Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supplementary Information

The Formation of Photodegradable Nitrophenylene Polymers via Ring-Opening Metathesis Polymerization

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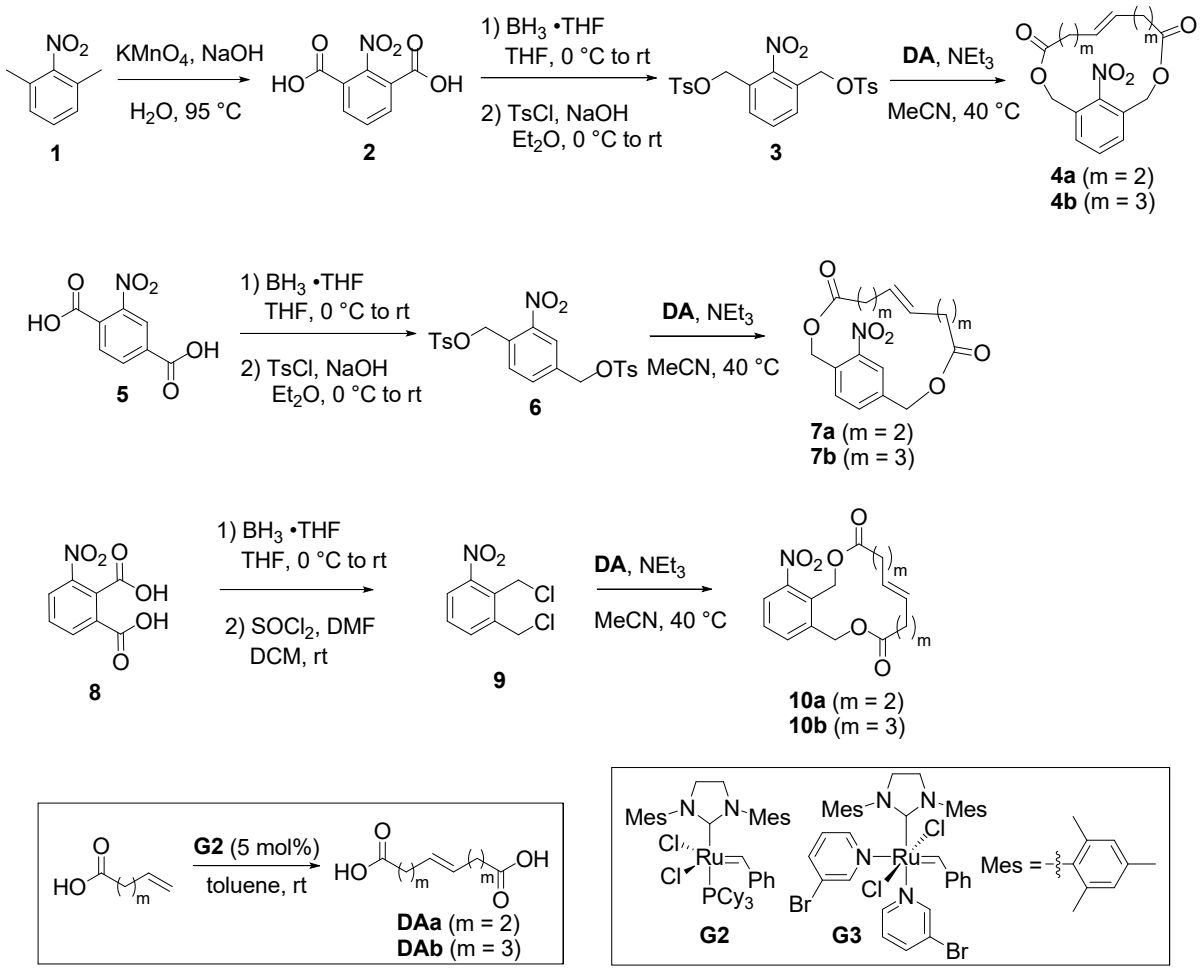
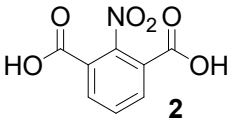
1. General information

All used commercially available chemicals were used without further purification. Dichloromethane (DCM) and tetrahydrofuran (THF) were obtained from a solvent purification system. All commercial reagents and solvents except DCM and THF were used directly without further purification. Analytical thin layer chromatography (TLC) analysis was carried out on the pre-coated silica gel 60 F254 glass plates, and flash column chromatography was performed on silica gel (400-630 mesh). ^{1}H NMR was recorded by Bruker AVANCE 400 (400 MHz) and AVANCE 500 (500 MHz) spectrometers. Chemical shifts for NMR were quoted in parts per million (ppm) referenced to the appropriate solvent peak ($CDCl_3$ = 7.26 ppm, CD_2Cl_2 = 5.30 ppm, DMSO =2.50 ppm). The abbreviation codes were used to describe ^{1}H NMR peak patterns; s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet and m = multiplet. Coupling constants, *J*, were reported in Hertz unit (Hz). ^{13}C NMR was recorded by Bruker AVANCE 400 (100 MHz) and 500 (125 MHz) and was fully decoupled by broad band decoupling. Chemical shifts of the ^{13}C NMR spectra were measured relative to $CDCl_3$ (77.00 ppm). Infrared (IR) spectra were recorded on Bruker Alpha FT-IR spectrometer. High-resolution (HR) ESI-MS measurements were performed using maXis 4G hybrid LC/Q-TOF system. High resolution mass spectra (HRMS) of compound **9** was obtained by electron impact (EI) ionization technique (magnetic sector – electric sector double focusing mass analyzer) from the KBSI (Korea Basic Science Institute Daegu Center). Gel permeation chromatography (GPC) analysis with refractive index (RI) detection was used to determine number average molecular weight (M_n), weight average molecular weight (M_w), and polydispersity (M_w/M_n). RI measurements were performed using a set of instruments consisting of a Waters 1515 isocratic pump, a 2414 differential refractive index detector, and a column heating module with Shodex KF-803, KF-804 and KF-805 columns connected in series. The column was eluted with tetrahydrofuran (preservative-free HPLC grade, Fisher) at 1.0 mL/min at 40 °C and calibrated against standard polystyrene (PS) (Sigma Aldrich, M_p 2,500-50,000). 36 W Osram Dulux® L BL UVA 36W/78 was used as UVA source for photodegradation. The data collection for single crystal structure analysis of samples was performed on a Bruker D8 QUEST diffractometer equipped with Iμs 3.0 Mo x-ray tube (λ = 0.71073Å) and Photon II detector. The selective crystals of samples were coated with Parabar oil for mounting on goniometer under a stream of N_2 (g) at 173 K. The diffraction data were integrated, scaled, and reduced by using the Bruker APEX4 software. The crystal structures of samples were solved by SHELX structure solution program and refined by full-matrix least-squares calculations with the SHELXL.

2. Preparation of monomers



2-Nitroisophthalic acid 2

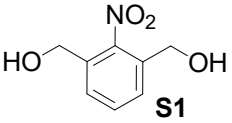


According to the literature,[1] a stirred mixture of 1,3-dimetyl-2-nitrobenzene **1** (6.00 g, 40.0 mmol, 1.0 equiv.) and sodium hydroxide (NaOH, 2.50 g, 62.5 mmol, 1.6 equiv.) in water (300 mL) was heated to 95 °C, then $KMnO_4$ (25.3 g, 160 mmol, 4.0 equiv.) was added in portions over a period of 3 h. The reaction mixture was refluxed for another 20 h and cooled to room temperature. The resulting mixture was filtered, and the filtrate was acidified with concentrated HCl. After drying the precipitate, the desired product **2** was obtained as white solid in 80% yield (6.77 g, 32.1 mmol).

^{1}H NMR (DMSO-d_6, 500 MHz, ppm) δ 14.14 (2H, br), 8.19 (2H, d, *J*= 7.8 Hz), 7.82 (1H, t, *J*= 7.8 Hz).

The spectral data are in complete agreement with the literature value.[1]

(2-Nitro-1,3-phenylene)bis(methylene) bis(4-methylbenzenesulfonate) 3

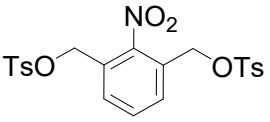


A solution of 2-nitroisophthalic acid **2** (4.22 g, 20.0 mmol, 1.0 equiv.) in anhydrous THF (250 mL) was cooled to 0 °C under N_2 atmosphere, and then borane tetrahydrofuran complex solution (1.0 M in THF, 100 mL, 100 mmol, 5.0 equiv.) was added dropwise over about 1 h. The reaction mixture was allowed to be warmed slowly to room temperature and stirred for another 48 h. Methanol (20 mL) was then added into the reaction system slowly using a syringe. The mixture was filtered, and the filtrate was evaporated with a rotary evaporator. The residue was redissolved in ethyl acetate and

washed with water (3 X 50 mL). The organic layer was dried with anhydrous $MgSO_4$ overnight before the solvent was removed by a rotary evaporator. The resulting yellow solid was further purified by silica gel chromatography (hexane/ ethyl acetate = 1:1) to obtain 2-nitro-1,3-benzenedimethanol **S1** (3.59 g, 19.6 mmol, 98%) as a white solid.[1]

^{1}H NMR (DMSO-d_6, 500 MHz, ppm) δ 7.58 (1H, dd, J_1= 8.8 Hz, J_2= 6.2 Hz), 7.54-7.51 (2H, m), 5.47 (2H, t, J= 5.3 Hz) 4.53 (2H, s), 4.52 (2H, s).

The spectral data are in complete agreement with the literature value.[1]



3

2-Nitro-1,3-benzenedimethanol **S1** (2.75 g, 15.0 mmol, 1.0 equiv.) was dissolved in diethyl ether (80 mL), and tosyl chloride (8.55 g, 44.8 mmol, 3.0 equiv.) was added. The reaction mixture was cooled to 0 °C, and powdered NaOH (1.80 g, 45.0 mmol, 3.0 equiv.) was added in portions under N_2. The reaction was stirred for 24 h at room temperature. After the reaction was completed, the reaction mixture was filtered for removal of solid remainders. The residue solution was concentrated under reduced pressure. The residue was washed with diethyl ether (3 X 20 mL), and the desired product **3** was obtained as a white solid in 83% yield (6.14 g, 12.5 mmol).

^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.76 (4H, d, J= 8.3 Hz), 7.60-7.52 (3H, m), 7.34 (4H, d, J= 8.0 Hz), 5.12 (4H, s), 2.45 (6H, s)

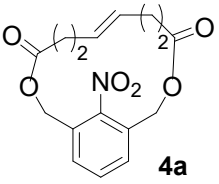
^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 147.6, 145.8, 132.5, 132.4, 130.5, 130.3, 128.6, 128.3, 67.2, 22.0

IR (cm^{-1}): 3083, 2879, 1597, 1531, 1466, 1353, 1171, 1094, 957, 939, 837, 808, 787, 764, 715, 703, 670, 608, 549, 479

Melting point: 128-129 °C

HRMS (ESI) m/z: $C_{22}H_{21}NNaO_8S_2$ $[M+Na]^+$ *calcd*: 514.0601, *found*: 514.0600.

Monomer 4a



4a

(2-Nitro-1,3-phenylene)bis(methylene) bis(4-methylbenzenesulfonate) **3** (2.00 g, 4.07 mmol, 1.0 equiv.), (E)-oct-4-enedioic acid **DAa** (758 mg, 4.40 mmol, 1.1 equiv.) and triethylamine (1.7 mL, 12.2 mmol, 3.0 equiv.) were dissolved in acetonitrile (400 mL). The reaction mixture was stirred for 24 h at 40 °C. After the reaction was completed, used solvent was removed under the reduced pressure, and the residue was extracted with ethyl acetate (3 X 50 mL). The organic was dried by anhydrous $MgSO_4$ and evaporated under the reduced pressure. The residue was purified by column chromatography on silica gel (eluted with hexane/ ethyl acetate = 7:3) to give the white solid **4a** (447 mg, 1.49 mmol, 37%).

^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.55 (2H, d, J= 7.5 Hz), 7.48 (1H, dd, J_1= 8.3 Hz, J_2= 6.9 Hz), 5.15 (4H, s), 5.12 (2H, t, J= 3.4 Hz), 2.36-2.30 (4H, m), 2.20-2.16 (4H, m)

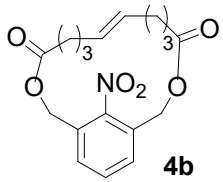
^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 172.5, 149.7, 133.3, 131.0, 130.3, 129.2, 63.0, 33.7, 27.7

IR (cm^{-1}): 2930, 1730, 1532, 1437, 1359, 1239, 1142, 965, 778

Melting point: 108.5-110 °C

HRMS (ESI) m/z: $C_{16}H_{17}NNaO_6$ $[M+Na]^+$ *calcd*: 342.0948, *found*: 342.0948.

Monomer 4b



4b

Using the procedure of compound **4a**, a mixture of (2-nitro-1,3-phenylene)bis(methylene) bis(4-methylbenzenesulfonate) **3** (1.47 g, 2.99 mmol, 1.0 equiv.), (E)-dec-5-enedioic acid **DAb** (660 mg, 3.30 mmol, 1.1 equiv.), and triethylamine (1.2 mL, 8.61 mmol, 2.9 equiv.) in acetonitrile (300 mL) was reacted to give the compound **4b** (380 mg, 1.09 mmol, 36%) as a white solid.

^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.58-7.54 (2H, m), 7.49 (1H, dd, *J*= 8.45, 6.8 Hz), 5.16-5.11 (6H, m), 2.27 (4H, t, *J*=6.6), 1.84 (4H, q, *J*= 6.3 Hz), 1.61 (4H, quint, *J*= 6.7 Hz)

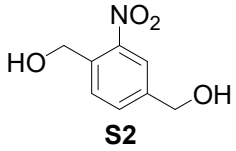
^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 173.2, 15.7, 133.2, 131.1, 130.3, 129.6, 62.3, 32.7, 31.1, 24.2

IR (cm^{-1}): 2932, 1737, 1536, 1455, 1439, 1364, 1231, 1145, 1100, 1043, 1010, 971, 853, 806, 779

Melting point: 81.5-83 °C

HRMS (ESI) m/z: $C_{18}H_{21}NNaO_6$ $[M+Na]^+$ *calcd*: 370.1261, *found*: 370.1261.

(2-Nitro-1,4-phenylene)bis(methylene) bis(4-methylbenzenesulfonate) 6

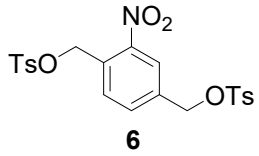


S2

Using the procedure of 2-nitro-1,3-benzenedimethanol **S1**, commercially available dicarboxylic acid **5** (4.22 g, 20.0 mmol, 1.0 equiv.) and borane tetrahydrofuran complex solution (1.0 M in THF, 100 mL, 100 mmol, 5.0 equiv.) in THF (30 mL) was reacted to give the compound **S2** (3.60 g, 19.7 mmol, 99%) as a white solid.

^{1}H NMR (DMSO-d_6, 500 MHz, ppm): δ 7.98 (1H, d, *J*= 1.48 Hz), 7.77 (1H, d, *J*= 7.96 Hz), 7.68 (1H, dd, J_1= 7.98 Hz, J_2= 1.62 Hz), 5.51 (1H, t, *J*= 5.56 Hz), 5.47 (1H, t, *J*= 5.74 Hz), 4.80 (2H, d, *J*= 5.5 Hz), 4.59 (2H, d, *J*= 5.72 Hz).

The spectral data are in complete agreement with the literature value.[2]



6

Using the procedure of (2-nitro-1,3-phenylene)bis(methylene) bis(4-methylbenzenesulfonate) **3**, (2-nitro-1,4-phenylene)dimethanol **S2** (3.30 g, 18.0 mmol, 1.0 equiv.), tosyl chloride (10.3 g, 54.0 mmol, 3.0 equiv.) and NaOH (2.16 g, 54.0 mmol, 3.0 equiv.) in diethyl ether (96 mL) was reacted to give the compound **6** (6.19 g, 12.6 mmol, 70%) as a pale yellow solid.

^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.96 (1H, d, *J*= 1.7 Hz), 7.83 (2H, d, *J*= 8.3 Hz), 7.78 (2H, d, *J*= 8.3 Hz), 7.74 (1H, d, *J*= 8.1 Hz), 7.59 (1H, dd, J_1= 8.1 Hz, J_2= 1.8 Hz), 7.35 (4H, dd, J_1= 11.0 Hz, J_2= 8.0 Hz), 5.42 (2H, s), 5.10 (2H, s), 2.46 (3H, s), 2.45 (3H, s)

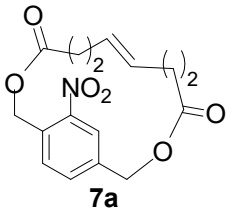
^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 146.8, 145.8, 135.8, 133.9, 132.9, 132.6, 131.5, 130.4, 130.4, 129.5, 128.3, 128.3, 124.9, 69.7, 68.0, 22.0, 22.0

IR (cm^{-1}): 1537, 1353, 1172, 1092, 970, 834, 810, 685, 580, 551, 526.

Melting point: 107.5-108 °C

HRMS (ESI) m/z: $C_{22}H_{21}NNaO_8S_2$ $[M+Na]^+$ *calcd*: 514.0601, *found*: 514.0600.

Monomer 7a



7a

Using the procedure of compound **4a**, a mixture of (2-nitro-1,4-phenylene)bis(methylene) bis(4-methylbenzenesulfonate) **6** (492 mg, 1.00 mmol, 1.0 equiv.), (E)-oct-4-enedioic acid **DAa** (190 mg, 1.10 mmol, 1.1 equiv.), and triethylamine (0.4 mL, 2.9 mmol, 2.9 equiv.) in acetonitrile (100 mL) was reacted to give the compound **7a** (89 mg, 0.28 mmol, 28%) as a white solid.

^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 8.03 (1H, s), 7.64 (1H, dd, J_1= 7.8 Hz, J_2= 1.6 Hz), 7.57 (1H, d, J= 7.8 Hz), 5.64 (1H, br), 5.26 (1H, br), 5.12 (2H, s), 4.61-4.42 (2H, m), 2.30-1.90 (8H, m)

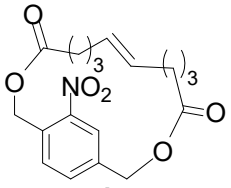
^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 172.6, 172.6, 149.9, 138.8, 134.9, 133.8, 131.8, 128.8, 128.7, 126.7, 65.0, 62.2, 34.4, 34.4, 28.6, 28.6

IR (cm^{-1}): 2917, 2852, 1731, 1527, 1450, 1360, 1233, 1130, 1058, 1019, 945, 882, 850, 810, 797, 749, 730, 677, 657, 602, 567, 513, 488, 446.

Melting point: 146.5-148 °C

HRMS (ESI) m/z: $C_{16}H_{17}NNaO_6$ $[M+Na]^+$ *calcd*: 342.0948, *found*: 342.0948.

Monomer 7b



7b

Using the procedure of compound **4a**, a mixture of (2-nitro-1,4-phenylene)bis(methylene) bis(4-methylbenzenesulfonate) **6** (492 mg, 1.00 mmol, 1.0 equiv.), (E)-dec-5-enedioic acid **DAb** (220 mg, 1.10 mmol, 1.1 equiv.), and triethylamine (0.4 mL, 2.9 mmol, 2.9 equiv.) in acetonitrile (100 mL) was reacted to give the compound **7b** (93 mg, 0.27 mmol, 27%) as a white solid.

^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 8.05 (1H, d, J= 1.7 Hz), 7.67 (1H, dd, J_1= 7.8 Hz, J_2= 1.7 Hz), 7.62 (1H, d, J= 7.8 Hz), 5.49 (2H, s), 5.16 (2H, s), 4.88-4.82 (2H, m), 2.31-2.22 (4H, m), 1.61-1.57 (4H, m), 1.55-1.47 (4H, m)

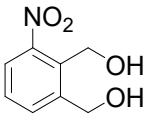
^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 173.4, 173.4, 149.3, 138.7, 134.5, 132.9, 131.8, 130.1, 129.8, 126.2, 64.3, 61.8, 33.8, 33.7, 31.9, 31.9, 24.7, 24.7

IR (cm^{-1}): 2928, 2848, 1726, 1525, 1417, 1342, 1234, 1131, 989, 962, 912, 882, 869, 846, 815, 800, 768, 756, 705, 664, 569, 554, 499, 405.

Melting point: 90.5-93 °C

HRMS (ESI) m/z: $C_{18}H_{21}NNaO_6$ $[M+Na]^+$ *calcd*: 370.1261, *found*: 370.1261.

1,2-Bis(chloromethyl)-3-nitrobenzene 9

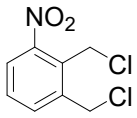


S3

Using the procedure of 2-nitro-1,3-benzenedimethanol **S1**, commercially available dicarboxylic acid **8** (4.22 g, 20.0 mmol, 1.0 equiv.) and borane tetrahydrofuran complex solution (1.0 M in THF, 100 mL, 100 mmol, 5.0 equiv.) in THF (30 mL) was reacted to give the compound **S3** (2.64 g, 14.4 mmol, 72%) as a brown solid.

^{1}H NMR (DMSO-d_6, 500 MHz, ppm): δ 7.72 (1H, d, *J*= 7.6 Hz), 7.67 (1H, d, *J*= 8.0 Hz), 7.48 (1H, d, *J*= 7.9 Hz), 5.39 (1H, t, *J*= 5.3 Hz), 5.22 (1H, t, *J*= 5.4 Hz), 4.68 (2H, d, *J*= 4.8 Hz), 4.63 (2H, d, *J*= 5.2 Hz).

The spectral data are in complete agreement with the literature value.[3]



9

According to the literature,[4] 3-nitrobenzene-1,2-dimethanol **S3** (0.915 g, 5 mmol, 1 equiv.) and DMF(0.5 mL, 6.5 mmol, 1.3 equiv.) were dissolved in DCM (25 mL). $SOCl_2$ (1 ml, 13 mmol, 2.6 eq) was added to the reaction solution over 15 h at room temperature. After the reaction was completed, the solvent and excess $SOCl_2$ were removed under reduced pressure. The residue was extracted with diethyl ether (3 X 50 mL). The organic was washed with water (50 mL) and dried by anhydrous $MgSO_4$. The resulting solution was concentrated by reduced pressure, and the residue was purified by column chromatography on silica gel (eluted with hexane/ ethyl acetate = 8:2) to give the pale yellow solid **9** (1.00 g, 4.54 mmol, 90.8%).

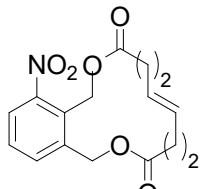
^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 7.89 (1H, dd, J_1= 8.2 Hz, J_2= 1.2 Hz), 7.68 (1H, dd, J_1=7.7 Hz, J_2= 1.2 Hz), 7.52 (1H, t, *J*= 7.9 Hz), 4.96 (2H, s), 4.8 (2H, s).

^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 150.2, 139.2, 135.1, 130.5, 130, 125.3, 42.3, 36.5

IR (cm^{-1}): 3090, 2882, 1528, 1464, 1440, 1349, 1271, 1254, 1213, 1191, 908, 871, 834, 819, 785, 760, 741, 696, 678, 643, 594.

HRMS (EI) m/z: C8H7Cl2NO2 $[M]^+$ *calcd*: 218.9854, *found*: 218.9850

Monomer 10a



10a

Using the procedure of compound **4a**, a mixture of 1,2-bis(chloromethyl)-3-nitrobenzene **9** (492 mg, 1.00 mmol, 1.0 equiv.), (E)-oct-4-enedioic acid **DAa** (190 mg, 1.10 mmol, 1.1 equiv.), and triethylamine (0.4 mL, 2.9 mmol, 2.9 equiv.) in acetonitrile (100 mL) was reacted to give the compound **10a** (130 mg, 0.41 mmol, 41%) as a white solid.

^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.85 (1H, dd, J_1= 8.1 Hz, J_2= 1.3 Hz), 7.67 (1H, dd, J_1= 7.7 Hz, J_2= 1.2 Hz), 7.52 (1H, t, *J*= 7.9 Hz), 5.45-5.26 (4H, m), 5.20 (2H, s), 2.42-2.35 (4H, m), 2.28-2.19 (4H, m)

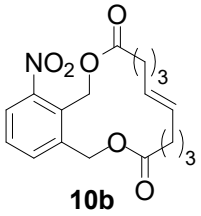
^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 173.2, 172.7, 151.6, 137.4, 136.3, 130.2, 130.1, 129.9, 129.2, 125.4, 64.6, 59.3, 35.2, 34.5, 27.9, 27.8

IR (cm^{-1}): 2918, 2849, 1721, 1529, 1459, 1438, 1340, 1304, 1243, 1134, 1075, 1013, 984, 960, 927, 892, 855, 822, 793, 744, 654.

Melting point: 142.5-144.5 °C

HRMS (ESI) m/z: $C_{16}H_{17}NNaO_6$ $[M+Na]^+$ *calcd*: 342.0948, *found*: 342.0950

Monomer 10b



10b

Using the procedure of compound **4a**, a mixture of 1,2-bis(chloromethyl)-3-nitrobenzene **9** (492 mg, 1.00 mmol, 1.0 equiv.), (E)-dec-5-enedioic acid **DAb** (220 mg, 1.10 mmol, 1.1 equiv.), and triethylamine (0.4 mL, 2.9 mmol, 2.9 equiv.) in acetonitrile (100 mL) was reacted to give the compound **10b** (170 mg, 0.49 mmol, 49%) as a white solid.

^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.84 (1H, dd, J_1= 8.1 Hz, J_2= 1.2 Hz), 7.67 (1H, dd, J_1= 7.7 Hz, J_2= 1.2 Hz), 7.5 (1H, t, J= 7.9 Hz), 5.35 (2H, s), 5.27-5.23 (2H, m), 5.20 (2H, s), 2.32 (4H, t, J= 7.1 Hz), 2.07-1.96 (4H, m), 1.78-1.68 (4H, m)

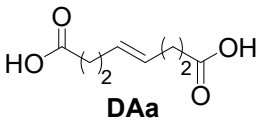
^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 173.5, 173.3, 151.7, 137.9, 135.5, 131.2, 131.1 129.9, 129.4, 125.2, 64.2, 59.2, 32.7, 32.2, 31.8, 31.3, 23.8, 22.7

IR (cm^{-1}): 2926, 2850, 1727, 1526, 1473, 1448, 1429, 1414, 1389, 1350, 1326, 1307, 1218, 1204, 1183, 1155, 1136, 1064, 1054, 1024, 996, 974, 955, 894, 883, 867, 819, 808, 792, 751, 661, 608.

Melting point: 85-87 °C

HRMS (ESI) m/z: $C_{18}H_{21}NNaO_6$ $[M+Na]^+$ *calcd*: 370.1261, *found*: 370.1261

(*E*)-Oct-4-enedioic acid DAa



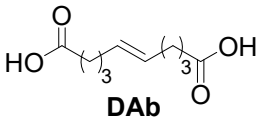
DAa

According to the literature,[5] a solution of 4-pentenoic acid (0.98 ml, 10 mmol, 1.00 equiv.) in dry toluene (10 mL) was added to Grubbs 2nd generation **G2** (43 mg, 0.05 mmol, 0.05 equiv). The reaction mixture was stirred for 20 h at room temperature. After the reaction was completed, the solvent was removed and recrystallized from 30% ethyl acetate in hexanes. The desired product **DAa** was obtained as a light purple solid in 46% yield (0.39 g, 2.3 mmol).

^{1}H NMR (DMSO-d_6, 500 MHz, ppm): δ 12.0 (2H, br), 5.48-5.39 (2H, m), 2.26-2.22 (4H, m), 2.19-2.14 (4H, m)

The spectral data are in complete agreement with the literature value.[5]

(*E*)-Dec-5-enedioic acid DAb



DAb

Using the procedure of (E)-oct-4-enedioic acid **DAa**, 5-hexenoic acid (1.2 ml, 10 mmol, 1 equiv.) and G2 (43 mg, 0.05 mmol, 0.05 equiv) in dry toluene (10 mL) was reacted to give the compound **DAb** (0.28 g, 1.4 mmol, 28%) as a purple solid.

^{1}H NMR (DMSO-d_6, 500 MHz, ppm): δ 12.0 (2H, br), 5.39-5.36 (2H, m), 2.18 (4H, t, J= 7.4 Hz), 1.98-1.94 (4H, m), 1.54 (4H, quin, J= 7.4 Hz).

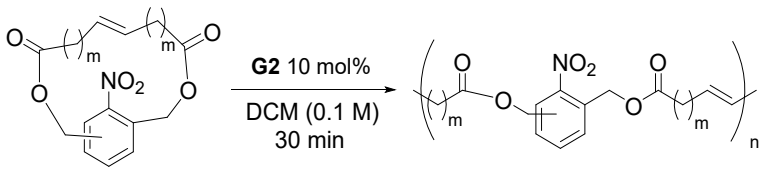
The spectral data are in complete agreement with the literature value.[6]

3. Polymerization

General procedure

A solution of monomer (0.025 mmol) in DCM (0.25 mL) was added into the Grubbs catalyst. The resulting solution was stirred at room temperature for 30 minutes. The reaction was quenched with ethyl vinyl ether (0.1 mL) and stirred for an additional 10 minutes at room temperature. The polymer was precipitated upon addition of methanol, and the polymer was isolated by centrifugation and decantation. The obtained polymer was dried under high vacuum. For the GPC analysis, the isolated polymer was diluted with THF (8 mg/mL), filtered, and then injected to GPC instrument.

