Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supplementary Materials

Multivalent Resorcinarene Clusters Decorated with DAB-1 Inhitopes: Targeting Golgi α-Mannosidase from Drosophila Melanogaster

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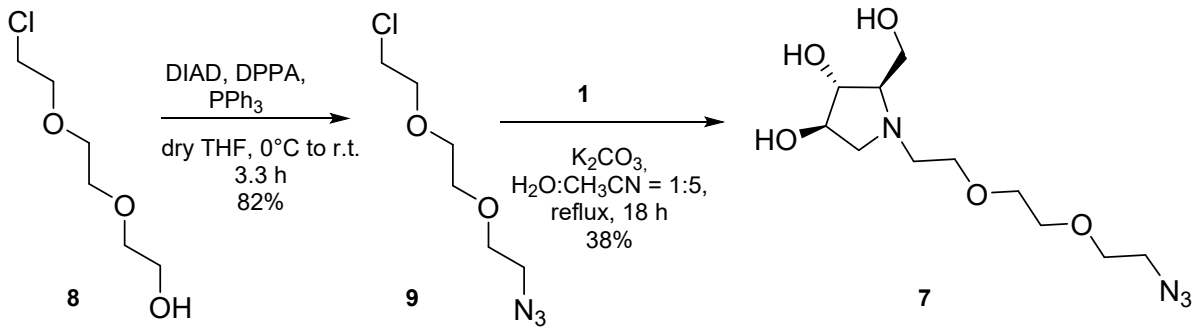
General Experimental Details

All chemicals were reagent grade and were used without further purification. Reaction temperatures were measured externally; reactions were monitored by TLC on Merck silica gel plates (0.25 mm) and visualized by UV light and spraying with H_2SO_4–$Ce(SO_4)_2$. Chromatography was carried out on Silica Gel. Yields refer to chromatographically and spectroscopically pure compounds unless otherwise stated. ^{1}H NMR spectra were recorded on a Varian Mercury-400 or on a Varian INOVA 400 instrument at 25 °C. ^{13}C NMR spectra were recorded on a Varian Gemini-200. 1D and 2D NMR spectra were also recorded on a Bruker Avance-600 [600 (^{1}H) and 150 MHz (^{13}C)], Avance-400 [400 (^{1}H) and 100 MHz (^{13}C)] or Avance-300 MHz [300 (^{1}H) and 75 MHz (^{13}C)]. Chemical shifts are reported relative to the residual solvent peak.[1] Standard pulse programs, provided by the manufacturer and integrals are in accordance with assignments, coupling constants are given in Hz. For detailed peak assignments 2D spectra were measured (COSY, HSQC). Small scale microwave assisted syntheses were carried out in a CEM Discover microwave apparatus for synthesis with an open reaction vessel and an external surface sensor. ESI-MS spectra were recorded with a Thermo Scientific™ LCQ Fleet Ion Trap Mass Spectrometer. Elemental analyses were performed with a PerkinElmer 2400 analyzer. HR MALDI mass spectra were recorded on a Bruker Solarix FT-ICR mass spectrometer equipped with a 7T magnet. All samples were recorded in MALDI (8 laser shots were used for each scan) and they were prepared by mixing 10 µL of analyte in methanol (1 mg/mL) with 10 µL of solution of 2,5-dihydroxybenzoic acid (10 mg/mL in Methanol). The mass spectra were calibrated externally, and a linear calibration was applied. Optical rotation measurements were performed on a JASCO DIP-370 polarimeter.

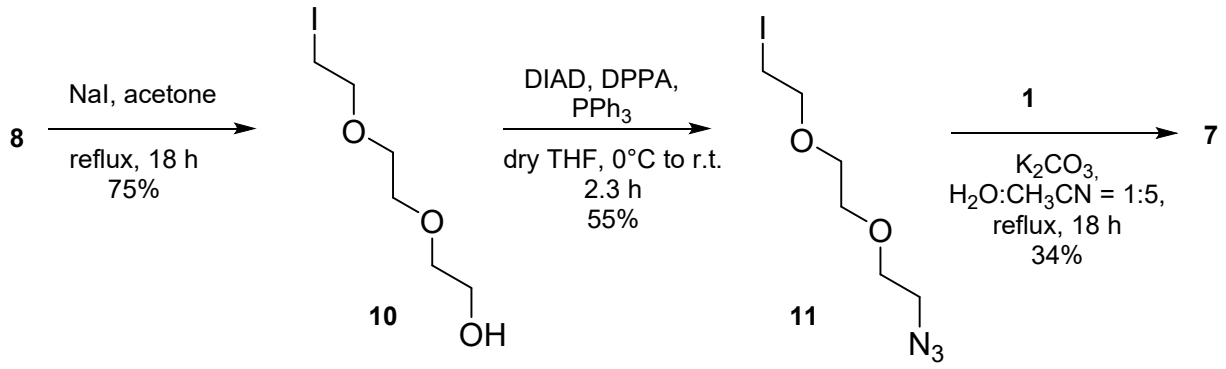
Synthetic strategies to access compound 7



Starting from commercially available 2-[2-(2-chloroethoxy)ethoxy)ethanol] (**8**), the azido moiety was introduced under Mitsunobu conditions through reaction with diphenyl phosphoryl azide (DPPA) in dry THF at room temperature, affording compound **9**[2] in 82% yield. Alkylation of DAB-1 (**1**)[3] with **9** was performed in a 1:5 CH_3CN/H_2O mixture in the

[1] G. R. Fulmer, A. J. M. Miller, N. H. Sherden, H. E. Gottlieb, A. Nudelman, B. M. Stoltz, J. E. Bercaw and K. I. Goldberg, NMR Chemical Shifts of Trace Impurities: Common Laboratory Solvents, Organics, and Gases in Deuterated Solvents Relevant to the Organometallic Chemist. *Organometallics*, 2010, **29**, 2176–2179.
[2] S. P. Amaral, M. Fernandez-Villamarin, J. Correa, R. Riguera and E. Fernandez-Megia, Efficient multigram synthesis of the repeating unit of gallic acid-triethylene glycol dendrimers. *Org. Lett.*, 2011, **13**, 4522–4525
[3] C. Parmeggiani, S. Catarzi, C. Matassini, G. D'Adamio, A. Morrone, A. Goti, P. Paoli, F. Cardona, Human Acid β-Glucosidase Inhibition by Carbohydrate Derived Iminosugars: Towards New Pharmacological

presence of K_2CO_3 as the base and heating at reflux for 18 h, thus affording compound **7** in 38% yield.



To improve the synthesis of the alkylation step, we tried an alternative strategy, namely replacement of alkylating reagent **9** with a compound bearing a better leaving group than chloride. Thus, compound **8** was converted into iodide **10**[4] through reaction with NaI in acetone at reflux, which proceeded with 75% yield. Azide introduction under Mitsunobu conditions, however, gave compound **11**[5] with a moderate 55% yield. The alkylation of DAB-1 (**1**) with iodide **11** also proceeded in moderate yield (34%), giving no advantage over the chloride derivative **9**.

Synthesis of compound 7

1-Azido-2-(2-(2-chloroethoxy)ethoxy)ethane (9): To a solution of **8** (280 mg, 1.66 mmol) in dry THF (15 mL) under a nitrogen atmosphere triphenylphosphine (1.30 g, 4.98 mmol) was added. The reaction mixture was cooled to 0 °C and DIAD (981 µL, 4.98 mmol) was added dropwise, forming a yellow precipitate. After addition of diphenylphosphorilazide (1.19 mL, 5.31 mmol), the suspension was raised to room temp. and stirred under a nitrogen atmosphere for 4 h, until TLC analysis (EtP:AcOEt=10:1) showed the disappearance of the starting material (R_f = 0.52) and formation of a new product (R_f = 0.78). The solvent was removed under reduced pressure and the crude was purified by FCC (EtP:Et_2O from 5:1 to 2:1) affording pure **9** (R_f = 0.31, 263 mg, 1.36 mmol, 82% yield) as a colorless oil. The spectrum is consistent with data reported in literature.[6] ^{1}H NMR (200 MHz, $CDCl_3$): δ 3.80-3.60 (m, 10H, from H-1 to H-5), 3.39 (t, *J*= 5.0 Hz, 2H, H-6) ppm.

2-[2-(2-Iodoethoxy)ethoxy]ethanol (10): 2-[2-(2-Chloroethoxy)ethoxy]ethanol (1.05 g, 6.23 mmol) and NaI (9 mg, 0.06 mmol) were refluxed overnight under stirring in acetone (6.3

Chaperones for Gaucher Disease. *ChemBioChem* 2015, **16**, 2054-2064.

[4] E. Ishow, A. Credi, V. Balzani, F. Spadola, L. Mandolini, A molecular-level plug/socket system: electronic energy transfer from a binaphthyl unit incorporated into a crown ether to an anthracenyl unit linked to an ammonium ion. *Chem. Eur. J.*, 1999, **5**, 984-989.

[5] L. Deng, O. Norberg, S. Uppalapati, M. Yan and O. Ramström, Stereoselective synthesis of light-activatable perfluorophenylazide-conjugated carbohydrates for glycoarray fabrication and evaluation of structural effects on protein binding by SPR imaging. *Org. Biomol. Chem.*, 2011, **9**, 3188-3198.

[6] S. P. Amaral, M. Fernandez-Villamarin, J. Correa, R. Riguera and E. Fernandez-Megia, Efficient multigram synthesis of the repeating unit of gallic acid-triethylene glycol dendrimers. *Org. Lett.*, 2011, **13**, 4522–4525

mL). After cooling, the slurry was taken up in the minimum amount of water and extracted with Et_2O (3x5 mL). The organic layers were dried (Na_2SO_4), filtered, and evaporated to dryness to yield compound **10** (1.21 g, 75% yield), as a colorless oil, which was used in the next step without further purification. The spectrum is consistent with data reported in literature.[4] ^{1}H NMR (200 MHz, $CDCl_3$): δ 3.79-3.59 (m, 12H, from H-1 to H-6), 2.46 (*br*s, 1H, OH) ppm.

1-Azido-2-(2-(2-iodoethoxy)ethoxy)ethane (11): To a solution of **10** (296 mg, 1.14 mmol) in dry THF (15 mL) under a nitrogen atmosphere triphenylphosphine (896 mg, 3.41 mmol) was added. The reaction mixture was cooled to 0 °C and DIAD (672 µL, 3.41 mmol) was added dropwise, forming a yellow precipitate. After addition of diphenylphosphorilazide (815 µL, 3.64 mmol), the suspension was raised to room temp. and stirred under a nitrogen atmosphere for 3 h, until TLC analysis (EtP:AcOEt=10:1) showed the disappearance of the starting material (R_f = 0.22) and formation of a new product (R_f = 0.75). The solvent was removed under reduced pressure and the crude was purified by FCC (EtP:Et_2O=10:1) affording pure 11 (R_f = 0.29, 178 mg, 0.62 mmol, 55% yield) as a colorless oil. The spectrum is consistent with data reported in literature.[5] ^{1}H NMR (200 MHz, $CDCl_3$) : δ 3.81-3.61 (m, 10H, from H-1 to H-5), 3.40 (t, *J*= 5.0 Hz, 2H, H-6) ppm.

Procedure A : (2*R*,3*R*,4*R*)-1-(2-(2-(2-azidoethoxy)ethoxy)ethyl)-2-(hydroxymethyl)pyrrolidine-3,4-diol (7): A solution of **1** (60 mg, 0.45 mmol), 2-[2-(2-azidoethoxy)ethoxy]ethanol **9** (175 mg, 0.90 mmol) and K_2CO_3 (93 mg, 0.68 mmol) in 2.4 mL of a mixture CH_3CN/H_2O 5:1 was stirred at reflux for 24 h, until a TLC analysis (CH_2Cl_2:MeOH:NH_3 2:1:0.2) showed the disappearance of the starting material (R_f = 0.10) and the formation of a new product (R_f = 0.79). After filtration through Celite®, the solvent was removed under reduced pressure and the crude was purified by FCC (CH_2Cl_2:MeOH:NH_3 from 6:1:0.1 to 2:1:0.1) affording pure 7 (R_f = 0.21, 50 mg, 0.17 mmol, 38% yield) as a yellow oil. $[\alpha]_{21}^{D}$= -41.5 (c = 0.68 in H_2O); ^{1}H NMR (400 MHz, D_2O): δ 4.00 (ps, 1H, H-4), 3.81 (ps, 1H, H-3), 3.61-3.54 (m, 10H, H-6, from H-2' to H-5'), 3.39 (t, *J* = 4.7 Hz, 2H, H-6'), 3.02-2.94 (m, 2H, Ha-5, Ha-1'), 2.71 (dd, *J* = 11.2, 5.7 Hz, 1H, Hb-5), 2.55-2.46 (m, 2H, H-2, Hb-1') ppm; ^{13}C{^{1}H} NMR (50 MHz, D_2O): δ= 78.9 (d, C-3), 75.5 (d, C-4), 72.0 (d, C-2), 69.6-68.7 (t, 4C, from C-2' to C-5'), 61.0 (t, C-6), 58.9 (t, C-5), 53.9 (t, C-1'), 50.2 (t, C-6') ppm; MS (ESI): *m/z* calcd (%) for $C_{11}H_{22}N_4O_5$ 290.16; found: 313.04 (55%, [M+ Na]$^+$), 291.06 (100%, [M+ H]$^+$). Elemental analysis: $C_{11}H_{22}N_4O_5$ (290.32) calcd.: C, 45.51; H, 7.64; N, 19.30; found C, 45.49; H, 7.48, N, 19.34.

Procedure B : (2*R*,3*R*,4*R*)-1-(2-(2-(2-azidoethoxy)ethoxy)ethyl)-2-(hydroxymethyl)pyrrolidine-3,4-diol (7): A solution of **1** (60 mg, 0.45 mmol), 1-Azido-2-(2-(2-iodoethoxy)ethoxy)ethane **11** (178 mg, 0.62 mmol) and K_2CO_3 (86 mg, 0.62 mmol) in 3.6 mL of a mixture CH_3CN/H_2O 5:1 was stirred at reflux for 72 h, until a TLC analysis (CH_2Cl_2:MeOH:NH_3=2:1:0.2) showed the disappearance of the starting material (R_f = 0.10) and the formation of a new product (R_f = 0.83). After filtration through Celite®, the solvent was removed under reduced pressure and the crude was purified by FCC (CH_2Cl_2:MeOH:NH_3 from 6:1:0.1 to 2:1:0.1) affording pure **7** (R_f = 0.21, 45 mg, 0.16 mmol, 34% yield) as a yellow oil.

Synthesis of derivatives 3a, 4a, 5a and 5b

The syntheses of derivatives **3c**,[7] **4c**,[8] **5c**,[8] and **3d** [9] were described in literature.

4d: A suspension of **4c** (0.44 g, 0.81 mmol) and K_2CO_3 (2.04 g, 14.7 mmol) in acetone (26 mL) was stirred at reflux for 1 h, then was cooled at 25 °C and propargyl bromide (0.74 mL, 9.89 mmol) was added. The reaction mixture was stirred at reflux for 24 h. Subsequently, the solvent was evaporated and the solid was dissolved in ethyl acetate (50 mL) and washed with an aqueous 1 M HCl solution (2 × 50 mL). The organic phase was dried with Na_2SO_4 and evaporated to obtain a pale-yellow solid. Derivative **4d** was obtained in 81 % yield (0.56 g). Mp: > 250 °C dec. *^{1}H NMR* (300 MHz, acetone-d_6): δ 6.22 (s, Ar*H*, 4H), 4.48 (d, *J*= 2.4 Hz, -OC*H*$_2$-, 16H), 3.98 (s, -C*H*$_2$-, 8H), 3.05 (t, *J*= 2.4 Hz, -C≡C*H*, 8H), 2.31 (s, -C*H*$_3$, 12H) ppm; ^{13}C{^{1}H} NMR (75 MHz, acetone-d_6): δ 155.3, 130.7, 129.6, 125.4, 80.4, 76.8, 61.2, 11.1 ppm; DEPT-135 (75 MHz, acetone-d_6): δ 129.6, 80.4, 76.8, 61.2, 30.8, 11.1; HRMS (MALDI) *m*/*z* [M+H]$^+$ calcd. for $[C_{56}H_{49}O_8]^+$: 849.3422; found: 849.3492.

5d: A suspension of **5c** (0.47 g, 0.58 mmol) and K_2CO_3 (2.16 g, 15.6 mmol) in acetone (27 mL) was stirred at reflux for 1 h, then was cooled at 25 °C and propargyl bromide (0.70 mL, 9.29 mmol) was added. The reaction mixture was stirred at reflux for 24 h, then an additional portion of propargyl bromide (0.70 mL, 9.29 mmol) was added. After further 24 h, the solvent was evaporated and the solid was dissolved in ethyl acetate (50 mL) and washed with an aqueous 1 M HCl solution (2 × 100 mL). The organic phase was dried with Na_2SO_4 and evaporated to obtain a pale-yellow solid. Derivative **5d** was obtained in 88 % yield (0.65 g). Mp: 210-215 °C dec. ^{1}H NMR (300 MHz, $CDCl_3$): δ 6.35 (s, Ar*H,* 6H), 4.40 (d, *J* = 2.4 Hz, -OC*H*$_2$-, 24H), 3.89 (s, -C*H*$_2$-, 12H), 3.03 (t, *J* = 2.4 Hz, -C≡C*H,* 12H), 2.24 (s, -C*H*$_3$*,* 18H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 154.2, 129.8, 129.2, 125.3, 79.4, 75.3, 60.5, 30.4, 10.9 ppm; HRMS (MALDI) *m*/*z* [M+H]$^+$ calcd. for $[C_{84}H_{73}O_{12}]^+$: 1273.5097; found: 1273.5142.

3a: Derivative **3d** (4.0 mg, 4.7 µmol) and derivative **6**[10] (11.0 mg, 42.6 µmol) were dissolved in a mixture of THF/H_2O (1.00 mL, 2:1 v/v) in an ACE pressure tube, and $Cu_2SO_4 \cdot 5\ H_2O$ (0.6 mg, 2.4 µmol) and sodium ascorbate (0.4 mg, 2.0 µmol) were added. The reaction mixture was heated under microwave irradiation for 45 min at 80 °C. The reaction mixture was filtered through a short pad of Celite® and the filtrate was concentrated under reduced pressure to give a yellow solid. The mixture was purified through chromatographic column (silica gel, gradient: from MeOH to ammonia solution 4 M in MeOH) to give derivative **3a** in 27 % of yield (3.7 mg). Mp: > 200 °C dec. ^{1}H NMR (600 MHz, CD_3OD): δ 8.09 (s, *H*-triazole,

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[8] P. Della Sala, C. Gaeta, W. Navarra, C. Talotta, M. De Rosa,G. Brancatelli, S. Geremia and P. Neri, Improved Synthesis of Larger Resorcinarenes. *J. Org. Chem.*, 2016, **81**, 5726-5731.

[9] W. Liu, H. Yang, H., W. Wu, H. Gao, S. Xu, Q. Guo, Y. Liu, S. Xu, S. Cao, Calix[4]resorcinarene-based branched macromolecules for all-optical photorefractive application. *J. Mater. Chem. C* 2016, **4**, 10684-10692.

[10] G. D'Adamio, C. Matassini, C. Parmeggiani, S. Catarzi, A. Morrone, A. Goti, P. Paoli, F. Cardona, Evidence for a multivalent effect in inhibition of sulfatases involved in lysosomal storage disorders (LSDs). *RSC Adv*. 2016, **6**, 64847-64851.

4H), 7.36 (s, *H*-triazole, 4H), 7.22 (s, Ar*H,* 2H), 6.99 (s, Ar*H,* 2H), 6.72 (s, Ar*H,* 2H), 5.98 (s, Ar*H,* 2H), 5.21 and 5.14 (AB, *J* = 12.0 Hz, -OC*H*$_2$-triazole, 8H), 4.89 (overlapped to signal of H_2O, -OC*H*$_2$-triazole, 8H), 4.55 (q, *J*= 7.2 Hz, Ar-C*H*(CH_3)-Ar, 4H), 4.45 (*broad*, 12H) 4.28 (*broad*, 8 H), 3.94-3.89 (overlapped, C*H*, 24H), 3.68-3.63 (overlapped, C*H*$_2$, 24H), 3.05-2.99 (m, C*H*$_2$, 12H), 2.86-2.79 (m, C*H*$_2$, 12H), 2.67-2.64 (m, C*H*$_2$, 12H), 2.45-2.33 (overlapped, 24H), 1.94-1.83 (overlapped, C*H*$_2$, 24H), 1.60-1.28 (overlapped to signal of grease C*H*$_2$,12H) ppm; $^{13}C\{^1H\}$ NMR (150 MHz, CD_3OD) : δ 148.0, 146.9, 137.9, 137.6, 125.5, 119.1, 119.0, 78.2, 75.0, 72.6, 62.9, 61.4, 61.4, 59.6, 56.0, 55.9, 52.1, 51.2, 32.7, 31.4, 30.5, 30.4, 29.7, 29.6, 29.4, 29.1, 22.6 ppm; HRMS (MALDI) *m*/*z* $[M+H]^+$ calcd. for $[C_{144}H_{225}N_{32}O_{32}]^+$: 2915.6991; found: 2915.7011; $[\alpha]_{25}^{D}$ (c: 3.7 mg/mL) = -20.99°.

4a: Derivative **4d** (4.06 mg, 4.80 µmol) and derivative **6**[10] (9.98 mg, 38.6 µmol) were dissolved in a mixture of THF/H_2O (1.00 mL, 2:1 v/v) in an ACE pressure tube and $Cu_2SO_4 \cdot 5\ H_2O$ (0.36 mg, 1.4 µmol) and sodium ascorbate (0.57 mg, 2.9 µmol) were added. The reaction mixture was heated under microwave irradiation for 45 min at 80° C. The reaction mixture was filtered through a short pad of Celite® and the filtrate was concentrated under reduced pressure to give a yellow solid. The mixture was purified through chromatographic column (silica gel, gradient: from MeOH to ammonia solution 4 M in MeOH) to give derivative **4a** with 44 % of yield (6.2 mg). Mp: > 230 °C dec. ^1H NMR (600 MHz, CD_3OD): δ 7.78 (s, *H*-triazole, 8H), 6.26 (s, Ar*H*, 4H), 4.82 (overlapped to signal of H_2O, -OC*H*$_2$-triazole, 16H), 4.34 (t, *J* = 7.4 Hz, triazole-C*H*$_2$, 16H), 3.95 (m, -C*H*OH, 8H), 3.90 (m, -C*H*OH, 8H), 3.80 (s, Ar-C*H*$_2$-Ar, 8H), 3.66 (m, N-CH-C*H*$_2$OH, 16H), 3.03 and 2.67 (AB, *J* = 10.2 Hz, N-C*H*$_2$-CHOH, 16H), 2.82 and 2.36 (AB, C*H*$_2$-N, 16H), 2.48 (m, -C*H*-CH_2OH, 8H), 2.31 (overlapped, Ar-C*H*$_3$, 12H), 1.86 (m, C*H*$_2$, 16H), 1.48 (m, C*H*$_2$, 16H), 1.36-1.29 (overlapped, C*H*$_2$, 32H) ppm; $^{13}C\{^1H\}$ NMR (100 MHz, CD_3OD): δ 155.7, 145.1, 131.1, 130.2, 125.8, 125.4, 80.6, 77.3, 74.7, 66.7, 62.5, 60.5, 56.6, 51.3, 31.2, 28.7, 27.8, 27.4, 11.4 ppm; HRMS (MALDI) *m*/*z* $[M + H]^+$ calcd. for $[C_{144}H_{225}N_{32}O_{32}]^+$: 2915.6991; found: 2915.6979; $[\alpha]_{25}^{D}$ (c: 4.1 mg/mL) = -21.01°.

5a: Derivative **5d** (12.3 mg, 9.70 µmol) and derivative **6**[10] (30.0 mg, 0.12 mmol) were dissolved in a mixture of THF/H_2O (1.00 mL, 2:1 v/v) in an ACE pressure tube and $Cu_2SO_4 \cdot 5\ H_2O$ (0.72 mg, 2.90 µmol) and sodium ascorbate (1.15 mg, 5.8 µmol) were added. The reaction mixture was heated under microwave irradiation for 90 min at 80° C. The reaction mixture was filtered through a pad of Celite® and the filtrate was concentrated under reduced pressure to give a yellow solid. The mixture was purified through chromatographic column (silica gel, gradient: from MeOH to ammonia solution 4 M in MeOH) to give derivative **5a** with 27 % of yield (11.5 mg). Mp: > 240 °C dec. ^1H NMR (400 MHz, CD_3OD): δ 7.89 (s, *H*-triazole, 12H), 6.42 (s, Ar*H*, 6H), 4.71 (s, -OC*H*$_2$-triazole, 24H), 4.32 (t, *J*= 7.1 Hz, triazole-C*H*$_2$-, 24H), 3.93-3.83 (overlapped, 36H), 3.63 (m, N-C*H*$_2$-CHOH, 24H), 2.97 (d, *J*= 10.3 Hz, N-C*H*$_2$-CHOH -, 12H), 2.77 (m, C*H*$_2$-N, 12H), 2.60 (m, N-C*H*$_2$-CHOH, 12H), 2.39 (m, -C*H*-CH_2OH, 12H), 2.28-2.17 (overlapped, Ar-C*H*$_3$ and C*H*$_2$-N, 30H), 2.03 (m, C*H*$_2$, 12H), 1.83 (m, C*H*$_2$, 24H), 1.60 (m, C*H*$_2$, 12H), 1.44 -1.29 (overlapped to signal of grease, C*H*$_2$, 36H). 0.90 (m, C*H*$_2$, 12H) ppm; $^{13}C\{^1H\}$ NMR (100 MHz, CD_3OD): δ 155.5, 145.0, 130.9, 126.3, 125.5, 80.9, 77.4, 74.4, 66.8, 62.6, 60.5, 56.4, 51.3, 31.3, 29.0, 27.9, 27.4, 11.2 ppm; HRMS (MALDI) *m*/*z* $[M]^+$ calcd. for $[C_{216}H_{336}N_{48}O_{48}]^+$: 4395.5286; found: 4395.5269; $[\alpha]_{25}^{D}$ (c: 1.9 mg/mL) = - 25.74°.

