Electronic Supplementary Material (ESI) for RSC Advances

Efficient Dispersion of Multi-walled Carbon Nanotubes in Aqueous Solution by Non-covalent Interaction with Perylene Bisimides

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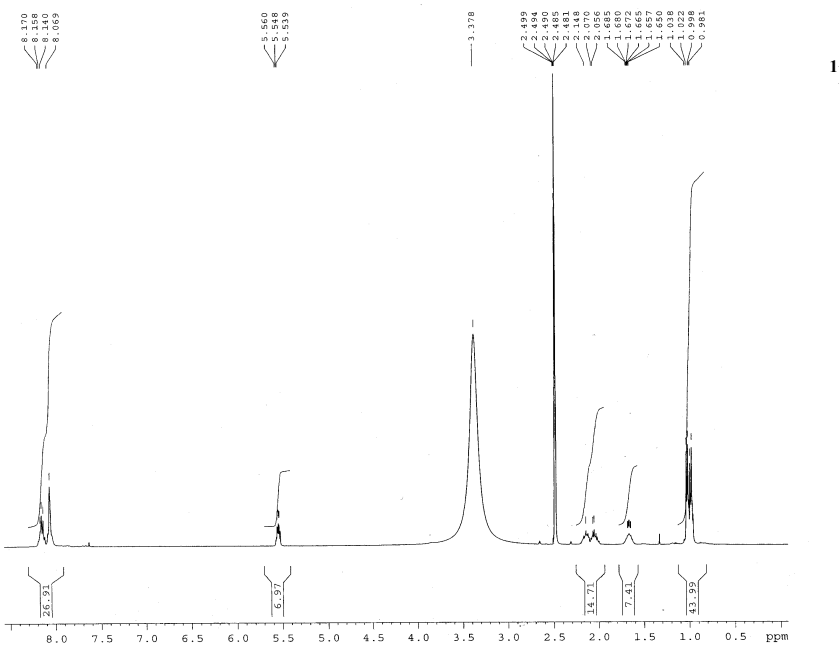
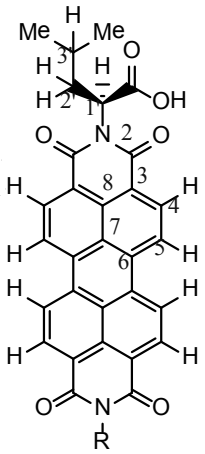
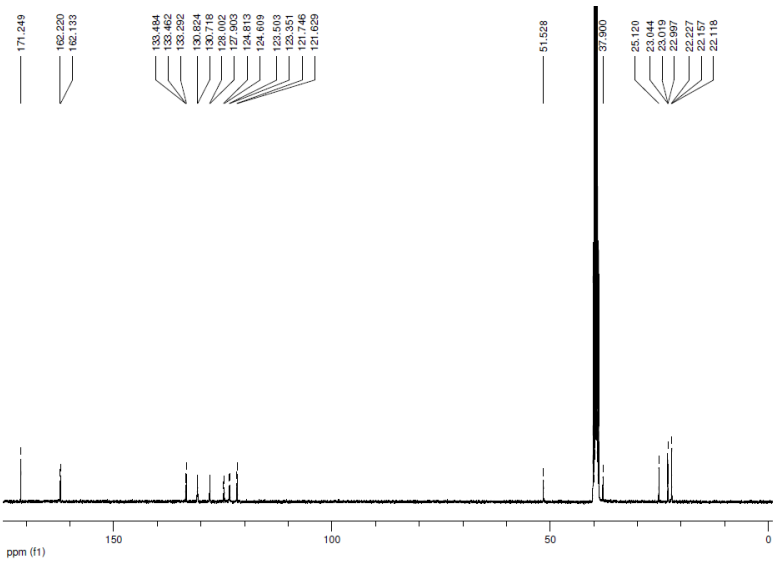
Compound **3a**



