Electronic Supplementary Information

Carbene functionalization of porphyrinoids through tosylhydrazones.

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Contents

Synthesis and characteristics of the synthesized compounds

General. Reactions were carried out under argon atmosphere using commercially available reagents that were purchased and used as received. Starting coprohemins I and II were synthesized according to the published procedure [1]. The heating of the reaction vessels was performed with oil bath. Column chromatography was performed using 40-63 μm silica gel, preparative thin layer chromatography (TLC) was performed using glass plates coated with 5-40 μm silica gel (5 mm thick). The reaction progress was monitored by TLC using aluminum-backed Silica Gel 60 F254 pre-coated plates. HPLC purification was performed on Agilent 1100 preparative system using the column YMC-Actus Triart C8 250×20 mm, 5 μm, 12 nm. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance III 600 MHz spectrometer at room temperature in $CDCl_3$. Chemical shifts were reported relative to signal of residual proton of $CDCl_3$ (7.26 ppm). High-resolution mass spectra (HRMS) were recorded using a Bruker microTOF II focus spectrometer (ESI). Electronic absorption spectra were recorded with U-2900 (Hitachi) spectrophotometer in quartz rectangular cells of 10 mm path length. Quantum-chemical calculations of geometry and electronic structure were made with the software package Gaussian 09W [2] using density functional theory (DFT) method with the hybrid correlation-exchange functional B3LYP. Fine integration grid was used for numerical integrations. All electron 6-31G(d) basis set was used for light atoms and LanL2DZ basis set was used for Ni atom. The geometry of all studied molecules was fully optimized, the absence of imaginary frequencies confirmed their stationary character. After the procedure of optimization of geometrical parameters wave function stability tests were carried out then calculation of thermochemical parameters was performed.

Starting *meso*-formyl-*β*-octaalkylporphyrinoids **5b**-**8b** were prepared from the corresponding *β*-octaalkylporphyrinoids **5a**-**8a** using reported procedures.[1, 2] Tosylhydrazones of the porphyrinoids were prepared using previously reported procedure with minor modifications.[2]

General procedure for the preparation of N-tosylhydrazones of pyropheophorbides on the example of the N-tosylhydrazone of methyl pyropheophorbide-*d* 3.

To a solution of methyl pyropheophorbide-*d* **1** (200 mg, 0.36 mmol) in CH_2Cl_2.(30 ml) *para*-toluenesulfonyl hydrazide (74 mg, 0.40 mmol) and trifluoroacetic acid (30 μl, 0.39 mmol) were added The reaction mixture was stirred at 45°C for 24 hours. The mixture was diluted with CH_2Cl_2 (100 ml), washed with water (2 x 50 ml), dried over Na_2SO_4 and concentrated *in vacuo*. The product was purified by preparative TLC (CH_2Cl_2/EtOH = 100:1) yielding N-tosylhydrazone of methyl pyropheophorbide-*d* **3** (196 mg, 76%) as a dark brown powder.

N-tosylhydrazone of methyl pyropheophorbide-*d* 3

^{1}H NMR (600 MHz, $CDCl_3$), δ, ppm: 9.62 (1H, s, 5-H), 9.21 (1H, s, 10-H), 8.89 (1H, s, CH=N), 8.47 (1H, s, 20-H), 8.15 (2H, m, 2,6-CH (Tosyl)), 7.31 (2H, m, 3,5-CH (Tosyl)), 6.75 (1H, s, 3^1-NH), 5.28 (1H, d, J = 19.0 Hz, 13^2-H^a), 5.12 (1H, d, J = 19.0 Hz, 13^2-H^b), 4.45 (1H, m, 18-H), 4.26 (1H, m, 17-H), 3.66 (3H, s, 12-CH_3), 3.60 (3H, s, 17^2-CO_2CH_3), 3.41 (2H, m, 8^1-CH_2), 3.33 (3H, s, 2-CH_3), 2.94 (3H, s, 7- CH_3), 2.71 (1H, m, 17^1-H^a), 2.60 (1H, m, 17^2-H^a), 2.36 (1H, m, 17^2-H^b), 2.31 (3H, s, CH_3(Tosyl)), 2.28 (1H, m, 17^1-H^b), 1.78 (3H, d, J = 7.4 Hz, 18-CH_3), 1.56 (3H, t, J = 7.7 Hz, 8^2-CH_3), -0.09 (1H, s, NH), -2.21 (1H, s, NH). ^{13}C NMR (150 MHz, $CDCl_3$), δ, ppm: 196.2, 173.6, 170.6, 160.7, 155.0, 151.1, 148.8, 144.5, 144.3, 142.5, 139.8, 138.4, 136, 7, 135.8, 135.2, 134.2, 130.8, 129.8, 128.8, 128.2, 128.1, 116.2, 106.4, 103.6, 98.9, 93.5, 51.9, 51.8, 49.7, 48.1, 31.0, 29.8, 29.7, 23.1, 21.5, 19.2, 17.2, 12, 0, 10.7, 10.9. HRMS (ESI), *m/z* found: 719.3001; calc. $C_{40}H_{43}N_6O_5S$: $[M+H]^+$, 719.3016. UV-Vis (CH_2Cl_2): λ_{max}, nm (log (ε [L mol^{-1} cm^{-1}])) 424 (5.03), 517 (4.17), 547 (4.12), 625 (3.96), 685 (4.81).

N-tosylhydrazone of methyl pyropheophorbide-*a* 4. The product (23 mg, 86%) was obtained as dark green solid from methyl pyropheophorbide-*a* **2** (20 mg, 0.037 mmol) and *para*-toluenesulfonyl hydrazide (15 mg, 0.12 mmol).

^{1}H NMR (600 MHz, $CDCl_3$), δ, ppm: 9.71 (1H, c, 5-H), 9.59 (1H, c, 10-H), 8.79 (1H, c, 20-H), 8.23 (2H, м, CH (Tosyl)) 8.14 (1H, дд, *J* = 17.8 Гц, *J* = 11.6 Гц, 3^1-H), 8.05 (1H, c, 13^1-NH) 7.46 (2H, м, CH(Tosyl)), 6.35 (1H, д, *J* = 17.8 Гц, 3^{2a}-H), 6.21 (1H, д, *J* = 11.6 Гц, 3^{2b}-H), 5.42 (1H, д, *J* = 18.2 Гц, 13^2-H^a), 5.29 (1H, д, *J* = 18.2 Гц, 13^2-H^b), 4.61 (1H, к, *J* = 7.4 Гц, 18-H), 4.39 (1H, м, 17-H), 3.79 (2H, к, *J* = 7.8 Гц, 8^1-CH_2), 3.66 (3H, c, 12-CH_3), 3.63 (3H, c, 17^2-CO_2CH_3), 3.52 (3H, c, 2-CH_3), 3.36 (3H, c, 7-CH_3), 2.75 (1H, м, 17^1-H^a), 2.65 (1H, м, 17^2-H^b), 2.47 (3H, c, CH_3(Tosyl)), 2.33 (2H, м, 17^1-H^b, 17^2-H^b), 1.85 (3H, д, *J* = 7.4 Гц, 18-CH_3), 1.75 (3H, т, *J* = 7.8 Гц, 8^2-CH_3), -0.6 (1H, s, NH), -2.6 (1H, s, NH). ^{13}C NMR (150 MHz, $CDCl_3$), δ, ppm: 173.7, 168.9, 160.8, 155.7, 152.4, 150.6, 144.2, 144.0, 139.6, 139.6, 136.2, 135.6, 135, 1, 134.0, 132.6, 130.1, 129.6, 128.5, 126.3, 122.0, 104.6, 101.6, 98.0, 93.1, 52.5, 51.7, 49.6, 38.9, 30.9, 29.7, 29.6, 23.5, 21.6, 19.6, 17.6, 11.2. HRMS (ESI), *m/z* found: 717.3206; calc. $C_{41}H_{45}N_6O_4S$: $[M+H]^+$, 717.3223. UV-Vis (CH_2Cl_2): λ_{max}, nm (log (ε [L mol^{-1} cm^{-1}])) 410 (5.13), 507 (4.2), 614 (0,04), 614 (3.82), 672 (4.82).

General procedure for the preparation of N-tosylhydrazones of the Ni (II) complexes of *meso*-formyl-*β*-octaalkyltetrapyrroles (porphyrins and chlorins) on the example of the N-tosylhydrazone of Ni (II) *meso*-formyl-*β*-octaethylporphyrin 5c.[2]

To a solution of Ni (II) *meso*-formyl-*β*-octaethylporphyrin **5a** (70 mg, 0.11 mmol) in CH_2Cl_2 (20 ml) *para*-toluenesulfonylhydrazide (22 mg, 0.11 mmol) was added followed by the addition of trifluoroacetic acid (8 μl, 0.1 mmol). The reaction mixture was stirred at 45°C for 24 hours. The resulting solution was cooled to room temperature and the solvent was evaporated *in vacuo*. The products were purified by column chromatography on silica gel (CH_2Cl_2 : MeOH = 100:1) yielding Z-isomer **Z-5c** (44 mg, 49% yield) and E-isomer **E-5c** (12 mg, 14% yield) of the N-tosylhydrazone of Ni (II) *meso*-formyl-*β*-octaethylporphyrin **1c** as green powders.

Ni (II) (*Z*)-N'-(2,3,7,8,12,13,17,18-octaethylporphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide Z-5c.

^{1}H NMR (600 MHz, $CDCl_3$), δ, ppm: 1.54 (7H, t, *β*-CH_3), 1.76 (7H, t, *β*-CH_3), 1.84 (13H, dt, *β*-CH_3), 2.46 (3H, s, CH_3(Tosyl)), 3.54 (2H, m, *β*-CH_2), 3.68 (3H, m, *β*-CH_2), 3.77 (2H, m, *β*-CH_2), 3.92 (11H, m, *β*-CH_2), 6.03 (1H, s, NH), 7.18 (2H, d, CH(Tosyl)), 7.40 (2H, d, CH(Tosyl)), 9.59 (2H, s, 10,20-CH), 9.62 (1H, s, 15-CH), 9.93 (1H, s, CH=N). ^{13}C NMR

(150 MHz, $CDCl_3$), δ, ppm: 143.7, 143.6, 143.2, 140.9, 140.5, 139.3, 136.0, 135.8, 129.3, 127.7, 98.8, 97.4, 97.3, 29.7, 21.6, 21.4, 19.6, 19.6, 19.5, 18.2, 18.1, 18.1, 16.9, 1.0.

Ni (II) (*E*)-N'-(2,3,7,8,12,13,17,18-octaethylporphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide E-5c.

^{1}H NMR (600 MHz, $CDCl_3$), δ, ppm: 1.41 (3H, t, *β*-CH_3), 1.72 (5H, t, *β*-CH_3), 1.80 (16H, t, *β*-CH_3), 2.28 (2H, s, CH_3(Tosyl)), 3.44 (4H, q, *β*-CH_2), 3.79 (4H, q, *β*-CH_2), 3.85 (8H, q, *β*-CH_2), 7.05 (2H, d, CH (Tosyl)), 7.60 (2H, d, CH(Tosyl)), 8.57 (1H, s, NH), 9.50 (2H, s, 10,20-CH), 9.50 (1H, s, 15-CH), 10.11 (1H, s, CH=N).

Ni (II) N'-(2,3,7,8,12,13,17,18-octaethyl-17,18-*trans*-dihydroporphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide 6c. Z- and E- isomers (46 mg, 61%, ratio 3:2) of the tosylhydrazone **6c** were prepared as emerald solid from Ni (II) 5-formyl-2,3,7,8,12,13,17,18-octaethyl-17,18-*trans*-dihydroporphyrin **6b** (60 mg, 0.096 mmol).

Isomer 1: ^{1}H NMR (600 MHz, $CDCl_3$), δ, ppm: 0.69 (3H, t, *J*=7.3 Hz, 18^2-CH_3), 0.97 (3H, t, *J*=7.3 Hz, 17^2-CH_3), 0.95 (1H, m, $17^{1b}CH_2$), 1.10 (1H, m, 17^{1a}-CH_2), 1.43 (3H, t, *J*=7.6 Hz, *β*-CH_3), 1.54 (3H, t, *J*=7.6 Hz, *β*-CH_3), 1.65 (12H, m, *β*-CH_3), 1.77 (2H, m, 17^1-CH_2), 2.38 (2H, s, CH_3(Tosyl)), 3.58 (12H, м, β-CH_2), 3.86 (1H, m, 17-CH), 3,93 (1H, м, 18-CH), 6.78 (1H, br.s, NH), 7.17 (2H, m, CH(Tosyl)), 7.52 (2H, m, CH(Tosyl)), 7.93 (1H, s, 10-CH), 8.85 (1H, s, CH=N), 8.96 (1H, s, 20-CH), 9.01(1H, s, 15-CH). ^{13}C NMR (150 MHz, $CDCl_3$), δ, ppm: 154.1, 152.4, 146.4, 145.4, 144.7, 143.9, 143.7, 140.6, 140.3, 139.2, 139.0, 137.9, 137, 3, 136.9, 135.8, 135.4, 129.3, 127.7, 103.2, 101.5, 93.5, 93.2, 53.7, 53.6, 29.7, 27.8, 25.5, 21.5, 19.6, 19.3, 19.2, 19.2, 19.2, 19.0, 18.9, 18.2, 18.1, 18, 0, 18.0, 17.9, 17.3, 17.3, 17.2, 11.4, 10.9. HRMS (ESI), *m/z* found: 789.3455; calc. $C_{44}H_{53}N_6NiO_2$: $[M+H]^+$, 789.3461. UV-Vis (CH_2Cl_2): λ_{max}, nm (log (ε [L mol^{-1} cm^{-1}])) 406 (5.17), 501 (3.98), 634 (4.82).

Isomer 2: 0.7 (3H, t, *J*=7.4 Hz, 18^2-CH_3), 1.02 (3H, t, *J*=7.4 Hz, 17^2-CH_3), 1.2 (2H, m, 18^1-CH_2), 1.57 (9H, m, *β*-CH_3), 1.65 (9H, m, *β*-CH_3), 1.77 (2H, m, 17^1-CH_2), 2.37 (2H, s, CH_3(Tosyl)), 3.16 (2H, m, *β*-CH_2), 3.56 (10H, m, *β*-CH_2), 3.92 (1H, t, *J*=7.0 Hz, 17-CH), 4.37 (1H, dd, *J*=4.2 Hz, *J*=9.0 Hz, 18-CH), 7.27 (2H, m, CH(Tosyl)), 7.82 (2H, m, CH(Tosyl)), 7.95 (1H, s, 10-CH), 8.07 (1H, br. S., NH), 8.89 (2H, s, 20-CH + CH=N), 8.93 (1H, s, 15-CH). ^{13}C NMR (150 MHz, $CDCl_3$), δ, ppm: 138.4, 137.7, 137.6, 137.0, 135.6, 135.1, 129.7, 127.9, 103.0, 101.3, 99.2, 93.4, 29, 7, 27.5, 25.3, 21.2, 20.4, 19.1, 19.1, 19.0, 19.0, 18.8, 17.9, 17.8, 17.7, 17.7, 17.0, 15.9, 11.2, 10.8. HRMS (ESI), *m/z* found: 789.3452; calc. $C_{44}H_{53}N_6NiO_2$: $[M+H]^+$, 789.3461. UV-Vis (CH_2Cl_2): λ_{max}, nm (log (ε [L mol^{-1} cm^{-1}])) 407 (5.13), 501 (3.94), 638 (4.7).

