (14 mg, 8 mol%), PhPF-*t*Bu (15 mg, 9 mol%) and *t*BuONa (86 mg, 0.9 mmol). The product was eluted with $CH_2Cl_2$–MeOH (50 : 1 v/v) mixture. Yield 65 mg (46%), yellow glassy solid. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 3.06 (t, $J$ = 4.9 Hz, 4H, $CH_2N$), 3.43 (t, $J$ = 4.9 Hz, 4H, $CH_2O$), 3.55–3.60 (m, 8H, $CH_2O$), 3.92 (br. s, 2H, NH), 6.55 (s, 2H, H2 (Ph)), 6.62 (dd, $J$ = 8.1, 1.2 Hz, 2H, H4 (Ph)), 7.06 (d, $J$ = 7.5 Hz, 2H, H5 (Ph)), 7.20 (t, $J$ = 7.8 Hz, 2H, H6 (Ph)), 7.71–7.75 (m, 2H, H6, H7 (Q)), 8.13–8.18 (m, 2H, H5, H8 (Q)). $^{13}$C NMR (400 MHz, $CDCl_3$): $\delta$ = 43.1 (2C, $CH_2N$), 68.7 (2C, $CH_2O$), 70.0 (2C, $CH_2O$), 70.7 (2C, $CH_2O$), 113.6 (2C), 114.8 (2C), 118.7 (2C), 129.1 (2C), 129.3 (2C), 129.6 (2C), 140.1 (2C), 141.0 (2C), 147.4 (2C), 154.1 (2C); IR (neat): $\nu_{max}$ (cm$^{-1}$) 3368 (w), 3056 (w), 2895 (w), 2865 (m), 1716 (w), 1653 (w), 1603 (vs), 1585 (s), 1559 (w), 1512 (m), 1473 (m), 1436 (m), 1394 (w), 1345 (s), 1265 (m), 1249 (m), 1205(w), 1169 (w), 1114 (s), 1098 (s), 1065 (s), 1031 (m), 1012 (w), 990 (m), 938 (w), 916 (w), 857(w), 763 (m), 732 (s), 701 (s), 612 (w); HRMS (MALDI-TOF): *m/z* [M+Na]$^+$ calcd. for $C_{28}H_{30}N_4O_3Na^+$: 493.2210; found: 493.2223.

**11,12,13,14,16,17,19,20,22,23,24,25-Dodecahydro-10.6:30.26-dimetheno[1,4,7,11,24]trioxa-diazacycloheptacosino[17,18-*b*]quinoxaline ($N_2C_{10}O_3Q$)**

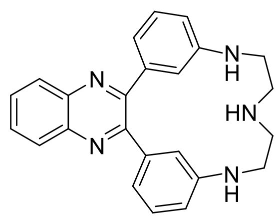


was synthesized according to the general procedure from 2,3-bis(3-bromophenyl)quinoxaline (132 mg, 0.3 mmol) and 3,3'-((oxybis(ethane-2,1-diyl))bis(oxy))bis(propan-1-amine) ($N_2C_{10}O_3$) (66 mg, 0.3 mmol) in dioxane (15 mL), in the presence Pd(dba)$_2$ (14 mg, 8 mol%), PhPF-*t*Bu (15 mg, 9 mol%) and *t*BuONa (86 mg, 0.9 mmol). The product was eluted with $CH_2Cl_2$–MeOH (50 : 1 v/v) mixture. Yield 78 mg (52%), yellow glassy solid. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 1.68 (quint., $J$ = 6.1 Hz, 4H, $CH_2$), 3.05 (t, $J$ = 6.4 Hz, 4 H, $CH_2N$), 3.51 (t, $J$ = 5.7 Hz, 4H, $CH_2O$), 3.56–3.58 (m, 4H, $CH_2O$), 3.61–3.63 (m, 4H, $CH_2O$), 4.11 (br. s, 2H, NH), 6.58–6.60 (m, 4H, H2, H4 (Ph)), 6.99 (d, $J$ = 7.6 Hz, 2H, H6 (Ph)), 7.17 (t, $J$ = 7.8 Hz, 2H, H5 (Ph)), 7.69–7.74 (m, 2H, H6, H7 (Q)), 8.12–8.17 (m, 2H, H5, H8 (Q)). $^{13}$C NMR (400 MHz, $CDCl_3$): $\delta$ = 28.7 (2C, $CH_2$), 41.7 (2C, $CH_2N$), 69.6 (2C, $CH_2O$), 70.2 (2C, $CH_2O$), 70.7 (2C, $CH_2O$), 113.9 (2C), 114.2 (2C), 118.5 (2C), 129.1 (4C), 129.5 (2C), 140.0 (2C),141.0 (2C),147.9 (2C), 154.1 (2C); IR (neat): $\nu_{max}$ (cm$^{-1}$) 3378 (w), 3049 (w), 2916 (w), 2862 (m), 1603 (s), 1584 (s), 1559 (w), 1512 (m), 1473 (m), 1429 (m), 1392 (w), 1345 (s), 1265 (s), 1202 (m), 1119 (s), 1062 (m), 1012 (m), 990 (m), 957 (w), 916 (w), 858 (m), 783 (m), 763 (m), 733 (s), 704 (s), 669 (w), 615 (w); HRMS (MALDI-TOF): *m/z* $[M+H]^+$ calcd. for $C_{30}H_{35}N_4O_3$: 499.2704; found: 499.2682.

**12,13,14,15-Tetrahydro-11*H*-10.6:20,16-dimetheno[1,5]diazacycloheptadecino[11,12-*b*]quinoxaline ($N_2C_3Q$)** was synthesized according to the general procedure from 2,3-bis(3-bromophenyl)quinoxaline (132 mg, 0.3 mmol) and propane-1,3-diamine ($N_2C_3$) (22 mg, 0.3 mmol) in dioxane (15 mL), in the presence Pd(dba)$_2$ (14 mg, 8 mol%), PhPF-*t*Bu (15 mg, 9 mol%) and *t*BuONa (86 mg, 0.9 mmol). The product was eluted with $CH_2Cl_2$–MeOH (50 : 1 v/v) mixture. Yield 175 mg (75%), yellow powder. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 1.75 (quint., $J$ = 6.7 Hz, 2H, $CH_2$), 3.21 (t, $J$ = 6.8 Hz, 4H, $CH_2$NH), 3.38 (br. s., 2H, NH), 6.72 (d, $J$ = 8.1 Hz, 2H, H4 (Ph)), 7.04 (s, 2H, H2 (Ph)), 7.10 (d, $J$ = 7.5 Hz, 2H, H6 (Ph)), 7.25 (t, $J$ = 7.9 Hz, 2H, H5 (Ph)), 7.76–7.78 (m, 2H, H6, H7 (Q)), 8.16–8.18 (m, 2H, H5, H8 (Q)). $^{13}$C NMR (400 MHz, $CDCl_3$): $\delta$ = 31.0 (1C, $CH_2$), 43.7 (2C, $CH_2$N), 118.4 (2C), 118.7 (2C), 121.2 (2C), 129.2 (2C), 129.7 (2C), 130.0 (2C), 139.4 (2C), 141.0 (2C), 146.4 (2C), 153.9 (2C); IR (neat): $\nu_{max}$ (cm$^{-1}$) 3334 (w), 3045 (w), 2934 (w), 2874 (w), 1709 (w), 1604 (s), 1583 (m), 1507 (w), 1469 (m), 1428 (m), 1394 (w), 1342 (s), 1263 (s), 1189 (m), 1165 (w), 1123 (w), 1051 (m), 996 (m), 958 (w), 898 (m), 869 (w), 851 (w), 790 (m), 762 (m), 733 (vs), 701 (s), 611 (w); HRMS (MALDI-TOF): *m/z* $[M+H]^+$ calcd. for $C_{23}H_{21}N_4$: 353.1761; found: 353.1735.

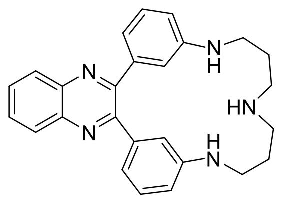


**12,13,14,15,16,17-Hexahydro-11*H*-10.6:22,18-dimetheno[1,4,7]triazacyclononadecino[13,14-*b*]quinoxaline ($N_3C_4Q$)** was synthesized according to the general procedure from 2,3-bis(3-bromophenyl)quinoxaline (132 mg, 0.3 mmol) and N$^1$-(2-aminoethyl)ethane-1,2-diamine ($N_3C_4$) (31 mg, 0.3 mmol) in dioxane (15 mL), in the presence Pd(dba)$_2$ (14 mg, 8 mol%), PhPF-*t*Bu (15 mg, 9 mol%) and *t*BuONa (86 mg, 0.9 mmol). The product was eluted with $CH_2Cl_2$–MeOH (5 : 1 v/v) mixture. Yield 105 mg (92%), yellow glassy solid. $^1$H NMR (400 MHz, $CDCl_3$–$CD_3OD$ (10 : 1 v/v)): $\delta$ = 2.37 (br. s, 1H, NH), 2.71 (t, $J$ = 5.8 Hz, 4H, C$\underline{H}_2$N), 3.32(t, $J$ = 5.8 Hz, 4H, C$\underline{H}_2$NHAr), 3.68 (br. s, 2H, NHAr), 6.48 (t, $J$ = 1.7 Hz, 2H, H2 (Ph)), 6.64 (dd, $J$ = 8.3, 1.6 Hz, 2H, H4 (Ph)), 7.00 (d, $J$ = 7.4 Hz, 2H, H6 (Ph)), 7.21 (t, $J$ = 7.7 Hz, 2H, H5 (Ph)), 7.71–7.76 (m, 2H, H6, H7 (Q)), 8.11–8.15 (m, 2H, H5, H8 (Q)). $^{13}$C NMR (400 MHz, $CDCl_3$): $\delta$ = 40.2 (2C, $CH_2$N), 46.4 (2C, $CH_2$NHAr), 113.8 (2C), 115.2 (2C), 119.1 (2C), 129.1 (2C), 129.7 (2C), 130.0 (2C), 140.1 (2C), 140.9 (2C), 145.2 (2C), 154.3 (2C); IR (neat): $\nu_{max}$ (cm$^{-1}$) 3302 (w), 3046 (vw), 2923 (w), 2850 (vw), 1604 (m), 1586 (m), 1519 (w), 1487 (w), 1473 (w), 1433 (w), 1394 (w), 1347 (m), 1263 (m), 1204 (w), 1168 (w), 1128 (w), 1099 (w), 1061 (w), 1011 (w), 992 (w), 957 (w), 918 (w), 857 (w), 787 (w),



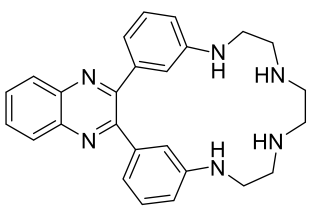
764 (m), 730 (vs), 698 (s), 670 (m), 612 (m); HRMS (MALDI-TOF): *m/z* $[M+H]^+$ calcd. for $C_{24}H_{24}N_5$: 382.2026; found: 382.2054.

**12,13,14,15,16,17,18,19-Octahydro-11*H*-10.6:24,20-dimetheno[1,5,9]triazacyclohenicosino**



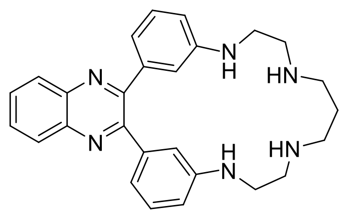

**[15,16-*b*]quinoxaline ($N_3C_6Q$)** was synthesized according to the general procedure from 2,3-bis(3-bromophenyl)quinoxaline (132 mg, 0.3 mmol) and $N^1$-(3-aminopropyl)propane-1,3-diamine ($N_3C_6$) (39 mg, 0.3 mmol) in dioxane (15 mL), in the presence Pd(dba)$_2$ (14 mg, 8 mol%), PhPF-*t*Bu (15 mg, 9 mol%) and *t*BuONa (86 mg, 0.9 mmol). The product was eluted with $CH_2Cl_2$–MeOH (5 : 1 v/v) mixture. Yield 92 mg (75%), yellow glassy solid. $^1$H NMR (400 MHz, $CD_3OD$): $\delta$ = 1.81 (quint., $J$ = 6.9 Hz, 4H, $CH_2$), 3.05 (t, $J$ = 7.3 Hz, 4H, $CH_2N$), 3.21 (t, $J$ = 6.2 Hz, 4H, C$\underline{H}_2$NHAr), 6.61 (t, $J$ = 1.9 Hz, 2H, H2 (Ph)), 6.74 (dd, $J$ = 8.0, 2.1 Hz, 2H, H4 (Ph)), 6.98 (d, $J$ = 7.6 Hz, 2H, H6 (Ph)), 7.22 (t, $J$ = 7.9 Hz, 2H, H5 (Ph)), 7.78–7.83 (m, 2H, H6, H7 (Q)), 8.09–8.13 (m, 2H, H5, H8 (Q)), NH-protons were not observed. $^{13}$C NMR (400 MHz, DMSO-*d6*): $\delta$ = 23.3 (2C, $CH_2$), 42.3 (2C, $CH_2$NHAr), 112.2 (2C), 114.0 (2C), 117.4 (2C), 128.7 (2C), 128.8 (2C), 130.3 (2C), 140.1 (2C), 140.4 (2C), 147.6 (2C), 154.6 (2C), one $CH_2$ signal overlaps with DMSO signal; IR (neat): $\nu_{max}$ (cm$^{-1}$) 3323 (w), 3043 (w), 2934 (w), 2849 (w), 2778 (w), 1603 (m), 1585 (m), 1514 (w), 1472 (w), 1429 (w), 1393 (w), 1347 (m), 1264 (m), 1202 (w), 1168 (w), 1127 (w), 1104 (w), 1056 (w), 1011 (w), 990 (w), 957 (w), 895 (w), 858 (w), 785 (w), 763 (w), 730 (vs), 700 (s), 669 (w), 614 (w); HRMS (MALDI-TOF): *m/z* $[M+H]^+$ calcd. for $C_{26}H_{28}N_5$: 410.2339; found: 410.2339.

**11,12,13,14,15,16,17,18,19,20-Decahydro-10,6:25,21-dimetheno[1,4,7,10]tetraazacyclodocosino**

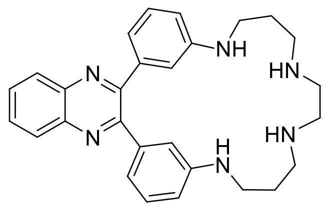



**[16,17-*b*]quinoxaline ($N_4C_6Q$)** was synthesized according to the general procedure from 2,3-bis(3-bromophenyl)quinoxaline (132 mg, 0.3 mmol) and $N^1$,$N^{1'}$-(ethane-1,2-diyl)bis(ethane-1,2-diamine) ($N_4C_6$) (44 mg, 0.3 mmol) in dioxane (15 mL), in the presence Pd(dba)$_2$ (14 mg, 8 mol%), PhPF-*t*Bu (15 mg, 9 mol%) and *t*BuONa (86 mg, 0.9 mmol). The product was eluted with $CH_2Cl_2$–MeOH (5 : 1 v/v) mixture. Yield 72 mg (57%), yellow glassy solid. $^1$H NMR (400 MHz, $CDCl_3$–$CD_3OD$ (5 : 1 v/v)): $\delta$ = 2.77 (t, $J$ = 6.2 Hz, 4H, C$\underline{H}_2$CH$_2$NHAr), 2.90 (s, 4H, $CH_2N$), 3.13 (t, $J$ = 6.2 Hz, 4H, C$\underline{H}_2$NHAr), 6.57–6.60 (m, 4H, H2, H4 (Ph)), 6.86 (d, $J$ = 7.6 Hz, 2H, H6 (Ph)), 7.09 (t, $J$ = 7.9 Hz, 2H, H5 (Ph)), 7.66–7.70 (m, 2H, H6, H7 (Q)), 8.03–8.07 (m, 2H, H5, H8 (Q)). $^{13}$C NMR (400 MHz, $CDCl_3$–$CD_3OD$ (5:1 v/v)): $\delta$ = 41.4 (2C, $CH_2N$), 44.6 (2C, $CH_2N$), 46.1 (2C, $CH_2$NHAr), 113.2 (2C), 113.9 (2C), 118.9 (2C), 128.6 (2C), 129.3 (2C), 130.0 (2C), 139.7 (2C), 140.7 (2C), 146.8 (2C), 153.8 (2C); IR (neat): $\nu_{max}$ (cm$^{-1}$) 3378 (w), 3051 (w), 2955 (w), 2918 (w), 2849 (w), 1653 (m), 1636 (m), 1616 (w), 1603 (m), 1582 (m), 1559 (m), 1540 (w), 1521 (w), 1507 (w), 1490 (w), 1473 (m), 1457 (m), 1436 (m), 1395 (w), 1347 (m), 1299 (w), 1269 (m), 1264 (m), 1249 (m), 1207 (w), 1168 (w), 1140 (w), 1127 (w), 1115 (w), 1061 (w), 1011 (w), 990 (w), 960 (w), 913 (w), 894 (w), 862 (w), 815 (w), 786 (m), 761 (w), 731 (s), 700 (s), 668 (m), 618 (w), 613 (w); HRMS (MALDI-TOF): *m/z* $[M+H]^+$ calcd. for $C_{26}H_{29}N_6$: 425.2448; found: 425.2496.

**12,13,14,15,16,17,18,19,20,21-Decahydro-11*H*-10.6:26.22-dimetheno[1,4,8,11]tetraazacyclo-tricosino[17,18-*b*]quinoxaline ($N_4C_7Q$)** was synthesized according to the general procedure from 2,3-bis(3-bromophenyl)quinoxaline (132 mg, 0.3 mmol) and $N^1$,$N^{1\prime}$-(propane-1,3-diyl)bis(ethane-1,2-diamine) ($N_4C_7$) (48 mg, 0.3 mmol) in dioxane (15 mL), in the presence Pd(dba)$_2$ (14 mg, 8 mol%), PhPF-*t*Bu (15 mg, 9 mol%) and *t*BuONa (86 mg, 0.9 mmol). The product was eluted with $CH_2Cl_2$–MeOH (5 : 1 v/v) mixture. Yield 85 mg (65%), yellow glassy solid. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 1.51 (quint., $J$ = 5.9 Hz, 2H, $CH_2$), 2.53 (t, $J$ = 5.9 Hz, 4H, C$\underline{H}_2$NH), 2.54 (t, $J$ = 5.9 Hz, 4H, C$\underline{H}_2$NH) 2.93 (t, $J$ = 5.9 Hz, 4H, C$\underline{H}_2$NHAr)), 6.53 (s, 2H, H3 (Ph)), 6.54 (d, $J$ = 8.1 Hz, 2H, H4 (Ph)), 6.85 (d, $J$ = 7.3 Hz, 2H, H6 (Ph)), 7.08 (t, $J$ = 7.8 Hz, 2H, H5 (Ph)), 7.64–7.70 (m, 2H, H6, H7 (Q)), 8.00–8.06 (m, 2H, H5, H8 (Q)), the signals of four NH-protons were not observed. $^{13}$C NMR (400 MHz, $CDCl_3$): $\delta$ = 23.4 (1C, $CH_2$), 41.1 (2C, $CH_2N$), 46.9 (2C, $CH_2N$), 49.3 (2C, $CH_2N$), 113.6 (2C), 113.7 (2C), 118.9 (2C), 129.0 (2C), 129.6 (2C), 129.9 (2C), 140.1 (2C), 140.9 (2C), 147.0 (2C), 153.8 (2C); IR (neat): $\nu_{max}$ (cm$^{-1}$) 3400 (w), 3314 (w), 3046 (w), 2925 (w), 2850 (w), 1675 (w), 1603 (m), 1585 (w), 1526 (w), 1490 (w), 1473 (w), 1430 (w), 1347 (m), 1264 (m), 1205 (w), 1169 (w), 1114 (w), 1059 (w), 1013 (w), 990 (w), 958 (w), 916 (w), 862 (w), 784 (w), 763 (w), 730 (s), 698 (s), 613 (w); HRMS (MALDI-TOF): *m/z* $[M+H]^+$ calcd. for $C_{27}H_{30}N_6Na$: 461.2424; found: 461.2379.

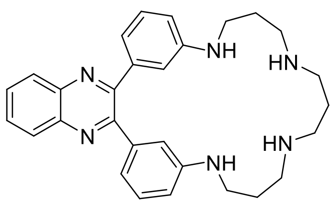



**11,12,13,14,15,16,17,18,19,20,21,22-Dodecahydro-10,6:27,23-dimetheno[1,4,8,21]tetraaza-cyclotetracosino[14,15-*b*]quinoxaline ($N_4C_8Q$)** was synthesized according to the general procedure from 2,3-bis(3-bromophenyl)quinoxaline (132 mg, 0.3 mmol) and $N^1$,$N^{1\prime}$-(ethane-1,2-diyl)bis(propane-1,3-diamine) ($N_4C_8$) (52 mg, 0.3 mmol) in dioxane (15 mL), in the presence Pd(dba)$_2$ (14 mg, 8 mol%), PhPF-*t*Bu (15 mg, 9 mol%) and *t*BuONa (86 mg, 0.9 mmol). The product was eluted with $CH_2Cl_2$–MeOH (5 : 1 v/v) mixture. Yield 65 mg (48%), yellow glassy solid. $^1$H NMR (400 MHz, $CDCl_3$–$CD_3OD$ (10 : 1 v/v)): $\delta$ = 1.57 (quint., $J$ = 6.0 Hz, 4H, C$\underline{H}_2$CH$_2$NHAr), 2.64 (t, $J$ = 5.9 Hz, 4H, $CH_2N$), 2.76 (s, 4H, $CH_2N$), 2.94 (t, $J$ = 6.2 Hz, 4H, C$\underline{H}_2$NHAr), 3.80 (br. s., 4H, NH), 6.56 (s, 2H, H3 (Ph)), 6.62 (d, $J$ = 8.1 Hz, 2H, H4 (Ph)), 7.01 (d, $J$ = 7.2 Hz, 2H, H6 (Ph)), 7.15 (t, $J$ = 7.8 Hz, 2H, H5 (Ph)), 7.68–7.73 (m, 2H, H6, H7 (Q)), 8.10–8.14 (m, 2H, H5, H8 (Q)). $^{13}$C NMR (400 MHz, $CDCl_3$–$CD_3OD$ (10:1 v/v)): $\delta$ = 27.9 (2C, CH$_2\underline{C}$H$_2$CH$_2$), 42.4 (2C, $CH_2N$), 47.2 (2C, $CH_2N$), 47.3 (2C, $CH_2N$), 112.9 (2 C), 115.1 (2 C), 118.9 (2 C), 129.0 (2



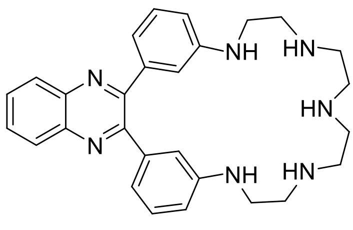
C), 129.2 (2 C), 129.6 (2 C), 140.0 (2 C), 141.0 (2 C), 147.6 (2 C), 154.0 (2 C); IR (neat): $\nu_{max}$ (cm$^{-1}$) 3310 (w), 3048 (w), 2921 (m), 2850 (m), 1732 (w), 1649 (w), 1602 (vs), 1585 (s), 1559 (m), 1514 (m), 1471 (m), 1431 (m), 1393 (m), 1346 (s), 1264 (s), 1203 (m), 1166 (w), 1140 (w), 1114 (m), 1060 (m), 1013 (w), 990 (w), 915 (vw), 858 (w), 785 (m), 762 (m), 732 (vs), 703 (vs), 670 (w), 614 (w); HRMS (MALDI-TOF): *m/z* [M+H]$^+$ calcd. for $C_{28}H_{33}N_6$: 453.2761; found: 453.2749.

**12,13,14,15,16,17,18,19,20,21,22,23-Dodecahydro-11*H*-10.6:28.24-dimetheno[1,5,9,13]**




**tetraazacyclopentacosino[19,20-*b*]quinoxaline ($N_4C_9Q$)** was synthesized according to the general procedure from 2,3-bis(3-bromophenyl)quinoxaline (132 mg, 0.3 mmol) and *N*[1],*N*[1']-(propane-1,3-diyl)bis(propane-1,3-diamine) ($N_4C_9$) (56 mg, 0.3 mmol) in dioxane (15 mL), in the presence Pd(dba)$_2$ (14 mg, 8 mol%), PhPF-*t*Bu (15 mg, 9 mol%) and *t*BuONa (86 mg, 0.9 mmol). The product was eluted with $CH_2Cl_2$–MeOH (5 : 1 v/v) mixture. Yield of 79 mg (57%), yellow glassy solid. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 1.59 (quint., *J* = 6.0 Hz, 4H, C$\underline{H_2}$CH$_2$NHAr), 1.80 (quint., *J* = 5.6 Hz, 2H, CH$_2$C$\underline{H_2}$CH$_2$), 2.68 (t, *J* = 6.4 Hz, 4H, CH$_2$N), 2.82 (t, *J* = 5.6 Hz, 4H, CH$_2$N), 3.00 (t, *J* = 5.9 Hz, 4H, C$\underline{H_2}$NHAr), 4.41 (br. s., 2H, NHAr), 6.53 (s, 2H, H2 (Ph)), 6.68 (d, *J* = 7.8 Hz, 2H, H4 (Ph)), 7.14 (d, *J* = 7.6 Hz, 2H, H6 (Ph)), 7.22 (t, *J* = 7.7, 2H, H5 (Ph)), 7.71–7.75 (m, 2H, H6, H7 (Q)), 8.13–8.17 (m, 2H, H5, H8 (Q)), the signals of two NH-protons were not observed. $^{13}$C NMR (400 MHz, $CDCl_3$–$CD_3OD$ (5 : 1 v/v)): $\delta$ = 22.9 (1C, CH$_2$), 24.4 (2C, CH$_2$), 41.8 (2C, CH$_2$N), 46.4 (2C, CH$_2$N), 47.2 (2C, CH$_2$N), 114.1 (2C), 115.3 (2C), 119.2 (2C), 128.9 (2C), 129.5 (2C), 129.9 (2C), 140.3 (2C), 140.9 (2C), 147.2 (2C), 154.0 (2C); IR (neat): $\nu_{max}$ (cm$^{-1}$) 3407 (w), 3321 (w), 3044 (w), 2952 (w), 2927 (w), 2852 (w), 1603 (m), 1586 (w), 1515 (w), 1474 (w), 1432 (w), 1394 (w), 1346 (w), 1264 (m), 1207 (w), 1167 (vw), 1114 (w), 1060 (w), 1012 (w), 991 (w), 894 (w), 858 (w), 786 (w), 763 (w), 730 (s), 698 (s), 611 (w); HRMS (MALDI-TOF): *m/z* [M+Na]$^+$ calcd. for $C_{29}H_{34}N_6Na$: 489.2737; found: 489.2707.

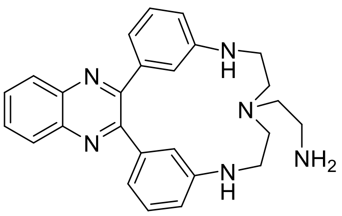
**12,13,14,15,16,17,18,19,20,21,22,23-Dodecahydro-11*H*-10.6:28.24-dimetheno[1,4,7,10,13]**



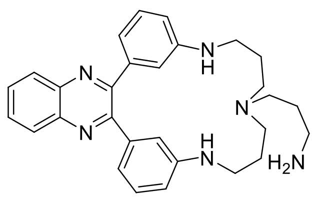

**pentaazacyclopentacosino[19,20-*b*]quinoxaline ($N_5C_8Q$)** was synthesized according to the general procedure from 2,3-bis(3-bromophenyl)quinoxaline (132 mg, 0.3 mmol) and *N*[1]-(2-aminoethyl)-*N*[2]-(2-((2-aminoethyl)amino)ethyl)ethane-1,2-diamine ($N_5C_8$) (57 mg, 0.3 mmol) in dioxane (15 mL), in the presence Pd(dba)$_2$ (14 mg, 8 mol%), PhPF-*t*Bu (15 mg, 9 mol%) and *t*BuONa (86 mg, 0.9 mmol). The product was eluted with $CH_2Cl_2$–MeOH–$NH_3$(aq.) (100:20:1 v/v/v) mixture. Yield 20 mg (14%), yellow glassy solid. $^1$H NMR (400 MHz, $CDCl_3$–$CD_3OD$ (1 : 1 v/v)): $\delta$ = 2.88–2.91 (m, 4H, CH$_2$N), 3.00–3.03 (m, 4H, CH$_2$N), 3.07–3.10 (m, 4H, CH$_2$N), 3.32 (t, *J* = 5.6 Hz, 4H, C$\underline{H_2}$NHAr), 6.59 (d, *J* = 7.8 Hz, 2H, H4

(Ph)), 6.63 (d, $J$ = 7.6 Hz, 2H, H6 (Ph)), 6.68 (s, 2H, H2 (Ph)), 6.93 (t, $J$ = 7.8 Hz, 2H, H5 (Ph)), 7.59–7.63 (m, 2H, H6, H7 (Q)), 7.93–7.97 (m, 2H, H5, H8 (Q)), the signals of NH-protons were not observed; $^{13}$C NMR (400 MHz, $CDCl_3$–$CD_3OD$ (1:1 v/v)): $\delta$ = 40.0 (2C, $CH_2N$), 44.0 (2C, $CH_2N$), 46.2 (2C, $CH_2N$), 46.6 (2C, $CH_2N$), 113.9 (2C), 114.2 (2C), 118.8 (2C), 128.2 (2C), 128.7 (2C), 129.9 (2C), 139.4 (2C), 140.4 (2C), 146.9 (2C), 154.4 (2C); IR (neat): $\nu_{max}$ (cm$^{-1}$) 3346 (w), 2957 (w), 2918 (w), 2850 (w), 1734 (w), 1722 (vw), 1653 (m), 1603 (s), 1586 (m), 1559 (m), 1540 (m), 1522 (w), 1464 (m), 1436 (m), 1394 (m), 1346 (s), 1275 (m), 1261 (s), 1204 (m), 1167 (w), 1125 (m), 1061 (m), 1030 (w), 990 (w), 916 (w), 860 (w), 764 (s), 751 (s), 701 (m), 669 (w); HRMS (MALDI-TOF): *m/z* [M+Na]$^+$ calcd. for $C_{28}H_{33}N_7Na$: 490.2690; found: 490.2655.

**2-(12,13,16,17-Tetrahydro-11*H*-10,6:22,18-dimetheno[1,4,7]triazacyclononadecino[13,14-*b*]quinoxalin-14(15*H*)-yl)ethanamine[2-(12,13,16,17-tetrahydro-11*H*-10,6:22,18-dimetheno[1,4,7]triazacyclononadecino[13,14-*b*]quinoxalin-14(15*H*)-yl)ethyl]amine (*pa*-$N_4C_6Q$)** was synthesized according to the general procedure from 2,3-bis(3-bromophenyl)quinoxaline (132 mg, 0.3 mmol) and $N^1$,$N^1$-bis(2-aminoethyl)ethane-1,2-diamine (***pa*-$N_4C_6$**) (66 mg, 0.45 mmol) in dioxane (15 mL), in the presence Pd(dba)$_2$ (28 mg, 16 mol%), PhPF-*t*Bu (29 mg, 18 mol%) and *t*BuONa (86 mg, 0.9 mmol). The product was eluted with $CH_2Cl_2$–MeOH (5 : 1 v/v) mixture. Yield 97 mg (76%), yellow glassy substance. $^1$H NMR (400 MHz, DMSO-*d6*): $\delta$ = 2.52 (br. s, 4H, $CH_2N$), 2.70 (br. s, 2H, C$\underline{H}_2NH_2$), 2.88 (br. s, 2H, C$\underline{H}_2CH_2NH_2$), 2.94 (br. s, 4H, C$\underline{H}_2$NHAr), 3.34 (br. s, 2H, $NH_2$), 6.57 (br. d, $J_{obs}$ = 7.9 Hz, 2H, H4 (Ph)), 6.61 (br. d, $J_{obs}$ = 7.4 Hz, 2H, H6 (Ph)), 6.76 (br. s, 2H, H2 (Ph)), 7.02 (t, $J$ = 7.8 Hz, 2H, H5 (Ph)), 7.74 (br. s, 2H, NHAr), 7.83–7.87 (m, 2H, H6, H7 (Q)), 8.09–8.13 (m, 2H, H5, H8 (Q)), the signals of two NH-protons were not assigned because of overlapping; $^{13}$C NMR (400 MHz, DMSO-*d6*): $\delta$ = 37.2 (1C, $CH_2NH_2$), 41.7 (1C, $CH_2N$), 51.9 (4C, $CH_2$), 113.4 (2C), 113.7 (2C), 116.4 (2C), 128.6 (2C), 128.8 (2C), 130.1 (2C), 139.9 (2C), 140.2 (2C), 148.1 (2C), 154.6 (2C); IR (neat): $\nu_{max}$ (cm$^{-1}$) 3401 (w), 3343 (w), 3056 (w), 2954 (m), 2922 (m), 2852 (m), 1653 (w), 1602 (s), 1584 (s), 1560 (s), 1520 (m), 1485 (m), 1452 (s), 1436 (m), 1426 (s), 1395 (m), 1345 (s), 1293 (m), 1278 (m), 1259 (m), 1204 (m), 1159 (m), 1108 (m), 1058 (m), 1048 (m), 1008 (m), 991 (m), 930 (w), 870 (w), 854 (w), 824 (w), 783 (m), 763 (s), 750 (m), 700 (s), 669 (w), 612 (w); HRMS (MALDI-TOF): *m/z* [M+Na]$^+$ calcd. for $C_{26}H_{28}N_6Na$: 447.2268; found: 447.2242.



**3-(11,12,13,14,16,17,18,19-Octahydro-15*H*-10,6:24,20-dimetheno[1,5,9]triazacyclohenicosino [15,16-*b*]quinoxalin-15-yl)propan-1-amine[3-(11,12,13,14,16,17,18,19-octahydro-15*H*-10.6:24.20-dimetheno[1,5,9]triazacyclohenicosino-[15,16-*b*]quinoxalin-15-yl)propyl]amine (*pa*-$N_4C_9$Q)** was synthesized according to the general procedure from 2,3-bis(3-bromophenyl)quinoxaline (132 mg, 0.3 mmol) and $N^1$,$N^1$-bis(3-aminopropyl)propane-1,3-diamine (*pa*-$N_4C_9$) (85 mg, 0.45 mmol) in dioxane (15 mL), in the presence Pd(dba)$_2$ (28 mg, 16 mol%), PhPF-*t*Bu (29 mg, 18 mol%) and *t*BuONa (86 mg, 0.9 mmol). The product was eluted with $CH_2Cl_2$–MeOH–$NH_3$(aq.) (100 : 20 : 3 v/v/v) mixture. Yield 107 mg (77%), yellow glassy solid. $^1$H NMR (400 MHz, $CDCl_3$–$CD_3OD$ (10 : 1 v/v)) : $\delta$ = 1.57 (quint., 4H, $J$ = 6.5 Hz, C<u>H</u>$_2$CH$_2$NHAr), 1.66 (quint., $J$ = 6.6 Hz, 2H, C<u>H</u>$_2$CH$_2$NH$_2$), 2.40 (t, $J$ = 6.6 Hz, 4H, CH$_2$N), 2.47 (t, $J$ = 6.6 Hz, 2H, CH$_2$N), 2.81 (t, $J$ = 6.2 Hz, 2H, C<u>H</u>$_2$NH$_2$), 3.04 (t, $J$ = 6.2 Hz, 4H, C<u>H</u>$_2$NHAr), 4.03 (br. s, 4H, NH), 6.57 (d, $J$ = 7.9 Hz, 2H, H4 (Ph)), 6.60 (s, 2H, H2 (Ph)), 6.88 (d, $J$ = 8.0 Hz, 2H, H6 (Ph)), 7.13 (t, $J$ = 7.8 Hz, 2H, H5 (Ph)), 7.68–7.72 (m, 2H, H6, H7 (Q)), 8.11–8.16 (m, 2H, H5, H8 (Q)). $^{13}$C NMR (400 MHz, $CDCl_3$–$CD_3OD$ (10:1 v/v)): $\delta$ = 25.1 (3C, <u>C</u>H$_2$CH$_2$N), 40.3 (1C, CH$_2$NH$_2$), 42.3 (2C, CH$_2$NHAr), 51.5 (2C, CH$_2$N), 53.2 (1C, CH$_2$N), 113.9 (2C), 114.1 (2C), 118.3 (2C), 129.1 (2C), 129.3 (2C), 129.7 (2C), 140.1 (2C), 140.9 (2C), 147.5 (2C), 154.5 (2C); IR (neat): $\nu_{max}$ (cm$^{-1}$) 3409 (w), 3301 (w), 3043 (w), 2925 (m), 2853 (w), 2818 (w), 1602 (s), 1584 (m), 1512 (m), 1471 (m), 1431 (m), 1391 (w), 1375 (w), 1345 (m), 1263 (m), 1202 (w), 1165 (w), 1111 (w), 1060 (w), 1012 (w), 990 (w), 957 (vw), 925 (w), 855 (w), 782 (m), 762 (m), 731 (s), 701 (s), 614 (w); HRMS (MALDI-TOF): *m/z* [M+Na]$^+$ calcd. for $C_{29}H_{34}N_6Na$: 489.2737; found: 489.2717.




**Cu-catalyzed synthesis of $N_2C_6O_3$Q.** In a two-necked flask, equipped with a magnetic stirrer and a reflux condenser, 2,3-bis(3-bromophenyl)quinoxaline (132 mg, 0.3 mmol) and CuI (12 mg, 20 mol%) were added. The flask was filled with argon. Dry DMF (2 mL) and 2-isobutyrylcyclohexanone (20 mg, 40 mol%) were added into the flask in a flow of dry argon. After stirring for 2–3 min, 0.3 mmol of $N_2C_6O_2$ (45 mg, 0.3 mmol) and cesium carbonate (391 mg, 1.2 mmol) were added and the reaction mixture was refluxed for 30 h under argon atmosphere. Upon completion of the reaction, the reaction mixture was diluted with $CH_2Cl_2$ (*ca.* 20 mL), the precipitate was separated by filtration, washed with dichloromethane and the combined filtrates were washed with $H_2O$ (10 mL), the water layer was also extracted with $CH_2Cl_2$. The organic phases were combined, dried over 3Å sieves and the concentrated under reduced pressure, the resulting residue was chromatographed on silica gel using the sequence of eluents $CH_2Cl_2$, $CH_2Cl_2$–MeOH (50:1–5:1 v/v). The product was eluted with $CH_2Cl_2$–MeOH (50 : 1 v/v) mixture. Yield 21 mg (16%), yellow glassy solid. The spectroscopic data of the obtained product were in agreement with those reported above.

## 3. DFT computations of the macrocyclization reaction

The structure of complexes was modeled by DFT calculations using the Firefly quantum chemistry package,[4] which is partially based on the GAMESS (US)[5] source code. The calculations were performed using the B3LYP functional with the 6-31G(d,p) basis set for all elements, at each step full optimization of geometry was achieved, and the minima were confirmed by computation of vibration frequencies. The optimized structures details are given in section 9.

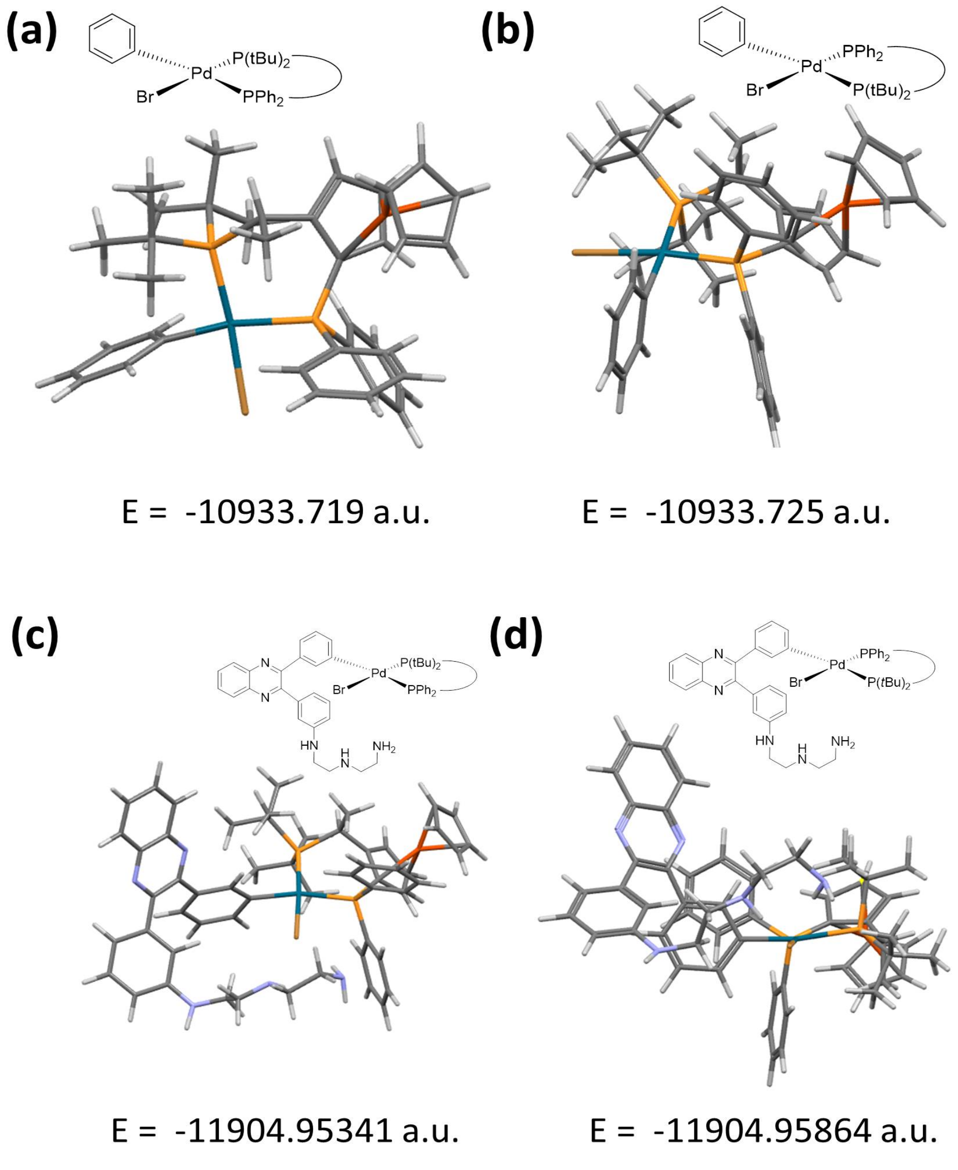



**Fig. S1.** DFT-optimized geometries of two isomers of (PhPF-*t*Bu)Pd(Ph)(Br) (a and b) and intermediate complex **A** (c and d). Color code for the atoms: C (dark grey), H (light grey), N (blue), P (yellow), Pd (blue-green), Fe (orange-red), Br (yellow-grey).

