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Electronic Supplementary Information

Fluoride-Mediated Alkoxylation and Alkylthio-Functionalization of Halogenated Perylenediimides

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1,6,7,12-tetraalkylthioperylene-3,4:9,10-tetracarboxydiimide (2d, 3d, 4d and 5c)
The thiol (0.6 mmol), KF (0.6 mmol) and 18-crown-6 (1.2 mmol) were added to a solution of 1,6,7,12-tetrachloroperylene-3,4:9,10-tetracarboxydiimide (0.06 mmol) in dry THF (0.5 mL) in a cone-shaped flask. The reaction was refluxed 8 hours under argon atmosphere, and after cooling, it was extracted with dichloromethane. The organic layer was dried over anhydrous sodium sulfate, filtered and evaporated. Purification was carried out by silica gel column chromatography using CH_2Cl_2:hexane 1:1 as eluent.

1,6,7-trihexylthio-12-chloroperylene-3,4:9,10-tetracarboxydiimide (2c)
Hexanethiol (0.18 mmol), KF (0.48 mmol) and 18-crown-6 (0.96 mmol) were added to a solution of 1,6,7,12-tetrachloroperylene-3,4:9,10-tetracarboxydiimide (0.06 mmol) in dry THF (1 mL) in a cone-shaped flask. The reaction was refluxed 24 hours under argon atmosphere, and after cooling, it was extracted with dichloromethane. The organic layer was dried over anhydrous sodium sulfate, filtered and evaporated. Purification was carried out by silica gel column chromatography using CH_2Cl_2:hexane 1:1 as eluent.

1-hexylthio-6,7,12-trichloroperylene-3,4:9,10-tetracarboxydiimide (2a)
Hexanethiol (0.06 mmol), KF (0.13 mmol) and 18-crown-6 (0.26 mmol) were added to a solution of 1,6,7,12-tetrachloroperylene-3,4:9,10-tetracarboxydiimide (0.06 mmol) in dry THF (2 mL) in a cone-shaped flask. The reaction was refluxed 24 hours under argon atmosphere, and after cooling, it was extracted with dichloromethane. The organic layer was dried over anhydrous sodium sulfate, filtered and evaporated. Purification was carried out by silica gel column chromatography using CH_2Cl_2:hexane 1:1 as eluent.

2,5,8,11-tetraalkylthioperylene-3,4:9,10-tetracarboxydiimide (13d, 14d, 15d and 16d)
The thiol (0.6 mmol), KF (0.6 mmol) and 18-crown-6 (1.2 mmol) were added to a solution of 2,5,8,11-tetrabromoperylene-3,4:9,10-tetracarboxydiimide (0.06 mmol) in dry THF (2 mL) in a cone-shaped flask. The reaction was refluxed 24 hours under argon atmosphere, and after cooling, it was extracted with dichloromethane. The organic layer was dried over anhydrous sodium sulfate, filtered and evaporated. Purification was carried out by silica gel column chromatography using CH_2Cl_2:hexane 1:1 as eluent.
The same procedure was followed with *p*-toluenethiol.

2,5,8-trihexylthio-11-bromoperylene-3,4:9,10-tetracarboxydiimide (13c)
Hexanethiol (0.3 mmol), KF (0.3 mmol) and 18-crown-6 (0.6 mmol) were added to a solution of 2,5,8,11-tetrabromoperylene-3,4:9,10-tetracarboxydiimide (0.06 mmol) in dry THF (2 mL) in a cone-shaped flask. The reaction was refluxed 24 hours under argon atmosphere, and after cooling, it was extracted with dichloromethane. The organic layer was dried over anhydrous sodium sulfate, filtered and evaporated. Purification was carried out by silica gel column chromatography using CH_2Cl_2:hexane 1:1 as eluent.

1,6,7,12-tetraalkoxyperylene-3,4:9,10-tetracarboxydiimide (6c and 8d)
The alcohol (0.6 mmol), CsF (0.6 mmol) and 18-crown-6 (2.4 mmol) were added to a solution of 1,6,7,12-tetrachloroperylene-3,4:9,10-tetracarboxydiimide (0.06 mmol) in

dry THF (2 mL) in a cone-shaped flask. The reaction was refluxed 24 hours under argon atmosphere, and after cooling, it was extracted with dichloromethane. The organic layer was dried over anhydrous sodium sulfate, filtered and evaporated. Purification was carried out by silica gel column chromatography using CH_2Cl_2:hexane 1:1 as eluent.
The same procedure was followed with dry butanol for obtaining 1,6,7-tributoxy-12-chloroperylene-3,4:9,10-tetracarboxydiimide (6c).

1-butoxy-6,7,12-trichloroperylene-3,4:9,10-tetracarboxydiimide (6a)
The alcohol (0.06 mmol), CsF (0.13 mmol) and 18-crown-6 (0.52 mmol) were added to a solution of 1,6,7,12-tetrachloroperylene-3,4:9,10-tetracarboxydiimide (0.06 mmol) in dry THF (2 mL) in a cone-shaped flask. The reaction was refluxed 24 hours under argon atmosphere, and after cooling, it was extracted with dichloromethane. The organic layer was dried over anhydrous sodium sulfate, filtered and evaporated. Purification was carried out by silica gel column chromatography using CH_2Cl_2:hexane 1:2 as eluent.

2,5,8,11-tetraalkoxy- and 2,5,8,11-tetraaryloxyperylene-3,4:9,10-tetracarboxydiimide (17d, 18d and 19d)
The alcohol or phenol (0.6 mmol), CsF (0.6 mmol) and 18-crown-6 (2.4 mmol) were added to a solution of 2,5,8,11-tetrabromoperylene-3,4:9,10-tetracarboxydiimide (0.06 mmol) in dry THF (2 mL) in a cone-shaped flask. The reaction was refluxed 24 hours under argon atmosphere, and after cooling, it was extracted with dichloromethane. The organic layer was dried over anhydrous sodium sulfate, filtered and evaporated. Purification was carried out by silica gel column chromatography using CH_2Cl_2:hexane 1:1 as eluent.

***N,N*'-di-(1'-hexylheptyl)-1,7(6)-dibutoxyperylene-3,4:9,10-tetracarboxydiimide (11)**
A mixture of 30 mg (0.4 mmol) of butanol, 76 mg (0.5 mmol) of CsF and 530 mg (2 mmol) of 18-crown-6 were added to a solution of 100 mg (0.1 mmol) of *N,N'*-di-(1'-hexylheptyl)-1,7(6)-dibromoperylene-3,4:9,10-tetracarboxydiimide in dry THF (2 mL). The reaction was refluxed 24 hours under argon atmosphere and, after cooling, it was extracted with dichloromethane and washed with water. The organic layer was dried over anhydrous sodium sulfate, filtered and evaporated. Purification was carried out by silica gel column chromatography using CH_2Cl_2:hexane 1:1 as eluent yielding 85 mg (95%) of a purple powder.

***N,N*'-di-(1'-hexylheptyl)-2-butoxy-5,8,11-trihexylthioperylene-3,4:9,10-tetracarboxydiimide (20)**
A mixture of 14 mg (0.18 mmol) of butanol, 29 mg (0.18 mmol) of CsF and 190 mg (0.72 mmol) of 18-crown-6 were added to a solution of 70 mg (0.06 mmol) of *N,N'*-di-(1'-hexylheptyl)-2-bromo-5,8,11-trihexylthioperylene-3,4:9,10-tetracarboxydiimide in dry THF (2 mL). The reaction was refluxed 24 hours under argon atmosphere and, after cooling, it was extracted with dichloromethane and washed with water. The organic layer was dried over anhydrous sodium sulfate, filtered and evaporated. Purification was

carried out by silica gel column chromatography using CH_2Cl_2:hexane 1:1 as eluent yielding 20 mg (28%) of an orange powder.

_N,N_'-di-(1'-hexylheptyl)-2,5,8-trihexylthio-11-phenoxyperylene-3,4:9,10-tetracarboxydiimide (21)

A mixture of 9 mg (0.09 mmol) of phenol, 14 mg (0.09 mmol) of CsF and 95 mg (0.36 mmol) of 18-crown-6 were added to a solution of 34 mg (0.03 mmol) of *N,N'*-di-(1'-hexylheptyl)-2-bromo-5,8,11-trihexylthioperylene-3,4:9,10-tetracarboxydiimide in dry THF (1 mL). The reaction was refluxed 24 hours under argon atmosphere and, after cooling, it was extracted with dichloromethane and washed with water. The organic layer was dried over anhydrous sodium sulfate, filtered and evaporated. Purification was carried out by silica gel column chromatography using CH_2Cl_2:hexane 1:1 as eluent yielding 30 mg (85%) of an orange powder.

_N,N_'-di-(1'-hexylheptyl)-2,5,8-tributoxy-11-hexylthioperylene-3,4:9,10-tetracarboxydiimide (22)

A mixture of 5 mg (0.039 mmol) of hexanethiol, 2,2 mg (0.039 mmol) of KF and 20 mg (0.078 mmol) of 18-crown-6 were added to a solution of 13 mg (0.013 mmol) of *N,N'*-di-(1'-hexylheptyl)-2-bromo-5,8,11-tributoxiperylene-3,4:9,10-tetracarboxydiimide in dry THF (0.5 mL). The reaction was refluxed 24 hours under argon atmosphere and, after cooling, it was extracted with dichloromethane and washed with water. The organic layer was dried over anhydrous sodium sulfate, filtered and evaporated. Purification was carried out by silica gel column chromatography using CH_2Cl_2:hexane 1:1 as eluent yielding 13 mg (92%) of an orange powder.

_N,N_'-di-(1'-hexylheptyl)-1-butoxy-6,7,12-trihexylthioperylene-3,4:9,10-tetracarboxydiimide (23)

Starting from 2c. A mixture of 14 mg (0.18 mmol) of butanol, 28 mg (0.18 mmol) of CsF and 190 mg (0.72 mmol) of 18-crown-6 were added to a solution of 70 mg (0.06 mmol) of *N,N'*-di-(1'-hexylheptyl)-1-chloro-6,7,12-trihexylthioperylene-3,4:9,10-tetracarboxydiimide in dry THF (2 mL). The reaction was refluxed 24 hours under argon atmosphere and, after cooling, it was extracted with dichloromethane and washed with water. The organic layer was dried over anhydrous sodium sulfate, filtered and evaporated. Purification was carried out by silica gel column chromatography using CH_2Cl_2:hexane 1:2 as eluent yielding 22 mg (31%) of a purple powder.

Starting from 6a. A mixture of 19 mg (0.16 mmol) of hexanethiol, 10 mg (0.16 mmol) of KF and 85 mg (0.32 mmol) of 18-crown-6 were added to a solution of 17 mg (0.018 mmol) of *N,N'*-di-(1'-hexylheptyl)-1-butoxi-6,7,12-trichloroperylene-3,4:9,10-tetracarboxydiimide in dry THF (0.5 mL). The reaction was refluxed 24 hours under argon atmosphere and, after cooling, it was extracted with dichloromethane and washed with water. The organic layer was dried over anhydrous sodium sulfate, filtered and evaporated. Purification was carried out by silica gel column chromatography using CH_2Cl_2:hexane 1:2 as eluent yielding 19 mg (89%) of a purple powder.

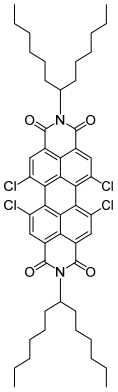
***N,N'*-di-(1'-hexylheptyl)-11,12-dichloro-4,5-dihydroperyleno[1,12b,12a,12-efg][1,4]dithiocine-1,14:8,9-tetracarboxydiimide (27)**

A mixture of 15 mg (0.24 mmol) of ethanedithiol, 19 mg (0.3 mmol) of KF and 160 mg (0.6 mmol) of 18-crown-6 were added to a solution of 54 mg (0.06 mmol) of *N,N'*-di-(1'-hexylheptyl)-1,6,7,12-tetrachloroperylene-3,4:9,10-tetracarboxydiimide in dry THF (6 mL). The reaction was refluxed 24 hours under argon atmosphere and, after cooling, it was extracted with dichloromethane and washed with water. The organic layer was dried over anhydrous sodium sulfate, filtered and evaporated. Purification was carried out by silica gel column chromatography using CH_2Cl_2:hexane 1:1 as eluent yielding 32 mg (59%) of a purple powder.

***N,N'*-di-(1'-hexylheptyl)-4,5,12,13-tetrahydroperyleno[1,12b,12a,12-efg:6,6a,6b,7-e'f'g']bis([1,4]dithiocine)-1,16:8,9-tetracarboxydiimide (28)**

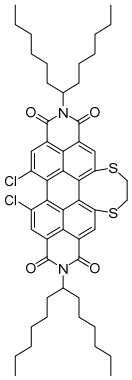
A mixture of 19 mg (0.3 mmol) of ethanedithiol, 38 mg (0.6 mmol) of KF and 320 mg (1.2 mmol) of 18-crown-6 were added to a solution of 54 mg (0.06 mmol) of *N,N'*-di-(1'-hexylheptyl)-1,6,7,12-tetrachloroperylene-3,4:9,10-tetracarboxydiimide in dry THF (3 mL). The reaction was refluxed 24 hours under argon atmosphere and, after cooling, it was extracted with dichloromethane and washed with water. The organic layer was dried over anhydrous sodium sulfate, filtered and evaporated. Purification was carried out by silica gel column chromatography using CH_2Cl_2:hexane 1:2 as eluent yielding 54 mg (96%) of a blue powder.

***N,N'*-di(1'-hexylheptyl)-1,6,7,12-tetrachloroperylene-3,4:9,10-tetracarboxydiimide (1)**



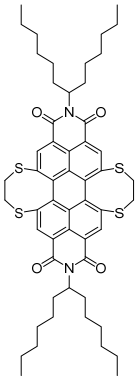
- The compound was prepared according to a described procedure (M. Queste, C. Cadiou, B. Pagoaga, L. Giraudet and N. Hoffmann, *New J. Chem.*, 2010, **34**, 2537-2545)
- Yield: 86%
- ^{1}H-NMR ($CDCl_3$) δ 0.83 (t, 12H), 1.23 (br, 32H), 1.85 (m, 4H), 2.22 (m, 4H), 5.17 (m, 2H), 8.66 (s, 4H)
- ^{13}C-NMR ($CDCl_3$) δ 163.47, 162.34, 135.29, 133.29, 132.73, 131.40, 128.41, 123.80, 123.46, 123.11, 55.23, 32.31, 32.24, 31.71, 31.71, 29.16, 26.84, 22.56, 14.01
- HRMS MALDI-TOF *m/z*: [M^+] calcd. for $C_{50}H_{58}N_2O_4Cl_4$ 890.3145, found: 890.3483
- IR (KBr): 2950, 2915, 2856, 1707, 1666, 1590, 1456, 1374, 1281, 1234, 1147, 803, 750, 674 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 431 (4.0), 492 (4.5), 522 (4.6)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 549

***N,N'*-di-(1'-hexylheptyl)-11,12-dichloro-4,5-dihydroperyleno[1,12b,12a,12-efg][1,4]dithiocine-1,14:8,9-tetracarboxydiimide (27)**



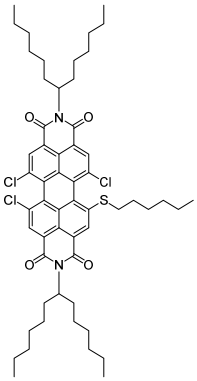
- Yield: 59%
- ^{1}H-NMR ($CDCl_3$) δ 0.84 (t, 12H), 1.25 (br, 32H), 1.85 (m, 4H), 2.22 (m, 4H), 3.35 (m, 4H), 5.18 (m, 2H), 8.64 (s, 2H), 8.92 (s, 2H)
- ^{13}C-NMR ($CDCl_3$) δ 134.90, 133.41, 129.54, 124.83, 55.10, 32.37, 31.74, 31.73, 30.86, 29.69, 29.20, 26.89, 22.59, 22.58, 14.03
- HRMS MALDI-TOF *m/z*: [M^+] calcd. for $C_{52}H_{62}N_2O_4Cl_2S_2$ 912.3528, found: 912.3435
- IR (KBr): 2920, 2844, 1695, 1660, 1578, 1456, 1380, 1275, 1246, 814, 744, 685 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 463 (4.1), 551 (4.2)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 537

***N,N'*-di-(1'-hexylheptyl)-4,5,12,13-tetrahydroperyleno[1,12b,12a,12-efg:6,6a,6b,7-e'f'g']bis([1,4]dithiocine)-1,16:8,9-tetracarboxydiimide (28)**



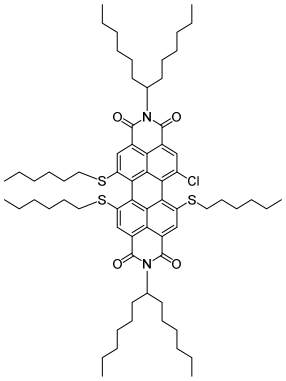
- Yield: 96%
- ^{1}H-NMR ($CDCl_3$) δ 0.83 (t, 12H), 1.25 (br, 32H), 1.84 (m, 4H), 2.25 (m, 4H), 3.35 (m, 8H), 5.19 (m, 2H), 8.85 (s, 2H), 8.88 (s, 2H)
- ^{13}C-NMR ($CDCl_3$) δ 164.17, 163.05, 138.86, 138.29, 136.95, 133.20, 127.89, 125.91, 122.76, 121.97, 54.80, 32.29, 31.63, 31.61, 30.66, 29.56, 29.12, 29.10, 26.78, 22.49, 22.47, 22.46, 22.45, 13.92
- HRMS MALDI-TOF *m/z*: [M^+] calcd. for $C_{54}H_{66}N_2O_4S_4$ 934.3905, found: 934.3590
- IR (KBr): 2914, 2856, 1695, 1660, 1584, 1374, 1269, 1234, 814 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 398 (4.0), 598 (4.2)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 649

***N,N'*-di-(1'-hexylheptyl)-1,6,7-trichloro-12-hexylthioperylene-3,4:9,10-tetracarboxydiimide (2a)**



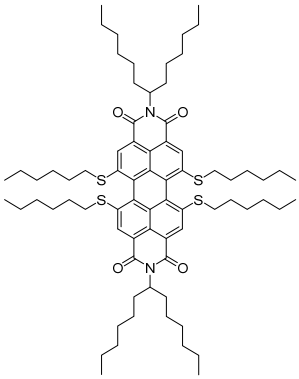
- Yield: 99%
- ^{1}H-NMR ($CDCl_3$) δ 0.78 (m, 3H), 0.83 (t, 12H), 1.14 (m, 4H), 1.24 (m, 34H), 1.50 (m, 2H), 1.85 (m, 4H), 2.25 (m, 4H), 3.01 (m, 2H), 5.17 (m, 2H), 8.66 (br, 4H)
- ^{13}C-NMR ($CDCl_3$) δ 163.68, 162.56, 141.97, 135.30, 134.83, 134.34, 133.04, 132.46, 131.40, 131.32, 130.40, 129.69, 129.04, 128.42, 127.98, 123.46, 123.42, 122.97, 55.15, 36.32, 32.33, 31.72, 31.15, 29.18, 29.16, 28.71, 28.35, 26.87, 22.57, 22.33, 14.01, 13.85
- HRMS MALDI-TOF *m/z*: [M^+] calcd. for $C_{56}H_{71}N_2O_4Cl_3S$ 972.4194, found: 972.4930
- IR (KBr): 2920, 2844, 1695, 1671, 1578, 1374, 1263, 1234, 808, 744, 680 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 483 (4.5), 525 (4.6)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 545

***N,N'*-di-(1'-hexylheptyl)-1-chloro-6,7,12-trihexylthioperylene-3,4:9,10-tetracarboxydiimide (2c)**



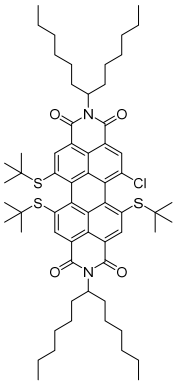
- Yield: 98%
- ^{1}H-NMR ($CDCl_3$) δ 0.76 (m, 9H), 0.84 (t, 12H), 1.12 (t, 6H), 1.25 (m, 44H), 1.46 (m, 6H), 1.87 (m, 4H), 2.26 (m, 4H), 2.99 (m, 6H), 5.19 (m, 2H), 8.62 (br, 1H), 8.71 (br, 3H)
- ^{13}C-NMR ($CDCl_3$) δ 164.65, 163.54, 144.59, 141.25, 140.37, 134.07, 134.02, 133.71, 131.17, 130.30, 130.24, 129.26, 123.39, 123.12, 122.99, 122.76, 122.57, 121.96, 121.93, 54.89, 36.63, 32.40, 31.75, 31.19, 31.18, 29.69, 29.23, 29.21, 28.70, 28.65, 28.60, 28.37, 28.35, 28.33, 26.92, 22.60, 22.37, 22.36, 22.35, 14.03, 13.88, 13.87
- HRMS MALDI-TOF *m/z*: [M^+] calcd. for $C_{68}H_{97}N_2O_4ClS_3$ 1136.6299, found: 1136.6529
- IR (KBr): 2926, 2833, 1701, 1666, 1584, 1467, 1368, 1269, 1251, 802, 750 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 550 (4.5)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 649

***N,N'*-di-(1'-hexylheptyl)-1,6,7,12-tetrahexylthioperylene-3,4:9,10-tetracarboxydiimide (2d)**



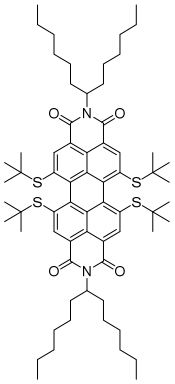
- Yield: 96%
- ^{1}H-NMR ($CDCl_3$) δ 0.75 (t, 12H), 0.84 (t, 12H), 1.24 (br, 64H), 1.87 (m, 4H), 2.26 (m, 4H), 2.95 (br, 8H), 5.20 (m, 2H), 8.68 (s, 2H), 8.72 (s, 2H)
- ^{13}C-NMR ($CDCl_3$) δ 164.65, 163.58, 139.27, 132.05, 131.20, 129.04, 122.83, 121.71, 54.69, 53.27, 36.65, 32.40, 32.34, 31.63, 31.07, 29.56, 29.14, 29.13, 28.49, 28.20, 26.85, 26.83, 22.48, 22.24, 13.91, 13.75
- HRMS MALDI-TOF *m/z*: [M^+] calcd. for $C_{74}H_{110}N_2O_4S_4$ 1218.7348, found: 1218.7791
- IR (KBr): 2926, 2838, 1701, 1660, 1585, 1462, 1362, 1275, 1234, 790 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 545 (4.3)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 680

***N,N'*-di-(1'-hexylheptyl)-1-chloro-6,7,12-tri-*t*-butylthioperylene-3,4:9,10-tetracarboxydiimide (4c)**



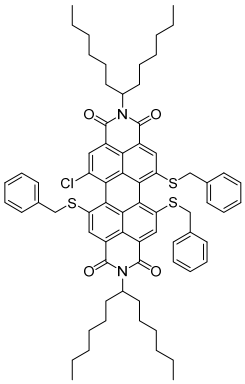
- Yield: 22%
- ^{1}H-NMR ($CDCl_3$) δ 0.77 (m, 39H), 1.25 (br, 32H), 1.93 (m, 4H), 2.23 (m, 4H), 5.18 (m, 2H), 8.62 (s, 1H), 8.84 (s, 3H)
- ^{13}C-NMR ($CDCl_3$) δ 136.91, 135.85, 135.25, 129.21, 128.28, 125.70, 124.19, 54.96, 49.97, 49.79, 49.74, 32.34, 31.92, 31.74, 31.71, 30.84, 30.58, 30.50, 29.69, 29.35, 29.19, 29.16, 27.03, 22.68, 22.57, 22.56, 14.10, 14.03
- HRMS MALDI-TOF *m/z*: [M^+] calcd. for $C_{62}H_{85}N_2O_4S_3Cl$ 1052.5360, found: 1052.5352
- IR (KBr): 2961, 2926, 2856, 1701, 1666, 1579, 1462, 1369, 1264, 1234, 1159, 820, 756 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 517 (4.6), 551 (4.7)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 619

***N,N'*-di-(1'-hexylheptyl)-1,6,7,12-tetra-*t*-butylthioperylene-3,4:9,10-tetracarboxydiimide (4d)**



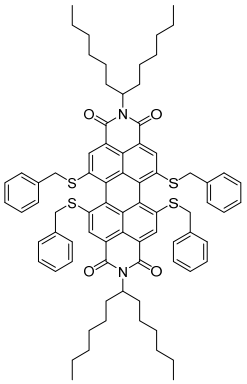
- Yield: 54%
- ^{1}H-NMR ($CDCl_3$) δ 0.76-0.83 (m, 48H), 1.25 (br, 32H), 1.97 (m, 4H), 2.18 (m, 4H), 5.18 (m, 2H), 8.86 (s, 4H)
- ^{13}C-NMR ($CDCl_3$) δ 164.47, 163.40, 139.97, 139.25, 137.85, 135.96, 127.80, 125.34, 54.97, 49.61, 32.43, 32.38, 31.72, 31.70, 30.47, 29.14, 27.12, 27.06, 22.54, 22.52, 14.02
- HRMS MALDI-TOF *m/z*: [M^+] calcd. for $C_{66}H_{94}N_2O_4S_4$ 1106.6090, found: 1106.6675
- IR (KBr): 2961, 2926, 2856, 1701, 1666, 1579, 1462, 1369, 1264, 1234, 1159, 820, 756 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 523 (4.3), 560 (4.4)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 616

