

Supporting Information

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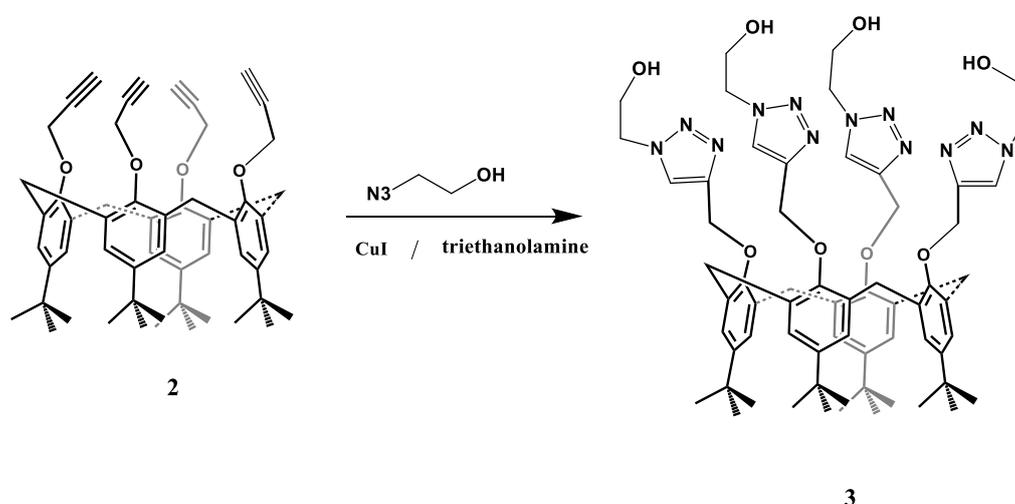
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Materials and Measurements

Deionised water passed from Millipore milli Q Plus water purification system was used for the preparation of aqueous solutions. Analytical TLC was performed on precoated silica gel plates (SiO_2 , Merck PF₂₅₄), while silica gel 60 (Merck, particle size 0.040–0.063 mm, 230–240 mesh) was used for preparative column chromatography. The analytical grade organic solvents and other reagents were commercially provided from Merck or Sigma-Aldrich and were used without any purification. Boron subphthalocyanine chloride was purchased from Sigma-Aldrich. 2-Azidoethanol was purchased from PubChem. Tebuconazole were purchased from Sigma-Aldrich.

The steady-state fluorescence excitation-emission measurements were recorded by a Varian Eclipse Spectrofluorometer and absorption properties were investigated by a Shimadzu 1800 UV-VIS Spectrophotometer. All spectral measurements were obtained at room temperature and using 1 cm path length cuvettes. The slit width of excitation and emission measurements was set as 5 nm for all fluorescence experiments. The three-dimensional (3-D) fluorescence time-resolved fluorescence measurements and excitation-emission matrix (EEM) analysis were performed using a 3-2iHR spectrofluorometer (Jobin-Yvon-SPEX, Horiba Fluorolog, France) equipped with CCD detector and signals were obtained by TCSPC (Single Photon Counting Controller module). The xenon lamp was used as the excitation source for 3D/EEM analysis. Fluorescence lifetime (τ_F) measurements were also recorded by Fluorolog 3-2iHR Spectrofluorometer equipped with a Single Photon Counting Control Module. For fluorescence lifetime (τ_F) measurements, the TCSPC module was used for signal acquisition and the NanoLed (310 nm) was used as an excitation source.