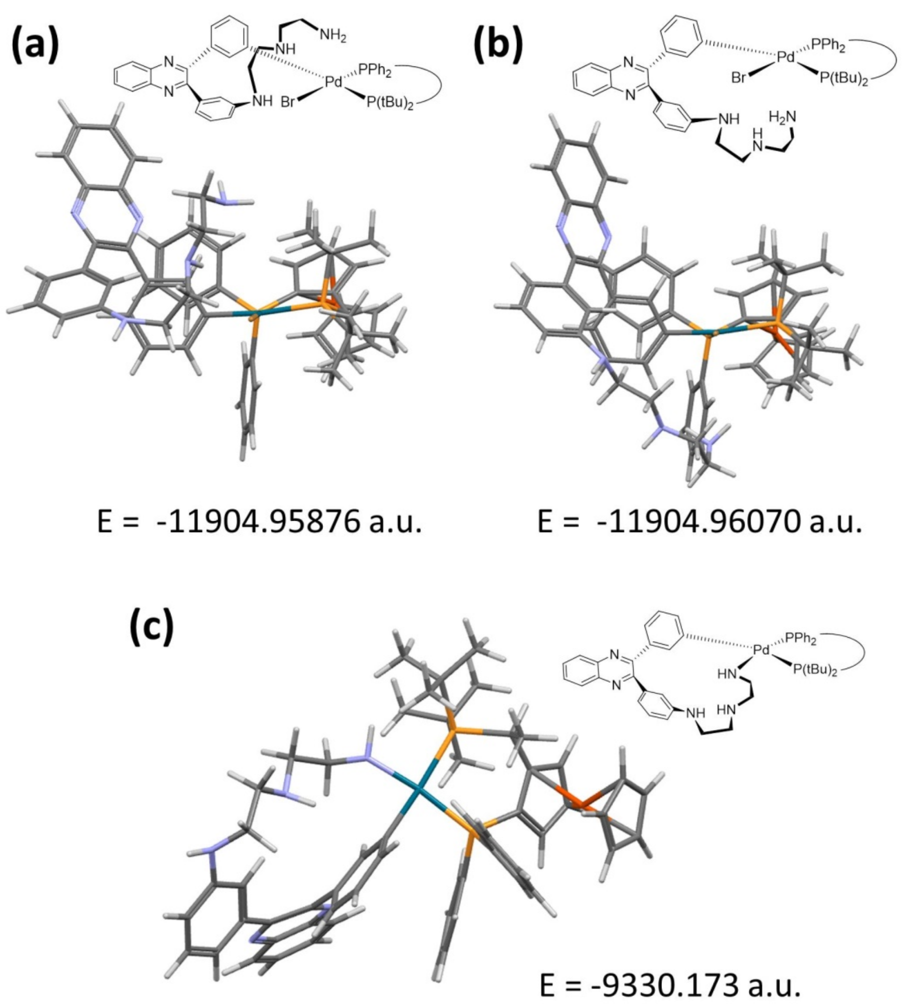



**Fig. S2.** DFT-optimized geometries of two isomers of intermediate complex **D** (a and b) and complex **E** (c). Color code for the atoms: C (dark grey), H (light grey), N (blue), P (yellow), Pd (blue-green), Fe (orange-red).

## 4. Photophysical studies in solution employing spectroscopic techniques and DFT computations

*Spectroscopic studies of macrocycles $N_2C_nO_xQ$ and $N_xC_nQ$.*

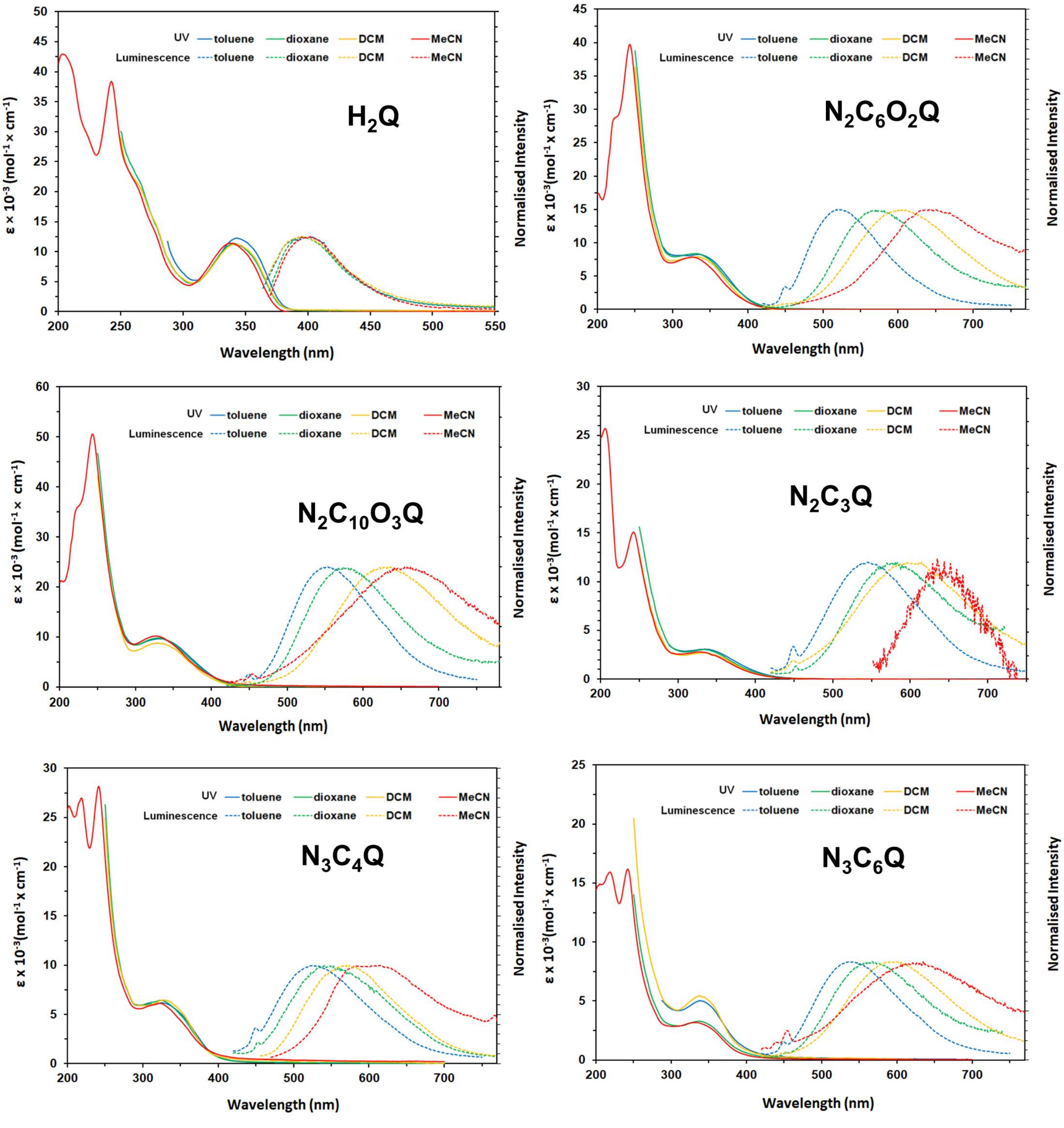



**Fig. S3.** Electronic absorbance (solid lines) and PL (dashed lines, $\lambda_{ex}$ = 395 nm) spectra of 2,3-diphenylquinoxaline ($H_2Q$, $\lambda_{ex}$ = 320 nm) and macrocycles $N_2C_3Q$, $N_2C_{10}O_3Q$, $N_3C_4Q$ and $N_3C_6Q$ in toluene (blue), dioxane (green), dichloromethane (yellow) and acetonitrile (red).

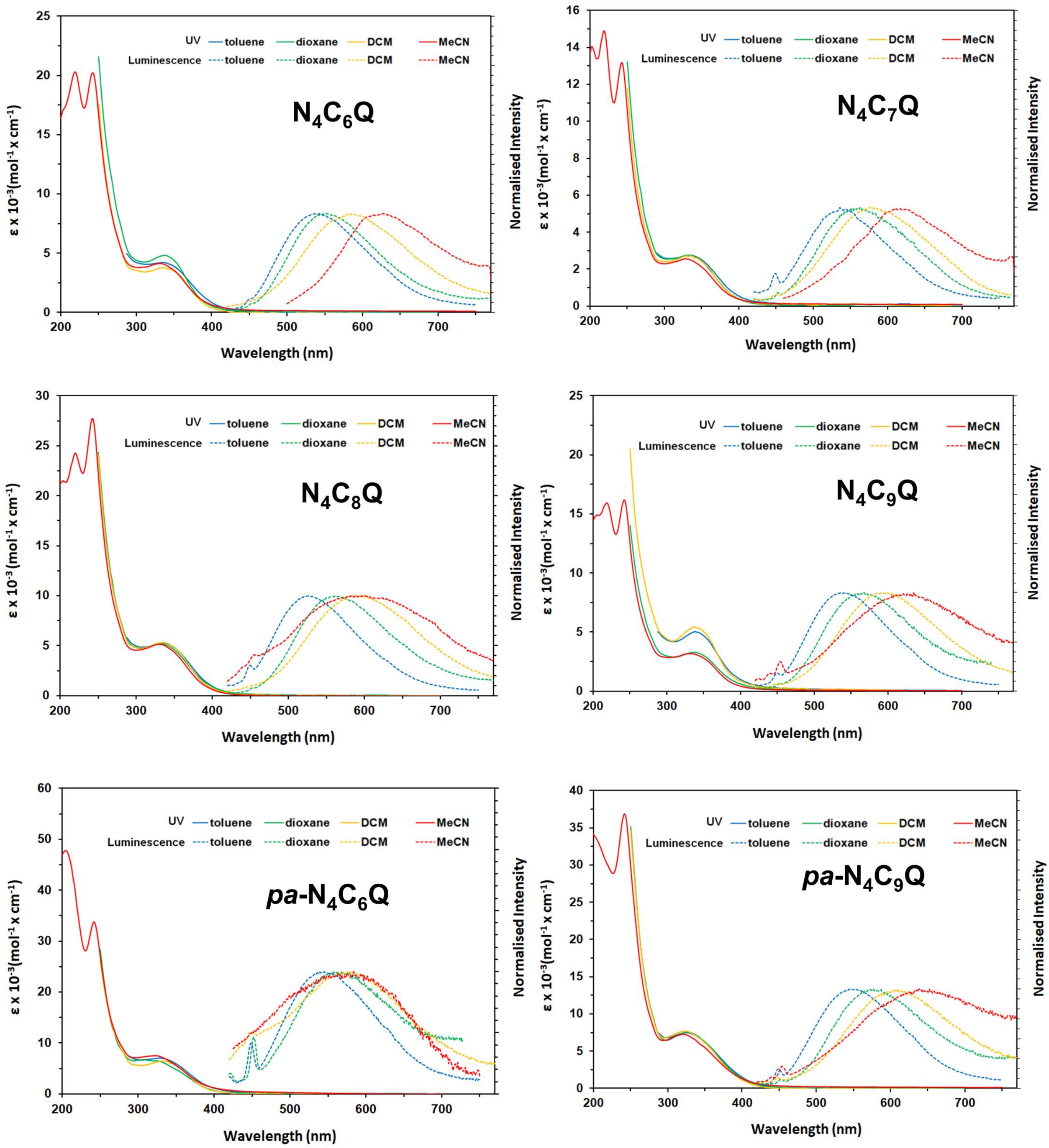



**Fig. S4.** Electronic absorbance (solid lines) and luminescence (dashed lines, $\lambda_{ex}$ = 395 nm) spectra of macrocycles $N_4C_6Q$, $N_4C_7Q$, $N_4C_8Q$, $N_4C_9Q$, *pa*-$N_4C_6Q$ and *pa*-$N_4C_9Q$ in toluene (blue), dioxane (green), dichloromethane (yellow) and acetonitrile (red).

**Table S1.** UV–vis absorption and photoluminescence of macrocycles $N_2C_nO_xQ$ and $N_xC_nQ$ in different organic solvents.

| Compound | Solvent | $\lambda_{abs}$ (nm) ($\varepsilon \times 10^{-3}$ ($M^{-1}$ $cm^{-1}$)) | $\lambda_{em}$ (nm)[a] |
|---|---|---|---|
| $H_2Q$ | MeCN | 204 (42.8), 242 (38.3), 338 (11.3) | 398 |
| | DCM | 341 (11.3) | 395 |
| | Dioxane | 341 (12.2) | 396 |
| | Toluene | 343 (12.3) | 395 |
| $N_2C_6O_2Q$ | MeCN | 227 (29.0), 243 (39.8), 325 (7.9) | 650 |
| | DCM | 333 (8.8) | 603 |
| | Dioxane | 330 (8.4) | 571 |
| | Toluene | 335 (8.3) | 522 |
| $N_2C_{10}O_3Q$ | MeCN | 224 (36.0), 244 (50.6), 326 (10.2) | 655 |
| | DCM | 329 (8.8) | 625 |
| | Dioxane | 330 (9.8) | 574 |
| | Toluene | 331 (9.6) | 554 |
| $N_2C_3Q$ | MeCN | 206 (25.7), 243 (15.1), 328 (2.6) | 635 |
| | DCM | 332 (2.8) | 602 |
| | Dioxane | 334 (3.1) | 581 |
| | Toluene | 335 (3.2) | 545 |
| $N_3C_4Q$ | MeCN | 202 (26.2), 242 (28.2), 321 (6.1) | 576 |
| | DCM | 328 (6.5) | 571 |
| | Dioxane | 324 (6.4) | 541 |
| | Toluene | 326 (6.2) | 526 |
| $N_3C_6Q$ | MeCN | 205 (14.9), 242 (16.2), 332 (3.2) | 635 |
| | DCM | 338 (5.4) | 597 |
| | Dioxane | 336 (3.3) | 567 |
| | Toluene | 338 (5.0) | 536 |
| $N_4C_6Q$ | MeCN | 219 (20.3), 242 (20.2), 329 (4.1) | 615 |
| | DCM | 337 (3.8) | 585 |
| | Dioxane | 338 (4.9) | 551 |
| | Toluene | 335 (4.3) | 543 |
| $N_4C_7Q$ | MeCN | 203 (14.1), 219 (14.9), 243 (13.2), 328 (2.6) | 617 |
| | DCM | 334 (2.8) | 577 |
| | Dioxane | 334 (2.6) | 563 |
| | Toluene | 335 (2.7) | 536 |
| $N_4C_8Q$ | MeCN | 220 (24.3), 243 (27.8), 329 (5.1) | 604 |
| | DCM | 335 (5.3) | 592 |
| | Dioxane | 333 (5.2) | 562 |
| | Toluene | 335 (5.3) | 527 |
| $N_4C_9Q$ | MeCN | 221 (20.5), 243 (20.5), 334 (4.2) | 605 |
| | DCM | 337 (4.4) | 600 |
| | Dioxane | 336 (4.4) | 569 |
| | Toluene | 337 (4.4) | 546 |
| *pa*-$N_4C_9Q$ | MeCN | 242 (37.0), 321 (7.3) | 648 |
| | DCM | 323 (7.7) | 609 |
| | Dioxane | 326 (7.5) | 577 |
| | Toluene | 324 (7.5) | 545 |
| *pa*-$N_4C_6Q$ | MeCN | 204 (47.8), 242 (33.8), 322 (7.5) | 584 |
| | DCM | 334 (7.4) | 578 |
| | Dioxane | 308 (7.6) | 563 |
| | Toluene | 328 (7.0) | 545 |

[a] $\lambda_{ex}$ = 320 nm for $H_2Q$ and *pa*-$N_4C_9Q$; 330 nm for $N_2C_{10}O_3Q$, $N_2C_6O_2Q$, $N_4C_9Q$, *pa*-$N_4C_6Q$, $N_4C_7Q$, $N_4C_8Q$, $N_3C_4Q$; 335 nm for $N_4C_6Q$; 340 nm for $N_3C_4Q$, $N_3C_6Q$.

*DFT computations of rotamers and rotation barriers in model compound $N_2Q$ and macrocycles $N_2C_nO_xQ$ and $N_xC_nQ$.*

The structures were modeled by DFT calculations using the Firefly quantum chemistry package,[4] which is partially based on the GAMESS (US)[5] source code. The calculations were performed using the B3LYP functional with the 6-31G(d,p) basis set for all elements, at each step full optimization of geometry was achieved. The atomic coordinates obtained by the computations are presented in Section 10 of the ESI.

The dihedral angle formed by the quinoxaline scaffold and the phenyl ring ($\Theta_1$) was fixed, and the geometry of the molecule was optimized. The calculations were repeated, systematically changing the value of $\Theta_1$ to obtain 1) the dihedral angle formed by the quinoxaline scaffold and the second phenyl ring ($\Theta_2$); 2) a rotamers relative energy diagram as a function of the dihedral angle $\Theta_1$; 3) the rotation barriers in the macrocycles. In the preliminary step of this study, the relative conformation energy diagram of 1,2-bis(3-aminophenyl)quinoxaline ($N_2Q$) was elucidated to validate this computational approach.

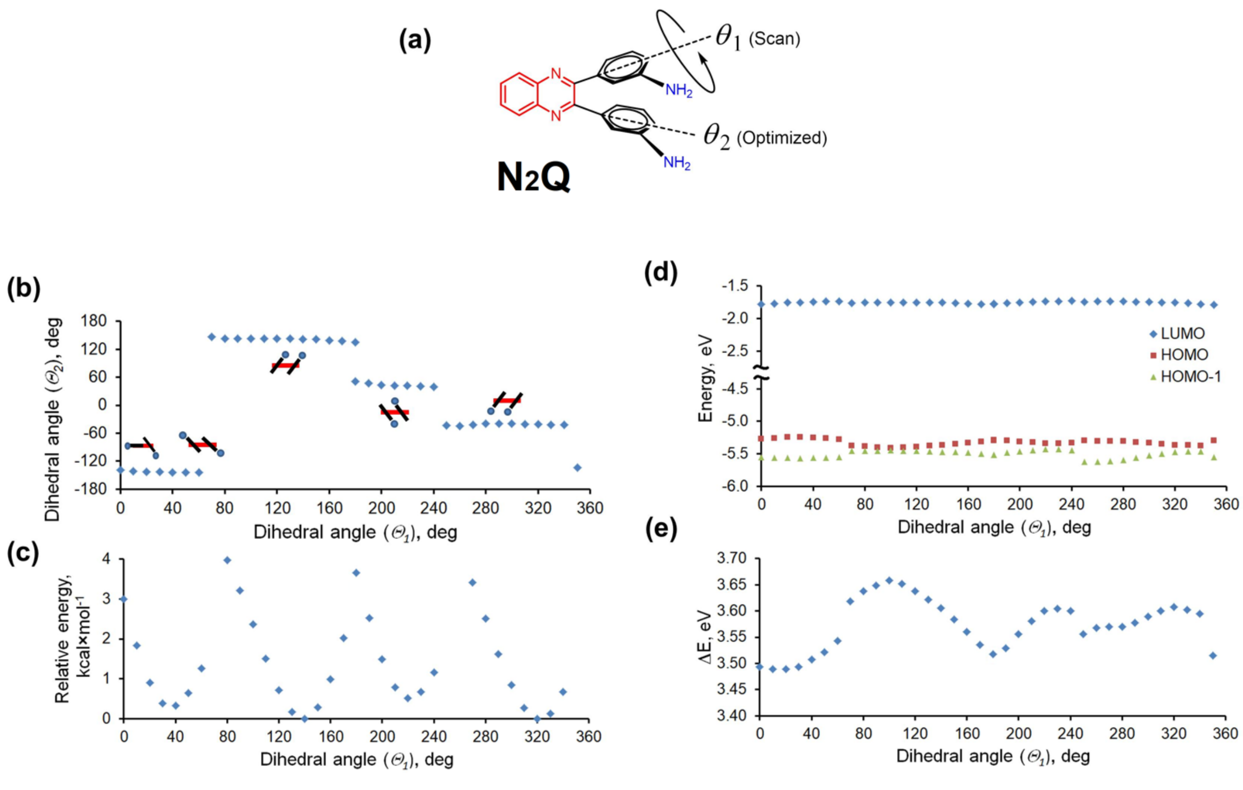



**Fig. S5**. Results of DFT calculations of 1,2-bis(3-aminophenyl)quinoxaline ($N_2Q$) molecules by geometry optimization with varying dihedral angle $\Theta_1$ shown on (a): (a) structure showing the rotation axes of aryl substituents relative to quinoxaline residue. (b) DFT-optimized values of dihedral angle $\Theta_2$ (color coding for schematic representation of the rotamers obtained is as such: quinoxaline plane (red line); phenyl plane (black line), the amino group positions (blue points)); (c) full energies of the optimized structures vs dihedral angle $\Theta_1$ being fixed; (d) energies of the $HOMO_{-1}$, HOMO and LUMO levels, and (e) the HOMO-LUMO energy gap.

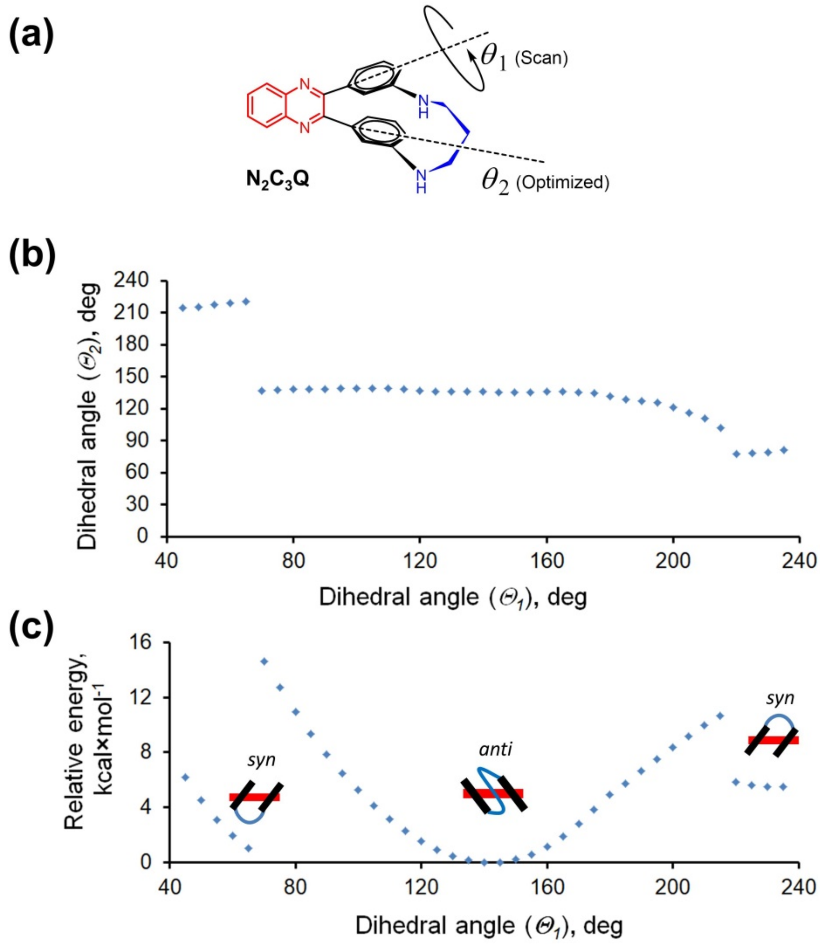



**Fig. S6**. Results of DFT calculations of $N_2C_3Q$ molecules by geometry optimization with varying dihedral angle $\Theta_1$ shown on (a): (a) structure showing the rotation axes of aryl substituents relative to quinoxaline residue. (b) DFT-optimized values of dihedral angle $\Theta_2$ (color coding for schematic representation of the rotamers obtained is as such: quinoxaline plane (red line); phenyl plane (black line), the amino group positions (blue points)); (c) full energies of the optimized structures vs dihedral angle $\Theta_1$ being fixed.

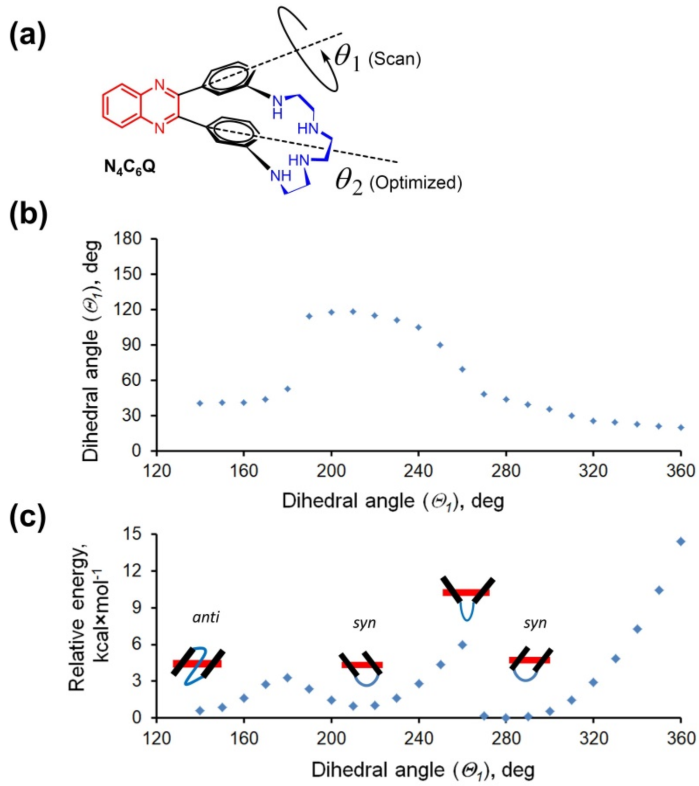



**Fig. S7.** Results of DFT calculations of $N_4C_6Q$ molecules by geometry optimization with varying dihedral angle $\Theta_1$ shown on (a): (a) structure showing the rotation axes of aryl substituents relative to quinoxaline residue. (b) DFT-optimized values of dihedral angle $\Theta_2$ (color coding for schematic representation of the rotamers obtained is as such: quinoxaline plane (red line); phenyl plane (black line), the amino group positions (blue points)); (c) full energies of the optimized structures vs dihedral angle $\Theta_1$ being fixed.

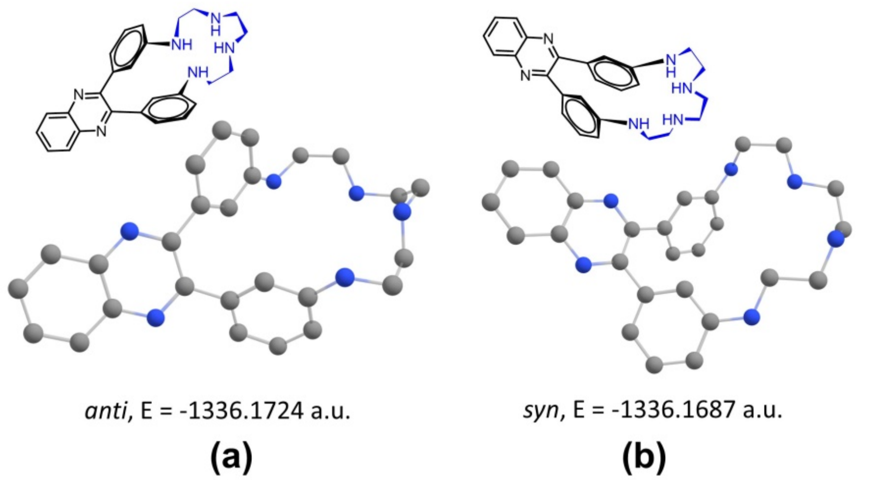



**Fig. S8.** DFT-optimized geometries for *anti*- (a) and *syn*- (b) rotamers of the $N_4C_6Q$.

**Table S2.** Selected parameters of DFT-optimized structures of macrocycles $N_2C_3Q$, $N_3C_4Q$, $N_4C_6Q$, $N_2C_6O_2Q$ and $N_2C_{10}O_3Q$ and experimental value of maxima of emission band in $CH_2Cl_2$.

| Macrocycle | Rotamer | Dihedral angle (deg) | | Orbitals energy (eV) | | | ΔE (eV) | $\lambda_{em}$ (nm)[a] |
|---|---|---|---|---|---|---|---|---|
| | | $\Theta_1$ | $\Theta_2$ | LUMO | HOMO | $HOMO_{-1}$ | | |
| $N_2C_3Q$ | *syn* | 99.3 | 54.5 | –2.00 | –5.53 | –6.01 | 3.53 | 602 |
| | *anti* | 42.6 | 40.6 | –2.04 | –5.43 | –5.67 | 3.39 | |
| $N_3C_4Q$ | *syn* | 67.5 | 28.4 | –1.70 | –5.08 | –5.36 | 3.38 | 571 |
| | *anti* | 45.1 | 36.0 | –1.71 | –5.12 | –5.29 | 3.41 | |
| $N_4C_6Q$ | *syn* | 47.1 | 37.3 | –1.64 | –5.05 | –5.17 | 3.41 | 585 |
| | *anti* | 40.9 | 39.9 | –1.64 | –5.06 | –5.17 | 3.42 | |
| $N_2C_6O_2Q$ | *syn* | 52.4 | 40.8 | –1.65 | –5.15 | –5.21 | 3.50 | 603 |
| | *anti* | 48.2 | 46.9 | –1.70 | –5.13 | –5.94 | 3.43 | |
| $N_2C_{10}O_3Q$ | *syn* | 44.9 | 40.6 | –1.75 | –5.17 | –5.35 | 3.42 | 635 |
| | *anti* | 49.4 | 40.6 | –1.73 | –5.16 | –5.25 | 3.43 | |

[a] Emission maxima in $CH_2Cl_2$, $\lambda_{ex}$ = 395 nm.

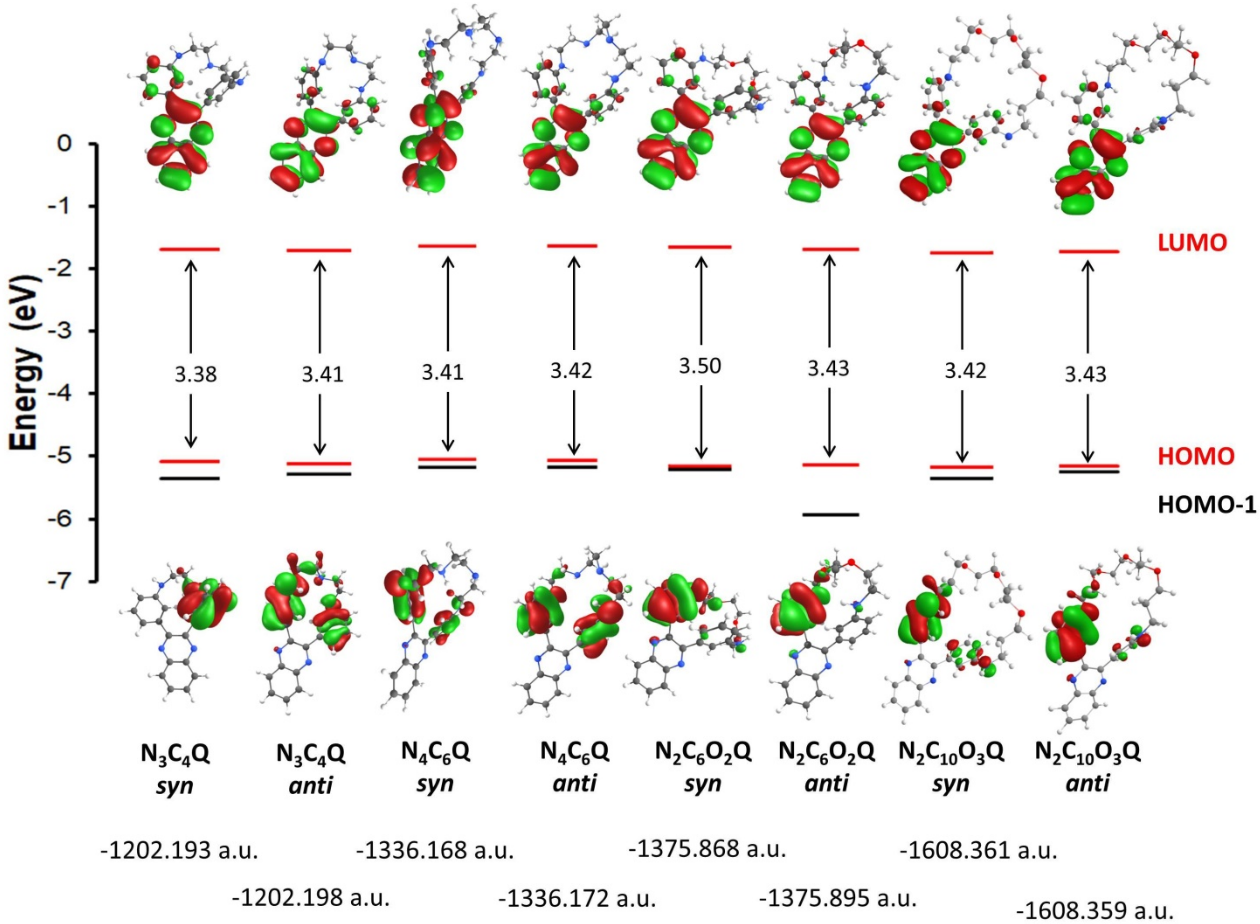



**Fig. S9.** Calculated isodensity plot of the LUMO, HOMO and HOMO$_{-1}$ orbitales for $N_2C_3Q$, $N_3C_4Q$, $N_4C_6Q$, $N_2C_6O_2Q$ and $N_2C_{10}O_3Q$ in *syn*- and *anti*-rotamers.

**Table S3.** Relative energies of DFT-optimized structures of macrocycles $N_2C_3Q$, $N_3C_4Q$, $N_4C_6Q$, $N_2C_6O_2Q$ and $N_2C_{10}O_3Q$.

| **Macrocycle** | **Rotamer** | **Relative energy (a.u.)** |
|---|---|---|
| $N_2C_3Q$ | *syn* | –1107.765 |
| | *anti* | –1107.773 |
| $N_3C_4Q$ | *syn* | –1202.193 |
| | *anti* | –1202.198 |
| $N_4C_6Q$ | *syn* | –1336.169 |
| | *anti* | –1336.172 |
| $N_2C_6O_2Q$ | *syn* | –1375.868 |
| | *anti* | –1375.895 |
| $N_2C_{10}O_3Q$ | *syn* | –1608.361 |
| | *anti* | –1608.359 |

## 5. Studies of aggregation-induced emission

*Preparation of nano-aggregates*

A solution of the ligand was prepared dissolving 0.008 mmol of the ligand in $CH_2Cl_2$ in a 5 mL volumetric flask. A $CH_2Cl_2$–hexane mixture (3 mL) with appropriate hexane fraction ($f_w$) was placed in a quartz fluorimeter cuvette, closed with a cap and stirred at room temperature. A solution of the macrocycle (30 μL) was added in this cuvette using a syringe. After 1 minute, the stirring was stopped, and the PL spectra were recorded ($\lambda_{ex}$ = 380 nm).

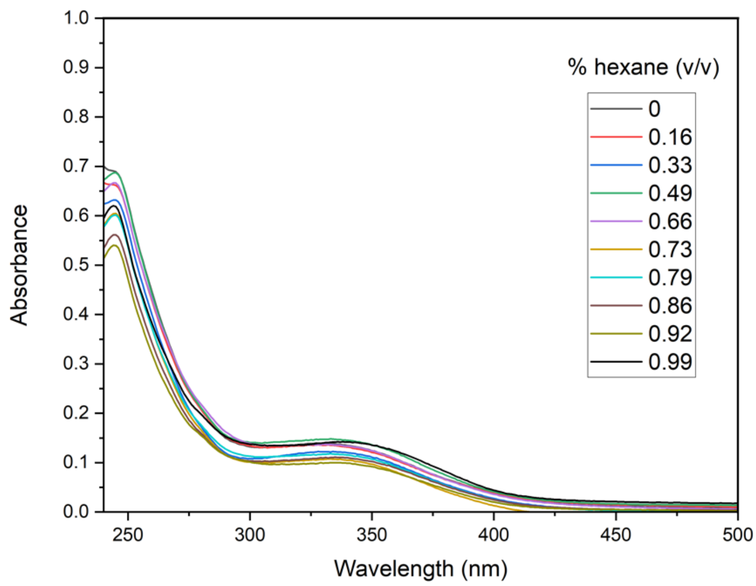
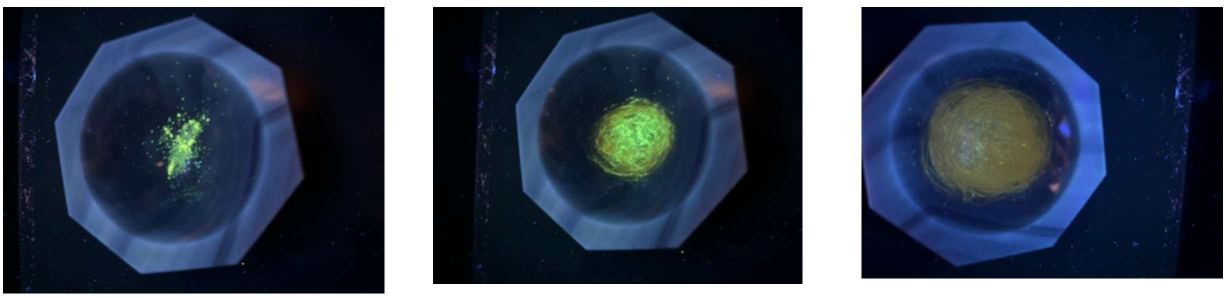
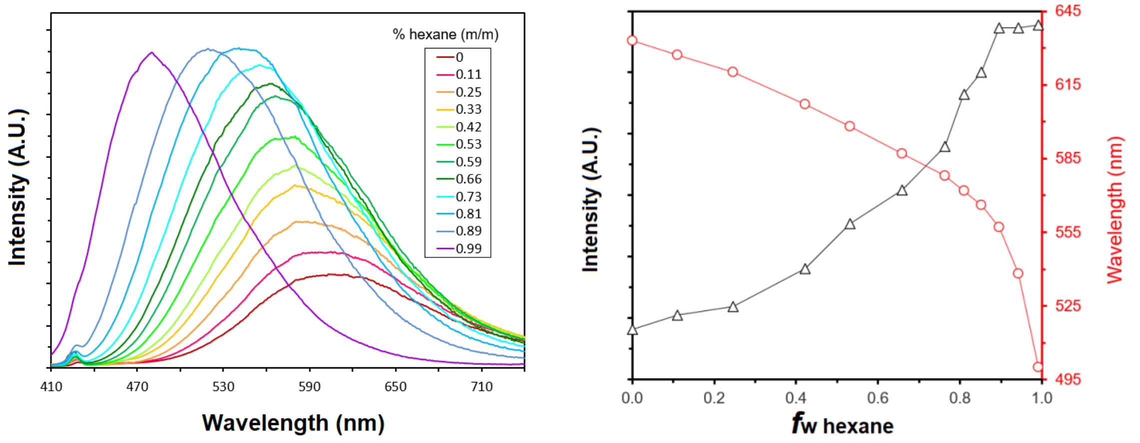



**Fig. S10.** UV–vis spectra of $N_2C_{10}O_3Q$ in $CH_2Cl_2$–hexane mixtures.



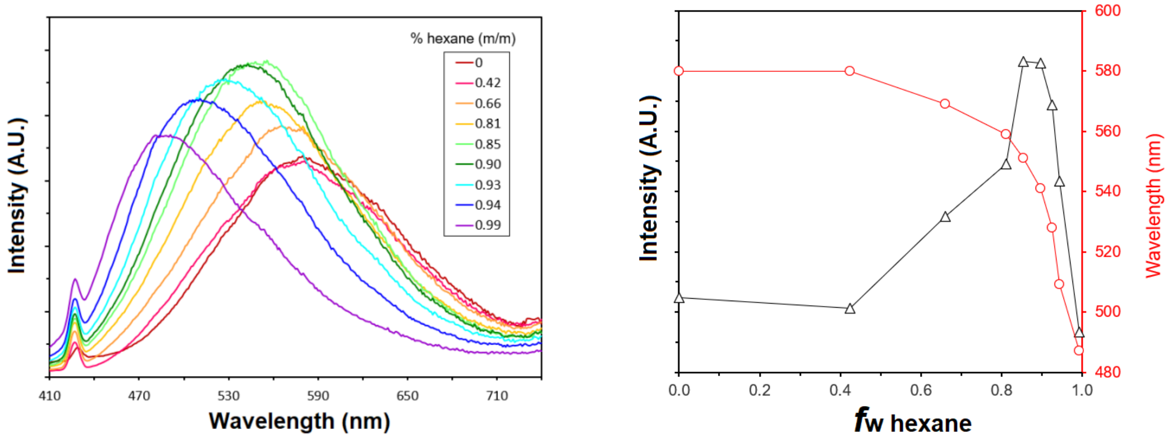
**(a)** **(b)** **(c)**

**Fig S11.** Images of the $N_2O_{10}O_3Q$ crystals: (a) before and (b and c) during grinding under a 365 nm UV lamp.




**(a)** **(b)**

**Fig. S12.** (a) Emission spectra of $N_2C_8O_3Q$ in $CH_2Cl_2$–hexane mixtures. (b) Evolution of the maximum and intensity of emission for $N_2C_8O_3Q$ with the composition of the solvent mixture.




