

Supplementary Information

Organic Photovoltaics Incorporating Fulleroisoquinolinones as n-Type Materials

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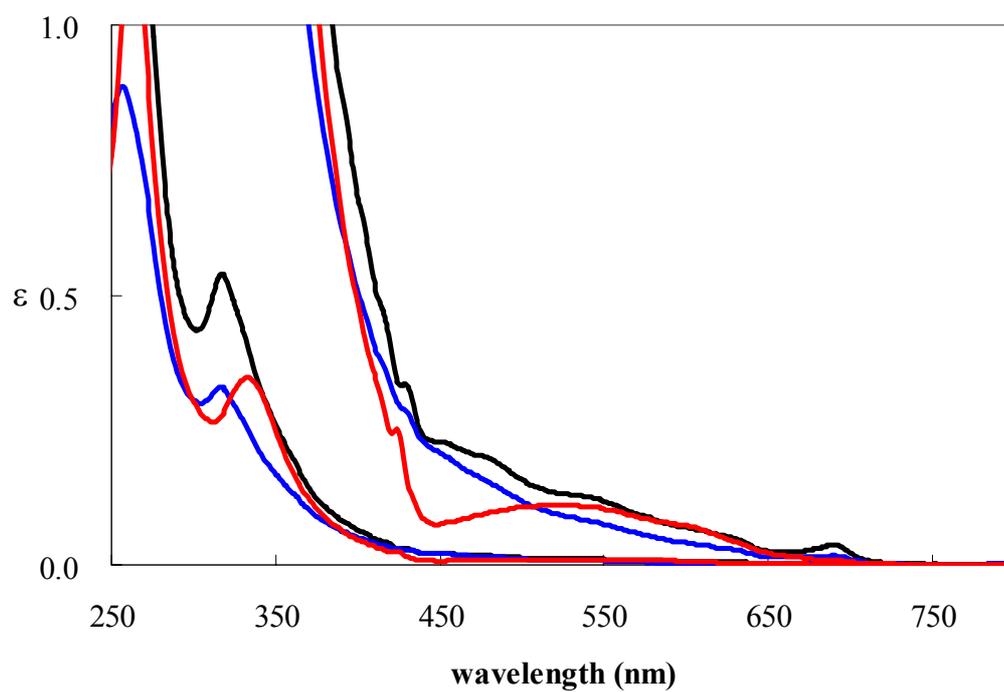


Figure S1. UV-Vis spectra of **2c** (black line, 5.9×10^{-5} M), **4c** (blue line, 5.0×10^{-5} M), and PCBM (red line, 5.1×10^{-5} M) in CHCl_3 .

Experimental

Materials and Equipment for Polymer Solar Cells

General methods. All reactions were performed under argon. Dry *o*-DCB was distilled from CaH₂ under argon. The chemical shifts of ¹H and ¹³C are with reference to TMS or CHCl₃. All chemicals were purchased and used as received unless otherwise specified.

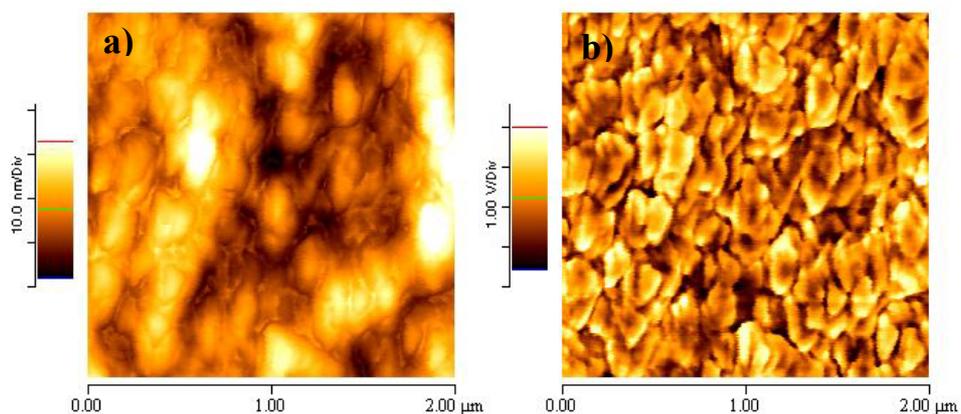
Photovoltaic Cells Fabrication and Testing

All the bulk-heterojunction photovoltaic cells were prepared using the same preparation procedures and device fabrication procedure referring as following: The glass-indium tin oxide (ITO) substrates (obtained from Sanyo, Japan (8Ω/□)) were first patterned by lithograph, then cleaned with detergent, and ultrasonicated in acetone and isopropyl alcohol, and subsequently dried on hot plate at 120 °C for 5 min, and finally treated with oxygen plasma for 5min. Poly(3,4-ethylene-dioxythiophene):poly(styrene-sulfonate) (PEDOT:PSS, Baytron P-VP AI4083) was filtered through a 0.45 μm filter before being deposited on ITO with a thickness around 30 nm by spin coating at 3000 rpm in the air and dried at 150 °C for 30 min inside glove box. The devices were fabricated using the fulleroisoquinolinones concentration of 15 mg/mL, a spin rate of 600 rpm for 30 s, and *o*-DCB as the solvent. The optimal thickness of the active layers obtained under these conditions was ~ 150 nm. Subsequently the device was completed by coating 30 nm thickness of Ca and an 80 nm thickness of Al in < 10⁻⁶ torr pressure respectively. The active area of the device is 5 mm². Finally the cell was encapsulated using UV-curing glue (purchased from Nagase, Japan). During the encapsulation process, the UV-glue was dispensed onto the edge of a piece of glass in the air. The UV-glue coated glass was transferred to the glove box to cover of the OPV device. The device was then sealed by pressing the UV-glue coated glass on top of the device and the device underwent UV curing (254nm) for 2 min. After encapsulation using UV-curing glue, we measured the I–V characteristics in air. I–V curves of the OPV devices were measured using a computer-controlled Keithley 2400 source measurement unit (SMU) equipped with a Peccell solar simulator under AM 1.5G illumination (100 mW cm⁻²). The illumination intensity was calibrated using a standard Si photodiode detector equipped with a KG-5 filter. The output photocurrent was adjusted to match the photocurrent of the Si reference cell to obtain a power density of 100 mW cm⁻². After encapsulation, all devices measurements were operated in an ambient atmosphere at 25 °C. The efficiency of 3.5% of a P3HT/PCBM reference cell measured under illumination in our laboratory was verified to be 3.4% under AM1.5G conditions (100 mW cm⁻²) in National Institute of Advanced Industrial Science and Technology (AIST, Japan).

Table 1. J-V characteristics of devices incorporating PCBM/P3HT (1:1, w/w).

<i>entry</i>	<i>compound</i>	J_{sc} (mA/cm ²)	V_{oc} (V)	<i>FF</i>	<i>PCE</i> (%)
1	PCBM	6.7	0.60	0.67	2.7
2	PCBM ^a	7.7	0.61	0.68	3.2
3	PCBM ^b	7.2	0.62	0.70	3.1
4	PCBM ^c	7.4	0.65	0.66	3.2

^aannealing at 140 °C, ^bannealing at 160 °C, ^cannealing at 180 °C



RMS=6.3nm

Figure S2. Tapping-mode AFM AFM (2×2 μ m) topography (a) and phase images (b) of P3HT: **4d** blend film (1:1, w/w)

