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All reagents and solvents were purchased from commercial sources and used without further purification. All solvents were dried before use according to standard literature protocols. Flash chromatography was performed on SiO₂ (0.018–0.032 mm). Thin-layer chromatography (TLC) was carried out on precoated silica gel 60 F₂₅₄ plates (Merck).

IR spectra (ATR) were recorded on a Perkin-Elmer-FT-IR 1725X spectrophotometer; ν values are given in cm⁻¹.

¹H and ¹³C NMR spectra were recorded on a Bruker Ultrashield Avance III (¹H at 500 MHz, ¹³C at 125 MHz) and Bruker Ascend 400 (400 MHz) (¹H at 400 MHz, ¹³C at 100 MHz) spectrometers using CDCl₃ as solvents and TMS as an internal standard. Chemical shifts (δ) are expressed in parts-per-million (ppm) and coupling constants (J) in Hz. The following abbreviations were used for signal multiplicities (s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, sex = sextet, m = multiplet, etc.). Homonuclear 2D (DQF-COSY and NOESY) and heteronuclear 2D ¹H-¹³C spectra (HSQC, HMBC) were recorded with the usual settings.

UV spectra were recorded with a COLO NOVEL4S UV-vis spectrophotometer.

UV spectra of thin films were recorded with a Thermo Scientific Evolution 60 UV-vis spectrophotometer.

The high-resolution MS spectra were taken with an Agilent 6210 LC ESI-MS TOF spectrometer.

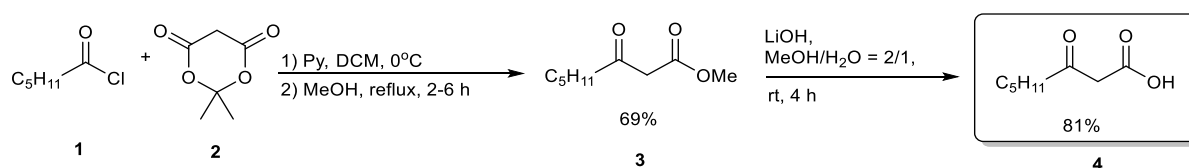
Cyclic Voltammetry and Linear sweep voltammetry measurements were recorded with METROHM Autolab PGSTAT128N, using a Glassy carbon electrode as a working electrode, Ag/AgCl as a reference electrode, and Platinum sheet electrode as a counter electrode. Tetrabutylammonium hexafluorophosphate (0.01 M) (98%, Sigma-Aldrich) was used as a supporting electrolyte.

Atomic force microscopy (AFM) was carried out using a NT-MTD, NTEGRA, microscope in tapping mode.

We deposited our compounds with Laurell WS-650MZ-23NPP spin coater.

Experimental protocols

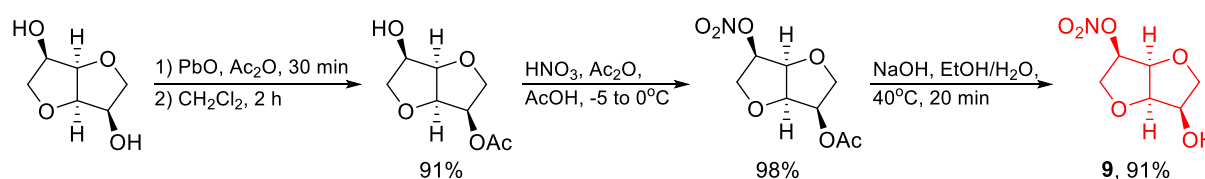
Synthesis of compound 4



Scheme S1. Synthesis of 3-oxooctanoic acid 4.

Anhydrous DCM (50 mL) was added to Meldrum's acid **2** (5.35 g, 40 mmol, 1 eq.) at 0°C under an argon atmosphere. Pyridine (6 mL, 70 mmol, 2 eq.) was added dropwise at 0°C over 20 min. Hexanoyl chloride **1** (5.2 mL, 40 mmol, 1 eq.) was added at 0°C and the mixture was left to stir for 2 h at 0°C and allowed to warm to room temperature with stirring over 1 h. The reaction mixture was diluted with 40 mL DCM and poured into 50 mL of an ice/HCl aq (2M) mixture. The resultant mixture was stirred for 10 min, the aqueous and organic phases separated, and the organic phase was washed with 80 mL HCl (2M) followed by saturated brine 80 mL. The resultant crude product material was dissolved in 140 mL methanol and heated to reflux under an argon atmosphere with stirring for 5 h. The solvent was removed under reduced pressure and the resultant product material was purified by column chromatography with petroleum ether/ethyl acetate (8:2 v/v) to give pure methyl 3-oxooctanoate **3** (4.76 g, 69%). The obtained spectra were in accordance with the reported in the literature.^[1]

Lithium hydroxide (834 mg, 34.8 mmol, 4 eq.) was added to the solution of methyl 3-oxooctanoate **3** (1.5 g, 8.7 mmol, 1 eq.) in 90 mL mixture of solvents methanol/water (2/1). The reaction mixture was stirred for 24 hours at room temperature, then solvents were evaporated under vacuum. The mixture was acidified to pH 2 using HCl, and the resulting solution was washed with ethyl acetate (3 × 30 mL) followed by washing with brine and drying over anhydrous Na₂SO₄. The solvent was evaporated under reduced pressure, and desired 3-oxooctanoic acid **4** (1.11 g, 81%) was obtained. The obtained spectra were in accordance with the reported in the literature.^[2]

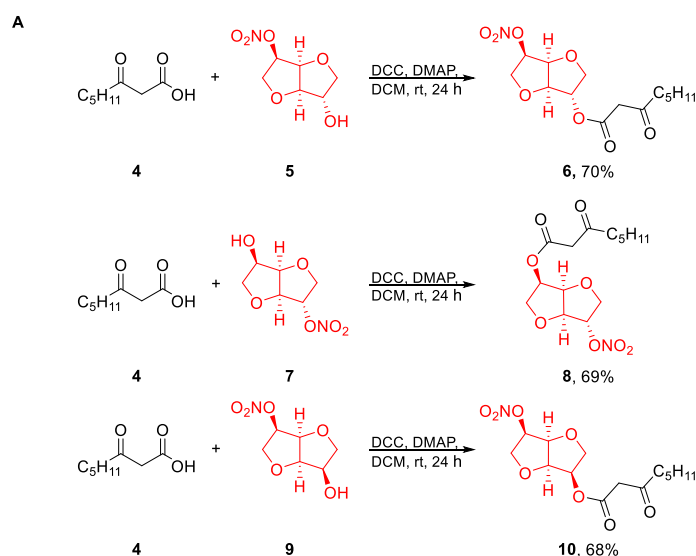


Scheme S2. Synthesis of compound 9.

To the neat isomannide (2.9 g, 20 mmol, 1 eq.) PbO (0.1 g, 0.45 mmol, 0.02 eq.) was added followed by acetic anhydride (2.5 mL, 26 mmol, 1.3 eq.). The mixture was stirred and became viscous after 30 min. Then anhydrous CH₂Cl₂ (3 mL) was added, and the mixture was stirred for a further 2 h. The mixture was concentrated in vacuo and the acetic acid was azeotropically removed with toluene under reduced pressure. Purification of the crude product by flash chromatography on silica gel (eluent: CHCl₃/MeOH, 100:0 to 95:5) afforded (3*R*,3*aR*,6*R*,6*aR*)-6-hydroxyhexahydrofuro[3,2-*b*]furan-3-yl acetate (3.4 g, 18 mmol, 91%) as a yellow oil. The obtained spectra were in accordance with the reported in the literature.³

The nitration mixture was prepared by adding 2 mL 86% fuming nitric acid in drops to a mixture of 4 mL acetic anhydride and 2 mL glacial acetic acid cooled to -5°C with vigorous stirring, the temperature was maintained at the interval of -5°C to 0°C . A 3.5 mL portion of the nitration mixture was added dropwise to a solution of (3*R*,3*aR*,6*R*,6*aR*)-6-hydroxyhexahydrofuro[3,2-*b*]furan-3-yl acetate (3.4 g, 18 mmol, 1 eq.) in 5 mL CH_2Cl_2 cooled to 0°C . The reaction mixture was left to stir for 1.5 h at 0°C to 10°C and allowed to warm to room temperature with stirring over 30 min. The remaining amount of 1.5 mL of the nitration mixture was added to the reaction mixture and stirred for 20 min. The reaction mixture was poured into 30 mL of an ice/ H_2O mixture. The resultant mixture was stirred for 10 min, the aqueous and organic phases separated, and the organic phase was washed with 30 mL saturated NaHCO_3 (aq) followed by water and saturated brine. The organic layer was dried over anhydrous Na_2SO_4 , and the solvent was removed under reduced pressure. Pure (3*R*,3*aR*,6*R*,6*aS*)-6-(nitrooxy)hexahydrofuro[3,2-*b*]furan-3-yl acetate (4.1 g, 13 mmol, 98%) was obtained.

The solution of NaOH (0.35 g, 8.8 mmol, 0.7 eq.) in 1.8 mL mixture of solvents ethanol/water (1/5) was added to solution of (3*R*,3*aR*,6*R*,6*aS*)-6-(nitrooxy)hexahydrofuro[3,2-*b*]furan-3-yl acetate (4.1 g, 13 mmol, 1 eq.) in 10 mL EtOH heated to 40°C . The ethanol solution was stirred for 20 min at 40°C . The reaction mixture was cooled to room temperature and extracted with CH_2Cl_2 (3 x 10 mL). The organic extracts were combined, dried over anhydrous Na_2SO_4 , evaporated and purified by column chromatography using ethyl acetate and petroleum ether to give (3*R*,3*aS*,6*R*,6*aR*)-6-hydroxyhexahydrofuro[3,2-*b*]furan-3-yl nitrate **9** (2.2 g, 11.8 mmol, 91%) as a white solid. The obtained spectra were in accordance with the reported in the literature.⁴



Scheme S3. Synthesis of β -keto ester-isohexide mononitrate derivatives **6**, **8**, **10**

Synthesis of compounds 6, 8, 10

N,N' -dicyclohexylcarbodiimide (DCC) (780 mg, 3.78 mmol, 1.5 eq.) and 4-dimethylaminopyridine (DMAP) (43 mg, 0.35 mmol) were added to the solution of 3-oxooctanoic acid **4** (400 mg, 2.52 mmol, 1 eq.) in 50 mL DCM and the mixture was left to stir for 5 min at 0°C . The appropriate isohexide (1,4:3,6-dianhydrohexitol) mononitrate **5**, **7**, **9** (482 mg, 2.52 mmol, 1 eq.) was added to the reaction mixture and stirring was continued for 24 h at room temperature. After the reaction was completed, the solvent was evaporated by increasing the temperature under reduced pressure. The residue was

dissolved in 50 mL of ethyl acetate and filtered under reduced pressure to remove the dicyclohexylurea (DCU). The filtrate was concentrated, and the crude product was chromatographed on a silica gel column with petroleum ether/ethyl acetate (7: 3 v/v) to give pure β -keto ester-isohexide mononitrate derivate **6**, **8**, **10**.

(3S,3aR,6R,6aS)-6-(nitrooxy)hexahydrofuro[3,2-b]furan-3-yl 3-oxooctanoate (6): 584 mg, 70%, white crystalline solid; ^1H NMR (500 MHz, CDCl_3): δ 11.84 (bs, 1H enol-OH), 5.35 (td, $J_1 = 5.5$ Hz, $J_2 = 2.8$ Hz, **C5-1H**), 5.28 (d, $J = 2.8$ Hz, **C2-1H**), 4.98 (s, 1H enol), 4.97 (t, $J = 5.2$ Hz, **C4-1H**), 4.53 (d, $J = 4.9$ Hz, **C3-1H**), 4.07 – 3.98 (m, **C1-2H**, **C6-1H**), 3.91 (dd, $J_1 = 11.3$ Hz, $J_2 = 5.5$ Hz, **C6-1H**), 3.47 (d (ABq), $J = 10.3$ Hz, 2H), 2.49 (t, $J = 7.4$ Hz, 2H), 2.19 (t, $J = 7.6$ Hz, 2H enol), 1.63 – 1.54 (m, 2H), 1.35 – 1.23 (m, 4H), 0.89 (t, $J = 7.0$ Hz, 3H) ppm; ^{13}C NMR (125 MHz, CDCl_3): δ 202.6 (keto) and 180.8 (enol), 170.8 (enol) and 166.5 (keto), 88.5 (enol), 86.9 (enol) and 86.6 (keto), 81.7, 81.4, 78.2, 73.7 (enol) and 73.4 (keto), 69.5 (keto) and 69.4 (enol), 49.0 (keto), 43.3 (keto) and 35.2 (enol), 31.33 (enol) and 31.27 (keto), 26.0 (enol) and 23.2 (keto), 22.5, 14.0 ppm; IR (ATR): ν 2958, 2934, 2874, 1750, 1716, 1644, 1283, 1099, 854 cm^{-1} ; $[\alpha]_{589}^{20} = 180^\circ$, t.t. 39.9-42.6°C, Elem. Anal. (calculated): C 50.75, H 6.39, N 4.23 %; Elem. Anal. (found): C 50.88, H 6.39, N 4.25 %.

(3R,3aR,6S,6aS)-6-(nitrooxy)hexahydrofuro[3,2-b]furan-3-yl 3-oxooctanoate (8): 576 mg, 69%, colorless oil; ^1H NMR (500 MHz, CDCl_3): δ 11.82 (bs, 1H enol-OH), 5.36 (d, $J = 2.6$ Hz, **C2-1H**), 5.25 – 5.20 (m, **C5-1H**), 5.05 (s, 1H enol), 4.86 (dd, $J_1 = 5.2$ Hz, $J_2 = 5.1$ Hz, **C4-1H**), 4.60 (d, $J = 5.0$ Hz, 1H enol), 4.58 (d, $J = 5.0$ Hz, **C3-1H**), 4.13 – 4.04 (m, **C1-2H**), 3.98 (dd, $J_1 = 10.2$ Hz, $J_2 = 5.9$ Hz, **C6-1H**), 3.87 (dd, $J_1 = 10.2$ Hz, $J_2 = 4.9$ Hz, **C6-1H**), 3.50 (d (ABq), $J = 4.9$ Hz, 2H), 2.55 (t, $J = 7.4$ Hz, 2H), 2.52 (t, $J = 7.6$ Hz, 2H enol), 1.62 – 1.56 (m, 2H), 1.35 – 1.24 (m, 4H), 0.88 (t, $J = 7.0$ Hz, 3H) ppm; ^{13}C NMR (125 MHz, CDCl_3): δ 202.4 (keto) and 180.7 (enol), 169.3 (enol) and 166.6 (keto), 88.3 (enol), 86.1, 84.6, 81.3 (enol) and 80.9 (keto), 74.5 (keto) and 73.2 (enol), 71.8 (enol) and 71.7 (keto), 70.80 (enol) and 70.76 (keto), 49.0 (keto), 43.1 (keto) and 35.3 (enol), 31.34 (enol) and 31.28 (keto), 26.0 (enol) and 23.2 (keto), 22.51 (keto) and 22.47 (enol), 14.0 ppm; IR (ATR): ν 3647, 2957, 2933, 2872, 1749, 1716, 1642, 1276, 1097, 856 cm^{-1} ; $[\alpha]_{589}^{20} = 87^\circ$; Elem. Anal. (calculated): C 50.75, H 6.39, N 4.23 %; Elem. Anal. (found): C 50.48, H 6.63, N 4.25 %.

(3R,3aR,6R,6aS)-6-(nitrooxy)hexahydrofuro[3,2-b]furan-3-yl 3-oxooctanoate (10): 568 mg, 68%, colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 11.79 (bs, 1H enol-OH), 5.34 – 5.29 (m, **C5-1H**), 5.14 – 5.07 (m, **C2-1H**), 5.06 (s, 1H enol), 4.86 (t, $J = 5.5$ Hz, **C4-1H**), 4.72 (t, $J = 5.3$ Hz, **C3-1H**), 4.12 (dd, $J_1 = 9.2$ Hz, $J_2 = 6.8$ Hz, **C1-1H**), 4.04 – 3.95 (m, **C6-2H**), 3.82 (t, $J = 8.6$ Hz, **C1-1H**), 3.50 (s, 2H), 2.54 (t, $J = 7.4$ Hz, 2H), 2.20 (t, $J = 7.6$ Hz, 2H enol), 1.63 – 1.55 (m, 2H), 1.36 – 1.21 (m, 4H), 0.88 (t, $J = 7.0$ Hz, 3H) ppm; ^{13}C NMR (101 MHz, CDCl_3): δ 202.3 (keto) and 180.7 (enol), 171.8 (enol) and 166.7 (keto), 88.3 (enol), 81.19 (enol) and 81.15 (keto), 81.02 (keto) and 81.00 (enol), 80.6, 73.8 (keto) and 72.6 (enol), 70.2, 69.63 (enol) and 69.55 (keto), 49.0 (keto), 43.1 (keto) and 35.2 (enol), 31.32 (enol) and 31.27 (keto), 26.0 (enol) and 23.2 (keto), 22.51 (keto) and 22.47 (enol), 14.03 (enol) and 14.01 (keto) ppm; IR (ATR): ν 2958, 2933, 2872, 1749, 1717, 1644, 1283, 1046, 856 cm^{-1} ; $[\alpha]_{589}^{20} = 163^\circ$; Elem. Anal. (calculated): C 50.75, H 6.39, N 4.23 %; Elem. Anal. (found): C 51.15, H 6.63, N 4.42 %.

Preparation of furan-fused fullerenes (13, 14, 15): DBU (40 μL , 0.26 mmol, 20 eq.) was added to the solution of C_{60} **11** (15 mg, 0.02 mmol, 1.5 eq.), β -keto ester-isohexide mononitrate derivate **6**, **8**, **10** (4.3 mg, 0.013 mmol, 1 eq.) and TEMPO (4.1 mg, 0.026 mmol, 2 eq.) in toluene (15 mL). The reaction mixture was stirred for 45 min at room temperature, under an argon atmosphere. After the reaction was completed, the reaction mixture was filtrated through a silica gel pad and washed with toluene. The solvent was removed under reduced pressure, and the residue was chromatographed on a silica

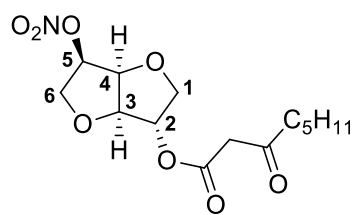
gel column with petrol ether as eluent, to recover unreacted C₆₀. Further elution with toluene/petroleum ether (7: 3 v/v, 5:5 v/v) and pure toluene gave pure product **13**, **14**, **15**.

Compound 13: 6.7 mg, 49%, brown solid; ¹H NMR (500 MHz, CDCl₃): δ 5.54 – 5.50 (m, **C2**-1H), 5.34 – 5.29 (m, **C5**-1H), 4.75 (t, *J* = 5.1 Hz, **C4**-1H), 4.52 (d, *J* = 4.2 Hz, **C3**-1H), 4.15 – 4.10 (m, **C1**-1H), 4.07 – 4.00 (m, **C1**-1H, **C6**-1H), 3.88 (dd, *J*₁ = 11.2 Hz, *J*₂ = 5.5 Hz, **C6**-1H), 3.28 (t, 2H, *J* = 6.5 Hz), 2.07 (quin, 2H, *J* = 7.2 Hz), 1.66 (quin, 2H, *J* = 7.3 Hz), 1.59 – 1.52 (m, 2H), 1.04 (t, 3H, *J* = 7.1 Hz) ppm; ¹³C NMR (125 MHz, CDCl₃): δ 175.2, 163.6, 148.4, 148.32, 148.31, 147.6, 147.2, 147.1, 146.7, 146.45, 146.41, 146.3, 146.2, 145.8, 145.7, 145.6, 145.44, 145.41, 145.28, 145.26, 144.9 (**2C**), 144.7, 144.5, 144.41, 144.36, 143.0, 142.9, 142.7 (**2C**), 142.65, 142.60, 142.5, 141.8, 141.7, 141.64, 141.62, 140.1, 139.54, 139.46, 137.7, 137.6, 135.61, 135.59, 104.3, 103.4 (*sp*³-C of C₆₀), 86.7, 81.9, 81.4, 77.4, 73.8, 72.0 (*sp*³-C of C₆₀), 69.5, 31.9, 29.3, 27.1, 22.7, 14.3 ppm; IR (ATR): ν 2956, 2929, 2869, 1706, 1644, 1542, 1460, 1280, 1123, 1101, 975, 848, 739, 528 cm⁻¹; UV-vis (CHCl₃): λ 429, 457, 483, 687 nm (ε = 2186, 1754, 1424, 130 dm³ mol⁻¹ cm⁻¹); Positive ESI FT-ICR MS: calcd for [M + Na]⁺ (C₇₄H₁₉NO₈Na)⁺: 1072.1003; found, 1072.0996.

