Supporting Information for Synthesis, linear and nonlinear optical properties of low-melting π-extended porphyrins

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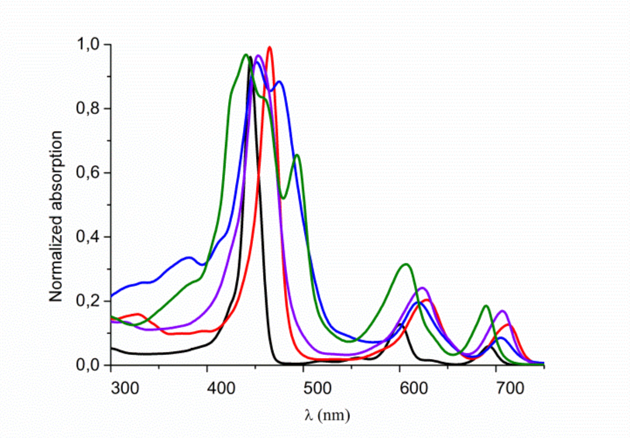

Fig. S-1 Normalized absorption spectra of *meso*-substituted porphyrins **6** (black), **8** (red), **10** (blue), **13** (violet), **15** (green) in CCl_4 at 298 K.

Experimental section:

General

All chemicals were used as received unless otherwise noted. Reagent grade solvents (CH_2Cl_2, hexanes) were distilled prior to use. All reported ^1H NMR spectra were collected using a 500 MHz spectrometer. Chemical shifts (δ ppm) were determined with TMS as the internal reference; *J* values are given in Hz. The UV/Vis absorption spectra were recorded in CCl_4. The absorption wavelengths are reported in nm with the extinction coefficient in $M^{-1}cm^{-1}$ in brackets. Purge gas is high purity argon. Chromatography was performed on silica (200–400 mesh) or alumina. Preparative scale size exclusion chromatography (SEC) was carried out using BioRad Bio-Beads S-X1 with toluene as an eluent. The mass spectra were obtained by field desorption MS

(FD-MS). 3-Perylenylacetylene, (4-ethynylphenyl)diphenylmethane and 5,15-dibromo-porphyrins were obtained according to literature procedure.[1-3]

5-bromo-10,20-bis-(3,4,5-tridecyloxyphenyl)-porphyrin (5). To the solution of A_2-porphyrin **1** (0.802 g, 0.57 mmol) in dichloromethane (30 mL) and methanol (3.3 mL) was added NBS (*N*-bromosuccinimide, 0.113 g, 0.63 mmol) at ambient temperature and stirred for 5 minutes. Bromination was quenched by addition of acetone (5 mL) and solvent was removed under reduced pressure. The crude material was purified by silica gel chromatography using hexanes/EtOAc as an eluent to give product **5** (0.535 g, 0.36 mmol) with 63% yield. ^{1}H NMR (500MHz, $CDCl_3$, 25 °C, TMS): δ = -2.99 (br s, 2H, NH), 0.83 (m, 12H, CH_3), 0.92 (m, 6H, CH_3), 1.22-1.54 (m, 80H, CH_2), 1.66-1.69 (m, 4H, CH_2), 1.87-189 (m, 8H, CH_2), 1.98-2.00 (m, 4H, CH_2), 4.12 (t, 8H, *J* = 6.4 Hz, OCH_2), 4.32 (t, 4H, *J* = 6.4 Hz, OCH_2), 7.42 (s, 4H, ArH), 9.04-9.07 (m, 4H), 9.27 (d, 2H, *J* = 5.0 Hz, β-H), 9.73 (d, 2H, *J* = 5.0 Hz, β-H), 10.14 (s, 1H, *meso*-H); R_f = 0.42 (hexanes/EtOAc, 95:5); LRMS (FD) calcd for $C_{92}H_{141}BrN_4O_6$ 1479.08; found 1479.0, isotope profiles agree; elemental analysis calcd (%) for $C_{92}H_{141}BrN_4O_6$ C 74.71, H 9.61, N 3.79; found C 74.77, H 9.69, N 3.63.

General procedure for mono-substituted A_2B-porphyrins synthesis. The mixture of 5-bromo-porphyrin (0.04 mmol) and corresponding alkyne (0.06 mmol) in THF (5 mL) with toluene (0.5 mL) and triethylamine (1 mL) was deoxygenated by freeze-pump-thaw cycles and purged with argon gas in a Schlenk flask. Triphenylarsine (6.5 mg, 0.02 mmol) and $Pd_2(dba)_3$ (25 mg, 30 μmol) were added and the reaction mixture was stirred at 30 °C in the dark for 24 hours. The crude mixture was filtered through celite. The organic layer separated was dried with Na_2SO_4 and solvent was removed under reduced pressure. The crude dark green product was first purified by silica gel chromatography using hexanes/EtOAc as an eluent, followed by size exclusion chromatography with toluene as an eluent.

5,15-Bis-(3,4,5-trisdecyloxyphenyl)-10-(4-*N*,*N*-dimethylaminophenylethynyl)-porphyrin (10). Product was obtained according to general procedure with 80 % yield (49 mg, 0.03 mmol). ^{1}H NMR (500MHz, $CDCl_3$, 25 °C, TMS): δ = -2.46 (br s, 2H, NH), 0.88-0.95 (m, 12H, CH_3), 0.96-0.98 (m, 6H, CH_3), 1.19-1.54 (m, 80H, CH_2), 1.68-1.70 (m, 4H, CH_2), 1.90-1,95 (m, 8H, CH_2), 2.00-2.10 (m, 4H, CH_2), 3.12 (s, 6H, NCH_3), 4.13 (t, 8H, *J* = 6.4 Hz, OCH_2), 4.38 (t, 4H, *J* = 6.4 Hz, OCH_2), 7.38 (d, 2H, *J* = 9.0 Hz, ArH), 7.44 (s, 4H, ArH), 7.92 (d, 2H, *J* = 9.0 Hz, ArH), 9.01-9.05 (m, 4H, β-H), 9.22 (d, 2H, *J* = 4.8 Hz, β-H), 9.81 (d, 2H, *J* = 5.0 Hz, β-H), 10.08 (s, 1H, *meso*-H); R_f = 0.39 (hexanes/ EtOAc, 95:5); UV/vis (CCl_4) λ (ε) = 421 (106 000), 444 (99 800), 351 (37 800), 589 (22 200), 675 nm (9700); LRMS (FD) calcd for $C_{102}H_{151}N_5O_6$ 1543.37, found 1543.2, isotope profiles agree; elemental analysis calcd (%) for $C_{102}H_{151}N_5O_6$ C 79.38, H 9.86, N 4.54; found C 79.08, H 10.06, N 4.50.

5,15-Bis-(3,4,5-trisdecyloxyphenyl)-10-(4-nitrophenylethynyl)porphyrin (15).

Product was obtained according to general procedure with 31 % yield (19 mg, 0.01 mmol). ^{1}H NMR (500MHz, $CDCl_3$, 25 °C, TMS): δ = -2.52 (br s, 2H, NH), 0.82-0.90 (m, 12H, CH_3), 0.92-0.98 (m, 6H, CH_3), 1.22-1.54 (m, 80H, CH_2), 1.68-1.70 (m, 4H, CH_2), 1.88-1.90 (m, 8H, CH_2), 2.00-2.05 (m, 4H, CH_2), 4.13 (t, 8H, *J* = 6.4 Hz, OCH_2), 4.32 (t, 4H, *J* = 6.4 Hz, OCH_2), 7.44 (s, 4H, ArH), 8.14 (d, 2H, *J* = 9.0 Hz, ArH), 8.42 (d, 2H, *J* = 9.0 Hz, ArH), 9.04 (d, 2H, *J* = 4.5 Hz, β-H), 9.10 (d, 2H, *J* = 4.5 Hz, β-H), 9.28 (d, 2H, *J* = 4.5 Hz, β-H), 9.76 (d, 2H, *J* = 4.5 Hz, β-H), 10.18 (s, 1H, *meso*-H), R_f = 0.39 (hexanes/EtOAc, 95:5); UV/vis (CCl_4) λ (ε) = 440 (124600), 574 nm (14900); LRMS (FD) calcd for $C_{100}H_{145}N_5O_8$ 1545.30; found 1545.0, isotope profiles agree.

General procedure for A_2B_2-porphyrins, 5-bromo-A_2B-porphyrins and unsymmetrically *meso*-substituted A_2BC-porphyrins synthesis. The mixture of 5,15-dibromo-porphyrin (0.04 mmol) and corresponding alkyne (0.1 mmol) in THF (5 mL) with toluene (0.5 mL) and triethylamine (1 mL) was deoxygenated by freeze-pump-thaw cycles and purged with argon gas in a Schlenk flask. Triphenylarsine (6.5 mg, 0.02 mmol) and $Pd_2(dba)_3$ (25 mg, 30 µmol) were added and the reaction mixture was stirred at 30 °C in the dark for 24 hours. The crude mixture was filtered through celite. The organic layer separated was dried with Na_2SO_4 and solvent was removed under reduced pressure. The crude green product was first purified by silica gel chromatography using hexanes/EtOAc as an eluent, followed by size exclusion chromatography with toluene as an eluent. In case of alkynes with electron-acceptor substituents at the *para*-position (cyano and nitro) as well as 1-ethynylperylene or 5-ethynyl-1-methyl-1*H*-imidazole, mono-substituted products were obtained exclusively which were applied again to Sonogashira reaction with alkynes (1.5 equiv.) including electron donating groups (-NMe_2 and -OMe). Corresponding, unsymmetrical porphyrins were purified by silica gel chromatography using hexanes/EtOAc as an eluent, followed by size exclusion chromatography with toluene as an eluent.

5,15-Bis-(3,4,5-trisundecyloxyphenyl)-10,20-bis-(phenylethynyl)-porphyrin (7). Product was obtained according to general procedure with 65 % yield (44 mg, 0.03 mmol). ^{1}H NMR (500MHz, $CDCl_3$, 25 °C, TMS): δ = -1.96 (br s, 2H, NH), 0.84-0.86 (m, 12H, CH_3), 0.87-0.91 (m, 6H, CH_3), 1.28-1.31 (m, 80H, CH_2), 1.35-1.40 (m, 12H, CH_2), 1.62-1.68 (m, 4H, CH_2), 1.85-1.91 (m, 8H, CH_2), 1.98-2.03 (m, 4H, CH_2), 4.13 (t, 8H, *J* = 6.5 Hz, CH_2), 4.31 (t, 4H, *J* = 6.5 Hz, CH_2), 7.42 (s, 4H, ArH), 7.48-7.54 (m, 2H, ArH), 7.56-7.60 (m, 4H, ArH), 8.00-8.06 (m, 4H, ArH), 8.95 (d, 4H, *J* = 5.0 Hz, β-H), 9.68 (d, 4H, *J* = 5.0 Hz, β-H), R_f = 0.43 (hexanes/EtOAc, 95:5); UV/vis (CCl_4) λ (ε) = 445 (393200), 600 (52000), 693 (24800), 556 (11600), 519 nm (8300); LRMS (FD) calcd for $C_{114}H_{162}N_4O_6$ 1684.59; found 1684.9, isotope profiles agree.

5,15-Bis-(3,4,5-trisundecyloxyphenyl)-10,20-bis-(4-methoxyphenylethynyl)-porphyrin (12). Product was obtained according to general procedure with 41 % yield (29 mg, 0.02 mmol). ^{1}H NMR (500MHz, $CDCl_3$, 25 °C, TMS): δ = -1.89 (br s, 2H, NH), 0.84-0.86 (m, 12H, CH_3), 0.87-0.91 (m, 6H, CH_3), 1.28-1.31 (m, 80H, CH_2), 1.35-1.40 (m, 12H, CH_2), 1.62-1.68 (m, 4H, CH_2), 1.85-1.91 (m, 8H, CH_2), 1.98-2.03 (m, 4H, CH_2), 3.94 (s, 6H, OCH_3), 4.13 (t, 8H, *J* = 6.5 Hz, OCH_2), 4.32 (t, 4H, *J* = 6.5 Hz, OCH_2), 7.09 (d, 4H, *J* = 8.5 Hz, ArH), 7.41 (s, 4H, ArH), 7.95 (d, 4H, *J* = 8.5 Hz, ArH), 8.92 (d, 4H, *J* = 5.0 Hz, β-H), 9.65 (d, 4H, *J* = 5.0 Hz, *β*-H), R_f = 0.42 (hexanes/EtOAc, 95:5); UV/vis (CCl_4) λ (ε) = 449 (419500), 607 (55600), 697 (27000), 523 nm (6400); LRMS (FD) calcd for $C_{116}H_{166}N_4O_8$ 1744.64, found 1744.1, isotope profiles agree; elemental analysis calcd (%) for $C_{116}H_{166}N_4O_8$ C 79.86, H 9.59, N 3.21; found C 79.57, H 9.68, N 2.88.

5-bromo-10,20-bis-(3,4,5-trisdecyloxyphenyl)-15-(4-cyanophenylethynyl)-porphyrin. Product was obtained according to general procedure with 28 % yield (18 mg, 0.01 mmol). ^{1}H NMR (500MHz, $CDCl_3$, 25 °C, TMS): *δ* = -2.29 (br s, 2H, NH), 0.85-0.93 (m, 12H, CH_3), 0.94-0.98 (m, 6H, CH_3), 1.22-1.54 (m, 80H, CH_2), 1.68-1.70 (m, 4H, CH_2), 1.88-1.90 (m, 8H, CH_2), 2.00-2.02 (m, 4H, CH_2), 4.11 (t, 8H, *J* = 6.4 Hz, OCH_2), 4.31 (t, 4H, *J* = 6.4 Hz, OCH_2), 7.40 (s, 4H, ArH), 7.85 (d, 2H, *J* = 8.3 Hz, ArH), 8.08 (d, 2H, *J* = 8.3 Hz, ArH), 8.92 (d, 2H, *J* = 4.6 Hz, *β*-H), 8.98 (d, 2H, *J* = 4.6 Hz, *β*-H), 9.61 (d, 2H, *J* = 4.8 Hz, *β*-H), 9.63 (d, 2H, *J* = 4.8 Hz, *β*-H); R_f = 0.38 (hexanes/EtOAc, 95:5); LRMS (FD) calcd for $C_{101}H_{144}BrN_5O_6$ 1604.16; found 1604.9, isotope profiles agree.

5,15-Bis-(3,4,5-trisdecyloxyphenyl)-10-(4-cyanophenylethynyl)-20-(4-ethynyl-*N*,*N*-dimethylaniline)-porphyrin (13). Product was obtained according to general procedure with 51 % yield (34 mg, 0.02 mmol). (starting from 5-bromo-10,20-bis-(3,4,5-trisdecyloxyphenyl)-15-(4-cyanophenylethynyl)-porphyrin). ^{1}H NMR (500MHz, $CDCl_3$, 25 °C, TMS): *δ* = -1.79 (br s, 2H, NH), 0.82-0.90 (m, 12H, CH_3), 0.92-0.98 (m, 6H, CH_3), 1.22-1.54 (m, 80H, CH_2), 1.69 (m, 4H, CH_2), 1.90 (m, 8H, CH_2), 2.00 (m, 4H, CH_2), 3.11 (s, 6H, NCH_3), 4.13 (t, 8H, *J* = 6.4 Hz, OCH_2), 4.32 (t, 4H, *J* = 6.4 Hz, OCH_2), 6.87 (d, 2H, *J* = 8.8 Hz, ArH), 7.40 (s, 4H, ArH), 7.84 (d, 2H, *J* = 8.5 Hz, ArH), 7.90 (d, 2H, *J* = 8.8 Hz, ArH), 8.08 (d, 2H, *J* = 8.5 Hz, ArH), 8.90 (d, 2H, *J* = 4.8 Hz, *β*-H), 8.94 (d, 2H, *J* = 4.8 Hz, *β*-H), 9.63 (d, 2H, *J* = 4.8 Hz, *β*-H), 9.67 (d, 2H, J = 4.8 Hz); R_f = 0.39 (hexanes/EtOAc, 95:5); UV/vis (CCl_4) λ (ε) = 453 (169000), 623 (42000), 706 nm (29600); LRMS (FD) calcd for $C_{111}H_{154}N_6O_6$ 1668.50; found 1668.1, isotope profiles agree.

5,15-Bis-(3,4,5-trisdecyloxyphenyl)-10-(4-methoxyphenylethynyl)-20-(4-cyanophenyl-ethynyl)-porphyrin (14). Product was obtained according to general procedure with 87 % yield (58 mg, 0.03 mmol) (starting from 5-bromo-10,20-bis-(3,4,5-trisdecyloxyphenyl)-15-(4-cyanophenylethynyl)-porphyrin). ^{1}H NMR (500MHz, $CDCl_3$, 25 °C, TMS): *δ* = -1.92 (br s, 2H, NH), 0.82-0.90 (m, 12H, CH_3), 0.92-0.98 (m, 6H, CH_3), 1.22-1.54 (m, 80H, CH_2), 1.69 (m, 4H, CH_2), 1.90 (m, 8H, CH_2), 2.00 (m, 4H, CH_2), 3.95 (s, 3H, OCH_3), 4.13 (t, 8H, *J* = 6.4 Hz, OCH_2), 4.32 (t, 4H, *J* = 6.4 Hz, OCH_2), 7.12 (d, 2H, *J* = 8.8 Hz, ArH), 7.41 (s, 4H, ArH), 7.85 (d, 2H, *J* = 8.5 Hz, ArH), 7.96 (d, 2H, *J* = 8.8 Hz, ArH), 8.09 (d, 2H, *J* = 8.5 Hz, ArH), 8.94 (d, 2H, J = 4.8 Hz, *β*-H), 8.97 (d, 2H, *J* = 4.8 Hz, *β*-H), 9.61 (d, 2H, *J* = 4.8 Hz, *β*-H), 9.68 (d, 2H, *J* = 4.8 Hz, *β*-H); R_f = 0.38 (hexanes/EtOAc, 95:5); UV/vis (CCl_4) λ (ε) = 449 (280000), 608 (38500), 696 (21000), 524 nm (8200); LRMS (FD) calcd for $C_{110}H_{151}N_5O_7$ 1655.46; found 1655.0, isotope profiles agree.

5,15-Bis-(3,4,5-trisdecyloxyphenyl)-10-(4-nitrophenylethynyl)porphyrin (15).