***N,N'*-di-(1'-hexylheptyl)-1,6,7-tribenzylthio-12-chloroperylene-3,4:9,10-tetracarboxydiimide (3c)**



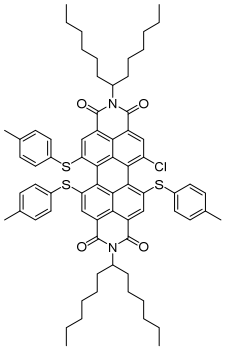
- Yield: 22%
- ^{1}H-NMR ($CDCl_3$) δ 0.80 (t, 12H), 1.23 (m, 32H), 1.87 (m, 4H), 2.26 (m, 4H), 3.46 (d, 1H), 3.71 (m, 2H), 3.89 (d, 1H), 4.01 (d, 1H), 4.23 (d, 1H), 5.19 (m, 2H), 6.18 (d, 2H), 6.34 (m, 3H), 6.58 (m, 5H), 6.98 (m, 5H), 8.47, (br, 1H), 8.76, (br, 3H)
- ^{13}C-NMR ($CDCl_3$) δ 164.43, 163.36, 147.67, 147.60, 147.05, 138.94, 138.53, 138.41, 137.57, 136.35, 136.18, 135.81, 135.51, 133.82, 130.49, 129.92, 129.09, 128.86, 128.45, 128.30, 127.54, 127.39, 126.91, 126.44, 125.98, 124.44, 124.06, 123.95, 123.68, 54.90, 43.54, 42.45, 41.24, 34.85, 34.50, 31.80, 31.42, 30.18, 29.68, 29.25, 29.21, 27.00, 26.99, 26.96, 22.61, 22.58, 14.05, 14.03
- HRMS MALDI-TOF *m/z*: [M+H$^+$] calcd. for $C_{71}H_{79}N_2ClO_4S_3$ 1155,4963 found: 1155.4981
- IR (KBr): 2956, 2938, 2839, 1689, 1660, 1590, 1456, 1386, 1258, 1088, 1030, 803 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 558 (4.4)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 603

***N,N'*-di-(1'-hexylheptyl)-1,6,7,12-tetrabenzylthioperylene-3,4:9,10-tetracarboxydiimide (3d)**



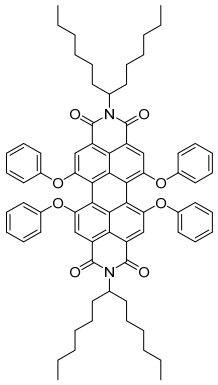
- Yield: 53%
- ^{1}H-NMR ($CDCl_3$) δ 0.84 (t, 12H), 1.28 (m, 32H), 1.90 (m, 4H), 2.29 (m, 4H), 3.93 (d, 4H), 4.07 (d, 4H), 5.24 (m, 2H), 6.81 (s, 20H), 8.72 (s, 2H), 8.76 (s, 2H)
- ^{13}C-NMR ($CDCl_3$) δ 164.65, 163.58, 147.67, 147.59, 147.06, 138.53, 138.41, 137.39, 135.75, 134.08, 133.28, 132.61, 128.86, 128.64, 128.52, 128.45, 128.29, 128.19, 127.86, 127.53, 127.39, 127.26, 126.83, 123.90, 121.98, 121.22, 54.80, 42.02, 34.86, 34.50, 32.49, 32.43, 31.81, 31.42, 30.18, 29.68, 29.25, 27.01, 26.99, 22.61, 14.05
- HRMS MALDI-TOF *m/z*: [M+H$^+$] calcd. for $C_{78}H_{86}N_2O_4S_4$ 1243.5470 found: 1243.5977
- IR (KBr): 2950, 2926, 2851, 1654, 1701, 1584, 1491, 1466, 1374, 1264, 1234, 1170, 692 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 521 (4.4), 585 (4.5)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 539

***N,N'*-di-(1'-hexylheptyl)-1-chloro-6,7,12-tri-*p*-tolylthioperylene-3,4:9,10-tetracarboxydiimide (5c)**



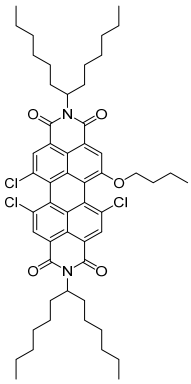
- Yield: 10%
- ^{1}H-NMR ($CDCl_3$) δ 0.84 (br, 12H), 1.24 (br, 32H), 1.83 (br, 4H), 2.26 (br, 13H), 5.14 (br, 2H), 7.10 (m, 12H), 8.52 (br, 4H)
- ^{13}C-NMR ($CDCl_3$) δ 141.08, 140.95, 139.12, 134.76, 133.90, 132.53, 130.88, 130.41, 130.35, 130.23, 130.18, 128.72, 123.23, 55.04, 54.74, 32.33, 31.70, 29.19, 29.17, 26.93, 22.57, 21.17, 14.02
- HRMS MALDI-TOF *m/z*: [M^+] calcd. for $C_{71}H_{79}N_2O_4ClS_3$ 1154.4885, found: 1154.4866
- IR (KBr): 2961, 2932, 2862, 1695, 1660, 1590, 1491, 1374, 1281, 1234, 1170, 820 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 491 (4.3), 555 (4.4)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 542

***N,N'*-di-(1'-hexylheptyl)-1,6,7,12-tetraphenoxyperylene-3,4:9,10-tetracarboxydiimide (8d)**



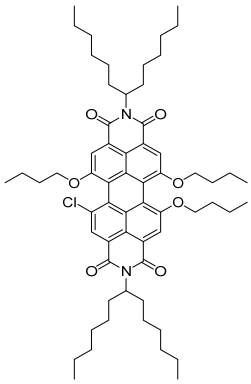
- Yield: 97%
- ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.81 (t, 12H), 1.20 (br, 32H), 1.76 (m, 4H), 2.11 (m, 4H), 5.07 (m, 2H), 6.95 (m, 8H), 7.11 (t, 4H), 7.27 (m, 8H), 8.16 (s, 2H), 8.20 (s, 2H)
- ^{13}C NMR ($CDCl_3$) δ 164.49, 163.38, 155.87, 155.27, 132.79, 132.64, 132.52, 130.33, 129.96, 129.52, 124.54, 123.30, 122.54, 120.33, 120.05, 119.81, 119.46, 116.45, 54.72, 32.38, 31.70, 29.15, 26.85, 22.54, 14.00
- HRMS MALDI-TOF *m/z*, [M^+] calc. for $C_{74}H_{78}N_2O_8$ 1122.5758 found: 1122.5100
- IR (KBr): 2956, 2926, 2839, 1701, 1672, 1596, 1497, 1415, 1334, 1304, 1211, 1170, 1071, 1030, 902, 808, 756, 686 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 443 (4.4), 533 (4.7), 570 (4.8)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 599

***N,N'*-di-(1'-hexylheptyl)-1-butoxy-6,7,12-trichloroperylene-3,4:9,10-tetracarboxydiimide (6a)**



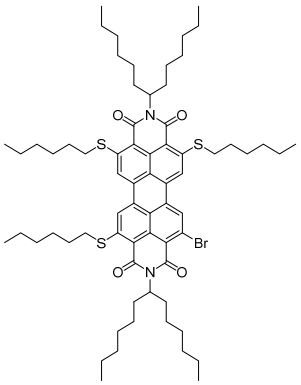
- Yield: 35%
- ^{1}H-RMN ($CDCl_3$) δ 0.84 (m, 12H), 1.02 (m, 3H), 1.25 (br, 32H), 1.48 (m, 2H), 1.85 (m, 6H), 2.25 (m, 4H), 4.44 (m, 2H), 5.18 (m, 2H), 8.43-8.65 (br, 4H)
- ^{13}C-RMN ($CDCl_3$) δ 157.45, 156.39, 135.31, 135.22, 134.39, 134.31, 131.90, 131.59, 131.42, 128.42, 123.78, 123.47, 120.57, 120.29, 69.92, 69.47, 69.25, 55.26, 55.09, 32.40, 32.33, 32.26, 31.74, 31.73, 31.16, 31.09, 29.69, 29.19, 29.17, 26.87, 22.58, 19.16, 19.10, 14.02, 13.80
- HRMS MALDI-TOF *m/z*: $[M+H]^+$ calc. for $C_{54}H_{67}N_2O_5Cl_3$ 929.4180, found: 929. 4508
- IR (KBr): 2956, 2926, 2839, 1701, 1656, 1590, 1415, 1374, 1275, 1252, 1240 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log λ): 424 (4.0), 482 (sh, 4.3), 517 (4.6), 550 (4.5)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 536

***N,N'*-di-(1'-hexylheptyl)-1,6,7-tributoxy-12-chloroperylene-3,4:9,10-tetracarboxydiimide (6c)**



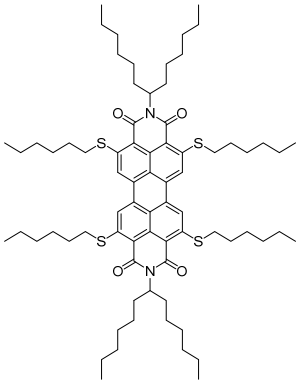
- Yield: 32%
- ^{1}H-RMN ($CDCl_3$) δ 0.83 (m, 12H), 0.98 (m, 9H), 1.25 (br, 32H), 1.44 (m, 6H), 1.81 (m, 10H), 2.29 (m, 4H), 4.07 (t, 1H), 4.36 (m, 5H), 5.21 (m, 2H), 8.28-8.65 (br, 4H)
- ^{13}C-RMN ($CDCl_3$) δ 157.19, 157.01, 156.96, 156.30, 132.15, 131.85, 131.83, 120.91, 120.58, 117.60, 69.21, 64.09, 54.81, 34.41, 32.49, 32.43, 31.91, 31.76, 31.50, 31.18, 30.70, 29.68, 29.35, 29.25, 26.92, 25.02, 22.68, 22.59, 19.20, 19.14, 19.07, 19.05, 14.10, 14.03, 13.86, 13.82, 13.70
- HRMS MALDI-TOF *m/z*: $[M]^+$ calc. for $C_{62}H_{85}N_2O_7Cl$ 1004.6045, found: 1004.6232
- IR (KBr): 2956, 2921, 2845, 1701, 1666, 1590, 1468, 1404, 1293, 1077cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log λ): 430 (4.2), 560 (4.6)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 650

***N,N'*-di-(1'-hexylheptyl)-2-bromo-5,8,11-trihexylthio-3,4:9,10-perylenetetracarboxydiimide (13c)**



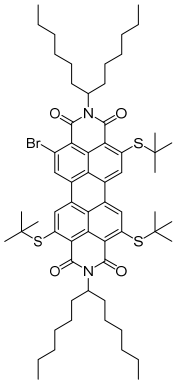
- Yield: 66%
- ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.83 (t, 12H), 0.93 (t, 9H), 1.32 (br, 46H), 1.65 (m, 4H), 1.93 (m, 10H), 2.22 (m, 4H), 3.17 (t, 6H), 5.20 (m, 2H), 8.13 (s, 1H), 8.22 (s,1H), 8.30 (s, 1H), 8.41 (s, 1H)
- ^{13}C NMR ($CDCl_3$) δ 163.29, 161.21, 151.15, 150.62, 133.29, 132.80, 132.30, 132.19, 132.09, 131.69, 131.30, 130.30, 128.95, 128.84, 122.43, 122.13, 120.08, 119.67, 119.36, 118.53, 117.96, 55.39, 55.00, 32.85, 32.77, 32.67, 32.54, 32.23, 31.77, 31.76, 31.64, 31.61, 31.60, 31.59, 31.57, 29.66, 29.25, 29.23, 29.18, 29.14, 28.07, 27.82, 27.20, 27.13, 22.59, 22.58, 22.51, 14.04, 14.02, 14.01
- HRMS MALDI-TOF *m/z*, [M+H$^+$] calc. for $C_{68}H_{97}N_2O_4S_3Br$ 1181.5794 found: 1181.5276
- IR (KBr): 2926, 2862, 1683, 1636, 1555, 1456, 1345, 1240, 814, 744 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 501 (4.7), 540 (4.8)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 569

***N,N'*-di-(1'-hexylheptyl)-2,5,8,11-tetrahexylthio-3,4:9,10-perylenetetracarboxydiimide (13d)**



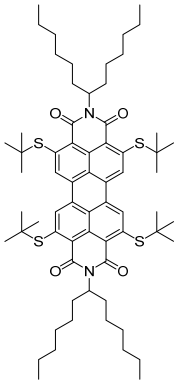
- Yield: 99%
- ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.83 (t, 12H), 0.93 (t, 12H), 1.30 (br, 52H), 1.65 (m, 4H), 1.94 (m, 12H), 2.25 (m, 4H), 3.20 (t, 8H), 5.23 (m, 2H), 8.37 (s, 4H)
- ^{13}C NMR ($CDCl_3$) δ 164.04, 163.30, 150.48, 131.93, 124.01, 120.13, 117.93, 116.77, 54.81, 32.63, 32.11, 31.64, 31.59, 31.46, 31.42, 29.12, 27.79, 26.99, 22.46, 22.41, 22.34, 13.93, 13.90, 13.89, 13.83
- HRMS MALDI-TOF *m/z*, [M+H$^+$] calc. for $C_{74}H_{110}N_2O_4S_4$ 1219.7348, found: 1219.7754
- IR (KBr): 2932, 2844, 1677, 1636, 1555, 1345, 1234, 849, 738 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 489 (5.1), 543 (5.1)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 556

***N,N'*-di-(1'-hexylheptyl)-2-bromo-5,8,11-tri-*t*-butylthioperylene-3,4:9,10-tetracarboxydiimide (15c)**



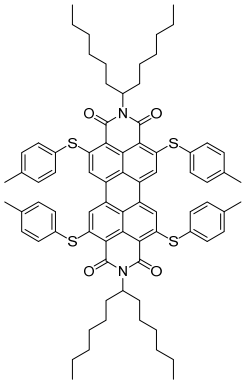
- Yield: 15%
- ^{1}H-NMR ($CDCl_3$) δ 0.82 (t, 12H), 1.22 (m, 32H), 1.77 (m, 27H), 1.92 (m, 4H), 2.22 (m, 4H), 5.23 (m, 2H), 8.59 (s, 1H), 8.73 (s, 2H), 8.81 (s, 1H)
- ^{13}C-NMR ($CDCl_3$) δ 133.70, 132.75, 132.37, 129.22, 123.03, 122.77, 121.15, 120.59, 55.40, 55.11, 47.28, 47.09, 46.89, 32.18, 31.77, 31.76, 31.75, 31.64, 31.63, 31.55, 29.23, 29.19, 27.03, 26.96, 22.57, 14.06
- HRMS MALDI-TOF *m/z*: [M^+] calcd. for $C_{62}H_{85}BrN_2O_4S_3$ 1096.4854 found: 1096.4369
- IR (KBr): 2961, 2915, 2839, 1643, 1476, 1334, 1294, 1053, 820 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 498 (4.5), 540 (4.48)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 540

***N,N'*-di-(1'-hexylheptyl)-2,5,8,11-tetra-*t*-butylthioperylene-3,4:9,10-tetracarboxydiimide (15d)**



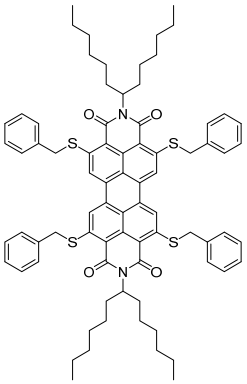
- Yield: 80%
- ^{1}H-NMR ($CDCl_3$) δ 0.82 (t, 12H), 1.22 (m, 32H), 1.75 (m, 36H), 1.91 (m, 4H), 2.23 (m, 4H), 5.19 (m, 2H), 8.72 (s, 4H)
- ^{13}C-NMR ($CDCl_3$) δ 163.60, 162.87, 149.91, 149.50, 132.34, 131.62, 122.70, 121.10, 119.45, 118.71, 55.03, 46.85, 32.16, 31.73, 31.61, 29.19, 26.97, 22.53, 14.03
- HRMS MALDI-TOF *m/z*: [M^+] calcd. for $C_{66}H_{94}N_2O_4S_4$ 1106.6096 found: 1106.6461
- IR (KBr): 2958, 2925, 2852, 1687, 1646, 1585, 1552, 1511, 1462, 1417, 1336, 1230, 1156, 821, 743 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 498 (4.6), 542 (4.6)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 574

***N,N'*-di-(1'-hexylheptyl)-2,5,8,11-tetra-*p*-tolylthioperylene-3,4:9,10-tetracarboxydiimide (16d)**



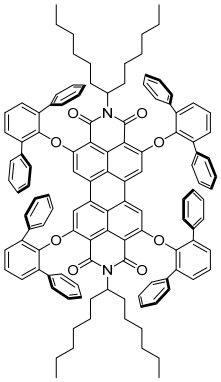
- Yield: 88%
- ^{1}H-NMR ($CDCl_3$) δ 0.83 (t, 12H), 1.23 (m, 32H), 1.93 (m, 4H), 2.23 (m, 4H), 2.51 (s, 12 H), 5.25 (m, 2H), 7.20 (d, 8H), 7.29 (d, 8H), 7.41 (s, 4H)
- ^{13}C-NMR ($CDCl_3$) δ 164.14, 163.42, 151.61, 151.03, 139.42, 137.31, 134.22, 133.79, 132.39, 130.86, 130.82, 129.67, 129.01, 128.40, 121.77, 120.85, 116.78, 116.16, 54.91, 32.20, 31.70, 31.68, 29.63, 29.15, 26.95, 22.54, 22.52, 21.42, 20.97, 14.01
- HRMS MALDI-TOF *m/z*: [M^+] calcd. for $C_{78}H_{86}N_2O_4S_4$ 1242.5470 found: 1242.5872
- IR (KBr): 2925, 2856, 1667, 1638, 1589, 1560, 1520, 1487, 1438, 1344, 1287, 1234, 1115, 1013, 800 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 463 (4.5), 495 (4.8), 532 (4.7)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 539

***N,N'*-di-(1'-hexylheptyl)-2,5,8,11-tetrabenzylthioperylene-3,4:9,10-tetracarboxydiimide (14d)**



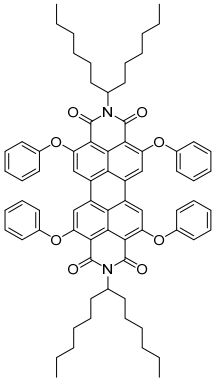
- Yield: 90%
- ^{1}H-NMR (C_2Cl_4) δ 0.82 (m, 12H), 1.21 (m, 32H), 1.90 (m, 4H), 2.16 (m, 4H), 4.22 (s, 8H), 5.17 (m, 2H), 7.32 (m, 12H), 7.45 (m, 8H), 8.22 (s, 4H)
- ^{13}C-NMR (C_2Cl_4) δ 163.94, 150.85, 135.12, 132.63, 132.07, 129.93, 129.64, 129.36, 129.30, 128.78, 128.24, 127.71, 121.03, 119.00, 55.35, 37.78, 32.61, 32.00, 29.46, 27.34, 22.82, 14.27
- HRMS MALDI-TOF *m/z*: [M+H$^+$] calcd. for $C_{78}H_{86}N_2O_4S_4$ 1243.5543 found: 1243.5520
- IR (KBr): 2915, 2856, 1672, 1631, 1549, 1520, 1450, 1345, 1246, 820, 715, 686 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 504 (4.2), 544 (4.2)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 557

***N,N'*-di-(1'-hexylheptyl)-2,5,8,11-tetrakis(diphenylphenoxy)perylene-3,4:9,10-tetracarboxydiimide (19d)**



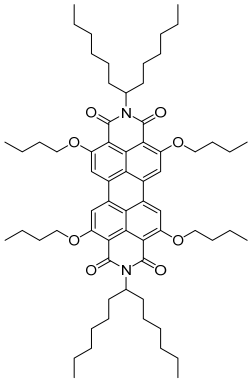
- Yield: 96%
- ^{1}H NMR ($CDCl_3$) δ 0.93 (m, 12H), 1.35 (m, 32H), 1.85 (m, 4H), 2.31 (m, 4H), 5.24 (m, 2H), 6.25 (s, 4H), 7.11 (m, 25H), 7.45 (m, 15H), 7.55 (m, 8H), 7.67 (m, 4H)
- ^{13}C NMR ($CDCl_3$) δ 159.51, 146.69, 136.83, 136.82, 136.81, 135.51, 133.31, 132.78, 130.83, 129.33, 129.01, 128.82, 128.04, 127.52, 127.01, 116.20, 109.29, 53.29, 32.31, 31.99, 30.89, 29.43, 26.83, 22.72, 14.18
- HRMS (MALDI-TOF): *m/z*: [M^+] calcd. for $C_{122}H_{110}N_2O_8$ 1730.8256; found: 1730.8291
- IR (KBr): 3078, 2921, 2845, 1689, 1654, 1549, 1404, 1369, 1299, 1188, 750, 698 cm^{-1}
- UV-Vis (CH_2Cl_2), λ_{max}/nm (log ε): 421 (4.3), 460 (4.2), 493 (4.6), 532 (4.8)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 540

***N,N'*-di-(1'-hexylheptyl)-2,5,8,11-tetraphenoxyperylene-3,4:9,10-tetracarboxydiimide (18d)**



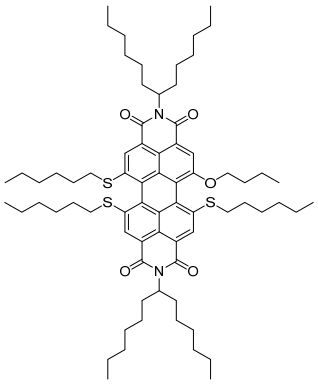
- Yield: 75%
- ^{1}H-NMR ($CDCl_3$) δ 0.81 (t, 12H), 1.19 (m, 32H), 1.78 (m, 4H), 2.08 (m, 4H), 5.09 (m, 2H), 7.08 (m, 8H), 7.22 (m, 4H), 7.36 (m, 8H), 7.56 (s, 4H)
- ^{13}C-NMR ($CDCl_3$) δ 160.87, 155.35, 134.37, 133.50, 130.06, 124.82, 119.55, 118.68, 114.98, 111.88, 54.44, 32.15, 31.73, 29.15, 26.94, 22.52, 14.01
- HRMS MALDI-TOF *m/z*: [M^+] calcd. for $C_{74}H_{78}N_2O_8$ 1122.5758 found: 1122.5442
- IR (KBr): 2938, 2845, 1689, 1660, 1596, 1485, 1363, 1328, 1211, 738 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 420 (4.3), 453 (4.4), 484 (4.7), 520 (4.8)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 533

***N,N'*-di(hexylheptyl)-2,5,8,11-tetrabutoxy-3,4:9,10-perylenetetracarboxydiimide (17d)**



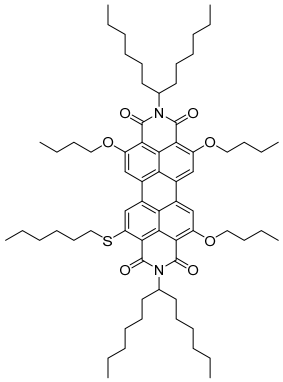
- Yield: 40%
- ^{1}H-RMN ($CDCl_3$) δ 0.83 (t, 12H), 1.05(t, 12H), 1.25 (br, 32H), 1.65 (m, 8H), 1.86 (m, 4H), 2.04 (m, 8H), 2.23 (m, 4H), 4.44 (m, 8H), 5.19 (m, 2H), 7.99 (s, 4H)
- ^{13}C-RMN ($CDCl_3$) δ 162.74, 133.87, 116.65, 109.73, 98.82, 70.37, 53.86, 53.27, 32.22, 31.70, 31.24, 29.56, 29.20, 26.90, 22.48, 19.08, 13.96, 13.76
- HRMS MALDI-TOF *m/z*: $[M+H]^+$ calc. for $C_{66}H_{95}N_2O_8$ 1043.7004, found: 1043.7092
- IR (KBr): 2973, 2920, 2844, 1689, 1648, 1590, 1351, 1257, 855 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 412 (4.2), 497 (4.5), 535 (4.6)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 548, 592

***N,N'*-di-(1'-hexylheptyl)-1-butoxy-6,7,12-trihexylthioperylene-3,4:9,10-tetracarboxydiimide (23)**



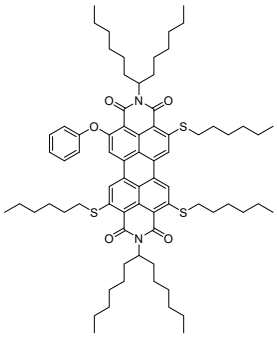
- Yield: 89%
- ^{1}H-RMN ($CDCl_3$) δ 0.75 (t, 9H), 0.84 (t, 12H), 0.96 (t, 3H), 1.09 (br, 12H), 1.25 (br, 38H), 1.41 (br, 6H), 1.87 (m, 4H), 2.26 (m, 4H), 2.95 (br, 6H), 4.32 (m, 1H), 4.49 (m, 1H), 5.20 (m, 2H), 8.38 (m, 1H), 8.70 (m, 3H)
- ^{13}C-RMN ($CDCl_3$) δ 164.83, 163.94, 163.73, 139.46, 139.39, 139.23, 132.21, 131.22, 129.17, 123.14, 122.96, 120.03, 54.82, 36.81, 32.53, 32.47, 31.76, 31.20, 31.17, 30.88, 29.69, 29.27, 28.62, 28.33, 28.27, 26.96, 22.61, 22.37, 22.35, 22.33, 19.15, 14.04, 13.88
- HRMS MALDI-TOF *m/z*: $[M]^+$ calc. for $C_{72}H_{106}N_2O_5S_3$ 1174.7264, found: 1174.7620
- IR (KBr): 2956, 2932, 2856, 1701, 1649, 1444, 1363, 1264, 1240, 1077, 1018, 797 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 549 (sh, 4.4), 585 (4.5)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 647