Ni (II) (*Z*)-N'-(3,8,13,18-tetramethyl-2,7,12,17-tetra(2-(ethoxycarbonyl)ethyl)porphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide 7**c.**[2] The product (27 mg, 78%) was obtained as a dark red solid from Ni (II) 5-formyl-3,8,13,18-tetramethyl-2,7,12,17-tetra(2-(ethoxycarbonyl)ethyl)porphyrin 7**b** (29 mg, 0.034 mmol).

^{1}H NMR (600 MHz, $CDCl_3$), δ, ppm: 1.22 (9H, m, $OCH_2\underline{CH_3}$), 1.46 (3H, t, *J*=7.18 Гц, $OCH_2\underline{CH_3}$), 2.28 (3H, s, CH_3(Tosyl)), 3.03 (2H, m, *β*-CH_2), 3.05 (3H, s, *β*-CH_3), 3,12 (4H, q, *J*=7.79 Hz, *β*-CH_2), 3.35 (3H, s, *β*-CH_3), 3.45 (6H, s, *β*-CH_3), 3.69 (2H, m, *β*-CH_2), 4.13 (2H, m, *β*-CH_2), 4.19 (10H, m, *β*-CH_2, $O\underline{CH_2}CH_3$), 4.40 (2H, q, *J*=7.18 Hz, $O\underline{CH_2}CH_3$), 7.01 (2H, m, CH(Tosyl)), 7.58 (2H, m, CH(Tosyl)), 9.51 (1H, s, NH), 9.57 (1H, s, 15-<u>CH</u>), 9.59 (1H, s, 20-<u>CH</u>), 9.61 (1H, s, 10-<u>CH</u>), 10.23 (1H, s, <u>CH</u>=N). ^{13}C NMR (150 MHz, $CDCl_3$), δ, ppm: 174.6, 173.0, 173.0, 150.7, 143.7, 141.9, 141.5, 141.4, 140.6,140.5, 129.2, 128.0, 106.4, 97.4, 97.3, 97.2, 61.6, 60.7, 58.5, 36.9, 35.0, 31.9, 29.7, 29.4, 24.7, 22.7, 17.4, 14.3, 14.1, 11.6, 11.5, 11.5, 1.0.

Ni (II) N'-(3,7,13,17-tetramethyl-2,8,12,18-tetra(2-(methoxycarbonyl)ethylm)porphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide 8c. The product (29 mg, 75%) was obtained as red powder from Ni (II) 5-formyl-3,7,13,17-tetramethyl-2,8,12,18-tetra(2-(methoxycarbonyl)ethyl)porphyrin **8b** (32 mg, 0.047 mmol).

Isomer 1: ^{1}H NMR (600 MHz, $CDCl_3$), δ, ppm: 10.36 (1H, s, CH=N), 9.66 (1H, s, 5-CH), 9.63 (1H, s, 20-CH), 9.53 (1H, s, 15-CH), 9.52 (1H, s, NH), 7.51 (2H, m, CH (Tosyl)), 7.01 (2H, m, CH (Tosyl)), 4.22 (14H, m, *β*-CH_2), 3.89 (6H, s, *β*-CH_3), 3.75 (3H, s, OCH_3), 3.69 (3H, s, OCH_3), 3.45 (6H, s, *β*-CH_3), 3.37 (3H, s, *β*-CH_3), 3.18 (4H, m, CH_2), 2.72 (4H, m, *β*-CH_2), 2.28 (3H, s, CH_3(Tosyl)). ^{13}C NMR (150 MHz, $CDCl_3$), δ, ppm: 174.2, 173.2, 150.3, 144.1, 141.1, 140.7, 140.6, 140.2, 140.1 , 139.8, 139.2, 138.2, 135.5, 129.2, 127.7, 97.7, 97.0, 52.0, 51.5, 36.5, 34.4, 24 , 3, 21.5, 21.1, 11.2, 11.2. HRMS (ESI), *m/z* found: 963.2878; calc. $C_{48}H_{53}N_6NiO_{10}S$: $[M+H]^+$, 963.2897. UV-Vis (CH_2Cl_2): λ_{max}, nm (log (ε [L mol^{-1} cm^{-1}])) 410 (4.8), 531 (3.47), 572 (3.84), 646 (3.09).

Isomer 2: ^{1}H NMR (600 MHz, $CDCl_3$), δ, ppm: 9.68 (1H, s, CH=N), 9.54 (3H, s, 5-CH, 20-CH, 15-CH), 8.92 (1H, s, NH), 7.68 (2H, m, CH (Tosyl)), 7.22 (2H, m, CH (Tosyl)), 4.15 (4H, m, *β*-CH_2), 3.98 (4H, m, *β*-CH_2), 3.70 (6H, s, OCH_3), 3,69 (6H, s, OCH_3), 3,38 (6H, s, *β*-CH_3), 3.14 (4H, m, *β*-CH_2), 2.96 (4H, m, *β*-CH_2), 2,68 (6H, s, *β*-CH_3), 2.41 (3H, s, CH_3 (Tosyl)). ^{13}C NMR (150 MHz, $CDCl_3$), δ, ppm: 173.2, 173.1, 150.4 144.6, 141.7, 141.4, 140.3, 140.0, 139.9, 139.4, 138.3, 137.6, 135.8 , 129.7, 127.8, 97.1, 51.5, 36.5, 36.4, 29.7, 21.5, 21.3, 21.2, 16.6, 11.2. HRMS (ESI), *m/z* found: 963.2883; calc. $C_{48}H_{53}N_6NiO_{10}S$: $[M+H]^+$, 963.2897. UV-Vis (CH_2Cl_2): λ_{max}, nm (log (ε [L mol^{-1} cm^{-1}])) 409 (5.22), 534 (3.98), 569 (4.29), 637 (3.83).

General cyclopropanation procedure on the example of the N-tosylhydrazone of methyl pyropheophorbide-*d* 3.

To a solution of tosylhydrazone **3** (50 mg, 0.070 mmol) in 1,4-dioxane (1 ml) styrene (2.0 ml, 17 mmol) and potassium carbonate (110 mg, 0.80 mmol) were added. The reaction mixture was refluxed for 1 hour, then the solvent was evaporated *in vacuo*. The resulting product was purified by column chromatography on silica gel (CH_2Cl_2:Et_2O = 90:1) yielding the mixture (36 mg, 71%) of two diastereomers of the cyclopropanated product **9** as a black powder. The mixture of diastereomers was separated using the RF-HPLC in a linear gradient from 85% to 100% (v/v) MeCN (Biosolve, HPLC-S gradient grade) in water affording two diastereomers of the cyclopropane conjugates with methyl pyropheophorbide-*d* **9a** (18 mg, 35 %) and **9b** (18 mg, 35 %).

Product 9a. ^{1}H NMR (600 MHz, $CDCl_3$), δ, ppm: 9.51 (1H, s, 10-H), 9.43 (1H, ds, 5-H), 8.50 (1H, s, 20-H), 7.58 (4H, m, Ph), 7.42 (1H, m, Ph), 5.27 (1H, d, J = 19.2 Hz, 13^2-H^a), 5.12 (1H, d, J = 19.2 Hz, 13^2-H^b), 4.49 (1H, m, 18-H), 4.30 (1H,

m, 17-H), 3.70 (2H, m, 8^1-CH_2), 3.69 (3H, s, 12-CH_3), 3.63 (3H, ds, 17^2-CO_2CH_3), 3.42 (3H, s, 2-CH_3), 3.13 (1H, m, cyclopropane), 3.42 (3H, s, 7-CH_3), 2.76 (1H, m, cyclopropane), 2.71 (1H, m, 17^1-H^a), 2.57 (1H, m, 17^2-H^a), 2.33 (2H, m, 17^1-H^b, 17^2-H^b), 2.07 (2H, m, cyclopropane), 1.83 (3H, d, J = 7.5 Hz, 18- CH_3), 1.70 (3H, t, J = 7.8 Hz, 8^2-CH_3), 0.10 (1H, s, NH), -1.62 (1H, s, NH). ^{13}C NMR (150 MHz, $CDCl_3$), δ, ppm: 196.2, 173.5, 171.7, 167.7, 159.9, 155.3, 150.7, 149.1, 145.0, 142.5, 142.0, 138.8, 138, 1, 137.7, 136.0, 133, 133.5, 130.9, 130.4, 128.9, 128.8, 128.0, 126.3, 126.0, 106.0, 104, 2, 97.3, 92.6, 68.2, 51.7, 51.6, 50.0, 48.0, 38.8, 30.9, 30.4, 29.9, 29.7, 28.9, 25.4, 25.3, 23.8, 23.1, 23.0, 20.3, 19.5, 17.4, 17.0, 17.0, 14.0, 12, 0, 11.6, 11.0, 10.6. HRMS (ESI), *m/z* found: 639.3351; calc. $C_{41}H_{43}N_4O_3$: $[M+H]^+$, 639.3335. UV-Vis (CH_2Cl_2): λ_{max}, nm (log (ε [L mol^{-1} cm^{-1}])) 410 (4.93), 505 (3.9), 536 (3.86), 605 (3.84), 660 (4.58).

Product 9b. ^{1}H NMR (600 MHz, $CDCl_3$), δ, ppm: 9.48 (1H, ds, 10-H), 9.44 (1H, ds, 5-H), 8.35 (1H, ds, 20-H), 6.87 (2H, m, Ph), 6.74 (3H, m, Ph), 5.25 (1H, dd, J = 19.2 Hz, 13^2-H^a), 5.10 (1H, dd, J = 19.2 Hz, 13^2-H^b), 4.43 (1H, m, 18-H), 4.27 (1H, m, 17-H), 3.71 (2H, m, 8^1-CH_2), 3.69 (3H, ds, 12-CH_3), 3.63 (3H, ds, 17^2-CO_2CH_3), 3.36 (1H, m, cyclopropane), 3.24 (3H, ds, 2-CH_3), 3.08 (3H, ds, 7-CH_3), 3.06 (1H, m cyclopropane), 2.70 (1H, m, 17^1-H^a), 2.55(1H, m, 17^2-H^a), 2.33 (2H, m, 17^1-H^b, 17^2-H^b), 2.21 (2H, m, cyclopropane), 1.79 (3H, m, 18-CH_3), 1.71 (3H, t, 8^2-CH_3), 0.10 (1H, s, NH), -1.7 (1H, s, NH). ^{13}C NMR (150 MHz, $CDCl_3$), δ, ppm: 196.2, 173.5, 171.5, 160.0, 159.9, 155.2, 150.6, 149.0, 144.9, 141.9, 141.8, 139.4, 138, 2, 137.6, 135.9, 135.7, 134.9, 134.8, 130.3, 127.9, 127.5, 126.8, 125.4, 105.8, 104.0, 97, 6, 97.6, 92.4, 92.4, 51.6, 50.0, 48.0, 45.4, 37.1, 34.3, 31.9, 31.4, 31.0, 31.0, 30.3, 30.2, 30.1, 29.9, 29.7, 29.2, 27.7, 27.4, 23.0, 22.7, 22.4, 22, 3, 21.5, 20.6, 19.7, 19.6, 19.5, 18.1, 17.4, 14.5, 14.1, 12.0, 11.5, 11.2. HRMS (ESI), *m/z* found: 639.3348; calc. $C_{41}H_{43}N_4O_3$: $[M+H]^+$, 639.3335. UV-Vis (CH_2Cl_2): λ_{max}, nm (log (ε [L mol^{-1} cm^{-1}])) 410 (4.56), 513 (3.48), 537 (3.19), 614 (3.49), 661 (4.22).

Product 10. The product (14 mg, 80%) was obtained as green black solid from N-tosylhydrazone of methyl pyropheophorbide-*a* **4** (20 mg, 0.028 mmol).

^{1}H NMR (600 MHz, $CDCl_3$), δ, ppm: 9.98-9.94 (1H, m, 10-H), 9.6-9.575, 9.405-9.38 (1H, m, 5-H), 9.01-8.97, 8.96-8.93 (1H, s, 20-H), 8,35-8.26 (1H, m, 3^1-H), 7.52-7.2 (5H, m, C_6H_5), 6.42-6.35 (1H, m, 3^{2a}-H), 6.21-6.16 (1H, m, 3^{2b}-H), 5.2-4.28 (4H, m,13^2-H^a + 13^2-H^b + 18-H + 17-H), 3.94-3.78 (2H, m, 8^1-CH_2), 3.68-3.44 (13H, m, 12-CH_3 +17^2-CO_2CH_3+2-CH_3+7-CH_3+CH(cyclopropane)), 2.85-2.06 (6H, m, 17^1-H^a+17^1-H^b+17^2-H^b+17^2-H^a +CH_2(cyclopropane)), 1.98-1.72 (6H, m, 8^2-CH_3+18-CH_3). ^{13}C NMR (150 MHz, $CDCl_3$), δ, ppm: 174.02, 173.9, 173.85, 173.55, 165.24, 165.2, 165.07, 162.6, 162.5, 162.32, 151.04, 150.9, 149.47, 149.44, 149.38, 146.2, 146.18, 144.9, 143.8, 143.76, 142.76, 142.64, 142.57, 142.56, 142.5, 142.22, 142.2, 139.47, 139.3, 136.8, 136.77, 136.7, 136.35, 133.45, 133.37, 131.35, 131.22, 131.15, 131.07, 130.34, 128.55, 128.53, 128.49, 128.44, 128.41, 127.76, 126.8, 126.39, 126.33, 121.23, 121.19, 120.84, 120.76, 111.17, 98.51, 97.21, 93.32, 53.54, 53.29, 53.06, 51.54, 51.47, 51.39, 49.16, 49.03, 42.1, 41.9, 32.75, 32.14, 31.92, 31.86, 31.66, 30.82, 30.54, 29.72, 29.39, 29.09, 28.93, 24.15, 24.06, 24.0, 23.9, 20.06, 20.0, 19.8, 19.7, 17.7, 17.6, 12.35, 11.52, 10.55, 10.09, 10.04. HRMS (ESI), *m/z* found: 637.3564; calc. $C_{42}H_{45}N_4O_2$: $[M+H]^+$, 637.3543. UV-Vis (CH_2Cl_2): λ_{max}, nm (log (ε [L mol^{-1} cm^{-1}])) 413 (4.9), 505 (3.91), 537 (3.19), 599 (3.41), 654 (4.37).

General procedure of the thermal decomposition of tosylhydrazones of the tetrapyrroles on the example of the N-tosylhydrazone of methyl pyropheophorbide-*d* 3.

To a solution of tosylhydrazone **3** (50 mg, 0.070 mmol) in 1,4-dioxane (3 ml) potassium carbonate (110 mg, 0.80 mmol) was added. The reaction mixture was refluxed for 4 hours, then the solvent was evaporated *in vacuo*. The resulting product was purified by column chromatography on silica gel (CH_2Cl_2:Et_2O = 90:1) yielding the mixture (25 mg, 58%) of two diastereomers of the conjugate of the methyl pyropheophorbide-*d* with 1,4-dioxane **11** as a black powder.