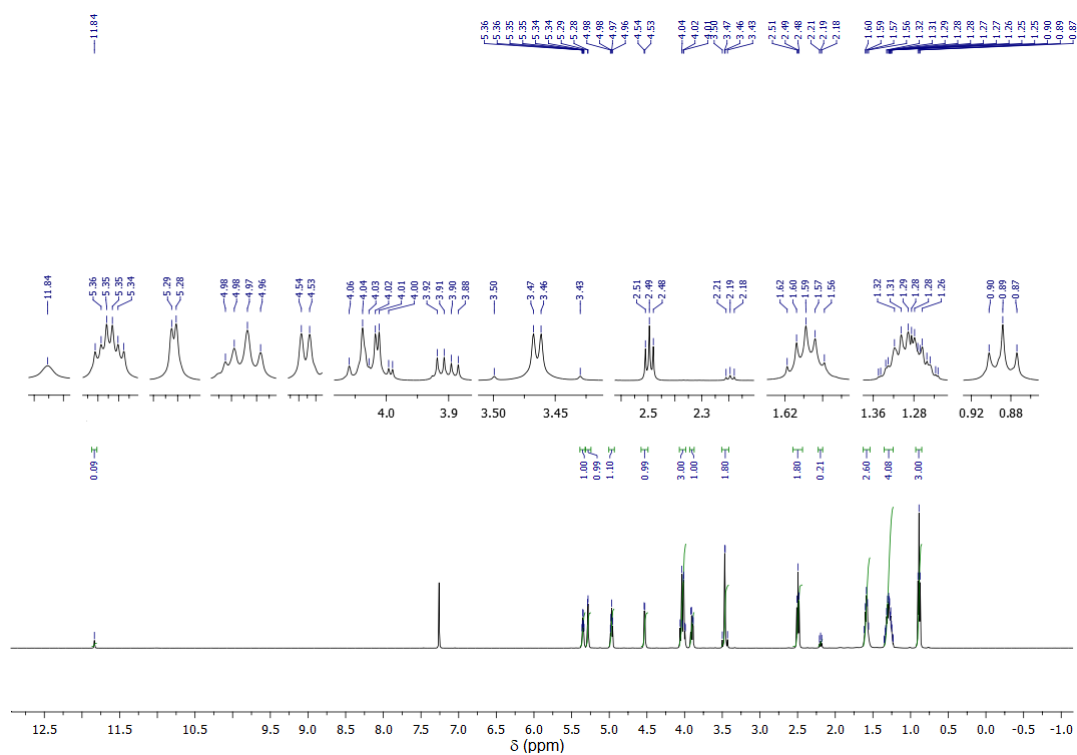
Compound 14: 6.7 mg, 49%, brown solid; ¹H NMR (500 MHz, CDCl₃): δ 5.40 (dd, *J*₁ = 11.8 Hz, *J*₂ = 6.2 Hz, **C5**-1H), 5.31 (d, *J* = 3.7 Hz, **C2**-1H), 4.93 (t, *J* = 5.0 Hz, **C4**-1H), 4.62 (d, *J* = 4.6 Hz, **C3**-1H), 4.06 (m, 2H), 3.96 (dd, *J*₁ = 11.4 Hz, *J*₂ = 4.0 Hz, **C1**-1H), 3.75 (dd, *J*₁ = 9.6 Hz, *J*₂ = 6.2 Hz, **C6**-1H), 3.39 – 3.27 (m, 2H), 2.13 – 2.05 (m, 2H), 1.70 – 1.64 (m, 2H), 1.59 – 1.51 (m, 2H), 1.04 (t, *J* = 7.3 Hz, 3H) ppm; ¹³C NMR (125 MHz, CDCl₃): δ 175.1, 164.0, 148.50, 148.48, 148.3, 147.6, 147.5, 147.3, 146.7, 146.5, 146.4, 146.3, 146.2, 145.9, 145.6, 145.5, 145.4 (**2C**), 145.3 (**2C**), 145.0, 144.9, 144.7, 144.5 (**3C**), 143.03, 142.95, 142.8, 142.7, 142.62, 142.55, 142.5, 141.8, 141.77, 141.7 (**2C**), 140.1, 139.6, 139.4, 137.7 (**2C**), 135.7, 135.6, 104.2, 103.4 (*sp*³-C of C₆₀), 86.3, 84.6, 81.1, 74.0, 72.1 (*sp*³-C of C₆₀), 71.5, 70.3, 31.9, 29.3, 27.1, 22.7, 14.3 ppm; IR (ATR): ν 2954, 2927, 2867, 1707, 1641, 1541, 1461, 1273, 1128, 1087, 971, 848, 746, 528 cm⁻¹; UV-vis (CHCl₃): λ 429, 457, 483, 687 nm (ε = 1955, 1624, 1376, 150 dm³ mol⁻¹ cm⁻¹). Positive HRMS (ESI): calcd for [M]⁺ (C₇₄H₁₉O₈N)⁺: 1049.11107; found, 1049.11542.

Compound 15: 8.2 mg, 60%, brown solid; ¹H NMR (500 MHz, CDCl₃): δ 5.37 – 5.29 (m, **C5**-1H, **C2**-1H), 4.91 (t, *J* = 5.3 Hz, **C4**-1H), 4.79 (t, *J* = 5.2 Hz, **C3**-1H), 4.19 (dd, *J*₁ = 8.7 Hz, *J*₂ = 7.1 Hz, **C1**-1H), 4.00 (dd, *J*₁ = 10.8 Hz, *J*₂ = 6.0 Hz, **C6**-1H), 3.91 (dd, *J*₁ = 10.8 Hz, *J*₂ = 4.3 Hz, **C6**-1H), 3.79 (t, *J* = 8.8 Hz, **C1**-1H), 3.31 (dd, *J*₁ = 8.5 Hz, *J*₂ = 6.6 Hz, 2H), 2.14 – 2.04 (m, 2H), 1.70 – 1.63 (m, 2H), 1.60 – 1.48 (m, 2H), 1.04 (t, *J* = 7.3 Hz, 3H) ppm; ¹³C NMR (125 MHz, CDCl₃): δ 175.0, 164.1, 148.5, 148.4, 148.3, 147.6, 147.4, 147.3, 146.7, 146.45, 146.38, 146.3, 146.2, 145.9, 145.65, 145.61, 145.4, 145.3, 144.98, 144.96, 144.8, 144.7, 144.5, 144.44, 144.43, 143.0, 142.9, 142.71, 142.68, 142.52, 142.48, 141.9, 141.8, 141.68, 141.66, 141.6, 140.1, 139.72, 139.67, 139.62, 139.57, 137.7, 135.6, 135.5, 104.2, 103.4 (*sp*³-C of C₆₀), 81.42, 81.35, 80.8, 73.3, 71.9 (*sp*³-C of C₆₀), 70.0, 69.5, 32.0, 29.4, 27.2, 22.7, 14.3 ppm. IR (ATR): ν 2956, 2927, 2867, 1706, 1644, 1462, 1430, 1280, 1130, 1044, 974, 852, 738, 528 cm⁻¹; UV-vis (CHCl₃): λ 429, 457, 483, 687 nm (ε = 2172, 1772, 1444, 128 dm³ mol⁻¹ cm⁻¹); Positive HRMS (ESI): calcd for [M]⁺ (C₇₄H₁₉O₈N)⁺: 1049.11107; found, 1049.11653.

NMR, UV / Vis and FTIR spectra



Compound 6:



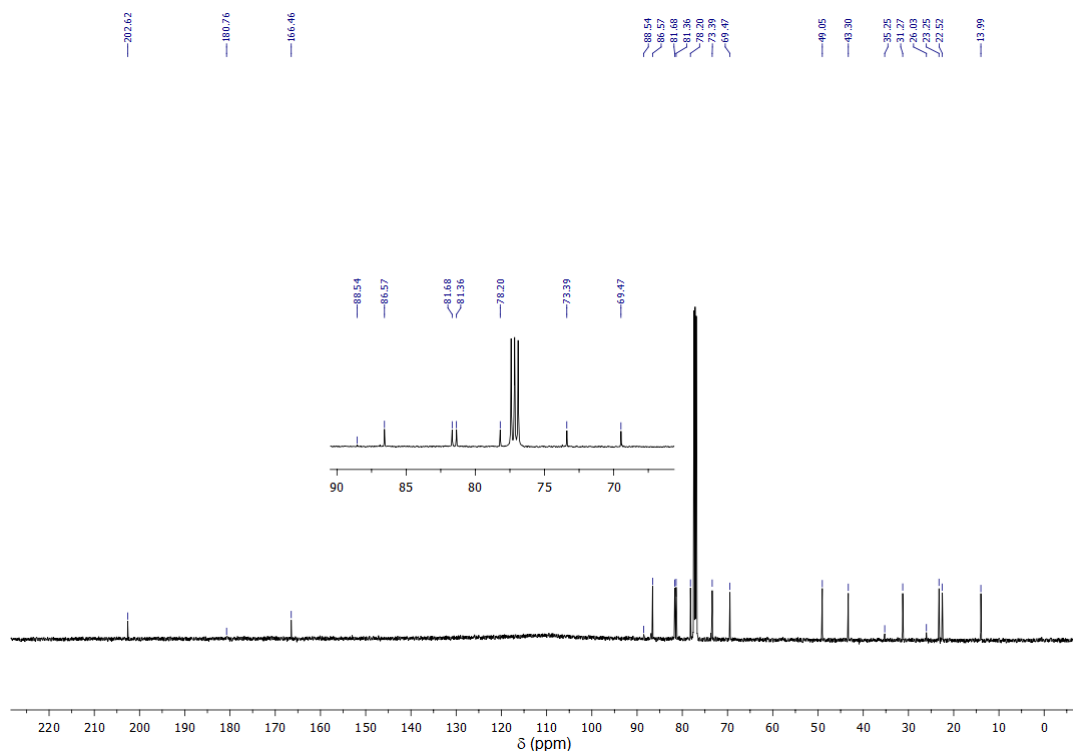


Figure S2. ^{13}C NMR spectrum (125 MHz) of **6** in CDCl_3 .

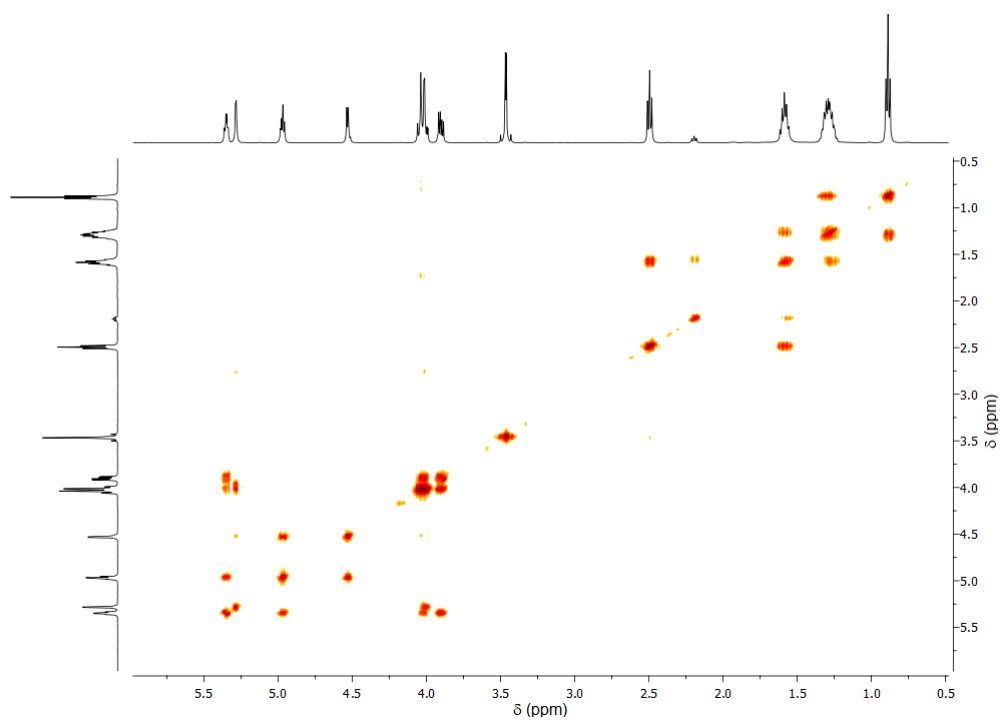


Figure S3. COSY spectrum of **6** in CDCl_3 .

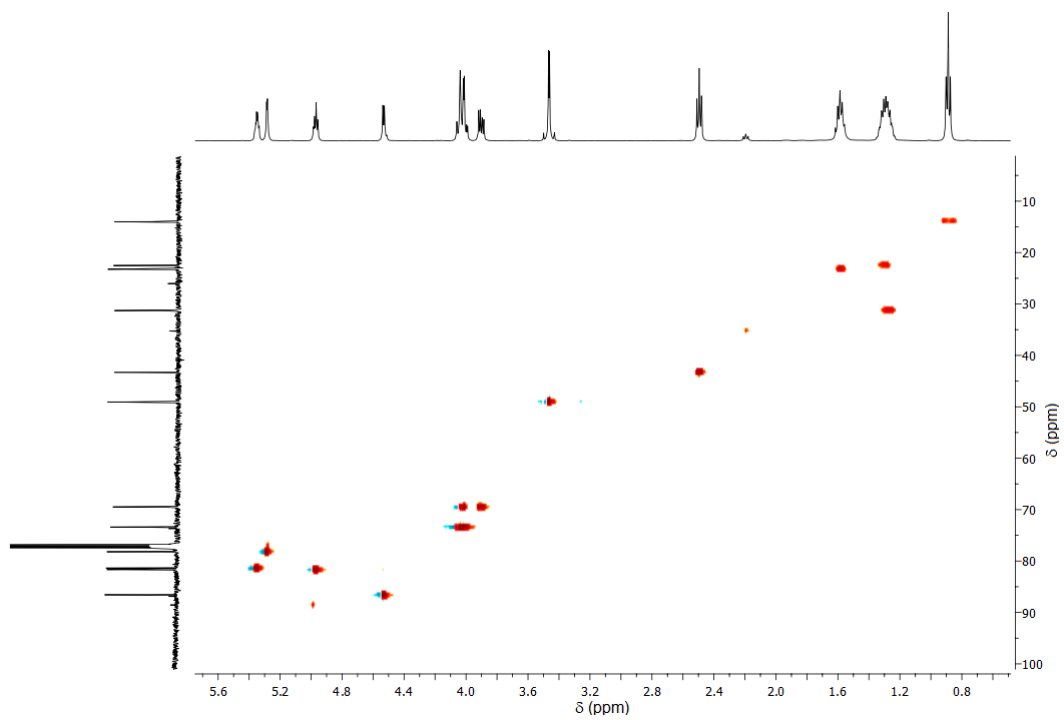


Figure S4. HSQC spectrum of **6** in CDCl₃.

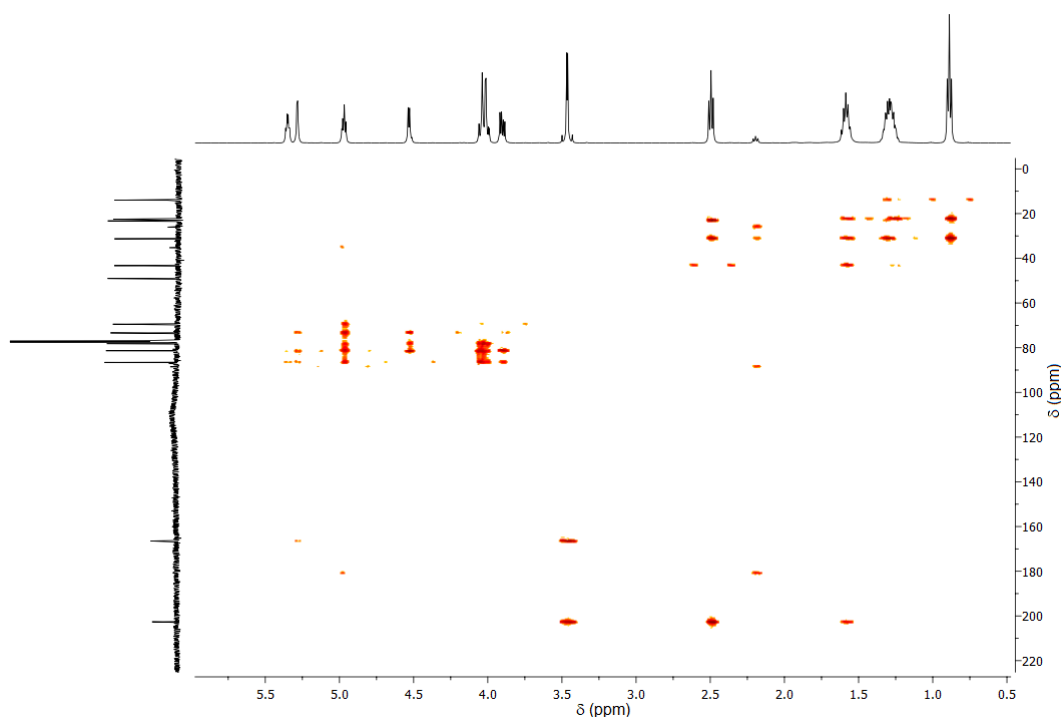


Figure S5. HMBC spectrum of **6** in CDCl₃.

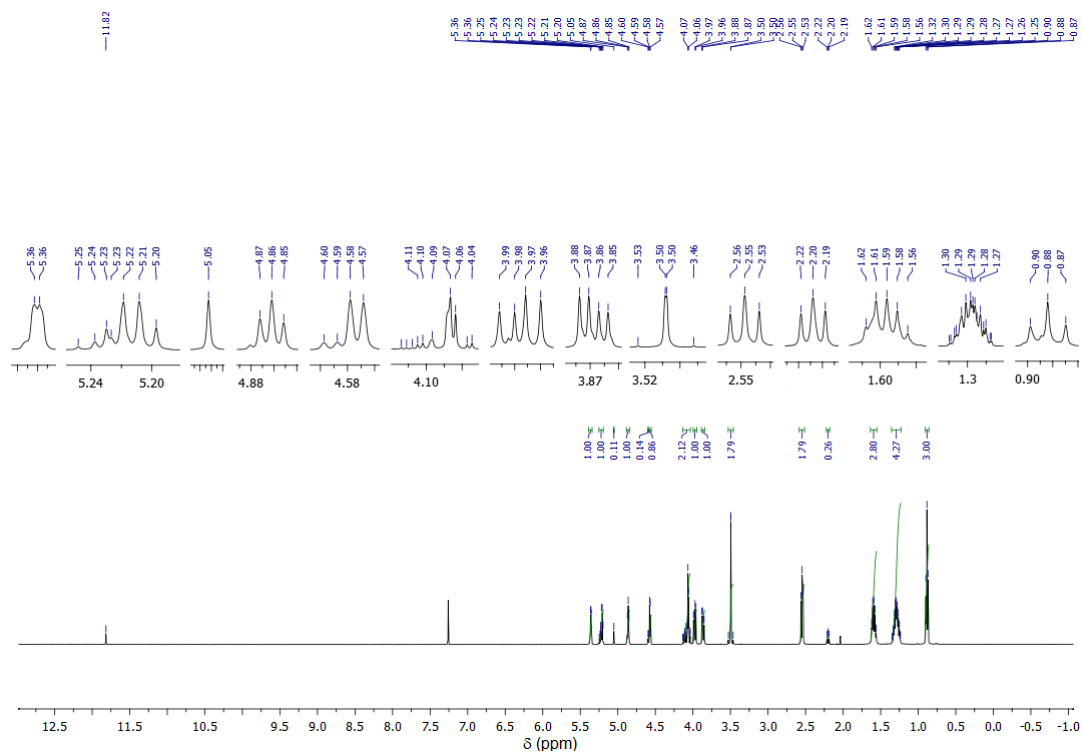
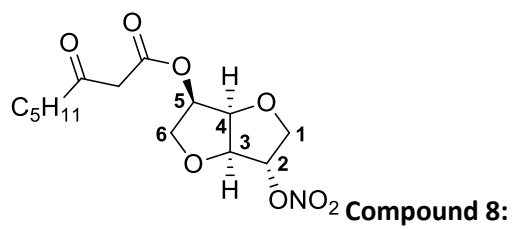


Figure S6. ^1H NMR spectrum (500 MHz) of **8** in CDCl_3 .

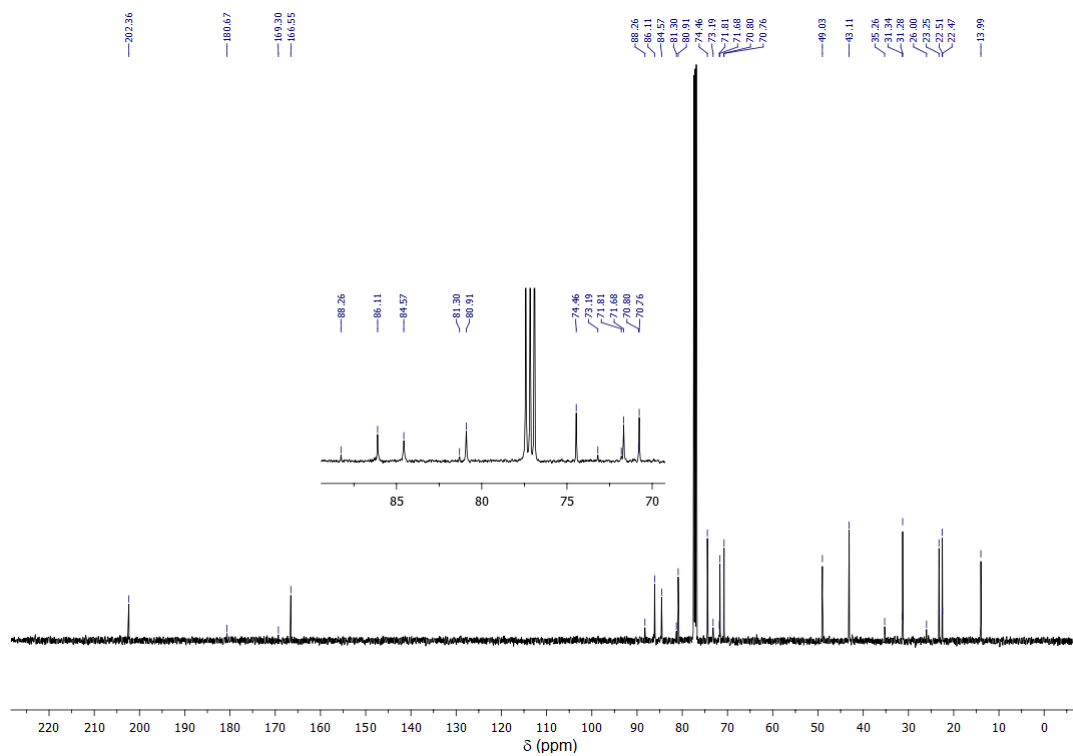


Figure S7. ^{13}C NMR spectrum (125 MHz) of **8** in CDCl_3 .