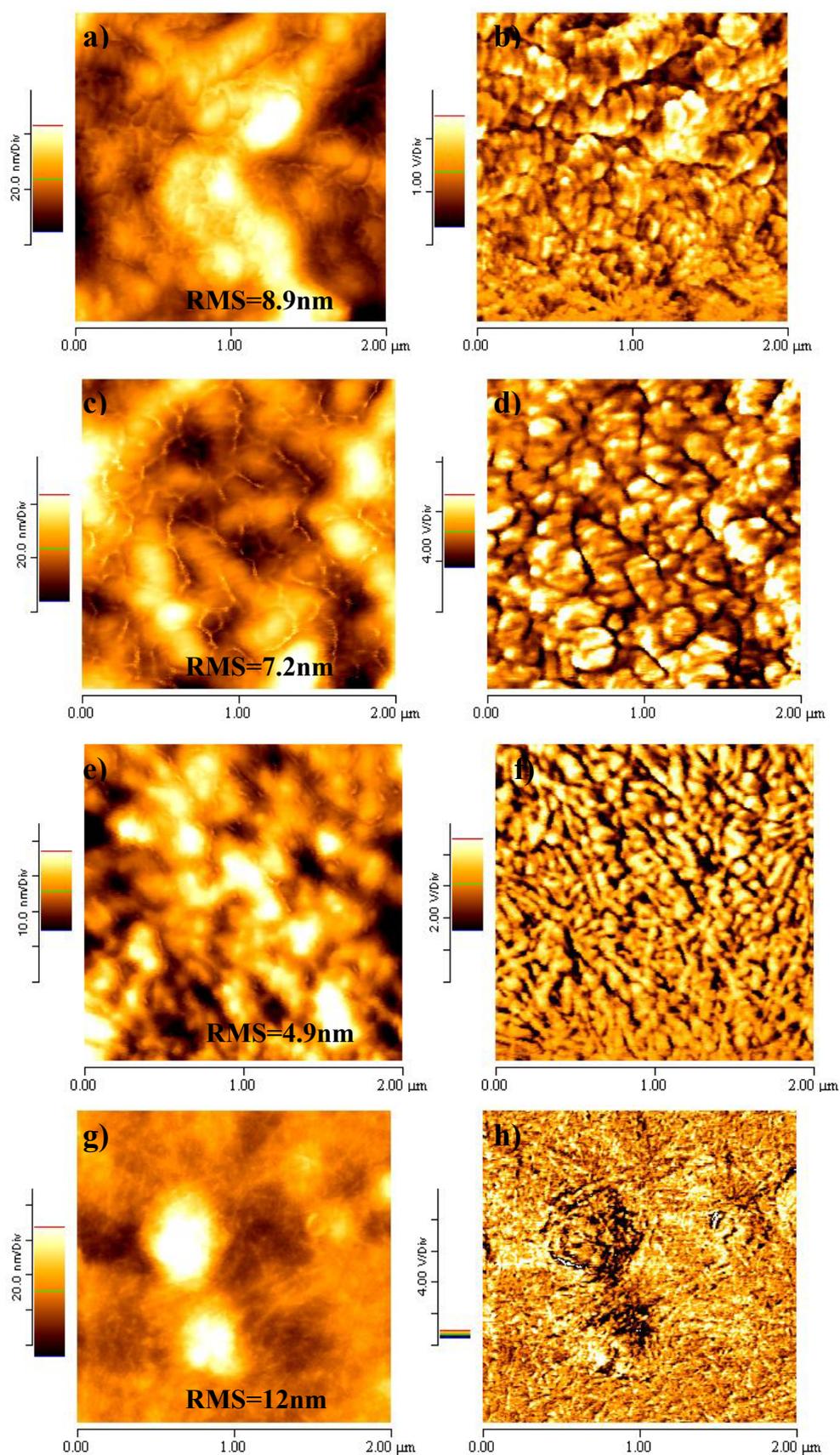


Figure S3. Tapping-mode AFM AFM (2×2 μ m) topography a), c), e), g) and phase images b), d), f), h) of P3HT: fullerisoquinolinones blend films (1:1, w/w): (a), (b) **2a**; (c), (d) **2b**; (e), (f) **2c**; and g), h) **2d**.

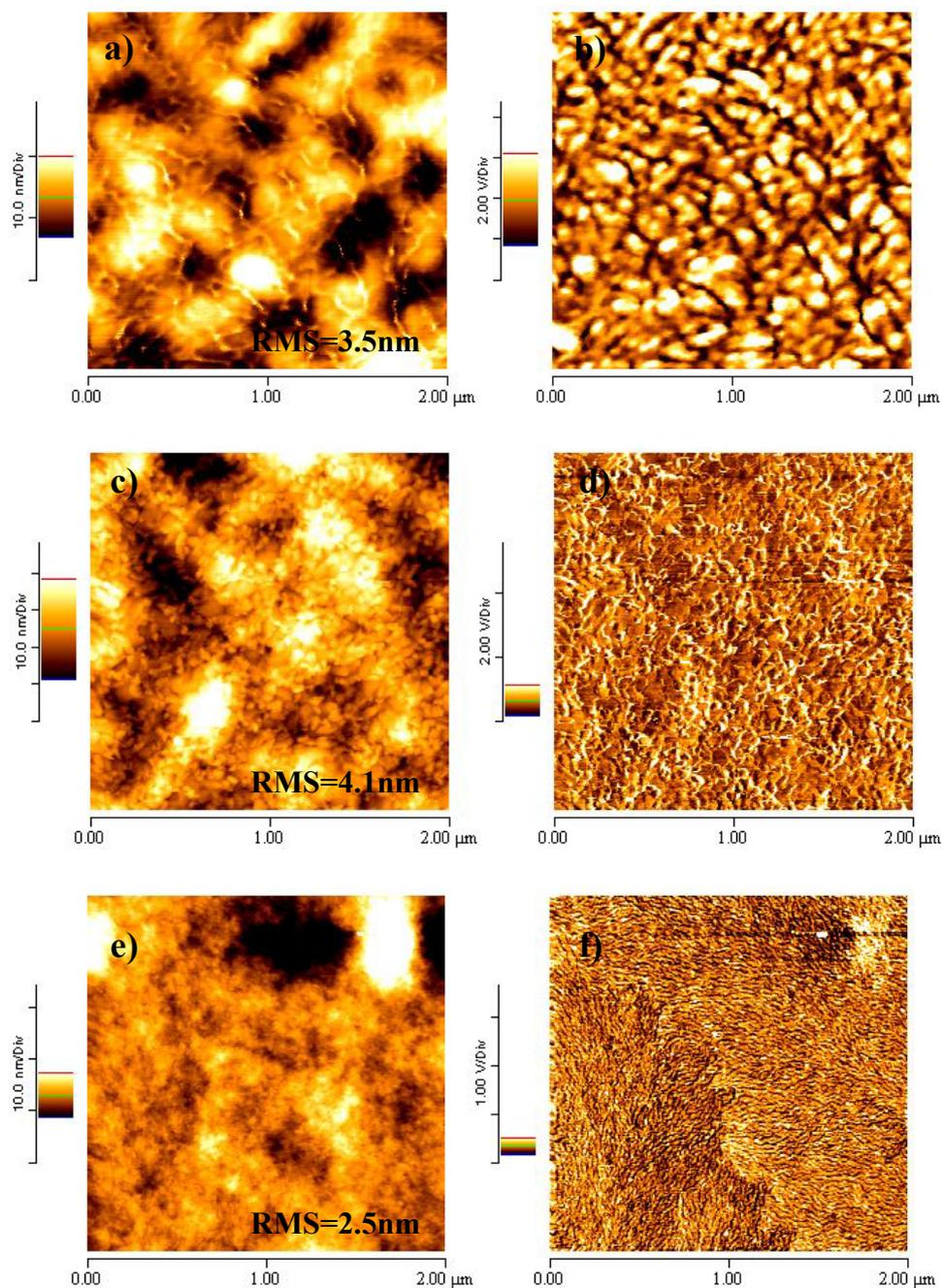


Figure S4. AFM ($2 \times 2 \mu\text{m}$) topography (a), (c), (e) and phase images (b), (d), (f) for P3HT:2c blend films (1:1, w/w): (a), (b) annealing at 140 °C for 20 min; (c), (d) annealing at 160 °C for 20 min; (e), (f) annealing at 180 °C for 20 min.

Synthetic procedure and spectral data for compound 2a-d and 4a-d

Compound 2a:

To a solution of C₆₀ (144 mg, 0.20 mmol) in a mixture of *o*-dichlorobenzene (18 mL) and CH₃CN (2 mL) was sequentially added N-hexylbenzamide (203 mg, 1.00 mmol), K₂S₂O₈ (290 mg, 1.10 mmol), PTSA (76 mg, 0.42 mmol), and Pd(OAc)₂ (4.4 mg, 0.02 mmol). After being stirred at 130 °C for 24 h, the reaction mixture was separated on a silica gel column with a mixture of hexanes and toluene (7:1) as eluent to give recovered C₆₀ (43 mg) and **2a** (58 mg) in 31% yield. (53% based on recovered C₆₀). *R_f* = 0.43 (hexanes:toluene = 1:1). ¹H NMR (300 MHz, CDCl₃): δ (ppm) 0.87 (m, 3H), 1.27 (m, 4H), 1.39 (m, 2H), 1.97 (m, 2H), 4.78 (t, *J* = 7.5 Hz, 2H), 7.66 (t, *J* = 7.2 Hz, 1H), 7.76 (t, *J* = 7.2 Hz, 1H), 8.71 (m, 2H); ¹³C NMR (150 MHz, CDCl₃): δ (ppm) 14.01, 22.55, 27.03, 29.44, 31.41, 45.77, 63.05, 79.59, 125.98, 128.19, 129.96, 130.14, 133.01, 133.93, 133.98, 135.68, 138.22, 139.51, 141.22, 141.45, 141.60, 141.92, 142.55, 142.58, 142.89, 142.98, 143.28, 144.63, 144.70, 144.87, 145.08, 145.30, 145.41, 145.94, 146.20, 146.27, 146.39, 146.70, 146.80, 147.79, 147.93, 148.42, 155.70, 161.73; HRMS (FAB): *m/z* calcd for C₇₃H₁₈NO (M+H⁺) 924.1388; found 924.1382; FT-IR ν (cm⁻¹) 527, 546, 576, 670, 688, 756, 821, 1032, 1052, 1087, 1214, 1320, 1368, 1400, 1463, 1585, 1597, 1648, 2854, 2925, 2953, 3011; UV-Vis λ_{max} (ε) (CHCl₃, 4.98×10⁻⁵ M): 230 (1.14×10⁴), 257 (1.26×10⁴), 317 (4.58×10³) nm.

Compound 2b:

To a solution of C₆₀ (75 mg, 0.10 mmol) in a mixture of *o*-dichlorobenzene (18 mL) and CH₃CN (2 mL) was sequentially added N-decylbenzamide (118 mg, 0.50 mmol), K₂S₂O₈ (140 mg, 0.50 mmol), PTSA (145 mg, 0.80 mmol), and Pd(OAc)₂ (2.2 mg, 0.01 mmol). After being stirred at 130 °C for 24 h, the reaction mixture was separated on a silica gel column with a mixture of hexanes and toluene (1:1) as eluent to give recovery C₆₀ (41 mg) and **2b** (16 mg) in 16% yield. (35% based on recovery C₆₀). ¹H NMR (600 MHz, CDCl₃): δ (ppm) 0.82 (t, *J* = 1.8 Hz, 3H), 1.21 (m, 4H), 1.28 (m, 4H), 1.38 (m, 2H), 1.97 (m, 2H), 4.76 (t, *J* = 2.1 Hz, 2H), 7.64 (m, 1H), 7.74 (m, 1H), 8.69 (m, 2H); ¹³C NMR (150 MHz, CDCl₃): δ (ppm) 14.12, 22.65, 27.35, 29.19 (2C), 29.47, 31.76, 45.78, 63.06, 79.60, 125.99, 128.20, 129.97, 130.14, 133.02, 133.95, 133.99, 135.69, 138.24, 139.51, 141.23, 141.45, 141.61, 141.94, 142.56, 142.59, 142.91, 142.99, 143.29, 144.65, 144.71, 144.88, 145.09, 145.31, 145.42, 145.94, 146.21, 146.28, 146.40, 146.71, 146.81, 147.80, 147.94, 148.34, 155.71, 161.74; HRMS (FAB): *m/z* calcd for C₇₇H₂₆NO (M+H⁺) 952.1701; found 952.1708; FT-IR ν (cm⁻¹) 527, 546, 576, 595, 622, 666, 688, 755, 819, 1031, 1090, 1214, 1320, 1374, 1399, 1463, 1584, 1651, 2852, 2923, 3011; UV-Vis (CHCl₃, 4.31×10⁻⁵ M): λ_{max} (ε) 230 (9.47×10³), 257 (1.02×10⁴), 318 (3.78×10³) nm.

