Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Predicting self-assembly and structure in diluted aqueous solutions of modified *mono*- and *bis*-βcyclodextrins that contain naphthoxy chromophore groups

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General Synthesis Protocols

Reactions were monitored by TLC on Merck 60 F254 (0.25 mm) plates, which were visualized by UV inspection and/or by heating after being sprayed with phosphomolybdic acid.

Reactions under combined MW/US irradiation were performed in a professional multimode oven, (Microsynth, Milestone), operating at 2.45 GHz, equipped with a high-power pyrex® US probe (20.5 kHz working frequency) and the temperature was strictly monitored by a fiber optic thermometer inside the reaction vessel.

Flash-chromatography purifications were performed on CombiFlash *Rf* (Teledyne ISCO), an automatic device with auto injection, fractions collector and UV detector.

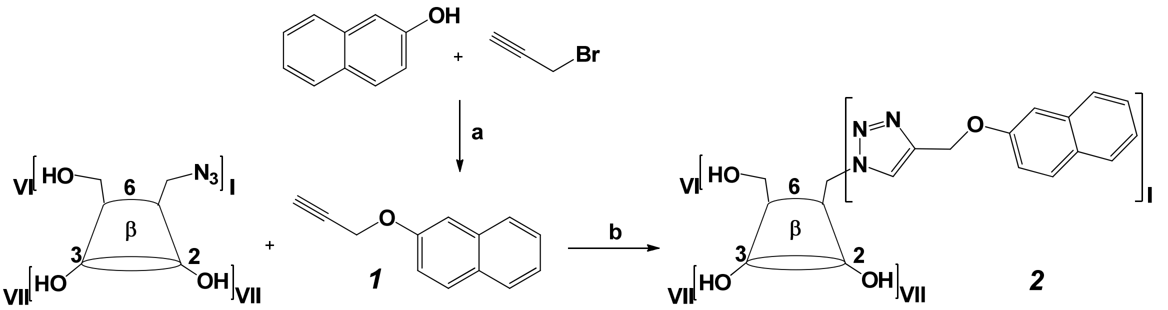
IR spectra were recorded with a Shimadzu FT-IR 8001 spectrophotometer.

NMR spectra were recorded on a Bruker 300 Avance (300 MHz and 75 MHz for ^{1}H and ^{13}C, respectively) at 25°C; chemical shifts were calibrated to residual proton and carbon resonances of the solvents, *viz.* $CDCl_3$ ($\delta_H = 7.27$, $\delta_C = 77.16$) and DMSO-d_6 ($\delta_H = 2.50$, $\delta_C = 39.52$). Chemical shifts (δ) are given in ppm and coupling constants (J) in Hz.

Low-resolution mass spectra were recorded on a Finnigan-MAT TSQ70 in electron impact (EI) and chemical ionization (CI) with isobutane as reactant gas; ESI-mass spectra were recorded on a Waters Micromass ZQ equipped with ESI source.

Scheme 1. Synthesis of β-CD (naphthyloxy)methyl triazolyl asymmetric derivative (**2, *mono*-NβCD**).

Reagents and conditions: a) K_2CO_3, acetone, 70°C (rfx); b) Cu powder, MW/US, 100°C, 1.5 h, DMF.



Synthesis of β-propargyloxynaphthalene (1)

In a two-necked round-bottomed flask (50 ml), 400 mg of β-naphthol (2.78 mmol, 1 eq) was dissolved in 10 ml of acetone and 1.53 g of K_2CO_3 (11.12 mmol, 4 eq) was added to the solution. The mixture was kept at 70°C for 30 min under magnetical stirring. Subsequently 360 μl of propargyl bromide (3.34 mmol, 1.2 eq) was added and the reaction was left at 70°C for 4 h.

Acetone was removed under vacuum. The crude product was extracted with CH_2Cl_2, dried under vacuum and purified on silica gel (flash chromatography) using a PE/EtOAc gradient. 325.1 mg of pure β-propargyloxynaphthalene was obtained (1.785 mmol, 64%).

Yellow powder. R*f* = 0.63 (PE/EtOAc 8:2).

IR (KBr, cm^{-1}): ν 3283, 3050, 2120 (alkyne), 1632, 1599, 1472, 1354, 1252, 1174, 1013, 837, 749, 687, 664, 478.

^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.81-7.76 (overlapped signals, 3H, H-1,5,8), 7.47 (t, *J* = 7.5 Hz, 1H, H-6), 7.37 (t, *J* = 7.5 Hz, 1H, H-7), 7.22 (d, *J* = 2.7 Hz, 1H, H-3), 7.19 (d, *J* = 2.7 Hz, 1H, H-4), 4.83 (d, *J* = 2.4 Hz, 2H, O-C*H*$_2$C≡CH), 2.50 (t, *J* = 2.4 Hz, 1H, O-CH$_2$C≡C*H*).

^{13}C NMR ($CDCl_3$, 75 MHz): δ 155.5 (C-2), 134.4 (C-8'), 129.7 (C-5), 129.4 (C-4'), 127.8 (C-1), 127.1 (C-8), 126.6 (C-6), 124.2 (C-7), 118.8 (C-4), 107.6 (C-3), 78.6 (O-$CH_2C≡CH$), 75.8 (O-$CH_2C≡CH$), 55.9 (O-$CH_2C≡CH$).

CI-MS (*m/z*, %) = 183 (100%) $[M + H]^+$.

Synthesis of 6^I-deoxy-6^I-(4-((2-naphthyloxy)methyl)-1*H*-1,2,3-triazol-1-yl)-β-CD (2, *mono*-NβCD).

In a three-necked pear-shaped reaction vessel (100 ml), 200 mg of 6^I-azido-6^I-deoxy-β-CD (0.172 mmol, 1 eq) and 126 mg of β-propargyloxynaphthalene (0.690 mmol, 4 eq) were dissolved in 10 ml of DMF and 100 mg of Cu powder was added to the solution. The reaction was carried out under combined MW/US irradiation at 100°C for 1.5 h (power of 100 W for MW, 35 W for US). The reaction outcome was monitored by TLC (*i*PrOH/H_2O/EtOAc/NH_4OH = 5:3:1:1).

The copper was filtered off on filter paper. After evaporation of DMF under vacuum, the crude product was crystallized in a water/acetone mixture and then purified on RP18 (flash-chromatography) using a H_2O/MeOH gradient. 173 mg of pure product was obtained (0.129 mmol, 75%).

White powder. R*f* = 0.77 (*i*PrOH/H_2O/EtOAc/NH_4OH = 5:3:1:1).

IR (KBr, cm^{-1}): ν 3400, 3283, 2926, 1632, 1510, 1213, 1155, 1078, 1028, 837, 478.

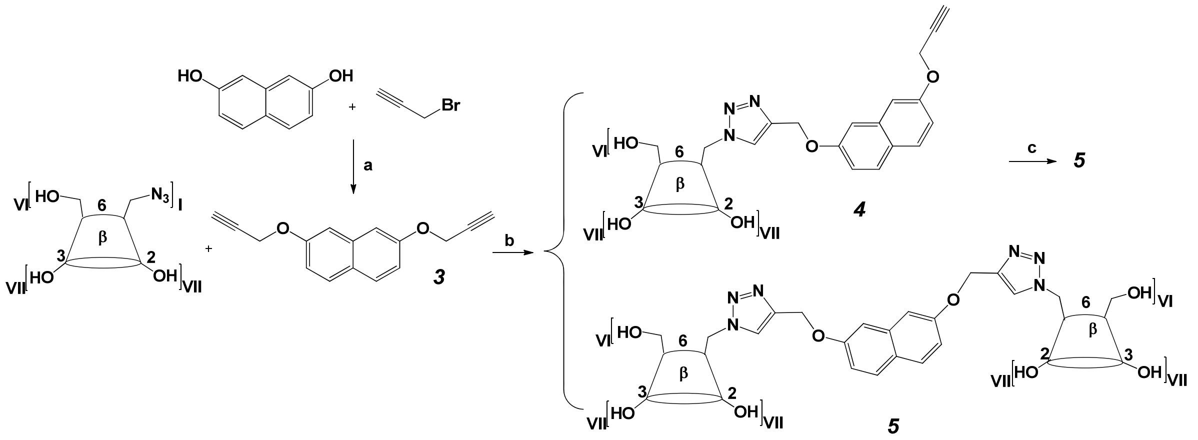
^1H NMR (DMSO-d_6, 300 MHz): δ 8.23 (s, 1H, H-5 Tz), 7.85-7.79 (overlapped signals, 3H, H-1,5,8 Npth), 7.50-7.17 (overlapped signals, 4H, H-7,6,4,3 Npth), 5.92-5.68 (overlapped signals, 14H, 2,3-OH), 5.22 (s, 4H, Tz-CH_2-O-Npth), 5.05 (s, 1H, H-1'), 4.96 (m, 1H, H-6'ab), 4.90-4.72 (m, 6H, H-1), 4.61 (m, 1H, H-6'ab), 4.59-4.31 (overlapped signals, 6H, 6-OH), 4.01 (m, 1H, H-5'), 3.82-3.49 (overlapped signals, 23H, H-3,5,6), 3.45-3.24 (overlapped signals, 14H, H-2,4), 3.14 (brm, 1H, H-6''ab), 2.88 (brm, 1H, H-6''ab).

^{13}C NMR (DMSO-d_6, 75 MHz): δ 156.1 (C-2 Npth), 142.4 (C-4 Tz), 134.2 (C-8' Npth), 129.4 (C-5 Npth), 129.3 (C-4' Npth), 128.6 (C-1 Npth), 127.5,126.8 (C-8,6 Npth), 126.4 (C-7 Npth), 125.6 (C-5 Tz), 118.7 (C-4 Npth), 107.1 (C-3 Npth), 102.3, 102.0, 101.9 (C-1), 83.5, 82.1 81.6, 81.5, 81.4, 81.0 (C-4), 73.2, 72.4, 72.3, 72.1, 71.8, 70.0 (C-2,3,5), 70.9 (C-5'), 61.0 (Tz-*C*H$_2$-O-Naf), 60.2, 60.0, 59.9 (C-6), 55.5 (C-6').

ESI-MS (*m/z*, %) calc. for $C_{55}H_{80}N_3O_{35}$ [M + H]$^+$ 1343.21, found 1342.87 (25%); for $C_{55}H_{79}N_3O_{35}Na$ [M + Na]$^+$ 1364.44, found 1364.81 (100%); for $C_{55}H_{79}N_3O_{35}K$ [M + K]$^+$ 1380.55, found 1380.78 (35%).

Scheme 2. Synthesis of 2,7-bis-((1-(6^I-deoxy-β-CD-6^I-yl)-1*H*-1,2,3-triazol-4-yl)methoxy)naphthalene (**5, *bis*-NβCD**).