***N,N'*-di(1'-hexylheptyl)-2,5,8-tributoxy-11-hexylthioperylene-3,4:9,10-tetracarboxydiimide (22)**



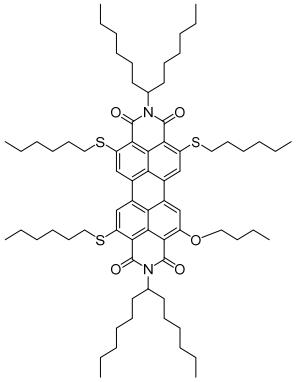
- Yield: 92%
- ^{1}H-RMN ($CDCl_3$) δ 0.83 (t, 12H), 0.92 (t, 3H), 1.05 (m, 9H), 1.22 (br, 32H), 1.39 (br, 6H), 1.65 (br, 8H), 1.91 (m, 4H), 2.04 (m, 6H), 2.23 (m, 4H), 3.19 (t, 2H), 4.45 (m, 6H), 5.21 (m, 2H), 7.99 (s, 1H), 8.03 (s, 2H), 8.29 (s, 1H)
- ^{13}C-RMN ($CDCl_3$) δ 162.92, 162.78, 162.73, 134.96, 134.66, 134.08, 132.99, 131.88, 118.33, 117.68, 116.86, 110.05, 109.51, 70.52, 70.24, 54.00, 32.57, 32.33, 32.27, 31.82, 31.79, 31.56, 31.36, 31.33, 29.33, 29.28, 28.23, 27.05, 27.02, 22.60, 22.59, 22.56, 19.24, 19.21, 14.05, 14.02, 13.89, 13.86
- HRMS MALDI-TOF *m/z*: $[M]^+$ calc. for $C_{68}H_{98}N_2O_7S$ 1086.7095, found: 1086.7812
- IR (KBr): 2950, 2929, 2852, 1695, 1646, 1601, 1573, 1544, 1471, 1409, 1344, 1299, 1250, 1103 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 430 (4.2), 472 (4.3), 502 (4.5), 541 (4.7)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 558

***N,N'*-di(1'-hexylheptyl)-2,5,8-trihexylthio-11-phenoxyperylene-3,4:9,10-tetracarboxydiimide (21)**



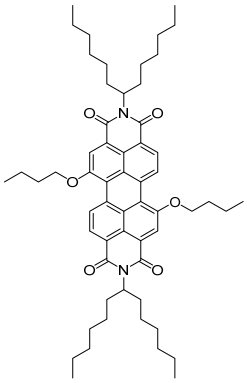
- Yield: 85%
- ^{1}H-RMN ($CDCl_3$) δ 0.83 (m, 12H), 0.93 (m, 9H), 1.21 (br, 32H), 1.36 (br, 12H), 1.50 (m, 3H), 1.64 (m, 3H), 1.74 (m, 3H), 1.95 (br, 7H), 2.18 (br, 4H), 2.85 (m, 3H), 3.21 (m, 3H), 5.20 (m, 2H), 7.26 (m, 4H), 7.48 (t, 2H), 7.88 (s, 1H), 7.96 (d, 1H), 8.42 (d, 1H)
- ^{13}C-RMN ($CDCl_3$) δ 161.06, 161.00, 155.51, 135.12, 134.89, 132.99, 132.84, 132.15, 131.97, 131.40, 130.19, 125.00, 54.88, 32.76, 32.36, 32.20, 31.77, 31.75, 31.73, 31.56, 31.52, 29.67, 29.23, 29.20, 29.05, 27.93, 27.69, 27.03, 22.57, 22.55, 22.52, 14.05, 14.03, 14.02
- HRMS MALDI-TOF *m/z*: $[M]^+$ calc. for $C_{74}H_{102}N_2O_5S_3$ 1194.6951, found: 1194.6512
- IR (KBr): 2956, 2921, 2845, 1695, 1654, 1573, 1456, 1421, 1339, 1293, 1229, 1199, 855, 750, 686 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 464 (4.5), 498 (4.6), 538 (4.7)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 581

***N,N'*-di-(1'-hexylheptyl)-2-butoxy-5,8,11-trihexylthioperylene-3,4:9,10-tetracarboxydiimide (20)**



- Yield: 28%
- ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.83 (t, 12H), 0.93 (t, 9H), 1.06 (t, 3H), 1.25 (br, 32H), 1.39 (br, 14H), 1.64 (m, 4H), 1.94 (br, 12H), 2.04 (m, 2H), 2.24 (m, 4H), 3.20 (br, 6H), 4.45 (t, 2H), 5.24 (m, 2H), 8.07 (s, 1H), 8.34 (s, 1H), 8.36 (s, 1H), 8.40 (s, 1H)
- ^{13}C NMR ($CDCl_3$) δ 164.15, 163.42, 162.59, 161.42, 133.03, 131.96, 131.86, 129.60, 125.13, 123.81, 123.10, 122.91, 120.08, 118.46, 118.05, 117.98, 117.52, 54.78, 32.62, 32.46, 32.15, 32.11, 31.79, 31.67, 31.63, 31.45, 31.43, 31.18, 29.56, 29.16, 29.11, 27.83, 27.80, 26.95, 22.47, 22.46, 22.44, 22.40, 19.12, 13.93, 13.90, 13.73
- HRMS MALDI-TOF *m/z*. [M+H$^+$] calc. for $C_{72}H_{106}N_2O_5S_3$ 1175.7264, found: 1175.7564
- IR (KBr): 2914, 2844, 1671, 1636, 1590, 1561, 1479, 1339, 1257, 802 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 473 (4.4), 501 (4.5), 540 (4.5)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 589

***N,N'*-di(1'-hexylheptyl)-1,7(6)-dibutoxyperylene-3,4:9,10-tetracarboxydiimide (11)**



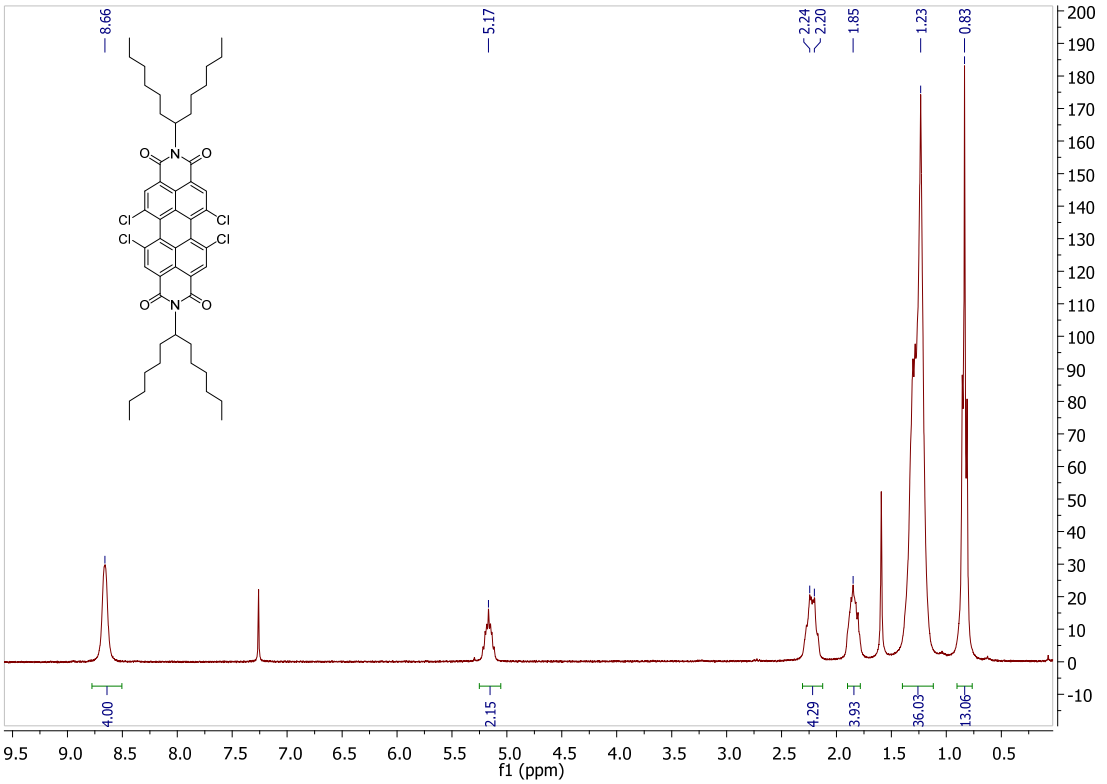
- Yield: 95% (70% isomer 1,7; 30% isomer 1,6)
- ^{1}H-RMN ($CDCl_3$) δ 0.83 (t, 12H), 1.08 (t, 6H), 1.23 (br, 32H), 1.67 (m, 4H), 1.87 (m, 4H), 2.06 (m, 4H), 2.26 (m, 4H), 4.48 (m, 4H), 5.19 (m, 2H), 8.46 (br, 4H), 9.51 (isomer 1,6) (d, 1H), 9.58 (isomer 1,7) (d, 1H)
- ^{13}C-RMN ($CDCl_3$) δ 164.82, 163.82, 157.96, 156.80, 134.25, 133.76, 130.69, 129.43, 129.20, 128.66, 128.50, 127.88, 127.11, 123.78, 123.11, 121.76, 121.40, 121.13, 120.61, 118.99, 117.98, 117.26, 70.25, 54.86, 54.57, 54.41, 32.39, 31.75, 31.42, 29.22, 26.91, 22.56, 19.56, 14.01, 13.85
- HRMS MALDI-TOF *m/z*: $[M]^+$ calc. for $C_{58}H_{78}N_2O_2$ 898.5860, found: 898.5826
- IR (KBr): 2955, 2920, 2844, 1695, 1649, 1596, 1467, 1327, 814, 744 cm^{-1}
- UV Vis (CH_2Cl_2), λ_{max}/nm (log ε): 531 (4.2), 568 (4.3)
- Fluorescence (CH_2Cl_2), λ_{em}/nm: 591

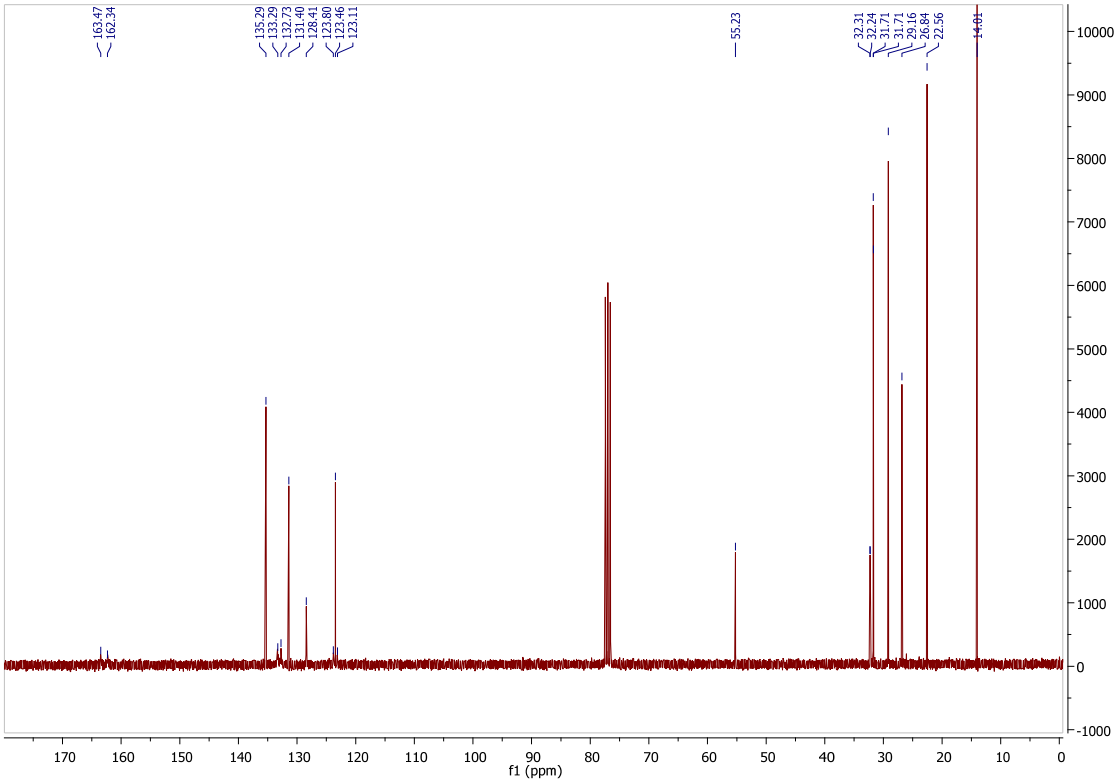
Electrochemical data of new compounds

PDI	E red 2	E red 1	E ox 1	E ox 2
1	-1.15	-0.88		
2a	-1.05	-0.83	0.51 irrev	1.27 irrev
2c	-1.29	-1.03	0.87 irrev	1.02 irrev
2d	-1.38	-1.11	0.78 irrev	0.88 irrev
3c		-1.01	0.98	
3d	-1.33	-1.07	0.88	1.35
4c	-1.25	-0.97	1.05	1.38
4d	-1.36	-1.03	0.99	1.13
5c	-1.13	-0.95		
6a	-0.99	-0.87	0.95	
6c	-1.40	-1.23	0.75	
8d	-1.32	-1.13	0.96	
11	-1.46	-1.26	0.87	
13c	-1.28	-1.09	1.45 irrev	
13d	-1.52	-1.09	1.32	1.71
14d	-1.35	-1.11		
15c	-1.33	-1.08	0.78 irrev	
15d	-1.39	-1.17	1.11 irrev	1.40
16d	-1.36	-1.16	1.07	1.35
17d		-1.34	0.68 irrev	1.05 irrev
18d	-1.30	-1.07	1.32 irrev	1.67 irrev
19d	-1.51	-1.33	1.32 irrev	1.84 irrev
20		-0.73	0.79	
21	-1.33	-1.13		
22		-1.36		
23	-1.37	-1.09	0.24	0.80
27	-1.19	-0.81	1.09 irrev	1.69 irrev
28	-1.19	-0.96	0.87 irrev	1.17 irrev

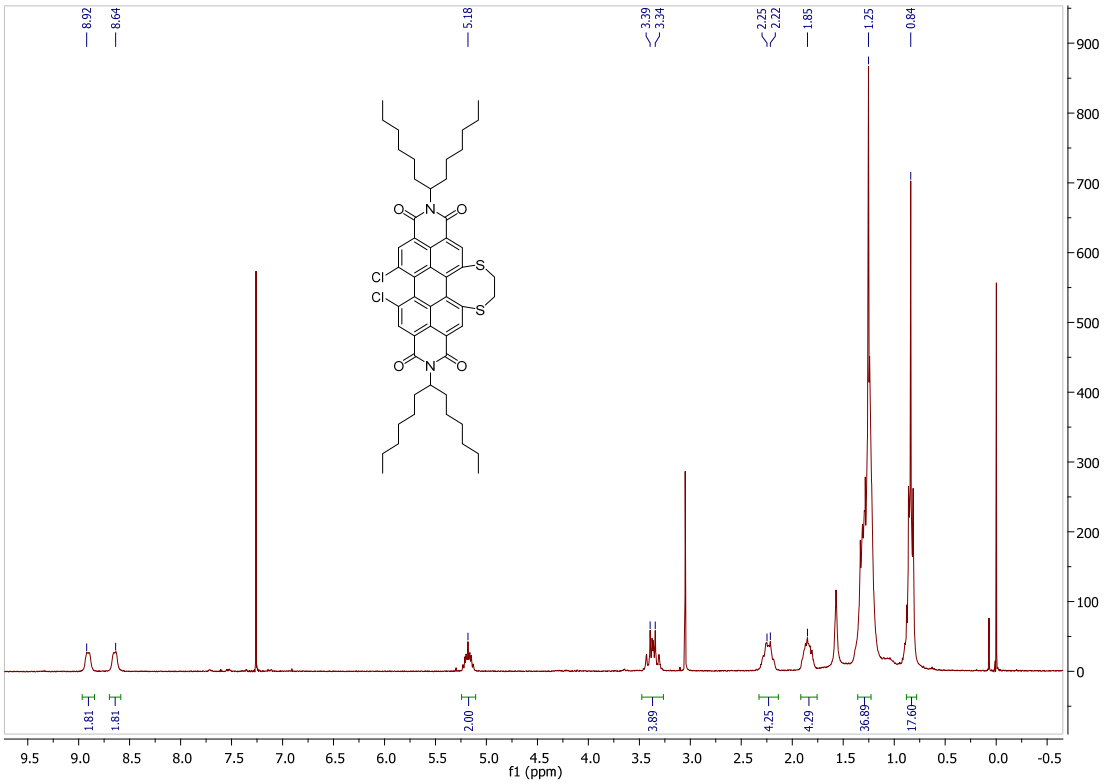
Redox potentials were measured in CH_2Cl_2 with 0.1 M $TBAPF_6$ *vs.* Fc/Fc^+. A glassy carbon working electrode, $Ag/AgNO_3$ reference electrode and a platinum wire counter electrode were employed.

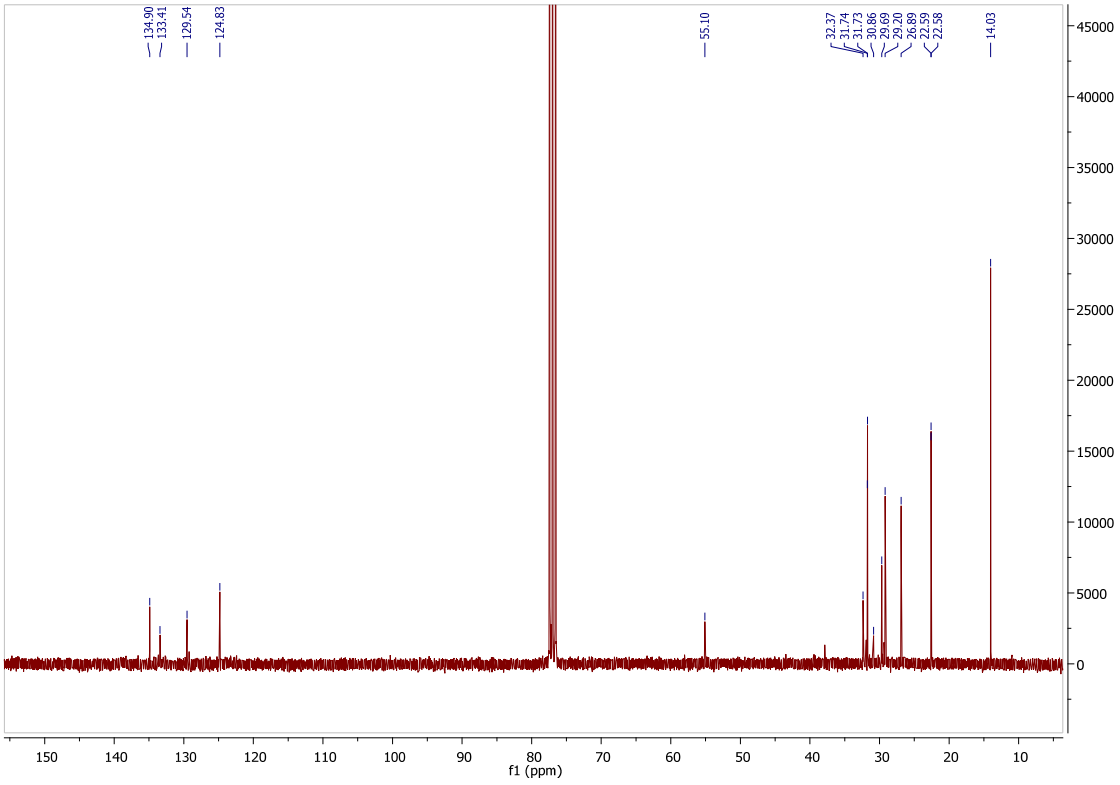
_N,N'_-di(1'-hexylheptyl)-1,6,7,12-tetrachloroperylene-3,4:9,10-tetracarboxydiimide (1)



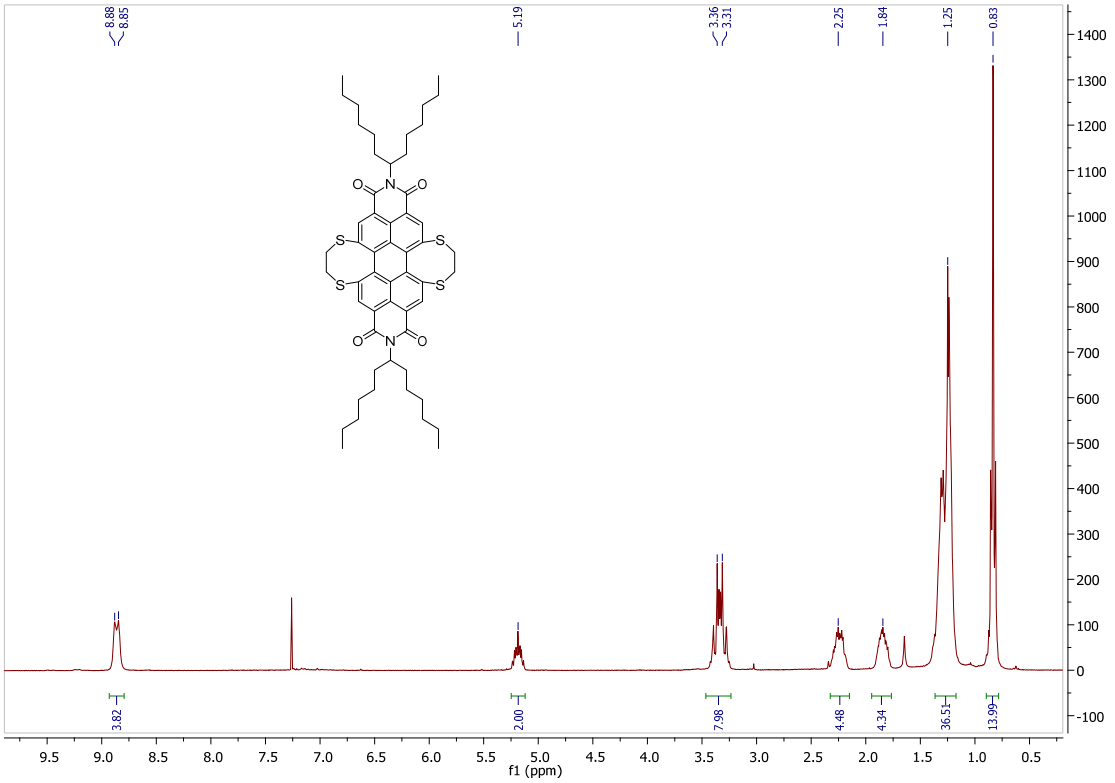


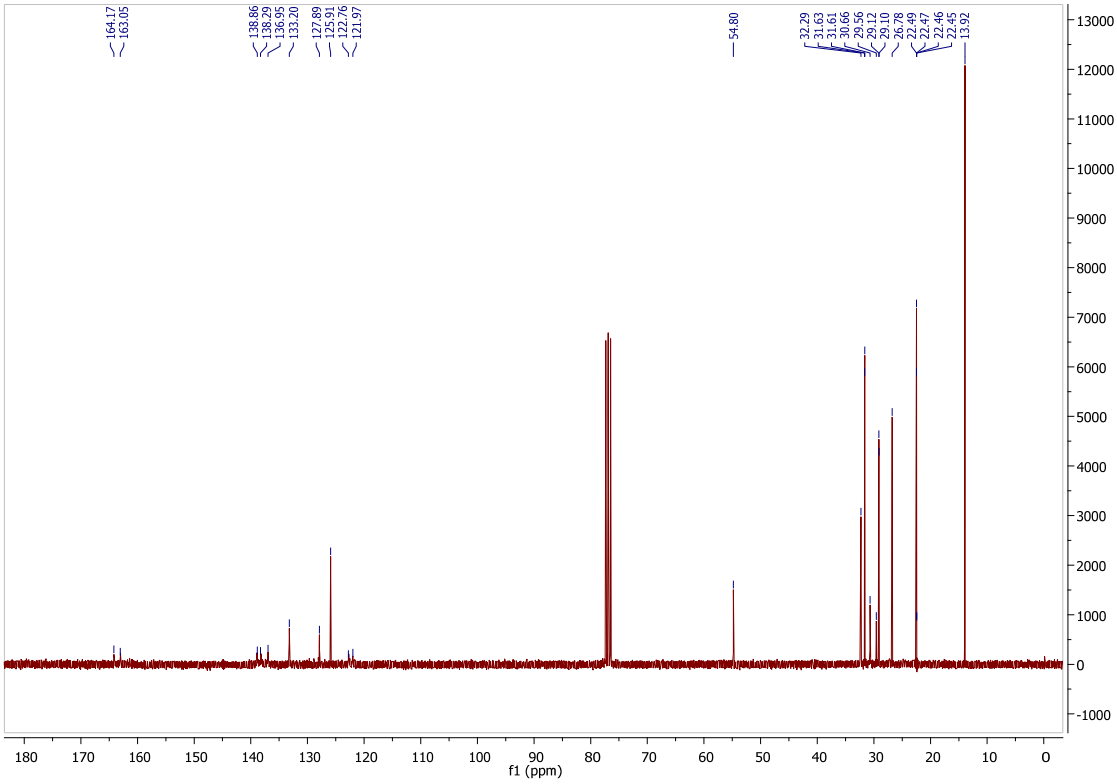
***N,N'*-di-(1'-hexylheptyl)-11,12-dichloro-4,5-dihydroperyleno[1,12b,12a,12-efg][1,4]dithiocine-1,14:8,9-tetracarboxydiimide (27)**