^{1}H NMR

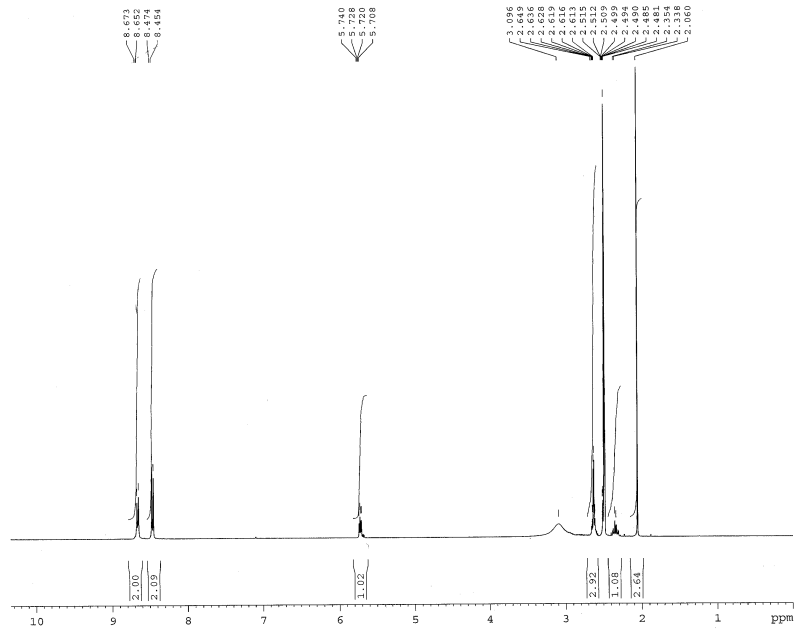




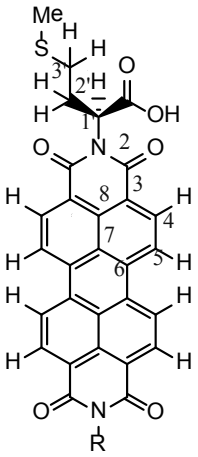
^{13}C NMR

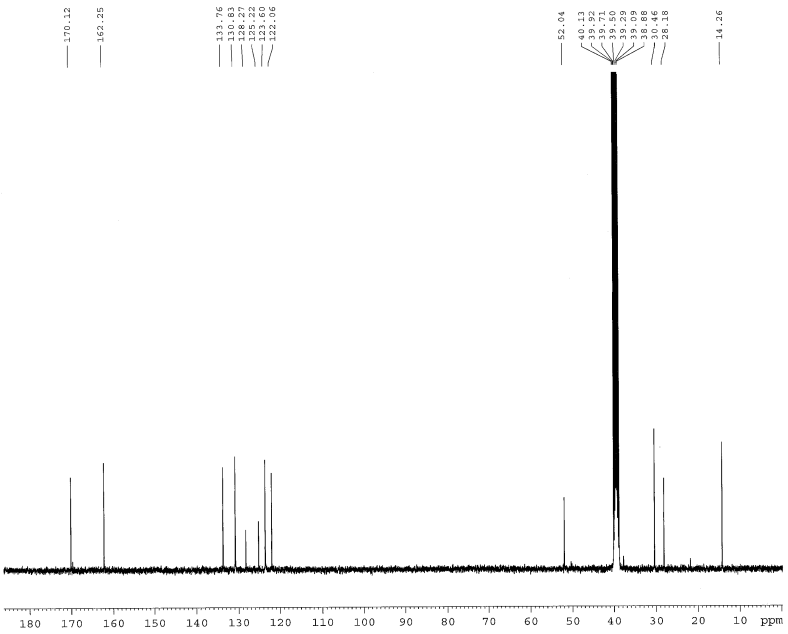
Compound **3a**, yield: 92 %, ^{1}HRMN (400 Mz, DMSO-d_6, 20 ºC): δ (ppm) 0.98 (d, 6H, J = 6.8 Hz, Me), 1.02 (d, 6H, J = 6.4 Hz, Me), 1.67 (m, 2H, J = 2.8 Hz, $C_{3'}$ – H), 2.06 (m, 2H, $C_{2'}$ – H), 2.15 (m, 2H, $C_{2'}$ – H), 5.55 (m, 2H, $C_{1'}$ – H), 8.06 (m, 4H, C – H perylene), 8.15 (m, 4H, C – H perylene). ^{13}CRMN (100 Mz, DMSO-d_6, 20 ºC): δ (ppm) 22.12 (Me), 22.16 (Me), 22.23 (Me), 23.00 (Me), 23.02 (Me), 23.04 (Me), 25.12 ($C_{3'}$), 37.90 ($C_{2'}$), 51.53 ($C_{1'}$), 121.63, 121.75, 123.35 e 123.50 (C from C – H of perylene), 124.61, 124.81, 127.90, 128.00, 130.80 e 130.82 (C from C – H of perylene), 133.29, 133.46, 133.48, 162.12 (C=O, perylene), 162.22 (C=O, perylene), 171.25 (COOH). FT – IR (KBr, cm^{-1}): 3467, 2958, 2935, 2869, 1731, 1697, 1658, 1593, 1434, 1404, 1361, 1346, 1253, 1176, 1130, 1022, 975, 810, 748, 713. Elemental analysis calcd (%) for $C_{36}H_{30}N_2O_8$: C 69.89, H 4.89, N 4.53; found: C 69.65, H 4.80, N 4.67.