5b: Derivative **5d** (10.9 mg, 8.60 μmol) and derivative **7** (30.0 mg, 0.10 mmol) were dissolved in a mixture of THF/H_2O (1.00 mL, 2:1 v/v) in an ACE pressure tube and $Cu_2SO_4 \cdot 5\ H_2O$ (0.64 mg, 2.60 μmol) and sodium ascorbate (1.00 mg, 5.20 μmol) were added. The reaction mixture was heated under microwave irradiation for 90 min at 80° C. The reaction mixture was filtered through a pad of Celite® and the filtrate was concentrated under reduced pressure to give a yellow solid. The mixture was purified through chromatographic column (silica gel, gradient: from MeOH to ammonia solution 4 M in MeOH) to give derivative **5b** with 31 % of yield (12.7 mg). Mp: > 210 °C dec. ^{1}H NMR (600 MHz, CD_3OD): δ 7.92 (s, *H*-triazole, 12H), 6.46 (s, Ar*H*, 6H), 4.72 (overlapped to signal of H_2O, 24H), 4.52 (overlapped to signal of H_2O, 24H), 3.90-3.84 (overlapped, 60H), 3.64-3.49 (overlapped, CH_2, 96H), 3.01-2.94 (overlapped, 24H), 2.66 (m, 12H), 2.46-2.42 (overlapped, 24H), 2.24 (s, Ar-CH_3, 18H) ppm; ^{13}C{^{1}H}NMR (150 MHz, CD_3OD): δ 155.6, 145.0, 130.9, 126.4, 126.2, 80.7, 77.4, 74.2, 71.3, 71.2, 70.7, 70.4, 66.8, 62.1, 61.1, 55.1, 51.4, 30.8,11.3 ppm; HRMS (MALDI) *m*/*z* [M+Na]$^+$ calcd. for $[C_{216}H_{336}N_{48}NaO_{72}]^+$: 4779.4065; found: 4779.3962; $[\alpha]_{25}^{D}$ (c: 1.1 mg/mL) = -10.74°.

Copies of 1D, 2D NMR and HR mass spectra

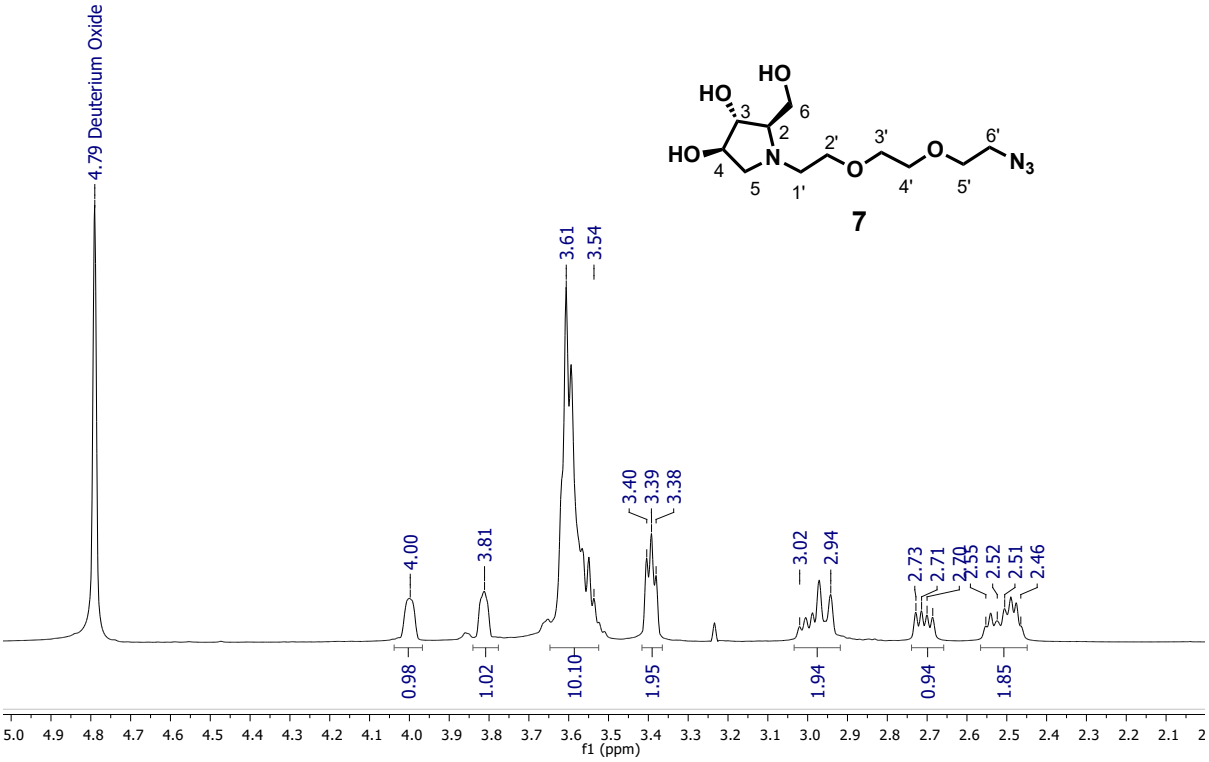

Figure S1: ^{1}H NMR spectrum of compound **7** (400 MHz, D_2O).

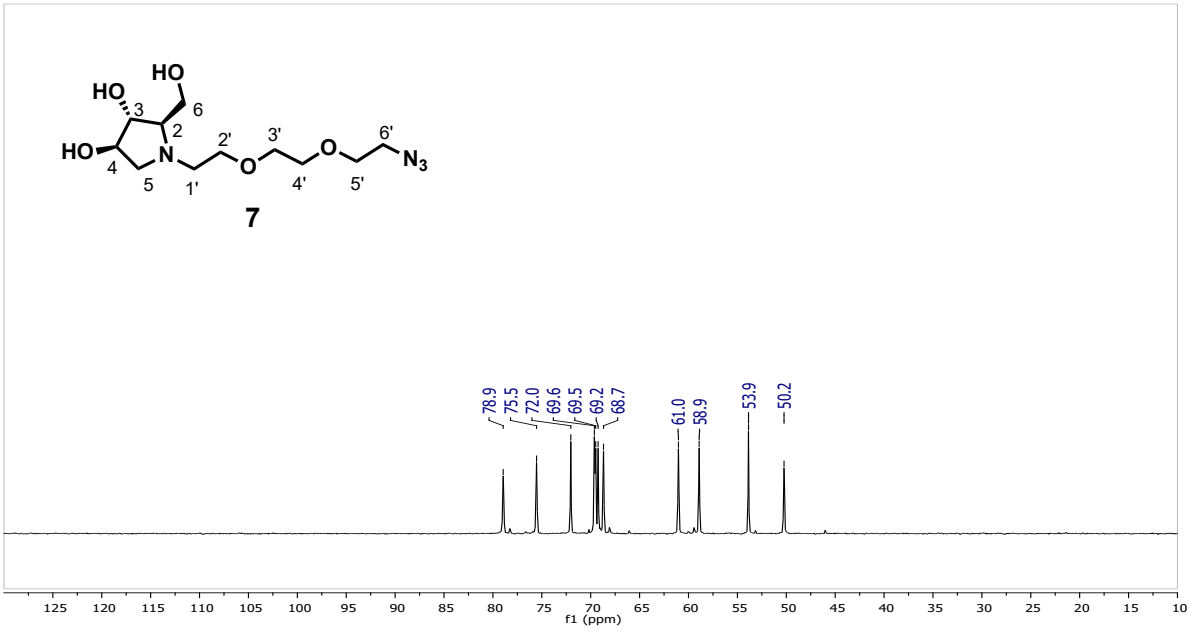

Figure S2: ^{13}C NMR spectrum of compound **7** (50 MHz, D_2O).

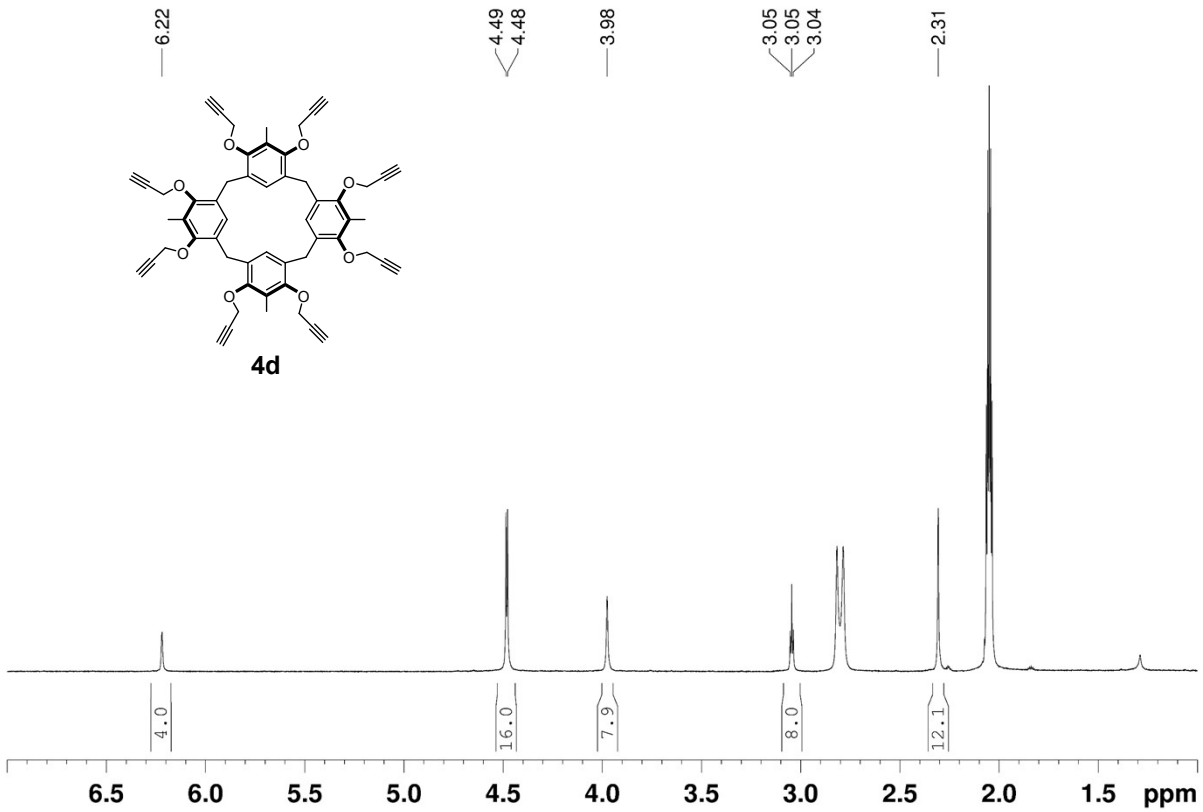

Figure S3: ^{1}H NMR spectrum of compound **4d** (300 MHz, Acetone-d_6).

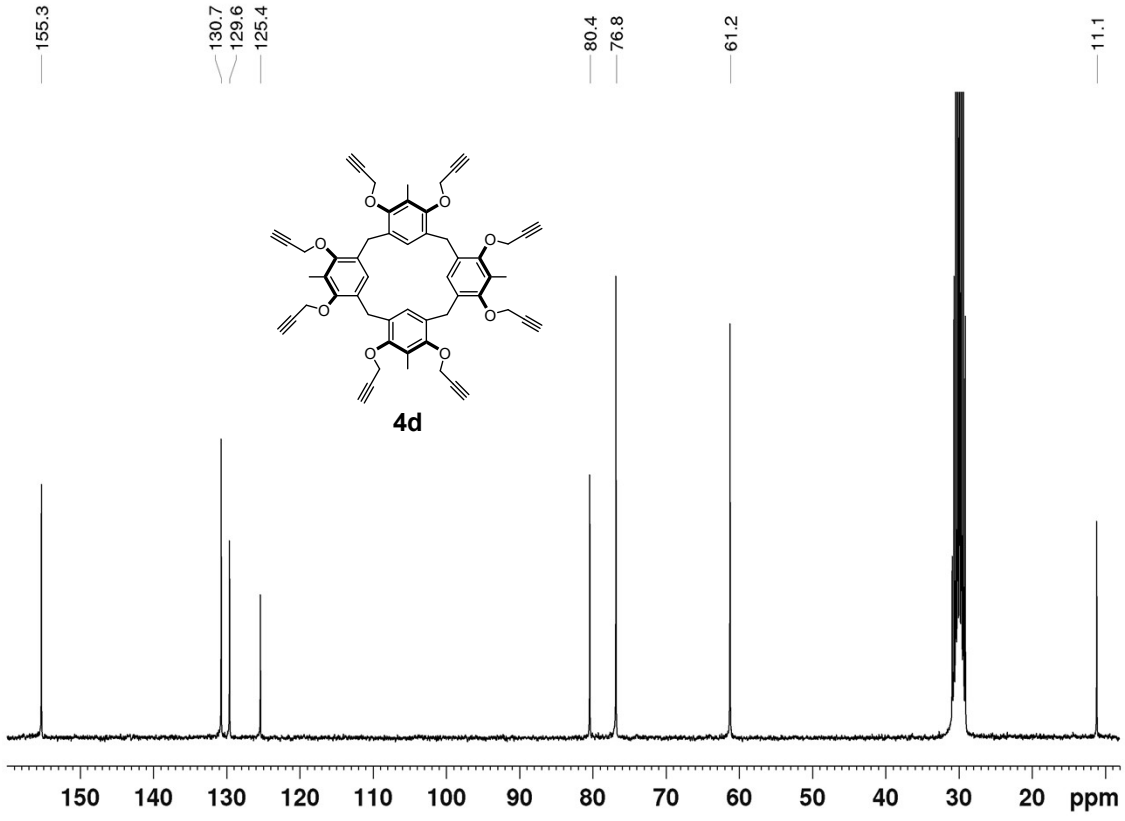

Figure S4: ^{13}C NMR spectrum of compound **4d** (75 MHz, Acetone-d_6).

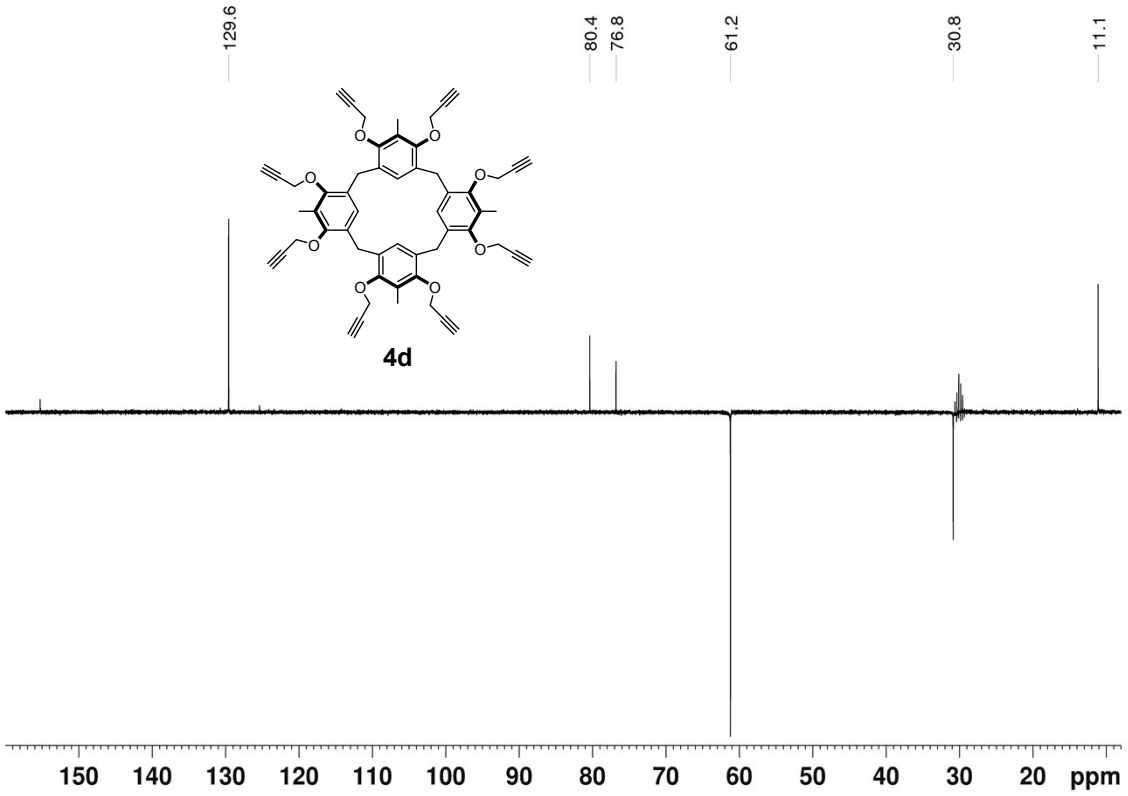

Figure S5: Dept 135 spectrum of compound **4d** (75 MHz, Acetone-d_6).

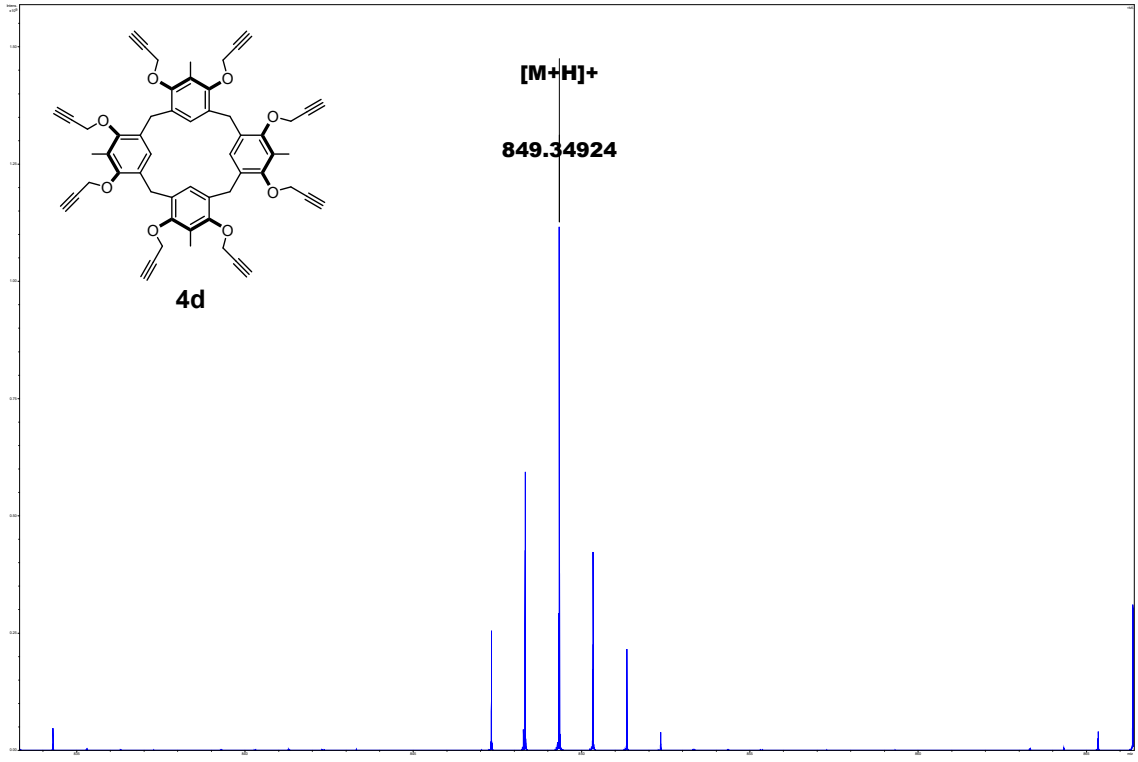

Figure S6: Significant portion of the MALDI FT-ICR mass spectrum of **4d** $[M+H]^+$, showing the isotopic envelop.

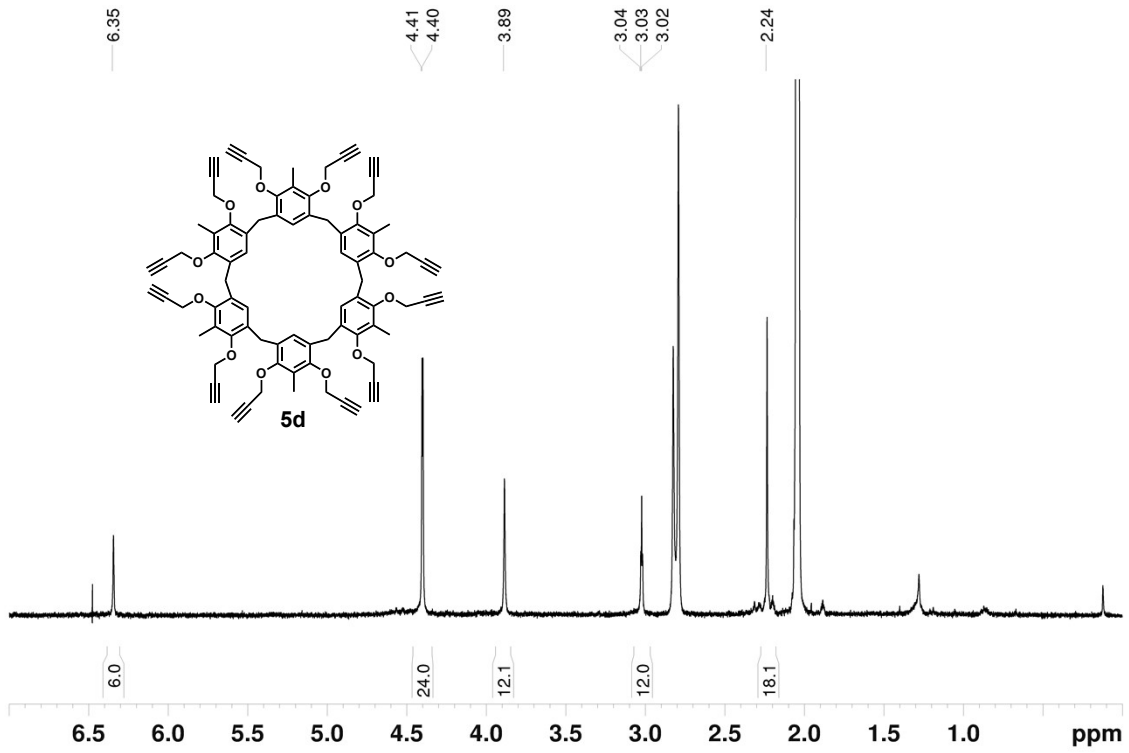

Figure S7: ^{1}H NMR spectrum of compound **5d** (300 MHz, Acetone-d_6).

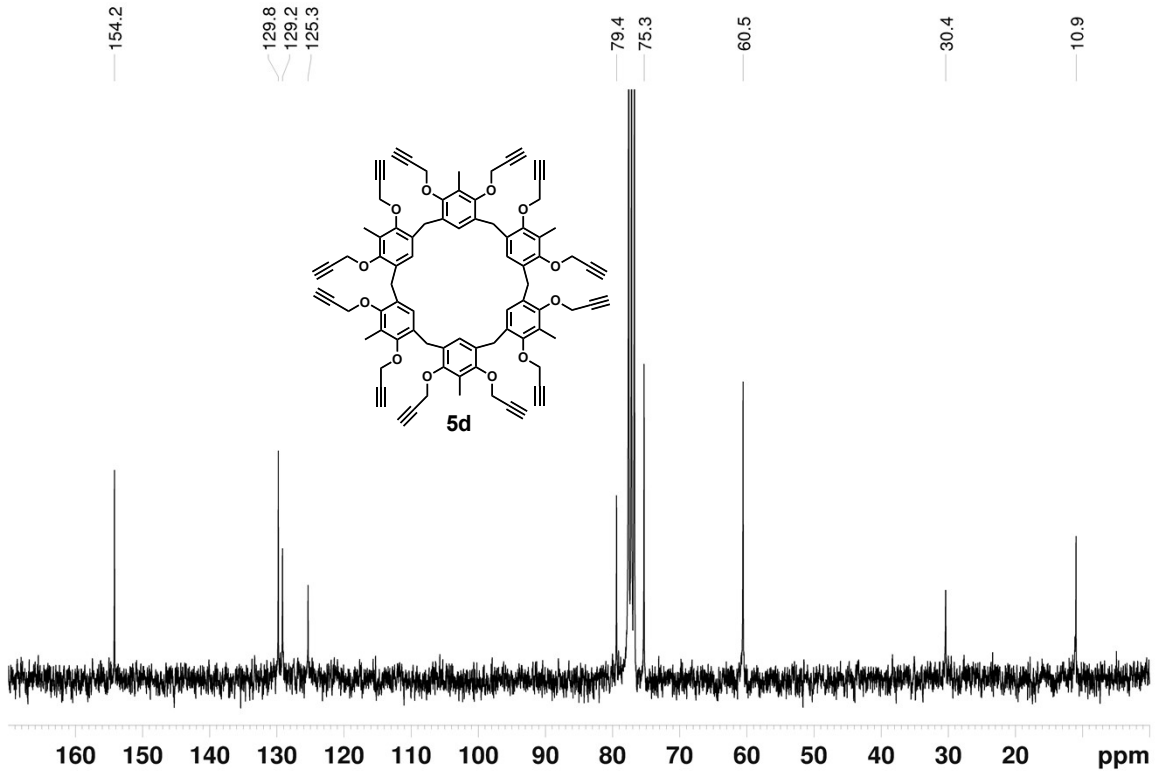

Figure S8: ^{13}C NMR spectrum of compound **5d** (100 MHz, Acetone-d_6).

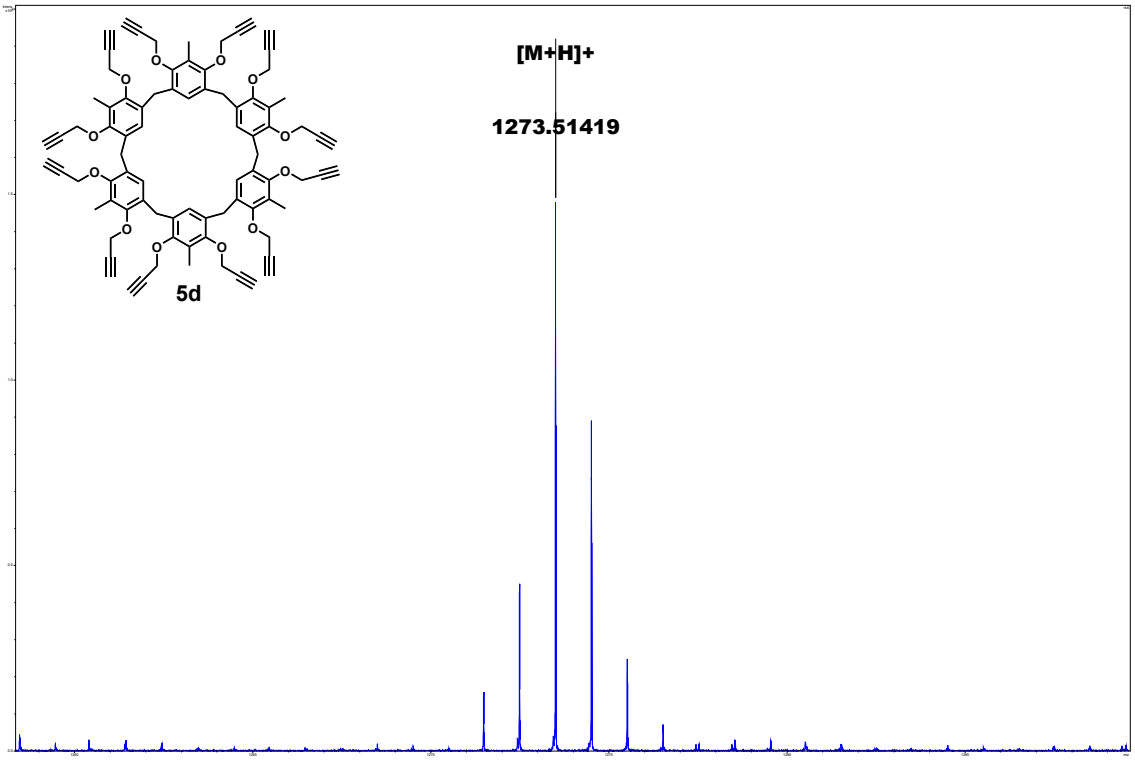

Figure S9: Significant portion of the MALDI FT-ICR mass spectrum of **5d** $[M+H]^+$, showing the isotopic envelop.