Reagents and conditions: a) K_2CO_3, acetone, 70°C (rfx); b) Cu powder, MW/US, 100°C, 1.5 h, DMF; c) 6^I-azido-6^I-deoxy-β-CD, Cu powder, MW/US, 100°C, 1.5 h, DMF.



Synthesis of 2,7-dipropargyloxynaphthalene (3)

In a two-necked round-bottomed flask (50 ml), 1 g of 2,7-dihydroxynaphtalene (6.24 mmol, 1 eq) was dissolved in 15 ml of acetone and 6.89 g of K_2CO_3 (49.9 mmol, 8 eq) was added to the solution. The mixture was kept at 70°C for 30 min under magnetical stirring. Subsequently 1.62 ml of propargyl bromide (14.98 mmol, 2.4 eq) was added and the reaction was left at 70°C for 20 h.

The acetone was removed under vacuum. The crude product was extracted with CH_2Cl_2, dried under vacuum and purified on silica gel (flash chromatography) using a PE/EtOAc gradient. 865 mg of pure 2,7-dipropargyloxynaphthalene was obtained (3.66 mmol, 59%).

Yellow powder. R*f* = 0.59 (PE/EtOAc 8:2).

IR (KBr, cm^{-1}): ν 3293, 2132 (alkyne), 1626, 1514, 1384, 1208, 1019, 839, 820, 685, 655, 628, 477.

^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.67 (d, *J* = 9 Hz, 2H, H-4,5), 7.18 (d, *J* = 2.4 Hz, 2H, H-1,8), 7.08 (dd, *J* = 9, 2.7 Hz, 2H, H-3,6), 4.81 (d, *J* = 2.4 Hz, 4H, O-C*H*$_2$C≡CH), 2.58 (t, *J* = 1.2 Hz, 2H, O-CH$_2$C≡C*H*).

^{13}C NMR ($CDCl_3$, 75 MHz): δ 156.3 (C-2,7), 135.5 (C-8'), 129.5 (C-4,5), 125.2 (C-4'), 116.7 (C-3,6), 107.1 (C-1,8), 78.6 (O-CH$_2$*C*≡CH), 75.8 (O-CH$_2$C≡*C*H), 55.9 (O-*C*H$_2$C≡CH).

CI-MS (*m/z*, %) = 237 (100%) $[M + H]^+$.

Synthesis of 6^{I}-deoxy-6^{I}-(4-((7-propargyloxynaphthalen-2-yloxy)methyl)-1*H*-1,2,3-triazol-1-yl)-β-CD (4)

In a three-necked pear-shaped reaction vessel (100 ml), 400 mg of 6^{I}-azido-6^{I}-deoxy-β-CD (0.345 mmol, 1 eq) and 244 mg of 2,7-dipropargyloxynaphtalene (1.033 mmol, 3 eq) were dissolved in 10 ml of DMF and afterwards 200 mg of Cu powder were added to the solution.

The reaction was carried out under combined MW/US irradiation at 100°C for 1.5 h (power of 100 W for MW, 35 W for US). The reaction outcome was monitored by TLC (*i*PrOH/H_2O/EtOAc/NH_4OH = 5:3:1:1).

The copper was filtered off on filter paper. After the evaporation of DMF under vacuum, the crude product was crystallized in water/acetone and then purified on RP18 (flash-chromatography) using a H_2O/MeOH gradient. 458.4 mg of pure monomeric product (**4**, 0.328 mmol, 76%) and 70 mg of pure dimeric product (**5**, 0.0274 mmol, 13%) were obtained.

6^{I}-deoxy-6^{I}-(4-((7-propargyloxynaphthalen-2-yloxy)methyl)-1*H*-1,2,3-triazol-1-yl)-β-CD (4) White powder. R*f* = 0.43 (*i*PrOH/H_2O/EtOAc/NH_4OH = 5:3:1:1).

IR (KBr, cm^{-1}): ν 3375, 2926, 1633, 1516, 1157, 1080, 1028, 754, 704, 581.

^{1}H NMR (DMSO-d_6, 300 MHz): δ 8.21 (s, 1H, H-5 Tz), 7.76 (d, *J* = 8.1 Hz, 2H, H-4,5 Npth overlapped), 7.40 (s, 1H, H-8 Npth), 7.30 (s, 1H, H-1 Npth), 7.02 (d, *J* = 9 Hz, 2H, H-3,6 Npth overlapped), 5.90-5.70 (overlapped signals, 14H, 2,3-OH), 5.20 (s, 2H, H-1, Tz-C*H*$_2$-O-Npth), 5.05 (s, 1H, H-1), 4.96 (m, 1H, H-6'ab), 4.95 (s, 2H, H-1, CHC-C*H*$_2$-O-Npth), 4.90-4.79 (m, 6H, H-1), 4.64 (m, 1H, H-6'ab), 4.59-4.34 (overlapped signals, 6H, 6-OH), 4.01 (m, 1H, H-5'), 3.64-3.50 (overlapped signals, 23H, H-3,5,6), 3.48-3.25 (overlapped signals, 14H, H-2,4), 3.15 (brm, 1H, H-6"ab), 2.91 (brm, 1H, H-6"ab).

^{13}C NMR (DMSO-*d*$_6$, 75 MHz): δ 156.8,155.7 (C-2,7 Npth), 142.4 (C-4 Tz), 135.5 (C-8' Npth), 129.2, 129.19 (C-4,5 Npth), 125.7 (C-5 Tz), 124.2 (C-4' Npth), 116.5, 115.9 (C-3,6 Npth), 107.0 (C-8 Npth), 106.6 (C-1 Npth), 102.2, 102.0, 101.9, 101.3 (C-1), 83.5, 82.2, 81.5, 81.4, 81.1 (C-4), 79.3 (C-2 propargyl), 78.4 (C-3 propargyl), 73.2, 73.1, 73.0, 72.9, 72.7, 72.5, 72.4, 72.1, 71.8 (C-2,3,5), 70.0 (C-5'), 61.1 (Tz-*C*H$_2$-O-Npth), 60.2, 60.0, 59.9 (C-6), 55.5 (C-1 propargyl), 50.5 (C-6$^{'ab}$).

ESI-MS (*m/z*, %) calc. for $C_{58}H_{82}N_3O_{36}$ [M + H]$^+$ 1397.27, found 1396.88 (40%); for $C_{58}H_{81}NaN_3O_{36}$ [M + Na]$^+$ 1418.45, found 1418.83 (100%); for $C_{58}H_{81}KN_3O_{36}$ [M + K]$^+$ 1434.56, found 1435.84 (50%).

Synthesis of 2,7-bis-((1-(6^{I}-deoxy-β-cyclodextrin-6^{I}-yl)-1*H*-1,2,3-triazol-4-yl) methoxy) naphthalene (5, *bis*-NβCD)

In order to increase the dimer yield, the same synthetic procedure described above was repeated on 0.150 mg of 6^{I}-azido-6^{I}-deoxy-β-CD (0.129 mmol, 1 eq) and 180 mg of 6^{I}-deoxy-6^{I}-(4-((7-propargyloxynaphthalen-2-yloxy)methyl)-1*H*-1,2,3-triazol-1-yl)-β-CD (**4**, 0.129 mmol, 1 eq). It yielded 92 mg of 2,7-bis-((1-(6^{I}-deoxy-β-cyclodextrin-6^{I}-yl)-1*H*-1,2,3-triazol-4-yl)methoxy)naphthalene (**5**, 0.036 mmol, 28%) after purification.

Yellow liquid. R*f* = 0.14 (*i*PrOH/H_2O/EtOAc/NH_4OH = 5:3:1:1).

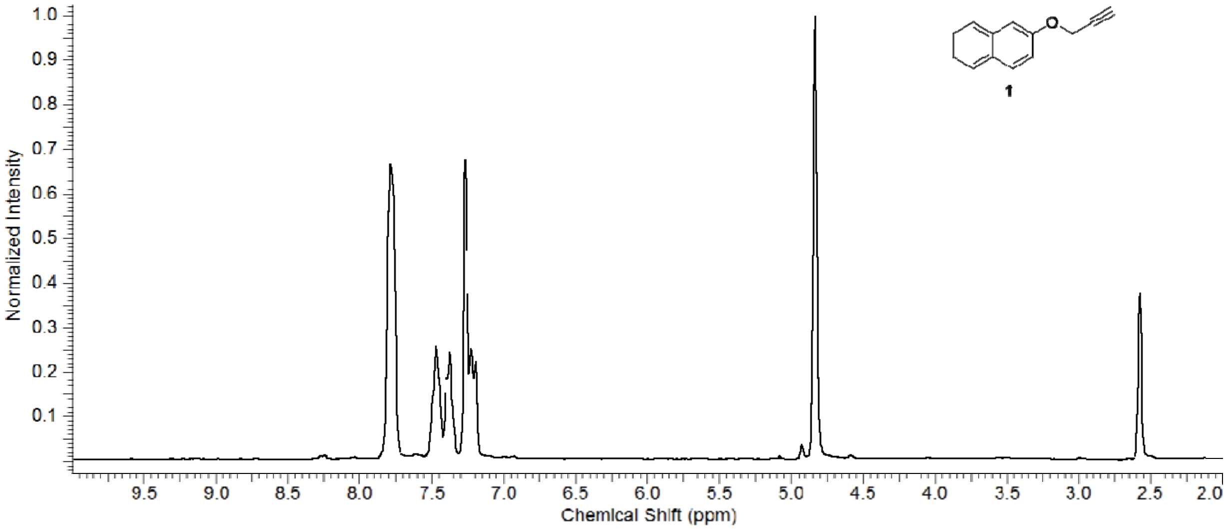
IR (KBr, cm^{-1}): ν 3380, 2924, 1640, 1516, 1159, 1080, 1026, 754, 841, 560.