Characterizations of Compound 3



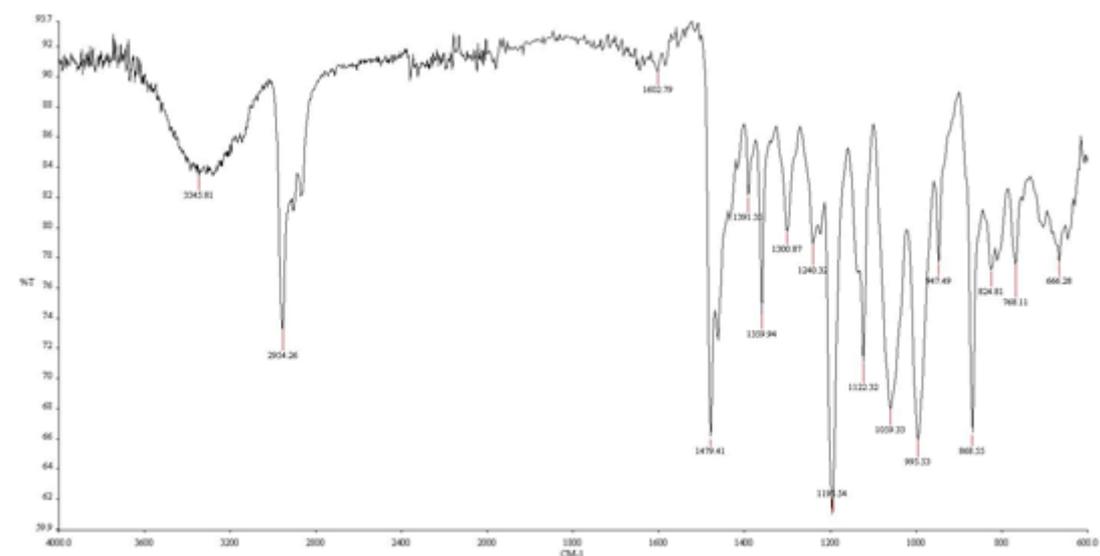


Figure S1. FT-IR Spectrum of Compound 3.

FT-IR: 3345 (OH stretching) 2954 (aromatic C–H), 2900–2854 (aliph. C–H).

FT-IR spectrum of the compound 3 showed that C≡C vibration peak at around 2117 cm^{-1} disappears (these vibrations belong to compounds 2). In addition, OH stretching at 3345 cm^{-1} , the aromatic -CH stretching at 2954 cm^{-1} , and the aliphatic -CH stretching around 2900-2854 cm^{-1} support the correctness of the structure of compound 3.