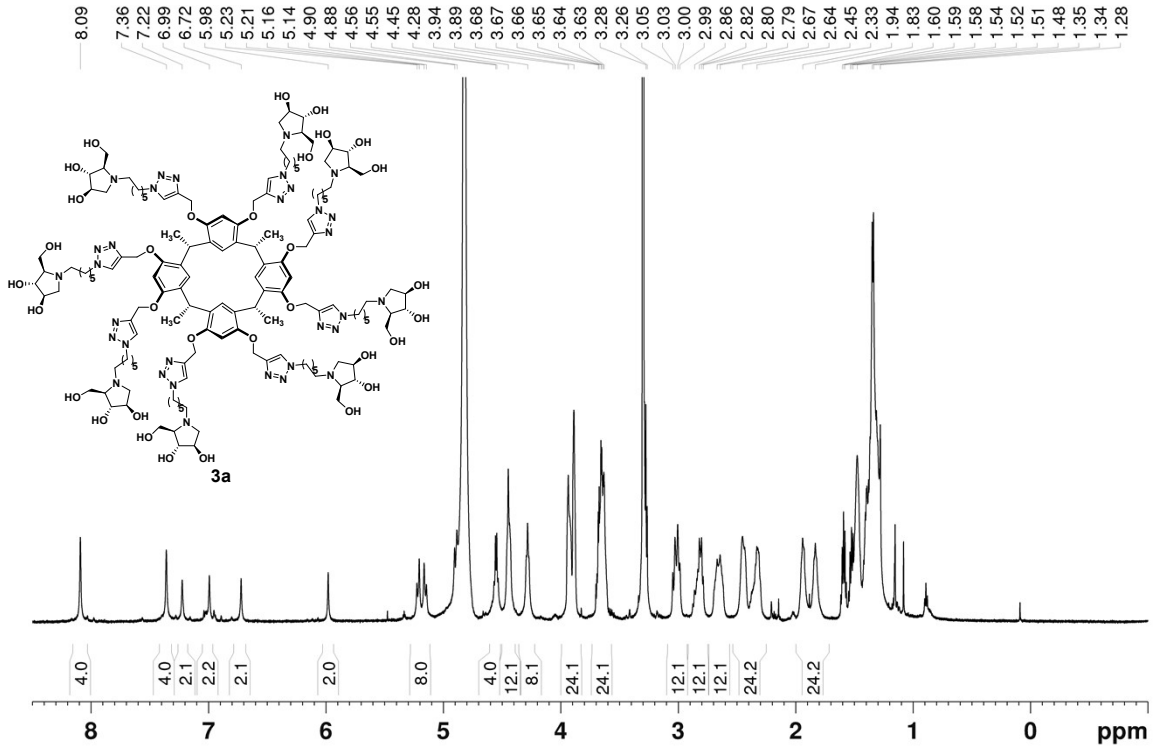

Figure S10: ^{1}H NMR spectrum of **3a** (CD_3OD, 600 MHz).

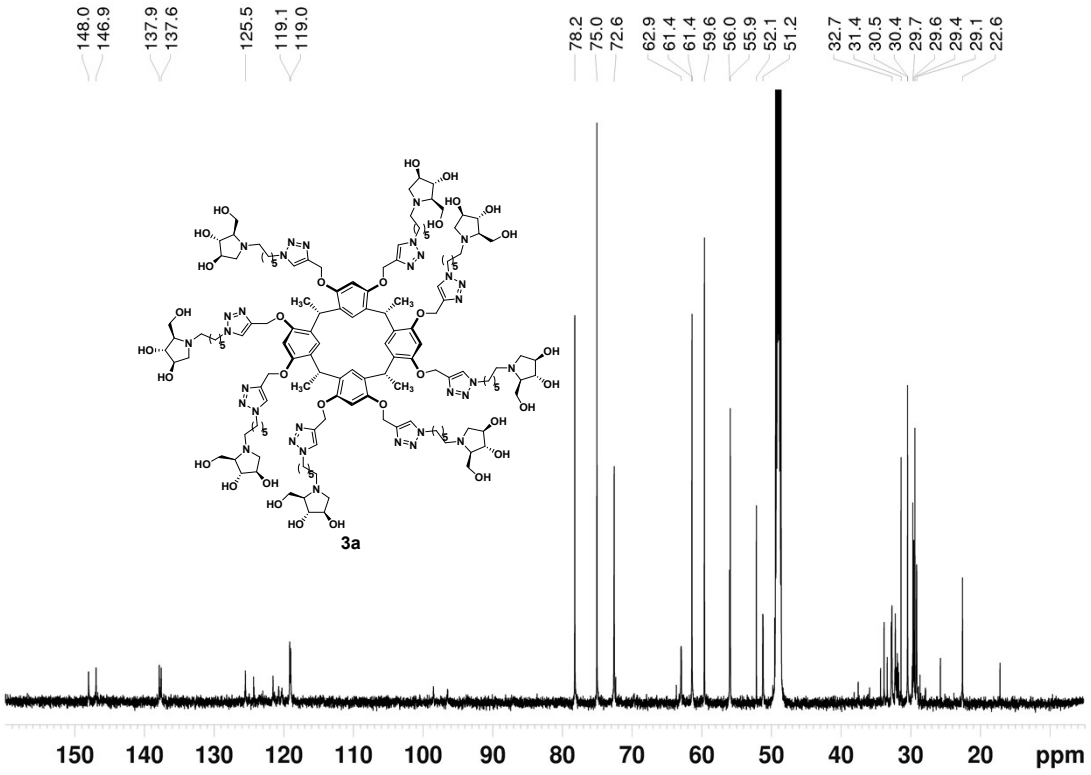

Figure S11: ^{13}C NMR spectrum of **3a** (CD_3OD, 150 MHz).

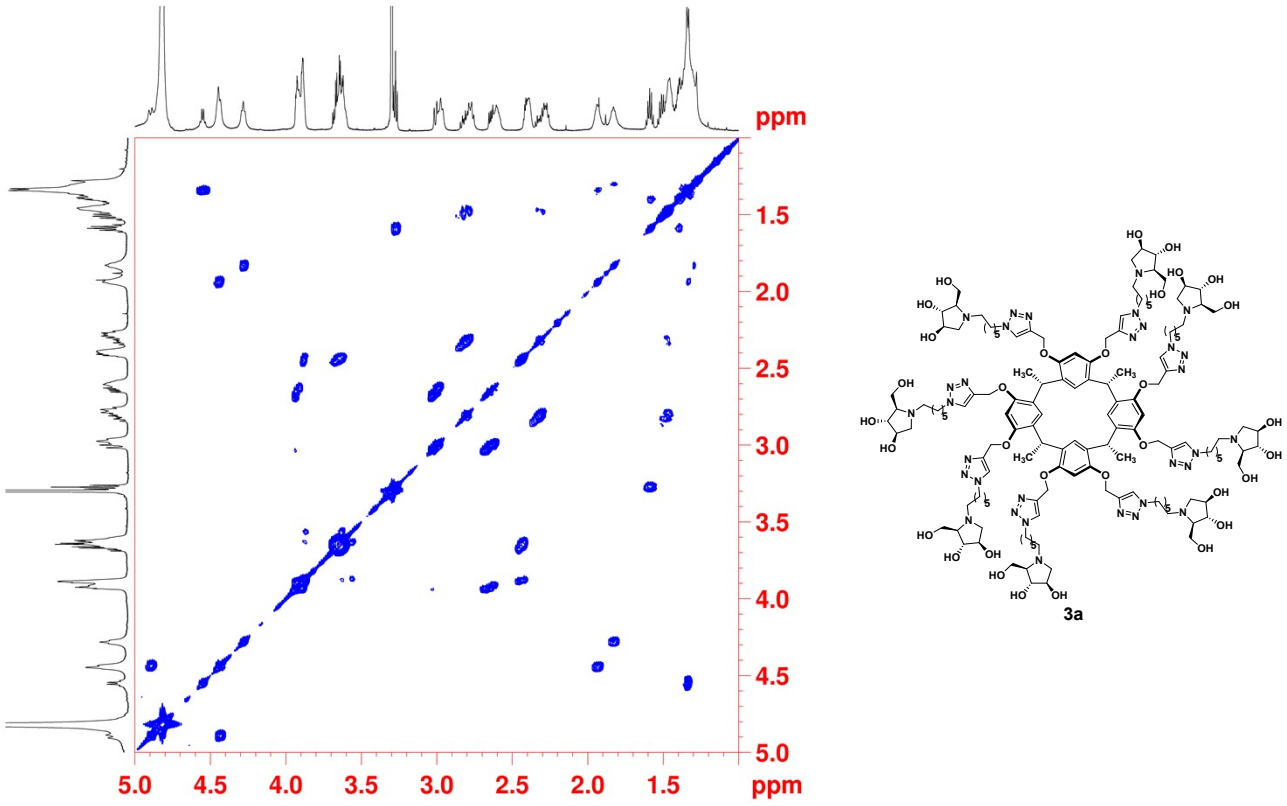

Figure S12: Significant portion of 2D COSY spectrum of **3a** (CD_3OD, 600 MHz).

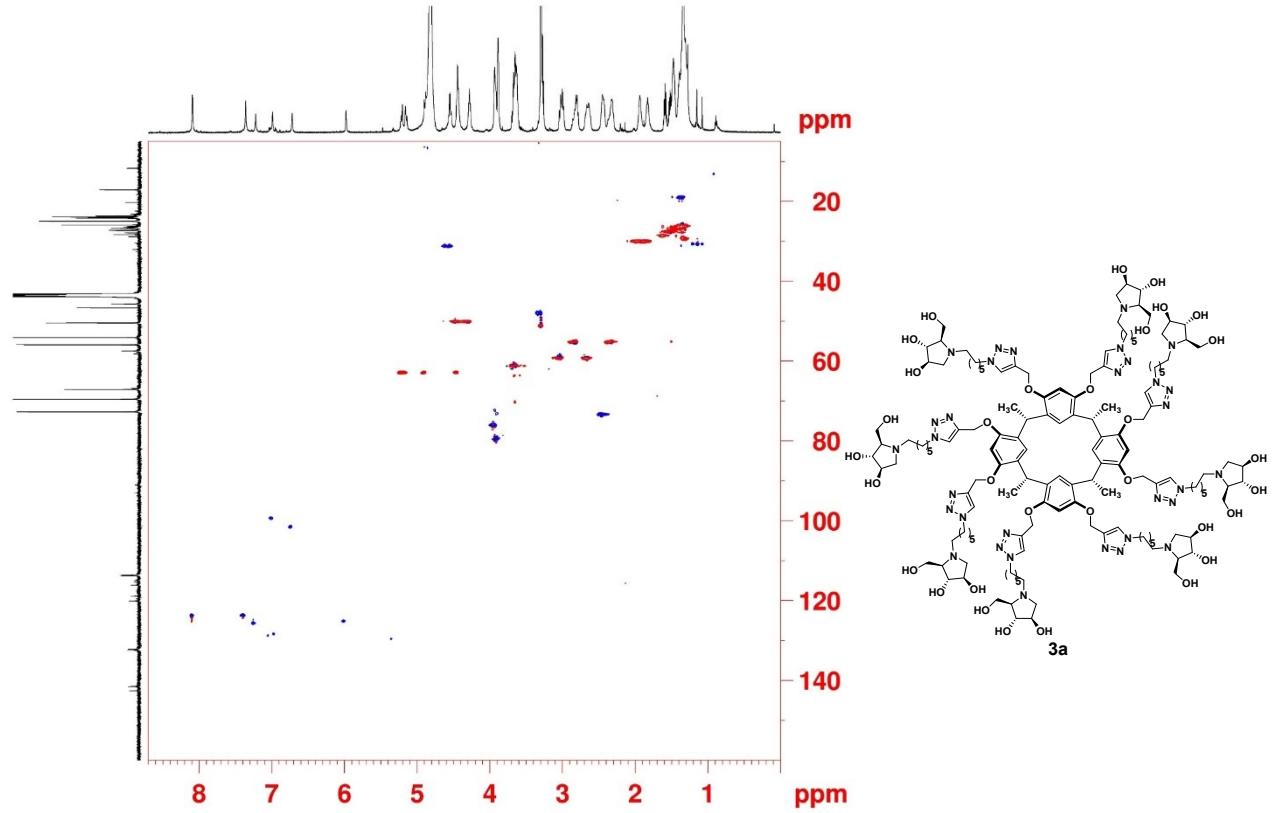

Figure S13: 2D HSQC spectrum of **3a** (CD_3OD, 600 MHz).

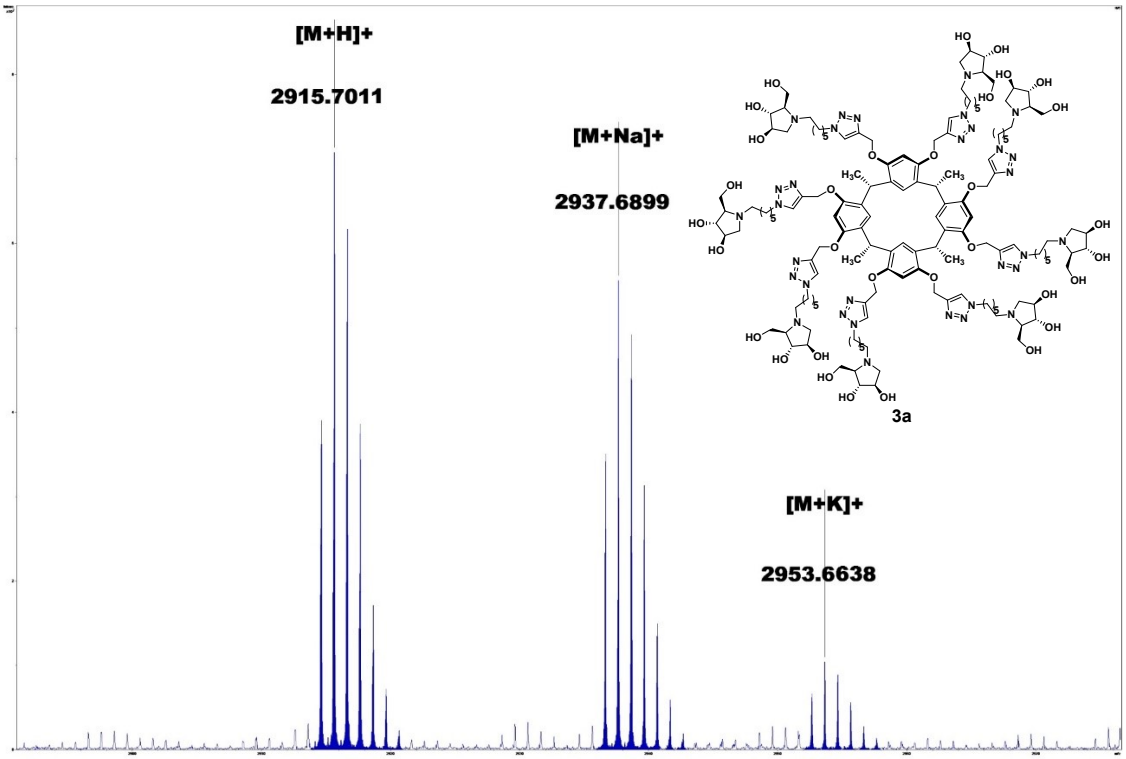

Figure S14: Significant portion of the MALDI FT-ICR mass spectrum of **3a**, showing the isotopic envelop of $[M+H]^+$, $[M+Na]^+$ and $[M+K]^+$.

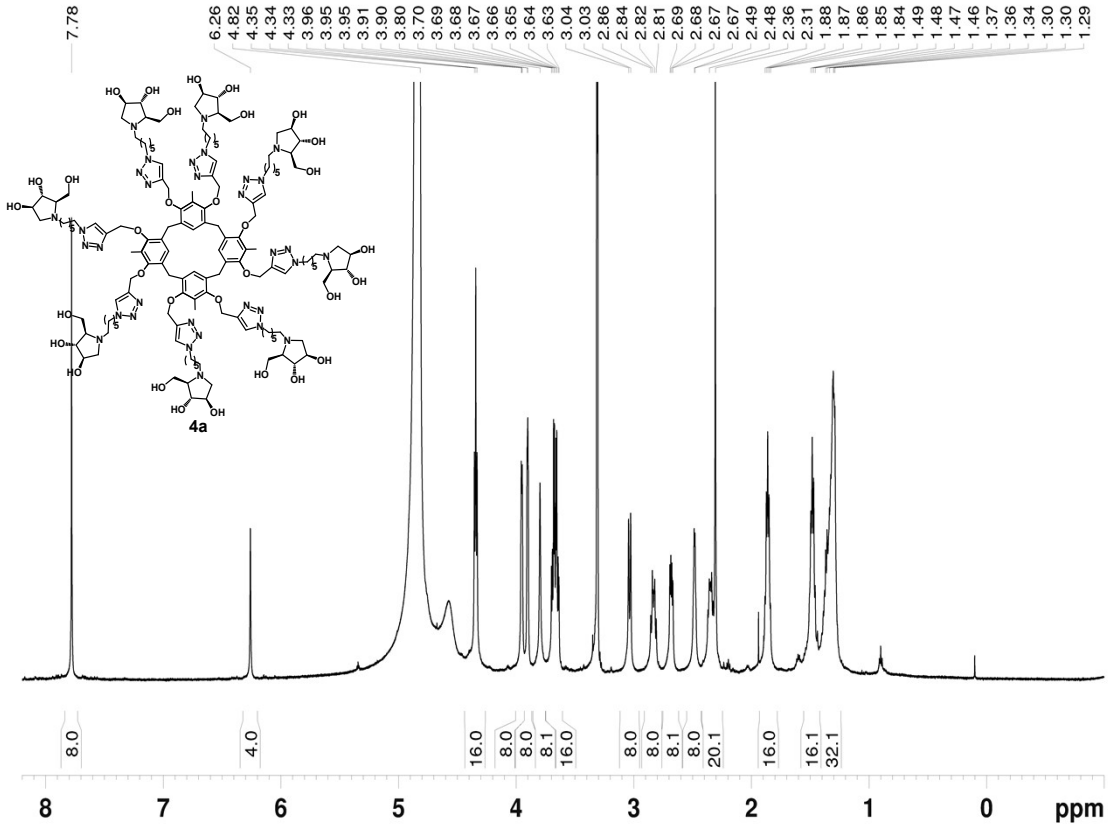

Figure S15: ^{1}H NMR spectrum of **4a** (CD_3OD, 600 MHz).

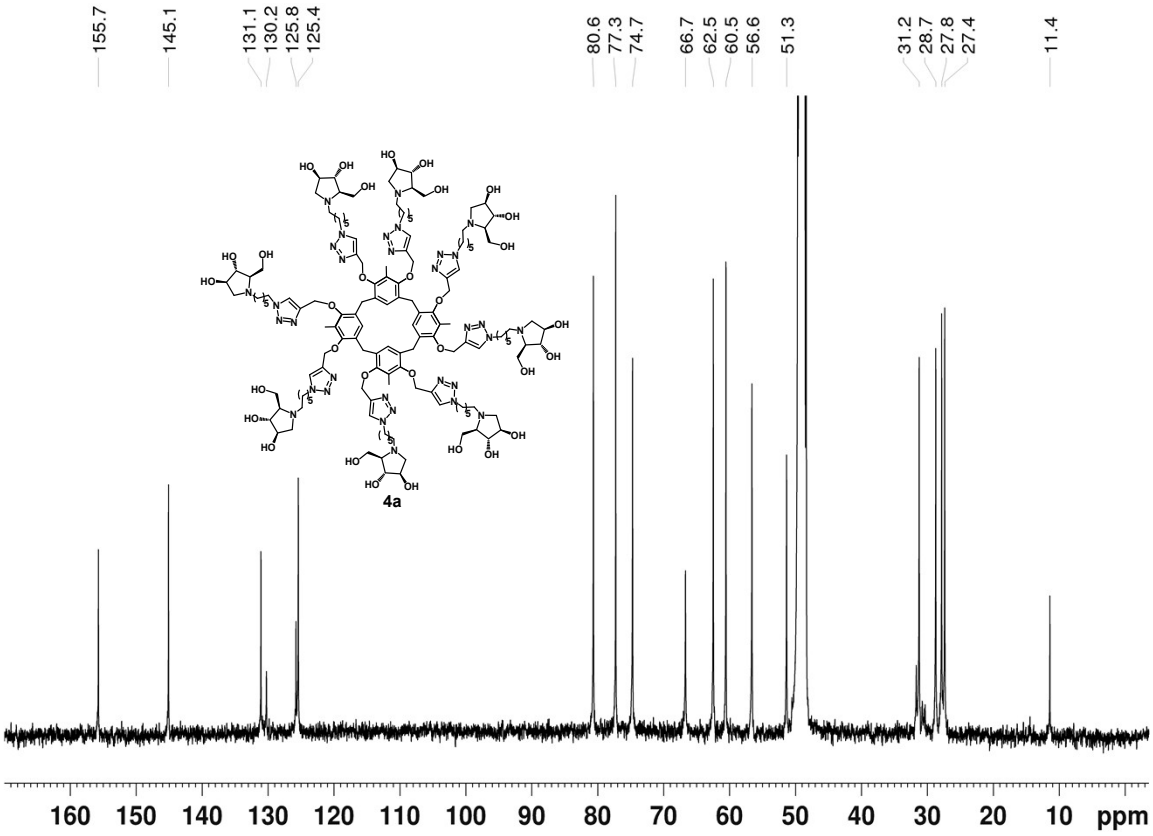

Figure S16: ^{13}C NMR spectrum of **4a** (CD_3OD, 100 MHz).

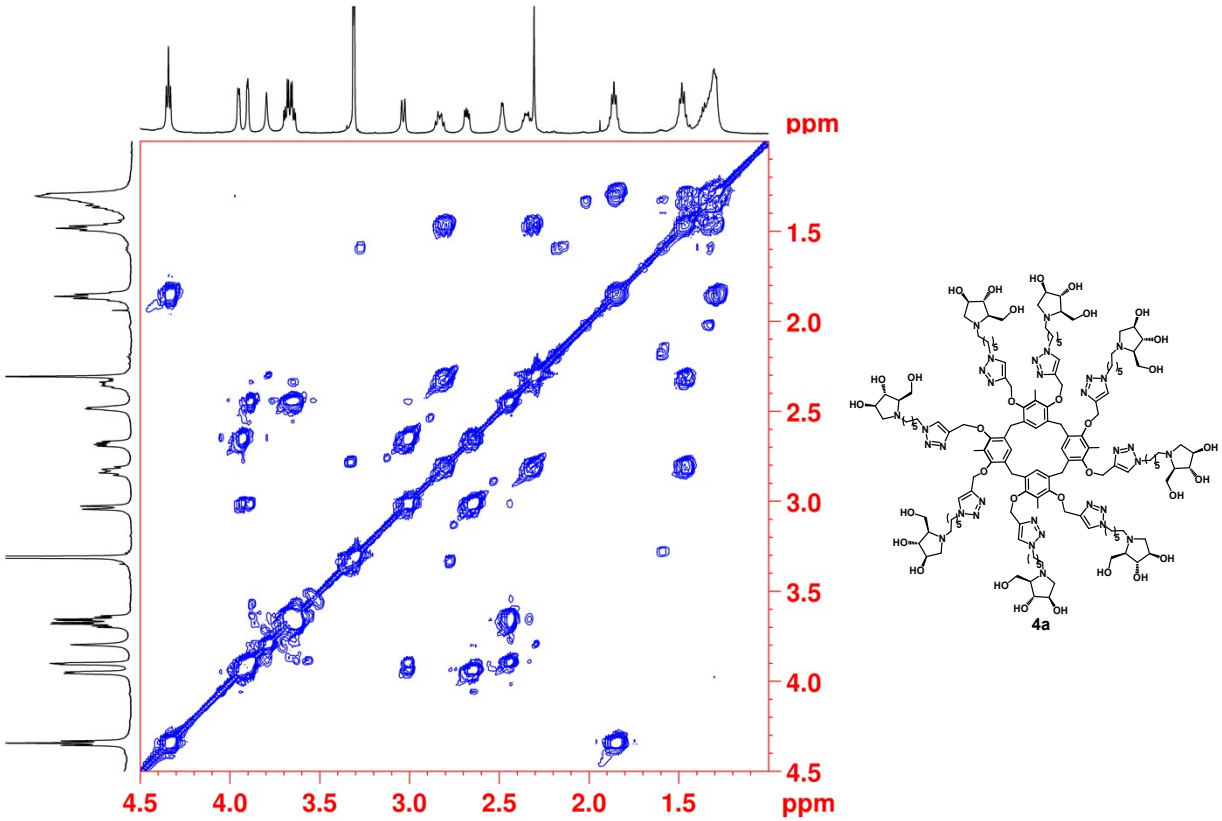

Figure S17: Significant portion of 2D COSY spectrum of **4a** (CD_3OD, 600 MHz).