Compound **3b**



^{1}H NMR

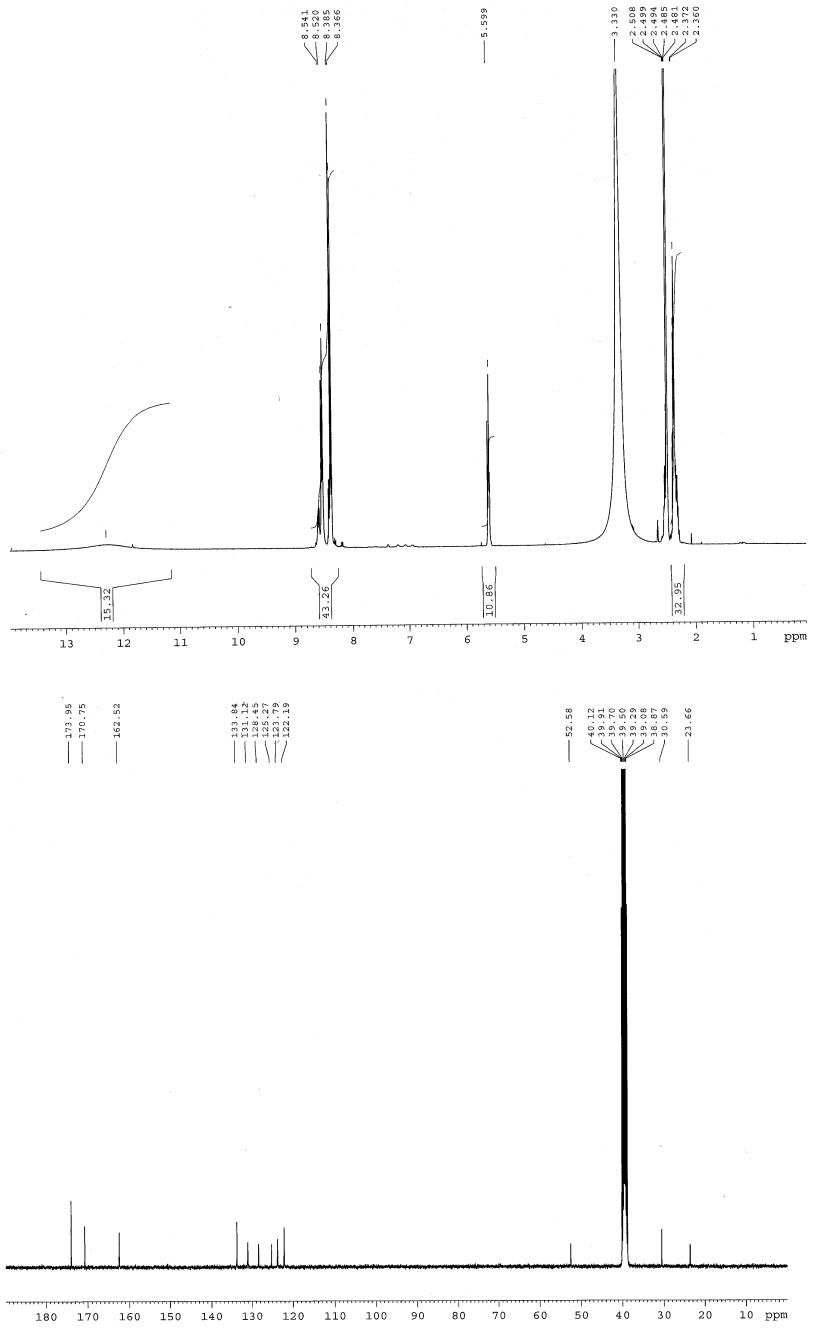




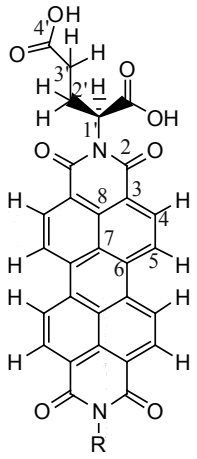
^{13}C NMR

Compound **3b**, yield: 96 %, ^{1}HRMN (400 Mz, DMSO-d_6, 70 ºC): δ (ppm) 2.06 (s, 6 H, Me), 2.35 (m, 2 H, $C_{2'}$ – H), 2.62 (m, 2 H, $C_{2'}$ – H), 2.62 (m, 4 H, $C_{3'}$ – H), 5.72 (dd, 2 H, J = 8 Hz, J = 4.8 Hz, $C_{1'}$ – H), 8.46 (d, 4 H, J = 8 Hz, C_4 – H), 8.66 (d, 4 H, J = 8.4 Hz, C_5 – H). ^{13}CRMN (100 Mz, DMSO-d_6, 70 ºC): δ (ppm) 14.26 (Me), 28.18 ($C_{2'}$), 30.46 ($C_{3'}$), 52.04 ($C_{1'}$), 122.06, 123.60 (C_5), 125.22, 128.27 (C_8), 130.83 (C_4), 133.76 (C_6), 162.25 (C_2), 170.12 (COOH). FT – IR (KBr, cm^{-1}): 3487, 2916, 1735, 1697, 1658, 1593, 1573, 1434, 1400, 1361, 1346, 1253, 1176, 1126, 860, 810, 748, 640. Elemental analysis calcd (%) for $C_{34}H_{26}N_2O_8S_2$: C 62.37, H 4.00, N 4.28, S 9.80; found: C 61.25, H 3.98, N 4.39, S 9.72.