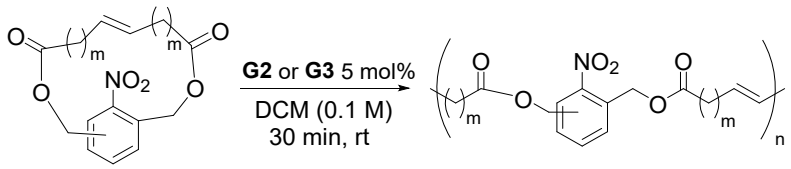
Table S1. Optimization of ROMP in the presence of **G2** 10 mol%



Entry	monomer	Temp (°C)	Yield (%)[a]
1	**4a**	rt	23
2	**4a**	40	92
3	**4b**	rt	99
4	**4b**	40	99
5	**7a**	rt	67
6	**7a**	40	85
7	**7b**	rt	99
8	**7b**	40	99

[a] Yields were determined by crude ^{1}H NMR using 1,3,5-trimethoxybenzene as an internal standard.

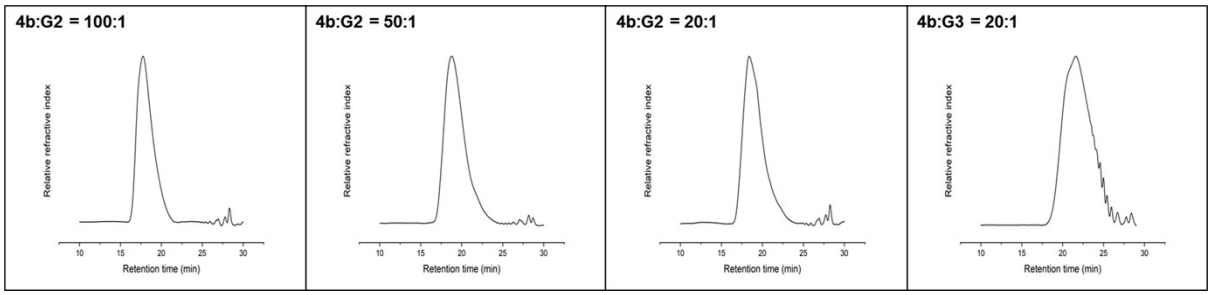
Table S2. Optimization of ROMP



Entry	monomer	Catalyst	Yield (%)[a]	M_n^{exp}(KDa) [b]	$Đ$ [b]
1	**4a**	**G2**	-	-	-
2	**4a**	**G3**	-	-	-
3[c]	**4a**	**G2**	54	5.98	1.28
4[c]	**4a**	**G3**	53	6.63	1.28
3	**4b**	**G2**	>95	18.5	1.41
4	**4b**	**G3**	>95	9.4	1.47
5	**7a**	**G2**	-	-	-
6	**7a**	**G3**	-	-	-
7[c]	**7a**	**G2**	21	-[d]	-[d]
8[c]	**7a**	**G3**	31	-[d]	-[d]
9	**7b**	**G2**	77	16.3	1.45
10	**7b**	**G3**	90	9.1	1.54
11	**10a**	**G2**	74	9.0	1.38
12	**10b**	**G2**	81	9.3	1.51
13[e]	**4b**	**G2**	>95	15.9	1.53
14[f]	**4b**	**G2**	>95	18.2	1.51

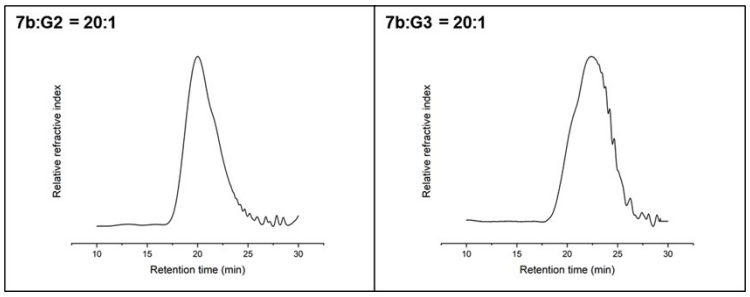
[a] Yields were determined by crude ^{1}H NMR using 1,3,5-trimethoxybenzene as an internal standard. [b] M_n^{exp}'s and $Đ$'s were determined by GPC (THF) using polystyrene standards (RI detection). [c] Reaction was carried out at 40 °C for 24 h. [d] Polymer was not isolated. [e] Using 2 mol% catalyst. [f] Using 1 mol% catalyst.

Table S3. GPC plot of polymer **4bP** at room temperature for 30 min in 0.1 M DCM.



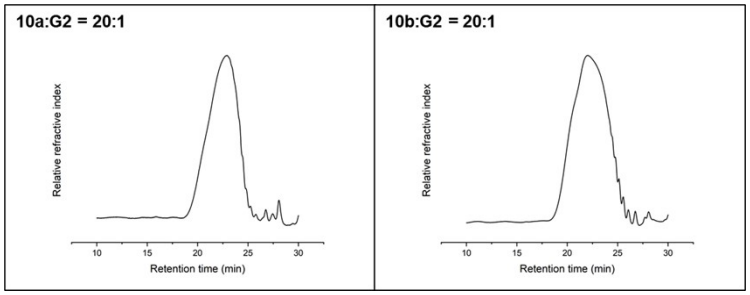
Catalyst	4b : cat.	M_n	M_w	PDI($Đ$)
G2	100 : 1	18215	27528	1.51
G2	50 : 1	15927	24421	1.53
G2	20 : 1	18521	26175	1.41
G3	20 : 1	9374	13764	1.47

Table S4. GPC plot of polymer **7bP** at room temperature for 30 min in 0.1 M DCM.



Catalyst	7b : cat.	M_n	M_w	PDI($Đ$)
G2	20 : 1	16346	23650	1.45
G3	20 : 1	9091	14012	1.54

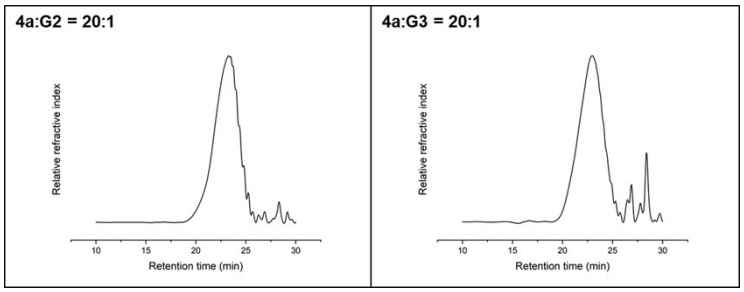
Table S5. GPC plot of polymers **10aP** and **10bP** at room temperature for 30 min in 0.1 M DCM.



Catalyst	10 : cat.	M_n	M_w	PDI($Đ$)
G2	20[a] : 1	9028	12429	1.38
G2	20[b] : 1	9301	14007	1.51

a. **10a** b. **10b** monomer.

Table S6. GPC plot of polymer **4aP** at 40 ºC for 24 h in 0.1 M DCM.



Catalyst	4a : cat.	M_n	M_w	PDI($Đ$)
G2	20 : 1	5975	7668	1.28
G3	20 : 1	6627	8488	1.28

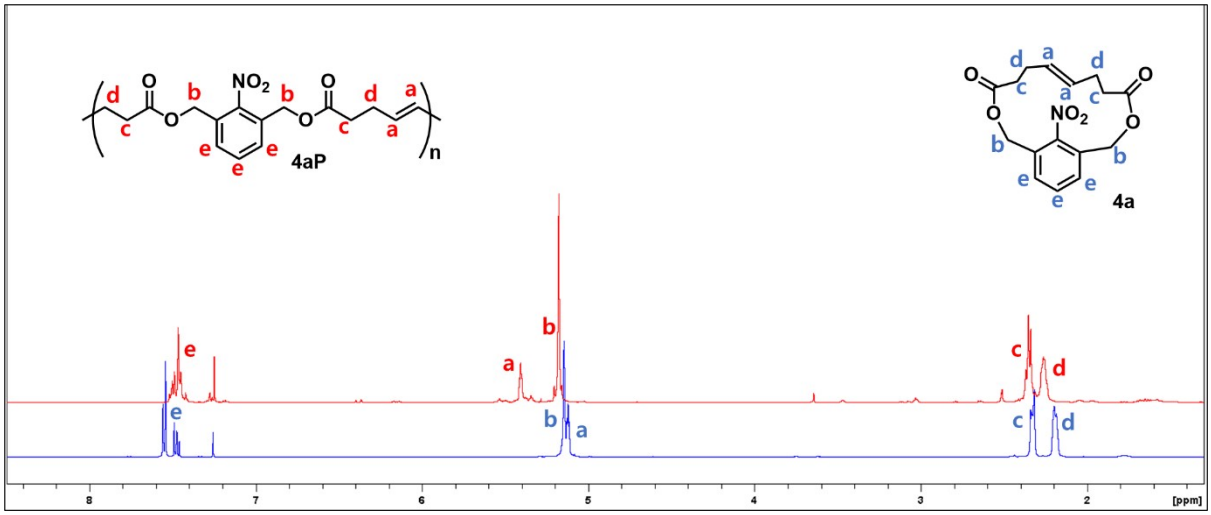


Fig. S1. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of polymer **4aP** (red line) and monomer **4a** (blue line).

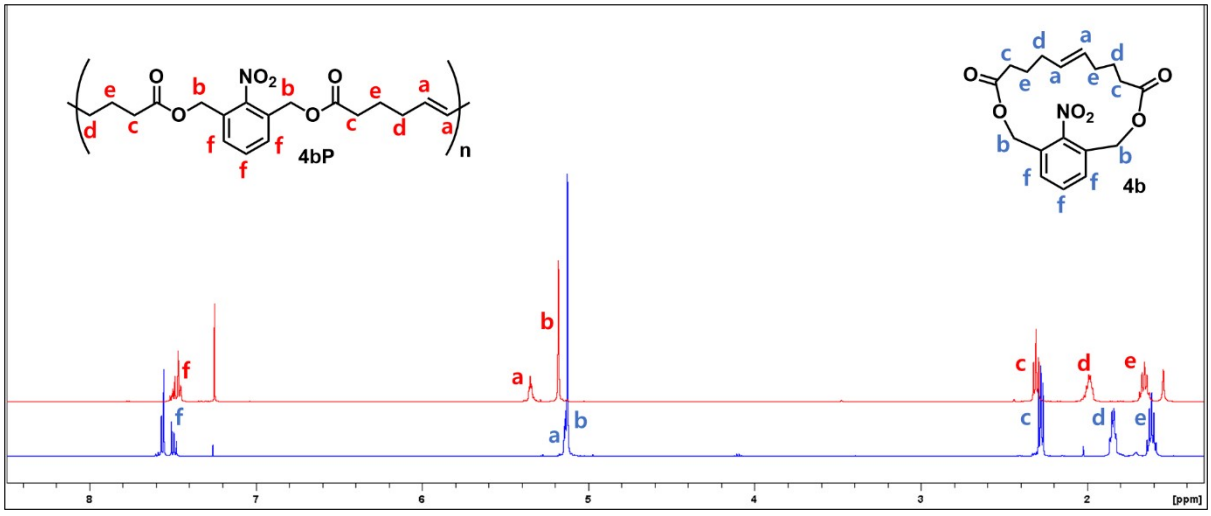


Fig. S2. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of polymer **4bP** (red line) and monomer **4b** (blue line).

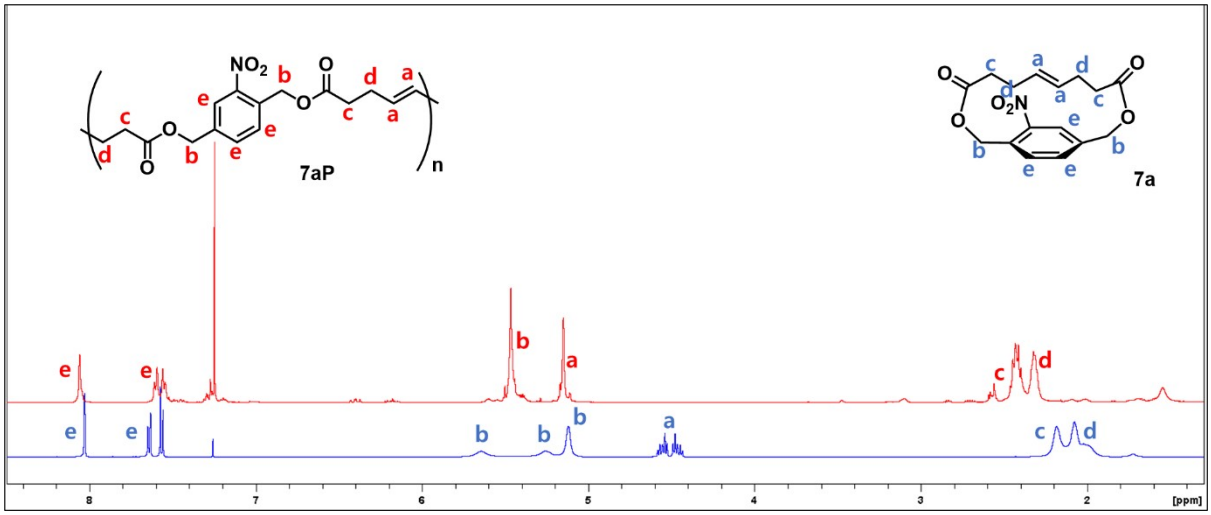


Fig. S3. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of polymer **7aP** (red line) and monomer **7a** (blue line).

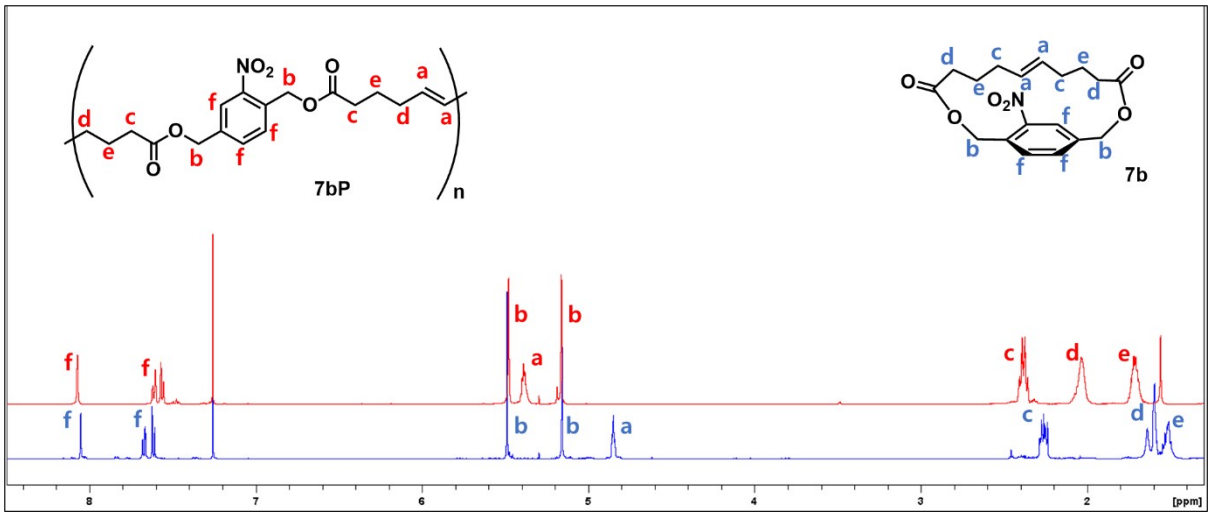


Fig. S4. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of polymer **7bP** (red line) and monomer **7b** (blue line).

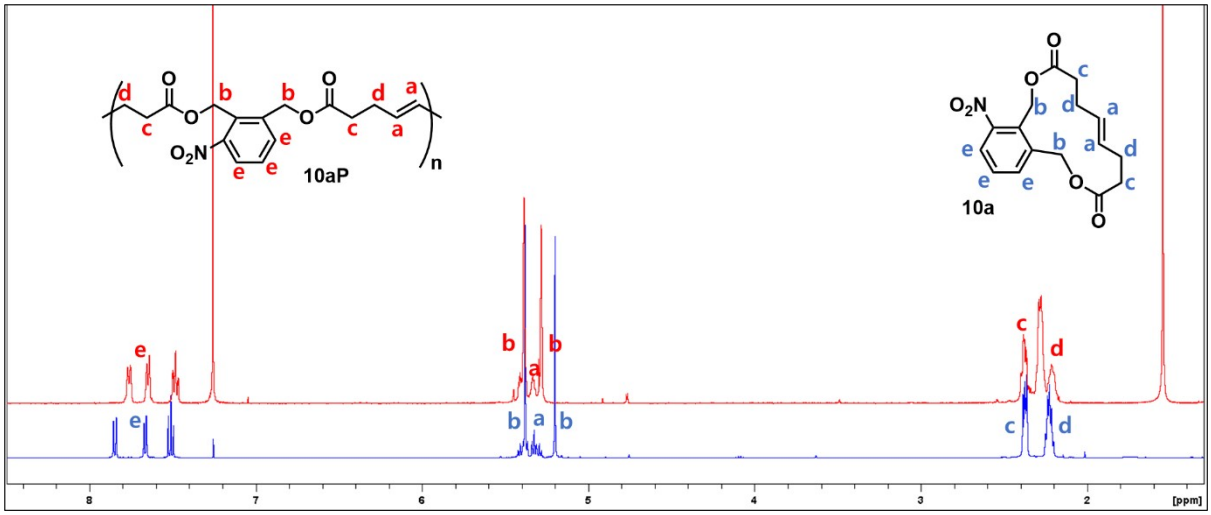


Fig. S5. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of polymer **10aP** (red line) and monomer **10a** (blue line).

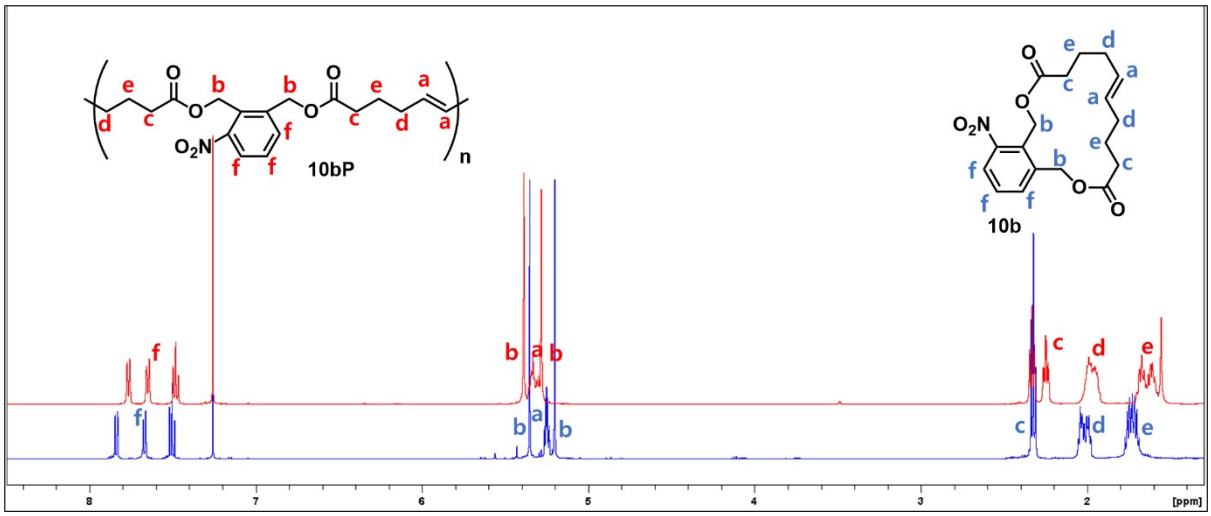


Fig. S6. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of polymer **10bP** (red line) and monomer **10b** (blue line).

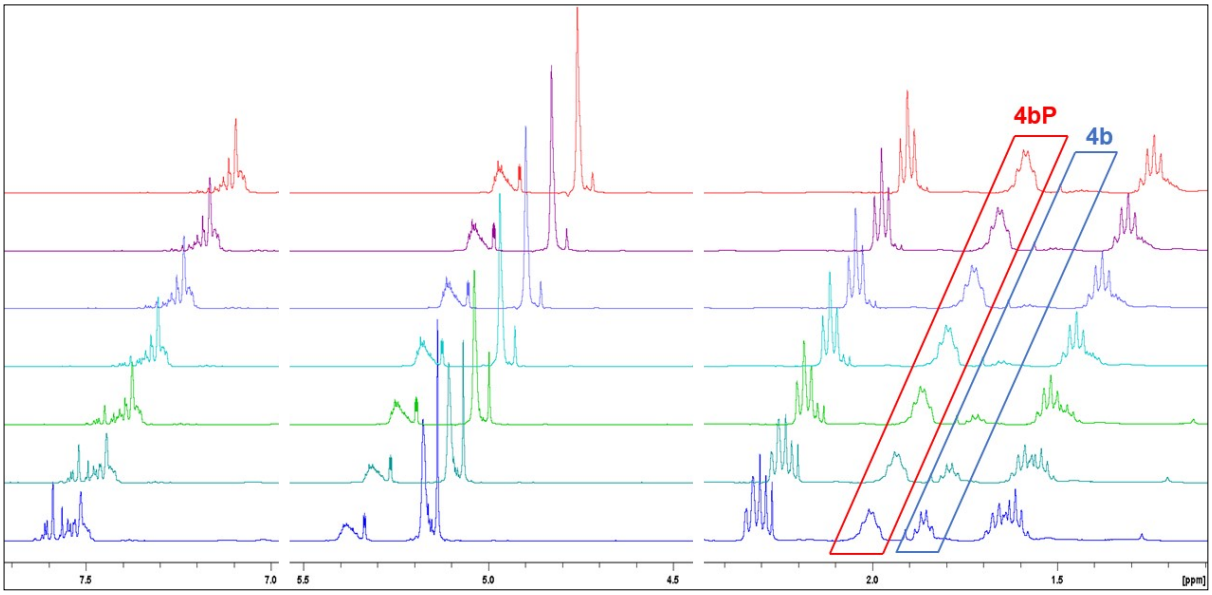


Fig. S7. (a) Polymerization of **4b**: 5.5 min, 7 min, 12 min, 17 min, 22 min, 27 min, 30 min (in CD_2Cl_2). (b) Plot of

Table S7. Monomer (**4b**) and Polymer (**4bP**) Ratio Comparison.

time (min)	Monomer **4b**	Polymer **4bP**	Conversion(%)
5.5	1.59	2.37	59.9
5.38	1.44	2.45	62.9
6	1.43	2.55	64.1
6.15	1.31	2.61	66.5
7	1.19	2.74	69.7
8	1.04	2.90	73.5
9	0.91	3.03	77.0
10	0.81	3.16	79.6
11	0.71	3.25	82.1
12	0.66	3.34	83.5
13	0.56	3.41	85.9
14	0.50	3.49	87.5
15	0.45	3.53	88.7
16	0.41	3.58	89.8
17	0.39	3.64	90.2
18	0.35	3.69	91.3
19	0.32	3.70	92.0
20	0.31	3.73	92.4
21	0.29	3.74	92.9
22	0.27	3.75	93.3
23	0.26	3.79	93.5
24	0.25	3.75	93.9
25	0.24	3.78	94.1
26	0.23	3.77	94.3
27	0.22	3.79	94.5
28	0.21	3.79	94.7
29	0.21	3.80	94.7
30	0.21	3.81	94.8

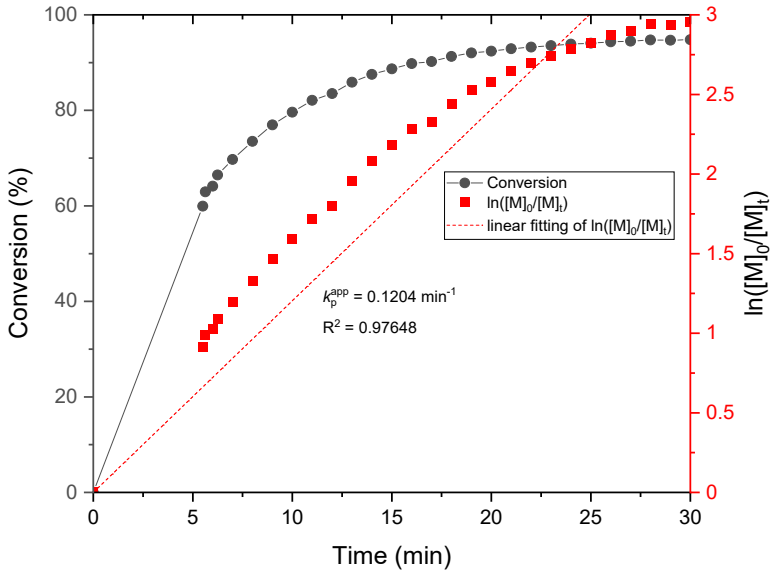
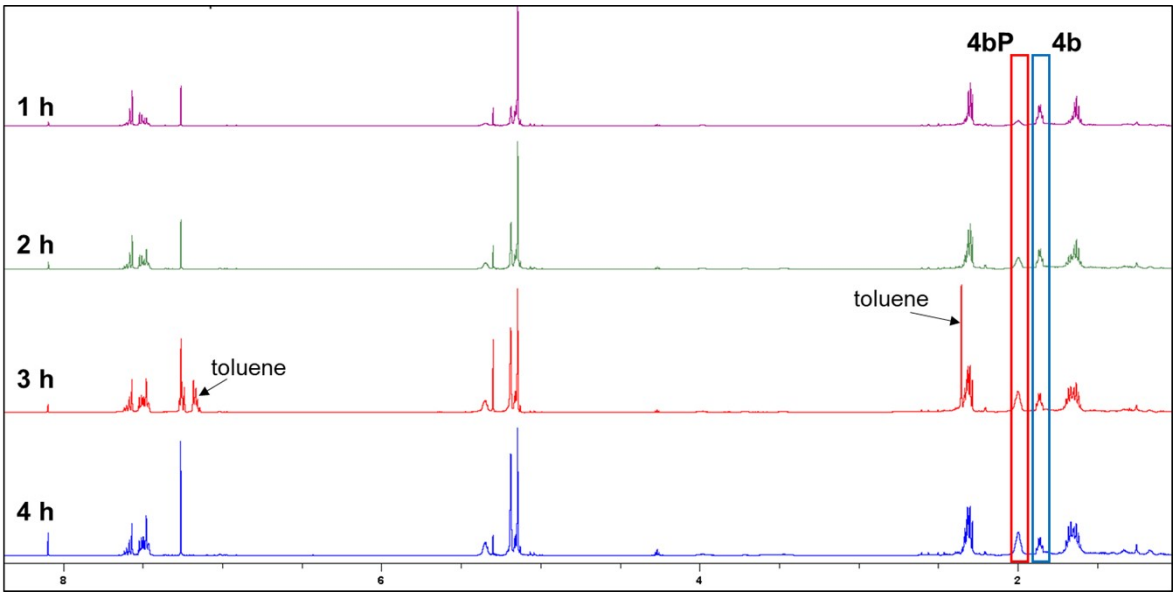
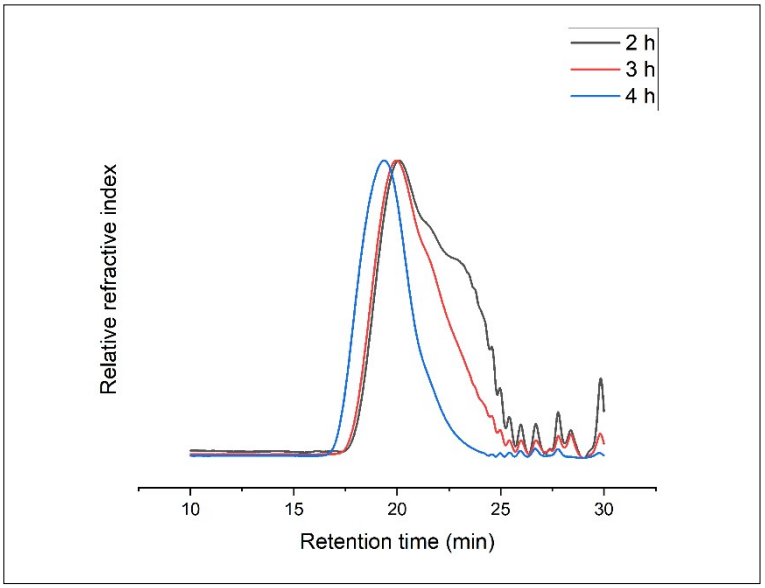


Fig. S8. Plots of conversion and ln([**4b**]$_0$/[**4b**]$_t$) over a length of time in polymerization of monomer **4b**.



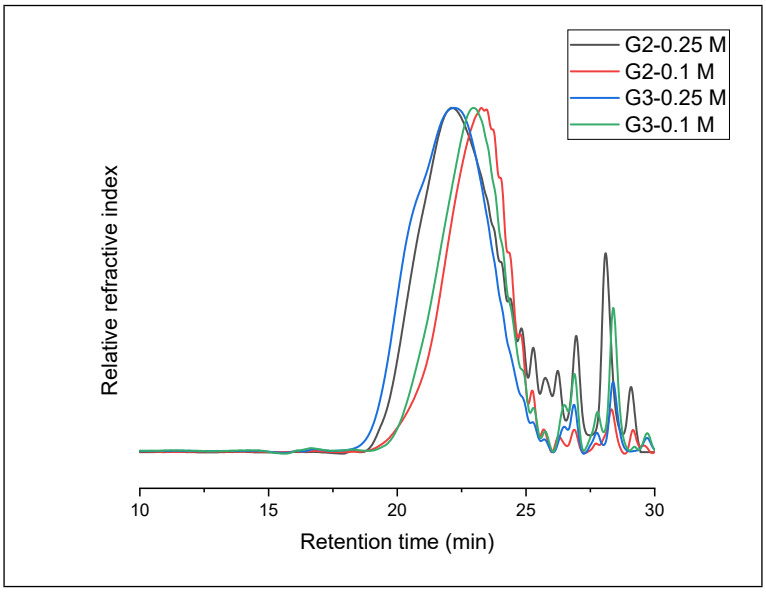
Reaction time (h)	Calculated conversion (%)
1	30.4
2	47.7
3	61.5
4	66.3

Fig. S9. Crude ^{1}H NMR of ROMP of **4b** with 5 mol % **G2** at 0 °C and calculated conversions in 0.1 M DCM.