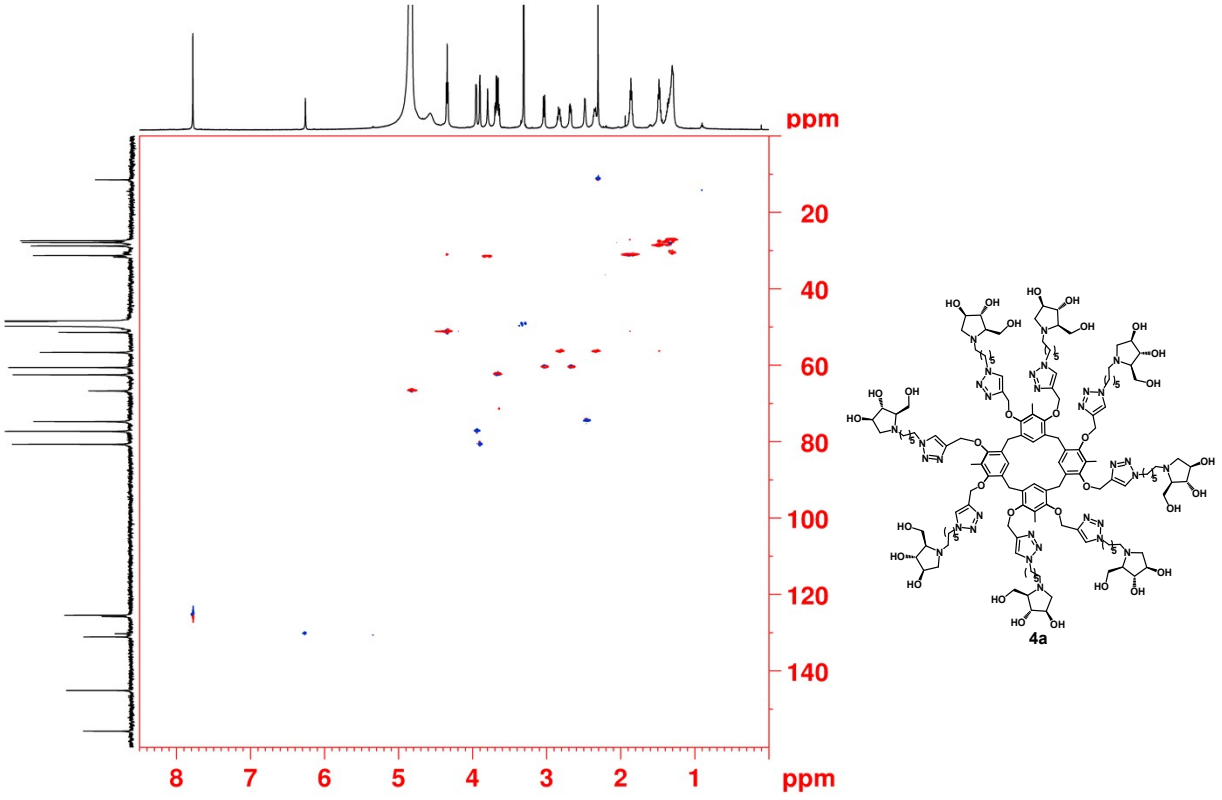

Figure S18: 2D HSQC spectrum of **4a** (CD_3OD, 600 MHz).

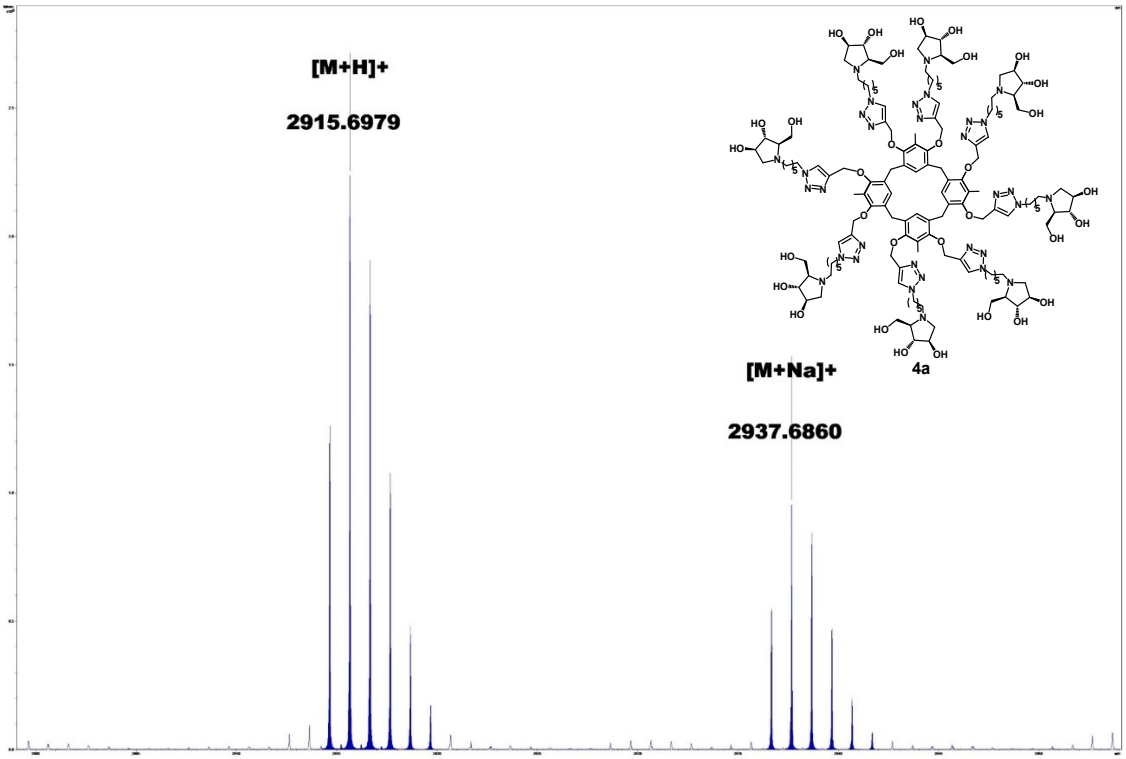

Figure S19: Significant portion of the MALDI FT-ICR mass spectrum of **4a,** showing the isotopic envelop of $[M+H]^+$ and $[M+Na]^+$.

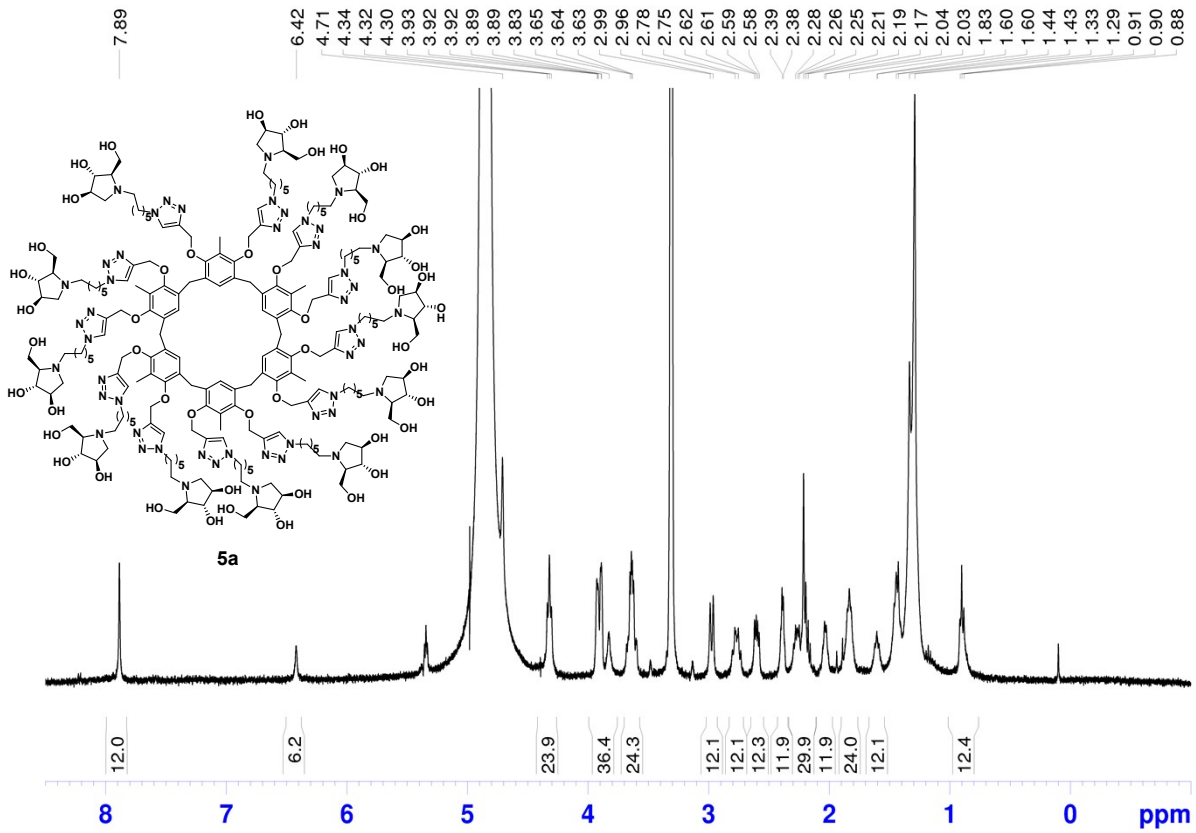

Figure S20: ^{1}H NMR spectrum of **5a** (CD_3OD, 400 MHz).

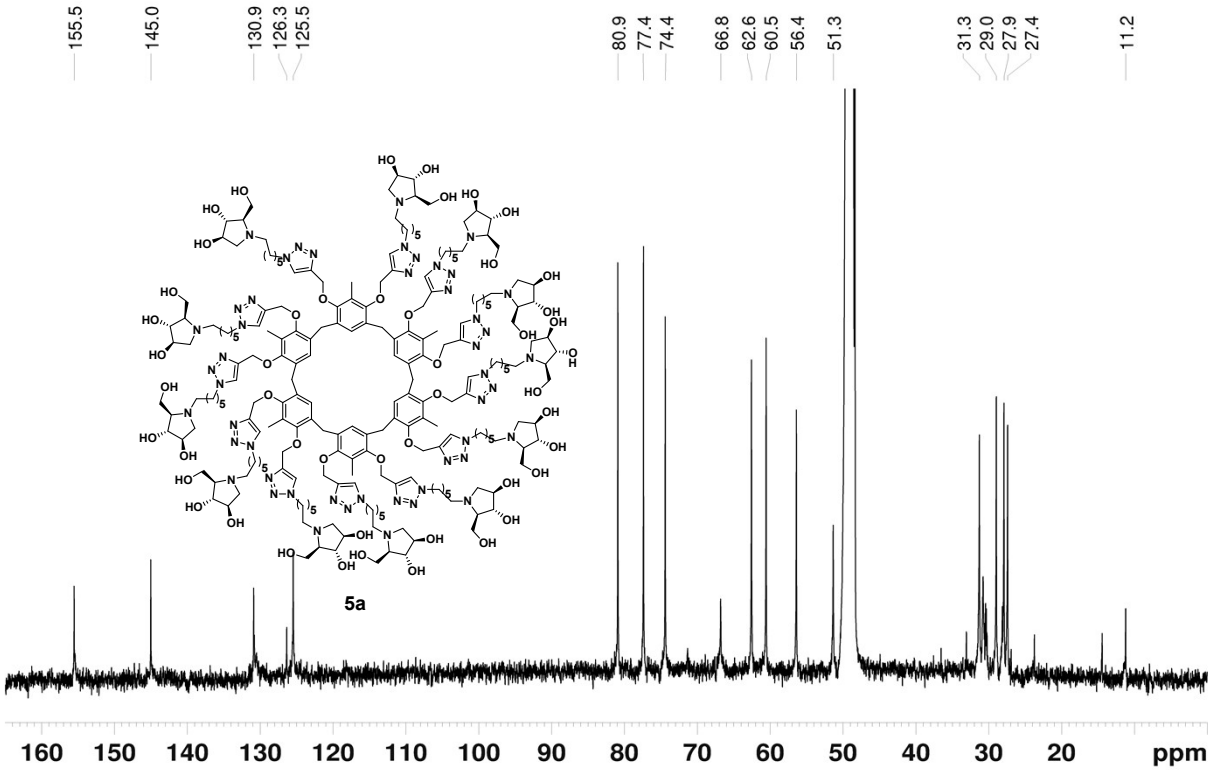

Figure S21: ^{13}C NMR spectrum of **5a** (CD_3OD, 100 MHz).

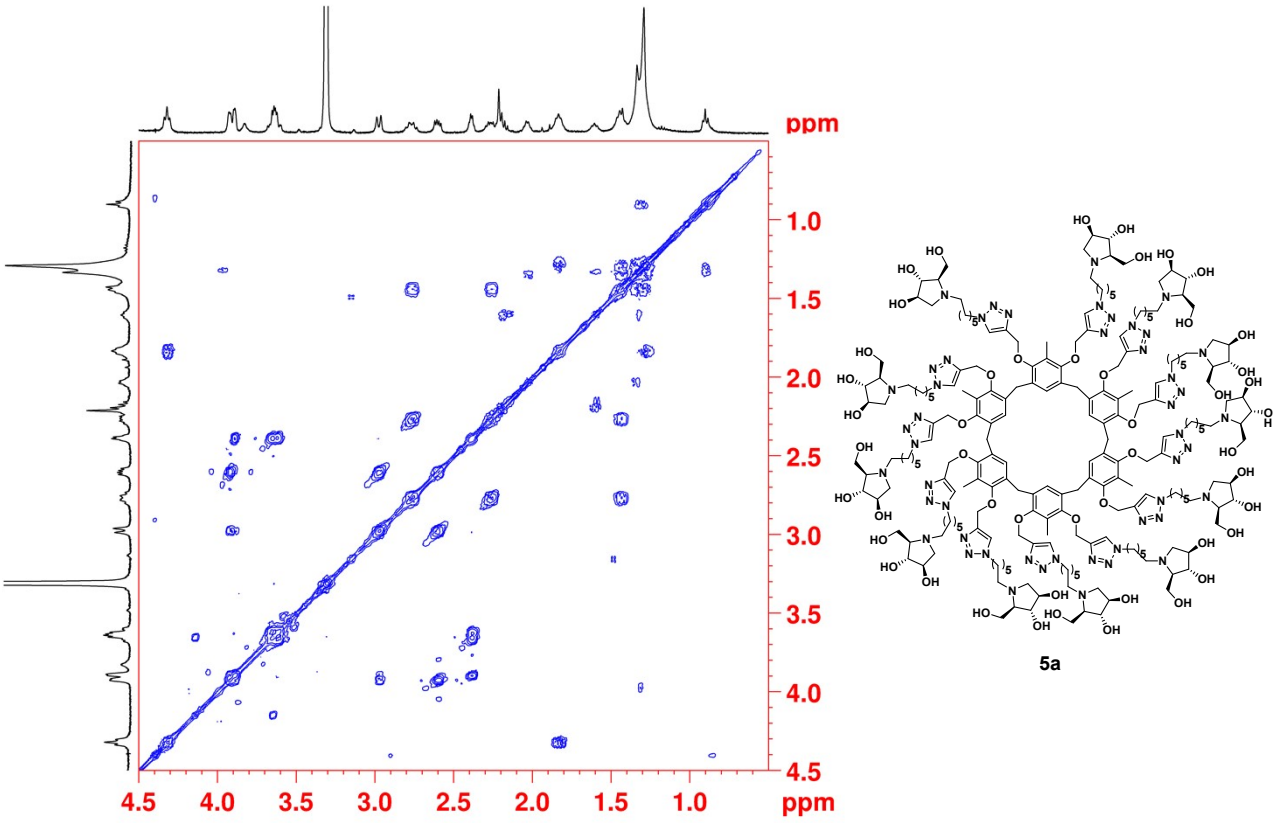

Figure S22: Significant portion of 2D COSY spectrum of **5a** (CD_3OD, 600 MHz).

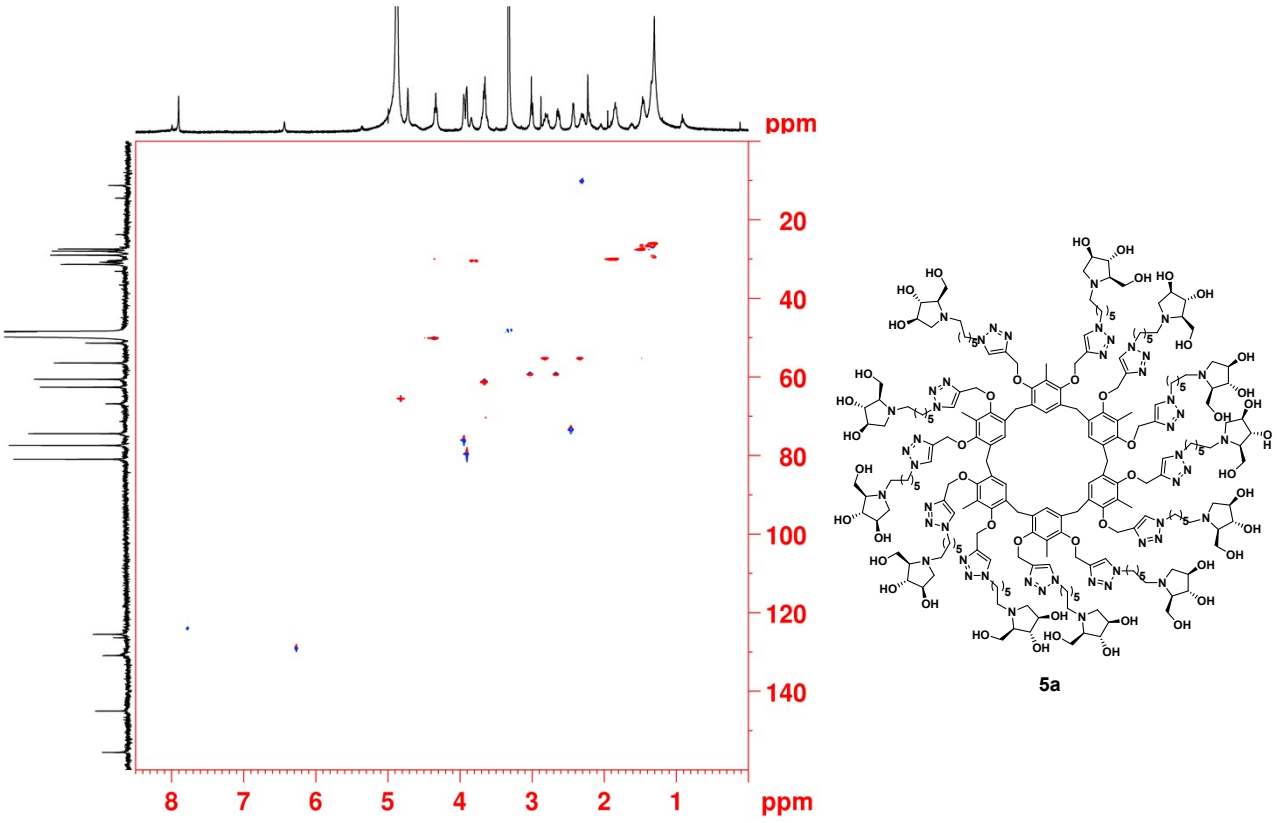

Figure S23: 2D HSQC spectrum of **5a** (CD_3OD, 600 MHz).

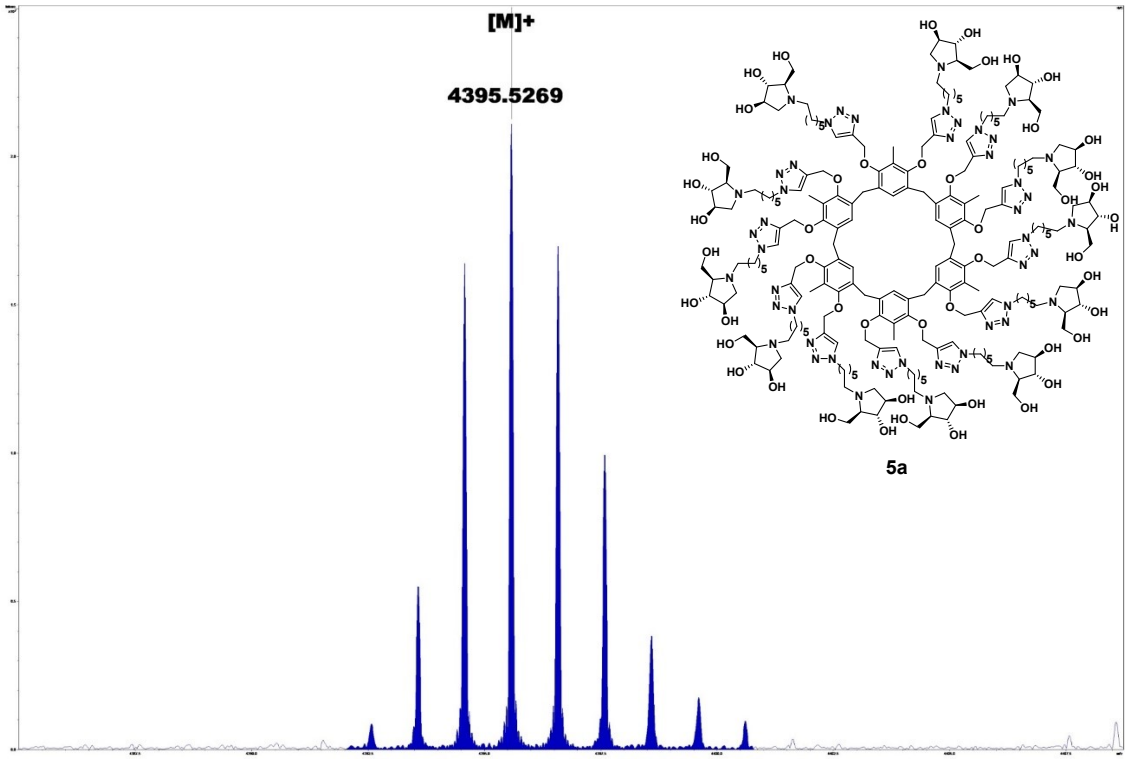

Figure S24: Significant portion of the MALDI FT-ICR mass spectrum of **5a** $[M]^+$, showing the isotopic envelop.

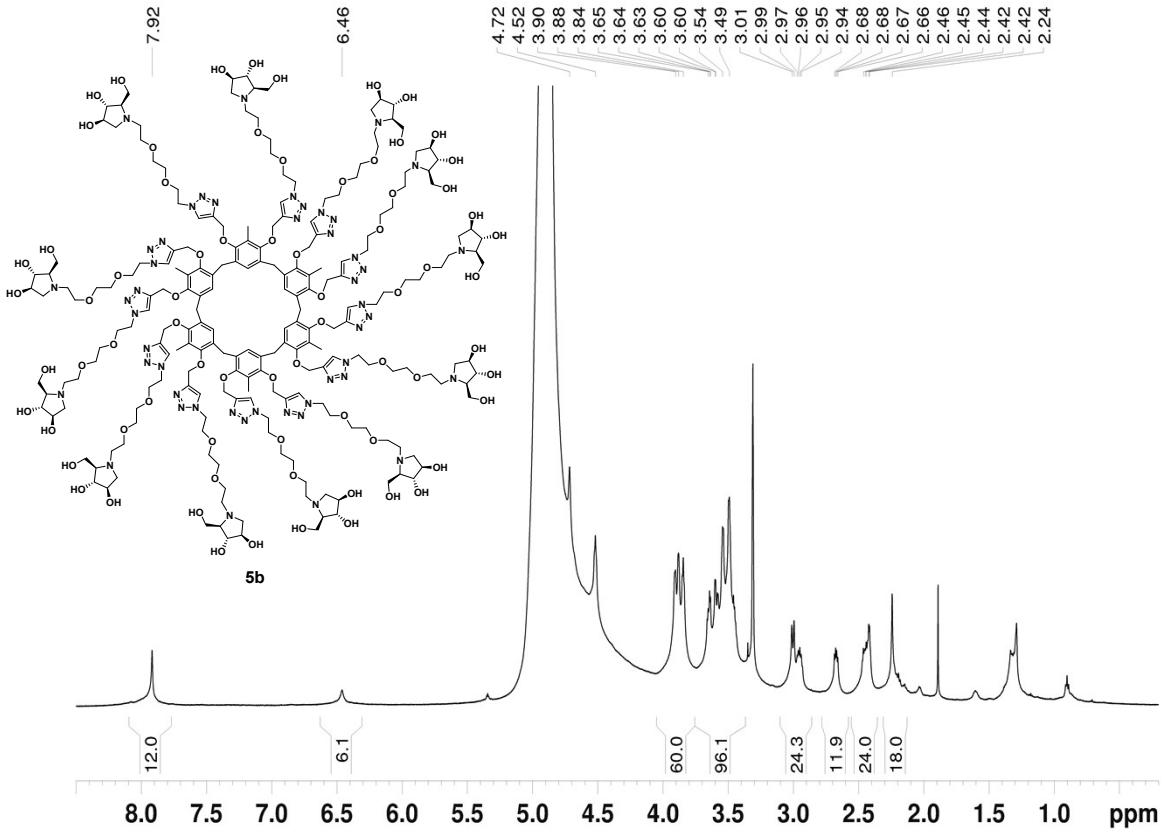

Figure S25: ^{1}H NMR spectrum of **5b** (CD_3OD, 600 MHz).

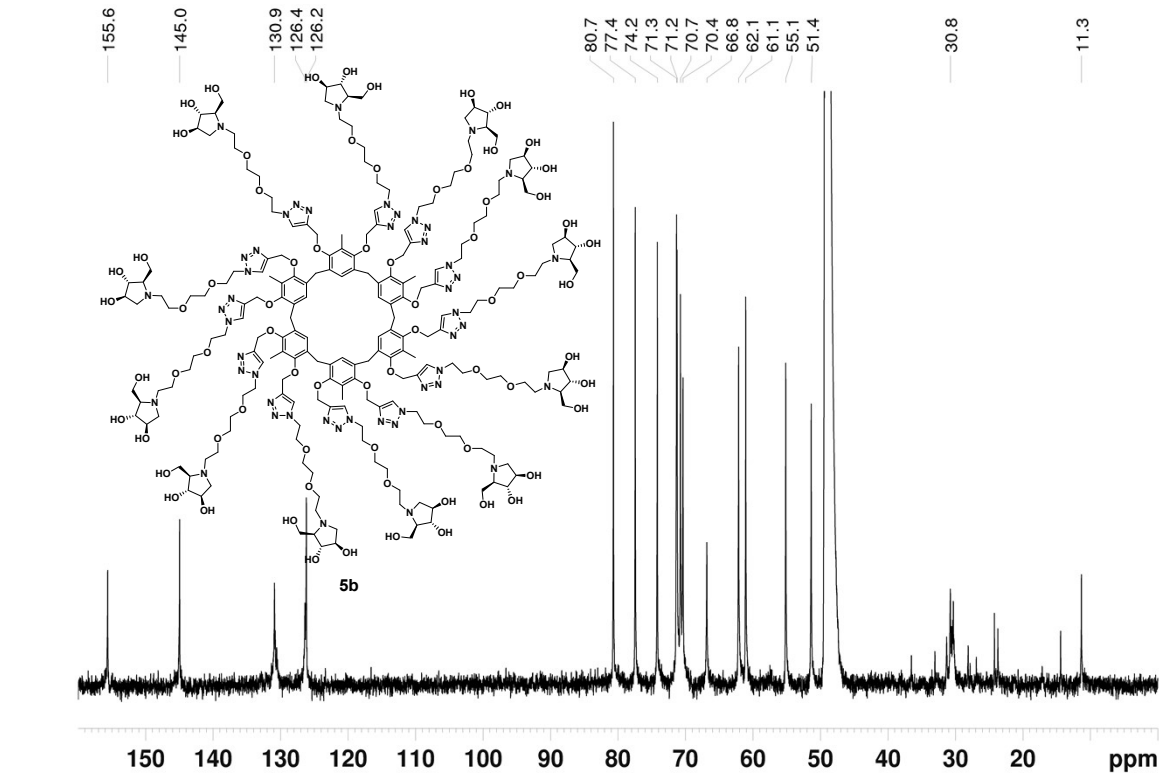

Figure S26: ^{13}C NMR spectrum of **5b** (CD_3OD, 150 MHz).