**(a)** **(b)**

**Fig. S13.** (a) Emission spectra of $N_2C_3Q$ in $CH_2Cl_2$–hexane mixtures. (a) Change of the position of the maximum of the emission band and its intensity for $N_2C_3Q$ with the composition of the solvent mixtures.

## 6. Single crystal X-ray analysis of $N_2C_8O_3Q$

Yellow greenish (clear green under a 365 nm diode, Fig. S38) needle-shaped crystals of $N_2C_8O_3Q$ suitable for single crystal X-ray diffraction analysis were obtained by slow diffusion of toluene to a solution of $N_2C_8O_3Q$ in $CH_2Cl_2$ at 4 °C. SCXRD analysis of $N_2C_8O_3Q$ was carried out on a Bruker D8 Quest diffractometer (Mo$K\alpha$ radiation, $\omega$ and $\varphi$-scan mode), the crystal data and refinement parameters are listed in Table S5. The structures were solved with direct methods and refined by least-squares method in the full-matrix anisotropic approximation on $F^2$. All hydrogens at carbon atoms were located in calculated positions and refined freely, and hydrogens at nitrogen atoms were localized from electron density difference map and refined freely. The asymmetric unit of the crystal contains one molecule of $N_2C_8O_3Q$ (Fig. S15). Two carbon atoms of the $C_8O_3$ fragment are disordered over two positions with occupancies of 0.7/0.3. All calculations were performed using the SHELXTL[7, 8] and Olex2[9] software packages. Atomic coordinates, bond lengths, angles, and thermal parameters have been deposited at the Cambridge Crystallographic Data Centre with deposition number CCDC 2312920, which are available free of charge at www.ccdc.cam.ac.uk.

**Table S4.** Crystal data and refinement parameters for macrocycle $N_2C_8O_3Q$.

| | |
|---|---|
| Molecular Formula | $C_{28}H_{30}N_4O_3$ |
| M | 470.56 |
| Temperature, K | 100(2) |
| System | Monoclinic |
| Space group | $P2_1/c$ |
| $a$, Å | 13.6697(5) |
| $b$, Å | 10.2676(4) |
| $c$, Å | 18.2714(7) |
| $\beta$, deg. | 109.3910(10) |
| $V$, Å$^3$ | 2419.01(16) |
| $Z$, $Z'$ | 4, 1 |
| $\rho_{calc}$, g/cm$^3$ | 1.292 |
| μ(Mo$K_\alpha$), mm$^{-1}$ | 0.085 |
| $F$(000) | 1000 |
| $\theta_{min}$–$\theta_{max}$, deg. | 1.579–30.585 |
| Number of measured reflections | 39741 |
| Number of unique reflections ($R_{int}$) | 7421 (0.0640) |
| Number of reflections with $I > 2\sigma(I)$ | 5697 |
| Number of refined parameters | 342 |
| $R$-factors ($I > 2\sigma(I)$) | $R_1 = 0.0585$<br>$\omega R_2 = 0.1528$ |
| $R$-factors (all reflections) | $R_1 = 0.0746$<br>$\omega R_2 = 0.1669$ |
| GOOF | 1.063 |
| $\Delta\rho_{max}$ / $\Delta\rho_{min}$, $e$/Å$^3$ | 0.643/–0.552 |

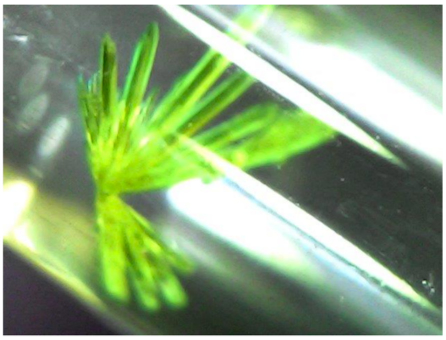
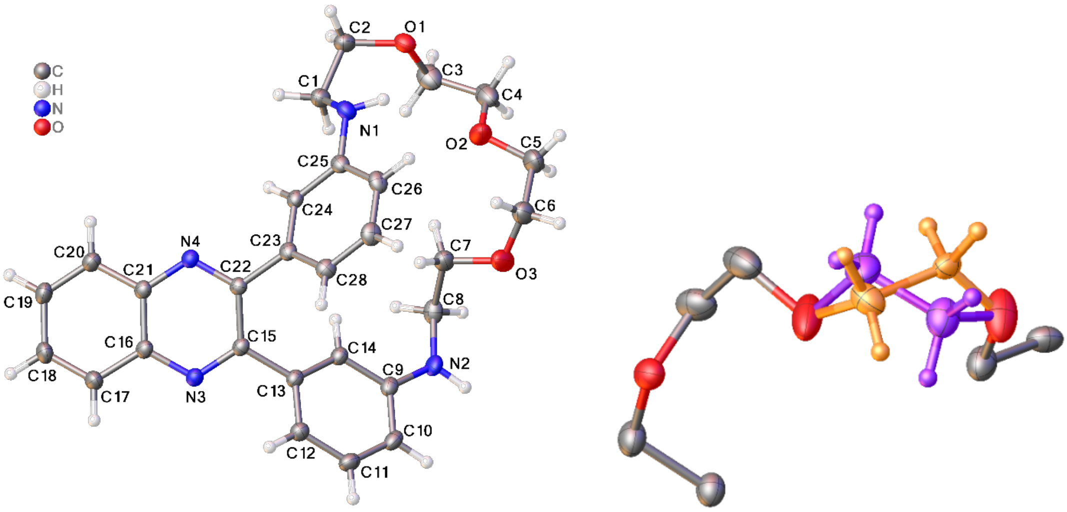
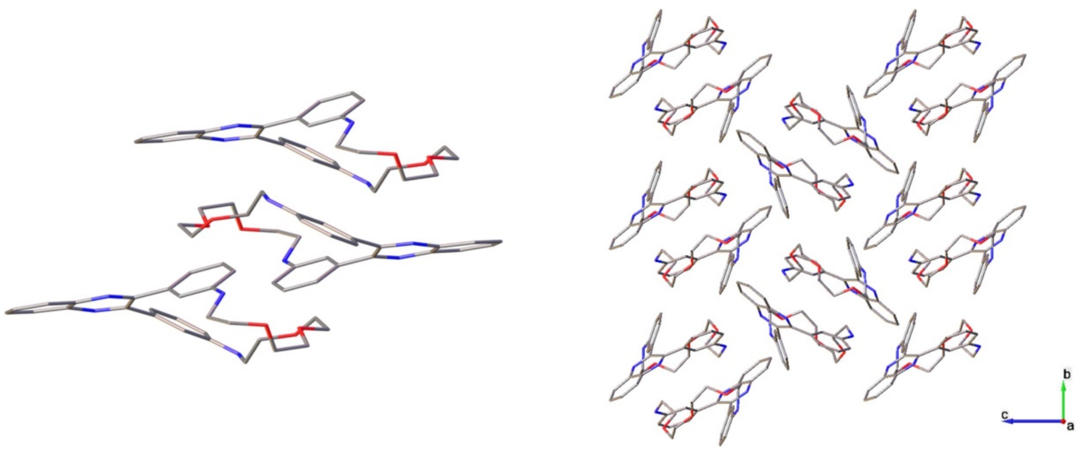


**Fig. S14**. Image of crystals of $N_2C_8O_3Q$ under a 365 nm UV lamp.




**(a)** **(b)**

**Fig. S15**. **(a)** General view of $N_2C_8O_3Q$ (left). Thermal ellipsoids of atomic displacement are shown at 50% probability. Disordered fragments were omitted for clarity; **(b)** view of the positional disorder of the $C_8O_3$ fragment in $N_2C_8O_3Q$. Non-disordered hydrogen atoms were omitted for clarity. Purple-colored illustrates the 70% occupied site of the disordered carbon and hydrogen atoms, and orange-colored atoms represents the 30% occupied site of the same carbon and hydrogen atoms. All thermal ellipsoids of atomic displacement are shown at 50% probability.




**(a)** **(b)**

**Fig. S16**. **(a)** General view packing in the crystal of $N_2C_8O_3Q$; **(b)** general view packing of $N_2C_8O_3Q$ in the crystal along the crystallographic axis. Thermal ellipsoids of atomic displacement, disordered fragments and hydrogen atoms are omitted for clarity.

## 7. Preparation of pH-sensitive paper test strips

The test strips were prepared by immersing cellulose filter paper ("Belaya lenta" Bashkhimservice, Ufa, Russia, with 8–12 μm pore size, or Whatman filter paper, cat N 1005-070) into a $CH_2Cl_2$ solution of $N_2C_{10}O_3Q$ (0.1–1 mM) with subsequent drying in air for 15 min. The procedure was repeated 3–4 times to obtain test strips (TS 1') with an intense color visible to the naked eye in daylight and under a 365 nm UV lamp (Fig. 5 and S19).

In the next series of experiments, Whatman filter paper (cat N 1005-070) was coated with a thin film of PVA. Initially, a 5% aqueous solution of PVA was prepared, and the paper was immersed in this solution. After drying at 80 °C for 2 h, this support was immersed in a $CH_2Cl_2$ solution of $N_2C_{10}O_3Q$ (0.1–1 mM) and dried in air for 15 min. The dye deposition process was repeated 3–4 times to obtain test strips TS 1 (Fig. 5).

The same procedures were employed to prepare AIE-exhibiting test strips (TS 2' and TS 2), with the only exception being that the $CH_2Cl_2$ solution of the $N_2C_{10}O_3Q$ dye was replaced by a suspension of $N_2C_{10}O_3Q$ in a $CH_2Cl_2$–heptane solvent mixture ($f_w$ = 0.9). The test strips prepared on PVA-covered paper (TS 2) were utilized for pH measurements.

Initially, test strips TS 1 and TS 2 were consistently exposed to HCl and $NH_3$ vapors for 10 seconds to successfully observe the color change in acidic vapors and the regeneration of PL in the basic vapors.

Then, a series of aqueous solutions with pH 1.0–5.0 was prepared by adding concentrated HCl to deionized water. pH was measured using a portable Ecotest 2000 pH-meter with a combined ESK-10601/7 glass electrode (Econix, Moscow, Russia). The electrode was calibrated with commercial buffers (pH = 4.01, 6.86, and 9.18) before determining the pH of the studied solutions. The test strips were immersed in deionized water with different pH for 1 sec. The color of the paper immediately changed and was different, as shown in Fig. S19.

The regeneration experiments were performed using a solution with pH 1 and a closed vial filled with $NH_3$ vapors. The color regeneration of test strips TS 1 and TS 2 in the vial with $NH_3$ vapors was observed after 10 sec. Repeating the measurements and regeneration for 5 times, we observed the excellent stability of both pH indicators.

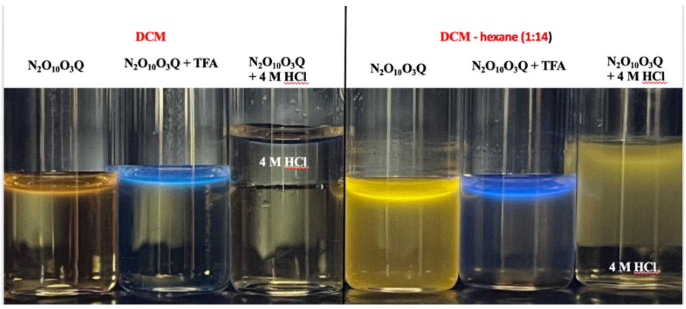



**Fig. S17.** Images of $N_2C_{10}O_3Q$ in $CH_2Cl_2$ (DCM) and $CH_2Cl_2$–hexane ($f_w$ = 0.9) solvent mixture under 365 nm UV lamp before and after addition of TFA and 4 M aqueous HCl.

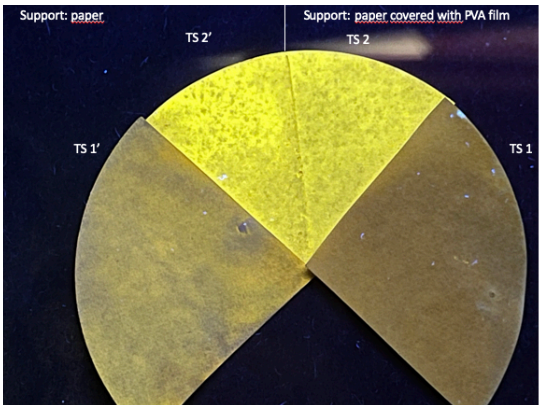



**Fig. S18**. Comparison of pH indicators prepared from the $N_2C_{10}O_3Q$ dyes using immersion of different paper supports in a $CH_2Cl_2$ solution (TS 1 and TS 1') and in a $CH_2Cl_2$–heptane solvent mixture (TS 2 and TS 2').

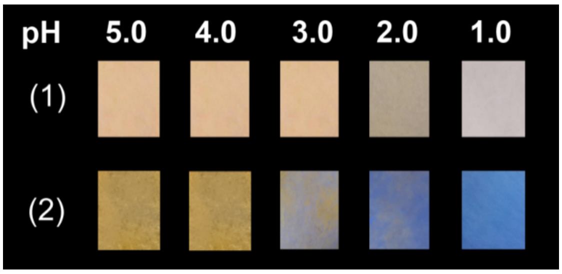



**Fig. S19**. Color changes of test strips TS 1 (1) in daylight and (2) under irradiation by LED ($\lambda$ = 365 nm) observed after immersion in aqueous solutions with different pH.