Compound 2c:

To a solution of C₆₀ (72 mg, 0.10 mmol) in a mixture of *o*-dichlorobenzene (8 mL) and CH₃CN (1 mL) was sequentially added N-decylbenzamide (131 mg, 0.50 mmol), K₂S₂O₈ (135 mg, 0.50 mmol), PTSA (31 mg, 0.18 mmol), and Pd(OAc)₂ (4.4 mg, 0.02 mmol). After being stirred at 130 °C for 24 h, the reaction mixture was separated on a silica gel column with a mixture of hexanes and toluene (7:1) as eluent to give unreacted C₆₀ (21 mg) and **2c** (18 mg) in 19% yield. (26% based on recovered C₆₀). ¹H NMR (600 MHz, CDCl₃): δ (ppm) 0.79 (t, *J* = 3.4 Hz, 3H), 1.20 (m, 12H), 1.21 (t, *J* = 1.8 Hz, 2H), 1.80 (t, *J* = 2.0 Hz, 2H), 4.56 (t, *J* = 2.0 Hz, 2H), 7.51 (m, 1 H), 7.61 (m, 1H), 8.49 (m, 2H); ¹³C NMR (150 MHz, CDCl₃): δ (ppm) 15.48, 24.16, 28.56, 30.51, 30.53, 30.61, 30.82, 30.83, 33.14, 46.21, 63.61, 80.10, 127.14, 128.29, 128.78, 130.43, 131.27, 133.30, 134.22, 134.72, 136.27, 138.97, 140.21, 141.94, 142.16, 142.39, 142.70, 143.26, 143.59, 143.68, 144.00, 145.35, 145.42, 145.56, 145.80, 145.96, 146.05, 146.12, 146.58, 146.93, 147.05, 147.38, 147.44, 148.57, 148.79, 149.04, 156.49, 160.76; HRMS (FAB): *m/z* calcd for C₇₇H₂₆NO (M+H⁺) 980.2014; found 980.2010; FT-IR ν (cm⁻¹) 526, 546, 595, 687, 737, 819, 1032, 1101, 1153, 1183, 1260, 1320, 1397, 1461, 1514, 1651, 2850, 2921, 2948; UV-Vis (CHCl₃, 5.92×10⁻⁵ M): λ_{max} (ε) 230 (1.34×10⁴), 257 (1.52×10⁴), 318 (5.39×10³) nm.

Compound 2d:

To a solution of C₆₀ (72 mg, 0.10 mmol) in a mixture of *o*-dichlorobenzene (18 mL) and CH₃CN (2 mL) was sequentially added N-decylbenzamide (145 mg, 0.50 mmol), K₂S₂O₈ (136 mg, 0.50 mmol), 2,5-dimethylbenzoic acid (279 mg, 0.18 mmol), and Pd(OAc)₂ (4.5 mg, 0.02 mmol). After being stirred at 130 °C for 24 h, the reaction mixture was separated on a silica gel column with a mixture of hexanes and toluene (7:1) as eluent to give unreacted C₆₀ (53 mg) and **2c** (4.6 mg) in 5% yield. (74% based on recovered C₆₀). Spectral Data: ¹H NMR (600 MHz, CDCl₃): δ (ppm) 0.84 (t, *J* = 6.7 Hz, 3H), 1.39-1.19 (m, 18H), 1.95 (m, 2H), 4.77 (t, *J* = 7.7 Hz, 2H), 7.65 (m, 1 H), 7.74 (m, 1H), 8.69 (m, 2H); ¹³C NMR (150 MHz, CDCl₃): δ (ppm) 14.12, 22.68, 27.31, 29.19, 29.35, 30.61, 29.41, 29.49, 29.55, 29.64(×2), 31.90, 45.76, 63.07, 79.61, 126.00, 128.19, 129.96, 130.12, 133.00, 133.98, 135.69, 138.23, 139.51, 141.23, 141.46, 141.62, 141.95, 142.57, 142.59, 142.91, 143.00, 143.29, 144.64, 144.72, 144.89, 145.10, 145.32, 145.43 (2C), 145.95, 146.22, 146.29, 146.41, 146.71, 146.81, 147.82, 147.95, 148.44, 155.73, 161.75; HRMS (FAB): *m/z* calcd for C₇₉H₃₀NO (M+H⁺) 1008.2327; found 1080.2318; FT-IR ν (cm⁻¹) 527, 547, 576, 688, 756, 1050, 1101, 1217, 1320, 1397, 1462, 1651, 2850, 2922; UV-Vis (CHCl₃, 5.16×10⁻⁵ M): λ_{max} (ε) 230 (1.30×10⁵), 257 (1.59×10⁵), 317 (5.31×10⁴) nm.

Compound 4a:

To a solution of C₆₀ (76 mg, 0.10 mmol) in a mixture of *o*-dichlorobenzene (18 mL) and CH₃CN (2 mL) was sequentially added N-phenylcaproamide (97 mg, 0.50 mmol), K₂S₂O₈ (141 mg, 0.50 mmol), PTSA (29 mg, 0.16 mmol), and Pd(OAc)₂ (3.0 mg,

0.01 mmol). After being stirred at 130 °C for 24 h, the reaction mixture was separated on a silica gel column with a mixture of hexanes and toluene (1:1) as eluent to give recovery C₆₀ (25 mg) and **4a** (33 mg) in 34% yield. (50% based on recovered C₆₀). *R_f* = 0.63 (hexanes:toluene = 1:1). ¹H NMR (300 MHz, CS₂/C₆D₁₂ as external lock solvent): δ (ppm) 0.87 (t, *J* = 6.6 Hz, 3H), 1.35 (m, 4H), 1.81 (m, 2H), 2.99 (t, *J* = 7.2 Hz, 2H), 7.24 (t, *J* = 7.3 Hz, 1H), 7.44 (t, *J* = 7.7 Hz, 1H), 7.61 (d, *J* = 8.4 Hz, 1H), 7.98 (d, *J* = 7.7 Hz, 1H); due to its poor solubility, ¹³C NMR was not measured; HRMS (FAB): *m/z* calcd for C₇₂H₁₆NO (M+H⁺) 910.1232; found 910.1234; FT-IR ν (cm⁻¹) 552, 574, 595, 667, 738, 784, 927, 1001, 1090, 1159, 1184, 1212, 1283, 1360, 1419, 1481, 1513, 1674, 2856, 2923, 2948; UV-Vis (CHCl₃, 4.73×10⁻⁵ M): λ_{max} (ε) 229 (1.15×10⁴), 256 (1.43×10⁴), 314 (4.42×10³) nm.

Compound 4b:

To a solution of C₆₀ (73 mg, 0.10 mmol) in a mixture of *o*-dichlorobenzene (8 mL) and CH₃CN (1 mL) was sequentially added N-phenyloctanamide (112 mg, 0.50 mmol), K₂S₂O₈ (141 mg, 0.50 mmol), PTSA (29 mg, 0.17 mmol), and Pd(OAc)₂ (2.5 mg, 0.01 mmol). After being stirred at 130 °C for 24 h, the reaction mixture was separated on a silica gel column with a mixture of hexanes and toluene (1:1) as eluent to give recovered C₆₀ (11 mg) and **4b** (25 mg) in 27% yield. (32% based on recovered C₆₀). *R_f* 0.68 (hexanes:toluene = 1:1). ¹H NMR (300 MHz, CS₂/C₆D₁₂ as external lock solvent): δ (ppm) 0.95 (br, 3H), 1.38-1.52 (br, 8H), 1.93 (t, *J* = 6.7 Hz, 2H), 3.11 (t, *J* = 6.6 Hz, 2H), 7.36 (t, *J* = 7.1 Hz, 1H), 7.56 (t, *J* = 7.0 Hz, 1H), 7.73 (d, *J* = 8.1 Hz, 1H), 8.10 (d, *J* = 7.0 Hz, 1H); ¹³C NMR (150 MHz, CS₂/C₆D₆ with Cr(acac)₃ as relaxation reagent): δ (ppm) 15.82, 24.48, 26.55, 30.90, 30.95, 33.38, 40.51, 72.28, 88.09, 117.16, 125.29, 130.84, 131.97, 136.09, 137.39, 138.41, 142.05, 142.08, 142.73, 142.78, 143.09, 143.14, 143.29, 143.81, 143.84, 143.91, 144.00, 144.11, 145.51, 145.59, 146.01, 146.10, 146.22 (2C), 146.29, 146.84, 146.90, 147.15, 147.26, 147.44, 147.50, 148.32, 148.79, 149.55, 154.12, 172.13; HRMS (FAB): *m/z* calcd for C₇₄H₂₀NO (M+H⁺) 938.1545; found 938.1543; FT-IR ν (cm⁻¹) 526, 543, 574, 596, 667, 740, 785, 901, 950, 1000, 1090, 1159, 1184, 1218, 1284, 1304, 1371, 1425, 1461, 1481, 1512, 1599, 1673, 2851, 2921, 2949; UV-Vis (CHCl₃, 4.80×10⁻⁵ M): λ_{max} (ε) 229 (1.34×10⁴), 256 (1.63×10⁴), 314 (5.13×10³) nm.