^{1}H NMR (600 MHz, $CDCl_3$), δ, ppm: 9.66 (1H, s, 5-H (isomer 2)), 9.515 (1H, s, 10-H (isomer 2)), 9.51 (1H, s, 10-H (isomer 1)), 9.25 (1H, s, 5-H (isomer 1)), 8.55 (1H, s, 20-H (isomer 2)), 8.52 (1H, s, 20-H (isomer 1)), 6.22 (1H, m, 3^2-H (isomer 2)), 5.28 (2H, m, 13^2-H^a (isomer 1 + isomer 2)), 5.13 (2H, m, 13^2-H^b (isomer 1 + isomer 2)), 4.49 (6H, m, 18-H (isomer 1 + isomer 2) + 3^4-CH_2 (isomer 1 + isomer 2)), 4.37 (1H, m, 3^2-H (isomer 1)), 4.3 (6H , m, 17-H (isomer 1 + isomer 2) + 3^5-CH_2 (isomer 1 + isomer 2)), 3.93 (3H, m, 3^7-CH_2 (isomer 2) + 1H, m, 3^{1a}-CH_2 (isomer 2)), 3.82 (1H, m, 3^{1b}-CH_2 (isomer 2)), 3.74 (2H , m, 3^1-CH_2, (isomer 1)), 3.72 (4H, m, 8^1-CH_2 (isomer 1 + isomer 2)), 3.68 (6H, s, 12-CH_3 (isomer 1 + isomer 2)), 3.64 (6H, s, 17^2-CO_2CH_3 (isomer 1 + isomer 2)), 3.45 (3H, s, 2-CH_3 (isomer 2)), 3.34 (3H, s, 2-CH_3 (isomer 1)), 3.30 (3H, s, 7-CH_3 (isomer 2)), 3.28 (3H, s, 7-CH_3 (isomer 1)), 2.95 (1H, m, 37^a-CH_2 isomer 2)), 2.72 (3H, m, 17^1-H^a (isomer 1 + isomer 2) + 3^{7b}-CH_2 (isomer 2)), 2.58 (1H, m, 17^2-H^a (isomer 1 + isomer 2)), 2.32 (4H, m, 17^1-H^b + 17^2-H^b (isomer 1 + isomer 2)). 1.84 (6H, d, J = 7.5 Hz, 18-CH_3 (isomer 1 + isomer 2)), 1.73 (6H, t, J = 7.8 Hz, 8^2-CH^3 (isomer 1 + isomer 2)), 0.10 (1H, s, NH), -1.64 (1H, s, NH). ^{13}C NMR (150 MHz, $CDCl_3$), δ, ppm: 196.2, 173.5, 171.6, 171.4, 160.3, 160.2, 155.0, 150.8, 150.6, 149.1, 145.1, 145.0, 141, 7, 141.4, 139.7, 137.8, 137.7, 137.2, 136.1, 135.9, 135.1, 134.6, 133.3, 131.1, 131.0, 130.4, 128.3, 128.3, 106.1, 104.2, 104.1, 98.1, 98.0, 96.5, 96.5, 92.8, 92.8, 73, 5, 73.4, 73.3, 71.3, 68.9, 67.1, 66.5, 51.7, 50.1, 48.0, 41.0, 30.9, 29.9, 28.8, 23.1, 23.1, 19.5, 17.4, 12.0, 11.7, 11.5, 11.3, 11.3. HRMS (ESI), *m/z* found: 623.3218; calc. $C_{37}H_{43}N_4O_5$: $[M+H]^+$ 623.3233. UV-Vis (CH_2Cl_2): λ_{max}, nm (log (ε [L mol^{-1} cm^{-1}])) 409 (5.17), 506 (4.19), 537 (4.15), 608 (4.04), 665 (4.82).

Ni(II) 3,5-(1-methylethylene)-2,7,8,12,13,17,18-heptaethylporphyrin 12. The product (17 mg, 75%) was obtained as a black solid from Ni (II) N'-(2,3,7,8,12,13,17,18-octaethylporphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide **5c** (30 mg, 0.038 mmol).

^{1}H NMR (600 MHz, $CDCl_3$), δ, ppm: 9.86 (1H, s, *meso*-H), 9.85 (1H, s, *meso*-H), 9.83 (1H, s, *meso*-H), 5.54 (1H, dd, J = 6.64, J = 15.78 Hz, 3^{1a}-CH_2), 4.79 (1H, dd, J = 2.26 Hz, J = 15.78, 3^{1b}-CH_2), 4.57 (1H, m, 4^1-CH), 3.99 (16H, m, $\underline{CH_2}$-CH_3), 2.0 (3H, d, J = 7.28 Hz, 3^2-CH_3), 1.94 (3H, t, J = 7.74 Hz, CH_2-$\underline{CH_3}$) , 1.89 (15H, m, CH_2-$\underline{CH_3}$), 1.76 (3H, t, J = 7.74 Hz, CH_2-$\underline{CH_3}$). ^{13}C NMR (150 MHz, $CDCl_3$), δ, ppm: 152.8, 148.60,145.30, 143.70, 142.60, 142.50, 142.40, 141.90, 141.60, 141.50, 141.20, 141.00, 141.05, 140.60, 140.40, 140.30, 138.80, 134.70, 117.40, 97.30, 97.41, 96.0, 46.90, 33.10, 29.70,

21.90, 20.80, 20.40, 19.80, 19.85, 19.70, 19.75, 18.70, 18.30, 18.35, 17.40, 17.20. HRMS (ESI), *m/z* found: 603.3016; calc. $C_{37}H_{45}N_4Ni$: $[M+H]^+$, 603.2998. UV-Vis (CH_2Cl_2): λ_{max}, nm (log (ε [L mol^{-1} cm^{-1}])) 393 (5.2), 514 (4.1), 551 (4.3).

Ni(II) 3,5-(1-methylethylene)-2,7,8,12,13,17,18-heptaethyl-17,18-*trans*-dihydroporphyrin 13. The product (14 mg, 59%) was obtained as a blue amorphous solid from Ni (II) N'-(2,3,7,8,12,13,17,18-octaethyl-17,18-*trans*-dihydroporphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide **6c** (31 mg, 0.035 mmol). The product **13** contained two diastereomers in a ratio of 8:1.

^{1}H NMR (600 MHz, $CDCl_3$), δ, ppm: 9.305 (2H, br.s, *meso*-H (isomer 2), 9.302 (1H, s, *meso*-H (isomer 1), 9.30 (1H , s, *meso*-H (isomer 1), 8.36 (1H, s, *meso*-H (isomer 2), 8.34 (1H, s, *meso*-H (isomer 1), 4.77 (1H, dd , J = 7.20, J = 15.0 3^{1a}-CH_2 (isomer 1)), 4.59 (1H, dd, J_1 = 7.17 Hz, J_2 = 15.0 Hz, 3^{1a}-CH_2 (isomer 2)), 4.37 (1H, dd, J_1 = 7.17 Hz, J_2 = 15.0 Hz, 3^2-CH (isomer 1)), 4.28 (3H, m, 8-CH (isomer 1 + isomer 2) + 3^2-CH (isomer 1)), 4.07 (2H, m, 7-CH (isomer 1 + isomer 2)), 4.03 (1H, dd, J_1 = 2.46 Hz, J_2 = 15.0 Hz, 3^{1b}-CH_2 (isomer 2)), 4.77 (1H, m, 3^{1b}-CH_2 (isomer 1)), 3.76 (20H, m, $\underline{CH_2}$-CH_3 (isomer 1 + isomer 2)), 2.04 (2H, m, 7^{1a}-$\underline{CH_2}$-CH_3 (isomer 1 + isomer 2)), 1.97 (2H , m, 8^{1a}-$\underline{CH_2}$-CH_3 (isomer 1 + isomer 2)), 1.91 (3H, d, J = 7.3 Hz, 3^1-CH-$\underline{CH_3}$ (isomer 1)), 1.89 (2H, m, 8^{1b}-$\underline{CH_2}$-CH_3 (isomer 1 + isomer 2)), 1.87 (2H, m, 7^{1b}-$\underline{CH_2}$-CH_3 (isomer 1 + isomer 2)), 1.83 (9H , m, 3^1-CH-$\underline{CH_3}$ (isomer 2) + CH_2-$\underline{CH_3}$ (isomer 1 + isomer 2)), 1.73 (24H, m, CH_2-$\underline{CH_3}$ (isomer 1 + isomer 2)), 1.07 (6H, m, 7^2-CH_3 (isomer 1 + isomer 2)), 1.01 (6H, m, 8^2-CH_3 (isomer 1 + isomer 2)). ^{13}C NMR (150 MHz, $CDCl_3$), δ, ppm: 139.4, 138.6, 137.8, 136.6, 100.4, 99.8, 93.1, 54.3, 50.2, 44.3, 44.2, 33.1, 32, 0, 30.2, 30.0, 29.8, 29.7, 29.4, 27.2, 22.7, 21.9, 21.8, 20.3, 19.5, 19.3, 18.3, 18.2, 17.7, 17.0, 16.9, 14.2, 11.0, 10.9, 10.8. HRMS (ESI), *m/z* found: 605.31671; calc. $C_{37}H_{47}N_4Ni$: $[M+H]^+$, 605.3154. UV-Vis (CH_2Cl_2): λ_{max}, nm (log (ε [L mol^{-1} cm^{-1}])) 399 (5.17), 490 (3.82), 610 (4.74).

Thermal decomposition of Ni (II) N'-(3,8,13,18-tetramethyl-2,7,12,17-tetra(2-(ethoxycarbonyl)ethyl)porphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide **7c** (42 mg,0.041 mmol) gave three products **14**-**16** with the total yield 76%.

Ni(II) 5,7-(2-((ethoxycarbonyl)methyl)ethylene)-3,8,13,18-tetramethyl-2,12,17-tri(2-(ethoxycarbonyl)ethyl)porphyrin 14. The product (15 mg, 44%) was obtained as red powder.

^{1}H NMR (600 MHz, $CDCl_3$), δ, ppm: 9.73 (1H, s, *meso*-H), 9.70 (1H, s, *meso*-H), 9.68 (1H, s, *meso*-H), 5.30 (1H, dd, J_1 = 7.2 Hz, J_2 = 16.6 Hz, 3^{1a}-CH_2), 4.72 (2H, m, 5^{1b}-CH_2 + 5^2-CH), 4.36 (2H, q, J = 7.2 Hz, 5^2-$CH_2COO\underline{CH_2}CH_3$), 4.21 (12H, m, -$O\underline{CH_2}CH_3$ + CH_2), 3.51 (3H, s, CH_3), 3.50 (3H, s, CH_3), 3.46 (1H, m, 5^{2a}-$CH_2COO\underline{CH_2}CH_3$), 3.45 (3H s, CH_3), 3.32 (3H, s, CH_3), 3.17 (4H, m, CH_2), 3.10 (2H, t, J = 7.9 Hz, CH_2), 2.96 (1H, m, 5^{2b}-$\underline{CH_2}COOCH_2CH_3$), 1.35 (3H, t, J = 7.2 Hz, $CHCOOCH_2\underline{CH_3}$), 1.22 (9H m, $OCH_2\underline{CH_3}$). ^{13}C NMR (150 MHz, $CDCl_3$), δ, ppm: 173.2, 173.1, 150.1, 148.2, 146.2, 142.1, 141.3, 141.3, 140.9, 140.6, 140.1, 139.3, 138, 8, 137.6, 136.5, 135.6, 128.5, 117.3, 97.3, 97.2, 96.1, 60.6, 45.4, 40.3, 37.4, 37.2, 37.2, 34.8, 29.7, 21.8, 21.8, 21.6, 14.2, 12.0, 11.7, 11.7. HRMS (ESI), *m/z* found: 835.3242; calc. $C_{45}H_{53}N_4NiO_8$: $[M+H]^+$, 835.3217. UV-Vis (CH_2Cl_2): λ_{max}, nm (log (ε [L mol^{-1} cm^{-1}])) 403 (5.36), 514 (4.11), 552 (4.39).

Ni(II) 5,7-(2-(ethoxycarbonyl)-1,3-propylene)-3,8,13,18-tetramethyl-2,12,17-tri(2-(ethoxycarbonyl)ethyl)porphyrin 15. The product (11 mg, 32%) was obtained as red powder. ^{1}H NMR (600 MHz, $CDCl_3$), δ, ppm: 9.66 (1H, s, *meso*-H), 9.62 (1H, s, *meso*-H), 9.60 (1H, s, *meso*-H), 4.95 (2H, m, 5^1-CH_2), 4.35 (2H q, J = 7.1 Hz, 5^2- $CH_2COO\underline{CH_2}CH_3$), 4.20 (12H, m, -$O\underline{CH_2}CH_3$ + CH_2), 4.08 (1H, m , 5^{3a}-CH_2), 3.95 (1H, m, 5^{3b}-CH_2), 3.49 (3H, s, CH_3), 3.47 (6H, s, CH_3), 3.43 (3H, s, CH_3), 3.36 (1H, m, 5^2-CH), 3.14 (6H, m, CH_2), 1.39 (3H, t, J = 7.1 Hz, $CHCOOCH_2\underline{CH_3}$), 1.22 (9H m, $OCH_2\underline{CH_3}$). ^{13}C NMR (150 MHz, $CDCl_3$), δ, ppm: 174.8, 173.1, 141.9, 141.4, 141.2, 141.0 140.7, 140.3, 139.8, 139.6, 139.1, 138.8, 137.6 , 137.4, 136.9, 133.9, 111.7, 97.1, 96.5, 95.8, 60.9, 60.6, 43.2, 37.2, 37.0, 33 , 9, 30.9, 29.7, 27.7, 21.7, 21.6, 16.8, 14.3, 14.2, 11.6, 11.6. HRMS (ESI), *m/z* found: 835.3238; calc. $C_{45}H_{53}N_4NiO_8$: $[M+H]^+$, 835.3217. UV-Vis (CH_2Cl_2): λ_{max}, nm (log (ε [L mol^{-1} cm^{-1}])) 407 (5.09), 520 (3.86), 555 (4.11).

Ni(II) 3,5-ethylene-8,13,18-trimethyl-2,7,12,17-tetra(2-(ethoxycarbonyl)ethyl)porphyrin 16.[3] The product was obtained in traces.

Ni(II) 3,5-ethylene-7,13,17-trimethyl-2,8,12,18-tetra(2-(methoxycarbonyl)ethyl)porphyrin 17.[3] The product (17 mg, 72%) was obtained as dark red powder from Ni (II) N'-(3,7,13,17-tetramethyl-2,8,12,18-tetra(2-(methoxycarbonyl)ethyl)porphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide **8c** (29 mg, 0.03 mmol).

^{1}H NMR (600 MHz, $CDCl_3$), δ, ppm: 9.70 (1H, s, *meso*-H), 9.63 (1H, s, *meso*-H), 9.53 (1H, s, *meso*-H), 4.74 (2H, m, 5^1-CH_2), 4.21 (4H, m, CH_2CH_2CO), 4.13 (2H, t, J = 7.7 Hz, CH_2CH_2CO), 4.07 (2H, t, J = 7.7 Hz, CH_2CH_2CO), 3.78 (3H, s, CH_3), 3.72 (3H, s, CH_3), 3.71 (3H, s, CH_3), 3.70 (3H, s, OCH_3), 3.65 (2H, m, 3^1-CH_2), 3.485 (3H, s, OCH_3), 3.48 (3H, s, OCH_3), 3.22 (3H, s, OCH_3), 3.17 (6H, m, CH_2CH_2CO), 3.11 (2H, t, J = 7.7 Hz, CH_2CH_2CO).