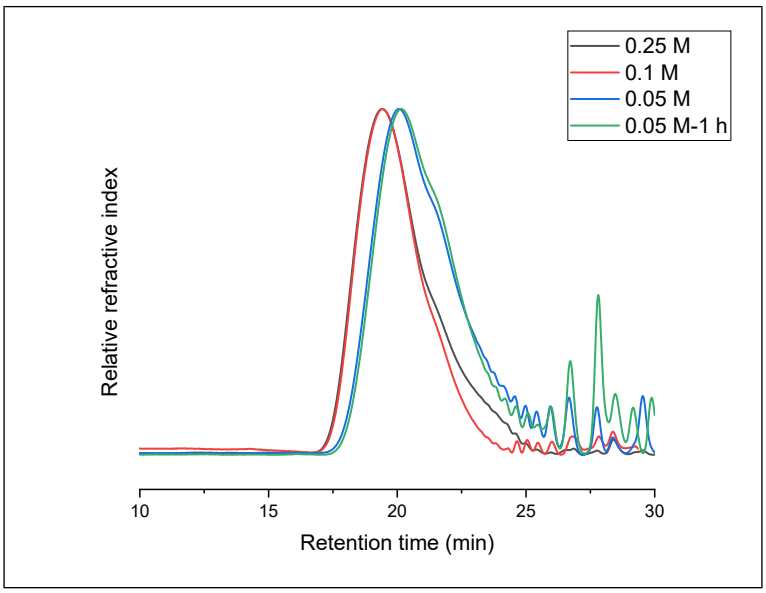
Reaction time (h)	M_n (kDa)	M_w (kDa)	$Đ$
2	11.8	19.5	1.65
3	15.3	22.9	1.50
4	19.5	28.0	1.44

Fig. S10. GPC plot of ROMP of **4b** with 5 mol % **G2** at 0 °C in 0.1 M DCM.



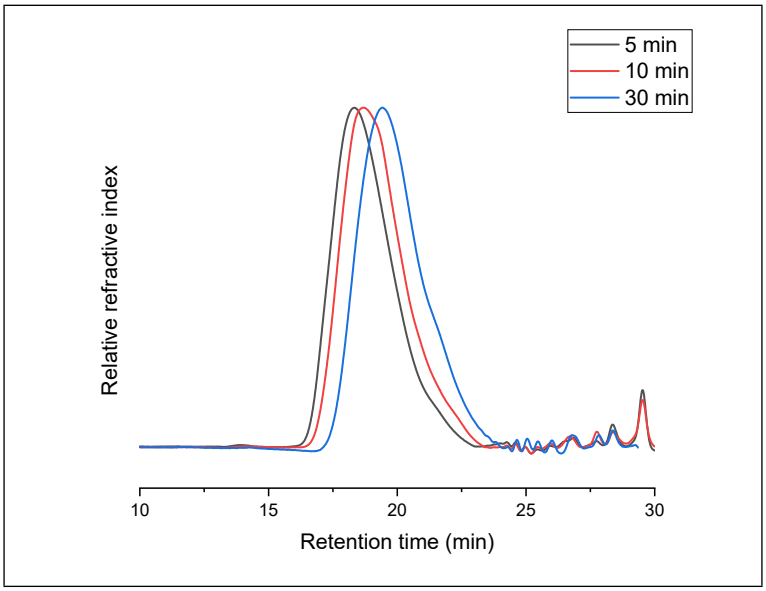
Catalyst	Concentration (M)	Conversion (%)	M_n (kDa)	M_w (kDa)	$Đ$
G2	0.25	64	7.66	10.3	1.35
	0.1	54	5.98	7.67	1.28
	0.05	47		Not isolated	
G3	0.25	53	8.69	12.1	1.39
	0.1	53	6.63	8.49	1.28
	0.05	41		Not isolated	

Fig. S11. GPC plot of ROMP of **4a** with 5 mol % catalyst at 40 °C for 24 h in various concentrations with DCM solvent.



Concentration (M)	Conversion (%)	M_n (kDa)	M_w (kDa)	$Đ$
0.25	> 95	16.7	24.4	1.46
0.1	> 95	18.5	26.2	1.41
0.05	> 95	13.6	20.0	1.47
0.05 (1h)	> 95	13.4	19.6	1.46

Fig. S12. GPC plot of ROMP of **4b** with 5 mol % **G2** at room temperature for 30 min in various concentrations with DCM solvent.



Reaction time	Conversion (%)	M_n (kDa)	M_w (kDa)	$Đ$
5 min	79	19.3	29.0	1.50
10 min	82	18.1	27.4	1.51
30 min	> 95	18.5	26.2	1.41

Fig. S13. GPC plot of ROMP of **4b** with 5 mol % **G2** at room temperature in 0.1 M DCM.

4. Photodegradations of polymers 4bP and 7bP

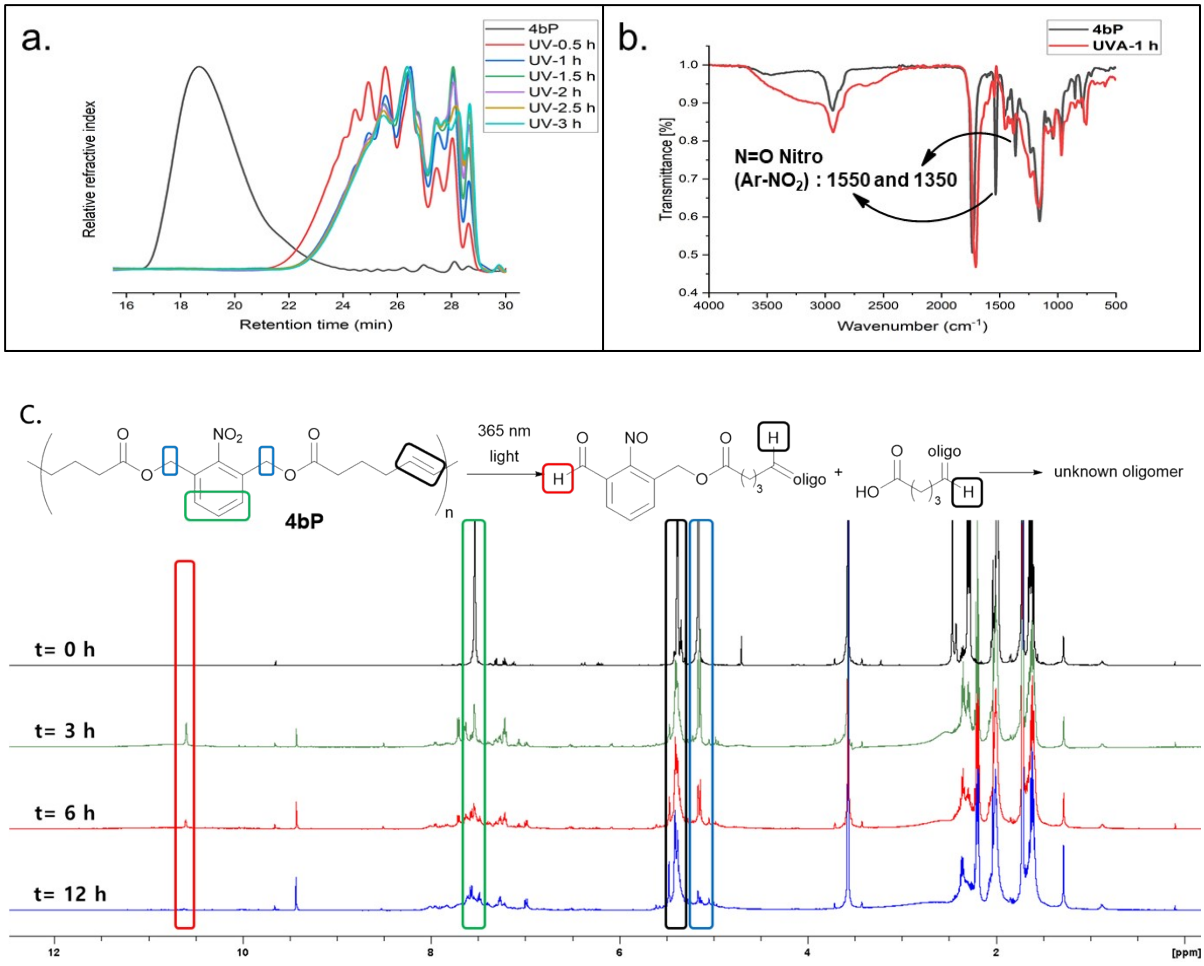


Fig. S14. Photodegradation study of polymer **4bP** under UVA light. GPC (a), FT-IR (b), NMR spectra (c) plots of polymer **4bP** and degraded polymer.

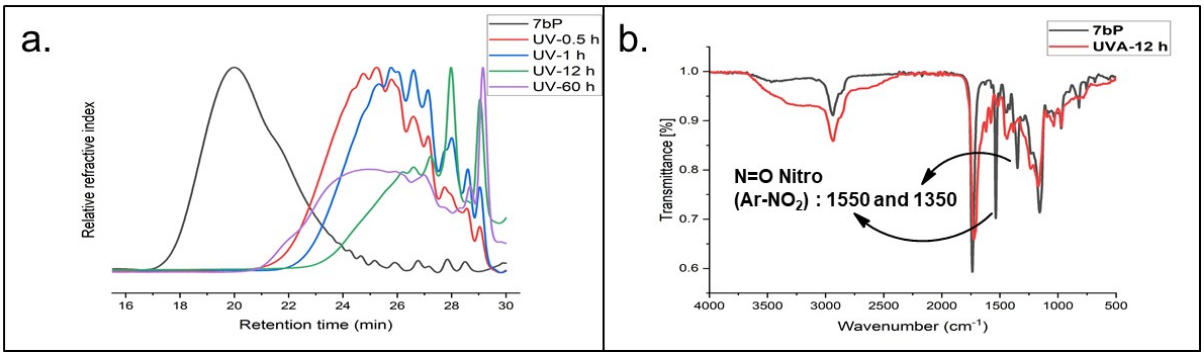
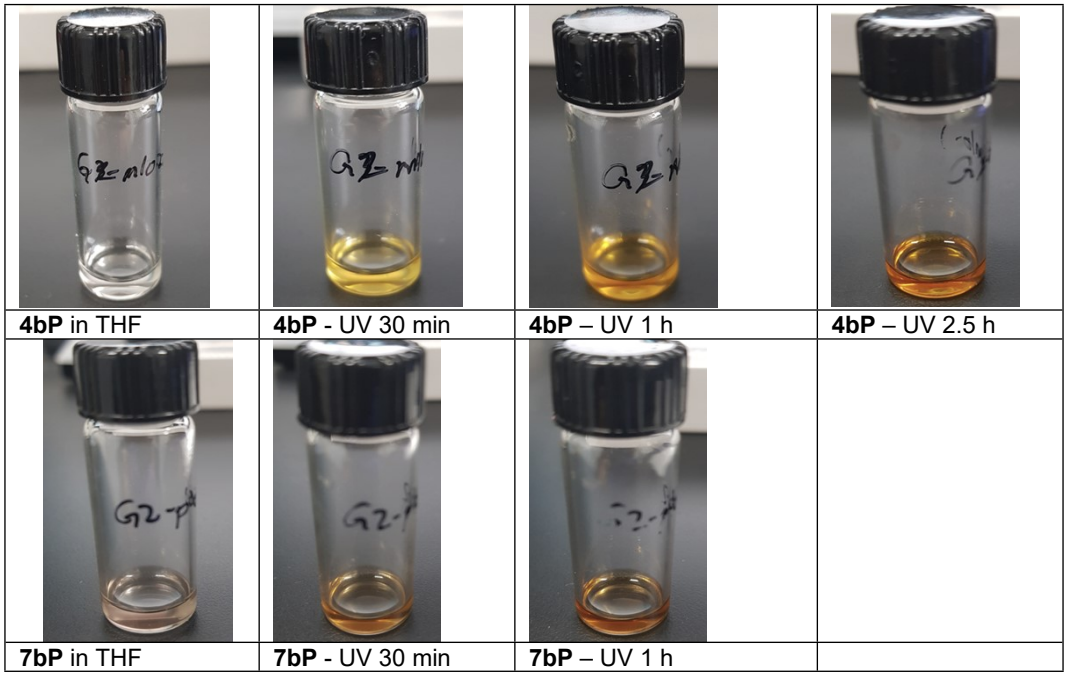


Fig. S15. Photodegradation study of polymer **7bP** under UVA light. GPC (a) and FT-IR (b) plots of polymer **7bP** and degraded polymer.



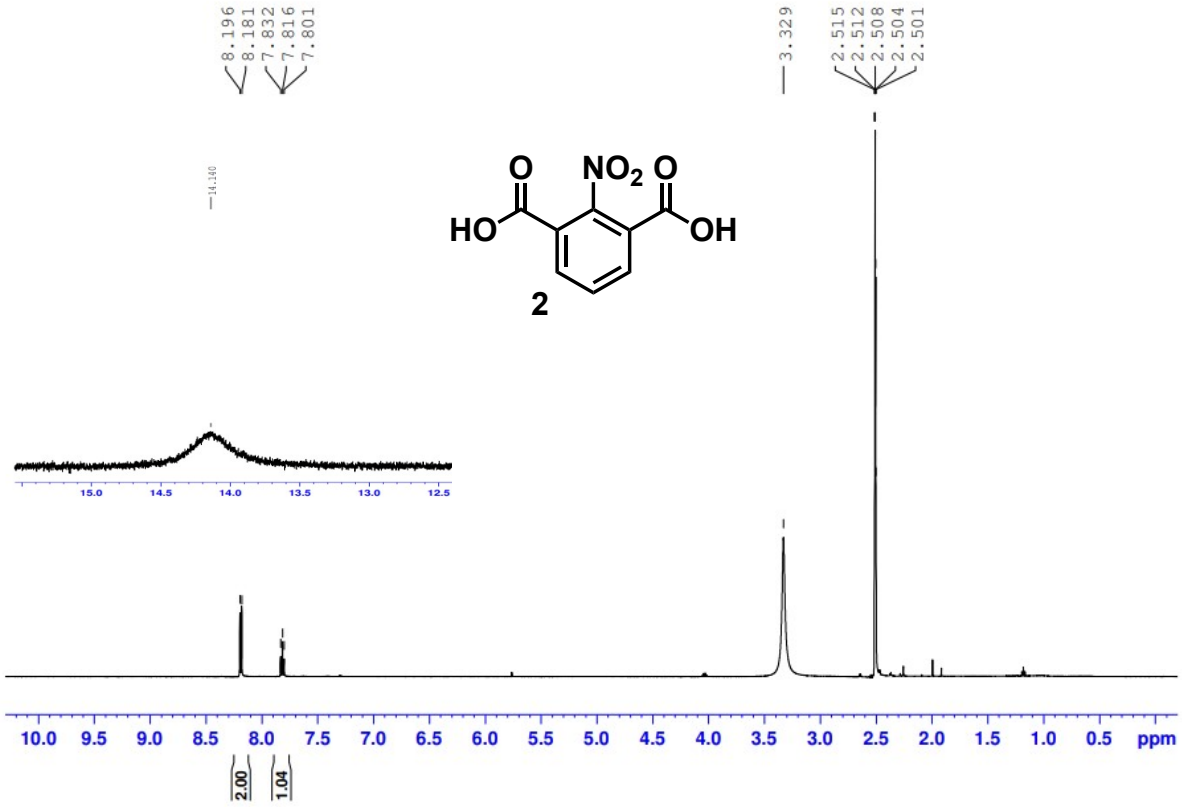
4bP in THF	**4bP** - UV 30 min	**4bP** – UV 1 h	**4bP** – UV 2.5 h
7bP in THF	**7bP** - UV 30 min	**7bP** – UV 1 h	

Fig. S16. Color changes of **4bP** and **7bP** under UVA light.

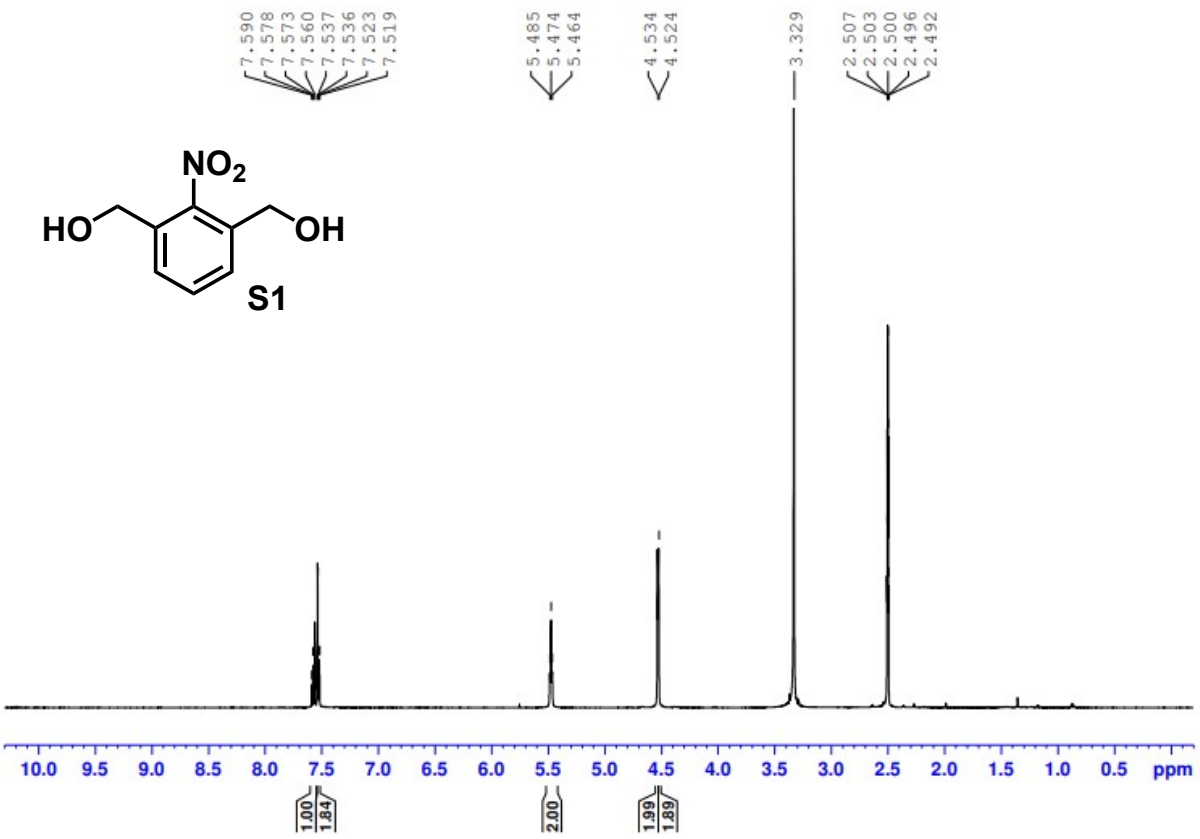
5. Computational Details

We optimized the geometries of the cyclic molecules at the B3LYP/6-31G(2df,p) level of theory based on the X-ray crystallographic structures. Such experimental structures were not available for linear molecules, and we performed the conformational searches as follows. First, we collected the lowest-energy conformations with the extended tight-binding (XTB) theory[7] using the software CREST.[8] The energy window for the conformational searches was 10.0 kcal/mol. Then, B3LYP/6-31G(2df,p) energies were calculated at all the geometries with the XTB energy within 0.003 E_h from the lowest-energy conformation (except for **7b**, in which we have employed 0.002 E_h). Finally, we performed free energy calculations for six molecular conformations with each species' lowest B3LYP/6-31G(2df,p) energies. In summary, the free energy calculations were performed at seven geometries (one and six for cyclic and linear molecules, respectively) for each species, resulting in 42 free energy calculations. The linear conformations with the lowest Gibbs free energies were used to compute the ΔG reported in Table 3 in the main text. The solvent effect due to the DCM solvent was considered in all DFT calculations using the SCRF theory.[9]

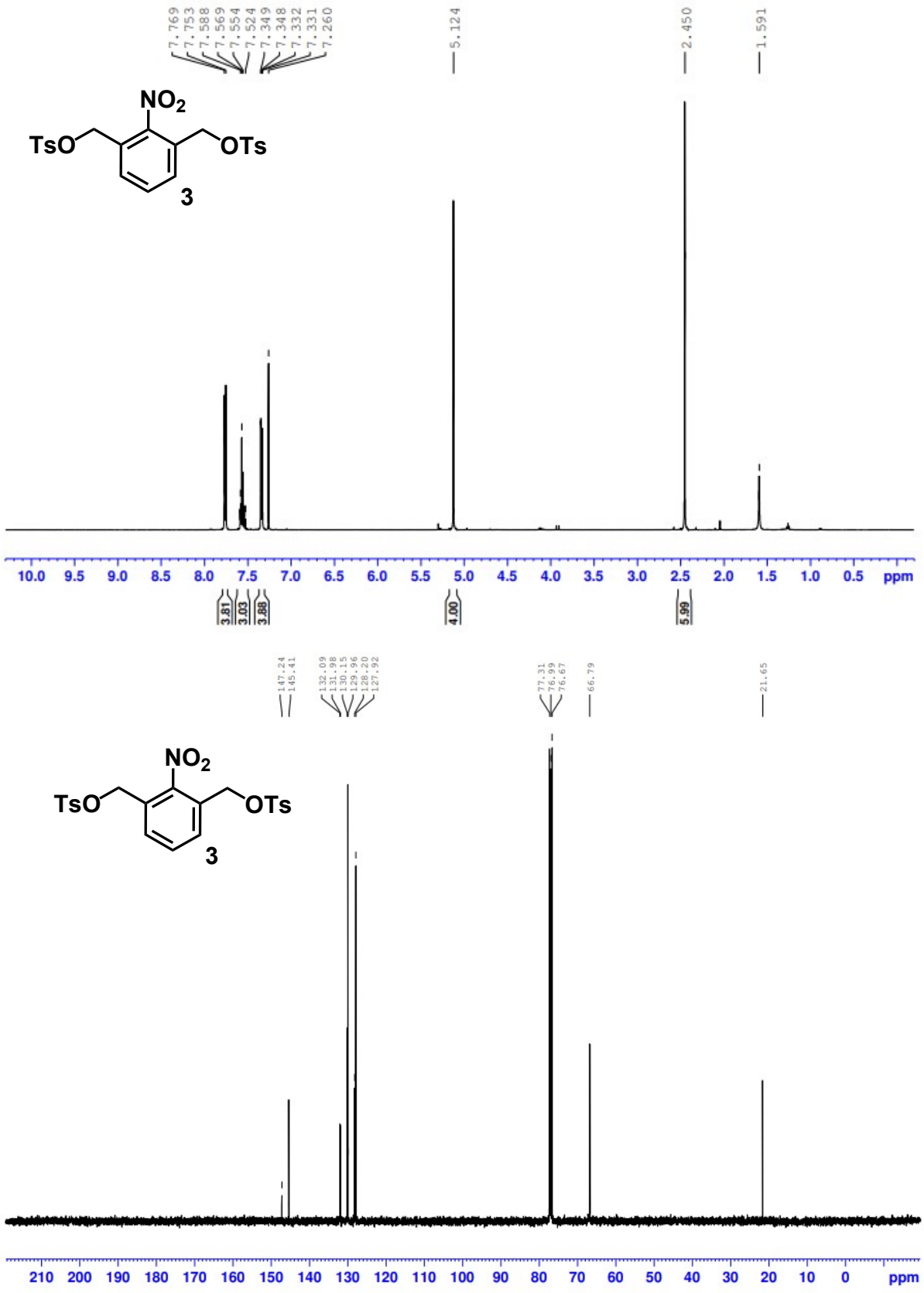
6. ^{1}H NMR and ^{13}C NMR spectra



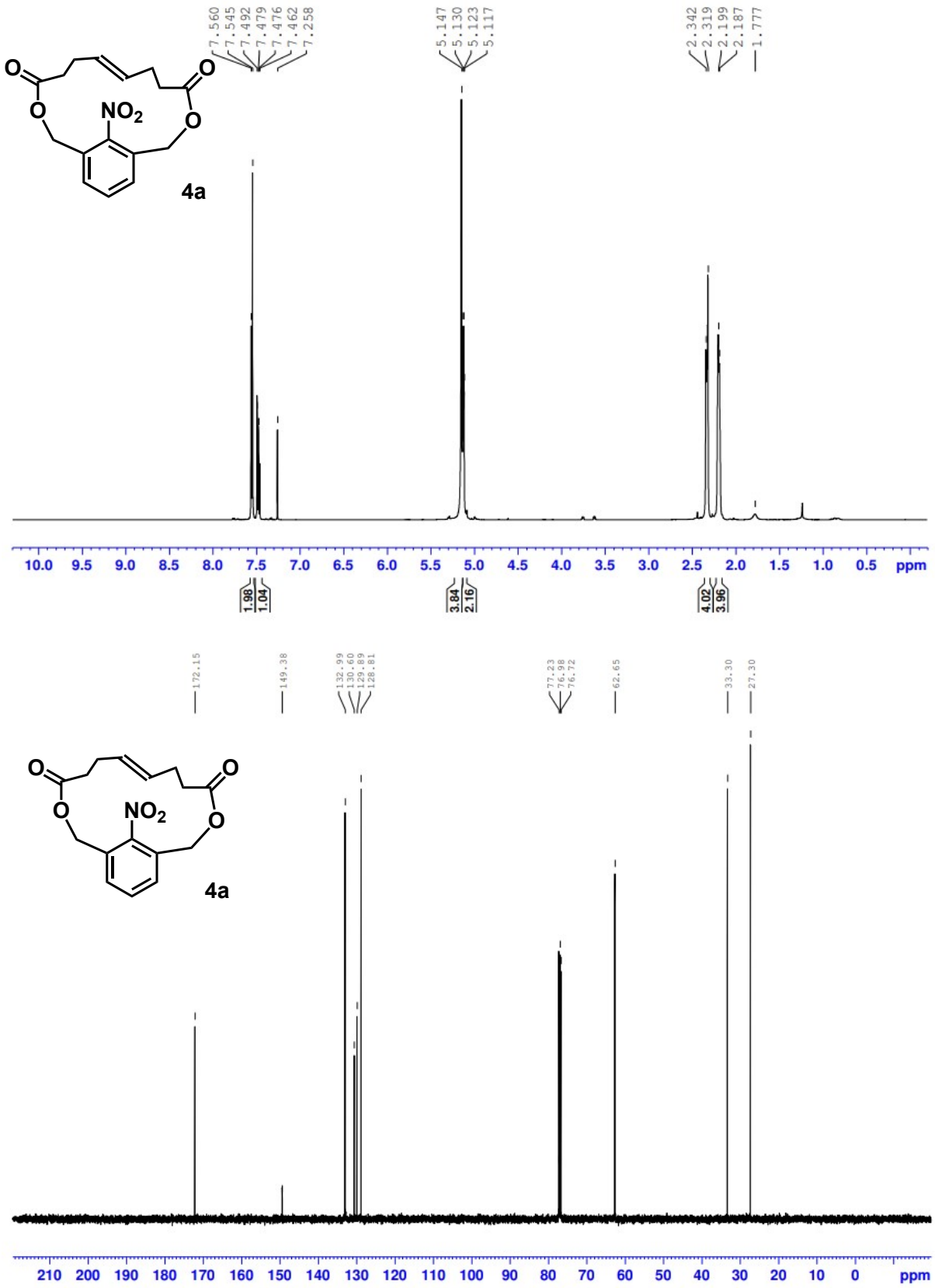
^{1}H NMR (DMSO-d_6, 500 MHz) spectra of compound **2**