Product was obtained according to general procedure with 31 % yield (19 mg, 0.01 mmol). ^{1}H NMR (500MHz, $CDCl_3$, 25 °C, TMS): δ = -2.52 (br s, 2H, NH), 0.82-0.90 (m, 12H, CH_3), 0.92-0.98 (m, 6H, CH_3), 1.22-1.54 (m, 80H, CH_2), 1.68-1.70 (m, 4H, CH_2), 1.88-1.90 (m, 8H, CH_2), 2.00-2.05 (m, 4H, CH_2), 4.13 (t, 8H, *J* = 6.4 Hz, OCH_2), 4.32 (t, 4H, *J* = 6.4 Hz, OCH_2), 7.44 (s, 4H, ArH), 8.14 (d, 2H, *J* = 9.0 Hz, ArH), 8.42 (d, 2H, *J* = 9.0 Hz, ArH), 9.04 (d, 2H, *J* = 4.5 Hz, *β*-H), 9.10 (d, 2H, *J* = 4.5 Hz, *β*-H), 9.28 (d, 2H, *J* = 4.5 Hz, *β*-H), 9.76 (d, 2H, *J* = 4.5 Hz, *β*-H), 10.18 (s, 1H, *meso*-H), R_f = 0.39 (hexanes/EtOAc, 95:5); UV/vis (CCl_4) λ (ε) = 440 (124600), 574 nm (14900); LRMS (FD) calcd for $C_{100}H_{145}N_5O_8$ 1545.30; found 1545.0, isotope profiles agree.

5-bromo-10,20-bis-(3,4,5-trisdecyloxyphenyl)-15-(4-nitrophenylethynyl)-porphyrin. Product was obtained according to general procedure with 32 % yield (21 mg, 0.01 mmol). ^{1}H NMR (500MHz, $CDCl_3$, 25 °C, TMS): δ = -2.25 (br s, 2H, NH), 0.85-0.93 (m, 12H, CH_3), 0.94-0.98 (m, 6H, CH_3), 1.22-1.54 (m, 80H, CH_2), 1.68-1.70 (m, 4H, CH_2), 1.88-1.90 (m, 8H, CH_2), 2.00-2.02 (m, 4H, CH_2), 4.11 (t, 8H, *J* = 6.4 Hz, OCH_2), 4.31 (t, 4H, *J* = 6.4 Hz, OCH_2), 7.40 (s, 4H, ArH), 7.98 (d, 2H, *J* = 9.2 Hz, ArH), 8.37 (d, 2H, *J* = 9.2 Hz, ArH), 8.92 (d, 2H, *J* = 4.6 Hz, *β*-H), 8.98 (d, 2H, *J* = 4.6 Hz, *β*-H), 9.61 (d, 2H, *J* = 4.8 Hz, *β*-H), 9.63 (d, 2H, *J* = 4.8 Hz, *β*-H); R_f = 0.39 (hexanes/EtOAc, 95:5); LRMS (FD) calcd for $C_{100}H_{144}BrN_5O_8$ 1624.20; found 1624.1, isotope profiles agree.

5,15-Bis-(3,4,5-trisdecyloxyphenyl)-10-(4-nitrophenylethynyl)-20-(4-*N*,*N*-dimethylaminophenylethynyl)-porphyrin (16). Product was obtained according to general procedure with 87 % yield (59 mg, 0.03 mmol) (starting from 5-bromo-10,20-bis-(3,4,5-trisdecyloxyphenyl)-15-(4-nitrophenylethynyl)-porphyrin). ^{1}H NMR (500MHz, $CDCl_3$, 25 °C, TMS): δ = -1.77 (br s, 2H, NH), 0.82-0.90 (m, 12H, CH_3), 0.92-0.98 (m, 6H, CH_3), 1.22-1.54 (m, 80H CH_2), 1.68-1.70 (m, 4H CH_2), 1.88-1.90 (m, 8H CH_2), 2.00-2.05 (m, 4H, CH_2), 3.13 (s, 6H, NCH_3), 4.13 (t, 8H, *J* = 6.4 Hz, OCH_2), 4.32 (t, 4H, *J* = 6.4 Hz, OCH_2), 6.87 (d, 2H, *J* = 8.8 Hz, ArH), 7.41 (s, 4H, ArH), 7.89 (d, 2H, *J* = 8.8 Hz, ArH), 8.11 (d, 2H, *J* = 9.2 Hz, ArH), 8.41 (d, 2H, J = 9.2 Hz, ArH), 8.90 (d, 2H, *J* = 4.8 Hz, *β*-H), 8.95 (d, 2H, *J* = 4.8 Hz, *β*-H), 9.58 (d, 2H, *J* = 4.8 Hz, *β*-H), 9.67 (d, 2H, *J* = 4.8 Hz, *β*-H); R_f = 0.39 (hexanes/EtOAc, 95:5); UV/vis (CCl_4) λ (ε) = 457 (154500), 623 (36000), 708 (28700), 804 nm (3000); LRMS (FD) calcd for $C_{110}H_{154}N_6O_8$ 1688.49; found 1688.0, isotope profiles agree.

5,15-Bis-(3,4,5-trisdecyloxyphenyl)-10-(4-nitrophenylethynyl)-20-(2-methoxynaphthalen-6-yl)-porphyrin (17). Product was obtained according to general procedure with 89 % yield (61 mg, 0.03 mmol) (starting from 5-bromo-10,20-bis-(3,4,5-trisdecyloxyphenyl)-15-(4-nitrophenylethynyl)-porphyrin. ^{1}H NMR (500MHz, $CDCl_3$, 25 °C, TMS): δ = -1.91 (br s, 2H, NH), 0.82-0.90 (m, 12H, CH_3), 0.92-0.98 (m, 6H, CH_3), 1.22-1.54 (m, 80H, CH_2), 1.68-1.70 (m, 4H, CH_2), 1.89-1.91 (m, 8H, CH_2), 2.00-2.02 (m, 4H, CH_2), 3.99 (s, 3H, OCH_3), 4.14 (t, 8H, *J* = 6.4 Hz, OCH_2), 4.33 (t, 4H, *J* = 6.4 Hz, OCH_2), 7.20-7.21 (m, 1H, ArH), 7.23-7.24 (m, 1H, ArH), 7.43 (s, 4H, ArH), 7.86 (d, *J* = 8.5 Hz, 2H, ArH), 7.99-8.01 (m, 1H, ArH), 8.08 (d, 2H, *J* = 9.0 Hz, ArH), 8.37 (d, 2H, *J* = 9.0 Hz, ArH), 8.41 (s, 1H, ArH), 8.94-9.02 (m, 4H, ArH), 9.61 (d, 2H, *J* = 5.0 Hz, *β*-H), 9.74 (d, 2H, *J* =

5.0 Hz, *β*-H); R_f = 0.39 (hexanes/EtOAc, 95:5); UV/vis (CCl_4) λ (ε) = 455 (295800), 613 (52400), 700 (32700), 524 nm (9500); LRMS (FD) calcd for $C_{113}H_{153}N_5O_9$ 1725.51; found 1725.1, isotope profiles agree.

5,15-Bis-(3,4,5-trisdecyloxyphenyl)-10,20-bis-(1-naphthylethynyl)-porphyrin (19). Product was obtained according to general procedure with 73 % yield (50 mg, 0.03 mmol). ^1H NMR (500MHz, $CDCl_3$, 25 °C, TMS): δ = -1.82 (br s, 2H, NH), 0.82-0.90 (m, 12H, CH_3), 0.92-0.98 (m, 6H, CH_3), 1.22-1.54 (m, 80H, CH_2), 1.68-1.70 (m, 4H, CH_2), 1.88-1.90 (m, 8H, CH_2), 2.00-2.05 (m, 4H, CH_2), 4.15 (t, 8H, *J* = 6.4 Hz, OCH_2), 4.33 (t, 4H, *J* = 6.4 Hz, OCH_2), 7.44 (s, 4H, ArH), 7.62-7.70 (m, 2H, ArH), 7.78-7.83 (m, 2H, ArH), 7.85-7.91 (m, 2H, ArH), 8.00-8.10 (m, 4H, ArH), 8.28-2.30 (m, 4H, ArH), 9.01 (d, 4H, *J* = 5.0 Hz, *β*-H), 9.81 (d, 4H, *J* = 5.0 Hz, *β*-H), R_f = 0.40 (hexanes/EtOAc, 95:5); UV/vis (CCl_4) λ (ε) = 451 (367700), 607 (49500), 697 (27100), 523 nm (7500); LRMS (FD) calcd for $C_{116}H_{154}N_4O_6$ 1700.54; found 1700.2, isotope profiles agree; elemental analysis calcd (%) for $C_{116}H_{154}N_4O_6$ C 81.93, H 9.13, N 3.29; found C 81.63, H 9.05, N 3.12.

5,15-Bis-(3,4,5-trisdecyloxyphenyl)-10,20-bis-(9-phenanthrylethynyl)-porphyrin (20). Product was obtained according to general procedure with 16 % yield (11 mg, 0.01 mmol). ^1H NMR (500MHz, $CDCl_3$, 25 °C, TMS): δ = -1.87 (br s, 2H, NH), 0.82-0.90 (m, 12H, CH_3), 0.92-0.98 (m, 6H, CH_3), 1.22-1.54 (m, 80H, CH_2), 1.68-1.70 (m, 4H, CH_2), 1.88-1.90 (m, 8H, CH_2), 2.00-2.02 (m, 4H, CH_2), 4.15 (t, 8H, *J* = 6.4 Hz, OCH_2), 4.32 (t, 4H, *J* = 6.4 Hz, OCH_2), 7.43 (s, 4H, ArH), 7.74-7.76 (m, 6H, ArH), 7.83-7.86 (m, 2H, ArH), 8.59 (s, 6H, ArH), 8.77-8.78 (m, 1H, ArH), 8.82-8.83 (m, 1H, ArH), 9.03 (d, 4H, *J* = 5.0 Hz, *β*-H), 9.12-9.14 (m, 2H, ArH), 9.86 (d, 4H, *J* = 5.0 Hz, *β*-H); R_f = 0.43 (hexanes/EtOAc, 95:5); UV/vis (CCl_4) λ (ε) = 454 (268000), 610 (28500), 698 nm (15200); LRMS (FD) calcd for $C_{124}H_{158}N_4O_6$ 1800.67; found 1800.1, isotope profiles agree.

5-Bromo-10,20-Bis-(3,4,5-trisdecyloxyphenyl)-15-(3-perylenylethynyl)-porphyrin (21). Product was obtained according to general procedure with 23 % yield (16 mg, 0.01 mmol). ^1H NMR (500MHz, $CDCl_3$, 25 °C, TMS): δ = -2.41 (br s, 2H, NH), 0.88-0.94 (m, 12H, CH_3), 0.95-0.98 (m, 6H, CH_3), 1.19-1.54 (m, 80H, CH_2), 1.68-1.70 (m, 4H, CH_2), 1.93-1.95 (m, 8H, CH_2), 1.98-2.00 (m, 4H, CH_2), 4.16 (t, 8H, *J* = 6.4 Hz, OCH_2), 4.34 (t, 4H, *J* = 6.4 Hz, OCH_2), 7. 32 (dt, 2H, *J* = 2.5, 7.9 Hz, ArH), 7.43 (s, 4H, ArH), 7.51 (t, 1H, *J* = 7.9 Hz, ArH), 7.51 (t, 1H, *J* = 7.9 Hz, ArH), 7.67-7.62 (m, 3H, ArH), 7.78-7.98 (m, 4H, ArH), 8.62 (d, 1H, *J* = 7.9 Hz, ArH), 8.88 (d, 2H, *J* = 4.5 Hz, *β*-H), 9.01 (d, 2H, *J* = 4.5 Hz, *β*-H), 9.52 (d, 2H, *J* = 4.5 Hz, *β*-H), 9.76 (d, 2H, *J* = 4.5 Hz, *β*-H), R_f = 0.42 (hexanes/EtOAc, 95:5); UV/vis (CCl_4) λ (ε) = 440 (117700), 493 (79800), 606 (38500), 689 nm (22500); LRMS (FD) calcd for $C_{114}H_{151}BrN_4O_6$ 1753.40; found 1753.1, isotope profiles agree; elemental analysis calcd (%) for $C_{114}H_{151}BrN_4O_6$ C 78.09, H 8.68, N 3.20; found C 78.30, H 8.61, N 3.05.

5,15-Bis-(3,4,5-trisdecyloxyphenyl)-10,20-bis-(pyridin-2-ylethynyl)-porphyrin (22). Product was obtained according to general procedure with 11 % yield (7 mg, 0.01 mmol). ^1H NMR (500MHz, $CDCl_3$, 25 °C, TMS): δ = -2.05 (br s, 2H, NH), 0.82-0.90 (m, 12H, CH_3), 0.92-0.98 (m, 6H, CH_3), 1.22-1.54 (m, 80H, CH_2), 1.68-1.70 (m, 4H, CH_2), 1.88-1.90 (m, 8H, CH_2), 2.00-

2.02 (m, 4H, CH_2), 4.13 (t, 8H, *J* = 6.4 Hz, OCH_2), 4.31 (t, 4H, *J* = 6.4 Hz, OCH_2), 7.40-7.42 (m, 2H, ArH), 7.41 (s, 4H, ArH), 7.88-7.93 (m, 2H, *J* = 8.5 Hz, ArH), 8.01-8.05 (m, 2H, ArH), 8.85-8.88 (m, 2H, ArH), 8.97 (d, 4H, *J* = 5.0 Hz, *β*-H), 9.76 (d, 4H, *J* = 5.0 Hz, *β*-H); R_f = 0.31 (hexanes/EtOAc, 95:5); UV/vis (CCl_4) λ (ε) = 445 (376000), 599 (52000), 691 (26800), 556 (11000), 519 nm (8500); LRMS (FD) calcd for $C_{106}H_{148}N_6O_6$ 1602.40; found 1602.0, isotope profiles agree.

5,15-Bis-(3,4,5-trisdecyloxyphenyl)-10,20-bis-(pyridin-4-ylethynyl)-porphyrin (23). Product was obtained according to general procedure with 15 % yield (10 mg, 0.01 mmol). ^{1}H NMR (500MHz, $CDCl_3$, 25 °C, TMS): *δ* = -2.04 (br s, 2H, NH), 0.82-0.90 (m, 12H, CH_3), 0.92-0.98 (m, 6H, CH_3), 1.22-1.54 (m, 80H, CH_2), 1.68-1.70 (m, 4H, CH_2), 1.88-1.90 (m, 8H, CH_2), 2.00-2.02 (m, 4H, CH_2), 4.13 (t, 8H, *J* = 6.4 Hz, OCH_2), 4.33 (t, 4H, *J* = 6.4 Hz, OCH_2), 7.41 (s, 4H, ArH), 7.86 (d, 4H, *J* = 8.5 Hz, ArH), 8.83 (d, 4H, *J* = 8.5 Hz, ArH), 8.99 (d, 4H, *J* = 5.0 Hz, *β*-H), 9.64 (d, 4H, *J* = 5.0 Hz, *β*-H); R_f = 0.31 (hexanes/EtOAc, 95:5); UV/vis (CCl_4) λ (ε) = 445 (266000), 599 (36600), 691 (18700), 555 (10000), 520 nm (9500); LRMS (FD) calcd for $C_{106}H_{148}N_6O_6$ 1602.40; found 1602.1, isotope profiles agree.

5,15-Bis-(3,4,5-trisdecyloxyphenyl)-10,20-bis-(4-(*N*,*N*-diphenylamino)-phenylethynyl)-porphyrin (24). Product was obtained according to general procedure with 53 % yield (41 mg, 0.02 mmol). ^{1}H NMR (500MHz, $CDCl_3$, 25 °C, TMS): *δ* = -1.83 (br s, 2H, NH), 0.82-0.90 (m, 12H, CH_3), 0.92-0.98 (m, 6H, CH_3), 1.22-1.54 (m, 80H, CH_2), 1.68-1.70 (m, 4H, CH_2), 1.88-1.90 (m, 8H, CH_2), 2.00-2.02 (m, 4H, CH_2), 4.12 (t, 8H, *J* = 6.5 Hz, OCH_2), 4.31 (t, 4H, *J* = 6.5 Hz, OCH_2), 7.13 (t, 4H, *J* = 7.5 Hz, ArH), 7.21-7.24 (m, 12H, ArH), 7.35 (t, 8H, *J* = 7.5 Hz, ArH), 7.39 (s, 4H, ArH), 7.86 (d, 4H, *J* = 8.7 Hz, ArH), 8.91 (d, 4H, *J* = 5.0 Hz, *β*-H), 9.63 (d, 4H, *J* = 5.0 Hz, *β*-H), R_f = 0.37 (hexanes/EtOAc, 95:5); UV/vis (CCl_4) λ (ε) = 464 (183700), 619 (45000), 706 nm (28500); LRMS (FD) calcd for $C_{132}H_{168}N_6O_6$ 1934.85; found 1934.2, isotope profiles agree; elemental analysis calcd (%) for $C_{132}H_{168}N_6O_6$ C 81.94, H 8.75, N 4.34; found C 81.27, H 8.93, N 4.18.

5,15-Bis-(3,4,5-trisdecyloxyphenyl)-10,20-bis-(3-ethynylthiophene)-porphyrin (25). Product was obtained according to general procedure with 58 % yield (37 mg, 0.02 mmol). ^{1}H NMR (500MHz, $CDCl_3$, 25 °C, TMS): *δ* = -1.98 (br s, 2H, NH), 0.82-0.90 (m, 12H, CH_3), 0.92-0.98 (m, 6H, CH_3), 1.22-1.54 (m, 80H, CH_2), 1.68-1.70 (m, 4H, CH_2), 1.88-1.90 (m, 8H, CH_2), 2.00-2.02 (m, 4H, CH_2), 4.12 (t, 8H, *J* = 6.4 Hz, OCH_2), 4.31 (t, 4H, *J* = 6.4 Hz, OCH_2), 7.41 (s, 4H, ArH), 7.53 (d, 2H, *J* = 1 Hz, ArH), 7.64 (d, 2H, *J* = 1 Hz, ArH), 7.96 (d, 2H, *J* = 1 Hz, ArH), 8.94 (d, 4H, *J* = 5.0 Hz, *β*-H), 9.64 (d, 4H, *J* = 5.0 Hz, *β*-H), R_f = 0.40 (hexanes/EtOAc, 95:5); UV/vis (CCl_4) λ (ε) = 444 (431000), 599 (53800), 692 (25400), 555 nm (13700); LRMS (FD) calcd for $C_{104}H_{146}N_4O_6S_2$ 1612.47; found 1612.0, isotope profiles agree; elemental analysis calcd (%) for $C_{104}H_{146}N_4O_6S_2$ C 77.47, H 9.13, N 3.47; found C 77.44, H 9.07, N 3.33.