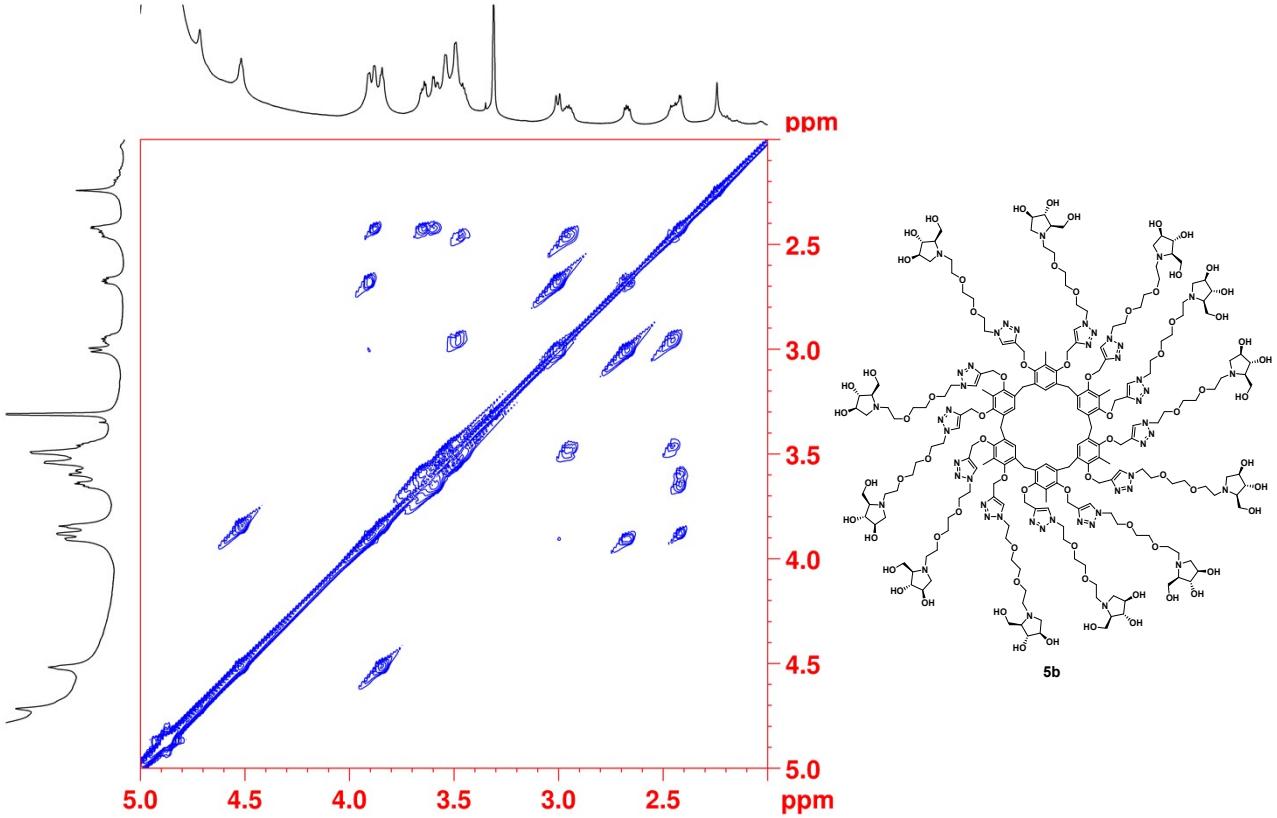

Figure S27: Significant portion of 2D COSY spectrum of **5b** (CD_3OD, 600 MHz).

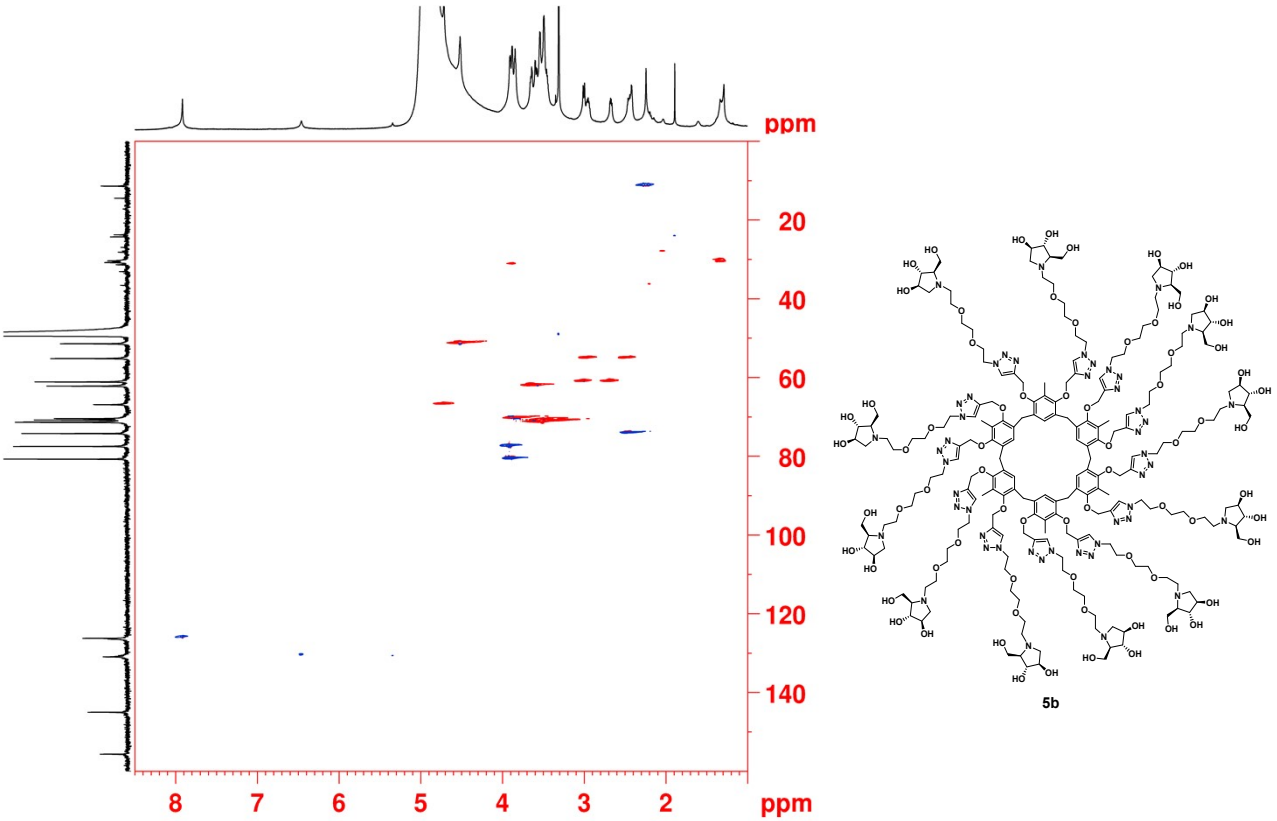

Figure S28: 2D HSQC spectrum of **5b** (CD_3OD, 600 MHz).

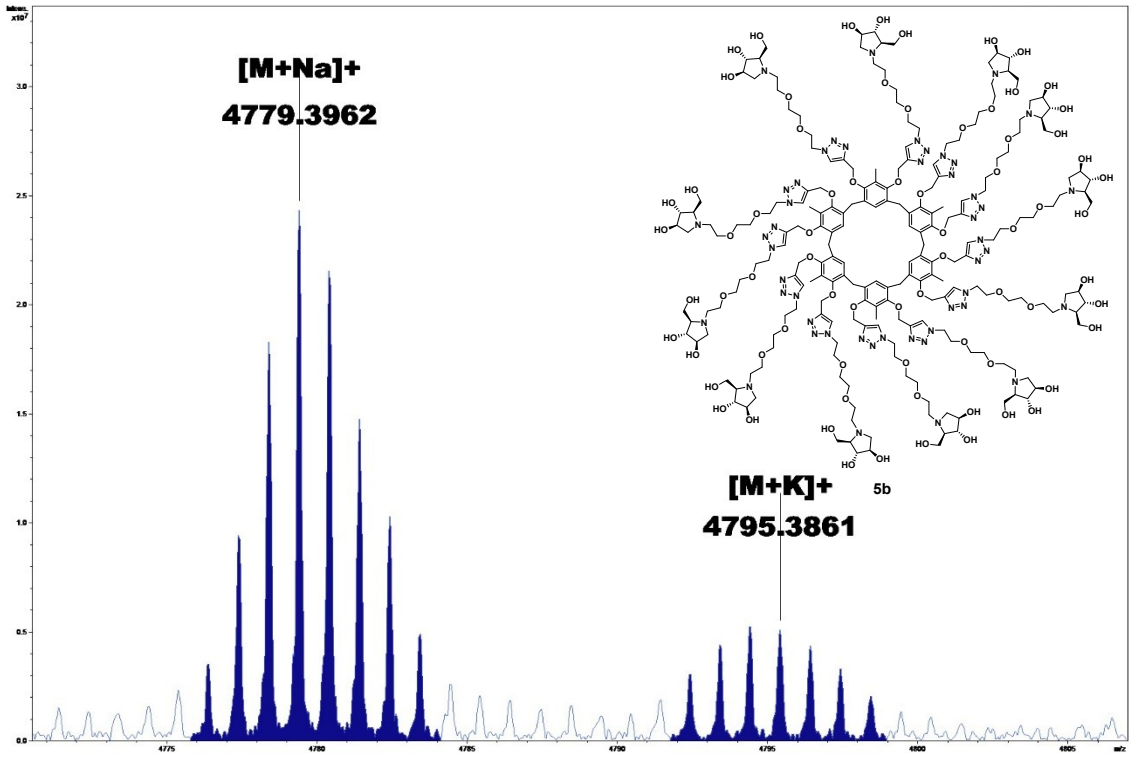

Figure S29: Significant portion of the MALDI FT-ICR mass spectrum of **5b**, showing the isotopic envelop of $[M+Na]^+$ and $[M+K]^+$.

In Silico Studies

VINA docking and molecular dynamics calculations were performed on Intel Xeon GOLD 5118 processors while Autodock calculation was carried out on an Intel Core i7-6700HQ. JBα-man high-resolution X-ray structure (Protein Data Bank, PDB entry 6B9O)[11] was used as the starting structure for molecular dynamics simulation and docking studies. The multivalent derivatives **3a**, **4a**, **5a** and **5b** were optimized through a molecular dynamics simulation performed with Yasara Software[12] package in a box of water (100 x 100 x 100 Å) and AMBER force field for 10 ns. The protein-ligand complexes were prepared for the molecular dynamics simulations on the dimeric protein structure $(LH)_2$ using Yasara Software package. Each complex was placed in a cubic box with periodic boundaries and water molecules, NaCl was added at the physiological conditions. The systems were simulated in NVT ensemble at 298 K for 10 ns. The systems were then energy minimized using first a steepest descent minimization and then by a simulated annealing minimization until convergence (<0.01 kcal/mol Å).

VINA calculation was performed with VINA docking software[13] (implemented in YASARA) performing 100 runs in a box (85 x 65 x 55 Å) sited in the center of tetramer $2x(LH)_2$ including all 4 active sites.

Autodock4[14] software and Autodock4_{Zn}[15] force field were used for docking calculations with **5a(DAB-1)$_1$** and **5b(DAB-1)$_1$** and the dimeric protein $(LH)_2$. A grid box size of 90 x 90 x 126 centered at -20 (x); 12(y); 0(z) was used. The spacing between the grid points was set to 0.55 Å to cover the two catalytic pockets. Lamarckian Genetic Algorithm was used (500 runs) for dockings. Results differing by less than 2.0 Å in positional RMSD were clustered together and represented by the result with the binding energies.

The optimizations of structures obtained by Autodock4 were performed with the Gaussian 16 [16] suite of programs at b3lyp/6-31G level of theory. The residues considered for DFT

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[11] E. Howard, A. Cousido-Siah, M. L. Lepage, J. P. Schneider, A. Bodlenner, A. Mitschler, A. Meli, I. Izzo, A. Alvarez, A. Podjarny, P. Compain, Structural Basis of Outstanding Multivalent Effects in Jack Bean α-Mannosidase Inhibition*. Angew. Chem., Int. Ed.* 2018, **57**, 8002–8006.

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[13] O. Trott and A. J. Olson, AutoDock Vina: Improving the Speed and Accuracy of Docking with a New Scoring Function, Efficient Optimization, and Multithreading. *J. Comput. Chem.* 2009, **31**, 455-461.

[14] G. M. Morris, R. Huey, W. Lindstrom, M. F. Sanner, R. K. Belew, D. S. Goodsell and A. J. Olson, AutoDock4 and AutoDockTools4: Automated Docking with Selective Receptor Flexibility. *J. Comput. Chem.,* 2009, **30**, 2785-2791.

[15] D. Santos-Martins, S. Forli, M. J. Ramos and A. J. Olson*,* AutoDock4Zn: An Improved AutoDock Force Field for Small-Molecule Docking to Zinc Metalloproteins. *J. Chem. Inf. Model.,* 2014, **54**, 2371–2379.

[16] Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

investigation were His 23, Asp 24, Asp 25, Trp 28, Asp 145, Phe 147, Arg 170, Tyr 210, Asp 268, Trp 333, His 385, His 386, Asp 387, Tyr 625, Arg 789 and Gly 790. Natural bond orbital (NBO) analyses were performed with NBO 3.1 version implemented in Gaussian 16 via single point energy calculations using the b3lyp/6-31G method. The non-covalent interaction (NCI) index was analyzed with the Multiwfn program, and its plot was graphed with Chemcraft (version 1.8).

Molecular Dynamics Optimized structures of 3a, 4a, 5a and 5b

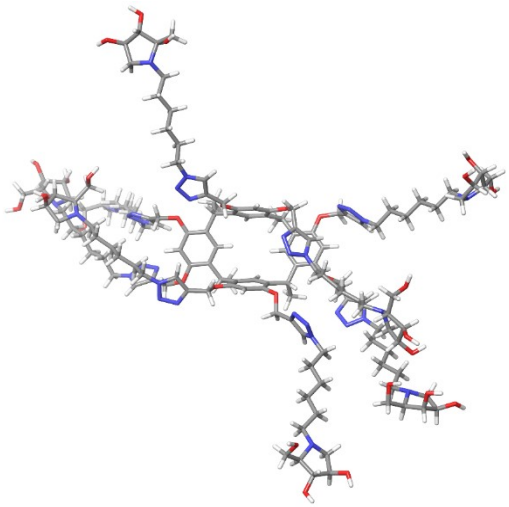

Figure S30: Lowest energy structure of **3a**

O	-15.49010000	15.57640000	-2.71110000
O	-16.18220000	16.78410000	-7.41280000
C	-15.12810000	15.53920000	-4.04920000
C	-15.79970000	16.26870000	-5.04270000
C	-15.49130000	16.12860000	-6.40220000
C	-14.45510000	15.25590000	-6.77450000
C	-13.73870000	14.57630000	-5.77910000
C	-14.07280000	14.69510000	-4.42800000
C	-14.12010000	15.05820000	-8.26430000
O	-8.56390000	9.55930000	-9.46100000
O	-6.52960000	10.18640000	-5.08630000
C	-8.57740000	10.03520000	-8.16050000
C	-7.57240000	9.75390000	-7.22290000
C	-7.60370000	10.30340000	-5.93980000
C	-8.69320000	11.09180000	-5.54230000
C	-9.69140000	11.38270000	-6.48180000
C	-9.64200000	10.87000000	-7.78460000
C	-8.75170000	11.60520000	-4.09080000
O	-7.58140000	14.11440000	-3.24610000
O	-11.89940000	16.23620000	-2.85930000
C	-8.94290000	14.06770000	-3.45030000
C	-9.70570000	15.20450000	-3.18930000
C	-11.10650000	15.15710000	-3.19430000
C	-11.75650000	13.95140000	-3.50300000
C	-10.98010000	12.82890000	-3.83290000
C	-9.57800000	12.87480000	-3.82460000
C	-13.29720000	13.87270000	-3.38400000
O	-12.05710000	16.83150000	-9.02010000
O	-8.91740000	13.11980000	-9.68520000
C	-11.68910000	15.49860000	-8.94050000
C	-10.40740000	15.02220000	-9.24960000
C	-10.11440000	13.65010000	-9.24230000
C	-11.09830000	12.73710000	-8.83470000
C	-12.37250000	13.21520000	-8.50640000
C	-12.68380000	14.58010000	-8.56690000
C	-10.75440000	11.23050000	-8.78700000
C	-15.18740000	14.18380000	-8.96100000
C	-9.14530000	10.47250000	-3.11850000
H	-10.14100000	10.08500000	-3.33410000
H	-8.44890000	9.63690000	-3.17970000
C	-11.96010000	10.28340000	-8.60160000
H	-11.65220000	9.24240000	-8.70270000
H	-12.40970000	10.39630000	-7.61470000
H	-9.17990000	16.10760000	-2.92830000
H	-11.46090000	11.89330000	-4.07470000
H	-12.92350000	13.91970000	-6.04280000
H	-16.60940000	16.91240000	-4.75490000
H	-13.14110000	12.52570000	-8.19450000
H	-9.64040000	15.71590000	-9.53440000
H	-7.72290000	11.85550000	-3.83520000
H	-14.22310000	16.03870000	-8.72890000
H	-13.49150000	14.30270000	-2.40010000
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H	-14.94950000	14.04310000	-10.01600000
H	-16.17220000	14.64660000	-8.91010000
H	-15.26910000	13.20000000	-8.49990000
H	-12.72890000	10.46660000	-9.35220000
H	-9.13880000	10.82170000	-2.08580000
C	-13.87210000	12.44180000	-3.30220000
H	-13.38180000	11.86010000	-2.52090000
H	-14.93640000	12.46670000	-3.06660000
H	-13.76010000	11.90910000	-4.24670000
C	-16.27620000	16.65840000	-2.19890000
H	-16.03200000	16.74190000	-1.14000000
H	-15.95030000	17.59980000	-2.64030000
C	-11.30450000	17.48870000	-2.53990000
H	-10.66650000	17.81500000	-3.36320000
H	-10.67300000	17.39640000	-1.65470000

C	-17.16260000	17.78520000	-7.12270000
H	-17.17380000	18.44850000	-7.98780000
H	-16.85720000	18.42040000	-6.29140000
C	-7.50840000	8.72570000	-9.94780000
H	-7.80330000	8.37340000	-10.93620000
H	-7.44250000	7.82740000	-9.33270000
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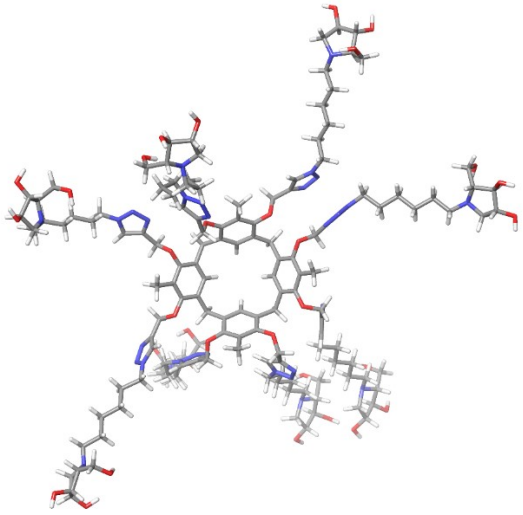

Figure S31: Lowest energy structure of **4a**

C	-17.55260000	13.91380000	-3.84970000
C	-17.30960000	13.74340000	-2.47610000
C	-18.36570000	13.82440000	-1.55780000
C	-19.67330000	13.96670000	-2.02770000
C	-19.93400000	14.07680000	-3.39580000
C	-18.86410000	14.12400000	-4.30220000
C	-16.39650000	13.87440000	-4.84450000
C	-21.37920000	14.18560000	-3.87170000
C	-22.59320000	10.95680000	-5.55390000
C	-22.00050000	12.21530000	-5.36790000
C	-22.02670000	12.82580000	-4.10700000
C	-22.67970000	12.19290000	-3.04970000
C	-23.30380000	10.95700000	-3.22910000
C	-23.29550000	10.35110000	-4.49620000
C	-22.44340000	10.25200000	-6.89930000
C	-22.19430000	7.57690000	-0.11040000
C	-22.95690000	8.22440000	-1.10170000
C	-23.13590000	9.61400000	-1.04070000
C	-22.54260000	10.34690000	-0.00980000
C	-21.80790000	9.70940000	0.99150000
C	-21.71170000	8.31140000	0.98570000
C	-24.03670000	10.33250000	-2.04600000
C	-21.83040000	6.09980000	-0.22940000
C	-17.33700000	10.83320000	2.13370000
C	-18.63610000	10.37500000	2.40730000
C	-19.74210000	11.00090000	1.81010000
C	-19.53800000	12.11040000	0.98470000
C	-18.25370000	12.61240000	0.75120000
C	-17.15130000	11.98000000	1.34780000
C	-16.12190000	10.10160000	2.69670000
C	-18.09180000	13.90090000	-0.05720000
C	-21.17280000	10.54420000	2.10390000
O	-21.38930000	12.84940000	-6.42400000
O	-23.95790000	9.15640000	-4.68080000
O	-15.87970000	12.47990000	1.18760000
C	-15.48090000	13.42320000	2.18370000
C	-25.16510000	9.21270000	-5.45060000
C	-22.28520000	13.54790000	-7.29130000
H	-20.49400000	14.00290000	-1.32640000
H	-15.48840000	14.29950000	-4.41600000
H	-16.60960000	14.42610000	-5.75880000
H	-16.19110000	12.84140000	-5.12590000
H	-21.96160000	14.74010000	-3.13480000
H	-21.44930000	14.78380000	-4.77700000
H	-22.70060000	12.66410000	-2.07820000
H	-22.57370000	9.17320000	-6.81130000
H	-21.44590000	10.41650000	-7.30970000
H	-23.16860000	10.63370000	-7.61730000
H	-22.66260000	11.42010000	0.01890000
H	-24.59080000	11.11760000	-1.52980000
H	-24.81030000	9.65000000	-2.39000000
H	-22.57960000	5.46890000	0.24720000
H	-20.86810000	5.89450000	0.24140000
H	-21.72830000	5.80550000	-1.27470000
H	-20.39070000	12.60030000	0.53860000
H	-15.77900000	10.57970000	3.61330000
H	-15.29900000	10.10980000	1.98050000
H	-16.34370000	9.05620000	2.91290000
H	-17.09990000	14.32590000	0.08380000
H	-18.75980000	14.64780000	0.37390000
H	-21.79210000	11.42290000	2.28980000
H	-21.19660000	9.99730000	3.04280000
O	-16.03120000	13.54080000	-2.01290000
O	-19.09610000	14.39980000	-5.62930000
O	-23.52970000	7.55410000	-2.16280000
O	-21.15050000	7.66330000	2.06310000
O	-18.82480000	9.32340000	3.27440000
C	-15.54680000	12.19900000	-2.13690000
C	-14.18150000	12.22070000	-2.79110000
C	-12.99960000	12.80750000	-2.35980000
N	-12.09070000	12.56280000	-3.35320000
N	-12.65160000	11.84410000	-4.32920000
N	-13.96070000	11.61880000	-3.94960000
C	-21.68230000	14.24010000	-12.27860000
C	-22.59940000	13.26050000	-13.04240000
C	-22.90240000	13.69680000	-14.48530000
C	-25.33170000	12.28170000	-17.24630000
N	-25.95880000	12.88830000	-18.42670000
C	-25.06170000	13.08000000	-19.59050000
C	-25.84180000	12.64400000	-20.84690000

C	-26.78870000	11.57480000	-20.29520000
C	-27.11480000	12.11390000	-18.89810000
C	-24.47500000	14.50920000	-19.70760000
O	-25.50130000	15.48530000	-19.65350000
O	-27.92200000	11.33540000	-21.12180000
O	-25.02960000	12.15890000	-21.90890000
C	-13.96970000	13.56130000	2.22630000
C	-13.12180000	13.58100000	3.32610000
N	-11.86710000	13.76640000	2.81320000
N	-11.90620000	13.81710000	1.48040000
N	-13.24030000	13.70000000	1.12910000
C	-10.60730000	13.89220000	3.53210000
C	-9.79110000	12.58350000	3.49670000
C	-8.53400000	12.67040000	4.38080000
C	-7.71840000	11.36660000	4.41400000
C	-6.51610000	11.45200000	5.37780000
N	-5.03440000	9.80880000	4.16290000
C	-4.00150000	10.76180000	3.69340000
C	-2.74950000	9.94380000	3.30100000
C	-2.86360000	8.72830000	4.22340000
C	-4.37590000	8.49630000	4.25580000
C	-4.49540000	11.71610000	2.57810000
O	-4.92000000	10.99380000	1.43690000
O	-2.10830000	7.60680000	3.79440000
O	-1.50680000	10.62760000	3.44110000
C	-18.78100000	9.69230000	4.65410000
C	-18.87470000	8.45860000	5.52880000
C	-18.60790000	7.12460000	5.24410000
N	-18.89350000	6.43820000	6.39510000
N	-19.31340000	7.28470000	7.34160000
N	-19.27620000	8.55090000	6.78680000
C	-27.79830000	8.13980000	1.60540000
C	-28.99950000	9.04080000	1.23520000
C	-29.91120000	9.38580000	2.42490000
C	-31.21130000	10.06500000	1.95850000
C	-32.21530000	10.33490000	3.09140000
C	-33.56960000	10.82020000	2.54120000
N	-34.52000000	11.14820000	3.60660000
C	-35.76520000	11.75590000	3.10640000
C	-36.82580000	11.48500000	4.18700000
C	-36.42930000	10.09240000	4.70150000
C	-34.91590000	10.00630000	4.44390000
C	-35.63140000	13.24520000	2.70480000
O	-35.05100000	14.00150000	3.75280000
O	-36.82310000	9.84550000	6.04320000
O	-38.16800000	11.51800000	3.71350000
C	-22.08630000	6.96180000	2.89450000
C	-22.56720000	7.83380000	4.04170000
C	-22.22500000	7.77320000	5.38070000
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C	-28.12750000	15.22790000	8.47350000
O	-26.90130000	15.93150000	8.58170000
O	-27.15450000	16.39730000	12.27690000
O	-30.47850000	15.80750000	10.98330000
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C	-25.68520000	6.92600000	-1.09250000
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O	-5.46220000	11.28740000	-9.96230000
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C	-19.11160000	15.79720000	-5.91840000
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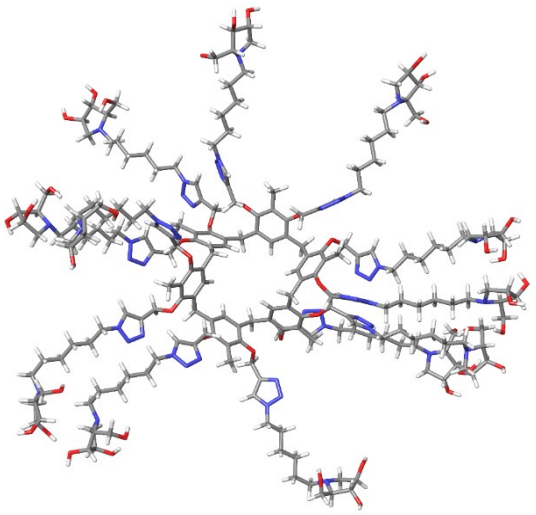