## 8. NMR and HR-mass spectra

*NMR spectra*

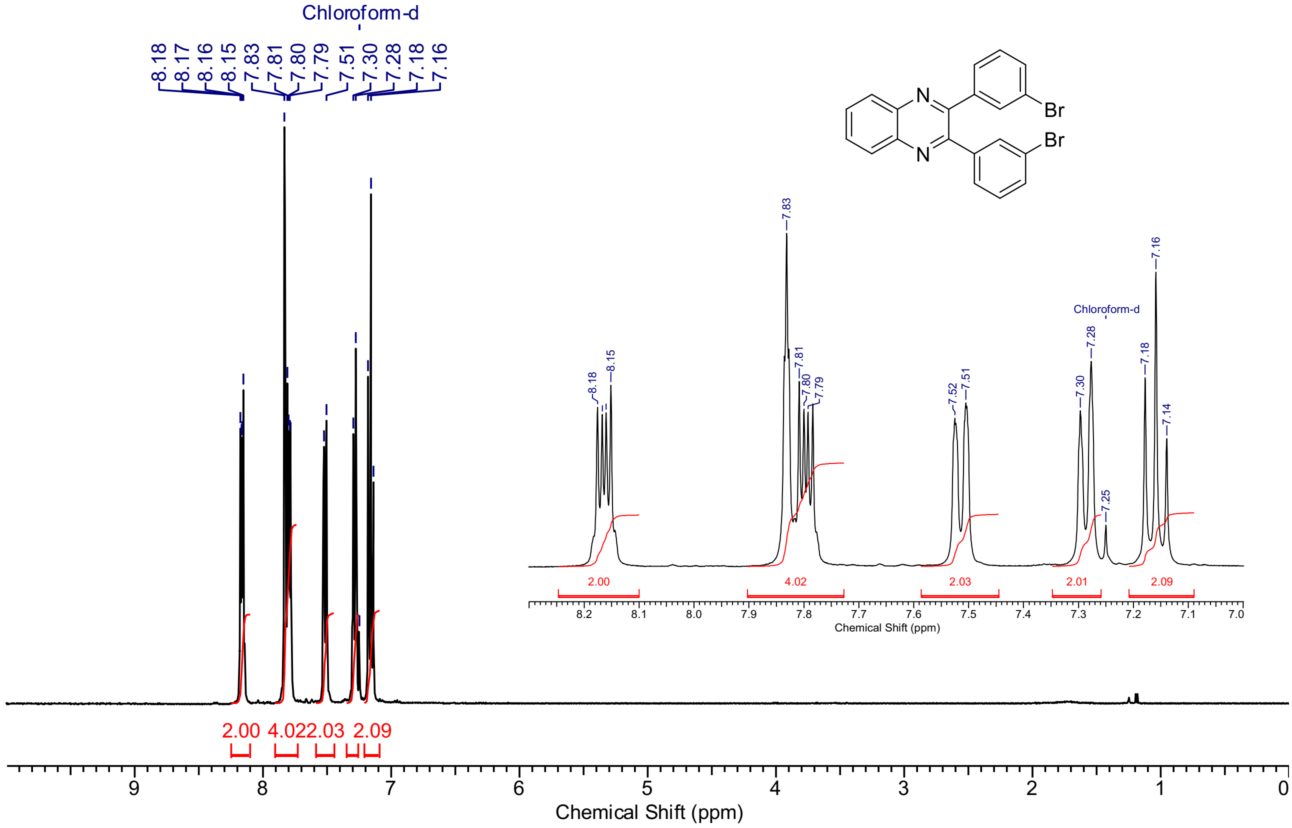



**Fig. S20.** $^{1}$H NMR spectrum of **3** ($CDCl_3$, 400 MHz, 300 K).

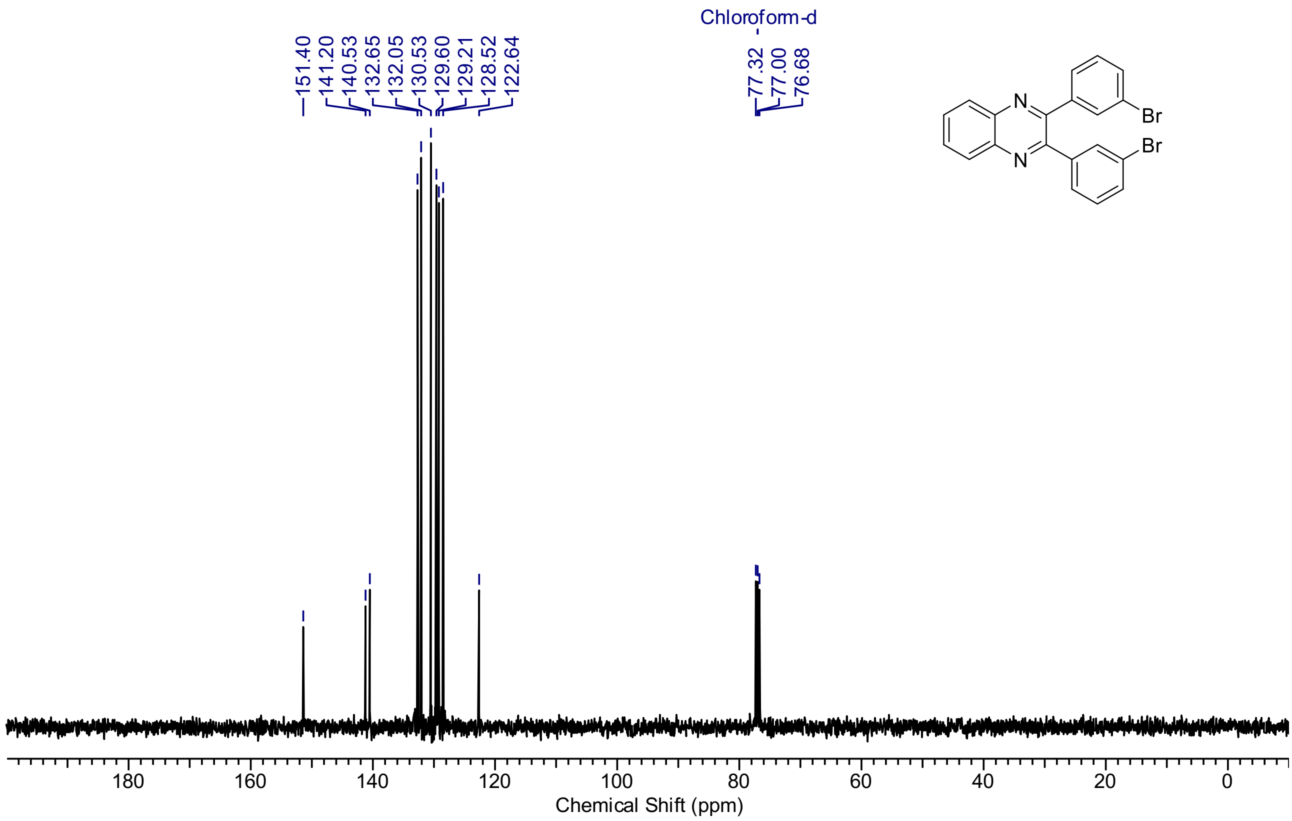



**Fig. S21.** $^{13}$C NMR spectrum of **3** ($CDCl_3$, 100.6 MHz, 300 K).

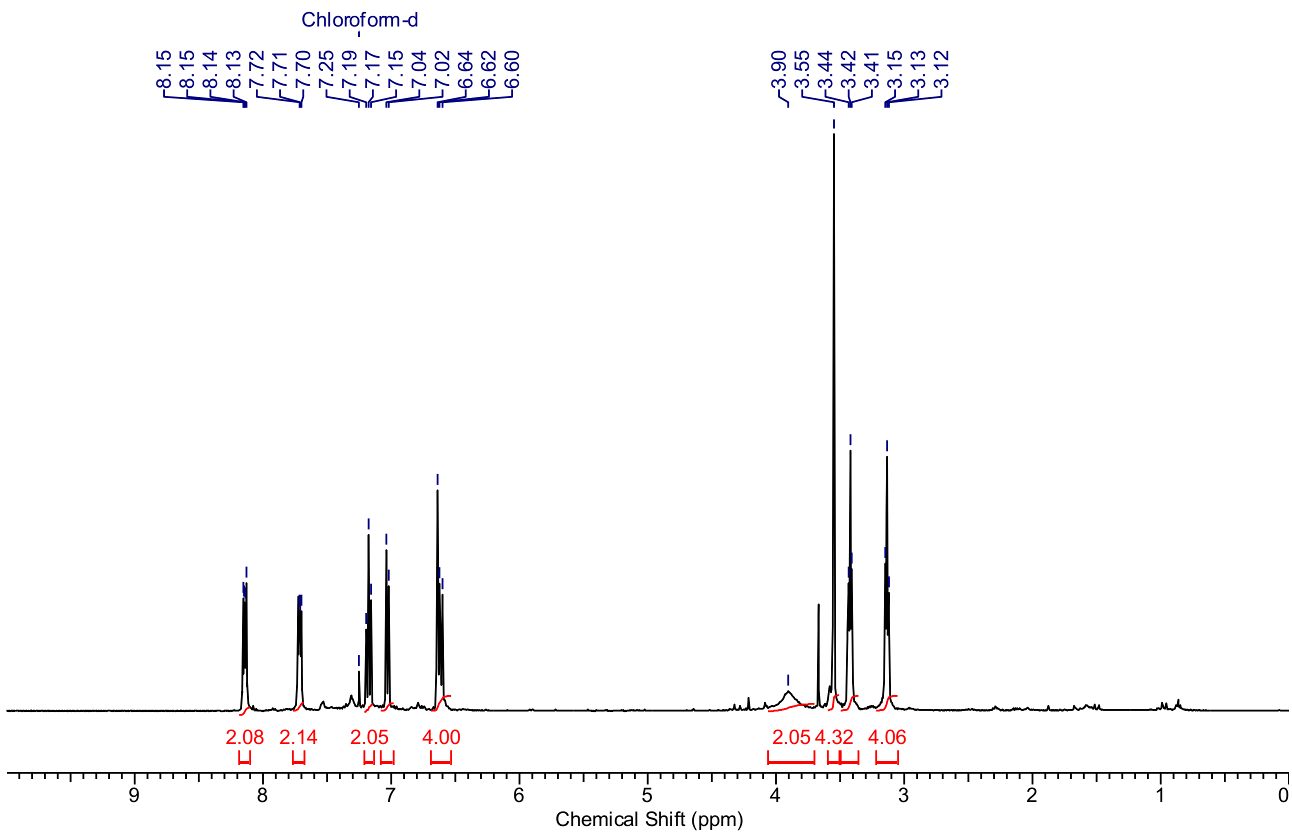



**Fig. S22.** $^1$H NMR spectrum of $N_2C_6O_2Q$ ($CDCl_3$, 400 MHz, 300 K).

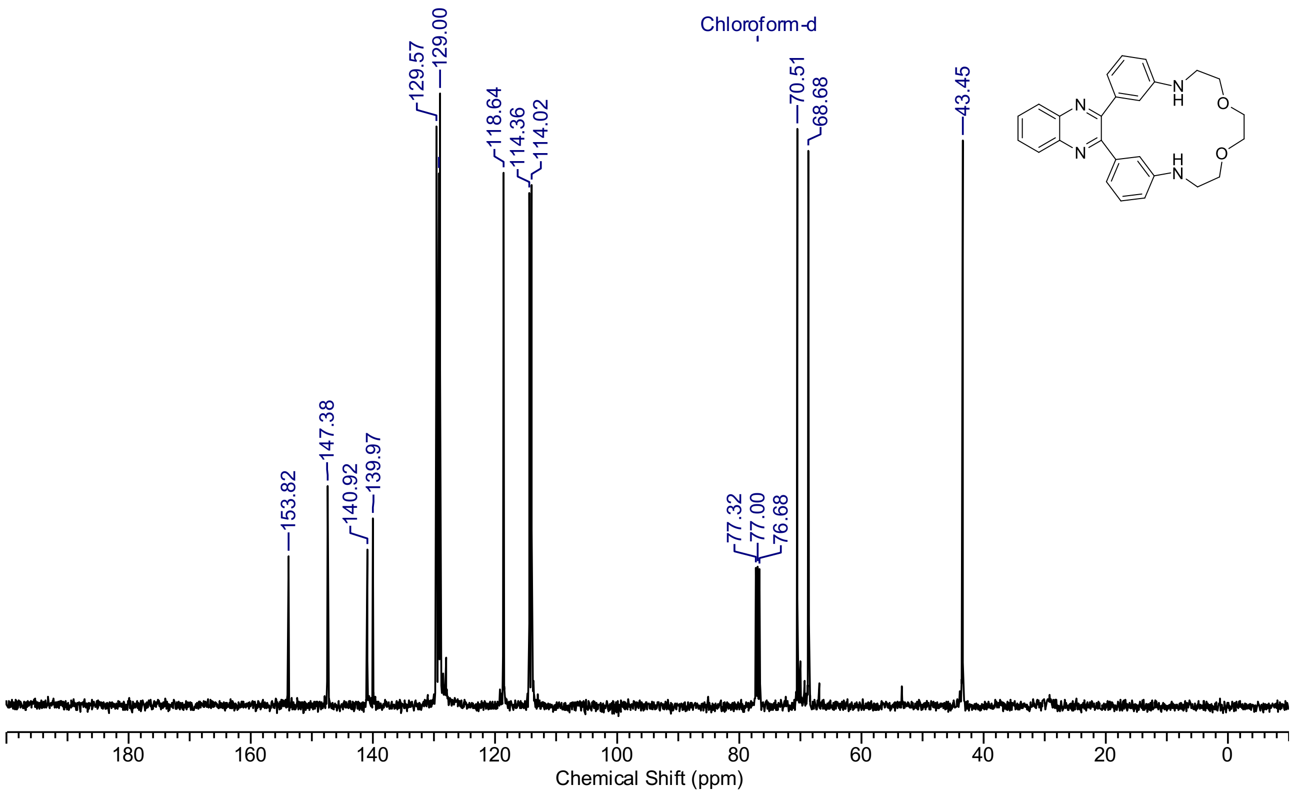



**Fig. S23.** $^{13}$C NMR spectrum of $N_2C_6O_2Q$ ($CDCl_3$, 100.6 MHz, 300 K).

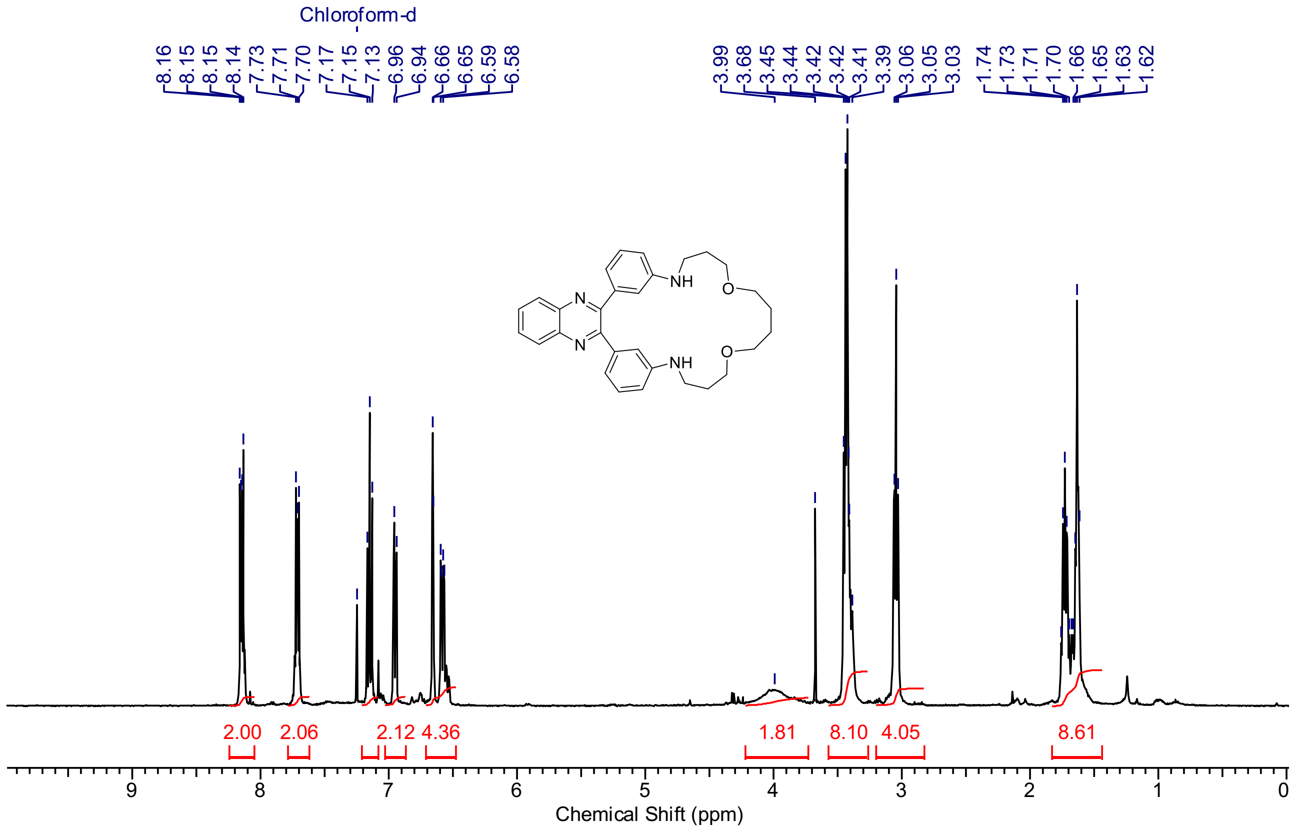



**Fig. S24.** [1]H NMR spectrum of $N_2C_{10}O_2Q$ ($CDCl_3$, 400 MHz, 300 K).

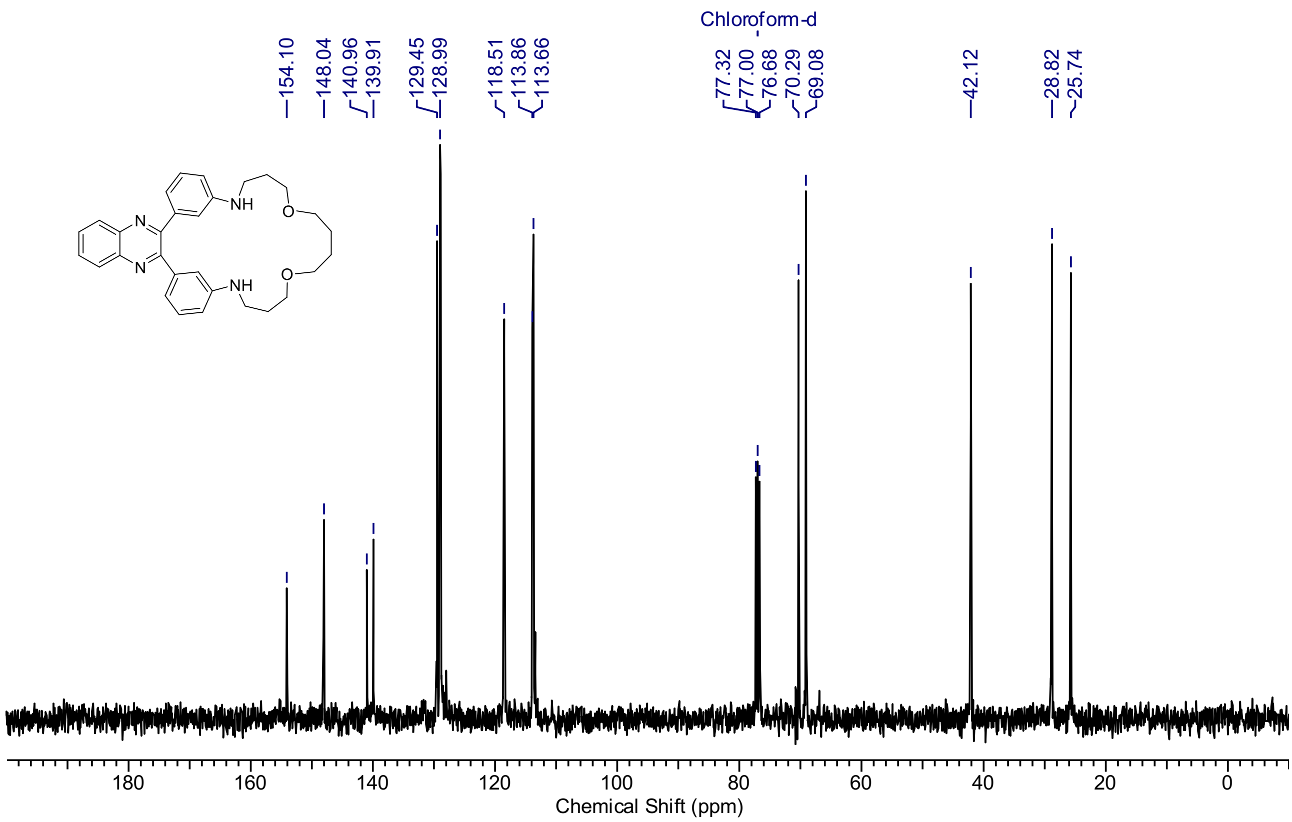



**Fig. S25.** [13]C NMR spectrum of $N_2C_{10}O_2Q$ ($CDCl_3$, 100.6 MHz, 300 K).

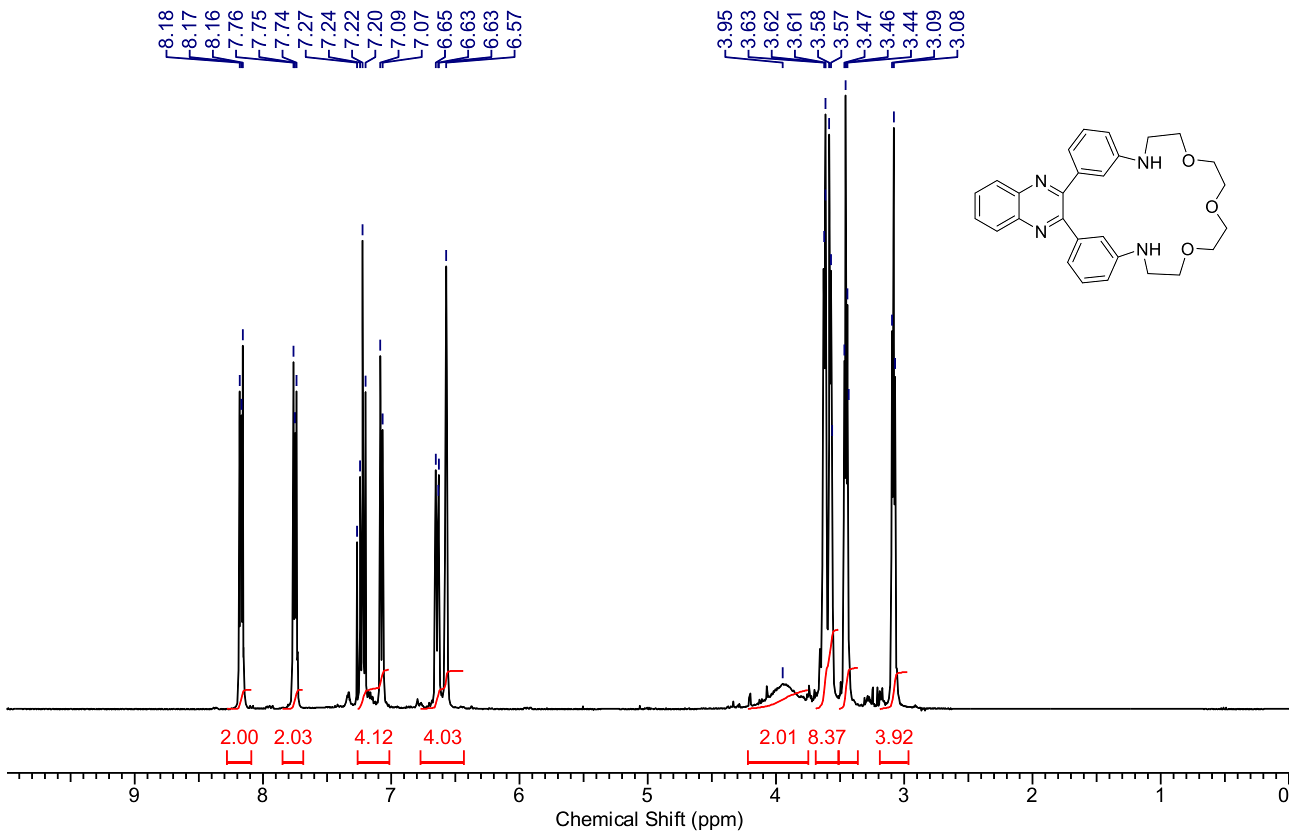



**Fig. S26.** $^{1}$H NMR spectrum of $N_2C_8O_3Q$ ($CDCl_3$, 400 MHz, 300 K).

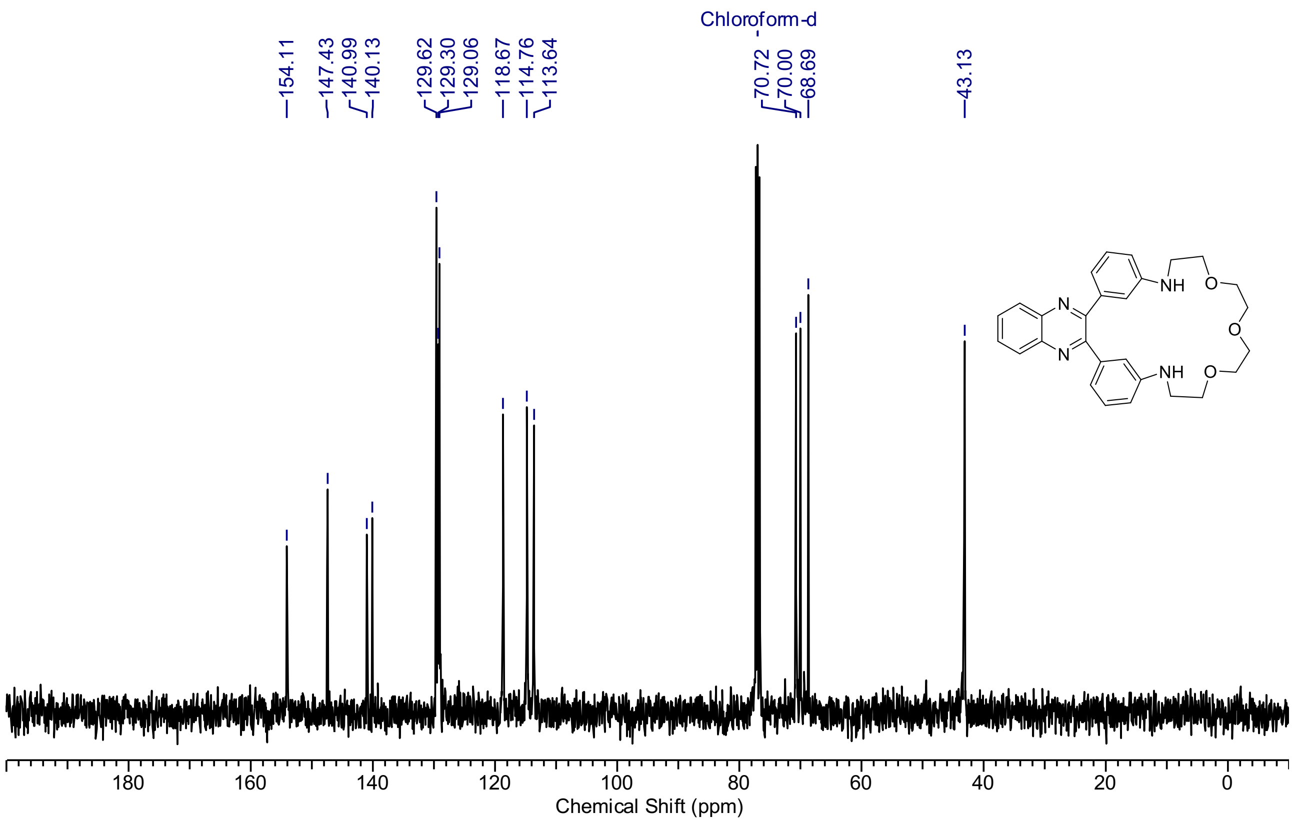



**Fig. S27.** $^{13}$C NMR spectrum of $N_2C_8O_3Q$ ($CDCl_3$, 100.6 MHz, 300 K).

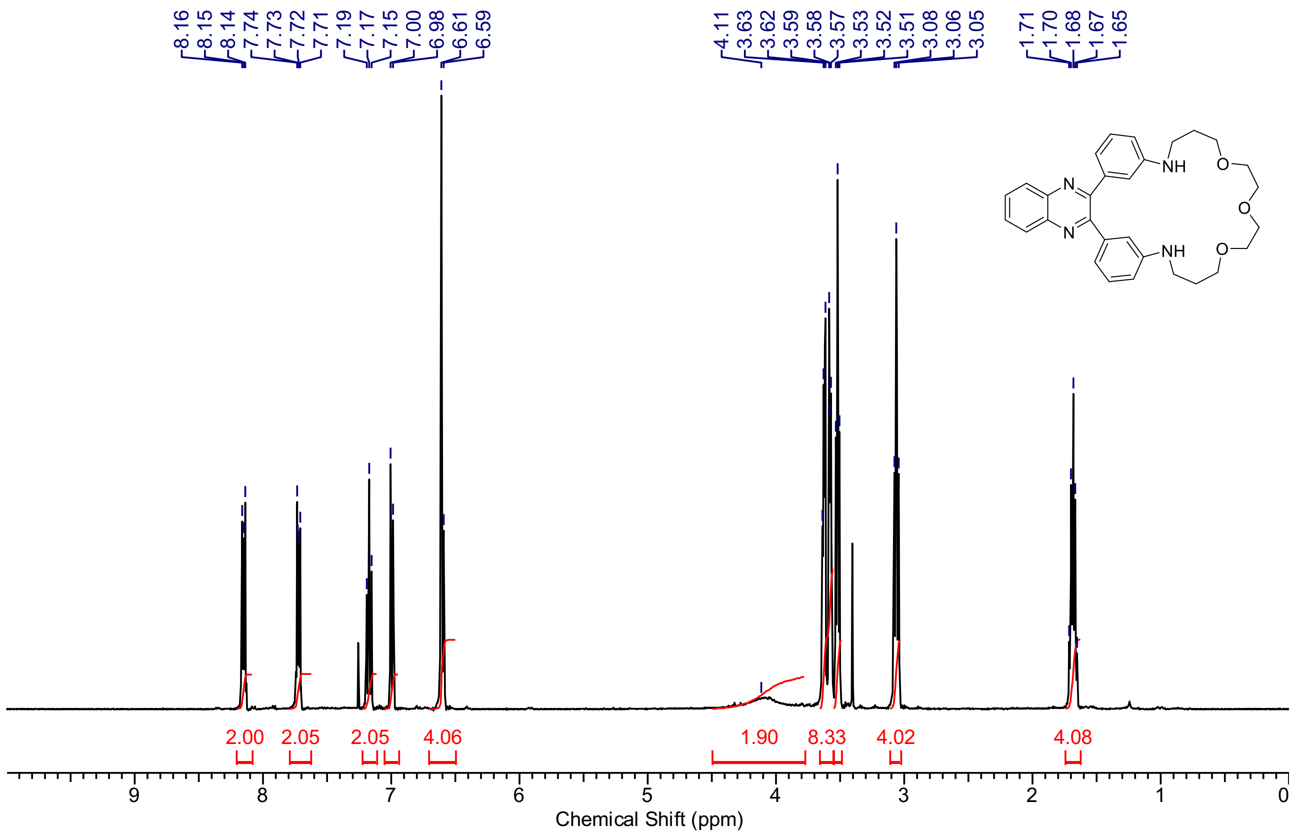



**Fig. S28.** [1]H NMR spectrum of $N_2C_{10}O_3Q$ ($CDCl_3$–$CD_3OD$, 400 MHz, 300 K).

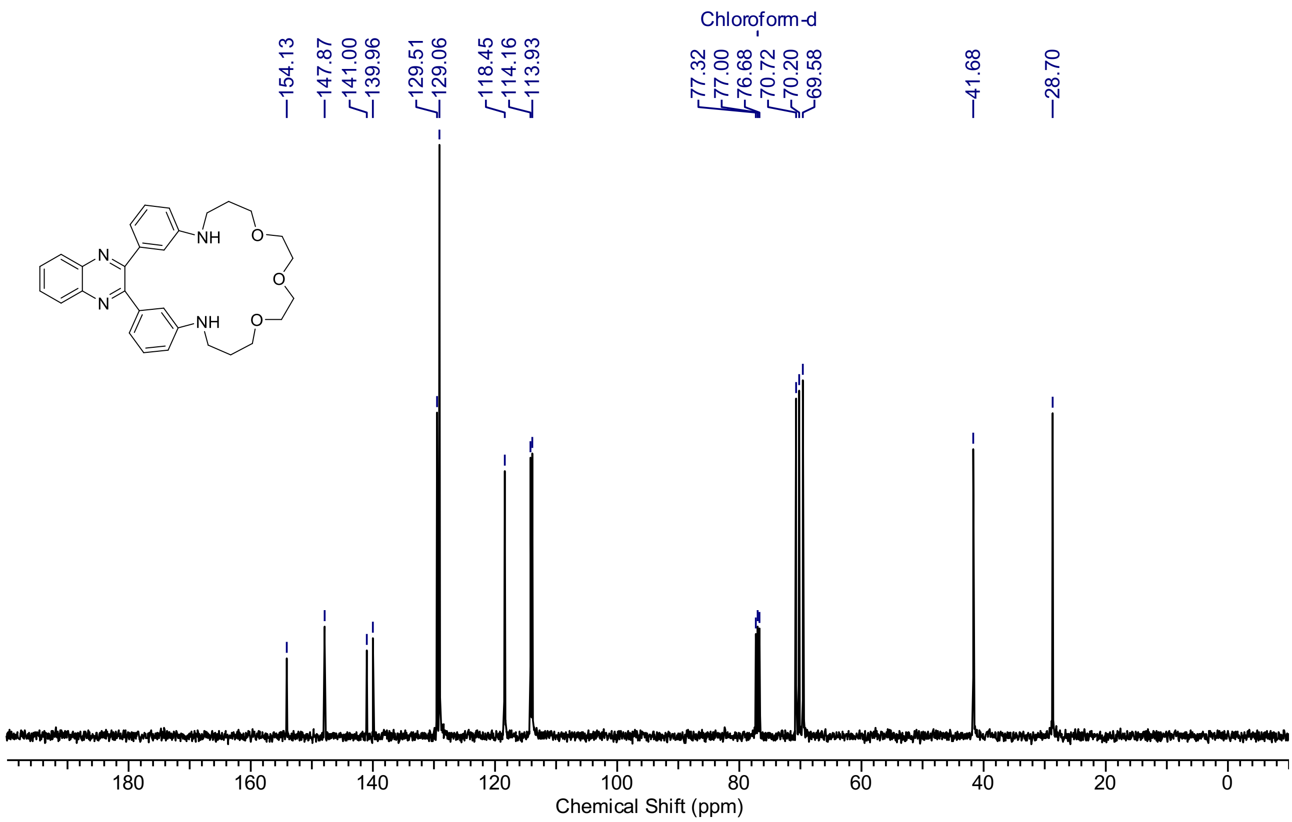



**Fig. S29.** [13]C NMR spectrum of $N_2C_{10}O_3Q$ ($CDCl_3$, 100.6 MHz, 300 K).

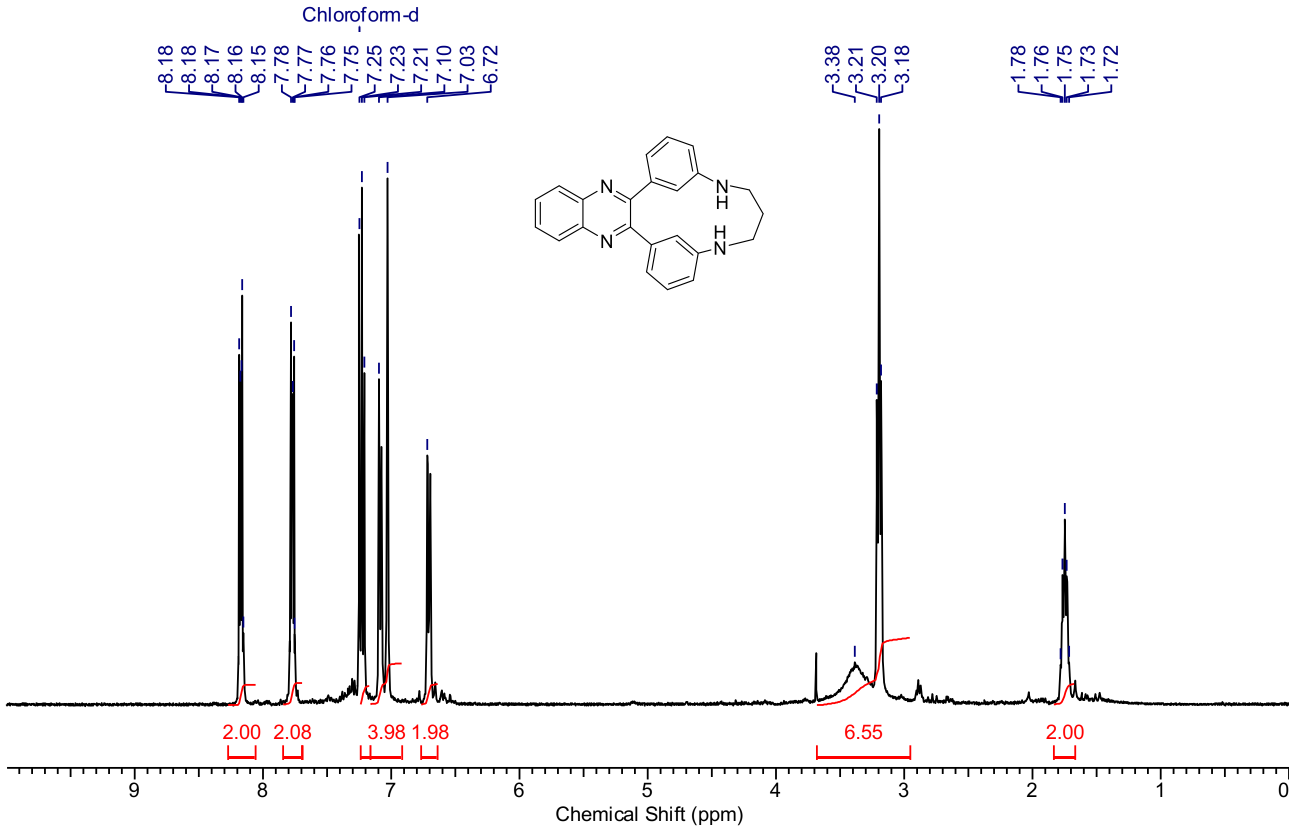



**Fig. S30.** $^{1}$H NMR spectrum of $N_2C_3Q$ ($CDCl_3$, 400 MHz, 300 K).

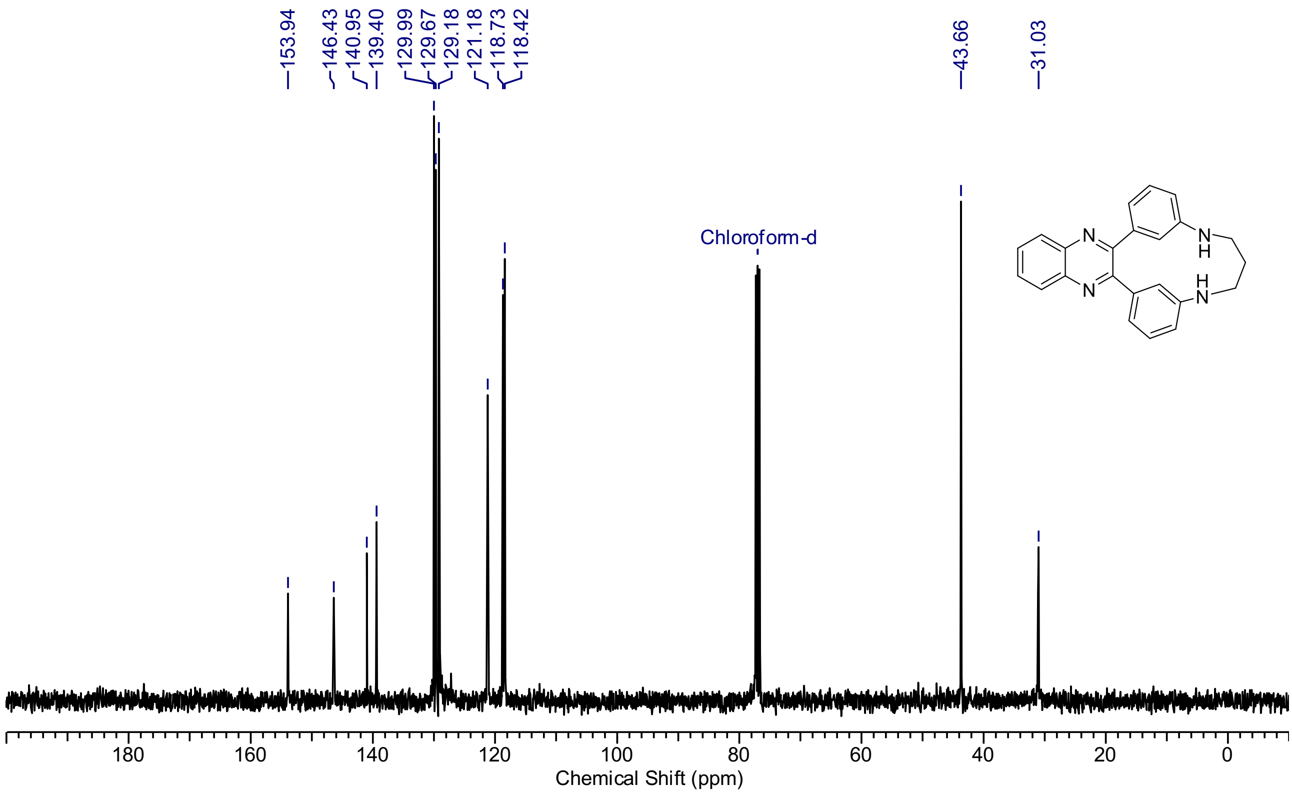



**Fig. S31.** $^{13}$C NMR spectrum of $N_2C_3Q$ ($CDCl_3$, 100.6 MHz, 300 K).

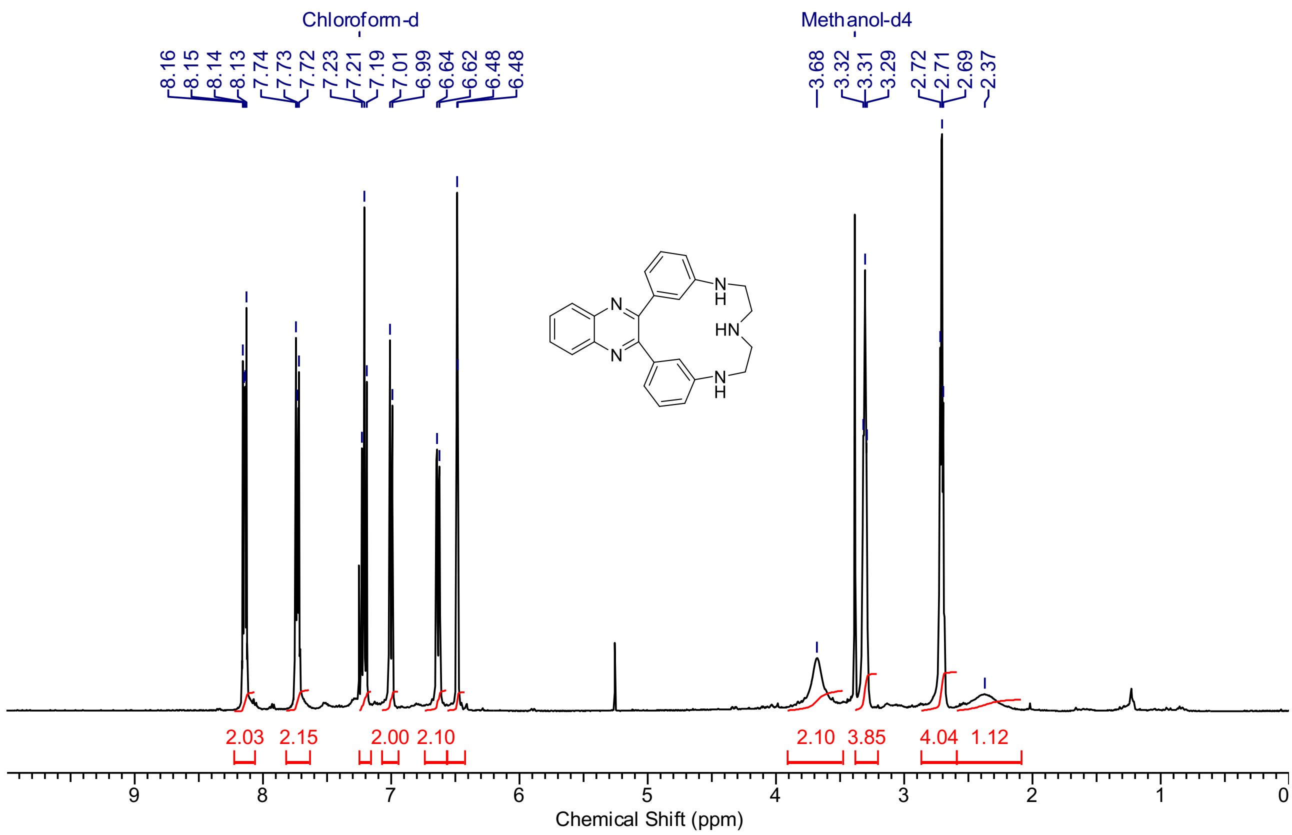



**Fig. S32.** $^{1}$H NMR spectrum of $N_3C_4Q$ ($CDCl_3$–$CD_3OD$ (10:1 v/v), 400 MHz, 300 K).

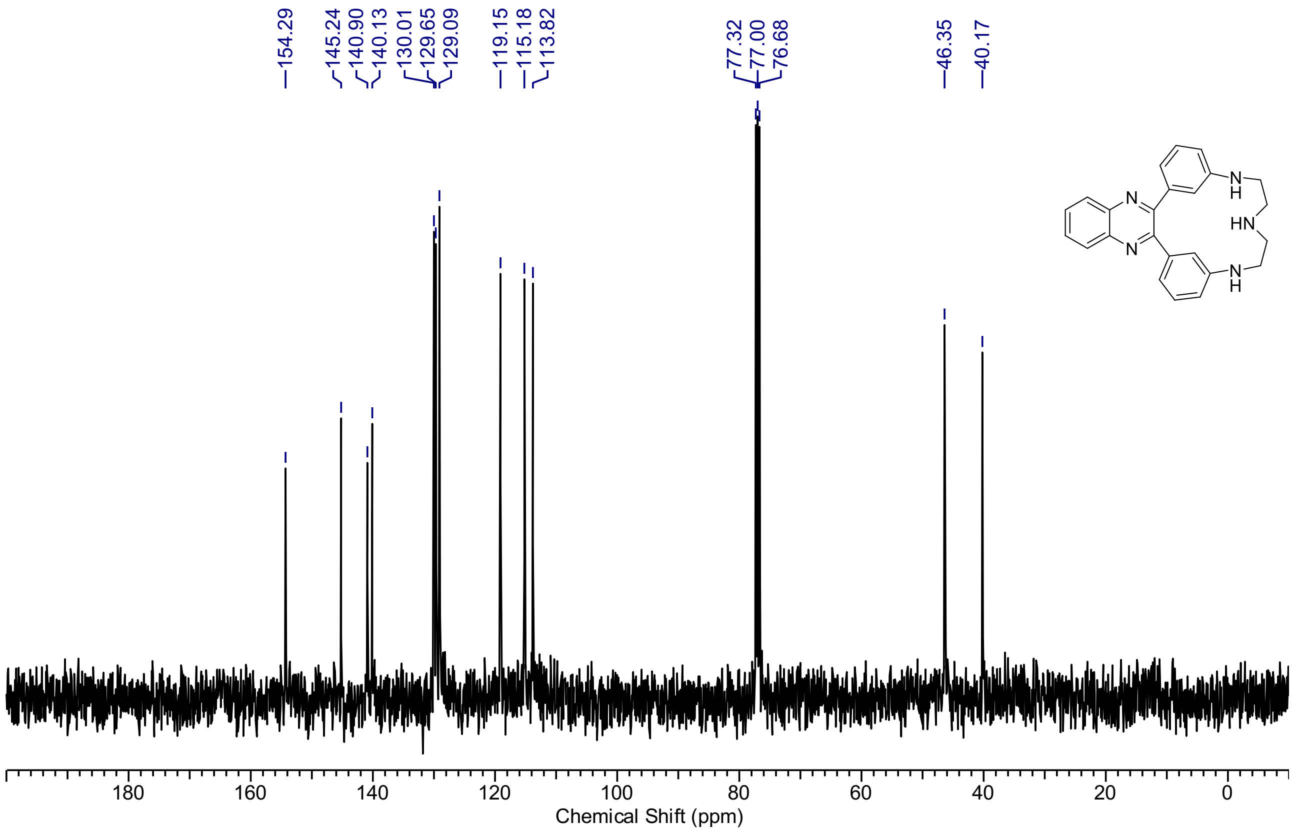



**Fig. S33.** $^{13}$C NMR spectrum of $N_3C_4Q$ ($CDCl_3$, 100.6 MHz, 300 K).

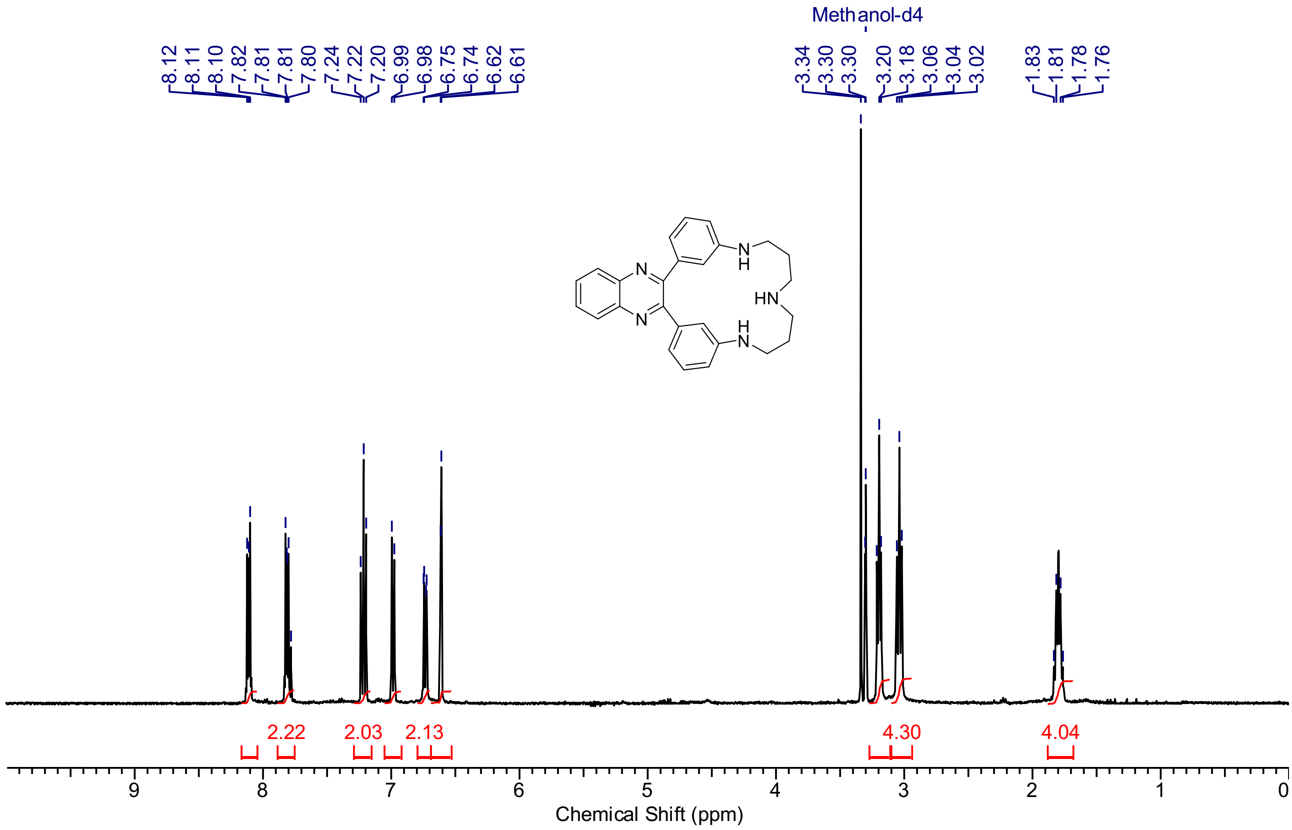