^{1}H NMR (DMSO-*d*$_6$, 300 MHz): δ 8.22 (s, 2H, H-5 Tz), 7.75 (d, *J* = 9 Hz, 2H, H-4,5 Npth), 7.44 (d, *J* = 17.1 Hz, 2H, H-1,8 Npth), 7.04 (d, *J* = 9 Hz, 2H, H-3,6 Npth), 5.90-

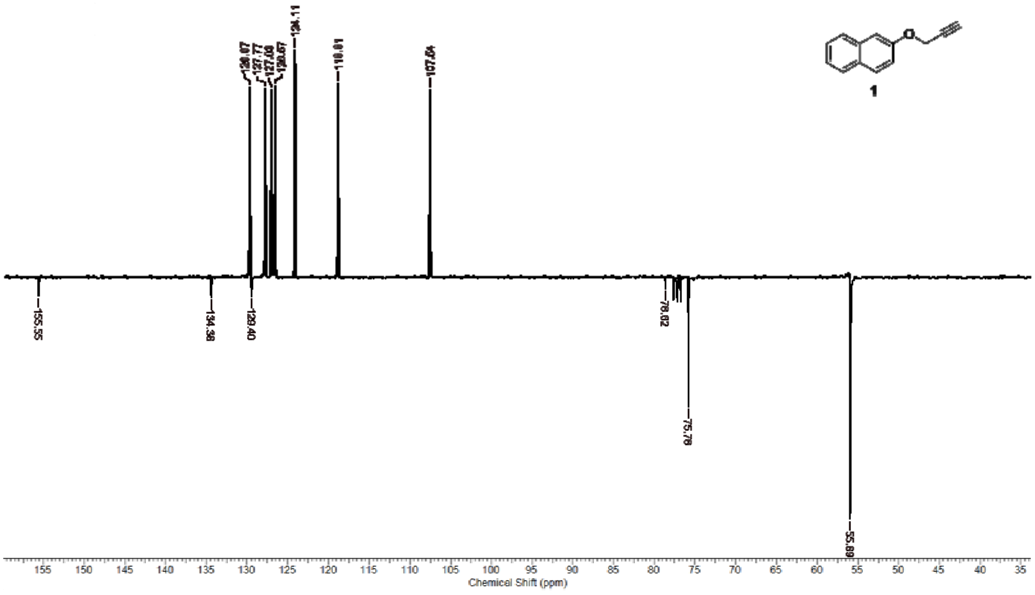
5.60 (overlapped signals, 28H, 2,3-OH), 5.20 (s, 4H, Tz-C*H*$_2$-O-Npth), 5.06 (s, 2H, H-1), 4.95 (m, 2H, H-6'ab), 4.90-4.72 (m, 12H, H-1), 4.62 (m, 2H, H-6'ab), 4.56-4.41 (overlapped signals, 12H, 6-OH), 4.01 (m, 2H, H-5'), 3.88-3.56 (overlapped signals, 46H, H-3,5,6), 3.47-3.22 (overlapped signals, 28H, H-2,4), 3.18 (brm, 2H, H-6''ab), 2.92 (brm, 2H, H-6''ab).

^{13}C NMR (DMSO-*d*$_6$, 75 MHz): δ 156.7 (C-2,7 Npth), 142.4 (C-4 Tz), 129.6 (C-4,5 Npth), 124.1 (C-4',8'Npth), 126.1 (C-5 Tz), 116.2 (C-3,6 Npth), 106.6 (C-1,8 Npth), 102.2, 102.0, 101.3 (C-1), 83.5, 82.0, 81.5, 81.4, 81.1 (C-4), 73.2, 73.1, 73.0, 72.9, 72.7, 72.4, 72.1, 71.8 (C-2,3,5), 70.0 (C-5'), 61.0 (Tz-*C*H$_2$-O-Npth), 60.0, 59.9, 59.1 (C-6), 50.4 (C-6').

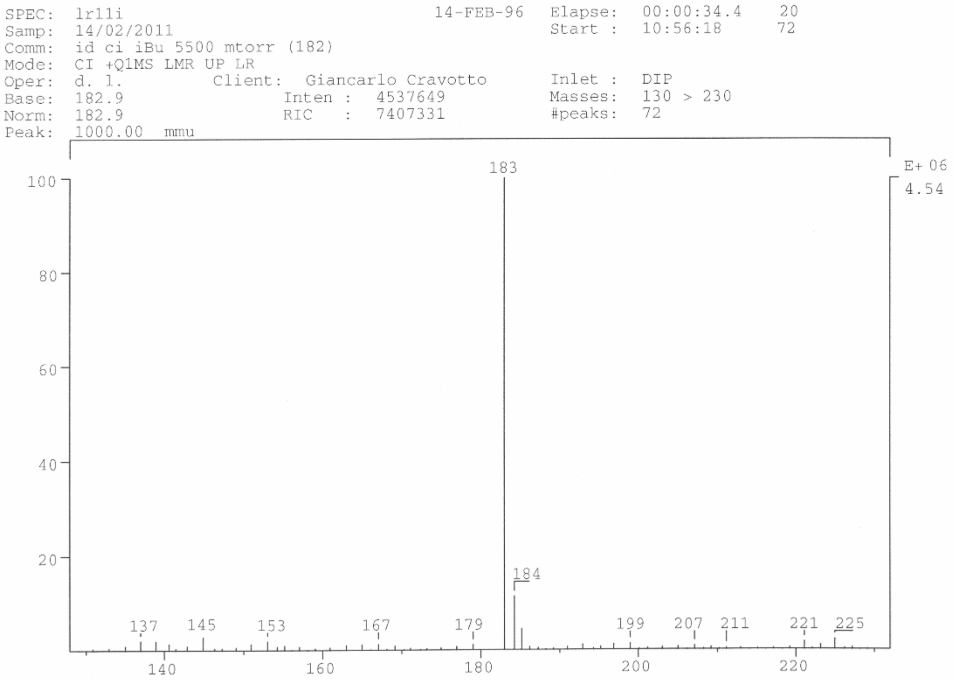
ESI-MS (*m/z*, %) calc. for $C_{100}H_{151}N_6O_{70}Na$ [M + H + Na]$^{2+}$ 1290.12, found 1290.23 (70%); for $C_{100}H_{151}N_6O_{70}K$ [M + H + K]$^{2+}$ 1298.18, found 1298.26 (100%).



^{1}H NMR spectra (300 MHz in $CDCl_3$)of compound 1



APT ^{13}C NMR spectra (75 MHz in $CDCl_3$) of compound 1



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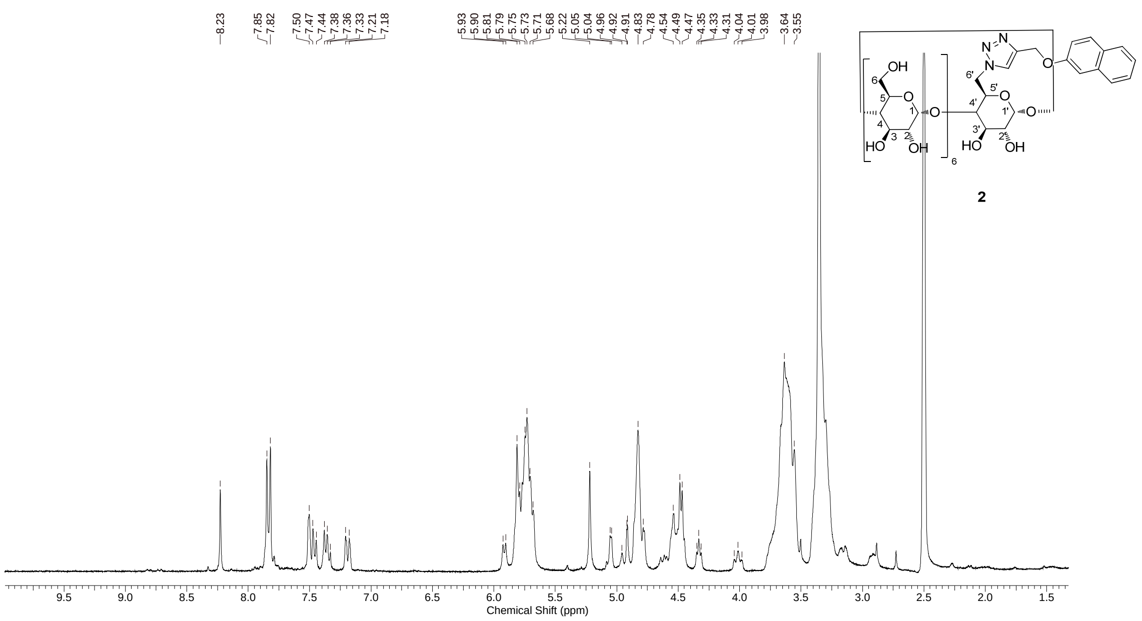
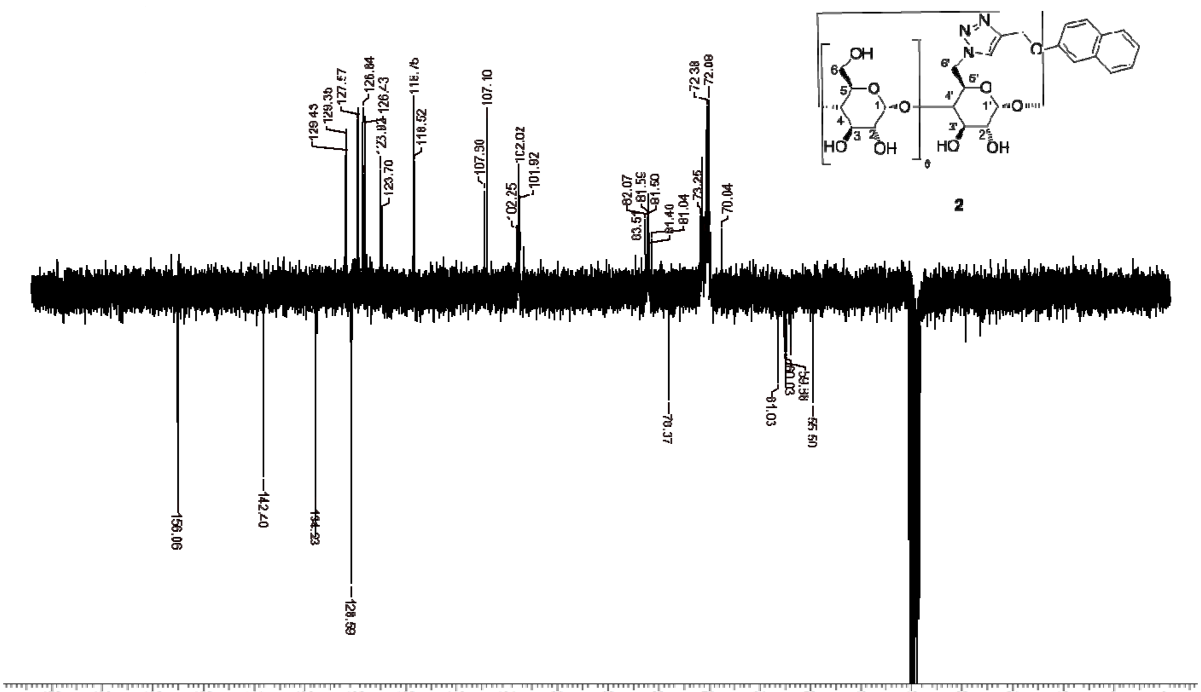
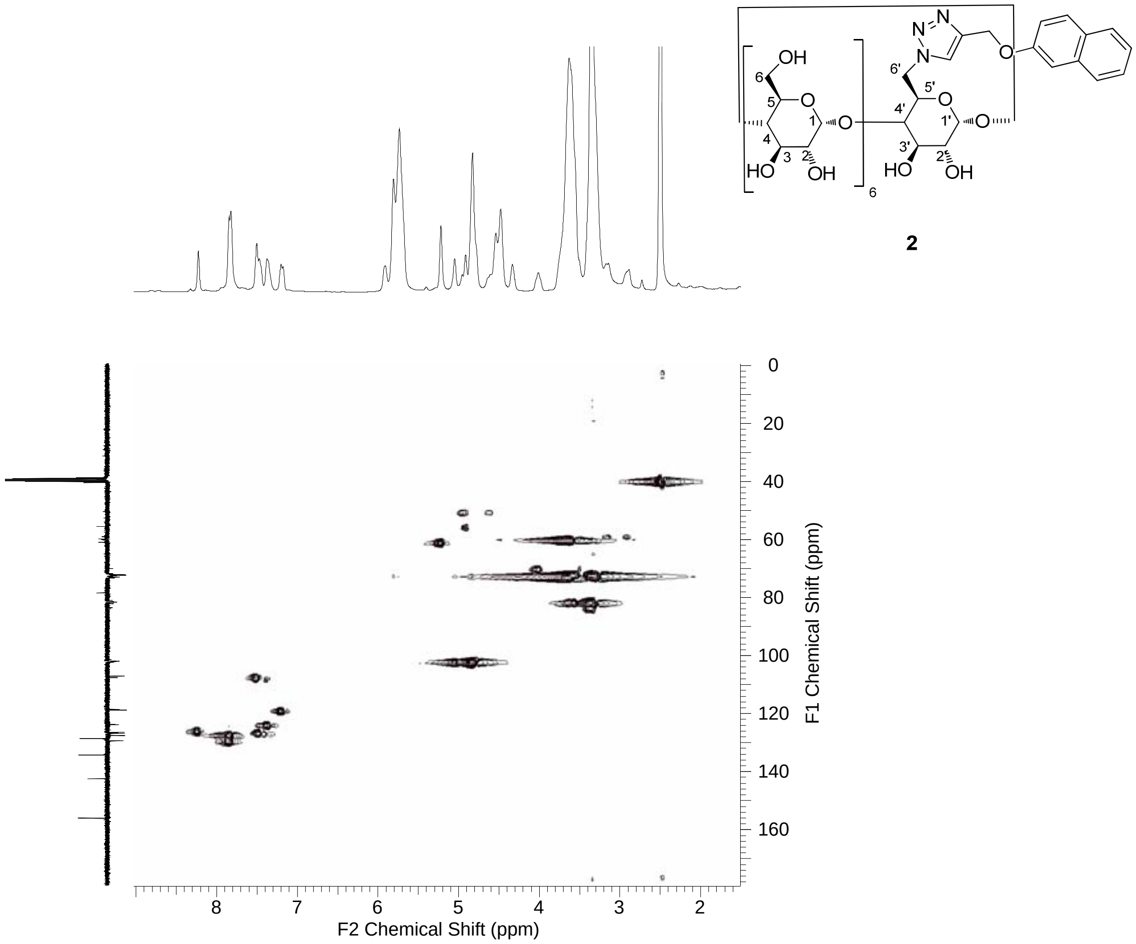
C.I. MS spectra of Compound **1**