5,15-Bis-(3,4,5-trisundecyloxyphenyl)-10,20-bis-(3-ethynylthiophene)porphyrin (26). Product was obtained according to general procedure with 52 % yield (35 mg, 0.02 mmol). ^{1}H NMR (500MHz, $CDCl_3$, 25 °C, TMS): *δ* = -1.97 (br s, 2H, NH), 0.84-

0.86 (m, 12H, CH_3), 0.87-0.91 (m, 6H, CH_3), 1.28-1.31 (m, 80H, CH_2), 1.35-1.40 (m, 12H, CH_2), 1.62-1.68 (m, 4H, CH_2), 1.85-1.91 (m, 8H, CH_2), 1.98-2.03 (m, 4H, CH_2), 4.12 (t, 8H, *J* = 6.5 Hz, OCH_2), 4.31 (t, 4H, *J* = 6.5 Hz, OCH_2), 7.41 (s, 4H, ArH), 7.53 (d, 2H, *J* = 1 Hz, ArH), 7.62 (d, 2H, *J* = 1 Hz, ArH), 7.97 (d, 2H, *J* = 1 Hz, ArH), 8.93 (d, 4H, *J* = 5.0 Hz, *β*-H), 9.64 (d, 4H, *J* = 5.0 Hz, *β*-H), R_f = 0.41 (hexanes/EtOAc, 95:5); UV/vis (CCl_4) λ (ε) = 444 (342000), 598 (42800), 692 (19800), 555 nm (10000); LRMS (FD) calcd for $C_{110}H_{158}N_4O_6S_2$ 1696.64; found 1696.1, isotope profiles agree; elemental analysis calcd (%) for $C_{110}H_{158}N_4O_6S_2$ C 77.87, H 9.39, N 3.30; found C 77.90, H 9.40, N 3.07.

5-Bromo-10,20-bis-(3,4,5-trisdecyloxyphenyl)-15-(5-ethynyl-1-methyl-1*H*-imidazole)-porphyrin (27). Product was obtained according to general procedure with 31 % yield (20 mg, 0.01 mmol). ^{1}H NMR (500MHz, $CDCl_3$, 25 °C, TMS): *δ* = -2.29 (br s, 2H, NH), 0.82-0.90 (m, 12H, CH_3), 0.92-0.98 (m, 6H, CH_3), 1.22-1.54 (m, 80H, CH_2), 1.68-1.70 (m, 4H, CH_2), 1.88-1.90 (m, 8H, CH_2), 2.00-2.02 (m, 4H, CH_2), 4.11 (t, 8H, *J* = 6.4 Hz, OCH_2), 4.21 (s, 3H, NCH_3), 4.31 (t, 4H, *J* = 6.4 Hz, OCH_2), 7.38 (s, 4H, ArH), 7.80 (s, 1H, ArH), 8.07 (s, 1H, ArH), 8.95 (dd, 4H, *J* = 26.5, 4.5 Hz, *β*-H), 9.58 (dd, 4H, *J* = 26.5, 4.5 Hz, *β*-H); R_f = 0.38 (hexanes/EtOAc, 95:5); UV/vis (CCl_4) λ (ε) = 441 (186700), 584 (16800), 679 nm (8000); LRMS (FD) calcd for $C_{98}H_{145}BrN_6O_6$ 1583.19; found 1583.9, isotope profiles agree.

Zinc 5,15-Bis-(3,5-dioctyloxy-phenyl)-10-[4-(*N*,*N*-dibutylamino)phenylethynyl]-20-trihexylsilanylethynyl-porphyrin (32). Zinc 5,15-Bis-(3,5-bis-octyloxy-phenyl)-10-ethynyl-20-trihexylsilanylethynyl-porphyrin (100 mg, 73 μmol), tris-(dibenzylideneacetone)-di-palladium(0) (4.5 mg, 4.9 μmol), PPh_3 (9.6 mg, 37 μmol) and CuI (3.5 mg, 19 μmol) were dried under vacuum before dry NEt_3 (6 mL) was added and the mixture degassed. *N*,*N*-Dibutyl-4-iodoaniline (4 eq., 97 mg, 292 μmol) was added and the reaction stirred at 50 °C for 1.5 hours when TLC (10:1:1 40-60 °C petroleum ether/EtOAc/pyridine, R_f = 0.75) showed the reaction to be complete. The volume was reduced and the mixture passed through a short silica gel column (CH_2Cl_2). Column chromatography (100:4:1 40-60 °C petroleum ether/EtOAc/pyridine) followed by recrystallization by layer addition (CH_2Cl_2/MeOH) gave a dark green solid (54 mg, 47 %); ^{1}H NMR (400 MHz, $CDCl_3$/5 % d^5-pyridine, 25 °C, TMS): *δ* = 0.46-0.40 (m, 27H, CH_3); 1.67-0.89 (m, 78H, CH_2), 1.94-1.76 (m, 8H, CH_2), 3.33 (t, 4H, *J* = 7.7 Hz, NCH_2), 4.16 (t, 8H, *J* = 6.6 Hz, OCH_2), 6.67 (d, 2H, *J* = 8.8 Hz, ArH), 6.91 (t, 2H, *J* = 2.2 Hz, ArH), 7.37 (d, 4H, *J* = 2.2 Hz, ArH), 7.74 (d, 2H, *J* = 8.8 Hz, ArH), 8.98 (d, 2H, *J* = 3.2 Hz, *β*-H), 8.99 (d, 2H, *J* = 3.2 Hz, *β*-H), 9.64 (d, 2H, *J* = 4.6 Hz, *β*-H), 9.72 (d, 2H, *J* = 4.6 Hz, *β*-H); UV/vis (CH_2Cl_2/1% pyridine) λ/nm (log ε) = 320 (4.24), 447 (4.92), 461 (4.98), 669 (4.58); LRMS (MALDI ToF MS^+) calcd for $C_{100}H_{144}N_5O_4SiZn$ ($[M+H]^{\bullet+}$ 1571.75; found 1571.03.

Zinc 5,15-Bis-(3,5-dioctyloxy-phenyl)-10-[4-(*N*-dibutylamino)phenylethynyl]-20-(4-nitrophenylethynyl)-porphyrin (33). Tetra-*n*-butylammonium fluoride (1 M solution in THF, 32 μL, 32 μmol) was added to a solution of zinc 5,15-bis-(3,5-bis-octyloxy-phenyl)-10-[4-(butyl-butyryl-amino)-phenylethynyl]-20-trihexylsilanylethynyl-porphyrin (50 mg, 32 μmol) in dry

CH_2Cl_2 (10 mL) and the reaction mixture stirred for 10 min. when TLC (10:1:1 40-60 °C petroleum ether/EtOAc/pyridine, R_f = 0.70) showed the reaction to be complete. CH_3COOH (4 μL, 64 μmol) was added, the reaction mixture passed through a short silica gel column (CH_2Cl_2) and the solvent removed. tris-(Dibenzylideneacetone)-di-palladium(0) (2.0 mg, 2.1 μmol), PPh_3 (4.2 mg, 16 μmol) and CuI (1.5 mg, 8.1 μmol) were added and the solids dried under vacuum before dry NEt_3 (6 mL) was added and the mixture degassed. 1-Iodo-4-nitrobenzene (4 eq., 64 mg, 256 μmol) was added and the reaction stirred at 50 °C for 0.5 hours when TLC (10:1:1 40-60 °C petroleum ether/EtOAc/pyridine, R_f = 0.65) showed the reaction to be complete. The volume was reduced and the mixture passed through a short silica gel column (CH_2Cl_2) followed by recrystallisation by layer addition (CH_2Cl_2/MeOH) to give a dark green solid (32 mg, 71 %); ^{1}H NMR (400 MHz, $CDCl_3$/5 % d^5 pyridine, 25 °C, TMS): δ = 0.88 (t, 12H, J = 6.7 Hz, CH_3); 1.03 (t, 6H, J = 7.4 Hz, CH_3), 1.57-1.27 (m, 4H, CH_2), 1.57-1.27 (m, 4H, CH_2), 1.71-1.64 (m, 4H, CH_2), 1.93-1.86 (m, 8H, CH_2), 3.39 (t, 4H, J = 7.7 Hz, NCH_2), 4.16 (t, 8H, J = 6.6 Hz, OCH_2), 6.79 (d, 2H, J = 8.7 Hz, ArH), 6.91 (s, 2H, ArH), 7.36 (d, 4H, J = 1.7 Hz, ArH), 7.85 (d, 2H, J = 8.7 Hz, ArH), 8.05 (d, 2H, J = 8.3 Hz, ArH), 8.35 (d, 2H, J = 8.3 Hz, ArH), 8.93 (d, 2H, J = 4.5 Hz, β-H), 8.99 (d, 2H, J = 4.5 Hz, β-H), 9.60 (d, 2H, J = 4.5 Hz, β-H), 9.69 (d, 2H, J = 4.5 Hz, β-H), UV/vis (CH_2Cl_2/1% pyridine) λ/nm (log ε) =314 (4.54), 465 (5.92), 600 (3.92), 692 (4.88); LRMS (MALDI ToF MS$^+$) calcd for $C_{88}H_{109}N_6O_6Zn$ ($[M+H]^{\bullet+}$) 1411.32; found 1409.77.

Photophysical measurements.

Two-photon absorption measurements were carried out using a wavelength-tunable femtosecond laser system that comprises a Ti:Sapphire femtosecond oscillator (Mira 900, Coherent Inc.) pumped by a CW frequency-doubled Nd:YAG laser (Verdi, Coherent Inc.) and a 1-kHz repetition rate Ti:Sapphire femtosecond regenerative amplifier (Legend H, Coherent Inc.). The pulses from the Ti:sapphire amplifier are down converted with an optical parametric amplifier, OPA (TOPAS-C, Quantronix), whose output signal (idler) is continuously tunable from 1100 to 1600 (1600 to 2200) nm. The second harmonic of idler was used for two-photon excitation in the λ_{ex} = 800 - 1100 nm region and the fundamental of signal in the 1100 - 1400 nm region. The OPA output signal pulse energy was 100–250 μJ (5–10 μJ after frequency doubling), and the pulse duration was 70–120 fs. A detailed description of the experimental procedure has been described earlier.[4] Briefly, the linearly polarized excitation laser beam was slightly focused with an f = 25-cm lens onto the sample solution contained in a 1x1 cm^2 spectroscopic cell and placed 15 cm behind the lens. A small fraction of the beam was split off by a thin glass plate placed just before the sample and directed to the reference detector (Molectron). The sample fluorescence was collected with a spherical mirror (f = 50 cm, diameter d = 10 cm) and focused with magnification ratio ~ 1 on the entrance slit of an imaging grating spectrometer (Jobin Yvon Triax 550). The 2PA spectrum (in relative units) was obtained by tuning the wavelength of OPA, and measuring the corresponding intensity of two-photon excited fluorescence. The wavelength tuning of OPA and data collection were computer-controlled with a LabView routine. At each wavelength, the fluorescence intensity was normalized to the square of the excitation photon flux, measured in the reference channel. The correction to the spectral variations of the OPA output (pulse duration and beam spatial profile) was done by using Rhodamine B in methanol as a standard, whose 2PA spectrum is well characterized.[4] To exclude possible artifacts, e.g. due to absorption at wavelengths close to the linear absorption, we checked that at each wavelength the fluorescence signal increased as a square of the excitation intensity. Absolute 2PA cross sections were measured using relative fluorescence technique as described with Rhodamine B as a standard.[4] To obtain absolute 2PA spectra in GM units, all relative 2PA spectra were calibrated to the known (at one wavelength in each spectral region) absolute cross section value. The 2PA properties were measured in CCl_4 solutions.

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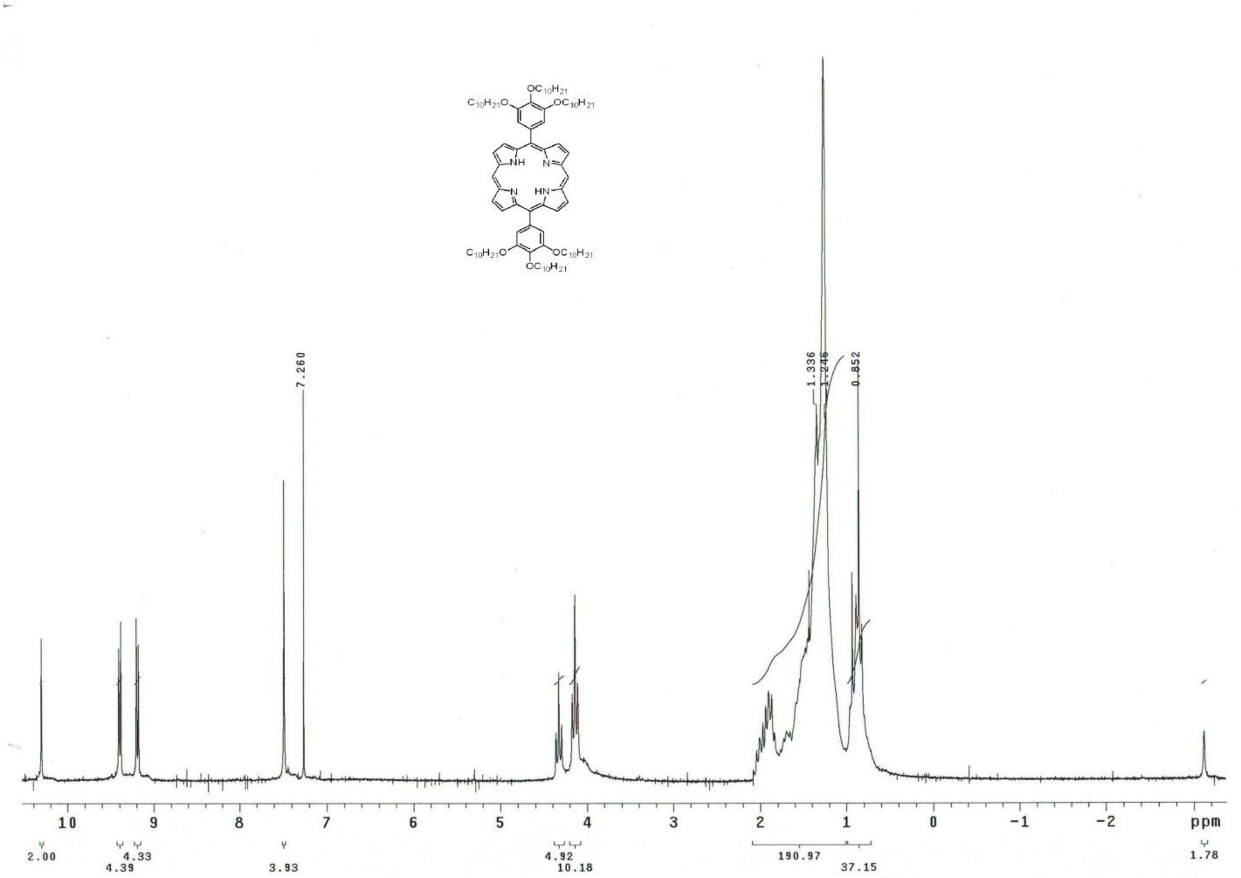