Compound **3c**



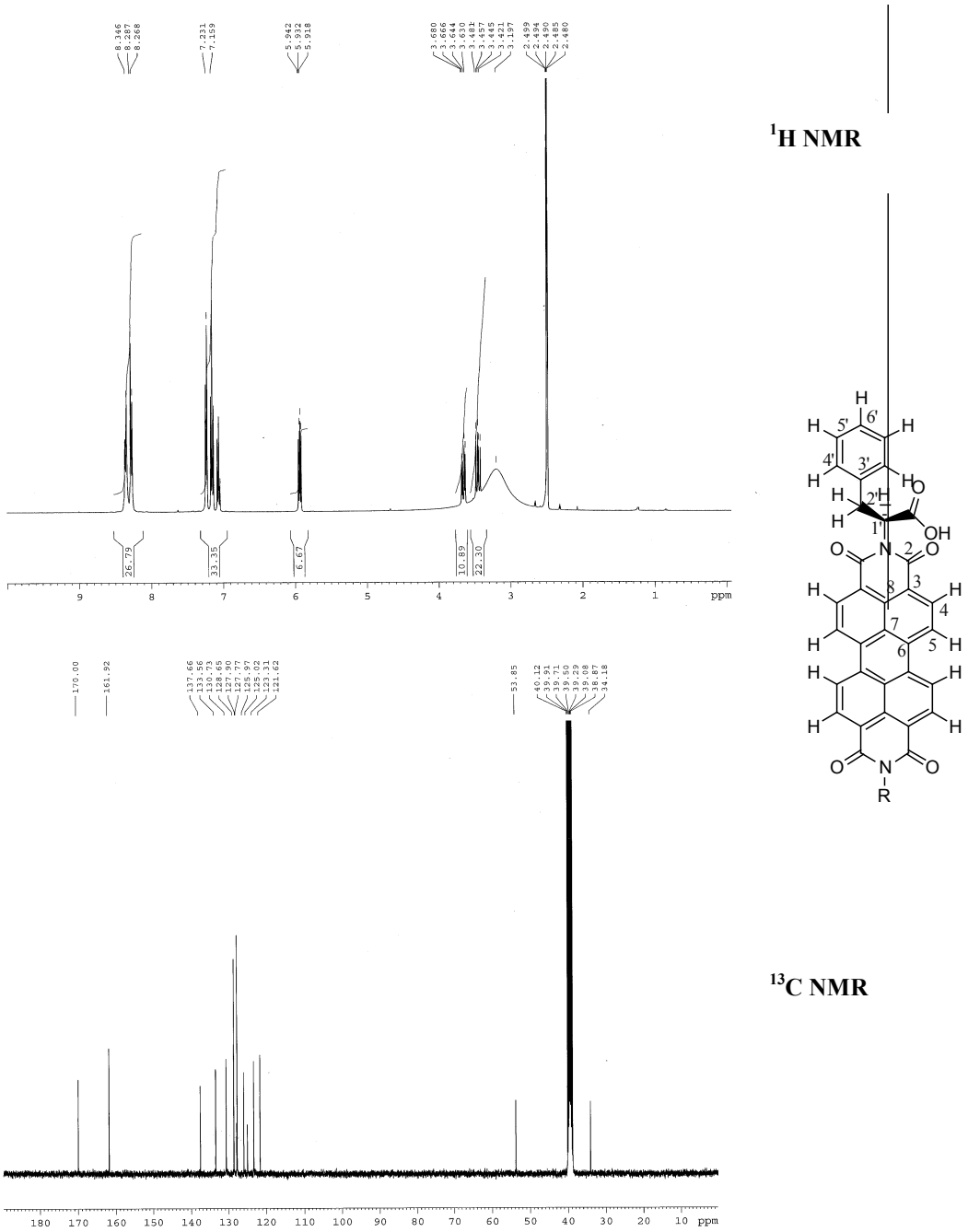
^{1}H NMR



^{13}C NMR

Compound **3c**, yield: 71 %, ^{1}HRMN (400 Mz, DMSO-d_6, 20 ºC): δ (ppm) 2.37 (m, 4 H, $C_{3'}$ – H), 2.37 (m, 2 H, $C_{2'}$ – H) 2.51 (m, 2 H, $C_{2'}$ – H), 5.61 (dd, 2 H, J = 9.2 Hz, J = 4.4 Hz, $C_{1'}$ – H), 8.38 (d, 4 H, J = 8.4 Hz, C_4 – H), 8.53 (d, 4 H, J = 8.4 Hz, C_5 – H), 12.30 (s broad, COOH). ^{13}CRMN (100 Mz, DMSO-d_6, 20 ºC): δ (ppm) 23.66 ($C_{2'}$), 30.59 ($C_{3'}$), 52.58 ($C_{1'}$), 122.19, 123.79 (C_5), 125.27, 128.45, 131.12 (C_4), 133.84, 162.52 (C_2), 170.75 (COOH), 173.95 ($C_{4'}$). FT – IR (KBr, cm^{-1}): 3440, 3163, 3116, 2927, 1747, 1697, 1647, 1593, 1573, 1438, 1384, 1365, 1342, 1257, 1180, 1134, 975, 864, 810, 748, 644. Elemental analysis calcd (%) for $C_{34}H_{22}N_2O_{12}$: C 62.77, H 3.41, N 4.31; found: C 63.34, H 3.35, N 4.29.