^{1}H NMR spectra (300 MHz in DMSO) of compound **2**

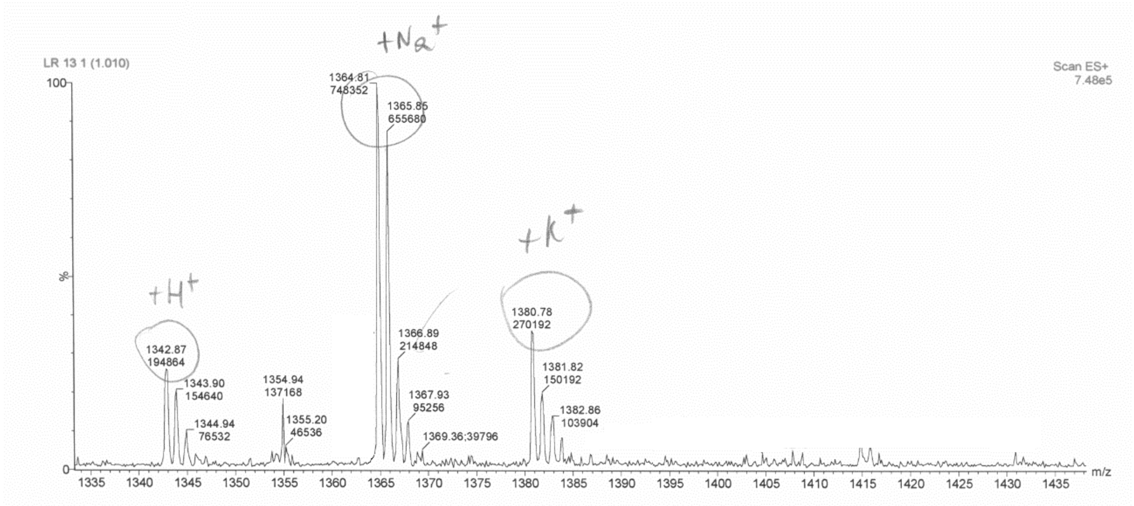


APT ^{13}C NMR spectra (75 MHz in DMSO-d_6)of compound **2**

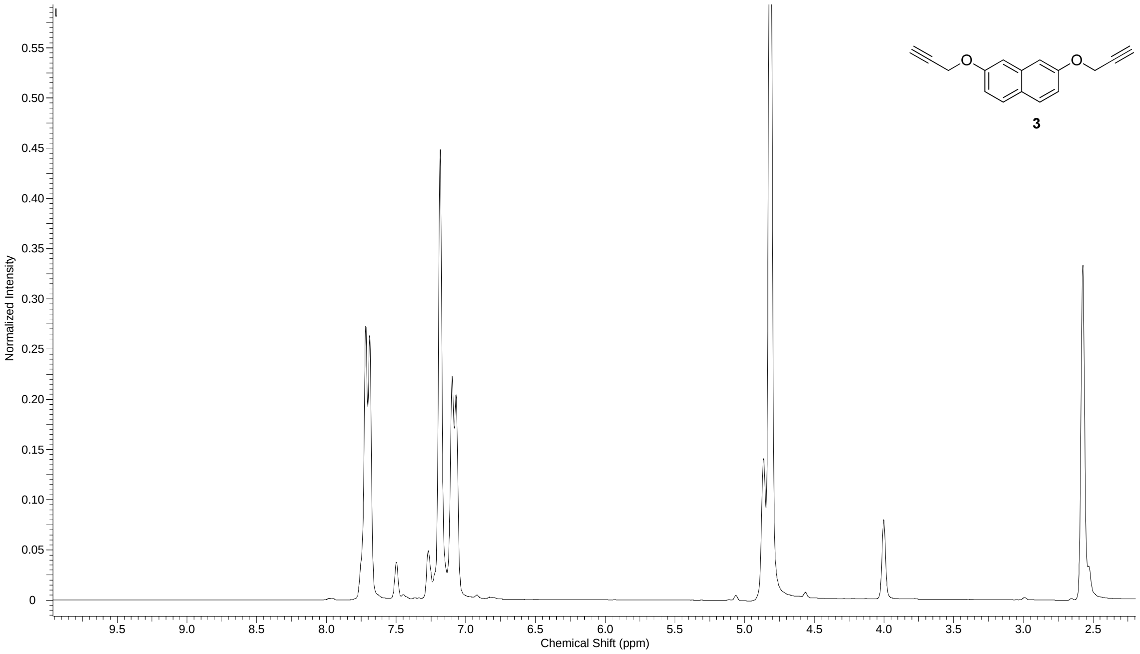


2

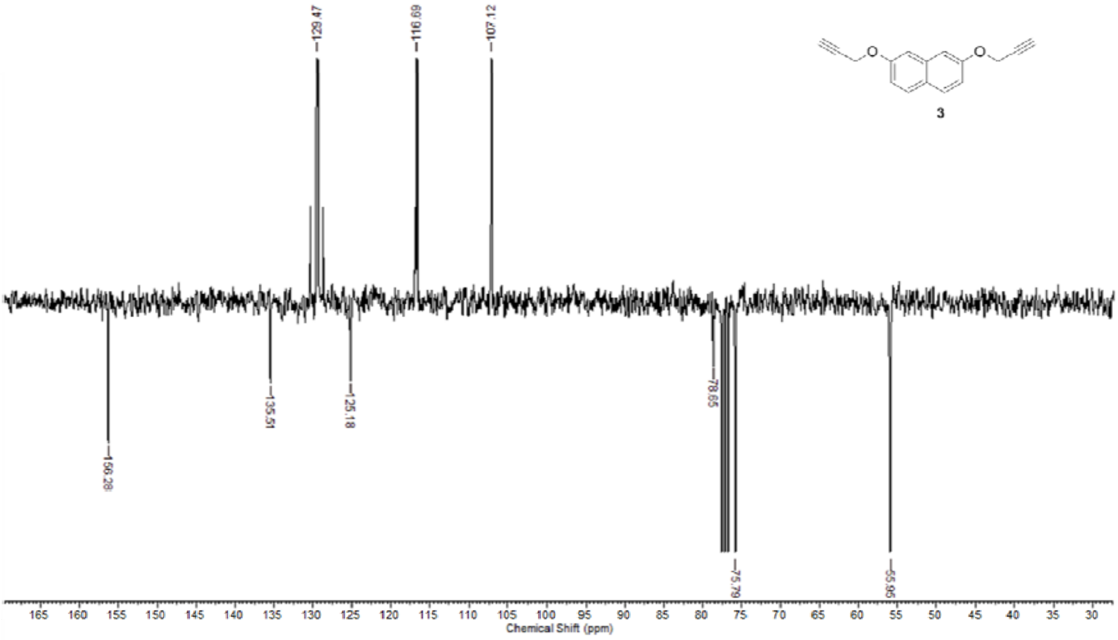
HSQC spectra (300 MHz for ^{1}H -^{13}C in DMSO-d_6) of Compound **2**