Compound 4c:

To a solution of C₆₀ (72 mg, 0.10 mmol) in a mixture of *o*-dichlorobenzene (8 mL) and CH₃CN (1 mL) was sequentially added N-phenyldecanamide (124 mg, 0.50 mmol), K₂S₂O₈ (140 mg, 0.50 mmol), PTSA (35 mg, 0.20 mmol), and Pd(OAc)₂ (2.0 mg, 0.01 mmol). After being stirred at 130 °C for 24 h, the reaction mixture was separated on a silica gel column with a mixture of hexanes and toluene (1:1) as eluent to give recovery C₆₀ (6.5 mg) and **21** (16 mg) in 16% yield. (18% based on recovered C₆₀). *R_f* = 0.70 (hexanes:toluene = 1:1). ¹H NMR (300 MHz, CS₂/C₆D₁₂ as external

lock solvent): δ (ppm) 0.98 (t, $J = 8.6$ Hz, 3H), 1.38-1.63 (m, 12H), 1.98 (m, 2H), 3.17 (t, $J = 7.1$ Hz, 2H), 7.42 (t, $J = 7.4$ Hz, 1H), 7.62 (t, $J = 7.4$ Hz, 1H), 7.79 (d, $J = 8.3$ Hz, 1H), 8.17 (d, $J = 7.6$ Hz, 1H); ^{13}C NMR (150 MHz, $\text{CS}_2/\text{C}_6\text{D}_6$ with $\text{Cr}(\text{acac})_3$ as relaxation reagent): δ (ppm) 14.12, 22.75, 25.03, 29.32, 29.37, 29.52, 29.55, 31.90, 39.29, 71.24, 87.09, 116.09, 124.22, 126.50, 129.60, 131.21, 134.92, 134.92, 136.42, 137.45, 140.68, 140.87, 141.51, 141.64, 141.90, 141.99, 142.07, 142.63, 142.71, 142.80, 144.37, 144.85, 144.94, 144.97, 145.02, 145.15, 145.69, 145.74, 145.99, 146.10, 146.27, 146.33, 147.17, 147.66, 147.96, 153.02, 172.62; HRMS (FAB): m/z calcd for $\text{C}_{76}\text{H}_{24}\text{NO}$ ($\text{M} + \text{H}^+$) 966.1858; found 966.1868; FT-IR ν (cm^{-1}) 527, 543, 554, 563, 575, 597, 667, 740, 786, 900, 927, 950, 1002, 1036, 1090, 1159, 1185, 1217, 1285, 1304, 1370, 1424, 1462, 1481, 1512, 1599, 1675, 2851, 2922; UV-Vis (CHCl_3 , 4.97×10^{-5} M): λ_{max} (ϵ) 230 (8.21×10^3), 256 (8.87×10^3), 316 (3.30×10^3) nm.

Compound 4d:

To a solution of C_{60} (74 mg, 0.10 mmol) in a mixture of *o*-dichlorobenzene (18 mL) and CH_3CN (2 mL) was sequentially added *N*-phenyldodecamide (275 mg, 1.00 mmol), $\text{K}_2\text{S}_2\text{O}_8$ (138 mg, 0.50 mmol), PTSA (144 mg, 0.80 mmol), and $\text{Pd}(\text{OAc})_2$ (3.0 mg, 0.01 mmol). After being stirred at 130 °C for 24 h, the reaction mixture was separated on a silica gel column with a mixture of hexanes and toluene (1:1) as eluent to give recovery C_{60} (25.7 mg) and **4d** (22 mg) in 22% yield. (27% based on recovered C_{60}). ^1H NMR (300 MHz, $\text{CS}_2/\text{C}_6\text{D}_{12}$ as external lock solvent): δ (ppm) 1.00 (m, 3H), 1.38-1.61 (m, 16H), 1.78 (m, 2H), 3.19 (t, $J = 7.2$ Hz, 2H), 7.44 (t, $J = 7.4$ Hz, 1H), 7.64 (t, $J = 8.4$ Hz, 1H), 7.81 (d, $J = 8.3$ Hz, 1H), 8.19 (d, $J = 7.6$ Hz, 1H); ^{13}C NMR (150 MHz, $\text{CS}_2/\text{C}_6\text{D}_6$ with $\text{Cr}(\text{acac})_3$ as relaxation reagent): δ (ppm) 15.81, 24.49, 26.53, 30.98 (2C), 31.21 (2C), 31.27 (2C), 33.49, 40.49, 72.27, 88.08, 117.14, 125.28, 127.68, 130.82, 131.95, 136.09, 137.38, 138.39, 142.03, 142.06, 142.72, 142.77, 143.08, 143.13, 143.28, 143.80, 143.82, 143.90, 143.99, 145.50, 145.57, 146.00, 146.09, 146.21, 146.27, 146.82, 146.89, 147.14, 147.25, 147.43, 147.49, 148.30, 148.78, 149.54, 154.10, 172.12; HRMS (FAB): m/z calcd for $\text{C}_{78}\text{H}_{28}\text{NO}$ ($\text{M} + \text{H}^+$) 994.2171; found 994.2188; FT-IR ν (cm^{-1}) 525, 562, 596, 741, 794, 901, 947, 1001, 1090, 1157, 1184, 1215, 1297, 1304, 1371, 1427, 1481, 1598, 1672, 2850, 2921; UV-Vis λ_{max} (ϵ) (CHCl_3 , 5.23×10^{-5} M): 229 (1.47×10^4), 256 (1.80×10^4), 314 (5.68×10^3) nm.

Figure S6. ^{13}C NMR spectra of compound **2a**

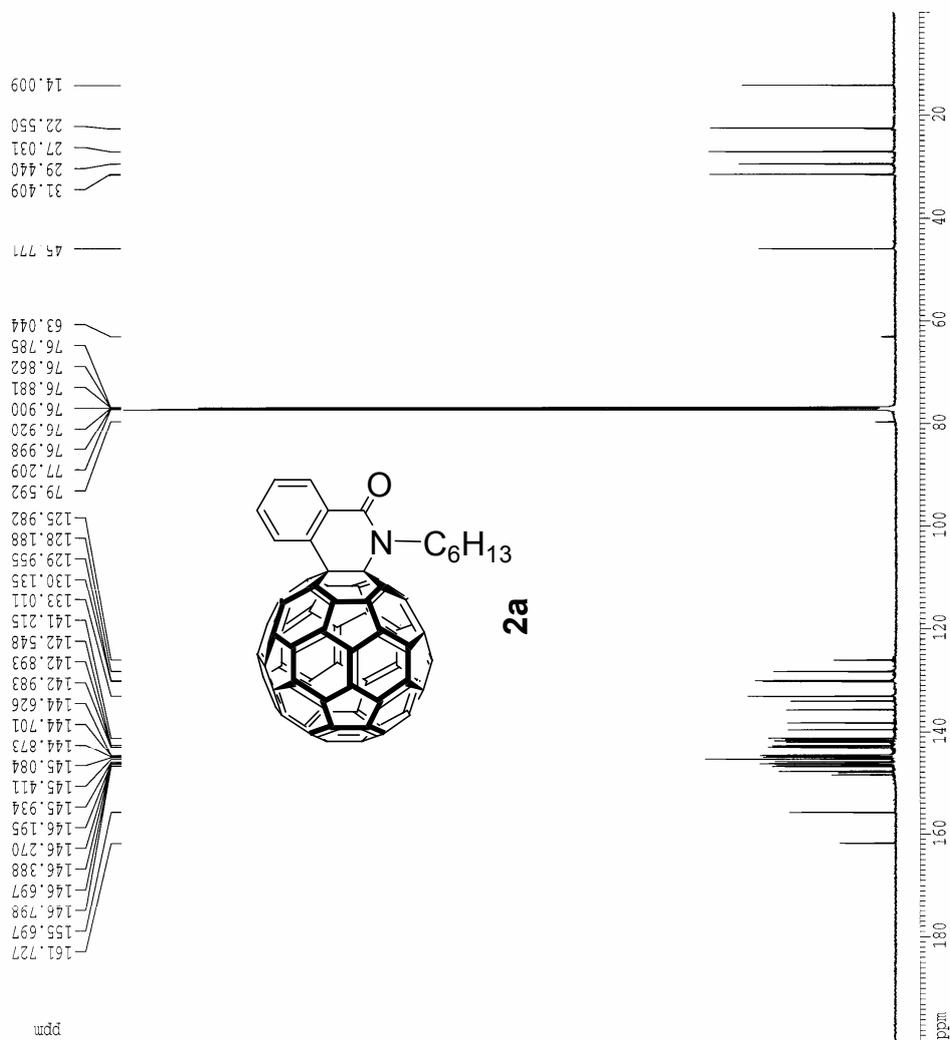


Figure S7. ^1H NMR spectra of compound **2b** (CDCl_3)