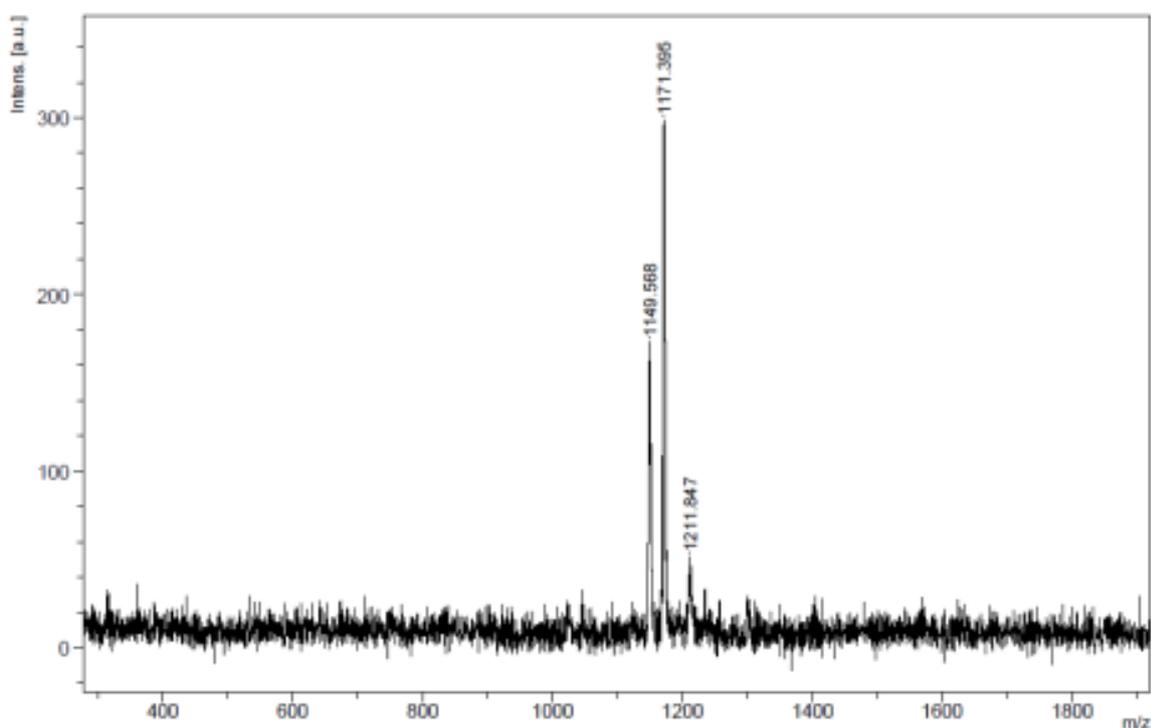


Figure S2. Mass spectrum of the compound 3.

MS (ES⁺), (m/z): Cal. for: C₆₄H₈₄O₈N₁₂, 1149.42; Found: 1149.56 [M+1]⁺, 1171.39 [M+Na]⁺ and 1211.84 [M+Cu]⁺

The mass spectrum of the compound **3** is given in Figure S2. When the spectrum is examined, it is seen that the product expected to be formed. The molecular weight was calculated as 1149.42 g/mol for C₆₄H₈₄O₈N₁₂. In the spectrum, the [M]⁺ peak was observed at 1149.56. In addition, [M+Na]⁺ peak was observed at 1171.39 and [M+Cu]⁺ peak was observed at 1211.84 m/z.