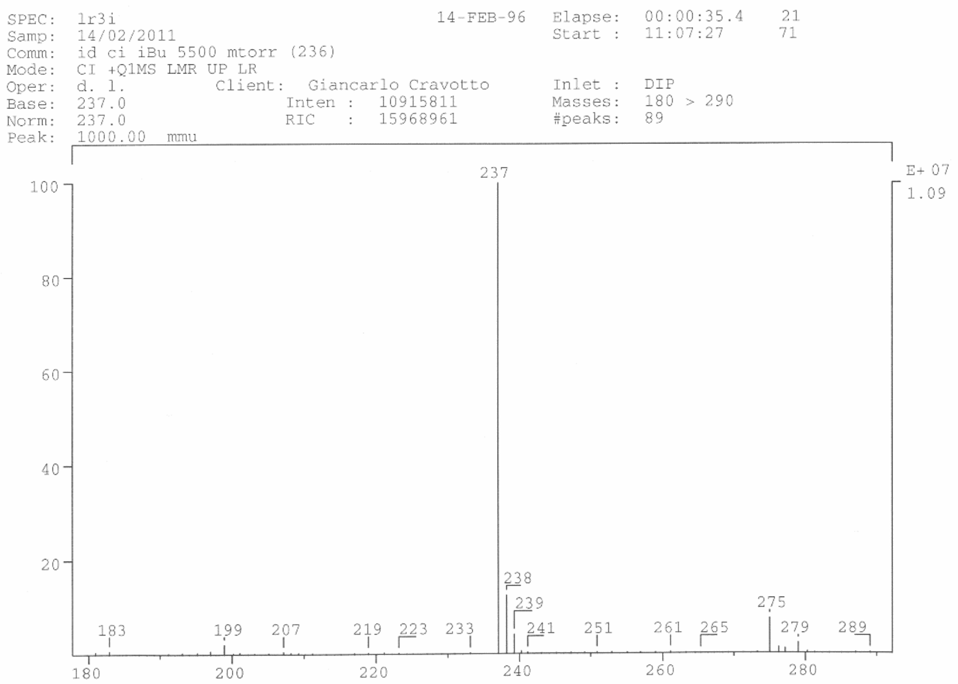
C.I. MS spectra of Compound **2**



^{1}H NMR spectra (300 MHz in CDCl3) of compound **3**



^{13}C NMR spectra (75 MHz in $CDCl_3$) of compound **3**



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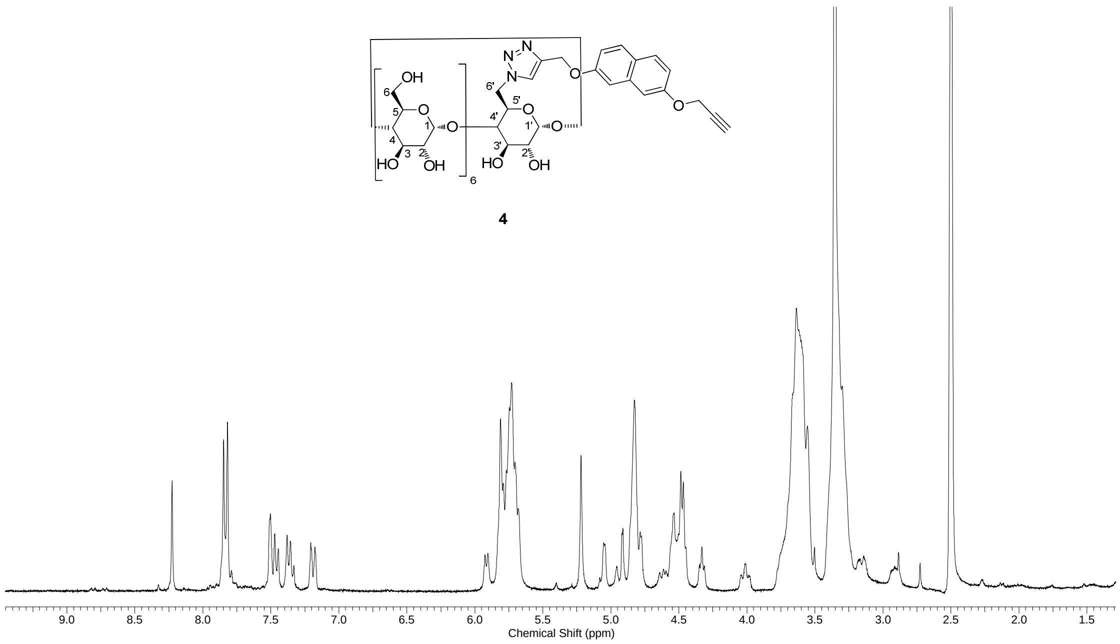
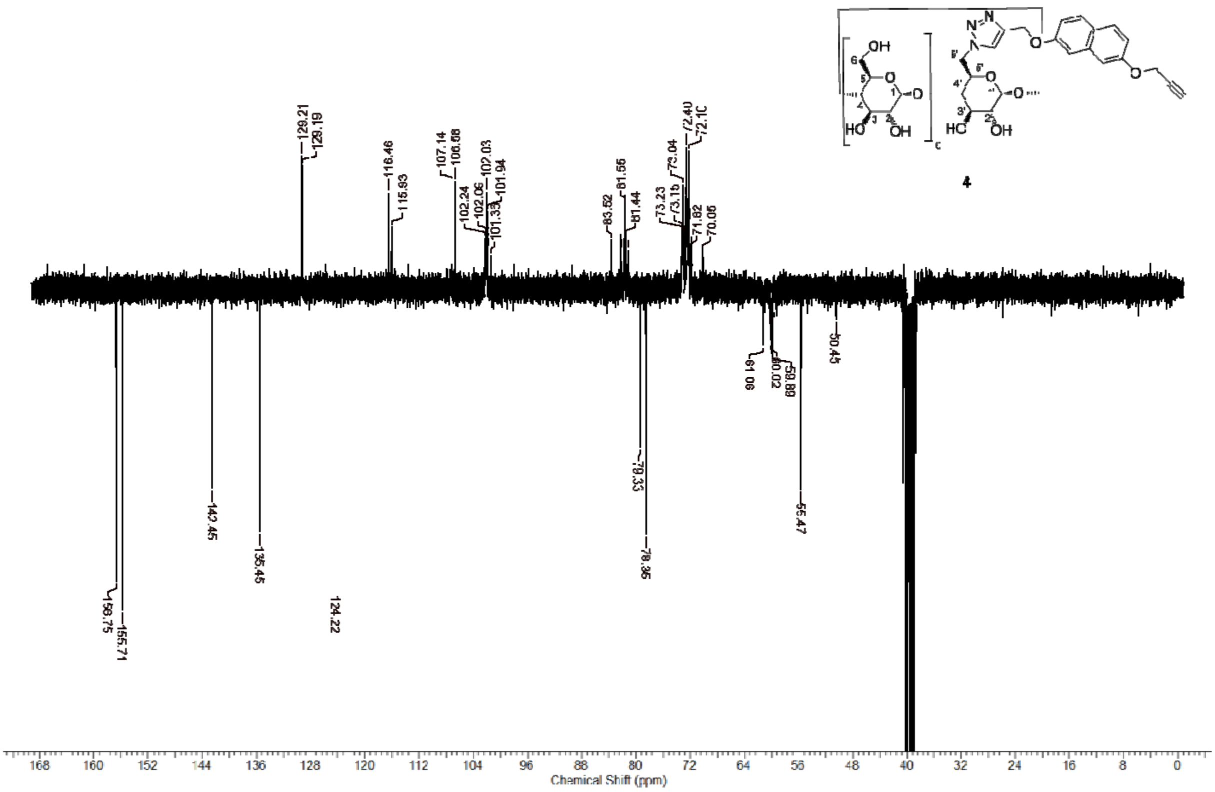
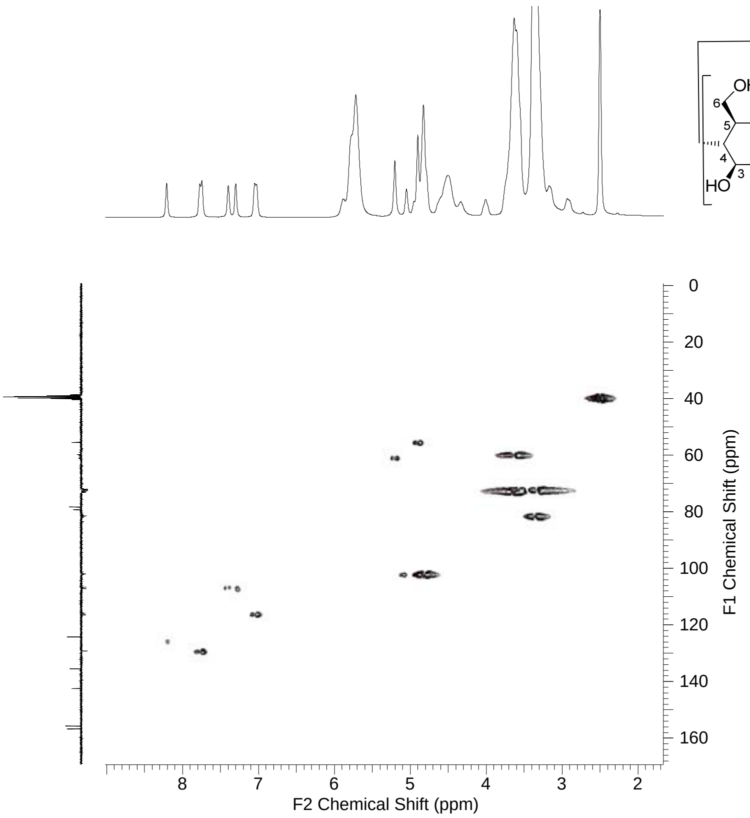
C.I. MS spectra of Compound **3**

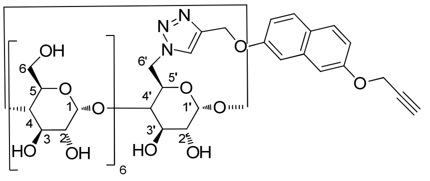


^{1}H NMR spectra (300 MHz in DMSO-d_6) of compound **4**



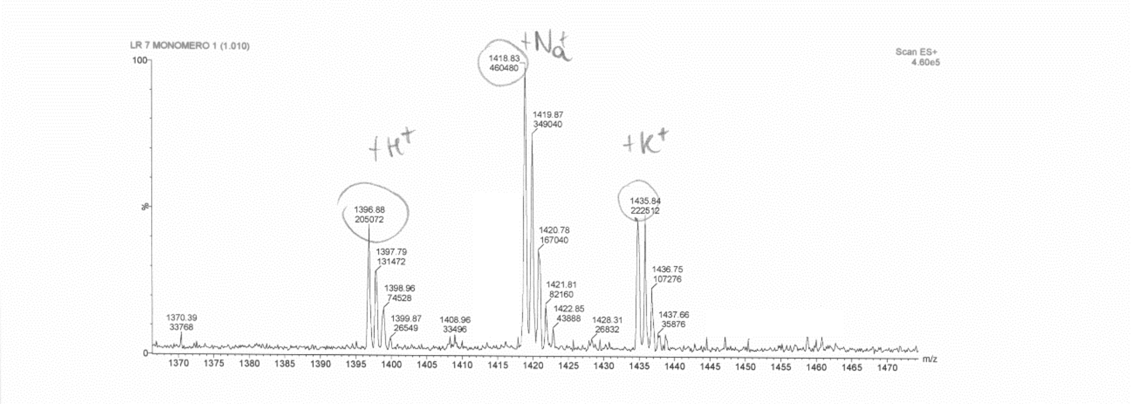
^{13}C NMR spectra (75 MHz in DMSO-d_6) of compound **4**