**Fig. S34.** $^{1}$H NMR spectrum of $N_3C_6Q$ ($CD_3OD$, 400 MHz, 300 K).

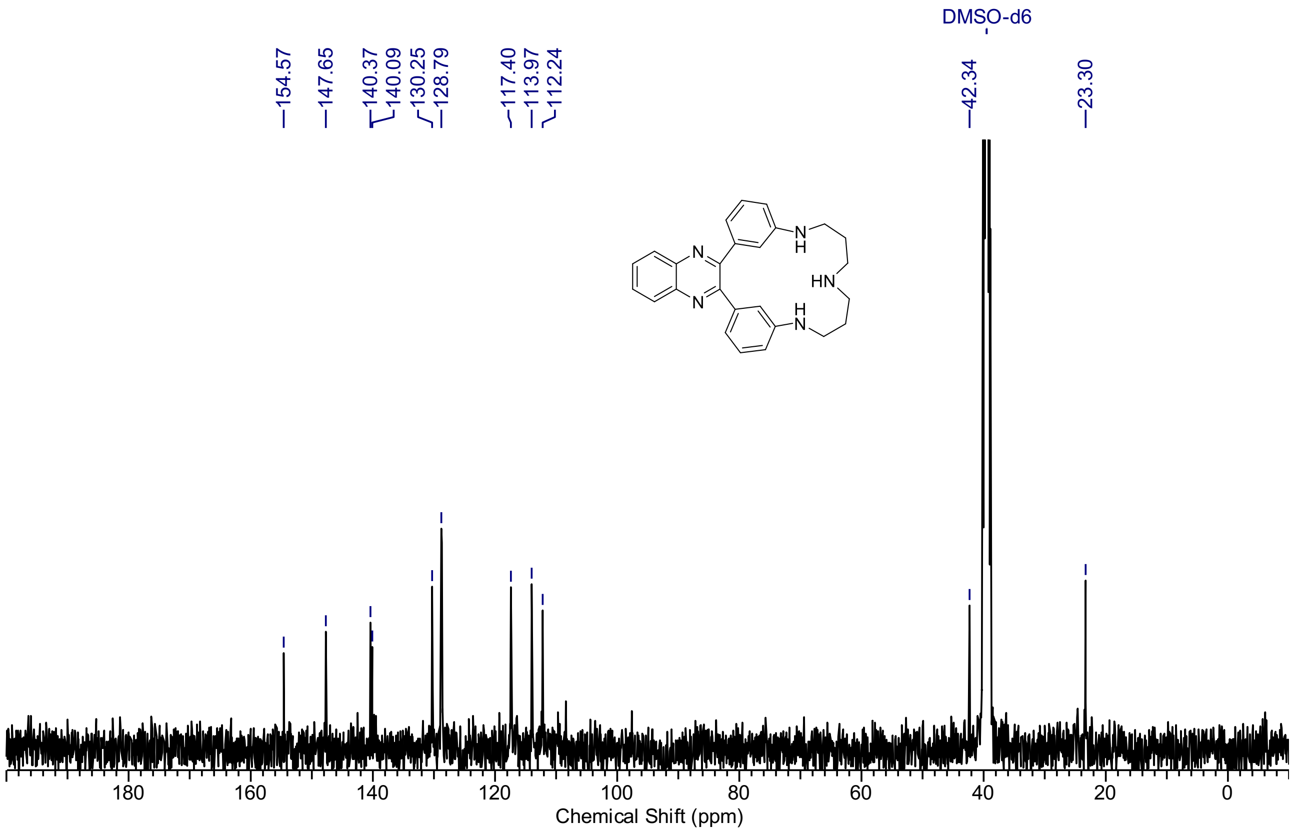



**Fig. S35.** $^{13}$C NMR spectrum of $N_3C_6Q$ (DMSO-D6, 100.6 MHz, 300 K).

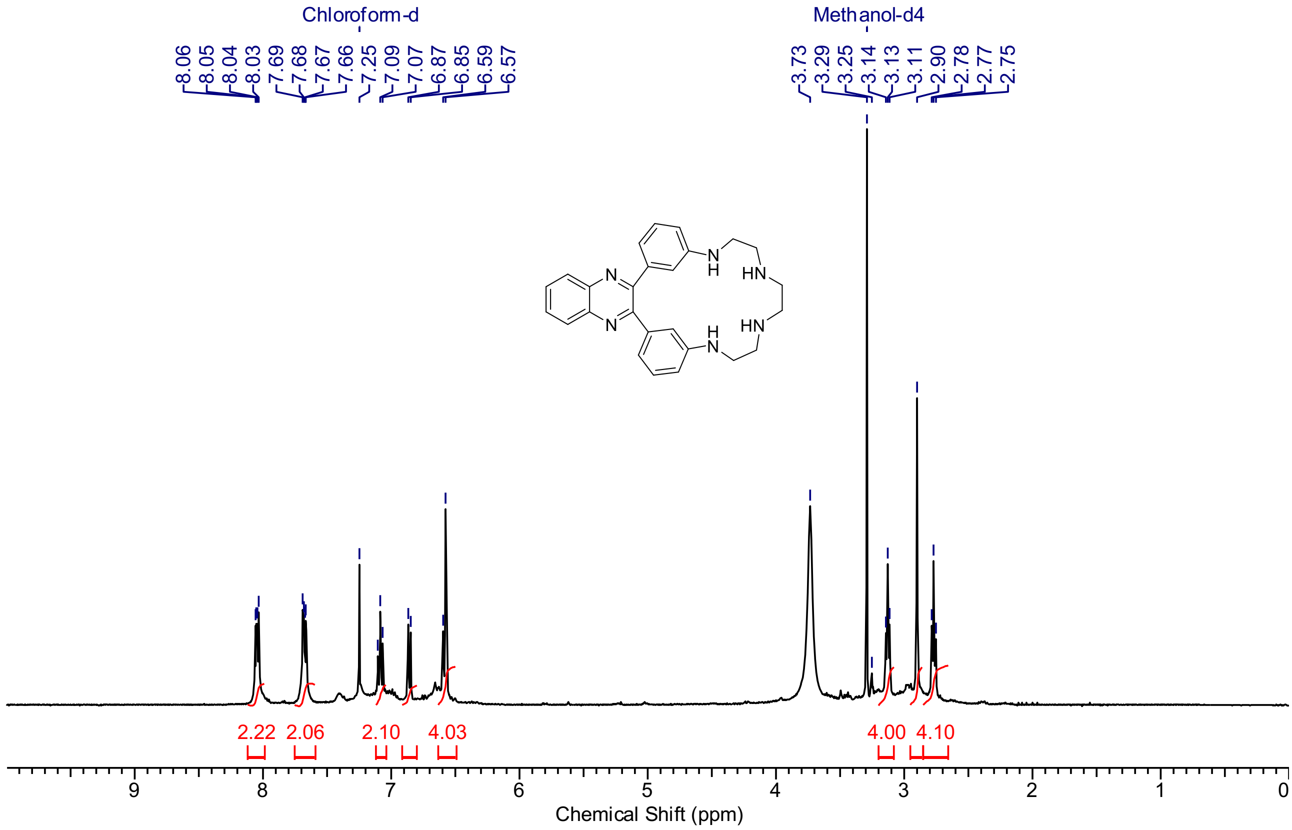



**Fig. S36.** $^{1}H$ NMR spectrum of $N_4C_6Q$ ($CDCl_3$–$CD_3OD$ (5:1 v/v), 400 MHz, 300 K).

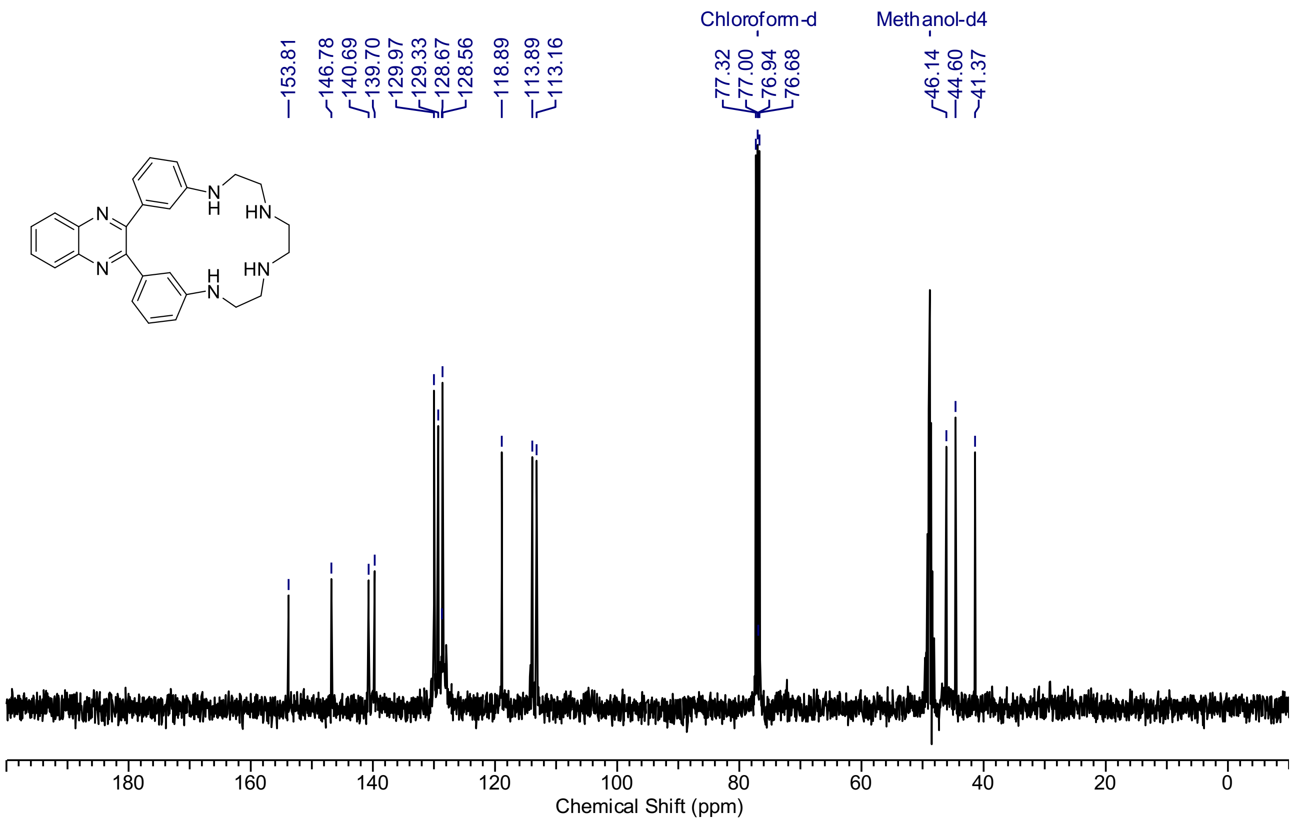



**Fig. S37.** $^{13}C$ NMR spectrum of $N_4C_6Q$ ($CDCl_3$–$CD_3OD$ (5:1 v/v), 100.6 MHz, 300 K).

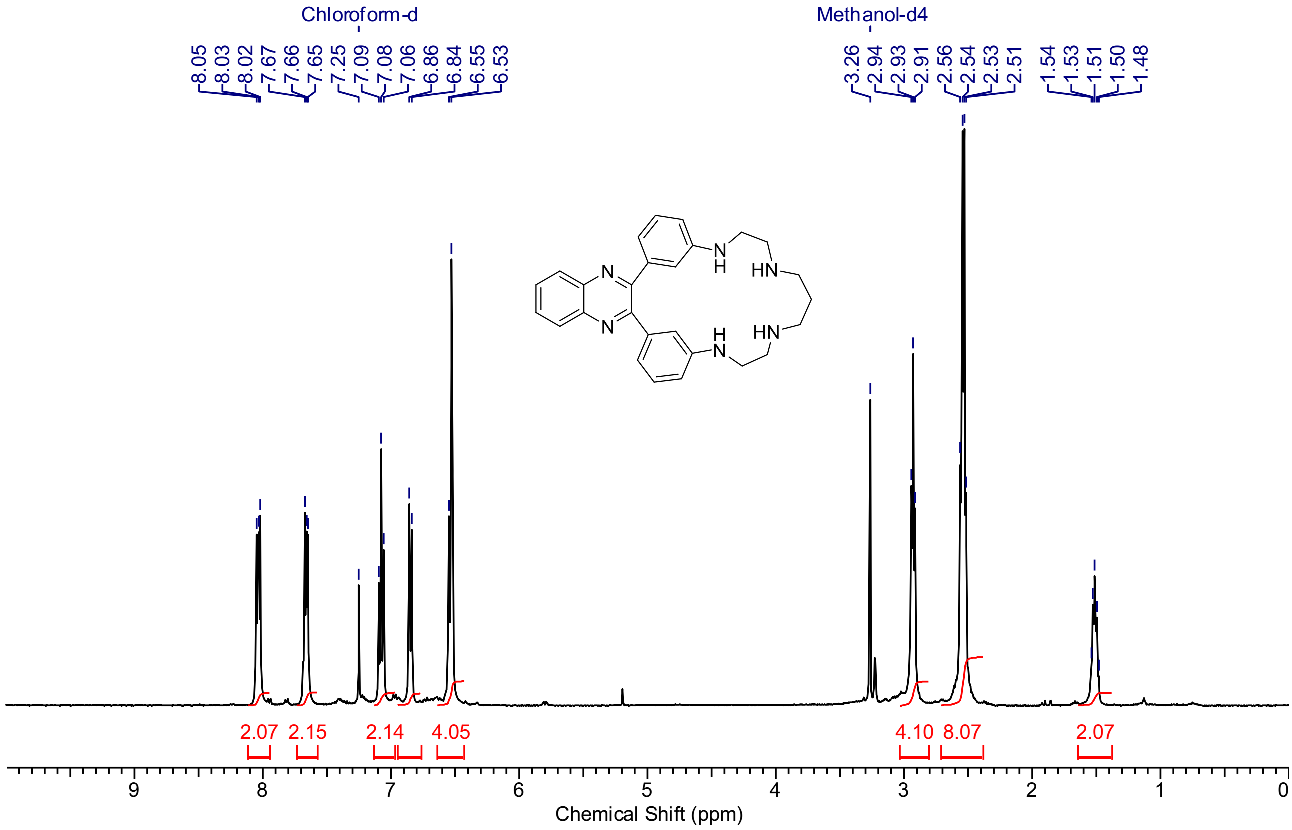



**Fig. S38.** $^{1}$H NMR spectrum of $N_4C_7Q$ ($CDCl_3$–$CD_3OD$ (10:1 v/v), 400 MHz, 300 K).

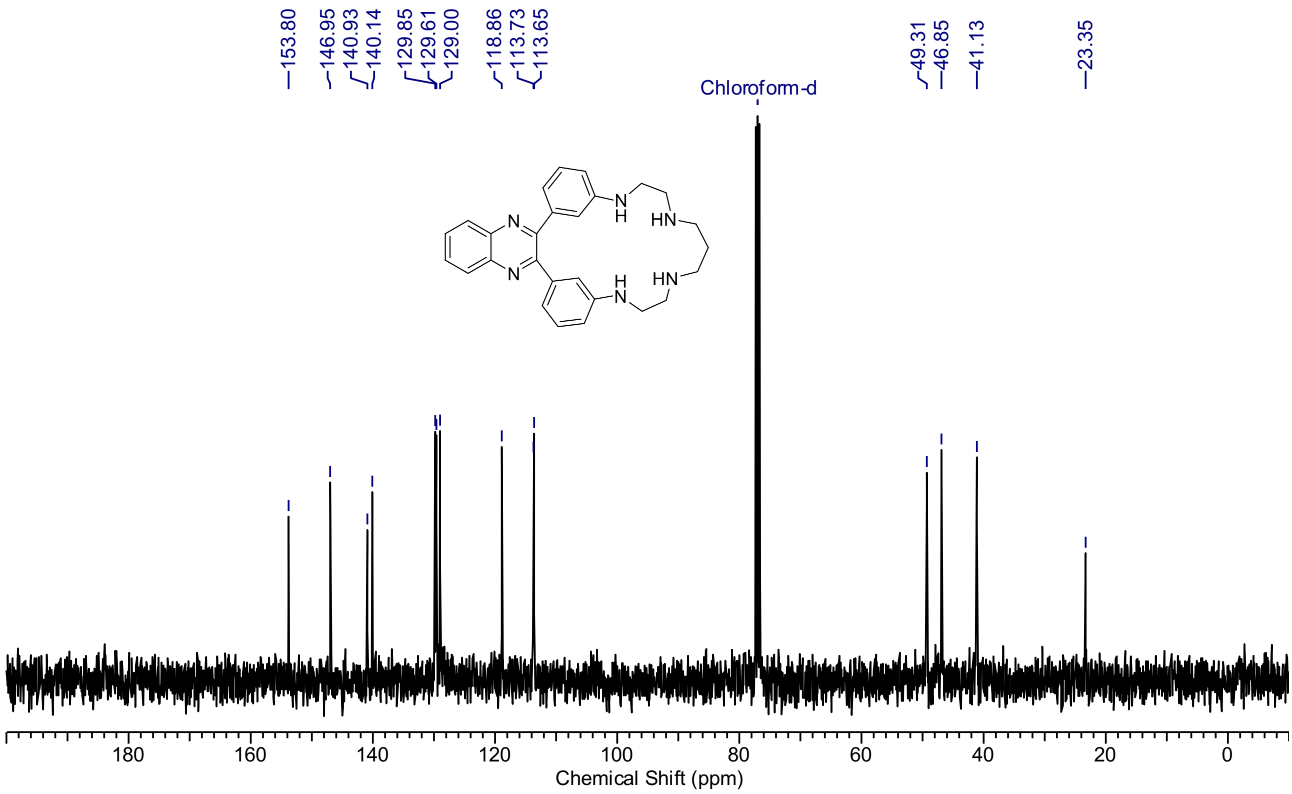



**Fig. S39.** $^{13}$C NMR spectrum of $N_4C_7Q$ ($CDCl_3$, 100.6 MHz, 300 K).

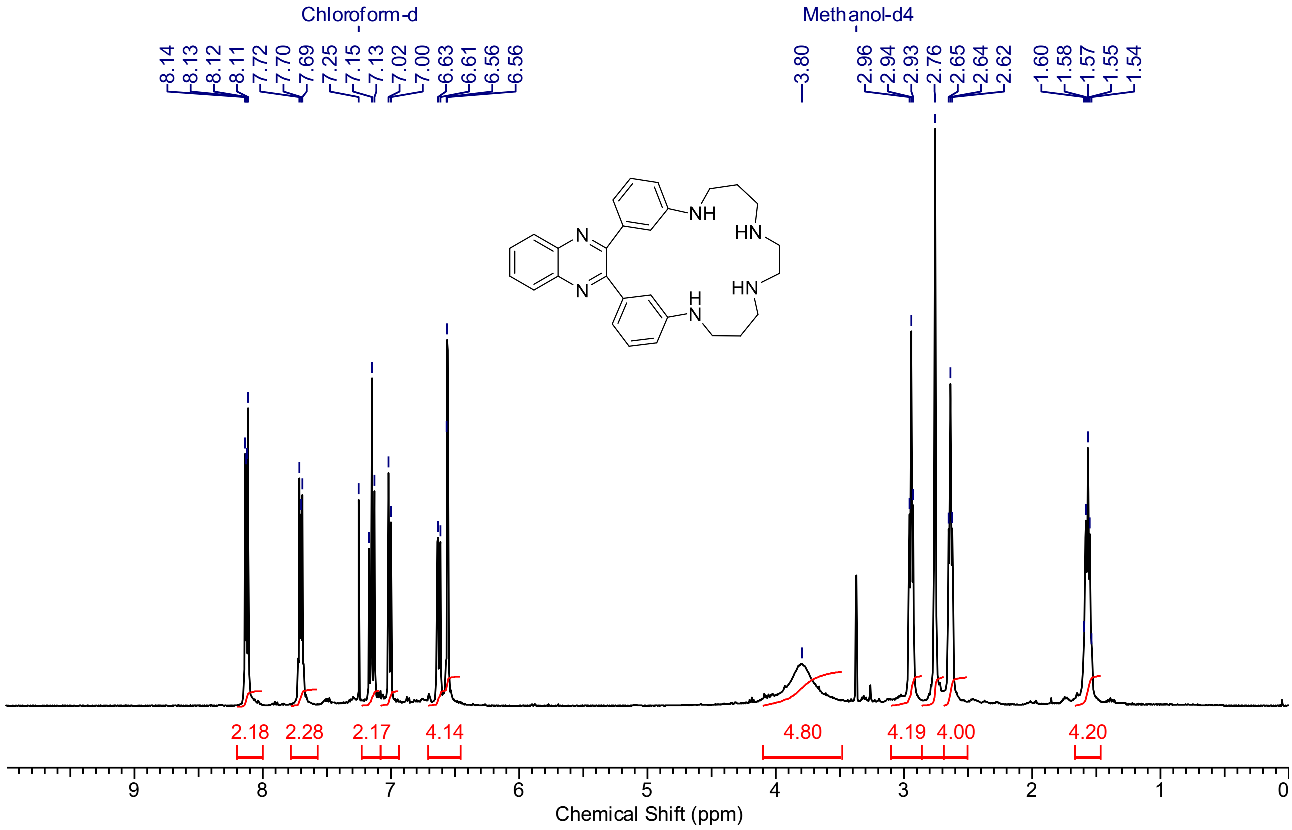



**Fig. S40.** $^{1}H$ NMR spectrum of $N_4C_8Q$ ($CDCl_3$–$CD_3OD$ (10:1 v/v), 400 MHz, 300 K).

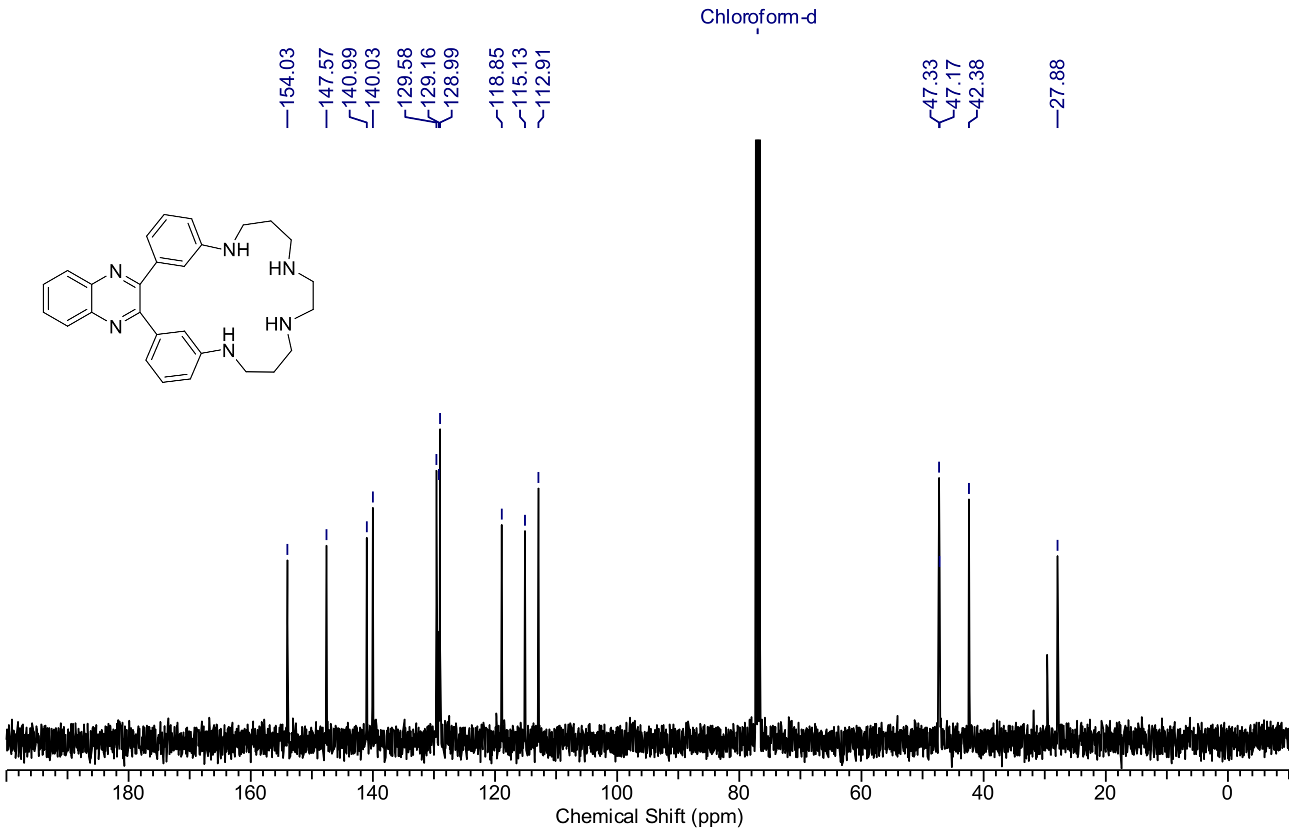



**Fig. S41.** $^{13}C$ NMR spectrum of $N_4C_8Q$ ($CDCl_3$–$CD_3OD$ (10:1 v/v), 100.6 MHz, 300 K).

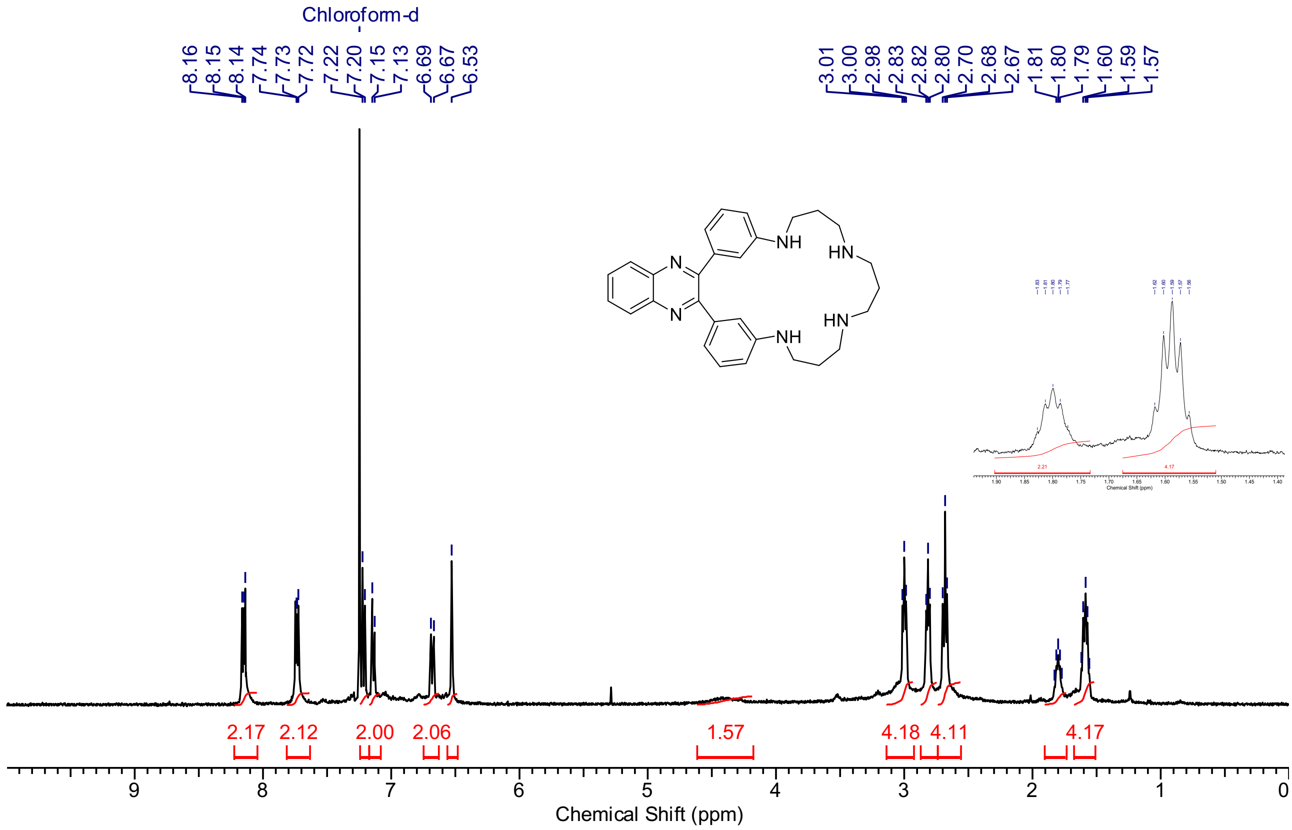



**Fig. S42.** $^{1}$H NMR spectrum of $N_4C_9Q$ ($CDCl_3$, 400 MHz, 300 K).

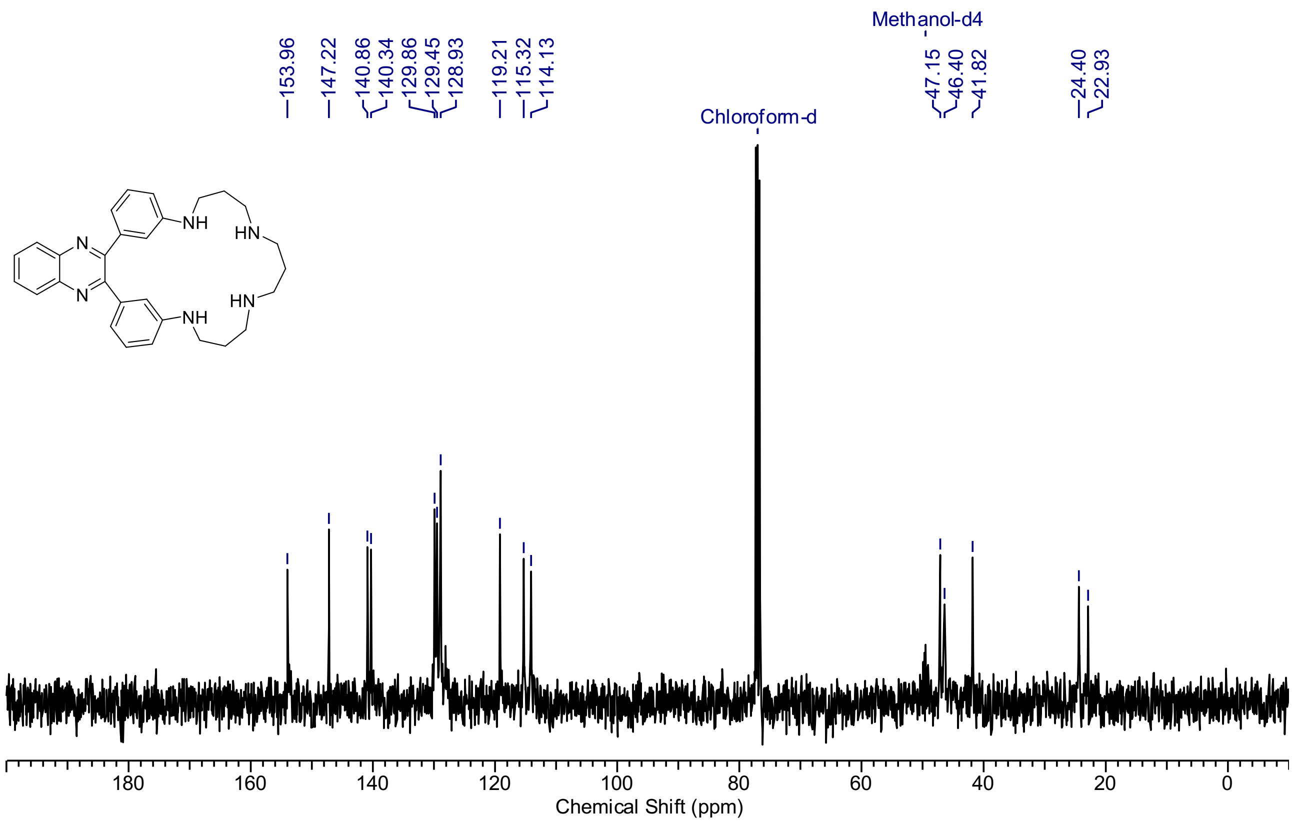



**Fig. S43.** $^{13}$C NMR spectrum of $N_4C_9Q$ ($CDCl_3$–$CD_3OD$ (5:1 v/v), 100.6 MHz, 300 K).

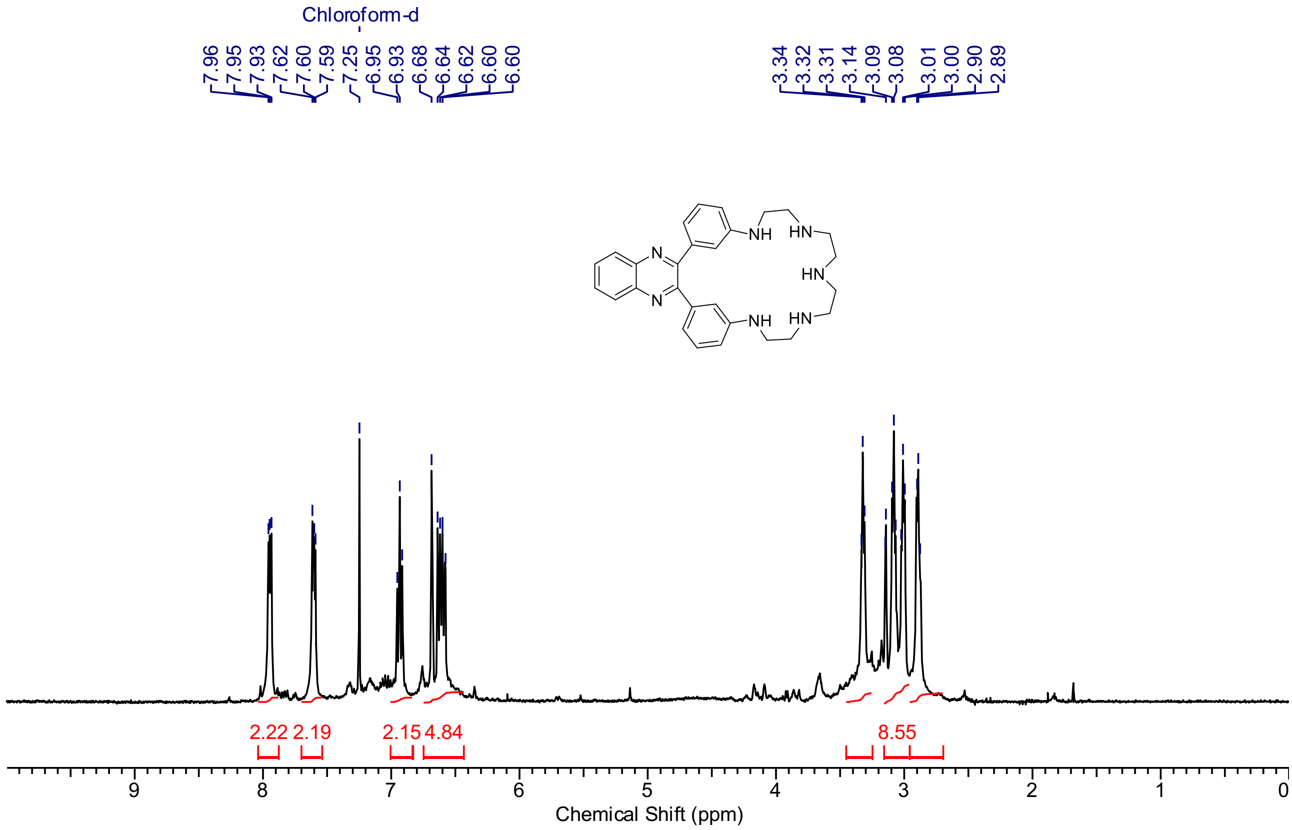



**Fig. S44.** $^{1}$H NMR spectrum of $N_5C_8Q$ ($CDCl_3$–$CD_3OD$ (1:1 v/v), 400 MHz, 300 K).

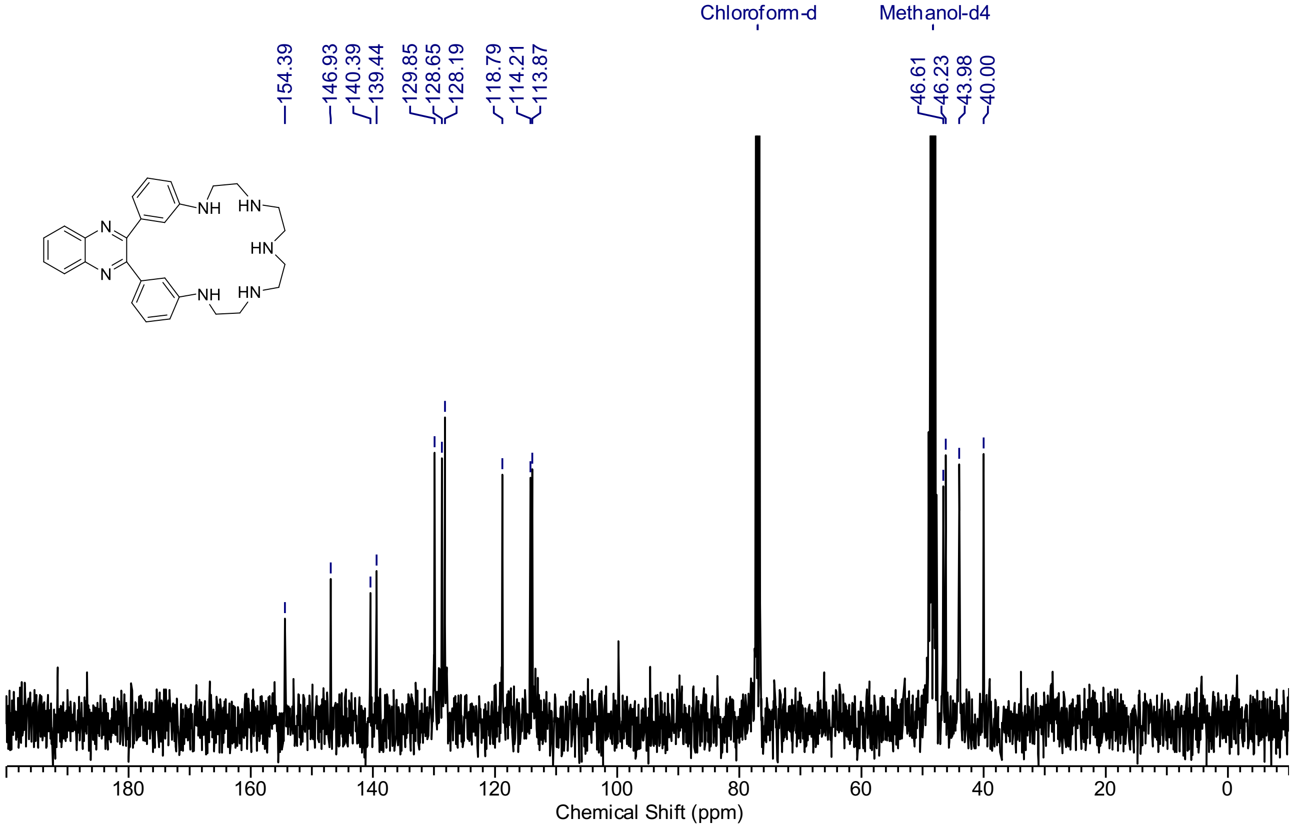



**Fig. S45.** $^{13}$C NMR spectrum of $N_5C_8Q$ ($CDCl_3$–$CD_3OD$ (1:1 v/v), 100.6 MHz, 300 K).

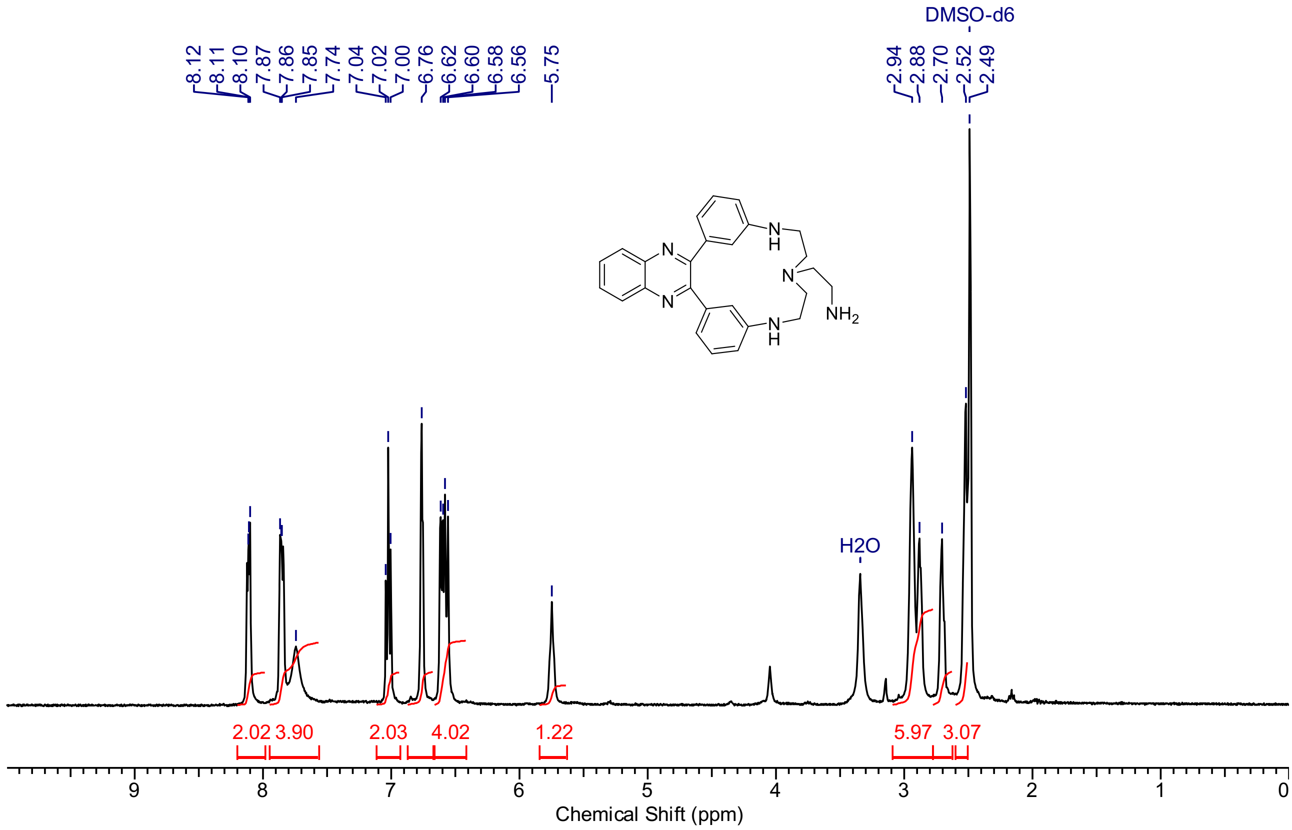



**Fig. S46.** [1]H NMR spectrum of *pa*-$N_4C_6$Q (DMSO-*d6*, 400 MHz, 300 K).

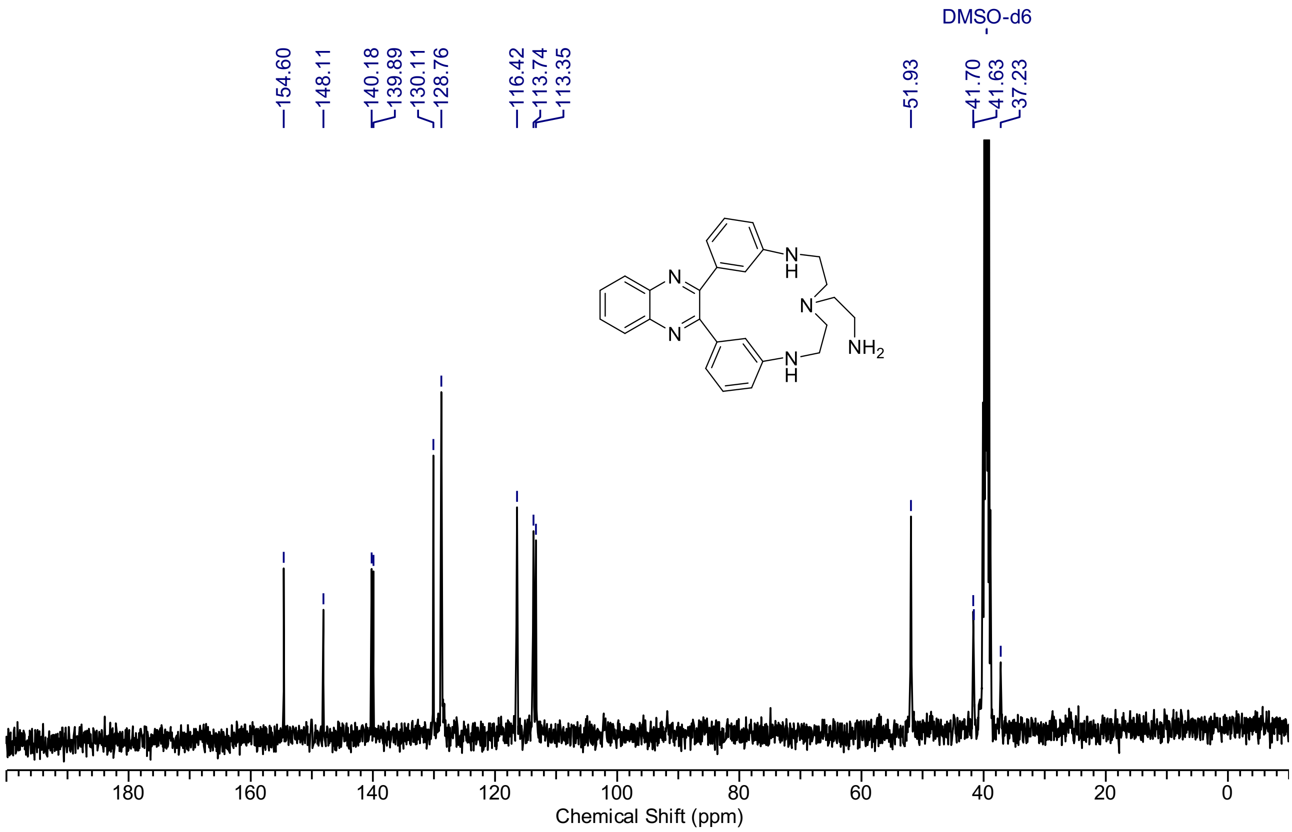



**Fig. S47.** [13]C NMR spectrum of *pa*-$N_4C_6$Q (DMSO-*d6*, 100.6 MHz, 300 K).

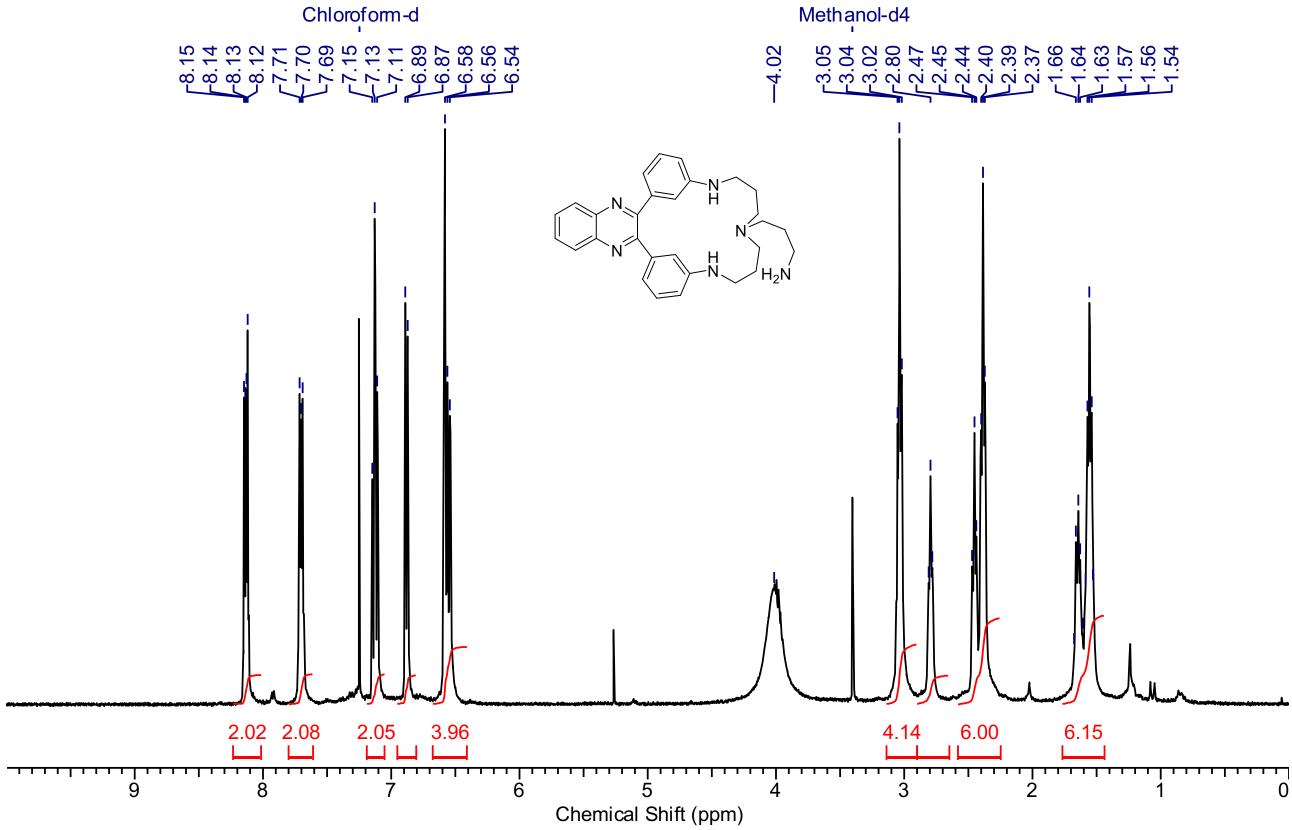