Figure S32: Lowest energy structure of **5a**

C	2.57250000	-4.60620000	10.28050000
C	2.15600000	-5.39790000	11.36390000
C	3.07260000	-5.73880000	12.37470000
C	4.39330000	-5.28810000	12.28700000
H	5.11090000	-5.57890000	13.04260000
C	4.81420000	-4.49280000	11.22010000
C	3.89060000	-4.12180000	10.23210000
C	1.61010000	-4.31810000	9.13100000
H	0.93650000	-5.15920000	8.96010000
H	2.14120000	-4.14630000	8.19400000
H	1.00810000	-3.43600000	9.34780000
C	6.29700000	-4.14160000	11.08830000
H	6.89950000	-4.85030000	11.66030000
H	6.58380000	-4.30940000	10.05070000
C	7.22100000	-0.41780000	11.06240000
C	7.02390000	-1.73550000	10.62260000
C	6.66360000	-2.73130000	11.54240000
C	6.67000000	-2.43870000	12.90710000
H	6.43790000	-3.21750000	13.62000000
C	7.00310000	-1.16180000	13.36670000
C	7.25950000	-0.14200000	12.43540000
C	7.40520000	0.72280000	10.06690000
H	8.43560000	1.07430000	10.07440000
H	6.76320000	1.56200000	10.33870000
H	7.14020000	0.43540000	9.04940000
C	7.07500000	-0.90610000	14.87300000
H	7.49680000	0.07460000	15.08710000
H	6.05060000	-0.85350000	15.24340000
C	9.98590000	-2.88440000	16.42160000
C	9.27020000	-2.00140000	15.59450000
C	7.87180000	-1.93970000	15.67550000
C	7.19710000	-2.79360000	16.55150000
H	6.12180000	-2.72770000	16.64370000
C	7.89450000	-3.72050000	17.33050000
C	9.29360000	-3.79070000	17.23680000
C	11.51180000	-2.83590000	16.45660000
H	11.90270000	-3.19110000	17.41060000
H	11.87000000	-1.81360000	16.33210000
H	11.93940000	-3.44490000	15.66150000
C	6.00000000	-2.14580000	21.03670000
C	6.82010000	-2.87570000	20.16580000
C	6.25950000	-3.84310000	19.31490000
C	4.89440000	-4.13080000	19.40460000
H	4.46820000	-4.90870000	18.78670000
C	4.07470000	-3.43680000	20.29760000
C	4.62290000	-2.41300000	21.08290000
C	7.11790000	-4.60460000	18.30590000
H	6.49920000	-5.27680000	17.71070000
H	7.78140000	-5.25370000	18.87360000
C	6.61450000	-1.07290000	21.93370000
H	7.58040000	-1.38600000	22.32730000
H	5.98460000	-0.83920000	22.79270000
H	6.76700000	-0.15550000	21.36460000
C	-0.30660000	-1.57250000	19.57730000
C	0.62940000	-2.29260000	20.33290000
C	1.57780000	-3.10560000	19.69520000
C	1.52060000	-3.26430000	18.30920000
H	2.22610000	-3.91980000	17.81800000
C	0.53800000	-2.61780000	17.55280000
C	-0.36130000	-1.74520000	18.18510000
C	-1.27160000	-0.61850000	20.27550000
H	-2.15280000	-1.16180000	20.61660000
H	-1.59620000	0.18420000	19.61210000
H	-0.80340000	-0.14650000	21.13960000
C	0.44790000	-2.89410000	16.05230000
H	-0.44490000	-2.44270000	15.62290000
H	1.27920000	-2.37020000	15.57920000
C	-0.61120000	-6.56120000	15.51330000
C	-0.60300000	-5.23790000	15.99170000
C	0.45020000	-4.37300000	15.64640000
C	1.50630000	-4.85450000	14.86940000
H	2.31980000	-4.19370000	14.59920000
C	1.52100000	-6.17450000	14.41150000
C	0.45770000	-7.03210000	14.73650000
C	-1.77910000	-7.49950000	15.80990000
H	-1.46670000	-8.27500000	16.51000000
H	-2.12090000	-7.98830000	14.89870000
H	-2.64300000	-6.98310000	16.22590000
C	2.68810000	-6.64870000	13.54480000
H	2.51170000	-7.64020000	13.13570000
H	3.53890000	-6.77800000	14.21490000
C	2.62600000	-3.88060000	20.49260000
H	2.53330000	-4.93570000	20.23110000
H	2.41100000	-3.84670000	21.56020000
O	0.87120000	-5.89370000	11.40160000
O	4.29830000	-3.32210000	9.19240000

O	7.19170000	-2.04200000	9.29060000
O	7.58320000	1.13050000	12.84460000
O	9.92930000	-1.17510000	14.71510000
O	10.00180000	-4.72600000	17.95950000
O	8.17310000	-2.62860000	20.15910000
O	3.80980000	-1.70480000	21.93090000
O	0.61290000	-2.18690000	21.70250000
O	-1.29310000	-1.05160000	17.44530000
O	-1.63710000	-4.77200000	16.77070000
O	0.46290000	-8.34750000	14.32850000
C	-0.15920000	-4.95810000	11.74860000
C	-1.43490000	-5.21570000	10.95820000
C	-2.34750000	-4.30350000	10.43940000
N	-3.34100000	-5.05950000	9.87630000
N	-3.05540000	-6.35910000	9.97900000
N	-1.86010000	-6.43940000	10.67170000
C	-4.57300000	-4.61710000	9.23540000
C	-4.40960000	-4.45480000	7.70890000
C	-5.73710000	-4.06820000	7.02770000
C	-5.59110000	-3.73550000	5.53160000
C	-6.94610000	-3.44000000	4.85560000
C	-6.80320000	-3.00290000	3.38420000
H	0.15910000	-3.92190000	11.61710000
H	-0.38210000	-5.05970000	12.80820000
H	-2.39520000	-3.22730000	10.44860000
H	-4.87090000	-3.67280000	9.69240000
H	-5.35570000	-5.34180000	9.46760000
H	-4.03590000	-5.38340000	7.27170000
H	-3.65610000	-3.69200000	7.50330000
H	-6.17350000	-3.20820000	7.53880000
H	-6.45210000	-4.88390000	7.15040000
H	-5.10360000	-4.56560000	5.01730000
H	-4.92980000	-2.87480000	5.41760000
H	-7.45930000	-2.67230000	5.42990000
H	-7.56960000	-4.33450000	4.91080000
N	-8.08260000	-3.01490000	2.66080000
C	-8.92660000	-1.80540000	2.77150000
C	-9.87710000	-1.88460000	1.56140000
C	-8.96840000	-2.44020000	0.45390000
C	-7.88850000	-3.22490000	1.22040000
C	-9.68450000	-1.61880000	4.11090000
O	-10.31530000	-2.82570000	4.50450000
O	-9.66380000	-3.18260000	-0.54010000
O	-10.48520000	-0.64900000	1.20370000
H	-8.29590000	-0.92610000	2.62030000
H	-10.64900000	-2.62430000	1.78680000
H	-8.47020000	-1.59260000	-0.02220000
H	-6.90430000	-2.88640000	0.89020000
H	-7.95680000	-4.29480000	1.02000000
H	-10.43350000	-0.82940000	4.02020000
H	-9.00710000	-1.28280000	4.89400000
H	-9.74140000	-3.53680000	4.19180000
H	-9.03770000	-3.51490000	-1.18900000
H	-11.07120000	-0.82820000	0.46060000
H	-6.12710000	-3.71760000	2.90870000
H	-6.31240000	-2.03040000	3.30560000
C	-0.01860000	-8.60250000	13.00280000
C	-1.07210000	-9.69580000	12.99520000
C	-2.24570000	-9.77820000	12.25610000
N	-2.81830000	-10.96740000	12.61880000
N	-2.07840000	-11.58130000	13.54400000
N	-0.97910000	-10.77140000	13.76350000
C	-4.06160000	-11.56740000	12.15440000
C	-5.16530000	-11.47510000	13.22950000
C	-6.45940000	-12.19890000	12.81750000
C	-7.59860000	-11.99370000	13.83370000
C	-8.90310000	-12.72950000	13.47110000
C	-8.81800000	-14.25800000	13.64770000
H	0.81860000	-8.90050000	12.37240000
H	-0.43620000	-7.70760000	12.54490000
H	-2.69490000	-9.12520000	11.52430000
H	-3.85230000	-12.60670000	11.89530000
H	-4.36800000	-11.06290000	11.23730000
H	-5.38130000	-10.42440000	13.43200000
H	-4.80630000	-11.90010000	14.16960000
H	-6.24940000	-13.26320000	12.70070000
H	-6.78370000	-11.84380000	11.83770000
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H	-7.27120000	-12.29720000	14.83000000
H	-9.19420000	-12.46170000	12.45680000
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N	-10.13190000	-14.88080000	13.45000000
C	-10.39810000	-15.41830000	12.10260000
C	-11.59890000	-16.36220000	12.30110000
C	-11.27970000	-17.02500000	13.65280000
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C	-10.62500000	-14.36400000	10.99180000
O	-11.63080000	-13.43920000	11.37040000
O	-12.42590000	-17.40430000	14.40410000
O	-11.79300000	-17.29800000	11.24390000
H	-9.55020000	-16.03910000	11.80290000
H	-12.49260000	-15.74370000	12.41780000
H	-10.67080000	-17.91130000	13.46080000
H	-9.43270000	-16.50290000	14.63930000
H	-10.82490000	-15.63140000	15.27760000
H	-10.91430000	-14.85160000	10.05930000
H	-9.69650000	-13.83650000	10.77440000
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C	-1.61580000	-5.21590000	18.13280000
C	-2.88990000	-4.77710000	18.82670000
C	-4.17830000	-4.63650000	18.32520000
N	-4.93490000	-4.19080000	19.37650000
N	-4.18240000	-4.08560000	20.47570000
N	-2.90050000	-4.45300000	20.11010000
C	-6.36760000	-3.90180000	19.40060000
C	-6.73050000	-2.66050000	20.25250000
C	-8.22690000	-2.30200000	20.17350000
C	-8.66720000	-1.31520000	21.27080000
C	-10.16270000	-0.95310000	21.19130000
C	-10.65750000	-0.20020000	22.44080000
H	-0.74120000	-4.80710000	18.63790000
H	-1.51490000	-6.29880000	18.20670000
H	-4.59820000	-4.80440000	17.34740000
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H	-6.13340000	-1.79820000	19.94930000
H	-6.46560000	-2.85970000	21.29310000
H	-8.82220000	-3.21260000	20.26650000
H	-8.45390000	-1.88920000	19.18880000
H	-8.06900000	-0.40360000	21.21450000
H	-8.45430000	-1.75640000	22.24660000
H	-10.74760000	-1.86530000	21.07070000
H	-10.33580000	-0.34990000	20.29850000
N	-12.00150000	0.35680000	22.26910000
C	-13.11430000	-0.58580000	22.02000000
C	-14.29270000	-0.16500000	22.94280000
C	-13.94290000	1.28650000	23.31870000
C	-12.41380000	1.20240000	23.39370000
C	-13.51570000	-0.62090000	20.52320000
O	-13.77310000	0.68890000	20.03680000
O	-14.38300000	2.23730000	22.35540000
O	-14.41720000	-1.02840000	24.07140000
H	-12.81580000	-1.59800000	22.30090000
H	-15.25040000	-0.18930000	22.41810000
H	-14.37350000	1.55090000	24.28620000
H	-12.13280000	0.74200000	24.34310000
H	-11.94740000	2.18770000	23.37620000
H	-14.39830000	-1.24690000	20.37910000
H	-12.72440000	-1.07350000	19.92510000
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H	-14.31530000	1.81700000	21.48230000
H	-13.59680000	-1.01690000	24.57050000
H	-9.97010000	0.62440000	22.64410000
H	-10.62060000	-0.85500000	23.31400000
C	-2.59550000	-1.63700000	17.42290000
C	-3.68880000	-0.61520000	17.16000000
C	-5.06470000	-0.80010000	17.20730000
N	-5.60880000	0.41610000	16.89890000
N	-4.65050000	1.31900000	16.69430000
N	-3.44820000	0.65070000	16.85160000

C	-7.01430000	0.78310000	16.81280000
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C	-8.98160000	1.87670000	18.01800000
C	-9.49830000	2.57820000	19.28610000
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C	-11.59960000	3.52410000	20.47480000
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H	-2.61350000	-2.40700000	16.65280000
H	-5.68370000	-1.65240000	17.42280000
H	-7.59420000	-0.12680000	16.65460000
H	-7.14860000	1.40720000	15.92740000
H	-6.90070000	2.42770000	18.22460000
H	-7.30210000	0.89360000	18.96170000
H	-9.56560000	0.97090000	17.84580000
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H	-8.92030000	3.48660000	19.46480000
H	-9.32850000	1.93990000	20.15480000
H	-11.54850000	2.01690000	18.95180000
H	-11.16740000	3.58280000	18.33610000
N	-10.97910000	4.79440000	20.86980000
C	-11.60880000	6.01840000	20.33430000
C	-11.08860000	7.14110000	21.25100000
C	-11.14620000	6.47590000	22.63530000
C	-10.99560000	4.97520000	22.32810000
C	-11.37210000	6.30470000	18.83150000
O	-9.99400000	6.21450000	18.51430000
O	-10.20680000	6.98310000	23.57490000
O	-11.82590000	8.35890000	21.18010000
H	-12.68840000	5.95350000	20.49230000
H	-10.04280000	7.32600000	20.99210000
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H	-11.82480000	4.43900000	22.79490000
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H	-11.74200000	7.29740000	18.56950000
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H	-10.44280000	7.89380000	23.77330000
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H	-11.42840000	2.78700000	21.25970000
H	-12.68420000	3.62750000	20.39640000
C	-0.23610000	-3.13100000	22.36010000
C	-0.77740000	-2.53870000	23.64500000
C	-2.09200000	-2.33160000	24.04610000
N	-2.00420000	-1.75170000	25.28390000
N	-0.72760000	-1.59950000	25.63650000
N	0.03060000	-2.10990000	24.60090000
C	-3.07620000	-1.29550000	26.16100000
C	-2.98650000	-1.92460000	27.57060000
C	-4.10090000	-1.42950000	28.50910000
C	-3.97580000	-1.98770000	29.93810000
C	-5.12020000	-1.52160000	30.86160000
C	-4.96310000	-1.96030000	32.33210000
H	0.32040000	-4.04570000	22.56400000
H	-1.07270000	-3.42590000	21.72640000
H	-3.04030000	-2.53270000	23.57570000
H	-4.03020000	-1.53730000	25.69170000
H	-3.01000000	-0.20790000	26.21800000
H	-2.01660000	-1.69330000	28.01600000
H	-3.03100000	-3.01250000	27.49270000
H	-5.07270000	-1.70120000	28.09340000
H	-4.08110000	-0.33860000	28.54990000
H	-3.01610000	-1.68690000	30.35990000
H	-3.95680000	-3.07840000	29.90800000
H	-6.05730000	-1.93220000	30.48350000
H	-5.23760000	-0.44260000	30.79140000
N	-3.78420000	-1.36340000	32.97580000
C	-3.99860000	-0.08800000	33.68580000
C	-2.77350000	0.05770000	34.61080000
C	-2.46780000	-1.39530000	35.02770000
C	-3.18900000	-2.25670000	33.97490000
C	-4.23490000	1.15490000	32.79150000
O	-3.26060000	1.23270000	31.76630000
O	-1.08950000	-1.70040000	35.15990000
O	-2.96890000	0.94310000	35.71250000
H	-4.87240000	-0.20070000	34.33140000
H	-1.94440000	0.42340000	34.00240000
H	-2.95700000	-1.58970000	35.98390000
H	-3.95230000	-2.85820000	34.47350000
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H	-4.20860000	2.06780000	33.38940000
H	-5.23020000	1.11890000	32.34950000
H	-3.15310000	0.33160000	31.43640000
H	-0.58630000	-0.86440000	35.20260000
H	-3.52040000	0.52100000	36.37560000
H	-4.86740000	-3.04890000	32.32870000
H	-5.86900000	-1.74600000	32.90260000
C	3.45250000	-0.40130000	21.46680000
C	3.00040000	0.42650000	22.64830000
C	1.76040000	0.47830000	23.26100000
N	1.91260000	1.33490000	24.31430000
N	3.15220000	1.83100000	24.34110000
N	3.82170000	1.25790000	23.27360000
C	0.94870000	1.66900000	25.35270000
C	1.30540000	0.95510000	26.67270000
C	0.21720000	1.08600000	27.75290000
C	0.52980000	0.21690000	28.98160000
C	-0.54780000	0.28540000	30.08230000
C	-0.26410000	-0.64780000	31.27730000
H	2.65930000	-0.48390000	20.72500000
H	4.28070000	0.09330000	20.95540000
H	0.83610000	-0.04460000	23.08610000
H	-0.03760000	1.36010000	25.00470000
H	0.92950000	2.75270000	25.47480000
H	2.25240000	1.33990000	27.05670000
H	1.47460000	-0.10460000	26.46840000
H	-0.74660000	0.78530000	27.33920000
H	0.11340000	2.13090000	28.04970000
H	1.49500000	0.51380000	29.39280000
H	0.64780000	-0.82150000	28.66560000
H	-1.50810000	0.00880000	29.64920000
H	-0.68220000	1.31030000	30.42670000
N	0.99550000	-0.31810000	31.95130000
C	0.98180000	0.90240000	32.78540000
C	1.63430000	0.54880000	34.15290000
C	2.39950000	-0.75110000	33.84680000
C	1.48610000	-1.40320000	32.80220000
C	1.69290000	2.08430000	32.07640000
O	3.00130000	1.71890000	31.65480000
O	3.71300000	-0.50420000	33.35900000
O	0.68550000	0.40680000	35.21360000
H	-0.04600000	1.21540000	32.97860000
H	2.33670000	1.32600000	34.46220000
H	2.47470000	-1.37870000	34.73610000
H	0.65650000	-1.89420000	33.31290000
H	2.00360000	-2.17430000	32.22960000
H	1.74890000	2.94710000	32.74220000
H	1.12040000	2.41460000	31.20980000
H	2.88060000	1.06730000	30.95040000
H	3.64340000	0.21110000	32.70560000
H	1.17200000	0.40230000	36.04600000
H	-0.20550000	-1.67000000	30.89700000
H	-1.09250000	-0.63710000	31.98820000
C	8.94800000	-3.50600000	20.97930000
C	10.13660000	-2.77730000	21.57900000
C	10.51550000	-2.65930000	22.91080000
N	11.67110000	-1.92550000	22.89790000
N	11.99240000	-1.58560000	21.64750000
N	11.02200000	-2.13770000	20.83010000
C	12.50420000	-1.52180000	24.02690000
C	13.98180000	-1.93420000	23.83350000
C	14.85760000	-1.64340000	25.06490000
C	16.34770000	-1.92830000	24.80550000
C	17.23580000	-1.68440000	26.04370000
C	18.74820000	-1.84870000	25.77950000
H	9.29040000	-4.35140000	20.38580000
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H	10.08590000	-3.02280000	23.82870000
H	12.09490000	-1.97580000	24.93020000
H	12.41120000	-0.44080000	24.13920000
H	14.39150000	-1.40500000	22.97000000
H	14.04190000	-2.99750000	23.59350000
H	14.50900000	-2.23960000	25.91000000
H	14.73930000	-0.59840000	25.35860000
H	16.68630000	-1.29860000	23.98080000

H	16.47600000	-2.95740000	24.46590000
H	16.94730000	-2.38830000	26.82530000
H	17.02160000	-0.70200000	26.45760000
N	19.23610000	-0.91310000	24.75790000
C	19.77680000	0.37020000	25.24180000
C	20.63140000	0.94200000	24.07930000
C	20.97690000	-0.29120000	23.21260000
C	20.34860000	-1.46270000	23.98580000
C	18.74150000	1.37700000	25.79740000
O	17.72220000	1.62590000	24.84720000
O	20.50100000	-0.18790000	21.87290000
O	21.78850000	1.64100000	24.53390000
H	20.46990000	0.14030000	26.05490000
H	20.01510000	1.61510000	23.47790000
H	22.05930000	-0.43330000	23.19320000
H	21.09770000	-1.88770000	24.65870000
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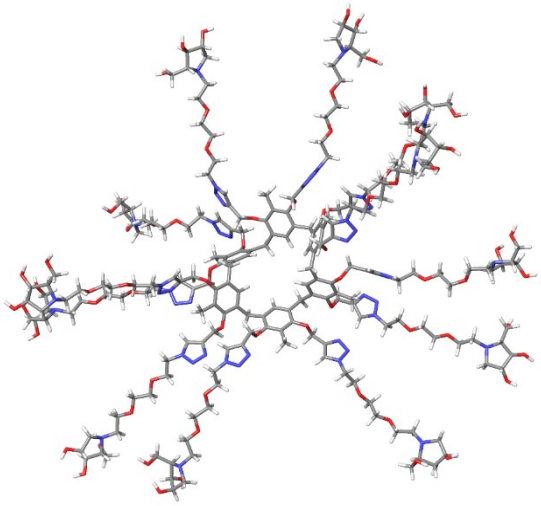

Figure S33: Lowest energy structure of **5b**

C	-12.74380000	15.79600000	-3.10540000
C	-12.72750000	16.19130000	-1.75530000
C	-13.58190000	17.21470000	-1.31380000
C	-14.47420000	17.80140000	-2.21650000
C	-14.49740000	17.42050000	-3.55990000
C	-13.63530000	16.40610000	-4.00330000
C	-11.73150000	14.77080000	-3.61030000
C	-15.33150000	18.23510000	-4.55100000
C	-18.20460000	16.55540000	-6.47460000
C	-16.95380000	17.12840000	-6.18910000
C	-16.69520000	17.64860000	-4.91340000
C	-17.72600000	17.69770000	-3.97650000
C	-19.01670000	17.26620000	-4.29920000
C	-19.26880000	16.69450000	-5.55780000
C	-18.38070000	15.79780000	-7.77910000
C	-20.13370000	17.44030000	-3.26480000
C	-21.01460000	21.13680000	-2.76720000
C	-20.90340000	19.86270000	-3.34690000
C	-20.22790000	18.84180000	-2.66530000
C	-19.68050000	19.09430000	-1.40350000
C	-19.75440000	20.36730000	-0.83340000
C	-20.38740000	21.40230000	-1.53930000
C	-21.84270000	22.22060000	-3.44600000
C	-21.77480000	19.10410000	2.92550000
C	-21.19130000	19.87430000	1.90890000
C	-19.80050000	19.83990000	1.70460000
C	-18.99670000	19.12960000	2.60510000
C	-19.56300000	18.42920000	3.67560000
C	-20.95680000	18.37370000	3.79900000
C	-19.14310000	20.60610000	0.55070000
C	-23.29170000	19.08150000	3.10440000
C	-18.44720000	14.09770000	5.54540000
C	-18.78060000	15.45670000	5.65890000
C	-18.33490000	16.37540000	4.69450000
C	-17.48370000	15.93990000	3.68100000
C	-17.06480000	14.60830000	3.61460000
C	-17.57910000	13.67150000	4.52630000
C	-19.00650000	13.09750000	6.55110000
C	-15.99910000	14.22370000	2.59060000
C	-12.76070000	16.11480000	3.46260000
C	-13.88730000	15.28060000	3.58760000
C	-14.80600000	15.18430000	2.52770000
C	-14.63700000	15.98290000	1.39160000
C	-13.56340000	16.87170000	1.29350000
C	-12.61230000	16.92240000	2.32560000
C	-11.68980000	16.16180000	4.55020000
C	-13.46780000	17.81470000	0.09210000
C	-18.66920000	17.86340000	4.78070000
O	-20.58890000	16.44720000	-5.89410000
O	-21.47890000	19.58750000	-4.56750000
O	-20.41240000	22.67120000	-1.00790000
O	-17.23860000	12.33970000	4.41090000
C	-19.41720000	23.56690000	-1.51220000
H	-18.83610000	23.92670000	-0.66350000
H	-18.69590000	23.06780000	-2.16520000
C	-20.75960000	20.04820000	-5.71710000
H	-19.86800000	20.62250000	-5.45160000
H	-20.39170000	19.18320000	-6.26710000
H	-15.10660000	18.61570000	-1.89030000
H	-10.78610000	14.85230000	-3.07320000
H	-11.50270000	14.91380000	-4.66650000
H	-12.11890000	13.76140000	-3.47750000
H	-15.49700000	19.23650000	-4.14980000
H	-14.72760000	18.40540000	-5.44140000
H	-17.53470000	18.12580000	-3.00280000
H	-19.03680000	16.33660000	-8.46310000
H	-18.76730000	14.80280000	-7.58610000
H	-17.43170000	15.60070000	-8.26830000
H	-21.10900000	17.18630000	-3.68110000
H	-19.97000000	16.71100000	-2.47080000
H	-19.19500000	18.29740000	-0.85850000
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H	-22.62830000	21.79550000	-4.06980000
H	-21.20920000	22.85060000	-4.06980000
H	-17.92140000	19.15790000	2.50010000
H	-18.08700000	20.34150000	0.48420000
H	-19.15170000	21.66420000	0.80860000
H	-23.76200000	20.00140000	2.76510000
H	-23.57170000	18.94660000	4.14980000
H	-23.71980000	18.25970000	2.53100000
H	-17.10050000	16.65710000	2.96830000
H	-18.33640000	13.01790000	7.40710000
H	-19.12550000	12.10840000	6.10970000
H	-19.98750000	13.40020000	6.91560000
H	-15.60500000	13.22790000	2.78930000
H	-16.48530000	14.15380000	1.61690000
H	-15.35870000	15.93750000	0.58780000
H	-10.73440000	15.83770000	4.14190000
H	-11.89880000	15.50940000	5.39570000
H	-11.57090000	17.17900000	4.92550000
H	-12.53560000	18.37690000	0.10870000
H	-14.24240000	18.56870000	0.23690000
H	-17.72860000	18.41570000	4.79830000
H	-19.13620000	18.10040000	5.73550000
C	-16.15520000	11.89780000	5.23320000
C	-21.03350000	15.13370000	-6.24110000
O	-11.80010000	15.65840000	-0.89030000
O	-13.58860000	16.10190000	-5.34310000
O	-15.97480000	17.17320000	-7.16000000
O	-21.98980000	20.70310000	1.15630000
O	-21.51660000	17.66100000	4.82840000
O	-19.55080000	15.87750000	6.71800000

