Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Synthesis of bay-triaminosubstituted perylenediimides

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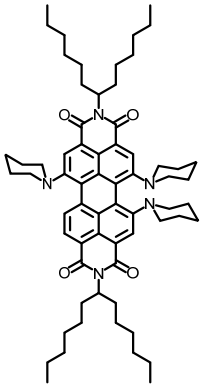
General Procedure for the Synthesis of Molecules 2-8 and 12-13.

The appropriate disubstituted PDI (**1a-f** or **11**, 0.2 mmol), TBAF (1.2 mL of a 1 M solution in THF, 1.2 mmol), the amine or the aromatic nitrogenated heterocycle (3.2 mmol) and dry THF (0.3 mL) were added to a 5 mL pear-shaped flask. The reaction was heated at 70 ^{o}C for 24 h under argon atmosphere. After cooling, the mixture was extracted with dichloromethane and washed with water. The organic phase was dried over anhydrous sodium sulfate, filtered and evaporated. Purification was carried out by silica gel column chromatography.

PDI 2



From **1a**

Eluent: Dichloromethane:Hexane (1:1). Yield: 75 %

^{1}H NMR ($CDCl_3$) δ 0.83 (br, 12H), 1.26 (br, 40H), 1.70 (m, 4H), 1.89 (m, 14H), 2.27 (m, 4H), 2.41 (m, 1H), 3.22 (m, 2H), 3.46 (m, 2H), 3.66 (m, 1H), 4.22 (m, 2H), 5.21 (m, 2H), 8.46 (m, 4H) and 9.84 ppm (d, *J* = 8.3 Hz, 1H)

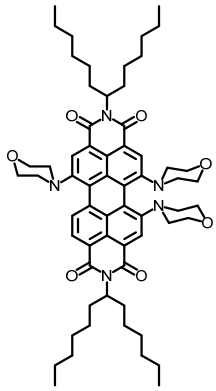
^{13}C NMR ($CDCl_3$) δ 166.11, 165.46, 165.44, 165.24, 151.84, 145.10, 143.70, 134.48, 132.83, 131.41, 126.63, 125.84, 124.12, 124.06, 123.32, 123.05, 122.64, 122.33, 122.19, 121.80, 120.85, 120.43, 119.91, 119.61, 119.26, 55.50, 54.65, 51.49, 51.33, 51.27, 51.16, 50.90, 32.82, 32.74, 31.95, 29.85, 29.49, 29.45, 27.23, 27.15, 26.49, 26.43, 26.35, 25.81, 24.79, 24.73, 24.15, 22.84, 22.78, 14.27 and 14.21 ppm

MALDI-TOF m/z [M^-] calc. for $C_{65}H_{89}N_5O_4$: 1003.6909, found: 1003.6931

IR (KBr): 2925, 2854, 1687, 1650, 1585, 1452, 1438, 1413, 1380, 1334, 1305, 1265, 1257, 1219, 1150, 1117, 1023, 920, 857 and 805 cm^{-1}

UV-vis ($CHCl_3$) λ_{max}/nm (log ε): 571 (4.2) and 708 (4.5)

PDI 3



From **1b**

Eluent: Dichloromethane:Ethyl acetate (9:1). Yield: 65 %

^{1}H NMR ($CDCl_3$) δ 0.84 (br, 12H), 1.25 (br, 32H), 1.48-2.11 (m, 8H), 2.27 (m, 4H), 2.47 (m, 1H), 2.65 (m, 1H), 3.05-3.62 (m, 7H), 3.63-4.25 (m, 11H), 5.22 (m, 2H), 8.48 (m, 4H) and 9.85 ppm (d, *J* = 8.3 Hz, 1H)

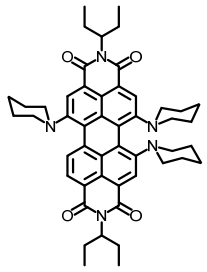
^{13}C NMR ($CDCl_3$) δ 165.66, 165.26, 165.06, 164.69, 164.24, 164.12, 150.73, 145.71, 144.49, 133.93, 132.80, 131.43, 129.93, 127.16, 126.36, 123.74, 123.29, 122.48, 122.28, 122.12, 121.70, 121.52, 120.95, 119.95, 119.86, 119.21, 66.51, 54.86, 53.59, 51.20, 50.84, 50.33, 50.15, 49.72, 32.59, 31.90, 31.55, 30.32, 29.80, 29.39, 29.37, 29.36, 27.16, 27.09, 22.72 and 14.17 ppm

MALDI-TOF m/z [M^-] calc. for $C_{62}H_{83}N_5O_7$: 1009.6287, found: 1009.6246

IR (KBr): 2954, 2923, 2853, 1689, 1651, 1585, 1457, 1415, 1364, 1332, 1305, 1254 and 1114 cm^{-1}

UV-vis ($CHCl_3$) λ_{max}/nm (log ε): 556 (4.2) and 681 (4.5)

PDI 4



From **1c**

Eluent: Dichloromethane. Yield: 69 %

^{1}H NMR ($CDCl_3$) δ 0.95 (m, 12H), 1.05-1.60 (br, 8H), 1.65 – 2.48 (br, 23H), 3.23 (m, 2H), 3.47 (m, 2H), 3.68 (m, 1H), 4.22 (m, 2H), 5.13 (m, 2H), 8.36 (s, 1H), 8.45 (d, *J* = 8.4 Hz, 1H), 8.45 (s, 1H), 8.56 (s, 1H) and 9.85 ppm (d, *J* = 8.4 Hz, 1H)

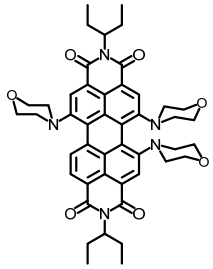
^{13}C NMR ($CDCl_3$) δ 166.12, 165.72, 165.42, 164.97, 151.86, 145.07, 143.68, 134.47, 132.83, 131.40, 124.08, 123.34, 123.07, 122.15, 119.88, 119.59, 119.27, 57.53, 57.39, 55.47, 51.50, 51.32, 51.26, 51.18, 50.89, 26.47, 26.42, 26.32, 25.78, 25.39, 25.31, 24.77, 24.73, 24.13, 11.63 and 11.55 ppm

MALDI-TOF m/z [M^-] calc. for $C_{49}H_{57}N_5O_4$: 779.4405, found: 779.4491

IR (KBr): 2927, 2853, 1688, 1652, 1584, 1510, 1458, 1415, 1379, 1335, 1305, 1258, 1206, 1153, 1114, 1066, 1023, 923 and 804 cm^{-1}

UV-vis ($CHCl_3$) λ_{max}/nm (log ε): 577 (4.1) and 707 (4.4)

PDI 5



From **1d**

Eluent: Dichloromethane:Ethyl acetate (9:1). Yield: 80 %

^{1}H NMR ($CDCl_3$) δ 0.95 (m, 12H), 1.52-1.85 (br, 4H), 1.96 (m, 4H), 2.27 (m, 4H), 2.48 (br, 1H), 2.65 (m, 1H), 3.05-3.62 (br, 7H), 3.80 (m, 4H), 4.00 (m, 7H), 5.10 (m, 2H), 8.36 (s, 1H), 8.40 (s, 1H), 8.47 (d, *J* = 8.4 Hz, 1H), 8.50 (s, 1H) and 9.83 ppm (d, *J* = 8.4 Hz, 1H)

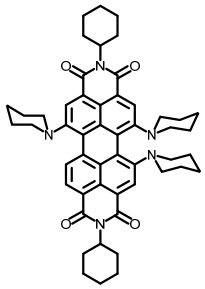
^{13}C NMR ($CDCl_3$) δ 163.50, 150.78, 145.73, 144.52, 137.85, 136.12, 133.97, 133.72, 133.70, 133.23, 132.84, 131.47, 129.63, 126.22, 123.79, 123.35, 119.97, 119.91, 119.29, 66.55, 62.25, 57.81, 53.60, 50.34, 32.08, 29.86, 29.52, 25.37, 25.27, 22.85, 11.63 and 11.55 ppm

MALDI-TOF m/z [M^-] calc. for $C_{46}H_{51}N_5O_7$: 785.3783, found: 785.3751

IR (KBr): 2960, 2925, 2854, 1734, 1689, 1653, 1585, 1541, 1510, 1458, 1450, 1417, 1398, 1383, 1365, 1333, 1306, 1257, 1205, 1161, 1114, 1068, 1039, 1024, 928, 908 and 804 cm^{-1}

UV-vis ($CHCl_3$) λ_{max}/nm (log ε): 557 (4.0) and 683 (4.3)

PDI 6



From **1e** or **1f**[1]

Eluent: Dichloromethane. Yield: 60 % from **1e** and 61 % from **1f**

^{1}H NMR ($CDCl_3$) δ 1.28-1.60 (br, 13H), 1.63-2.08 (br, 24H), 2.14 (m, 1H), 2.41 (m, 1H), 2.62 (m, 4H), 3.22 (m, 2H), 3.47 (m, 2H), 3.66 (m, 1H), 4.19 (m, 2H), 5.10 (m, 2H), 8.35 (s, 1H), 8.44 (m, 2H), 8.55 (s, 1H) and 9.83 ppm (d, *J* = 8.4 Hz, 1H)

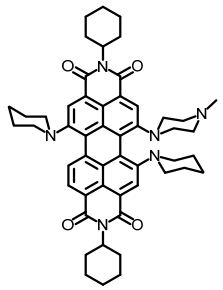
^{13}C NMR ($CDCl_3$) δ 165.40, 165.31, 164.93, 164.70, 151.83, 145.10, 143.71, 134.41, 132.76, 131.34, 126.15, 123.98, 123.32, 122.89, 122.79, 122.16, 121.86, 120.74, 120.45, 120.16, 119.78, 119.58, 119.35, 119.08, 55.45, 53.90, 53.76, 51.45, 51.28, 51.17, 50.88, 32.05, 29.82, 29.41, 29.38, 29.32, 26.78, 26.44, 26.39, 26.26, 25.73, 24.75, 24.70, 24.12, 22.81 and 14.24 ppm

MALDI-TOF m/z [M^-] calc. for $C_{51}H_{57}N_5O_4$: 803.4405, found: 803.4458

IR (KBr): 2927, 2852, 1687, 1650, 1581, 1450, 1440, 1413, 1334, 1305, 1259, 1022 and 804 cm^{-1}

UV-vis ($CHCl_3$) λ_{max}/nm (log ε): 577 (4.0) and 706 (4.4)

PDI 7



From **1f**[1]

Eluent: Dichloromethane. Yield: 65 %

^{1}H NMR ($CDCl_3$) δ 1.30 (m, 6H), 1.48 (br, 7H), 1.76 (br, 10H), 1.91 (br, 7H), 2.09 (m, 4H), 2.24 (s, 3H), 2.41 (m, 1H), 2.61 (m, 5H), 2.81 (br, 1H), 3.21 (m, 2H), 3.54 (m, 1H), 3.66 (m, 2H), 4.17 (m, 2H), 5.09 (m, 2H), 8.36 (s, 1H), 8.38 (s, 1H), 8.44 (d, *J* = 8.2 Hz, 1H), 8.54 (s, 1H) and 9.82 ppm (d, *J* = 8.2, 1H)

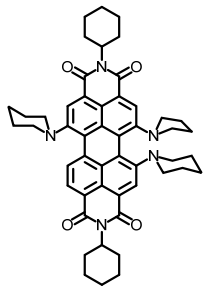
^{13}C NMR ($CDCl_3$) δ 165.27, 165.21, 164.83, 164.65, 151.78, 144.56, 144.43, 134.29, 132.74, 131.44, 126.13, 124.05, 123.47, 122.77, 122.74, 122.18, 121.33, 121.17, 121.09, 120.69, 120.38, 119.96, 119.38, 118.43, 63.48, 55.41, 54.81, 53.94, 53.83, 53.11, 51.41, 51.24, 49.99, 49.62, 46.07, 34.62, 34.20, 32.06, 29.84, 29.40, 29.33, 26.78, 26.48, 26.37, 26.26, 25.72, 24.67, 24.09, 22.82 and 14.25 ppm

MALDI-TOF m/z [M^-] calc. for $C_{51}H_{58}N_6O_4$: 818.4514, found: 818.4533

IR (KBr): 2927, 2852, 2796, 1687, 1651, 1581, 1556, 1450, 1414, 1371, 1334, 1306, 1259, 1198, 1090, 1022 and 804 cm^{-1}

UV-vis ($CHCl_3$) λ_{max}/nm (log ε): 565 (4.0) and 703 (4.3)

PDI 8



From **1f**[1]

Eluent: Toluene:Dichloromethane (1:1). Yield: 40 %

^{1}H NMR ($CDCl_3$) δ 1.04-1.56 (br, 15H), 1.70-2.16 (br, 20H), 2.24 (m, 1H), 2.40 (m, 1H), 2.63 (m, 4H), 3.22 (m, 2H), 3.57 (m, 3H), 4.00 (m, 2H), 5.10 (m, 2H), 8.34 (s, 1H), 8.39 (s, 1H), 8.51 (d, *J* = 8.4, 1H), 8.55 (s, 1H) and 9.88 ppm (d, *J* = 8.4 Hz, 1H)

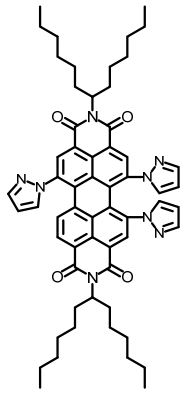
^{13}C NMR ($CDCl_3$) δ 165.47, 165.26, 165.09, 164.69, 152.59, 144.91, 144.67, 134.70, 131.81, 131.46, 126.92, 123.98, 123.53, 123.49, 123.42, 123.05, 122.57, 121.06, 119.93, 119.58, 118.67, 118.61, 118.41, 115.49, 55.52, 53.94, 53.74, 52.18, 51.48, 50.25, 29.51, 29.37, 29.27, 26.80, 26.43, 26.27, 25.75, 25.61, 24.30 and 24.14 ppm

MALDI-TOF m/z [M^-] calc. for $C_{50}H_{55}N_5O_4$: 789.4248, found: 789.4218

IR (KBr): 2927, 2852, 2804, 1687, 1651, 1581, 1556, 1539, 1510, 1433, 1415, 1396, 1377, 1331, 1300, 1257, 1225, 1198, 1151, 1109, 1086, 1034, 985 and 804 cm^{-1}

UV-vis ($CHCl_3$) λ_{max}/nm (log ε): 555 (4.1) and 703 (4.4)