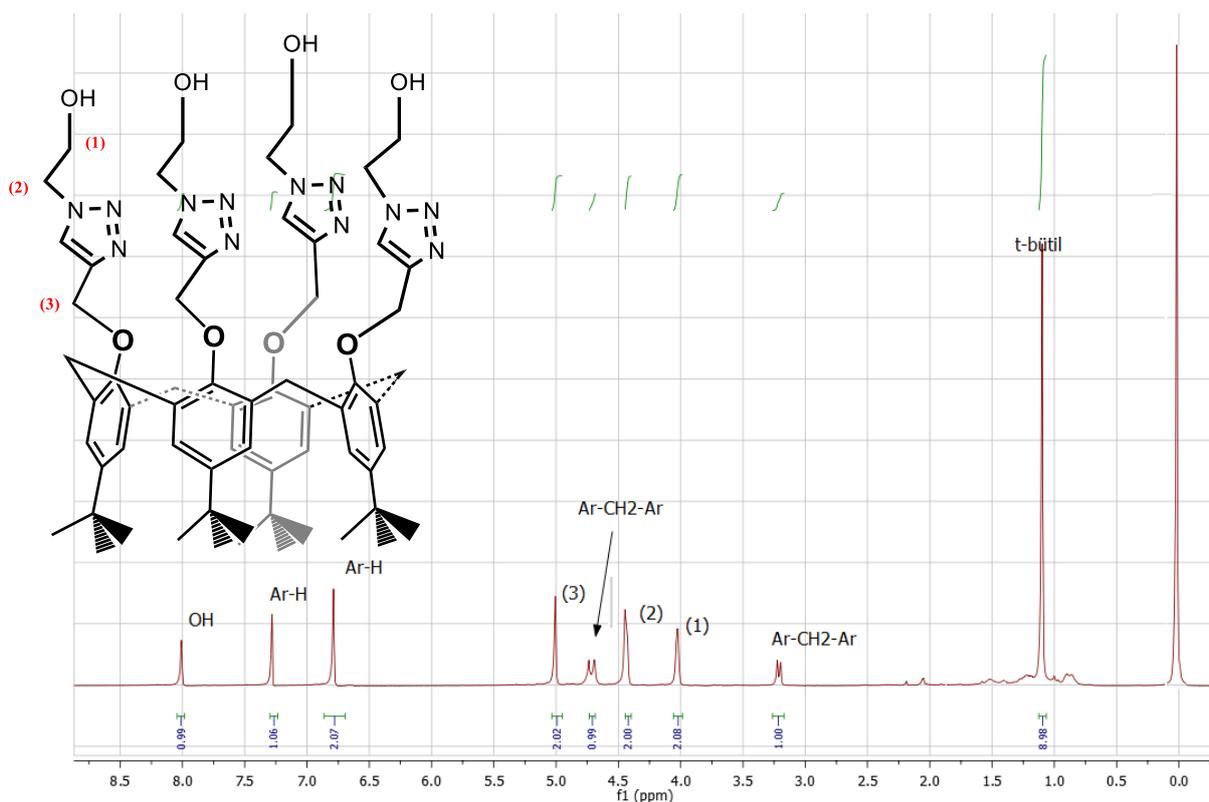


Figure S3. ¹H-NMR spectrum of the compound **3**.

¹H NMR (500 MHz; δH, ppm, DMSO-d₆): 1.08 (s, 36H, t-Bu), 3.25 (d, j:1.8 Hz, 4H, Ar-CH₂-Ar), 4.05 (m, 8H, C-H), 4.92 (m, 8H, C-H), 4.76 (d, j:2.2 Hz, 4H, Ar-CH₂-Ar), 5.02 (s, 8H, C-H), 6.80 (s, 8H, Ar-H), 7.25 (s, 4H, Ar-H), 8.02 (s, 4H, OH).

In the ¹H-NMR spectrum of the compound **3** recorded in DMSO-d₆, the signals belonging to the OH protons were observed as singlet peaks at 8.02 ppm. The signals belonging to the aromatic protons (C-CH-N) were observed as singlet peaks at 7.25 ppm and the signals belonging to the aromatic hydrogens of calixarene were observed as singlet peaks at 6.80 ppm. The peaks belonging to the protons