Compound **3d**



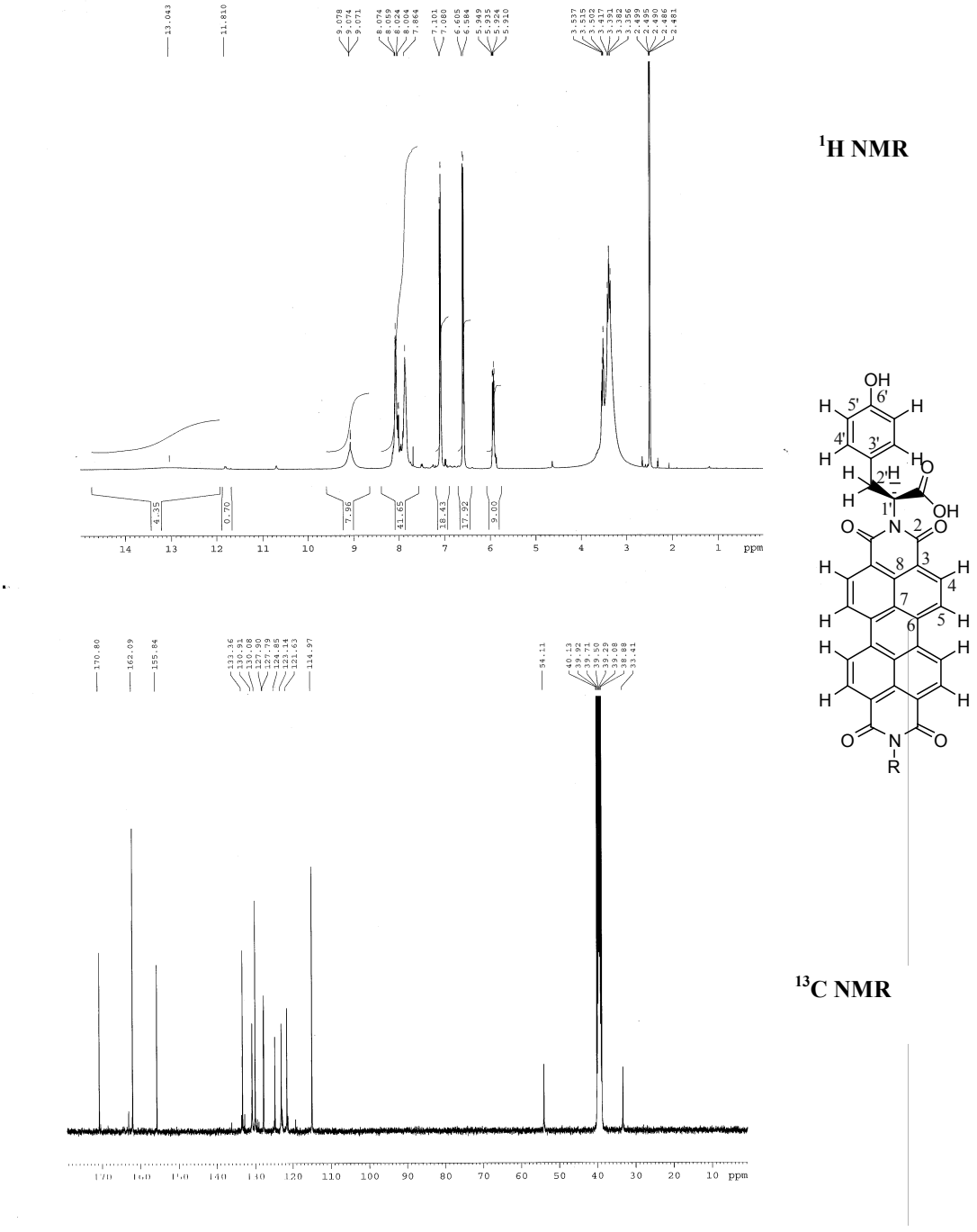
^{1}H NMR

^{13}C NMR

Compound **3d**, yield: 97 %. ^{1}HRMN (400 Mz, DMSO-d_6, 70 ºC): δ (ppm) 3.45 (dd, 2 H, J = 14.4 Hz, J = 9.6 Hz, $C_{2'}$ – H), 3.66 (dd, 2 H, J = 14.4 Hz, J = 5.6 Hz, $C_{2'}$ – H), 5.94 (dd, 2 H, J = 9.6 Hz, J = 5.6 Hz, $C_{1'}$ – H), 7.07 (t, 2 H, J = 7.2 HZ, $C_{6'}$ – H), 7.16 (t, 4 H, J = 6.6 Hz, $C_{5'}$ – H), 7.24 (d, 4H, J = 7.6 Hz, $C_{4'}$ – H) 8.28 (d, 4H, J = 8.28, C_4 – H), 8.36 (d, 4H, J = 8.36, C_5 – H). ^{13}CRMN (100 Mz, DMSO-d_6, 70 ºC): 34.18 ($C_{2'}$), 53.85 ($C_{1'}$), 121.62, 123.31 (C_5), 125.02, 125.97 ($C_{6'}$), 127.77 ($C_{5'}$), 127.90 (C_8), 128.65 ($C_{4'}$), 130.73 (C_4), 133.56 (C_6), 137.66 ($C_{3'}$), 161.92 (C_2), 170.00 (COOH). FT – IR (KBr, cm^{-1}): 3502, 3028, 2935, 1735, 1697, 1658, 1593, 1573, 1496, 1434, 1400, 1365, 1342, 1253, 1168, 1126, 979, 952, 856, 810, 748,

698, 648, 601. Elemental analysis calcd (%) for $C_{42}H_{26}N_2O_8$: C 73.46, H 3.82, N 4.08; found: C 72.34, H 3.75, N 4.15.