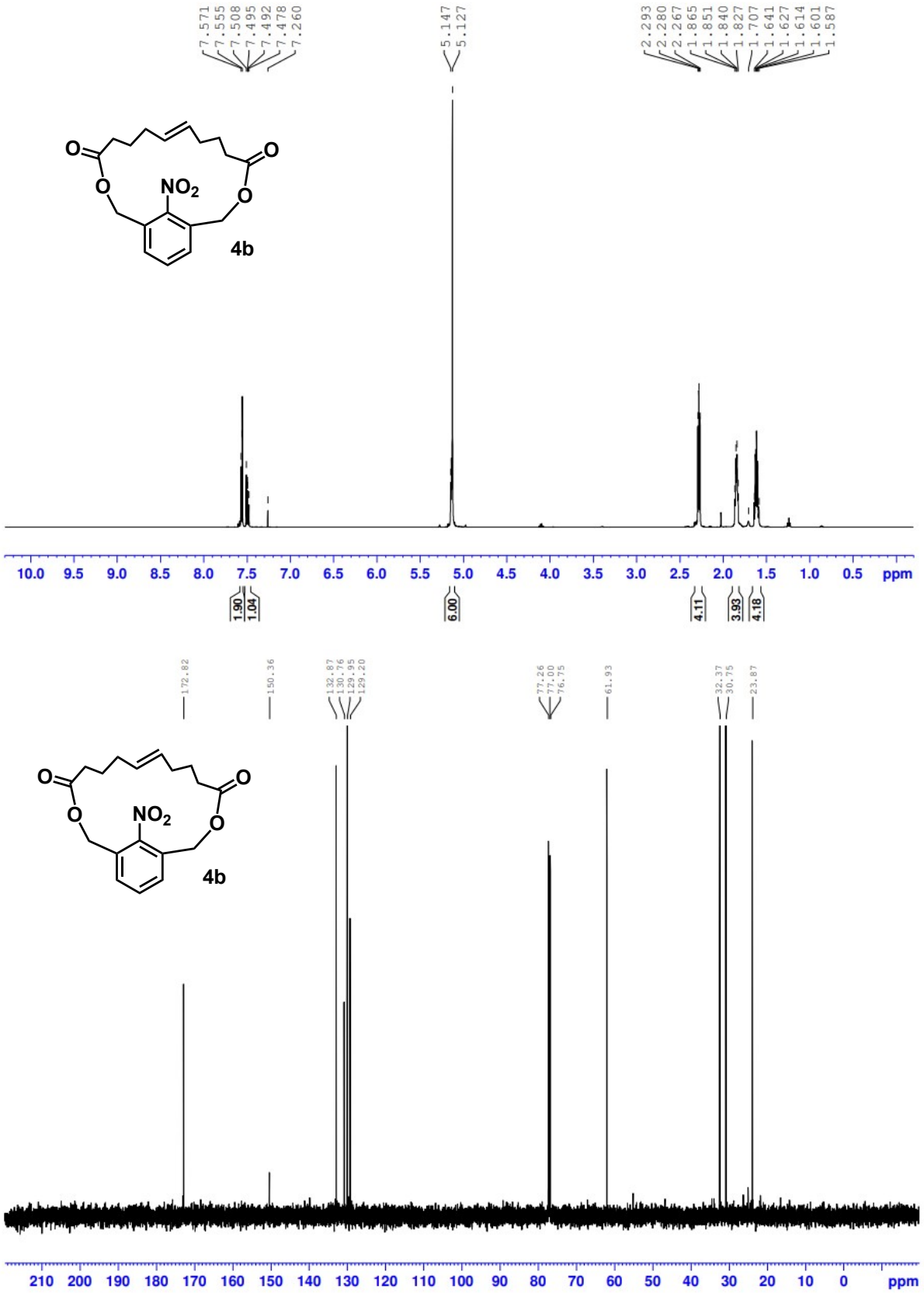
^{1}H NMR (DMSO-d_6, 500 MHz) spectra of compound **S1**



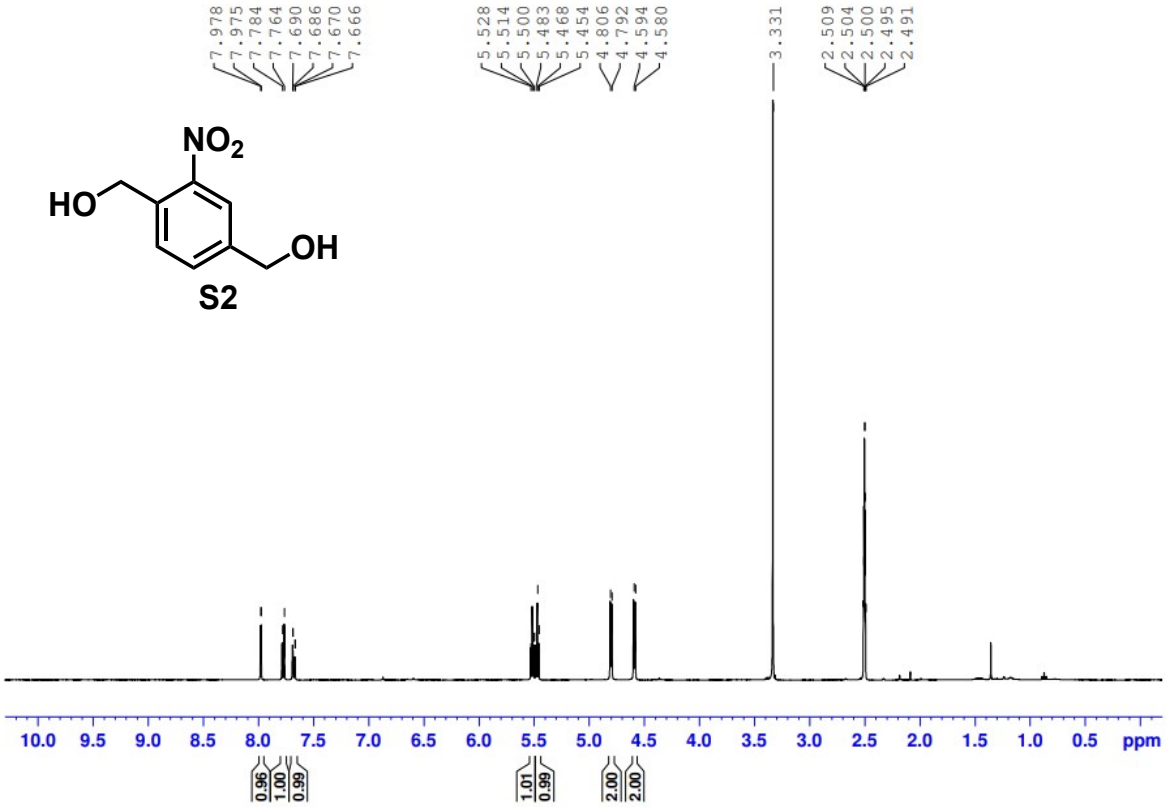
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of compound **3**



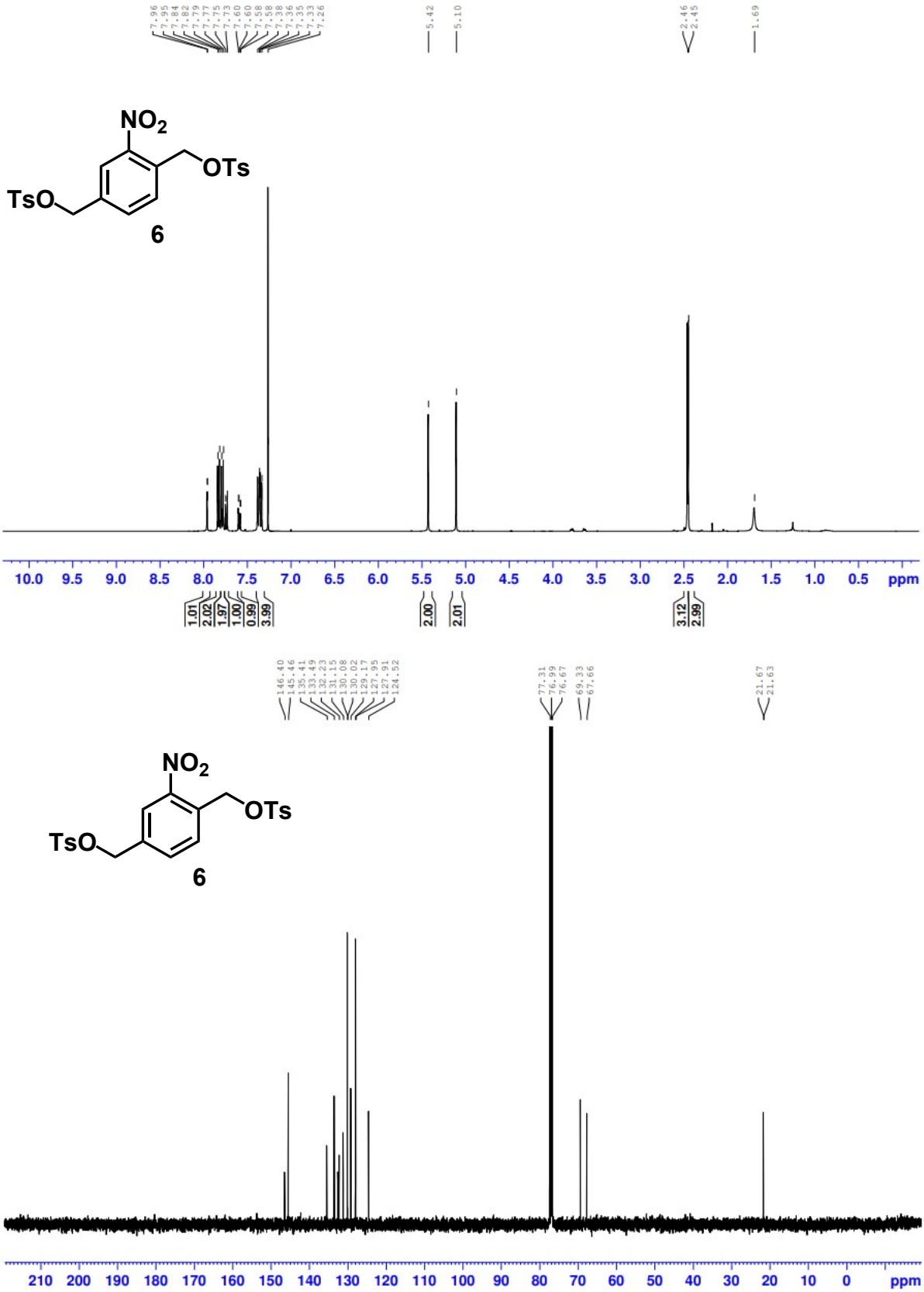
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 125 MHz) spectra of compound **4a**



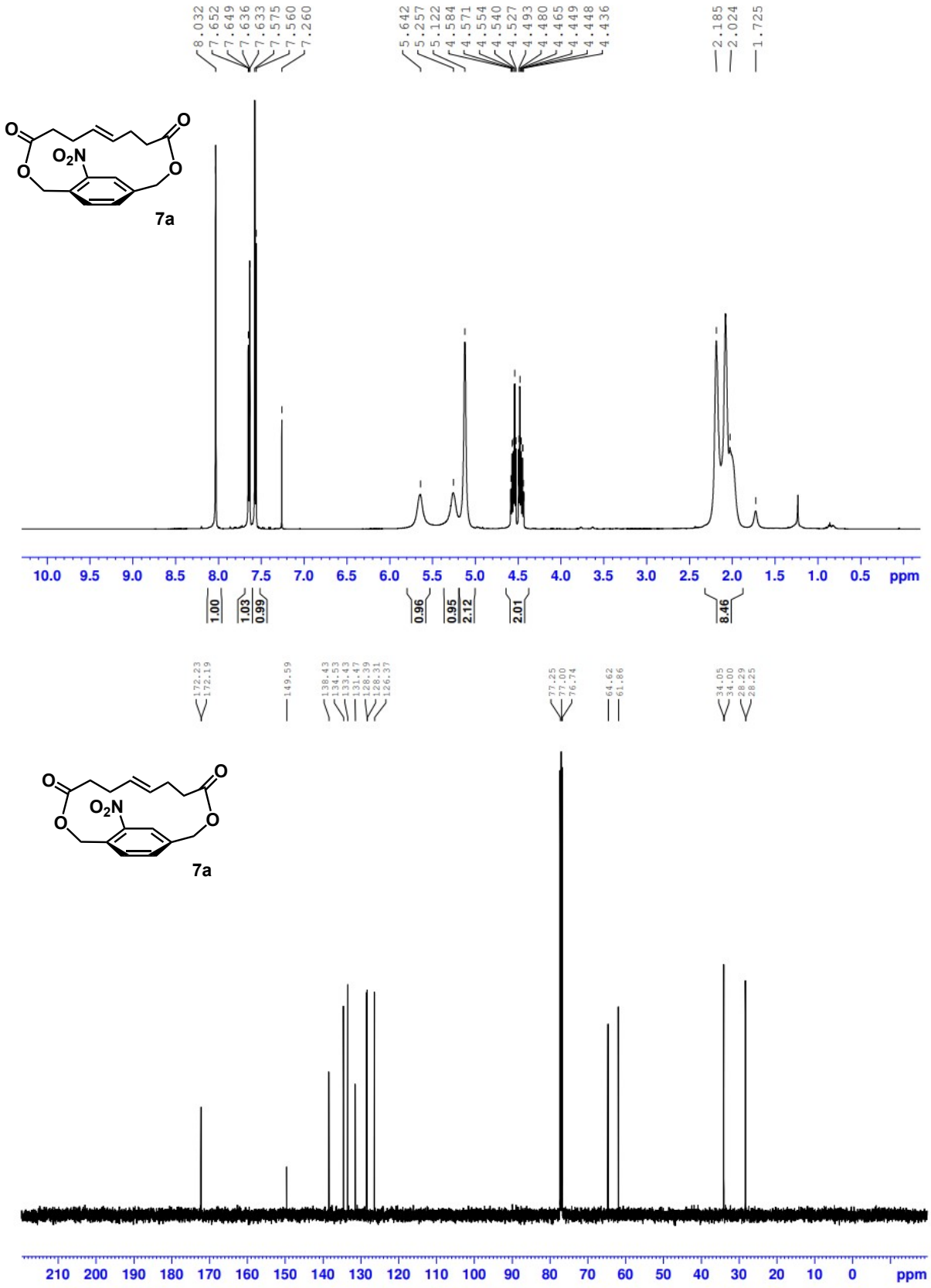
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 125 MHz) spectra of compound **4b**



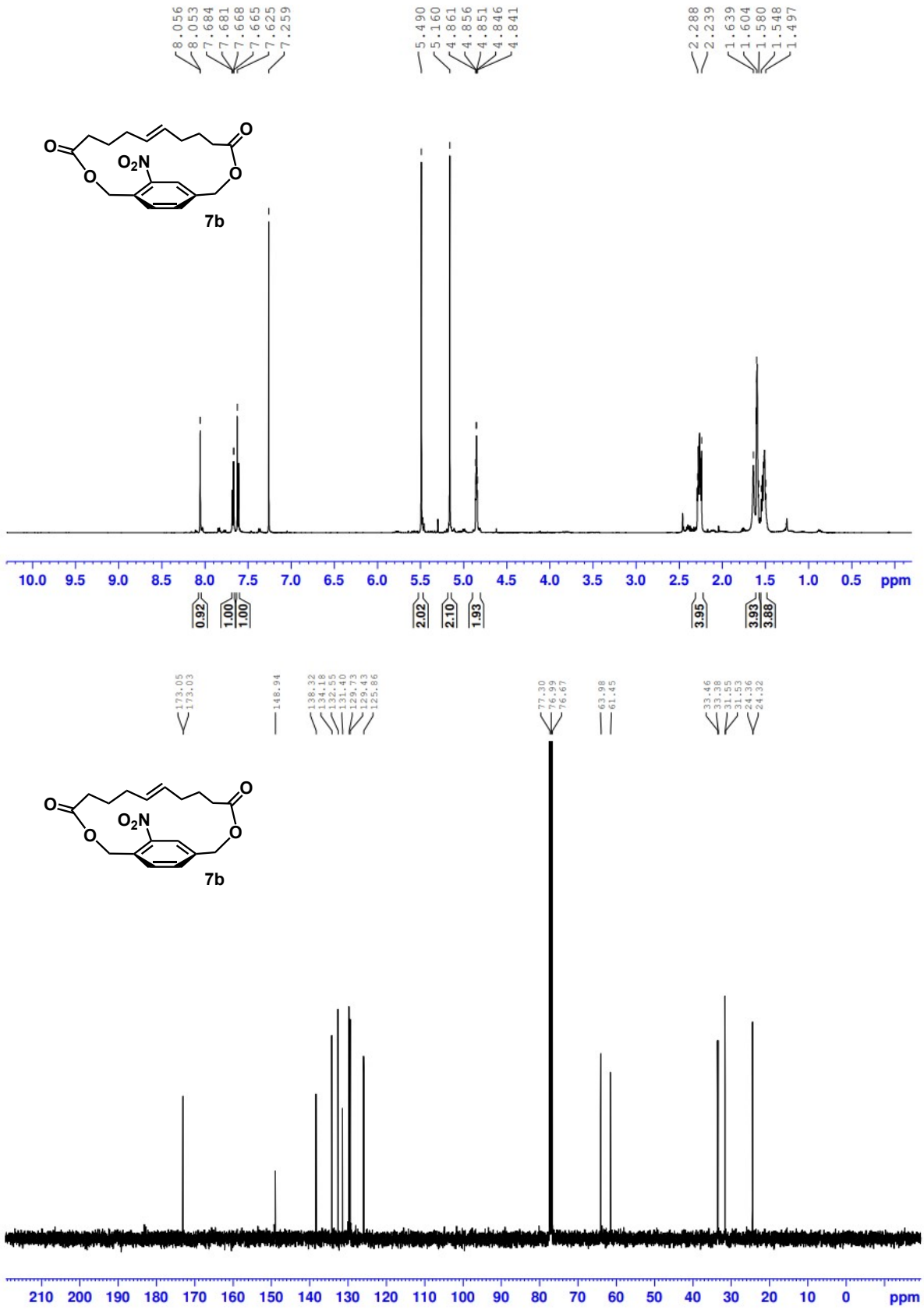
^{1}H NMR (DMSO-d_6, 500 MHz) spectra of compound **S2**



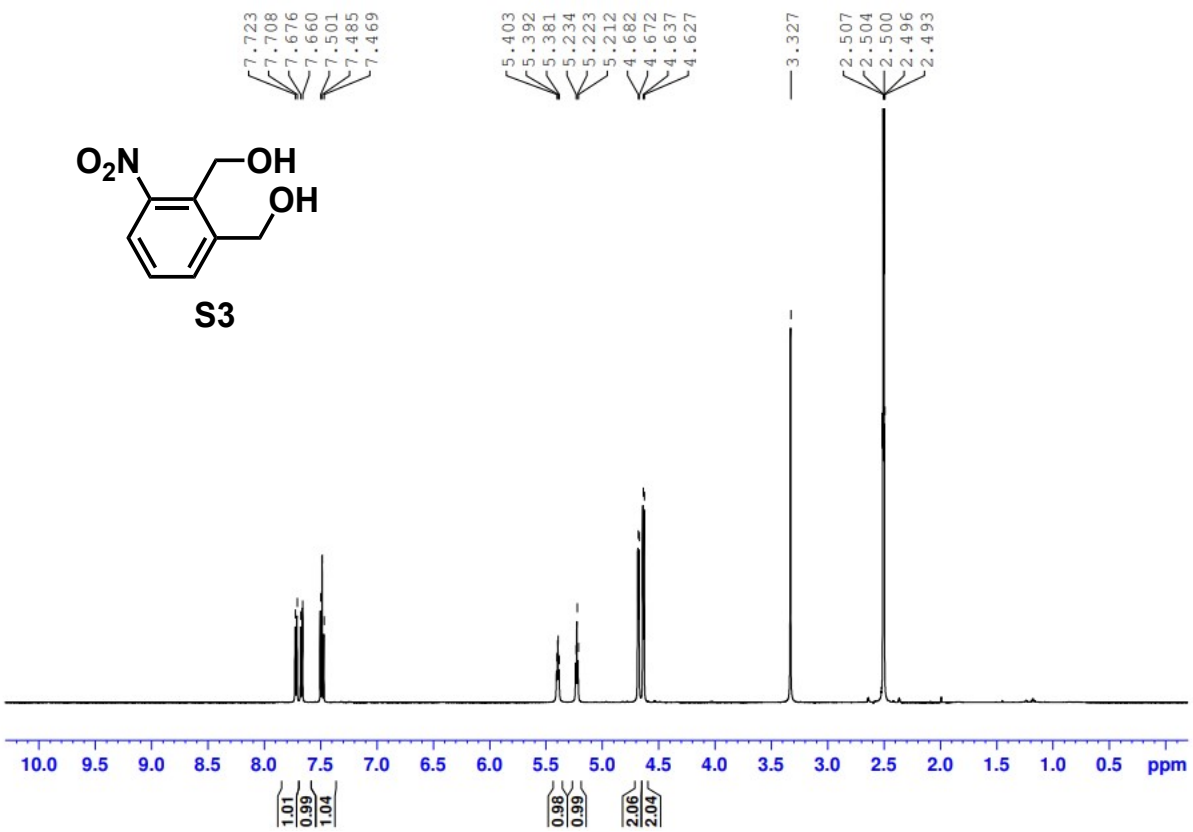
^{1}H NMR ($CDCl_3$, 400 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of compound **6**



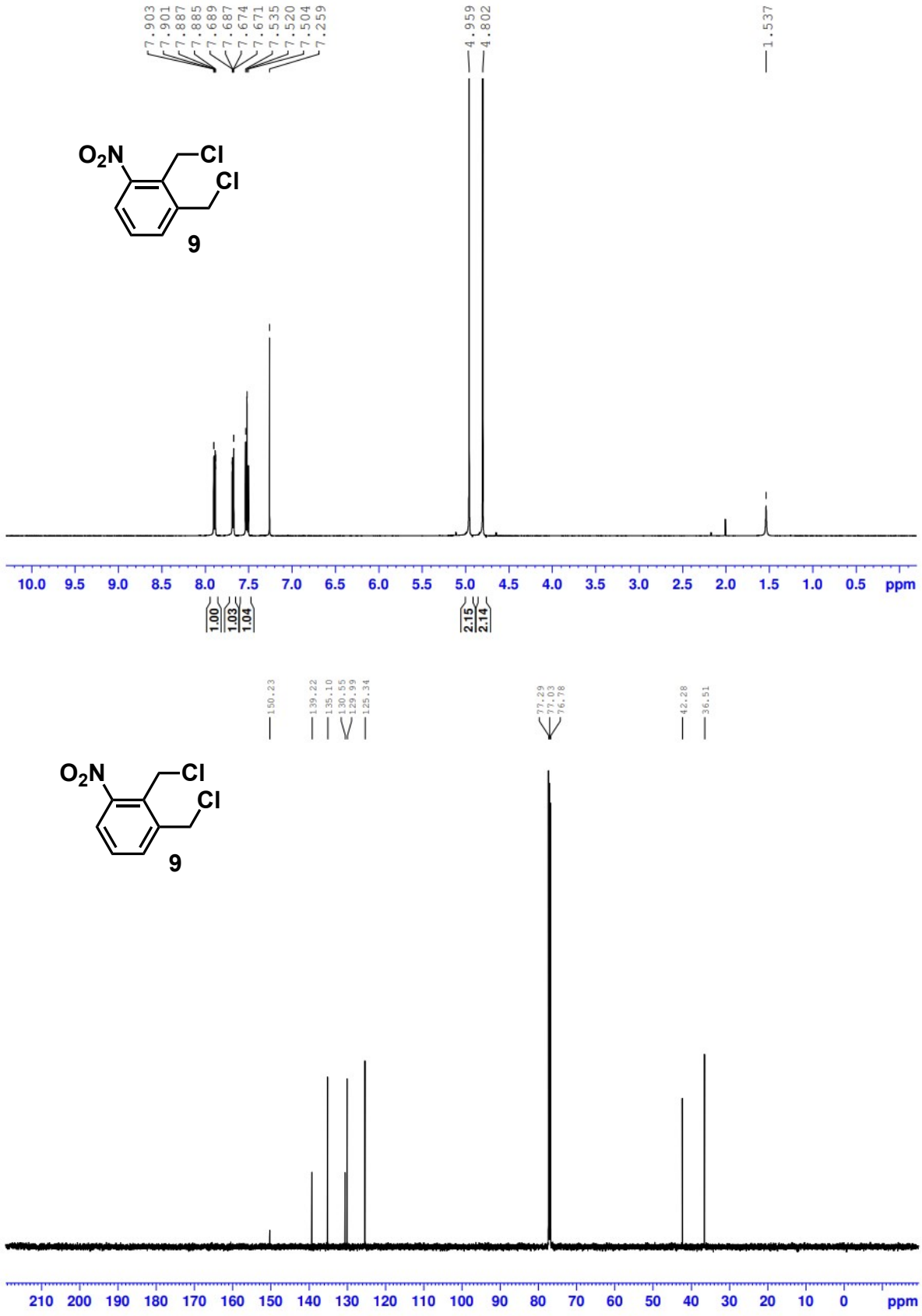
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 125 MHz) spectra of compound **7a**



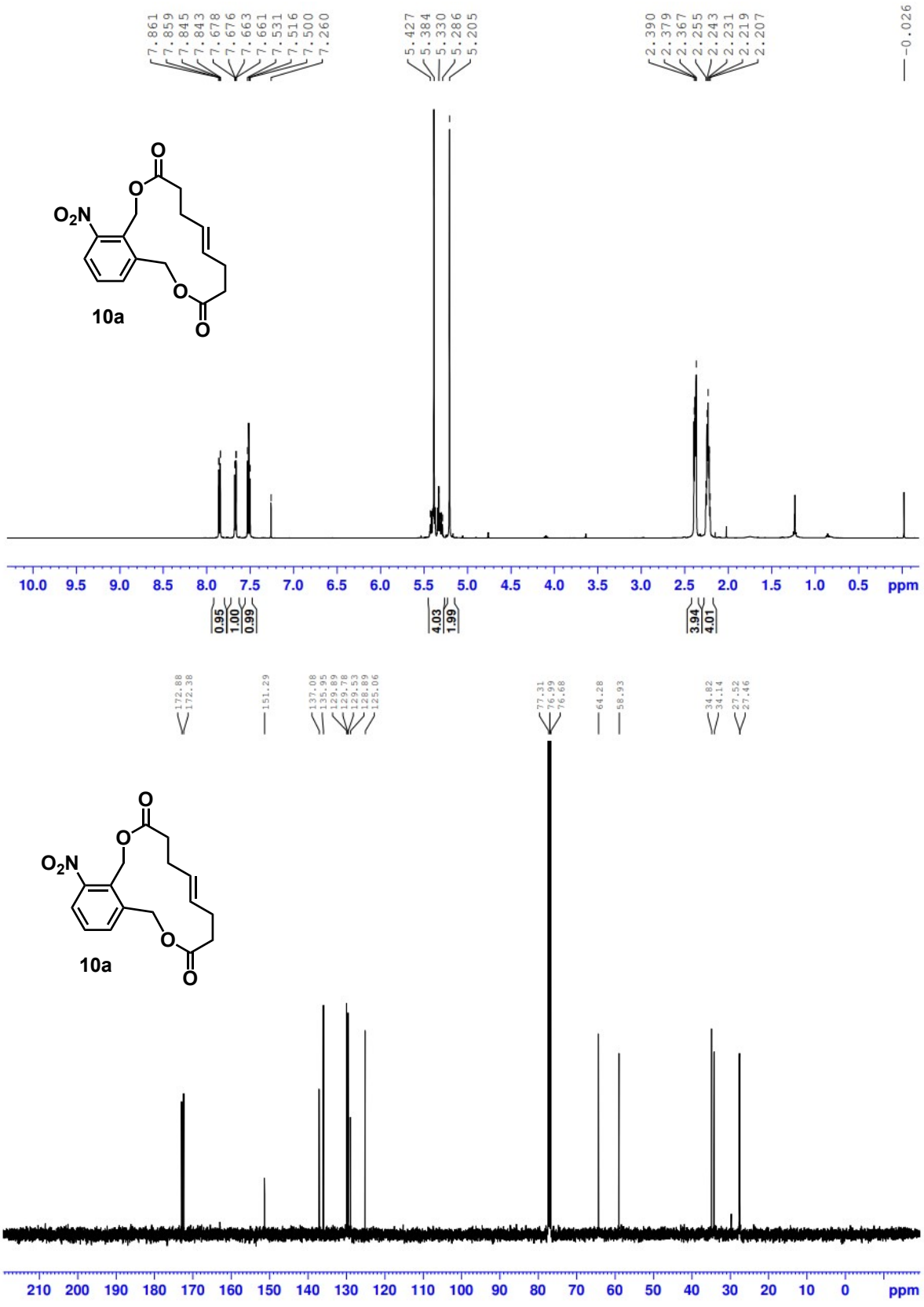
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of compound **7b**