**Fig. S48.** $^{1}H$ NMR spectrum of *pa*-$N_4C_9Q$ ($CDCl_3$–$CD_3OD$ (10:1 v/v), 400 MHz, 300 K).

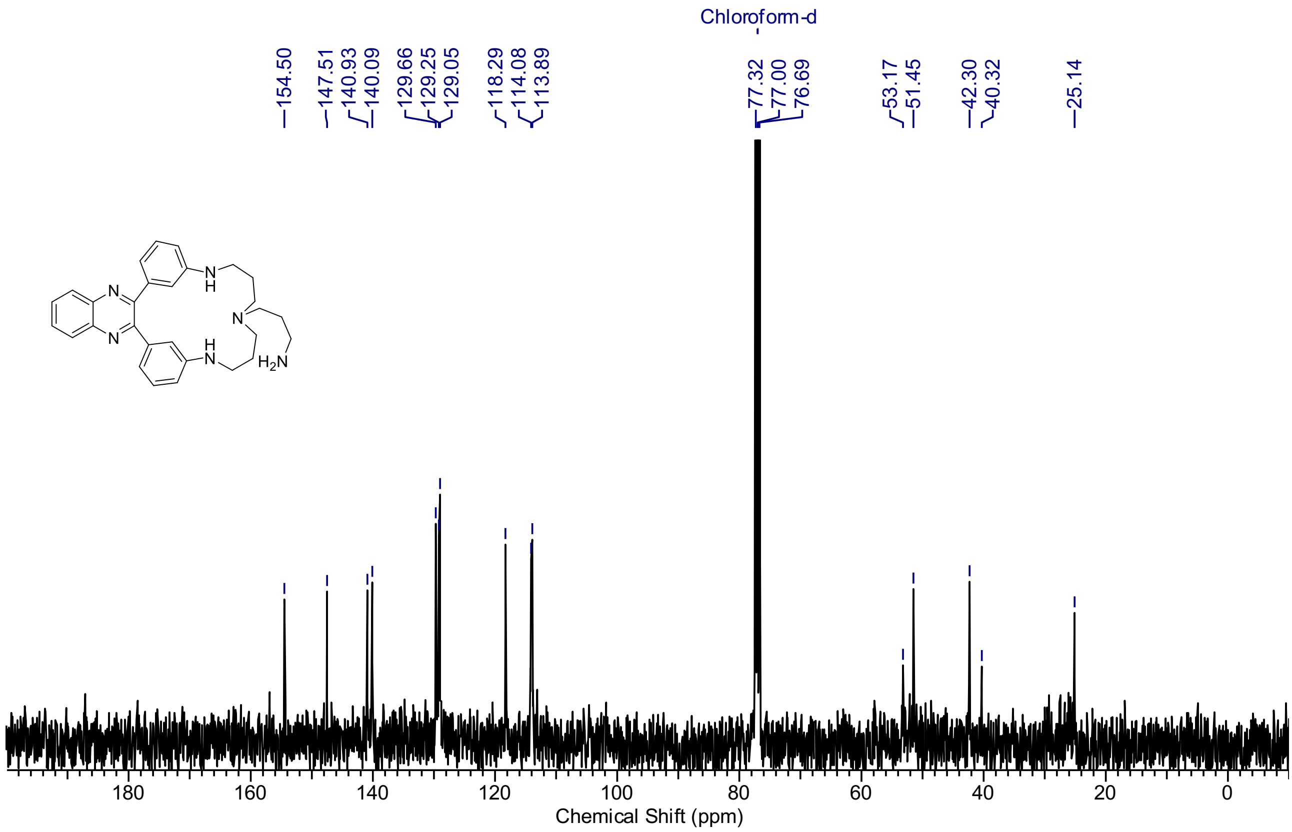


**Fig. S49.** $^{13}C$ NMR spectrum of *pa*-$N_4C_9Q$ ($CDCl_3$–$CD_3OD$ (10:1 v/v), 100.6 MHz, 300 K).

*MALDI-TOF spectra*

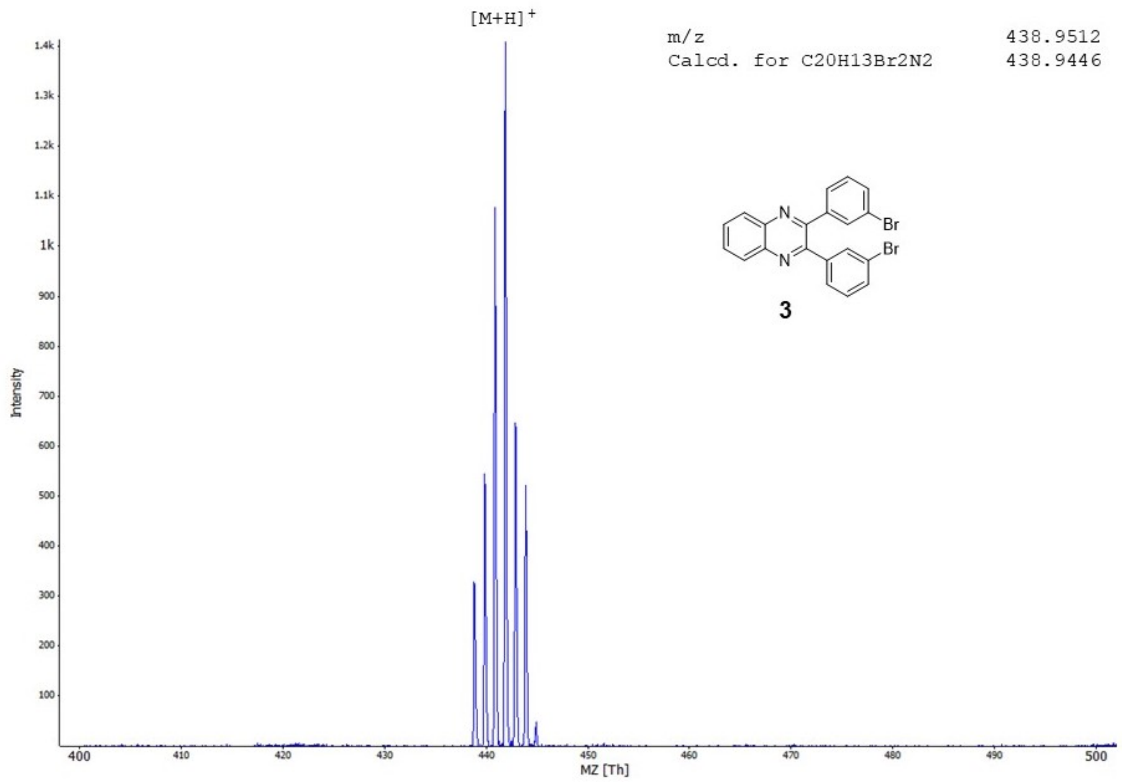



**Fig. S50.** MALDI-TOF spectrum of **3**. Matrix: 1,8,9-trihydroxyanthracene. Calibration standard: PEG-400.

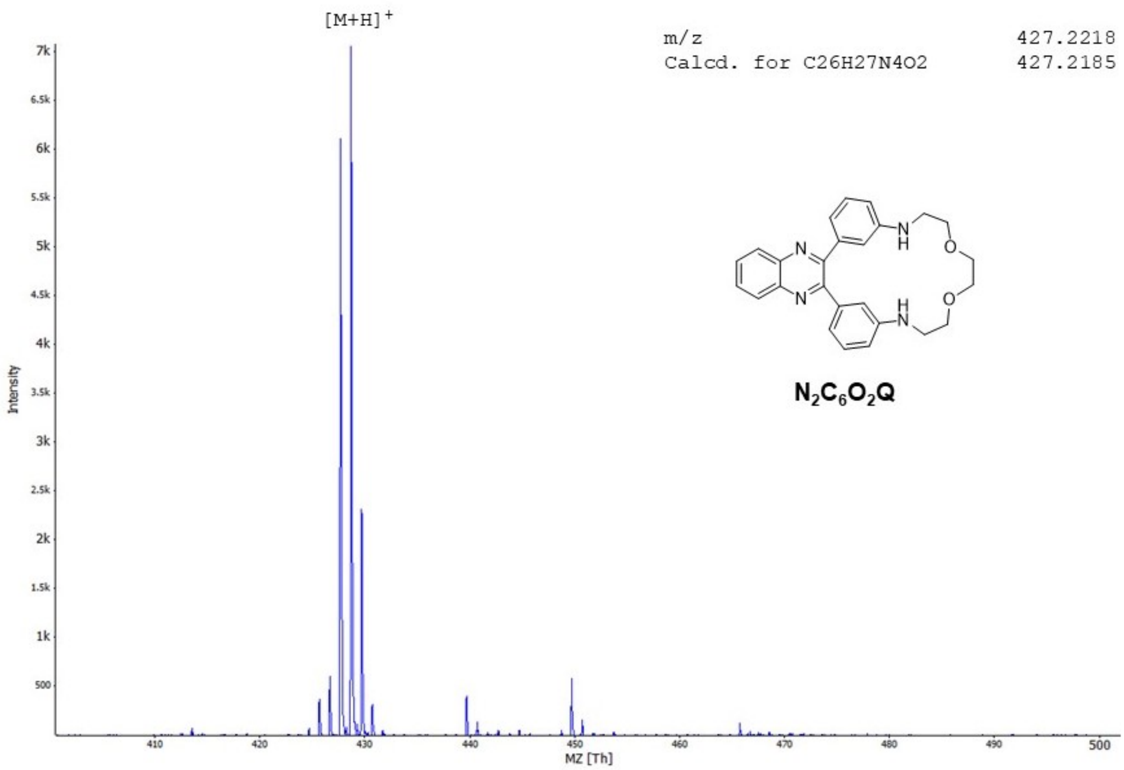



**Fig. S51.** MALDI-TOF spectrum of $N_2C_6O_2Q$. Matrix: 1,8,9-trihydroxyanthracene. Calibration standard: PEG-400.

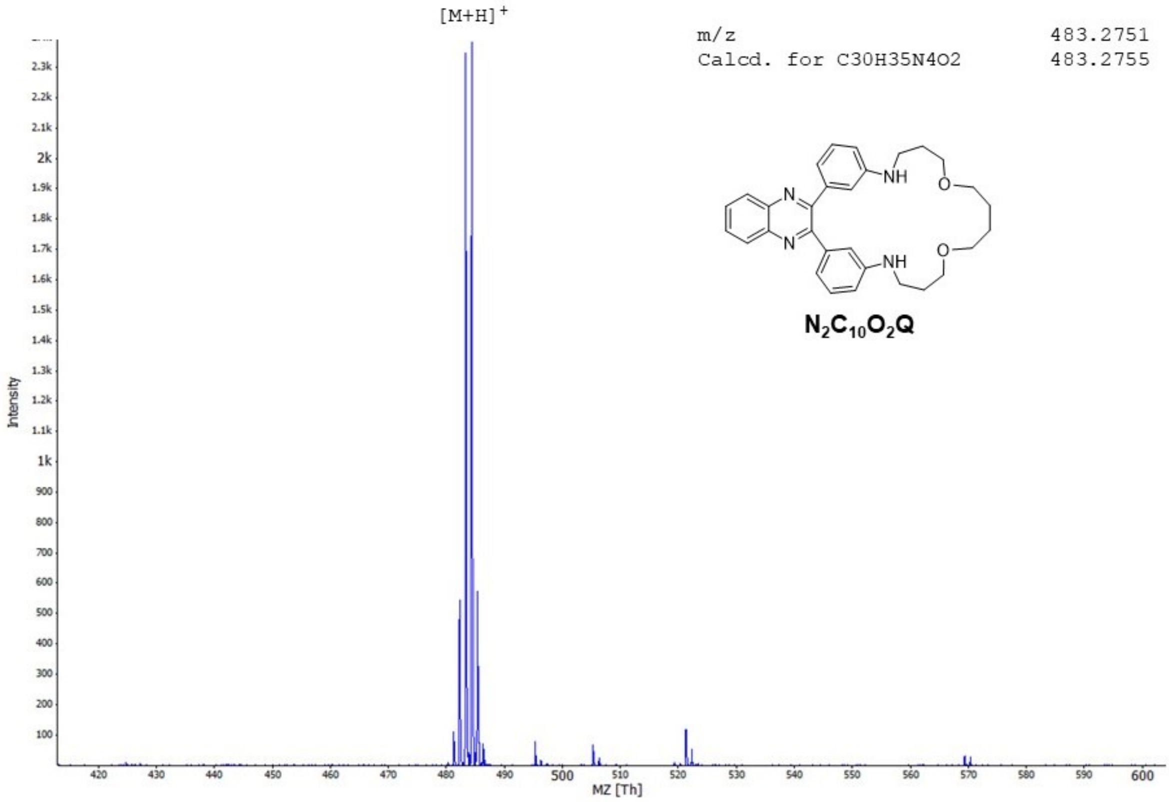



**Fig. S52.** MALDI-TOF spectrum of $N_2C_{10}O_2Q$. Matrix: 1,8,9-trihydroxyanthracene. Calibration standard: PEG-500.

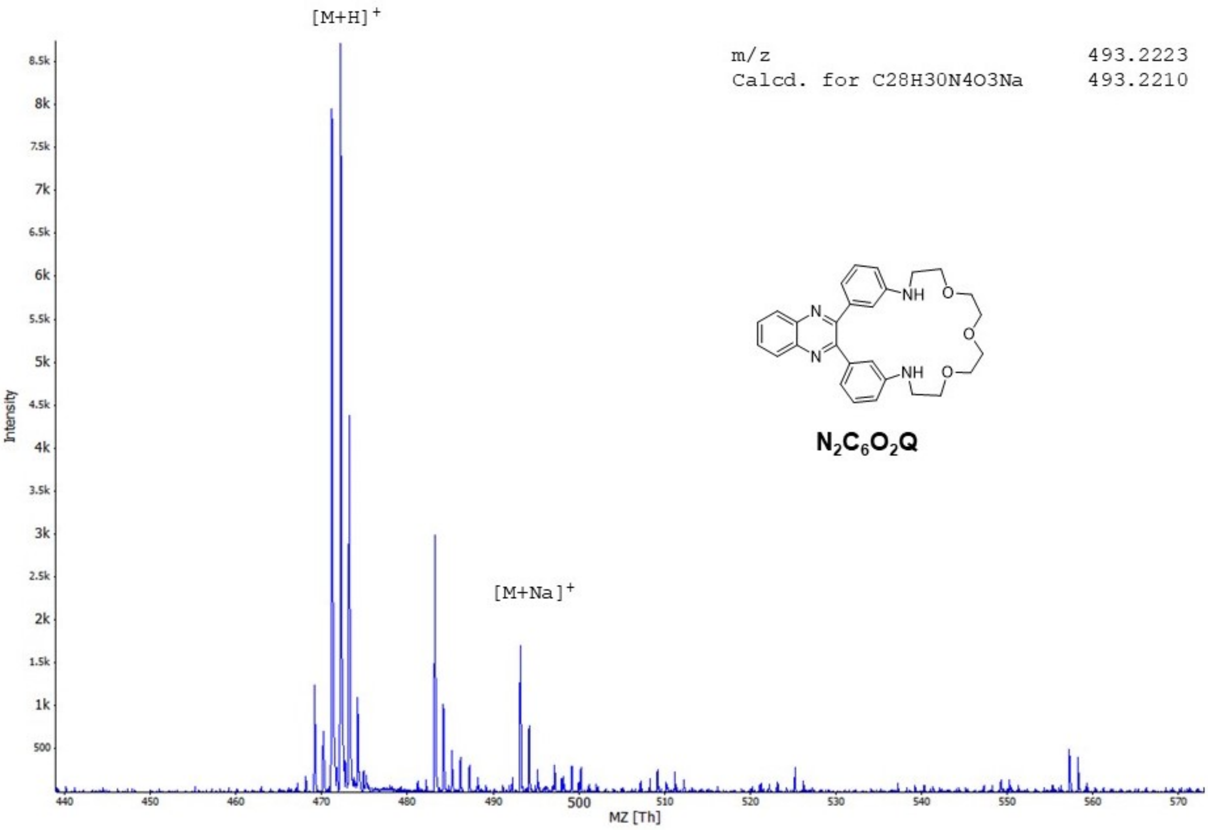



**Fig. S53.** MALDI-TOF spectrum of $N_2C_8O_3Q$. Matrix: 1,8,9-trihydroxyanthracene. Calibration standard: PEG-500.

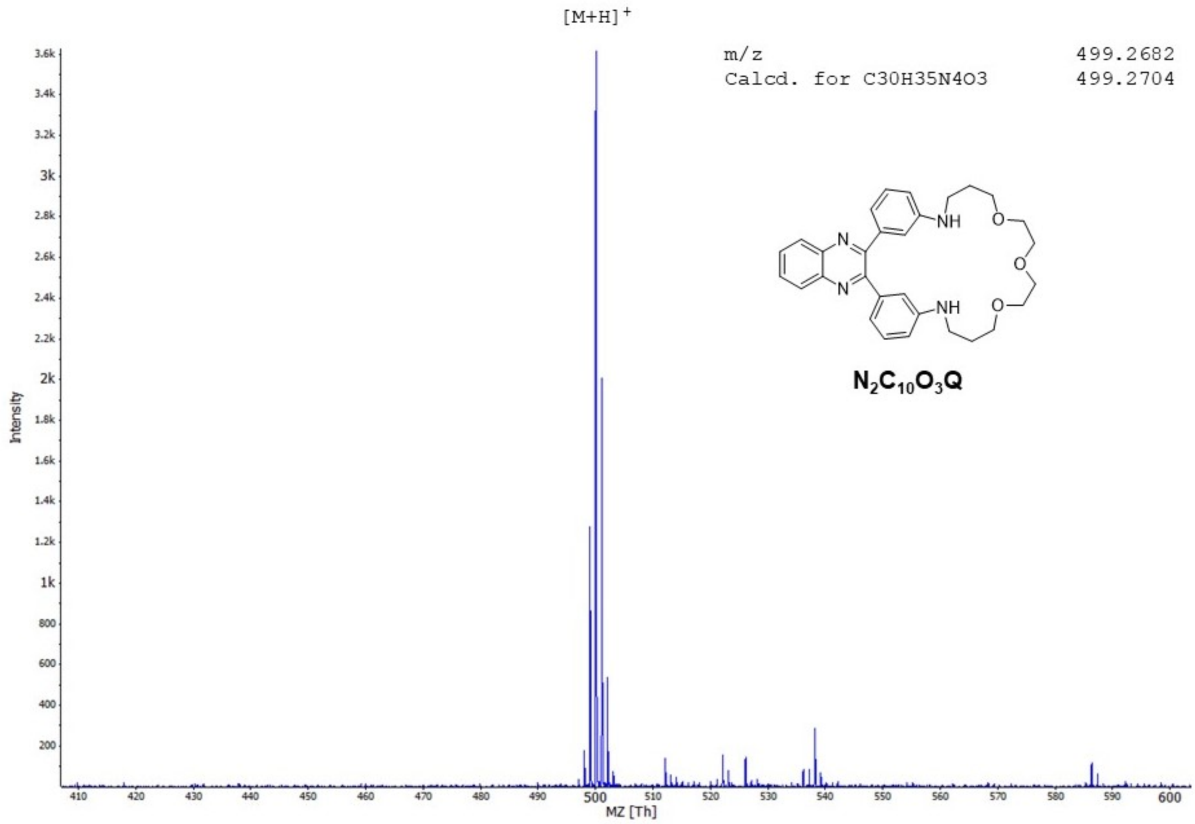



**Fig. S54.** MALDI-TOF spectrum of $N_2C_{10}O_3Q$. Matrix: 1,8,9-trihydroxyanthracene. Calibration standard: PEG-500.

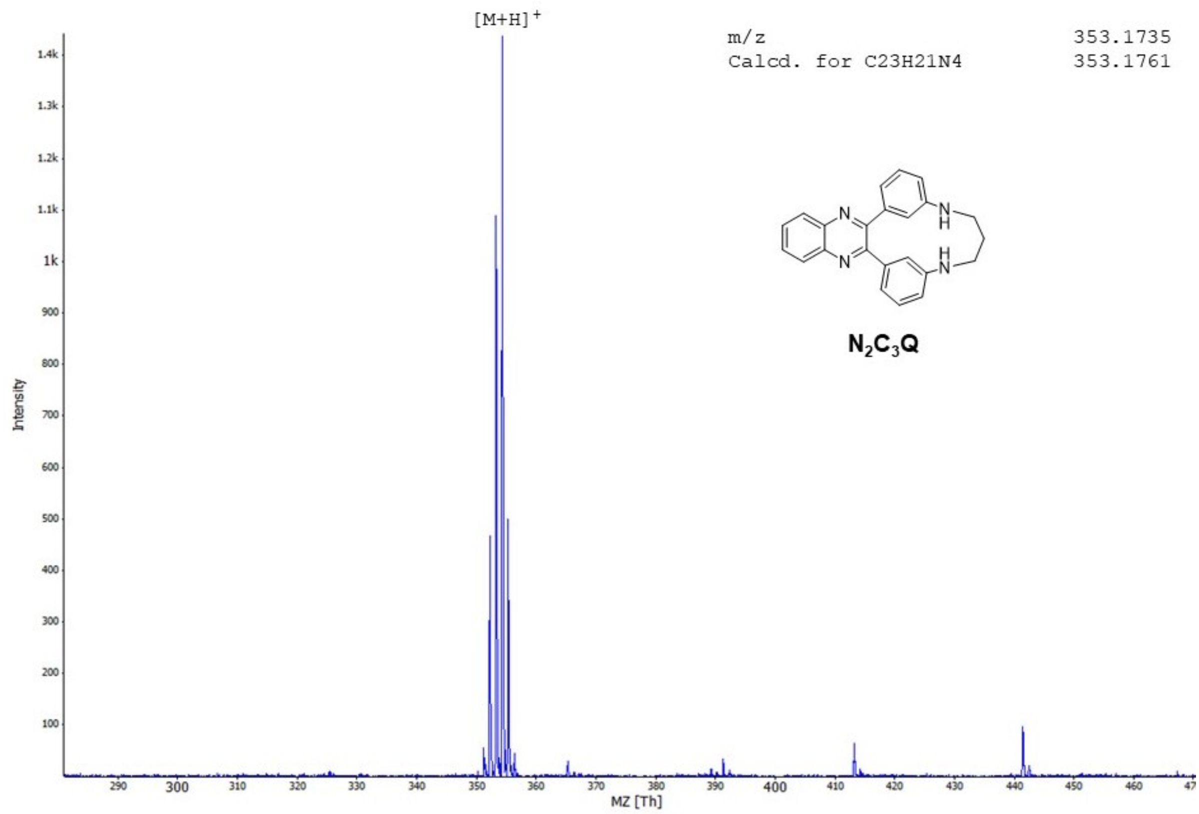



**Fig. S55.** MALDI-TOF spectrum of $N_2C_3Q$. Matrix: 1,8,9-trihydroxyanthracene. Calibration standard: PEG-400.

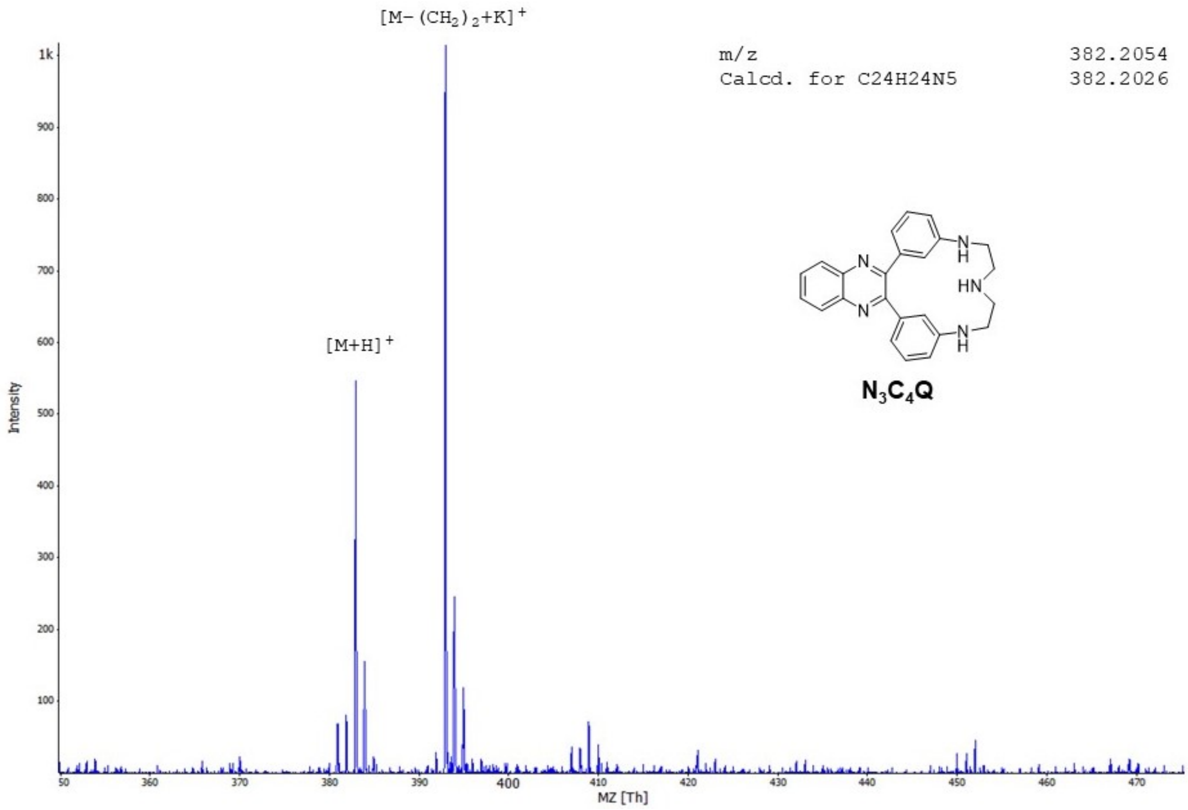



**Fig. S56.** MALDI-TOF spectrum of $N_3C_4Q$. Matrix: 1,8,9-trihydroxyanthracene. Calibration standard: PEG-400.

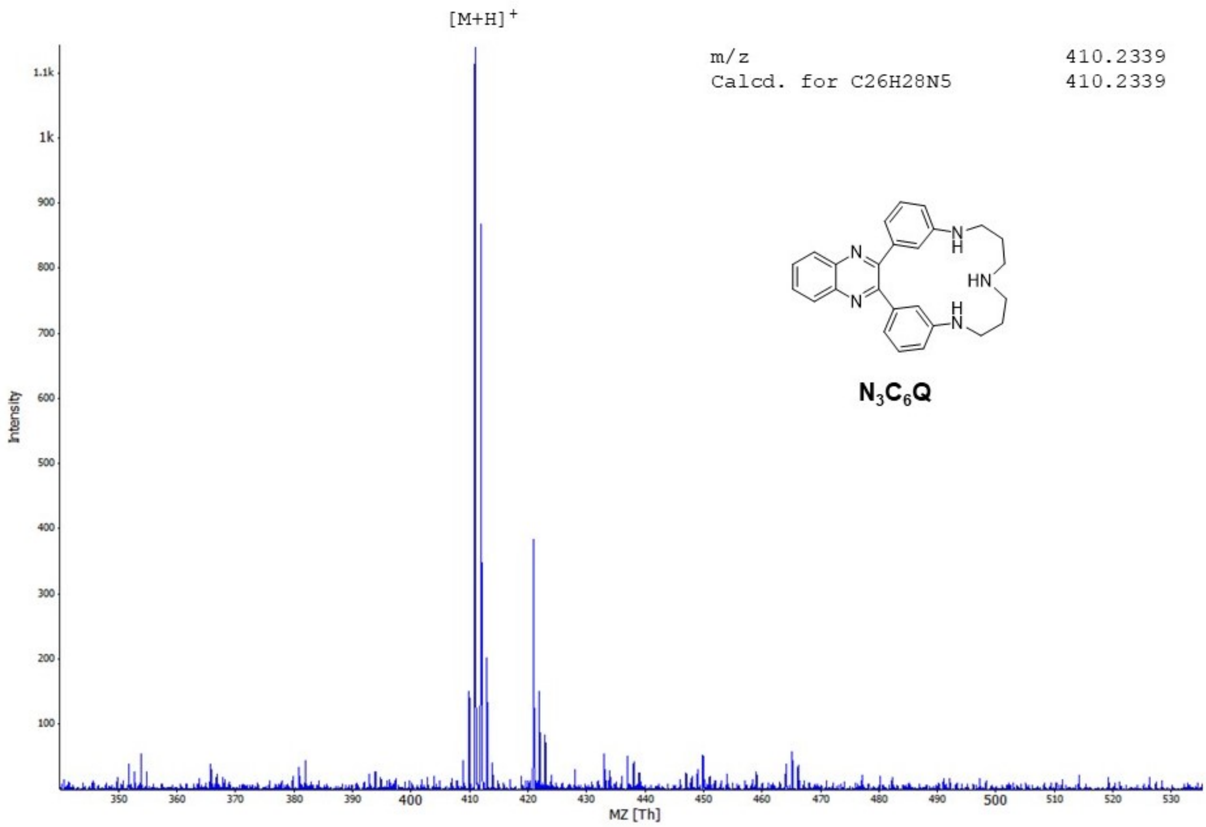



**Fig. S57.** MALDI-TOF spectrum of $N_3C_6Q$. Matrix: 1,8,9-trihydroxyanthracene. Calibration standard: PEG-400.

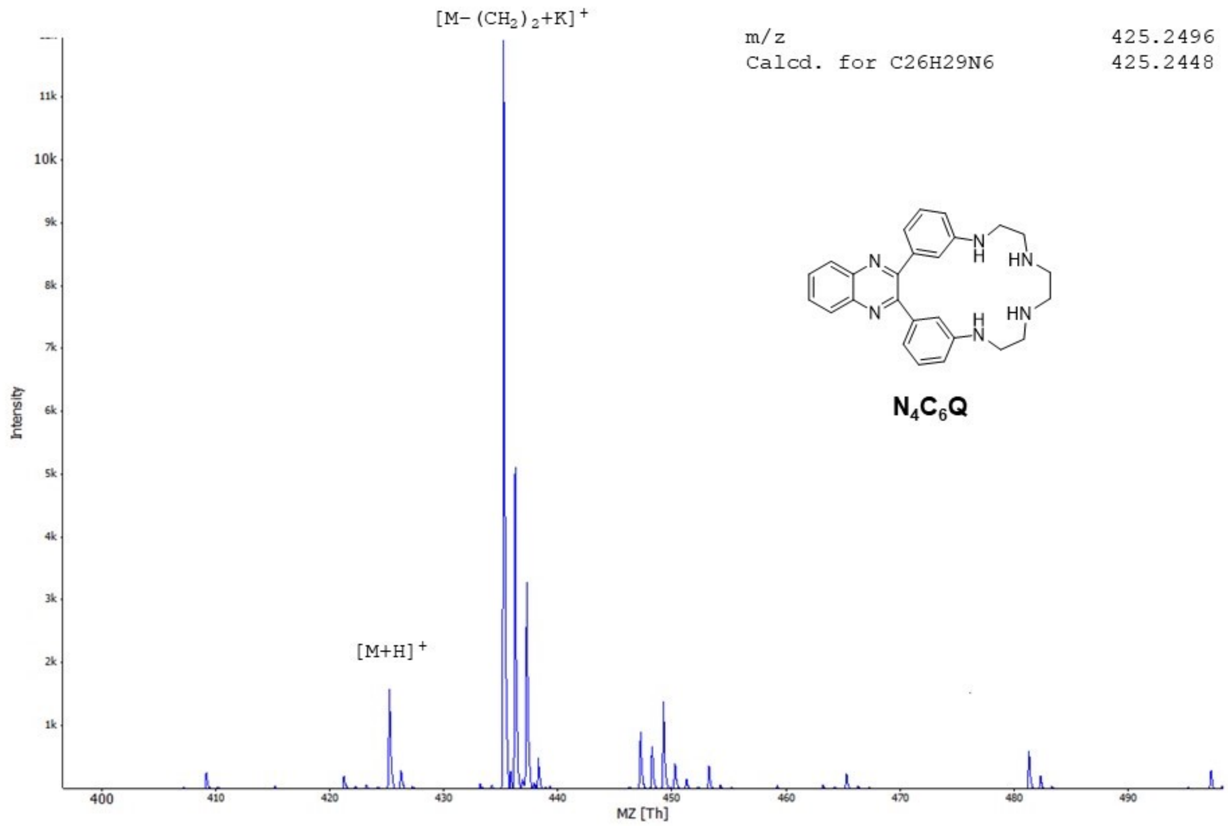



**Fig. S58.** MALDI-TOF spectrum of $N_4C_6Q$. Matrix: 1,8,9-trihydroxyanthracene. Calibration standard: PEG-400.

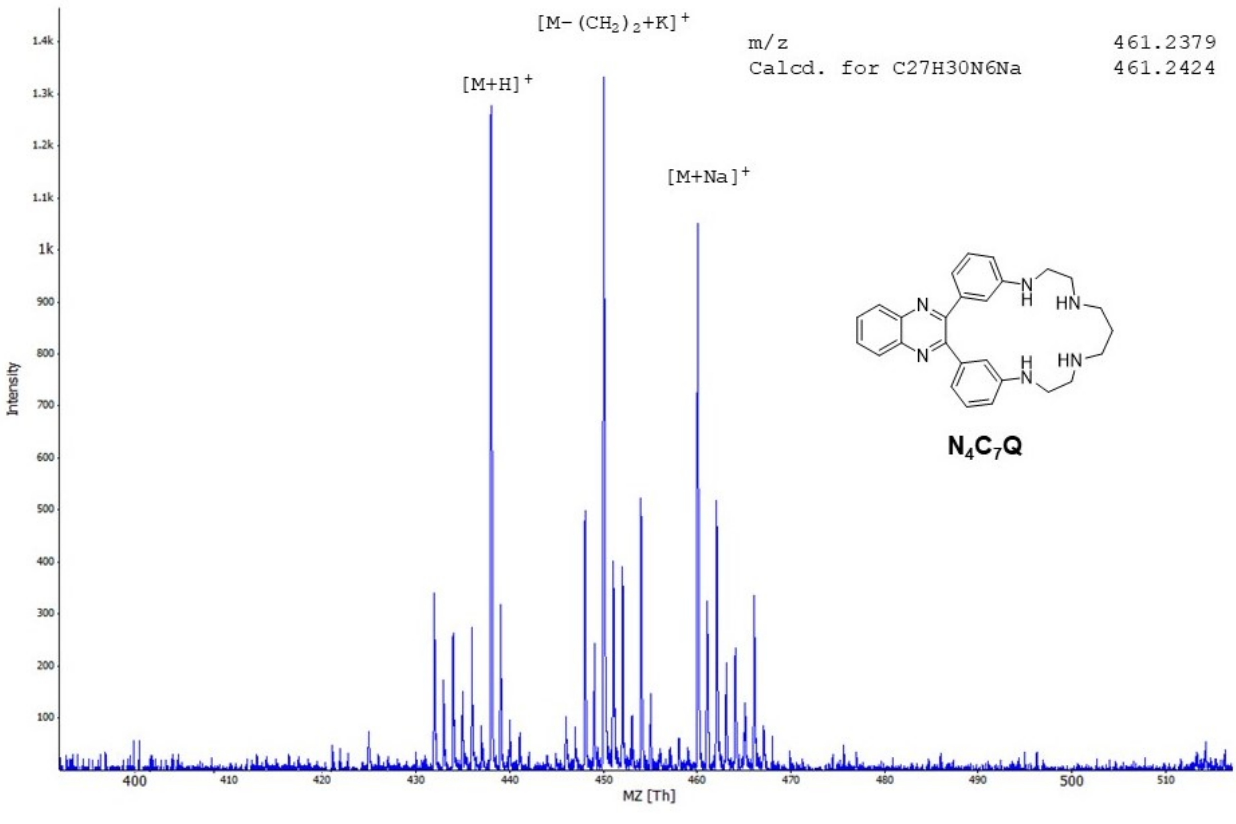



**Fig. S59.** MALDI-TOF spectrum of the compound $N_4C_7Q$. Matrix: 1,8,9-trihydroxyanthracene. Calibration standard: PEG-500.