Compound **3e**



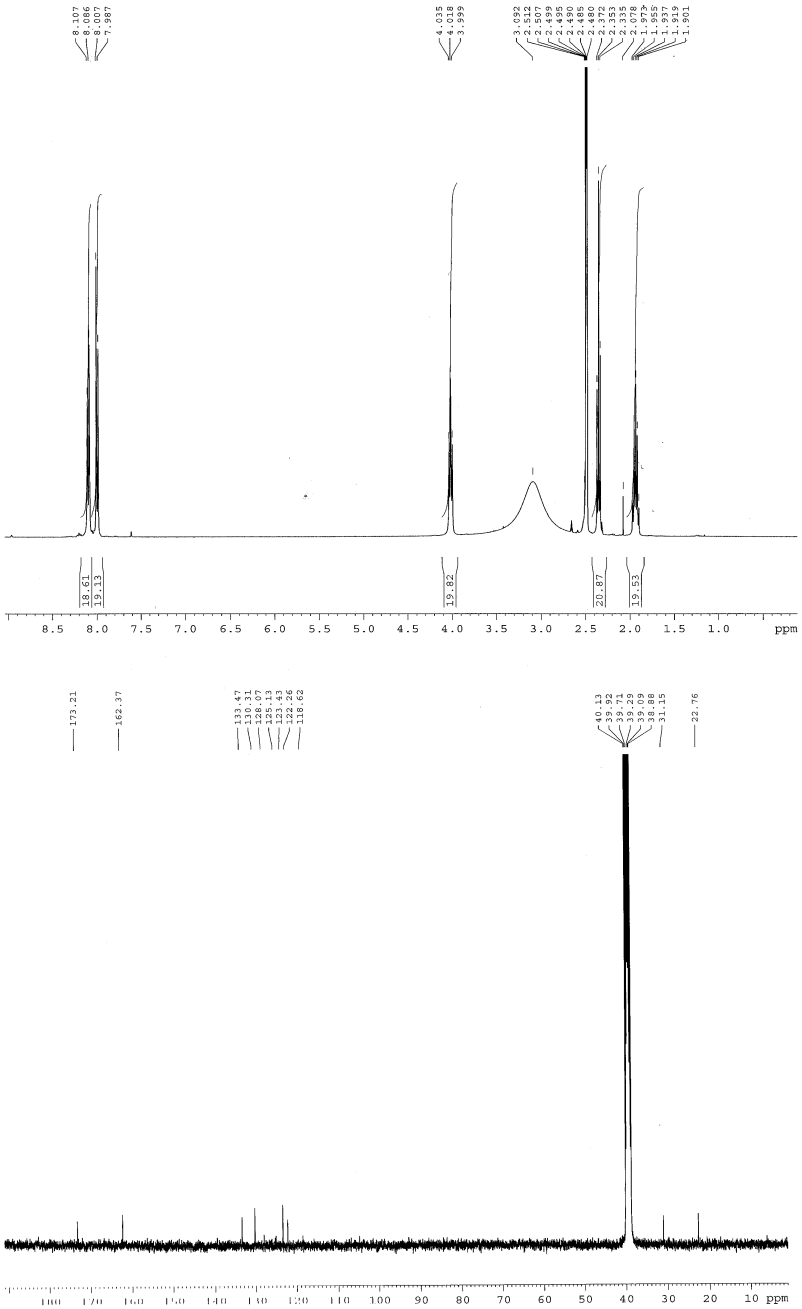
^{1}H NMR

^{13}C NMR

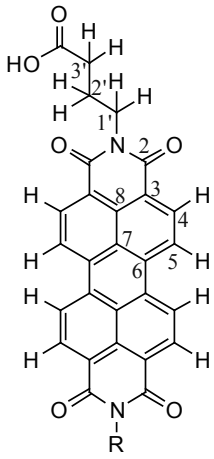
Compound **3e**, yiled: 85 %, ^{1}HRMN (400 Mz, DMSO-d_6, 20 ºC): δ (ppm) 3.39 (dd, 2 H, J = 14 Hz, J = 10.4 Hz, $C_{2'}$ – H), 3.53 (dd, 2 H, J = 14 Hz, J = 5.2 Hz, $C_{2'}$ – H), 5.93 (dd, 2 H, J = 10Hz, J = 5.6 Hz, $C_{1'}$), 6.59 (d, 4 H, J = 8.4 Hz, $C_{5'}$ – H), 7.09 (d, 4 H, J = 8.4 Hz, $C_{4'}$ – H), 7.86 (s broad, 4 H, C_5 – H), 8.07 (s broad, 4 H, C_4 – H). ^{13}CRMN (100 Mz, DMSO-d_6, 20 ºC): δ (ppm) 33.41 ($C_{2'}$), 54.11 ($C_{1'}$) 114.97 ($C_{5'}$), 121.63, 123.14 (C_5), 124.85, 127.79 ($C_{3'}$), 127,90, 130.08 ($C_{4'}$), 130.91 (C_4), 133.36 (C_6), 155.84 ($C_{6'}$), 162.09 (C_2), 170.80 (COOH). FT – IR (KBr, cm^{-1}): 3379, 2935, 1731, 1697, 1650, 1593, 1573, 1512, 1434,

1400, 1365, 1342, 1253, 1222, 1168, 1130, 952, 860, 810, 748, 644, 597. Elemental analysis calcd (%) for $C_{42}H_{26}N_2O_{10}$: C 70.19, H 3.65, N 3.90; found: C 69.85, H 3.81, N 4.20.