PDI 12



From **11**

Eluent: Chloroform:Ethyl acetate (60:1). Yield: 11 %

^{1}H NMR ($CDCl_3$) δ 0.83 (br, 12H), 1.25 (br, 32H), 1.83 (m, 4H), 2.22 (m, 4H), 5.15 (m, 2H), 6.33 (m, 2H), 6.63 (m, 1H), 6.76 (d, *J* = 8.1 Hz, 1H), 7.19 (d, *J* =2.3, 1H), 7.24 (d, *J* = 2.6 Hz, 1H), 7.50 (m, 2H), 7.66 (d, *J* = 2.3 Hz, 1H), 7.89 (m, 1H), 8.22-8.47 (br, 3H) and 8.71 ppm (m, 1H)

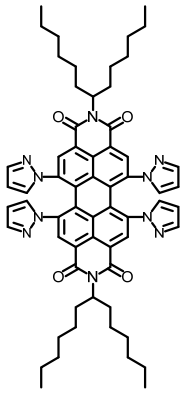
^{13}C NMR (CD_2Cl_2) δ 163.20, 143.15, 142.95, 142.89, 142.57, 139.81, 139.29, 138.83, 138.56, 137.87, 132.20, 130.90, 130.47, 129.11, 128.17, 127.06, 126.86, 124.76, 117.42, 113.99, 110.01, 109.70, 32.92, 32.35, 30.26, 29.79, 27.43, 23.18 and 14.38 ppm

MALDI-TOF m/z [M^-] calc. for $C_{59}H_{68}N_8O_4$: 952.5358, found: 952.5344

IR (KBr): 2954, 2924, 2854, 1703, 1662, 1603, 1522, 1456, 1400, 1319, 1261, 1180, 1084, 1041, 810 and 754 cm^{-1}

UV-vis ($CHCl_3$) λ_{max}/nm (log ε): 429 (4.1), 535 (4.4), 564 (4.4) and 675 (sh, 3.6)

PDI 13



From **11** as a by-product in the synthesis of **PDI 12**

Eluent: Chloroform:Ethyl acetate (60:1). Yield: 1 %

^{1}H NMR (CD_2Cl_2) δ 0.85 (t, *J* = 6.8 Hz, 12H), 1.26 (br, 32H), 1.85 (m, 4H), 2.23 (m, 4H), 5.18 (m, 2H), 6.31 (dd, *J* = 2.5 Hz, *J* = 1.6 Hz, 4H), 7.26 (d, *J* = 2.5 Hz, 4H), 7.45 (d, *J* = 1.6 Hz, 4H) and 8.40 ppm (s, 4H)

^{13}C NMR (CD_2Cl_2) δ 164.48, 163.41, 150.28, 142.89, 139.64, 132.42, 131.50, 130.75, 129.34, 127.58, 126.94, 125.43, 124.55, 109.63, 32.98, 32.90, 32.35, 32.32, 30.26, 29.83, 29.80, 27.46, 23.20 and 14.39 ppm

MALDI-TOF m/z [M^-] calc. for $C_{62}H_{70}N_{10}O_4$: 1018.5576, found: 1018.5575

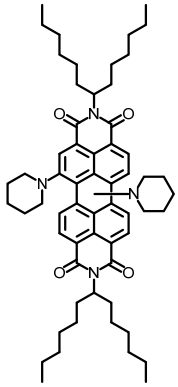
IR (KBr): 3147, 3128, 3103, 2952, 2925, 2856, 1699, 1660, 1595, 1525, 1456, 1421, 1396, 1360, 1321, 1304, 1269, 1236, 1186, 1119, 1078, 1041, 930, 756 and 746 cm^{-1}

UV-vis ($CHCl_3$) λ_{max}/nm (log ε): 457 (4.2), 550 (4.2) and 591 (4.3)

General Procedure for the Synthesis of Molecules 1a-d.

A 25 mL round-bottomed flask was charged with 0.55 mmol of dibromoperylenediimide **9a**[2] or **9b**[3] (as mixture of 1,6 and 1,7 regioisomers) and 0.20 mol of the amine (piperidine or morfoline). The reaction was heated at 60 ^{o}C for 48 h under argon atmosphere. After cooling, 150 mL of dichloromethane were added and the organic phase was washed with HCl 2 M three times. The organic phase was dried over anhydrous sodium sulfate, filtered and evaporated. The solid was purified by column chromatography on silica gel.

PDI 1a



From *N*,*N'*-di(hexylheptyl)-1,7(6)-dibromoperylenediimide **9a**[2]

Eluent: Dichloromethane:Hexane (1:1). Yield: 86 % (80 % 1,7 isomer; 20% 1,6 isomer)

^{1}H NMR ($CDCl_3$) δ 0.83 (t, *J* = 6.6 Hz, 12H), 1.23 (m, 32H), 1.46 (br, 2H), 1.82 (m, 14H), 2.27 (m, 4H), 2.96 (m, 4H), 3.39 (m, 1H), 3.53 (m, 3H), 5.19 (m, 2H), 8.49 (m, 4H), 9.67 (1,7 isomer; d, *J* = 8.4 Hz, 2H) and 9.74 ppm (1,6 isomer; d, *J* = 8.2 Hz, 2H)

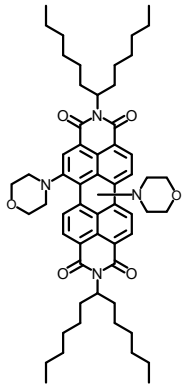
^{13}C NMR ($CDCl_3$) δ 165.11, 164.86, 164.06, 163.87, 153.33, 151.00, 135.75, 131.71, 131.20, 130.23, 128.90, 128.11, 128.01, 124.81, 124.53, 123.86, 123.77, 123.38, 122.45, 120.93, 54.50, 53.14, 52.93, 32.47, 31.78, 29.26, 27.00, 26.93, 25.80, 23.83, 22.59 and 14.05 ppm

MALDI-TOF m/z [M^-] calc. for $C_{60}H_{80}N_4O_4$: 920.6174, found: 920.6197

IR (KBr): 2925, 2854, 2814, 1693, 1655, 1595, 1583, 1512, 1452, 1412, 1377, 1338, 1325, 1250, 1207, 1111, 1082, 926 and 810 cm^{-1}

UV-vis ($CHCl_3$) λ_{max}/nm (log ε): 413 (4.1), 435 (4.2) and 676 (4.4)

PDI 1b



From *N*,*N'*-di(hexylheptyl)-1,7(6)-dibromoperylenediimide **9a**[2]

Eluent: Dichloromethane:Ethyl Acetate (100:1). Yield: 68 % (71 % 1,7 isomer; 29 % 1,6 isomer)

^{1}H NMR ($CDCl_3$) δ 0.83 (t, *J* = 6.7 Hz, 12H), 1.28 (m, 32H), 1.85 (m, 4H), 2.25 (m, 4H), 3.15 (m, 4H), 3.30 (m, 1H), 3.46 (m, 3H), 3.94 (m, 8H), 5.18 (m, 2H), 8.46 (br, 3H), 8.59 (br, 1H), 9.83 (1,7 isomer; d, *J* = 8.3 Hz, 2H) and 9.89 ppm (1,6 isomer; d, *J* = 8.3 Hz, 2H)

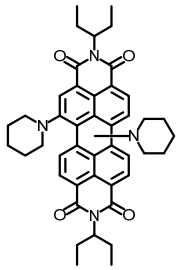
^{13}C NMR ($CDCl_3$) δ 164.90, 164.62, 163.78, 163.55, 152.06, 150.08, 135.24, 131.75, 130.28, 129.13, 128.95, 128.39, 128.25, 125.19, 124.39, 123.90, 123.58, 122.92, 121.82, 66.61, 66.53, 54.87, 54.67, 51.73, 51.55, 32.43, 31.77, 31.76, 29.26, 29.23, 29.20, 26.98, 26.92, 22.60, 22.59 and 14.05 ppm

MALDI-TOF m/z [M^-] calc. for $C_{58}H_{76}N_4O_6$: 924.5759, found: 924.5761

IR (KBr): 2954, 2925, 2854, 1693, 1655, 1595, 1585, 1562, 1512, 1460, 1414, 1363, 1334, 1325, 1252, 1205, 1198, 1120, 931 and 810 cm^{-1}

UV-vis ($CHCl_3$) λ_{max}/nm (log ε): 404 (4.1), 426 (4.2) and 646 (4.5)

PDI 1c



From *N*,*N'*-di(ethylpropyl)-1,7(6)-dibromoperylenediimide **9b**[3]

Eluent: Dichloromethane:Ethyl acetate (100:1). Yield: 79 % (90 % 1,7 isomer; 10 % 1,6 isomer)

^{1}H NMR ($CDCl_3$) δ 0.93 (t, *J* = 7.5 Hz, 12H), 1.46 (br, 2 H), 1.88 (m, 14H), 2.27 (m, 4H), 2.95 (m, 4H), 3.53 (m, 4H), 5.08 (m, 2H), 8.42 (d, *J* = 8.3 Hz, 2H), 8.50 (s, 2H), 9.67 (1,7 isomer; d, *J* = 8.3 Hz, 2H) and 9.74 ppm (1,6 isomer; d, *J* = 8.4 Hz, 2H)

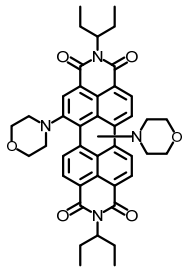
^{13}C NMR ($CDCl_3$) δ 165.01, 164.70, 164.55, 164.50, 153.49, 151.16, 135.90, 130.38, 128.70, 124.98, 123.55, 123.49, 122.99, 57.56, 53.07, 25.94, 25.25, 23.98, 11.58 and 11.49 ppm

MALDI-TOF m/z [M^-] calc. for $C_{44}H_{48}N_4O_4$: 696.3670, found: 696.3628

IR (KBr): 2960, 2931, 2873, 2856, 2806, 1695, 1657, 1597, 1585, 1562, 1512, 1458, 1412, 1390, 1381, 1342, 1325, 1250, 1227, 1205, 1163, 1138, 1111, 1074, 1034, 1012, 987, 933, 906, 879 and 812 cm^{-1}

UV-vis ($CHCl_3$) λ_{max}/nm (log ε): 415 (sh, 4.0), 435 (4.1) and 679 (4.2)

PDI 1d



From *N*,*N'*-di(ethylpropyl)-1,7(6)-dibromoperylenediimide **9b**[3]

Eluent: Dichloromethane:Ethyl acetate (9:1). Yield: 55 % (77 % 1,7 isomer; 23 % 1,6 isomer)

^{1}H NMR ($CDCl_3$) δ 0.92 (t, *J* = 7.5 Hz, 12H), 1.93 (m, 4H), 2.27 (m, 4H), 3.14 (m, 4H), 3.28 (m, 1H), 3.46 (m, 3H), 3.93 (m, 8H), 5.07 (m, 2H), 8.39-8.61 (m, 4H), 9.84 (1,7 isomer; d, *J* = 8.3 Hz, 2H) and 9.90 ppm (1,6 isomer; d, *J* = 8.4 Hz, 2H)

^{13}C NMR ($CDCl_3$) δ 164.55, 152.24, 150.25, 135.42, 130.45, 125.37, 124.55, 124.09, 123.88, 123.76, 66.76, 66.69, 57.75, 51.89, 51.71, 25.22, 11.56 and 11.48 ppm

MALDI-TOF m/z [M^-] calc. for $C_{42}H_{44}N_4O_6$: 700.3255, found: 700.3222

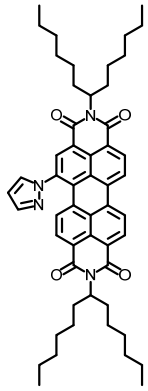
IR (KBr): 2964, 2933, 2875, 2854, 1693, 1655, 1595, 1585, 1512, 1460, 1414, 1363, 1334, 1325, 1254, 1203, 1120, 1078, 1026, 935 and 810 cm^{-1}

UV-vis ($CHCl_3$) λ_{max}/nm (log ε): 404 (4.9), 426 (5.1) and 647 (5.4)

General Procedure for the Synthesis of Molecules 10-11.[4]

9a (274 mg, 0.3 mmol) was added to a stirred mixture of pyrazole (204 mg, 3 mmol), anhydrous potassium carbonate (83 mg, 0.6 mmol), and 18-crown-6 (158 mg, 0.6 mmol) in toluene (75 mL) at room temperature. The reaction mixture was heated at reflux under nitrogen with stirring for 19 h. After the system had cooled to room temperature, the solvent was removed under reduced pressure and the solid was purified by column chromatography on silica gel with chloroform:ethyl acetate (100:1) to give **11** (231 mg, 87%) and **10** (12 mg, 5%).