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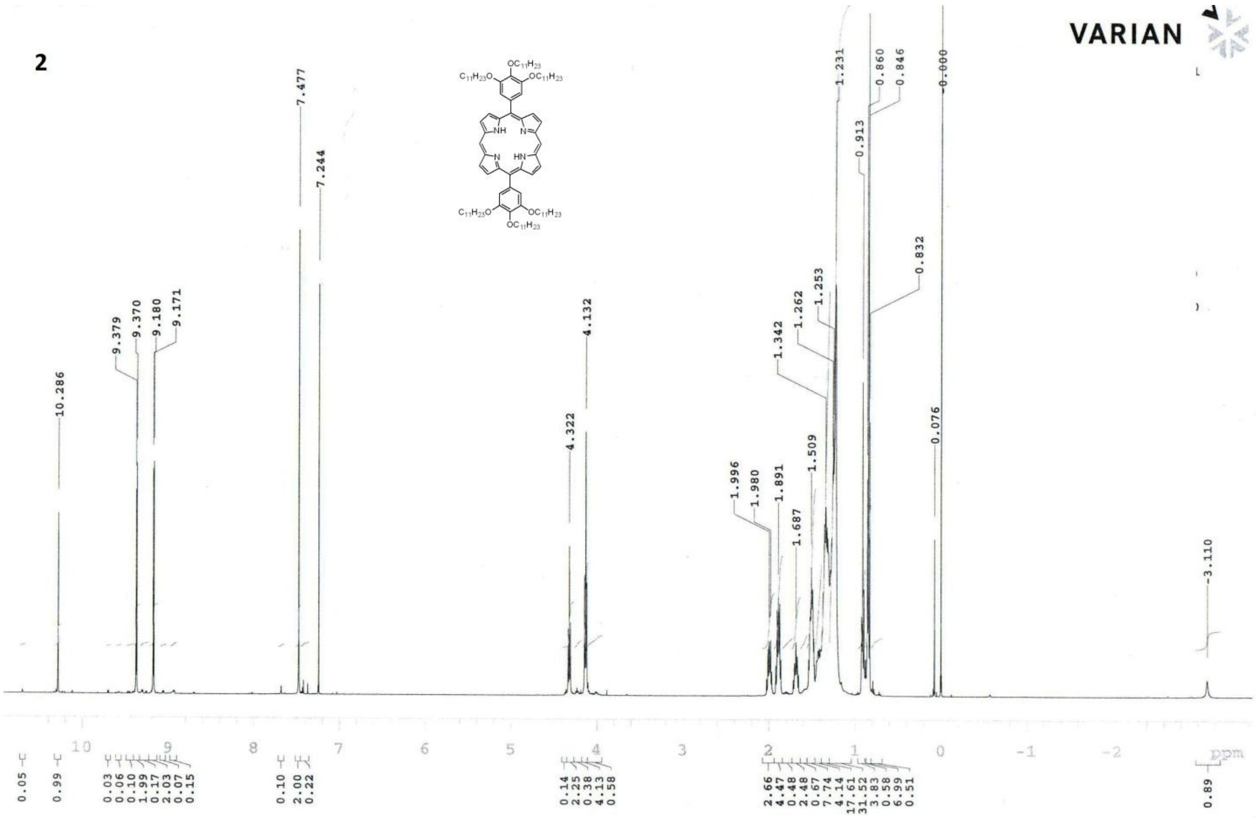
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1.231
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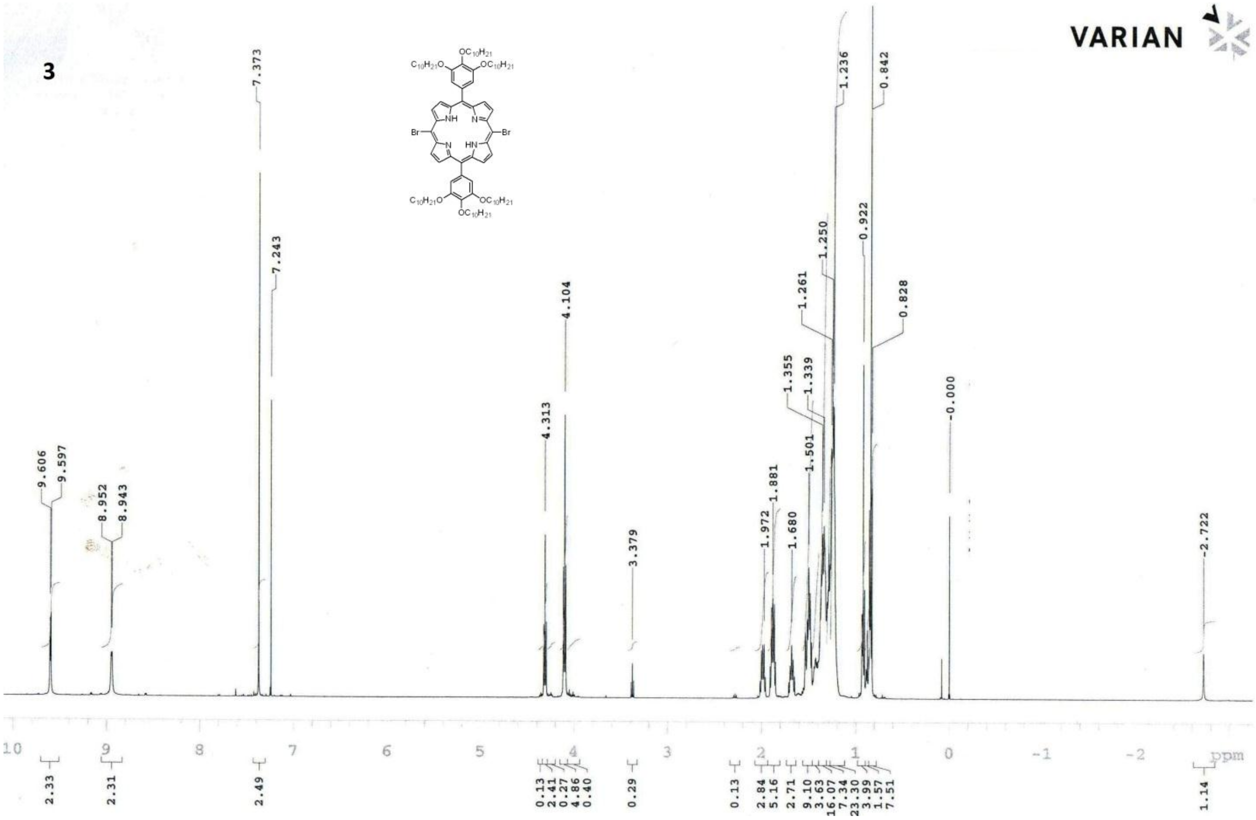
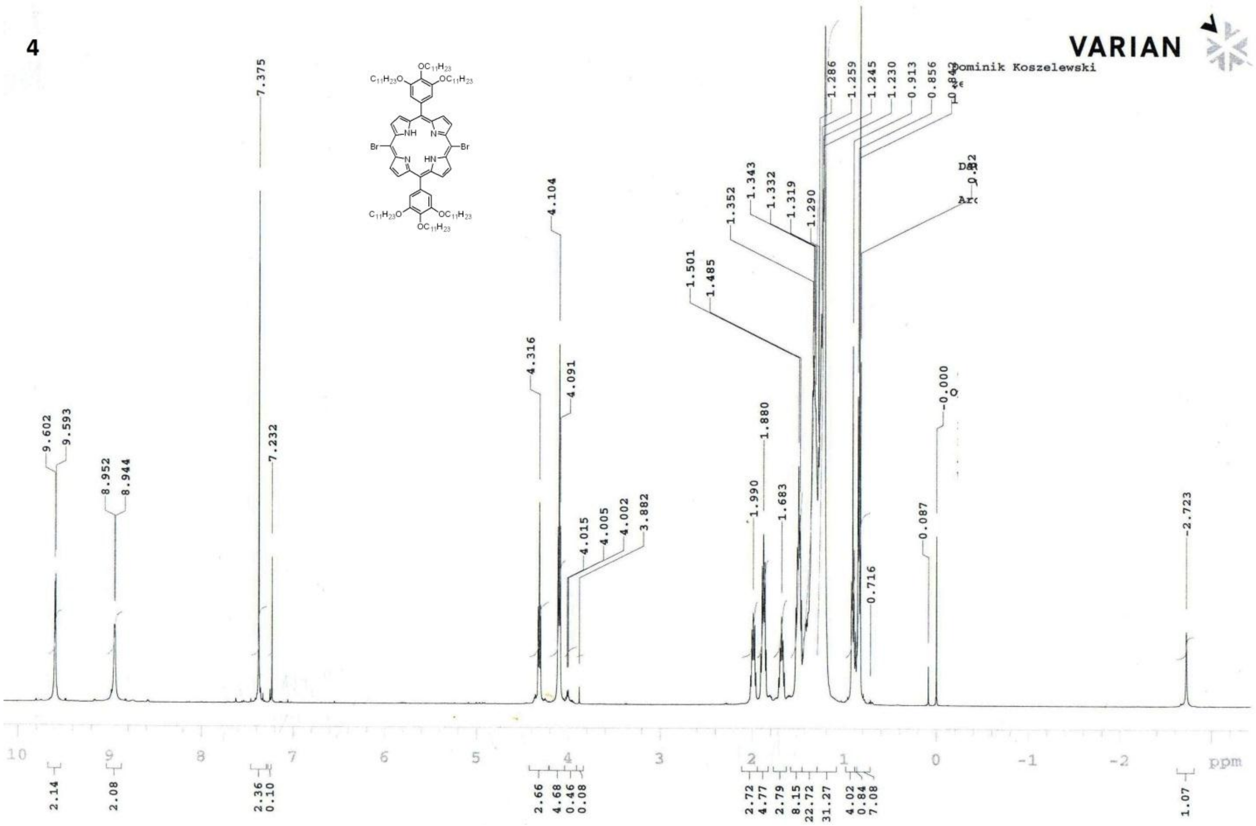
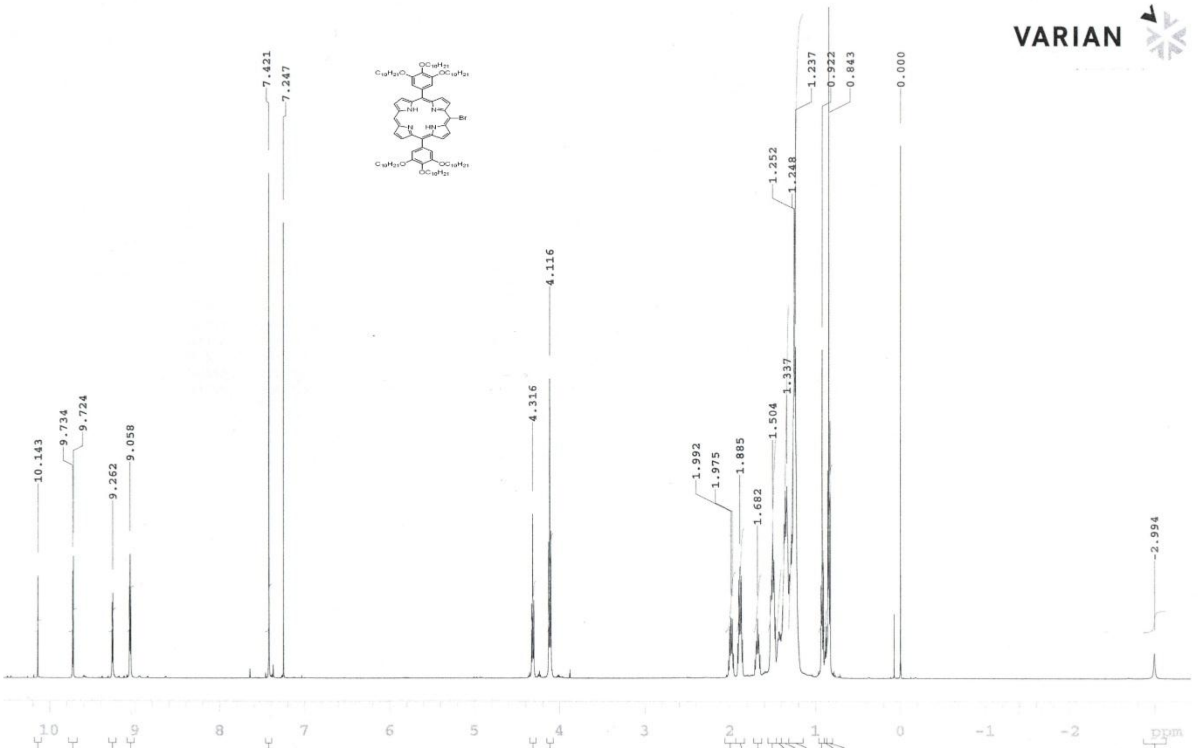
0.05
0.99
0.03
0.06
0.10
1.99
0.17
2.03
0.07
0.15
0.10
2.00
0.22
0.14
2.25
0.38
4.13
0.58
2.66
4.47
0.48
2.48
0.67
7.74
4.14
17.61
31.52
3.83
0.58
6.59
0.51
0.89

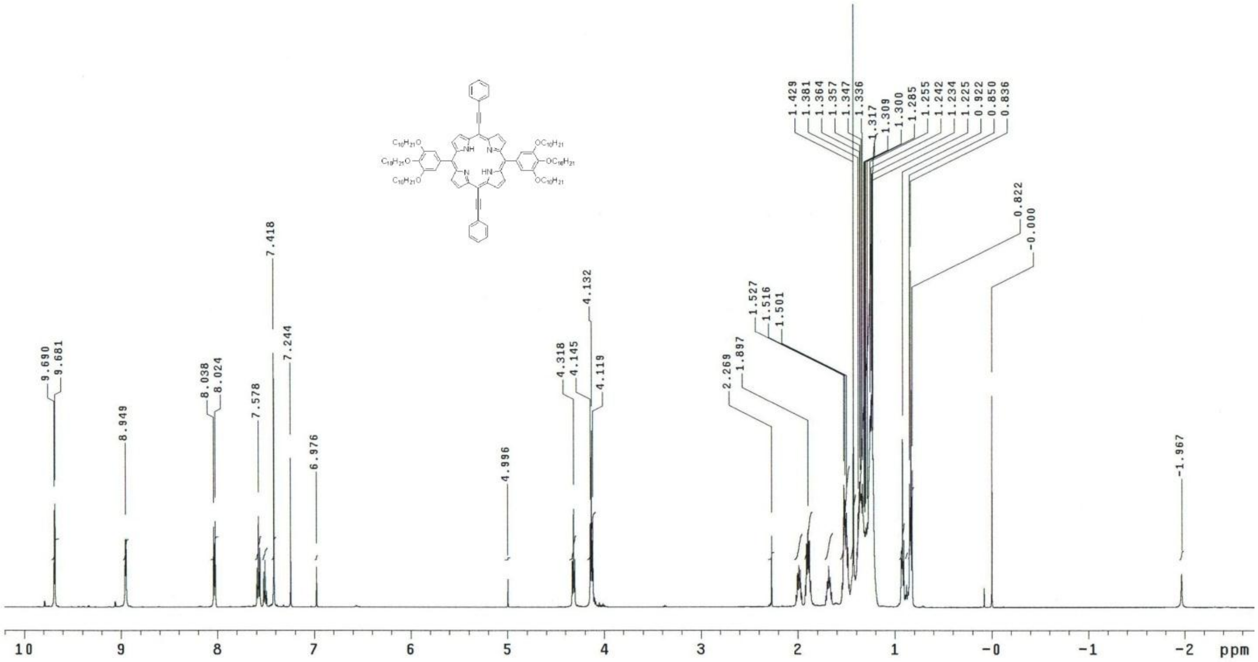
3

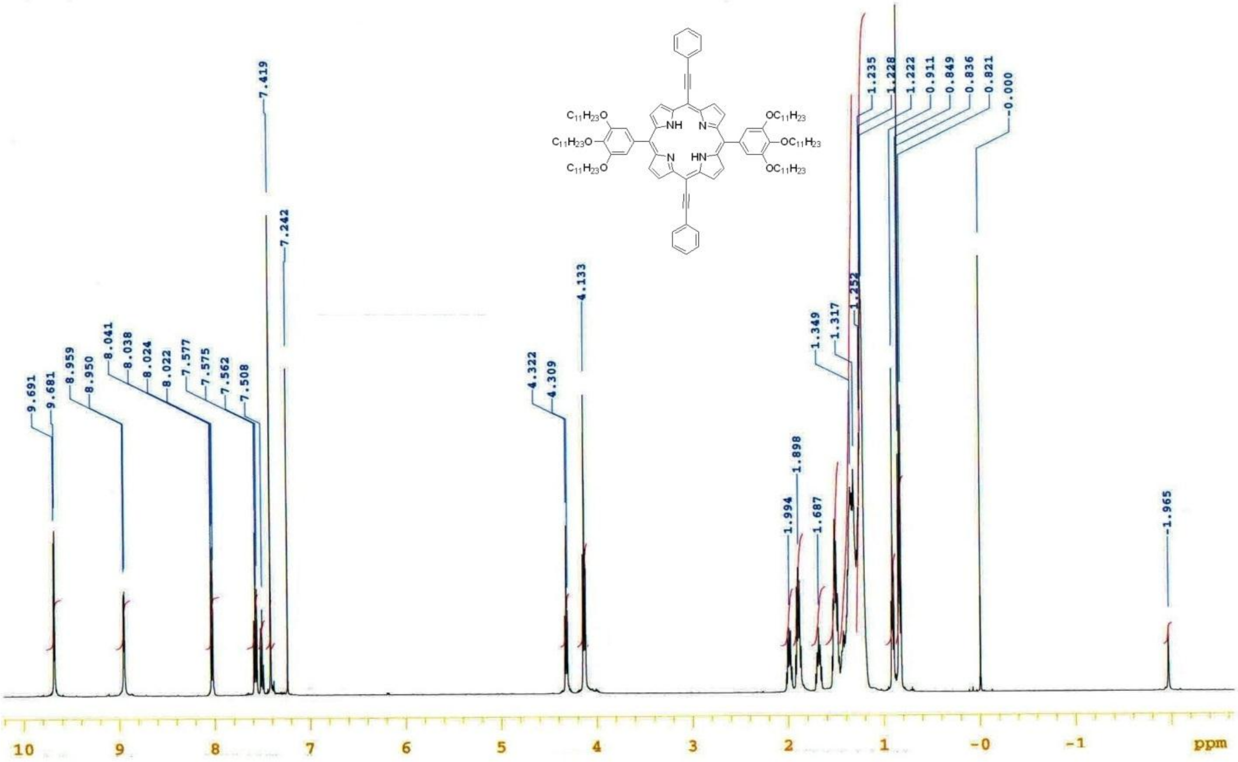

VARIAN
OC10H21
C10H21O
OC10H21
NH
N
Br
Br
N
HN
9.606
9.597
8.952
8.943
7.373
7.243
4.313
4.104
3.379
1.972
1.881
1.680
1.501
1.355
1.339
1.261
1.250
1.236
0.922
0.842
0.828
-0.000
-2.722
10
9
8
7
6
5
4
3
2
1
0
-1
-2
ppm
2.33
2.31
2.49
0.13
2.41
0.27
4.86
0.40
0.29
0.13
2.84
5.16
2.71
9.10
3.63
16.07
7.34
23.30
3.99
1.57
7.51
1.14