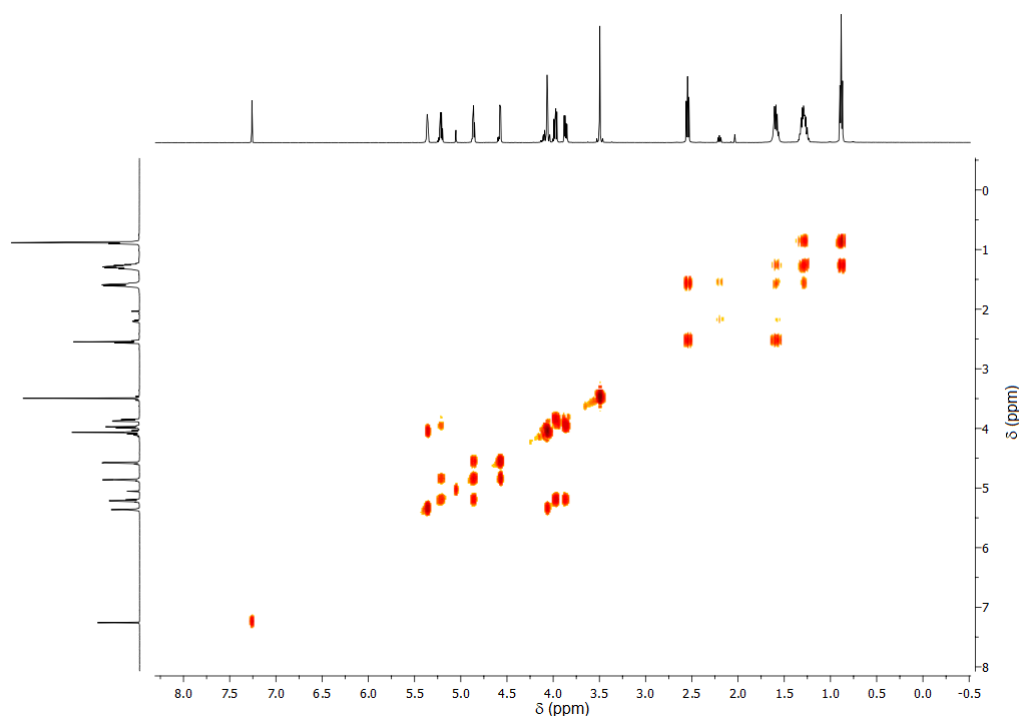


Figure S8. The COSY spectrum of **8** in CDCl_3 .

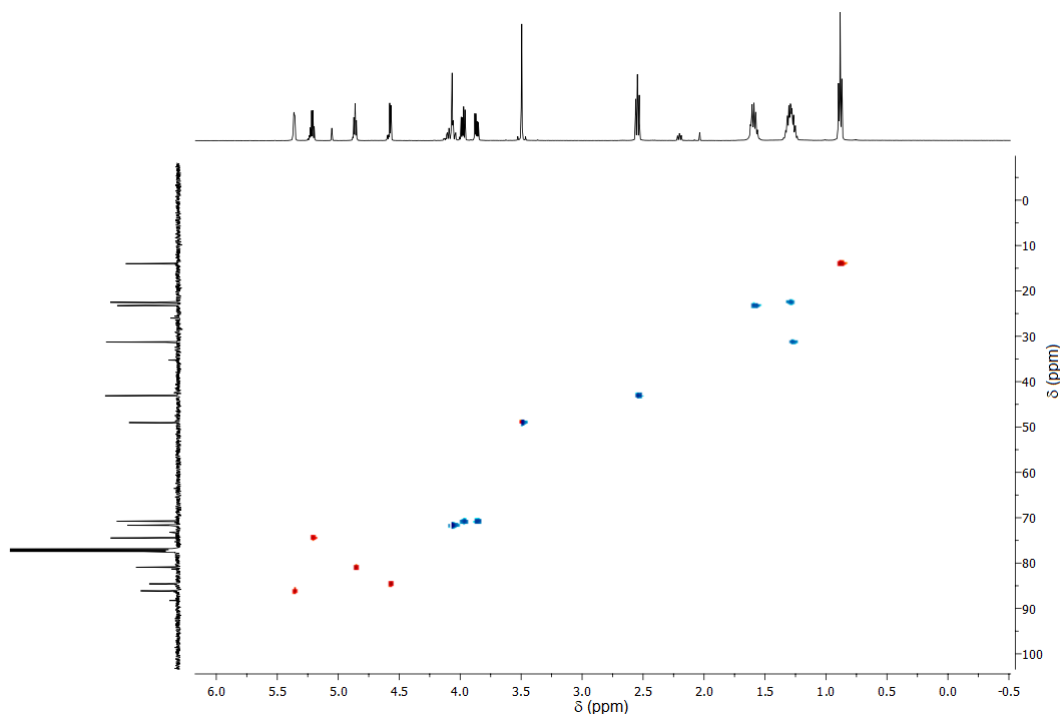


Figure S9. HSQC spectrum of **8** in CDCl₃.

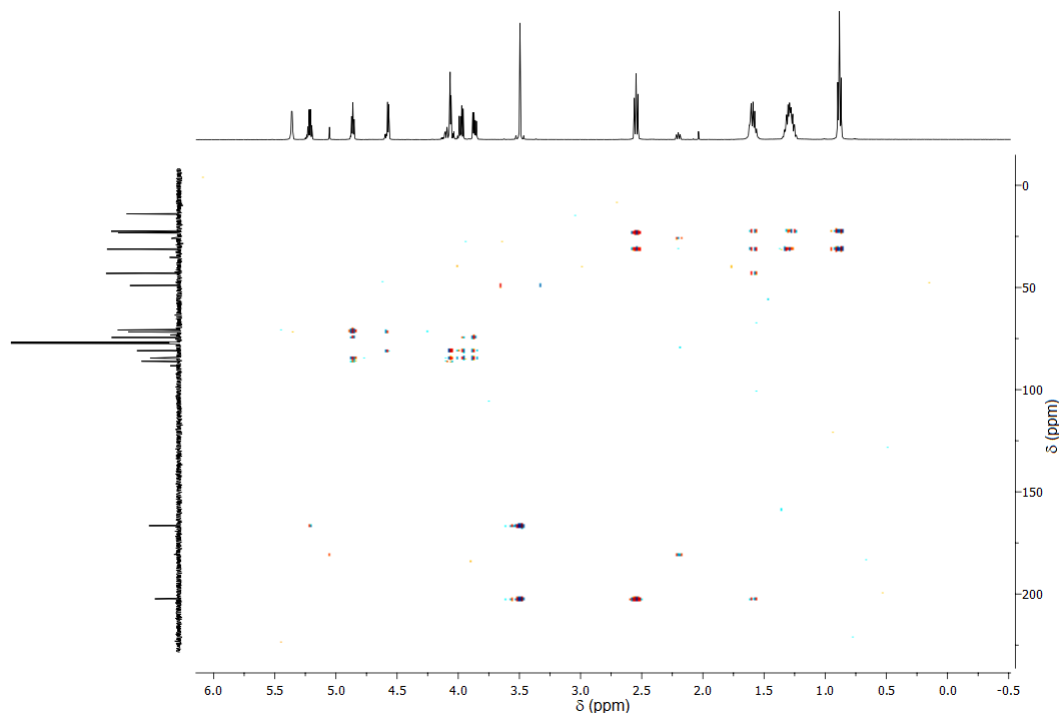
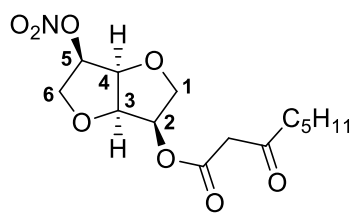


Figure S10. HMBC spectrum of **8** in CDCl₃.



Compound 10:

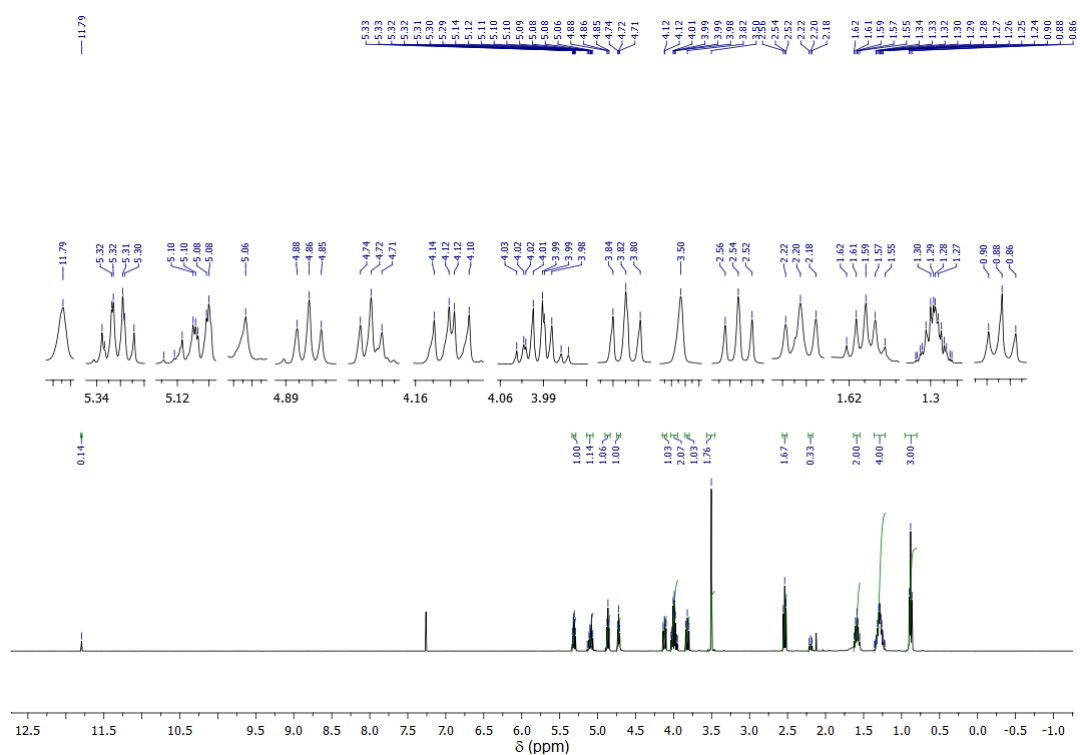


Figure S11. ^1H NMR spectrum (400 MHz) of **10** in CDCl_3 .

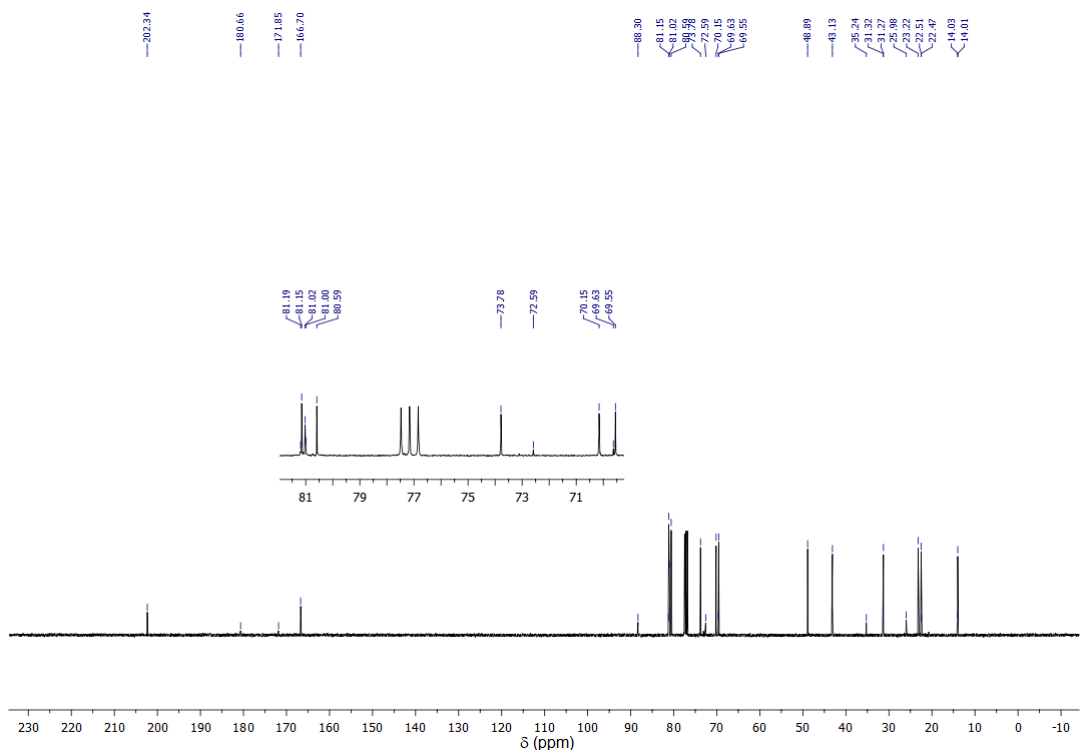


Figure S12. ^{13}C NMR spectrum (100 MHz) of **10** in CDCl_3 .

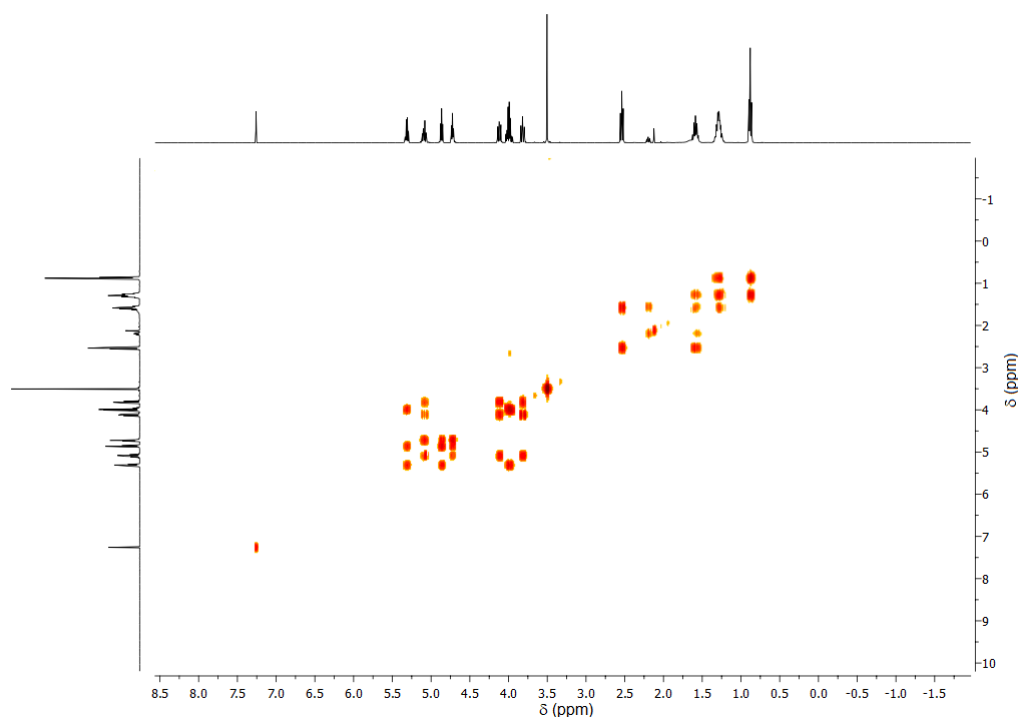


Figure S13. The COSY spectrum of **10** in CDCl_3 .

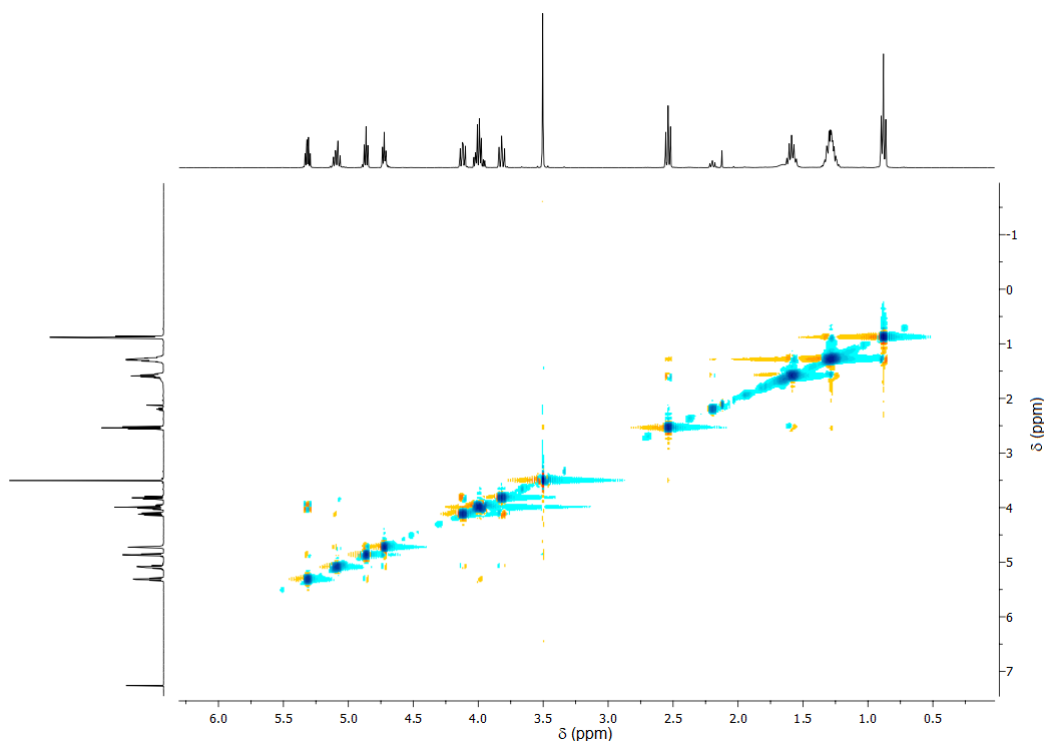


Figure S14. NOESY spectrum of **10** in CDCl_3 .

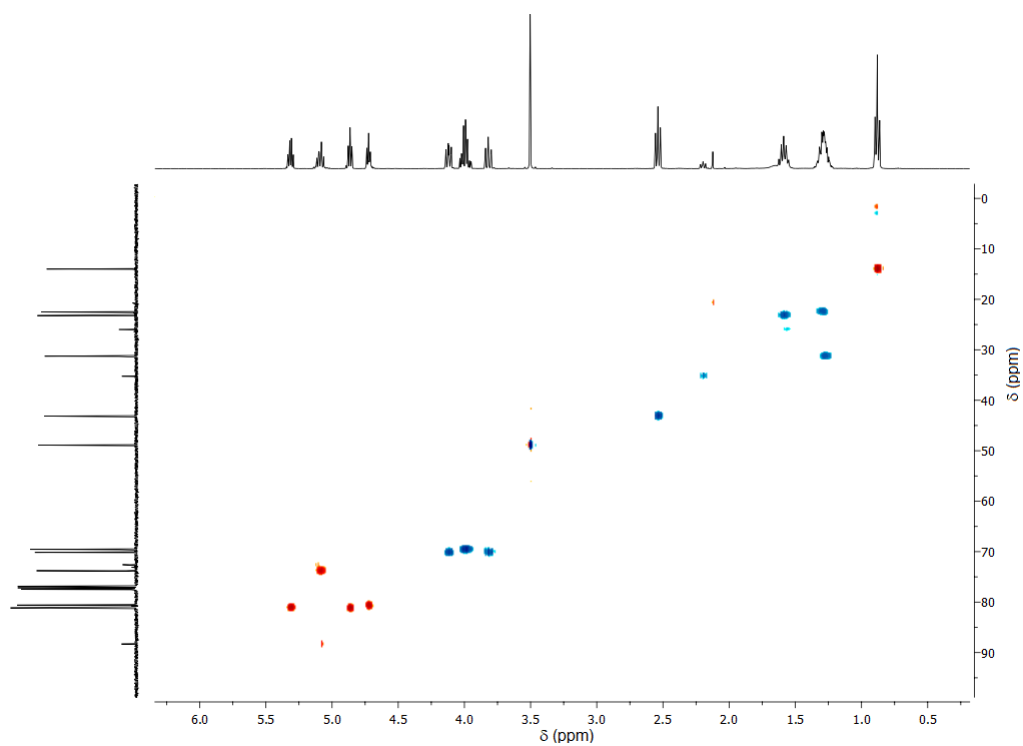


Figure S15. HSQC spectrum of **10** in CDCl_3 .

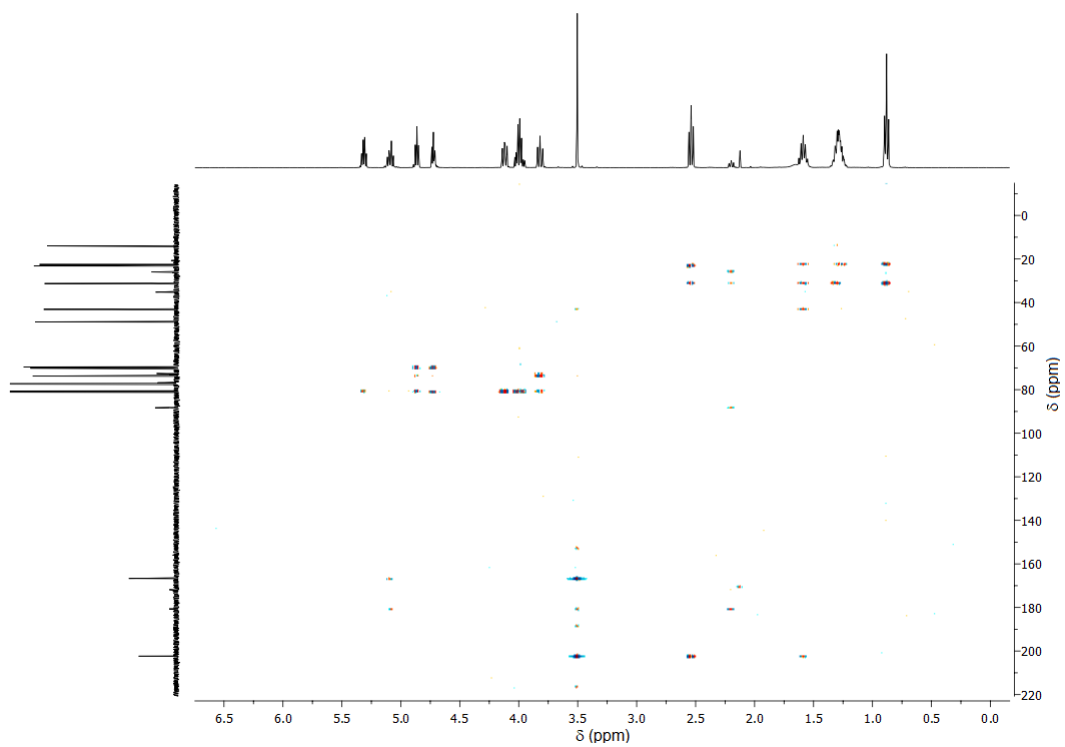
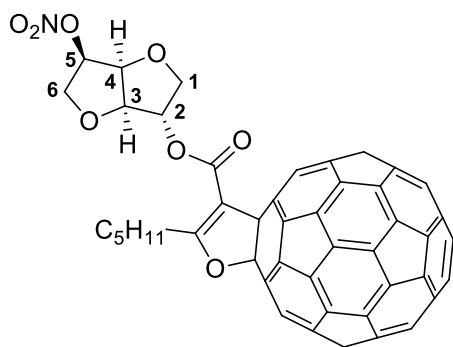


Figure S16. HMBC spectrum of **10** in CDCl_3 .