PDI 10



^{1}H NMR ($CDCl_3$) δ 0.83 (m, 12H), 1.26 (m, 32H), 1.86 (m, 4H), 2.23 (m, 4H), 5.19 (m, 2H), 6.60 (d, *J* = 8.3 Hz, 1H), 6.70 (dd, *J* = 2.3 Hz, *J* = 1.5 Hz, 1H), 7.74 (d, *J* = 2.3 Hz, 1H), 7.94 (d, *J* = 1.5 Hz, 1H), 8.29 (br, 1H) and 8.70 ppm (m, 5H)

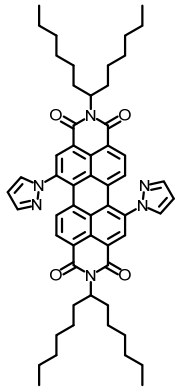
^{13}C NMR ($CDCl_3$) δ 164.67, 164.19, 163.69, 163.49, 143.05, 137.83, 135.37, 133.93, 132.15, 131.61, 130.85, 129.73, 129.16, 129.05, 128.33, 128.01, 127.23, 124.08, 123.32, 109.90, 55.12, 54.90, 39.03, 33.38, 32.49, 32.08, 31.90, 30.32, 30.19, 29.86, 29.52, 29.35, 27.03, 26.91, 22.85, 22.73, 14.27 and 14.19 ppm

MALDI-TOF m/z [M^-] calc. for $C_{53}H_{64}N_4O_4$: 820.4922, found: 820.4942

IR (KBr): 2956, 2925, 2854, 1699, 1657, 1595, 1458, 1422, 1404, 1335, 1261, 1178, 1110, 1041, 812 and 750 cm^{-1}

UV-vis ($CHCl_3$) λ_{max}/nm (log ε): 461 (sh 4.0), 492 (4.4) and 527 (4.6)

PDI 11



^{1}H NMR ($CDCl_3$) δ 0.83 (t, *J* = 6.8 Hz, 12H), 1.25 (m, 32H), 1.82 (m, 4H), 2.23 (m, 4H), 5.15 (m, 2H), 6.67 (m, 2H), 6.75 (d, *J* = 8.2, 2H), 7.74 (m, 2H), 7.90 (m, 2H), 8.32 (br, 2H) and 8.69 ppm (br, 2H)

^{13}C NMR ($CDCl_3$) δ 164.31, 163.96, 163.21, 162.78, 143.14, 143.03, 138.48, 137.78, 132.91, 131.14, 130.86, 130.54, 130.03, 129.93, 129.55, 129.06, 128.41, 128.23, 128.11, 128.07, 127.92, 127.80, 124.55, 123.51, 122.79, 109.99, 109.90, 55.29, 55.06, 54.86, 32.42, 32.06, 31.87, 31.65, 29.83, 29.32, 26.98, 22.71 and 14.17 ppm

MALDI-TOF m/z [M^-] calc. for $C_{56}H_{66}N_6O_4$: 886.5140, found: 886.5155

IR (KBr): 2954, 2925, 2854, 1699, 1657, 1599, 1591, 1520, 1421, 1402, 1333, 1261, 1244, 1182, 1113, 1080, 1041, 812 and 758 cm^{-1}

UV-vis ($CHCl_3$) λ_{max}/nm (log ε): 394 (3.8), 501 (sh, 4.4) and 536 (4.5)