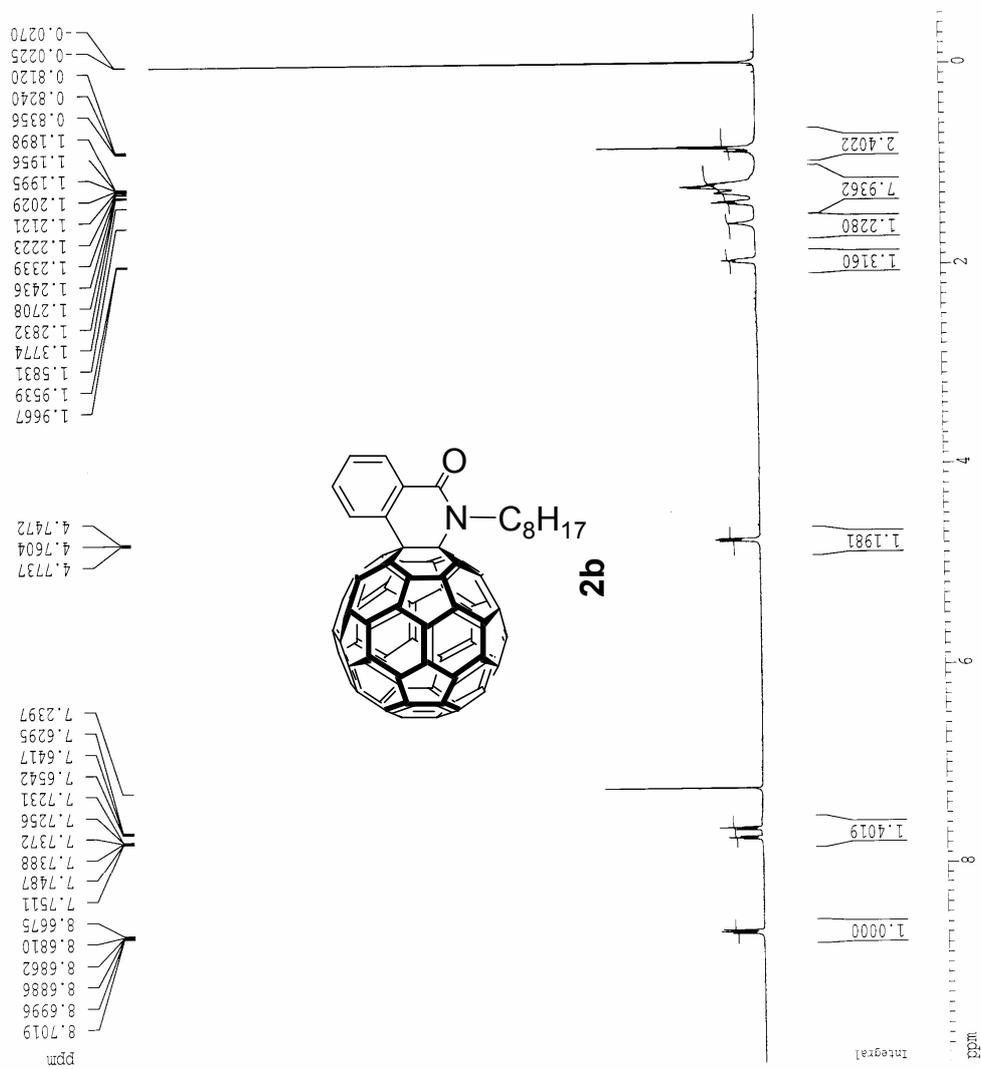


Figure S8. ^{13}C NMR spectra of compound **2b** (CDCl_3)

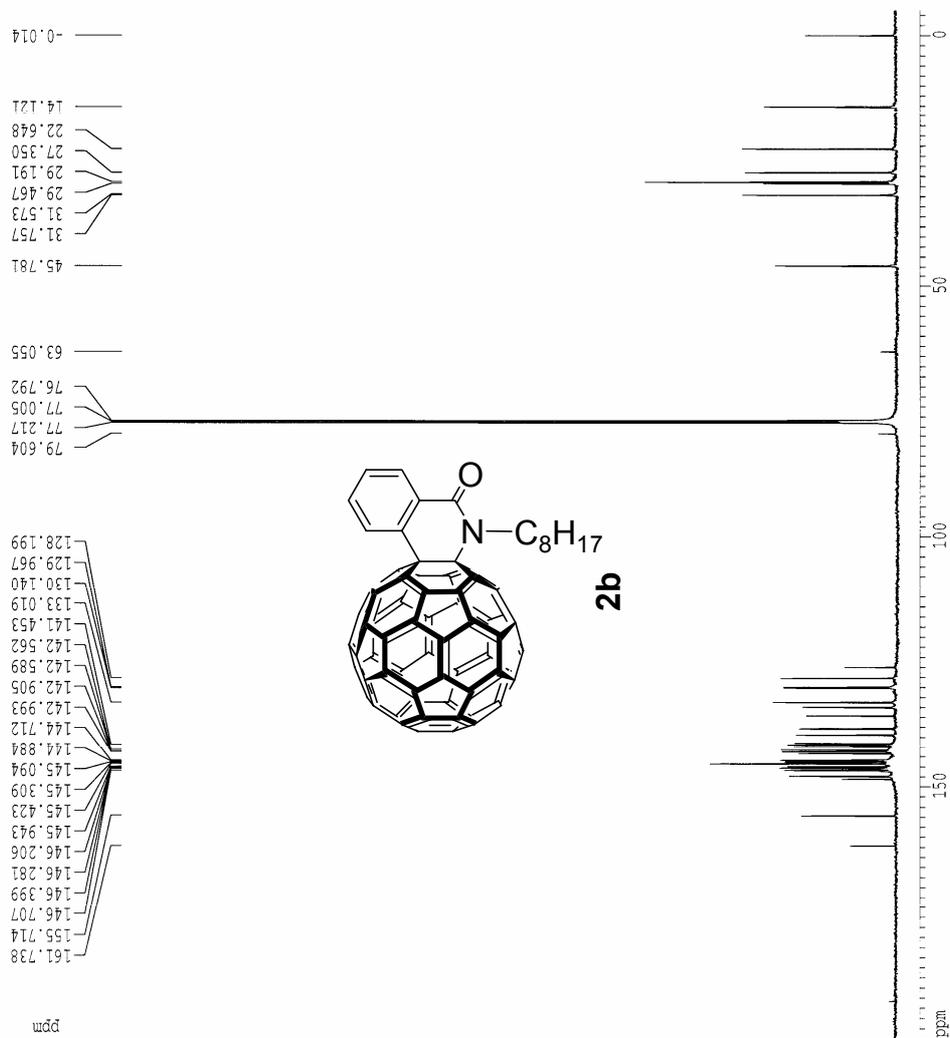


Figure S9. ^1H NMR spectra of compound **2c** (CDCl_3)

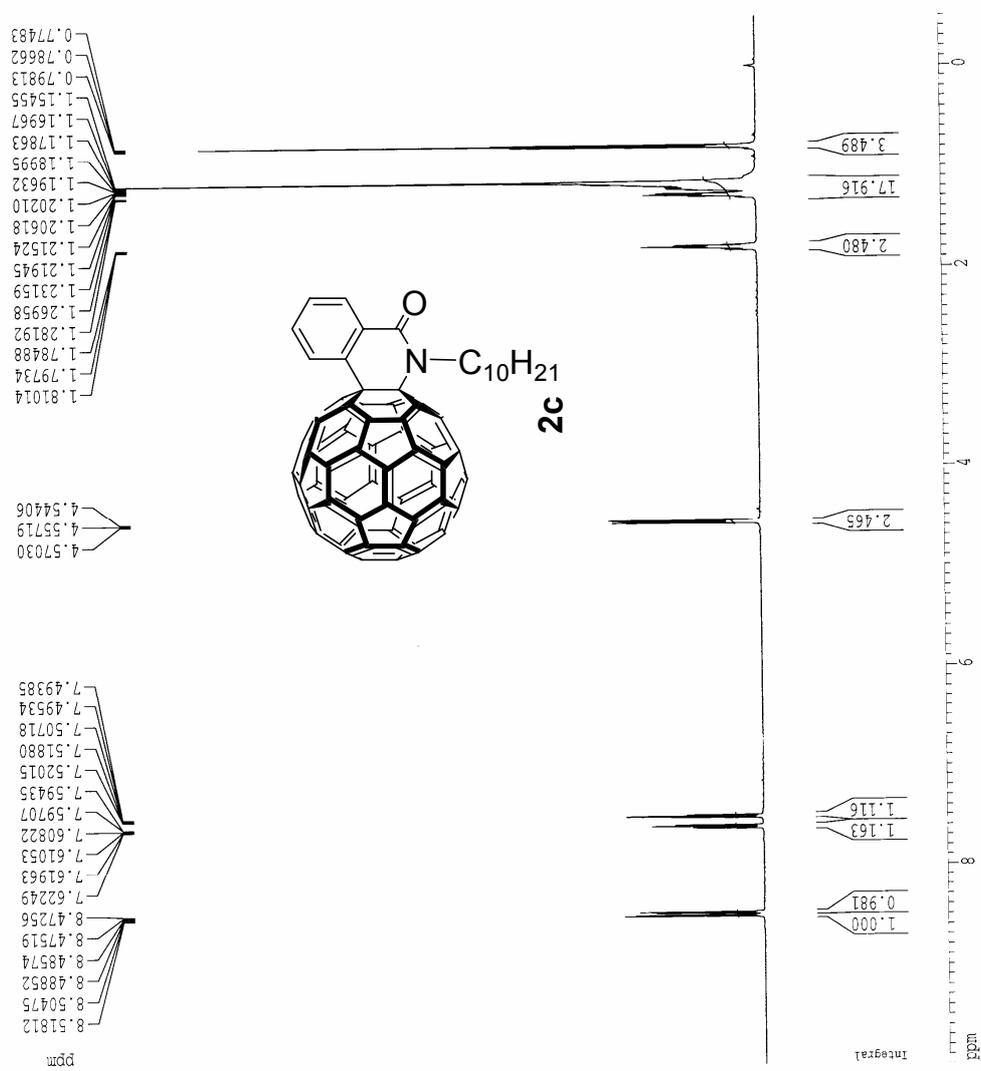


Figure S10. ^{13}C NMR spectra of compound **2c** (CDCl_3)