X-ray diffraction study

Single-crystal X-ray data of the red needle crystal of **9a** were collected by using STOE diffractometer Pilatus100K detector, focusing mirror collimation CuK_{α} (1.54086 Å) radiation, rotation method mode. STOE X-AREA software was used for cells refinement and data reduction. Data collection and image processing was performed with X-Area 1.67 (STOE & Cie GmbH, Darmstadt, Germany, 2013). Intensity data were scaled with LANA (part of X-Area) in order to minimize differences of intensities of symmetry-equivalent reflections (multi-scan method). All hydrogen atoms were placed in the calculated positions and allowed to ride on their parent atoms [C-H 0.93-0.98; Uiso (H) = 1.2 Ueq(parent atom)]. The crystal structure was solved and refined with SHELX[22] program. The non-hydrogen atoms were refined by using the anisotropic full matrix least-square procedure. Refinement was made against 4491 reflections, 401 parameters were refined using 84 restraints. The final R 0.1407 against I>2σ(I), Rw = 0.3023. Molecular geometry calculations were performed with the SHELX program, and the molecular graphics were prepared by using DIAMOND[23] software. Crystal data and structure refinement parameters are in the table S1. Structure parameters are in the tables S2-S4. The plot of the molecular structure of the **9a** is in the Figure S1. CCDC-2092020 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

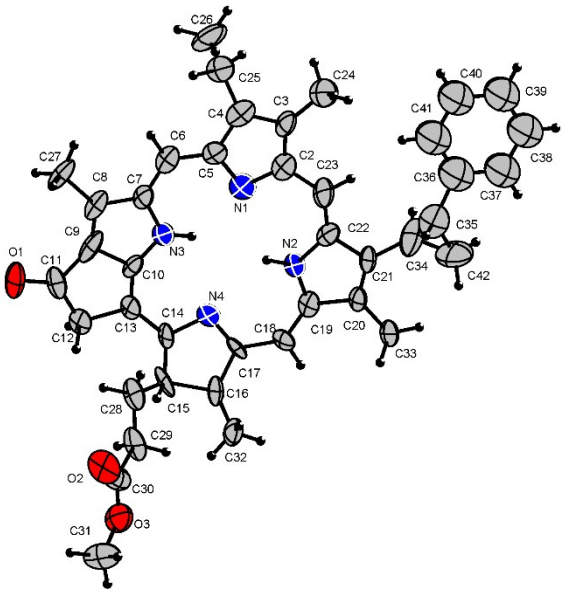

Figure S1. The thermal ellipsoid plot of **9a**. Displacement ellipsoids are drawn at 50% probability level at 295 K.

Table S1. Crystal data and structure refinement for **9a**.

Identification code	shelx	
Empirical formula	C41 H42 N4 O3	
Formula weight	638.78	
Temperature	293(2) K	
Wavelength	1.54186 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 5.5160(10) Å	α= 90°.
	b = 19.977(3) Å	β= 90°.
	c = 30.800(10) Å	γ = 90°.
Volume	3393.9(14) $Å^3$	
Z	4	
Density (calculated)	1.250 Mg/m^3	
Absorption coefficient	0.627 mm^{-1}	
F(000)	1360	
Crystal size	.01 x .01 x .3 mm^3	
Theta range for data collection	4.427 to 59.996°.	
Index ranges	-6<=h<=5, -10<=k<=22, -34<=l<=34	
Reflections collected	16576	
Independent reflections	4491 [R(int) = 0.4735]	
Completeness to theta = 59.996°	93.6 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4491 / 83 / 401	
Goodness-of-fit on F^2	0.878	
Final R indices [I>2sigma(I)]	R1 = 0.1407, wR2 = 0.3318	
R indices (all data)	R1 = 0.3023, wR2 = 0.4251	
Absolute structure parameter	-3.1(10)	
Largest diff. peak and hole	0.356 and -0.452 e. $Å^{-3}$	

Table S2. Bond lengths [Å] and angles [°] for porf.

O(1)-C(11)	1.25(3)
O(2)-C(30)	1.17(2)
O(3)-C(30)	1.30(2)
O(3)-C(31)	1.48(3)
N(1)-C(2)	1.36(2)
N(1)-C(5)	1.386(19)
N(2)-C(22)	1.368(19)
N(2)-C(19)	1.371(18)
N(2)-H(2)	0.8600
N(3)-C(10)	1.346(19)
N(3)-C(7)	1.378(18)
N(3)-H(3)	0.8600
N(4)-C(17)	1.372(18)
N(4)-C(14)	1.398(17)
C(2)-C(3)	1.38(2)
C(2)-C(23)	1.44(3)
C(3)-C(4)	1.39(3)
C(3)-C(24)	1.47(3)
C(4)-C(5)	1.44(3)
C(4)-C(25)	1.53(3)
C(5)-C(6)	1.42(2)
C(6)-C(7)	1.36(2)
C(6)-H(6)	0.9300
C(7)-C(8)	1.42(3)
C(8)-C(9)	1.35(3)
C(8)-C(27)	1.49(2)
C(9)-C(10)	1.44(3)
C(9)-C(11)	1.51(4)
C(10)-C(13)	1.33(3)
C(11)-C(12)	1.50(3)
C(12)-C(13)	1.55(3)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(13)-C(14)	1.41(3)
C(14)-C(15)	1.45(2)
C(15)-C(28)	1.47(2)
C(15)-C(16)	1.55(2)
C(15)-H(15)	0.8(3)
C(16)-C(17)	1.45(3)
C(16)-C(32)	1.48(2)
C(16)-H(16)	1.01(4)
C(17)-C(18)	1.42(2)
C(18)-C(19)	1.33(2)
C(18)-H(18)	0.9300
C(19)-C(20)	1.46(3)
C(20)-C(21)	1.31(2)
C(20)-C(33)	1.48(2)
C(21)-C(22)	1.43(3)
C(21)-C(34)	1.47(3)
C(22)-C(23)	1.37(3)
C(23)-H(23)	0.9300
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(25)-C(26)	1.49(3)
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600

C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
C(28)-C(29)	1.56(3)
C(28)-H(28A)	0.9700
C(28)-H(28B)	0.9700
C(29)-C(30)	1.53(3)
C(29)-H(29A)	0.9700
C(29)-H(29B)	0.9700
C(31)-H(31A)	0.9600
C(31)-H(31B)	0.9600
C(31)-H(31C)	0.9600
C(32)-H(32A)	0.9600
C(32)-H(32B)	0.9600
C(32)-H(32C)	0.9600
C(33)-H(33A)	0.9600
C(33)-H(33B)	0.9600
C(33)-H(33C)	0.9600
C(34)-C(35)	1.35(3)
C(34)-C(42)	1.35(3)
C(34)-H(34)	1.01(4)
C(35)-C(36)	1.56(3)
C(35)-C(42)	1.58(3)
C(35)-H(35)	1.03(3)
C(36)-C(37)	1.3900
C(36)-C(41)	1.3900
C(37)-C(38)	1.3900
C(37)-H(37)	0.9300
C(38)-C(39)	1.3900
C(38)-H(38)	0.9300
C(39)-C(40)	1.3900
C(39)-H(39)	0.9300
C(40)-C(41)	1.3900
C(40)-H(40)	0.9300
C(41)-H(41)	0.9300
C(42)-H(42A)	0.9700
C(42)-H(42B)	0.9700

C(30)-O(3)-C(31)	117.8(18)
C(2)-N(1)-C(5)	102.1(19)
C(22)-N(2)-C(19)	114.8(17)
C(22)-N(2)-H(2)	122.6
C(19)-N(2)-H(2)	122.6
C(10)-N(3)-C(7)	112.0(18)
C(10)-N(3)-H(3)	124.0
C(7)-N(3)-H(3)	124.0
C(17)-N(4)-C(14)	102.6(15)
N(1)-C(2)-C(3)	117(2)
N(1)-C(2)-C(23)	120(2)
C(3)-C(2)-C(23)	123(2)
C(2)-C(3)-C(4)	103(2)
C(2)-C(3)-C(24)	132(2)
C(4)-C(3)-C(24)	125(2)
C(3)-C(4)-C(5)	107.4(19)
C(3)-C(4)-C(25)	128(2)
C(5)-C(4)-C(25)	124(2)
N(1)-C(5)-C(6)	121(2)
N(1)-C(5)-C(4)	110(2)
C(6)-C(5)-C(4)	129(2)
C(7)-C(6)-C(5)	128(2)
C(7)-C(6)-H(6)	116.0
C(5)-C(6)-H(6)	116.0

C(6)-C(7)-N(3)	122(2)
C(6)-C(7)-C(8)	130(2)
N(3)-C(7)-C(8)	108.5(19)
C(9)-C(8)-C(7)	103.8(18)
C(9)-C(8)-C(27)	129(2)
C(7)-C(8)-C(27)	127(2)
C(8)-C(9)-C(10)	113(3)
C(8)-C(9)-C(11)	143(2)
C(10)-C(9)-C(11)	104(2)
C(13)-C(10)-N(3)	141.2(19)
C(13)-C(10)-C(9)	116(2)
N(3)-C(10)-C(9)	103(2)
O(1)-C(11)-C(12)	125(2)
O(1)-C(11)-C(9)	127(3)
C(12)-C(11)-C(9)	108(2)
C(11)-C(12)-C(13)	104.3(18)
C(11)-C(12)-H(12A)	110.9
C(13)-C(12)-H(12A)	110.9
C(11)-C(12)-H(12B)	110.9
C(13)-C(12)-H(12B)	110.9
H(12A)-C(12)-H(12B)	108.9
C(10)-C(13)-C(14)	128.2(18)
C(10)-C(13)-C(12)	108(2)
C(14)-C(13)-C(12)	124.2(19)
N(4)-C(14)-C(13)	113.4(18)
N(4)-C(14)-C(15)	117.0(17)
C(13)-C(14)-C(15)	129.5(15)
C(14)-C(15)-C(28)	121(2)
C(14)-C(15)-C(16)	100.7(15)
C(28)-C(15)-C(16)	116.7(16)
C(14)-C(15)-H(15)	105.9
C(28)-C(15)-H(15)	105.9
C(16)-C(15)-H(15)	105.9
C(17)-C(16)-C(32)	118.5(16)
C(17)-C(16)-C(15)	103.6(17)
C(32)-C(16)-C(15)	115.1(18)
C(17)-C(16)-H(16)	106.3
C(32)-C(16)-H(16)	106.3
C(15)-C(16)-H(16)	106.3
N(4)-C(17)-C(18)	118.9(16)
N(4)-C(17)-C(16)	115.8(15)
C(18)-C(17)-C(16)	124.8(18)
C(19)-C(18)-C(17)	133.4(19)
C(19)-C(18)-H(18)	113.3
C(17)-C(18)-H(18)	113.3
C(18)-C(19)-N(2)	126.5(19)
C(18)-C(19)-C(20)	130.1(19)
N(2)-C(19)-C(20)	102.5(18)
C(21)-C(20)-C(19)	108.7(18)
C(21)-C(20)-C(33)	127.5(18)
C(19)-C(20)-C(33)	124(2)
C(20)-C(21)-C(22)	111.6(18)
C(20)-C(21)-C(34)	131(2)
C(22)-C(21)-C(34)	118(2)
N(2)-C(22)-C(23)	127(2)
N(2)-C(22)-C(21)	102.1(18)
C(23)-C(22)-C(21)	130(2)
C(22)-C(23)-C(2)	131(2)
C(22)-C(23)-H(23)	114.5
C(2)-C(23)-H(23)	114.5
C(3)-C(24)-H(24A)	109.5
C(3)-C(24)-H(24B)	109.5

H(24A)-C(24)-H(24B)	109.5
C(3)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(26)-C(25)-C(4)	112.6(18)
C(26)-C(25)-H(25A)	109.1
C(4)-C(25)-H(25A)	109.1
C(26)-C(25)-H(25B)	109.1
C(4)-C(25)-H(25B)	109.1
H(25A)-C(25)-H(25B)	107.8
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(8)-C(27)-H(27A)	109.5
C(8)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(8)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(15)-C(28)-C(29)	118(2)
C(15)-C(28)-H(28A)	107.8
C(29)-C(28)-H(28A)	107.8
C(15)-C(28)-H(28B)	107.8
C(29)-C(28)-H(28B)	107.8
H(28A)-C(28)-H(28B)	107.2
C(30)-C(29)-C(28)	113.3(19)
C(30)-C(29)-H(29A)	108.9
C(28)-C(29)-H(29A)	108.9
C(30)-C(29)-H(29B)	108.9
C(28)-C(29)-H(29B)	108.9
H(29A)-C(29)-H(29B)	107.7
O(2)-C(30)-O(3)	129(2)
O(2)-C(30)-C(29)	122(2)
O(3)-C(30)-C(29)	108(2)
O(3)-C(31)-H(31A)	109.5
O(3)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
O(3)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(16)-C(32)-H(32A)	109.5
C(16)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(16)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(20)-C(33)-H(33A)	109.5
C(20)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(20)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(35)-C(34)-C(42)	71.6(19)
C(35)-C(34)-C(21)	135(3)
C(42)-C(34)-C(21)	131(3)
C(35)-C(34)-H(34)	104.7
C(42)-C(34)-H(34)	104.7
C(21)-C(34)-H(34)	104.7
C(34)-C(35)-C(36)	125(3)

C(34)-C(35)-C(42)	54.2(15)
C(36)-C(35)-C(42)	117(3)
C(34)-C(35)-H(35)	115.3
C(36)-C(35)-H(35)	115.3
C(42)-C(35)-H(35)	115.3
C(37)-C(36)-C(41)	120.0
C(37)-C(36)-C(35)	118(2)
C(41)-C(36)-C(35)	121(2)
C(36)-C(37)-C(38)	120.00(5)
C(36)-C(37)-H(37)	120.0
C(38)-C(37)-H(37)	120.0
C(39)-C(38)-C(37)	120.00(8)
C(39)-C(38)-H(38)	120.0
C(37)-C(38)-H(38)	120.0
C(40)-C(39)-C(38)	120.0
C(40)-C(39)-H(39)	120.0
C(38)-C(39)-H(39)	120.0
C(41)-C(40)-C(39)	120.00(8)
C(41)-C(40)-H(40)	120.0
C(39)-C(40)-H(40)	120.0
C(40)-C(41)-C(36)	120.00(9)
C(40)-C(41)-H(41)	120.0
C(36)-C(41)-H(41)	120.0
C(34)-C(42)-C(35)	54.2(15)
C(34)-C(42)-H(42A)	118.3
C(35)-C(42)-H(42A)	118.3
C(34)-C(42)-H(42B)	118.3
C(35)-C(42)-H(42B)	118.3
H(42A)-C(42)-H(42B)	115.6

Symmetry transformations used to generate equivalent atoms:

Table S3. Torsion angles [°] for **9a**.