Compound **3f**



^{1}H NMR

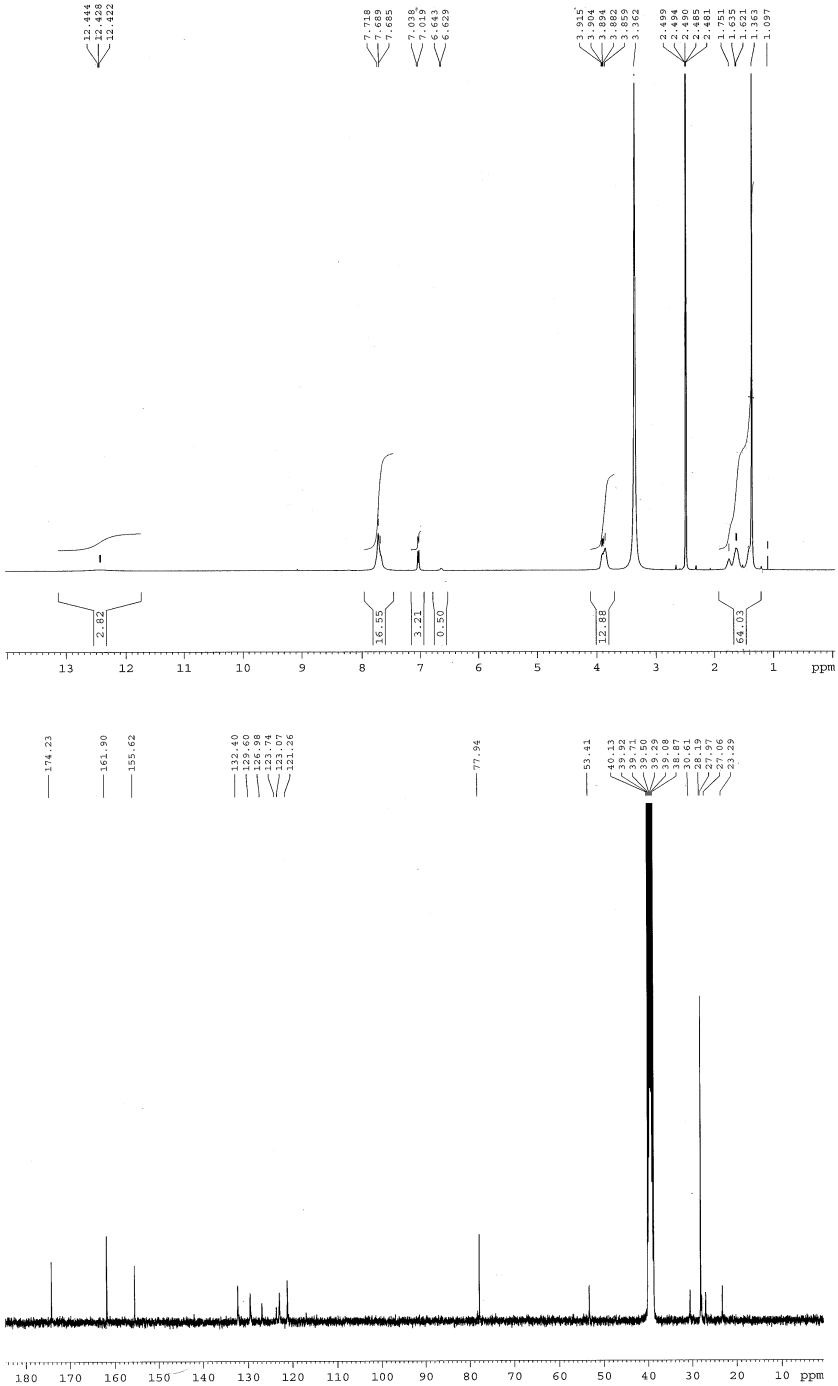


^{13}C NMR

Compound **3f**, yield: 81 %, ^{1}H RMN (400 Mz, DMSO-d_6, 80 ºC): δ (ppm) 1.94 (m, 4 H, $C_{2'}$ – H), 2.35 (t, 4 H, J = 7.4 Hz, $C_{3'}$ – H), 4.02 (t, 4 H, J = 7.2 Hz, $C_{1'}$ – H), 8.00 (d, 4 H, J = 8 Hz, C_4 – H), 8.10 (d, 4 H, J = 8.4 Hz, C_5 – H). ^{13}CRMN (100 Mz, DMSO-d_6, 80 ºC): δ (ppm) 22.76 ($C_{3'}$), 31.15 ($C_{2'}$), 39.29 ($C_{1'}$), 122.26, 123.43 (C_5), 125.13, 128.07 (C_8), 130.31 (C_4), 133.47 (C_6), 162.37 (C_2), 173.21 (COOH). FT – IR (KBr, cm^{-1}): 3552, 2927, 2869, 1731, 1693, 1650, 1593, 1577, 1442, 1400, 1384, 1342, 1249, 1164, 1126,

1056, 856, 810, 744. Elemental analysis calcd (%) for $C_{32}H_{22}N_2O_8$: C 68.32, H 3.94, N 4.98; found: C 69.95, H 3.37, N 4.66.

Compound **3g**



^{1}H NMR

^{13}C NMR