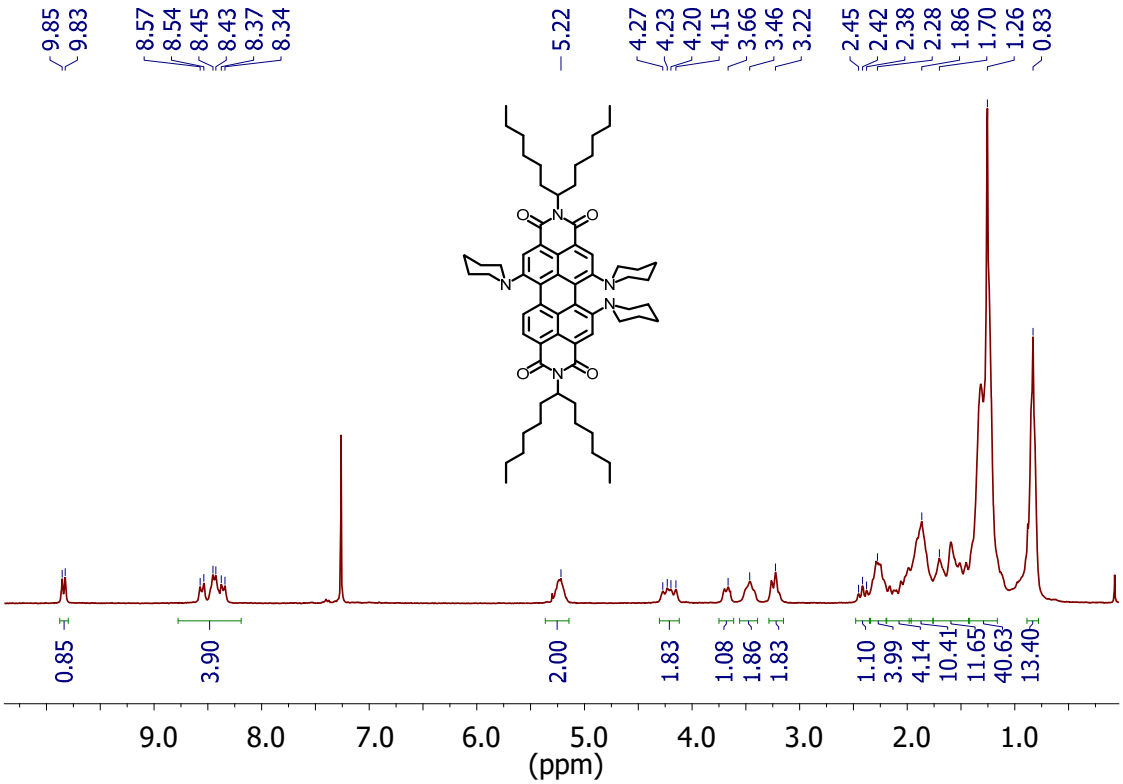
References

1 L. Fan, Y. Xu, H. Tian, *Tetrahedron Lett.* **2005**, *46*, 4443-4447.

2 Q. Yan, D. Zhao, *Org. Lett.* **2009**, *11*, 3426-3429.

3 P. Rajasingh, R. Cohen, E. Shirman, L. J. W. Shimon, B. Rybtchinski, *J. Org. Chem.* **2007**, *72*, 5973-5979.

4 Y. Li, Y. Li, J. Li, C. Li, X. Liu, M. Yuan, H. Liu, S. Wang, *Chem. Eur. J.* **2006**, *12*, 8378-8385.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3.66
3.46
3.22
2.45
2.42
2.38
2.28
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1.70
1.26
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0.85
3.90
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1.08
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1.83
1.10
3.99
4.14
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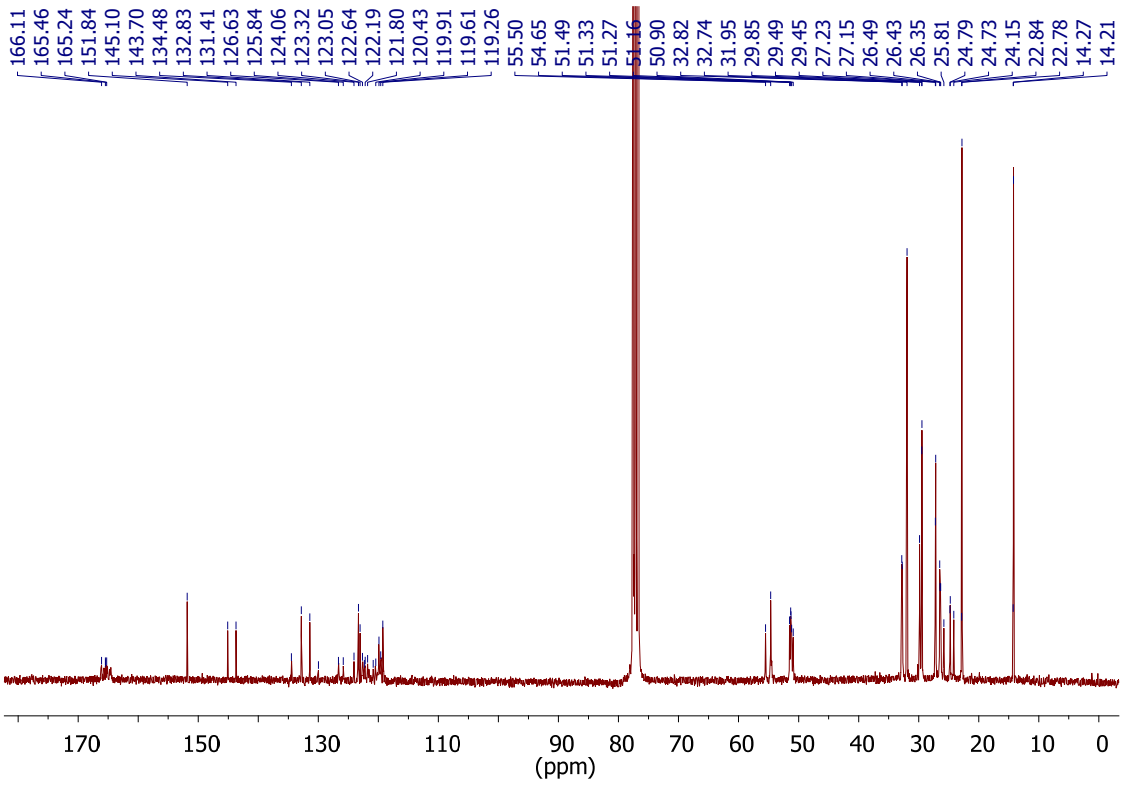
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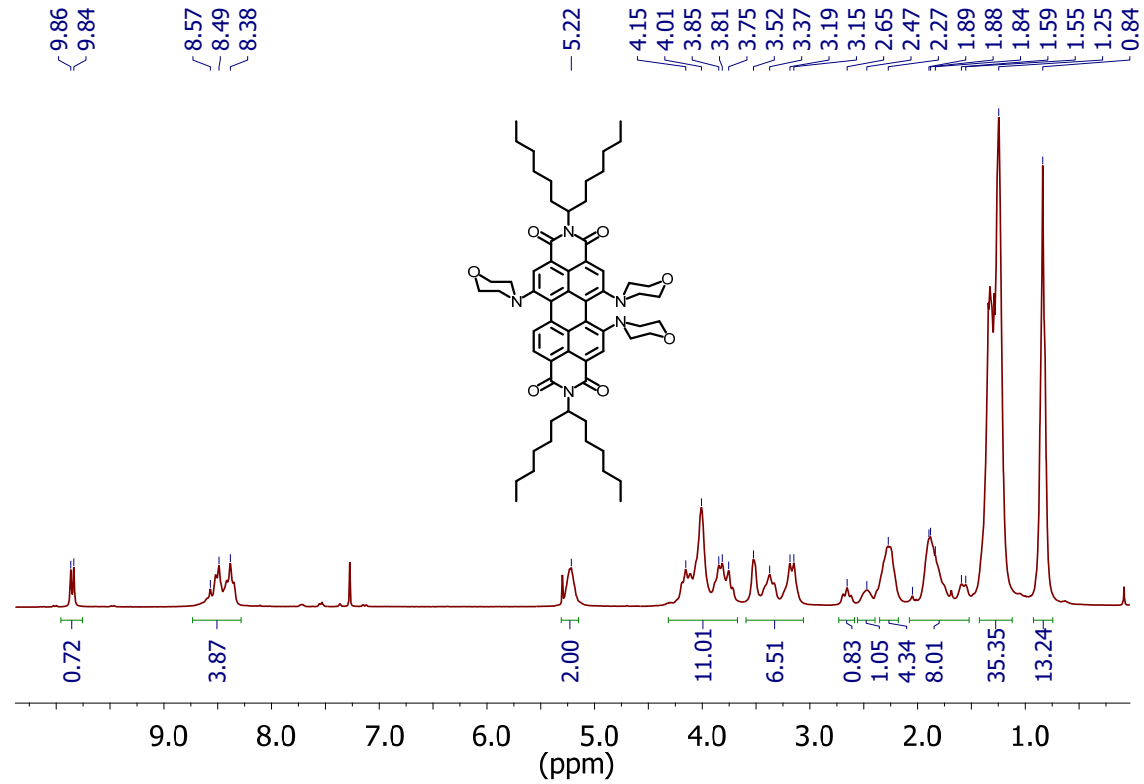
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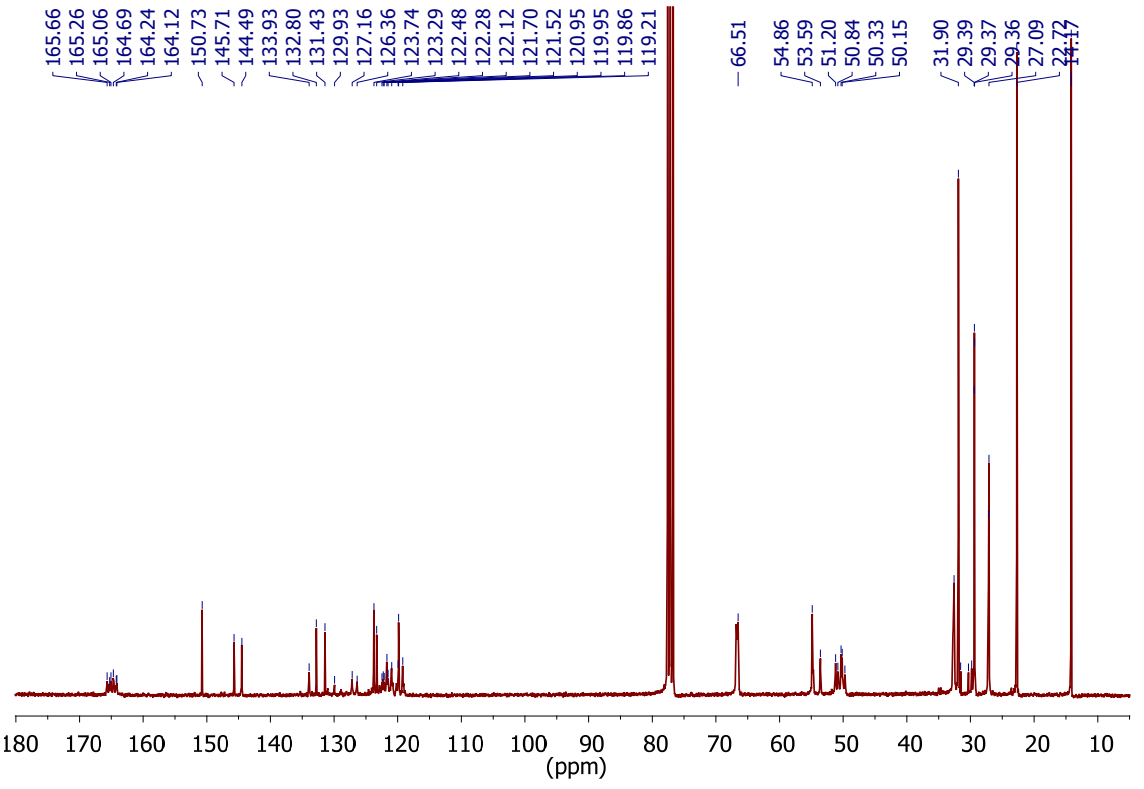
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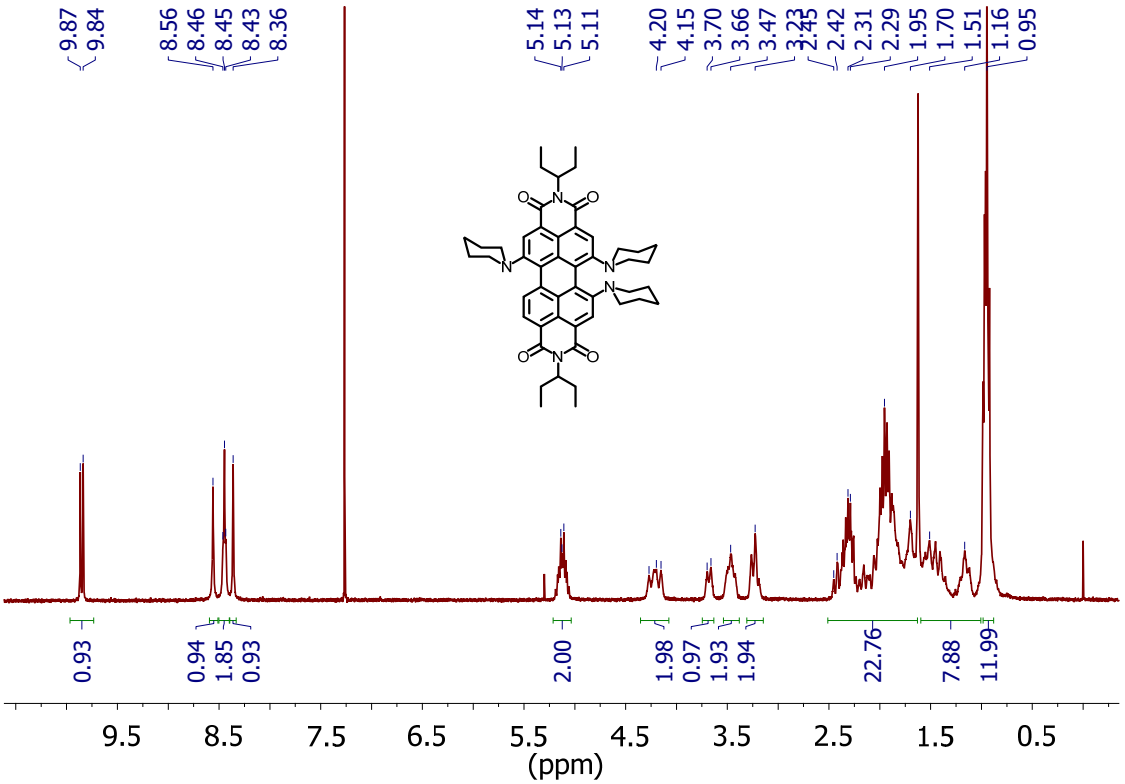
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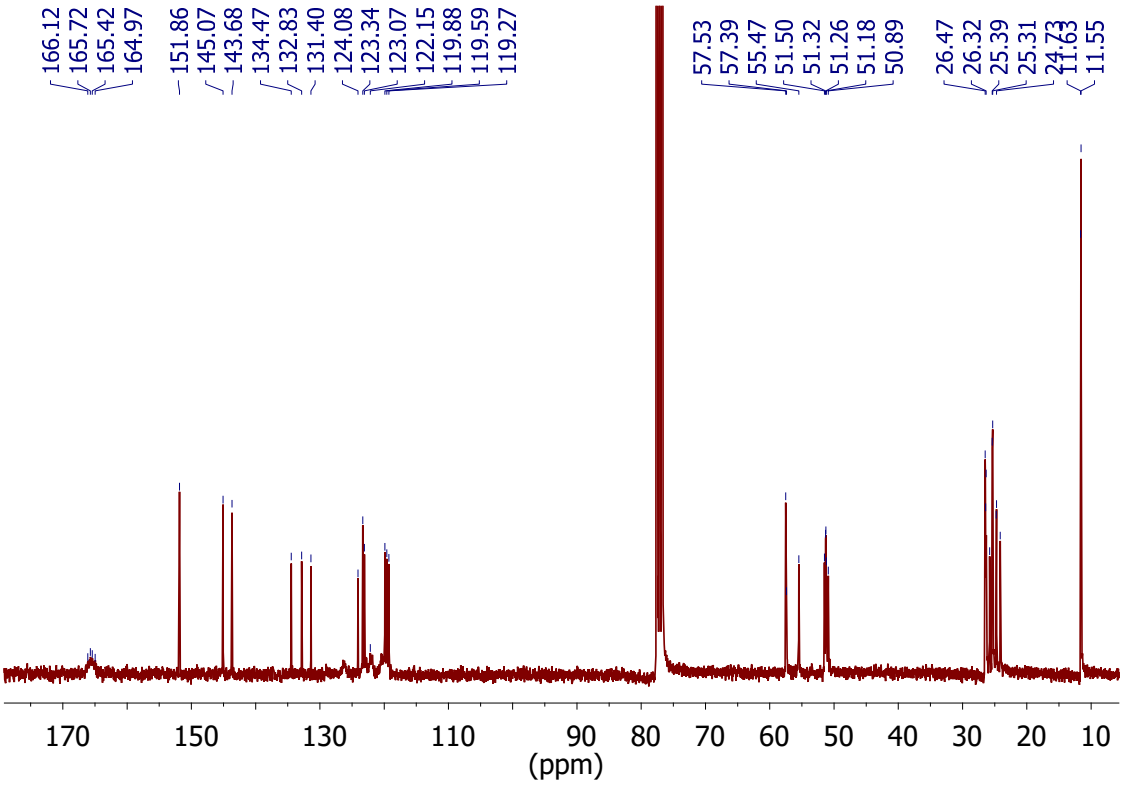
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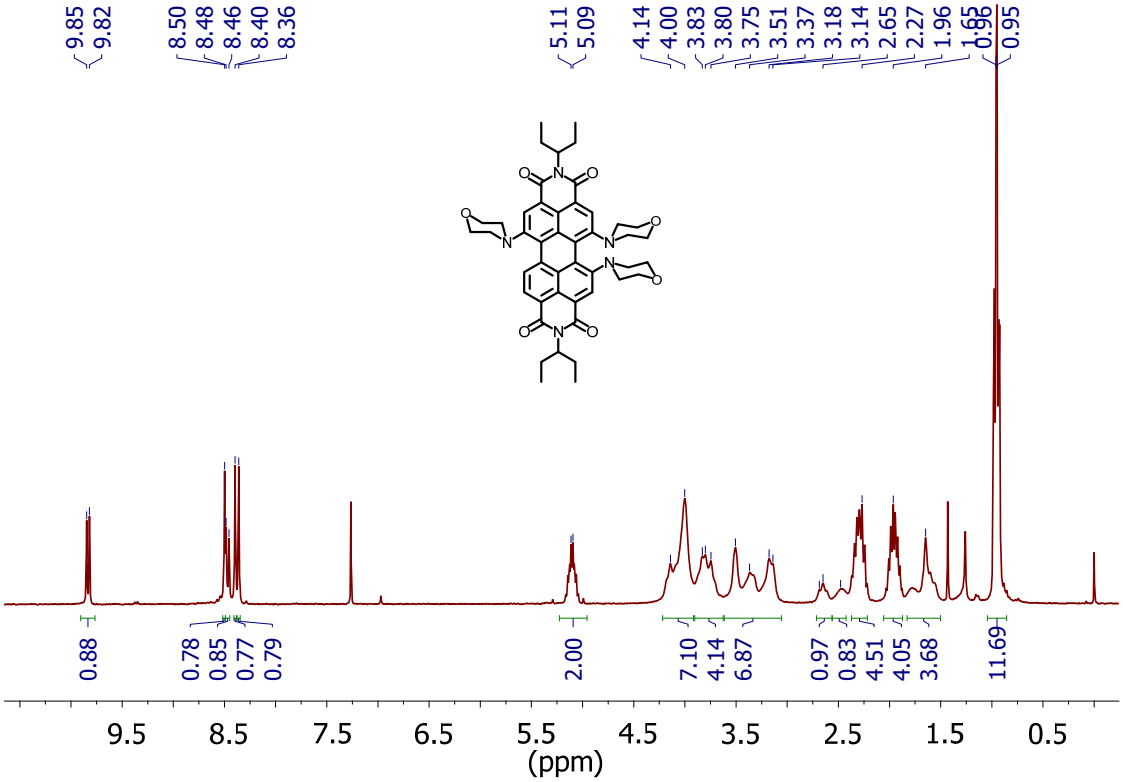