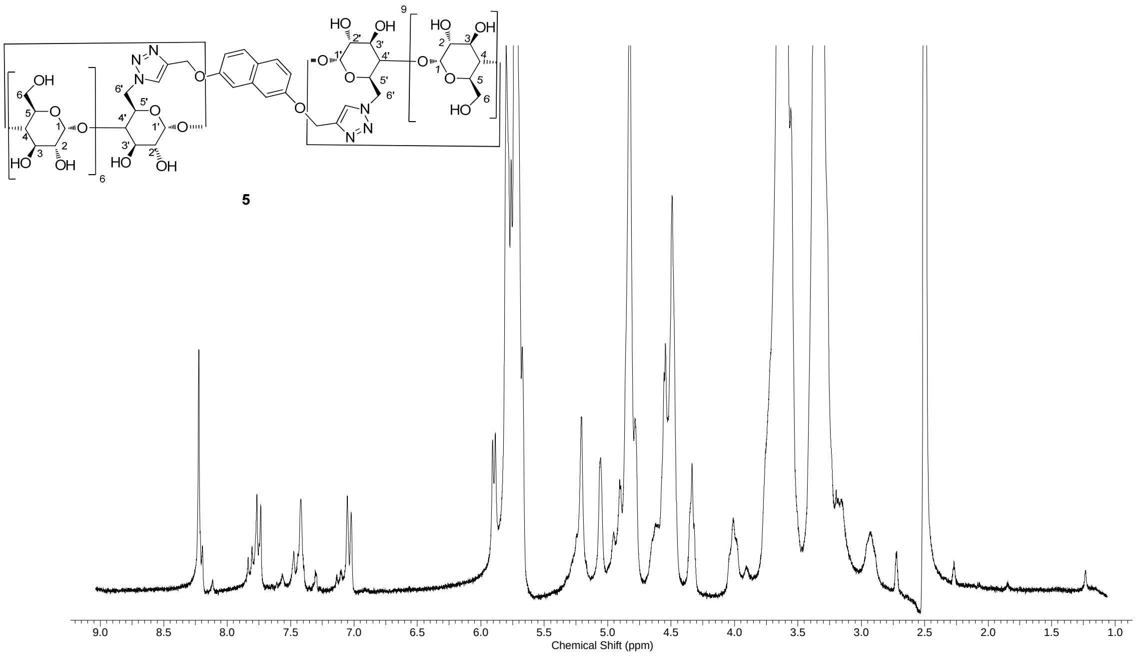


4

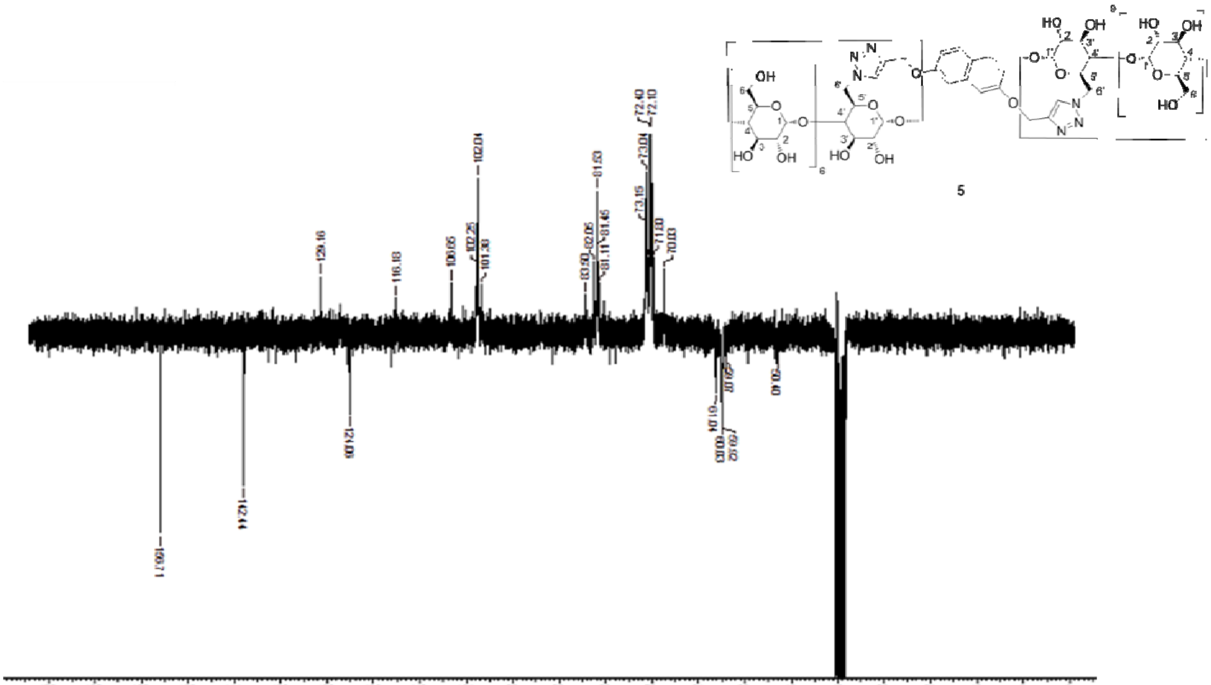
HSQC spectra (300 MHz for ^{1}H -^{13}C in DMSO-d_6) of Compound **4**