Compound 1

3:

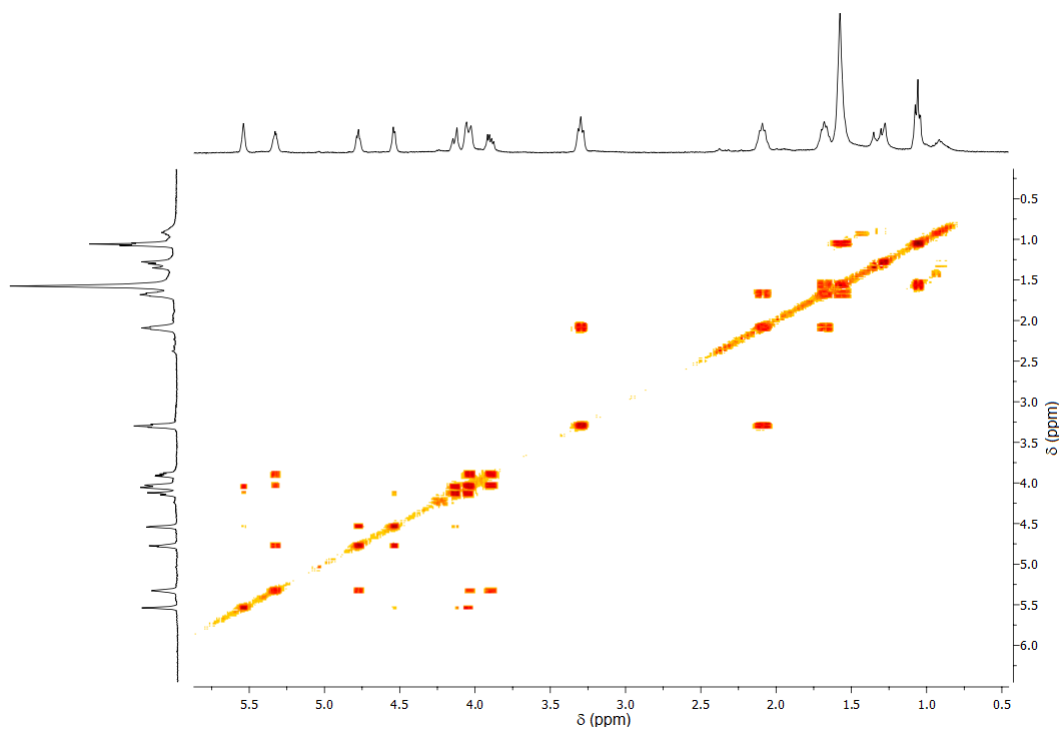


Figure S19. COSY spectrum of **13** in CDCl_3 .

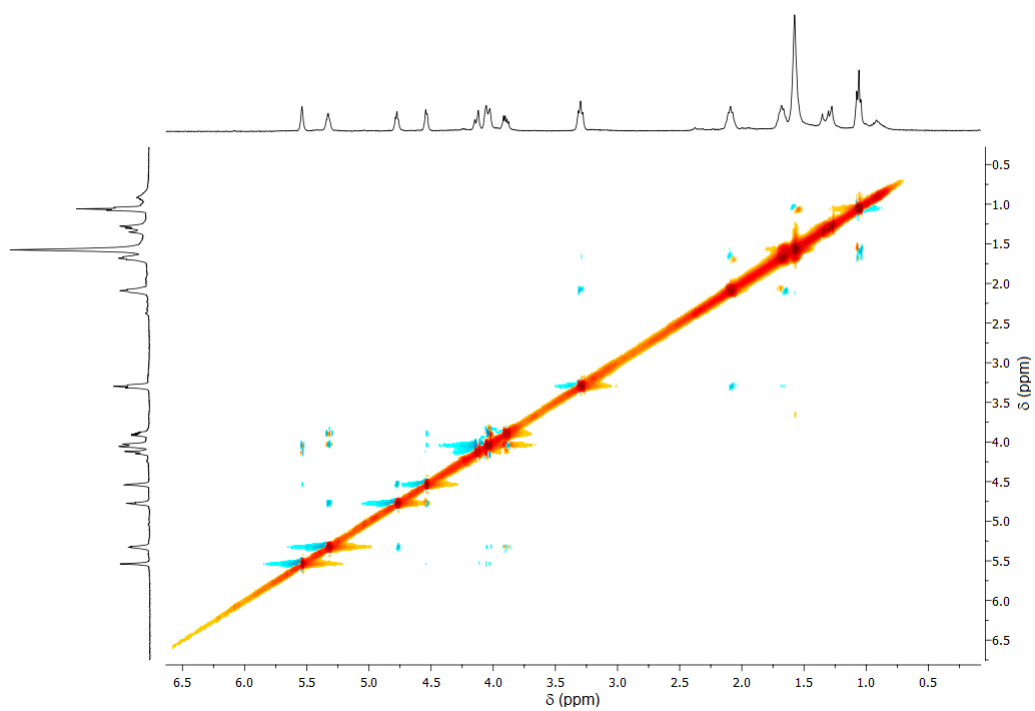


Figure S20. NOESY spectrum of **13** in CDCl_3 .

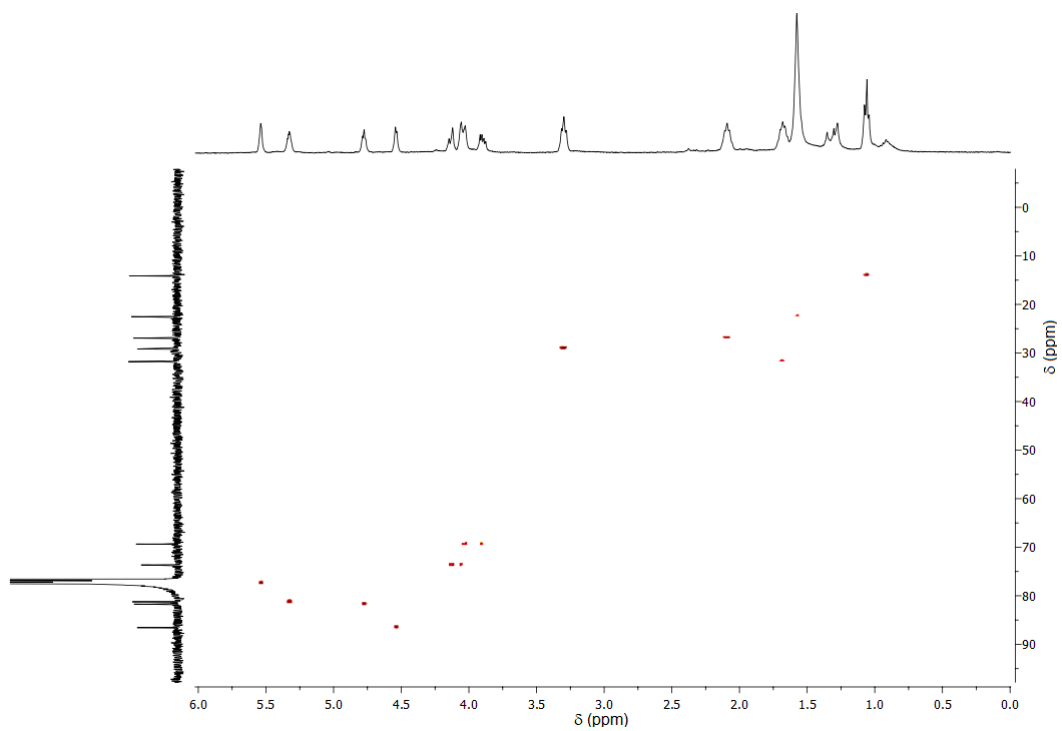


Figure S21. HSQC spectrum of **13** in CDCl_3 .

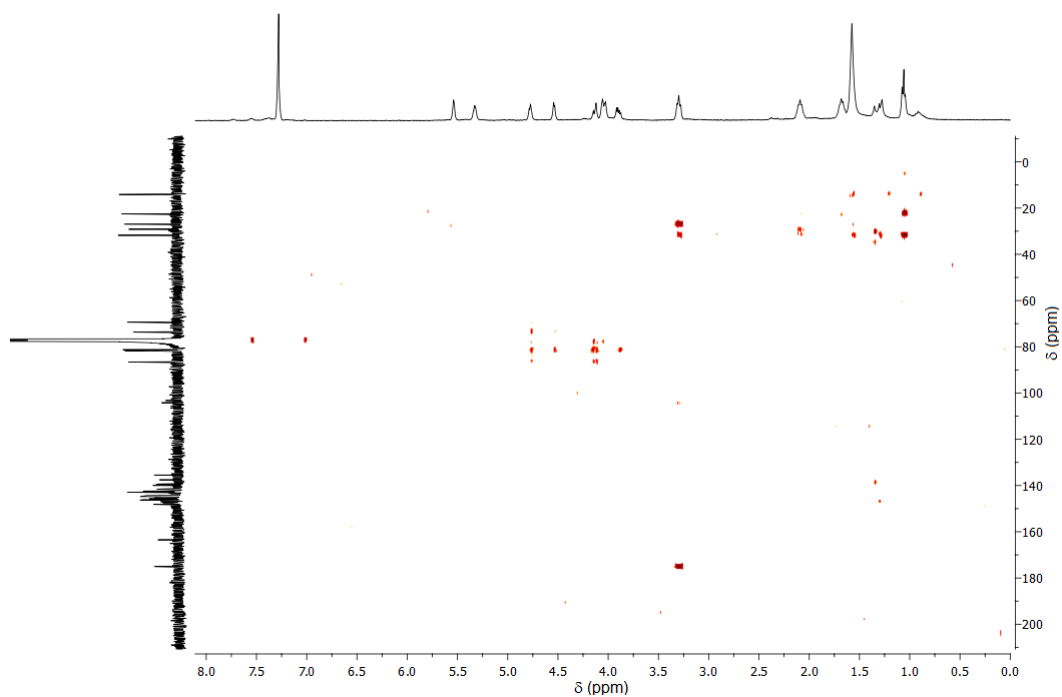
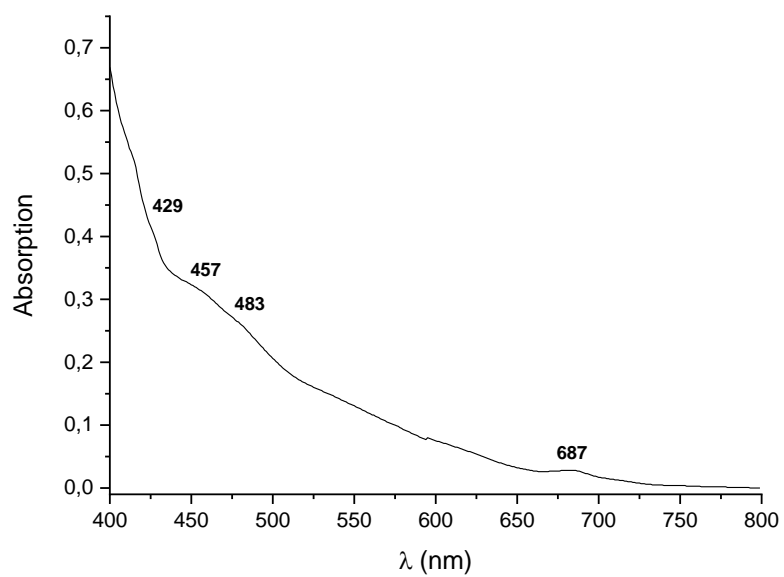


Figure S22. HMBC spectrum of **13** in CDCl_3 .

a)



λ (nm)	ϵ ($\text{dm}^3 \text{ mol}^{-1} \text{ cm}^{-1}$)
429	2186
457	1754
483	1424
687	130

b)

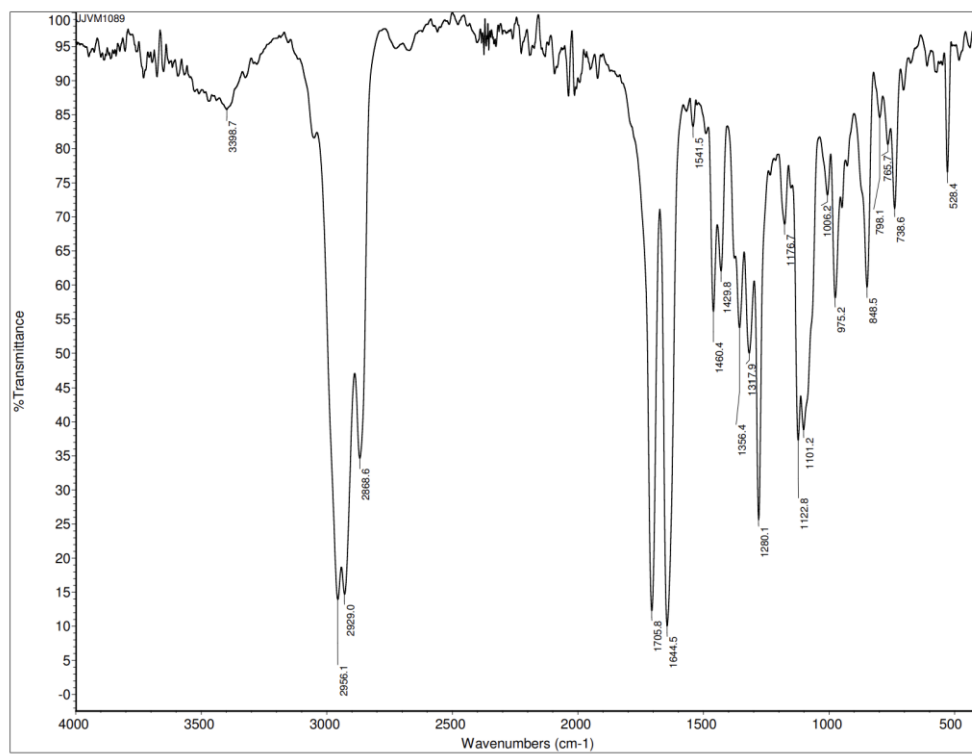


Figure S23. a) UV-vis absorption spectrum of compound **13** in CHCl_3 . b) FTIR-ATR of **13**.

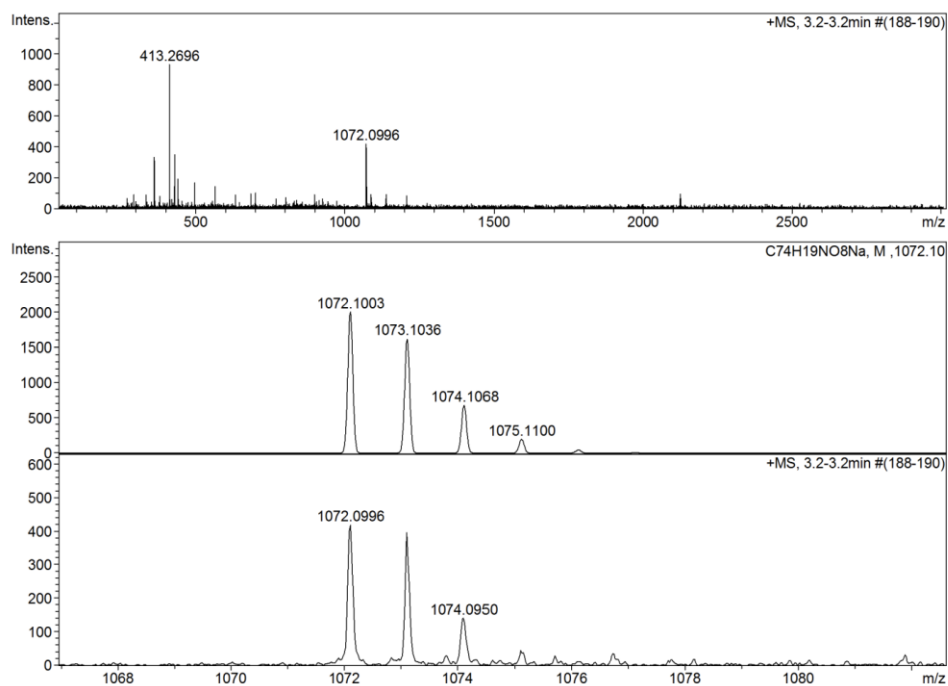
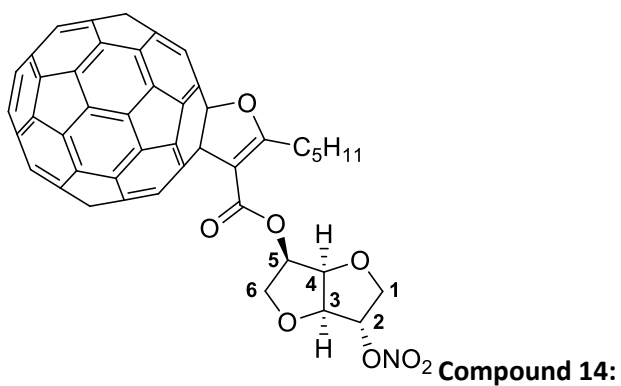


Figure S24. HRMS spectra of **13**.



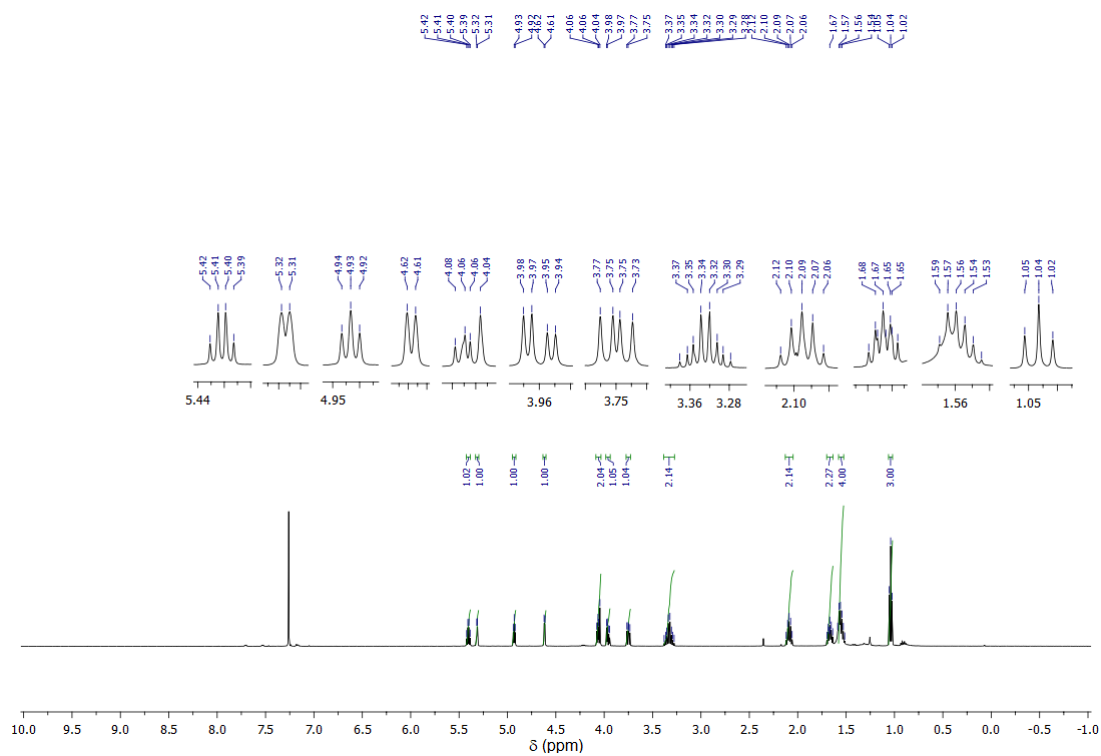


Figure S25. ^1H NMR spectrum (500 MHz) of **14** in CDCl_3 .

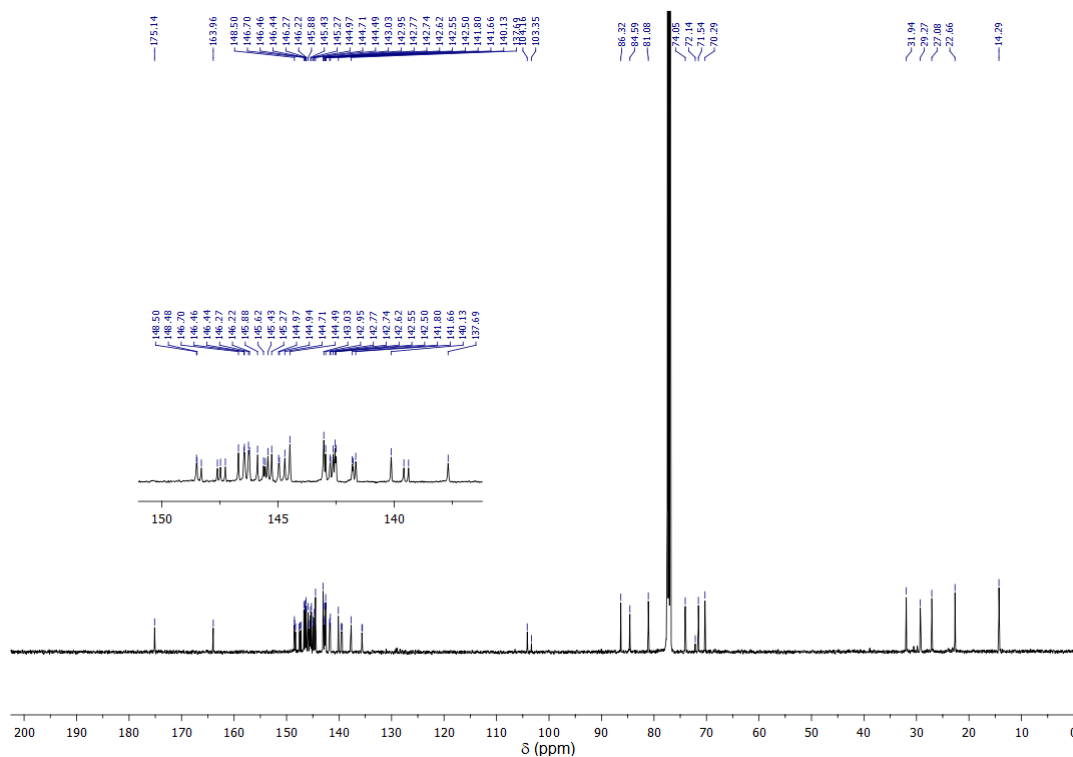


Figure S26. ^{13}C NMR spectrum (125 MHz) of **14** in CDCl_3 .