C(5)-N(1)-C(2)-C(3)	0(2)
C(5)-N(1)-C(2)-C(23)	-173.8(19)
N(1)-C(2)-C(3)-C(4)	4(2)
C(23)-C(2)-C(3)-C(4)	176.7(19)
N(1)-C(2)-C(3)-C(24)	-178(2)
C(23)-C(2)-C(3)-C(24)	-5(4)
C(2)-C(3)-C(4)-C(5)	-5(2)
C(24)-C(3)-C(4)-C(5)	176(2)
C(2)-C(3)-C(4)-C(25)	176(2)
C(24)-C(3)-C(4)-C(25)	-2(3)
C(2)-N(1)-C(5)-C(6)	-178.3(17)
C(2)-N(1)-C(5)-C(4)	-3(2)
C(3)-C(4)-C(5)-N(1)	5(2)
C(25)-C(4)-C(5)-N(1)	-176.1(19)
C(3)-C(4)-C(5)-C(6)	-179.9(19)
C(25)-C(4)-C(5)-C(6)	-1(3)
N(1)-C(5)-C(6)-C(7)	-3(3)
C(4)-C(5)-C(6)-C(7)	-177(2)
C(5)-C(6)-C(7)-N(3)	5(3)
C(5)-C(6)-C(7)-C(8)	-178.7(18)
C(10)-N(3)-C(7)-C(6)	176.8(18)
C(10)-N(3)-C(7)-C(8)	0(2)
C(6)-C(7)-C(8)-C(9)	-177(2)
N(3)-C(7)-C(8)-C(9)	0(2)
C(6)-C(7)-C(8)-C(27)	5(3)
N(3)-C(7)-C(8)-C(27)	-178.2(18)
C(7)-C(8)-C(9)-C(10)	1(2)
C(27)-C(8)-C(9)-C(10)	178.4(18)
C(7)-C(8)-C(9)-C(11)	-176(3)
C(27)-C(8)-C(9)-C(11)	1(4)
C(7)-N(3)-C(10)-C(13)	178(2)
C(7)-N(3)-C(10)-C(9)	0(2)
C(8)-C(9)-C(10)-C(13)	-178.8(18)
C(11)-C(9)-C(10)-C(13)	-1(2)
C(8)-C(9)-C(10)-N(3)	-1(2)
C(11)-C(9)-C(10)-N(3)	177.5(16)
C(8)-C(9)-C(11)-O(1)	-6(4)
C(10)-C(9)-C(11)-O(1)	177(2)
C(8)-C(9)-C(11)-C(12)	180(3)
C(10)-C(9)-C(11)-C(12)	3(2)
O(1)-C(11)-C(12)-C(13)	-177(2)
C(9)-C(11)-C(12)-C(13)	-3(2)
N(3)-C(10)-C(13)-C(14)	-3(4)
C(9)-C(10)-C(13)-C(14)	174.5(18)
N(3)-C(10)-C(13)-C(12)	-179(2)
C(9)-C(10)-C(13)-C(12)	-1(2)
C(11)-C(12)-C(13)-C(10)	3(2)
C(11)-C(12)-C(13)-C(14)	-173.3(19)
C(17)-N(4)-C(14)-C(13)	177.6(17)
C(17)-N(4)-C(14)-C(15)	-2(2)
C(10)-C(13)-C(14)-N(4)	4(3)
C(12)-C(13)-C(14)-N(4)	179.1(16)
C(10)-C(13)-C(14)-C(15)	-176(2)
C(12)-C(13)-C(14)-C(15)	-1(3)
N(4)-C(14)-C(15)-C(28)	129.0(17)
C(13)-C(14)-C(15)-C(28)	-51(3)
N(4)-C(14)-C(15)-C(16)	-1(2)
C(13)-C(14)-C(15)-C(16)	179.1(19)
C(14)-C(15)-C(16)-C(17)	4(2)
C(28)-C(15)-C(16)-C(17)	-129(2)

C(14)-C(15)-C(16)-C(32)	-127(2)
C(28)-C(15)-C(16)-C(32)	100(2)
C(14)-N(4)-C(17)-C(18)	177.5(15)
C(14)-N(4)-C(17)-C(16)	5(2)
C(32)-C(16)-C(17)-N(4)	123(2)
C(15)-C(16)-C(17)-N(4)	-6(2)
C(32)-C(16)-C(17)-C(18)	-49(3)
C(15)-C(16)-C(17)-C(18)	-177.8(17)
N(4)-C(17)-C(18)-C(19)	6(3)
C(16)-C(17)-C(18)-C(19)	178(2)
C(17)-C(18)-C(19)-N(2)	-10(3)
C(17)-C(18)-C(19)-C(20)	-177.2(19)
C(22)-N(2)-C(19)-C(18)	-175.8(19)
C(22)-N(2)-C(19)-C(20)	-6(2)
C(18)-C(19)-C(20)-C(21)	173(2)
N(2)-C(19)-C(20)-C(21)	3(2)
C(18)-C(19)-C(20)-C(33)	-10(3)
N(2)-C(19)-C(20)-C(33)	-179.6(19)
C(19)-C(20)-C(21)-C(22)	0(2)
C(33)-C(20)-C(21)-C(22)	-177(2)
C(19)-C(20)-C(21)-C(34)	180(3)
C(33)-C(20)-C(21)-C(34)	3(4)
C(19)-N(2)-C(22)-C(23)	-179(2)
C(19)-N(2)-C(22)-C(21)	6(2)
C(20)-C(21)-C(22)-N(2)	-3(2)
C(34)-C(21)-C(22)-N(2)	177(2)
C(20)-C(21)-C(22)-C(23)	-178(2)
C(34)-C(21)-C(22)-C(23)	2(4)
N(2)-C(22)-C(23)-C(2)	9(4)
C(21)-C(22)-C(23)-C(2)	-178(2)
N(1)-C(2)-C(23)-C(22)	-10(4)
C(3)-C(2)-C(23)-C(22)	177(3)
C(3)-C(4)-C(25)-C(26)	-89(3)
C(5)-C(4)-C(25)-C(26)	93(3)
C(14)-C(15)-C(28)-C(29)	-178.5(16)
C(16)-C(15)-C(28)-C(29)	-56(3)
C(15)-C(28)-C(29)-C(30)	-69(2)
C(31)-O(3)-C(30)-O(2)	-4(4)
C(31)-O(3)-C(30)-C(29)	179(2)
C(28)-C(29)-C(30)-O(2)	2(4)
C(28)-C(29)-C(30)-O(3)	179.6(19)
C(20)-C(21)-C(34)-C(35)	119(4)
C(22)-C(21)-C(34)-C(35)	-61(5)
C(20)-C(21)-C(34)-C(42)	14(6)
C(22)-C(21)-C(34)-C(42)	-167(4)
C(42)-C(34)-C(35)-C(36)	-99(4)
C(21)-C(34)-C(35)-C(36)	131(4)
C(21)-C(34)-C(35)-C(42)	-130(5)
C(34)-C(35)-C(36)-C(37)	96(3)
C(42)-C(35)-C(36)-C(37)	33(4)
C(34)-C(35)-C(36)-C(41)	-94(3)
C(42)-C(35)-C(36)-C(41)	-158(3)
C(41)-C(36)-C(37)-C(38)	0.0
C(35)-C(36)-C(37)-C(38)	170(3)
C(36)-C(37)-C(38)-C(39)	0.0
C(37)-C(38)-C(39)-C(40)	0.0
C(38)-C(39)-C(40)-C(41)	0.0
C(39)-C(40)-C(41)-C(36)	0.0
C(37)-C(36)-C(41)-C(40)	0.0
C(35)-C(36)-C(41)-C(40)	-170(3)
C(21)-C(34)-C(42)-C(35)	134(4)
C(36)-C(35)-C(42)-C(34)	116(4)

Symmetry transformations used to generate equivalent atoms:

Table S4. Hydrogen bonds for **9a** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2)...N(1)	0.86	2.47	3.01(3)	121.1
N(2)-H(2)...N(4)	0.86	2.44	2.98(2)	120.8
N(3)-H(3)...N(1)	0.86	2.15	2.75(3)	126.3
C(15)-H(15)...O(2)	0.83	2.59	3.14(3)	124.1
C(16)-H(16)...O(2)#1	1.01	2.57	3.53(3)	159.2
C(29)-H(29A)...O(2)#1	0.97	2.57	3.40(2)	143.6

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z

NMR Spectra

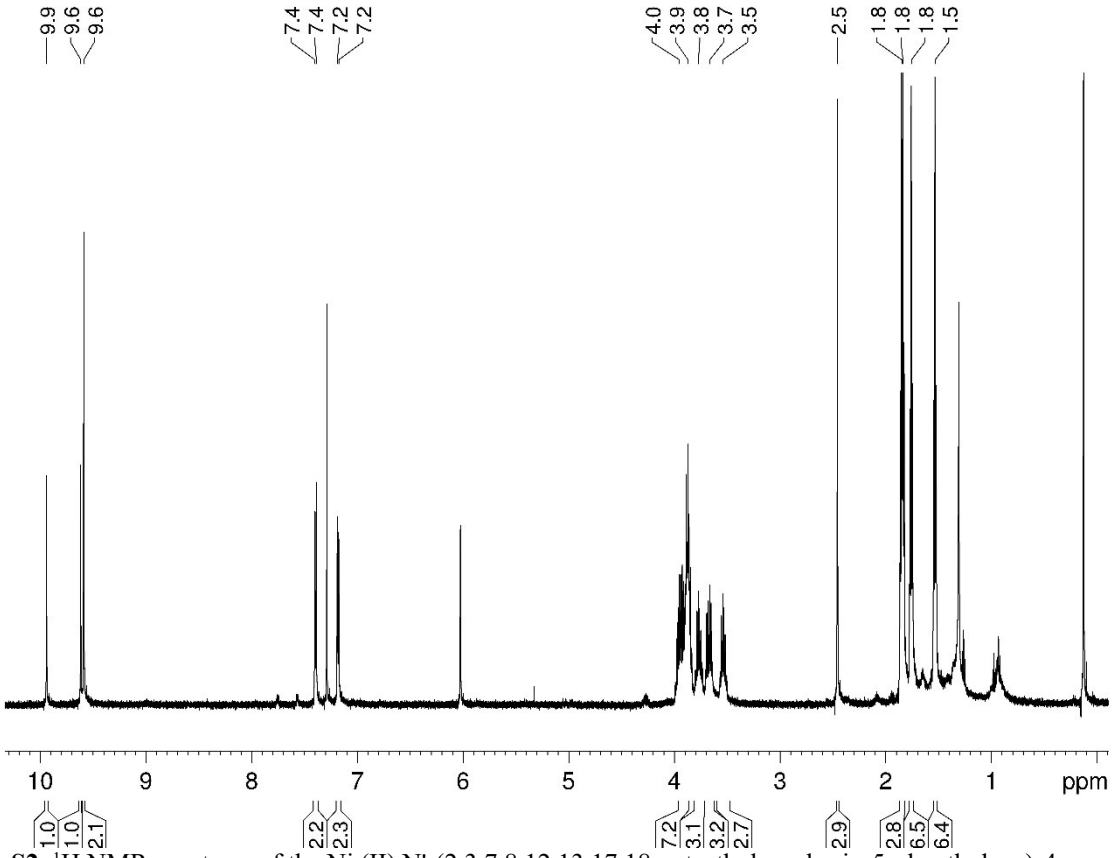

Figure S2. ^{1}H NMR spectrum of the Ni (II) N'-(2,3,7,8,12,13,17,18-octaethylporphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide (**5c**) isomer 1 in $CDCl_3$.

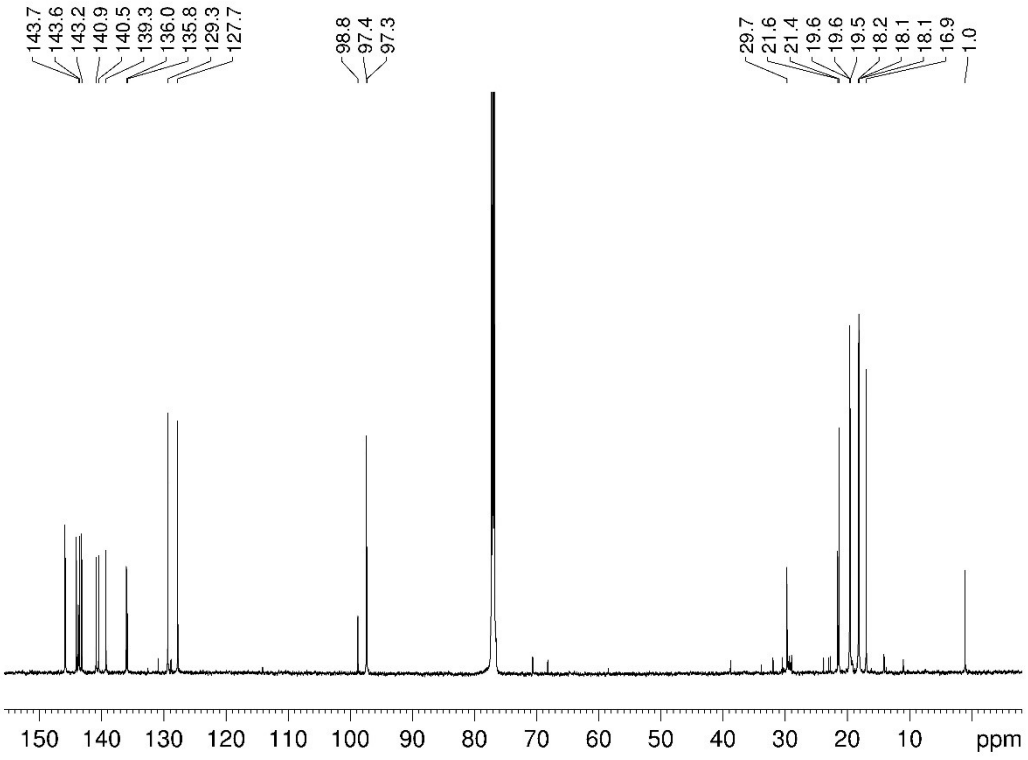

Figure S3. ^{13}C NMR spectrum of the Ni (II) N'-(2,3,7,8,12,13,17,18-octaethylporphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide (**5c**) isomer 1 in $CDCl_3$.

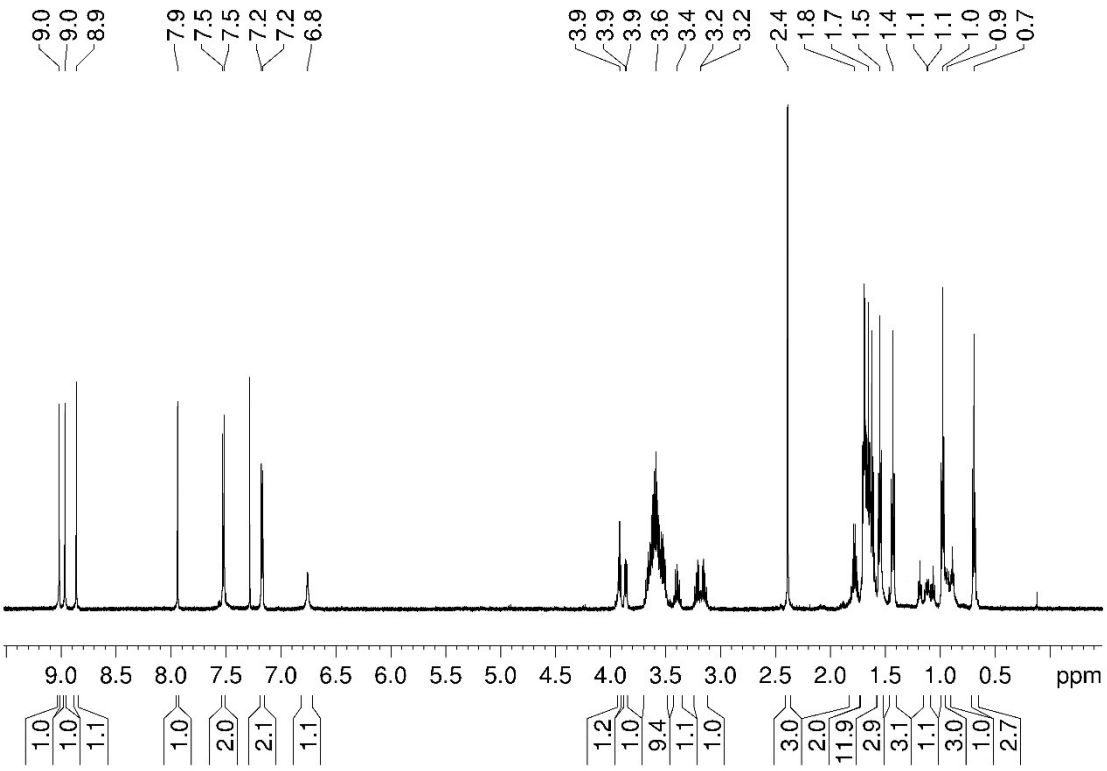

Figure S4. [1]H NMR spectrum of the Ni (II) N'-(2,3,7,8,12,13,17,18-octaethyl-17,18-*trans*-dihydroporphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide (**6c**) isomer 1 in $CDCl_3$.