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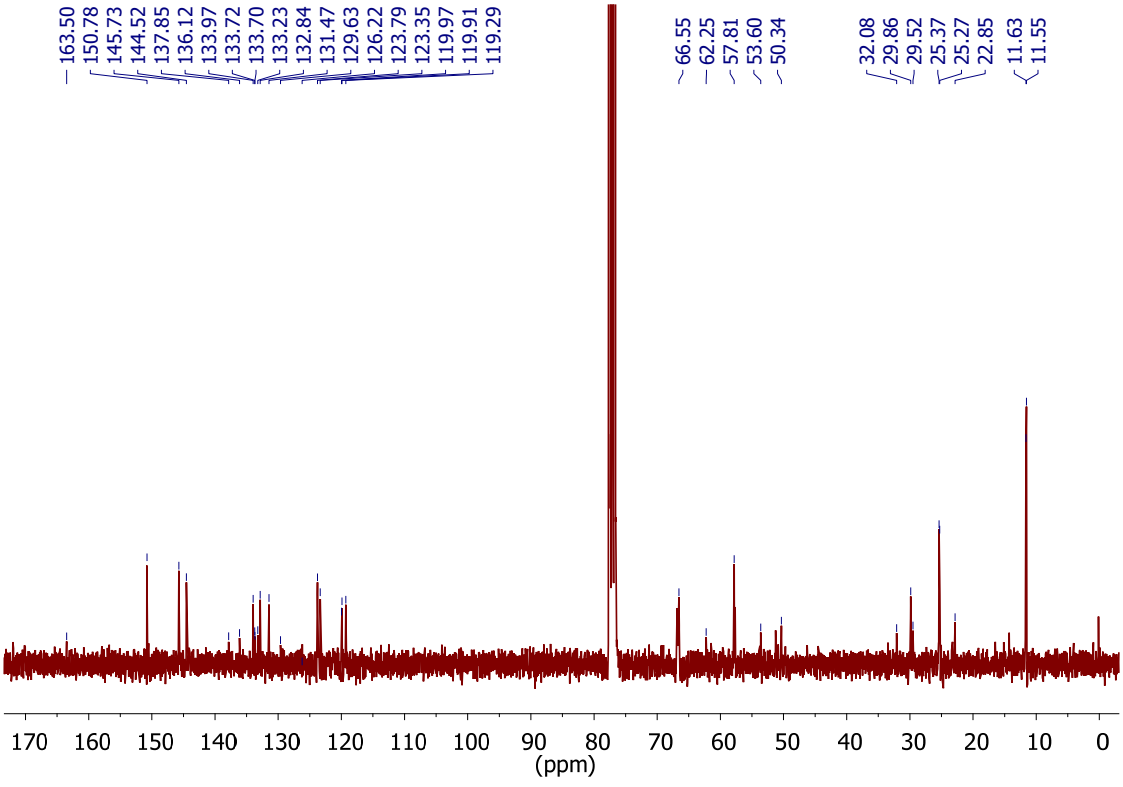
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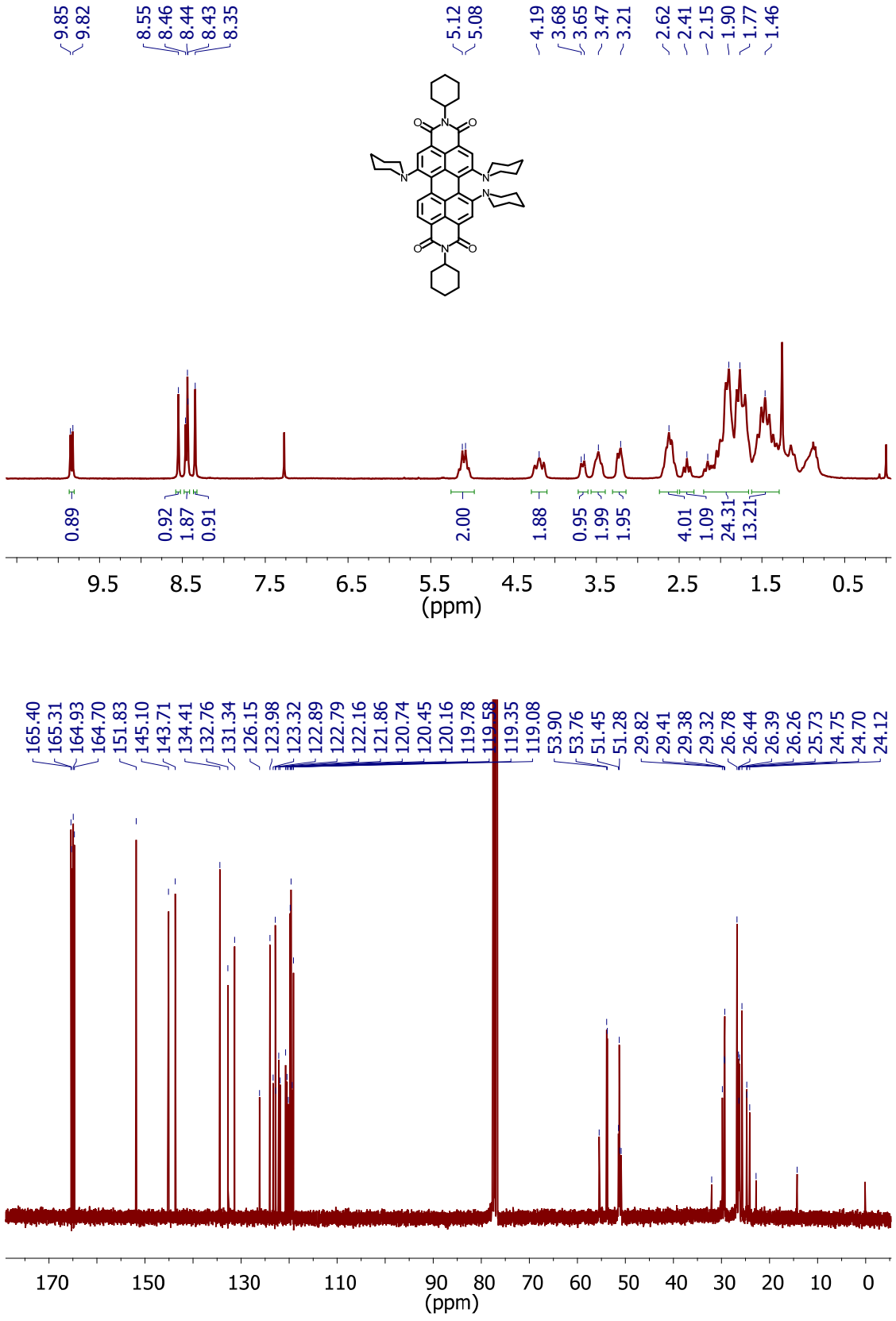
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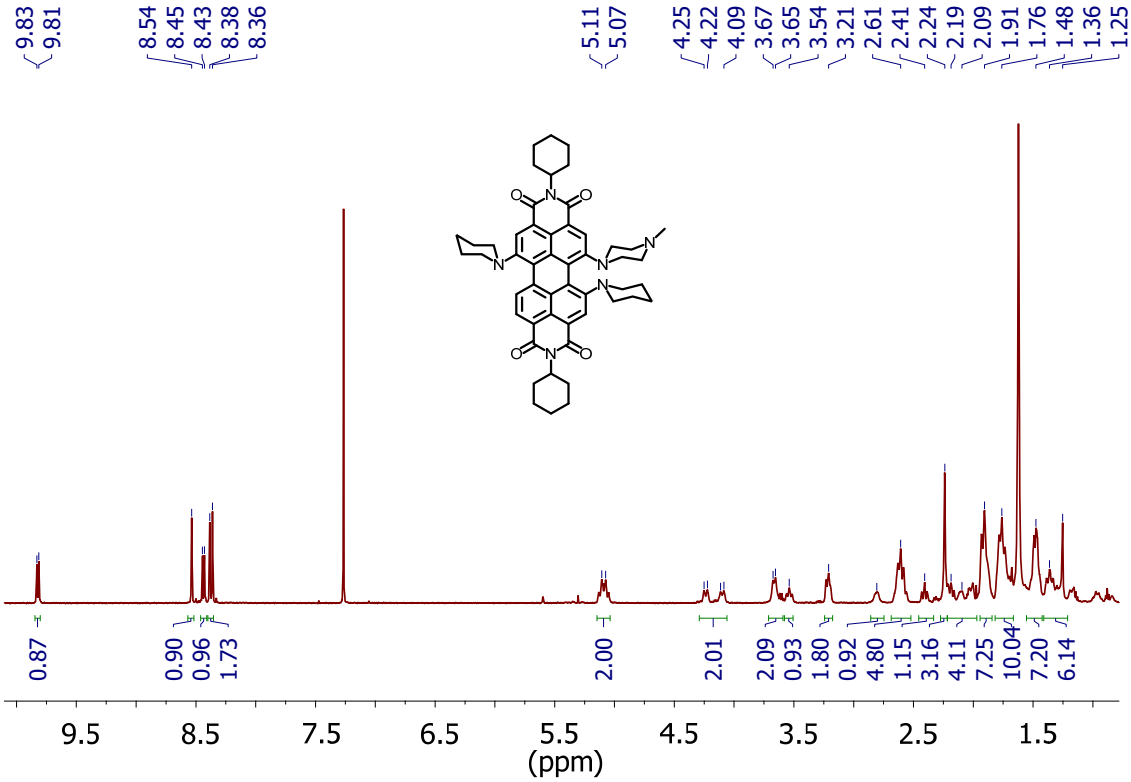
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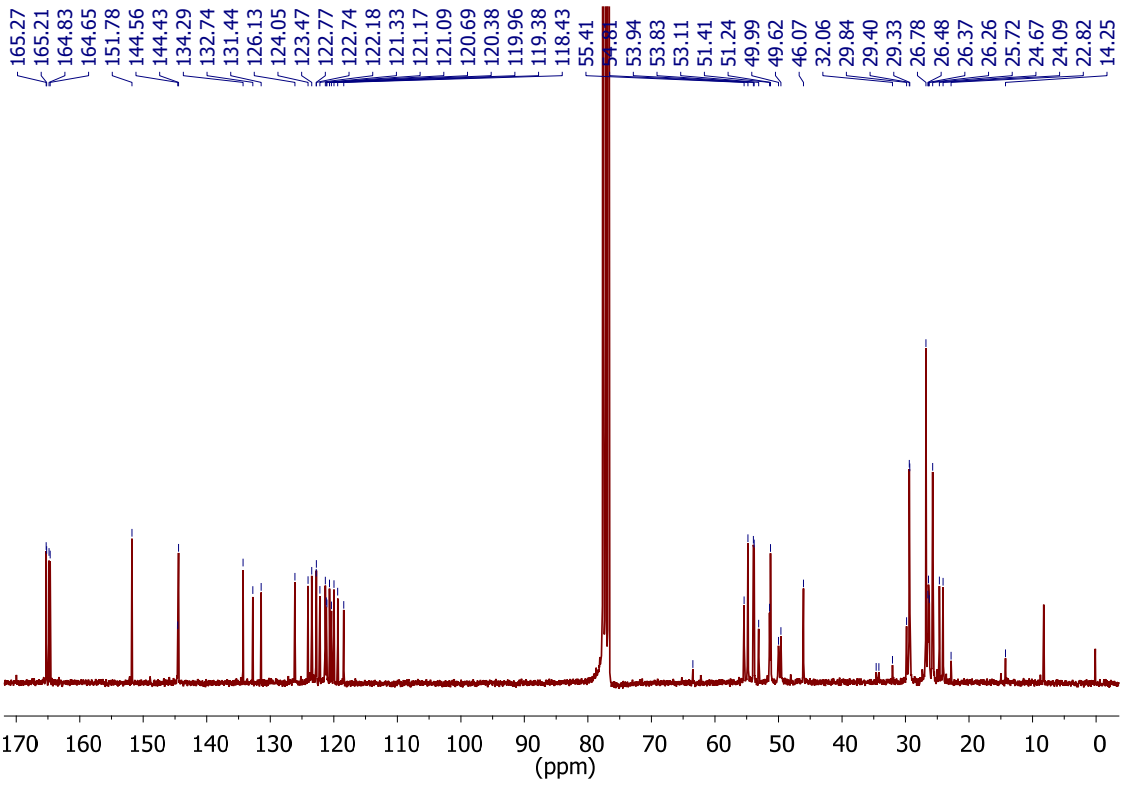
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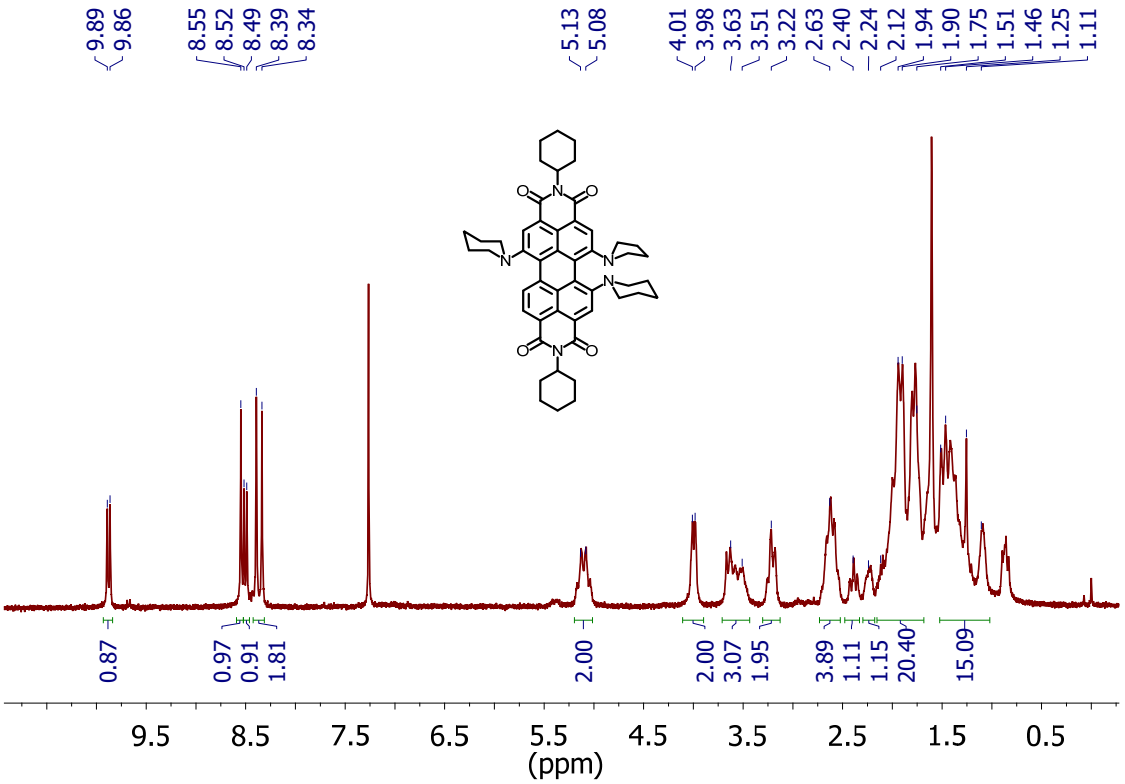
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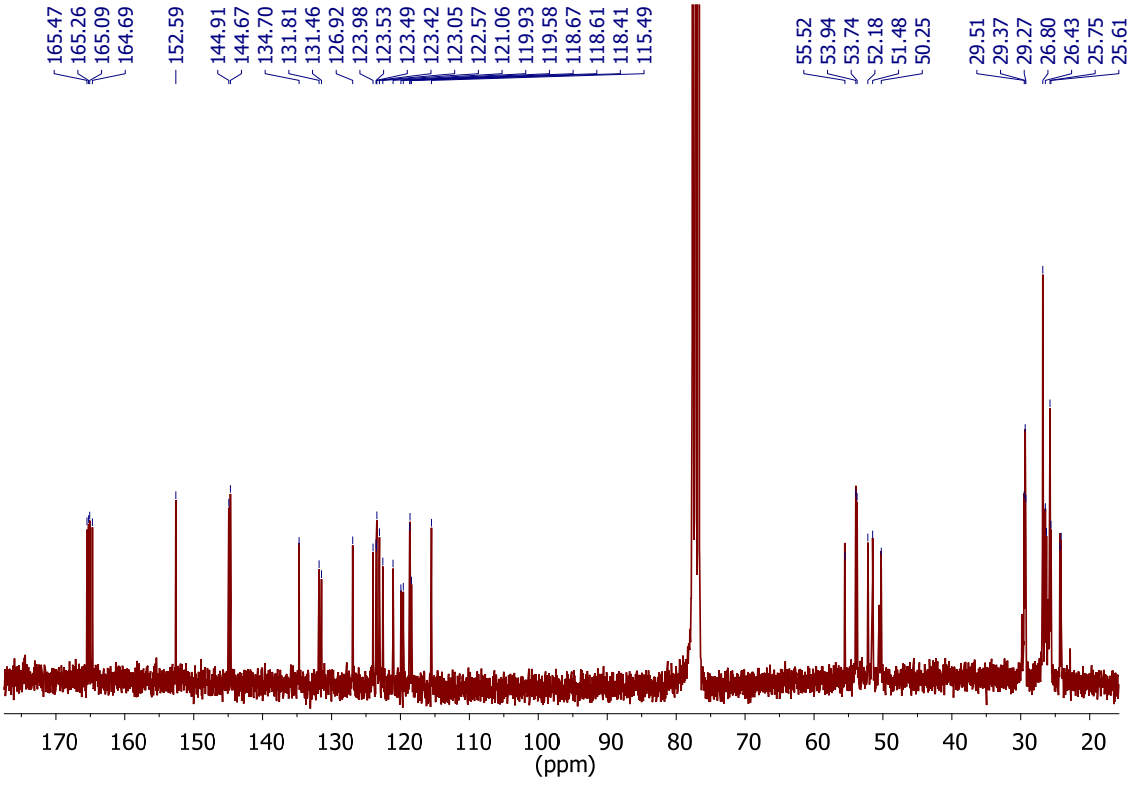
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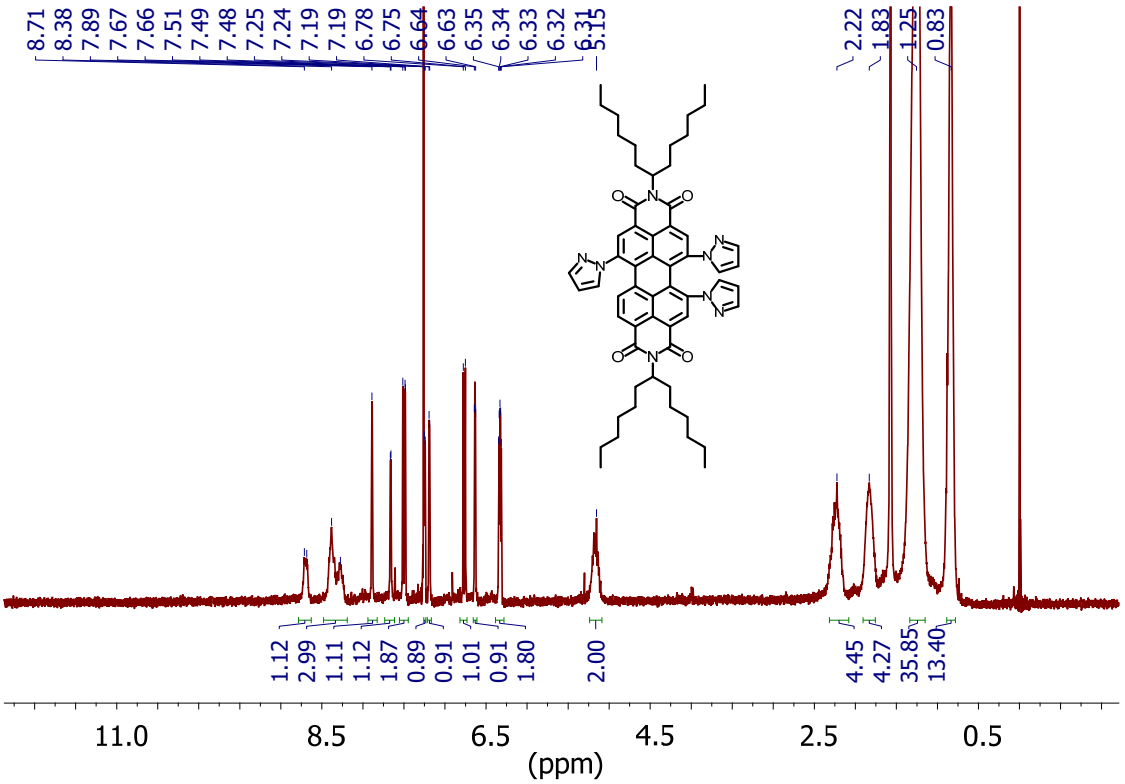
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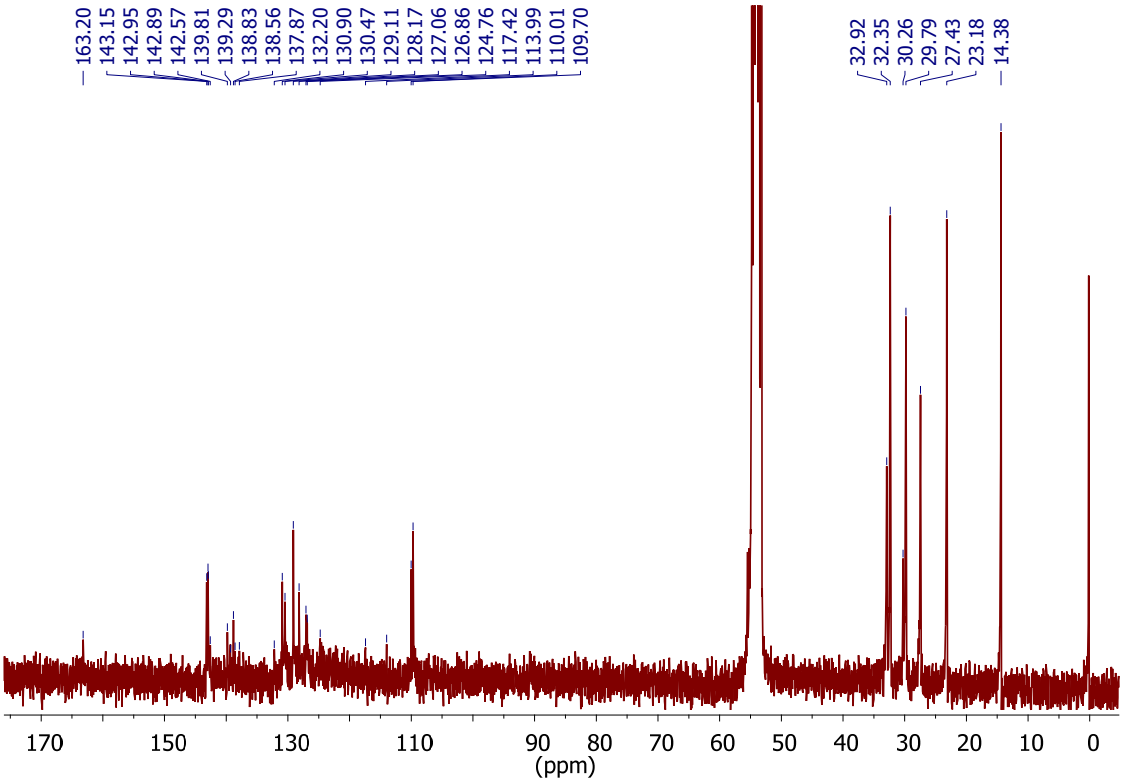
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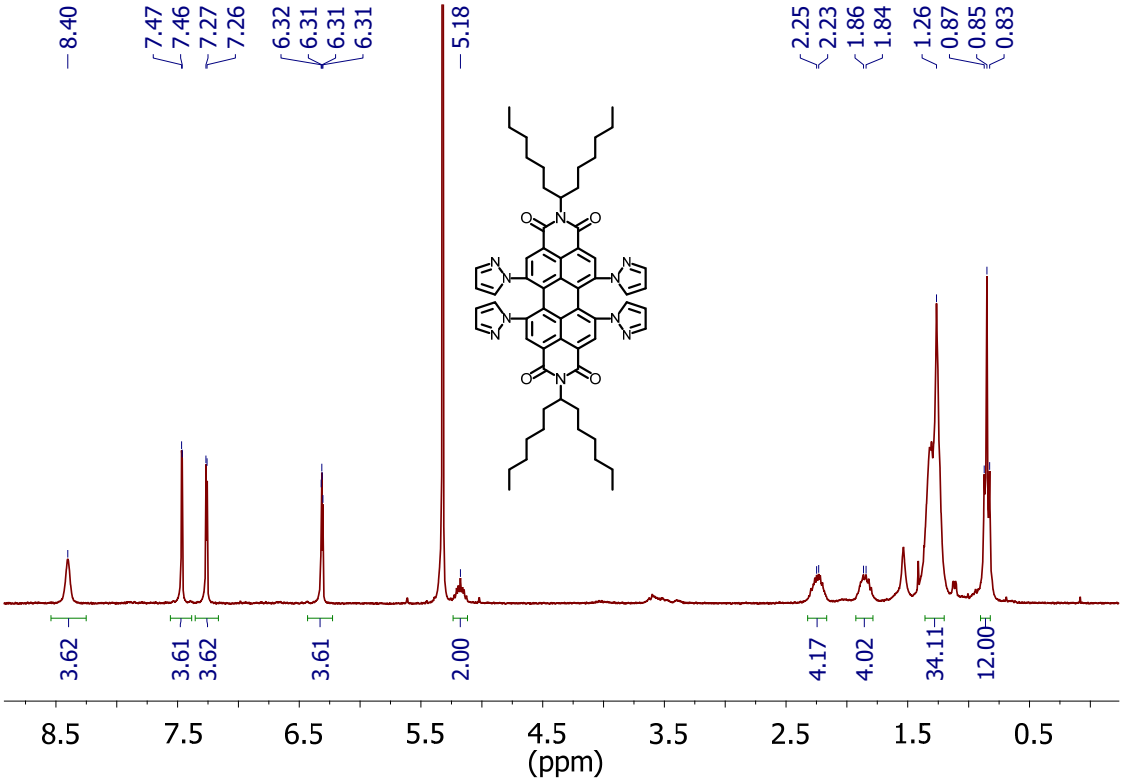
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1.26
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0.83
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3.61
3.62
3.61
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4.17
4.02
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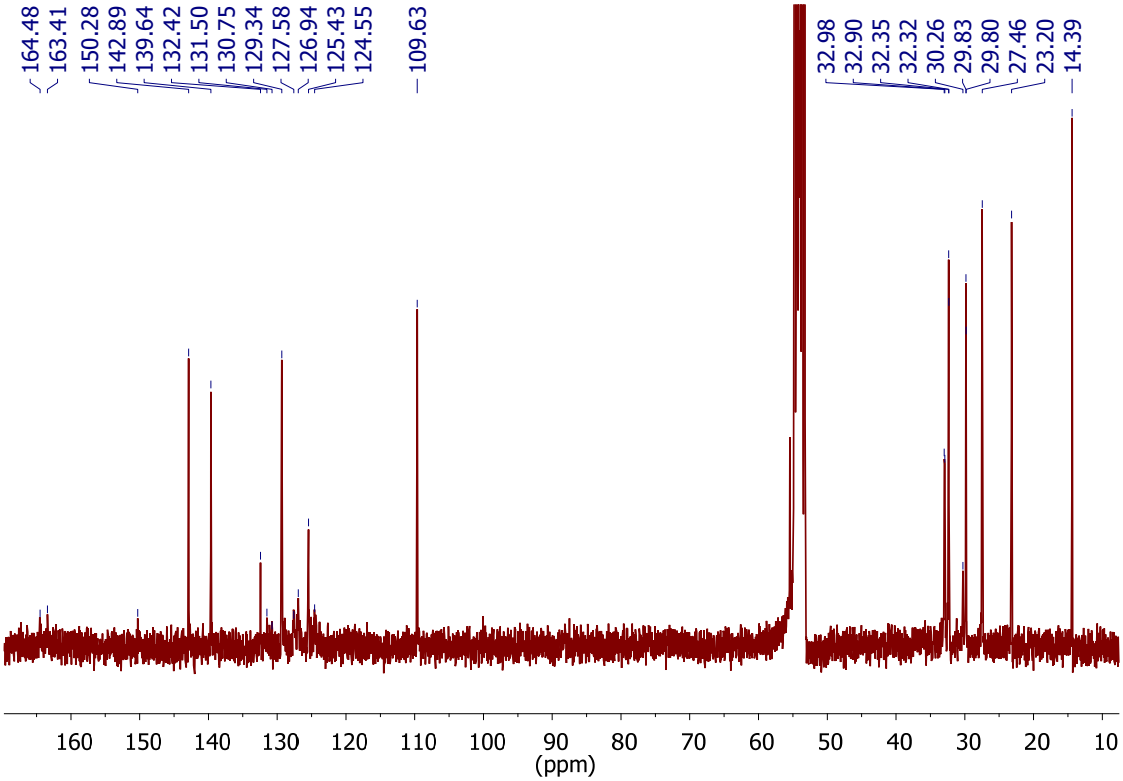
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32.98
32.90
32.35
32.32