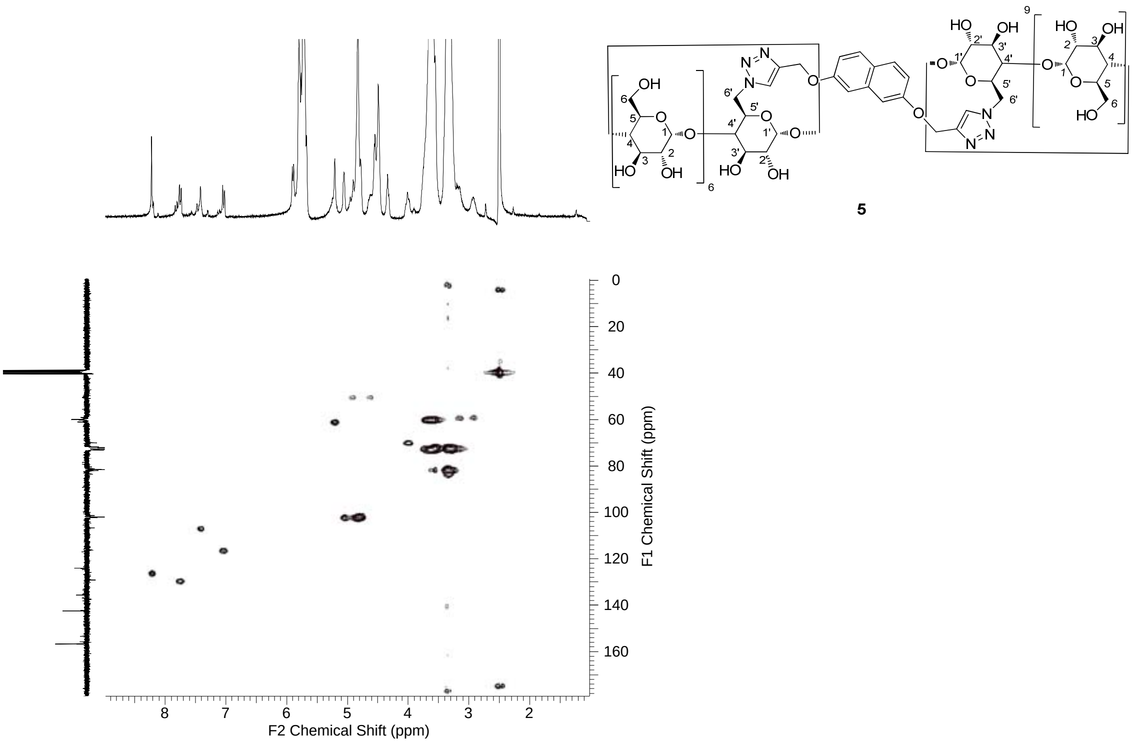
C.I. MS spectra of Compound **4**



^{1}H NMR spectra (300 MHz in DMSO-d_6) of compound **5**

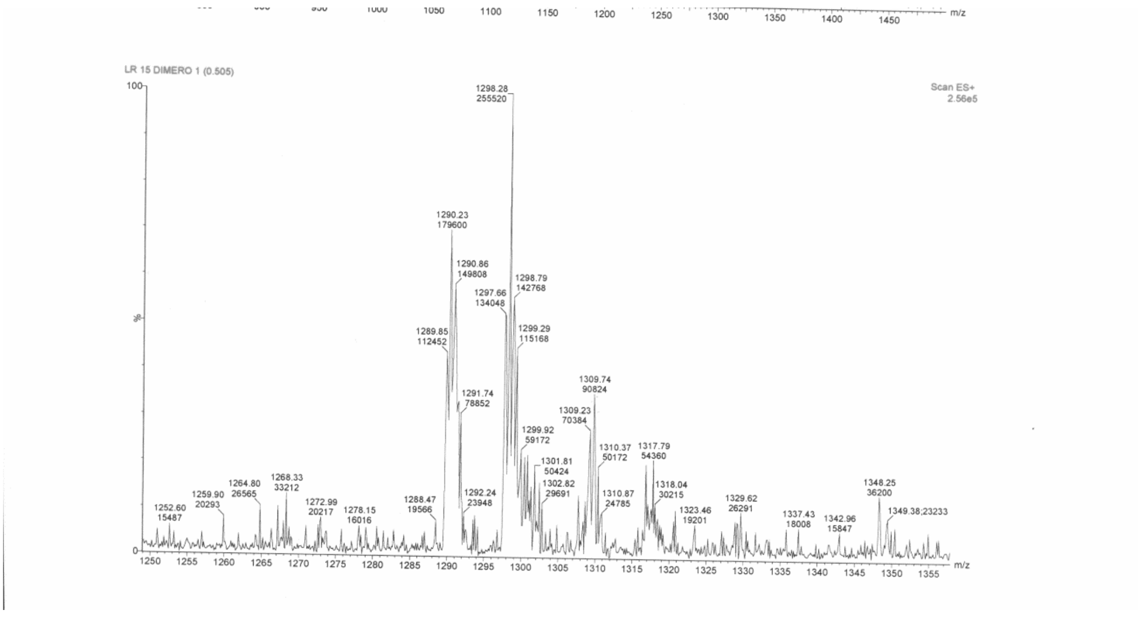


^{13}C NMR spectra (75 MHz in DMSO-d_6) of compound **5**



5

HSQC spectra (300 MHz for ^1H -^{13}C in DMSO-d_6) of Compound **5**



C.I. MS spectra of Compound **5**

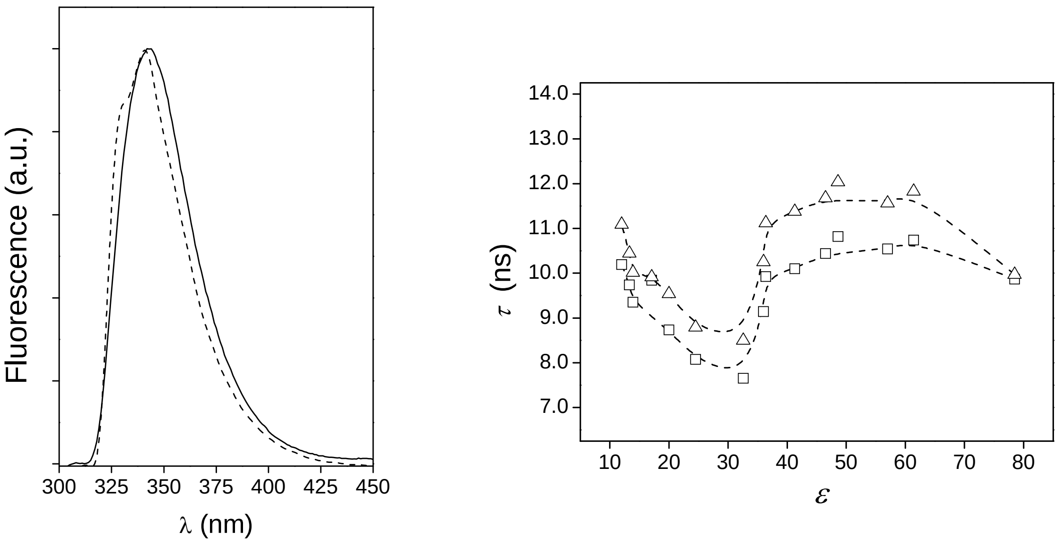


Figure 1S. (left) Emission spectra for MON and dMON (dashed) in water at 25ºC, (right) Lifetime as a function of solvent polarity, *ε*, for model compounds MON (□) and dMON (△) at 25ºC in linear water *n*-alcohols from methanol to *n*-heptanol and some methanol and ethanol:water mixtures.

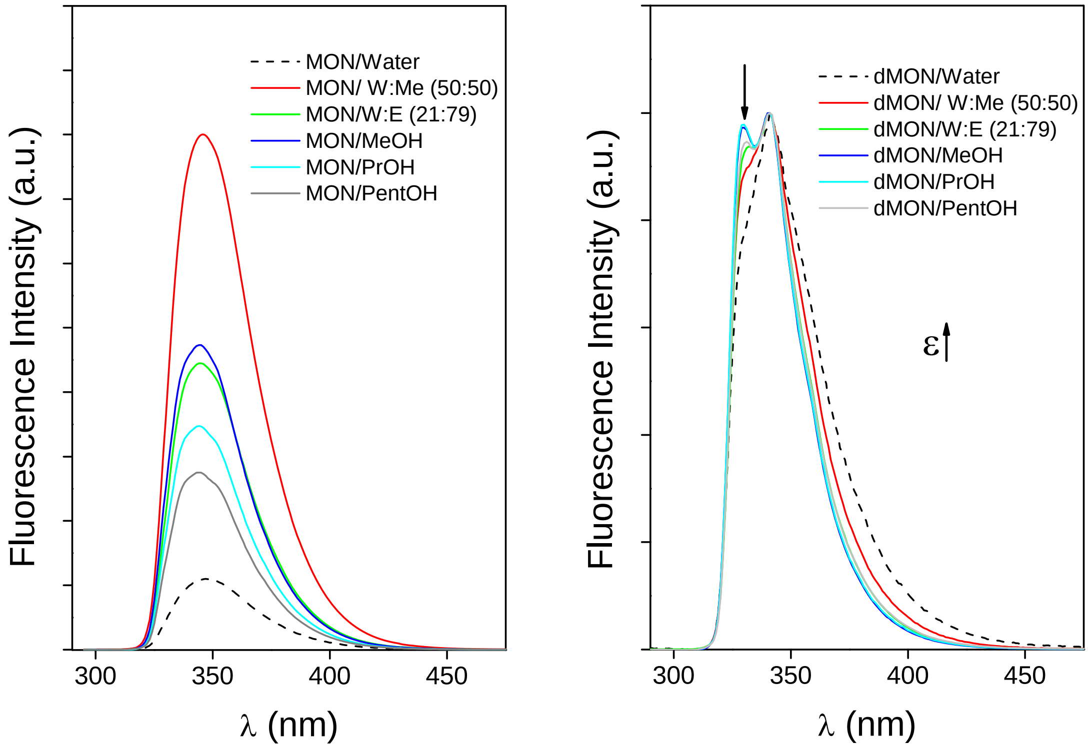


Figure 2S. Emission spectra for MON (left) and dMON (right) in some solvents of different polarities at 25ºC. Spectra for dMON were normalized at the maximum of the low energy emission band. Intensity of the high energy band significantly decreases with the polarity of the solvent.

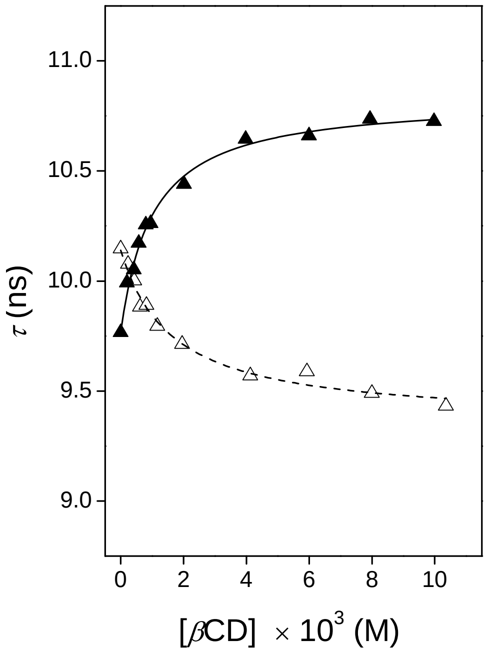


Figure 3S. Lifetime variation with [βCD] at 25 ºC for MON (▲) and dMON (△). [βCD] were 0, 0.2, 0.4, 0.6, 0.8, 1.0, 2.0, 4.0, 6.0, 8.0 y 10×10^{-3} M and 0, 0.2, 0.4, 0.6, 0.8, 1.0, 2.0, 4.1, 5.9, 8.0 y 10×10^{-3} M respectively. Chromophore concentrations were fixed at 10^{-5} M.

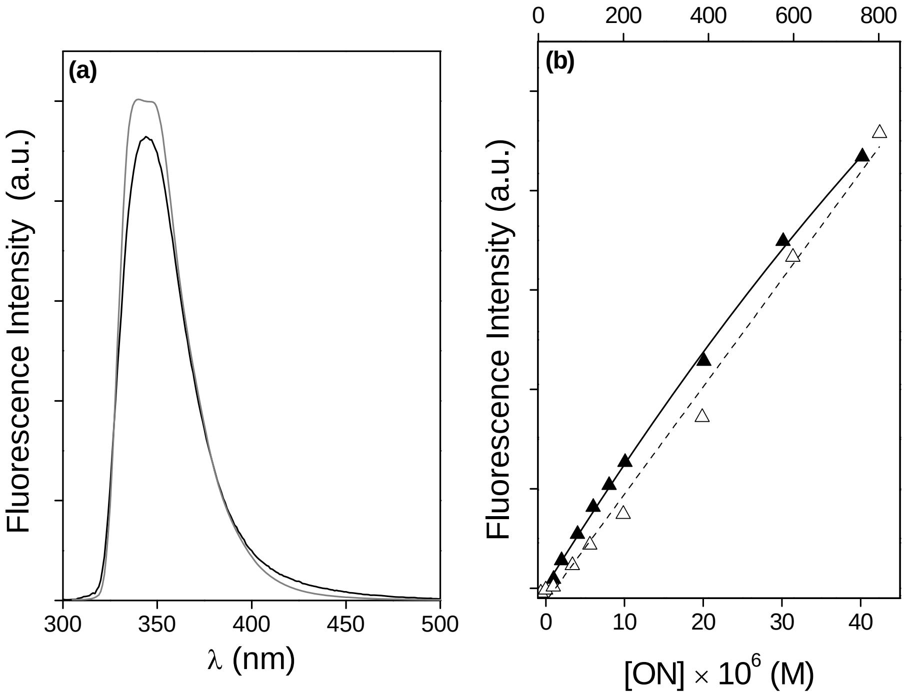


Figure 4S. (a) Emission spectra for *mono*-NβCD (—) and *bis*-NβCD (—) aqueous solutions of concentrations 1.0×10^{-6} M and 0.6×10^{-6} M respectively upon excitation of 285 nm at 25ºC; **(b)** Corrected fluorescence intensity using equation 2 as a function of the concentration of naphthoxy or binaphthoxy groups. Concentrations were 1, 2, 4, 6, 8, 10, 20, 30 y 40×10^{-6} M for *mono*-NβCD (▲) and 6, 17, 35, 80,121, 200, 385, 599 y 802×10^{-6} M for *bis*-NβCD (Δ).

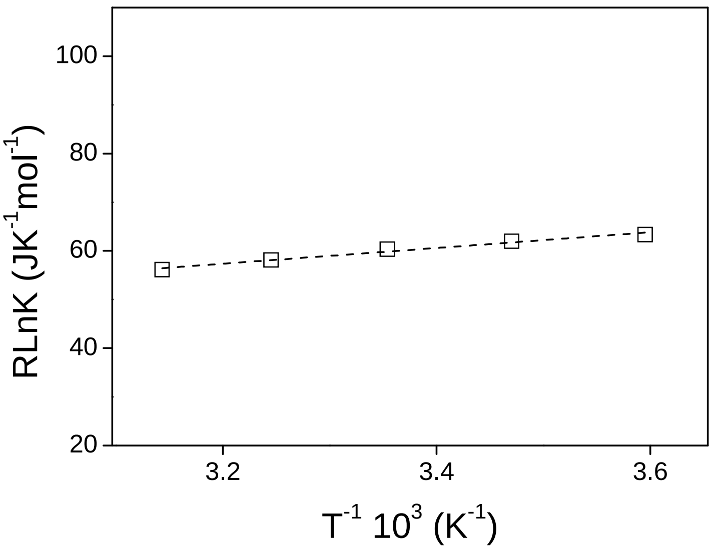


Figure 5S. van't Hoff plot for the *mono*-NβCD heteroassociation with βCD.