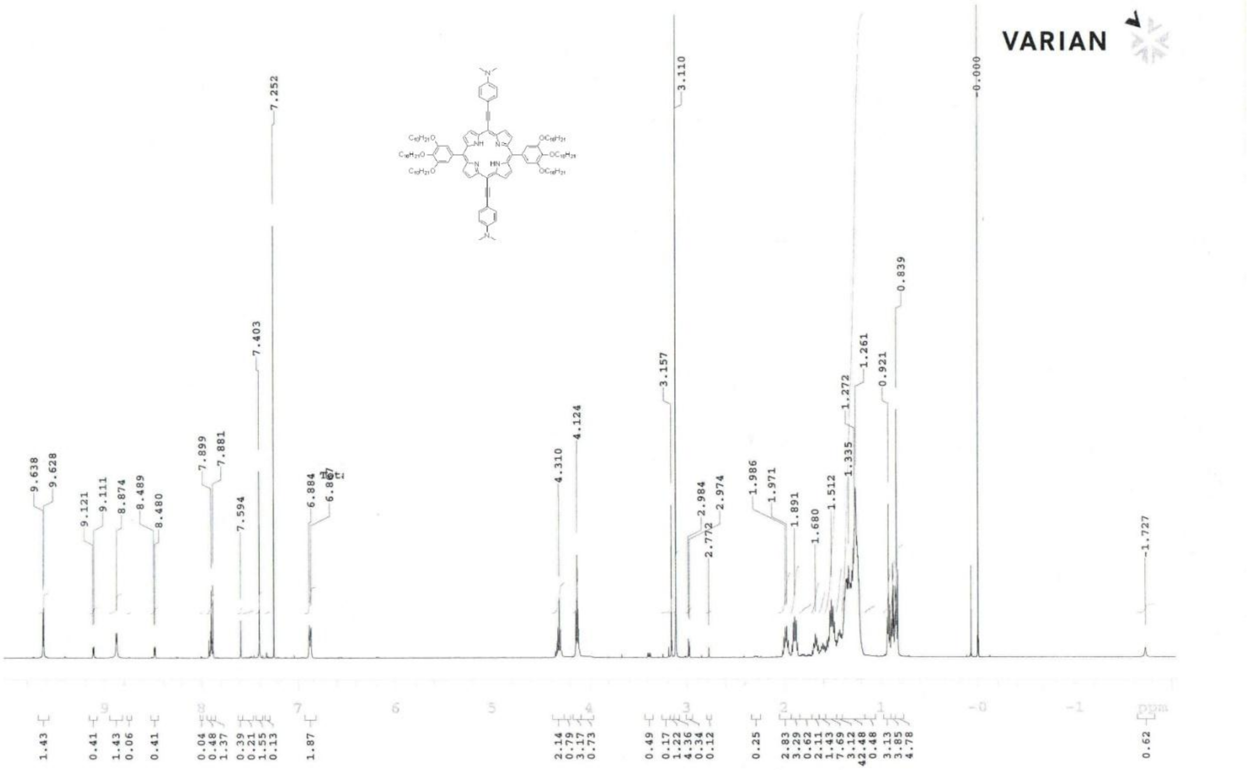
4

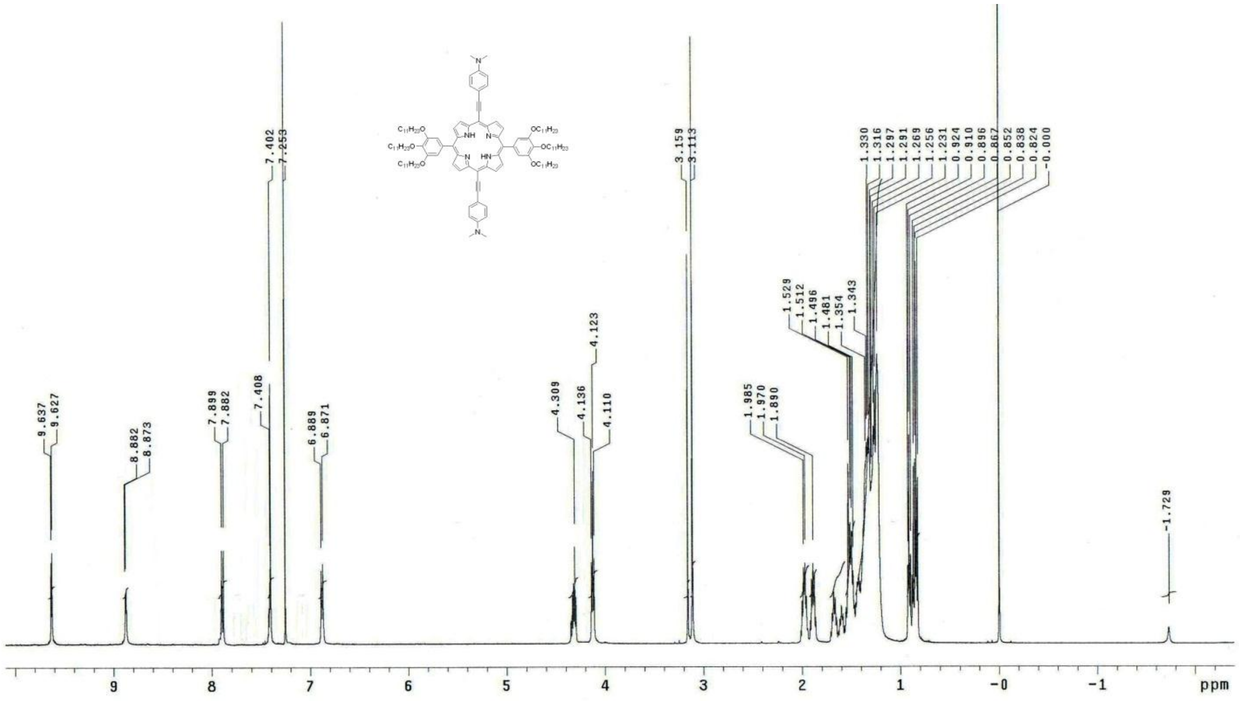

VARIAN
Dominik Koszelewski
9.602
9.593
8.952
8.944
7.375
7.232
4.316
4.104
4.091
4.015
4.005
4.002
3.882
1.990
1.880
1.683
1.501
1.485
1.352
1.343
1.332
1.319
1.290
1.286
1.259
1.245
1.230
0.913
0.856
0.843
0.716
0.087
0.000
-2.723
ppm
10
9
8
7
6
5
4
3
2
1
0
-1
-2
2.14
2.08
2.36
0.10
2.66
4.68
0.46
0.08
2.72
4.77
2.79
8.15
22.72
31.27
4.02
0.84
7.08
1.07
$OC_{11}H_{23}$
$C_{11}H_{23}O$
NH
N
HN
Br

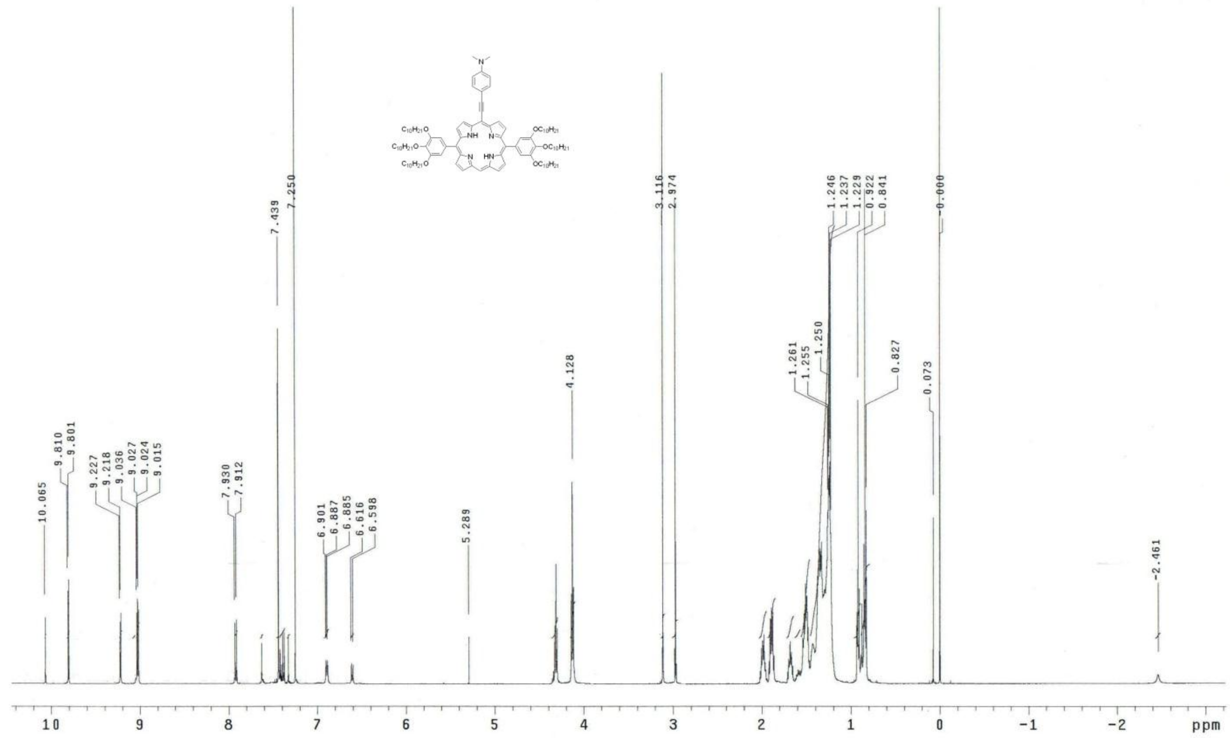

VARIAN
10.143
9.734
9.724
9.262
9.058
7.421
7.247
4.316
4.116
1.992
1.975
1.885
1.682
1.504
1.337
1.252
1.248
1.237
0.922
0.843
0.000
-2.994
ppm
10
9
8
7
6
5
4
3
2
1
0
-1
-2
$OC_{10}H_{21}$
$C_{10}H_{21}O$
NH
N
HN
Br

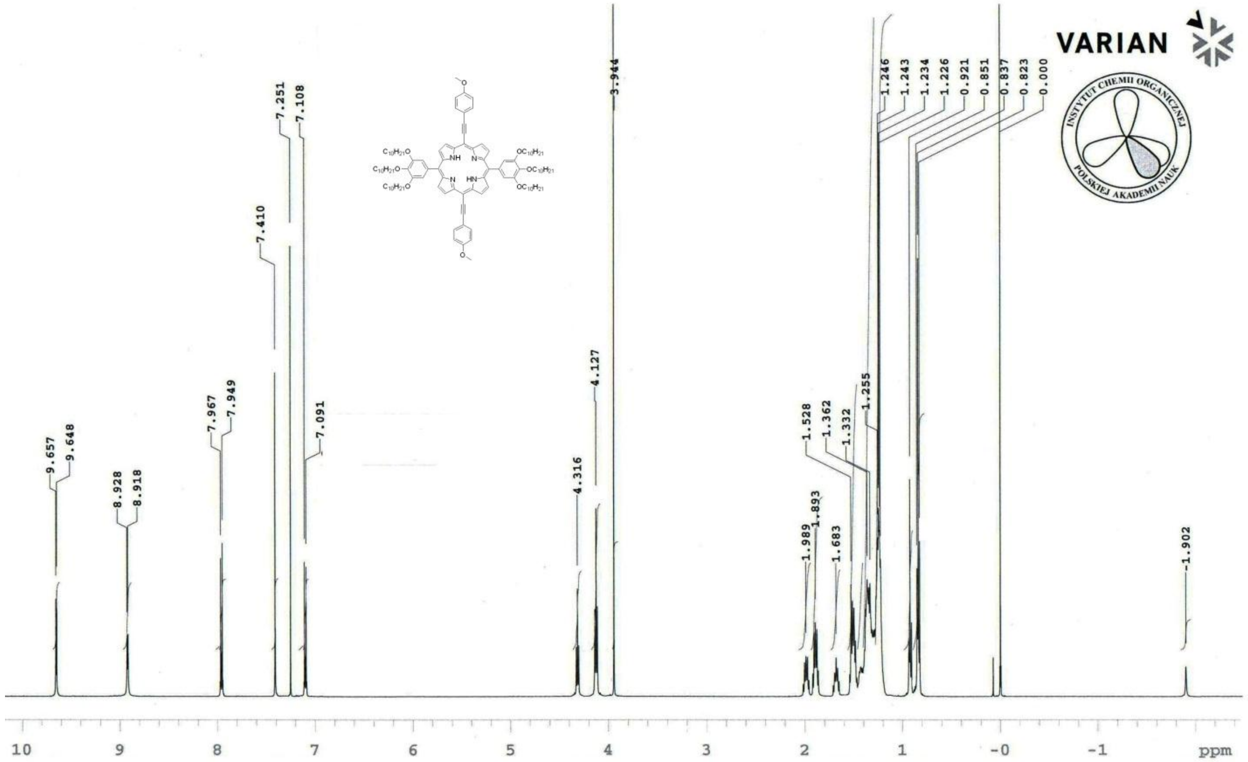

9.690
9.681
8.949
8.038
8.024
7.578
7.418
7.244
6.976
4.996
4.318
4.145
4.132
4.119
2.269
1.897
1.527
1.516
1.501
1.429
1.381
1.364
1.357
1.347
1.336
1.317
1.309
1.300
1.285
1.255
1.242
1.234
1.225
0.922
0.850
0.836
0.822
-0.000
-1.967
$C_{10}H_{21}O$
$OC_{10}H_{21}$
NH
N
HN
10
9
8
7
6
5
4
3
2
1
-0
-1
-2
ppm

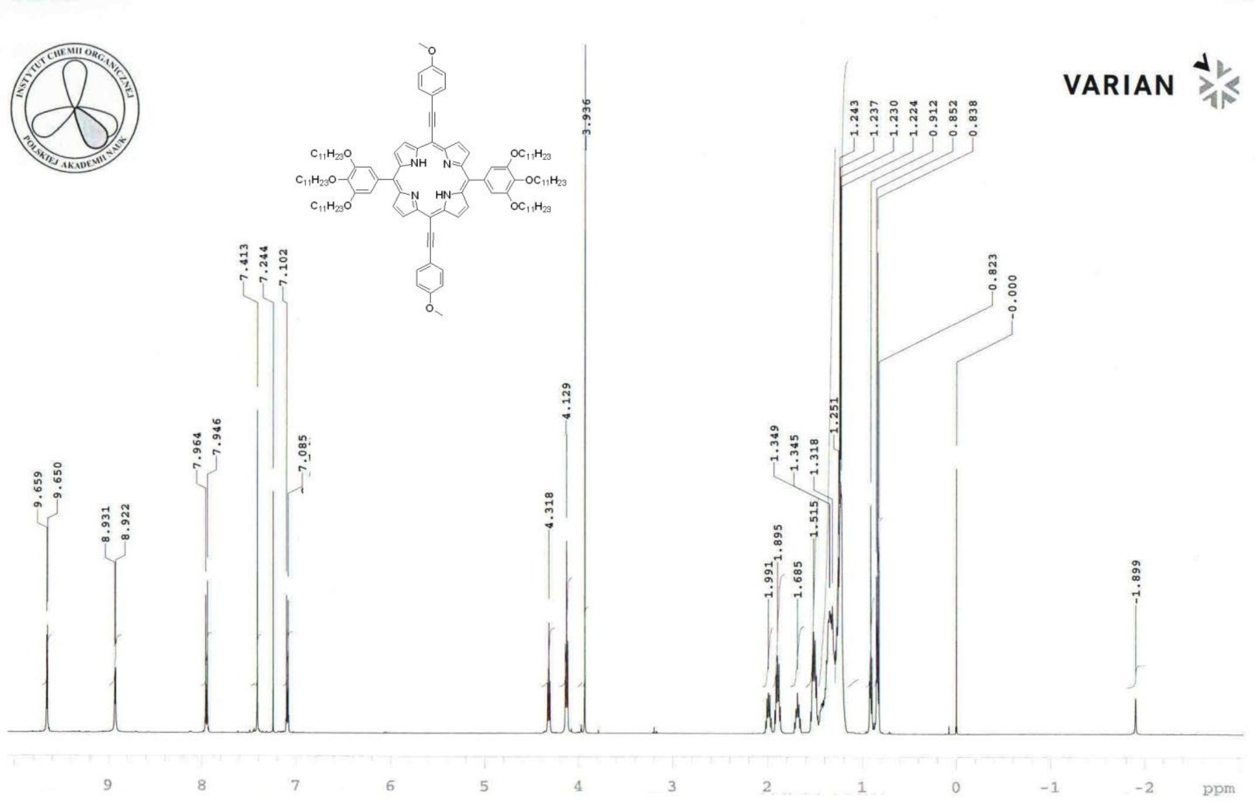

9.691
9.681
8.959
8.950
8.041
8.038
8.024
8.022
7.577
7.575
7.562
7.508
7.419
7.242
4.322
4.309
4.133
1.994
1.898
1.687
1.349
1.317
1.252
1.235
1.228
1.222
0.911
0.849
0.836
0.821
-0.000
-1.965
$C_{11}H_{23}O$
$OC_{11}H_{23}$
NH
N
HN
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm

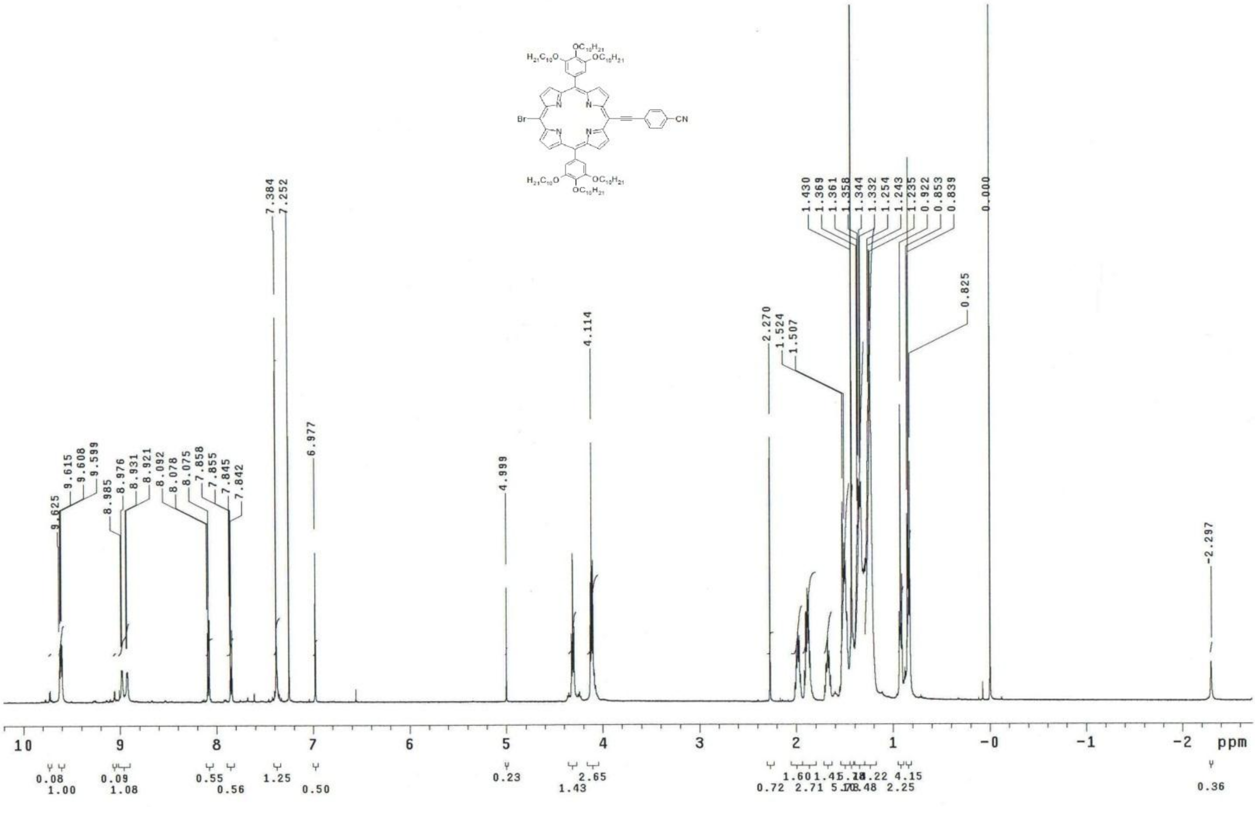

VARIAN
7.252
3.110
-0.000
0.839
7.403
3.157
1.261
0.921
1.272
4.124
9.638
9.628
9.121
9.111
8.874
8.489
8.480
7.899
7.881
7.594
6.884
6.867
4.310
2.984
2.974
2.772
1.986
1.971
1.891
1.680
1.512
1.335
-1.727
NH
N
HN
1.43
0.41
1.43
0.06
0.41
0.04
0.48
1.37
0.39
0.21
1.55
0.13
1.87
2.14
0.79
3.17
0.73
0.49
0.17
1.22
4.36
0.34
0.12
0.25
2.83
3.29
0.62
2.11
1.43
7.69
3.12
42.48
0.48
3.13
3.85
4.78
0.62
9
8
7
6
5
4
3
2
1
-0
-1
ppm