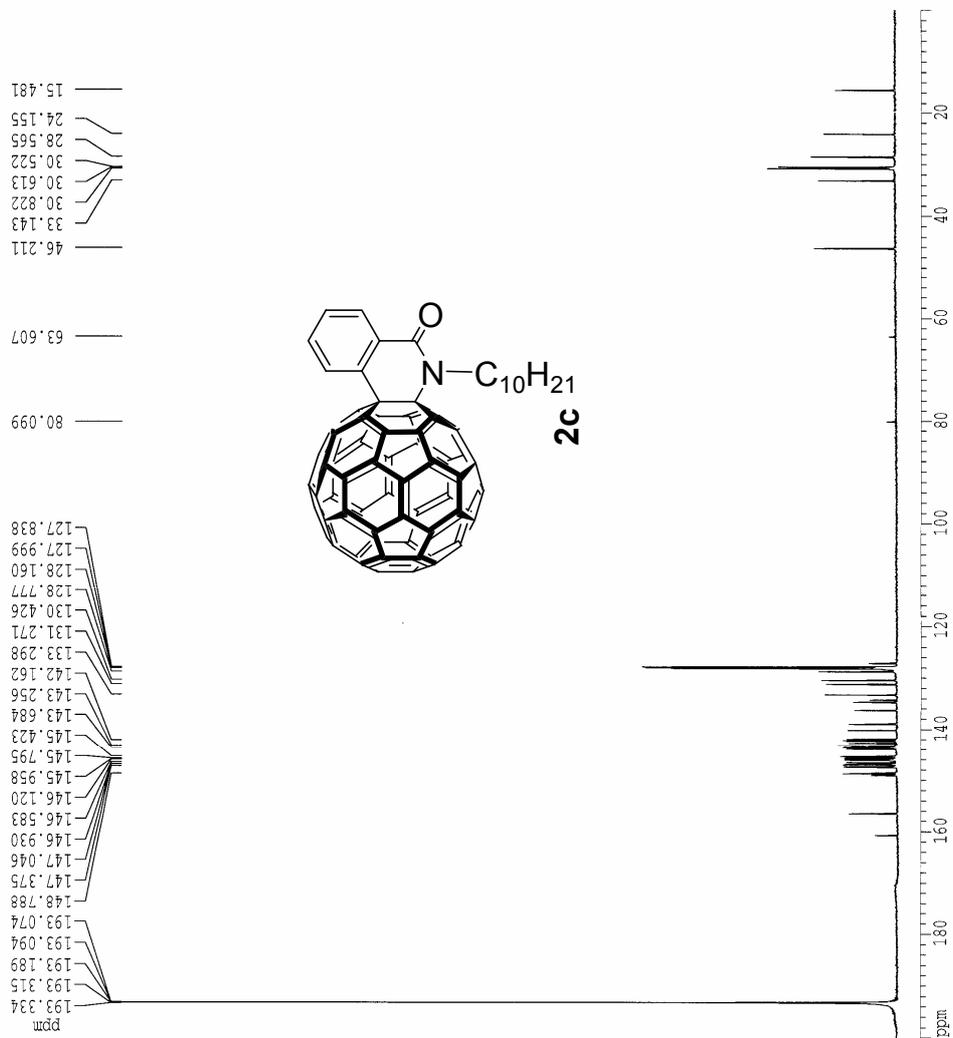


Figure S11. ^1H NMR spectra of compound **2d** (CDCl_3)

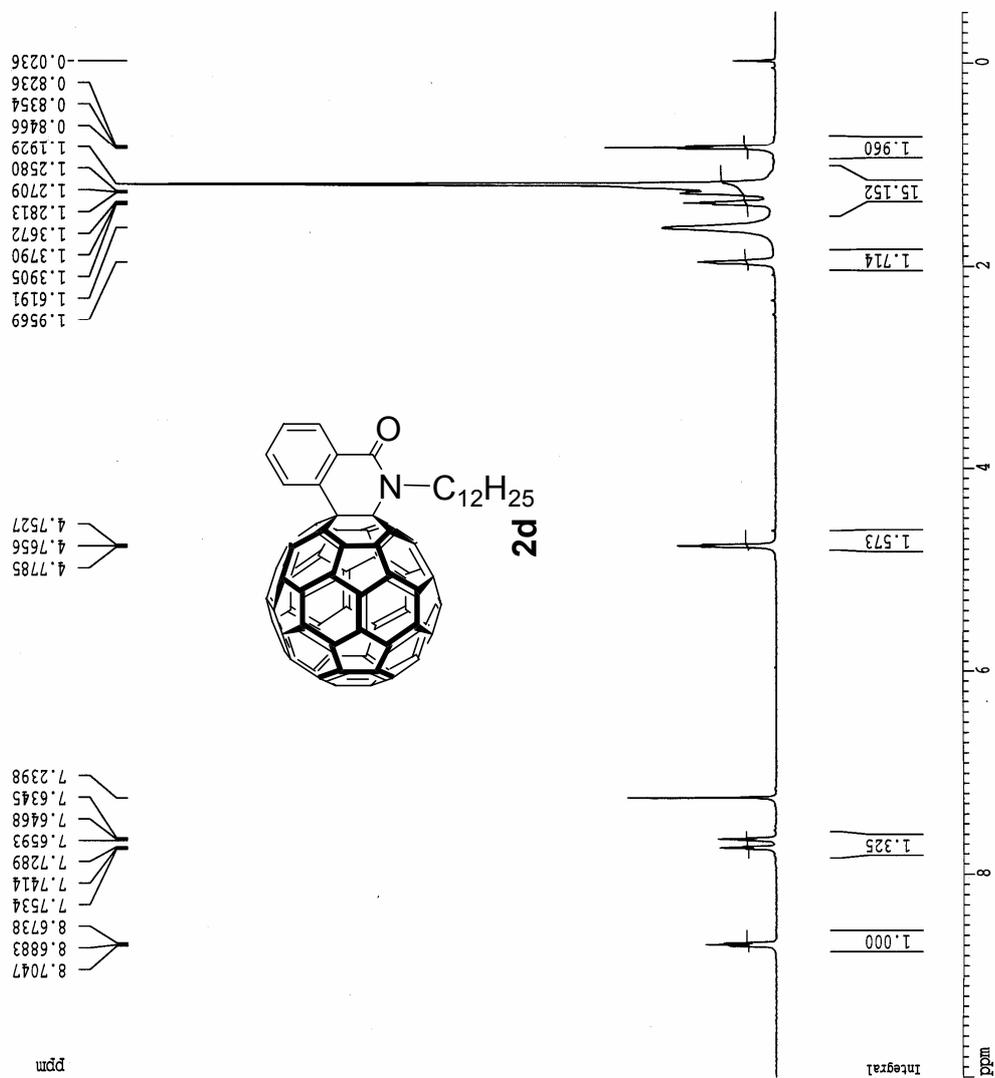


Figure S12. ^{13}C NMR spectra of compound **2d** (CDCl_3)

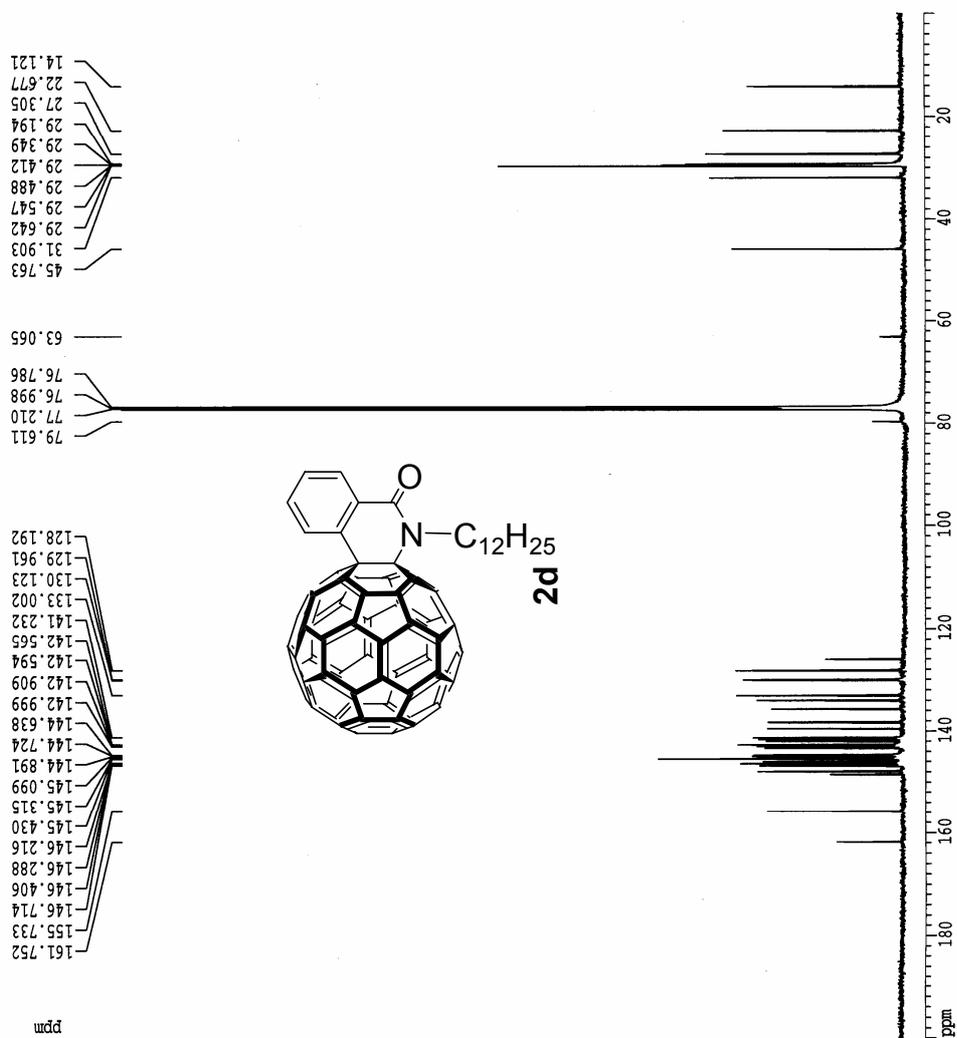


Figure S13. ^1H NMR spectra of compound **4a** (CS_2 with C_6D_{12} as external standard)