30.26
29.83
29.80
27.46
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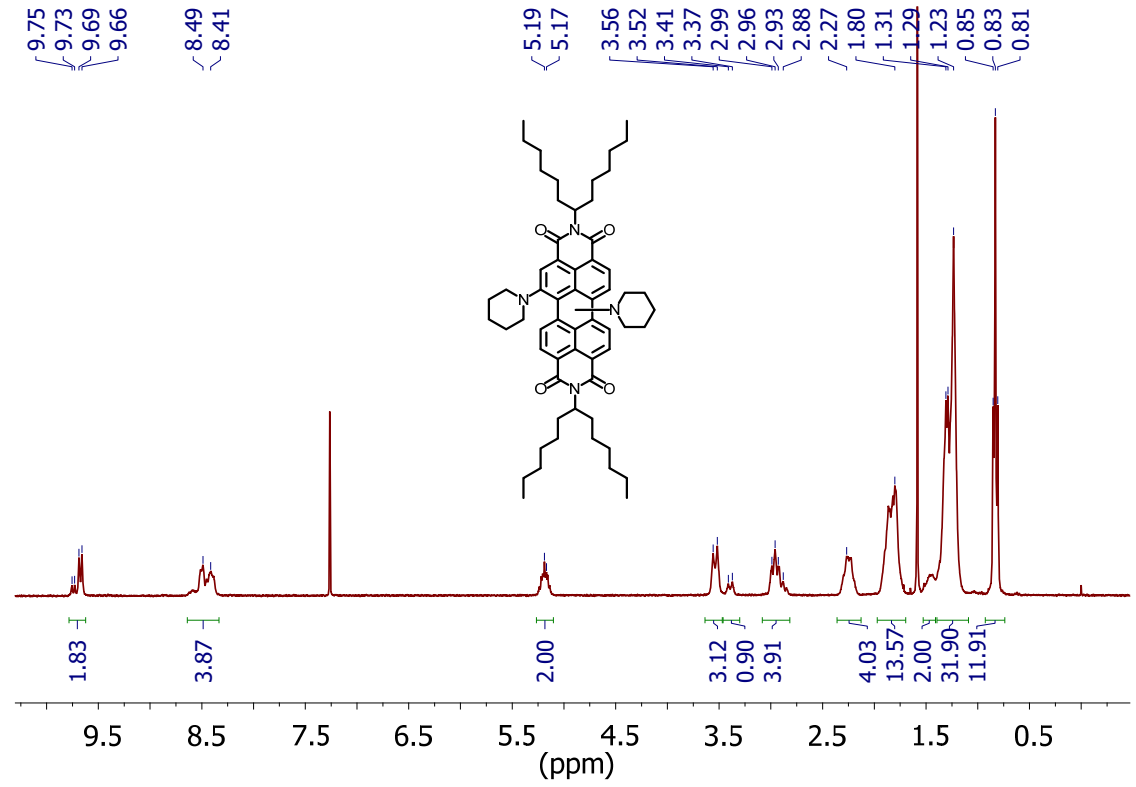
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2.96
2.93
2.88
2.27
1.80
1.31
1.29
1.23
0.85
0.83
0.81
1.83
3.87
2.00
3.12
0.90
3.91
4.03
13.57
2.00
31.90
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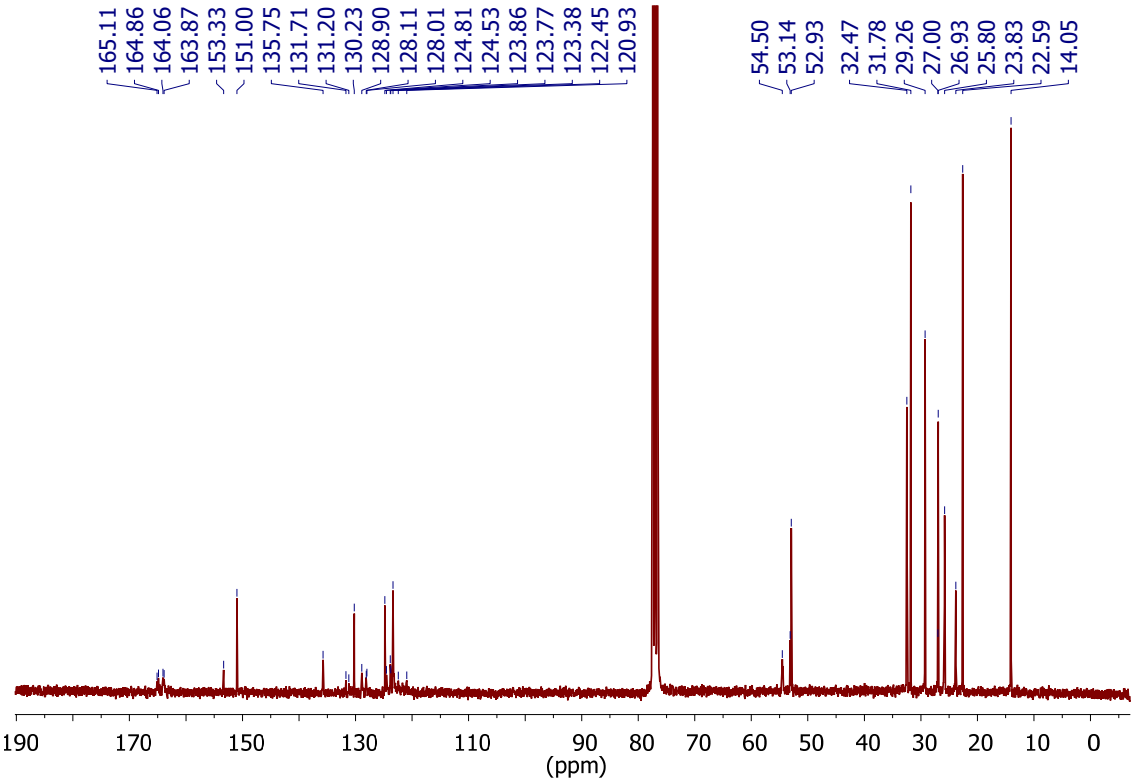
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53.14
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32.47
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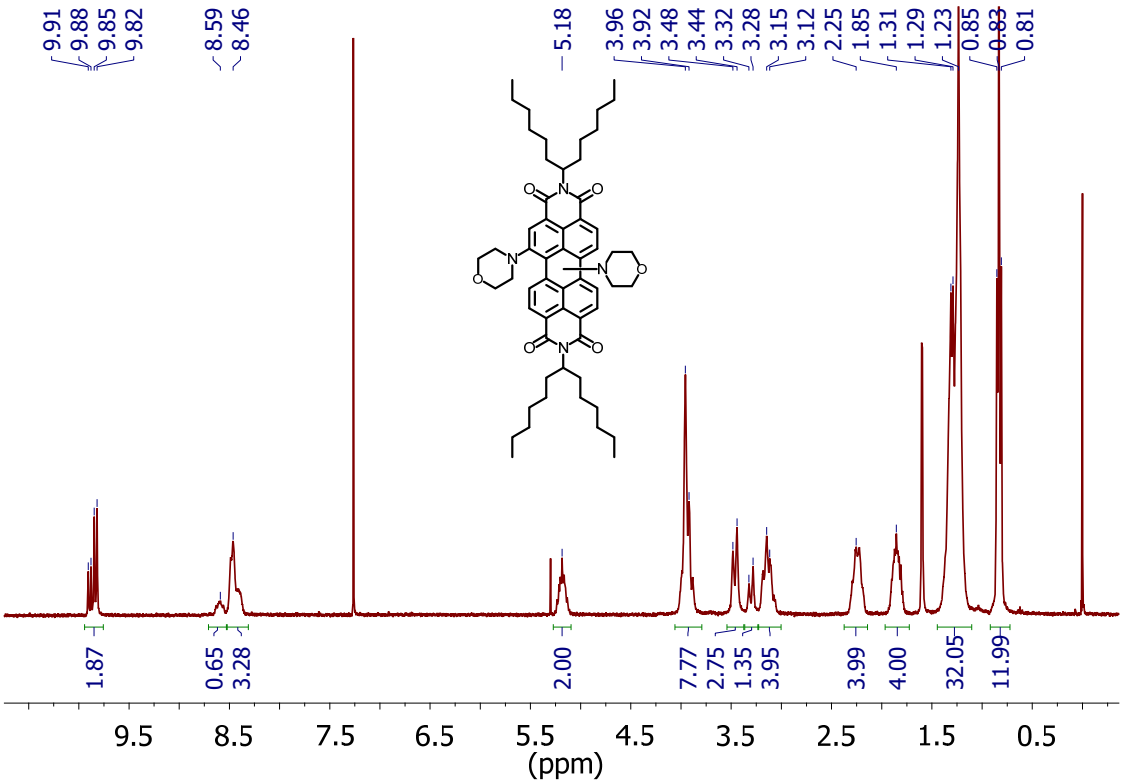
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1.31
1.29
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0.83
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3.28
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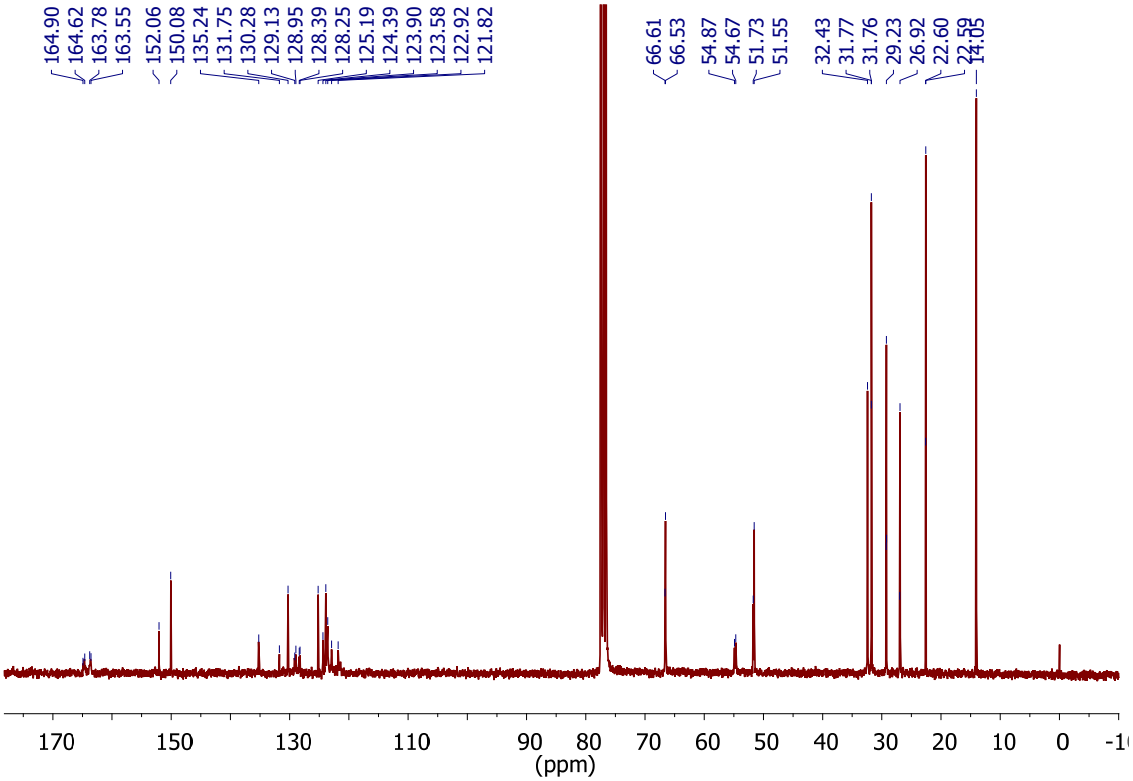
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31.77
31.76
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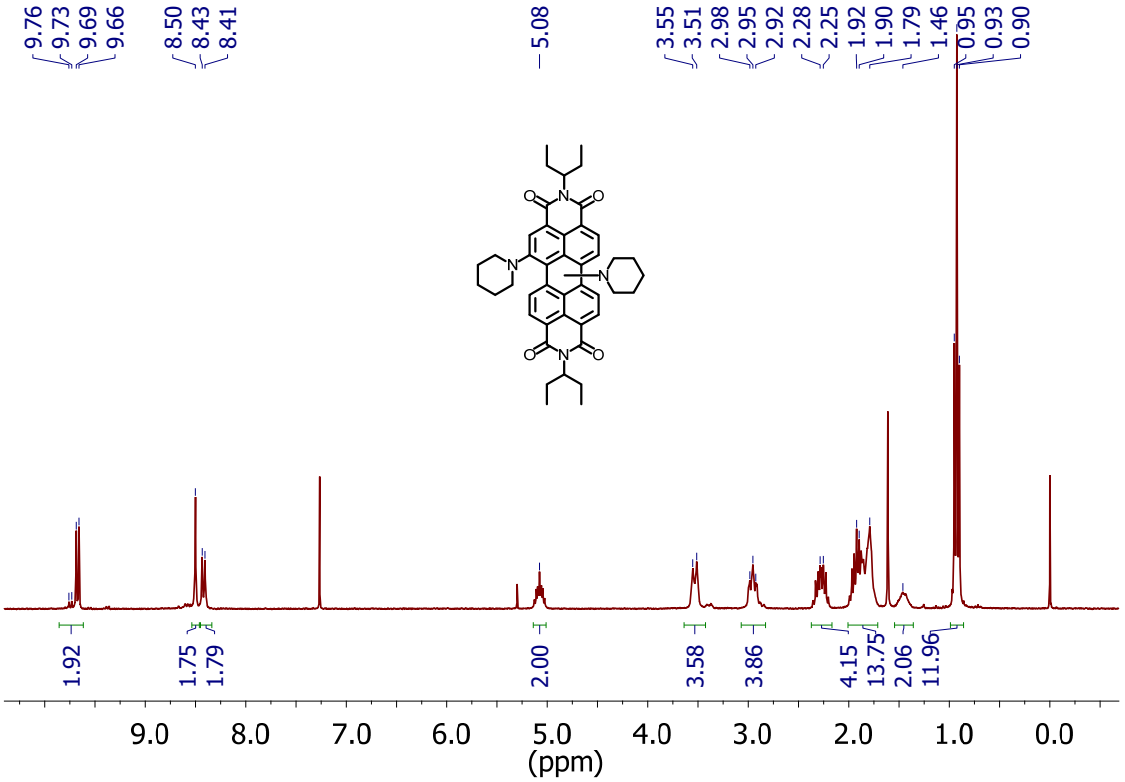
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2.28
2.25
1.92
1.90
1.79
1.46
0.95
0.93
0.90
1.92
1.75
1.79
2.00
3.58
3.86
4.15
13.75
2.06
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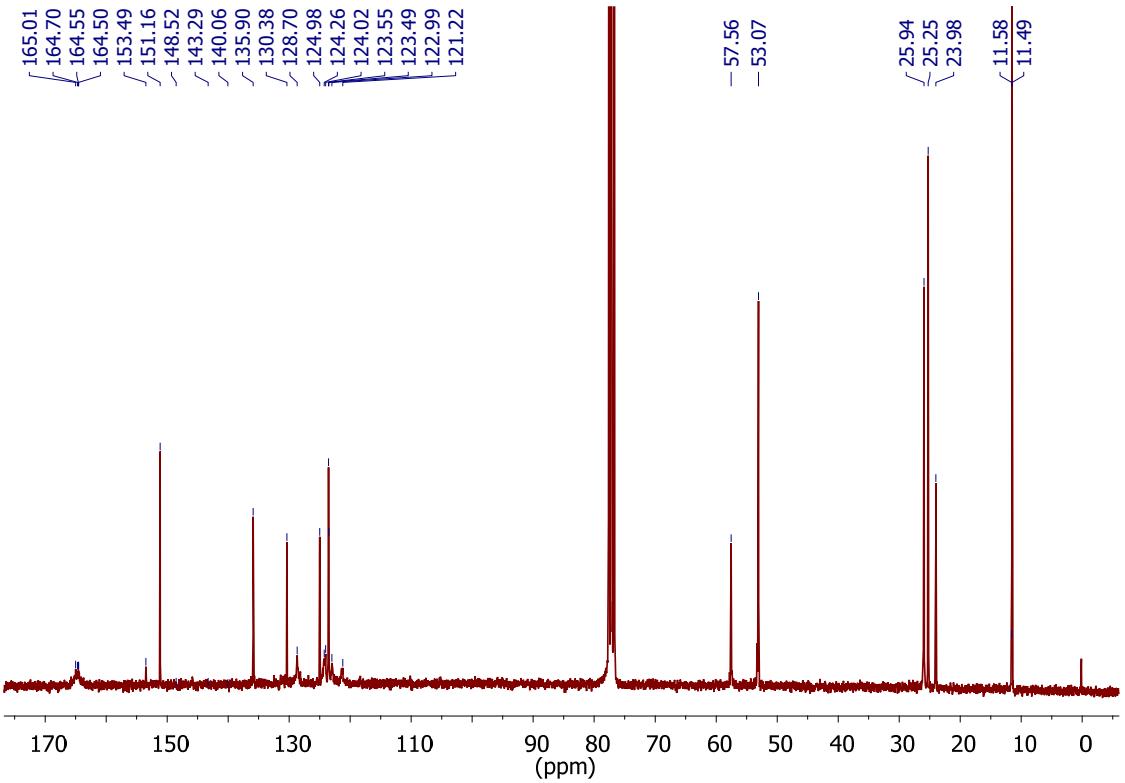
(ppm)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124.02