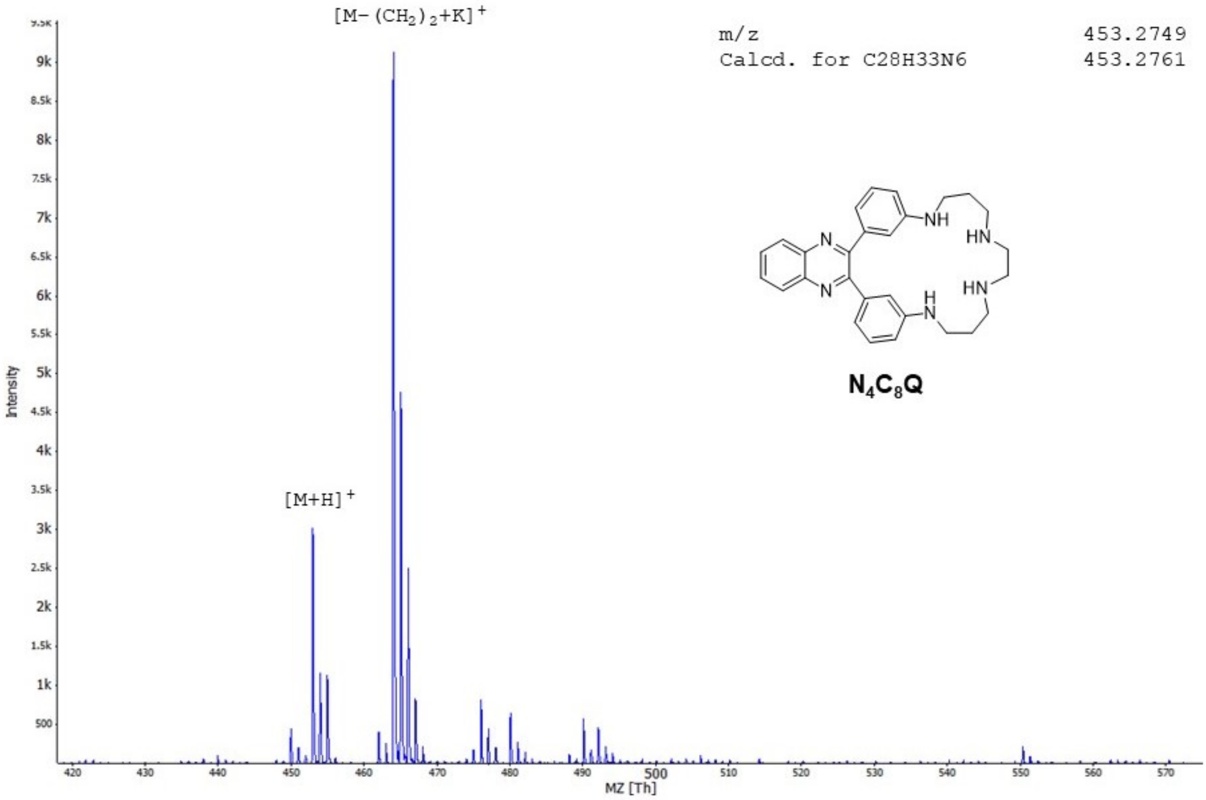



**Fig. S60.** MALDI-TOF spectrum of $N_4C_8Q$. Matrix: 1,8,9-trihydroxyanthracene. Calibration standard: PEG-500.

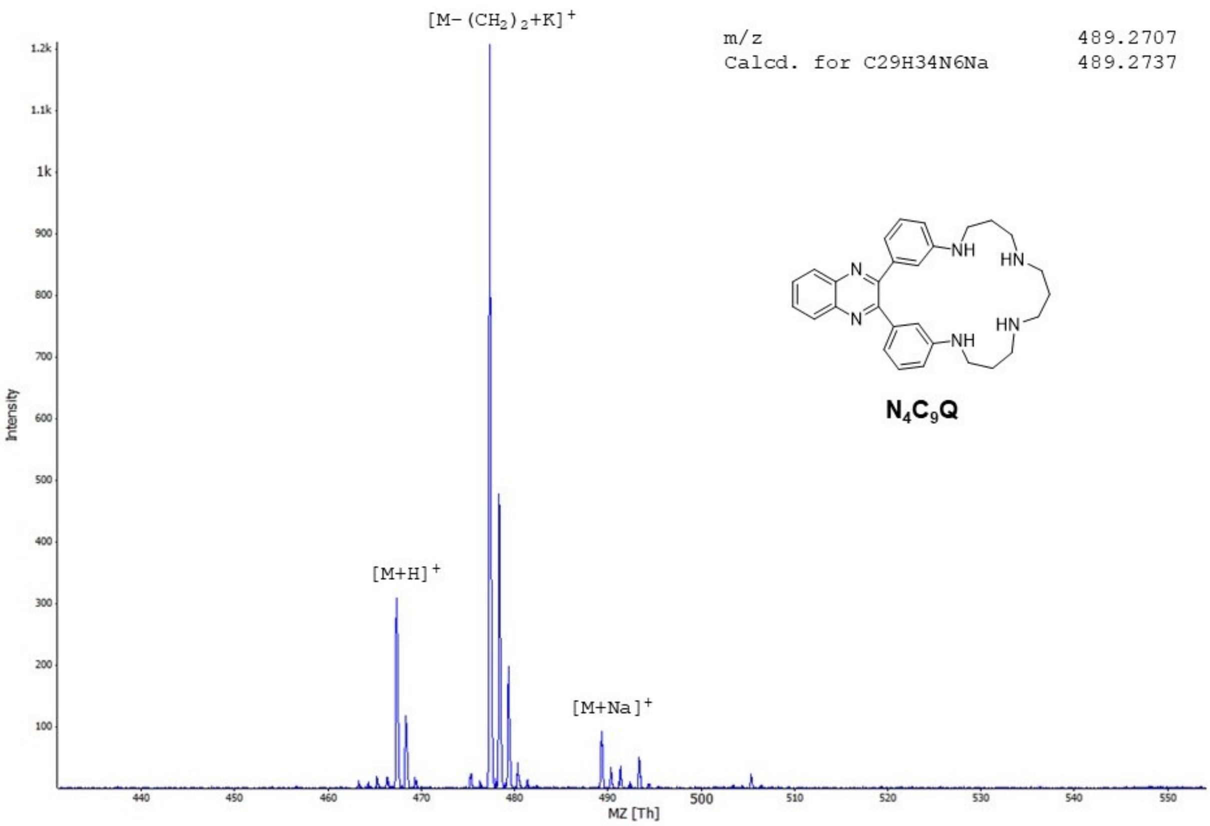



**Fig. S61.** MALDI-TOF spectrum of $N_4C_9Q$. Matrix: 1,8,9-trihydroxyanthracene. Calibration standard: PEG-500.

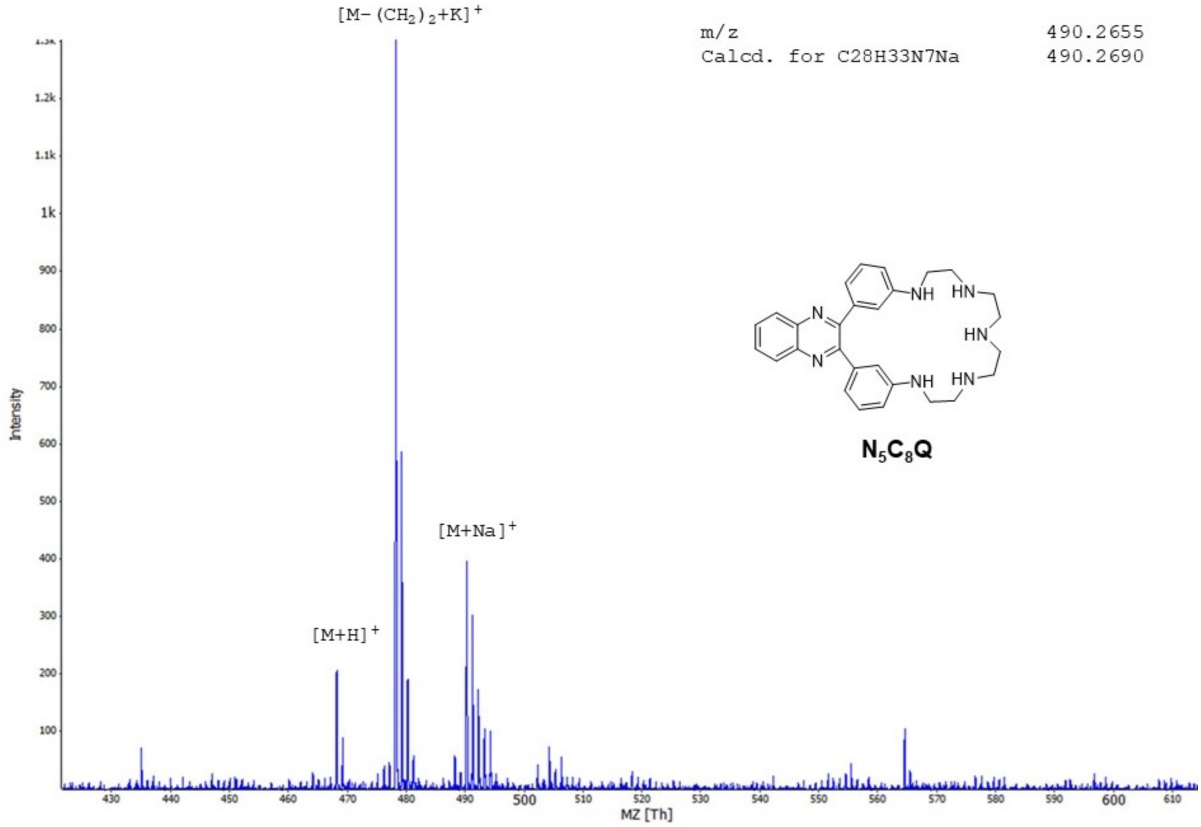



**Fig. S62.** MALDI-TOF spectrum of $N_5C_8Q$. Matrix: 1,8,9-trihydroxyanthracene. Calibration standard: PEG-500.

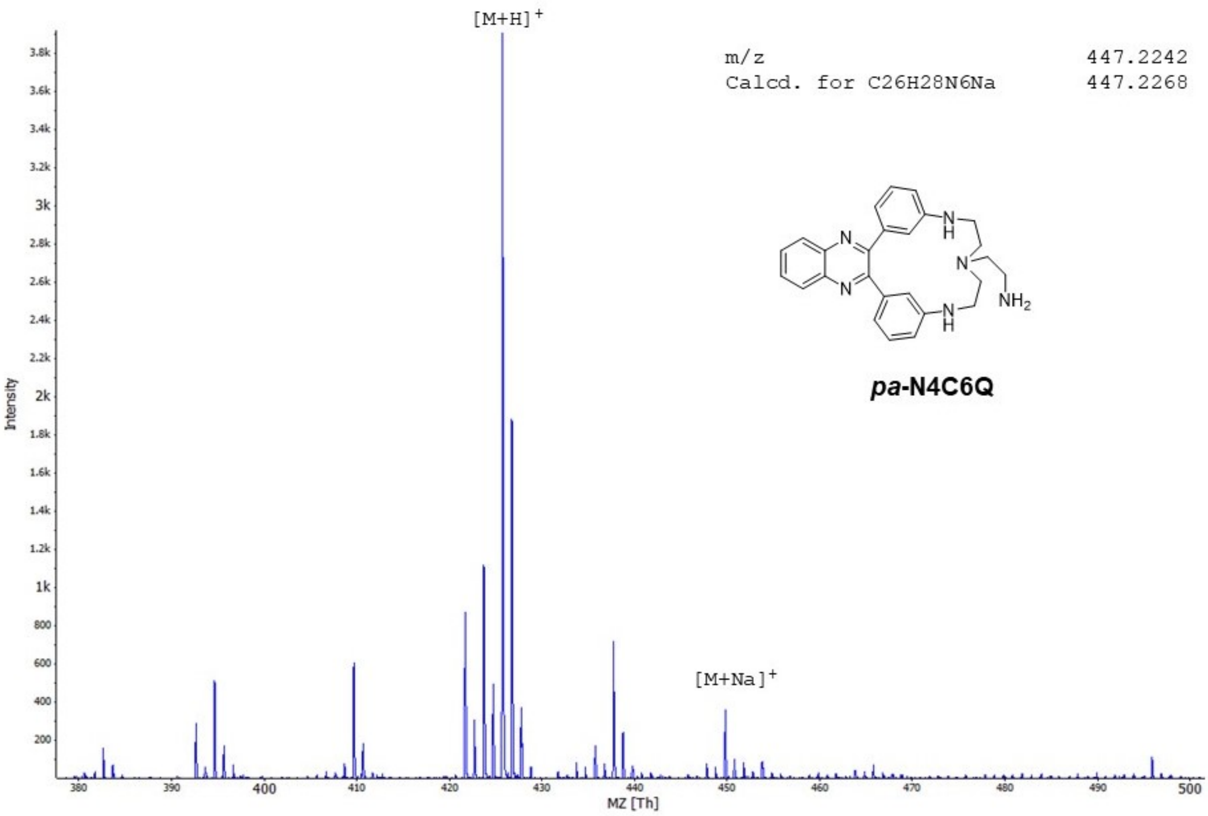



**Fig. S63.** MALDI-TOF spectrum of *pa*-$N_4C_6Q$. Matrix: 1,8,9-trihydroxyanthracene. Calibration standard: PEG-400.

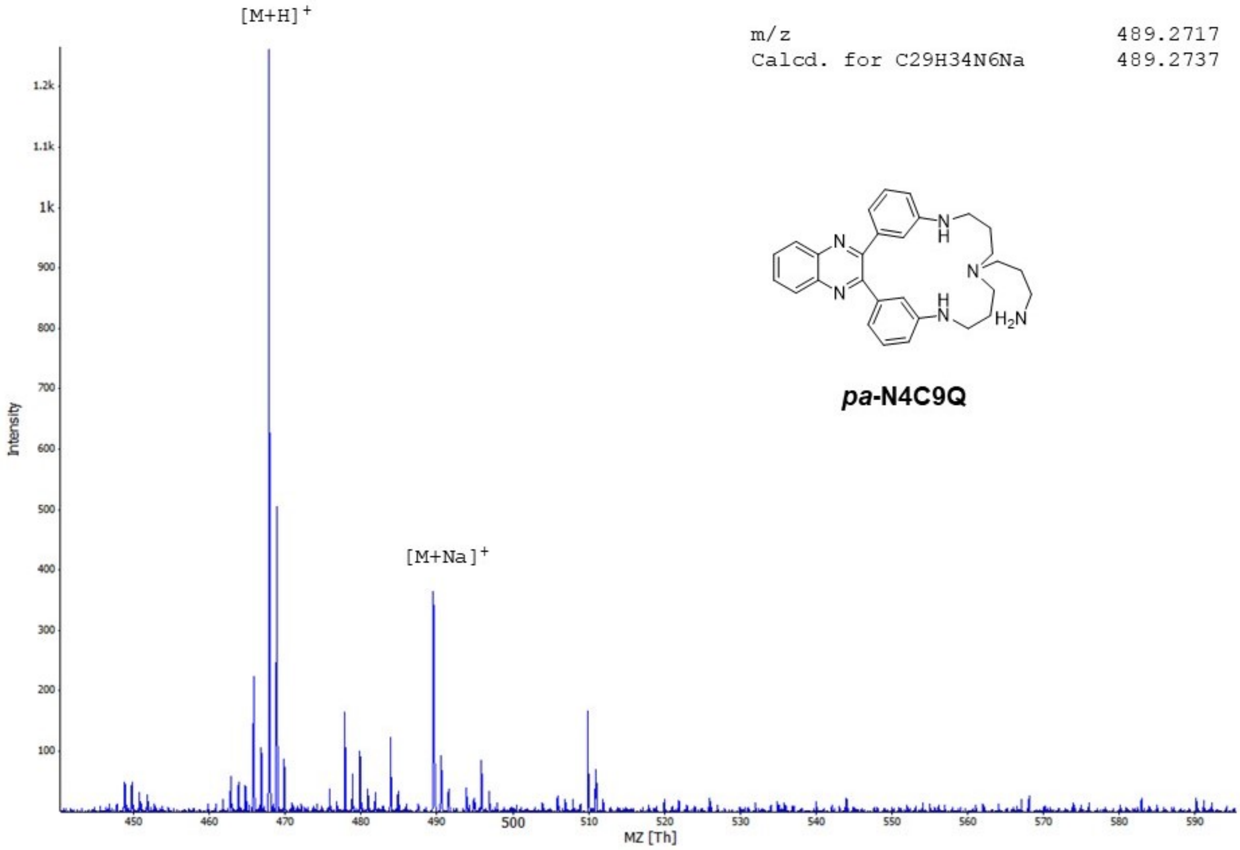
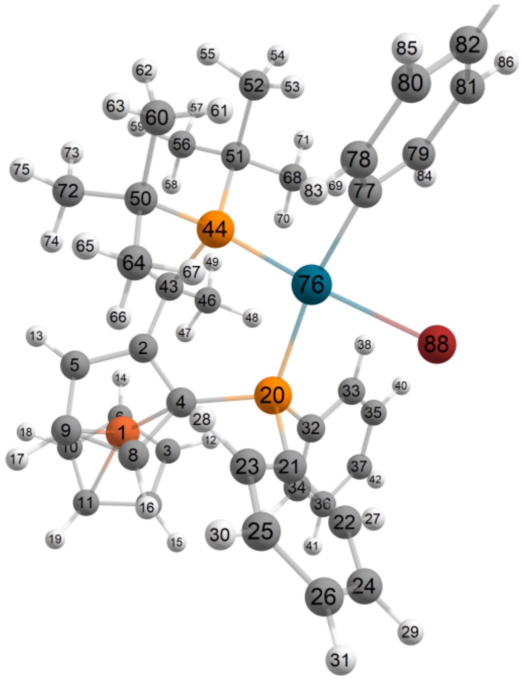



**Fig. S64.** MALDI-TOF spectrum of *pa*-$N_4C_9$Q. Matrix: 1,8,9-trihydroxyanthracene. Calibration standard: PEG-500.

## 10. Atomic coordinates obtained by DFT computations

*Molecular structures of DFT-optimized intermediates of the macrocyclization reaction*

**PhPdBr(PhPF-tBu)**

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| 3 | 6 | -3.937611665 | -3.613004471 | 0.778888742 |
| 4 | 6 | -1.269459286 | -1.851628493 | -0.819428815 |
| 5 | 6 | -2.368259671 | 0.004124529 | 0.033916341 |
| 6 | 6 | -4.737196658 | -2.440655377 | 0.950206923 |
| 7 | 6 | -2.982974073 | -3.653051042 | 1.843141502 |
| 8 | 6 | -0.710229013 | -1.535741153 | 0.470915269 |
| 9 | 6 | -1.373408252 | -0.382664734 | 0.985281690 |
| 10 | 6 | -4.270529777 | -1.750585009 | 2.112316946 |
| 11 | 6 | -3.187539011 | -2.502839338 | 2.665798847 |
| 12 | 1 | -4.024346757 | -4.343429661 | -0.024007315 |
| 13 | 1 | -3.072866999 | 0.827836110 | 0.148514595 |
| 14 | 1 | -5.557862999 | -2.120223132 | 0.308544675 |
| 15 | 1 | -2.224684536 | -4.419192986 | 1.997405049 |
| 16 | 1 | 0.099366142 | -2.077880331 | 0.955174203 |
| 17 | 1 | -1.184565047 | 0.090779602 | 1.948565682 |
| 18 | 1 | -4.659880212 | -0.808090590 | 2.498166928 |
| 19 | 1 | -2.602956614 | -2.232364825 | 3.545531837 |
| 20 | 15 | -0.529601594 | -2.932101845 | -2.124100905 |
| 21 | 6 | 1.185390593 | -3.187951717 | -1.456355418 |
| 22 | 6 | 1.758284188 | -4.462132347 | -1.322450055 |
| 23 | 6 | 1.969775684 | -2.058901991 | -1.160142527 |
| 24 | 6 | 3.074347703 | -4.603973191 | -0.866734543 |
| 25 | 6 | 3.284756511 | -2.202104135 | -0.708687932 |
| 26 | 6 | 3.841157373 | -3.477369077 | -0.553984933 |
| 27 | 1 | 1.187004265 | -5.351827806 | -1.592217052 |
| 28 | 1 | 1.554604494 | -1.056553720 | -1.285178008 |
| 29 | 1 | 3.503178202 | -5.606347306 | -0.768586998 |
| 30 | 1 | 3.878041933 | -1.310186171 | -0.482812047 |
| 31 | 1 | 4.871552484 | -3.590601752 | -0.201898879 |
| 32 | 6 | -1.338982473 | -4.591587146 | -1.990865690 |
| 33 | 6 | -1.950129450 | -5.145435057 | -3.126136654 |
| 34 | 6 | -1.354012447 | -5.314478721 | -0.786288830 |
| 35 | 6 | -2.584328088 | -6.391159636 | -3.053660175 |

| | | | | |
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| 37 | 6 | -2.600222603 | -7.103336143 | -1.849510168 |
| 38 | 1 | -1.902280606 | -4.600842907 | -4.072262930 |
| 39 | 1 | -0.868634360 | -4.901986299 | 0.101564777 |
| 40 | 1 | -3.054952145 | -6.810101148 | -3.948736305 |
| 41 | 1 | -1.975740025 | -7.120441037 | 0.227193914 |
| 42 | 1 | -3.088676878 | -8.081678277 | -1.794605168 |
| 43 | 6 | -3.099034716 | -0.744940365 | -2.369885793 |
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| 45 | 1 | -3.752105296 | 0.133869530 | -2.252389399 |
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| 50 | 6 | -1.190389925 | 1.382771315 | -3.417278199 |
| 51 | 6 | -3.272883799 | -0.128830237 | -5.327868686 |
| 52 | 6 | -2.698265570 | 0.663508522 | -6.523614507 |
| 53 | 1 | -1.687642402 | 0.342994782 | -6.808177102 |
| 54 | 1 | -3.356740616 | 0.487604592 | -7.393888708 |
| 55 | 1 | -2.694372736 | 1.746380344 | -6.340261033 |
| 56 | 6 | -4.559171757 | 0.594575457 | -4.878038841 |
| 57 | 1 | -5.234972435 | 0.675982261 | -5.749882143 |
| 58 | 1 | -5.117569789 | 0.067456440 | -4.089745060 |
| 59 | 1 | -4.360402374 | 1.621413888 | -4.530764676 |
| 60 | 6 | -0.675510445 | 2.158179878 | -4.649583477 |
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| 62 | 1 | -1.485448321 | 2.685145595 | -5.172523249 |
| 63 | 1 | 0.032090898 | 2.930317595 | -4.294534174 |
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| 65 | 1 | 0.538336927 | 2.031967632 | -2.278010174 |
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| 69 | 1 | -2.726316581 | -2.060396673 | -6.212048155 |
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| 74 | 1 | -2.464963227 | 1.910586818 | -1.684317580 |
| 75 | 1 | -1.638241501 | 3.270049158 | -2.462983614 |
| 76 | 46 | -0.447758248 | -1.989278180 | -4.223589234 |
| 77 | 6 | 0.122165583 | -1.331892435 | -6.037044353 |
| 78 | 6 | 1.181569159 | -0.402334012 | -6.131859904 |
| 79 | 6 | -0.321166611 | -1.889624385 | -7.256550781 |
| 80 | 6 | 1.736349993 | -0.022312772 | -7.362848700 |
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| 84 | 1 | -1.087800042 | -2.670613623 | -7.252818514 |
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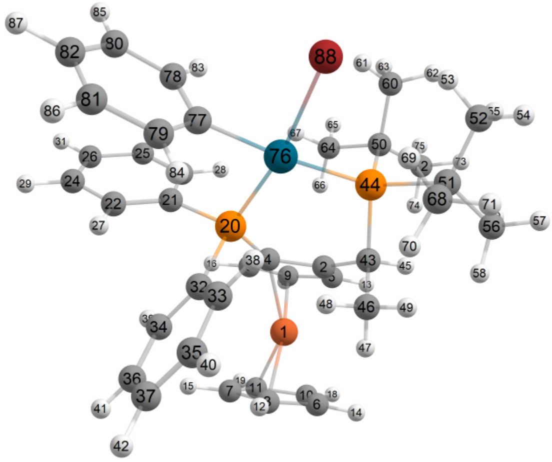
| 86 | 1 | -0.158857134 | -1.974667246 | -9.409865850 |
| 87 | 1 | 1.672908469 | -0.264985747 | -9.520352819 |
| 88 | 35 | 0.982937989 | -3.994663893 | -4.817686960 |

**PhPdBr(PhPF-tBu)**

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| 3 | 6 | -3.992765294 | -3.608084272 | 0.762684049 |
| 4 | 6 | -1.315968872 | -1.828770332 | -0.792430864 |
| 5 | 6 | -2.443251876 | 0.022205689 | 0.040716870 |
| 6 | 6 | -4.798777569 | -2.445184060 | 0.961721321 |
| 7 | 6 | -3.031948566 | -3.662625032 | 1.821133034 |
| 8 | 6 | -0.780729208 | -1.502452168 | 0.507177745 |
| 9 | 6 | -1.460197573 | -0.352791786 | 1.007685947 |
| 10 | 6 | -4.329993396 | -1.774200323 | 2.133954269 |
| 11 | 6 | -3.240054536 | -2.530522937 | 2.667622610 |
| 12 | 1 | -4.080636392 | -4.322735109 | -0.054080262 |
| 13 | 1 | -3.149485525 | 0.848445905 | 0.130205603 |
| 14 | 1 | -5.626172687 | -2.118115870 | 0.332572433 |
| 15 | 1 | -2.268012802 | -4.426909187 | 1.954483209 |
| 16 | 1 | 0.018840840 | -2.039554647 | 1.012336503 |
| 17 | 1 | -1.288102353 | 0.124526073 | 1.972126838 |
| 18 | 1 | -4.723915424 | -0.842075716 | 2.539838473 |
| 19 | 1 | -2.652704908 | -2.273581553 | 3.549597326 |
| 20 | 15 | -0.537905251 | -2.946697427 | -2.051084915 |
| 21 | 6 | 1.141139195 | -3.247895509 | -1.313652557 |
| 22 | 6 | 1.711198202 | -4.530771841 | -1.280983036 |
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| 36 | 6 | -2.020901832 | -6.578482596 | -0.661194108 |
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| 44 | 15 | -2.042712741 | -0.435574903 | -3.879307593 |

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| 45 | 1 | -3.792553880 | 0.163584031 | -2.236388118 |
| 46 | 6 | -4.093578520 | -1.943851406 | -2.553685683 |
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| 55 | 1 | -2.787458847 | 1.834551091 | -6.115905171 |
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| 61 | 1 | 0.278041757 | 0.875323268 | -5.223706181 |
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| 63 | 1 | 0.430929543 | 2.463398599 | -4.420935416 |
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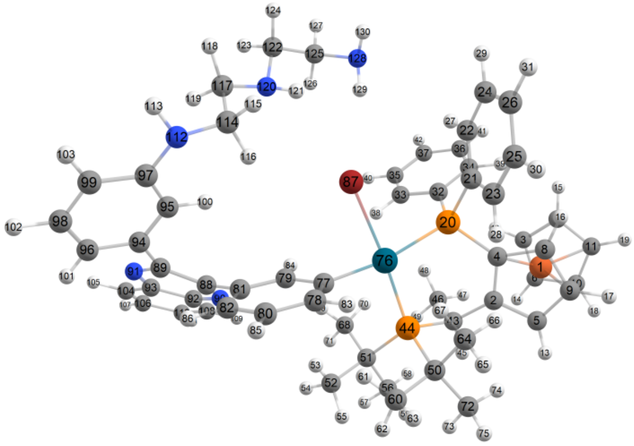
| 71 | 1 | -4.565553580 | -1.340871287 | -6.627346880 |
| 72 | 6 | -2.001327997 | 2.363297226 | -3.035252089 |
| 73 | 1 | -2.711756667 | 2.683555814 | -3.814321514 |
| 74 | 1 | -2.571501459 | 2.103800461 | -2.127852755 |
| 75 | 1 | -1.379663739 | 3.244083405 | -2.785889701 |
| 76 | 46 | -0.487720355 | -2.164533405 | -4.137120834 |
| 77 | 6 | 0.972217133 | -3.510842795 | -4.459986069 |
| 78 | 6 | 2.319960721 | -3.101145781 | -4.367266699 |
| 79 | 6 | 0.742121663 | -4.834794184 | -4.882561237 |
| 80 | 6 | 3.377771495 | -3.963162186 | -4.675920457 |
| 81 | 6 | 1.797303517 | -5.707493366 | -5.189050838 |
| 82 | 6 | 3.123993626 | -5.278935683 | -5.083938947 |
| 83 | 1 | 2.557404417 | -2.077858290 | -4.057864160 |
| 84 | 1 | -0.280137860 | -5.205484956 | -5.001416693 |
| 85 | 1 | 4.409324106 | -3.601312989 | -4.597555788 |
| 86 | 1 | 1.573384317 | -6.728446341 | -5.519923591 |
| 87 | 1 | 3.949505986 | -5.956855857 | -5.326037046 |
| 88 | 35 | -0.094078479 | -1.609871808 | -6.572314149 |

## Intermediate A isomer



| | | | | |
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| 3 | 6 | 0.431839605 | -0.323655603 | 0.873578934 |
| 4 | 6 | 1.078307810 | 1.926937032 | -1.828245643 |
| 5 | 6 | -0.615703795 | 3.153014347 | -0.825805348 |
| 6 | 6 | -0.805785948 | 0.298536993 | 1.225186540 |
| 7 | 6 | 1.489502748 | 0.437765214 | 1.463275806 |
| 8 | 6 | 1.669826540 | 2.866087172 | -0.908628379 |
| 9 | 6 | 0.627738309 | 3.631533489 | -0.307377664 |
| 10 | 6 | -0.514189190 | 1.448734568 | 2.023014379 |
| 11 | 6 | 0.905601681 | 1.532024560 | 2.172951518 |
| 12 | 1 | 0.556210295 | -1.211150616 | 0.255098839 |
| 13 | 1 | -1.604936758 | 3.506126824 | -0.534206079 |
| 14 | 1 | -1.801401048 | -0.036925153 | 0.935174279 |
| 15 | 1 | 2.555077247 | 0.229118203 | 1.380527813 |
| 16 | 1 | 2.736175829 | 2.981467668 | -0.725259612 |
| 17 | 1 | 0.754706127 | 4.410419058 | 0.444324841 |
| 18 | 1 | -1.244458073 | 2.149542297 | 2.428381690 |
| 19 | 1 | 1.448494077 | 2.310299328 | 2.709973323 |
| 20 | 15 | 1.931272852 | 1.015776146 | -3.188287772 |
| 21 | 6 | 3.603742467 | 1.825520276 | -3.190005936 |
| 22 | 6 | 4.798768709 | 1.093016506 | -3.112573261 |
| 23 | 6 | 3.672704390 | 3.219008129 | -3.367191491 |
| 24 | 6 | 6.035262106 | 1.747349807 | -3.174705930 |
| 25 | 6 | 4.907879222 | 3.869424427 | -3.434235664 |
| 26 | 6 | 6.095943091 | 3.135451231 | -3.331935820 |
| 27 | 1 | 4.778938821 | 0.004830729 | -3.026760078 |
| 28 | 1 | 2.753918106 | 3.802776911 | -3.460224612 |
| 29 | 1 | 6.955669895 | 1.158349087 | -3.108219215 |
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| 31 | 1 | 7.064154704 | 3.643607009 | -3.385324135 |
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| 33 | 6 | 1.790152995 | -1.780743609 | -3.403671562 |
| 34 | 6 | 2.940663500 | -0.990399706 | -1.425339475 |
| 35 | 6 | 2.011702672 | -3.103504000 | -3.003968611 |
| 36 | 6 | 3.170557013 | -2.311641401 | -1.030442077 |
| 37 | 6 | 2.702139297 | -3.372159324 | -1.817431417 |
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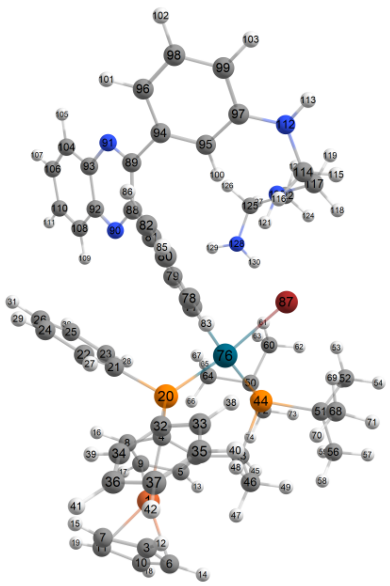
| 128 | 7 | 6.189606855 | -1.998519839 | -5.363177154 |
| 129 | 1 | 5.392189478 | -1.360682323 | -5.470017116 |
| 130 | 1 | 7.038791828 | -1.444147740 | -5.519852963 |

## Intermediate A isomer



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| 3 | 6 | 0.374200790 | 5.761196301 | -0.516460281 |
| 4 | 6 | 0.489539303 | 4.081330981 | -3.686089607 |
| 5 | 6 | -1.727552770 | 4.767646185 | -3.771637096 |
| 6 | 6 | -1.048948373 | 5.889678963 | -0.518236322 |
| 7 | 6 | 0.911159093 | 6.812067858 | -1.325536649 |
| 8 | 6 | 0.419616765 | 5.352389669 | -4.366011346 |
| 9 | 6 | -0.944422531 | 5.760749080 | -4.436941559 |
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| 11 | 6 | -0.179702930 | 7.584212488 | -1.830332376 |
| 12 | 1 | 0.952191260 | 4.993932238 | -0.003636441 |
| 13 | 1 | -2.808314215 | 4.792028617 | -3.627613897 |
| 14 | 1 | -1.755915524 | 5.243863191 | 0.002094752 |

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| 15 | 1 | 1.965339210 | 6.991258190 | -1.530778577 |
| 16 | 1 | 1.268459648 | 5.898457518 | -4.770015460 |
| 17 | 1 | -1.315102475 | 6.684261885 | -4.881458039 |
| 18 | 1 | -2.402821116 | 7.358644396 | -1.554978214 |
| 19 | 1 | -0.102415561 | 8.442486465 | -2.498410734 |
| 20 | 15 | 1.924608698 | 2.906324650 | -3.710305910 |
| 21 | 6 | 3.079286781 | 3.732753262 | -4.904698586 |
| 22 | 6 | 4.442624026 | 3.906955001 | -4.618880126 |
| 23 | 6 | 2.603939640 | 4.096816636 | -6.177432237 |
| 24 | 6 | 5.300786498 | 4.473572213 | -5.568364331 |
| 25 | 6 | 3.461610654 | 4.665701691 | -7.121130848 |
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| 27 | 1 | 4.850473961 | 3.583166601 | -3.660116637 |
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| 29 | 1 | 6.360892853 | 4.597826923 | -5.326384257 |
| 30 | 1 | 3.072473299 | 4.942651095 | -8.105209755 |
| 31 | 1 | 5.485937919 | 5.301272761 | -7.562285365 |
| 32 | 6 | 2.778831901 | 3.050615139 | -2.069712491 |
| 33 | 6 | 2.871155328 | 1.914745933 | -1.250792290 |
| 34 | 6 | 3.329002242 | 4.262237514 | -1.619163559 |
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| 37 | 6 | 4.037627156 | 3.197956781 | 0.443055073 |
| 38 | 1 | 2.446205044 | 0.972267022 | -1.610604988 |
| 39 | 1 | 3.273624793 | 5.152107123 | -2.250393123 |
| 40 | 1 | 3.551805193 | 1.093194524 | 0.629215870 |
| 41 | 1 | 4.389532938 | 5.283202073 | -0.036381784 |
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| 43 | 6 | -1.321204956 | 2.445270691 | -2.656200336 |
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| 56 | 6 | -3.033408549 | -0.042424881 | -1.955962225 |
| 57 | 1 | -3.496568108 | -0.916413078 | -1.461757591 |
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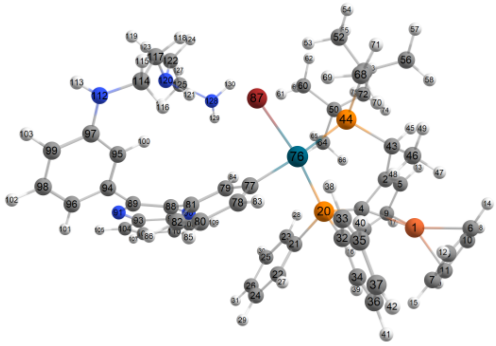
## Intermediate D isomer



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| 41 | 1 | 4.389532938 | 5.283202073 | -0.036381784 |
| 42 | 1 | 4.529413258 | 3.255917044 | 1.419283065 |
| 43 | 6 | -1.321204956 | 2.445270691 | -2.656200336 |
| 44 | 15 | -0.887989103 | 0.901740622 | -3.715486954 |
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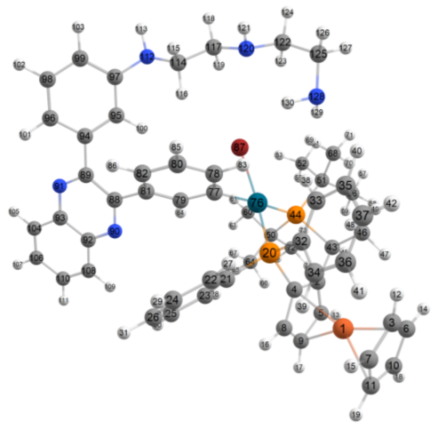
## Intermediate D isomer



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| 20 | 15 | 1.368158375 | 3.360950997 | -3.715181190 |
| 21 | 6 | 2.379991649 | 3.902193674 | -5.174547271 |
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| 23 | 6 | 1.714895783 | 4.277851537 | -6.355828559 |
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| 26 | 6 | 3.834675598 | 4.577472934 | -7.492841617 |

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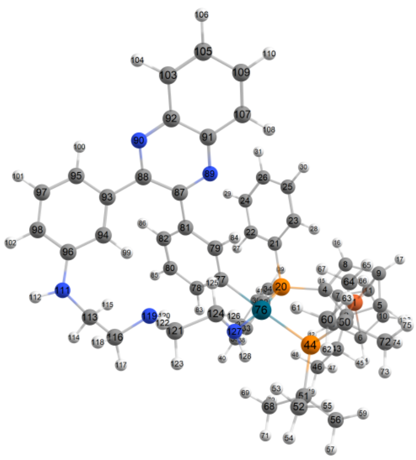
## Intermediate E



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| 51 | 6 | -2.232526149 | -0.781938533 | -3.504621590 |
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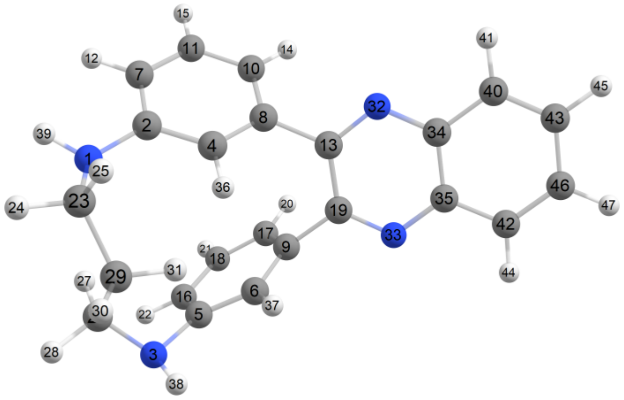
| 53 | 1 | -1.924664857 | -2.140951557 | -5.252454954 |
| 54 | 1 | -3.079848378 | -2.700578136 | -4.024297614 |
| 55 | 1 | -3.549550938 | -1.421780223 | -5.158690334 |
| 56 | 6 | -3.505838193 | -0.345695098 | -2.743783219 |
| 57 | 1 | -4.033180324 | -1.254133889 | -2.397502718 |
| 58 | 1 | -3.306153254 | 0.264430530 | -1.852217250 |
| 59 | 1 | -4.207633207 | 0.209887966 | -3.386032280 |
| 60 | 6 | -2.008221504 | 0.177153620 | -6.987499001 |
| 61 | 1 | -0.978691929 | -0.198929538 | -7.082617574 |
| 62 | 1 | -2.675309302 | -0.672868280 | -6.800405239 |
| 63 | 1 | -2.301033807 | 0.608561179 | -7.962327061 |

| | | | | |
|---|---|---|---|---|
| 64 | 6 | -1.315026788 | 2.483270727 | -6.502856905 |
| 65 | 1 | -1.709351420 | 2.703222129 | -7.512064889 |
| 66 | 1 | -1.401388800 | 3.397863230 | -5.904315063 |
| 67 | 1 | -0.248929574 | 2.222416761 | -6.601252534 |
| 68 | 6 | -1.278013643 | -1.524362296 | -2.538730618 |
| 69 | 1 | -0.414010280 | -1.959214645 | -3.064546345 |
| 70 | 1 | -0.878313867 | -0.877222245 | -1.745134377 |
| 71 | 1 | -1.833565679 | -2.346831939 | -2.049383036 |
| 72 | 6 | -3.580035061 | 1.696612731 | -5.736608575 |
| 73 | 1 | -4.215132041 | 0.851681222 | -5.424224385 |
| 74 | 1 | -3.707071857 | 2.514614411 | -5.008384251 |
| 75 | 1 | -3.979936903 | 2.059756140 | -6.702445544 |
| 76 | 46 | 1.039821000 | 0.480999861 | -4.652067594 |
| 77 | 6 | 2.975659981 | 0.207047353 | -5.160223225 |
| 78 | 6 | 3.950425712 | -0.207575959 | -4.226660069 |
| 79 | 6 | 3.421552528 | 0.361839232 | -6.487176696 |
| 80 | 6 | 5.288915222 | -0.415300637 | -4.593412022 |
| 81 | 6 | 4.742478458 | 0.085529326 | -6.891191134 |
| 82 | 6 | 5.693620856 | -0.274993617 | -5.921093667 |
| 83 | 1 | 3.677450693 | -0.367653136 | -3.180242703 |
| 84 | 1 | 2.729730917 | 0.695742066 | -7.264555078 |
| 85 | 1 | 6.022139009 | -0.699796964 | -3.830153659 |
| 86 | 1 | 6.735277198 | -0.448175882 | -6.200379830 |
| 87 | 6 | 5.083740711 | 0.217376835 | -8.335472462 |
| 88 | 6 | 6.005819490 | -0.663807165 | -9.052221615 |
| 89 | 7 | 4.483479594 | 1.214700157 | -8.968934483 |
| 90 | 7 | 6.343466210 | -0.393532124 | -10.305224632 |
| 91 | 6 | 4.785902717 | 1.451926582 | -10.271731702 |
| 92 | 6 | 5.772184971 | 0.665347629 | -10.936777794 |
| 93 | 6 | 6.626809898 | -1.912868058 | -8.504345537 |
| 94 | 6 | 5.927084181 | -2.818850199 | -7.686686717 |
| 95 | 6 | 7.935824080 | -2.219628410 | -8.926659467 |
| 96 | 6 | 6.535494902 | -4.022752633 | -7.272317899 |
| 97 | 6 | 8.535081140 | -3.413156329 | -8.523619080 |
| 98 | 6 | 7.848684460 | -4.308387736 | -7.701778281 |
| 99 | 1 | 4.894856844 | -2.632658818 | -7.376747834 |
| 100 | 1 | 8.461756109 | -1.522279276 | -9.581307213 |
| 101 | 1 | 9.554828019 | -3.647322182 | -8.847355548 |
| 102 | 1 | 8.330906721 | -5.239259104 | -7.378726546 |
| 103 | 6 | 6.124687793 | 0.971445108 | -12.279912432 |
| 104 | 1 | 6.886234109 | 0.354517080 | -12.766776451 |
| 105 | 6 | 5.498559462 | 2.015476925 | -12.934777798 |
| 106 | 1 | 5.765301065 | 2.250709899 | -13.970096652 |
| 107 | 6 | 4.147355918 | 2.512698530 | -10.970353363 |

*Molecular structures of DFT-optimized conformers of macrocycles*

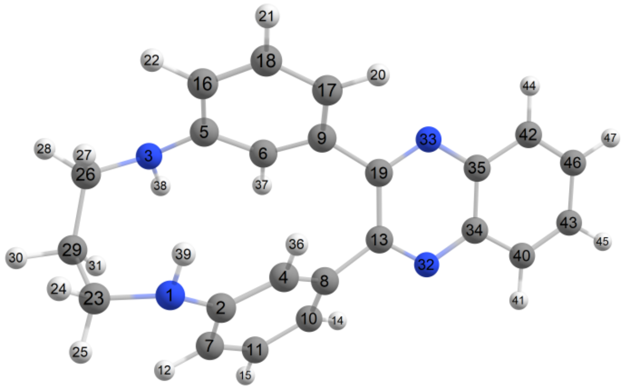
**$N_2C_3Q$ (*syn*-conformer)**




| | | | | |
|---|---|---|---|---|
| 1 | 7 | -0.255606765 | 0.261087946 | -5.478346110 |
| 2 | 6 | 0.553014478 | -0.250616656 | -4.461474174 |
| 3 | 7 | -3.568484030 | 1.686822966 | -3.294937429 |
| 4 | 6 | 0.710687973 | 0.386175048 | -3.223703453 |
| 5 | 6 | -2.949137355 | 0.832016736 | -2.333234279 |
| 6 | 6 | -1.903169520 | 1.259813997 | -1.508430784 |
| 7 | 6 | 1.183591968 | -1.497027903 | -4.639443563 |
| 8 | 6 | 1.397912191 | -0.223351758 | -2.170041046 |
| 9 | 6 | -1.154762697 | 0.341780000 | -0.768966837 |
| 10 | 6 | 2.034758622 | -1.449115757 | -2.371508615 |
| 11 | 6 | 1.922126817 | -2.071770983 | -3.613833791 |
| 12 | 1 | 1.086235829 | -2.012829830 | -5.590194469 |
| 13 | 6 | 1.393852697 | 0.413975255 | -0.818786303 |
| 14 | 1 | 2.586873969 | -1.910382802 | -1.562640807 |
| 15 | 1 | 2.406551893 | -3.027327432 | -3.782134774 |
| 16 | 6 | -3.332376394 | -0.513487970 | -2.291220235 |
| 17 | 6 | -1.538443706 | -1.000171177 | -0.749738454 |
| 18 | 6 | -2.645677719 | -1.414818739 | -1.486303680 |
| 19 | 6 | 0.146704766 | 0.751879056 | -0.152568203 |
| 20 | 1 | -0.959879473 | -1.718473837 | -0.180813750 |
| 21 | 1 | -2.954766558 | -2.453586618 | -1.455429463 |
| 22 | 1 | -4.165186003 | -0.835141442 | -2.905599772 |
| 23 | 6 | -0.539066954 | 1.680603365 | -5.694048070 |
| 24 | 1 | -0.887081273 | 1.761580826 | -6.727661066 |
| 25 | 1 | 0.380201303 | 2.280745300 | -5.624371751 |
| 26 | 6 | -2.948945334 | 1.581864989 | -4.640277657 |
| 27 | 1 | -2.810561585 | 0.519846927 | -4.849427058 |
| 28 | 1 | -3.661847841 | 1.967655964 | -5.374808111 |
| 29 | 6 | -1.593273904 | 2.315024567 | -4.763043725 |
| 30 | 1 | -1.754688801 | 3.340740636 | -5.114615400 |
| 31 | 1 | -1.168067300 | 2.411318826 | -3.765161083 |
| 32 | 7 | 2.552710565 | 0.642632447 | -0.240819847 |
| 33 | 7 | 0.132011448 | 1.380521637 | 0.998982051 |
| 34 | 6 | 2.550577317 | 1.264178028 | 0.970288454 |
| 35 | 6 | 1.330510787 | 1.668984401 | 1.580603351 |
| 36 | 1 | 0.256601702 | 1.347598568 | -3.053928112 |
| 37 | 1 | -1.601760589 | 2.302362945 | -1.517699482 |
| 38 | 1 | -3.538195323 | 2.652237795 | -2.982684974 |
| 39 | 1 | -0.161739884 | -0.253384779 | -6.340199779 |
| 40 | 6 | 3.777811380 | 1.535628138 | 1.622116960 |
| 41 | 1 | 4.691300489 | 1.215894125 | 1.135557319 |
| 42 | 6 | 1.363334527 | 2.350377196 | 2.820483042 |
| 43 | 6 | 3.782441286 | 2.195084080 | 2.828161306 |
| 44 | 1 | 0.419038000 | 2.645755885 | 3.261627659 |
| 45 | 1 | 4.721769042 | 2.406270461 | 3.326339161 |

| | | | | |
|---|---|---|---|---|
| 46 | 6 | 2.568660561 | 2.607311441 | 3.429593056 |
| 47 | 1 | 2.595532092 | 3.126800470 | 4.380616583 |

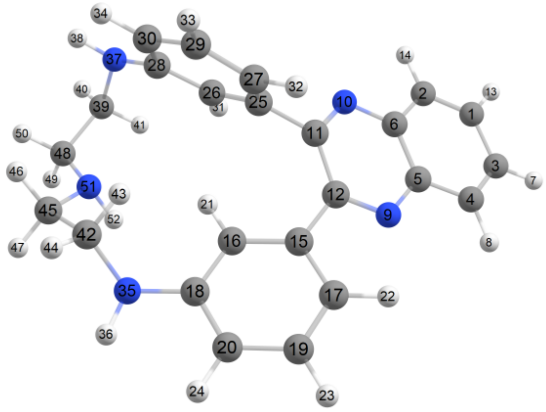
## $N_2C_3Q$ (*anti*-conformer)



| | | | | |
|---|---|---|---|---|
| 1 | 7 | -0.721820910 | -1.209723188 | -4.708171072 |
| 2 | 6 | 0.369685913 | -0.513365826 | -4.192337670 |
| 3 | 7 | -2.478183906 | 1.737698264 | -4.052327320 |
| 4 | 6 | 0.521974478 | -0.451416849 | -2.799627956 |
| 5 | 6 | -2.442338372 | 1.261816045 | -2.742708725 |
| 6 | 6 | -1.311436945 | 1.521093250 | -1.953698578 |
| 7 | 6 | 1.311127511 | 0.154017987 | -4.992501344 |
| 8 | 6 | 1.479291430 | 0.365269063 | -2.203462395 |
| 9 | 6 | -1.141130836 | 0.927974351 | -0.704688145 |
| 10 | 6 | 2.424200712 | 1.012924701 | -3.011964627 |
| 11 | 6 | 2.339604273 | 0.881675923 | -4.394141053 |
| 12 | 1 | 1.242412370 | 0.111638735 | -6.072642786 |
| 13 | 6 | 1.434577073 | 0.661335260 | -0.740741352 |
| 14 | 1 | 3.186416512 | 1.627727133 | -2.551725208 |
| 15 | 1 | 3.065932096 | 1.382477463 | -5.024927399 |
| 16 | 6 | -3.484325990 | 0.505802272 | -2.178783761 |
| 17 | 6 | -2.191565194 | 0.184259781 | -0.149494079 |
| 18 | 6 | -3.356078464 | -0.003010425 | -0.887411091 |
| 19 | 6 | 0.189293037 | 0.931400287 | -0.026220325 |
| 20 | 1 | -2.071434822 | -0.257420781 | 0.831115283 |
| 21 | 1 | -4.174997079 | -0.572673760 | -0.461850149 |
| 22 | 1 | -4.395071262 | 0.330622378 | -2.738800927 |
| 23 | 6 | -1.329473573 | -0.898683876 | -5.994804694 |
| 24 | 1 | -2.111332019 | -1.647778905 | -6.151821930 |
| 25 | 1 | -0.593955494 | -1.068483743 | -6.787852166 |
| 26 | 6 | -3.015768217 | 0.965332526 | -5.176727806 |
| 27 | 1 | -3.553233113 | 0.099204457 | -4.780406790 |
| 28 | 1 | -3.758533035 | 1.572088587 | -5.705822691 |
| 29 | 6 | -1.941725654 | 0.508309626 | -6.193181764 |
| 30 | 1 | -2.392561304 | 0.504735794 | -7.192368295 |
| 31 | 1 | -1.146839390 | 1.261170422 | -6.230180979 |
| 32 | 7 | 2.590596966 | 0.709677825 | -0.114183219 |
| 33 | 7 | 0.191247433 | 1.136023804 | 1.273381856 |
| 34 | 6 | 2.599517449 | 0.957853491 | 1.221601409 |
| 35 | 6 | 1.380690039 | 1.142455499 | 1.931101736 |
| 36 | 1 | -0.193462209 | -0.977879752 | -2.180660804 |
| 37 | 1 | -0.504643019 | 2.101606024 | -2.384321919 |
| 38 | 1 | -1.640356767 | 2.244288859 | -4.300058202 |
| 39 | 1 | -1.394594864 | -1.456236492 | -3.996676215 |
| 40 | 6 | 3.828625690 | 1.004043496 | 1.922497153 |
| 41 | 1 | 4.741620113 | 0.859702704 | 1.357570087 |
| 42 | 6 | 1.413921753 | 1.355626145 | 3.330298422 |
| 43 | 6 | 3.834258417 | 1.215640762 | 3.280743435 |
| 44 | 1 | 0.471380296 | 1.493341363 | 3.846298234 |

| | | | | |
|---|---|---|---|---|
| 45 | 1 | 4.774009376 | 1.247136379 | 3.820161500 |
| 46 | 6 | 2.620290236 | 1.389719236 | 3.988823374 |
| 47 | 1 | 2.648429765 | 1.553501336 | 5.060009943 |