Compound **3g**, yield: 90 %, ^{1}HRMN (400 Mz, DMSO-d_6, 20 ºC): δ (ppm) 1.36 (s, 18 H, Me from Boc), 1.40 (m, 4 H), 1.63 (m, 4 H), 1.63 (m, 2 H, $C_{4'}$ – H), 1.75 (m, 2H, $C_{4'}$ – H), 3.89 (m, 6 H, $C_{1'}$ – H e $C_{5'}$ – H), 7.03 (d, 2 H, J = 7.6 Hz, N – H), 7.69 (s broad, 8 H, C_4 – H e C_5 – H). ^{13}C RMN (100 Mz, DMSO-d_6, 20 ºC): δ (ppm) 23.29 ($C_{3'}$), 27.06, 28.19 (Me from Boc), 30.61 ($C_{4'}$), 39.71 ($C_{1'}$ ou $C_{5'}$), 53.41 ($C_{1'}$ ou $C_{5'}$), 77.94 ($C(Me)_3$ from Boc), 121.26, 123.07 (C_4 ou C_5), 123.74, 126.98, 129.60 (C_4 ou C_5), 132.40, 155.62

(2C, C=O from Boc), 161.90 (C_2), 174.23 (COOH). FT – IR (KBr, cm^{-1}): 3506, 3355, 2970, 2931, 2866, 1697, 1650, 1593, 1577, 1508, 1442, 1400, 1342, 1249, 1164, 1126, 1087, 1068, 1049, 1018, 856, 810, 744, 628. Elemental analysis calcd (%) for $C_{46}H_{50}N_4O_{12}$: C 64.93, H 5.92, N 6.58; found: C 63.76, H 5.50, N 6.71.