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121.22
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53.07
25.94
25.25
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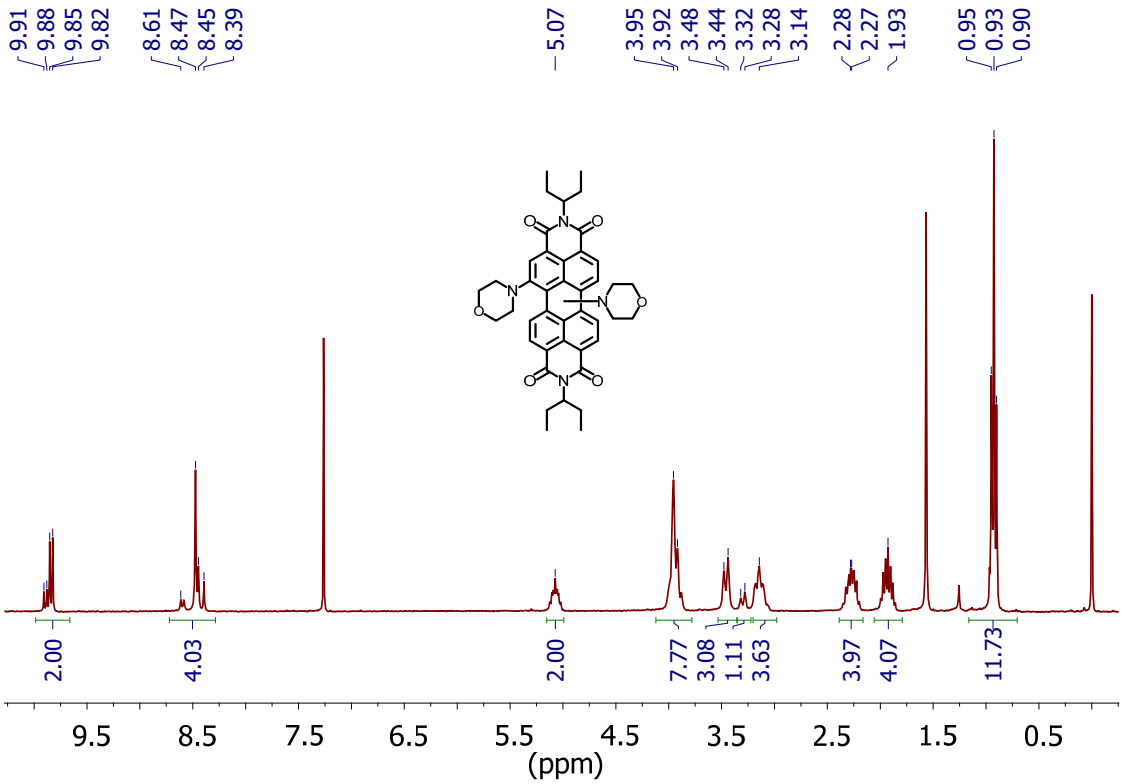
(ppm)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3.28
3.14
2.28
2.27
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4.03
2.00
7.77
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1.11
3.63
3.97
4.07
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3.5
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1.5
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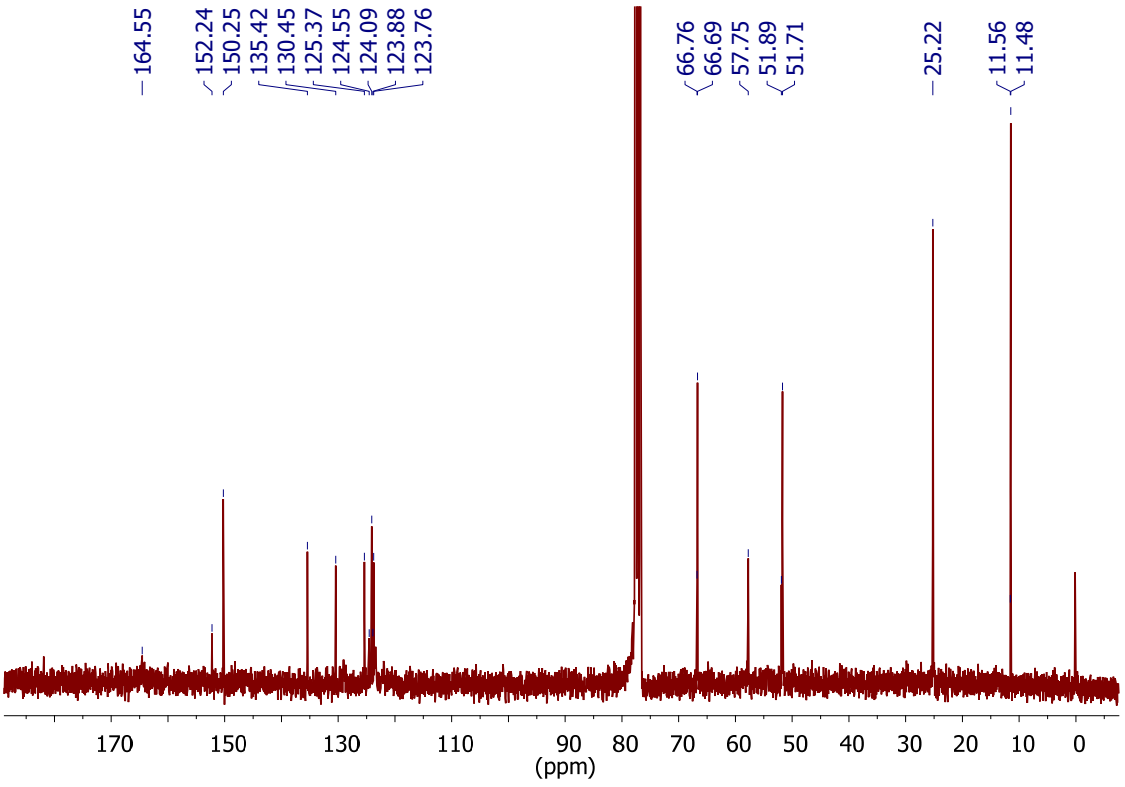
(ppm)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51.71
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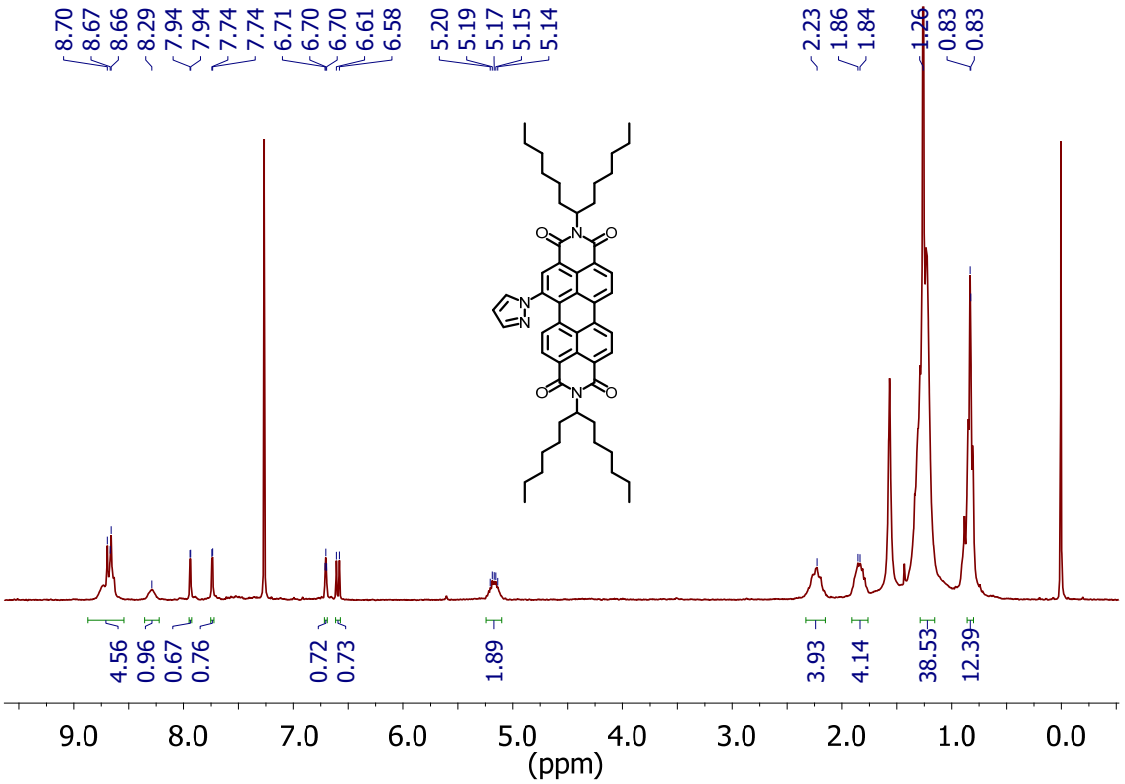
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5.19
5.17
5.15
5.14
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0.83
4.56
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0.67
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0.73
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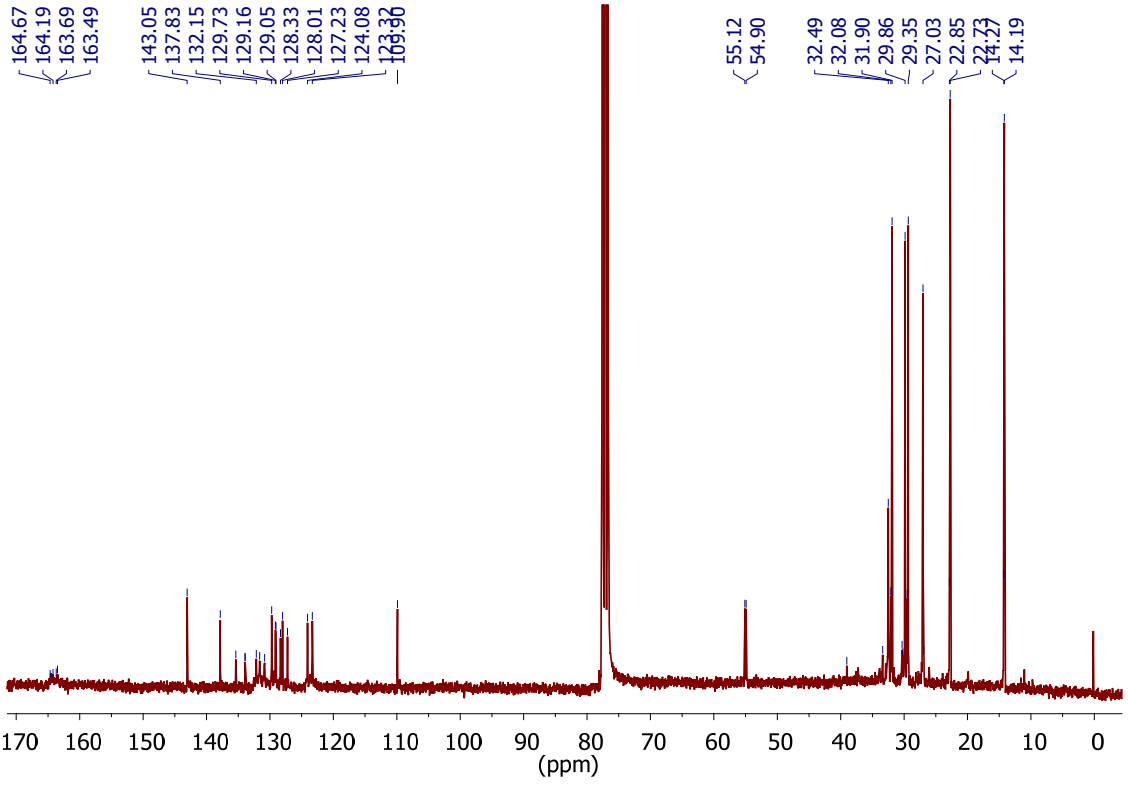
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128.33
128.01
127.23
124.08
55.12
54.90
32.49
32.08