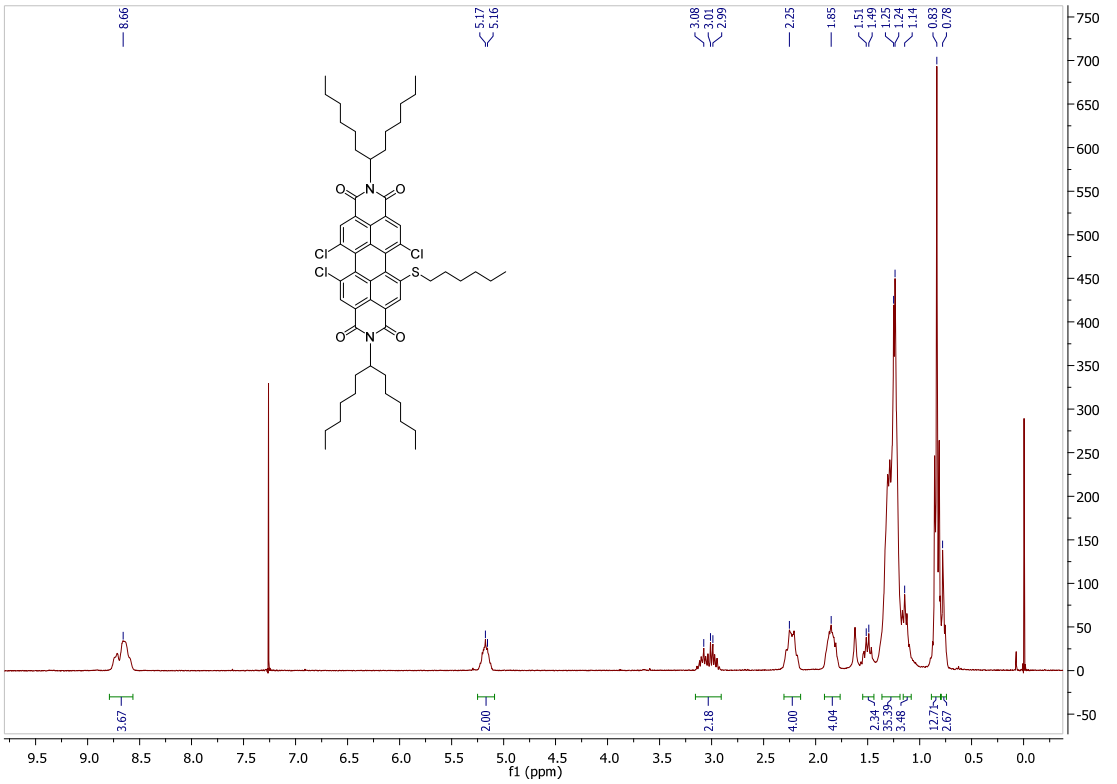


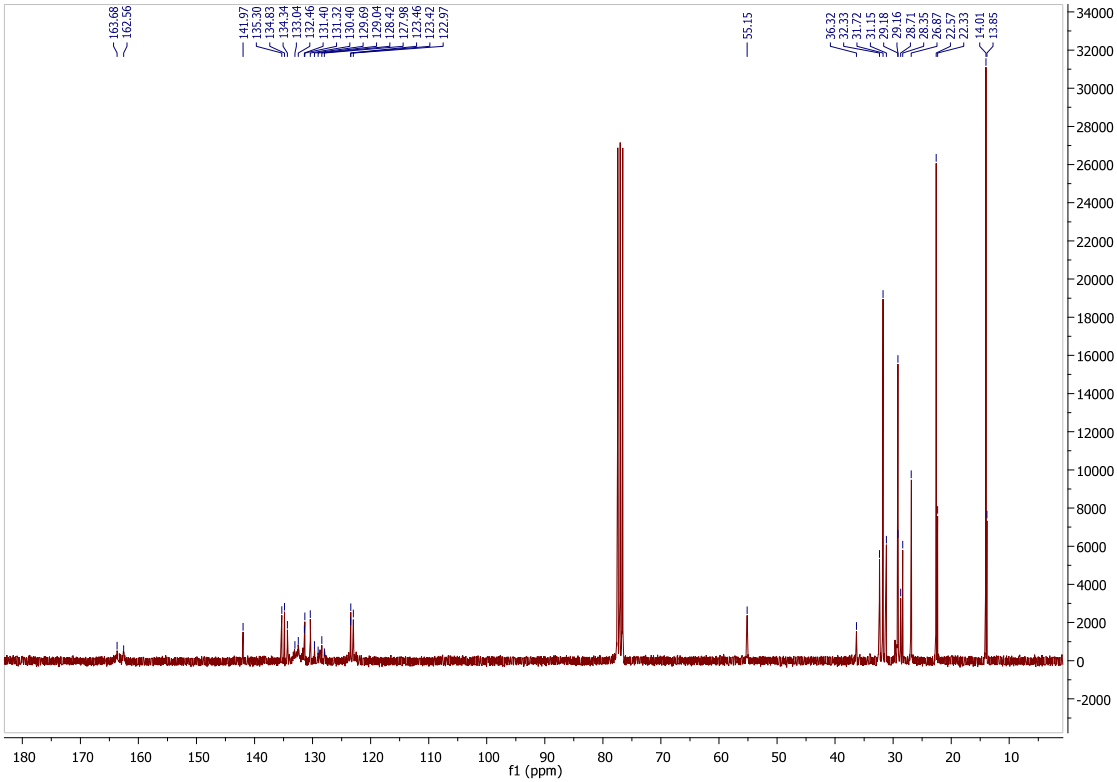
***N,N'*-di-(1'-hexylheptyl)-4,5,12,13-tetrahydroperyleno[1,12b,12a,12-efg:6,6a,6b,7-e'f'g']bis([1,4]dithiocine)-1,16:8,9-tetracarboxydiimide (28)**



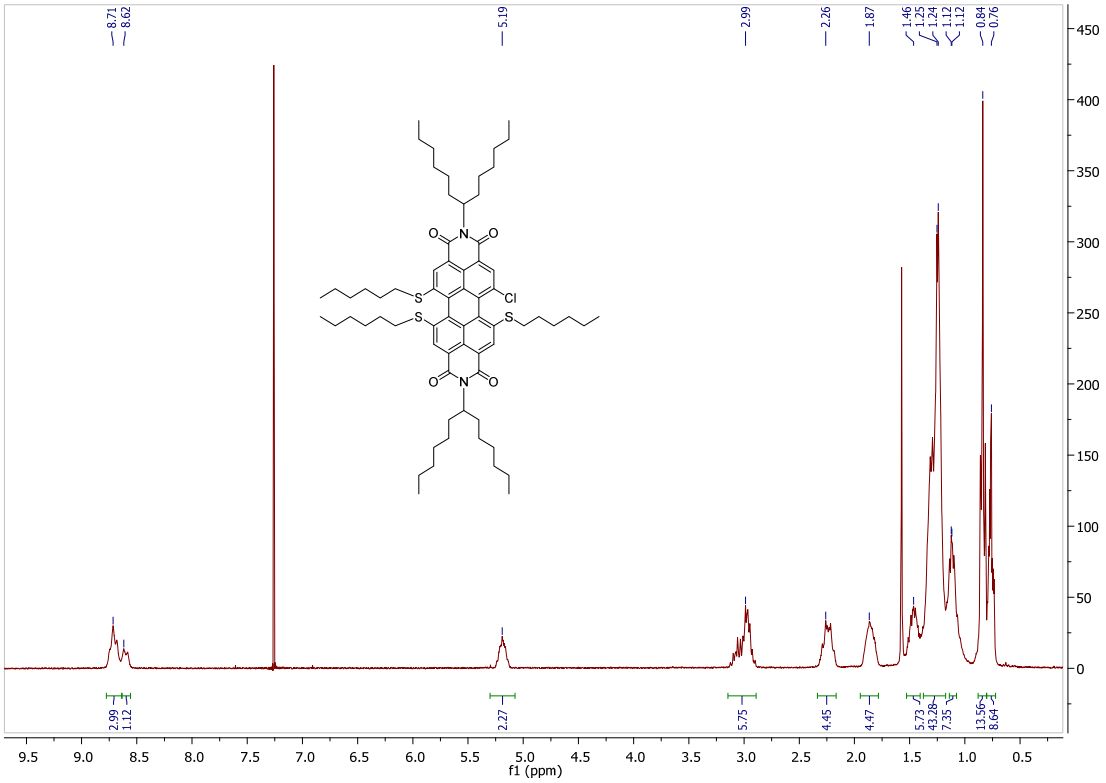


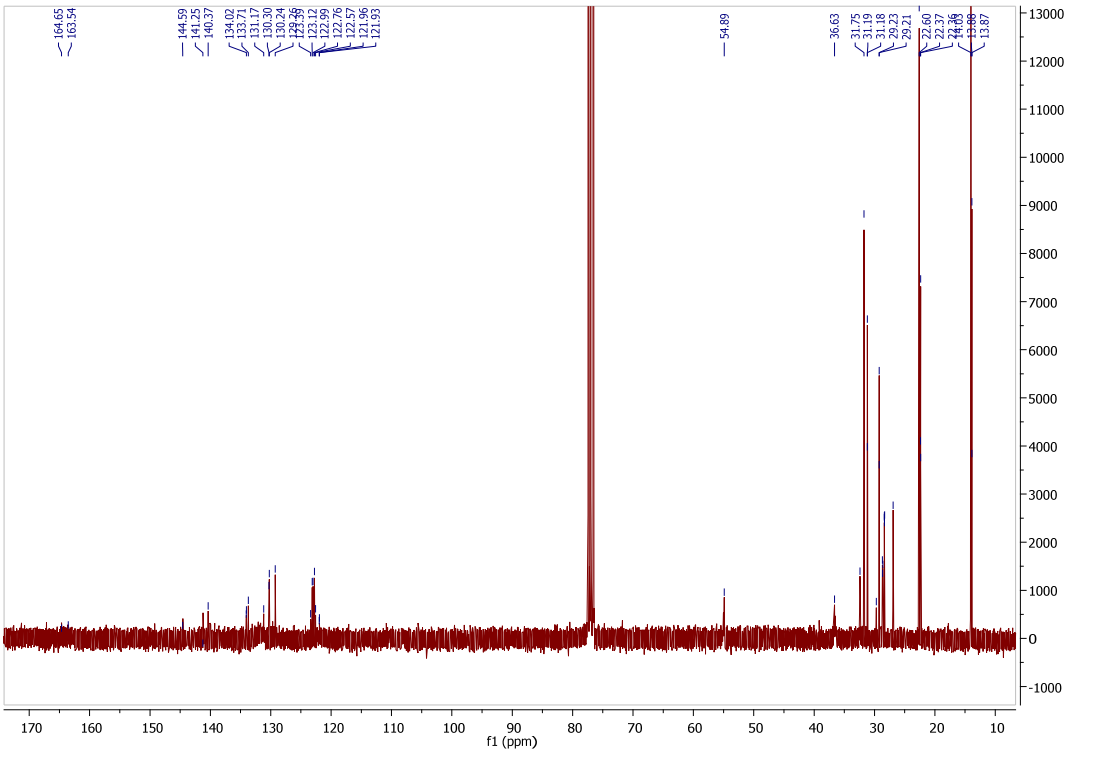
***N,N'*-di-(1'-hexylheptyl)-1,6,7-trichloro-12-hexylthioperylene-3,4:9,10-tetracarboxydiimide (2a)**



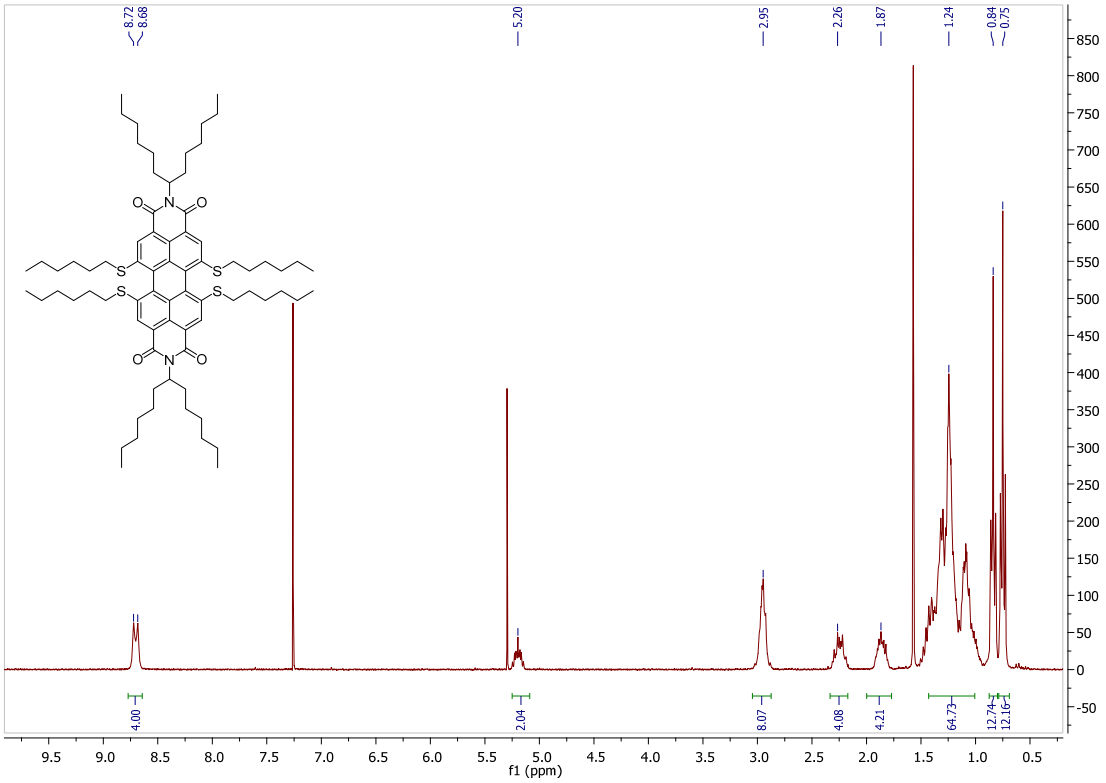


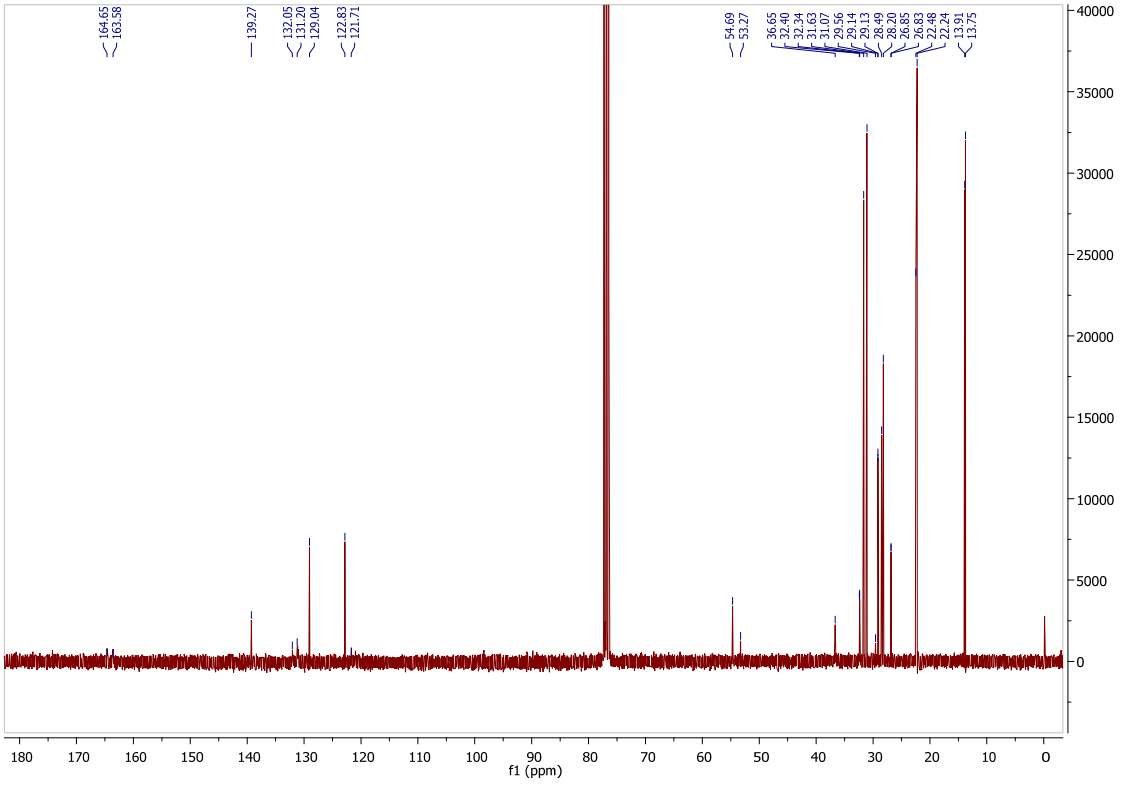
***N,N'*-di-(1'-hexylheptyl)-1-chloro-6,7,12-trihexylthioperylene-3,4:9,10-tetracarboxydiimide (2c)**



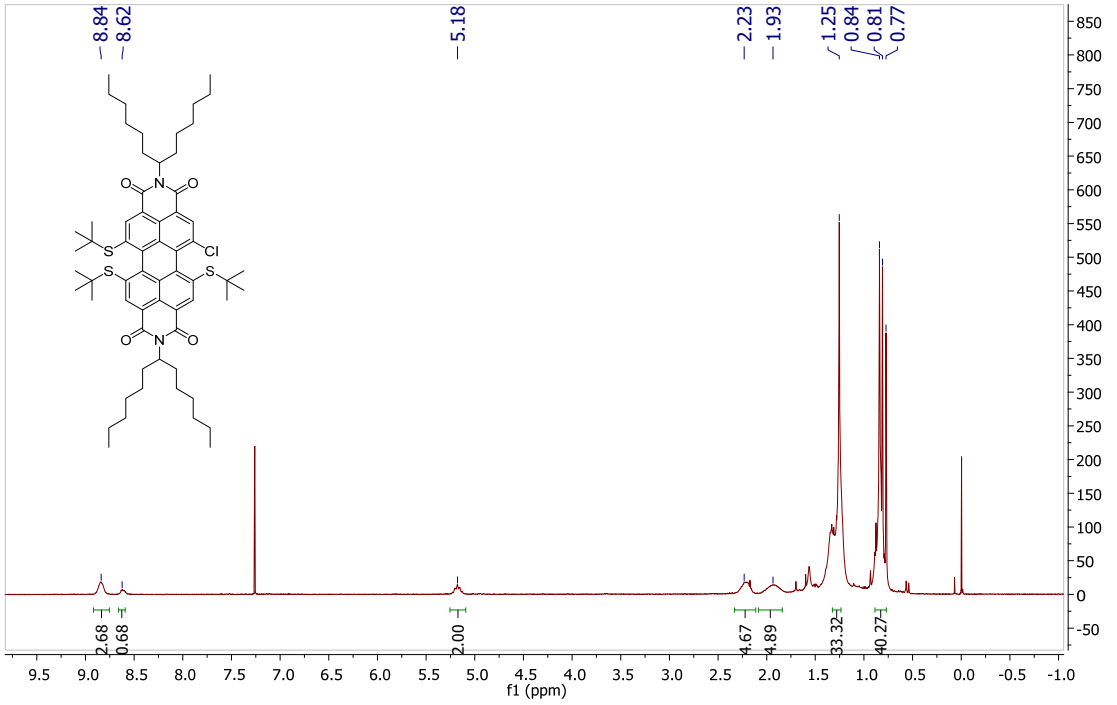


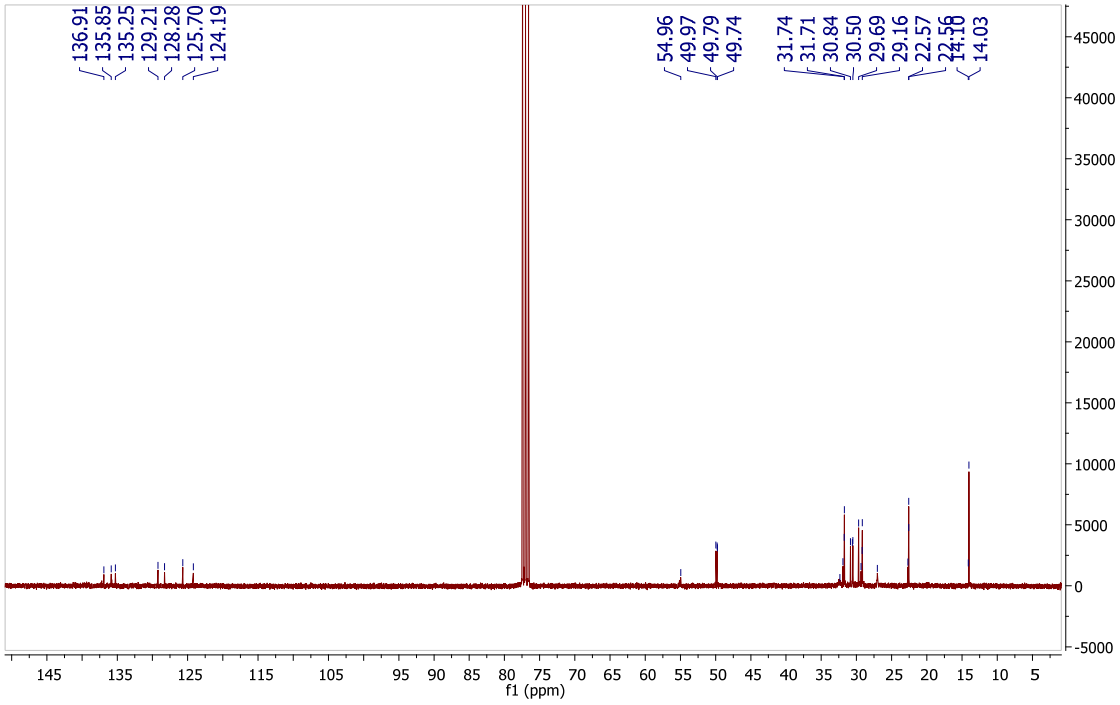
***N,N'*-di-(1'-hexylheptyl)-1,6,7,12-tetrahexylthioperylene-3,4:9,10-tetracarboxydiimide (2d)**



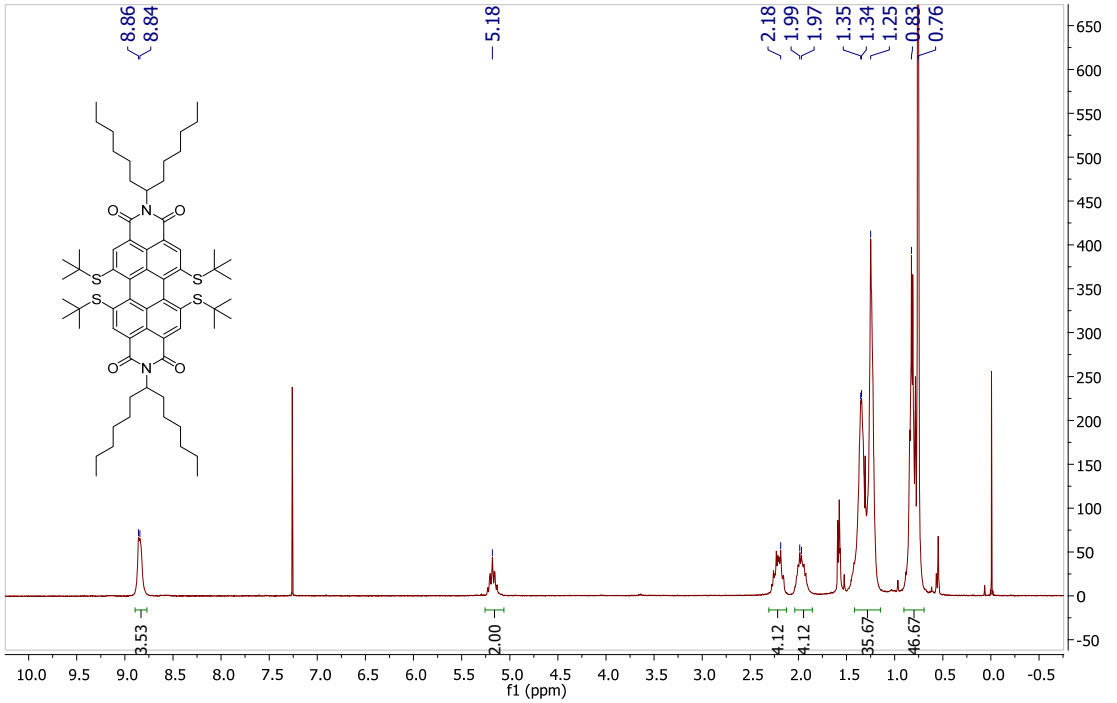


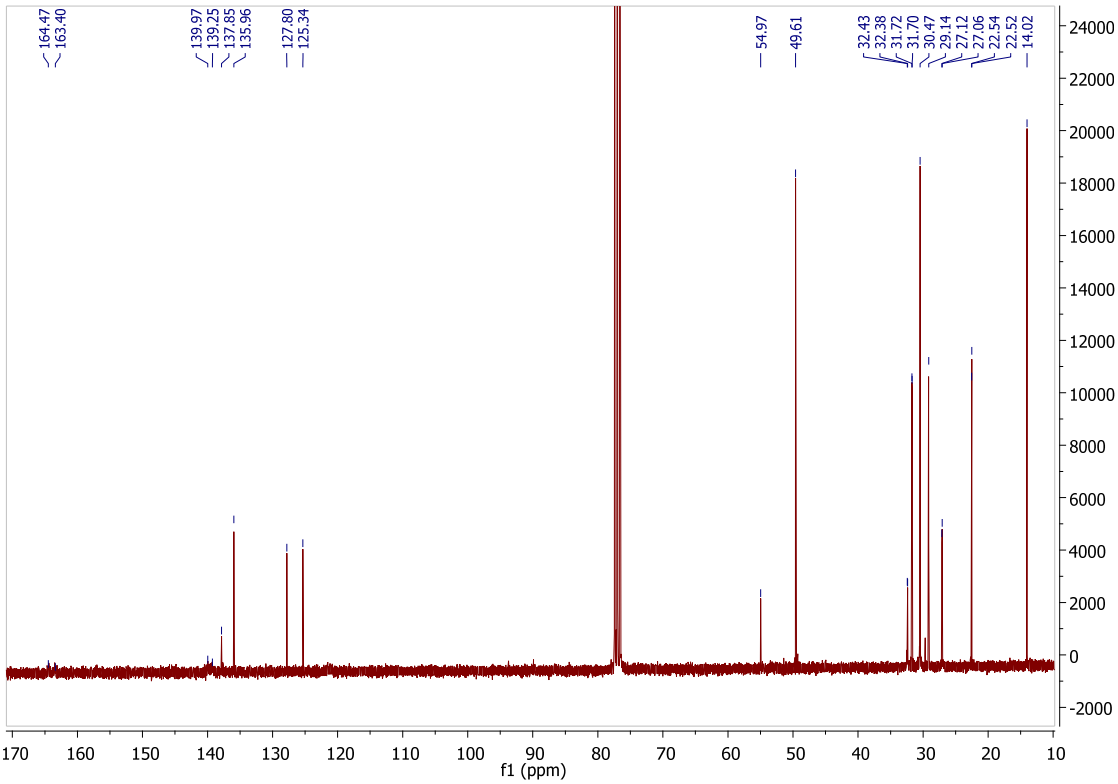
***N,N'*-di-(1'-hexylheptyl)-1-chloro-6,7,12-tri-*t*-butylthioperylene-3,4:9,10-tetracarboxydiimide (4c)**