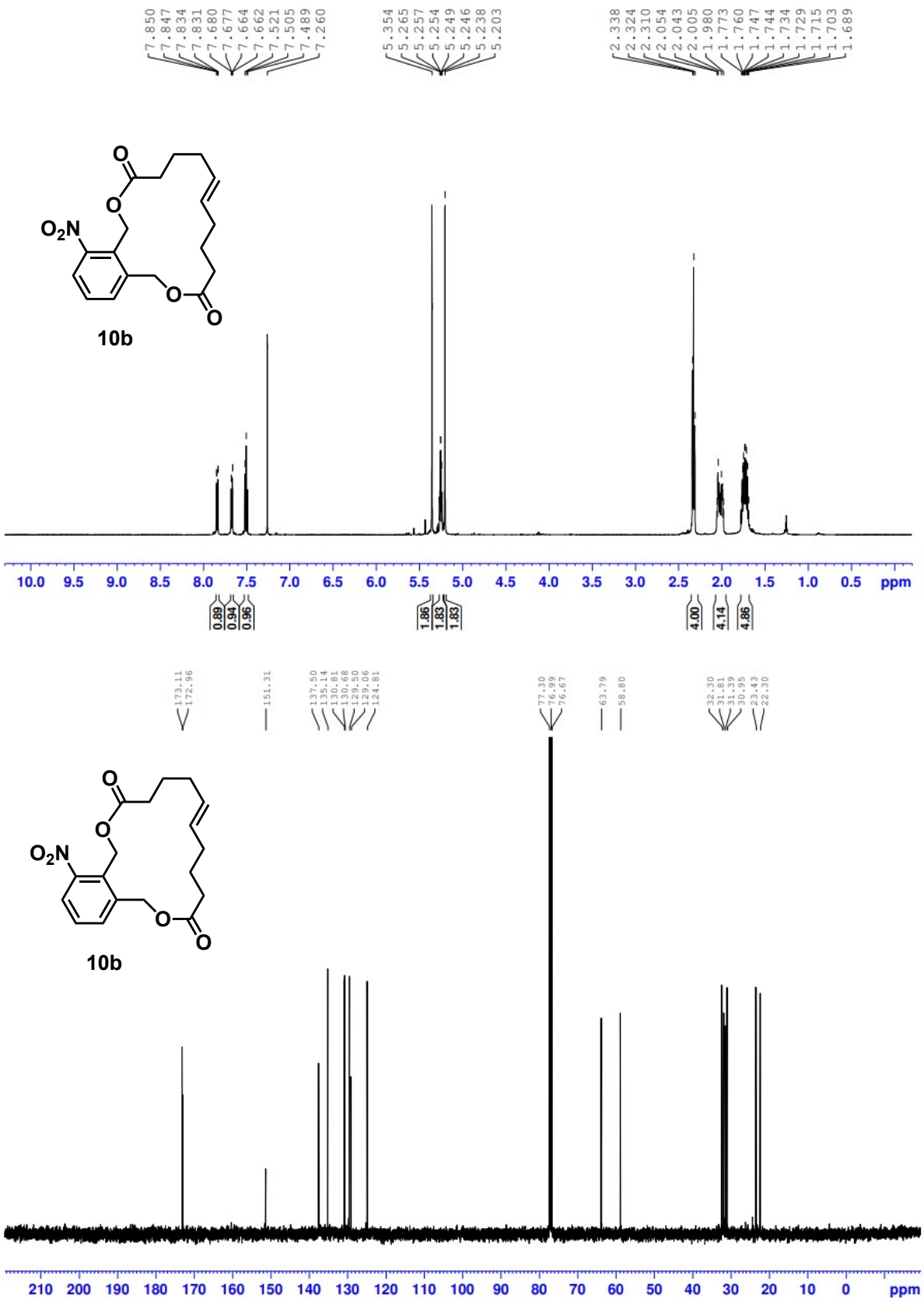
^{1}H NMR (DMSO-d_6, 500 MHz) spectra of compound **S3**



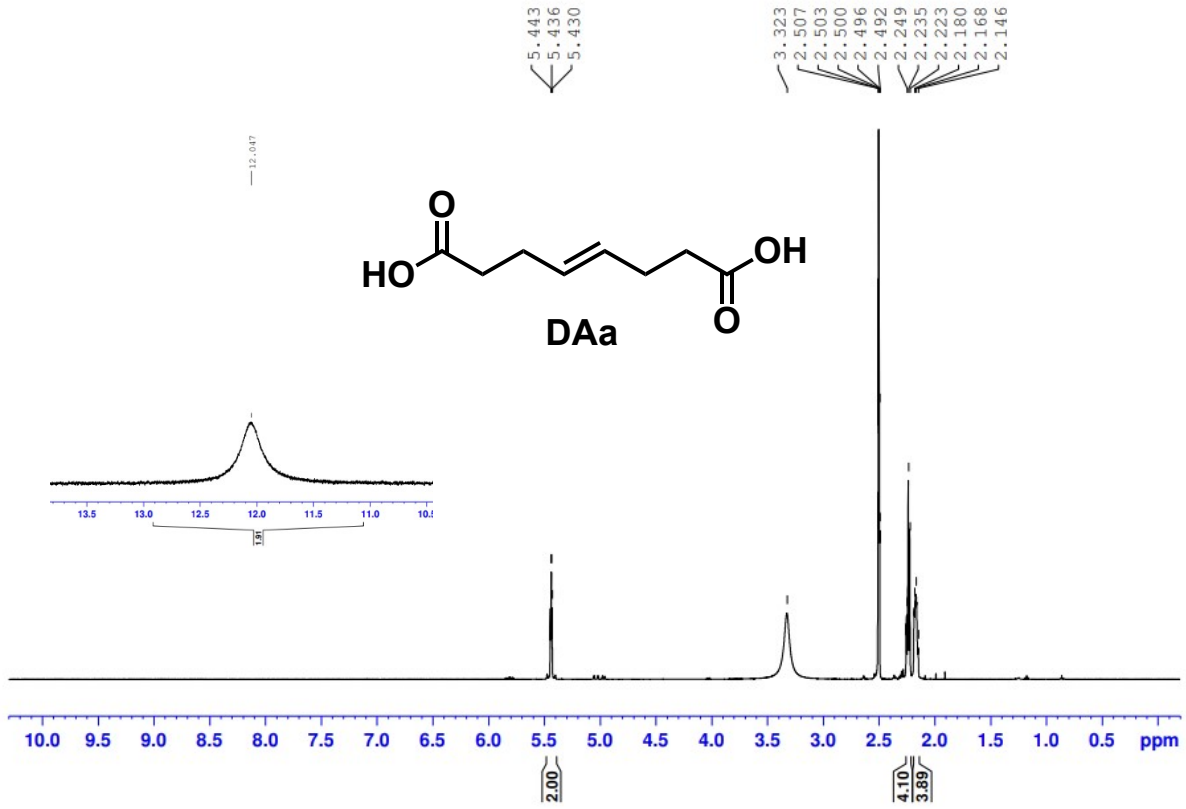
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 125 MHz) spectra of compound **9**



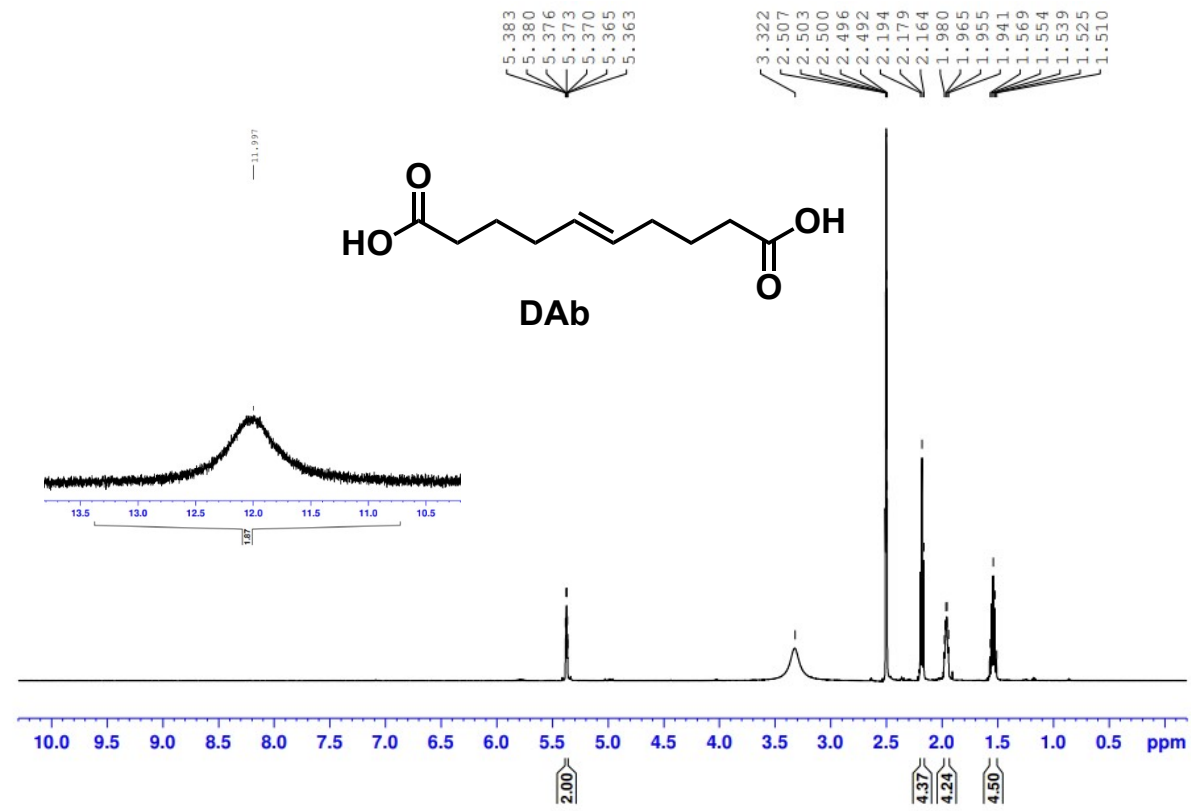
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of compound **10a**



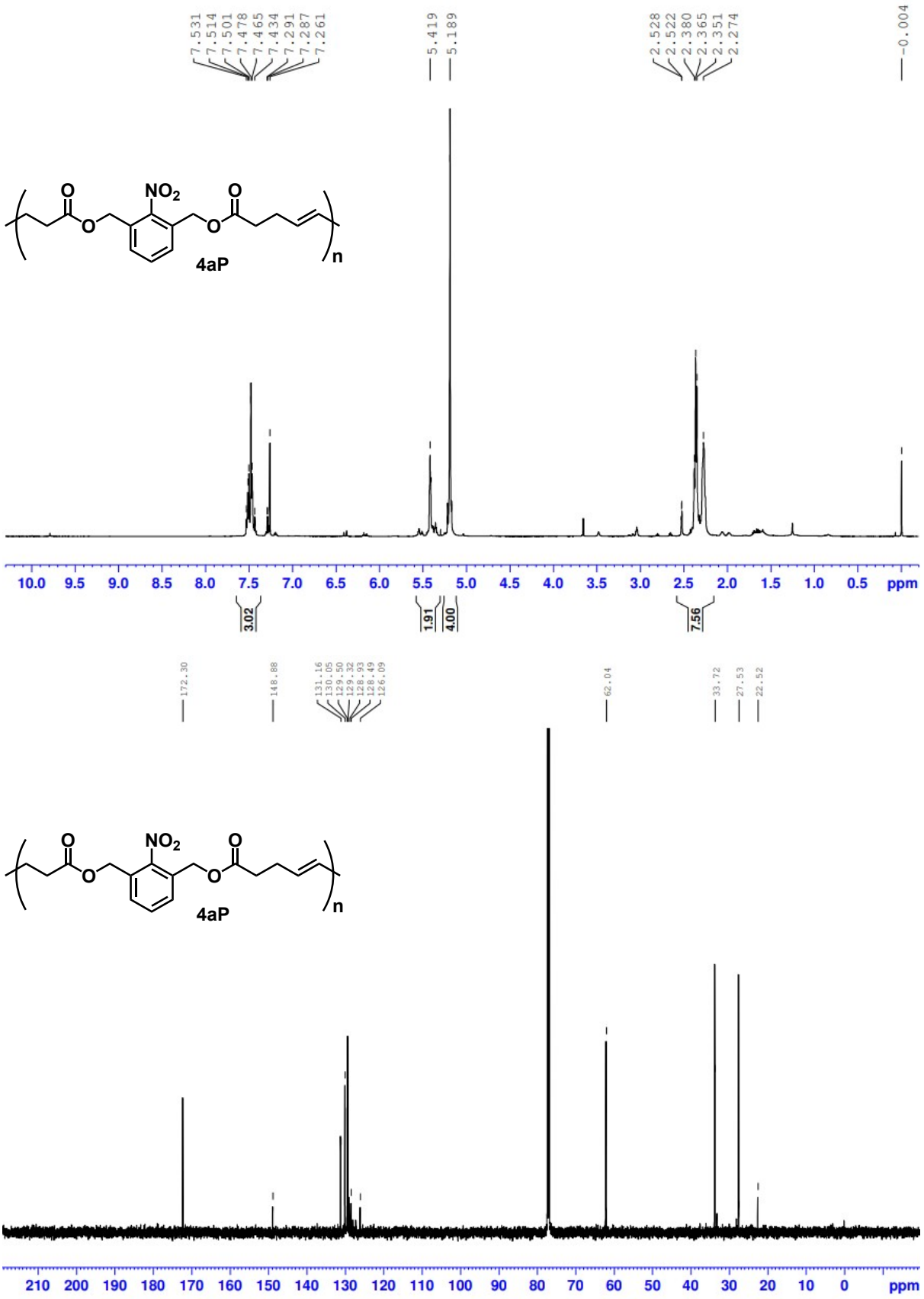
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of compound **10b**



^{1}H NMR (DMSO-d_6, 500 MHz) spectra of compound **DAa**

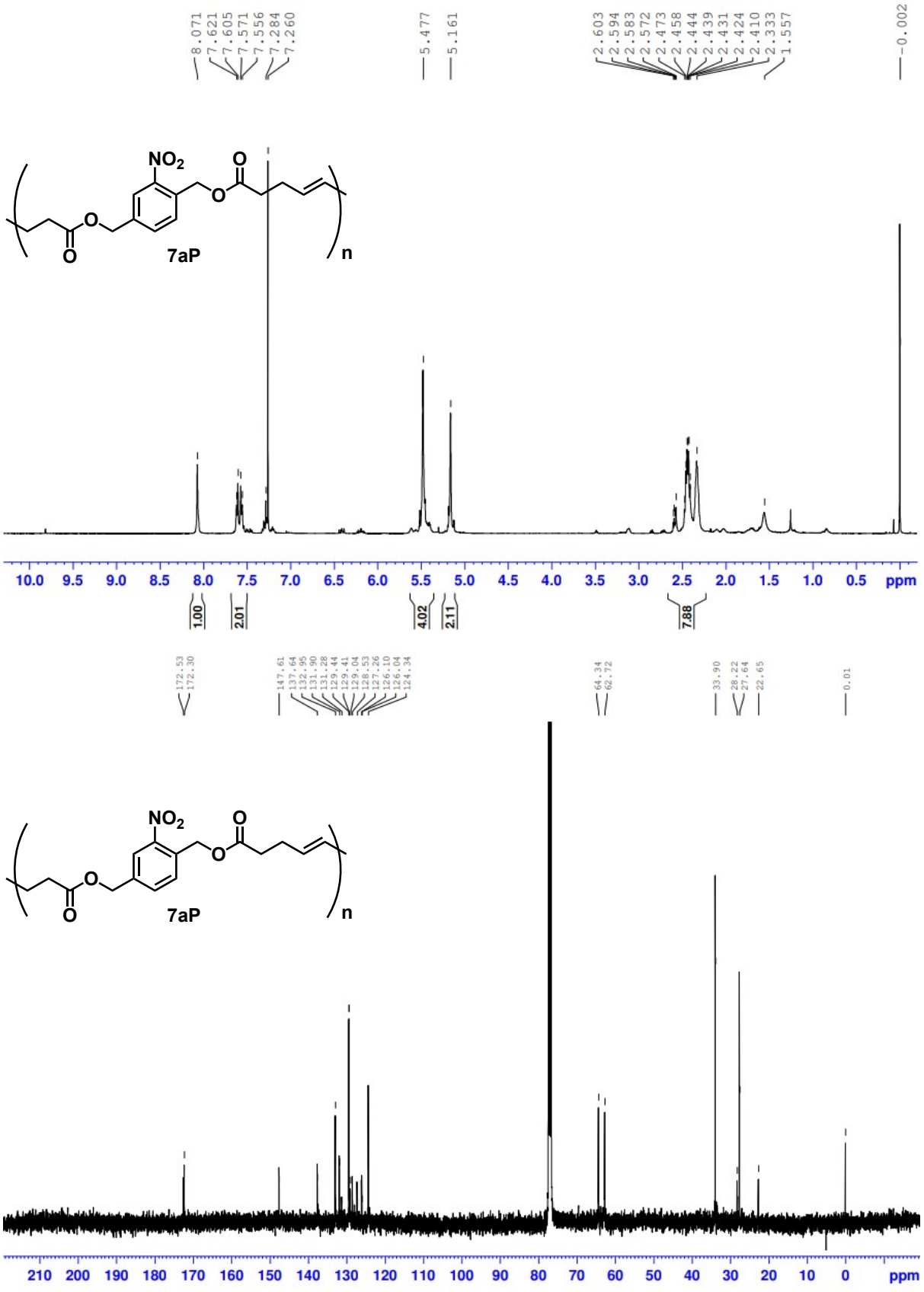


^{1}H NMR (DMSO-d_6, 500 MHz) spectra of compound **Dab**.

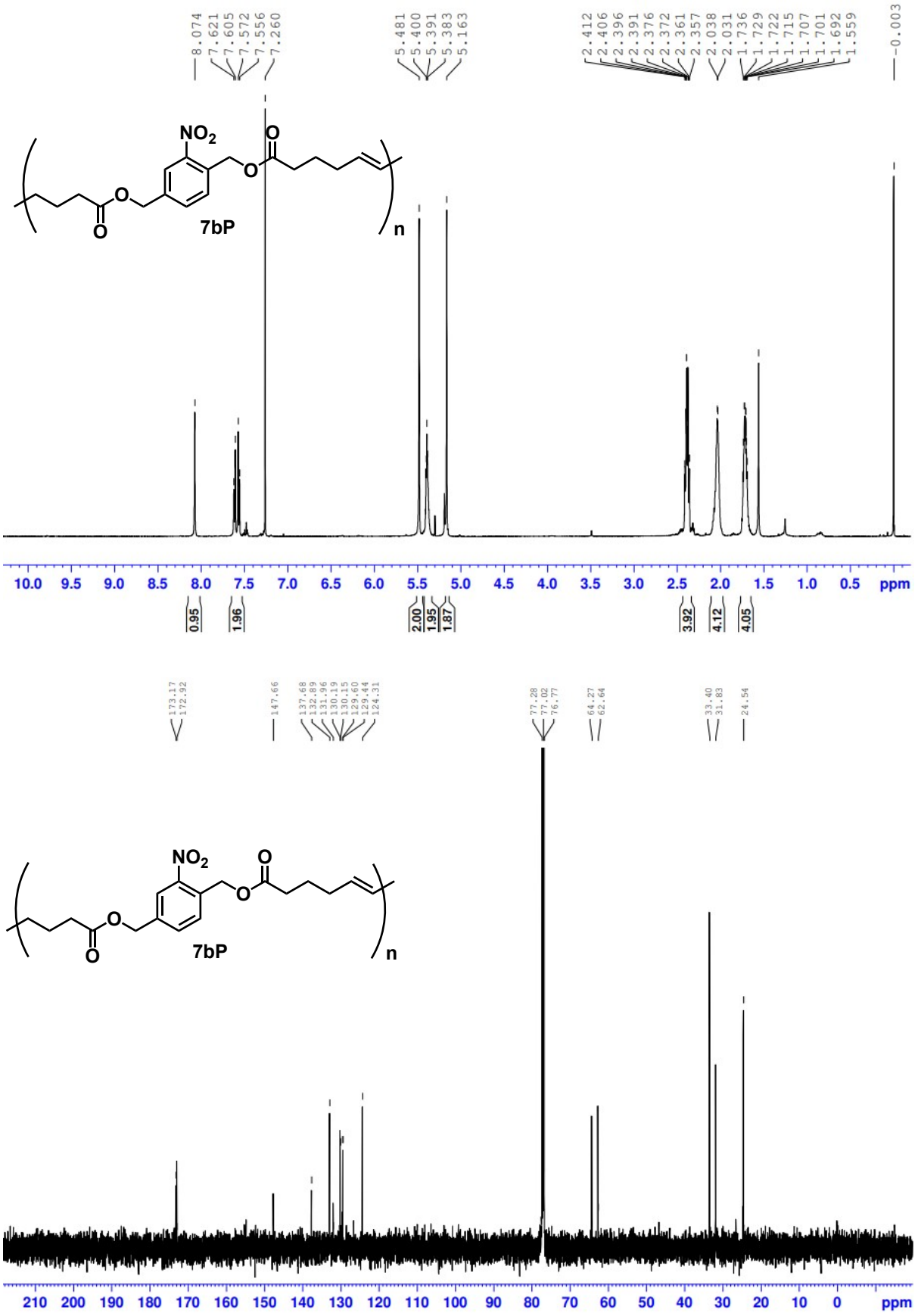


^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 125 MHz) spectra of compound **4aP.**

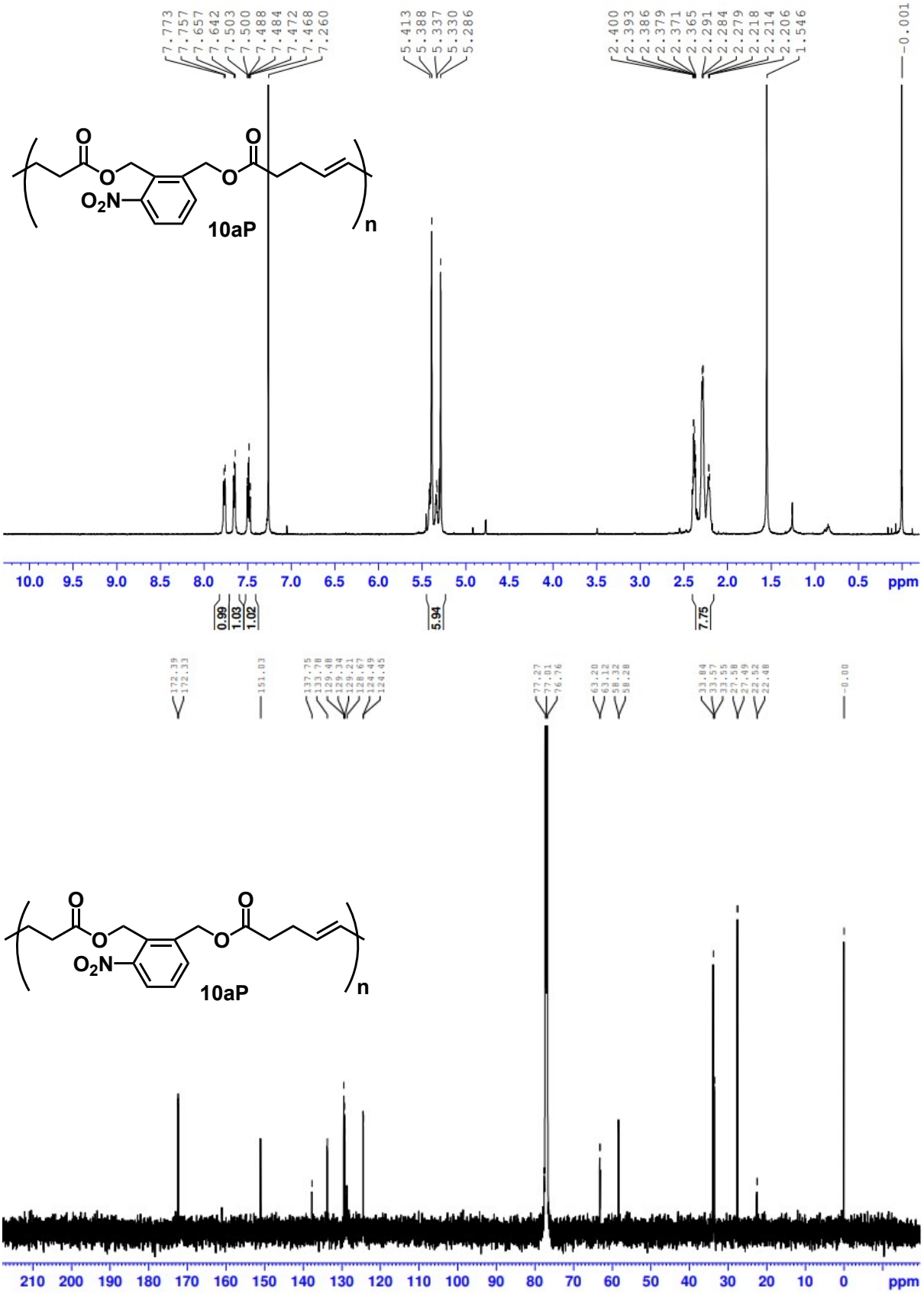
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of compound **4bP.**



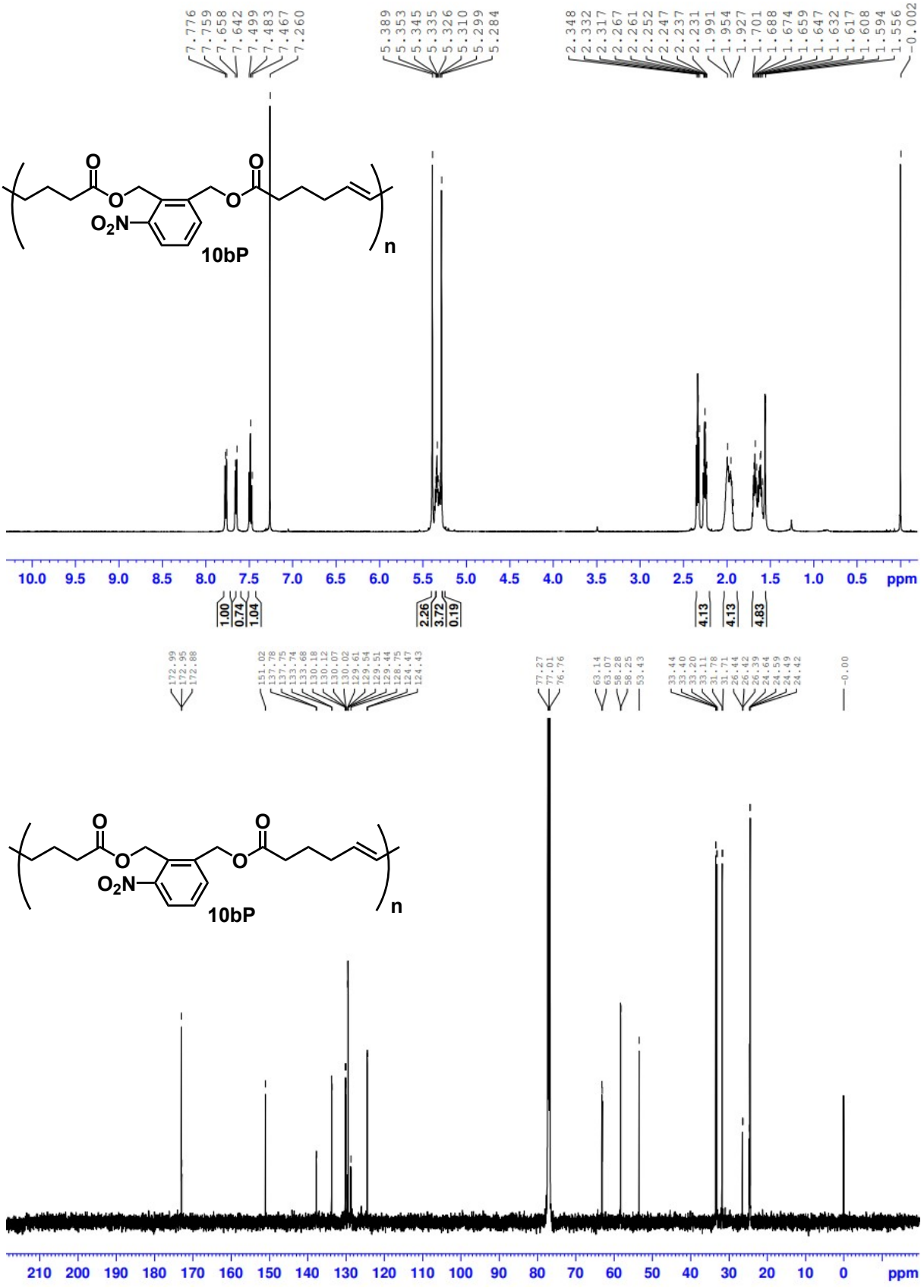
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 100 MHz) spectra of compound **7aP.**



^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 125 MHz) spectra of compound **7bP.**

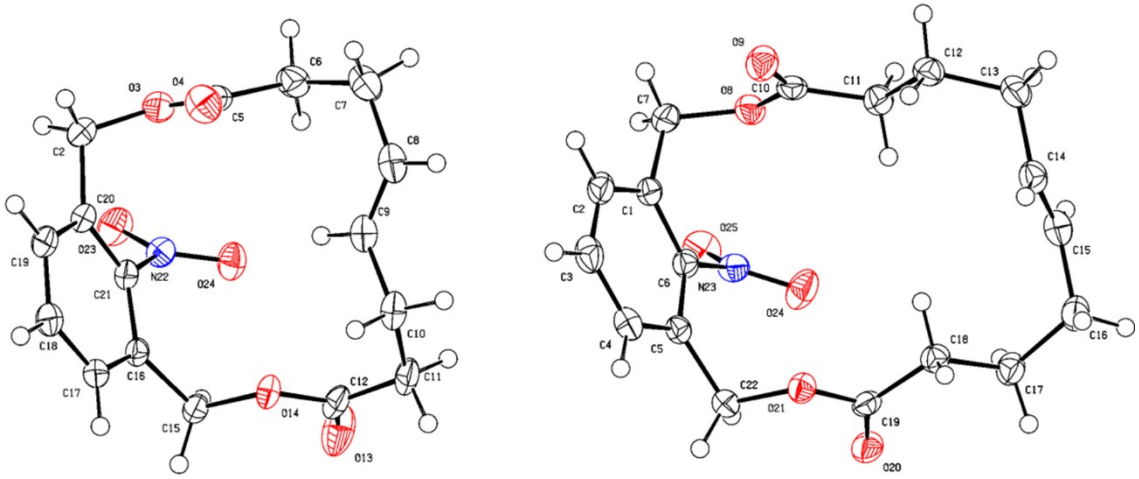


^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 125 MHz) spectra of compound **10aP.**



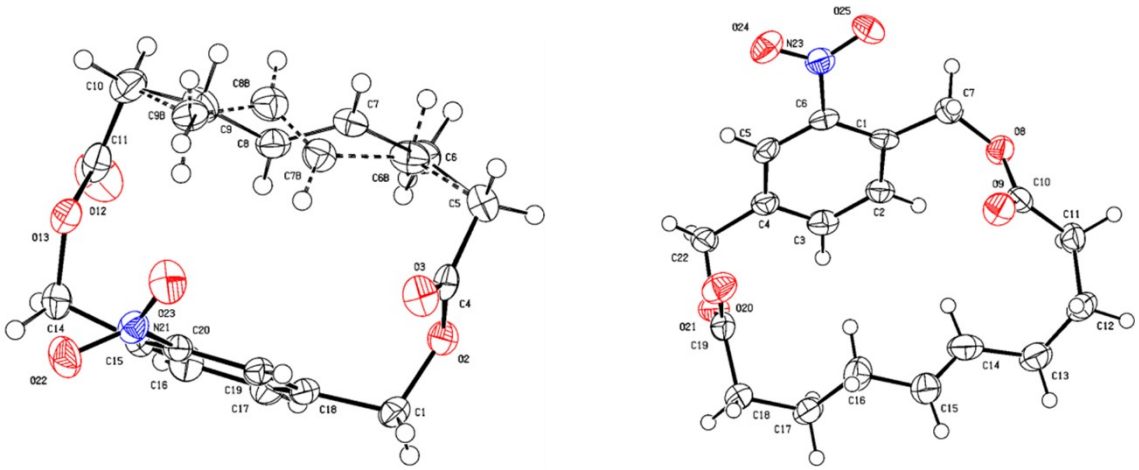
^{1}H NMR ($CDCl_3$, 500 MHz) and ^{13}C NMR ($CDCl_3$, 125 MHz) spectra of compound **10bP.**

7. Data tables for the obtained X-ray crystal structures of monomers



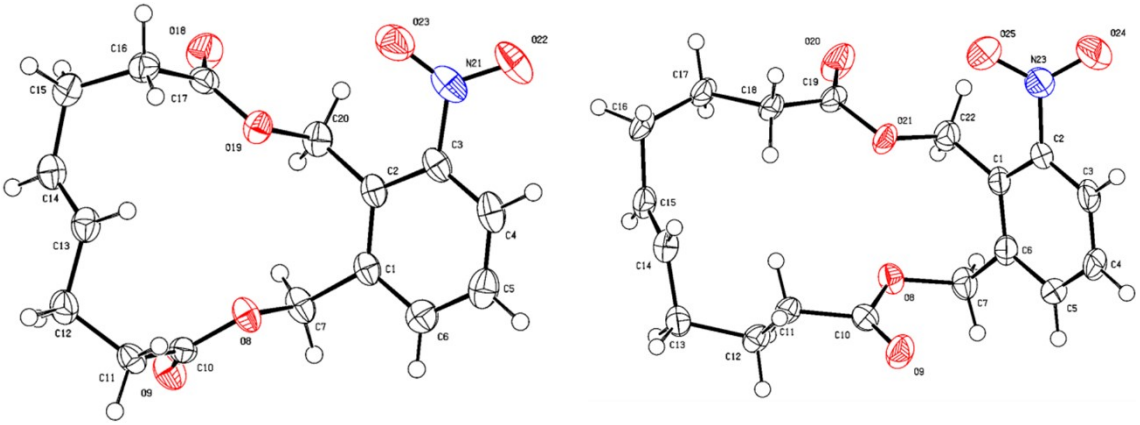
4a **4b**

Fig. S17. X-ray structures of **4a**, **4b**.