31.90
29.86
29.35
27.03
22.85
14.19
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120
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100
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80
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50
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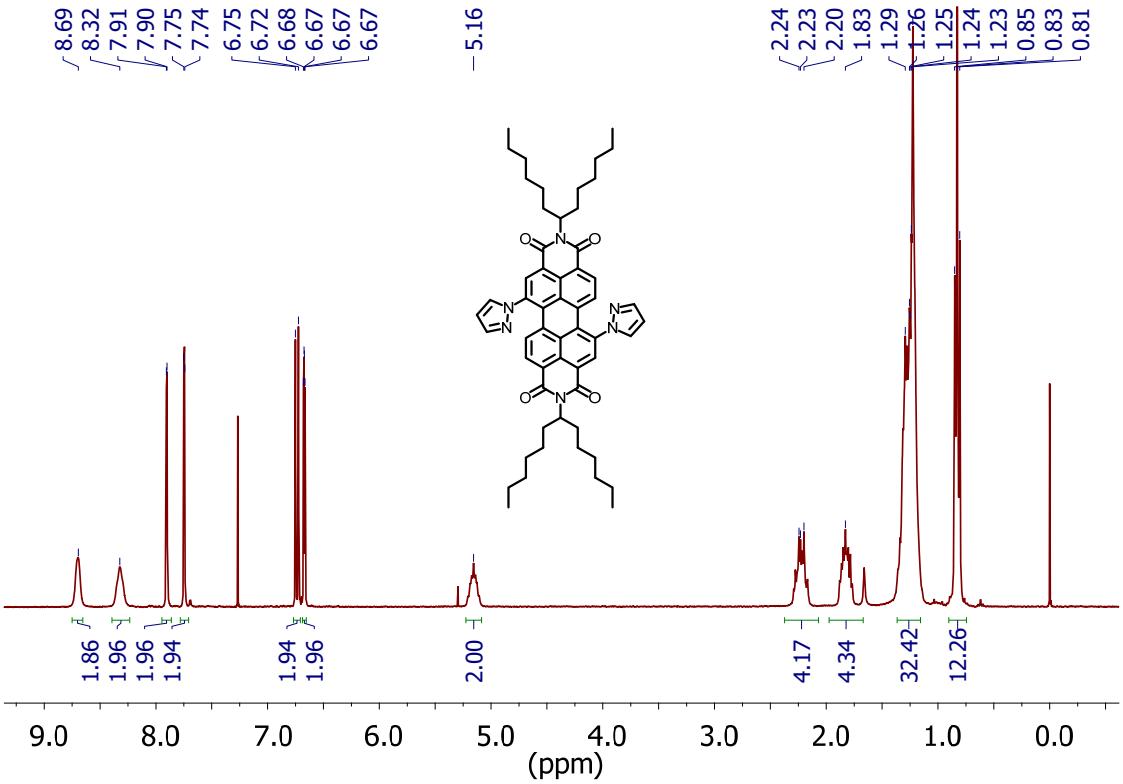
(ppm)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6.72
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6.67
6.67
5.16
2.24
2.23
2.20
1.83
1.29
1.26
1.25
1.24
1.23
0.85
0.83
0.81
1.86
1.96
1.96
1.94
1.94
1.96
2.00
4.17
4.34
32.42
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7.0
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4.0
3.0
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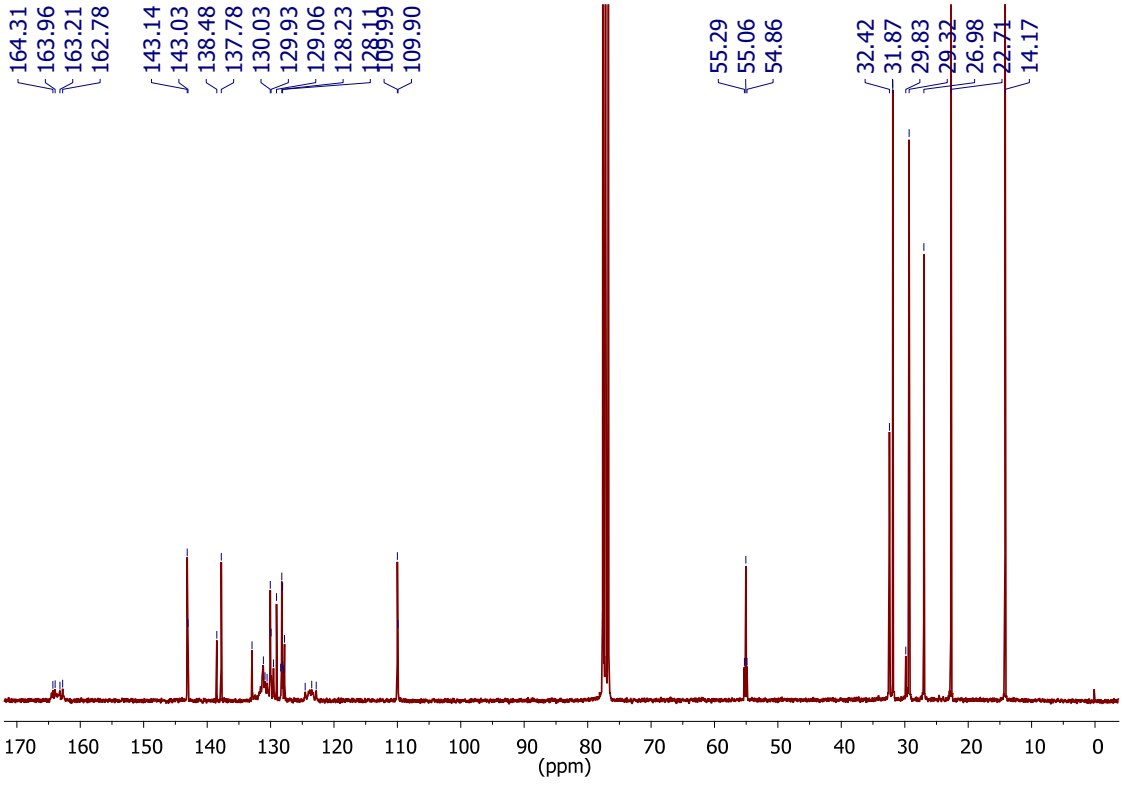
(ppm)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143.03
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137.78
130.03
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129.06
128.23
109.99
109.90
55.29
55.06
54.86
32.42
31.87
29.83
29.32
26.98
22.71
14.17
170
160
150
140
130
120
110
100
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80
70
60
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30
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0
(ppm)