O	-14.10100000	14.56770000	4.74810000
O	-11.57100000	17.82250000	2.27090000
C	-12.05980000	14.33630000	-0.40840000
C	-10.77030000	13.53530000	-0.35720000
C	-10.45630000	12.32280000	-0.95820000
N	-9.16350000	12.06080000	-0.59110000
N	-8.68640000	13.03820000	0.18240000
N	-9.71360000	13.95310000	0.32620000
C	-8.32840000	10.92840000	-0.95290000
C	-7.23200000	11.34850000	-1.94230000
O	-6.47910000	10.18320000	-2.25020000
C	-5.50170000	10.36690000	-3.26790000
C	-4.70650000	9.06140000	-3.42360000
C	-2.41540000	8.04620000	-6.15380000
N	-1.33340000	6.95570000	-6.36970000
C	-1.81550000	5.48250000	-6.28180000
C	-0.94860000	4.74030000	-7.30880000
C	-0.73640000	5.75410000	-8.44250000
C	-0.59310000	7.10390000	-7.72520000
C	-1.74370000	4.84090000	-4.88040000
O	-0.51800000	5.25350000	-4.29990000
O	0.36730000	5.44030000	-9.27510000
O	-1.55060000	3.52050000	-7.70130000
C	-10.40580000	17.41040000	1.54810000
C	-9.19620000	17.33610000	2.46110000
C	-8.26820000	16.31480000	2.61600000
N	-7.41430000	16.74890000	3.59470000
N	-7.77320000	17.95880000	4.02800000
N	-8.89290000	18.31590000	3.30130000
C	-6.28400000	16.06220000	4.19630000
C	-6.61530000	15.66530000	5.64240000
O	-5.46810000	15.05730000	6.22250000
C	-5.72280000	14.47400000	7.49670000
C	-4.40480000	14.04560000	8.16210000
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N	-0.84840000	15.99990000	10.93950000
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C	0.56480000	13.87280000	10.33060000
O	-0.11690000	13.31640000	11.44140000
O	1.42880000	17.89210000	13.08200000
O	2.84220000	15.81440000	11.11960000
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C	-14.51800000	14.56120000	7.13840000
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C	-14.37150000	9.26850000	11.56790000
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C	-11.27140000	5.39170000	16.76340000
O	-11.19510000	4.01450000	16.43690000
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C	-21.31450000	16.29030000	23.55630000
O	-19.92660000	16.02970000	23.67060000
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C	-22.00940000	16.37010000	4.46810000
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O	-36.41760000	31.03110000	-1.05660000
O	-34.39020000	33.11290000	1.19470000
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C	-21.27830000	25.37560000	-1.96180000
N	-21.37910000	26.35890000	-2.90540000
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C	-25.51900000	29.61450000	-5.88120000
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O	-30.70560000	33.71990000	-11.31150000
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N	-22.56340000	22.65190000	-7.54100000
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O	-25.57930000	22.89210000	-10.47890000
C	-25.55210000	23.66940000	-11.66890000
C	-26.98080000	24.17460000	-11.94450000
C	-27.71040000	25.04180000	-15.48930000
N	-26.71220000	26.13630000	-15.94780000
C	-27.21640000	27.01760000	-17.12360000
C	-26.51760000	28.39450000	-16.92030000
C	-25.54660000	28.20320000	-15.72860000
C	-26.26080000	27.15260000	-14.88130000
C	-27.03080000	26.41190000	-18.52820000
O	-25.67550000	26.03400000	-18.64130000
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Molecular Dynamics of Ligand-Protein Complexes

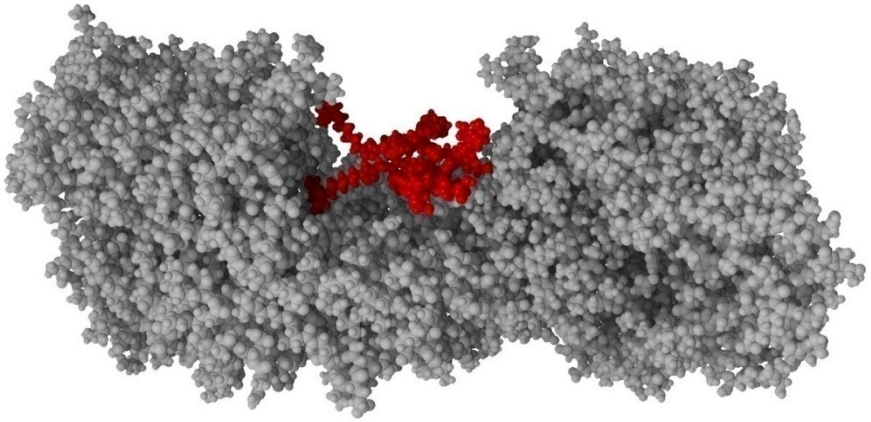

Figure S34: Lowest energy structure of the complex **3a@(LH)$_2$**

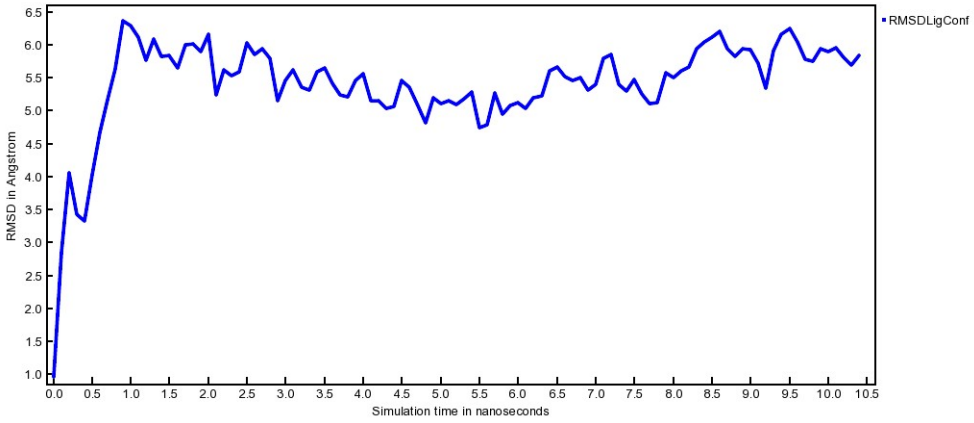

Figure S35: Variation of RMSD values calculated for the conformation **3a** during the MD simulation with respect to its starting conformation to summarize conformational changes.

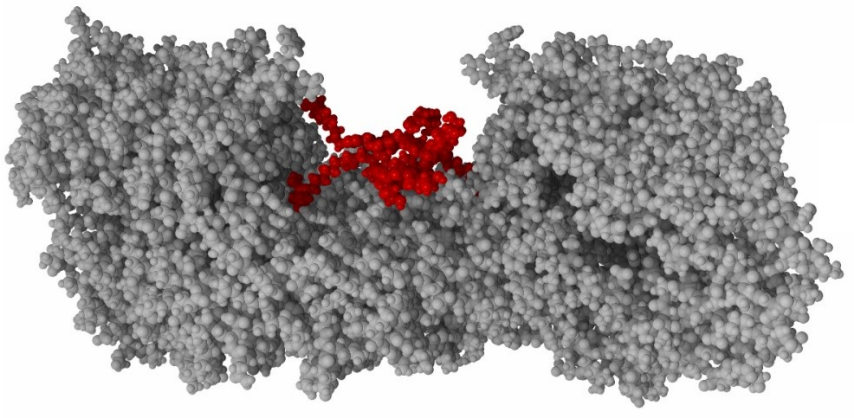

Figure S36: Lowest energy structure of the complex **4a@(LH)$_2$**

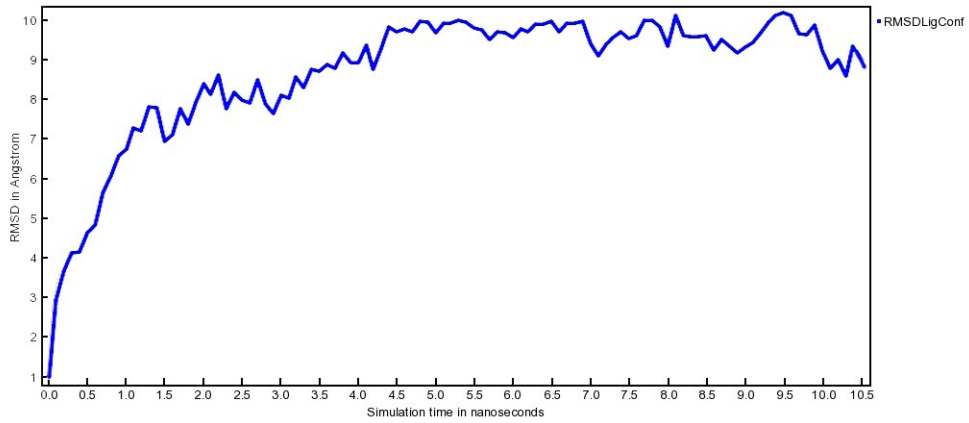

Figure S37: Variation of RMSD values calculated for the conformation **4a** during the MD simulation with respect to its starting conformation to summarize conformational changes.

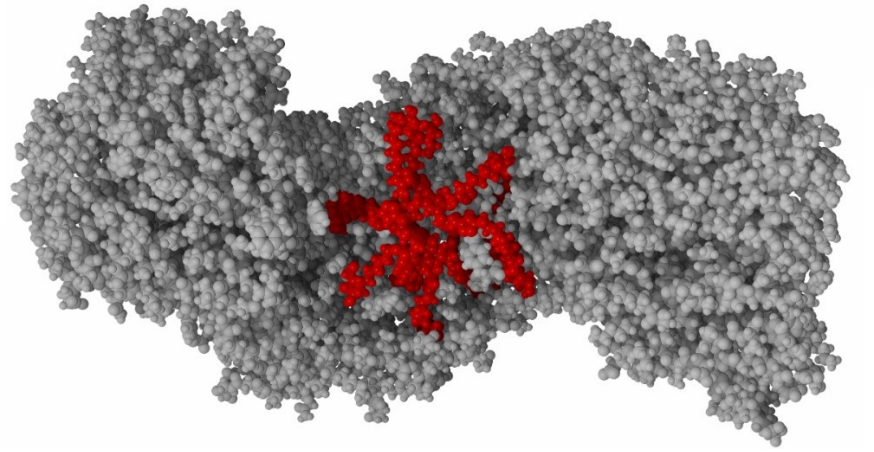

Figure S38: Lowest energy structure of the complex **5a@(LH)$_2$**

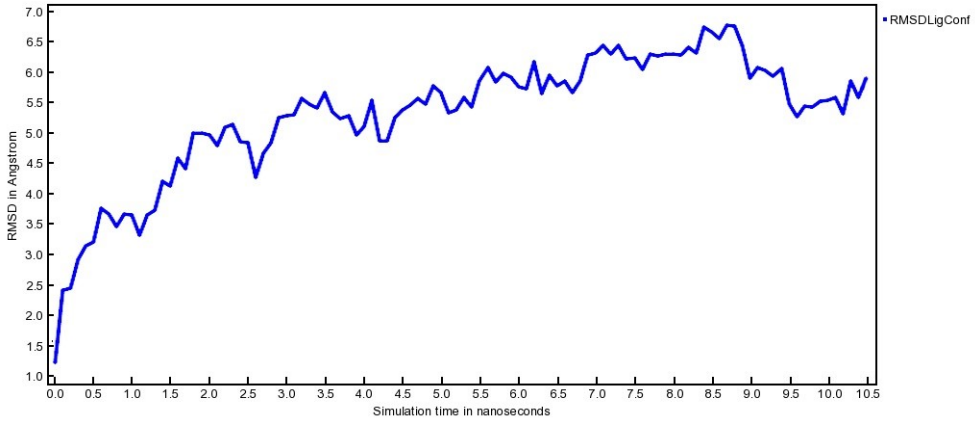

Figure S39: Variation of RMSD values calculated for the conformation **5a** during the MD simulation with respect to its starting conformation to summarize conformational changes.

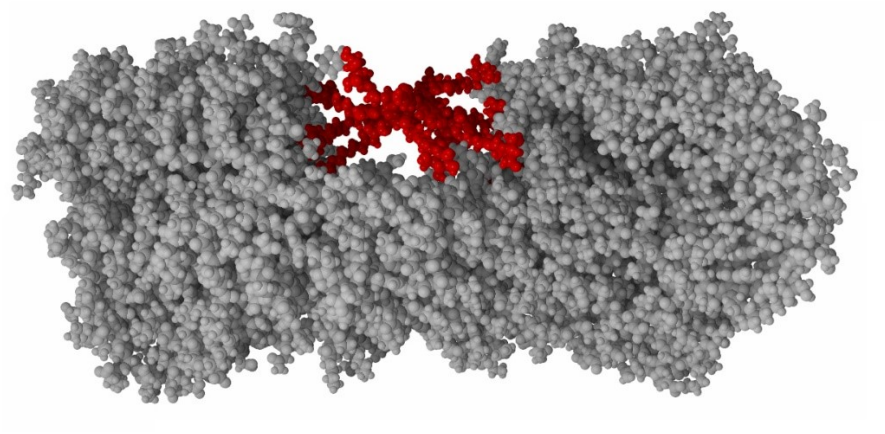

Figure S40: Lowest energy structure of the complex **5b@(LH)$_2$**

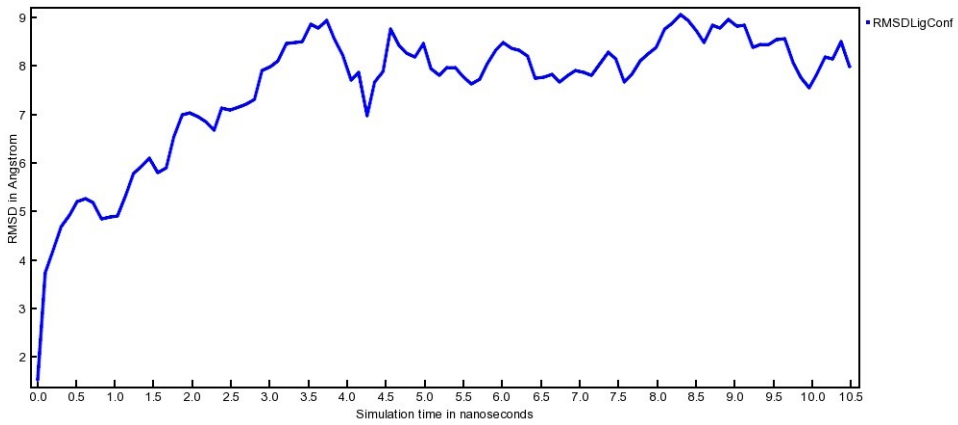

Figure S41: Variation of RMSD values calculated for the conformation **5b** during the MD simulation with respect to its starting conformation to summarize conformational changes.

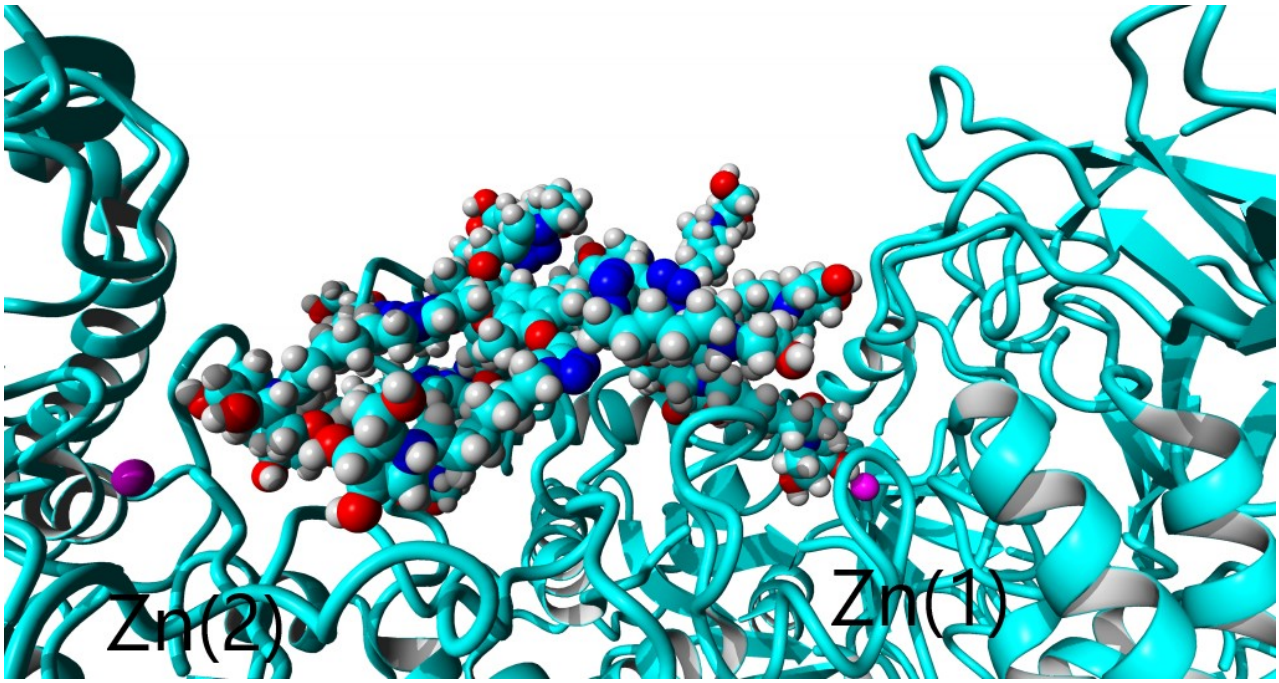

Figure S42: Detailed view of the lowest energy structure of the complex **5a**@(**LH**)$_2$ obtained by MD simulation, in which the resorcinarene cluster **5a** is mono-coordinated to Zn(1) atom, see also figure 5 in the main text.

Stabilizing secondary interactions between the DAB-1 and the side chains of amino acids were detected during the MD (SI). In details, the side chain of Asp267 acts as bidentate acceptor of two H-bonds with 4-OH and 6-CH_2OH groups of a free (non-chelating) DAB-1 unit (Figure S43). Interestingly, other stabilizing H-bonding interactions were detected during the MD between free DAB-1 units and the side chains of Asp268 (Figure S43), Gln228 (Figures S44-45), Asp229 (Figures S44-45) and Glu49 (Figure S45). In addition, a relevant O–H···π interaction was detected between the 4-OH of a DAB-1 unit and the aromatic side chain of Trp28 during the MD simulation (Figure S46).

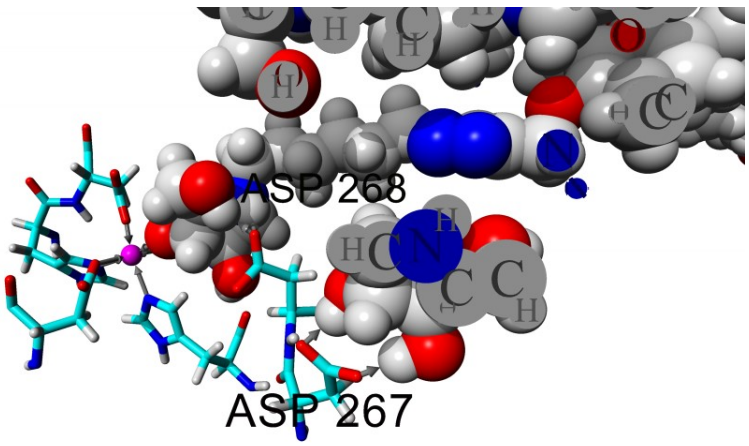

Figure S43: The side chain of Asp267 acts as bidentate acceptor of two H-bonds with 4-OH and 6-CH_2OH groups of a free (non-chelating) DAB-1 unit.

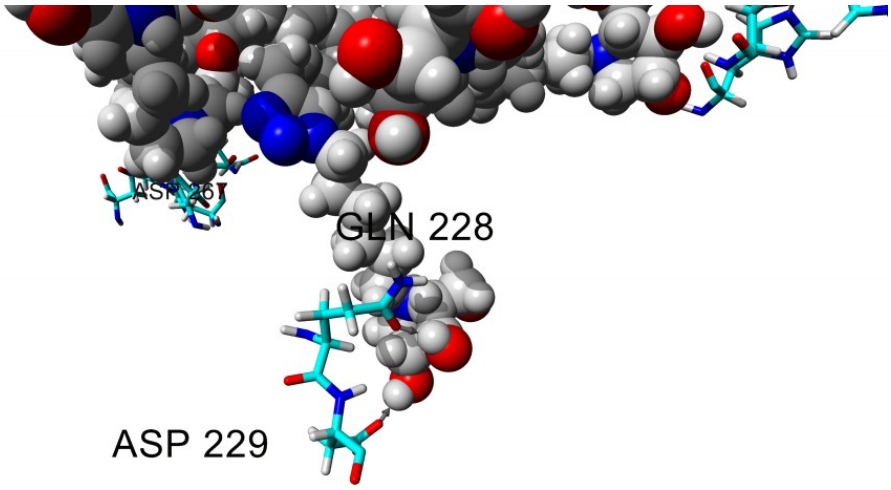

Figure S44: The side chain of Asp229 and Gln 228 establish H-bonds with OH groups of a free (non-chelating) DAB-1 unit.

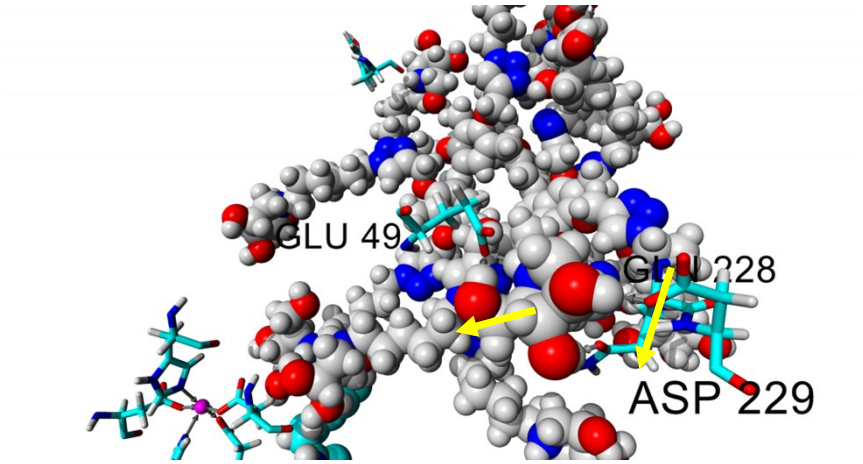

Figure S45: The side chain of Glu 49 establishes an H-bond with an OH group of a free (non-chelating) DAB-1 unit.

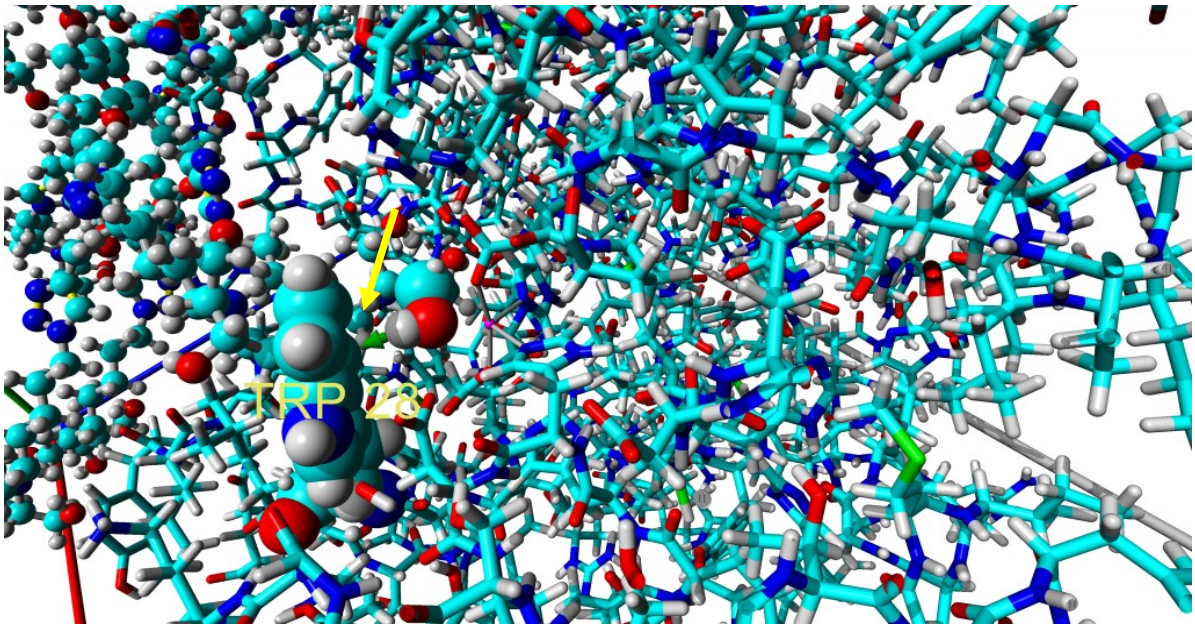

Figure S46: The side chain of Trp 28 establishes an OH···π interaction with an OH group of a free (non-chelating) DAB-1 unit.

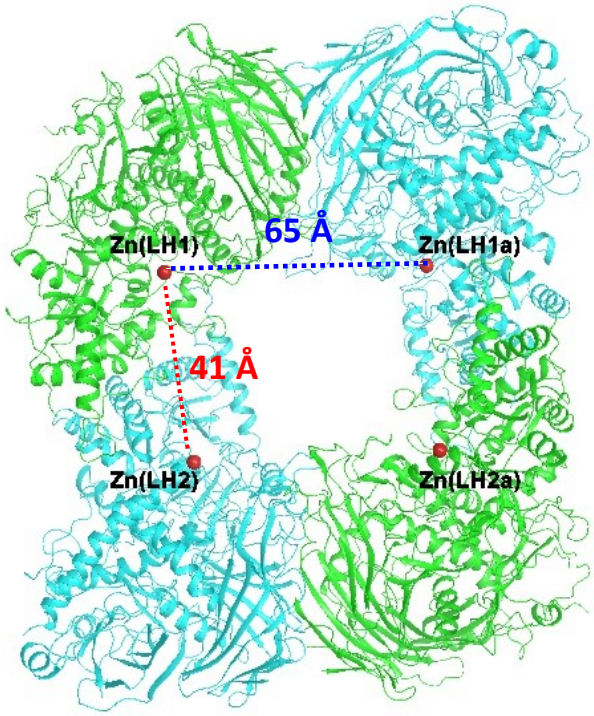

Figure S47: Representation of the tetrameric protein 2x(LH)2 formed by four LH dimers. Intradimeric Zn···Zn mean distance = 41 Å (measured between LH1/LH2 and LH1a/LH2a); interdimeric Zn···Zn mean distance = 65 Å (measured between LH1/LH1a and LH2/LH2a).