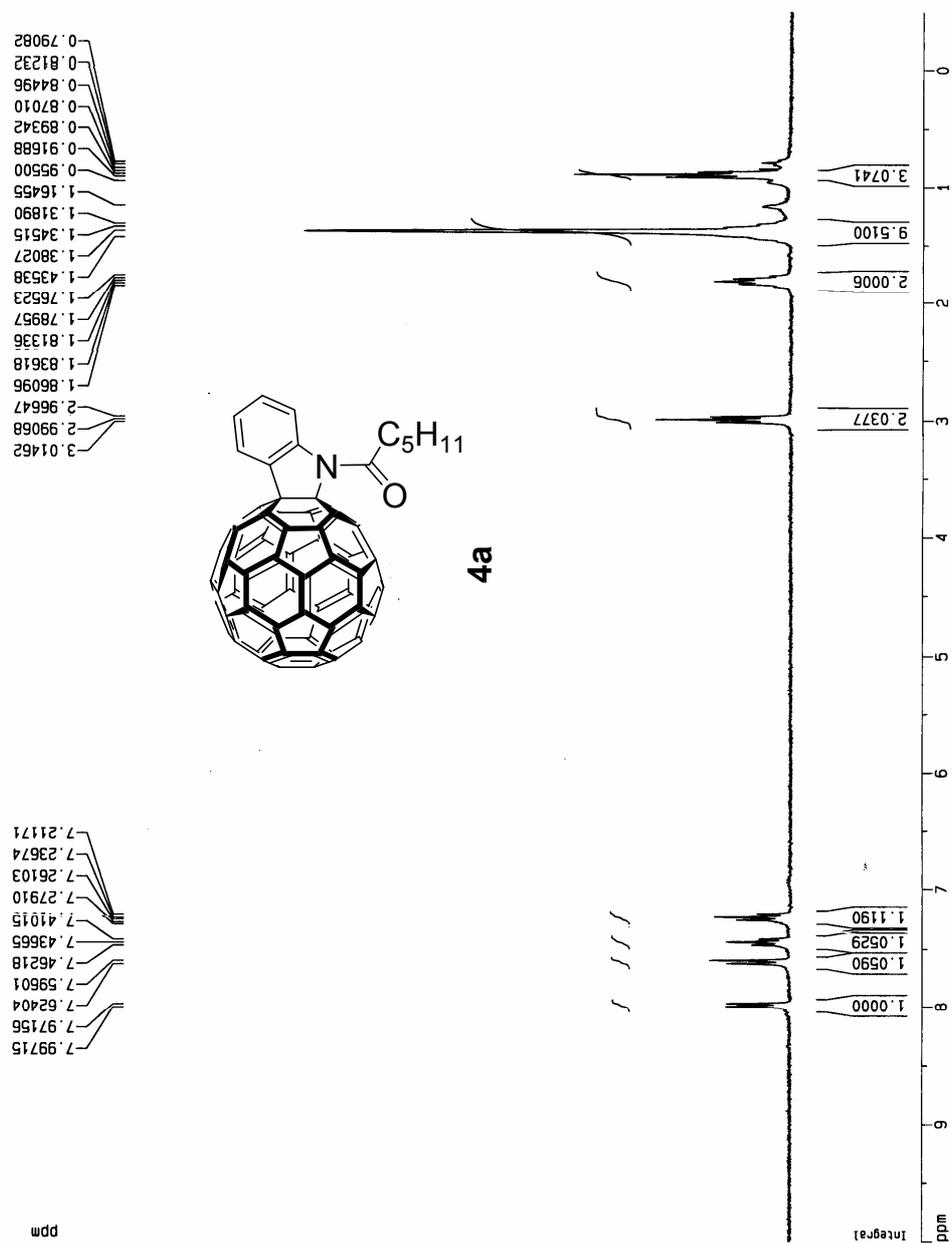


Figure S14. ^1H NMR spectra of compound **4b** (CS_2 with C_6D_{12} as external standard)

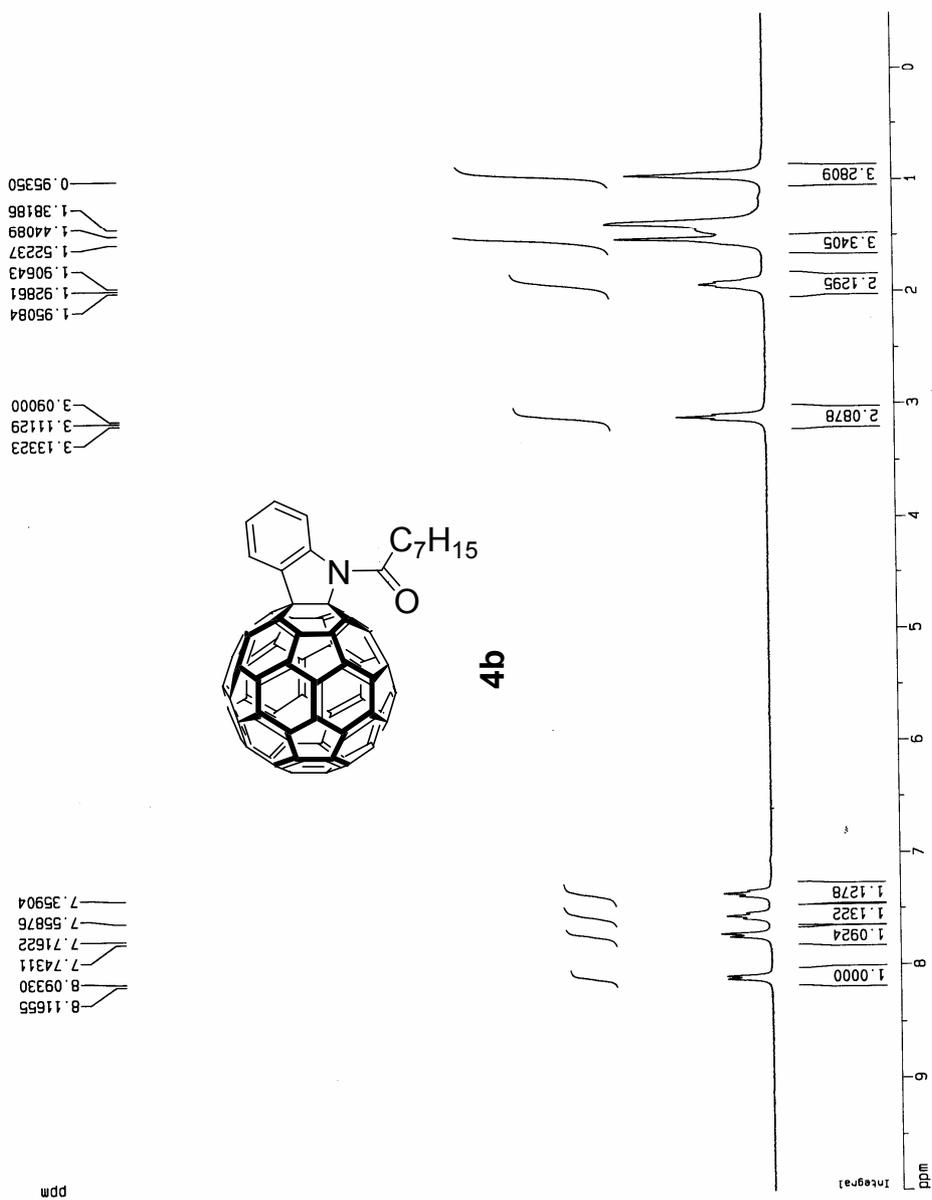


Figure S15. ^{13}C NMR spectra of compound **4b** (CS_2 with C_6D_6 as external standard)