on the carbon number 3 position were observed as singlet peaks at 5.02 ppm, and the peaks belonging to the protons on the carbon number 2 and 1 positions were observed as multiplet peaks at 4.92 and 4.05 ppm because they caused splitting

in each other's peaks. The peaks belonging to the protons on the calixarene bridging CH₂ hydrogen atoms were observed at 4.76 ppm and 3.25 ppm, in accordance with the cone conformation of calixarene. All chemical shift values (δ), coupling constants (J) and integration values observed for this compound prove the validity of the structure.

Characterizations of Calix-Sub Compound

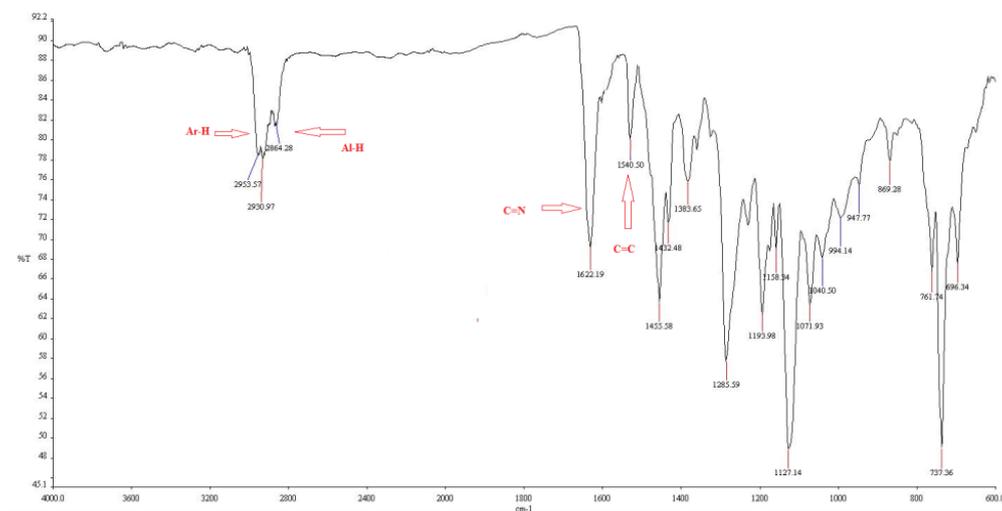


Figure S4. FT-IR Spectrum of the **Calix-Sub** Compound.