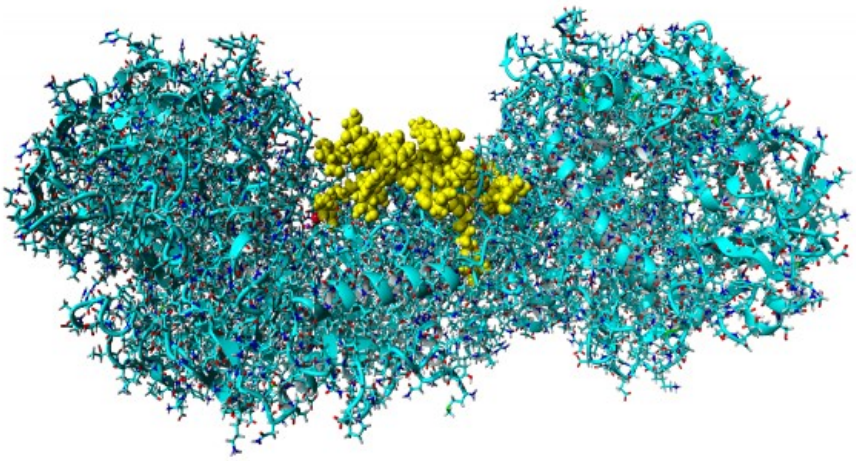

Figure S48: Lowest energy structure of the complex **5a**@(**LH**)$_2$ obtained by MD simulation.

Docking Studies with VINA

At this point a docking study (Figure S48) was performed starting by the tetrameric 2×(LH)$_2$ protein with the aim to confirm the results of MD simulations. Following a protocol previously reported by some of us, the resorcinarene-based multivalent architectures **3a-5a** and **5b** were optimized by molecular mechanics calculations and molecular dynamics simulations in a box of water molecules using the YASARA program and AMBER force field.

Regarding the resorcin[6]arene-based compound **5a**, docking studies performed with VINA[17] (Figure S48) showed that the 12-valent cluster binds only one active site of the tetrameric enzyme with one DAB-1 unit inside the active site pocket (SI) to establish interactions with the catalytically active zinc ion. Analogously, VINA calculations indicated a mono-coordination for the multivalent compounds **3a**, **4a** and **5b**.

NBO and NCI Calculations

The energy contribution of noncovalent interactions (NCI) was evaluated by a second order perturbation theory (SOPT) analysis of the Fock matrix in the natural bond orbital (NBO) basis. SOPT analyses were performed on simplified models of the complex **5a**@JBMan and **5b**@JBMan as obtained by AutoDock4$_{Zn}$ calculations (Figure S49)**.** and considering the 16 most significant amino acid residues[18] surrounding the chain armed with DAB-1 unit coordinated to the Zn atom. DFT NBO and NCI analysis was performed at the B3LYP/6-31G level of theory with Gaussian 16.

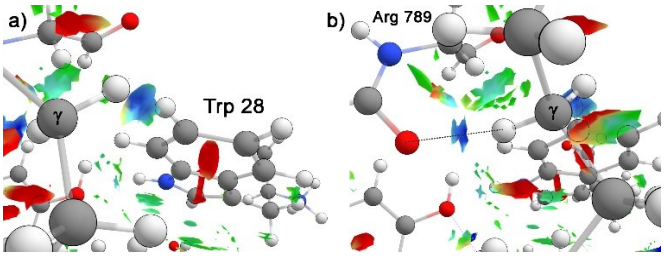

Figure S49: Non-covalent interaction plots by the sign of the second Hessian eigenvalue (gradient isosurfaces (s = 0.6 a.u.) for: (a) interaction between the CH_2 in γ position of **5a**, and the aromatic ring of the

[17] O. Trott and A. J. Olson, AutoDock Vina: Improving the Speed and Accuracy of Docking with a New Scoring Function, Efficient Optimization, and Multithreading. *J. Comput. Chem.* 2009, **31**, 455-461

[18] The residues involved in DFT analysis were: His 23, Asp 24, Asp 25, Trp 28, Asp 145, Phe 147, Arg 170, Tyr 210, Asp 268, Trp 333, His 385, His 386, Asp 387, Tyr 625, Arg 789 and Gly 790

TRP28. (b) Moderate C–H···O=C^{Arg789} H-bonding interaction. The $^{\gamma}$C–H···O=C^{Arg789} H-bond computed by DFT NBO calculations shows a C···O distance of 3.00 Å and a C–H···O angle of 131°. NBO calculations evidenced a LP→σ* donation of the lone pair on the oxygen atom of the carbonyl of Arg789 to the antibonding orbital of the $^{\gamma}$C–H bond. In addition, the γ–CH_2 was involved in a C–H···π^{Trp28} interaction with the aromatic side chain of Trp28, and finally, hydrophobic contacts between the alkyl chain of **5a** and GLY788 and GLY790 were detected. All these interactions accounted for 93% of the total NBO-stabilization energy between alkyl chain and active site pocket. In the coloring isosurface blue and green colors represent strong and medium interactions (H-bonding and van der Waals).

DFT structures of simplified models of the complex 5a@ JBα-man

N	-28.51800000	3.06600000	-19.94900000
H	-29.27000000	2.46900000	-20.23000000
H	-27.78000000	2.51300000	-19.56300000
H	-28.92200000	3.38400000	-19.06800000
C	-28.09900000	4.03700000	-20.94800000
H	-28.34200000	3.66700000	-21.84400000
C	-26.59600000	4.21500000	-20.81500000
O	-26.11400000	4.75200000	-19.81500000
C	-28.83100000	5.36600000	-20.78300000
H	-29.81500000	5.21100000	-20.87300000
H	-28.63400000	5.73700000	-19.87600000
C	-28.42100000	6.38100000	-21.80400000
N	-28.49100000	6.13100000	-23.16000000
H	-28.83500000	5.27000000	-23.58400000
C	-27.89200000	7.62300000	-21.67500000
H	-27.70700000	8.10400000	-20.81800000
C	-28.04100000	7.18400000	-23.82200000
H	-27.99800000	7.27400000	-24.81700000
N	-27.65700000	8.09700000	-22.94700000
N	-25.84800000	3.75300000	-21.80400000
H	-26.30000000	3.42600000	-22.65800000
C	-24.39000000	3.69900000	-21.70300000
H	-24.12700000	4.02300000	-20.79400000
C	-23.77400000	4.62200000	-22.75000000
O	-23.71200000	4.28400000	-23.93900000
C	-23.92400000	2.26000000	-21.85200000
H	-24.18200000	1.92900000	-22.76000000
H	-22.92900000	2.23100000	-21.75700000
C	-24.54200000	1.35100000	-20.80600000
O	-24.91600000	1.85900000	-19.71200000
O	-24.66100000	0.13300000	-21.08600000
N	-23.32600000	5.79400000	-22.31200000
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C	-18.91900000	11.47700000	-22.13600000
H	-18.91000000	12.03600000	-22.96500000
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H	-32.04500000	16.52200000	-21.35500000
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DFT structures of simplified models of the complex 5b@ JBα-man

N	-18.22400000	-7.98400000	6.68100000
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O	-22.55700000	-10.19400000	6.05000000
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Molecular Docking of 5a(DAB-1)$_1$ and 5b(DAB-1)$_1$

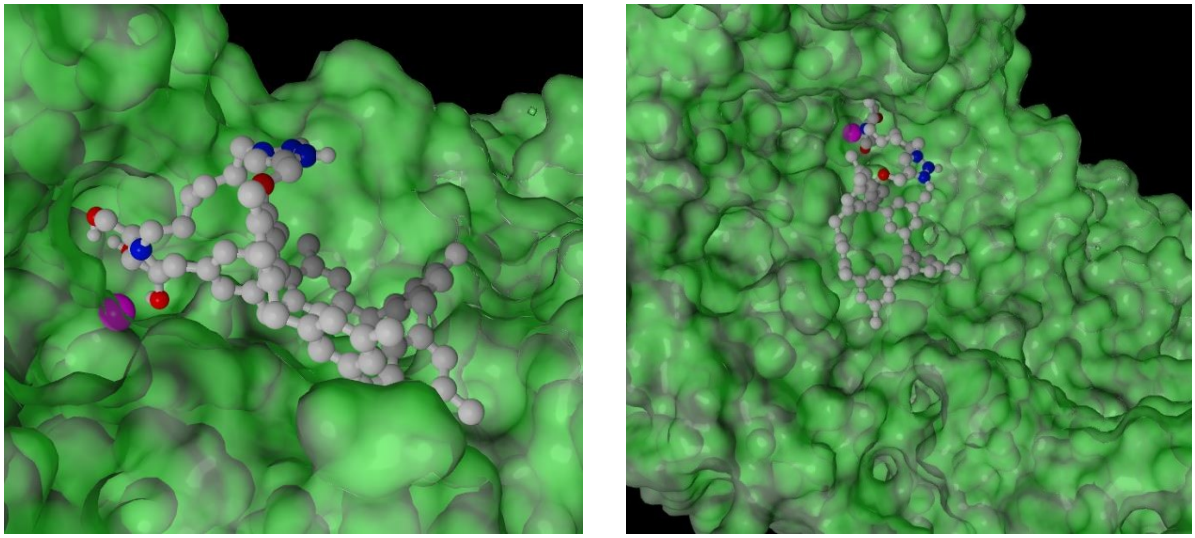

Figure S50: 3D model of the interaction between **5a(DAB-1)$_1$** and Zn atom (magenta). The protein is represented by green molecular surface.

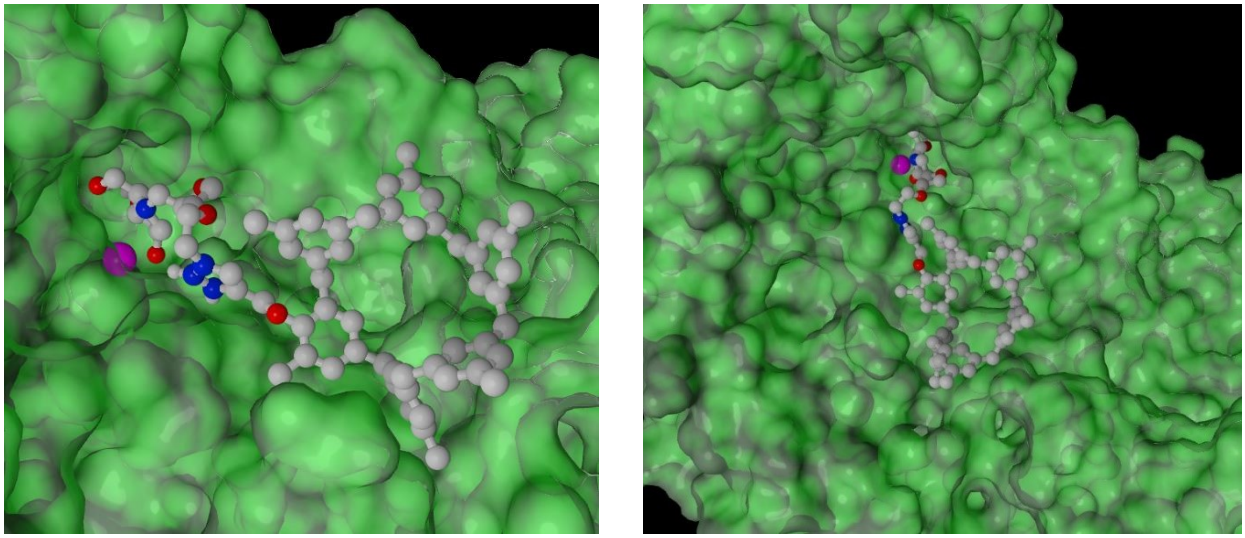

Figure S51: 3D model of the interaction between **5b(DAB-1)$_1$** and Zn atom (magenta). The protein is represented by green molecular surface.

Biological Assays

Enzyme assay

The enzyme assays of commercial enzymes were made following manufacturer recommendation using *p*-nitrophenyl-α-D-mannopyranoside (pNP-Man) in α-mannosidase activity and *p*-nitrophenyl-α-D-glucopyranoside (pNP-Glc) in α-glucosidase activity. The mannosidase assay of recombinant α-mannosidases GMIIb and LManII were performed as described earlier. [19,20] The absorbance reading of released *p*-nitrophenol (pNP) at 405 nm was used for quantification of enzyme activity.

[19] I. Nemčovičová, S. Šesták, D. Rendič, M. Plšková, J. Mucha, I. B. H. Wilson, Characterisation of class I and II α-mannosidases from Drosophila melanogaster. *Glycoconjugate J.* 2013, **9**, 899-909.

[20] S. Mirabella, G. D'Adamio, C. Matassini, A. Goti, S. Delgado, A. Gimeno, I. Robina, A. J. Moreno-Vargas, S. Šesták, J. Jimenez-Barbero, F. Cardona, Mechanistic Insight into the Binding of Multivalent Pyrrolidines to α-Mannosidases. *Chem. Eur. J.* 2017, **23**, 14585-14596

Kinetic studies

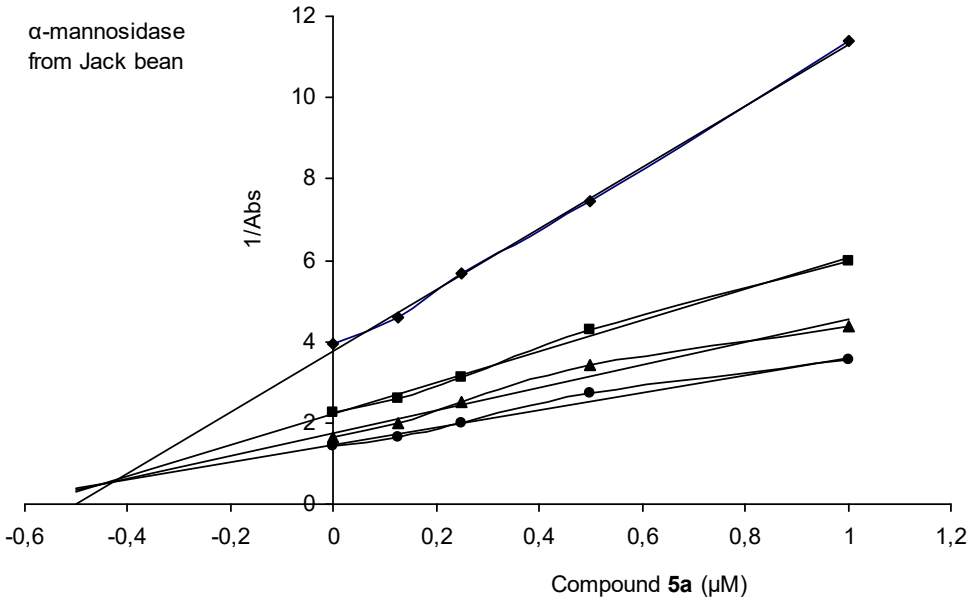

Figure S52. Dixon plot of the inhibition of commercial α-mannosidase by the compound **5a** in the presence of *p*-nitrophenyl-α-D-mannopyranoside (pNP-Man). 0.5 mM (♦), 1 mM (■), 2 mM (▲), 4 mM (●).

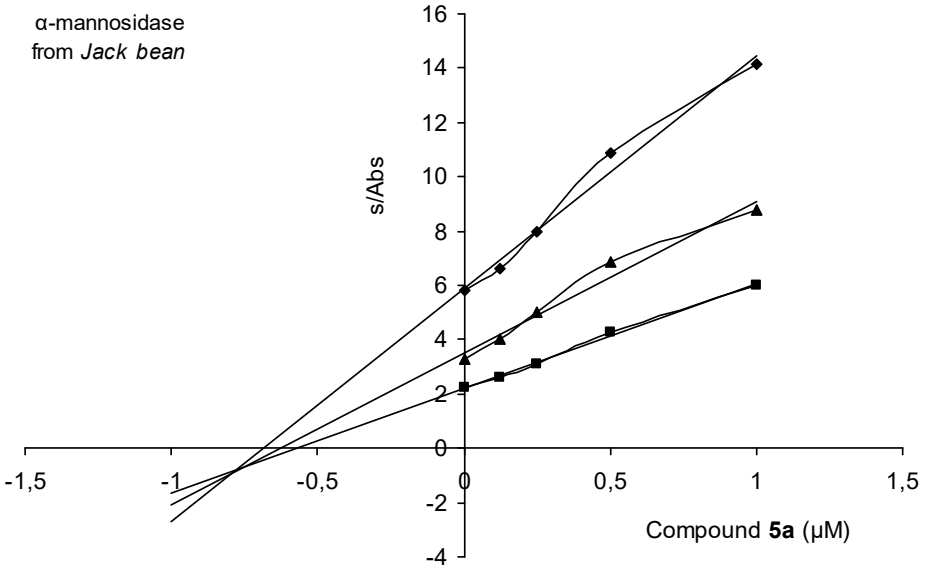

Figure S53. Cornish-Bowden plot[21] of the inhibition of commercial α-mannosidase by the compound **5a** in the presence of *p*-nitrophenyl-α-D-mannopyranoside (pNP-Man). 0.5 mM (■), 1 mM (▲), 2 mM (♦).

[21] A. Cornish-Bowden, A Simple Graphical Method for Determining the Inhibition Constants of Mixed, Uncompetitive and Non-Competitive Inhibitors. *Biochem. J.* 1974, **137**,143-144.

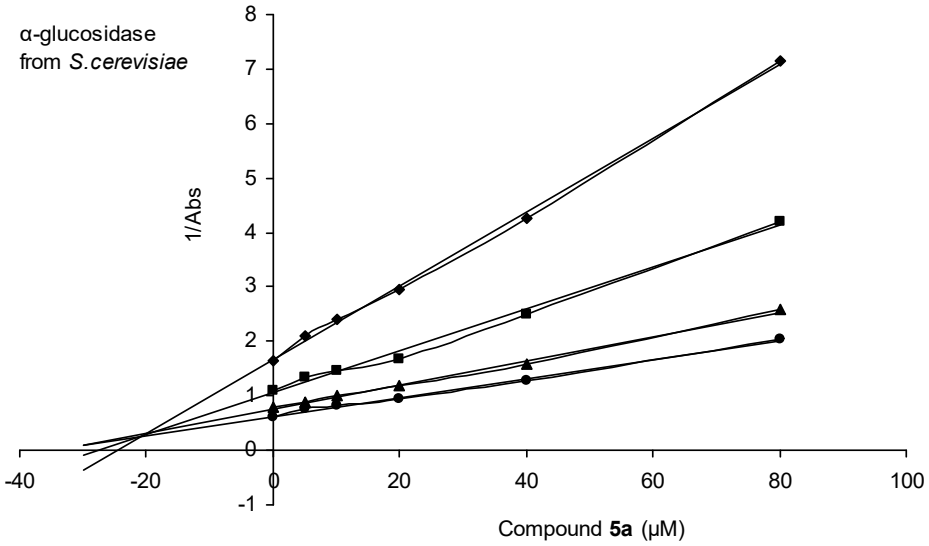

Figure S54. Dixon plot of the inhibition of α-glucosidase by the compound **5a** in the presence of *p*-nitrophenyl-α-D-glucopyranoside (pNP-Glc). 0.5 mM (♦), 1 mM (■), 2 mM (▲), 4 mM (●).

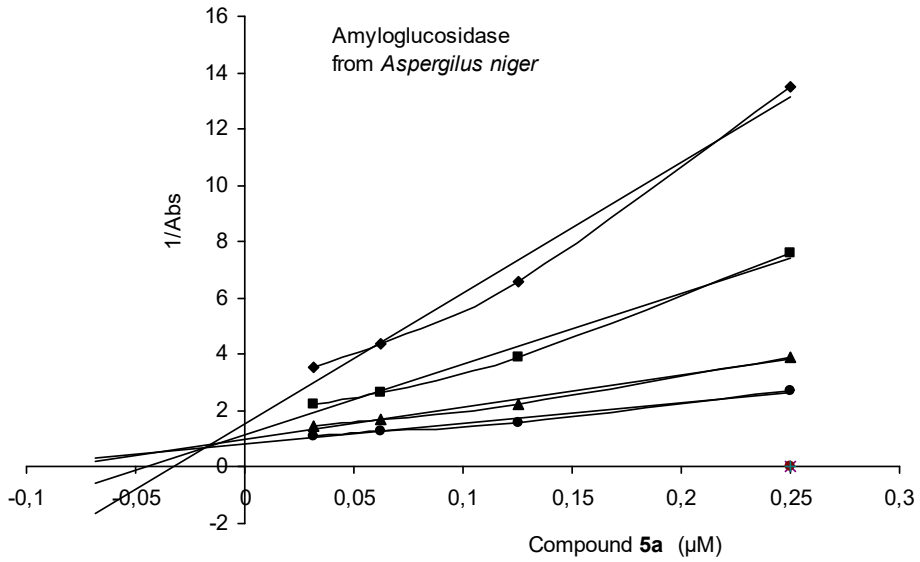

Figure S55. Dixon plot of the inhibition of commercial amyloglucosidase by the compound **5a** in the presence of *p*-nitrophenyl-α-D-glucopyranoside (pNP-Glc) 0.5 mM (♦), 1 mM (■), 2 mM (▲), 4 mM (●).

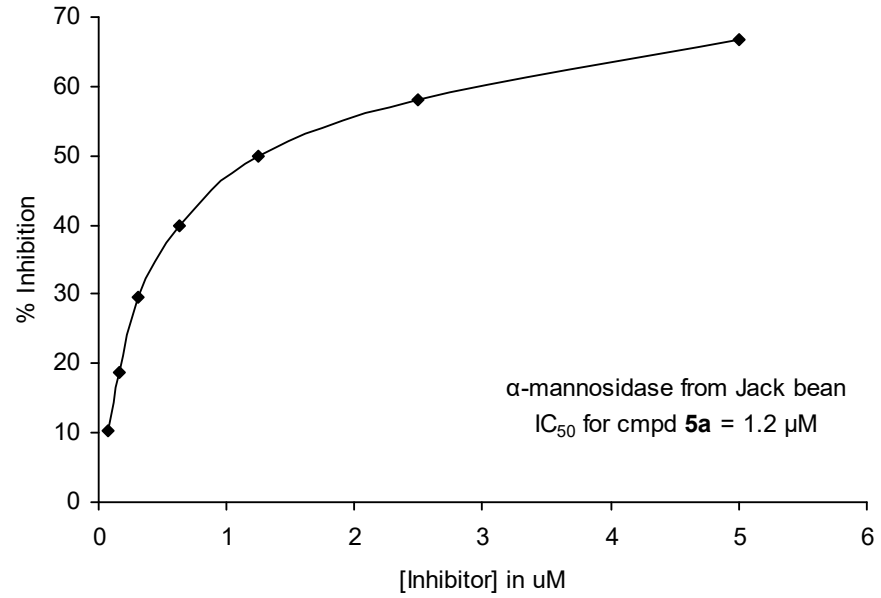

Figure S56. Inhibitory activity of compound **5a** toward α-mannosidase expressed in IC_{50}.

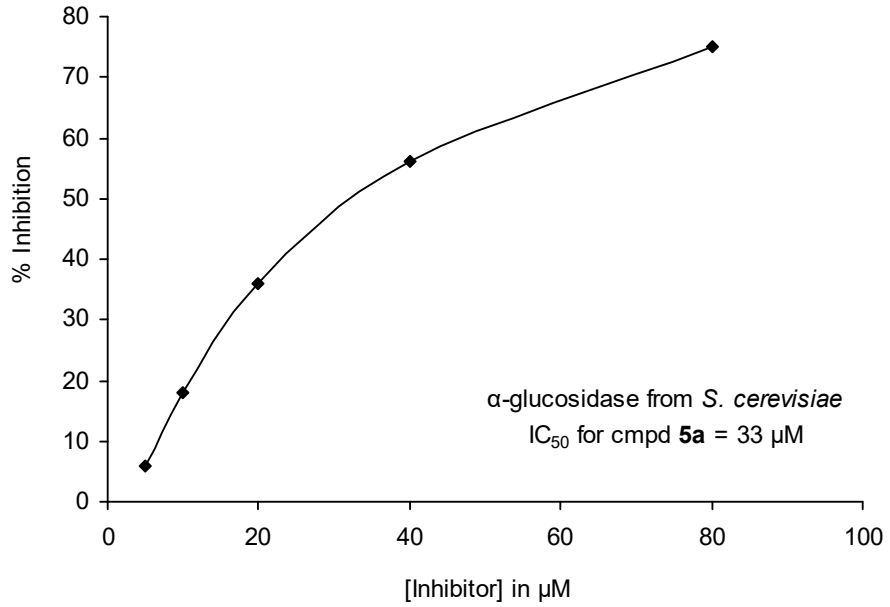

Figure S57. Inhibitory activity of compound **5a** toward α-glucosidase expressed in IC_{50}.

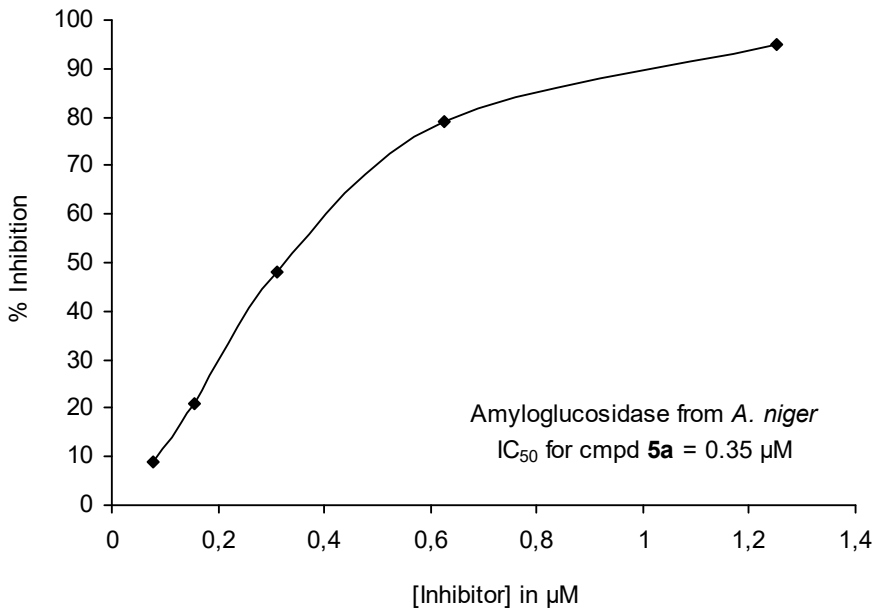

Figure S58. Inhibitory activity of compound **5a** toward amyloglucosidase expressed in IC_{50}.