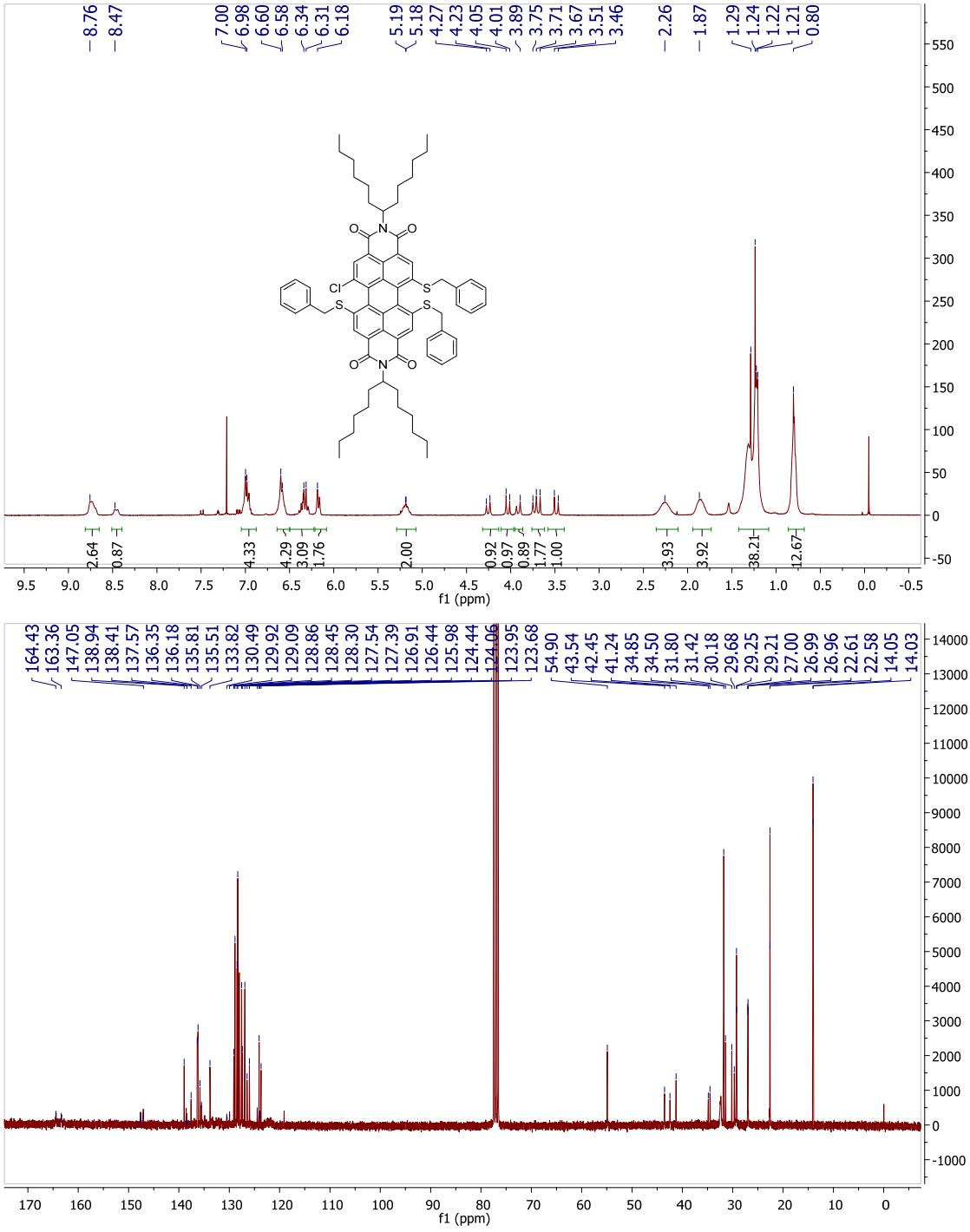


***N,N'*-di-(1'-hexylheptyl)-1,6,7,12-tetra-*t*-butylthioperylene-3,4:9,10-tetracarboxydiimide (4d)**

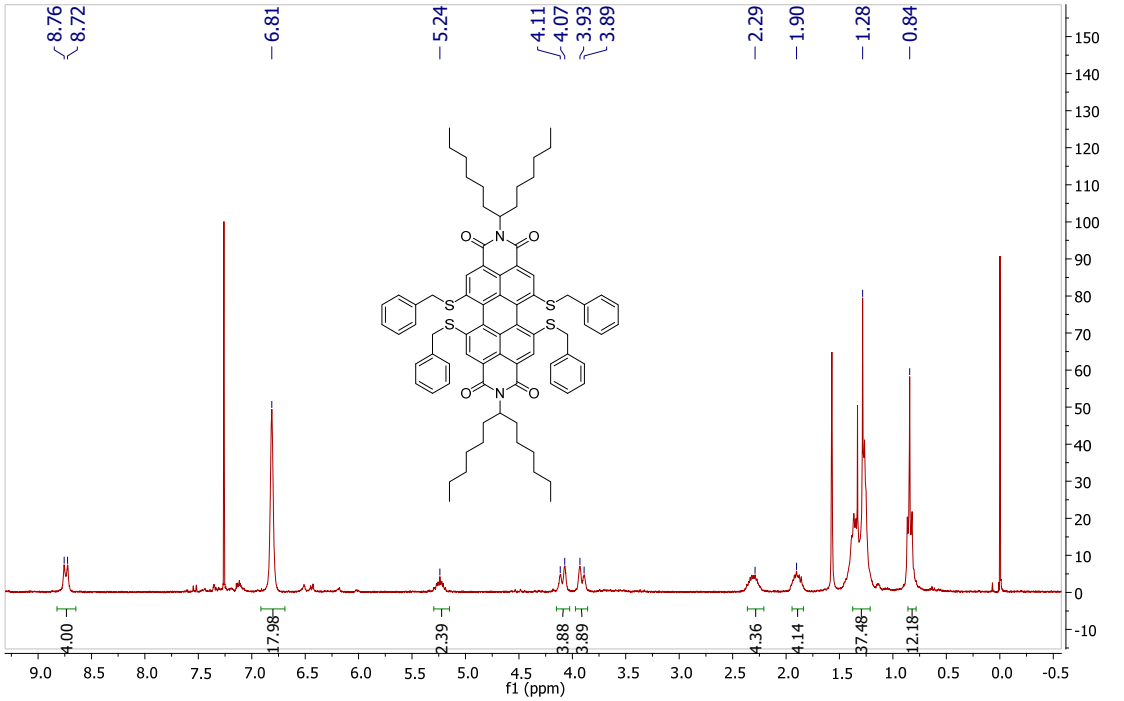


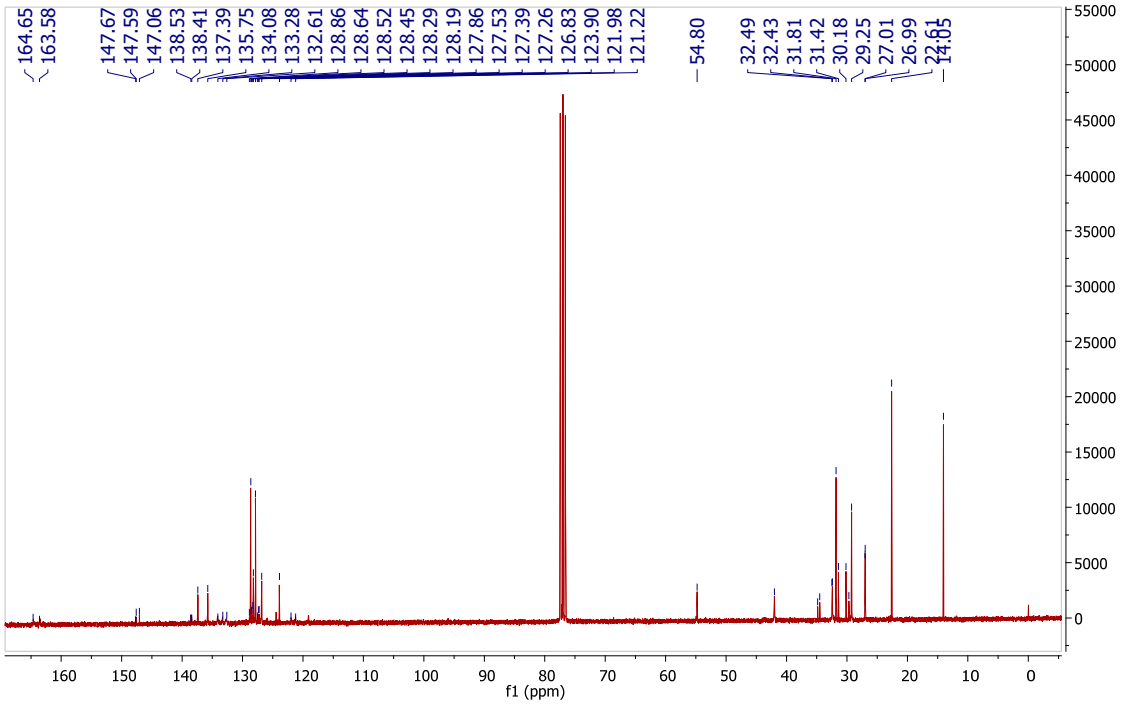


***N,N'*-di-(1'-hexylheptyl)-1,6,7-tribenzylthio-12-chloroperylene-3,4:9,10-tetracarboxydiimide (3c)**

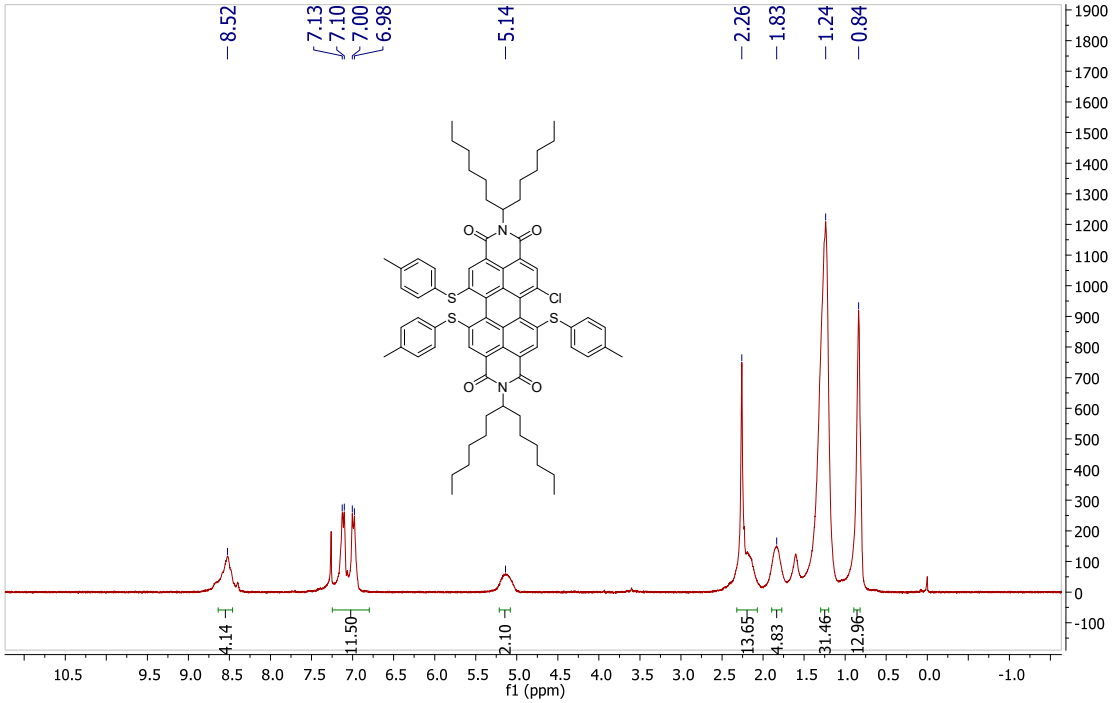


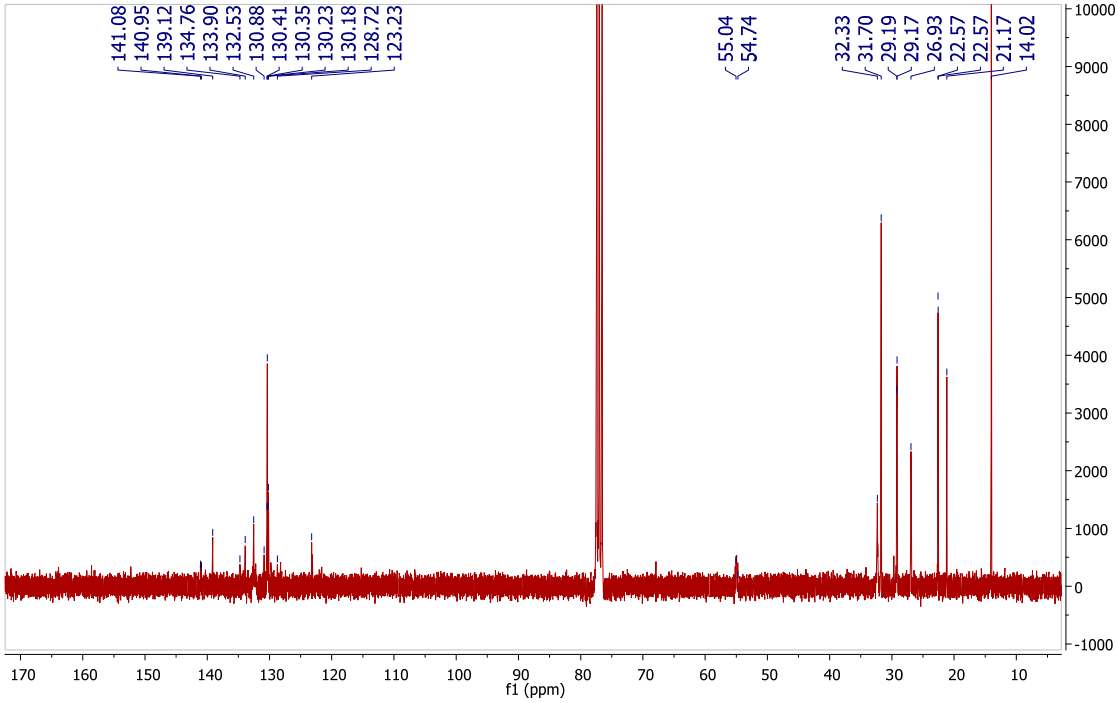
***N,N'*-di-(1'-hexylheptyl)-1,6,7,12-tetrabenzylthioperylene-3,4:9,10-tetracarboxydiimide (3d)**



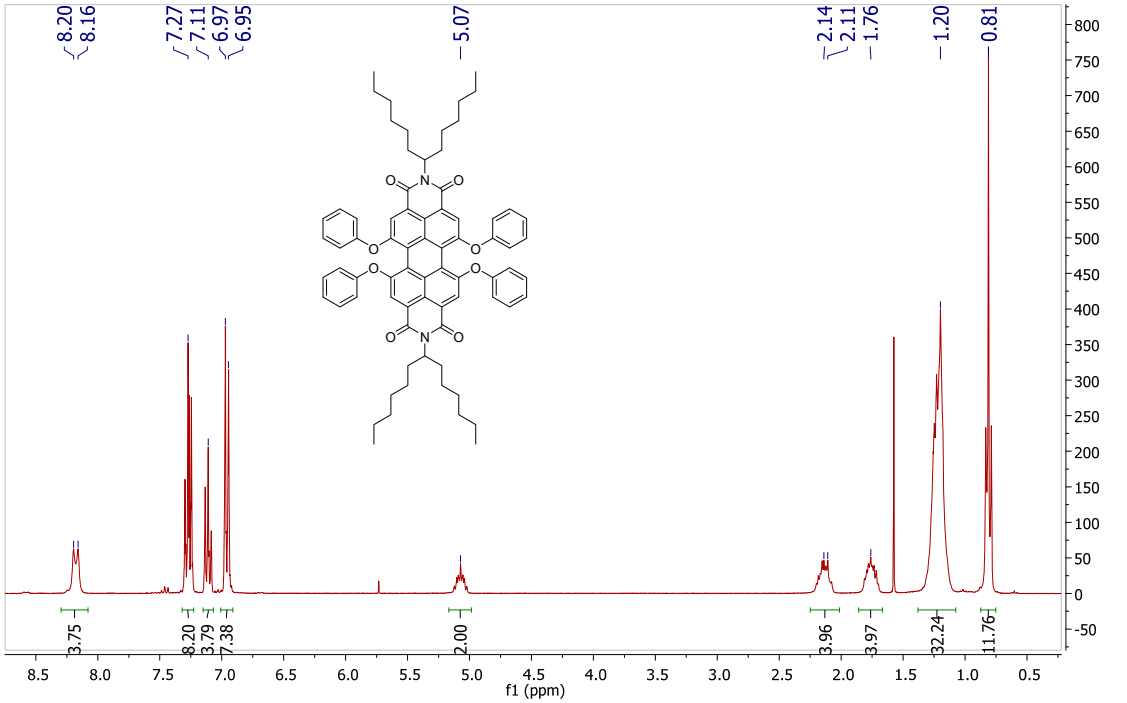


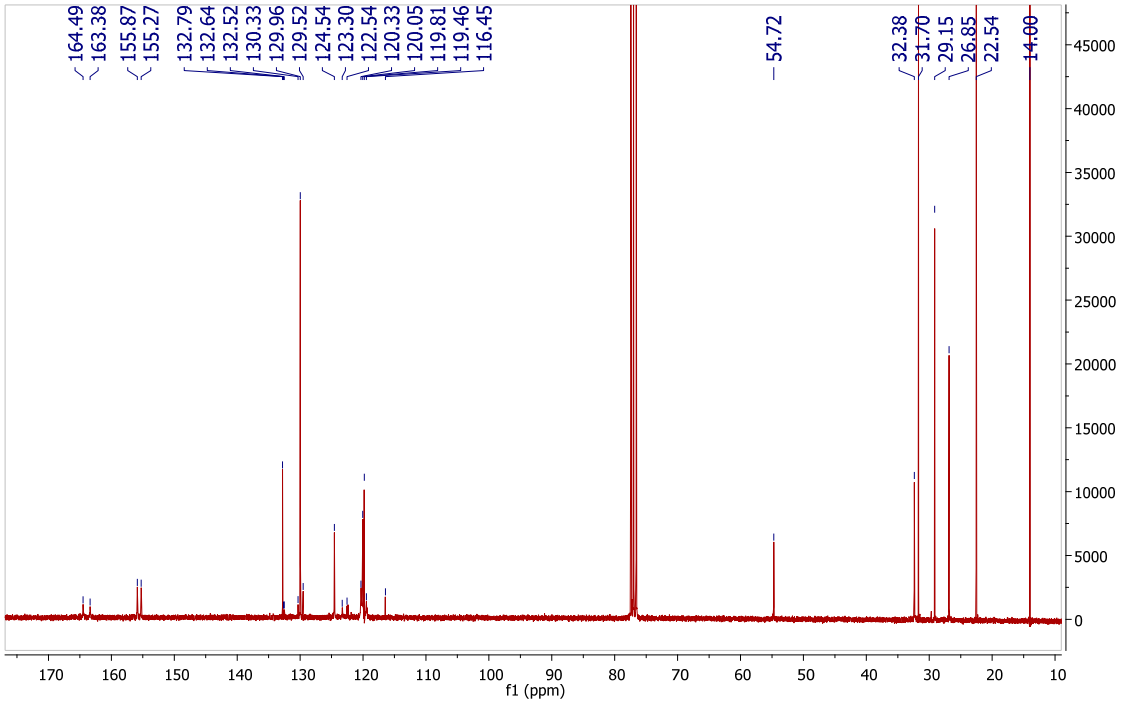
***N,N'*-di-(1'-hexylheptyl)-1-chloro-6,7,12-tri-*p*-tolylthioperylene-3,4:9,10-tetracarboxydiimide (5c)**



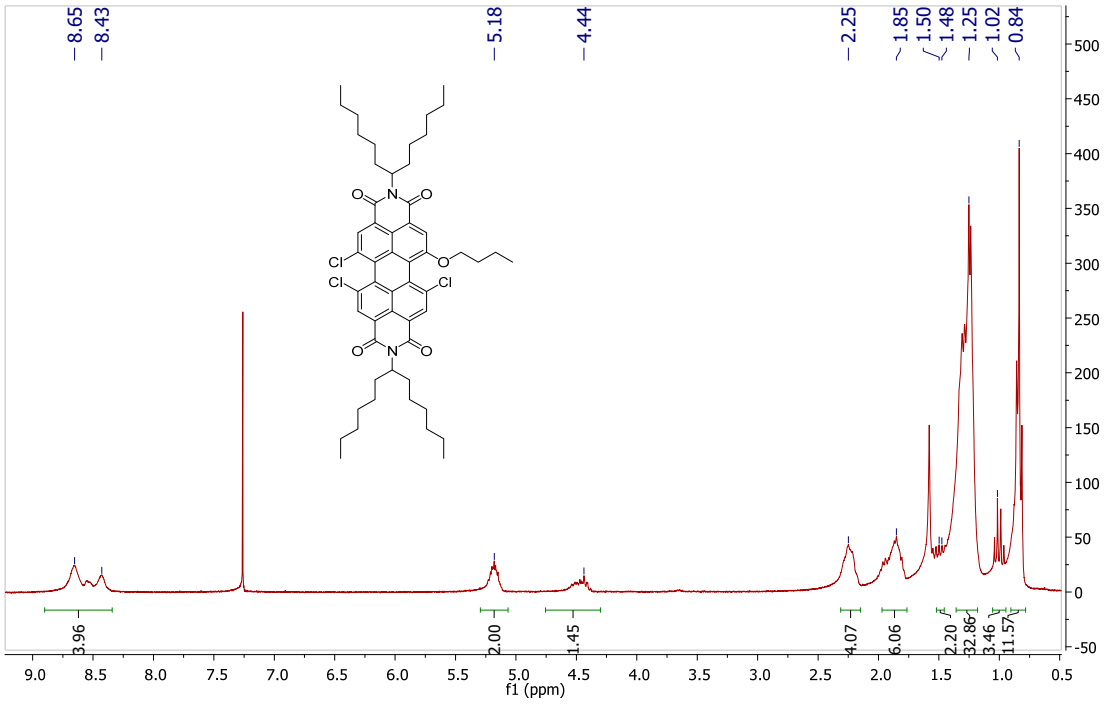


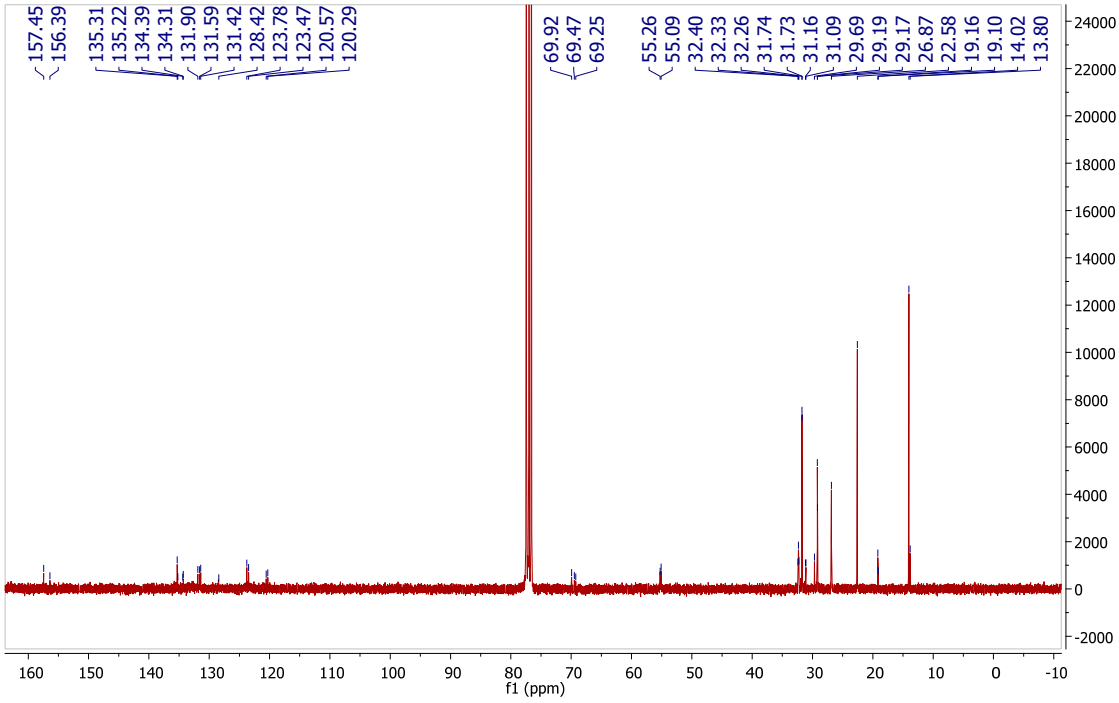
***N,N'*-di-(1'-hexylheptyl)-1,6,7,12-tetraphenoxyperylene-3,4:9,10-tetracarboxydiimide (8d)**