7a **7b**

Fig. S18. X-ray structures of **7a**, **7b.**



10a **10b**

Fig. S19. X-ray structures of **10a**, **10b.**

Table S8. Crystal data and structure refinement for **4a**.

Empirical formula	$C_{16}\ H_{17}\ N\ O_6$	
Formula weight	319.30	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 12.9980(5) Å	α = 90°
	b = 7.7936(3) Å	β = 106.5061(12)°
	c = 15.3862(6) Å	γ = 90°
Volume	1494.41(10) $Å^3$	
Z	4	
Density (calculated)	1.419 Mg/m^3	
Absorption coefficient	0.110 mm^{-1}	
F(000)	672	
Crystal size	0.317 x 0.288 x 0.132 mm^3	
Theta range for data collection	2.761 to 27.494°.	
Index ranges	–16<=h<=16, –10<=k<=10, –19<=l<=18	
Reflections collected	25507	
Independent reflections	3360 [R(int) = 0.0714]	
Completeness to theta = 25.242°	97.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6093	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3360 / 0 / 208	
Goodness-of-fit on F^2	1.054	
Final R indices [I>2sigma(I)]	R1 = 0.0382, wR2 = 0.0908	
R indices (all data)	R1 = 0.0461, wR2 = 0.0991	
Largest diff. peak and hole	0.240 and –0.227 $e·Å^{-3}$	

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **4a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(2)	4198(1)	4027(2)	7285(1)	32(1)
O(3)	3077(1)	4493(1)	7045(1)	31(1)
O(4)	3409(1)	6845(1)	6317(1)	38(1)
C(5)	2776(1)	5907(2)	6514(1)	29(1)
C(6)	1572(1)	6071(2)	6243(1)	33(1)
C(7)	1108(1)	7436(2)	5535(1)	37(1)
C(8)	1120(1)	7054(2)	4578(1)	34(1)
C(9)	1452(1)	5649(2)	4260(1)	30(1)
C(10)	1469(1)	5411(2)	3292(1)	31(1)
C(11)	1008(1)	3707(2)	2858(1)	32(1)
C(12)	1551(1)	2104(2)	3309(1)	29(1)
O(13)	1125(1)	732(1)	3282(1)	49(1)
O(14)	2597(1)	2365(1)	3739(1)	26(1)
C(15)	3184(1)	948(2)	4260(1)	25(1)
C(16)	4011(1)	1802(1)	5023(1)	22(1)
C(17)	4993(1)	2292(2)	4903(1)	25(1)
C(18)	5719(1)	3267(2)	5545(1)	29(1)
C(19)	5461(1)	3826(2)	6315(1)	29(1)
C(20)	4501(1)	3341(2)	6474(1)	26(1)
C(21)	3816(1)	2285(2)	5835(1)	23(1)
N(22)	2849(1)	1617(1)	6043(1)	26(1)
O(23)	2994(1)	816(1)	6753(1)	37(1)
O(24)	1967(1)	1864(1)	5501(1)	33(1)

Table S10. Bond lengths [Å] and angles [°] for **4a**.

C(2)-O(3)	1.4442(15)
C(2)-C(20)	1.5098(16)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
O(3)-C(5)	1.3607(15)
O(4)-C(5)	1.2020(16)
C(5)-C(6)	1.5058(17)
C(6)-C(7)	1.5199(19)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.505(2)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.3212(19)
C(8)-H(8)	0.9500
C(9)-C(10)	1.5081(18)
C(9)-H(9)	0.9500
C(10)-C(11)	1.5297(19)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.5035(18)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-O(13)	1.1999(16)
C(12)-O(14)	1.3474(14)
O(14)-C(15)	1.4483(14)
C(15)-C(16)	1.5027(15)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.3934(16)
C(16)-C(21)	1.3971(16)
C(17)-C(18)	1.3835(17)
C(17)-H(17)	0.9500
C(18)-C(19)	1.3903(17)
C(18)-H(18)	0.9500
C(19)-C(20)	1.3905(17)

C(19)-H(19)	0.9500
C(20)-C(21)	1.3924(16)
C(21)-N(22)	1.4760(15)
N(22)-O(24)	1.2258(13)
N(22)-O(23)	1.2264(13)

O(3)-C(2)-C(20)	111.05(9)
O(3)-C(2)-H(2A)	109.4
C(20)-C(2)-H(2A)	109.4
O(3)-C(2)-H(2B)	109.4
C(20)-C(2)-H(2B)	109.4
H(2A)-C(2)-H(2B)	108.0
C(5)-O(3)-C(2)	117.01(10)
O(4)-C(5)-O(3)	122.89(12)
O(4)-C(5)-C(6)	127.61(12)
O(3)-C(5)-C(6)	109.50(10)
C(5)-C(6)-C(7)	115.28(11)
C(5)-C(6)-H(6A)	108.5
C(7)-C(6)-H(6A)	108.5
C(5)-C(6)-H(6B)	108.5
C(7)-C(6)-H(6B)	108.5
H(6A)-C(6)-H(6B)	107.5
C(8)-C(7)-C(6)	116.83(11)
C(8)-C(7)-H(7A)	108.1
C(6)-C(7)-H(7A)	108.1
C(8)-C(7)-H(7B)	108.1
C(6)-C(7)-H(7B)	108.1
H(7A)-C(7)-H(7B)	107.3
C(9)-C(8)-C(7)	128.35(12)
C(9)-C(8)-H(8)	115.8
C(7)-C(8)-H(8)	115.8
C(8)-C(9)-C(10)	124.47(12)
C(8)-C(9)-H(9)	117.8
C(10)-C(9)-H(9)	117.8
C(9)-C(10)-C(11)	115.14(11)
C(9)-C(10)-H(10A)	108.5
C(11)-C(10)-H(10A)	108.5
C(9)-C(10)-H(10B)	108.5

C(11)-C(10)-H(10B)	108.5
H(10A)-C(10)-H(10B)	107.5
C(12)-C(11)-C(10)	116.46(10)
C(12)-C(11)-H(11A)	108.2
C(10)-C(11)-H(11A)	108.2
C(12)-C(11)-H(11B)	108.2
C(10)-C(11)-H(11B)	108.2
H(11A)-C(11)-H(11B)	107.3
O(13)-C(12)-O(14)	122.87(12)
O(13)-C(12)-C(11)	124.97(11)
O(14)-C(12)-C(11)	112.14(10)
C(12)-O(14)-C(15)	117.20(9)
O(14)-C(15)-C(16)	104.06(9)
O(14)-C(15)-H(15A)	110.9
C(16)-C(15)-H(15A)	110.9
O(14)-C(15)-H(15B)	110.9
C(16)-C(15)-H(15B)	110.9
H(15A)-C(15)-H(15B)	109.0
C(17)-C(16)-C(21)	116.84(10)
C(17)-C(16)-C(15)	119.78(10)
C(21)-C(16)-C(15)	123.12(10)
C(18)-C(17)-C(16)	121.35(11)
C(18)-C(17)-H(17)	119.3
C(16)-C(17)-H(17)	119.3
C(17)-C(18)-C(19)	120.03(11)
C(17)-C(18)-H(18)	120.0
C(19)-C(18)-H(18)	120.0
C(18)-C(19)-C(20)	120.67(11)
C(18)-C(19)-H(19)	119.7
C(20)-C(19)-H(19)	119.7
C(19)-C(20)-C(21)	117.61(11)
C(19)-C(20)-C(2)	120.47(11)
C(21)-C(20)-C(2)	121.83(11)
C(20)-C(21)-C(16)	123.22(11)
C(20)-C(21)-N(22)	118.01(10)
C(16)-C(21)-N(22)	118.76(10)
O(24)-N(22)-O(23)	124.29(10)
O(24)-N(22)-C(21)	119.10(9)

O(23)-N(22)-C(21)	116.60(10)

Symmetry transformations used to generate equivalent atoms:

Table S11. Anisotropic displacement parameters ($Å^2$ x 10^3) for **4a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(2)	29(1)	42(1)	22(1)	-5(1)	3(1)	4(1)
O(3)	30(1)	37(1)	27(1)	-1(1)	10(1)	3(1)
O(4)	31(1)	39(1)	45(1)	1(1)	14(1)	-4(1)
C(5)	30(1)	31(1)	26(1)	-6(1)	10(1)	0(1)
C(6)	29(1)	38(1)	35(1)	-3(1)	13(1)	1(1)
C(7)	30(1)	32(1)	50(1)	-2(1)	11(1)	4(1)
C(8)	26(1)	31(1)	41(1)	8(1)	5(1)	2(1)
C(9)	24(1)	31(1)	32(1)	7(1)	4(1)	1(1)
C(10)	23(1)	37(1)	31(1)	10(1)	2(1)	1(1)
C(11)	19(1)	44(1)	26(1)	4(1)	-2(1)	1(1)
C(12)	22(1)	39(1)	21(1)	0(1)	-1(1)	-5(1)
O(13)	36(1)	44(1)	53(1)	8(1)	-11(1)	-16(1)
O(14)	20(1)	30(1)	24(1)	3(1)	-2(1)	-1(1)
C(15)	24(1)	26(1)	21(1)	0(1)	1(1)	1(1)
C(16)	22(1)	22(1)	20(1)	2(1)	2(1)	3(1)
C(17)	23(1)	29(1)	22(1)	0(1)	4(1)	5(1)
C(18)	19(1)	35(1)	31(1)	-1(1)	4(1)	1(1)
C(19)	20(1)	34(1)	28(1)	-5(1)	-1(1)	-1(1)
C(20)	24(1)	30(1)	20(1)	-1(1)	1(1)	3(1)
C(21)	20(1)	25(1)	21(1)	3(1)	2(1)	2(1)
N(22)	27(1)	27(1)	23(1)	1(1)	6(1)	-1(1)
O(23)	43(1)	40(1)	28(1)	10(1)	11(1)	-2(1)
O(24)	22(1)	41(1)	33(1)	4(1)	3(1)	-2(1)

Table S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **4a**.

	x	y	z	U(eq)
H(2A)	43453144	776739		
H(2B)	46425047	752639		
H(6A)	13476331	679340		
H(6B)	12564949	600840		
H(7A)	3567647	553045		
H(7B)	15108514	572845		
H(8)	8537938	414841		
H(9)	16984726	467036		
H(10A)	22205506	326938		
H(10B)	10576358	292338		
H(11A)	2433653	284338		
H(11B)	10373706	222138		
H(15A)	3530242	388730		
H(15B)	2704210	449530		
H(17)	51671950	436930		
H(18)	63943555	545935		
H(19)	59464547	673835		

Table S13. Crystal data and structure refinement for **4b**.

Empirical formula	$C_{18}\ H_{21}\ N\ O_6$	
Formula weight	347.36	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 8.1602(3) Å	α = 88.2151(14)°
	b = 10.1021(4) Å	β = 69.4794(14)°
	c = 11.5212(4) Å	γ = 72.0806(13)°
Volume	843.20(5) $Å^3$	
Z	2	
Density (calculated)	1.368 Mg/m^3	
Absorption coefficient	0.103 mm^{-1}	
F(000)	368	
Crystal size	0.243 x 0.191 x 0.077 mm^3	
Theta range for data collection	2.724 to 27.513°.	
Index ranges	–10<=h<=10, –13<=k<=13, –14<=l<=14	
Reflections collected	20654	
Independent reflections	3808 [R(int) = 0.0650]	
Completeness to theta = 25.242°	98.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.5000	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3808 / 0 / 226	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2sigma(I)]	R1 = 0.0392, wR2 = 0.0935	
R indices (all data)	R1 = 0.0489, wR2 = 0.1027	
Largest diff. peak and hole	0.281 and –0.189 $e·Å^{-3}$	

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **4b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6023(2)	299(1)	6130(1)	26(1)
C(2)	7337(2)	-824(1)	5315(1)	32(1)
C(3)	8574(2)	-604(1)	4208(1)	34(1)
C(4)	8573(2)	737(1)	3918(1)	29(1)
C(5)	7303(2)	1895(1)	4713(1)	23(1)
C(6)	6015(2)	1641(1)	5787(1)	23(1)
C(7)	4752(2)	58(1)	7370(1)	32(1)
O(8)	4758(1)	917(1)	8355(1)	29(1)
O(9)	7466(1)	-610(1)	8279(1)	35(1)
C(10)	6306(2)	509(1)	8640(1)	25(1)
C(11)	6368(2)	1638(1)	9422(1)	28(1)
C(12)	8016(2)	1201(1)	9838(1)	29(1)
C(13)	8173(2)	2405(2)	10524(1)	33(1)
C(14)	8833(2)	3435(1)	9673(1)	30(1)
C(15)	7884(2)	4752(1)	9655(1)	31(1)
C(16)	8598(2)	5756(1)	8794(1)	33(1)
C(17)	7878(2)	6004(1)	7717(1)	30(1)
C(18)	8623(2)	4706(1)	6832(1)	26(1)
C(19)	7796(2)	4821(1)	5845(1)	24(1)
O(20)	6665(1)	5832(1)	5691(1)	33(1)
O(21)	8499(1)	3593(1)	5137(1)	26(1)
C(22)	7466(2)	3321(1)	4424(1)	26(1)
N(23)	4545(2)	2835(1)	6621(1)	27(1)
O(24)	4996(1)	3722(1)	7019(1)	41(1)
O(25)	2952(1)	2866(1)	6865(1)	37(1)

Table S15. Bond lengths [Å] and angles [°] for **4b**.

C(1)-C(2)	1.3894(19)
C(1)-C(6)	1.3996(16)
C(1)-C(7)	1.5065(18)
C(2)-C(3)	1.383(2)
C(2)-H(2)	0.9500
C(3)-C(4)	1.3853(19)
C(3)-H(3)	0.9500
C(4)-C(5)	1.3917(17)
C(4)-H(4)	0.9500
C(5)-C(6)	1.3908(17)
C(5)-C(22)	1.5039(16)
C(6)-N(23)	1.4803(15)
C(7)-O(8)	1.4530(15)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
O(8)-C(10)	1.3545(15)
O(9)-C(10)	1.2010(16)
C(10)-C(11)	1.4992(17)
C(11)-C(12)	1.5181(17)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.5332(18)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.4985(19)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.3212(19)
C(14)-H(14)	0.9500
C(15)-C(16)	1.500(2)
C(15)-H(15)	0.9500
C(16)-C(17)	1.5336(18)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.5123(17)
C(17)-H(17A)	0.9900

C(17)-H(17B)	0.9900
C(18)-C(19)	1.4984(17)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-O(20)	1.2036(15)
C(19)-O(21)	1.3528(15)
O(21)-C(22)	1.4500(14)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
N(23)-O(25)	1.2208(14)
N(23)-O(24)	1.2217(14)

C(2)-C(1)-C(6)	117.44(12)
C(2)-C(1)-C(7)	120.46(11)
C(6)-C(1)-C(7)	121.98(12)
C(3)-C(2)-C(1)	120.55(12)
C(3)-C(2)-H(2)	119.7
C(1)-C(2)-H(2)	119.7
C(2)-C(3)-C(4)	120.53(12)
C(2)-C(3)-H(3)	119.7
C(4)-C(3)-H(3)	119.7
C(3)-C(4)-C(5)	121.04(12)
C(3)-C(4)-H(4)	119.5
C(5)-C(4)-H(4)	119.5
C(6)-C(5)-C(4)	116.97(11)
C(6)-C(5)-C(22)	123.63(11)
C(4)-C(5)-C(22)	119.26(11)
C(5)-C(6)-C(1)	123.32(11)
C(5)-C(6)-N(23)	119.36(10)
C(1)-C(6)-N(23)	117.31(11)
O(8)-C(7)-C(1)	109.95(10)
O(8)-C(7)-H(7A)	109.7
C(1)-C(7)-H(7A)	109.7
O(8)-C(7)-H(7B)	109.7
C(1)-C(7)-H(7B)	109.7
H(7A)-C(7)-H(7B)	108.2
C(10)-O(8)-C(7)	115.76(10)
O(9)-C(10)-O(8)	122.93(11)

O(9)-C(10)-C(11)	125.96(12)
O(8)-C(10)-C(11)	111.10(11)
C(10)-C(11)-C(12)	113.25(11)
C(10)-C(11)-H(11A)	108.9
C(12)-C(11)-H(11A)	108.9
C(10)-C(11)-H(11B)	108.9
C(12)-C(11)-H(11B)	108.9
H(11A)-C(11)-H(11B)	107.7
C(11)-C(12)-C(13)	112.80(11)
C(11)-C(12)-H(12A)	109.0
C(13)-C(12)-H(12A)	109.0
C(11)-C(12)-H(12B)	109.0
C(13)-C(12)-H(12B)	109.0
H(12A)-C(12)-H(12B)	107.8
C(14)-C(13)-C(12)	112.93(11)
C(14)-C(13)-H(13A)	109.0
C(12)-C(13)-H(13A)	109.0
C(14)-C(13)-H(13B)	109.0
C(12)-C(13)-H(13B)	109.0
H(13A)-C(13)-H(13B)	107.8
C(15)-C(14)-C(13)	126.59(13)
C(15)-C(14)-H(14)	116.7
C(13)-C(14)-H(14)	116.7
C(14)-C(15)-C(16)	125.06(13)
C(14)-C(15)-H(15)	117.5
C(16)-C(15)-H(15)	117.5
C(15)-C(16)-C(17)	113.27(11)
C(15)-C(16)-H(16A)	108.9
C(17)-C(16)-H(16A)	108.9
C(15)-C(16)-H(16B)	108.9
C(17)-C(16)-H(16B)	108.9
H(16A)-C(16)-H(16B)	107.7
C(18)-C(17)-C(16)	111.53(11)
C(18)-C(17)-H(17A)	109.3
C(16)-C(17)-H(17A)	109.3
C(18)-C(17)-H(17B)	109.3
C(16)-C(17)-H(17B)	109.3
H(17A)-C(17)-H(17B)	108.0

C(19)-C(18)-C(17)	114.25(10)
C(19)-C(18)-H(18A)	108.7
C(17)-C(18)-H(18A)	108.7
C(19)-C(18)-H(18B)	108.7
C(17)-C(18)-H(18B)	108.7
H(18A)-C(18)-H(18B)	107.6
O(20)-C(19)-O(21)	123.96(11)
O(20)-C(19)-C(18)	126.48(11)
O(21)-C(19)-C(18)	109.56(10)
C(19)-O(21)-C(22)	117.81(9)
O(21)-C(22)-C(5)	105.82(9)
O(21)-C(22)-H(22A)	110.6
C(5)-C(22)-H(22A)	110.6
O(21)-C(22)-H(22B)	110.6
C(5)-C(22)-H(22B)	110.6
H(22A)-C(22)-H(22B)	108.7
O(25)-N(23)-O(24)	124.30(11)
O(25)-N(23)-C(6)	117.24(10)
O(24)-N(23)-C(6)	118.45(10)

Symmetry transformations used to generate equivalent atoms:

Table S16. Anisotropic displacement parameters ($Å^2$ x 10^3) for **4b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	33(1)	27(1)	28(1)	6(1)	-19(1)	-14(1)
C(2)	46(1)	21(1)	38(1)	4(1)	-27(1)	-10(1)
C(3)	39(1)	26(1)	35(1)	-6(1)	-19(1)	0(1)
C(4)	30(1)	32(1)	24(1)	-1(1)	-12(1)	-6(1)
C(5)	26(1)	24(1)	23(1)	3(1)	-13(1)	-8(1)
C(6)	25(1)	22(1)	25(1)	1(1)	-12(1)	-7(1)
C(7)	42(1)	34(1)	34(1)	11(1)	-21(1)	-24(1)
O(8)	30(1)	35(1)	28(1)	7(1)	-13(1)	-15(1)
O(9)	39(1)	28(1)	40(1)	1(1)	-18(1)	-8(1)
C(10)	27(1)	29(1)	23(1)	10(1)	-9(1)	-14(1)
C(11)	29(1)	28(1)	29(1)	3(1)	-12(1)	-9(1)
C(12)	31(1)	31(1)	29(1)	8(1)	-14(1)	-12(1)
C(13)	37(1)	39(1)	28(1)	5(1)	-16(1)	-14(1)
C(14)	30(1)	35(1)	29(1)	2(1)	-14(1)	-13(1)
C(15)	32(1)	35(1)	30(1)	-2(1)	-15(1)	-10(1)
C(16)	39(1)	28(1)	39(1)	0(1)	-22(1)	-11(1)
C(17)	35(1)	23(1)	37(1)	2(1)	-19(1)	-8(1)
C(18)	27(1)	22(1)	29(1)	4(1)	-12(1)	-8(1)
C(19)	26(1)	22(1)	27(1)	7(1)	-10(1)	-12(1)
O(20)	41(1)	23(1)	42(1)	8(1)	-25(1)	-9(1)
O(21)	26(1)	25(1)	29(1)	2(1)	-12(1)	-9(1)
C(22)	31(1)	28(1)	24(1)	5(1)	-13(1)	-12(1)
N(23)	27(1)	25(1)	26(1)	4(1)	-7(1)	-8(1)
O(24)	42(1)	32(1)	41(1)	-11(1)	-1(1)	-17(1)
O(25)	24(1)	45(1)	39(1)	4(1)	-10(1)	-8(1)

Table S17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **4b**.

	x	y	z	U(eq)
H(2)	7386-1750	551939		
H(3)	9430-1379	364240		
H(4)	9453869	316434		
H(7A)	3484295	736438		
H(7B)	5162-940	752138		
H(11A)	52221917	1016733		
H(11B)	64062465	894133		
H(12A)	9156832	909935		
H(12B)	7910439	1039235		
H(13A)	69512897	1115639		
H(13B)	90392018	1096639		
H(14)	100593108	908735		
H(15)	66535089	1023338		
H(16A)	99635391	844939		
H(16B)	82386660	927639		
H(17A)	65136292	805436		
H(17B)	82476773	725736		
H(18A)	99754490	642631		
H(18B)	83973913	731931		
H(22A)	81253338	352431		
H(22B)	62294031	467131		

Table S18. Crystal data and structure refinement for **7a**.

Empirical formula	$C_{16}\ H_{17}\ N\ O_6$	
Formula weight	319.30	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 7.8712(4) Å	α = 90°
	b = 16.4752(7) Å	β = 91.5968(14)°
	c = 11.7570(5) Å	γ = 90°
Volume	1524.05(12) $Å^3$	
Z	4	
Density (calculated)	1.392 Mg/m^3	
Absorption coefficient	0.107 mm^{-1}	
F(000)	672	
Crystal size	0.291 x 0.183 x 0.096 mm^3	
Theta range for data collection	2.869 to 27.499°.	
Index ranges	-10<=h<=10, -21<=k<=21, -15<=l<=15	
Reflections collected	20523	
Independent reflections	3447 [R(int) = 0.0547]	
Completeness to theta = 25.242°	98.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6508	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3447 / 148 / 245	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2sigma(I)]	R1 = 0.0369, wR2 = 0.0841	
R indices (all data)	R1 = 0.0495, wR2 = 0.0932	
Largest diff. peak and hole	0.242 and -0.201 $e.Å^{-3}$	

Table S19. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **7a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4152(2)	5527(1)	6452(1)	31(1)
O(2)	5914(1)	5280(1)	6314(1)	30(1)
O(3)	6610(1)	5785(1)	8042(1)	36(1)
C(4)	7034(2)	5499(1)	7150(1)	27(1)
C(5)	8819(2)	5359(1)	6793(1)	32(1)
C(6)	9330(4)	5983(1)	5888(2)	31(1)
C(7)	9542(2)	6821(1)	6375(1)	29(1)
C(8)	8630(3)	7462(1)	6055(1)	30(1)
C(9)	8914(4)	8312(2)	6503(2)	35(1)
C(6B)	9240(50)	6128(10)	6080(20)	33(3)
C(7B)	8700(30)	7012(11)	6317(16)	30(2)
C(8B)	9380(30)	7618(13)	6034(17)	34(2)
C(9B)	8650(60)	8387(13)	6586(19)	31(3)
C(10)	8820(2)	8967(1)	5565(1)	37(1)
C(11)	7110(2)	8976(1)	4969(1)	32(1)
O(12)	6834(2)	8817(1)	3985(1)	53(1)
O(13)	5866(1)	9168(1)	5692(1)	29(1)
C(14)	4139(2)	8961(1)	5317(1)	32(1)
C(15)	3883(2)	8080(1)	5613(1)	25(1)
C(16)	3748(2)	7491(1)	4770(1)	31(1)
C(17)	3785(2)	6669(1)	5039(1)	30(1)
C(18)	3973(1)	6413(1)	6159(1)	25(1)
C(19)	4077(1)	6991(1)	7021(1)	24(1)
C(20)	4015(1)	7803(1)	6732(1)	22(1)
N(21)	4142(1)	8380(1)	7687(1)	27(1)
O(22)	3118(1)	8941(1)	7714(1)	41(1)
O(23)	5255(1)	8263(1)	8414(1)	39(1)

Table S20. Bond lengths [Å] and angles [°] for **7a**.