FT-IR: 2953 (aromatic. C–H), 2930–2864 (aliph. C–H), 1622 (C=N), 1540 (C=C)

In the FT-IR spectrum, the disappearance of the broad peak belonging to OH group at 3345 cm⁻¹ for compound **2**, the observation of the peak belonging to the aromatic -CH group at 2953 cm⁻¹, the aliphatic -CH group at 2864-2930 cm⁻¹, the C=N group at 1622 cm⁻¹, and the C=C group at 1540 cm⁻¹ confirmed the structure of this compound.

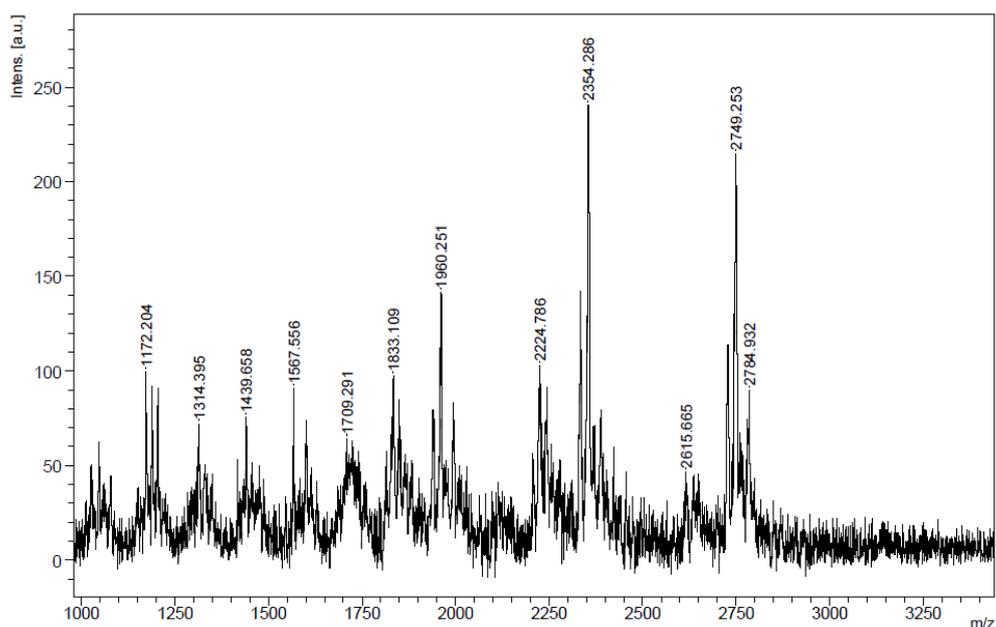
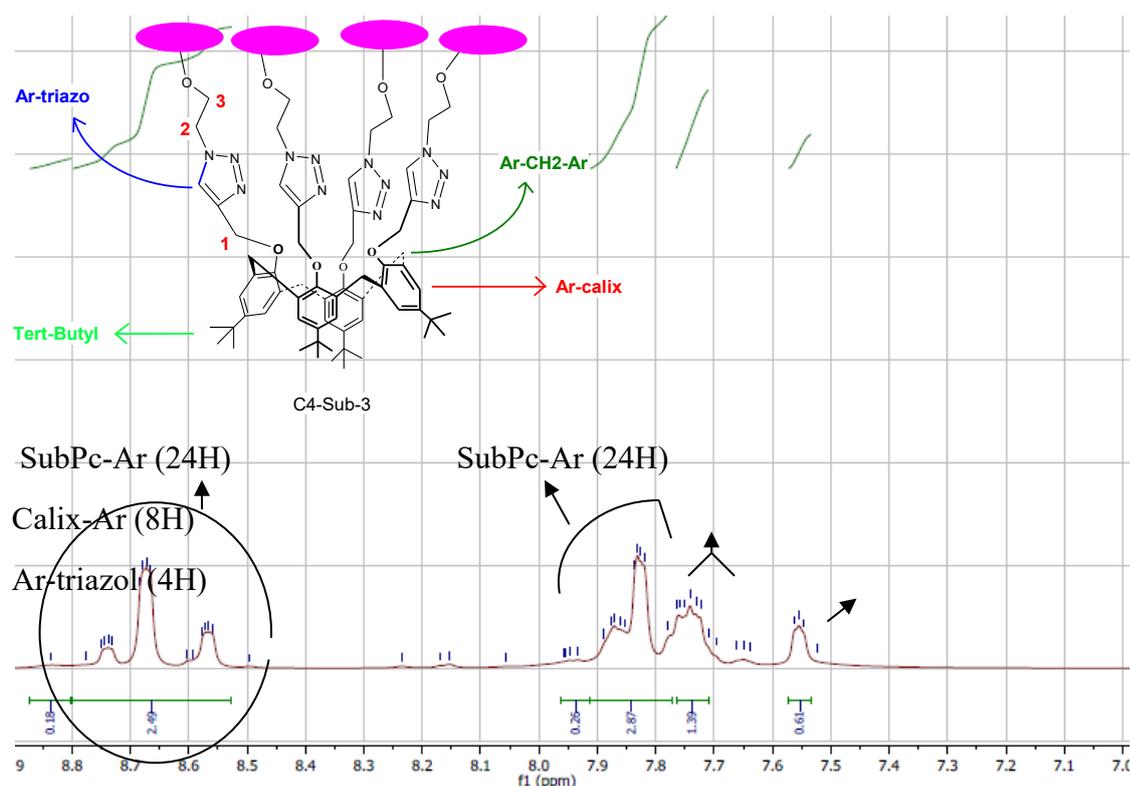