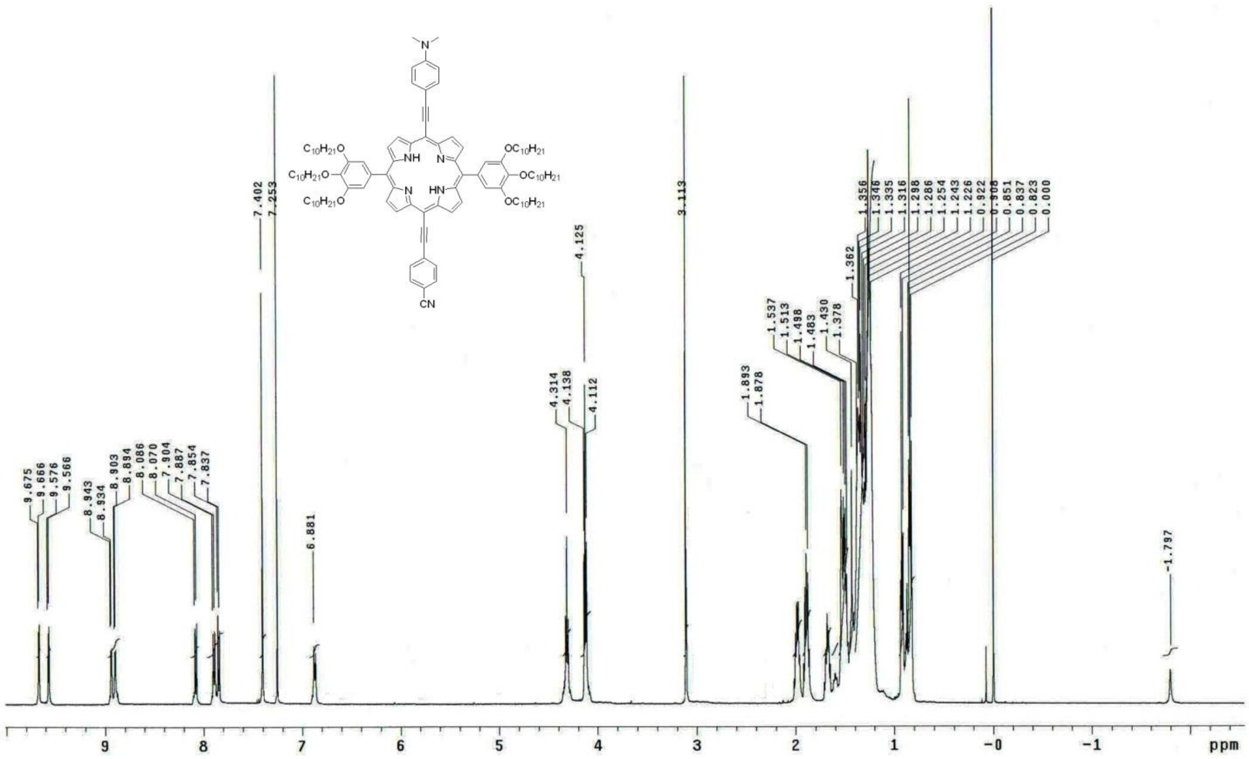

C11H23O
OC11H23
NH
N
HN
9.637
9.627
8.882
8.873
7.899
7.882
7.408
7.402
7.253
6.889
6.871
4.309
4.136
4.123
4.110
3.159
3.113
1.985
1.970
1.890
1.529
1.512
1.496
1.481
1.354
1.343
1.330
1.316
1.297
1.291
1.269
1.256
1.231
0.924
0.910
0.896
0.867
0.852
0.838
0.824
-0.000
-1.729
9
8
7
6
5
4
3
2
1
-0
-1
ppm

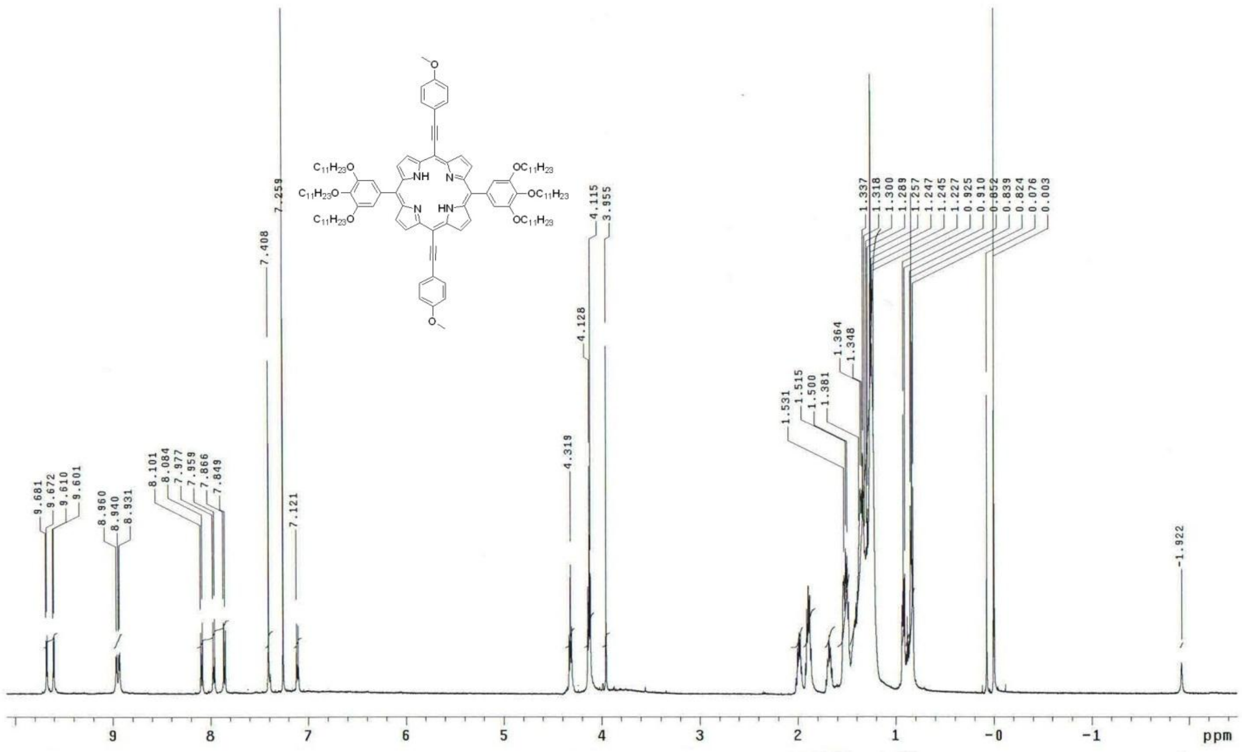

C10H21O
NH
N
HN
OC10H21
10.065
9.810
9.801
9.227
9.218
9.036
9.027
9.024
9.015
7.930
7.912
7.439
7.250
6.901
6.887
6.885
6.616
6.598
5.289
4.128
3.116
2.974
1.261
1.255
1.250
1.246
1.237
1.229
0.922
0.841
0.827
0.073
0.000
-2.461
10
9
8
7
6
5
4
3
2
1
0
-1
-2
ppm

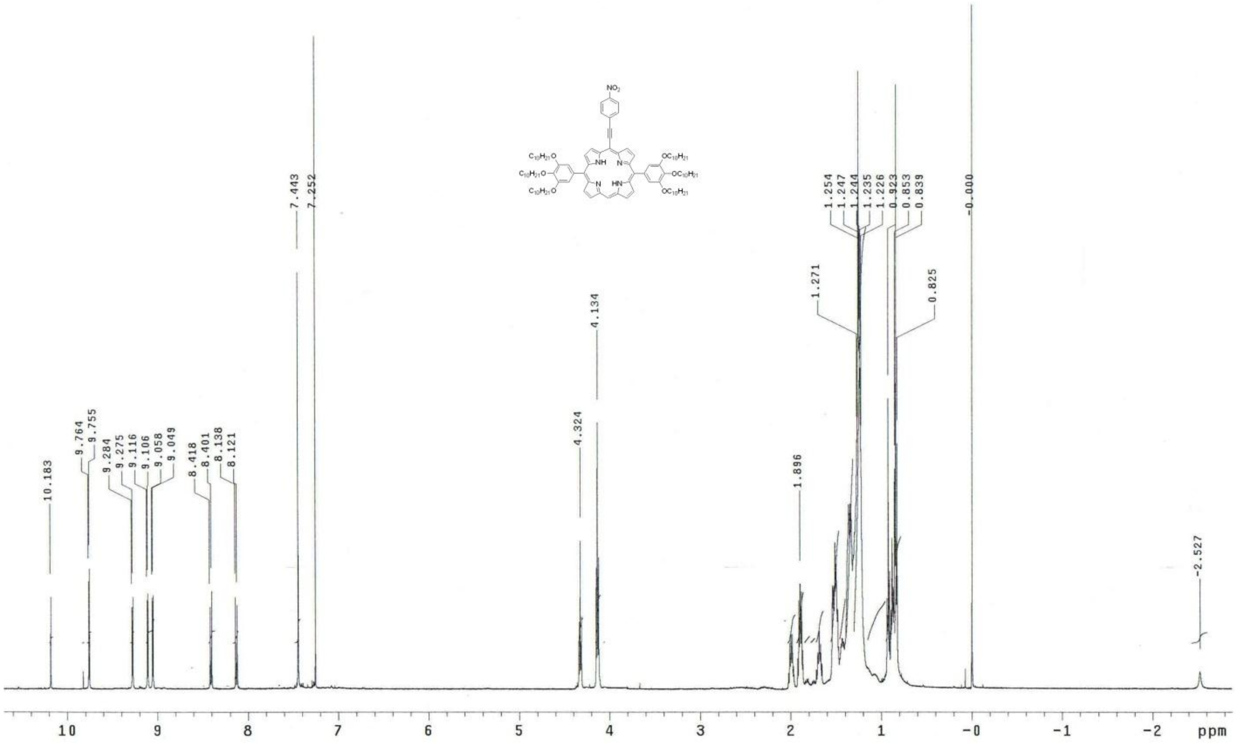

VARIAN
INSTYTUT CHEMII ORGANICZNEJ POLSKIEJ AKADEMII NAUK
C10H21O
NH
N
HN
OC10H21
9.657
9.648
8.928
8.918
7.967
7.949
7.410
7.251
7.108
7.091
4.316
4.127
3.944
1.989
1.893
1.683
1.528
1.362
1.332
1.255
1.246
1.243
1.234
1.226
0.921
0.851
0.837
0.823
0.000
-1.902
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm

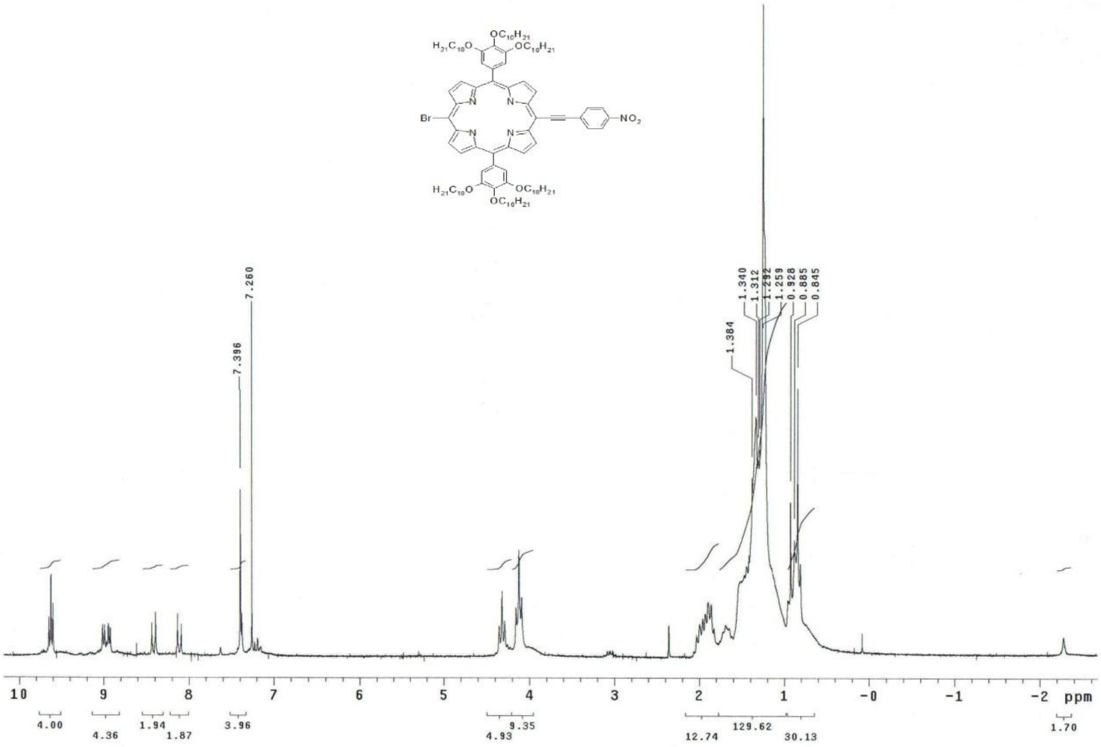

VARIAN
9.659
9.650
8.931
8.922
7.964
7.946
7.413
7.244
7.102
7.085
4.318
4.129
3.936
1.991
1.895
1.685
1.515
1.349
1.345
1.318
1.251
1.243
1.237
1.230
1.224
0.912
0.852
0.838
0.823
0.000
-1.899
9
8
7
6
5
4
3
2
1
0
-1
-2
ppm

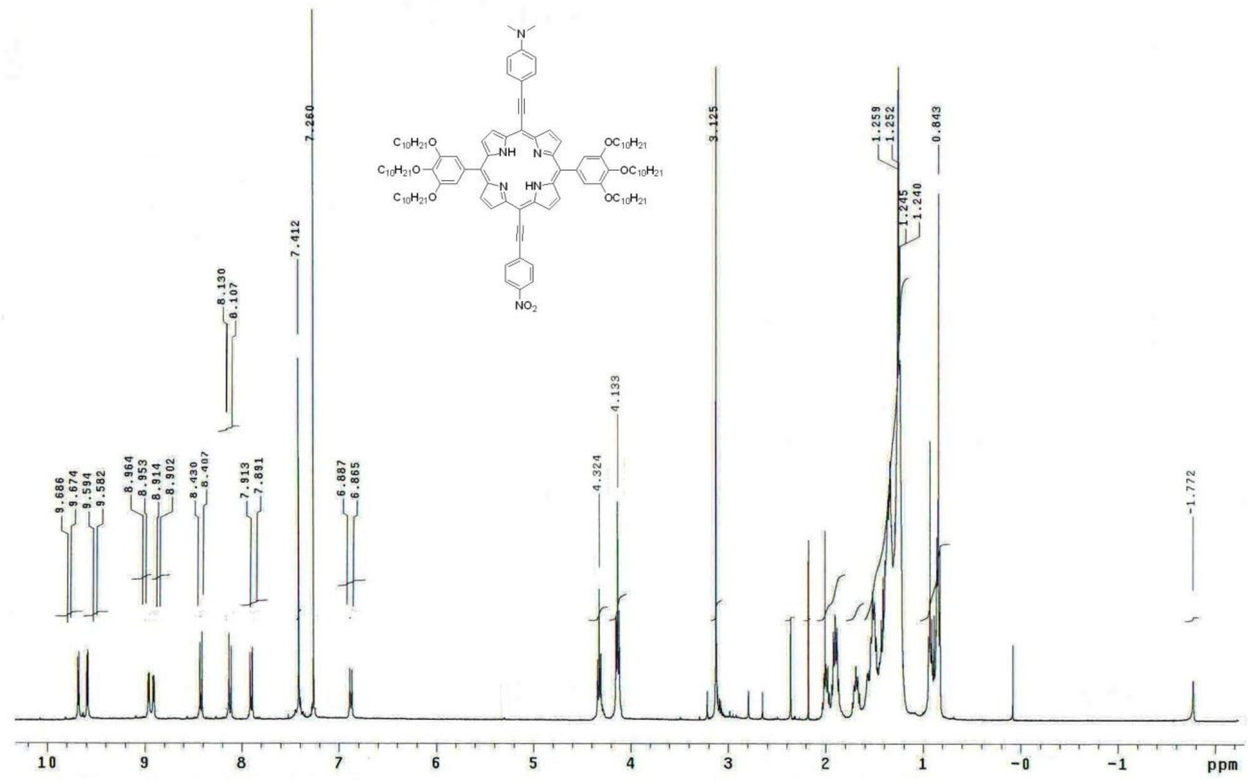

9.625
9.615
9.608
9.599
8.985
8.976
8.931
8.921
8.092
8.078
8.075
7.858
7.855
7.845
7.842
7.384
7.252
6.977
4.999
4.114
2.270
1.524
1.507
1.430
1.369
1.361
1.358
1.344
1.332
1.254
1.243
1.235
0.922
0.853
0.839
0.825
0.000
-2.297
10
9
8
7
6
5
4
3
2
1
-0
-1
-2
ppm
0.08
1.00
0.09
1.08
0.55
0.56
1.25
0.50
0.23
1.43
2.65
0.72
2.71
1.60
1.41
5.18
5.70
8.48
8.22
2.25
4.15
0.36

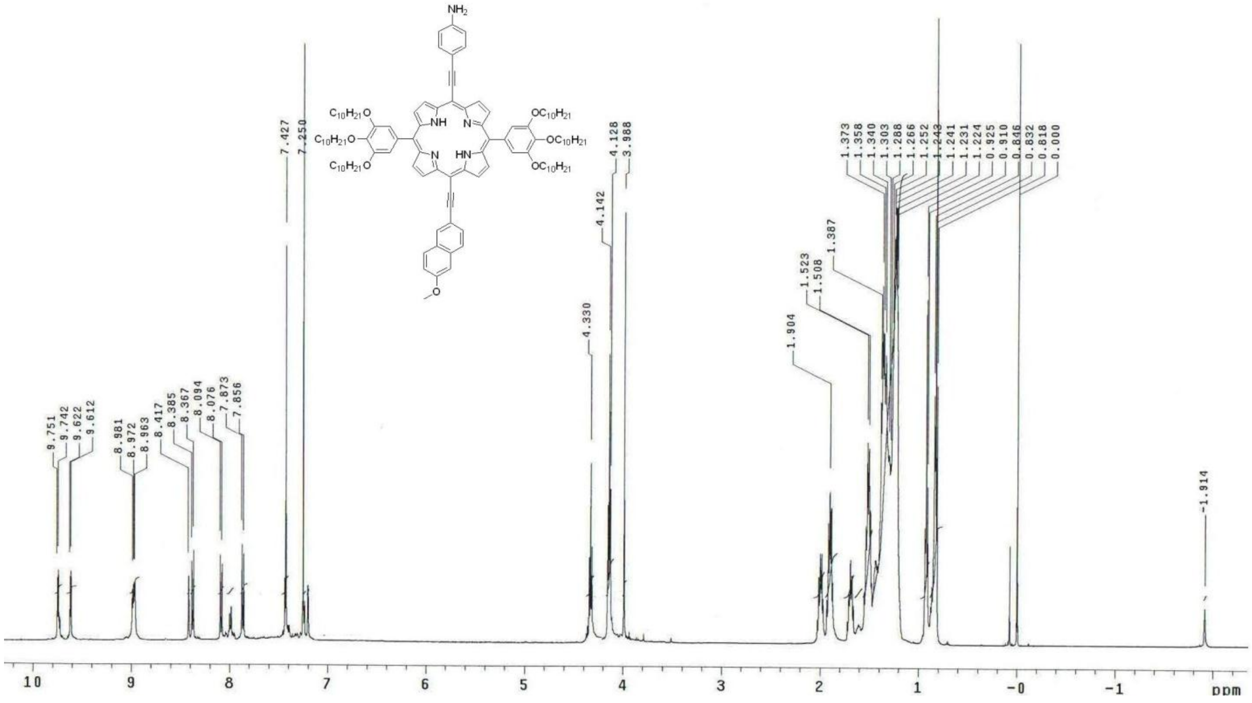

9.675
9.666
9.576
9.566
8.943
8.934
8.903
8.894
8.086
8.070
7.904
7.887
7.854
7.837
7.402
7.253
6.881
4.314
4.138
4.125
4.112
3.113
1.893
1.878
1.537
1.513
1.498
1.483
1.430
1.378
1.362
1.356
1.346
1.335
1.316
1.298
1.286
1.254
1.243
1.226
0.922
0.908
0.851
0.837
0.823
0.000
-1.797
C10H21O
OC10H21
NH
N
HN
CN
9
8
7
6
5
4
3
2
1
-0
-1
ppm