C(1)-O(2)	1.4581(15)
C(1)-C(18)	1.5062(16)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
O(2)-C(4)	1.3510(15)
O(3)-C(4)	1.2052(15)
C(4)-C(5)	1.4958(18)
C(5)-C(6)	1.540(2)
C(5)-C(6B)	1.558(10)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.503(2)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.324(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.511(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.543(2)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(6B)-C(7B)	1.542(10)
C(6B)-H(6BA)	0.9900
C(6B)-H(6BB)	0.9900
C(7B)-C(8B)	1.18(3)
C(7B)-H(7B)	0.9500
C(8B)-C(9B)	1.539(10)
C(8B)-H(8B)	0.9500
C(9B)-C(10)	1.542(10)
C(9B)-H(9BA)	0.9900
C(9B)-H(9BB)	0.9900
C(10)-C(11)	1.500(2)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-O(12)	1.1995(17)
C(11)-O(13)	1.3522(15)

O(13)-C(14)	1.4582(16)
C(14)-C(15)	1.5074(16)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.3896(17)
C(15)-C(20)	1.3938(16)
C(16)-C(17)	1.3901(18)
C(16)-H(16)	0.9500
C(17)-C(18)	1.3867(18)
C(17)-H(17)	0.9500
C(18)-C(19)	1.3917(16)
C(19)-C(20)	1.3799(16)
C(19)-H(19)	0.9500
C(20)-N(21)	1.4728(14)
N(21)-O(23)	1.2226(14)
N(21)-O(22)	1.2269(13)

O(2)-C(1)-C(18)	109.18(9)
O(2)-C(1)-H(1A)	109.8
C(18)-C(1)-H(1A)	109.8
O(2)-C(1)-H(1B)	109.8
C(18)-C(1)-H(1B)	109.8
H(1A)-C(1)-H(1B)	108.3
C(4)-O(2)-C(1)	116.60(9)
O(3)-C(4)-O(2)	123.10(12)
O(3)-C(4)-C(5)	126.15(12)
O(2)-C(4)-C(5)	110.73(10)
C(4)-C(5)-C(6)	110.85(14)
C(4)-C(5)-C(6B)	103.8(13)
C(4)-C(5)-H(5A)	109.5
C(6)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5B)	109.5
C(6)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	108.1
C(7)-C(6)-C(5)	112.26(14)
C(7)-C(6)-H(6A)	109.2
C(5)-C(6)-H(6A)	109.2
C(7)-C(6)-H(6B)	109.2

C(5)-C(6)-H(6B)	109.2
H(6A)-C(6)-H(6B)	107.9
C(8)-C(7)-C(6)	124.81(19)
C(8)-C(7)-H(7)	117.6
C(6)-C(7)-H(7)	117.6
C(7)-C(8)-C(9)	124.5(2)
C(7)-C(8)-H(8)	117.8
C(9)-C(8)-H(8)	117.8
C(8)-C(9)-C(10)	113.2(2)
C(8)-C(9)-H(9A)	108.9
C(10)-C(9)-H(9A)	108.9
C(8)-C(9)-H(9B)	108.9
C(10)-C(9)-H(9B)	108.9
H(9A)-C(9)-H(9B)	107.7
C(7B)-C(6B)-C(5)	127.5(17)
C(7B)-C(6B)-H(6BA)	105.4
C(5)-C(6B)-H(6BA)	105.4
C(7B)-C(6B)-H(6BB)	105.4
C(5)-C(6B)-H(6BB)	105.4
H(6BA)-C(6B)-H(6BB)	106.0
C(8B)-C(7B)-C(6B)	128(2)
C(8B)-C(7B)-H(7B)	115.8
C(6B)-C(7B)-H(7B)	115.8
C(7B)-C(8B)-C(9B)	114(3)
C(7B)-C(8B)-H(8B)	123.1
C(9B)-C(8B)-H(8B)	123.1
C(8B)-C(9B)-C(10)	98.1(13)
C(8B)-C(9B)-H(9BA)	112.1
C(10)-C(9B)-H(9BA)	112.1
C(8B)-C(9B)-H(9BB)	112.1
C(10)-C(9B)-H(9BB)	112.1
H(9BA)-C(9B)-H(9BB)	109.8
C(11)-C(10)-C(9B)	106.0(19)
C(11)-C(10)-C(9)	111.45(17)
C(11)-C(10)-H(10A)	109.3
C(9)-C(10)-H(10A)	109.3
C(11)-C(10)-H(10B)	109.3
C(9)-C(10)-H(10B)	109.3

H(10A)-C(10)-H(10B)	108.0
O(12)-C(11)-O(13)	122.88(13)
O(12)-C(11)-C(10)	125.73(13)
O(13)-C(11)-C(10)	111.37(11)
C(11)-O(13)-C(14)	116.12(10)
O(13)-C(14)-C(15)	106.57(10)
O(13)-C(14)-H(14A)	110.4
C(15)-C(14)-H(14A)	110.4
O(13)-C(14)-H(14B)	110.4
C(15)-C(14)-H(14B)	110.4
H(14A)-C(14)-H(14B)	108.6
C(16)-C(15)-C(20)	116.48(11)
C(16)-C(15)-C(14)	121.12(11)
C(20)-C(15)-C(14)	121.77(11)
C(15)-C(16)-C(17)	121.18(12)
C(15)-C(16)-H(16)	119.4
C(17)-C(16)-H(16)	119.4
C(18)-C(17)-C(16)	120.87(11)
C(18)-C(17)-H(17)	119.6
C(16)-C(17)-H(17)	119.6
C(17)-C(18)-C(19)	119.07(11)
C(17)-C(18)-C(1)	121.26(11)
C(19)-C(18)-C(1)	119.60(11)
C(20)-C(19)-C(18)	118.86(11)
C(20)-C(19)-H(19)	120.6
C(18)-C(19)-H(19)	120.6
C(19)-C(20)-C(15)	123.48(10)
C(19)-C(20)-N(21)	115.89(10)
C(15)-C(20)-N(21)	120.62(10)
O(23)-N(21)-O(22)	123.98(10)
O(23)-N(21)-C(20)	117.62(10)
O(22)-N(21)-C(20)	118.39(10)

Symmetry transformations used to generate equivalent atoms:

Table S21. Anisotropic displacement parameters ($Å^2$ x 10^3) for **7a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	29(1)	23(1)	41(1)	-4(1)	4(1)	-5(1)
O(2)	32(1)	24(1)	34(1)	-5(1)	1(1)	1(1)
O(3)	42(1)	38(1)	27(1)	-1(1)	2(1)	6(1)
C(4)	36(1)	18(1)	26(1)	5(1)	2(1)	2(1)
C(5)	33(1)	32(1)	32(1)	1(1)	-1(1)	7(1)
C(6)	31(1)	34(1)	28(1)	-4(1)	6(1)	0(1)
C(7)	21(1)	35(1)	32(1)	-1(1)	2(1)	-1(1)
C(8)	25(1)	33(1)	33(1)	1(1)	-1(1)	-4(1)
C(9)	31(1)	39(1)	35(1)	-7(1)	1(1)	5(1)
C(6B)	29(5)	44(5)	26(5)	-4(5)	11(5)	0(5)
C(7B)	29(4)	33(4)	29(4)	2(4)	1(4)	1(4)
C(8B)	31(4)	40(4)	30(4)	3(4)	-4(4)	-1(4)
C(9B)	29(5)	34(5)	30(5)	-3(5)	-3(5)	-5(5)
C(10)	37(1)	31(1)	43(1)	-7(1)	12(1)	-7(1)
C(11)	45(1)	22(1)	30(1)	2(1)	10(1)	2(1)
O(12)	59(1)	73(1)	28(1)	-5(1)	6(1)	16(1)
O(13)	36(1)	23(1)	29(1)	-1(1)	7(1)	-2(1)
C(14)	36(1)	27(1)	32(1)	5(1)	-1(1)	3(1)
C(15)	24(1)	25(1)	27(1)	1(1)	-1(1)	2(1)
C(16)	36(1)	34(1)	24(1)	-1(1)	-4(1)	0(1)
C(17)	31(1)	30(1)	30(1)	-8(1)	-3(1)	-3(1)
C(18)	20(1)	23(1)	33(1)	-2(1)	3(1)	-3(1)
C(19)	22(1)	24(1)	25(1)	1(1)	4(1)	-2(1)
C(20)	19(1)	23(1)	24(1)	-3(1)	1(1)	-1(1)
N(21)	30(1)	24(1)	27(1)	-2(1)	6(1)	-1(1)
O(22)	41(1)	32(1)	49(1)	-12(1)	4(1)	12(1)
O(23)	51(1)	39(1)	28(1)	-7(1)	-10(1)	5(1)

Table S22. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **7a**.

	x	y	z	U(eq)
H(1A)	38205434	724837		
H(1B)	33955199	594637		
H(5A)	89204804	647939		
H(5B)	96025403	746439		
H(6A)	104125811	555237		
H(6B)	84485995	527237		
H(7)	103916898	695535		
H(8)	77377381	550736		
H(9A)	100448339	689342		
H(9B)	80488433	707442		
H(6BA)	104916140	604439		
H(6BB)	88096009	530039		
H(7B)	77037077	674336		
H(8B)	102797629	551540		
H(9BA)	93478565	725537		
H(9BB)	74568316	680437		
H(10A)	90479506	590844		
H(10B)	97078859	500444		
H(14A)	39909045	448738		
H(14B)	33069305	571038		
H(16)	36297652	399638		
H(17)	36816278	444836		
H(19)	41906830	779628		

Table S23. Crystal data and structure refinement for **7b**.

Empirical formula	$C_{18}\ H_{21}\ N\ O_6$	
Formula weight	347.36	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 17.150(4) Å	α = 90°
	b = 9.733(3) Å	β = 106.541(7)°
	c = 10.702(3) Å	γ = 90°
Volume	1712.6(8) $Å^3$	
Z	4	
Density (calculated)	1.347 Mg/m^3	
Absorption coefficient	0.102 mm^{-1}	
F(000)	736	
Crystal size	0.132 x 0.089 x 0.028 mm^3	
Theta range for data collection	2.478 to 25.499°.	
Index ranges	–20<=h<=20, –11<=k<=11, –12<=l<=12	
Reflections collected	20258	
Independent reflections	3188 [R(int) = 0.1536]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7455 and 0.3322	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3188 / 0 / 226	
Goodness-of-fit on F^2	1.182	
Final R indices [I>2sigma(I)]	R1 = 0.1112, wR2 = 0.2192	
R indices (all data)	R1 = 0.1464, wR2 = 0.2349	
Largest diff. peak and hole	0.400 and –0.316 $e \cdot Å^{-3}$	

Table S24. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **7b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3831(3)	3716(5)	4416(4)	29(1)
C(2)	3494(3)	4503(5)	3303(5)	33(1)
C(3)	3441(3)	5924(5)	3327(5)	36(1)
C(4)	3731(3)	6647(5)	4486(5)	32(1)
C(5)	4104(3)	5913(5)	5601(5)	31(1)
C(6)	4157(2)	4501(5)	5556(4)	29(1)
C(7)	3817(3)	2171(5)	4328(5)	35(1)
O(8)	3318(2)	1734(3)	3070(3)	37(1)
O(9)	2230(2)	1767(4)	3837(3)	43(1)
C(10)	2512(3)	1599(5)	2956(5)	33(1)
C(11)	2051(3)	1161(5)	1583(5)	37(1)
C(12)	1140(3)	1462(6)	1203(5)	43(1)
C(13)	908(3)	2921(6)	732(5)	45(1)
C(14)	1193(3)	4030(6)	1756(6)	50(2)
C(15)	773(3)	4983(6)	2098(6)	50(1)
C(16)	1104(4)	6000(5)	3157(5)	47(1)
C(17)	1083(3)	7470(5)	2689(5)	39(1)
C(18)	1395(3)	8495(5)	3810(5)	38(1)
C(19)	2255(3)	8190(5)	4570(5)	35(1)
O(20)	2472(2)	7661(4)	5625(3)	47(1)
O(21)	2785(2)	8556(3)	3897(3)	38(1)
C(22)	3633(3)	8173(5)	4499(5)	37(1)
N(23)	4605(2)	3813(4)	6787(4)	35(1)
O(24)	4851(2)	4539(4)	7770(3)	44(1)
O(25)	4723(2)	2588(4)	6770(3)	48(1)

Table S25. Bond lengths [Å] and angles [°] for **7b**

C(1)-C(2)	1.395(6)
C(1)-C(6)	1.413(7)
C(1)-C(7)	1.506(7)
C(2)-C(3)	1.387(7)
C(2)-H(2)	0.9500
C(3)-C(4)	1.389(7)
C(3)-H(3)	0.9500
C(4)-C(5)	1.382(6)
C(4)-C(22)	1.495(7)
C(5)-C(6)	1.379(7)
C(5)-H(5)	0.9500
C(6)-N(23)	1.482(6)
C(7)-O(8)	1.440(6)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
O(8)-C(10)	1.359(5)
O(9)-C(10)	1.188(6)
C(10)-C(11)	1.517(7)
C(11)-C(12)	1.526(7)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.521(8)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.517(8)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.289(8)
C(14)-H(14)	0.9500
C(15)-C(16)	1.489(8)
C(15)-H(15)	0.9500
C(16)-C(17)	1.513(7)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.535(7)
C(17)-H(17A)	0.9900

C(17)-H(17B)	0.9900
C(18)-C(19)	1.497(7)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-O(20)	1.200(6)
C(19)-O(21)	1.359(6)
O(21)-C(22)	1.461(5)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
N(23)-O(25)	1.211(5)
N(23)-O(24)	1.237(5)

C(2)-C(1)-C(6)	114.0(4)
C(2)-C(1)-C(7)	120.0(4)
C(6)-C(1)-C(7)	126.1(4)
C(3)-C(2)-C(1)	123.0(5)
C(3)-C(2)-H(2)	118.5
C(1)-C(2)-H(2)	118.5
C(2)-C(3)-C(4)	120.9(5)
C(2)-C(3)-H(3)	119.6
C(4)-C(3)-H(3)	119.6
C(5)-C(4)-C(3)	118.0(4)
C(5)-C(4)-C(22)	122.1(4)
C(3)-C(4)-C(22)	119.9(4)
C(6)-C(5)-C(4)	120.3(4)
C(6)-C(5)-H(5)	119.9
C(4)-C(5)-H(5)	119.9
C(5)-C(6)-C(1)	123.7(4)
C(5)-C(6)-N(23)	116.2(4)
C(1)-C(6)-N(23)	120.1(4)
O(8)-C(7)-C(1)	110.3(4)
O(8)-C(7)-H(7A)	109.6
C(1)-C(7)-H(7A)	109.6
O(8)-C(7)-H(7B)	109.6
C(1)-C(7)-H(7B)	109.6
H(7A)-C(7)-H(7B)	108.1
C(10)-O(8)-C(7)	115.6(4)
O(9)-C(10)-O(8)	123.3(4)

O(9)-C(10)-C(11)	126.1(4)
O(8)-C(10)-C(11)	110.5(4)
C(10)-C(11)-C(12)	114.6(4)
C(10)-C(11)-H(11A)	108.6
C(12)-C(11)-H(11A)	108.6
C(10)-C(11)-H(11B)	108.6
C(12)-C(11)-H(11B)	108.6
H(11A)-C(11)-H(11B)	107.6
C(13)-C(12)-C(11)	114.8(4)
C(13)-C(12)-H(12A)	108.6
C(11)-C(12)-H(12A)	108.6
C(13)-C(12)-H(12B)	108.6
C(11)-C(12)-H(12B)	108.6
H(12A)-C(12)-H(12B)	107.6
C(14)-C(13)-C(12)	115.1(4)
C(14)-C(13)-H(13A)	108.5
C(12)-C(13)-H(13A)	108.5
C(14)-C(13)-H(13B)	108.5
C(12)-C(13)-H(13B)	108.5
H(13A)-C(13)-H(13B)	107.5
C(15)-C(14)-C(13)	128.8(5)
C(15)-C(14)-H(14)	115.6
C(13)-C(14)-H(14)	115.6
C(14)-C(15)-C(16)	124.8(5)
C(14)-C(15)-H(15)	117.6
C(16)-C(15)-H(15)	117.6
C(15)-C(16)-C(17)	114.1(4)
C(15)-C(16)-H(16A)	108.7
C(17)-C(16)-H(16A)	108.7
C(15)-C(16)-H(16B)	108.7
C(17)-C(16)-H(16B)	108.7
H(16A)-C(16)-H(16B)	107.6
C(16)-C(17)-C(18)	112.7(4)
C(16)-C(17)-H(17A)	109.1
C(18)-C(17)-H(17A)	109.1
C(16)-C(17)-H(17B)	109.1
C(18)-C(17)-H(17B)	109.1
H(17A)-C(17)-H(17B)	107.8

C(19)-C(18)-C(17)	111.5(4)
C(19)-C(18)-H(18A)	109.3
C(17)-C(18)-H(18A)	109.3
C(19)-C(18)-H(18B)	109.3
C(17)-C(18)-H(18B)	109.3
H(18A)-C(18)-H(18B)	108.0
O(20)-C(19)-O(21)	122.5(4)
O(20)-C(19)-C(18)	126.1(5)
O(21)-C(19)-C(18)	111.4(4)
C(19)-O(21)-C(22)	115.6(4)
O(21)-C(22)-C(4)	110.5(4)
O(21)-C(22)-H(22A)	109.6
C(4)-C(22)-H(22A)	109.6
O(21)-C(22)-H(22B)	109.6
C(4)-C(22)-H(22B)	109.6
H(22A)-C(22)-H(22B)	108.1
O(25)-N(23)-O(24)	123.9(4)
O(25)-N(23)-C(6)	118.5(4)
O(24)-N(23)-C(6)	117.6(4)

Symmetry transformations used to generate equivalent atoms:

Table S26. Anisotropic displacement parameters ($Å^2$ x 10^3) for **7b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	18(2)	34(3)	36(3)	4(2)	9(2)	7(2)
C(2)	27(2)	36(3)	34(3)	0(2)	6(2)	6(2)
C(3)	31(3)	40(3)	36(3)	8(2)	6(2)	3(2)
C(4)	22(2)	33(3)	39(3)	3(2)	5(2)	0(2)
C(5)	19(2)	39(3)	34(3)	-5(2)	5(2)	-5(2)
C(6)	18(2)	39(3)	29(2)	6(2)	4(2)	2(2)
C(7)	29(2)	33(3)	43(3)	1(2)	8(2)	0(2)
O(8)	28(2)	41(2)	42(2)	-9(2)	12(2)	-2(2)
O(9)	38(2)	52(2)	44(2)	-6(2)	18(2)	-2(2)
C(10)	28(2)	24(3)	47(3)	0(2)	13(2)	2(2)
C(11)	36(3)	33(3)	44(3)	-11(2)	13(2)	-1(2)
C(12)	30(3)	52(3)	43(3)	-8(3)	3(2)	-4(2)
C(13)	33(3)	55(4)	44(3)	-4(3)	5(2)	1(2)
C(14)	35(3)	57(4)	52(3)	3(3)	3(3)	12(3)
C(15)	44(3)	36(3)	61(4)	4(3)	3(3)	-5(3)
C(16)	52(3)	38(3)	47(3)	-1(3)	5(3)	-10(3)
C(17)	31(3)	44(3)	37(3)	0(2)	1(2)	-2(2)
C(18)	28(2)	37(3)	45(3)	-4(2)	5(2)	-1(2)
C(19)	35(3)	31(3)	36(3)	-8(2)	8(2)	-1(2)
O(20)	42(2)	63(3)	33(2)	-2(2)	6(2)	1(2)
O(21)	29(2)	38(2)	43(2)	7(2)	6(2)	3(2)
C(22)	26(2)	28(3)	52(3)	3(2)	6(2)	-1(2)
N(23)	30(2)	36(3)	39(2)	5(2)	6(2)	-1(2)
O(24)	43(2)	52(2)	33(2)	4(2)	2(2)	-11(2)
O(25)	53(2)	32(2)	52(2)	10(2)	6(2)	11(2)

Table S27. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **7b**.

	x	y	z	U(eq)
H(2)	32924044	249139		
H(3)	32036410	254144		
H(5)	43246382	640338		
H(7A)	43781823	447042		
H(7B)	36011785	501842		
H(11A)	2129161	149745		
H(11B)	22901635	96145		
H(12A)	860815	50652		
H(12B)	9381282	196752		
H(13A)	11373117	-1	54	
H(13B)	3092974	38954		
H(14)	17574021	220860		
H(15)	2115042	163960		
H(16A)	16735751	361357		
H(16B)	7875937	379757		
H(17A)	5177713	220446		
H(17B)	14207547	207946		
H(18A)	13649437	345245		
H(18B)	10438453	440045		
H(22A)	38098510	540944		
H(22B)	39828608	401744		

Table S28. Crystal data and structure refinement for **10a**.

Empirical formula	$C_{16}\,H_{17}\,N\,O_6$	
Formula weight	319.30	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 8.1387(4) Å	α = 90°
	b = 24.2934(10) Å	β = 117.4138(13)°
	c = 8.5069(4) Å	γ = 90°
Volume	1493.08(12) Å^3	
Z	4	
Density (calculated)	1.420 Mg/m^3	
Absorption coefficient	0.110 mm^{-1}	
F(000)	672	
Crystal size	0.211 x 0.138 x 0.125 mm^3	
Theta range for data collection	2.825 to 28.293°.	
Index ranges	–10<=h<=10, –32<=k<=32, –11<=l<=11	
Reflections collected	34884	
Independent reflections	3658 [R(int) = 0.0607]	
Completeness to theta = 25.242°	98.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6131	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3658 / 0 / 208	
Goodness-of-fit on F^2	1.025	
Final R indices [I>2sigma(I)]	R1 = 0.0443, wR2 = 0.1139	
R indices (all data)	R1 = 0.0494, wR2 = 0.1190	
Largest diff. peak and hole	0.484 and –0.244 e·Å^{-3}	

Table S29. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **10a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3548(2)	3963(1)	4928(2)	27(1)
C(2)	4779(2)	4219(1)	6513(2)	26(1)
C(3)	4354(2)	4764(1)	6755(2)	30(1)
C(4)	2805(2)	5041(1)	5534(2)	37(1)
C(5)	1611(2)	4777(1)	3998(2)	40(1)
C(6)	1985(2)	4242(1)	3700(2)	34(1)
C(7)	3877(2)	3395(1)	4421(2)	32(1)
O(8)	5011(1)	3477(1)	3526(1)	30(1)
O(9)	4910(2)	2569(1)	3040(1)	36(1)
C(10)	5406(2)	3022(1)	2871(2)	25(1)
C(11)	6550(2)	3148(1)	1947(2)	28(1)
C(12)	8529(2)	2939(1)	3019(2)	34(1)
C(13)	9531(2)	3232(1)	4786(2)	33(1)
C(14)	10778(2)	3004(1)	6244(2)	33(1)
C(15)	11893(2)	3285(1)	7978(2)	34(1)
C(16)	11125(2)	3828(1)	8265(2)	33(1)
C(17)	9526(2)	3734(1)	8659(2)	28(1)
O(18)	9622(2)	3466(1)	9889(1)	43(1)
O(19)	7957(1)	3980(1)	7502(1)	30(1)
C(20)	6404(2)	3909(1)	7888(2)	31(1)
N(21)	5579(2)	5083(1)	8342(2)	38(1)
O(22)	4863(2)	5452(1)	8811(2)	50(1)
O(23)	7232(2)	4976(1)	9100(2)	51(1)

Table S30. Bond lengths [Å] and angles [°] for **10a**.

C(1)-C(6)	1.3946(19)
C(1)-C(2)	1.4018(18)
C(1)-C(7)	1.5060(17)
C(2)-C(3)	1.4057(17)
C(2)-C(20)	1.5040(18)
C(3)-C(4)	1.384(2)
C(3)-N(21)	1.4765(18)
C(4)-C(5)	1.376(2)
C(4)-H(4)	0.9500
C(5)-C(6)	1.384(2)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-O(8)	1.4554(14)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
O(8)-C(10)	1.3418(14)
O(9)-C(10)	1.2024(15)
C(10)-C(11)	1.5003(17)
C(11)-C(12)	1.5259(18)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.5169(19)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.3094(19)
C(13)-H(13)	0.9500
C(14)-C(15)	1.4944(19)
C(14)-H(14)	0.9500
C(15)-C(16)	1.5262(19)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.5035(18)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-O(18)	1.2038(16)
C(17)-O(19)	1.3418(15)

O(19)-C(20)	1.4552(14)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
N(21)-O(23)	1.2219(18)
N(21)-O(22)	1.2314(16)

C(6)-C(1)-C(2)	120.43(11)
C(6)-C(1)-C(7)	116.83(12)
C(2)-C(1)-C(7)	122.66(12)
C(1)-C(2)-C(3)	116.31(11)
C(1)-C(2)-C(20)	120.55(11)
C(3)-C(2)-C(20)	123.08(12)
C(4)-C(3)-C(2)	123.25(12)
C(4)-C(3)-N(21)	115.44(12)
C(2)-C(3)-N(21)	121.30(12)
C(5)-C(4)-C(3)	119.13(12)
C(5)-C(4)-H(4)	120.4
C(3)-C(4)-H(4)	120.4
C(4)-C(5)-C(6)	119.55(13)
C(4)-C(5)-H(5)	120.2
C(6)-C(5)-H(5)	120.2
C(5)-C(6)-C(1)	121.32(13)
C(5)-C(6)-H(6)	119.3
C(1)-C(6)-H(6)	119.3
O(8)-C(7)-C(1)	105.34(9)
O(8)-C(7)-H(7A)	110.7
C(1)-C(7)-H(7A)	110.7
O(8)-C(7)-H(7B)	110.7
C(1)-C(7)-H(7B)	110.7
H(7A)-C(7)-H(7B)	108.8
C(10)-O(8)-C(7)	115.83(9)
O(9)-C(10)-O(8)	123.09(11)
O(9)-C(10)-C(11)	124.90(11)
O(8)-C(10)-C(11)	112.01(10)
C(10)-C(11)-C(12)	110.99(10)
C(10)-C(11)-H(11A)	109.4
C(12)-C(11)-H(11A)	109.4
C(10)-C(11)-H(11B)	109.4

C(12)-C(11)-H(11B)	109.4
H(11A)-C(11)-H(11B)	108.0
C(13)-C(12)-C(11)	112.02(11)
C(13)-C(12)-H(12A)	109.2
C(11)-C(12)-H(12A)	109.2
C(13)-C(12)-H(12B)	109.2
C(11)-C(12)-H(12B)	109.2
H(12A)-C(12)-H(12B)	107.9
C(14)-C(13)-C(12)	124.72(12)
C(14)-C(13)-H(13)	117.6
C(12)-C(13)-H(13)	117.6
C(13)-C(14)-C(15)	126.58(12)
C(13)-C(14)-H(14)	116.7
C(15)-C(14)-H(14)	116.7
C(14)-C(15)-C(16)	116.44(11)
C(14)-C(15)-H(15A)	108.2
C(16)-C(15)-H(15A)	108.2
C(14)-C(15)-H(15B)	108.2
C(16)-C(15)-H(15B)	108.2
H(15A)-C(15)-H(15B)	107.3
C(17)-C(16)-C(15)	111.33(11)
C(17)-C(16)-H(16A)	109.4
C(15)-C(16)-H(16A)	109.4
C(17)-C(16)-H(16B)	109.4
C(15)-C(16)-H(16B)	109.4
H(16A)-C(16)-H(16B)	108.0
O(18)-C(17)-O(19)	122.51(12)
O(18)-C(17)-C(16)	124.06(12)
O(19)-C(17)-C(16)	113.43(11)
C(17)-O(19)-C(20)	114.44(10)
O(19)-C(20)-C(2)	107.98(9)
O(19)-C(20)-H(20A)	110.1
C(2)-C(20)-H(20A)	110.1
O(19)-C(20)-H(20B)	110.1
C(2)-C(20)-H(20B)	110.1
H(20A)-C(20)-H(20B)	108.4
O(23)-N(21)-O(22)	123.63(13)
O(23)-N(21)-C(3)	119.15(11)

O(22)-N(21)-C(3)	117.21(13)

Symmetry transformations used to generate equivalent atoms:

Table S31. Anisotropic displacement parameters ($Å^2$ x 10^3) for **10a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	32(1)	24(1)	34(1)	0(1)	23(1)	-2(1)
C(2)	31(1)	24(1)	33(1)	2(1)	23(1)	-1(1)
C(3)	41(1)	25(1)	35(1)	-1(1)	27(1)	-2(1)
C(4)	49(1)	26(1)	49(1)	5(1)	34(1)	8(1)
C(5)	40(1)	39(1)	46(1)	11(1)	24(1)	11(1)
C(6)	34(1)	37(1)	35(1)	2(1)	19(1)	-1(1)
C(7)	41(1)	25(1)	42(1)	-3(1)	30(1)	-4(1)
O(8)	40(1)	23(1)	38(1)	-3(1)	27(1)	-3(1)
O(9)	47(1)	24(1)	46(1)	-4(1)	28(1)	-5(1)
C(10)	26(1)	24(1)	22(1)	-1(1)	9(1)	1(1)
C(11)	37(1)	28(1)	24(1)	1(1)	18(1)	2(1)
C(12)	34(1)	38(1)	36(1)	0(1)	22(1)	3(1)
C(13)	32(1)	27(1)	43(1)	0(1)	20(1)	0(1)
C(14)	35(1)	31(1)	40(1)	1(1)	22(1)	2(1)
C(15)	29(1)	38(1)	37(1)	2(1)	15(1)	3(1)
C(16)	27(1)	31(1)	37(1)	-4(1)	13(1)	-4(1)
C(17)	31(1)	25(1)	26(1)	-5(1)	12(1)	-2(1)
O(18)	45(1)	50(1)	35(1)	13(1)	19(1)	8(1)
O(19)	28(1)	33(1)	32(1)	6(1)	17(1)	2(1)
C(20)	33(1)	33(1)	35(1)	6(1)	22(1)	1(1)
N(21)	57(1)	29(1)	41(1)	-5(1)	34(1)	-9(1)
O(22)	82(1)	29(1)	51(1)	-7(1)	42(1)	2(1)
O(23)	46(1)	58(1)	54(1)	-19(1)	28(1)	-15(1)

Table S32. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **10a**.

	x	y	z	U(eq)
H(4)	25695408	575344		
H(5)	5384960	314948		
H(6)	11594061	263641		
H(7A)	45313162	548539		
H(7B)	26903216	362039		
H(11A)	65673550	177534		
H(11B)	59842971	76534		
H(12A)	85032539	322740		
H(12B)	92172996	232840		
H(13)	92333607	483840		
H(14)	109962622	619440		
H(15A)	131463355	810441		
H(15B)	120303029	893541		
H(16A)	121174029	926339		
H(16B)	107124059	719039		
H(20A)	67254052	908337		
H(20B)	60953513	785337		

Table S33. Crystal data and structure refinement for **10b**.