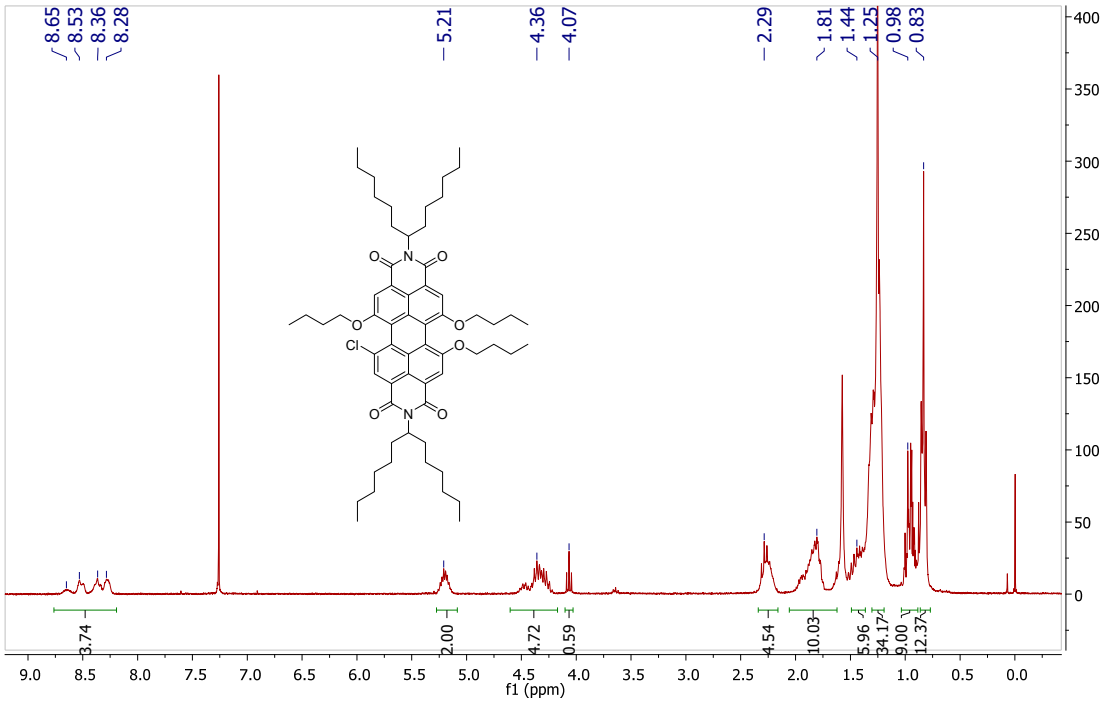


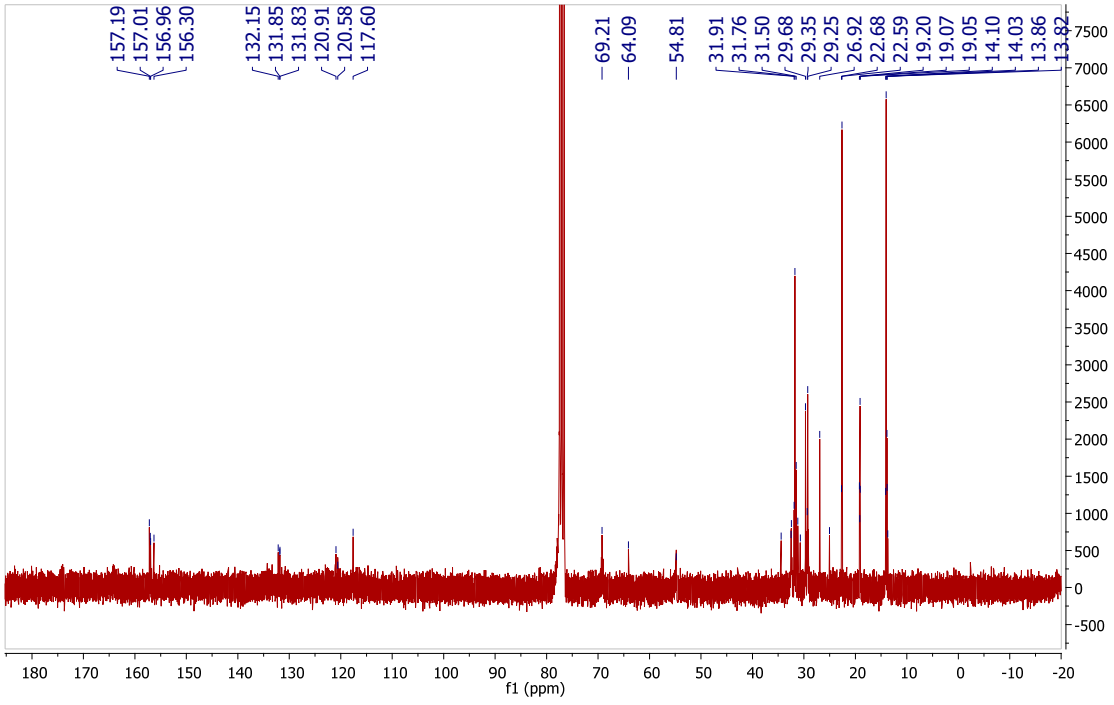
***N,N'*-di-(1'-hexylheptyl)-1-butoxy-6,7,12-trichloroperylene-3,4:9,10-tetracarboxydiimide (6a)**



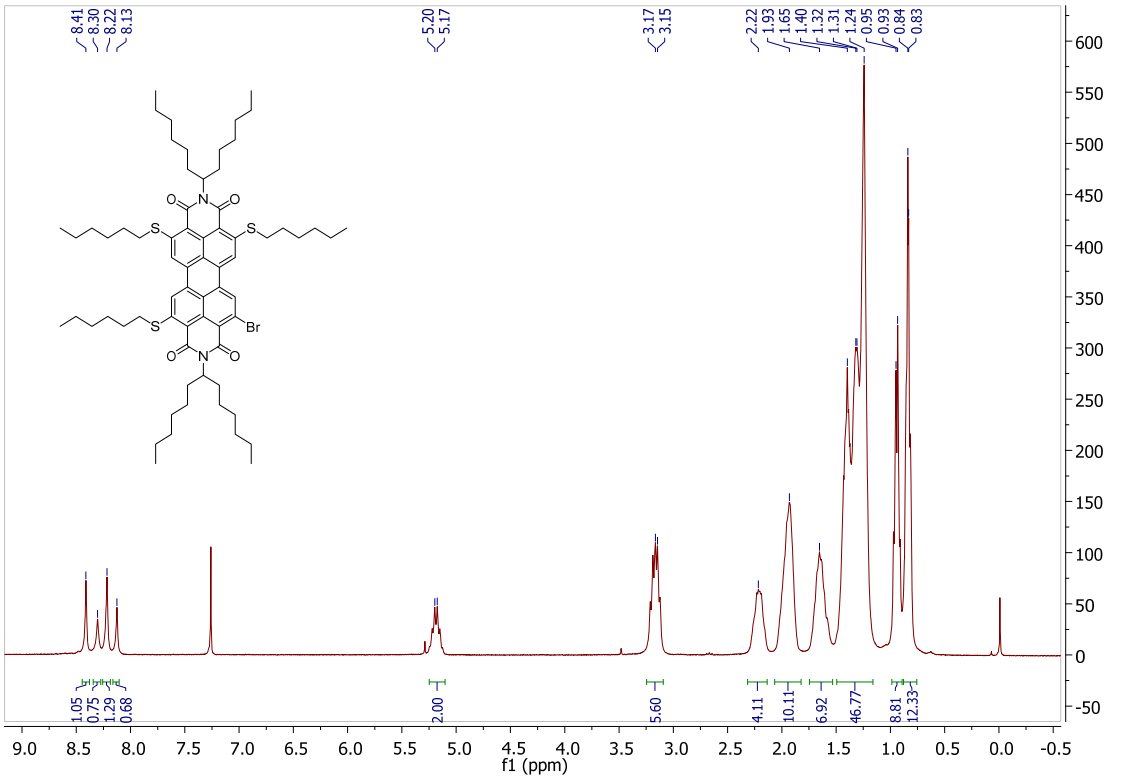


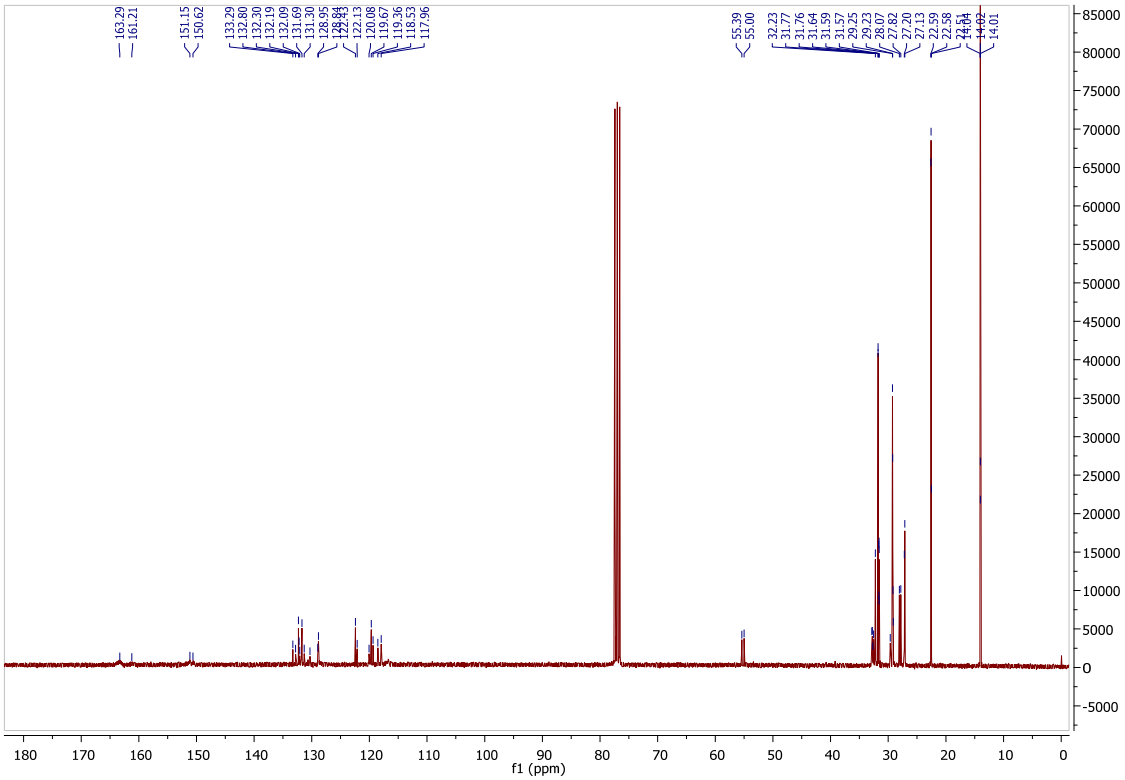
***N,N'*-di-(1'-hexylheptyl)-1,6,7-tributoxy-12-chloroperylene-3,4:9,10-tetracarboxydiimide (6c)**



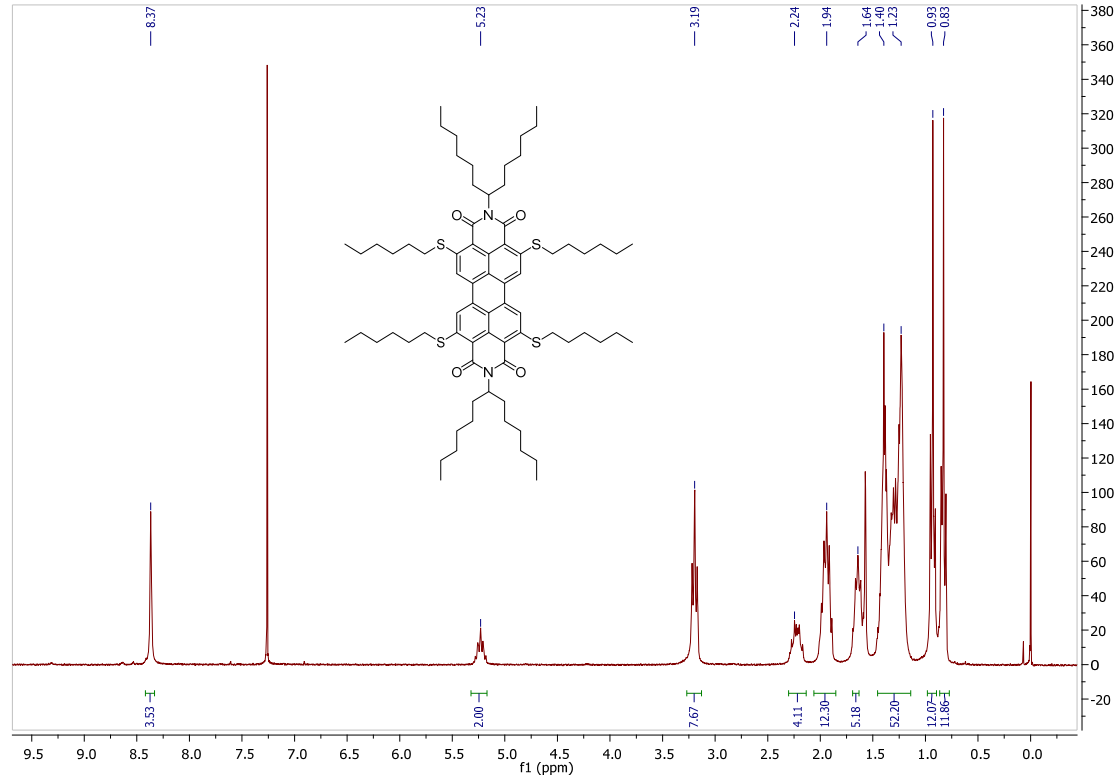


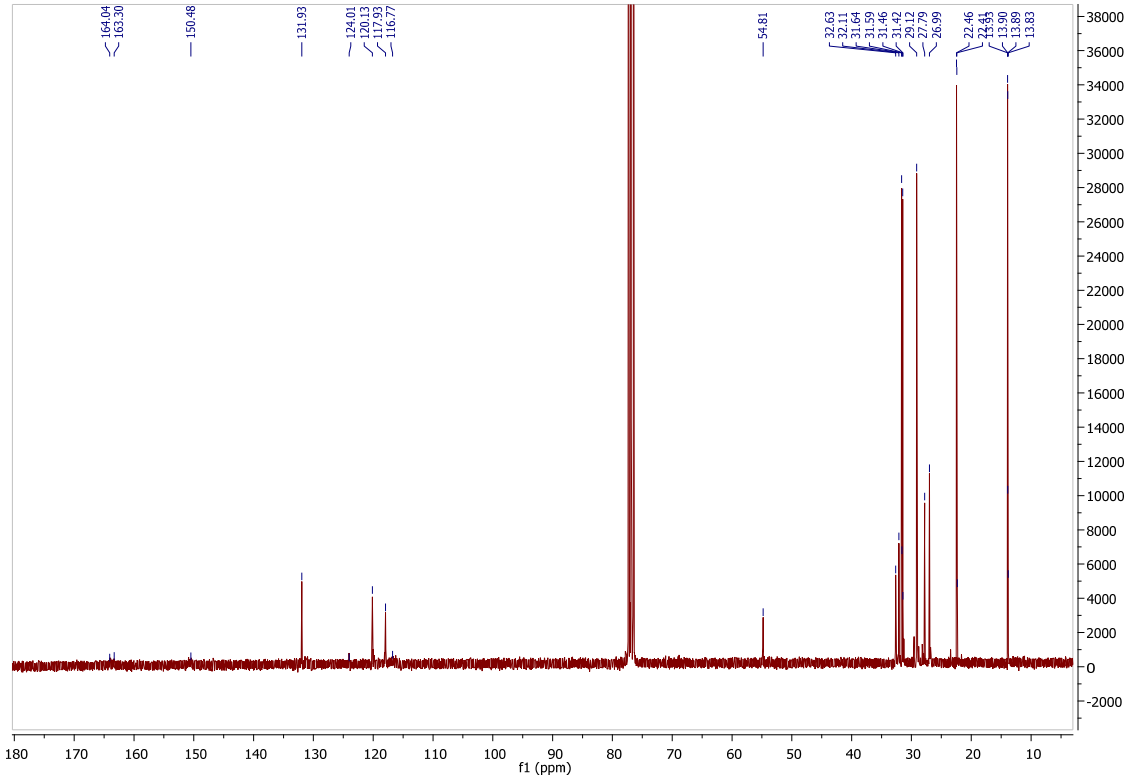
***N,N'*-di-(1'-hexylheptyl)-2-bromo-5,8,11-trihexylthio-3,4:9,10-perylenetetracarboxydiimide (13c)**



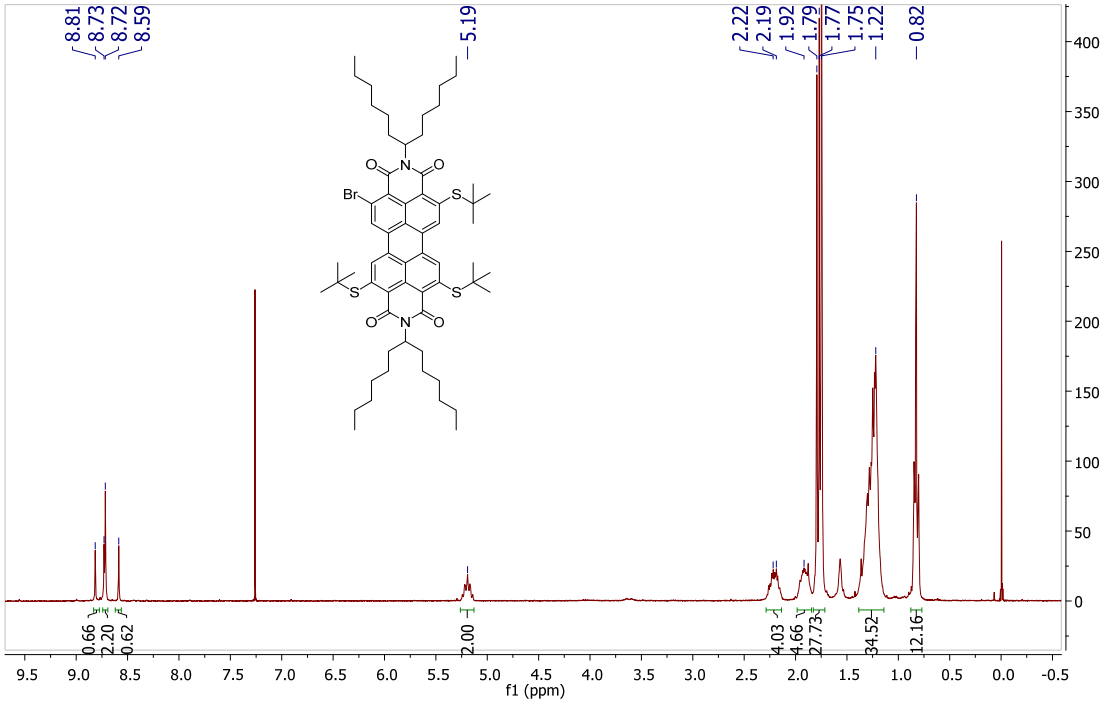


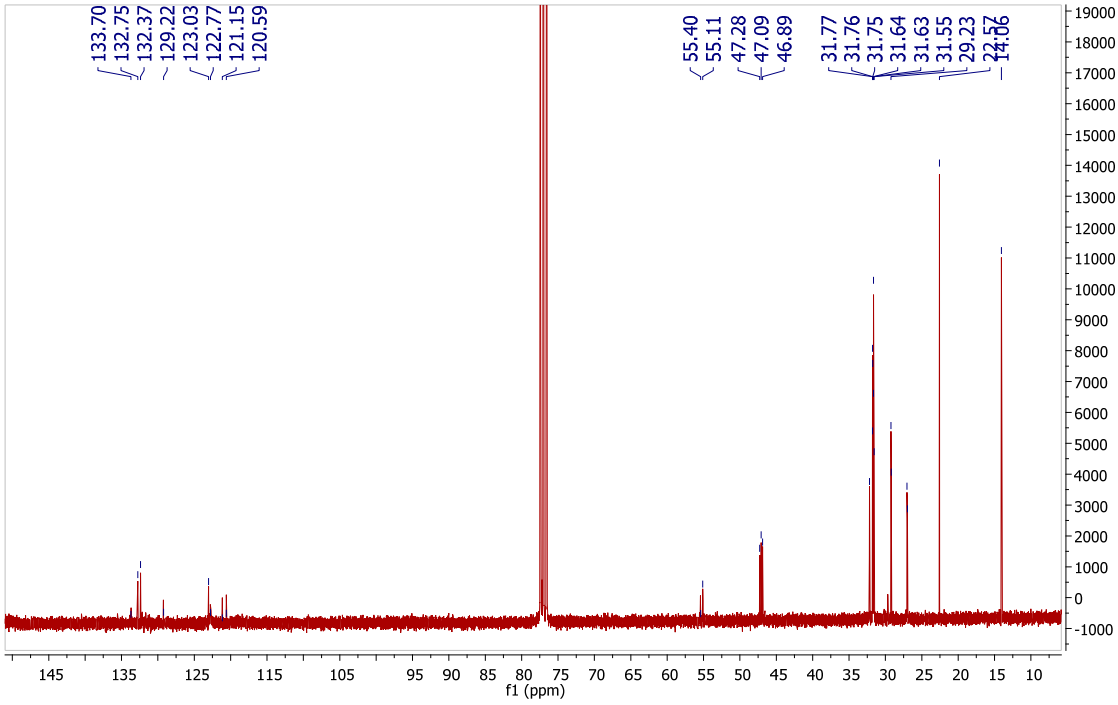
_N,N'_-di-(1'-hexylheptyl)-2,5,8,11-tetrahexylthio-3,4:9,10-perylenetetracarboxydiimide (13d)