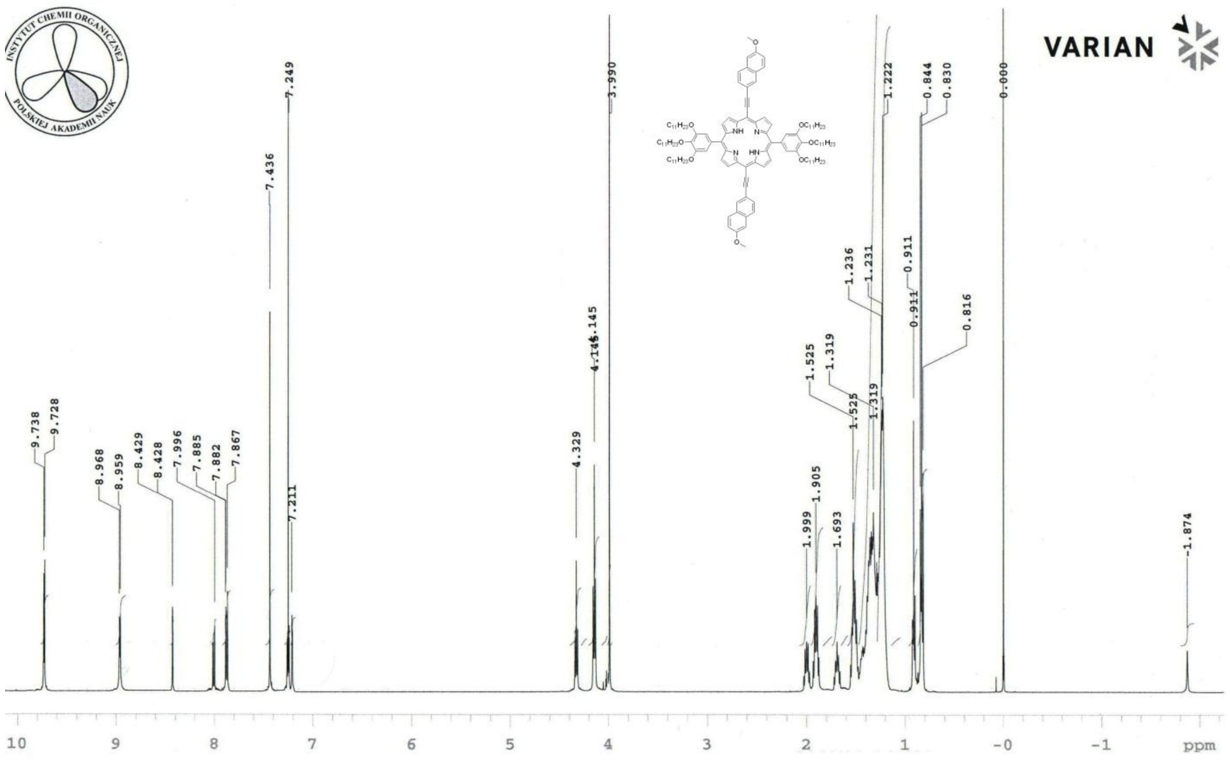

9.681
9.672
9.610
9.601
8.960
8.940
8.931
8.101
8.084
7.977
7.959
7.866
7.849
7.408
7.259
7.121
4.319
4.128
4.115
3.955
1.531
1.515
1.500
1.381
1.364
1.348
1.337
1.318
1.300
1.289
1.257
1.247
1.245
1.227
0.925
0.910
0.852
0.839
0.824
0.076
0.003
-1.922
C11H23O
OC11H23
NH
N
HN
9
8
7
6
5
4
3
2
1
-0
-1
ppm

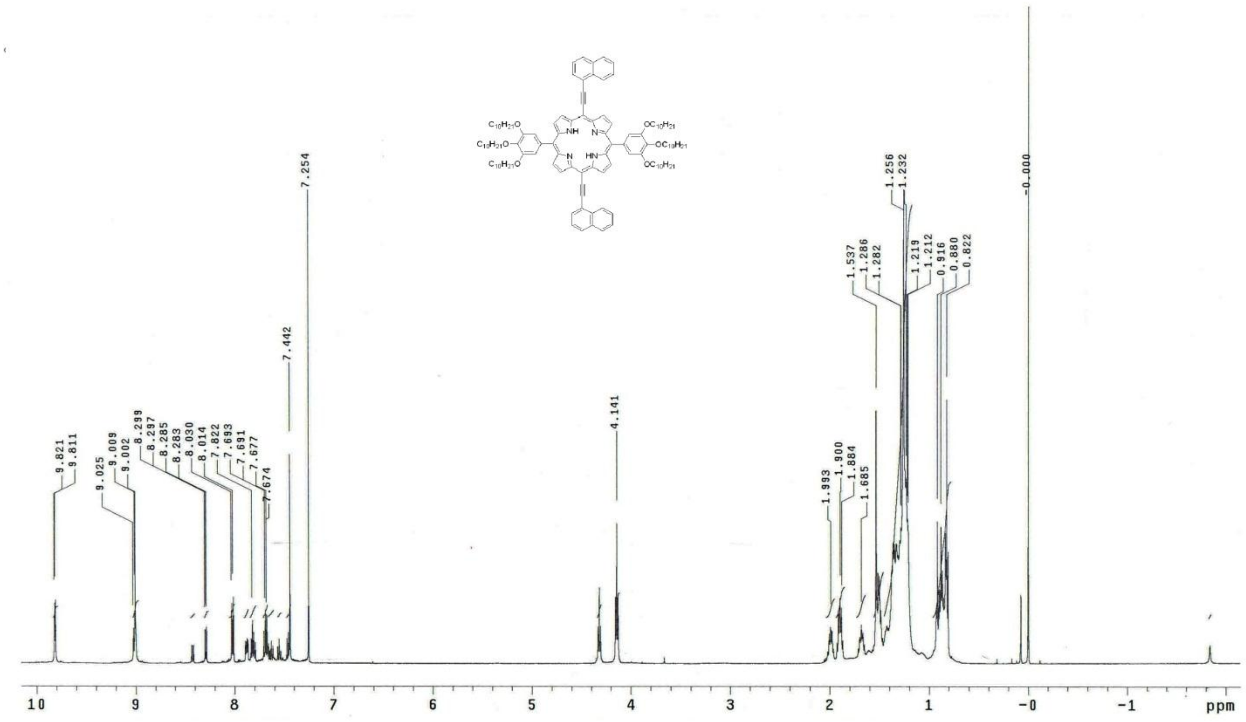

NO$_2$
C$_{10}$H$_{21}$O
NH
N
HN
OC$_{10}$H$_{21}$
10.183
9.764
9.755
9.284
9.275
9.116
9.106
9.058
9.049
8.418
8.401
8.138
8.121
7.443
7.252
4.324
4.134
1.896
1.271
1.254
1.247
1.244
1.235
1.226
0.923
0.853
0.839
0.825
-0.000
-2.527
10
9
8
7
6
5
4
3
2
1
-0
-1
-2
ppm

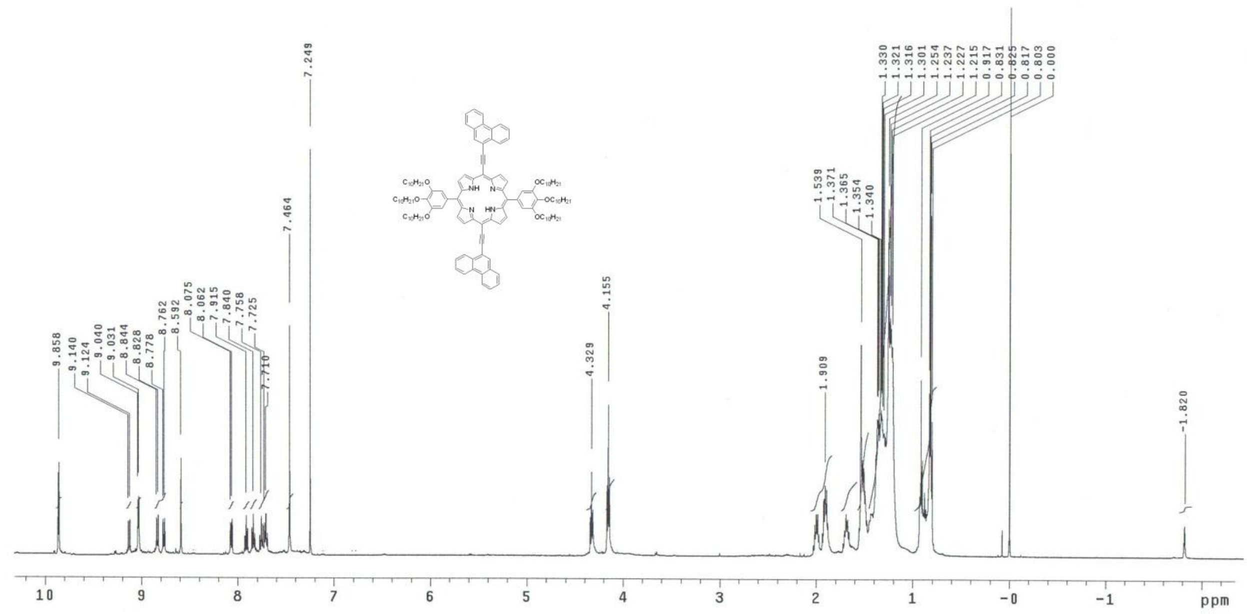

OC$_{10}$H$_{21}$
H$_{21}$C$_{10}$O
Br
N
NO$_2$
7.396
7.260
1.384
1.340
1.312
1.292
1.259
0.928
0.885
0.845
10
9
8
7
6
5
4
3
2
1
-0
-1
-2
ppm
4.00
4.36
1.94
1.87
3.96
4.93
9.35
12.74
129.62
30.13
1.70

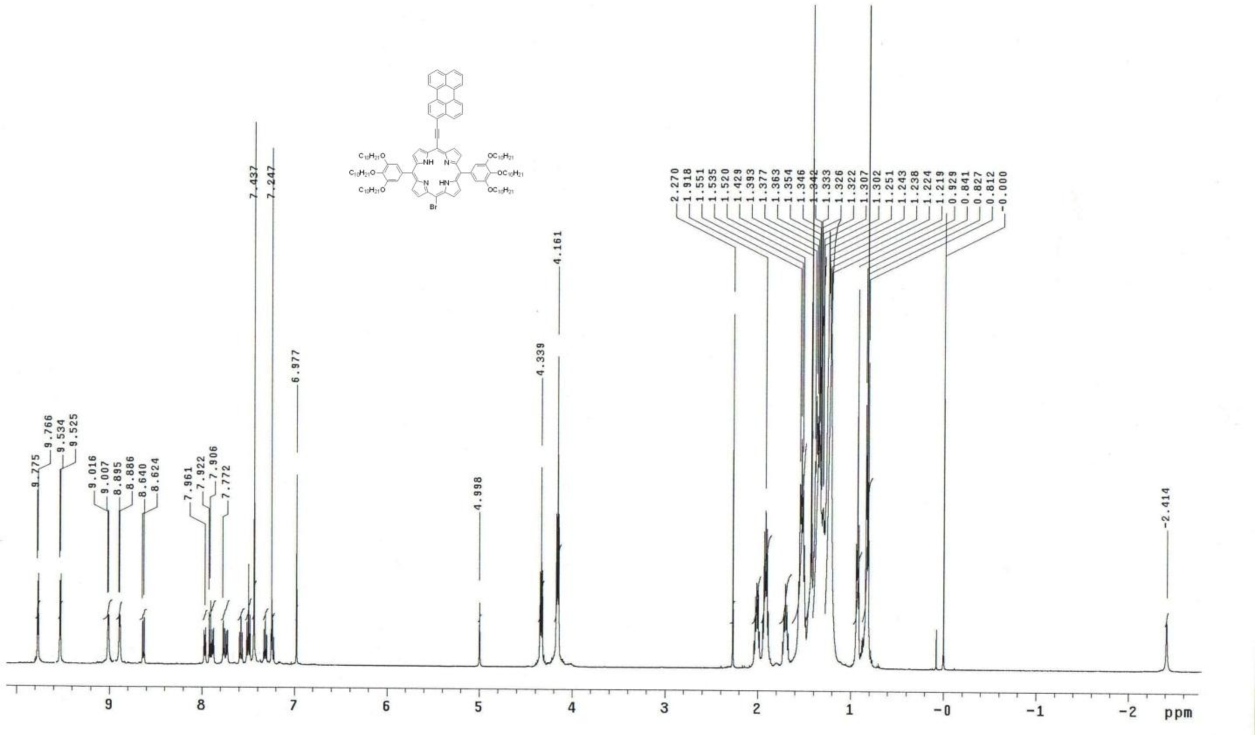

N
$C_{10}H_{21}O$
NH
N
HN
$OC_{10}H_{21}$
NO_2
9.686
9.674
9.594
9.582
8.964
8.953
8.914
8.902
8.430
8.407
8.130
8.107
7.913
7.891
7.412
7.260
6.887
6.865
4.324
4.133
3.125
1.259
1.252
1.245
1.240
0.843
-1.772
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm

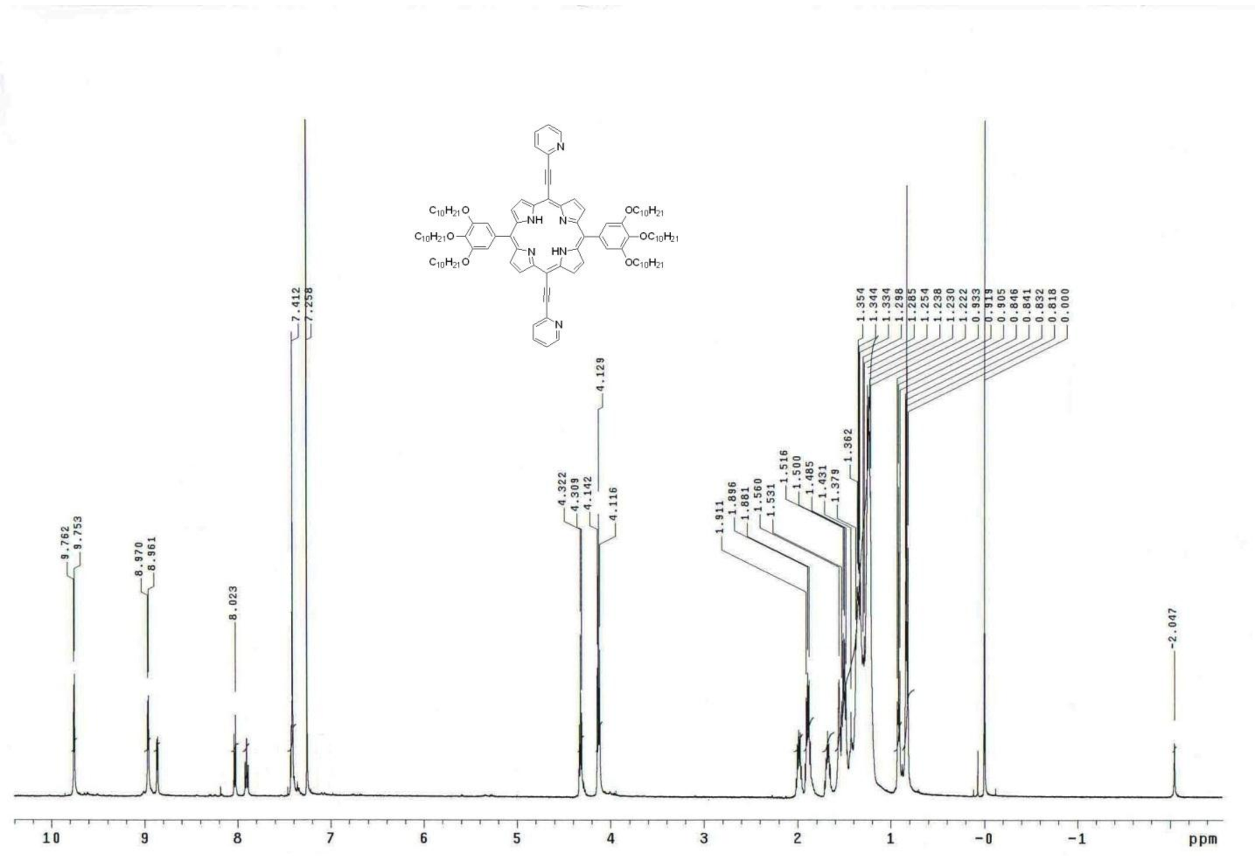

NH_2
$C_{10}H_{21}O$
NH
N
HN
$OC_{10}H_{21}$
O
9.751
9.742
9.622
9.612
8.981
8.972
8.963
8.417
8.385
8.367
8.094
8.076
7.873
7.856
7.427
7.250
4.330
4.142
4.128
3.988
1.904
1.523
1.508
1.387
1.373
1.358
1.340
1.303
1.288
1.266
1.252
1.248
1.241
1.231
1.224
0.925
0.910
0.846
0.832
0.818
0.000
-1.914
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm

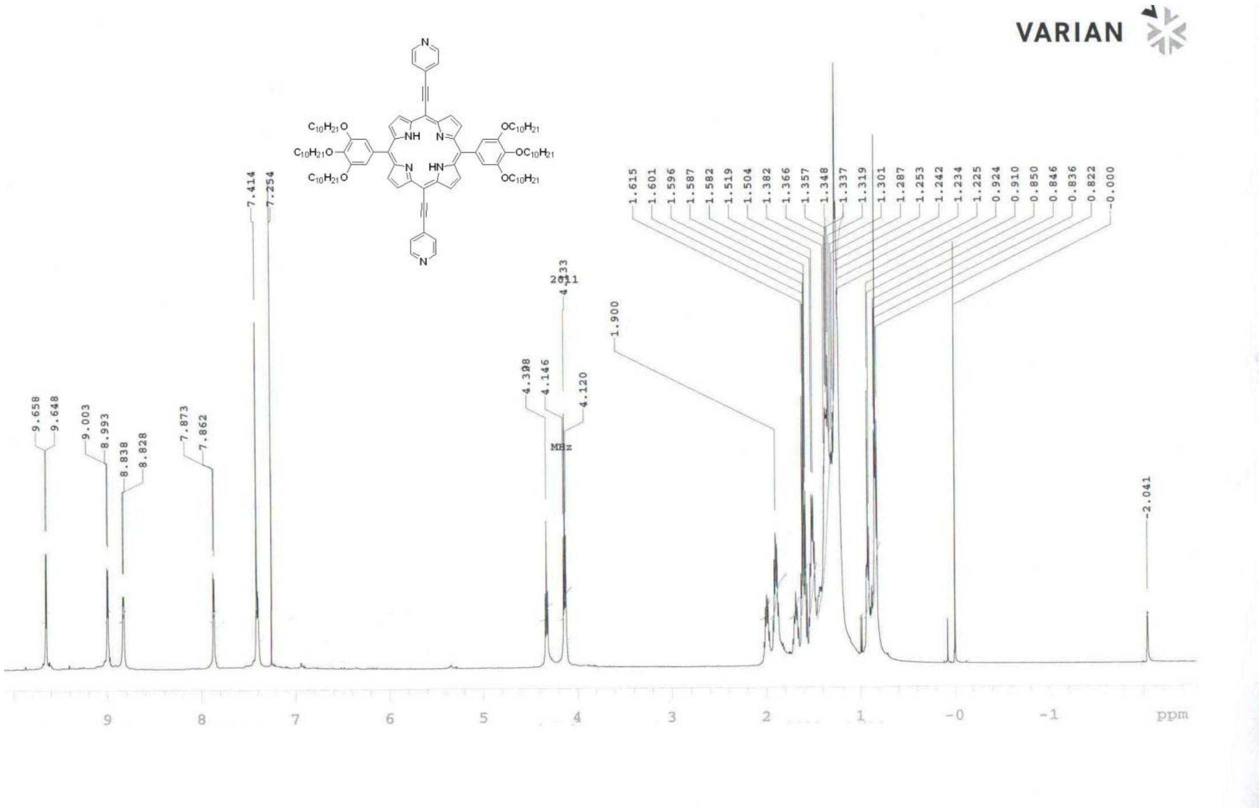

INSTYTUT CHEMII ORGANICZNEJ POLSKIEJ AKADEMII NAUK
VARIAN
$C_{11}H_{23}O$
NH
N
HN
$OC_{11}H_{23}$
9.738
9.728
8.968
8.959
8.429
8.428
7.996
7.885
7.882
7.867
7.436
7.249
7.211
4.329
4.146
4.145
3.990
1.999
1.905
1.693
1.525
1.319
1.525
1.319
1.236
1.231
1.222
0.911
0.911
0.844
0.830
0.816
0.000
-1.874
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm

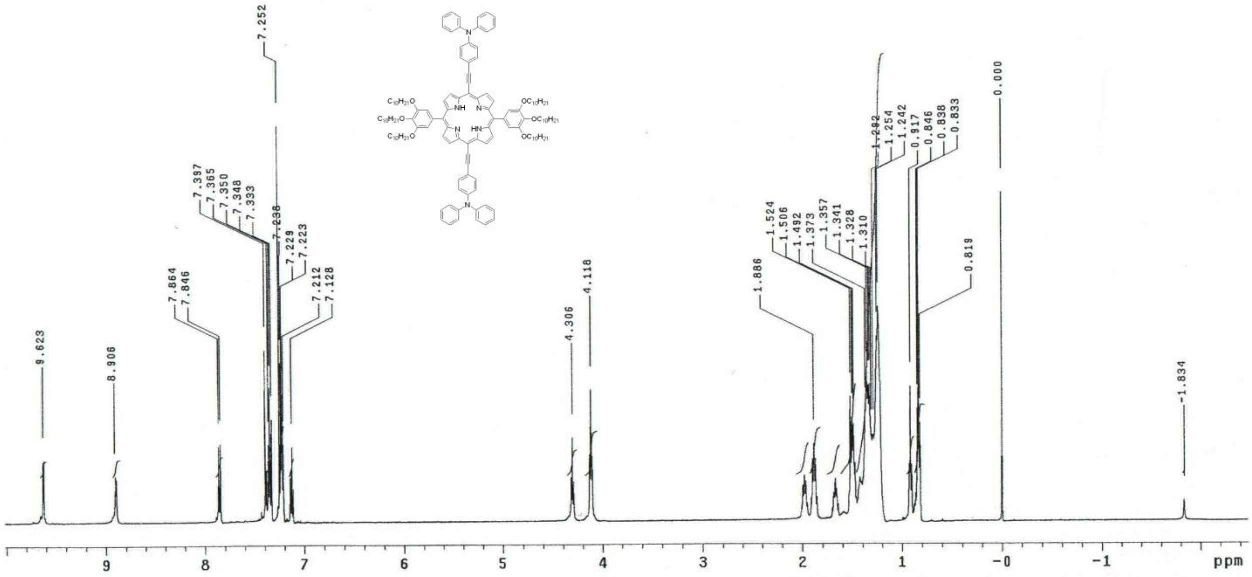

$C_{10}H_{21}O$
NH
N
HN
$OC_{10}H_{21}$
9.821
9.811
9.025
9.009
9.002
8.299
8.297
8.285
8.283
8.030
8.014
7.822
7.693
7.691
7.677
7.674
7.442
7.254
4.141
1.993
1.900
1.884
1.685
1.537
1.286
1.282
1.256
1.232
1.219
1.212
0.916
0.880
0.822
-0.000
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm

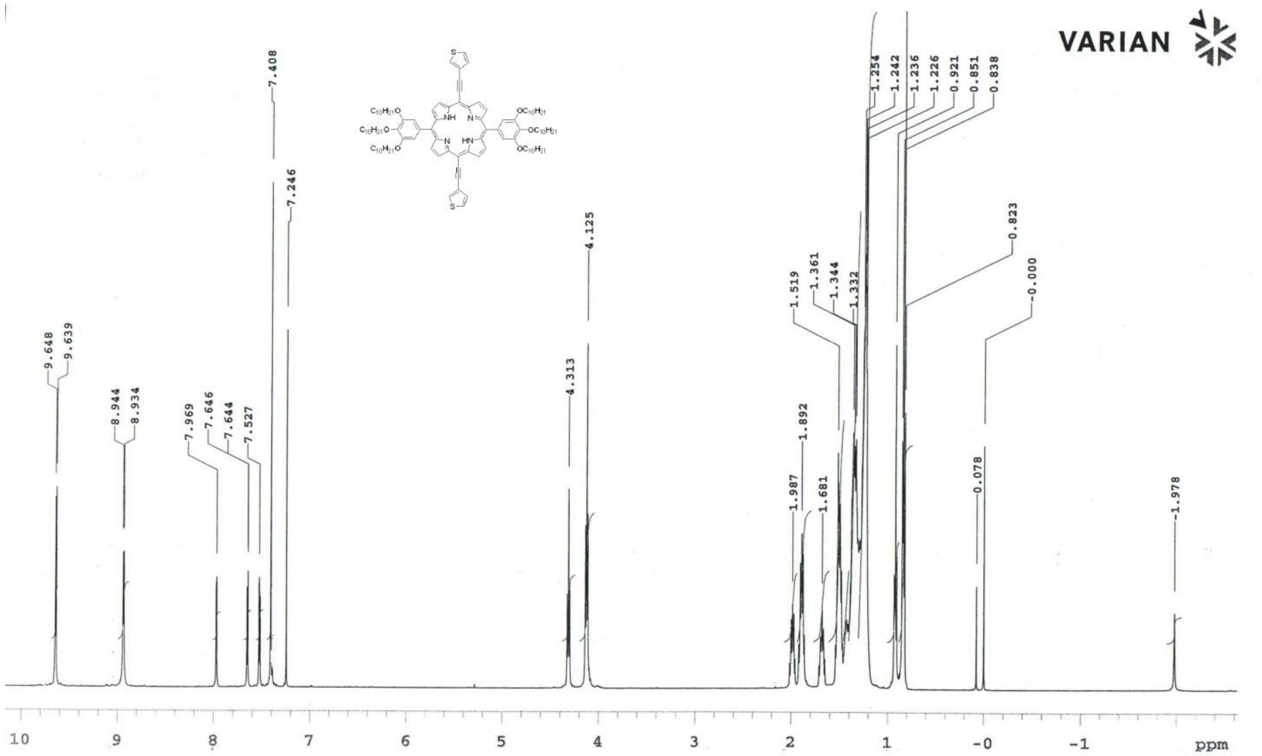

9.858
9.140
9.124
9.040
9.031
8.844
8.828
8.778
8.762
8.592
8.075
8.062
7.915
7.840
7.758
7.725
7.710
7.464
7.249
4.329
4.155
1.909
1.539
1.371
1.365
1.354
1.340
1.330
1.321
1.316
1.301
1.254
1.237
1.227
1.215
0.917
0.831
0.825
0.817
0.803
0.000
-1.820
C10H21O
OC10H21
NH
N
HN
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm

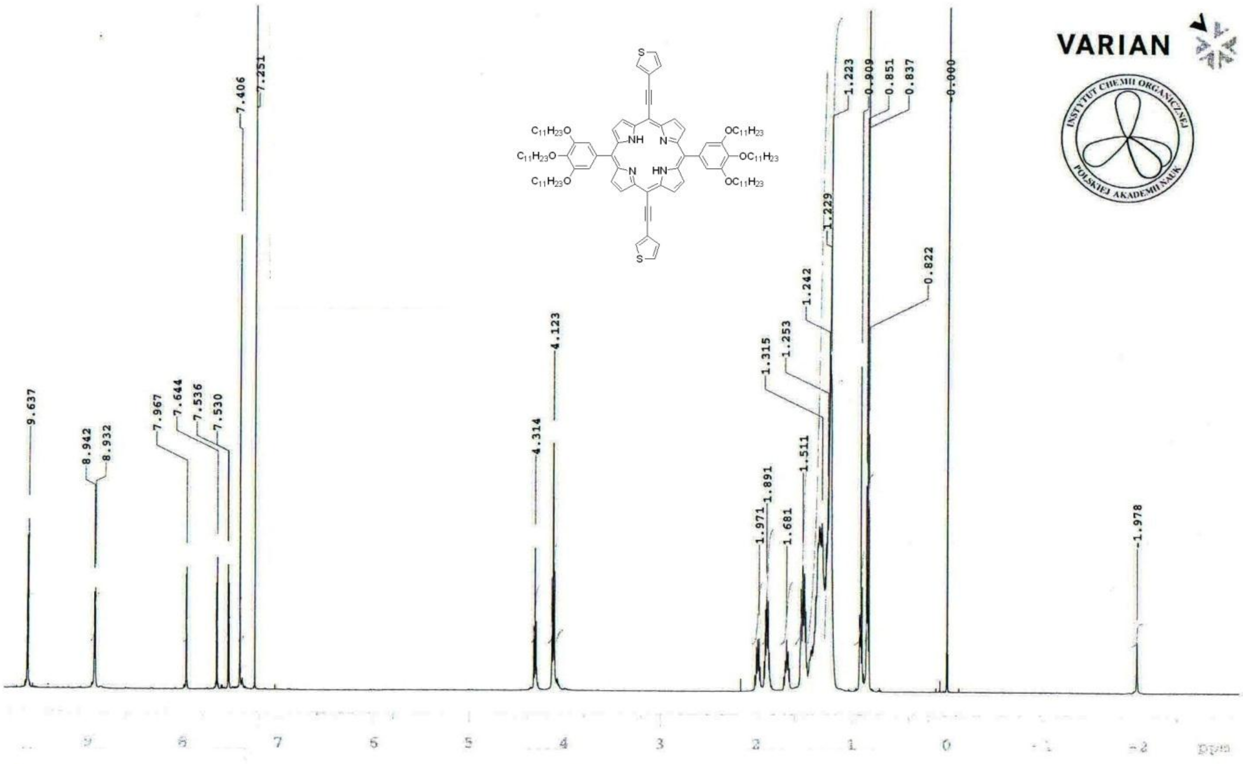

9.775
9.766
9.534
9.525
9.016
9.007
8.895
8.886
8.640
8.624
7.961
7.922
7.906
7.772
7.437
7.247
6.977
4.998
4.339
4.161
2.270
1.918
1.551
1.535
1.520
1.429
1.393
1.377
1.363
1.354
1.346
1.342
1.333
1.326
1.322
1.307
1.302
1.251
1.243
1.238
1.224
1.219
0.929
0.841
0.827
0.812
-0.000
-2.414
C10H21O
OC10H21
NH
N
HN
Br
9
8
7
6
5
4
3
2
1
-0
-1
-2
ppm


C10H21O
C10H21O
C10H21O
OC10H21
OC10H21
OC10H21
NH
N
N
HN
N
N
9.762
9.753
8.970
8.961
8.023
7.412
7.258
4.322
4.309
4.142
4.129
4.116
1.911
1.896
1.881
1.560
1.531
1.516
1.500
1.485
1.431
1.379
1.362
1.354
1.344
1.334
1.298
1.285
1.254
1.238
1.230
1.222
0.933
0.919
0.905
0.846
0.841
0.832
0.818
0.000
-2.047
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm

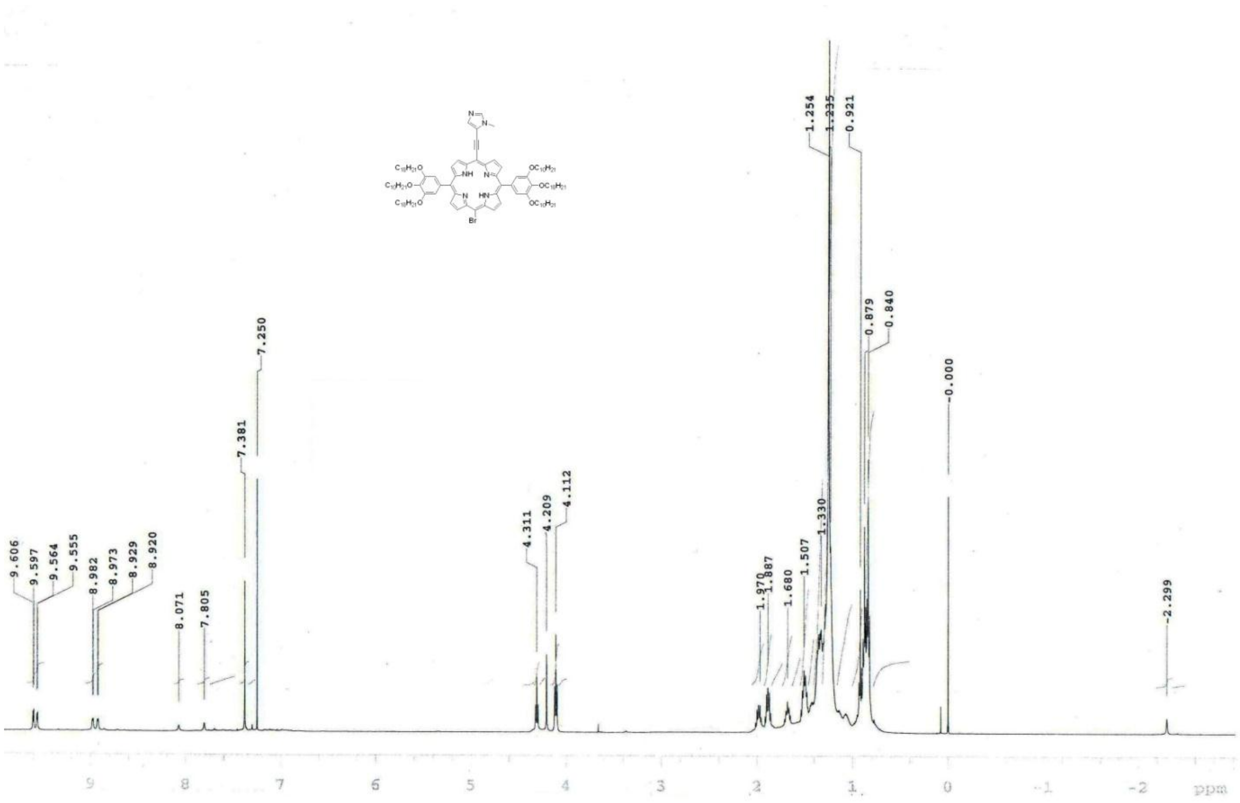

VARIAN
N
NH
HN
$C_{10}H_{21}O$
$OC_{10}H_{21}$
9.658
9.648
9.003
8.993
8.838
8.828
7.873
7.862
7.414
7.254
4.338
4.146
4.133
2011
4.120
MHz
1.900
1.615
1.601
1.596
1.587
1.582
1.519
1.504
1.382
1.366
1.357
1.348
1.337
1.319
1.301
1.287
1.253
1.242
1.234
1.225
0.924
0.910
0.850
0.846
0.836
0.822
0.000
-2.041
9
8
7
6
5
4
3
2
1
-0
-1
ppm


N
NH
HN
$C_{10}H_{21}O$
$OC_{10}H_{21}$
9.623
8.906
7.864
7.846
7.397
7.365
7.350
7.348
7.333
7.252
7.238
7.229
7.223
7.212
7.128
4.306
4.118
1.886
1.524
1.506
1.492
1.373
1.357
1.341
1.328
1.310
1.292
1.254
1.242
0.917
0.846
0.838
0.833
0.819
0.000
-1.834
9
8
7
6
5
4
3
2
1
-0
-1
ppm





INSTYTUT CHEMII ORGANICZNEJ POLSKIEJ AKADEMII NAUK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9.597
9.564
9.555
8.982
8.973
8.929
8.920
8.071
7.805
7.381
7.250
4.311
4.209
4.112
1.970
1.887
1.680
1.507
1.330
1.254
1.235
0.921
0.879
0.840
-0.000
-2.299
9
8
7
6
5
4
3
2
1
0
-1
-2
ppm
N
N
NH
N
N
HN
Br
$C_{10}H_{21}O$
$C_{10}H_{21}O$
$C_{10}H_{21}O$
$OC_{10}H_{21}$
$OC_{10}H_{21}$
$OC_{10}H_{21}$