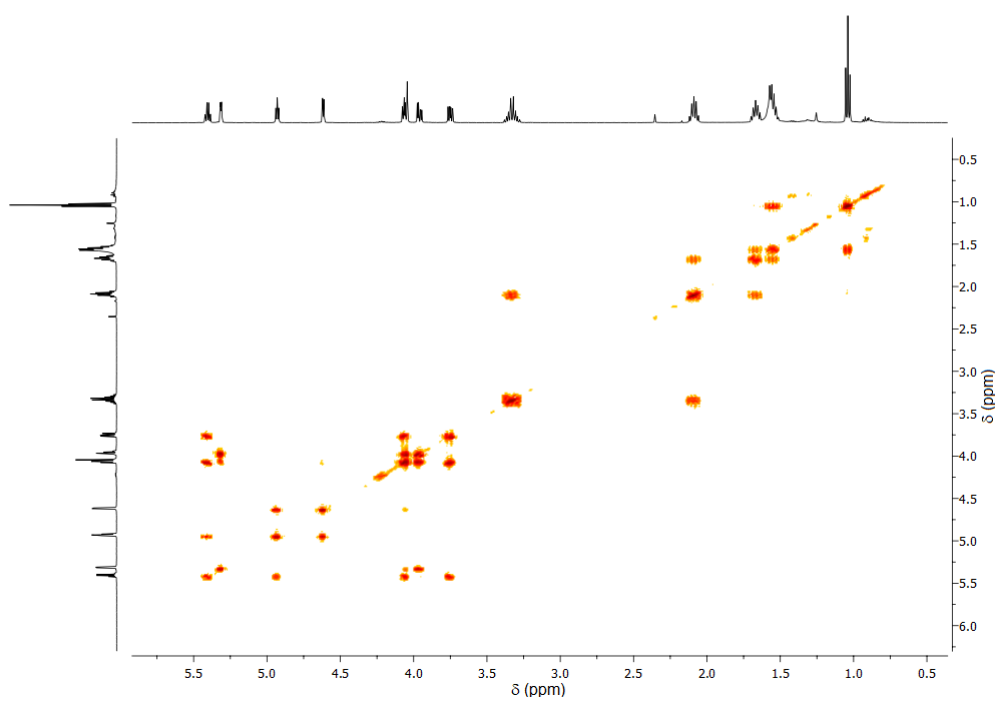


Figure S27. The COSY spectrum of **14** in CDCl_3 .

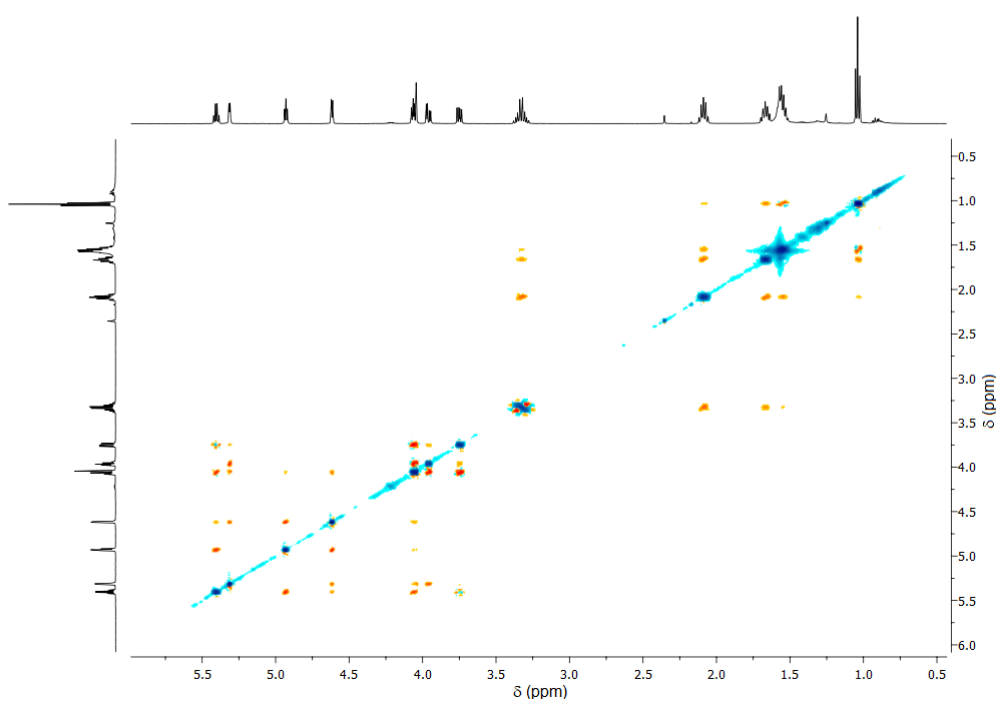


Figure S28. NOESY spectrum of **14** in CDCl_3 .

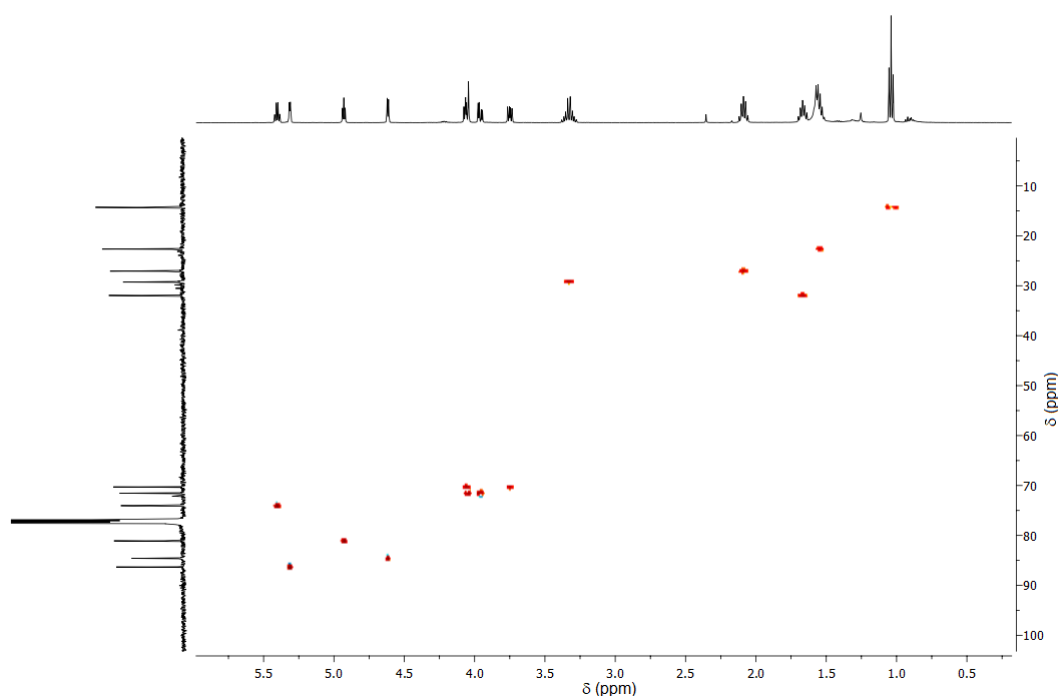


Figure S29. HSQC spectrum of **14** in CDCl₃.

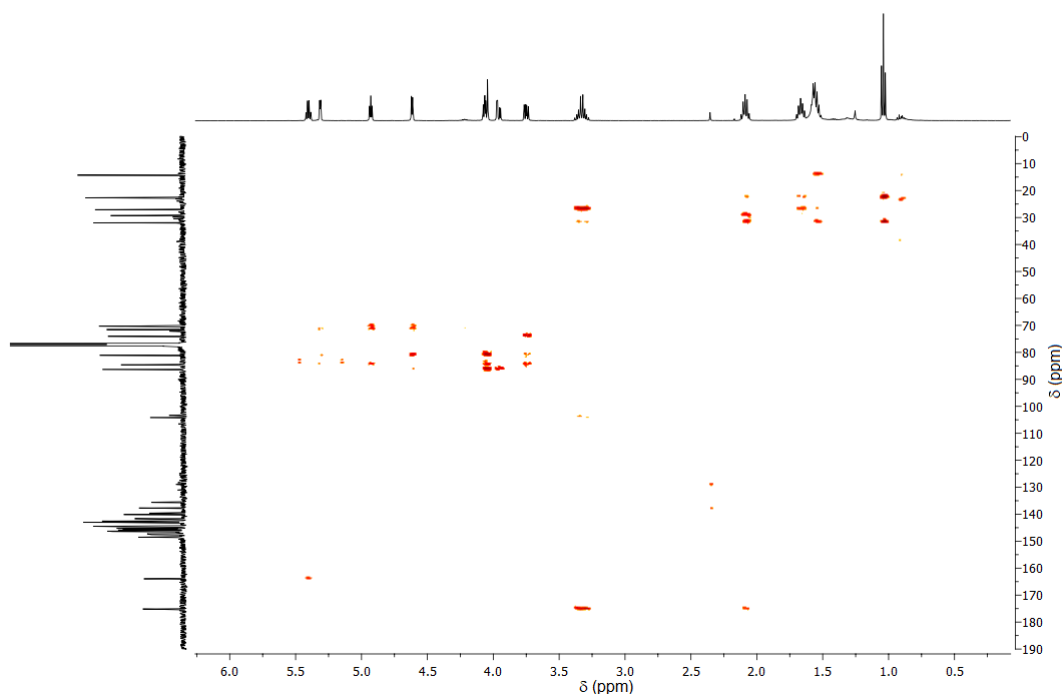
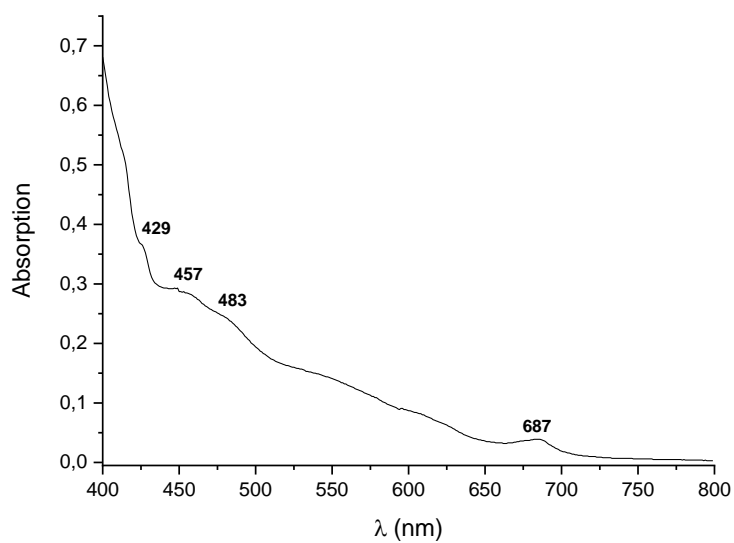


Figure S30. HMBC spectrum of **14** in CDCl₃.

a)



λ (nm)	ϵ ($\text{dm}^3 \text{ mol}^{-1} \text{ cm}^{-1}$)
429	1955
457	1624
483	1376
687	150

b)

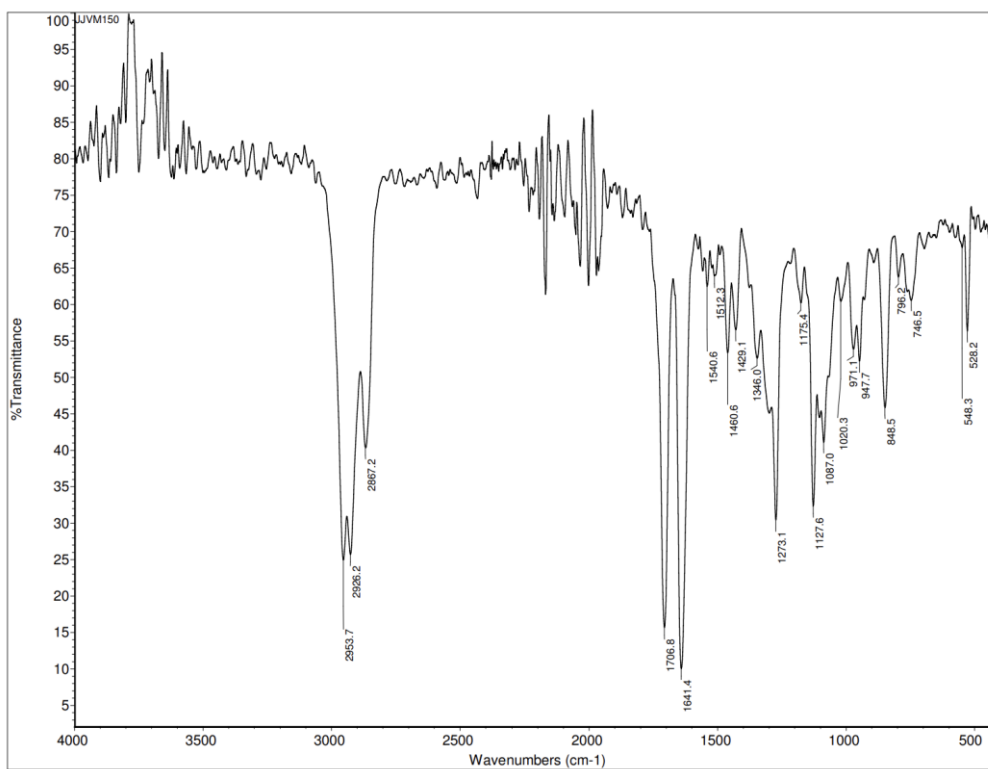


Figure S31. a) UV-vis absorption spectrum of **14** compound in CHCl_3 . b) FTIR-ATR of **14**.

OB7057 #1-54 RT: 0.00-0.50 AV: 54 NL: 9.41E4
T: FTMS + p ESI Full ms [1000.00-1200.00]

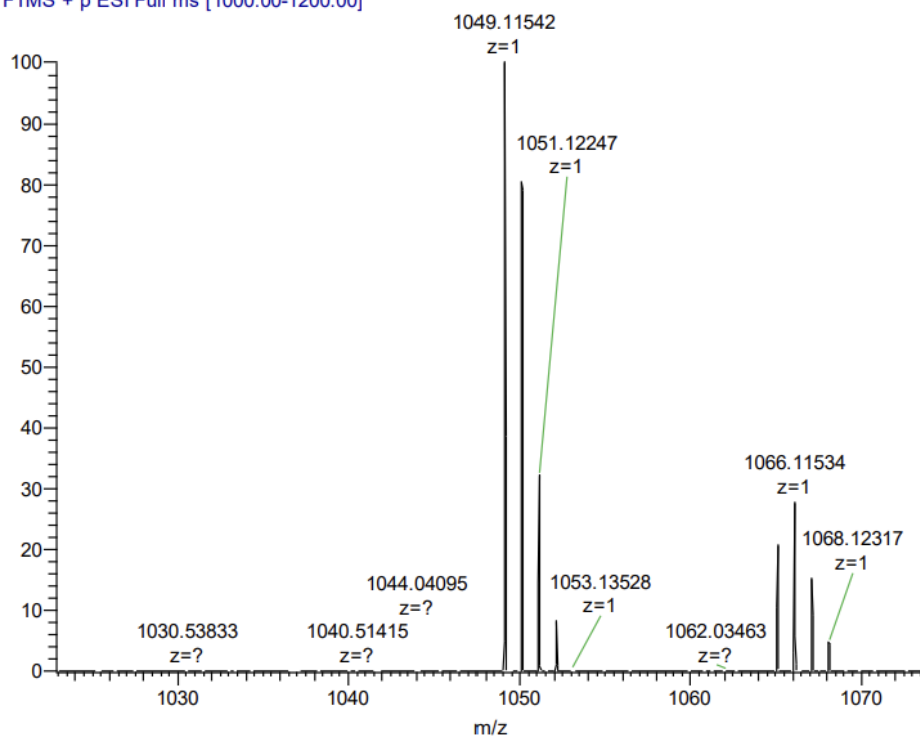
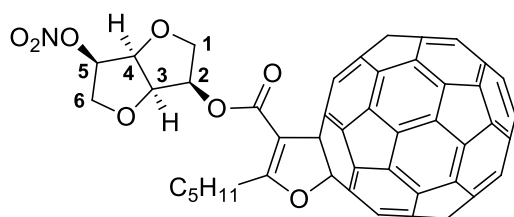


Figure S32. HRMS spectra of **14**.

Compound 15:



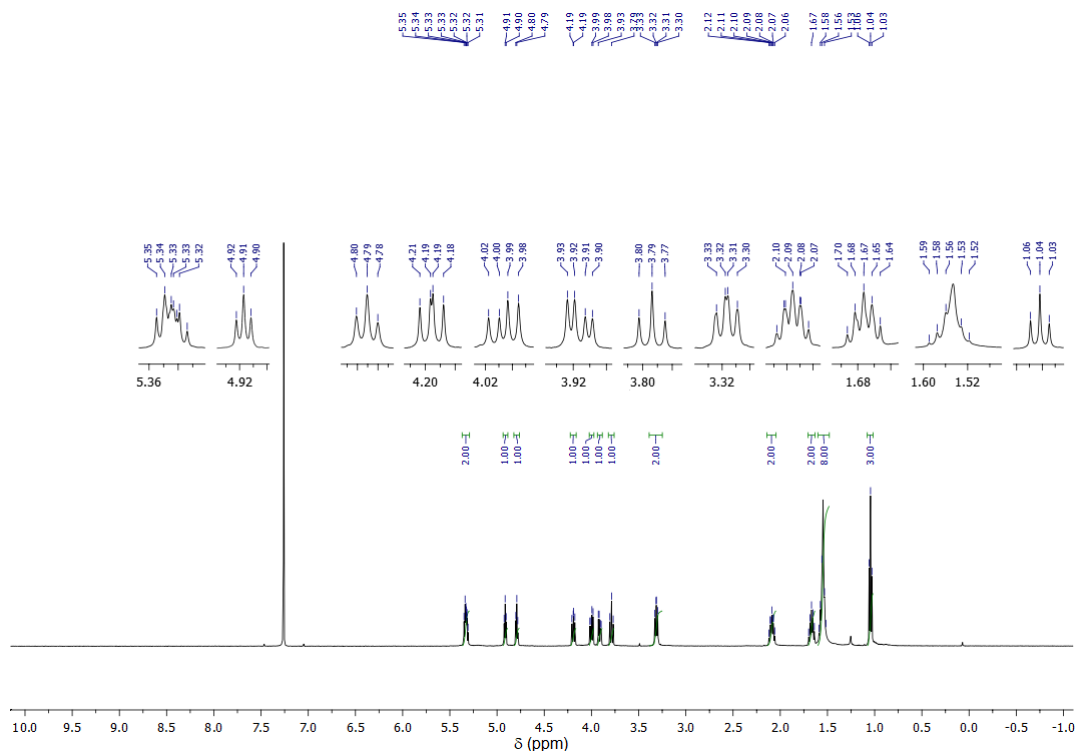


Figure S33. ^1H NMR spectrum (500 MHz) of **15** in CDCl_3 .

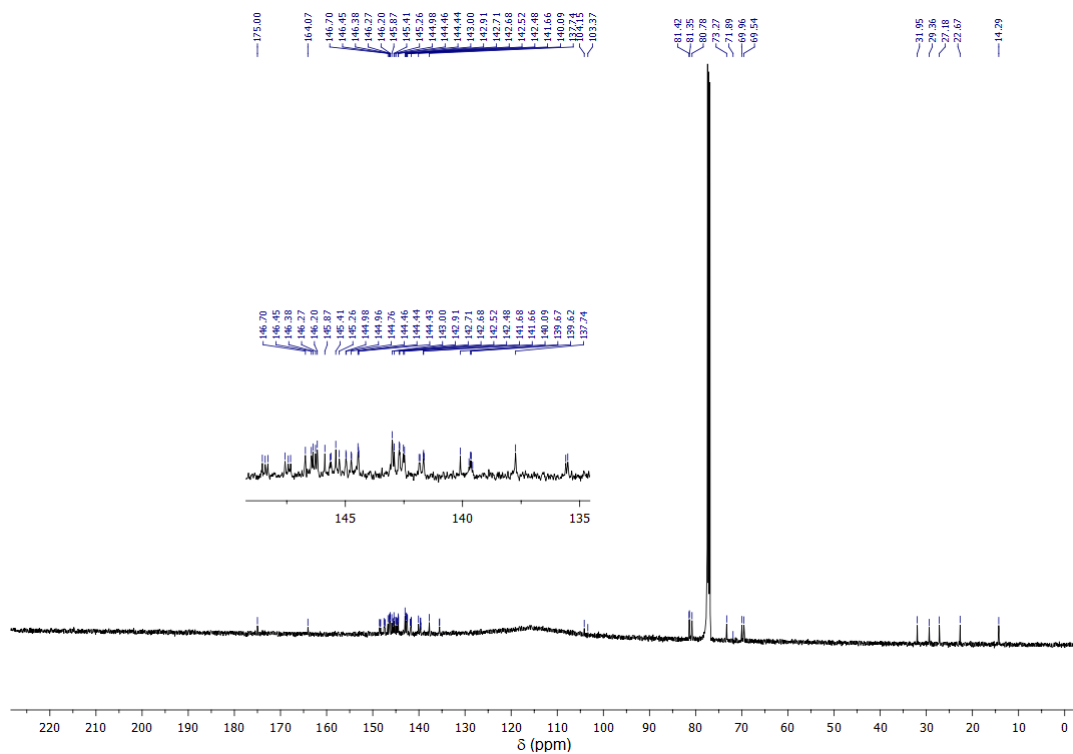


Figure S34. ^{13}C NMR spectrum (125 MHz) of **15** in CDCl_3 .