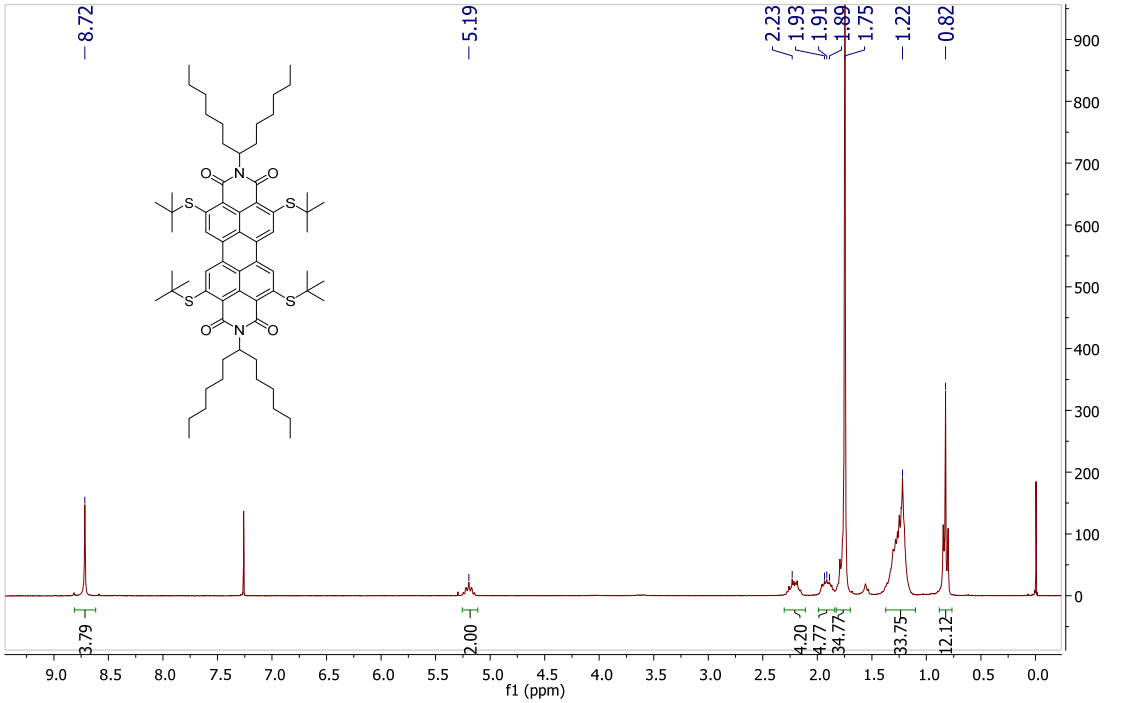


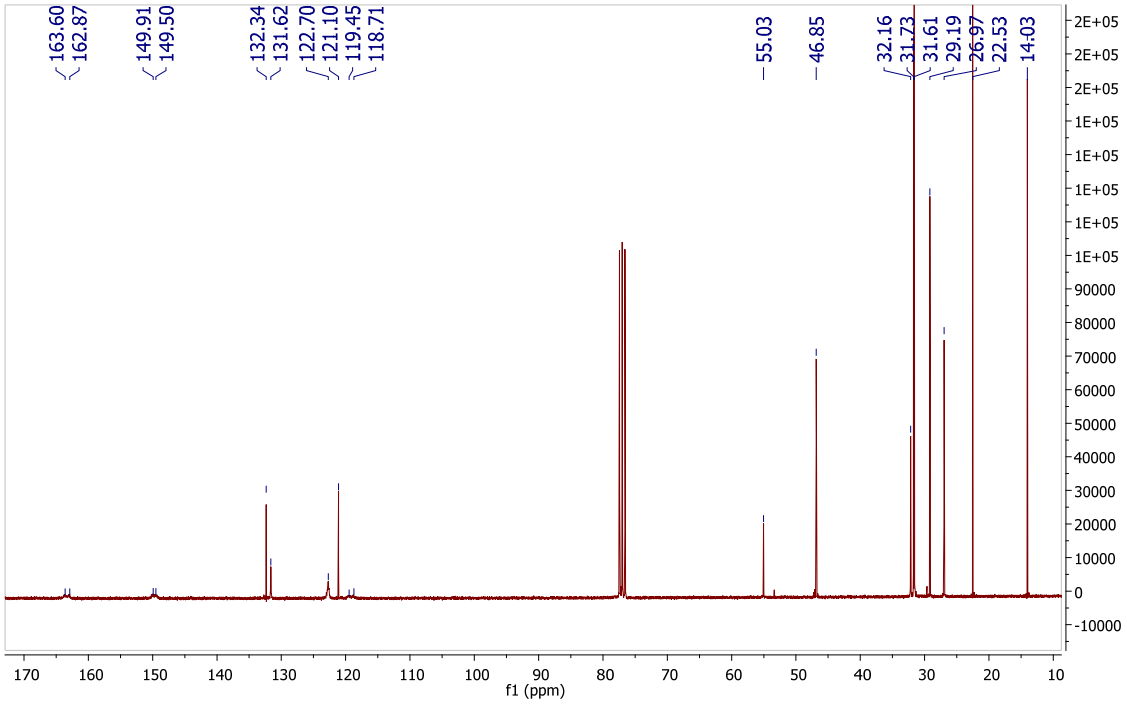
***N,N'*-di-(1'-hexylheptyl)-2-bromo-5,8,11-tri-*t*-butylthioperylene-3,4:9,10-tetracarboxydiimide (15c)**



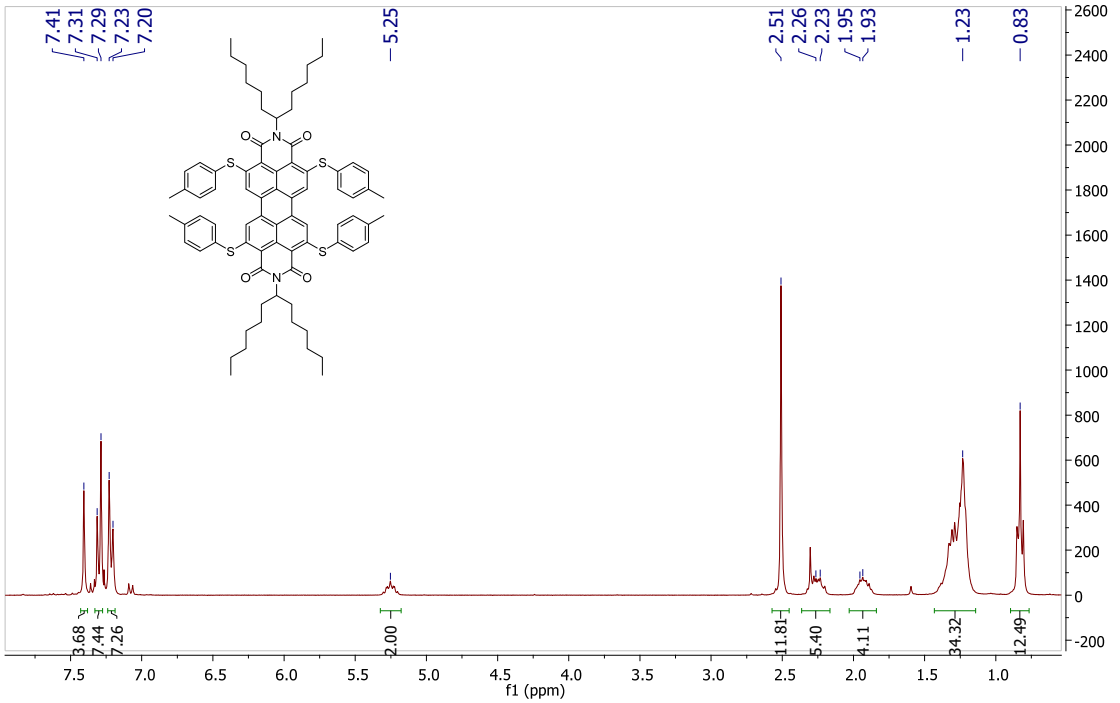


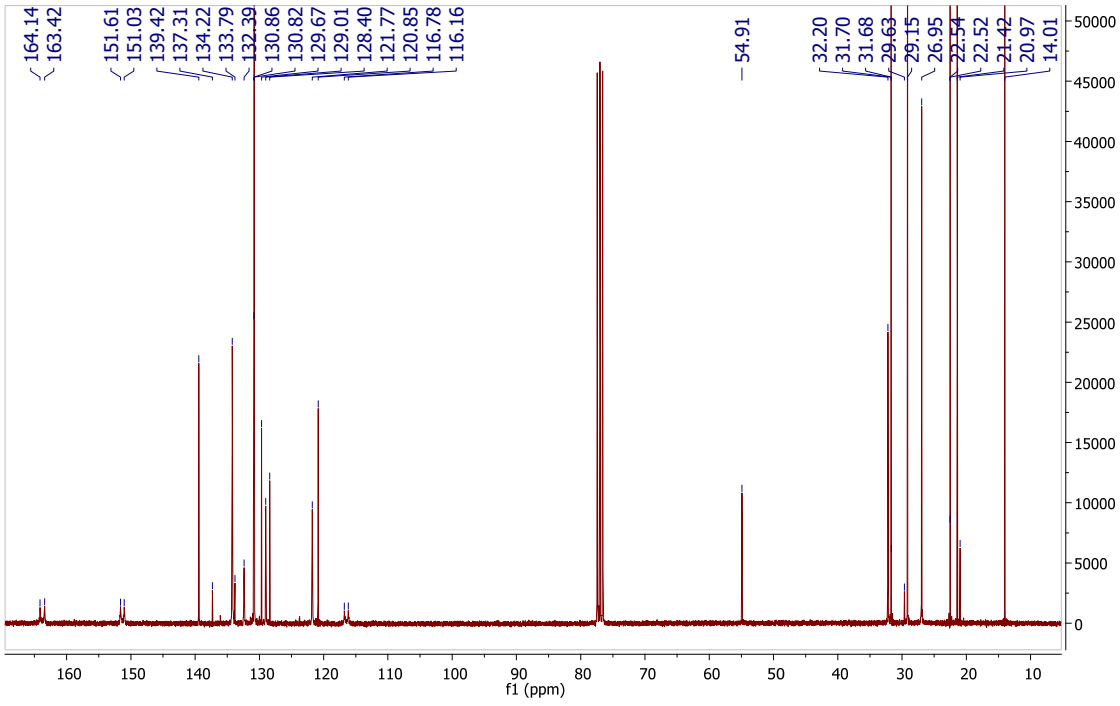
***N,N'*-di-(1'-hexylheptyl)-2,5,8,11-tetra-*t*-butylthioperylene-3,4:9,10-tetracarboxydiimide (15d)**



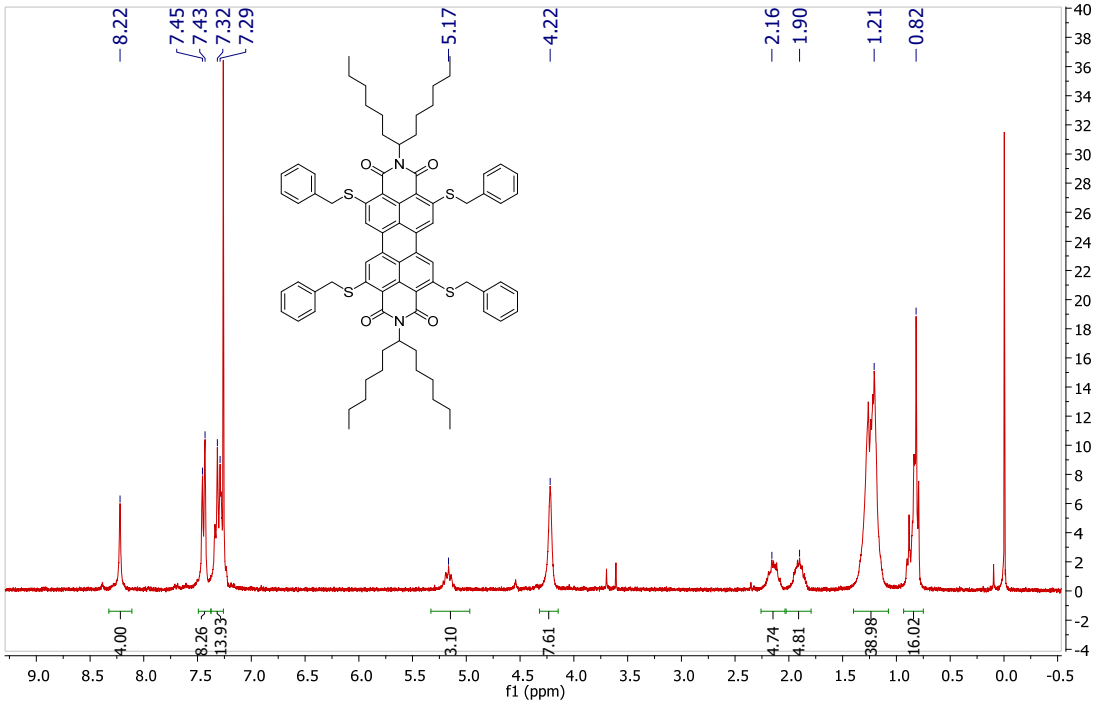


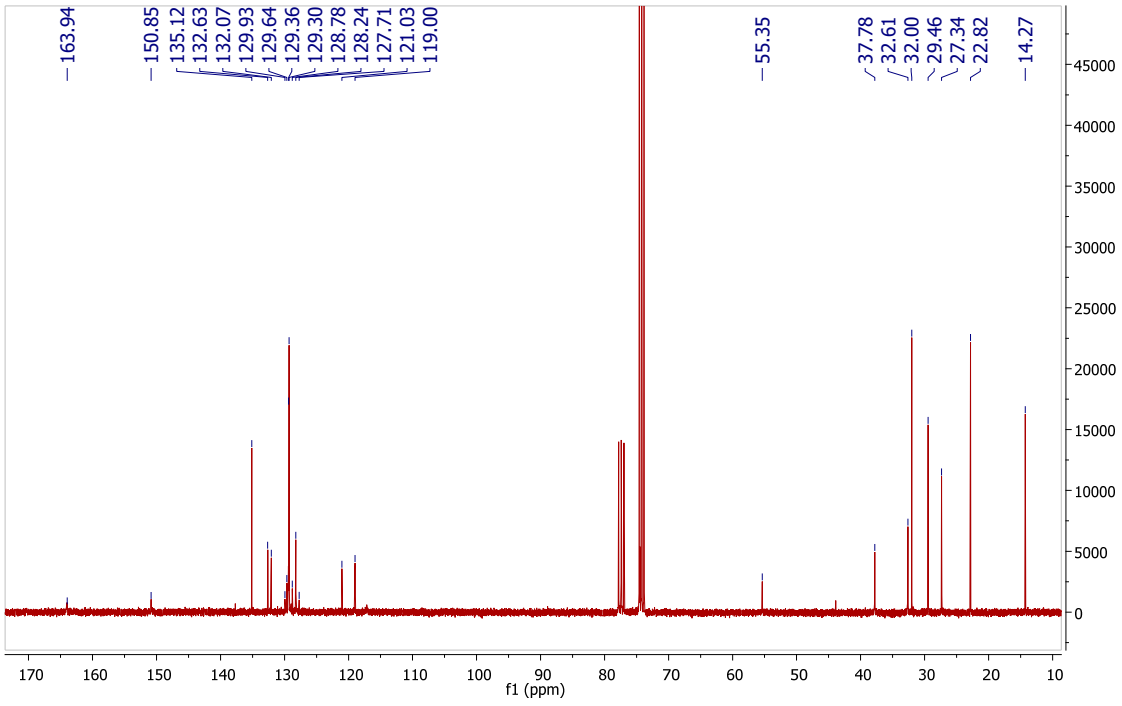
***N,N'*-di-(1'-hexylheptyl)-2,5,8,11-tetra-*p*-tolylthioperylene-3,4:9,10-tetracarboxydiimide (16d)**



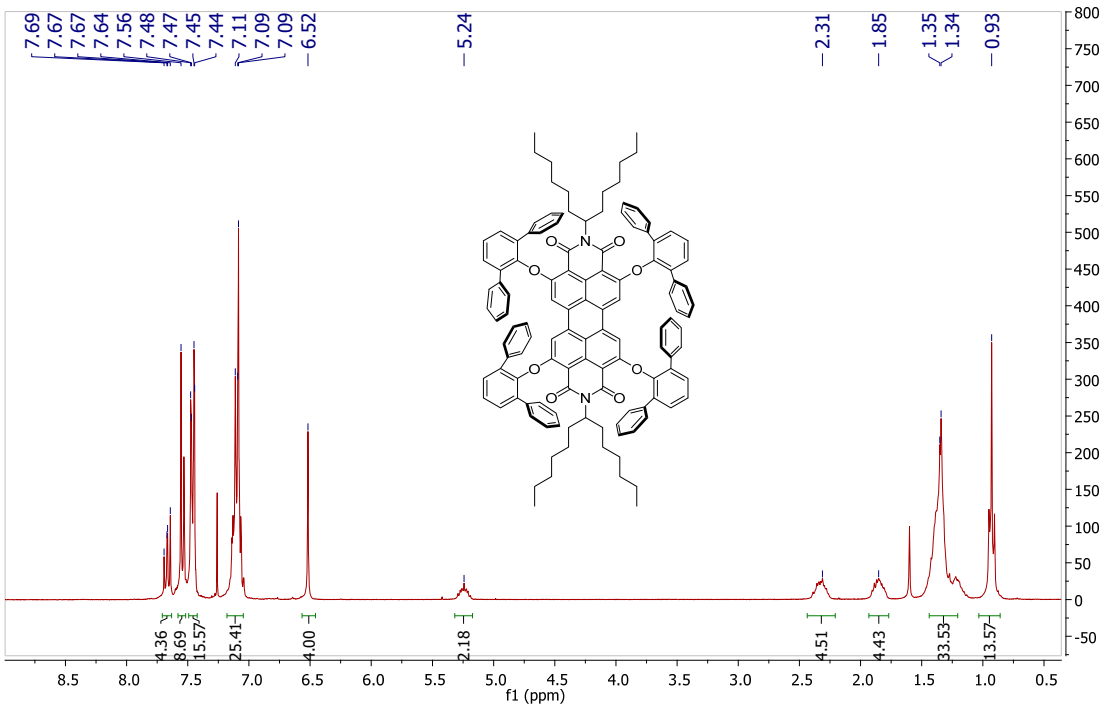


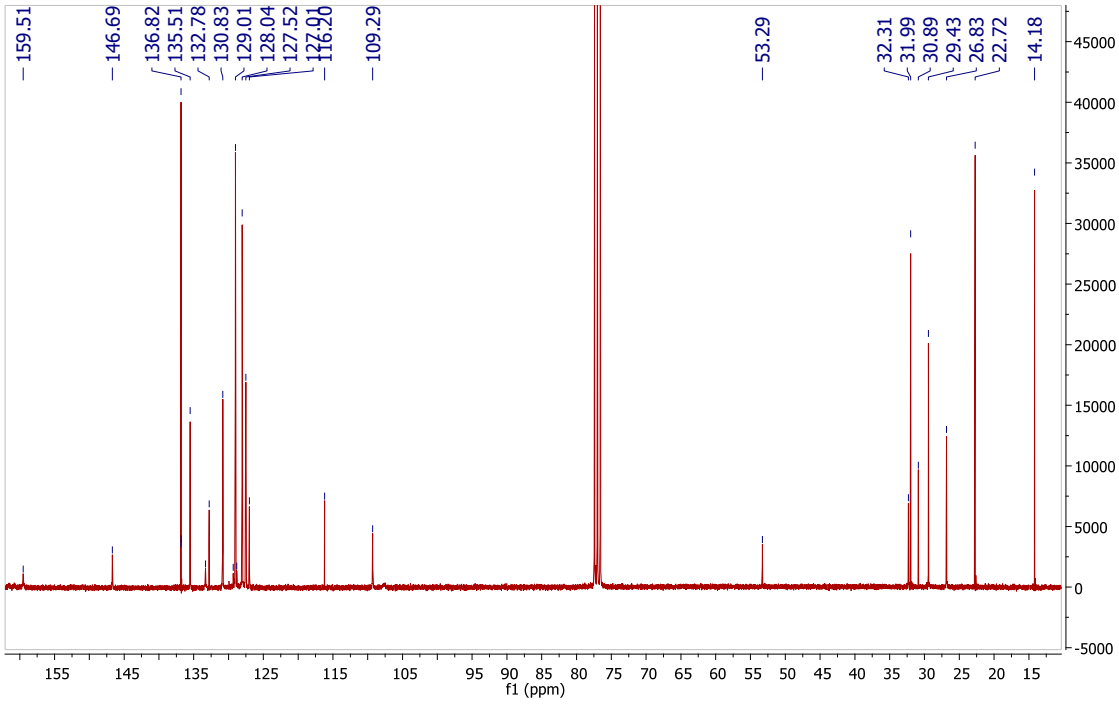
***N,N'*-di-(1'-hexylheptyl)-2,5,8,11-tetrabenzylthioperylene-3,4:9,10-tetracarboxydiimide (14d)**



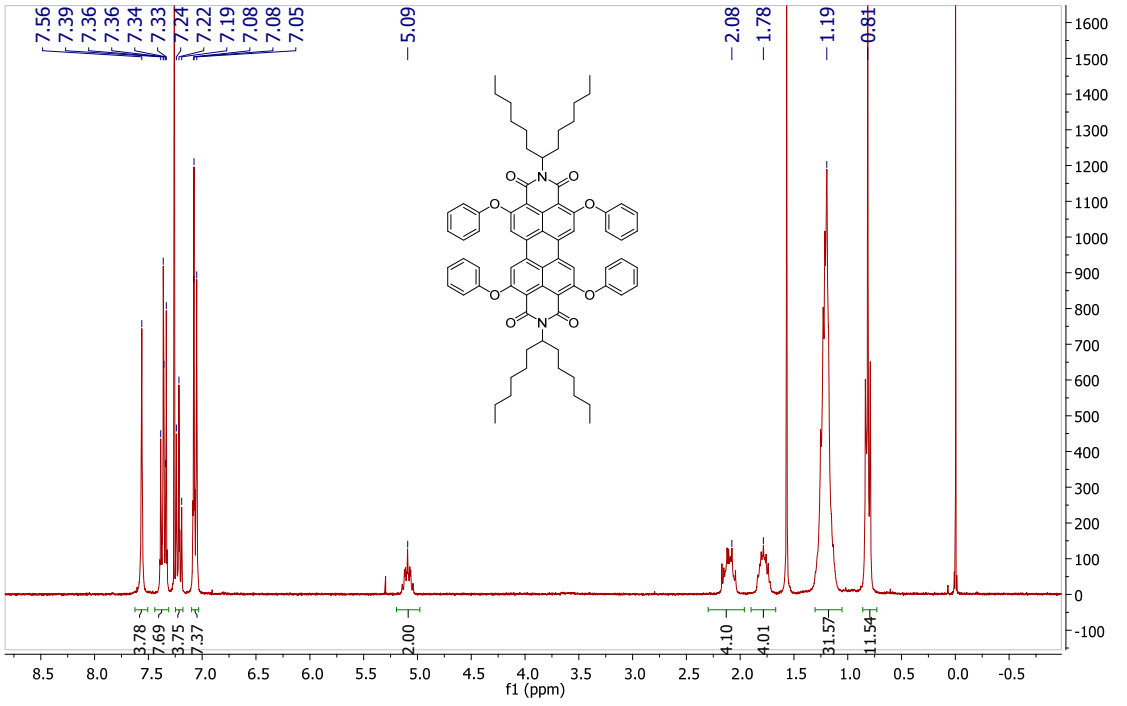


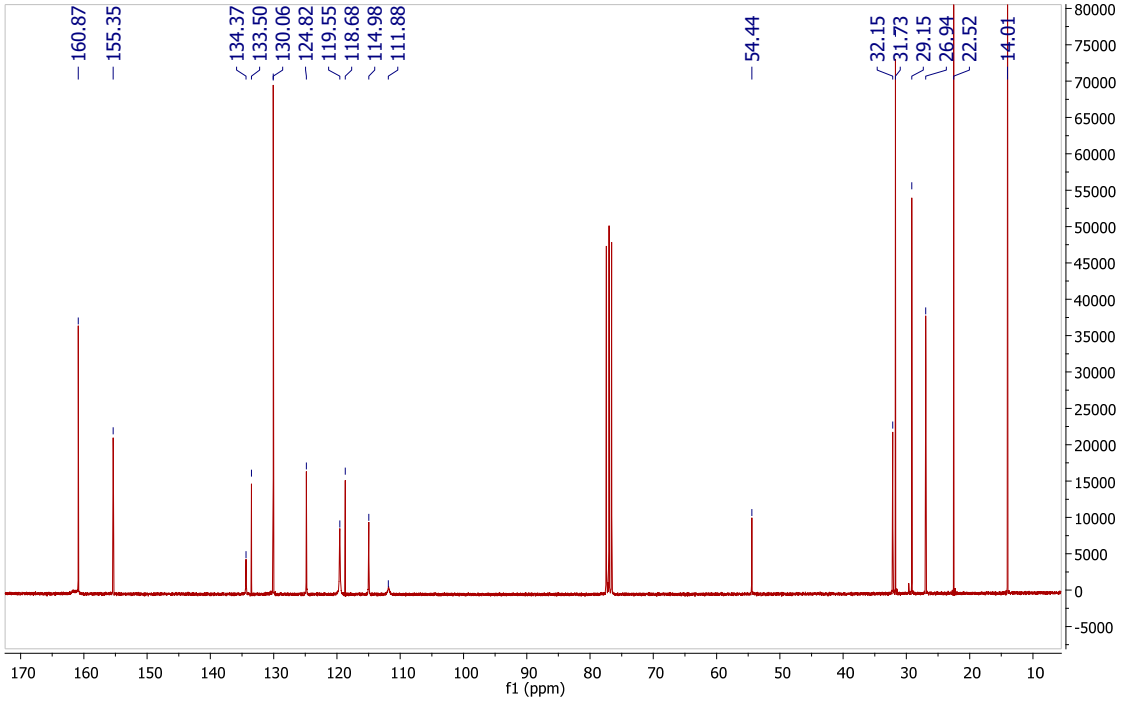
***N,N'*-di-(1'-hexylheptyl)-2,5,8,11-tetrakis(diphenylphenoxy)perylene-3,4:9,10-tetracarboxydiimide (19d)**