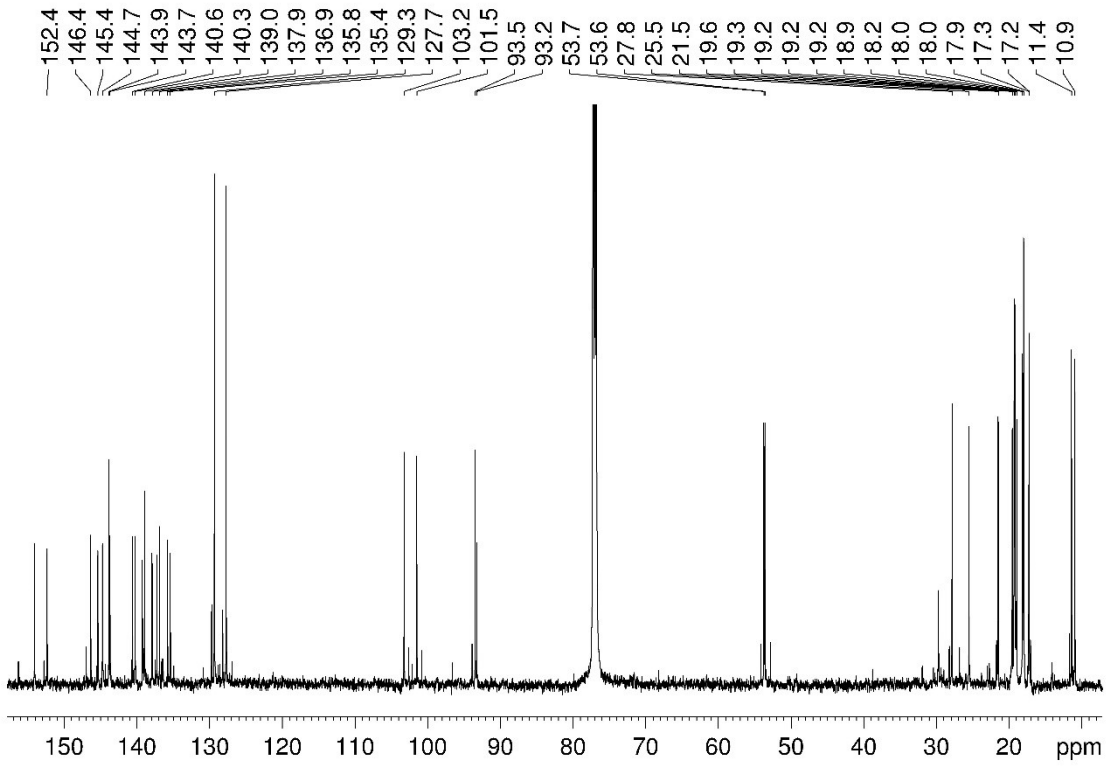

Figure S5. [13]C NMR spectrum of the Ni (II) N'-(2,3,7,8,12,13,17,18-octaethyl-17,18-*trans*-dihydroporphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide (**6c**) isomer 1 in $CDCl_3$.

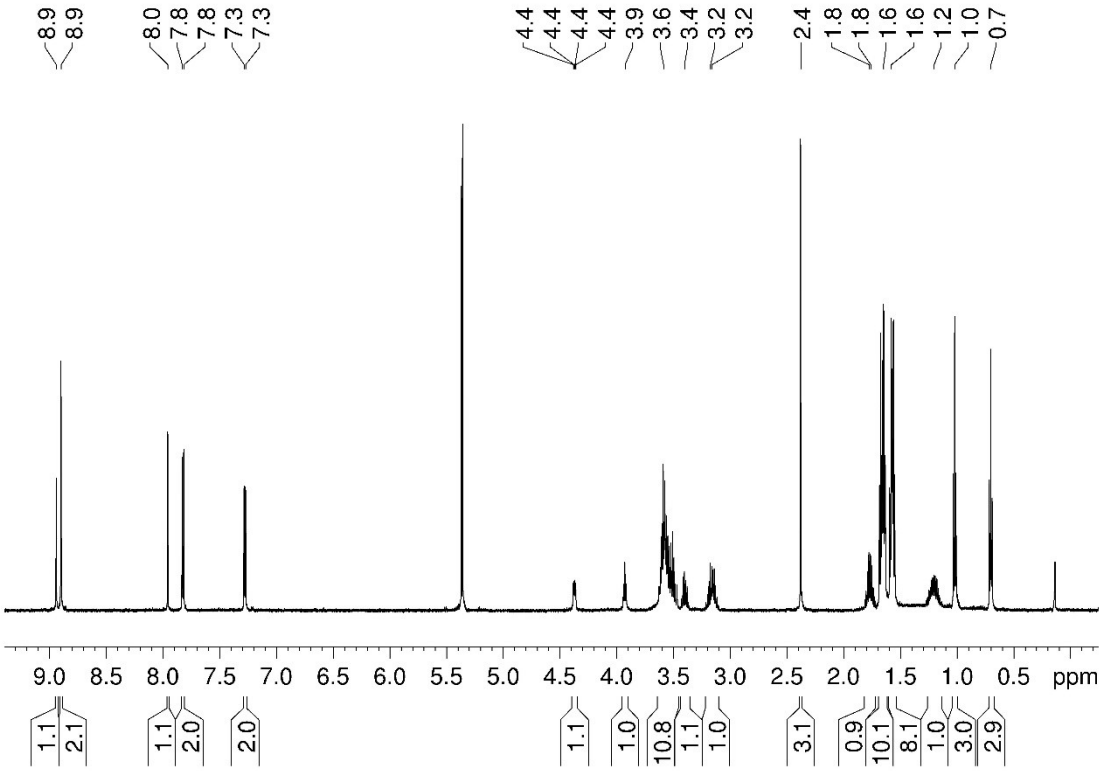

Figure S6. ^{1}H NMR spectrum of the Ni (II) N'-(2,3,7,8,12,13,17,18-octaethyl-17,18-*trans*-dihydroporphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide (**6c**) isomer 2 in $CDCl_3$.

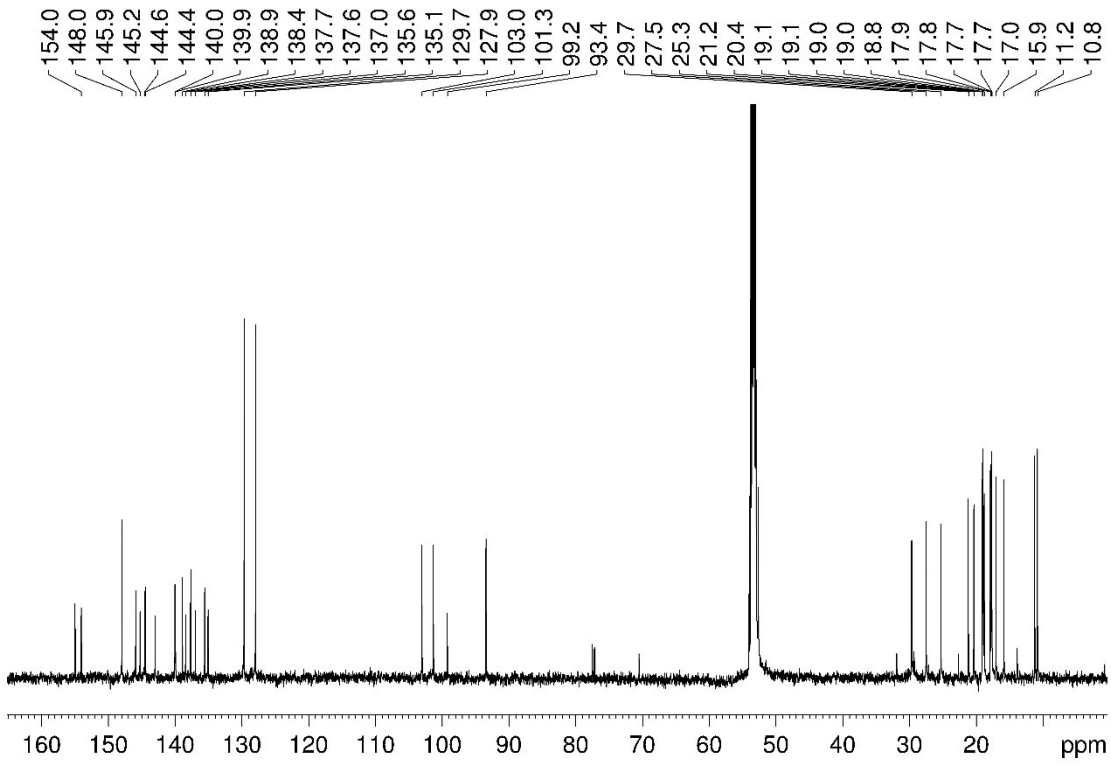

Figure S7. ^{13}C NMR spectrum of the Ni (II) N'-(2,3,7,8,12,13,17,18-octaethyl-17,18-*trans*-dihydroporphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide (**6c**) isomer 2 in $CDCl_3$.

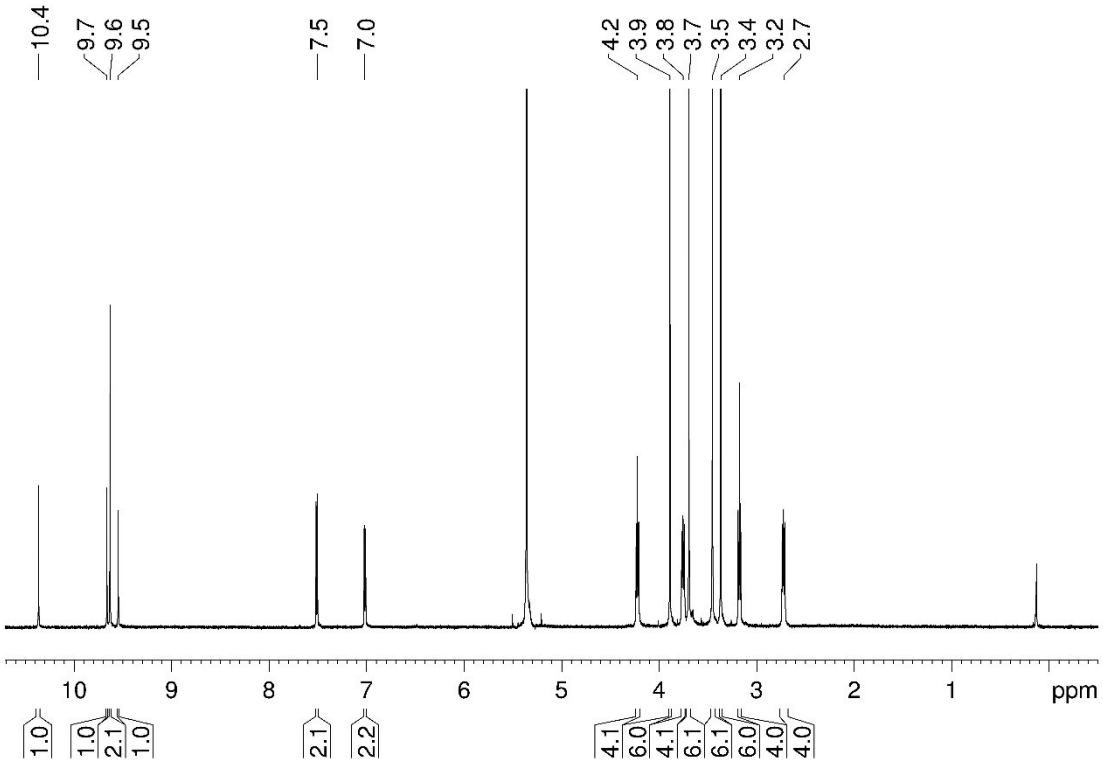

Figure S8. ^{1}H NMR spectrum of the Ni (II) (*Z*)-N'-(3,8,13,18-tetramethyl-2,7,12,17-tetra(2-(ethoxycarbonyl)ethyl)porphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide (**7c**) isomer 1 in $CDCl_3$.

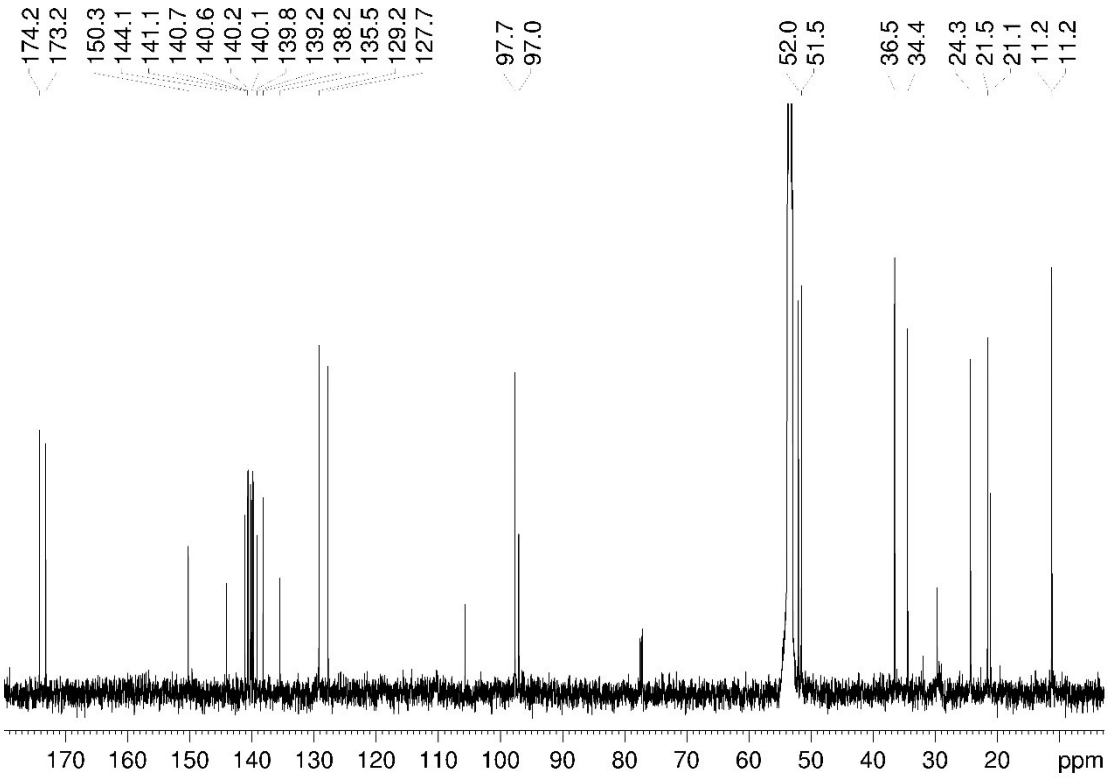

Figure S9. ^{13}C NMR spectrum of the Ni (II) N'-(2,3,7,8,12,13,17,18-octaethyl-17,18-*trans*-dihydroporphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide (**7c**) isomer 1 in $CDCl_3$.