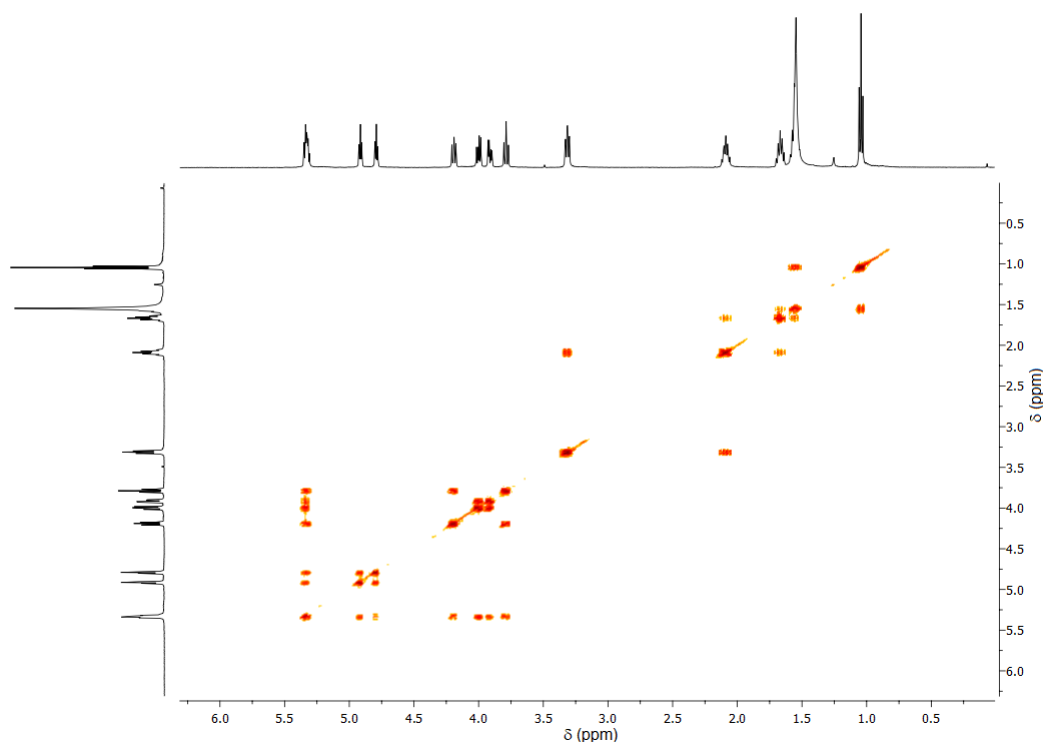


Figure S35. The COSY spectrum of **15** in CDCl_3 .

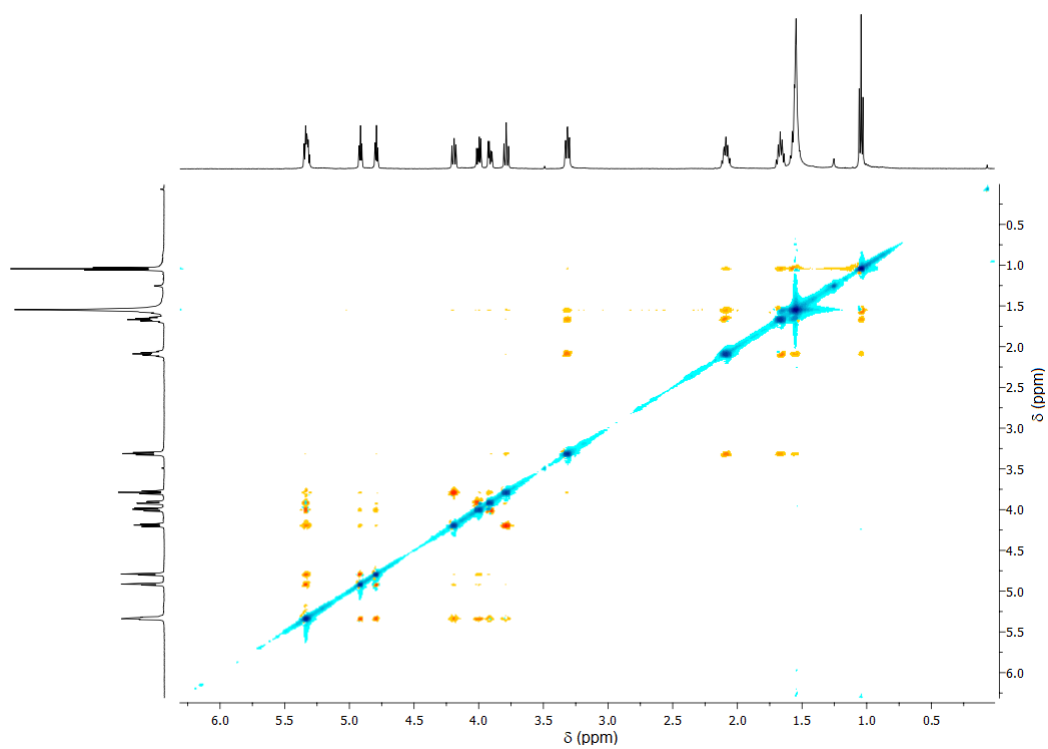


Figure S36. NOESY spectrum of **15** in CDCl_3 .

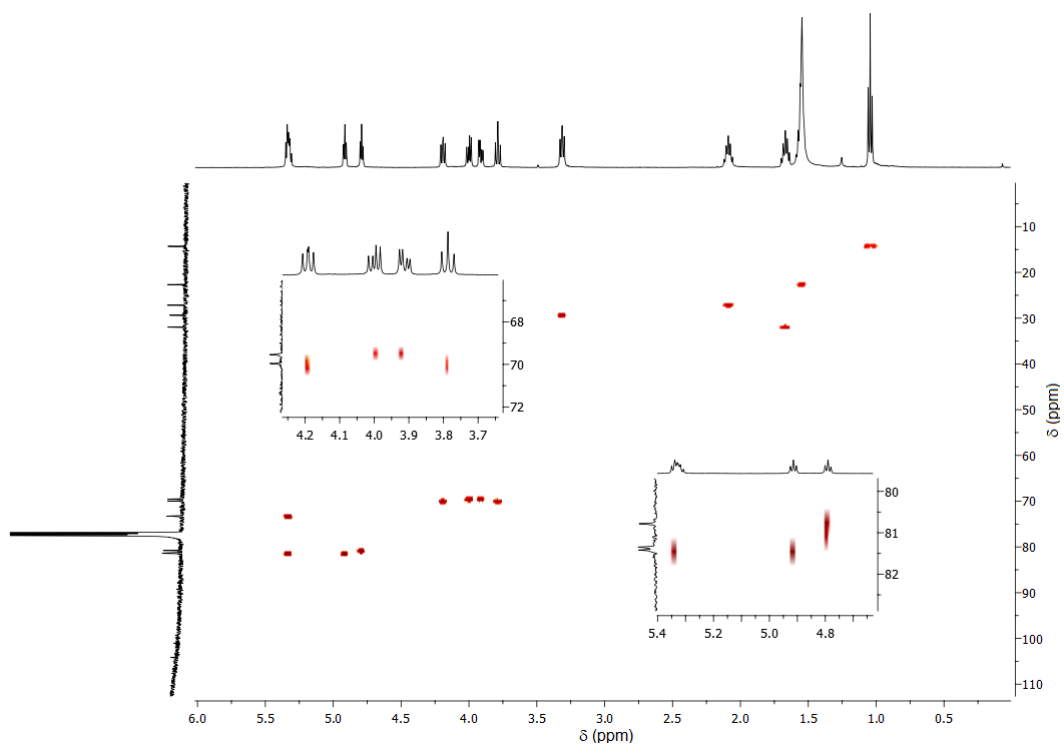


Figure S37. HSQC spectrum of **15** in CDCl₃.

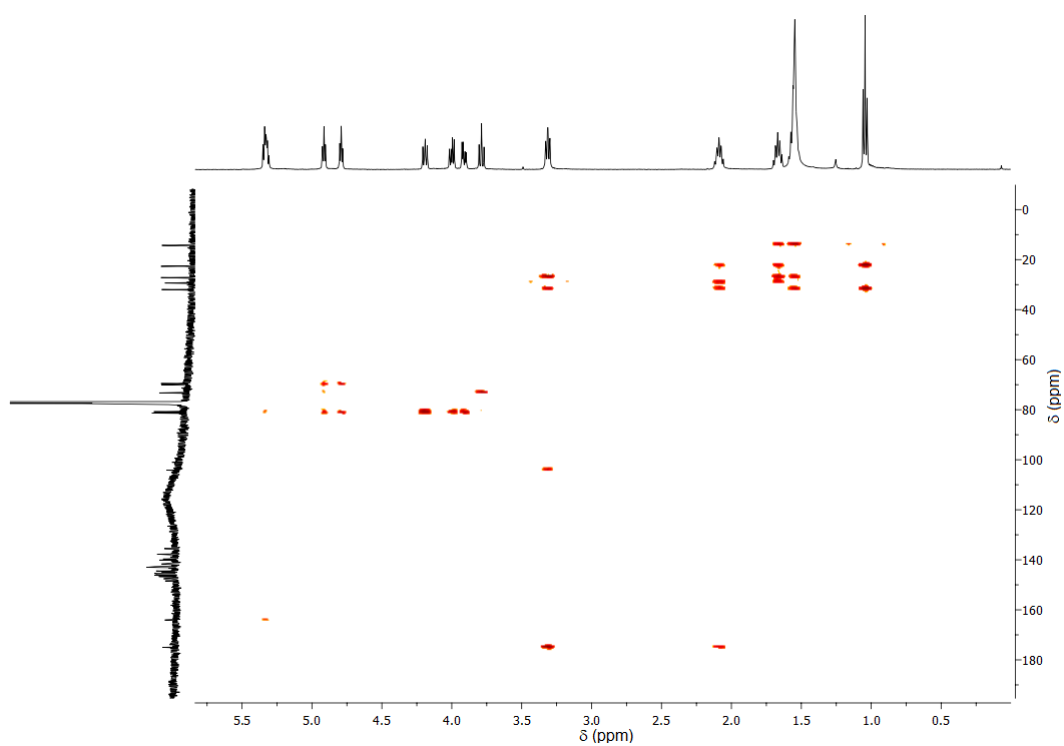
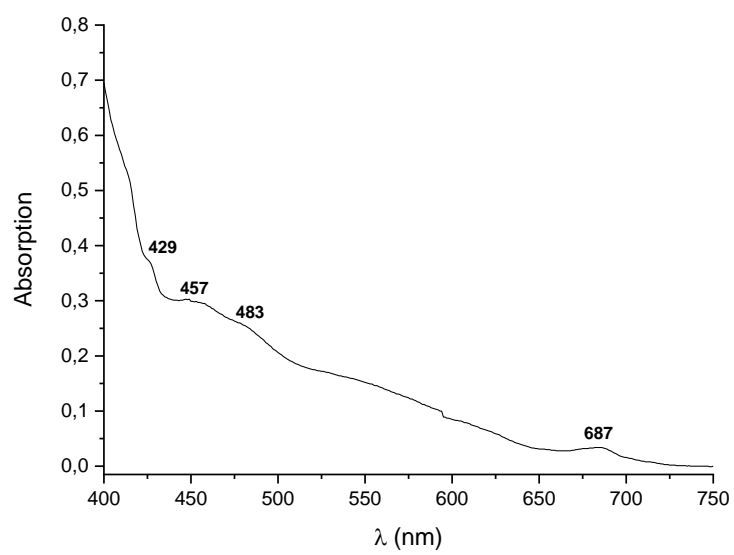


Figure S38. HMBC spectrum of **15** in CDCl₃.

a)



λ (nm)	ϵ ($\text{dm}^3 \text{mol}^{-1} \text{cm}^{-1}$)
429	2172
457	1772
483	1444
687	128

b)

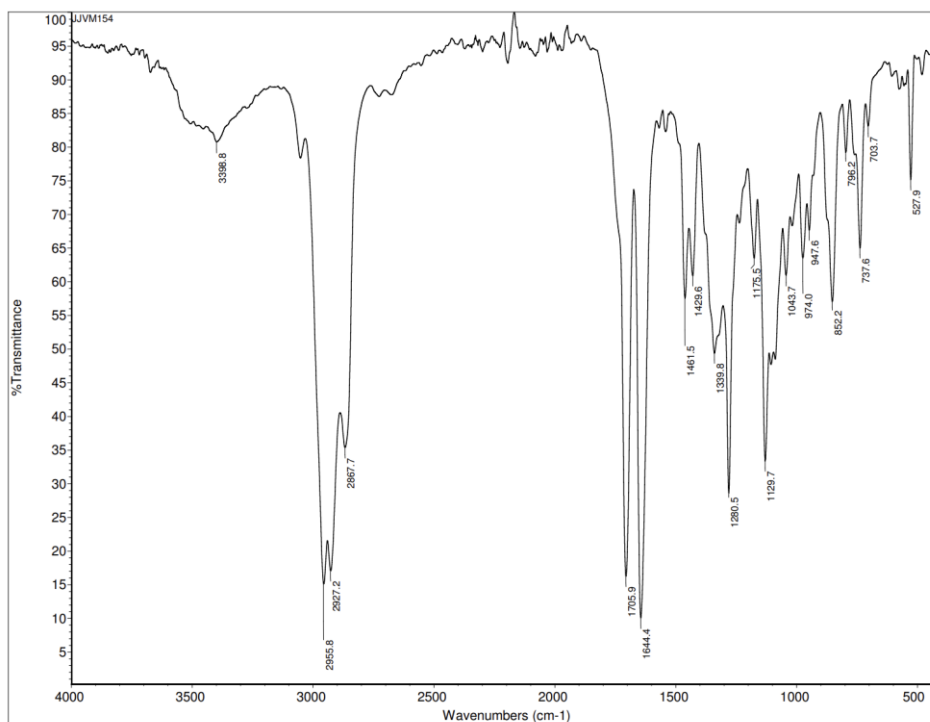


Figure S39. a) UV-vis absorption spectrum of **15** compound in CHCl_3 . b) FTIR-ATR of **15**.

OB7062 #35-50 RT: 0.33-0.47 AV: 16 NL: 3.15E4
T: FTMS + p ESI Full ms [1000.00-1200.00]

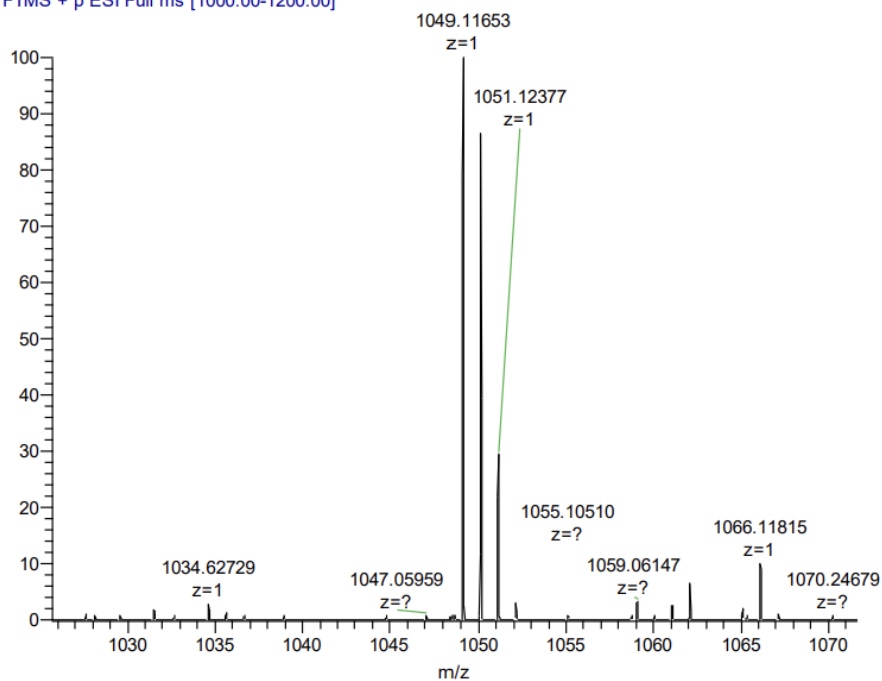


Figure S40. HRMS spectra of **15**.

Cyclic Voltammetry measurements in solution

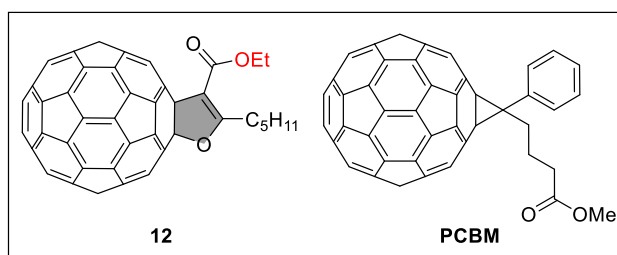


Table S1. Half-wave reduction potentials (V vs. Fc/Fc⁺) of C₆₀, PCBM and furan-fused fullerenes **12**, **13**, **14**, **15**^a

Compound	E _{red} ¹ (V) ^b	E _{red} ² (V) ^b	E _{red} ³ (V) ^b	E _{red} ⁴ (V) ^b	LUMO (eV) ^b	E _g (eV) ^c	HOMO (eV) ^d	λ _{abs} (nm) ^f
C ₆₀	-1.14	-1.51	-1.98	-2.49	-3.66	1.70	-5.36	729
12	-1.16	-1.48	-1.95	-2.32	-3.64	1.76	-5.40	704
13	-1.12	-1.46	-1.92	-2.30	-3.68	1.75	-5.43	708
14	-1.15	-1.48	-1.98	-2.31	-3.65	1.77	-5.42	700
15	-1.14	-1.46	-1.94	-2.31	-3.66	1.77	-5.43	700
PCBM	-1.24	-1.64	-1.81	-2.18	-3.56	1.73	-5.29	717

^aExperimental conditions: V vs ferrocene/ferrocenium (Fc/Fc⁺); the reference electrode is Ag/AgCl; the working electrode is a glassy carbon electrode (GCE); 0.1 M *n*Bu₄NPF₆; scan rate: 50 mVs⁻¹; measured in *o*-dichlorobenzene/dimethylformamide (100:1 v/v) at room temperature. ^bMeasured by CV; LUMO energy calculated using equation $E(\text{LUMO}) = -(E_{1/2}^1 + 4.8)$ (eV)^[3]. ^cDetermined from the Tauc plot calculated from the UV-Vis spectra in toluene. ^dCalculated using the equation: $E(\text{HOMO}) = E(\text{LUMO}) - \text{Energy gap (eV)}$. ^fUV-vis spectra in toluene.

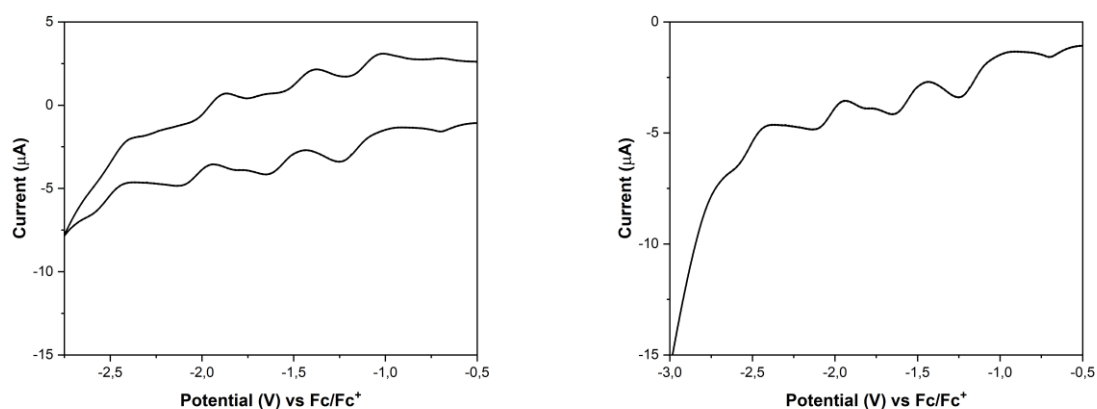


Figure S41. (left) CV, (right) Linear sweep voltammetry (LSV) of **11** (0.4 mg mL⁻¹) recorded in ODCB/DMF 100/1, at 50 mVs⁻¹, at room temperature, under Argon. Potentials are shown versus Fc/Fc⁺.

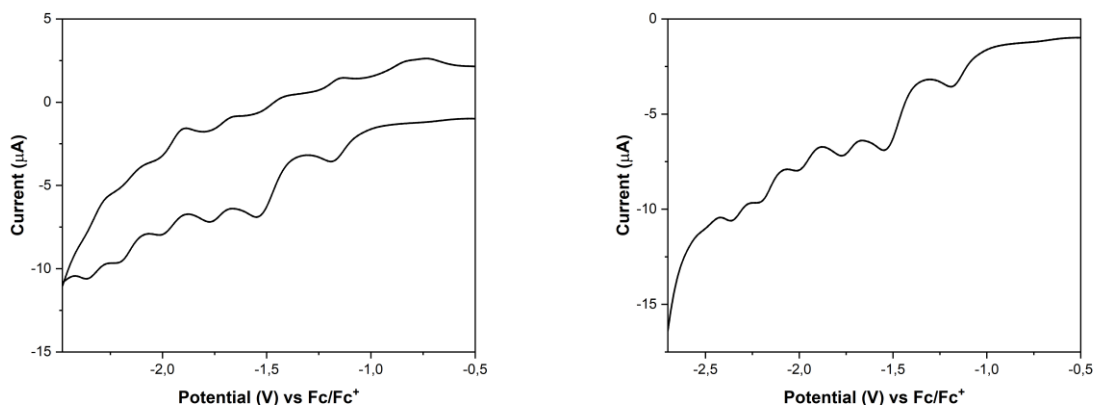


Figure S42. (left) CV, (right) Linear sweep voltammetry (LSV) of **12** (0.4 mg mL^{-1}) recorded in ODCB/DMF 100/1, at 50 mVs^{-1} , at room temperature, under Argon. Potentials are shown versus Fc/Fc^+ .

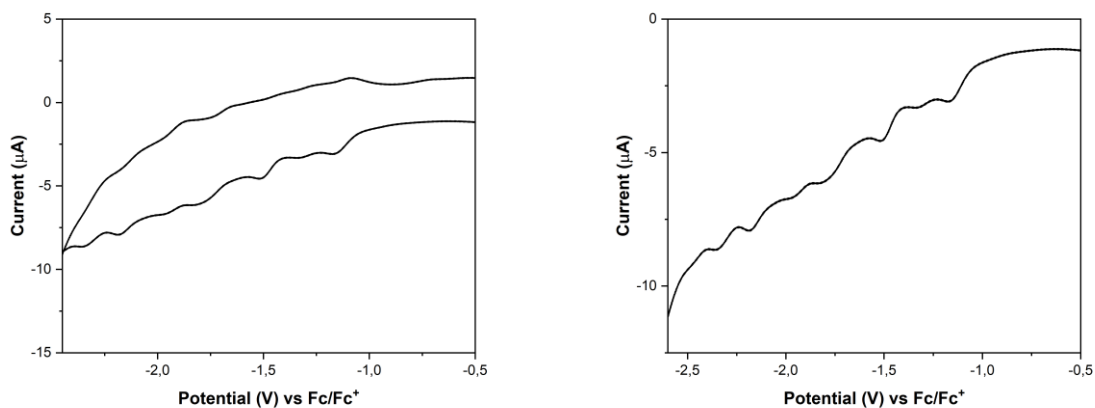


Figure S43. (left) CV, (right) Linear sweep voltammetry (LSV) of **13** (0.4 mg mL^{-1}) recorded in ODCB/DMF 100/1, at 50 mVs^{-1} , at room temperature, under Argon. Potentials are shown versus Fc/Fc^+ .