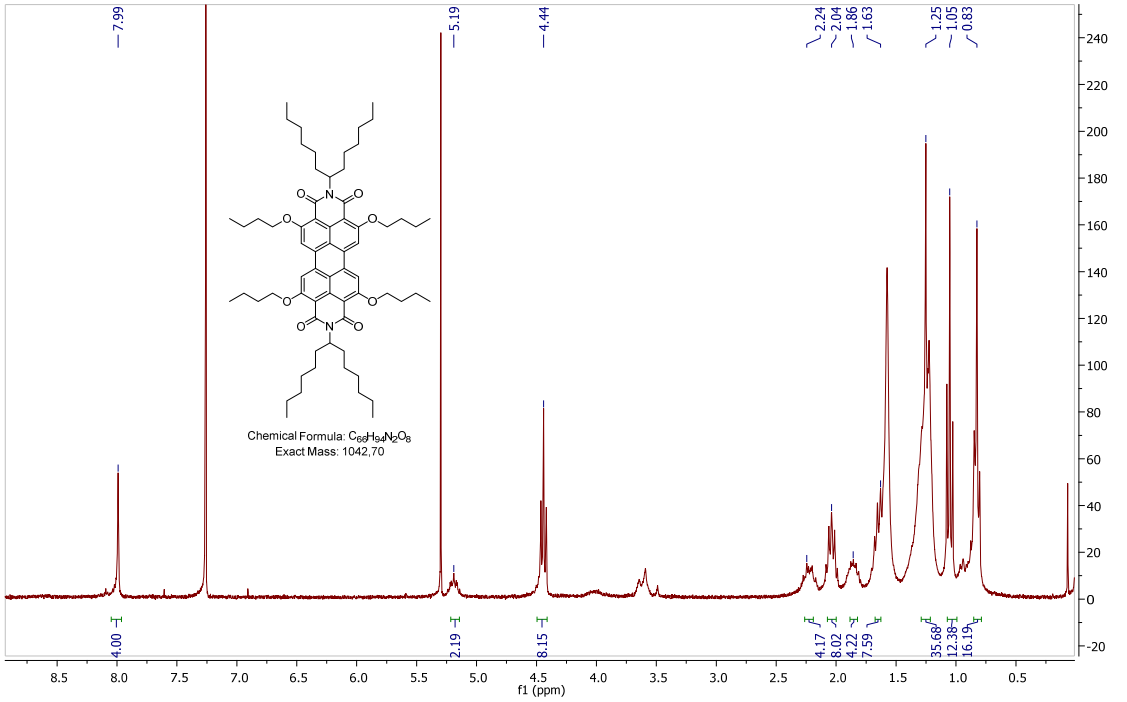


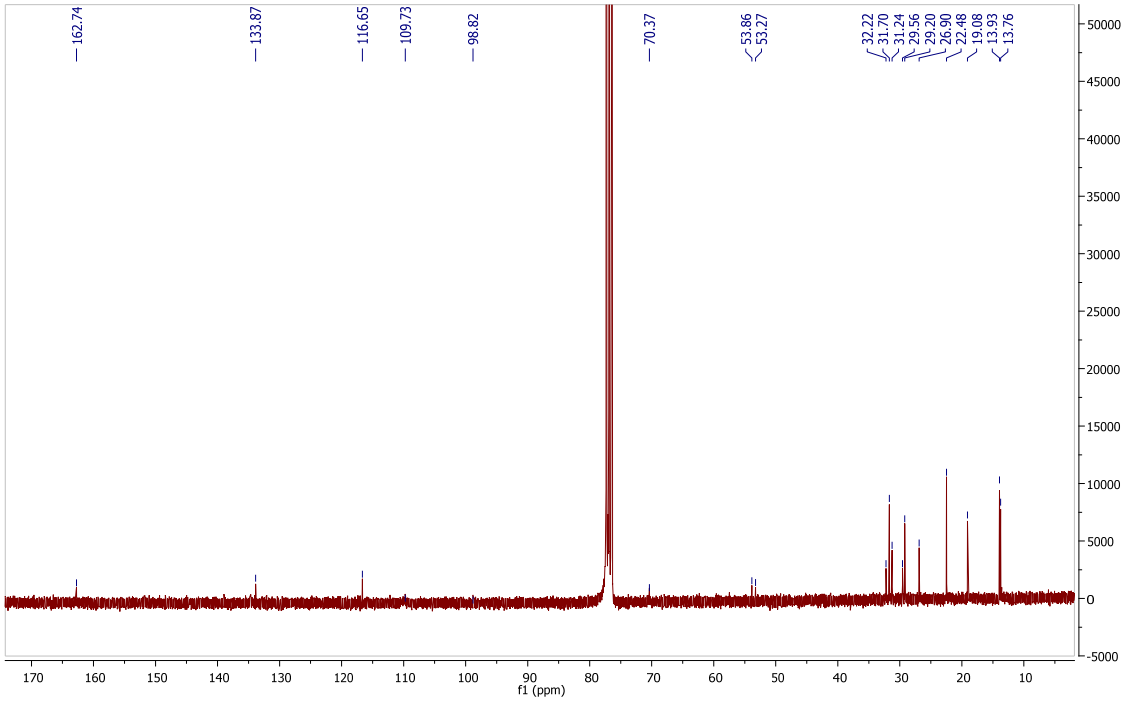
***N,N'*-di-(1'-hexylheptyl)-2,5,8,11-tetraphenoxyperylene-3,4:9,10-tetracarboxydiimide (18d)**



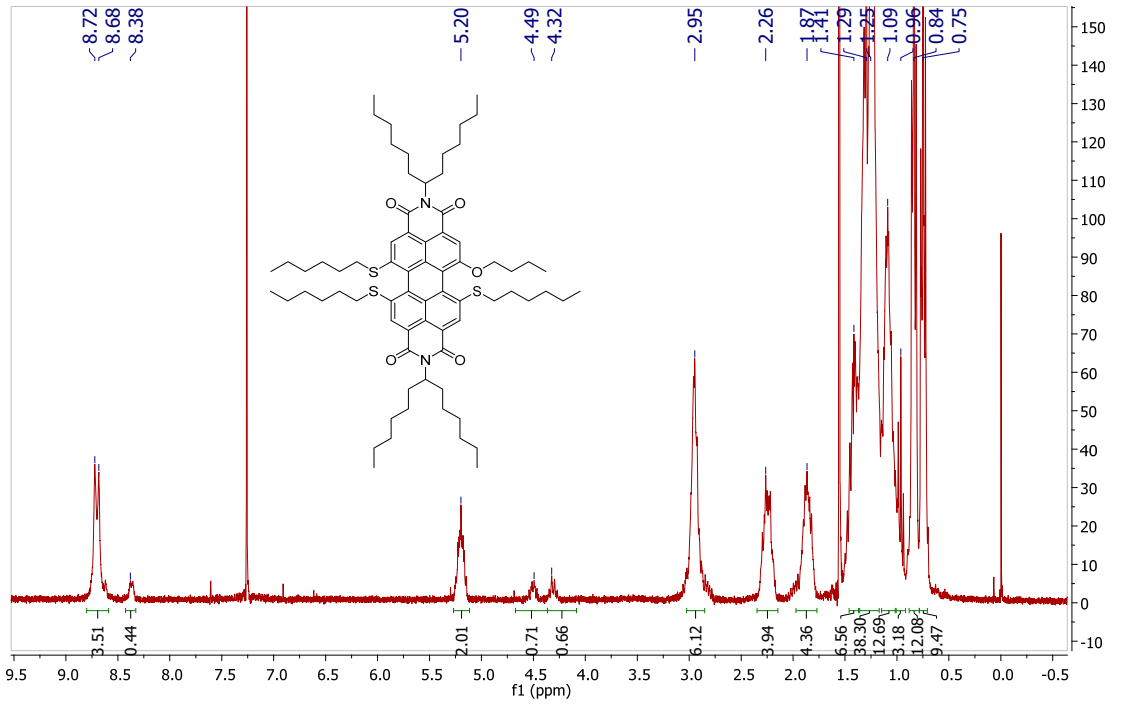


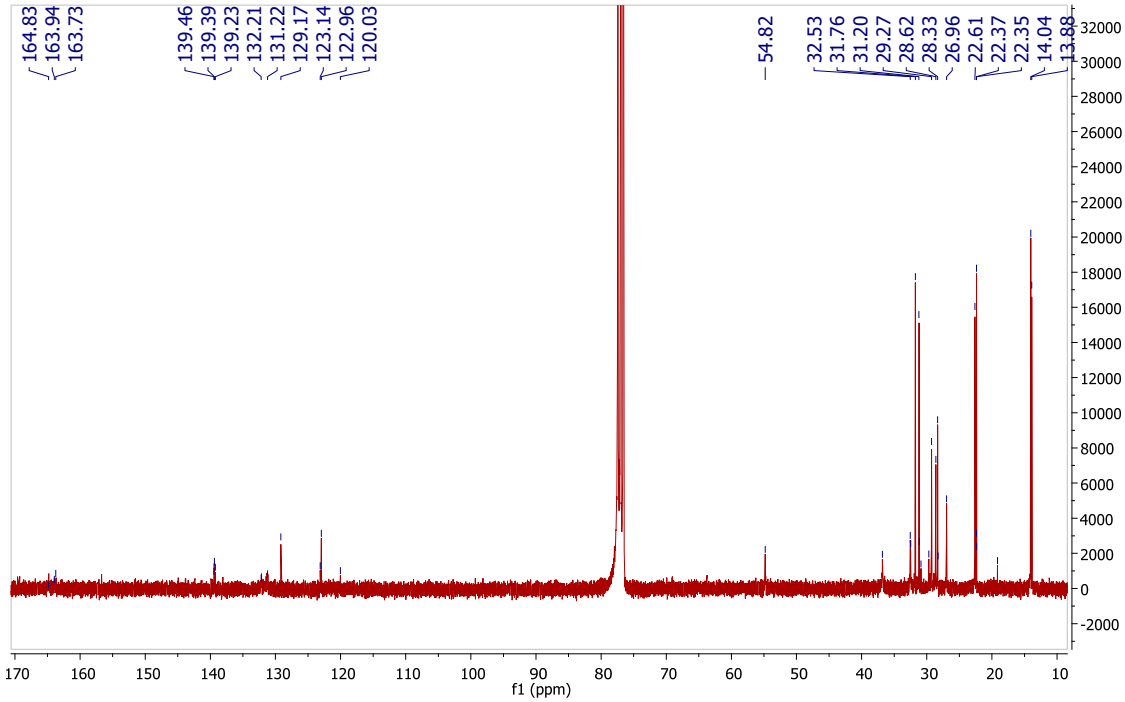
***N,N'*-di(hexylheptyl)-2,5,8,11-tetrabutoxy-3,4:9,10-perylenetetracarboxydiimide (17d)**



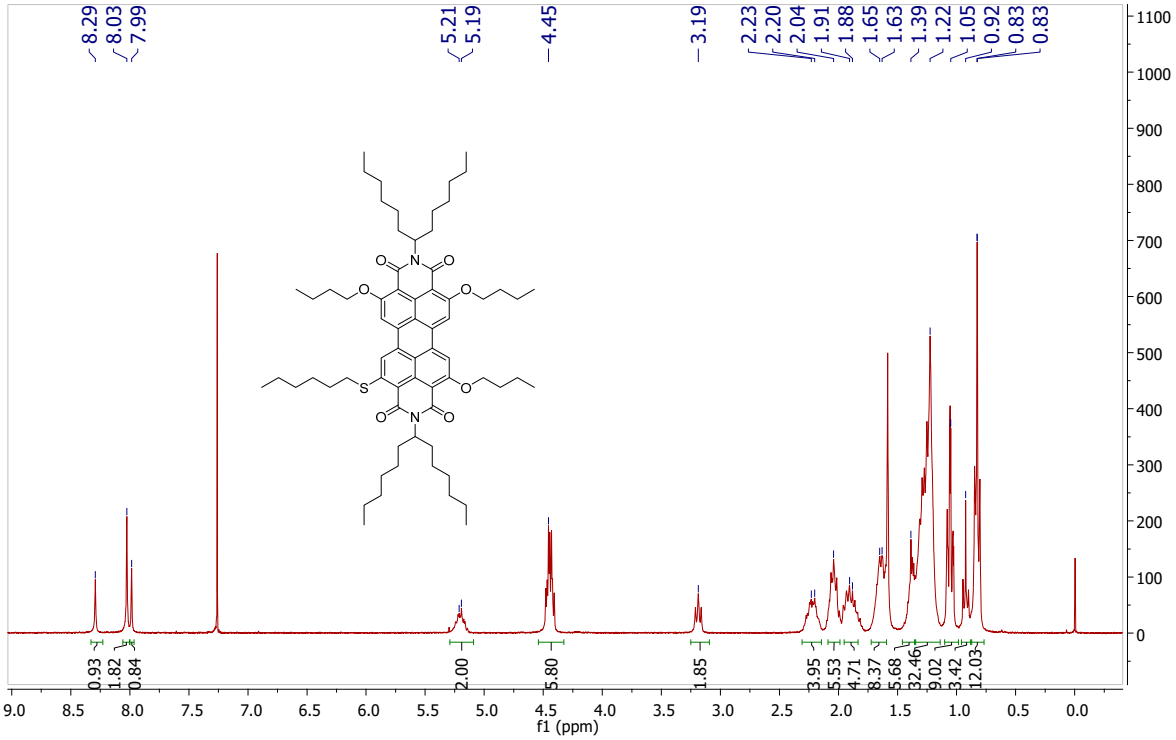


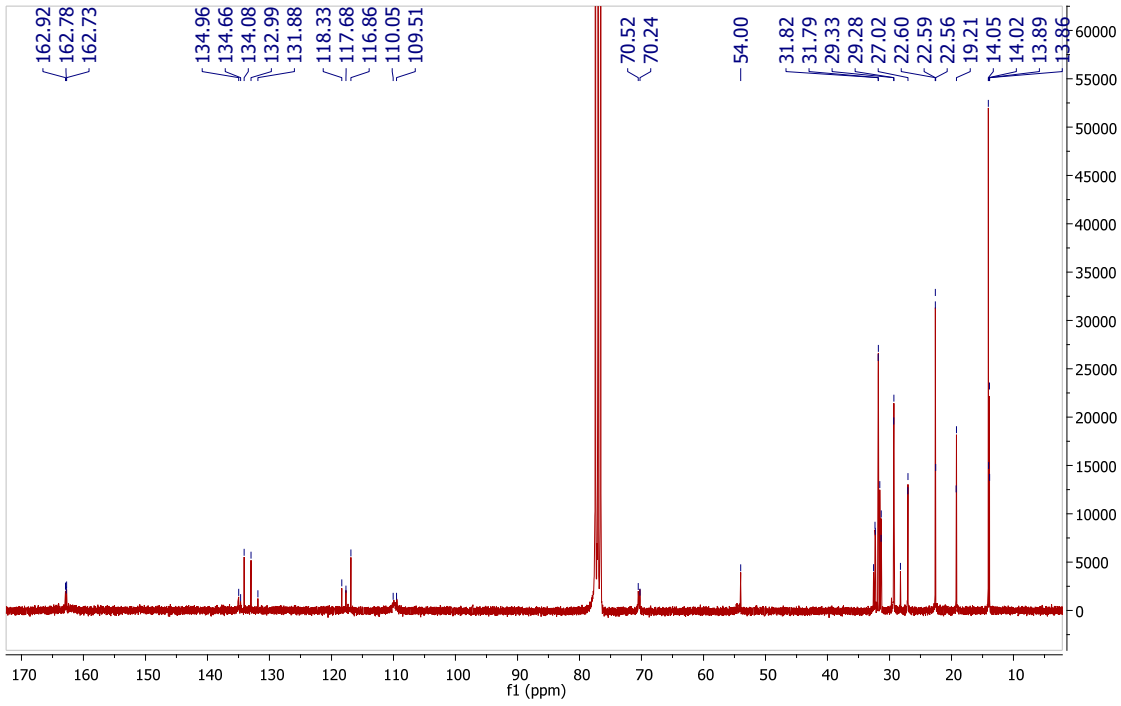
***N,N'*-di-(1'-hexylheptyl)-1-butoxy-6,7,12-trihexylthioperylene-3,4:9,10-tetracarboxydiimide (23)**



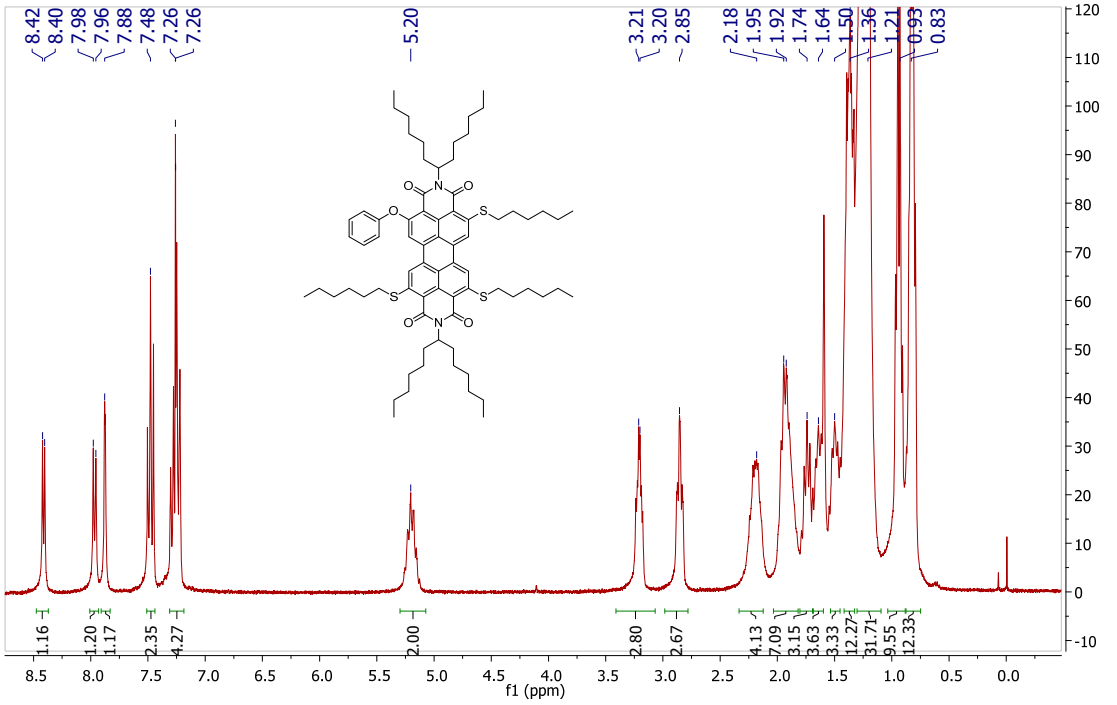


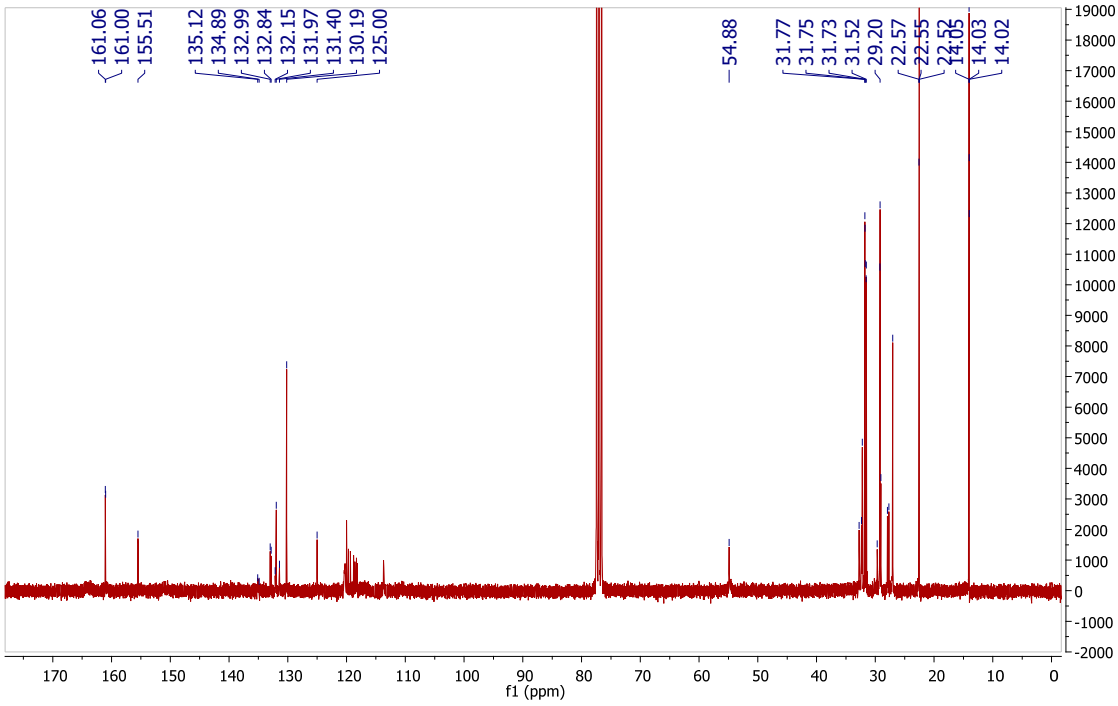
***N,N'*-di(1'-hexylheptyl)-2,5,8-tributoxy-11-hexylthioperylene-3,4:9,10-tetracarboxydiimide (22)**



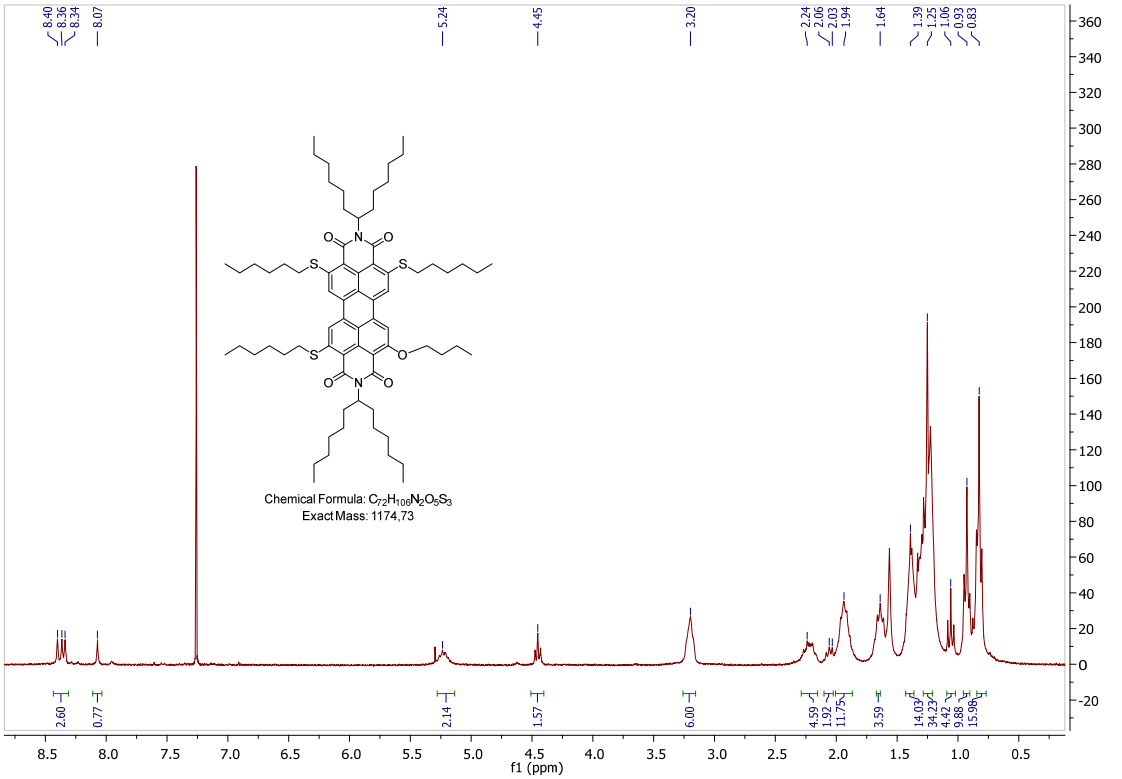


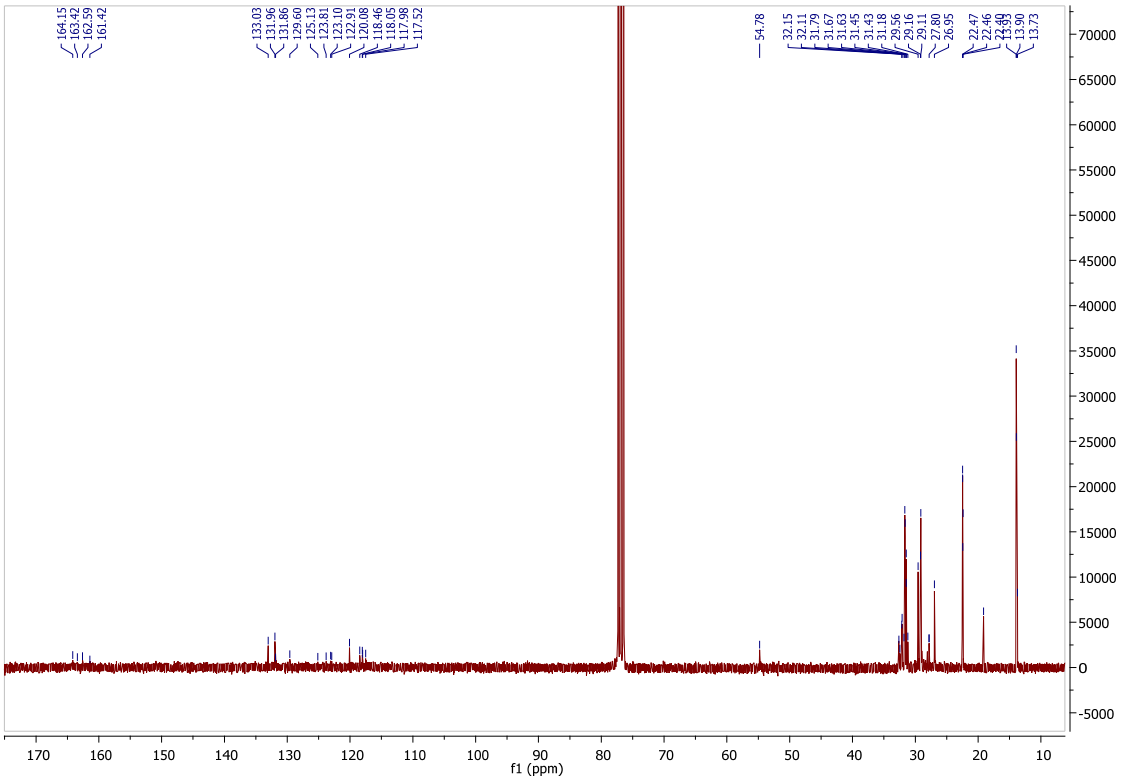
***N,N'*-di(1'-hexylheptyl)-2,5,8-trihexylthio-11-phenoxyperylene-3,4:9,10-tetracarboxydiimide (21)**





***N,N'*-di-(1'-hexylheptyl)-2-butoxy-5,8,11-trihexylthioperylene-3,4:9,10-tetracarboxydiimide (20)**





***N,N'*-di(1'-hexylheptyl)-1,7(6)-dibutoxyperylene-3,4:9,10-tetracarboxydiimide (11)**