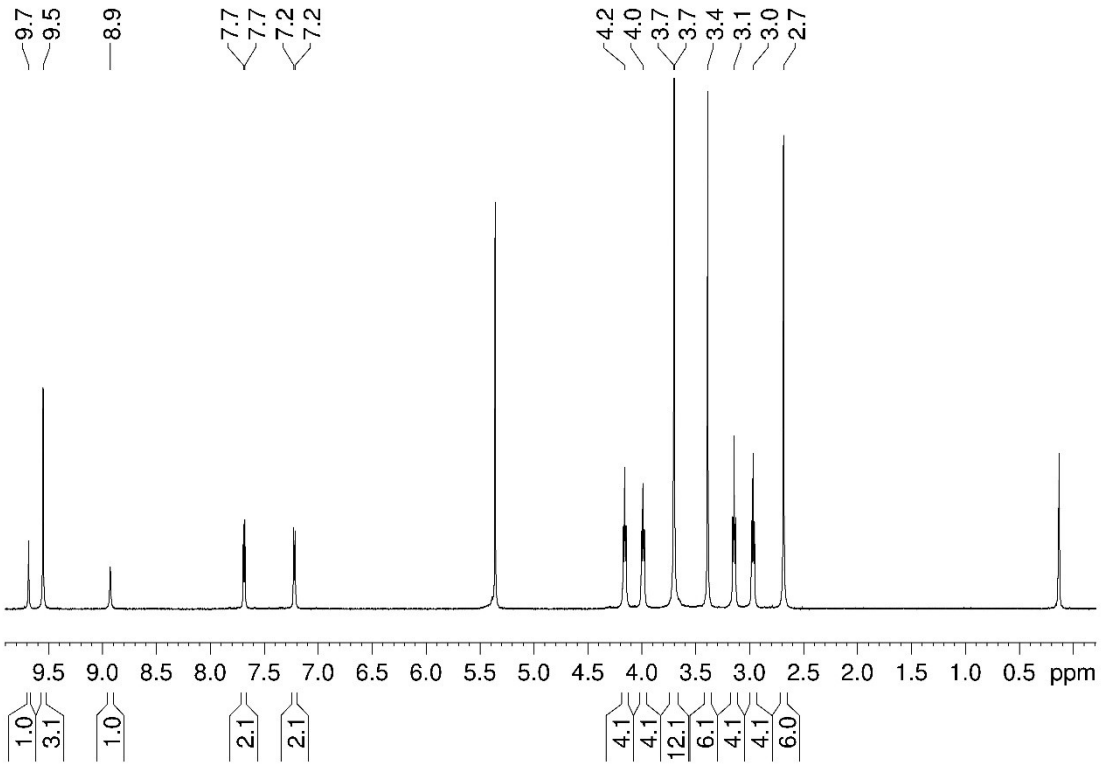

Figure S10. ^{1}H NMR spectrum of the Ni (II) (*Z*)-N'-(3,8,13,18-tetramethyl-2,7,12,17-tetra(2-(ethoxycarbonyl)ethyl)porphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide (**7c**) isomer 2 in $CDCl_3$.

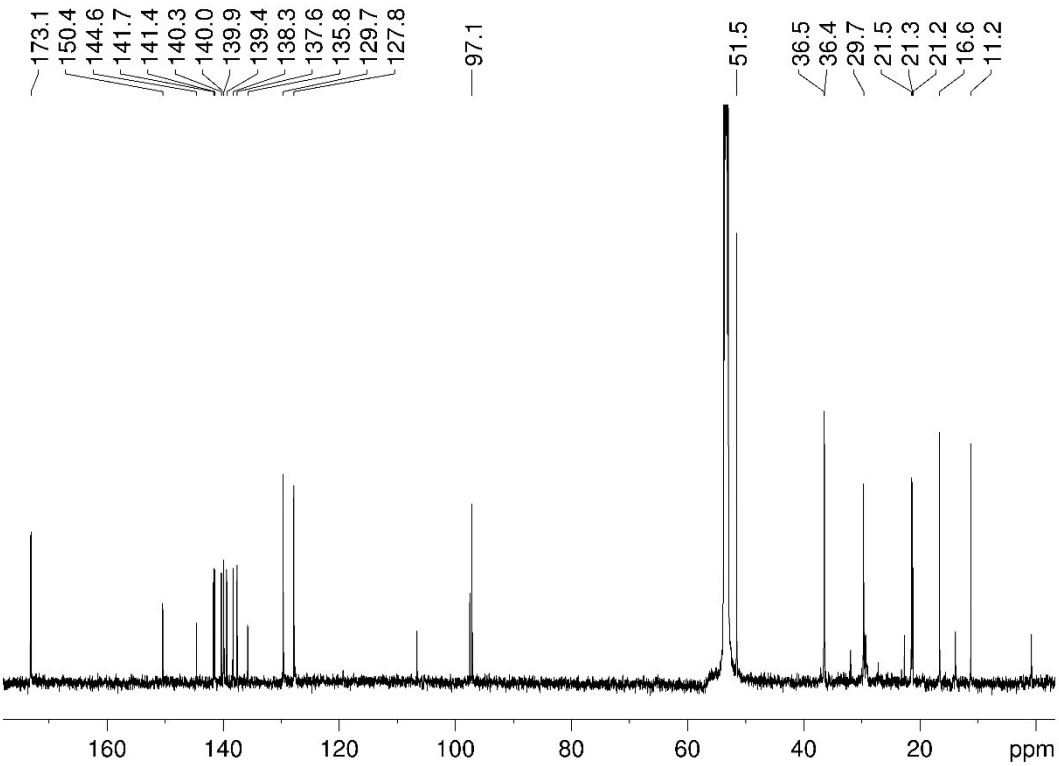

Figure S11. ^{13}C NMR spectrum of the Ni (II) N'-(2,3,7,8,12,13,17,18-octaethyl-17,18-*trans*-dihydroporphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide (**7c**) isomer 2 in $CDCl_3$.

Figure S12. ^{1}H NMR spectrum of the Ni (II) N'-(3,7,13,17-tetramethyl-2,8,12,18-tetra(2-(methoxycarbonyl)ethyl)porphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide (**8c**) isomer 1 in $CDCl_3$.

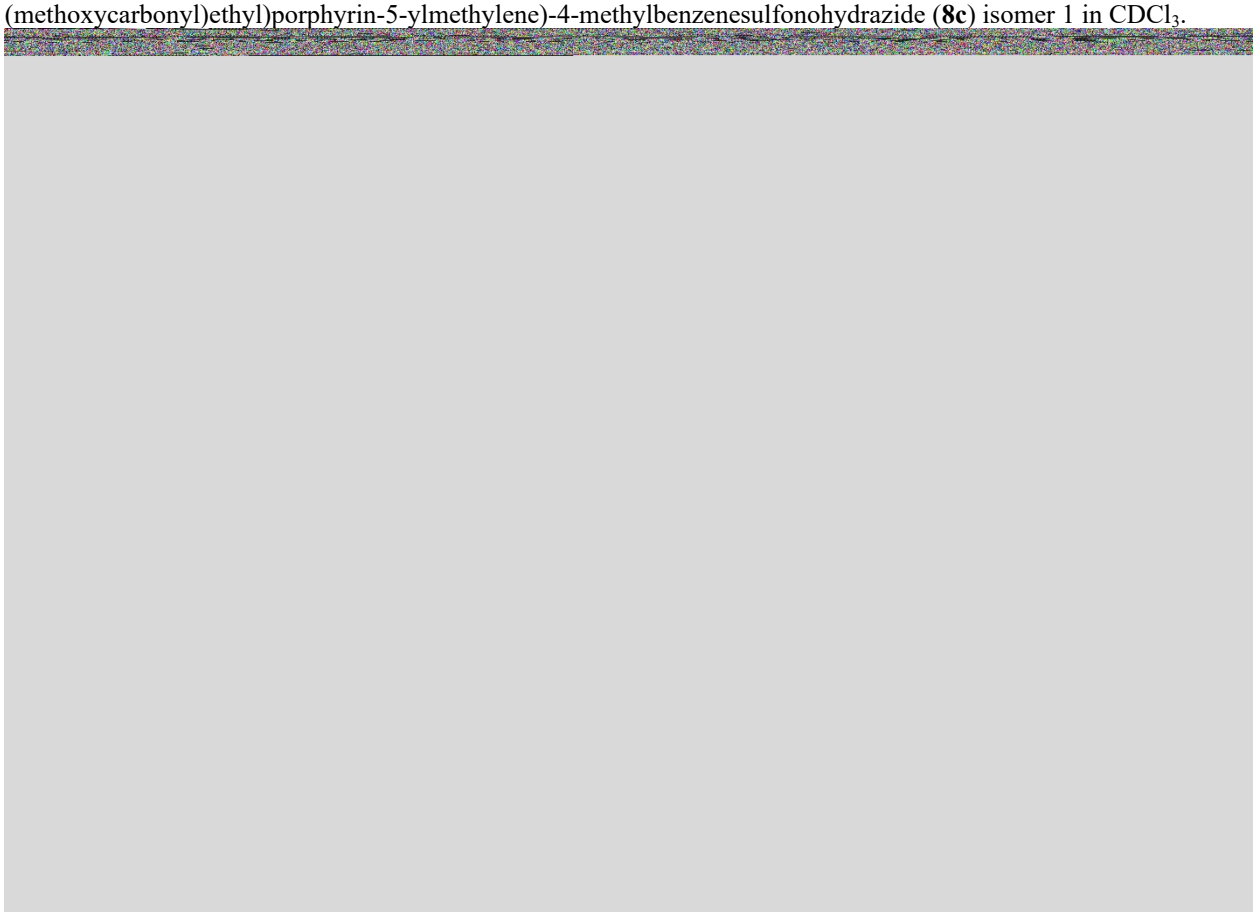

Figure S13. ^{13}C NMR spectrum of the Ni (II) N'-(3,7,13,17-tetramethyl-2,8,12,18-tetra(2-(methoxycarbonyl)ethyl)porphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide (**8c**) isomer 1 in $CDCl_3$.

Figure S14. ^{1}H NMR spectrum of the Ni (II) N'-(3,7,13,17-tetramethyl-2,8,12,18-tetra(2-(methoxycarbonyl)ethyl)porphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide (**8c**) isomer 2 in $CDCl_3$.

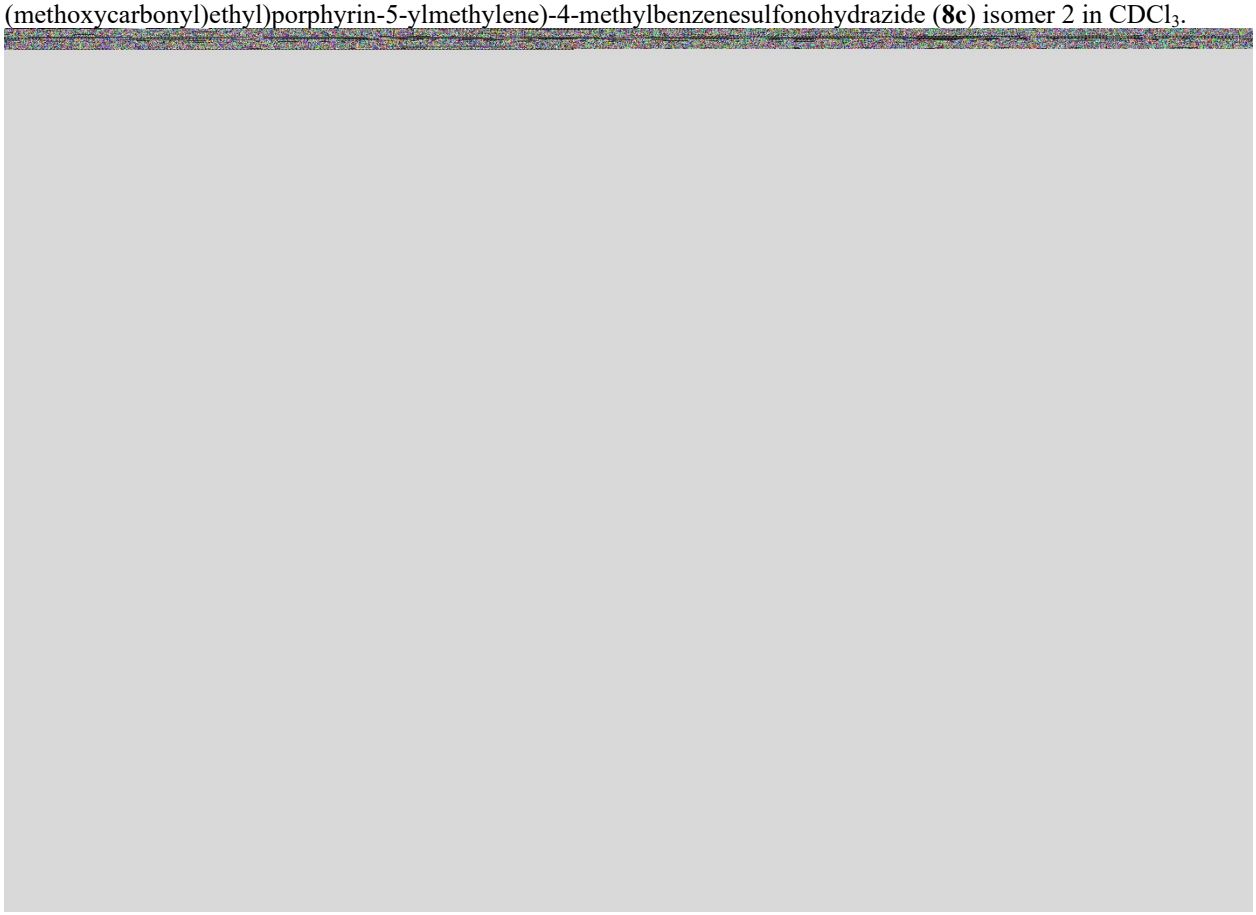

Figure S15. ^{13}C NMR spectrum of the Ni (II) N'-(3,7,13,17-tetramethyl-2,8,12,18-tetra(2-(methoxycarbonyl)ethyl)porphyrin-5-ylmethylene)-4-methylbenzenesulfonohydrazide (**8c**) isomer 2 in $CDCl_3$.

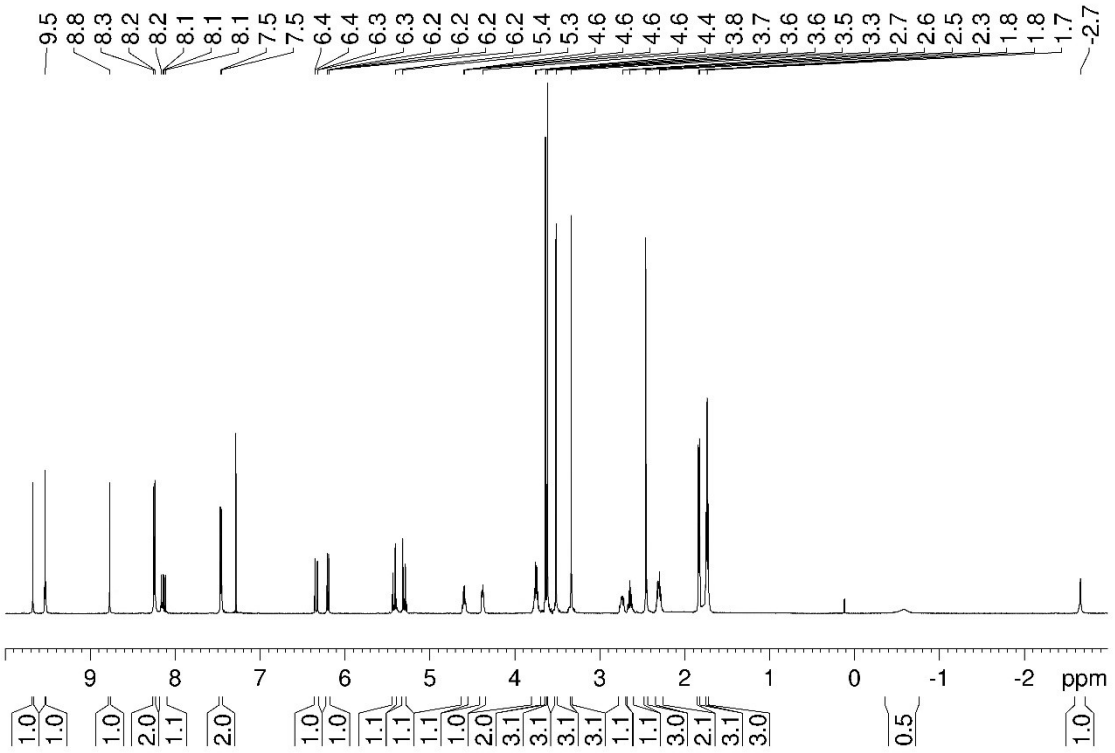

Figure S16. ^{1}H NMR spectrum of the N-tosylhydrazone of methyl pyropheophorbide-*a* (**4**) in $CDCl_3$.