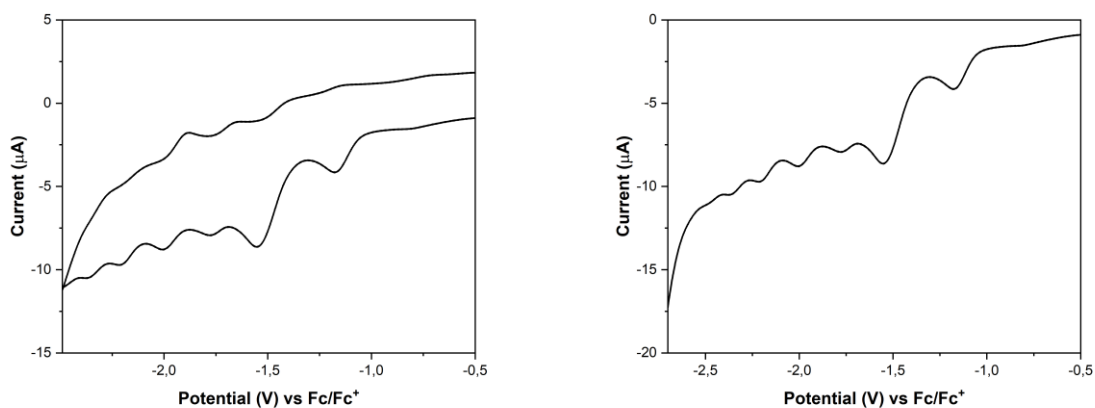


Figure S44. (left) CV, (right) Linear sweep voltammetry (LSV) of **14** (0.4 mg mL^{-1}) recorded in ODCB/DMF 100/1, at 50 mVs^{-1} , at room temperature, under Argon. Potentials are shown versus Fc/Fc^+ .

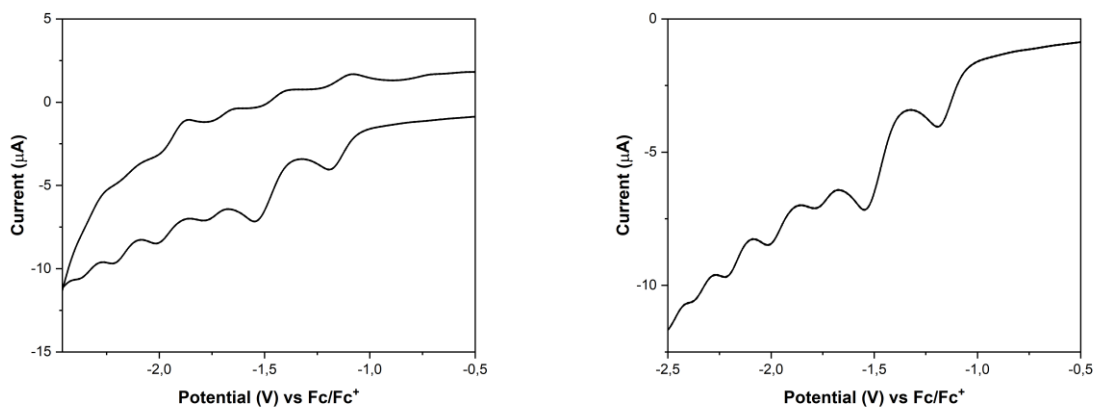


Figure S45. (left) CV, (right) Linear sweep voltammetry (LSV) of **15** (0.4 mg mL^{-1}) recorded in ODCB/DMF 100/1, at 50 mVs^{-1} , at room temperature, under Argon. Potentials are shown versus Fc/Fc^+ .

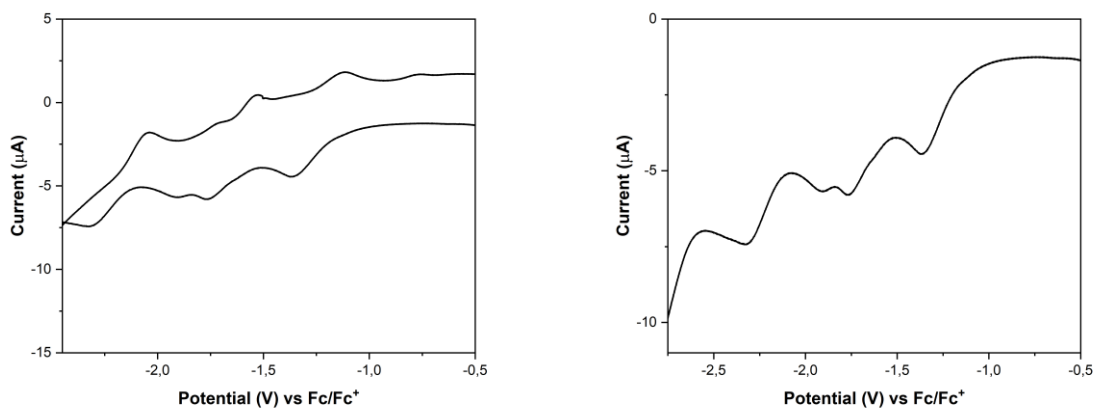


Figure S46. (left) CV, (right) Linear sweep voltammetry (LSV) of **PCBM** (0.4 mg mL^{-1}) recorded in ODCB/DMF 100/1, at 50 mVs^{-1} , at room temperature, under Argon. Potentials are shown versus Fc/Fc^+ .

UV-vis in solution

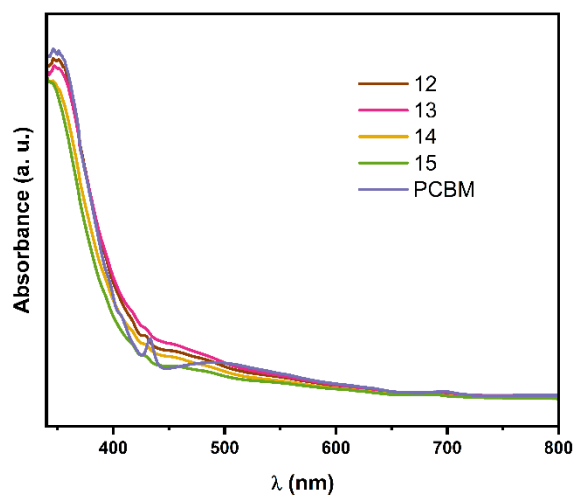


Figure S47. UV-vis of PCBM, 11, 12, 13, 14, 15 (0.2 mg mL^{-1}) in toluene.

UV-vis of thin films

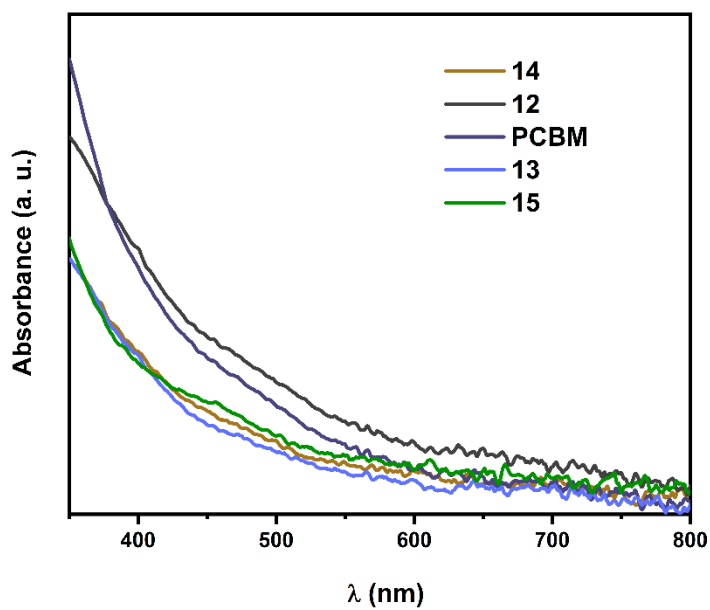


Figure S48. UV-vis of 12, 13, 14, 15, and PCBM on a thin film.

Determination of the energy gap by UV-vis in solution

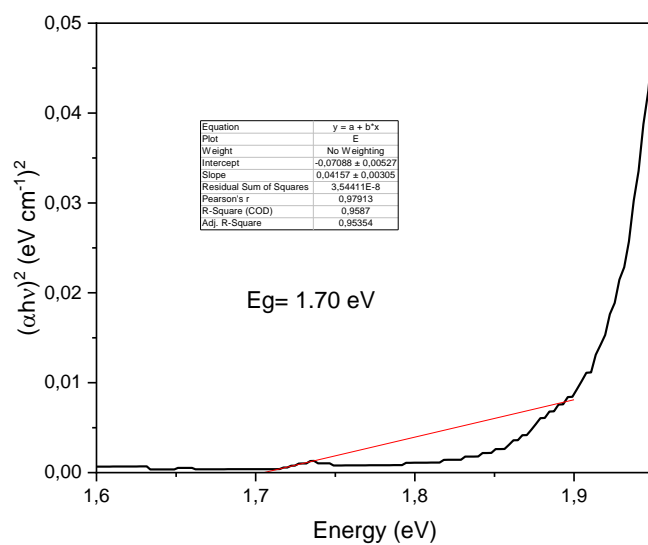


Figure S49. Band gap energy from absorption data of **11** in toluene using the Tauc plot method.

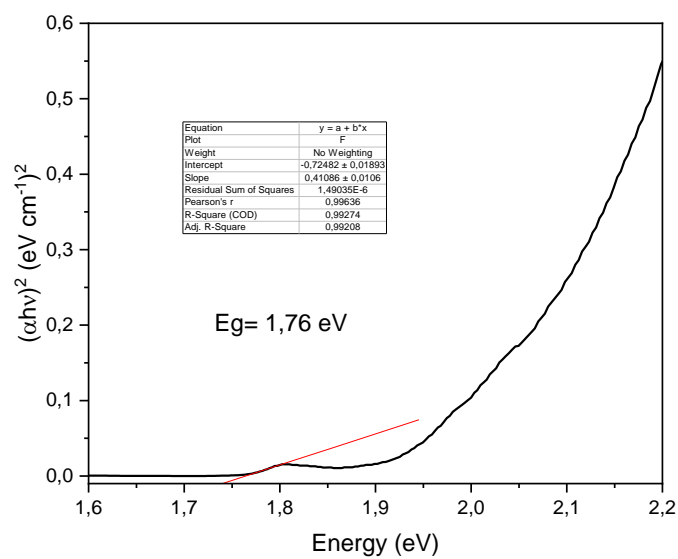


Figure S50. Band gap energy from absorption data of **12** in toluene using the Tauc plot method.

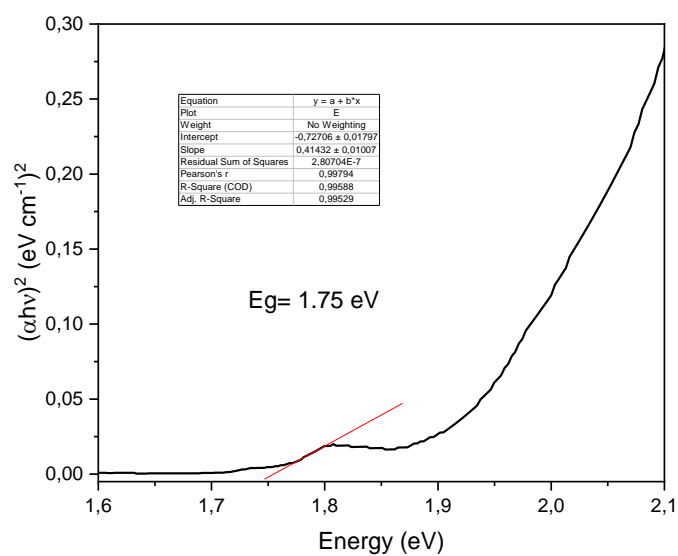


Figure S51. Band gap energy from absorption data of **13** in toluene using the Tauc plot method.

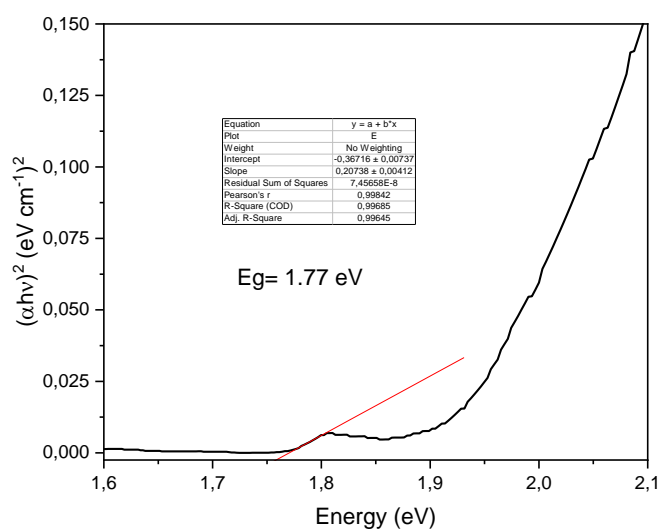


Figure S52. Band gap energy from absorption data of **14** in toluene using the Tauc plot method.

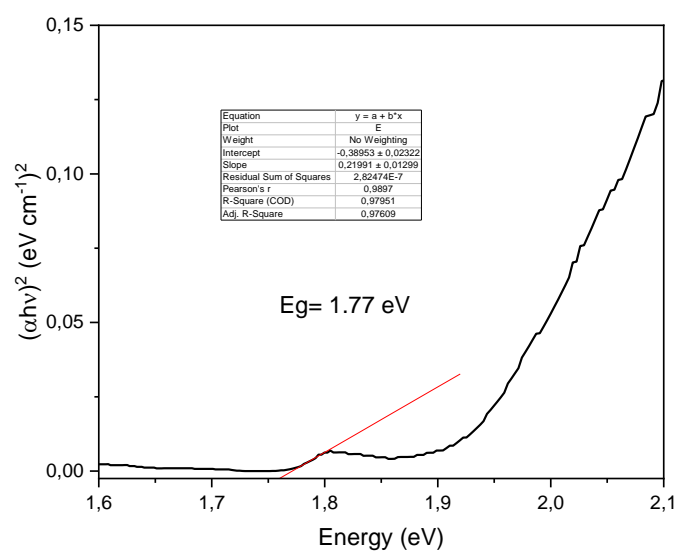


Figure S53. Band gap energy from absorption data of **15** in toluene using the Tauc plot method.

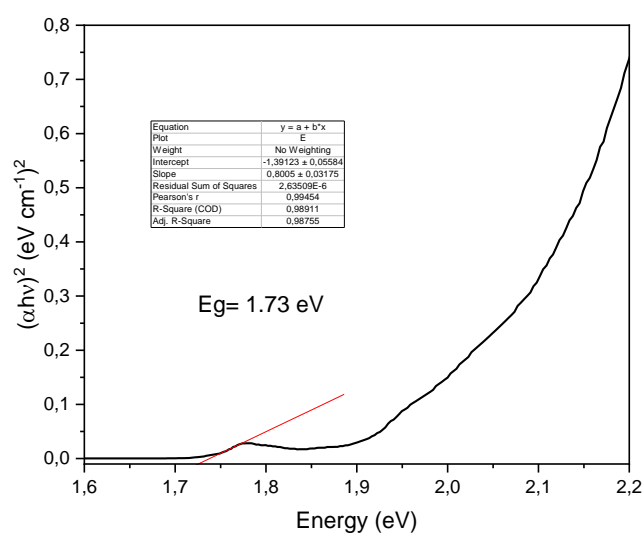


Figure S54. Band gap energy from absorption data of **PCBM** in toluene using the Tauc plot method.

Cyclic Voltammetry measurements on a thin film

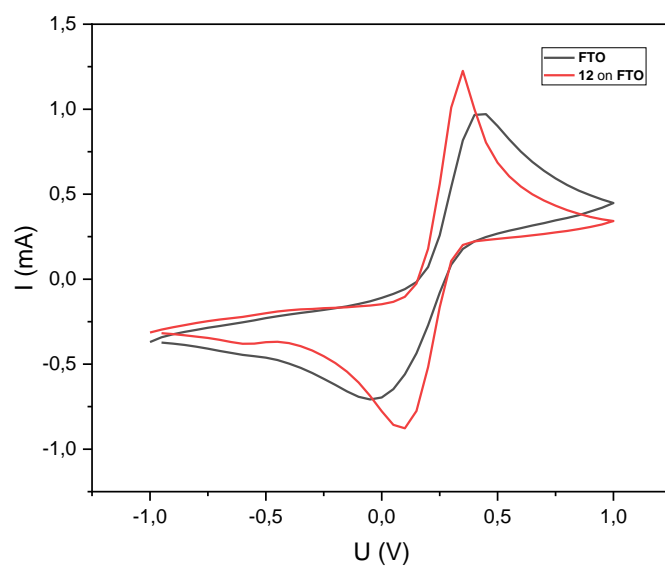


Figure S55. CV of **12** in water solution with inorganic electrolyte $K_3[Fe(CN)_6]$ (5×10^{-4} M), $K_4[Fe(CN)_6]$ (5×10^{-4} M) and KCl (0.1 M).

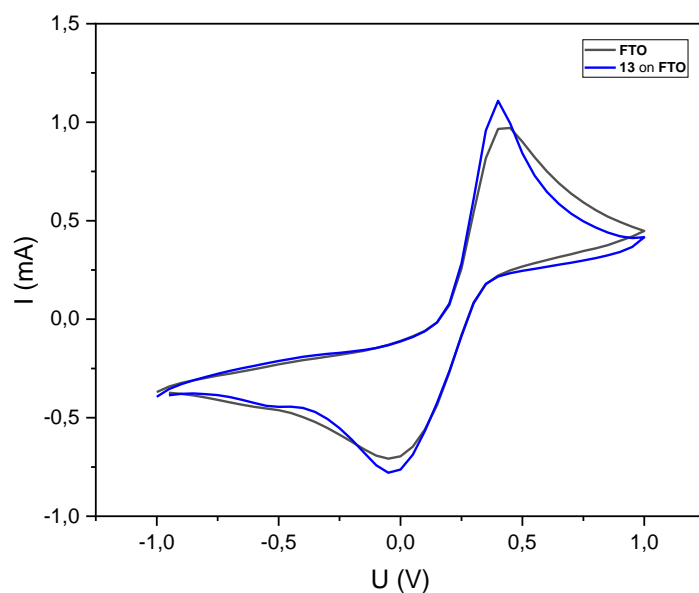


Figure S56. CV of **13** in water solution with inorganic electrolyte $K_3[Fe(CN)_6]$ (5×10^{-4} M), $K_4[Fe(CN)_6]$ (5×10^{-4} M) and KCl (0.1 M).

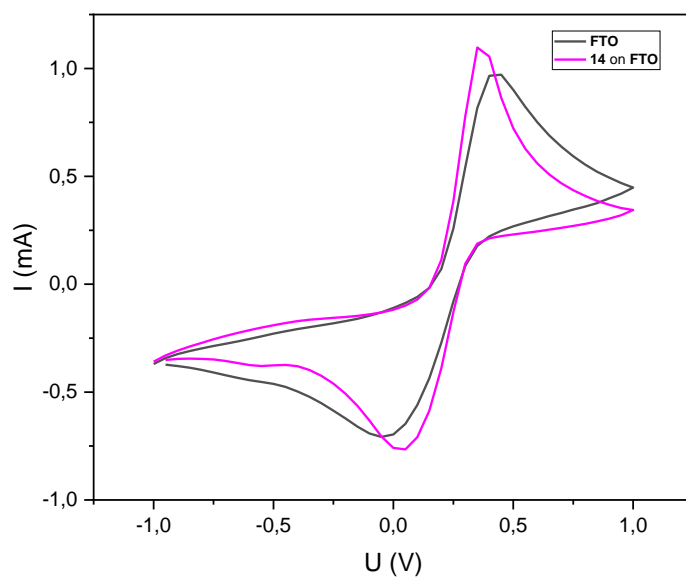


Figure S57. CV of **14** in water solution with inorganic electrolyte $K_3[Fe(CN)_6]$ (5×10^{-4} M), $K_4[Fe(CN)_6]$ (5×10^{-4} M) and KCl (0.1 M).

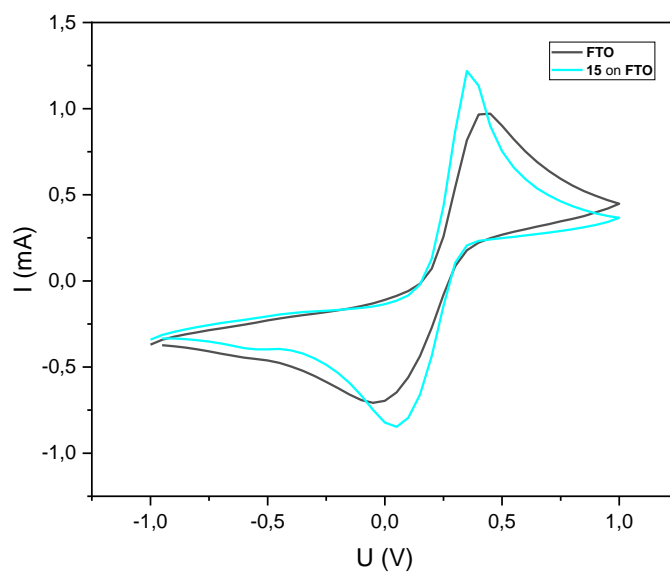


Figure S58. CV of **15** in water solution with inorganic electrolyte $K_3[Fe(CN)_6]$ (5×10^{-4} M), $K_4[Fe(CN)_6]$ (5×10^{-4} M) and KCl (0.1 M).