Empirical formula	$C_{18}\ H_{21}\ N\ O_6$	
Formula weight	347.36	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*Cc*	
Unit cell dimensions	a = 5.0300(3) Å	α = 90°
	b = 20.5537(12) Å	β = 97.379(2)°
	c = 16.8829(10) Å	γ = 90°
Volume	1730.98(18) $Å^3$	
Z	4	
Density (calculated)	1.333 Mg/m^3	
Absorption coefficient	0.100 mm^{-1}	
F(000)	736	
Crystal size	0.268 x 0.065 x 0.054 mm^3	
Theta range for data collection	3.139 to 26.992°.	
Index ranges	–6<=h<=6, –26<=k<=26, –21<=l<=21	
Reflections collected	10870	
Independent reflections	3487 [R(int) = 0.0750]	
Completeness to theta = 25.242°	98.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.2627	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3487 / 2 / 226	
Goodness-of-fit on F^2	1.076	
Final R indices [I>2sigma(I)]	R1 = 0.0782, wR2 = 0.2076	
R indices (all data)	R1 = 0.0829, wR2 = 0.2152	
Absolute structure parameter	0.1(8)	
Largest diff. peak and hole	0.569 and –0.348 $e \cdot Å^{-3}$	

Table S34. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **10b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4030(9)	7123(2)	4041(3)	28(1)
C(2)	5757(9)	7563(2)	3735(3)	29(1)
C(3)	6313(12)	7547(2)	2953(3)	37(1)
C(4)	5109(13)	7081(2)	2448(3)	40(1)
C(5)	3350(12)	6639(2)	2729(3)	39(1)
C(6)	2812(9)	6656(2)	3521(3)	30(1)
C(7)	832(10)	6163(2)	3771(3)	34(1)
O(8)	1930(6)	5762(2)	4437(2)	31(1)
O(9)	4611(8)	5281(2)	3650(2)	41(1)
C(10)	3843(8)	5323(2)	4279(3)	28(1)
C(11)	4686(9)	4917(2)	5012(3)	27(1)
C(12)	7195(9)	4520(2)	4957(3)	29(1)
C(13)	8150(11)	4183(2)	5770(3)	35(1)
C(14)	9180(10)	4662(2)	6397(3)	33(1)
C(15)	7933(11)	4854(2)	6999(3)	34(1)
C(16)	8834(10)	5406(2)	7557(3)	33(1)
C(17)	7142(10)	6012(2)	7327(3)	32(1)
C(18)	7784(10)	6308(2)	6536(3)	29(1)
C(19)	5614(9)	6738(2)	6136(3)	28(1)
O(20)	3999(9)	7033(2)	6464(2)	49(1)
O(21)	5610(7)	6751(2)	5348(2)	33(1)
C(22)	3515(10)	7143(2)	4906(3)	34(1)
N(23)	7072(10)	8085(2)	4235(3)	41(1)
O(24)	7093(16)	8629(2)	3948(3)	83(2)
O(25)	8012(11)	7971(2)	4928(3)	59(1)

Table S35. Bond lengths [Å] and angles [°] for **10b**.

C(1)-C(6)	1.388(7)
C(1)-C(2)	1.398(7)
C(1)-C(22)	1.517(7)
C(2)-C(3)	1.384(7)
C(2)-N(23)	1.471(6)
C(3)-C(4)	1.371(8)
C(3)-H(3)	0.9500
C(4)-C(5)	1.395(8)
C(4)-H(4)	0.9500
C(5)-C(6)	1.398(7)
C(5)-H(5)	0.9500
C(6)-C(7)	1.518(7)
C(7)-O(8)	1.445(6)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
O(8)-C(10)	1.370(5)
O(9)-C(10)	1.179(6)
C(10)-C(11)	1.509(6)
C(11)-C(12)	1.516(6)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.558(6)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.489(7)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.322(8)
C(14)-H(14)	0.9500
C(15)-C(16)	1.506(7)
C(15)-H(15)	0.9500
C(16)-C(17)	1.531(7)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.539(6)
C(17)-H(17A)	0.9900

C(17)-H(17B)	0.9900
C(18)-C(19)	1.496(7)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-O(20)	1.204(6)
C(19)-O(21)	1.331(5)
O(21)-C(22)	1.454(6)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
N(23)-O(24)	1.218(6)
N(23)-O(25)	1.227(6)

C(6)-C(1)-C(2)	117.3(4)
C(6)-C(1)-C(22)	120.8(4)
C(2)-C(1)-C(22)	121.9(4)
C(3)-C(2)-C(1)	123.3(4)
C(3)-C(2)-N(23)	115.7(4)
C(1)-C(2)-N(23)	121.0(4)
C(4)-C(3)-C(2)	118.9(5)
C(4)-C(3)-H(3)	120.6
C(2)-C(3)-H(3)	120.6
C(3)-C(4)-C(5)	119.5(5)
C(3)-C(4)-H(4)	120.3
C(5)-C(4)-H(4)	120.3
C(4)-C(5)-C(6)	121.2(5)
C(4)-C(5)-H(5)	119.4
C(6)-C(5)-H(5)	119.4
C(1)-C(6)-C(5)	119.9(4)
C(1)-C(6)-C(7)	122.6(4)
C(5)-C(6)-C(7)	117.5(4)
O(8)-C(7)-C(6)	113.4(4)
O(8)-C(7)-H(7A)	108.9
C(6)-C(7)-H(7A)	108.9
O(8)-C(7)-H(7B)	108.9
C(6)-C(7)-H(7B)	108.9
H(7A)-C(7)-H(7B)	107.7
C(10)-O(8)-C(7)	115.5(4)
O(9)-C(10)-O(8)	123.0(4)

O(9)-C(10)-C(11)	127.5(4)
O(8)-C(10)-C(11)	109.6(4)
C(10)-C(11)-C(12)	113.3(4)
C(10)-C(11)-H(11A)	108.9
C(12)-C(11)-H(11A)	108.9
C(10)-C(11)-H(11B)	108.9
C(12)-C(11)-H(11B)	108.9
H(11A)-C(11)-H(11B)	107.7
C(11)-C(12)-C(13)	110.5(4)
C(11)-C(12)-H(12A)	109.6
C(13)-C(12)-H(12A)	109.6
C(11)-C(12)-H(12B)	109.6
C(13)-C(12)-H(12B)	109.6
H(12A)-C(12)-H(12B)	108.1
C(14)-C(13)-C(12)	111.8(4)
C(14)-C(13)-H(13A)	109.3
C(12)-C(13)-H(13A)	109.3
C(14)-C(13)-H(13B)	109.3
C(12)-C(13)-H(13B)	109.3
H(13A)-C(13)-H(13B)	107.9
C(15)-C(14)-C(13)	126.0(5)
C(15)-C(14)-H(14)	117.0
C(13)-C(14)-H(14)	117.0
C(14)-C(15)-C(16)	124.8(5)
C(14)-C(15)-H(15)	117.6
C(16)-C(15)-H(15)	117.6
C(15)-C(16)-C(17)	110.0(4)
C(15)-C(16)-H(16A)	109.7
C(17)-C(16)-H(16A)	109.7
C(15)-C(16)-H(16B)	109.7
C(17)-C(16)-H(16B)	109.7
H(16A)-C(16)-H(16B)	108.2
C(16)-C(17)-C(18)	111.7(4)
C(16)-C(17)-H(17A)	109.3
C(18)-C(17)-H(17A)	109.3
C(16)-C(17)-H(17B)	109.3
C(18)-C(17)-H(17B)	109.3
H(17A)-C(17)-H(17B)	107.9

C(19)-C(18)-C(17)	113.7(4)
C(19)-C(18)-H(18A)	108.8
C(17)-C(18)-H(18A)	108.8
C(19)-C(18)-H(18B)	108.8
C(17)-C(18)-H(18B)	108.8
H(18A)-C(18)-H(18B)	107.7
O(20)-C(19)-O(21)	122.3(4)
O(20)-C(19)-C(18)	125.9(4)
O(21)-C(19)-C(18)	111.7(4)
C(19)-O(21)-C(22)	115.6(4)
O(21)-C(22)-C(1)	106.0(4)
O(21)-C(22)-H(22A)	110.5
C(1)-C(22)-H(22A)	110.5
O(21)-C(22)-H(22B)	110.5
C(1)-C(22)-H(22B)	110.5
H(22A)-C(22)-H(22B)	108.7
O(24)-N(23)-O(25)	122.2(5)
O(24)-N(23)-C(2)	117.9(4)
O(25)-N(23)-C(2)	119.8(4)

Symmetry transformations used to generate equivalent atoms:

Table S36. Anisotropic displacement parameters ($Å^2$ x 10^3) for **10b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	34(2)	25(2)	25(2)	6(2)	3(2)	5(2)
C(2)	39(2)	21(2)	27(2)	4(2)	1(2)	1(2)
C(3)	50(3)	30(2)	31(3)	13(2)	11(2)	2(2)
C(4)	65(4)	37(2)	19(2)	7(2)	15(2)	6(2)
C(5)	61(3)	27(2)	26(2)	-1(2)	-3(2)	3(2)
C(6)	34(2)	30(2)	26(2)	6(2)	5(2)	6(2)
C(7)	31(2)	33(2)	36(3)	8(2)	-1(2)	3(2)
O(8)	33(2)	28(1)	32(2)	6(1)	10(1)	4(1)
O(9)	53(2)	47(2)	26(2)	3(2)	10(2)	13(2)
C(10)	27(2)	25(2)	31(3)	0(2)	5(2)	1(2)
C(11)	30(2)	31(2)	21(2)	-1(2)	9(2)	0(2)
C(12)	28(2)	36(2)	23(2)	-2(2)	6(2)	5(2)
C(13)	44(2)	30(2)	30(2)	6(2)	5(2)	4(2)
C(14)	33(2)	38(2)	29(2)	8(2)	5(2)	2(2)
C(15)	42(2)	36(2)	24(2)	10(2)	4(2)	-2(2)
C(16)	39(2)	45(3)	16(2)	4(2)	5(2)	-4(2)
C(17)	40(2)	39(2)	17(2)	1(2)	6(2)	-3(2)
C(18)	37(2)	34(2)	16(2)	0(2)	9(2)	-2(2)
C(19)	32(2)	35(2)	18(2)	-1(2)	11(2)	-5(2)
O(20)	54(2)	69(3)	26(2)	-2(2)	15(2)	19(2)
O(21)	44(2)	39(2)	17(2)	2(1)	6(1)	11(1)
C(22)	39(2)	35(2)	27(2)	2(2)	6(2)	10(2)
N(23)	44(2)	33(2)	41(3)	1(2)	-6(2)	-2(2)
O(24)	131(5)	35(2)	72(4)	4(2)	-32(3)	-20(3)
O(25)	74(3)	53(2)	44(2)	-3(2)	-19(2)	-3(2)

Table S37. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **10b**.

	x	y	z	U(eq)
H(3)	75097853	277044		
H(4)	54707060	190948		
H(5)	25016319	237747		
H(7A)	-7576396	391640		
H(7B)	2265878	331040		
H(11A)	32034618	509732		
H(11B)	50035207	548332		
H(12A)	86324808	481035		
H(12B)	68214186	453435		
H(13A)	66343939	594842		
H(13B)	95843867	569742		
H(14)	108904847	636040		
H(15)	63524627	708741		
H(16A)	107475502	752840		
H(16B)	86445279	811340		
H(17A)	74856340	775738		
H(17B)	52185895	727438		
H(18A)	94596564	664234		
H(18B)	81055951	616734		
H(22A)	35977597	510740		
H(22B)	17256962	496240		

8. Calculated open-structures of monomers

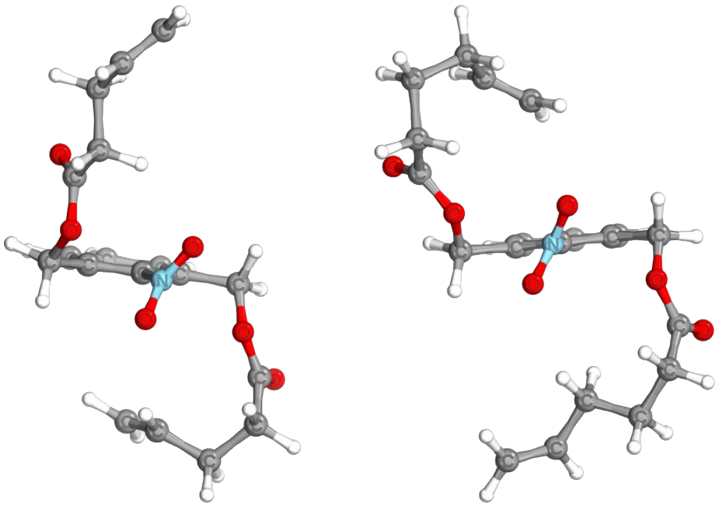


Fig. S20. Calculated structures of **4a'** and **4b'**.

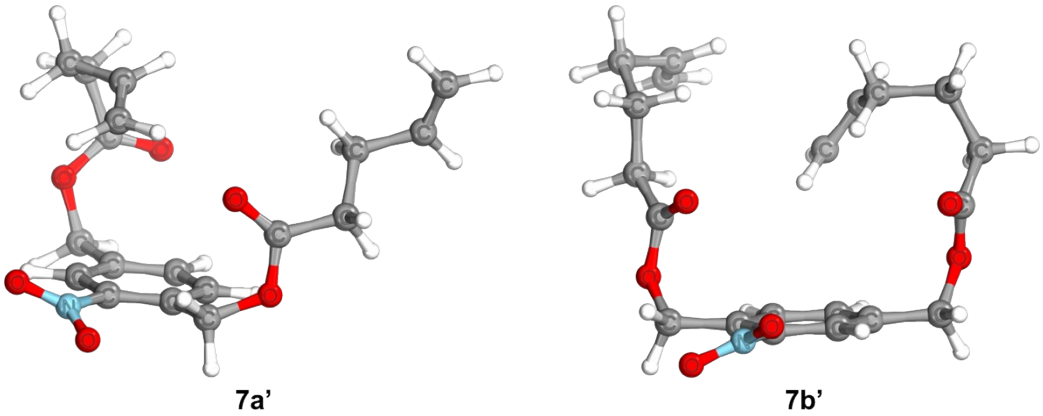


Fig. S21. Calculated structures of **7a'** and **7b'**.

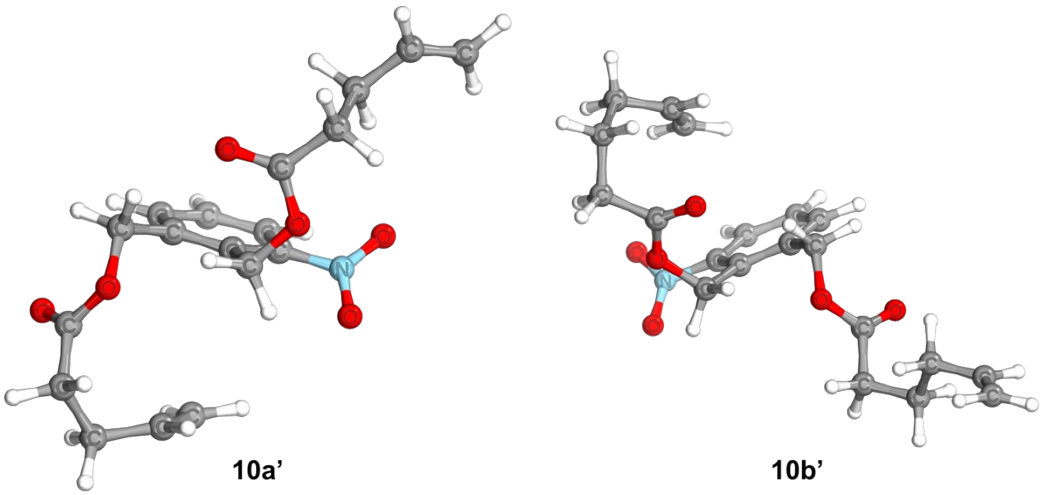


Fig. S22. Calculated structures of **10a'** and **10b'**.

Table S38. Calculated atomic coordinates for **4a'**.

	x	y	z
O	-0.56705	-1.61984	0.757895
O	0.392309	-1.21205	-1.12046
O	-2.48963	-0.31415	-1.32707
O	-4.36775	0.896582	-1.54106
O	3.437485	0.923168	0.6893
O	2.119884	-0.7541	1.37896
N	-0.1135	-0.86673	-0.07321
C	-3.48835	0.715047	2.219204
C	6.0096	-1.90774	-2.8632
C	-0.17811	0.552692	0.200019
C	0.504087	1.064971	1.301778
C	0.421264	2.427533	1.554909
C	-0.33573	3.248163	0.737668
C	-1.00737	2.724829	-0.35454
C	-0.92572	1.371364	-0.64637
C	-1.68021	0.767676	-1.80216
C	-3.80699	-0.11269	-1.19511
C	-4.46322	-1.29553	-0.53118
C	-4.86518	-0.88877	0.899281
C	-3.66538	-0.48541	1.699805
C	5.764738	-1.93792	-1.56703
C	5.102711	-0.83467	-0.80261
C	3.826453	-1.3295	-0.11865
C	3.14494	-0.24499	0.6723
C	1.347877	0.160403	2.161998
H	-2.90936	-1.25161	1.817783
H	-2.60794	0.969416	2.785234
H	-4.22345	1.495686	2.104537
H	6.043749	-2.80327	-0.97894
H	5.741277	-1.05866	-3.47092
H	6.492163	-2.72493	-3.3725
H	0.957298	2.841436	2.394525
H	-0.39986	4.30394	0.950139
H	-1.59978	3.366059	-0.98843
H	-0.99285	0.341195	-2.53948
H	-2.32303	1.514482	-2.27677
H	-5.35433	-1.57126	-1.09626
H	-3.76082	-2.12858	-0.50861
H	-5.35081	-1.74495	1.374008

H	-5.5782	-0.06381	0.849777
H	5.788067	-0.45981	-0.03676
H	4.85882	-0.00451	-1.46705
H	4.034889	-2.16416	0.554219
H	3.109329	-1.68649	-0.86415
H	0.720425	-0.47583	2.792834
H	2.01867	0.761357	2.783504

Table S39. Calculated atomic coordinates for **4b'**.

	x	y	z
O	0.476339	1.550635	1.271157
O	-0.55851	1.584296	-0.6095
O	-2.32232	0.622863	1.824792
O	-3.99575	-0.8707	1.796941
O	3.961853	-0.37325	-1.8801
O	2.071775	0.655686	-1.24037
N	-0.04924	1.007036	0.32521
C	3.19708	-0.9309	1.823987
C	-3.65033	0.58614	-3.94254
C	-1.44101	-0.33181	2.427197
C	-3.56529	0.220852	1.520592
C	-4.31366	1.307473	0.792299
C	-4.80657	0.801626	-0.56896
C	-3.64712	0.344736	-1.46179
C	-4.11871	0.022614	-2.84508
C	4.353238	-0.60939	1.273549
C	5.018792	0.722066	1.417136
C	5.341348	1.365541	0.065097
C	4.07698	1.741423	-0.7099
C	3.404976	0.543044	-1.32945
C	1.256247	-0.37135	-1.81328
C	-0.08116	-0.43994	0.31564
C	-0.72774	-1.11269	1.353272
C	-0.76803	-2.49911	1.320334
C	-0.15888	-3.19398	0.288878
C	0.490641	-2.51398	-0.72695
C	0.531076	-1.12632	-0.73159
H	4.895405	-1.33495	0.680085
H	2.636379	-0.22528	2.416312
H	2.761863	-1.91008	1.711298
H	-4.90045	-0.72448	-2.90349
H	-4.01715	0.326278	-4.92146
H	-2.87311	1.332823	-3.90581
H	-0.7382	0.252426	3.027085
H	-2.01789	-1.00491	3.067714
H	-5.17171	1.597589	1.402299
H	-3.65255	2.165658	0.669423
H	-5.49557	-0.03059	-0.4118
H	-5.34866	1.609213	-1.06432

H	-3.19847	-0.55428	-1.02486
H	-2.88084	1.12162	-1.50313
H	4.384496	1.391841	2.001887
H	5.957858	0.581788	1.96154
H	5.932934	0.676562	-0.54127
H	5.930839	2.268263	0.233687
H	4.341776	2.405612	-1.53778
H	3.358783	2.258165	-0.07249
H	0.54028	0.128128	-2.47577
H	1.891479	-1.04631	-2.39457
H	-1.28421	-3.03037	2.104675
H	-0.19119	-4.27239	0.27726
H	0.971916	-3.0578	-1.5248

Table S40. Calculated atomic coordinates for **7a'**.

	x	y	z
O	-1.45722	-3.82431	-0.59812
O	0.530473	-3.74379	-1.40266
O	-3.0996	-0.34885	0.786039
O	-2.32627	0.416247	-1.17376
O	3.112657	1.713171	1.352439
O	3.835988	-0.25783	0.566971
N	-0.33097	-3.35985	-0.63345
C	-4.3332	5.134993	-0.96675
C	1.089585	0.399337	-2.03912
C	0.009254	-2.31459	0.284591
C	1.363466	-2.14066	0.562497
C	1.783838	-1.16412	1.447522
C	0.825868	-0.3567	2.052566
C	-0.51609	-0.52273	1.765858
C	-0.96028	-1.49412	0.87489
C	-2.43092	-1.58805	0.565269
C	-2.97443	0.582652	-0.1703
C	-3.75468	1.823736	0.179152
C	-3.05491	3.092275	-0.32574
C	-3.87992	4.308909	-0.04312
C	2.015188	1.326092	-1.87772
C	3.488173	1.07678	-1.99376
C	4.248099	1.627167	-0.77539
C	3.665239	1.064567	0.497334
C	3.255307	-0.94181	1.684393
H	-4.1003	4.484095	1.002302
H	-4.1268	4.982549	-2.01396
H	-4.9228	6.001532	-0.71867
H	1.733344	2.344366	-1.64102
H	1.349932	-0.61953	-2.2814
H	0.037392	0.610868	-1.94944
H	2.077188	-2.78617	0.071784
H	1.135104	0.415618	2.740072
H	-1.2447	0.11806	2.23837
H	-2.91475	-2.30967	1.229805
H	-2.59457	-1.90222	-0.47089
H	-4.73364	1.736652	-0.30146
H	-3.90925	1.852844	1.258135
H	-2.87096	2.997014	-1.39695

H	-2.0869	3.18575	0.175871
H	3.674974	0.006525	-2.09213
H	3.87106	1.576892	-2.88802
H	4.168171	2.714001	-0.73195
H	5.298786	1.341523	-0.84175
H	3.795706	-1.88803	1.747589
H	3.412905	-0.34757	2.590017

Table S41. Calculated atomic coordinates for **7b'**.

	x	y	z
O	3.038572	3.506771	0.402507
O	1.206431	4.09434	1.351243
O	-3.28906	1.304601	-1.34439
O	-3.36742	1.823216	0.836973
O	1.919643	-0.36383	1.234819
O	3.11791	-0.43568	-0.6569
N	1.827249	3.446784	0.53024
C	1.21245	-5.80054	-0.55282
C	-1.40392	-2.23516	-0.52333
C	-2.4943	2.462809	-1.618
C	-3.64675	1.08245	-0.07226
C	-4.46334	-0.18249	0.033884
C	-4.19201	-0.9343	1.338071
C	-2.75158	-1.45231	1.418678
C	-2.42299	-2.39017	0.300858
C	1.027018	-5.12171	0.56411
C	2.11795	-4.69414	1.494742
C	2.175079	-3.16946	1.636384
C	2.610653	-2.50353	0.33359
C	2.497158	-1.00351	0.390337
C	3.071463	0.990506	-0.71849
C	1.089407	2.588424	-0.34792
C	-0.25282	2.908806	-0.55169
C	-1.03355	2.157811	-1.40888
C	-0.4544	1.072454	-2.06328
C	0.86651	0.740359	-1.83832
C	1.669543	1.479007	-0.97236
H	0.029496	-4.82516	0.863305
H	0.39264	-6.08868	-1.18977
H	2.194838	-6.10815	-0.87437
H	-3.08857	-3.2385	0.196543
H	-0.73076	-1.39822	-0.42579
H	-1.18915	-2.93636	-1.31259
H	-2.69484	2.706144	-2.66471
H	-2.81218	3.285006	-0.96973
H	-5.51546	0.113453	-0.00408
H	-4.25005	-0.8068	-0.834
H	-4.88687	-1.77323	1.41007
H	-4.37406	-0.26228	2.178549

H	-2.63135	-1.98051	2.369832
H	-2.05524	-0.6107	1.416184
H	1.925916	-5.12473	2.481433
H	3.081106	-5.06815	1.142275
H	1.192032	-2.78664	1.918187
H	2.873638	-2.8995	2.430769
H	1.97547	-2.84925	-0.48698
H	3.639714	-2.76243	0.077776
H	3.4785	1.402414	0.209133
H	3.729878	1.266309	-1.5464
H	-0.66325	3.756623	-0.02336
H	-1.05384	0.479376	-2.73748
H	1.296898	-0.11744	-2.33364

Table S42. Calculated atomic coordinates for **10a'**.

	x	y	z
O	2.337413	-2.53972	0.607559
O	0.732206	-2.03446	1.941644
O	1.437394	0.787264	1.303416
O	1.482943	2.438402	-0.21182
O	-4.00943	0.756733	-1.75145
O	-2.50351	1.624828	-0.33251
N	1.24991	-2.0525	0.844934
C	-3.25317	-1.91611	1.049354
C	6.487997	-0.07699	0.394615
C	0.042662	0.568133	1.045975
C	2.050181	1.739555	0.593304
C	3.522234	1.782858	0.900908
C	4.2724	0.925026	-0.13762
C	5.749139	0.976318	0.101723
C	-3.78196	-0.81595	1.550877
C	-4.99985	-0.13574	1.00792
C	-4.67055	1.282871	0.508568
C	-3.72341	1.184744	-0.66085
C	-1.48134	1.532884	-1.33162
C	-0.87737	-0.61589	-2.46034
C	-0.23228	-1.83866	-2.52005
C	0.485098	-2.28589	-1.42725
C	0.517548	-1.51208	-0.27435
C	-0.12358	-0.27211	-0.19531
C	-0.81144	0.182217	-1.32244
H	-3.33084	-0.33717	2.410883
H	-2.37842	-2.37574	1.47801
H	-3.67985	-2.40997	0.190956
H	6.196101	1.959217	0.026013
H	7.549669	-0.00163	0.558771
H	6.059644	-1.06316	0.477151
H	-0.3319	0.043933	1.927192
H	-0.4634	1.528415	0.94215
H	3.867112	2.815593	0.839207
H	3.697774	1.3863	1.900654
H	4.048838	1.312511	-1.13603
H	3.925214	-0.10845	-0.08082
H	-5.41907	-0.71563	0.183919
H	-5.75172	-0.05526	1.797027

H	-4.20714	1.871653	1.299494
H	-5.58774	1.768165	0.171642
H	-1.92953	1.717121	-2.31241
H	-0.75637	2.318963	-1.1014
H	-1.43696	-0.26451	-3.31371
H	-0.28361	-2.43852	-3.41477
H	1.007637	-3.23044	-1.4443

Table S43. Calculated atomic coordinates for **10b'**.

	x	y	z
O	3.452722	2.960817	0.096884
O	1.923099	2.922182	1.602304
O	2.078136	-0.06447	1.485982
O	1.570991	-2.11038	0.720243
O	-3.34941	0.629878	-1.17379
O	-2.00648	-0.4889	0.231448
N	2.336422	2.682839	0.48667
C	-7.6497	-2.76896	1.124036
C	3.621914	-0.40746	-1.91673
C	0.736218	0.384419	1.249364
C	2.367778	-1.33889	1.195736
C	3.776819	-1.66997	1.615681
C	4.44117	-2.70608	0.708568
C	4.915958	-2.09621	-0.61417
C	3.779033	-1.64022	-1.47151
C	-6.95844	-1.92357	0.382974
C	-5.53968	-1.52632	0.645264
C	-5.42048	-0.01543	0.871434
C	-3.97437	0.404436	1.151191
C	-3.10564	0.214305	-0.06818
C	-1.07398	-0.73807	-0.82749
C	-0.20339	0.460176	-1.11202
C	-0.22998	1.033297	-2.37978
C	0.584698	2.1048	-2.70128
C	1.439015	2.623083	-1.74711
C	1.441531	2.07893	-0.46896
C	0.626059	0.996691	-0.12436
H	-7.4146	-1.45528	-0.48031
H	-7.21976	-3.24853	1.988914
H	-8.67128	-3.02476	0.897781
H	3.059816	-2.40722	-1.72996
H	4.317639	0.380161	-1.67314
H	2.79504	-0.13094	-2.54923
H	0.053069	-0.45834	1.361549
H	0.53558	1.129556	2.022988
H	4.354955	-0.74628	1.659937
H	3.700977	-2.06903	2.631792
H	3.727599	-3.50824	0.5099
H	5.299959	-3.1313	1.230494

H	5.47726	-2.85991	-1.16106
H	5.589099	-1.25978	-0.41384
H	-5.15946	-2.0614	1.517932
H	-4.92718	-1.80339	-0.21867
H	-6.04553	0.272015	1.718843
H	-5.77633	0.516425	-0.01326
H	-3.55207	-0.16576	1.978527
H	-3.94954	1.467409	1.403477
H	-0.46671	-1.58357	-0.49069
H	-1.62862	-1.01265	-1.72965
H	-0.89608	0.626065	-3.12494
H	0.559162	2.530111	-3.69206
H	2.096432	3.449948	-1.9695

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