Table 1S. Binding constants for the *mono*-NβCD heteroassociation with βCD at different temperatures

T (ºC)	K (M^{-1})
5	2020 ± 350
15	1730 ± 300
25	1410 ± 100
35	1080 ± 110
45	850 ± 45

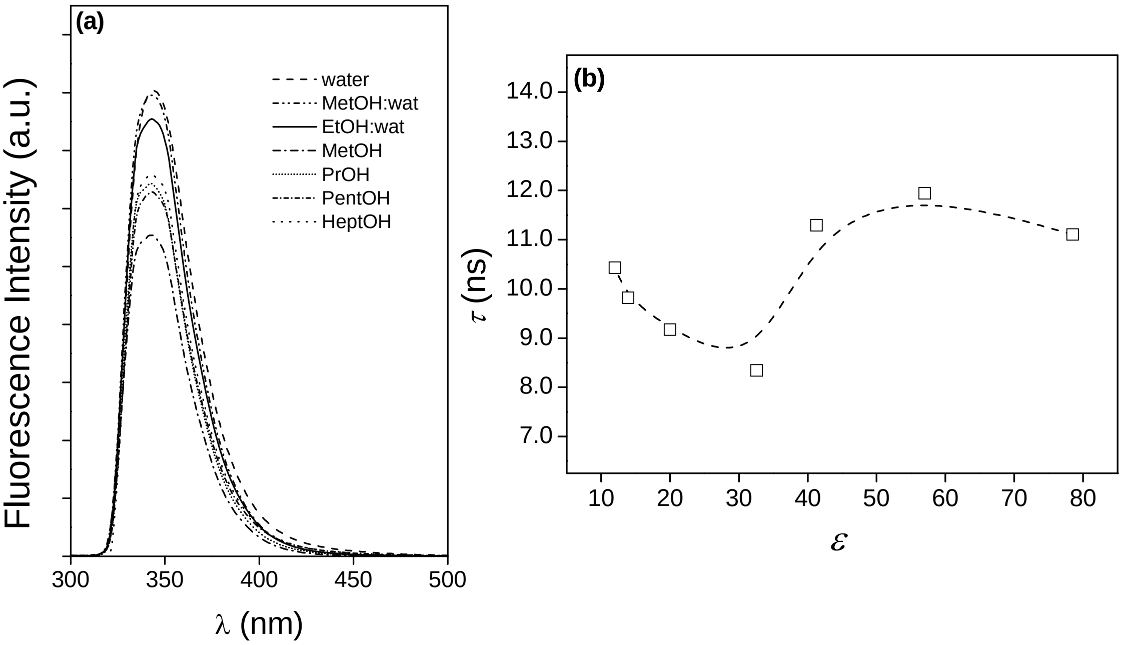


Figura 6S. (a) Emission spectra and **(b)** lifetimes, τ, for dilute solutions of *mono*-NβCD in different *n*-alcohols (methanol, *n*-propanol, *n*-penthanol y *n*-hepthanol) and methanol:water (50%) and ethanol:water (79 %) (v/v) mixtures as a function of the medium dielectric permitivity, ε at 25 ºC.

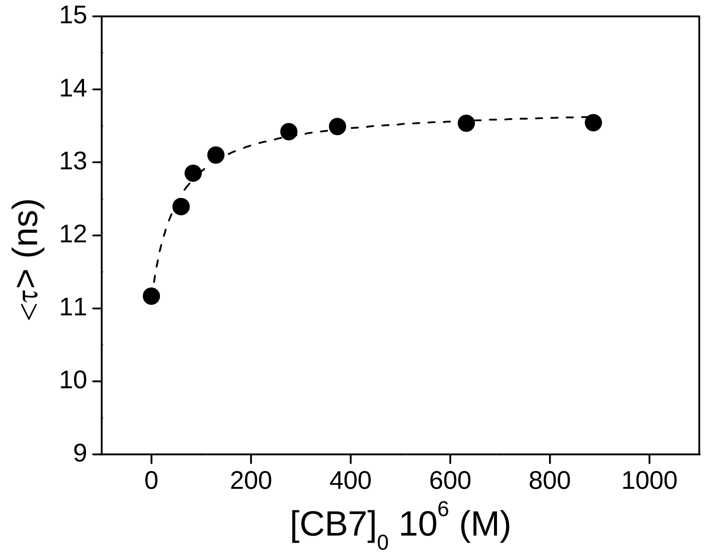


Figure 7S. Weighted average fluorescence lifetime, <*τ*> variation with CB7 concentration at 25 °C. [*mono*-NβCD] was 1.4×10^{-5} M.

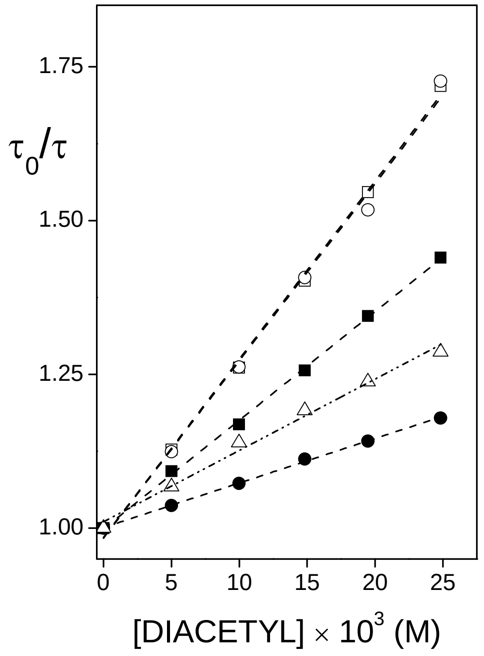


Figura 8S. Stern-Volmer plots obtained from fluorescence lifetime measurements on aqueous MON (□), dMON (○), *mono*-NβCD (■) and *bis*-NβCD (●) solutions at 10^{-5} M concentration and *mono*-NβCD (△) at 8×10^{-5} M concentration.

Table 2S. Geometrical parameters, the averages of some distances and angles between transition moments and the CD main axis, from the analysis of the MD trajectories on *mono*- and *bis*-NβCDs. The probabilities of finding angles smaller than 54.7° for different transitions appear in bold and in parentheses. The values for energy conformation minima appear simply between parentheses.

Parameter	*mono*-NβCD	*bis*-NβCD
Distance (Å)		
CD1–CD2	---	13.2 ± 2.6 (12.2)
CD$_1$–dON	9.6 ± 2.2 (6.7)	9.2 ± 2.2 (10.9)
CD$_2$–dON	---	9.4 ± 1.8 (6.5)
Tri$_1$–dON	6.0 ± 0.9 (5.6)	5.8 ± 0.9 (5.3)
Tri$_2$–dON	---	6.1 ± 1.0 (5.2)
CD$_{\text{main axis}}$ – Transition (°)		
CD$_1$–dON (^1L_a)	84 ± 31 (119) (**0.01**)	89 ± 33 (77) (**0.21**)
CD$_1$–dON (^1B_b)	92 ± 22 (67) (**0.01**)	92 ± 20 (104) (**0.04**)
CD$_2$–dON (^1L_a)	---	87 ± 28 (54) (**0.15**)
CD$_2$–dON (^1B_b)	---	94 ± 23 (111) (**0.06**)

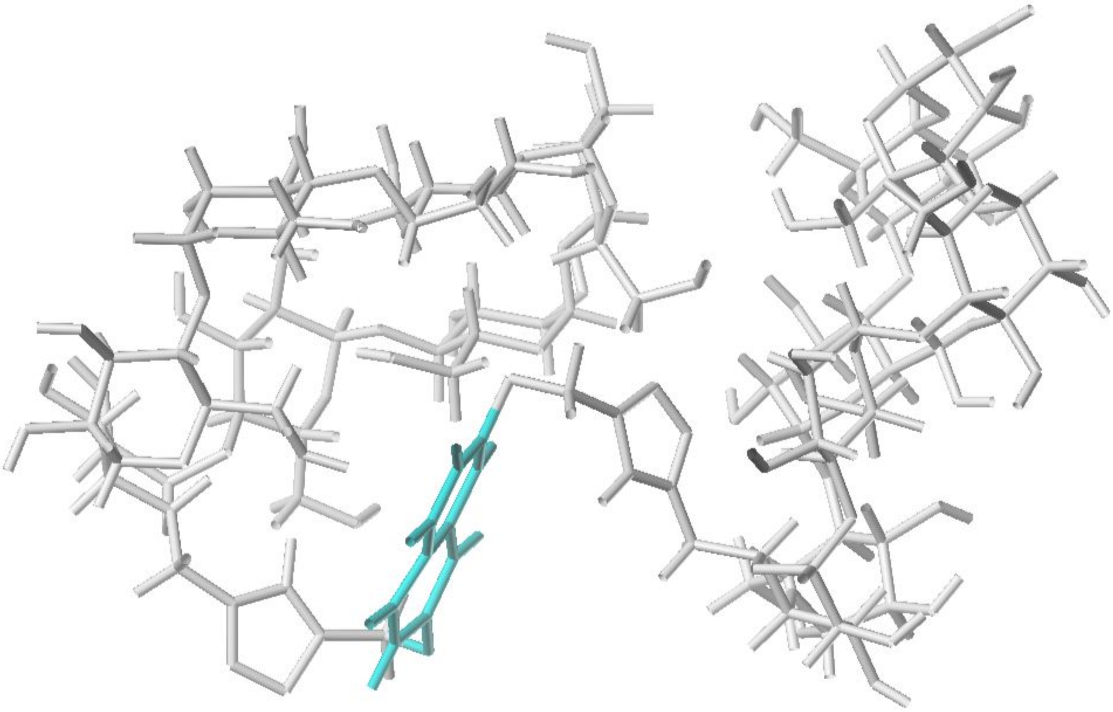


Figure 9S. Minimum binding energy structure for *bis*NβCD obtained from the analysis of the MD trajectory.

Table 3S. Averages for several distances, angles between naphthoate ON group transition moments and the main βCD axis for each CD, as well as binding energies and contributions obtained from the analysis of the 2ns MD trajectories in TH and TT arrangements of the non-covalent (*mono*-NβCD)$_2$ dimers. Values for the minima binding energy structures are found in parentheses.

Parameter	**TH *(axial)***	**TT *(axial)***
Distance (Å)		
CD_1–CD_2	13.0 ± 2.8	10.9 ± 0.3 (9.9)
CD_1–ON_2	7.9 ± 3.0	1.0 ± 0.3 (1.2)
CD_2–ON_1	18.3 ± 1.9	2.6 ± 0.3 (1.6)
TRI_2–ON_1	15.5 ± 2.1	4.5 ± 0.4 (3.7)
TRI_1–ON_2	9.2 ± 0.6	6.1 ± 0.3 (6.1)
ON_2–ON_1	13.1 ± 1.4	9.4 ± 0.4 (9.6)
CD_{axis}–transition angle (°)		
CD_1–ON_2 (^1B_b)	---	10 ± 6 (14)
CD_1–ON_2 (^1L_a)	---	97 ± 7 (96)
CD_2–ON_1 (^1B_b)	---	31 ± 8 (13)
CD_2–ON_1 (^1L_a)	---	72 ± 8 (81)
Binding Energy (kJmol^{-1})		
Total	−37.7 ± 24.0 (−104.9)	−175.39 ± 13.6 (−225.9)
Electrostatic	−1.6 ± 1.7 (-6.5)	−7.1 ± 1.8 (−5.8)
van der Waals	−36.2 ± 22.7 (−98.3)	−168.2 ± 13.7 (−219.1)