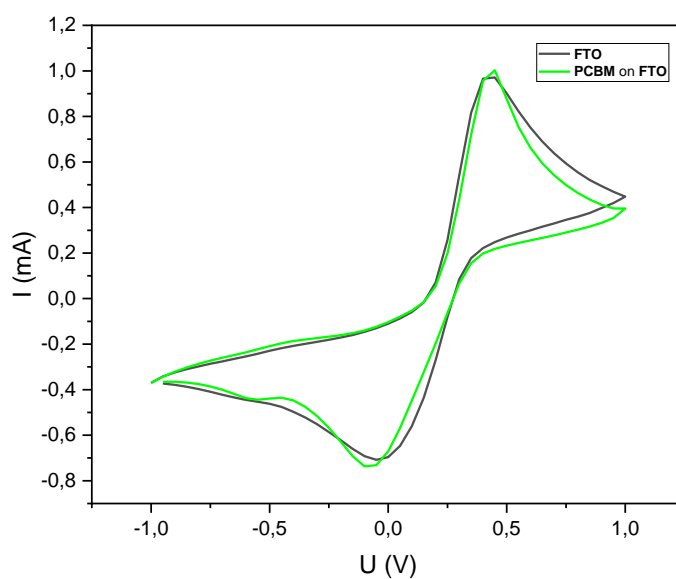


Figure S59. CV of PCBM in water solution with inorganic electrolyte $K_3[Fe(CN)_6]$ (5×10^{-4} M), $K_4[Fe(CN)_6]$ (5×10^{-4} M) and KCl (0.1 M).

Atomic Force Microscopy

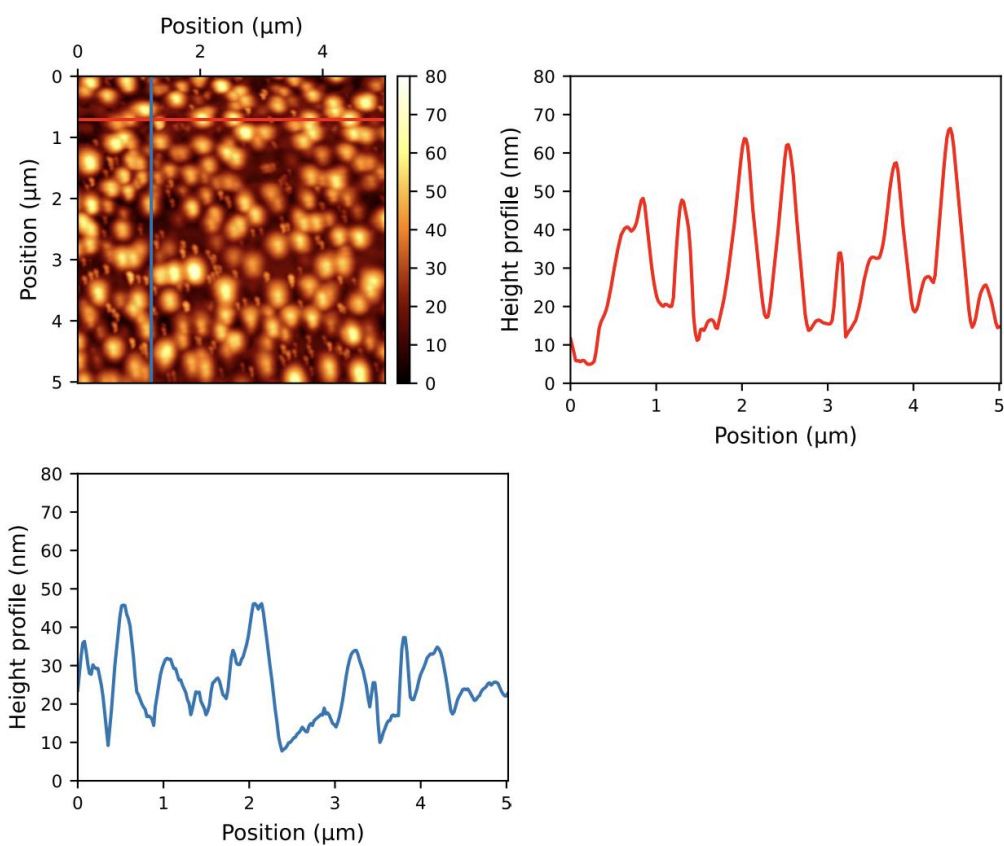


Figure S60. AFM of 12.

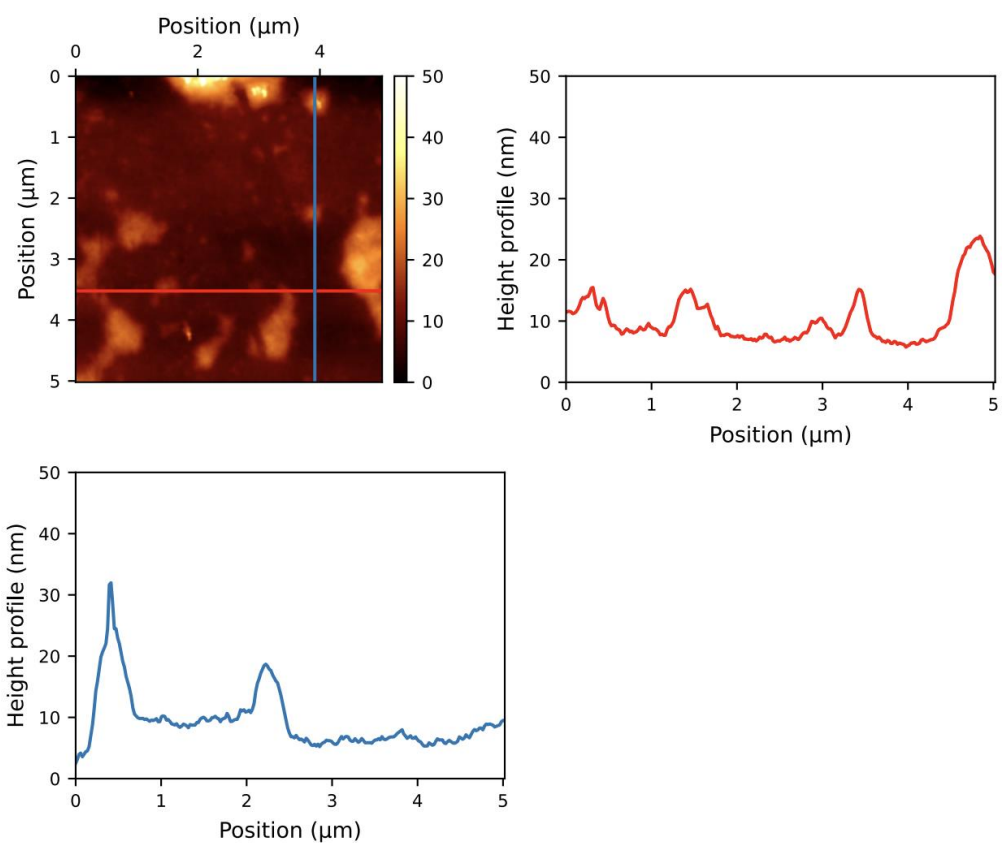


Figure S61. AFM of 13.

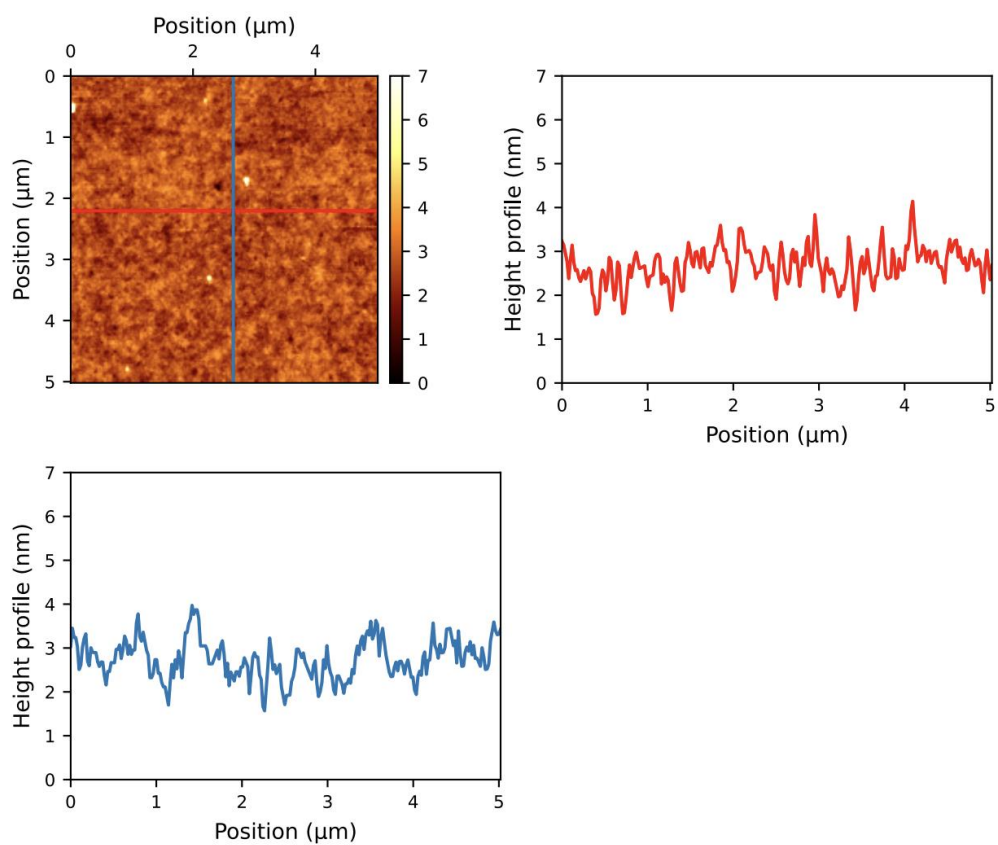


Figure S62. AFM of 14.

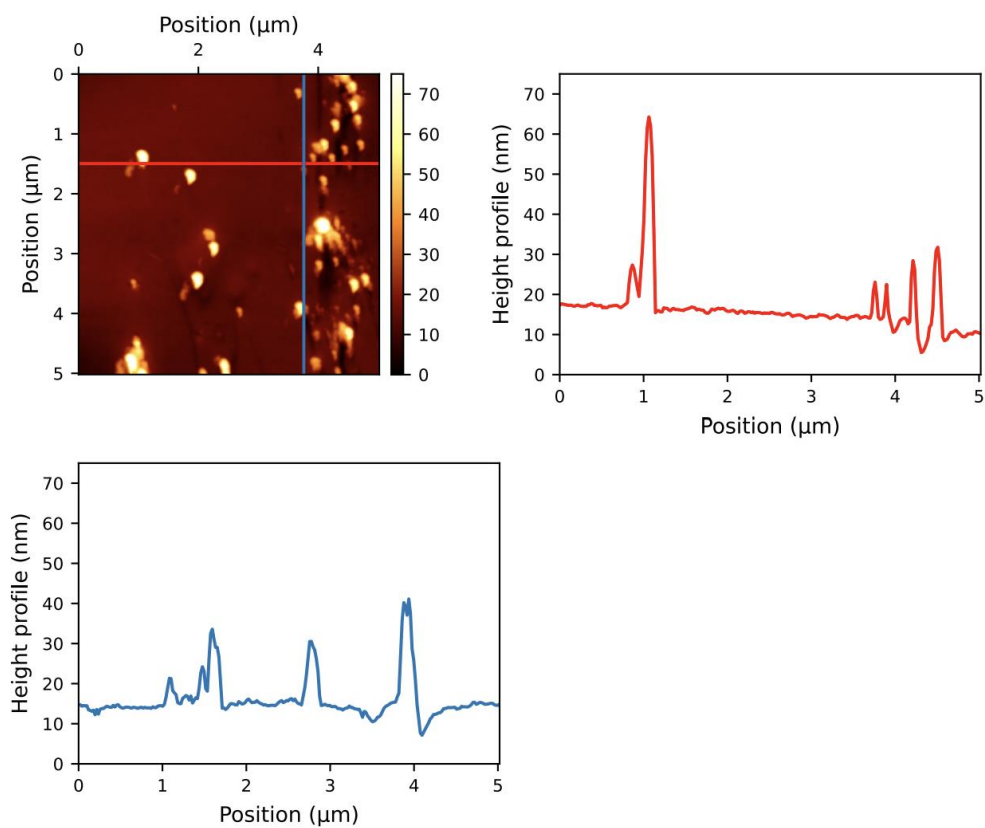


Figure S63. AFM of 15.

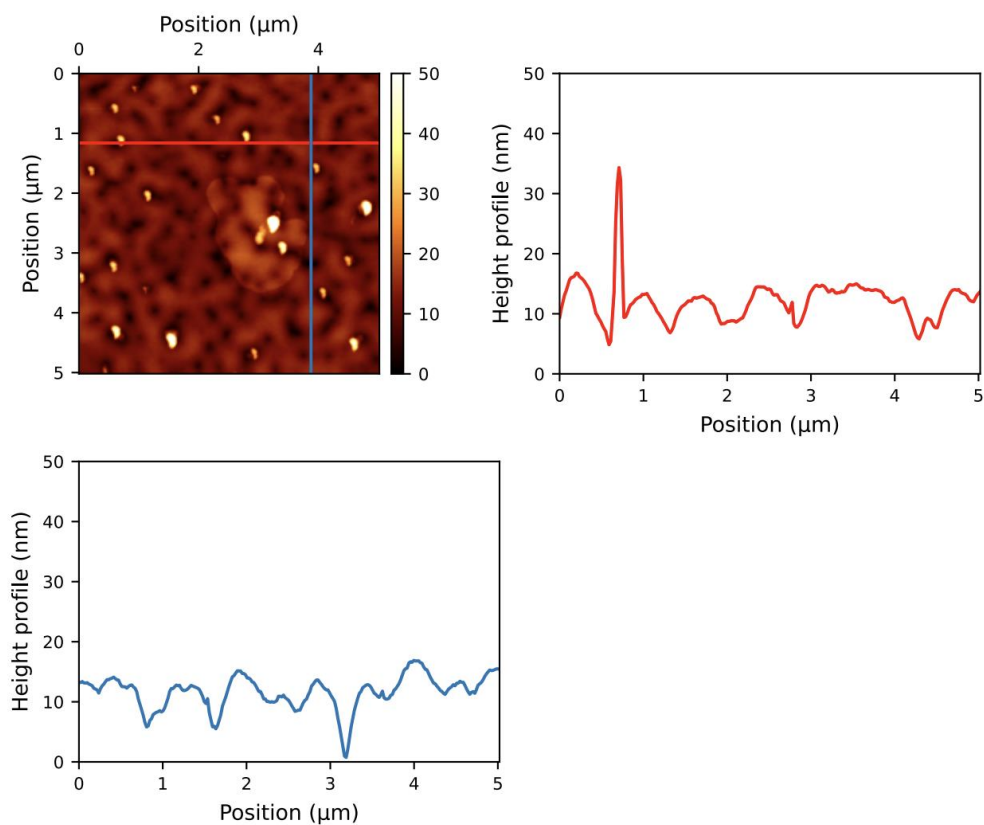


Figure S64. AFM of PCBM.

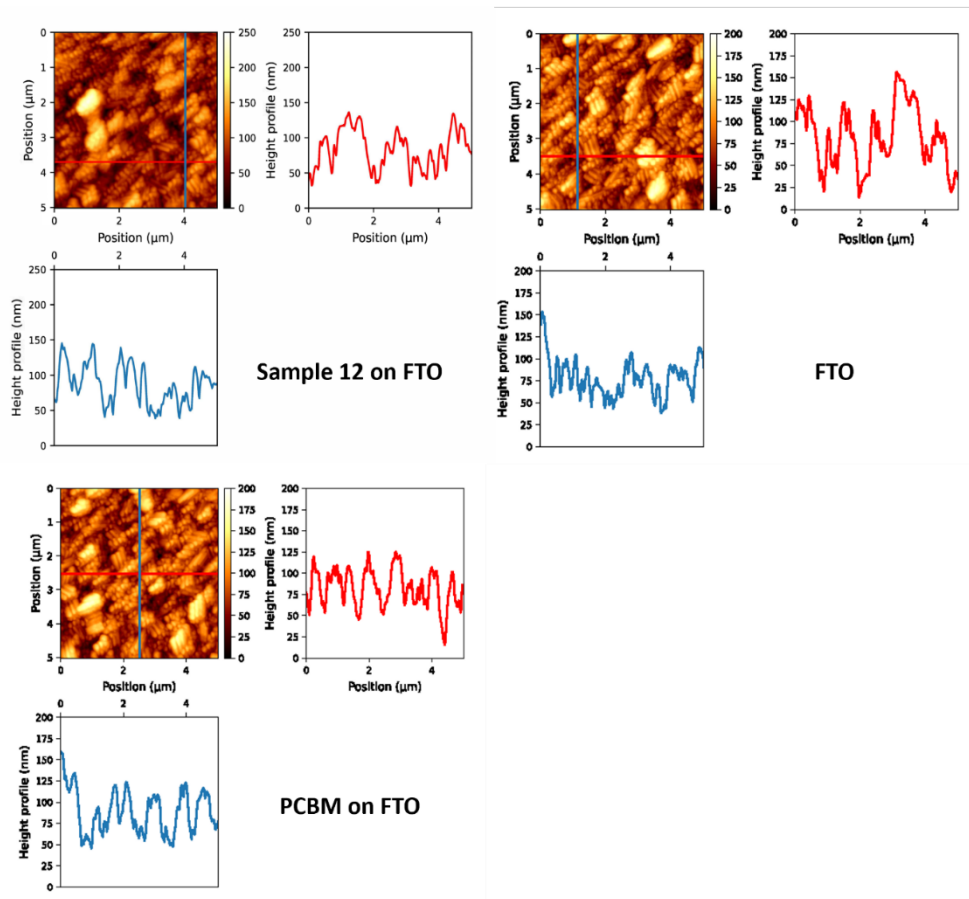


Figure S65. AFM measurements performed on FTO alone, as well as on samples **12** and **PCBM** dropcasted on FTO.

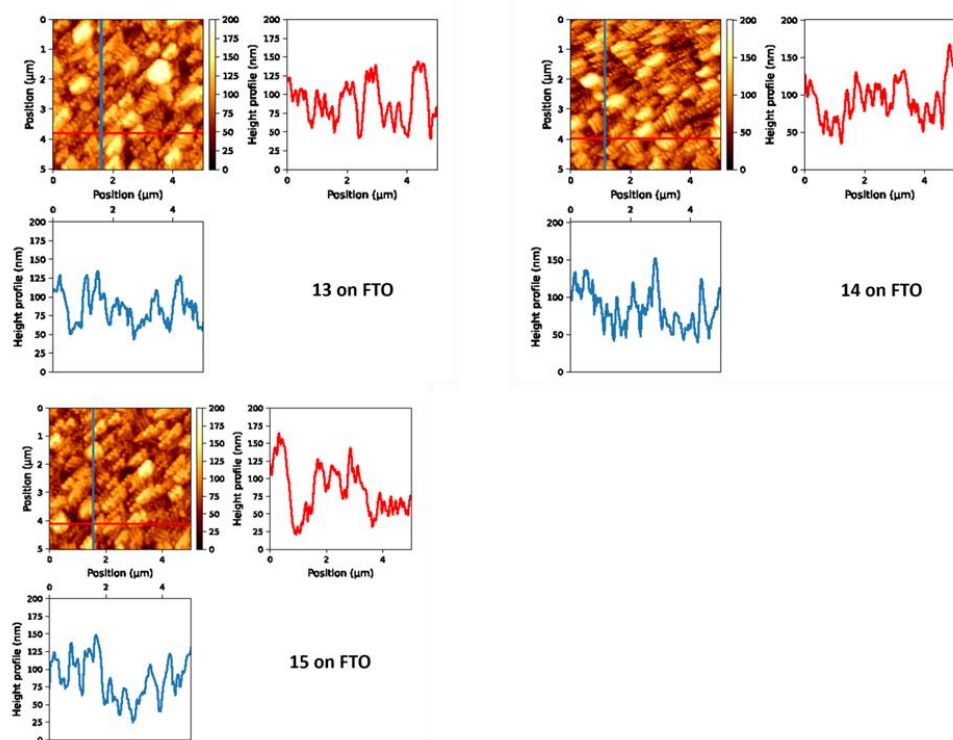


Figure S66. AFM measurements performed on samples **13**, **14**, and **15** dropcasted on FTO.

Bode diagrams

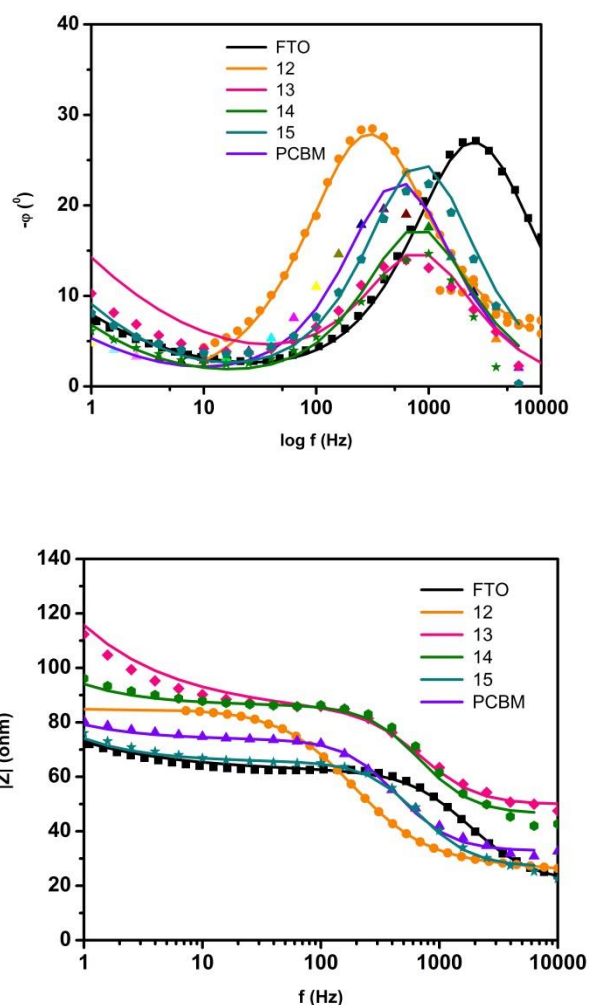


Figure S67. EIS diagrams were obtained by fitting the experimental result with equivalent circuits: (top) phase, (down) impedance magnitude - Bode diagrams of the samples. Measured in water solution with inorganic electrolyte $K_3[Fe(CN)_6]$ (5×10^{-4} M), $K_4[Fe(CN)_6]$ (5×10^{-4} M) and KCl (0.1 M). Symbols represent experimental data, while the straight lines represent data obtained by fitting with an equivalent circuit from Fig. 3.

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