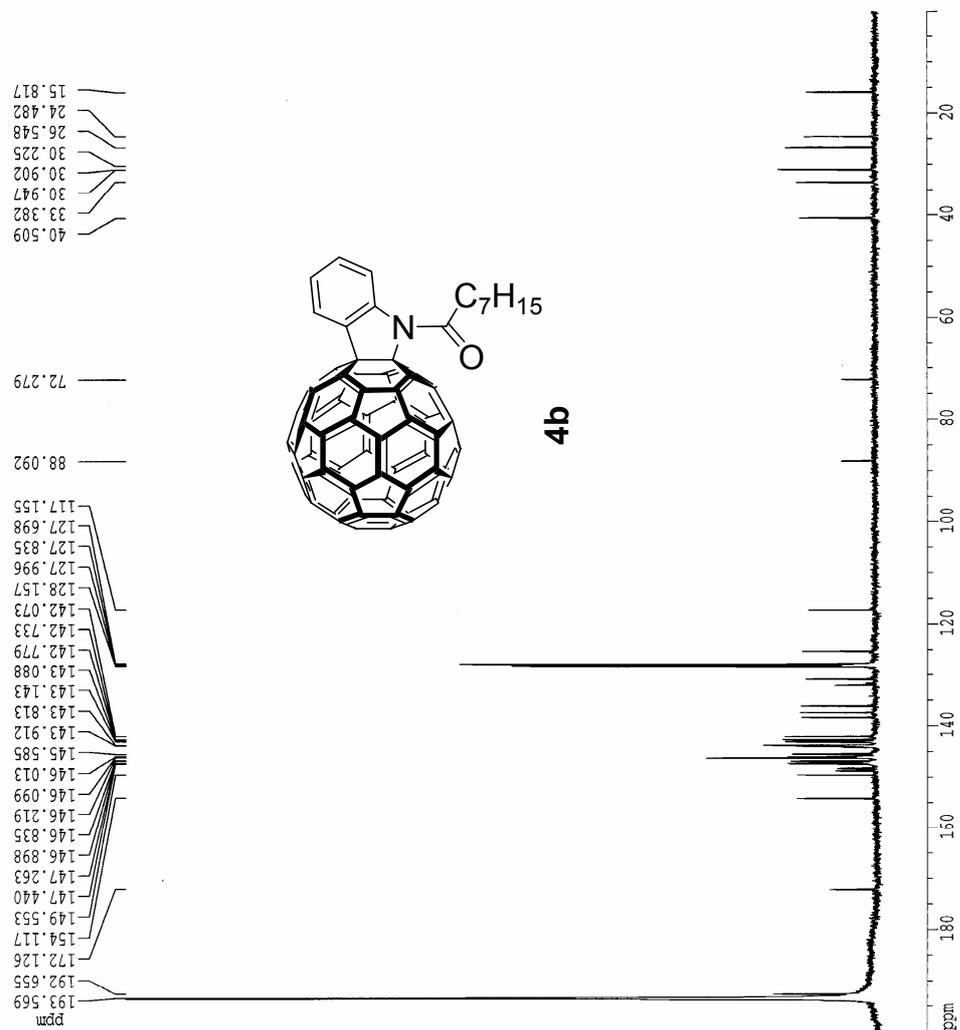


Figure S16. ^1H NMR spectra of compound **4c** (CS_2 with C_6D_{12} as external standard)

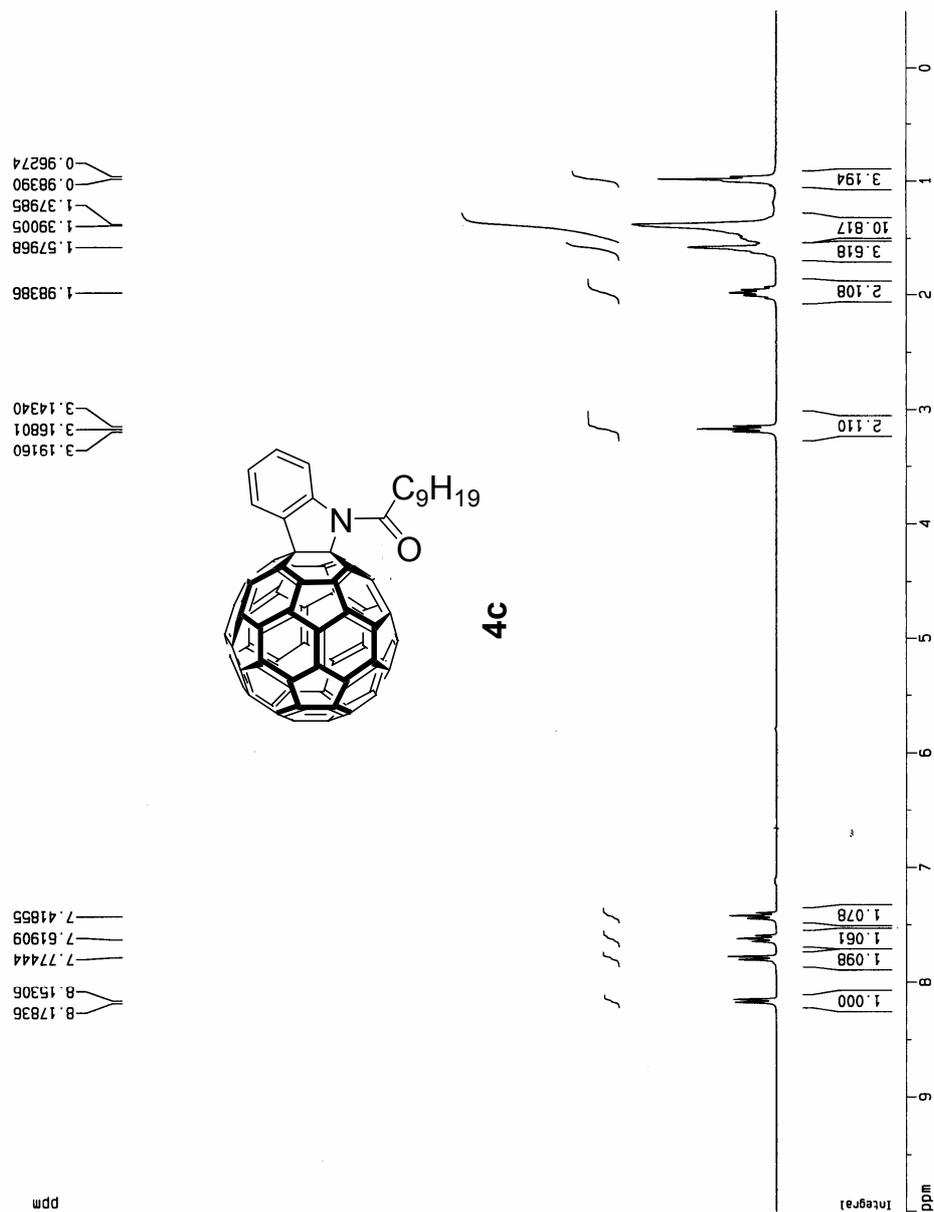


Figure S17. ^{13}C NMR spectra of compound **4c** (CS_2 with C_6D_6 as external standard)

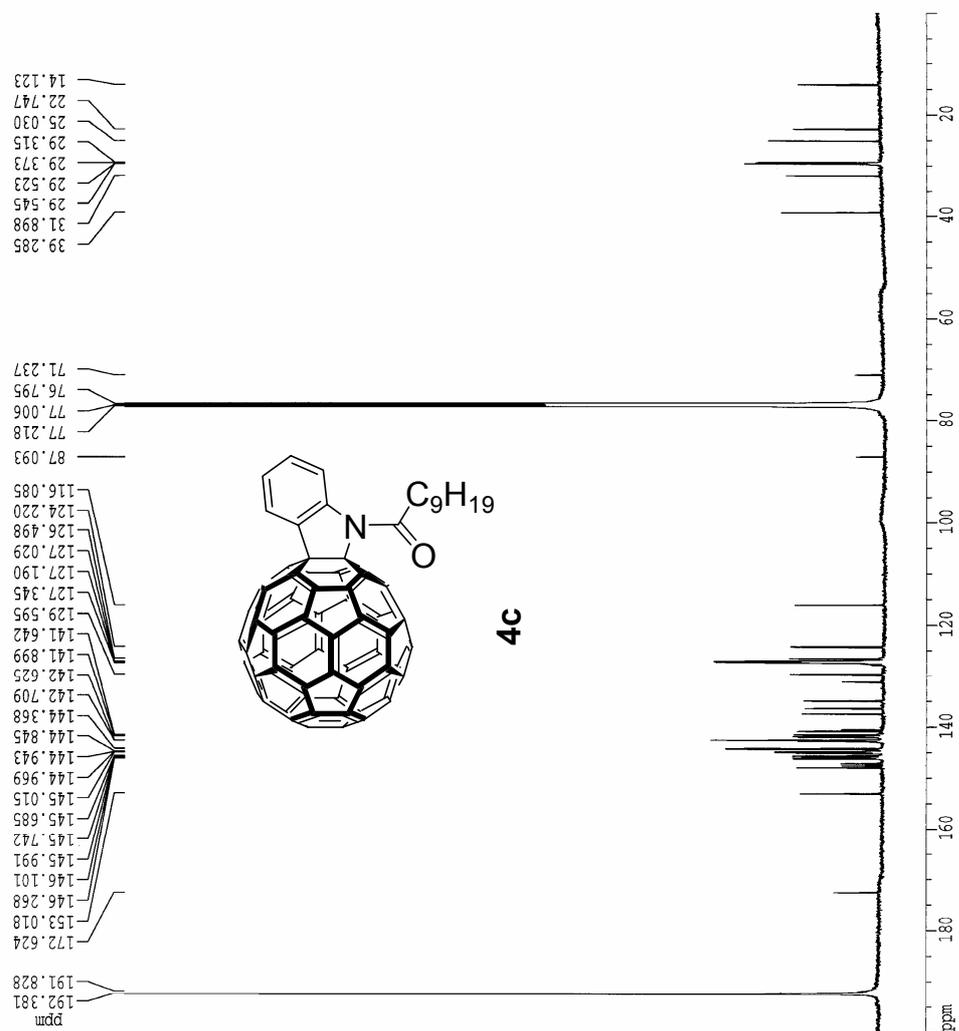


Figure S19. ^{13}C NMR spectra of compound **4d** (CS_2 with C_6D_6 as external standard)