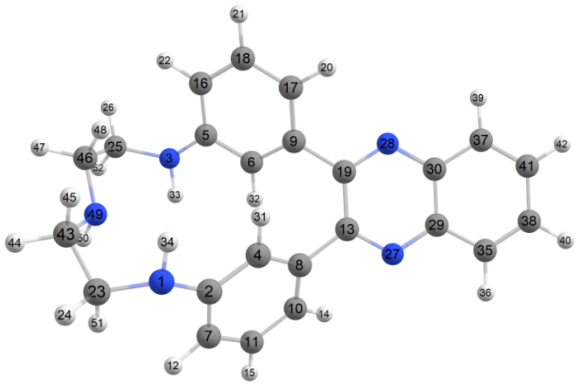
## $N_3C_4Q$ (*syn*-conformer)




| | | | | |
|---|---|---|---|---|
| 1 | 6 | -5.087917720 | -7.053274919 | 8.753818671 |
| 2 | 6 | -5.102989218 | -5.686045988 | 8.586585940 |
| 3 | 6 | -4.573736966 | -7.630087674 | 9.943646708 |
| 4 | 6 | -4.086443772 | -6.834967537 | 10.956862538 |
| 5 | 6 | -4.093742357 | -5.423346482 | 10.810853379 |
| 6 | 6 | -4.597030697 | -4.846357834 | 9.610209961 |
| 7 | 1 | -4.570220155 | -8.710606011 | 10.052864054 |
| 8 | 1 | -3.697067078 | -7.251538567 | 11.880124859 |
| 9 | 7 | -3.655225848 | -4.633735026 | 11.823957308 |
| 10 | 7 | -4.560801984 | -3.497949541 | 9.428273200 |
| 11 | 6 | -4.075666052 | -2.743718344 | 10.396970883 |
| 12 | 6 | -3.658742037 | -3.318405959 | 11.664528153 |
| 13 | 1 | -5.468321861 | -7.700693868 | 7.969314452 |
| 14 | 1 | -5.481336729 | -5.218874577 | 7.683221412 |
| 15 | 6 | -3.266070850 | -2.531194284 | 12.872723266 |
| 16 | 6 | -3.774681725 | -1.251823860 | 13.137081893 |
| 17 | 6 | -2.448647624 | -3.152170662 | 13.835597621 |
| 18 | 6 | -3.475894157 | -0.585351180 | 14.336919157 |
| 19 | 6 | -2.156913870 | -2.498183408 | 15.027087316 |
| 20 | 6 | -2.659711859 | -1.222488917 | 15.282290337 |
| 21 | 1 | -4.438350723 | -0.764938050 | 12.435305674 |
| 22 | 1 | -2.074119671 | -4.149515971 | 13.641626794 |
| 23 | 1 | -1.521528924 | -2.979645250 | 15.765224530 |
| 24 | 1 | -2.412503034 | -0.712986115 | 16.210972654 |
| 25 | 6 | -3.971421952 | -1.286933247 | 10.077064380 |
| 26 | 6 | -5.140083761 | -0.548651661 | 9.885883433 |
| 27 | 6 | -2.718832760 | -0.675896840 | 9.932053910 |
| 28 | 6 | -5.087947108 | 0.829399253 | 9.618766531 |
| 29 | 6 | -2.661011891 | 0.672043286 | 9.579778478 |
| 30 | 6 | -3.826310231 | 1.421765290 | 9.433283203 |
| 31 | 1 | -6.097023592 | -1.050807349 | 9.974139349 |
| 32 | 1 | -1.810191964 | -1.251145121 | 10.075203356 |
| 33 | 1 | -1.696899715 | 1.151820111 | 9.434960043 |
| 34 | 1 | -3.764150440 | 2.482038602 | 9.197994864 |
| 35 | 7 | -4.039425603 | 0.679803804 | 14.605394022 |
| 36 | 1 | -3.849711281 | 0.967522481 | 15.557344018 |
| 37 | 7 | -6.256399343 | 1.589880174 | 9.478980908 |
| 38 | 1 | -6.047567134 | 2.561039445 | 9.277596203 |
| 39 | 6 | -7.363934282 | 1.468250313 | 10.425894148 |
| 40 | 1 | -8.261157095 | 1.891188901 | 9.956766356 |
| 41 | 1 | -7.573900483 | 0.408203358 | 10.590972960 |
| 42 | 6 | -3.851260158 | 1.790064283 | 13.657020711 |

| | | | | |
|---|---|---|---|---|
| 43 | 1 | -3.390137442 | 1.402808328 | 12.744622441 |
| 44 | 1 | -3.163374817 | 2.535467108 | 14.082707669 |
| 45 | 6 | -5.161132859 | 2.484038391 | 13.276500249 |
| 46 | 1 | -4.911860036 | 3.345158495 | 12.643277928 |
| 47 | 1 | -5.643978721 | 2.889057009 | 14.186576479 |
| 48 | 6 | -7.128582903 | 2.171892216 | 11.777851207 |
| 49 | 1 | -8.075808450 | 2.173264854 | 12.347222013 |
| 50 | 1 | -6.897565418 | 3.226449088 | 11.577738458 |
| 51 | 7 | -6.008878861 | 1.587988148 | 12.504718150 |
| 52 | 1 | -6.303461370 | 0.809429033 | 13.085861117 |

## $N_3C_4Q$ (*anti*-conformer)



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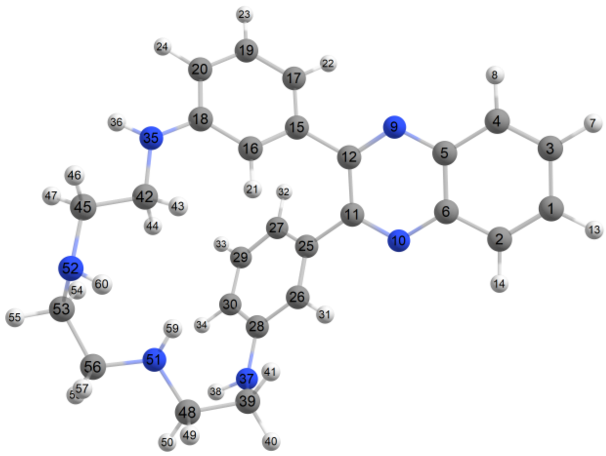
| 1 | 7 | -0.200678761 | -2.108781880 | -4.719289551 |
| 2 | 6 | 0.547324364 | -1.037370994 | -4.228828409 |
| 3 | 7 | -3.112879831 | 1.818508331 | -3.750003663 |
| 4 | 6 | 0.499327934 | -0.738026918 | -2.855903251 |
| 5 | 6 | -2.930851146 | 1.226239396 | -2.493760591 |
| 6 | 6 | -1.652728630 | 1.276923795 | -1.912803362 |
| 7 | 6 | 1.409000818 | -0.281378243 | -5.045030530 |
| 8 | 6 | 1.267937780 | 0.290423939 | -2.304373850 |
| 9 | 6 | -1.385589829 | 0.693469591 | -0.672866437 |
| 10 | 6 | 2.130476015 | 1.027150167 | -3.130966035 |
| 11 | 6 | 2.183725673 | 0.736326291 | -4.492035557 |
| 12 | 1 | 1.496821678 | -0.505046795 | -6.102997844 |
| 13 | 6 | 1.211641387 | 0.613886619 | -0.847601637 |
| 14 | 1 | 2.743793376 | 1.809222430 | -2.699118234 |
| 15 | 1 | 2.849344984 | 1.302964570 | -5.137366581 |
| 16 | 6 | -3.969605689 | 0.613767858 | -1.772528582 |
| 17 | 6 | -2.437197273 | 0.090877277 | 0.039962706 |
| 18 | 6 | -3.712576788 | 0.063145077 | -0.515181537 |
| 19 | 6 | -0.018681602 | 0.722222448 | -0.076032774 |
| 20 | 1 | -2.238795635 | -0.343571122 | 1.012484065 |
| 21 | 1 | -4.526146276 | -0.404731024 | 0.032344637 |
| 22 | 1 | -4.972733265 | 0.567442950 | -2.183531982 |
| 23 | 6 | -0.837594102 | -2.122012328 | -6.029675031 |
| 24 | 1 | -0.718102219 | -3.114204516 | -6.486420951 |
| 25 | 6 | -4.115702645 | 1.317204929 | -4.681061436 |
| 26 | 1 | -5.116495834 | 1.447427395 | -4.255196182 |
| 27 | 7 | 2.387192665 | 0.793092763 | -0.270677171 |
| 28 | 7 | 0.025015823 | 0.881676554 | 1.236548984 |
| 29 | 6 | 2.432099154 | 1.010390084 | 1.070504333 |
| 30 | 6 | 1.235073694 | 1.008681812 | 1.842336293 |
| 31 | 1 | -0.170779592 | -1.307168140 | -2.218404290 |
| 32 | 1 | -0.855582831 | 1.765940261 | -2.461903320 |
| 33 | 1 | -2.221428783 | 1.937423818 | -4.215028336 |
| 34 | 1 | -0.786189223 | -2.523899261 | -4.005517276 |
| 35 | 6 | 3.680582767 | 1.203187345 | 1.713693201 |
| 36 | 1 | 4.576195317 | 1.199814172 | 1.101021226 |

| | | | | |
|---|---|---|---|---|
| 37 | 6 | 1.310937492 | 1.180915456 | 3.248061860 |
| 38 | 6 | 3.727187530 | 1.374186107 | 3.079618166 |
| 39 | 1 | 0.385246282 | 1.177090439 | 3.814158368 |
| 40 | 1 | 4.682240370 | 1.518301438 | 3.575904945 |
| 41 | 6 | 2.536709922 | 1.359593646 | 3.850764141 |
| 42 | 1 | 2.597627942 | 1.495450200 | 4.926512557 |
| 43 | 6 | -2.338114658 | -1.790142352 | -5.990443904 |
| 44 | 1 | -2.791544214 | -2.078263852 | -6.957639226 |
| 45 | 1 | -2.812293680 | -2.432715285 | -5.236368395 |
| 46 | 6 | -3.943660968 | -0.149556279 | -5.114279350 |
| 47 | 1 | -4.746737345 | -0.394409591 | -5.836161483 |
| 48 | 1 | -4.092866875 | -0.799486661 | -4.244407301 |
| 49 | 7 | -2.596961721 | -0.402457310 | -5.618863953 |
| 50 | 1 | -2.408554018 | 0.200063516 | -6.417944826 |
| 51 | 1 | -0.320604551 | -1.416385738 | -6.685450087 |
| 52 | 1 | -4.080191001 | 1.968176069 | -5.563449500 |

## $N_4C_6Q$ (*syn*-conformer)



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| 3 | 6 | -0.251535135 | 2.750898114 | 6.150899653 |
| 4 | 6 | -0.092259921 | 2.183011100 | 7.395764405 |
| 5 | 6 | -0.545174842 | 2.873084122 | 8.548728768 |
| 6 | 6 | -1.143472064 | 4.158952512 | 8.407429108 |
| 7 | 1 | 0.089103005 | 2.221883147 | 5.265779086 |
| 8 | 1 | 0.361706725 | 1.206635190 | 7.530709419 |
| 9 | 7 | -0.451663033 | 2.285554443 | 9.771865487 |
| 10 | 7 | -1.519612679 | 4.869152936 | 9.505054476 |
| 11 | 6 | -1.357605749 | 4.321061496 | 10.696596205 |
| 12 | 6 | -0.880298482 | 2.954835338 | 10.828180932 |
| 13 | 1 | -0.981280028 | 4.449598654 | 5.017423895 |
| 14 | 1 | -1.762849902 | 5.697306505 | 7.033854768 |
| 15 | 6 | -0.894029839 | 2.198783480 | 12.113017350 |
| 16 | 6 | -2.002443583 | 2.273069728 | 12.968285523 |
| 17 | 6 | 0.179095924 | 1.358237652 | 12.433517495 |
| 18 | 6 | -2.056013224 | 1.517544324 | 14.149856287 |
| 19 | 6 | 0.141807053 | 0.625746352 | 13.620586421 |
| 20 | 6 | -0.954752147 | 0.699426128 | 14.471818862 |
| 21 | 1 | -2.826764493 | 2.923379240 | 12.706405788 |
| 22 | 1 | 1.022522029 | 1.287145341 | 11.756786086 |
| 23 | 1 | 0.977488701 | -0.016235790 | 13.884924801 |
| 24 | 1 | -0.975380297 | 0.113896373 | 15.387973512 |
| 25 | 6 | -1.650912459 | 5.200928201 | 11.864109736 |
| 26 | 6 | -2.796547638 | 6.005918507 | 11.835020253 |
| 27 | 6 | -0.761179049 | 5.288126477 | 12.944068873 |
| 28 | 6 | -3.102346928 | 6.868772662 | 12.900774314 |

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| 29 | 6 | -1.037238739 | 6.175597177 | 13.982939502 |
| 30 | 6 | -2.196065131 | 6.944927598 | 13.975989625 |
| 31 | 1 | -3.426838517 | 5.968929990 | 10.953709145 |
| 32 | 1 | 0.135792230 | 4.679817675 | 12.965789466 |
| 33 | 1 | -0.348233068 | 6.258126880 | 14.818826474 |
| 34 | 1 | -2.415545472 | 7.606279630 | 14.810811609 |
| 35 | 7 | -3.175239203 | 1.523654184 | 14.980269254 |
| 36 | 1 | -2.978612250 | 1.250747470 | 15.934137067 |
| 37 | 7 | -4.234600372 | 7.687406399 | 12.891337660 |
| 38 | 1 | -4.333476614 | 8.197123376 | 13.760503134 |
| 39 | 6 | -5.524483044 | 7.229210434 | 12.384918418 |
| 40 | 1 | -5.967651302 | 7.986295587 | 11.724270040 |
| 41 | 1 | -5.364230981 | 6.338257586 | 11.770274269 |
| 42 | 6 | -4.231078452 | 2.512562907 | 14.849387881 |
| 43 | 1 | -4.639500721 | 2.450927885 | 13.831598851 |
| 44 | 1 | -3.865805708 | 3.545097448 | 14.983395038 |
| 45 | 6 | -5.376969390 | 2.213576980 | 15.832196322 |
| 46 | 1 | -5.733405500 | 1.193231663 | 15.644648922 |
| 47 | 1 | -4.994432792 | 2.222103813 | 16.861874723 |
| 48 | 6 | -6.532858572 | 6.906498455 | 13.496679903 |
| 49 | 1 | -7.501317946 | 6.646251871 | 13.025820685 |
| 50 | 1 | -6.721267943 | 7.816006419 | 14.085866746 |
| 51 | 7 | -6.024487707 | 5.886998079 | 14.402762813 |
| 52 | 7 | -6.503000314 | 3.131624800 | 15.768543644 |
| 53 | 6 | -6.338295093 | 4.452130307 | 16.389543296 |
| 54 | 1 | -5.279821928 | 4.676940088 | 16.582886252 |
| 55 | 1 | -6.853010273 | 4.463028345 | 17.361380792 |
| 56 | 6 | -6.901439555 | 5.583686808 | 15.530444834 |
| 57 | 1 | -7.935135284 | 5.323136613 | 15.225925206 |
| 58 | 1 | -6.982582747 | 6.487777082 | 16.146849797 |
| 59 | 1 | -5.824931693 | 5.037001604 | 13.880491591 |
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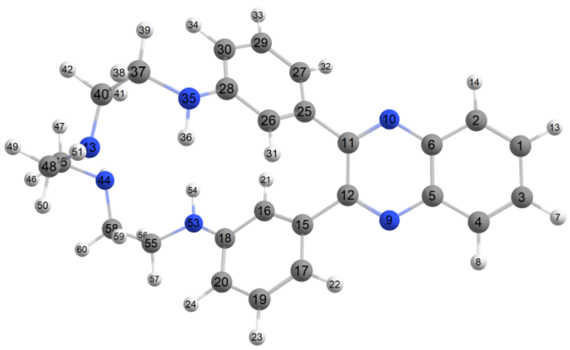
## $N_4C_6Q$ (*anti*-conformer)



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| 3 | 6 | 24.797043618 | 56.836498827 | 55.803373894 |
| 4 | 6 | 23.896727110 | 55.881506869 | 56.221326415 |
| 5 | 6 | 22.532184795 | 55.990135430 | 55.851193437 |
| 6 | 6 | 22.103066329 | 57.098704329 | 55.066324138 |
| 7 | 1 | 25.843671053 | 56.753316578 | 56.080686861 |
| 8 | 1 | 24.196857940 | 55.029323279 | 56.822401715 |
| 9 | 7 | 21.651948224 | 55.018373958 | 56.207886963 |
| 10 | 7 | 20.788051484 | 57.256954206 | 54.760836380 |
| 11 | 6 | 19.924446825 | 56.341143553 | 55.166318144 |
| 12 | 6 | 20.384192568 | 55.143665720 | 55.852451276 |
| 13 | 1 | 25.101788681 | 58.668879712 | 54.684429083 |
| 14 | 1 | 22.699300720 | 58.896796481 | 54.042255712 |
| 15 | 6 | 19.519816062 | 53.970185011 | 56.168637951 |

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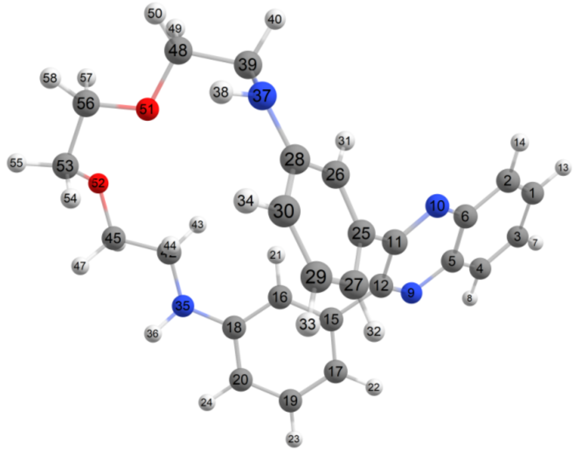
|---|---|---|---|---|
| 16 | 6 | 18.561836094 | 53.506869613 | 55.265126507 |
| 17 | 6 | 19.731837510 | 53.269972754 | 57.369158314 |
| 18 | 6 | 17.785022460 | 52.364143351 | 55.534870408 |
| 19 | 6 | 18.963615980 | 52.144825683 | 57.645747640 |
| 20 | 6 | 17.992413649 | 51.690677656 | 56.751678818 |
| 21 | 1 | 18.415784608 | 54.021905545 | 54.320994705 |
| 22 | 1 | 20.495419486 | 53.613356117 | 58.056725456 |
| 23 | 1 | 19.113337932 | 51.607319850 | 58.578123306 |
| 24 | 1 | 17.402847602 | 50.817832221 | 57.008440784 |
| 25 | 6 | 18.491125457 | 56.662816670 | 54.906512613 |
| 26 | 6 | 17.510627853 | 56.428278823 | 55.871733382 |
| 27 | 6 | 18.135497068 | 57.287117167 | 53.698267227 |
| 28 | 6 | 16.165818651 | 56.786843363 | 55.660164625 |
| 29 | 6 | 16.807206813 | 57.633496663 | 53.477041153 |
| 30 | 6 | 15.822390983 | 57.385702724 | 54.434972905 |
| 31 | 1 | 17.784601435 | 55.974688838 | 56.818983818 |
| 32 | 1 | 18.901253708 | 57.493841418 | 52.960021438 |
| 33 | 1 | 16.522321094 | 58.101111149 | 52.538469005 |
| 34 | 1 | 14.795208795 | 57.658357638 | 54.220412720 |
| 35 | 7 | 15.260296008 | 56.579012117 | 56.701368340 |
| 36 | 1 | 15.511687872 | 55.795967348 | 57.290788287 |
| 37 | 6 | 13.825228017 | 56.725748287 | 56.550147737 |
| 38 | 1 | 13.404919423 | 56.917373166 | 57.548265893 |
| 39 | 1 | 13.617273073 | 57.625039184 | 55.964145413 |
| 40 | 6 | 13.096462409 | 55.522581641 | 55.934649730 |
| 41 | 1 | 13.519768147 | 55.301578424 | 54.949114852 |
| 42 | 1 | 12.032981465 | 55.798576737 | 55.786338281 |
| 43 | 7 | 13.266000842 | 54.344208912 | 56.783623613 |
| 44 | 7 | 13.927382980 | 52.361666519 | 54.636743961 |
| 45 | 6 | 12.553423666 | 52.663294807 | 55.034669994 |
| 46 | 1 | 11.890200392 | 51.777232189 | 54.984353407 |
| 47 | 1 | 12.157026349 | 53.387814100 | 54.313559216 |
| 48 | 6 | 12.393179713 | 53.218179437 | 56.454839757 |
| 49 | 1 | 11.318702692 | 53.467618028 | 56.557681929 |
| 50 | 1 | 12.596901651 | 52.424004010 | 57.182578971 |
| 51 | 1 | 13.064839249 | 54.610129669 | 57.746480566 |
| 52 | 1 | 13.895175689 | 52.018509210 | 53.677828561 |
| 53 | 7 | 16.892800610 | 51.931728543 | 54.553152176 |
| 54 | 1 | 16.548929234 | 52.686392683 | 53.973826771 |
| 55 | 6 | 15.897996307 | 50.900319269 | 54.776360554 |
| 56 | 1 | 15.640798915 | 50.471777300 | 53.796747783 |
| 57 | 1 | 16.349224735 | 50.084066632 | 55.346623769 |
| 58 | 6 | 14.603113564 | 51.361185675 | 55.461718980 |
| 59 | 1 | 14.839285814 | 51.813514476 | 56.430895447 |
| 60 | 1 | 13.976197373 | 50.467476187 | 55.655462136 |

## $N_2C_6O_2Q$ (*syn*-conformer)



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| 3 | 6 | -0.272388806 | 2.667614773 | 6.118646938 |
| 4 | 6 | -0.135208457 | 2.119797640 | 7.374767069 |
| 5 | 6 | -0.541002995 | 2.860410708 | 8.514115860 |
| 6 | 6 | -1.069897618 | 4.173597684 | 8.348766885 |
| 7 | 1 | 0.032148117 | 2.100944365 | 5.243781357 |
| 8 | 1 | 0.263255606 | 1.122149456 | 7.529767811 |
| 9 | 7 | -0.468700106 | 2.295366053 | 9.747898965 |
| 10 | 7 | -1.410476362 | 4.923924520 | 9.433383039 |
| 11 | 6 | -1.276252143 | 4.386980362 | 10.632229596 |
| 12 | 6 | -0.861942131 | 3.005018455 | 10.791795744 |
| 13 | 1 | -0.914518469 | 4.377951728 | 4.951533819 |
| 14 | 1 | -1.614455722 | 5.711319176 | 6.945937304 |
| 15 | 6 | -0.909287666 | 2.271366953 | 12.088115989 |
| 16 | 6 | -1.997464058 | 2.422732090 | 12.960717599 |
| 17 | 6 | 0.110628028 | 1.360129184 | 12.392124257 |
| 18 | 6 | -2.088639060 | 1.660063754 | 14.135691375 |
| 19 | 6 | 0.039513562 | 0.624835272 | 13.575029463 |
| 20 | 6 | -1.040656328 | 0.766960511 | 14.438906386 |
| 21 | 1 | -2.778530084 | 3.132108201 | 12.717783183 |
| 22 | 1 | 0.935017887 | 1.232767506 | 11.700052442 |
| 23 | 1 | 0.828983483 | -0.080794090 | 13.818221711 |
| 24 | 1 | -1.094854630 | 0.171868588 | 15.347513374 |
| 25 | 6 | -1.535047145 | 5.280905834 | 11.797436516 |
| 26 | 6 | -2.737598626 | 5.995157325 | 11.864603060 |
| 27 | 6 | -0.571674998 | 5.427541207 | 12.803605798 |
| 28 | 6 | -3.025033087 | 6.817965493 | 12.967749942 |
| 29 | 6 | -0.822256489 | 6.301126795 | 13.861327487 |
| 30 | 6 | -2.030398861 | 6.982623159 | 13.953300731 |
| 31 | 1 | -3.439875252 | 5.903304273 | 11.044526245 |
| 32 | 1 | 0.355634799 | 4.867713831 | 12.758216985 |
| 33 | 1 | -0.071493106 | 6.442531359 | 14.634630818 |
| 34 | 1 | -2.221175736 | 7.636038872 | 14.801702752 |
| 35 | 7 | -3.195046776 | 1.720268931 | 14.981555071 |
| 36 | 1 | -2.997176678 | 1.437607531 | 15.931628578 |
| 37 | 7 | -4.242042214 | 7.484882271 | 13.096684549 |
| 38 | 1 | -4.369395321 | 7.875436871 | 14.021451732 |
| 39 | 6 | -5.477159280 | 6.947950755 | 12.533662120 |
| 40 | 1 | -5.859056606 | 7.584122013 | 11.722157736 |
| 41 | 1 | -5.287606011 | 5.957212455 | 12.108542371 |
| 42 | 6 | -4.245738095 | 2.714392889 | 14.852382995 |
| 43 | 1 | -4.607794363 | 2.727012536 | 13.819626918 |
| 44 | 1 | -3.904964737 | 3.738131259 | 15.077192146 |
| 45 | 6 | -5.428412657 | 2.323706576 | 15.749511540 |
| 46 | 1 | -5.773436136 | 1.324185985 | 15.466355532 |

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| 47 | 1 | -5.114673858 | 2.275198400 | 16.806474767 |
| 48 | 6 | -6.563655026 | 6.789549308 | 13.589332596 |
| 49 | 1 | -7.491189712 | 6.440042960 | 13.107487683 |
| 50 | 1 | -6.789819536 | 7.759512036 | 14.068668977 |
| 51 | 8 | -6.107843521 | 5.854585074 | 14.546975397 |
| 52 | 8 | -6.533484322 | 3.193407919 | 15.585498185 |
| 53 | 6 | -6.520638912 | 4.377909526 | 16.366711121 |
| 54 | 1 | -5.506045404 | 4.628910752 | 16.704307747 |
| 55 | 1 | -7.154367255 | 4.251443846 | 17.260106783 |
| 56 | 6 | -7.063606326 | 5.525269212 | 15.535534611 |
| 57 | 1 | -8.014335783 | 5.215300931 | 15.073284149 |
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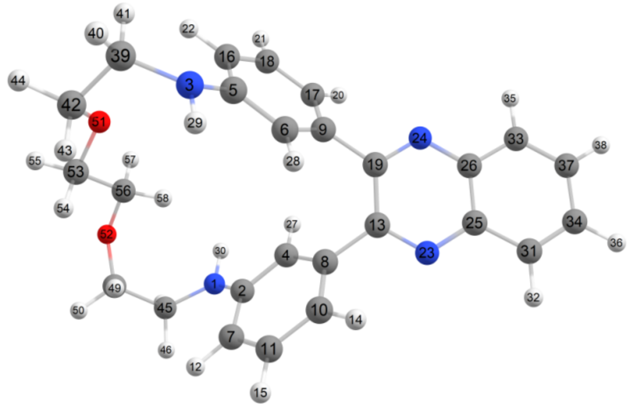
## $N_2C_6O_2Q$ (*anti*-conformer)



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| 3 | 7 | 0.782222385 | -3.869929032 | -3.681862253 |
| 4 | 6 | -0.306073459 | 1.205747592 | -3.281143231 |
| 5 | 6 | -0.016267441 | -3.159765719 | -2.787354347 |
| 6 | 6 | 0.503598302 | -1.989562846 | -2.203419729 |
| 7 | 6 | 0.662387935 | 1.833721187 | -5.404103307 |
| 8 | 6 | 0.961970896 | 1.177858958 | -2.696564565 |
| 9 | 6 | -0.190539400 | -1.300587441 | -1.204424568 |
| 10 | 6 | 2.091678407 | 1.486495155 | -3.470253954 |
| 11 | 6 | 1.927498045 | 1.794425884 | -4.817197573 |
| 12 | 1 | 0.571255788 | 2.096536461 | -6.452032762 |
| 13 | 6 | 1.107979348 | 0.939363242 | -1.231073105 |
| 14 | 1 | 3.072048325 | 1.490319843 | -3.007842085 |
| 15 | 1 | 2.797620758 | 2.019999685 | -5.427712607 |
| 16 | 6 | -1.291216959 | -3.593435595 | -2.378143358 |
| 17 | 6 | -1.440194367 | -1.771360072 | -0.776414749 |
| 18 | 6 | -1.980535166 | -2.901912733 | -1.384052870 |
| 19 | 6 | 0.436244369 | -0.133162847 | -0.522473594 |
| 20 | 1 | -1.965510484 | -1.253779377 | 0.018003508 |
| 21 | 1 | -2.959597714 | -3.260345436 | -1.078005209 |
| 22 | 1 | -1.750128713 | -4.460421475 | -2.837013523 |
| 23 | 7 | 1.845178854 | 1.823647109 | -0.582356301 |
| 24 | 7 | 0.404139426 | -0.153144137 | 0.798934368 |
| 25 | 6 | 1.881025153 | 1.762634378 | 0.776311039 |
| 26 | 6 | 1.094807307 | 0.802373879 | 1.477583114 |
| 27 | 1 | -1.180352689 | 0.983839145 | -2.675117499 |
| 28 | 1 | 1.480436679 | -1.632171528 | -2.518893794 |
| 29 | 1 | 1.591203662 | -3.357265651 | -4.004567320 |
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| 31 | 6 | 2.662342679 | 2.694057229 | 1.506030496 |
| 32 | 1 | 3.253263562 | 3.412688718 | 0.947575022 |
| 33 | 6 | 1.077968629 | 0.815486966 | 2.895507646 |

| | | | | |
|---|---|---|---|---|
| 34 | 6 | 2.638188742 | 2.677880723 | 2.883096507 |
| 35 | 1 | 0.468381117 | 0.076584405 | 3.405275749 |
| 36 | 1 | 3.232018297 | 3.392892948 | 3.444756416 |
| 37 | 6 | 1.836796998 | 1.738232076 | 3.581088862 |
| 38 | 1 | 1.829224270 | 1.747519150 | 4.667021204 |
| 39 | 6 | 0.310845606 | -4.885661340 | -4.602494214 |
| 40 | 1 | 1.146695774 | -5.556291433 | -4.839258420 |
| 41 | 1 | -0.444397827 | -5.499145598 | -4.104905855 |
| 42 | 6 | -0.252410235 | -4.346594584 | -5.919260435 |
| 43 | 1 | 0.523202747 | -3.753091789 | -6.433280024 |
| 44 | 1 | -0.515820194 | -5.187096071 | -6.584901623 |
| 45 | 6 | -2.097771184 | 1.751341353 | -6.548665663 |
| 46 | 1 | -1.476611845 | 2.518016971 | -7.027699132 |
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| 48 | 6 | -1.963920001 | 0.433519890 | -7.323014329 |
| 49 | 1 | -0.947302485 | 0.032388805 | -7.215577878 |
| 50 | 1 | -2.134697524 | 0.628303383 | -8.389411933 |
| 51 | 8 | -1.374342292 | -3.541539496 | -5.630299794 |
| 52 | 8 | -2.942581385 | -0.516379461 | -6.910407328 |
| 53 | 6 | -1.783927766 | -2.659103297 | -6.659655159 |
| 54 | 1 | -0.912320903 | -2.288301403 | -7.221694331 |
| 55 | 1 | -2.453457512 | -3.156215350 | -7.377841715 |
| 56 | 6 | -2.498416190 | -1.492351420 | -5.976648971 |
| 57 | 1 | -3.389726334 | -1.863098236 | -5.461136511 |
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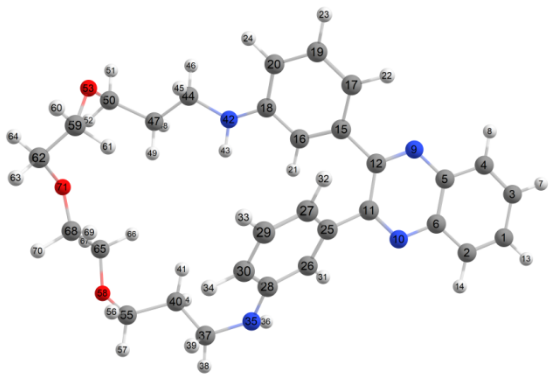
## $N_2C_{10}O_3Q$ (*syn*-conformer)



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| 2 | 6 | 21.492180481 | 58.875822506 | 55.883160554 |
| 3 | 6 | 23.102927200 | 58.408221164 | 57.640565034 |
| 4 | 6 | 22.830941973 | 57.059243786 | 57.579373769 |
| 5 | 6 | 21.865612322 | 56.575600813 | 56.660194116 |
| 6 | 6 | 21.201491390 | 57.491154739 | 55.792743378 |
| 7 | 1 | 23.838514287 | 58.781949382 | 58.346635728 |
| 8 | 1 | 23.325715247 | 56.340873079 | 58.224766909 |
| 9 | 7 | 21.548646572 | 55.253109628 | 56.642993386 |
| 10 | 7 | 20.328586097 | 57.039906193 | 54.851215470 |
| 11 | 6 | 20.081550379 | 55.743428215 | 54.792236054 |
| 12 | 6 | 20.650591635 | 54.830418584 | 55.770222339 |
| 13 | 1 | 22.653958948 | 60.381245913 | 56.860887562 |
| 14 | 1 | 20.971370641 | 59.552142844 | 55.213155496 |
| 15 | 6 | 20.243045084 | 53.402591616 | 55.889008425 |
| 16 | 6 | 18.902187450 | 53.033301036 | 55.772903877 |
| 17 | 6 | 21.209279694 | 52.418939253 | 56.158433739 |
| 18 | 6 | 18.496894924 | 51.691552047 | 55.881551375 |
| 19 | 6 | 20.814685741 | 51.088810465 | 56.266940043 |
| 20 | 6 | 19.477646341 | 50.713471782 | 56.123607950 |
| 21 | 1 | 18.148868925 | 53.791875700 | 55.582830997 |

| | | | | |
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| 22 | 1 | 22.247103809 | 52.709352286 | 56.272432807 |
| 23 | 1 | 21.559615388 | 50.321933472 | 56.459924395 |
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| 25 | 6 | 19.238641236 | 55.291851533 | 53.646540273 |
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| 40 | 6 | 14.179773522 | 54.819019678 | 51.821401029 |
| 41 | 1 | 14.841737066 | 54.072959883 | 52.275146608 |
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| 43 | 1 | 16.614018191 | 52.122483377 | 55.319083669 |
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| 45 | 1 | 17.257590907 | 49.639769761 | 54.555709798 |
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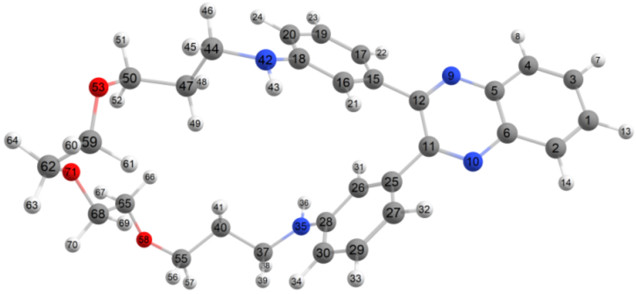
| 53 | 8 | 15.310495320 | 48.108018908 | 53.553401043 |
| 54 | 1 | 13.603100692 | 55.279396520 | 52.633018184 |
| 55 | 6 | 13.211823670 | 54.156691336 | 50.835231463 |
| 56 | 1 | 13.778488848 | 53.543799039 | 50.115784891 |
| 57 | 1 | 12.692754518 | 54.926847620 | 50.253387717 |
| 58 | 8 | 12.161859449 | 53.405282790 | 51.434051826 |
| 59 | 6 | 15.242367946 | 48.735029371 | 52.281563033 |
| 60 | 1 | 15.838430808 | 48.089989869 | 51.626480692 |
| 61 | 1 | 15.720670027 | 49.727404107 | 52.288617206 |
| 62 | 6 | 13.831923572 | 48.861822880 | 51.703440499 |
| 63 | 1 | 13.889008437 | 48.921525262 | 50.606967037 |
| 64 | 1 | 13.260000551 | 47.962128778 | 51.957931889 |
| 65 | 6 | 12.532270577 | 52.278715456 | 52.210622360 |
| 66 | 1 | 13.215094571 | 52.550009349 | 53.028475555 |
| 67 | 1 | 11.605134953 | 51.917228538 | 52.664427160 |
| 68 | 6 | 13.133831470 | 51.133233808 | 51.392584319 |
| 69 | 1 | 14.160399308 | 51.369624357 | 51.071491032 |
| 70 | 1 | 12.527526254 | 50.973512372 | 50.486926619 |
| 71 | 8 | 13.115470019 | 49.981830326 | 52.223323026 |

## $N_2C_{10}O_3Q$ (*anti*-conformer)



| | | | | |
|---|---|---|---|---|
| 1 | 6 | 24.288788187 | 58.018221393 | 55.213197218 |
| 2 | 6 | 23.008660556 | 58.039355915 | 54.705235242 |
| 3 | 6 | 24.667937404 | 57.049618608 | 56.177743728 |
| 4 | 6 | 23.768117575 | 56.102549418 | 56.614334668 |
| 5 | 6 | 22.447499489 | 56.093909200 | 56.097669659 |
| 6 | 6 | 22.059514042 | 57.083999980 | 55.148154536 |
| 7 | 1 | 25.681313270 | 57.055153834 | 56.568069401 |
| 8 | 1 | 24.038633166 | 55.340491287 | 57.337884536 |
| 9 | 7 | 21.579230260 | 55.115080029 | 56.468674538 |
| 10 | 7 | 20.774913516 | 57.147480618 | 54.704385862 |
| 11 | 6 | 19.917593299 | 56.238345974 | 55.132241032 |
| 12 | 6 | 20.354254320 | 55.137661610 | 55.971780272 |
| 13 | 1 | 25.017086784 | 58.751408280 | 54.879638366 |
| 14 | 1 | 22.688263717 | 58.778681328 | 53.978367130 |
| 15 | 6 | 19.509822829 | 53.945872598 | 56.264660337 |
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| 17 | 6 | 19.559802072 | 53.341525076 | 57.531634393 |
| 18 | 6 | 17.998603652 | 52.189186177 | 55.475952026 |
| 19 | 6 | 18.815745403 | 52.188201426 | 57.762106455 |
| 20 | 6 | 18.038863891 | 51.609011065 | 56.757578663 |
| 21 | 1 | 18.708888081 | 53.823456490 | 54.271605670 |
| 22 | 1 | 20.180831959 | 53.775122336 | 58.306844386 |
| 23 | 1 | 18.839377929 | 51.721146639 | 58.742898878 |
| 24 | 1 | 17.480479847 | 50.703385169 | 56.967810288 |
| 25 | 6 | 18.494397516 | 56.466745659 | 54.746984413 |
| 26 | 6 | 17.492882814 | 56.461831611 | 55.719080059 |
| 27 | 6 | 18.172341098 | 56.772836959 | 53.416009733 |
| 28 | 6 | 16.156001503 | 56.774281737 | 55.401705540 |
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| 30 | 6 | 15.841507236 | 57.035231579 | 54.053917189 |
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| 32 | 1 | 18.956251377 | 56.806328915 | 52.668272572 |
| 33 | 1 | 16.581588198 | 57.256655063 | 52.055920725 |
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| 35 | 7 | 15.231834164 | 56.867811893 | 56.434413809 |
| 36 | 1 | 15.561773553 | 56.538227304 | 57.329934212 |
| 37 | 6 | 13.791684394 | 56.932525302 | 56.292318294 |
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| 39 | 1 | 13.556807698 | 57.362743761 | 55.315334233 |
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| 42 | 7 | 17.312330927 | 51.621886289 | 54.407417116 |
| 43 | 1 | 17.205448562 | 52.245352632 | 53.619539365 |
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| 50 | 6 | 13.782802430 | 50.219196669 | 55.129035602 |
| 51 | 1 | 14.080895236 | 49.240142527 | 55.522048230 |

| | | | | |
|---|---|---|---|---|
| 52 | 1 | 12.933875651 | 50.573855847 | 55.720841711 |
| 53 | 8 | 13.378922953 | 49.962013545 | 53.777496022 |
| 54 | 1 | 13.154876258 | 55.258380006 | 57.510484855 |
| 55 | 6 | 11.580580984 | 55.705233709 | 56.107356051 |
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| 58 | 8 | 10.731799848 | 54.718813633 | 56.682535579 |
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| 64 | 1 | 10.764400607 | 49.962459553 | 53.651062528 |
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| 70 | 1 | 9.827258839 | 53.277178660 | 54.606878498 |
| 71 | 8 | 10.943100872 | 51.543311994 | 54.906112279 |

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