Figure S5. Mass spectrum of the **Calix-Sub** compound.

MS (ES⁺), (m/z): Cal. for: C₁₆₀H₁₂₈B₄N₃₆O₈, 2726.20; Found: 2726.24 [M]⁺, 2749.25 [M+Na]⁺ and 2784.93 [M+Cu]⁺

The mass spectrum of the compound is given in Figure S5. When the spectrum is examined, the molecular ion peaks were observed at 2726.24 m/z as [M]⁺, 2749.25 m/z as [M+Na]⁺ and 2784.93 m/z as [M+Cu]⁺ of the **Calix-Sub** compound which is in accordance the calculated molecular weight of 2726.20 g/mol for with the closed formula C₁₆₀H₁₂₈B₄N₃₆O₈. These results support the accuracy of the expected structure.



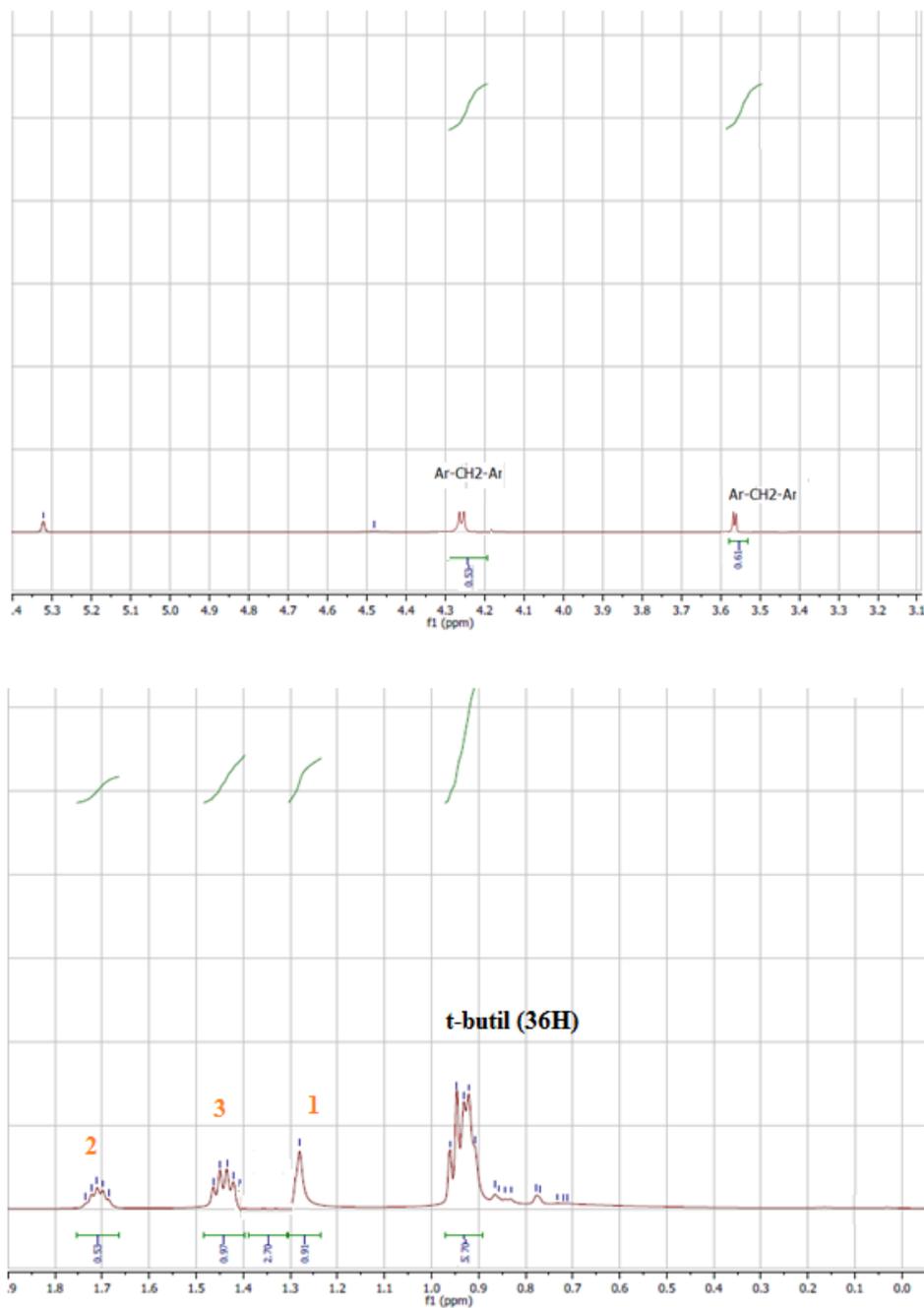


Figure S6. ¹H-NMR spectra of the **Calix-Sub** compound.

¹H NMR (500 MHz, δ H, ppm DMSO- d_6): 0.90 (s, 36H, t-butyl), 1.42 (m, 8H), 1.28 (s, 8H), 1.70 (m, 8H), 3.56 (d, j :1.6 Hz, 4H, Ar-CH₂-Ar), 4.25 (d, j :2.0 Hz, 4H, Ar-CH₂-Ar), 7.55 (s, triazole, 4H), 7.7-7.8 (Calix Ar-H, 8H), 7.8-7.9 (Sub-Pc, 24H), 8.55-8.75 (Sub-Pc, 24H).

The structure of the **Calix-Sub** compound is very huge and it has a lot of aromatic structures. Therefore, in order to better elucidate the structure, the ¹H-NMR spectra were given in parts and the H numbers are written directly on it. The protons belonging to subphthalocyanine are

found in two different regions as split from each other as expected. The aromatic protons belonging to the calixarene moiety are found at 7.7-7.8 ppm and the aromatic protons belonging to the triazole ring are found at 7.55 ppm. The bridge protons (Ar-CH₂-Ar) belonging to calixarene are found in two different regions and as doublets. This is also evidence that calixarene is in the cone conformation. All chemical shift values (δ), coupling constants (J) and integration values observed for this compound prove the correctness of the structure.