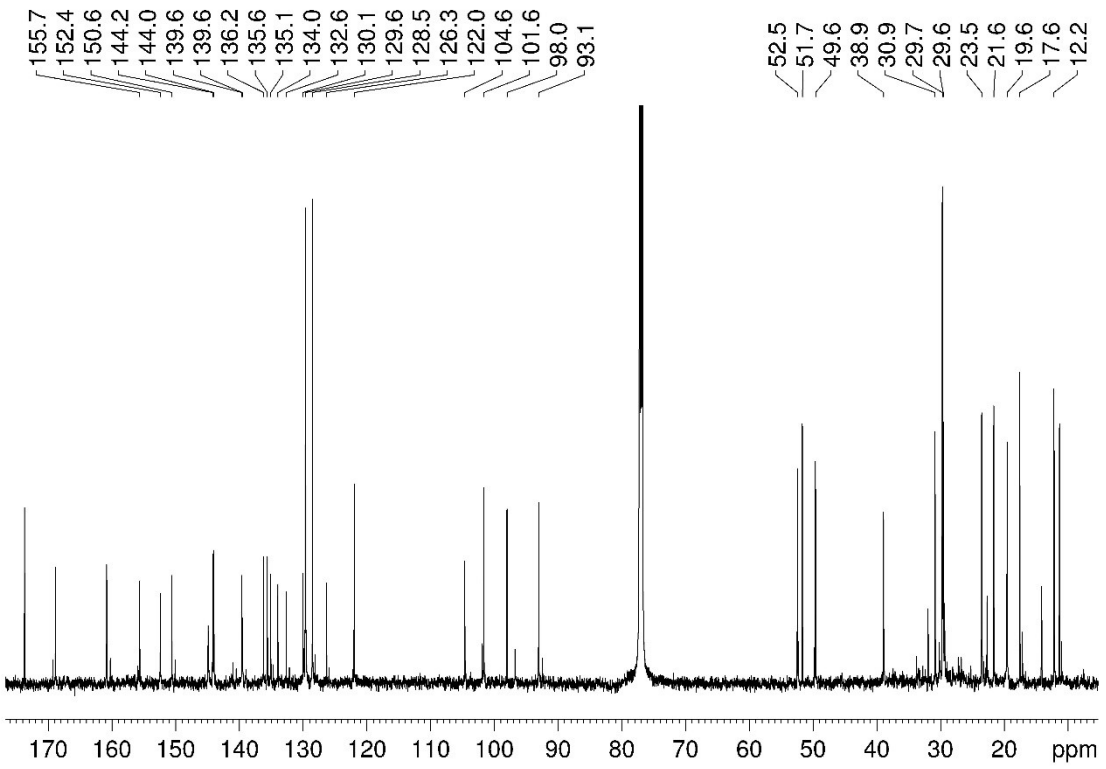

Figure S17. ^{13}C NMR spectrum of the N-tosylhydrazone of methyl pyropheophorbide-*a* (**4**) in $CDCl_3$.

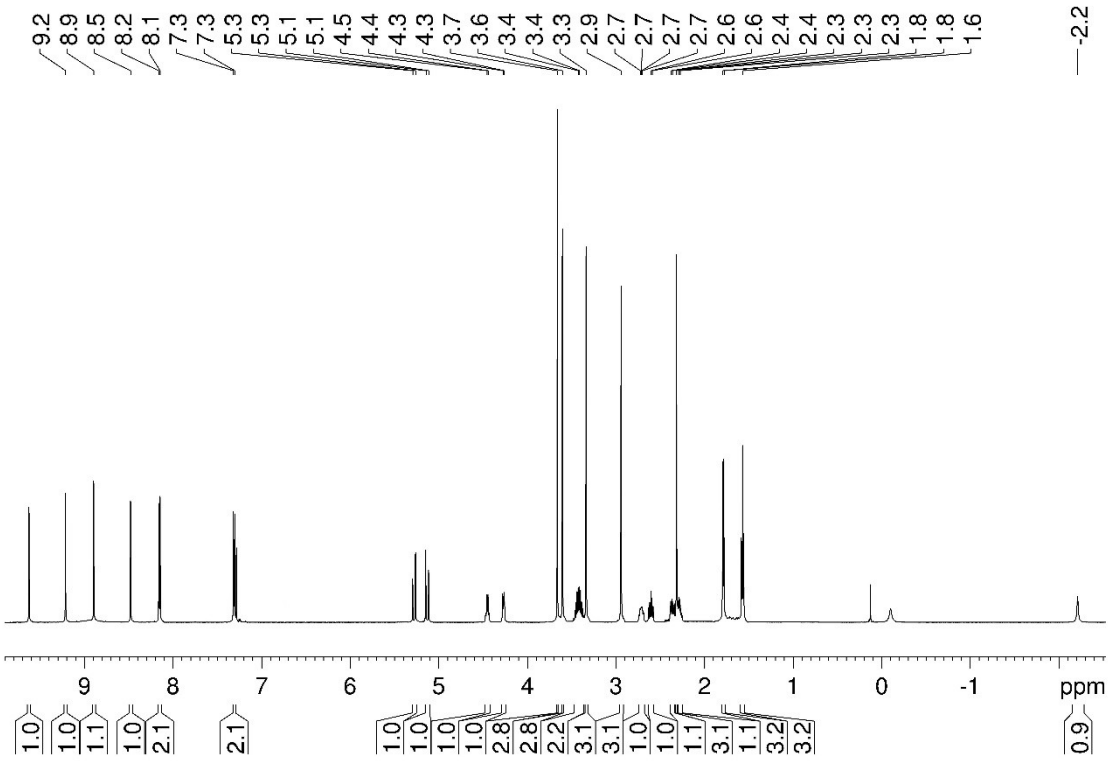

Figure S18. ^{1}H NMR spectrum of the N-tosylhydrazone of methyl pyropheophorbide-*d* (**3**) in $CDCl_3$.

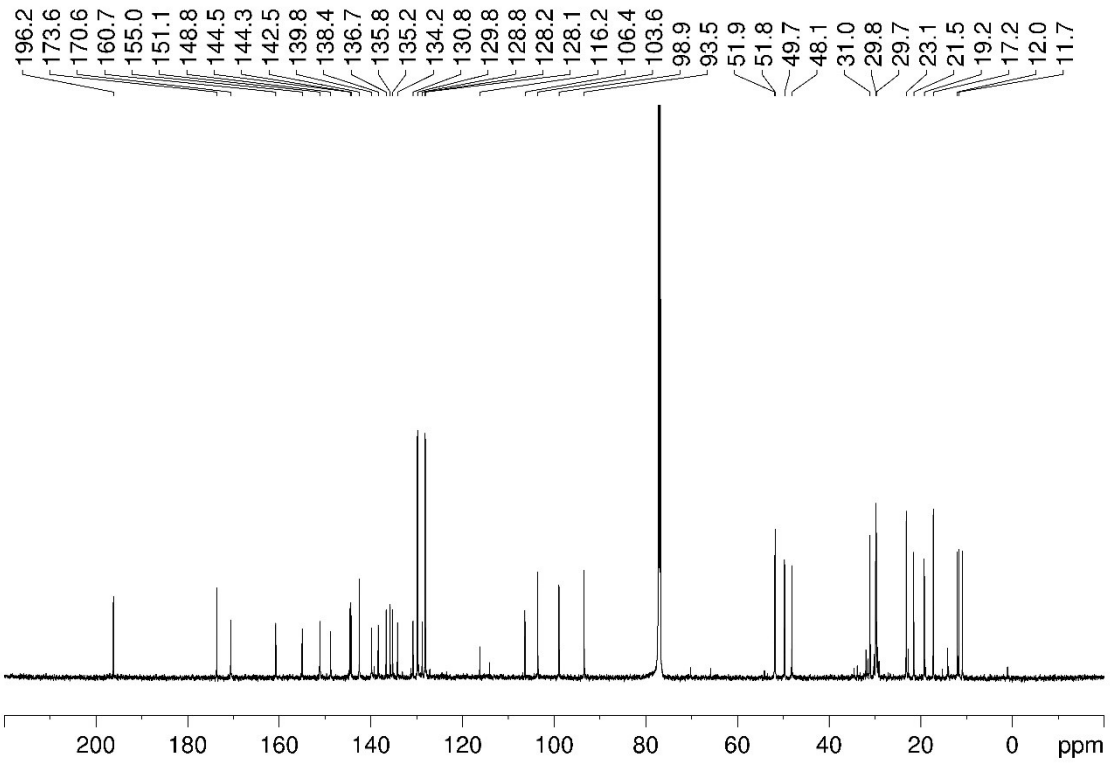

Figure S19. ^{13}C NMR spectrum of the N-tosylhydrazone of methyl pyropheophorbide-*d* (**3**) in $CDCl_3$.

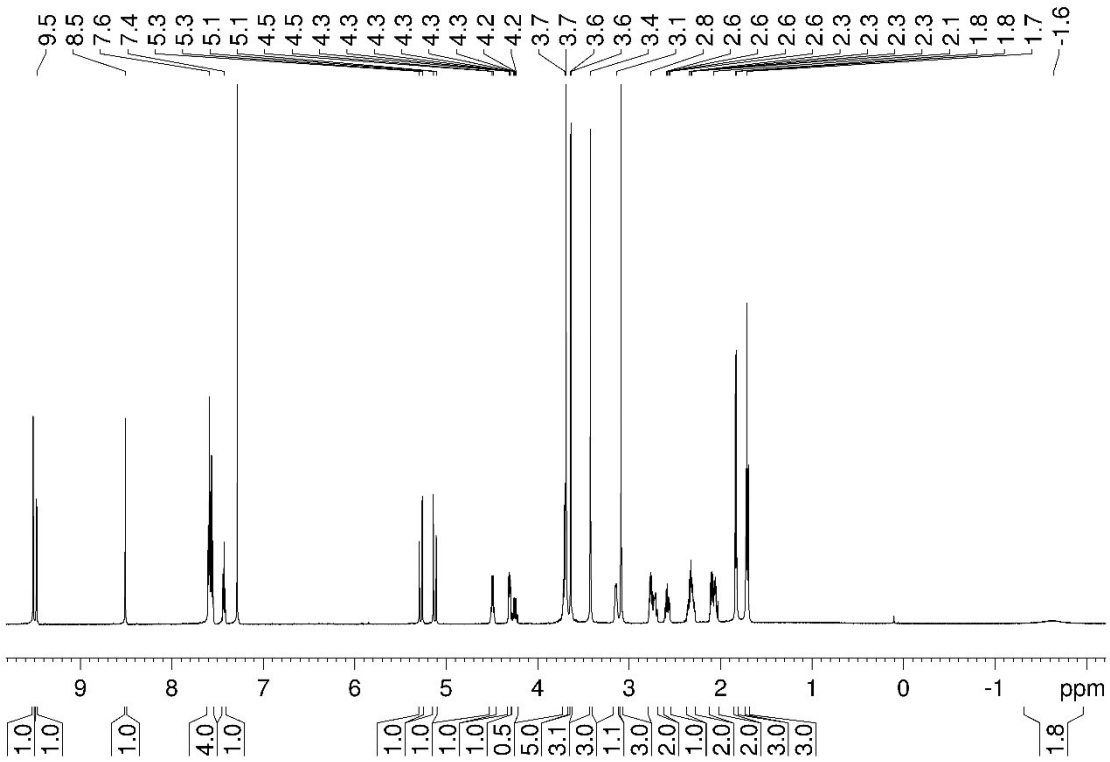

Figure S20. ^{1}H NMR spectrum of the cyclopropane conjugate with methyl pyropheophorbide-d (**9a**) in $CDCl_3$.

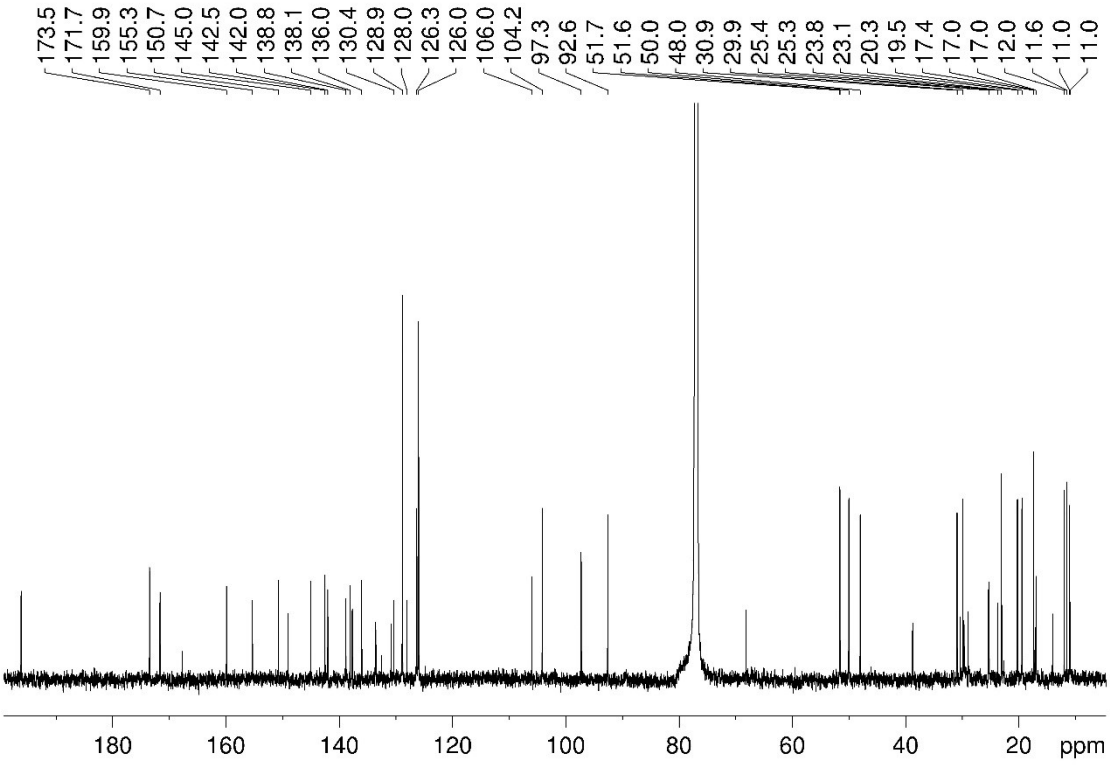

Figure S21. ^{13}C NMR spectrum of the cyclopropane conjugate with methyl pyropheophorbide-d (**9a**) in $CDCl_3$.

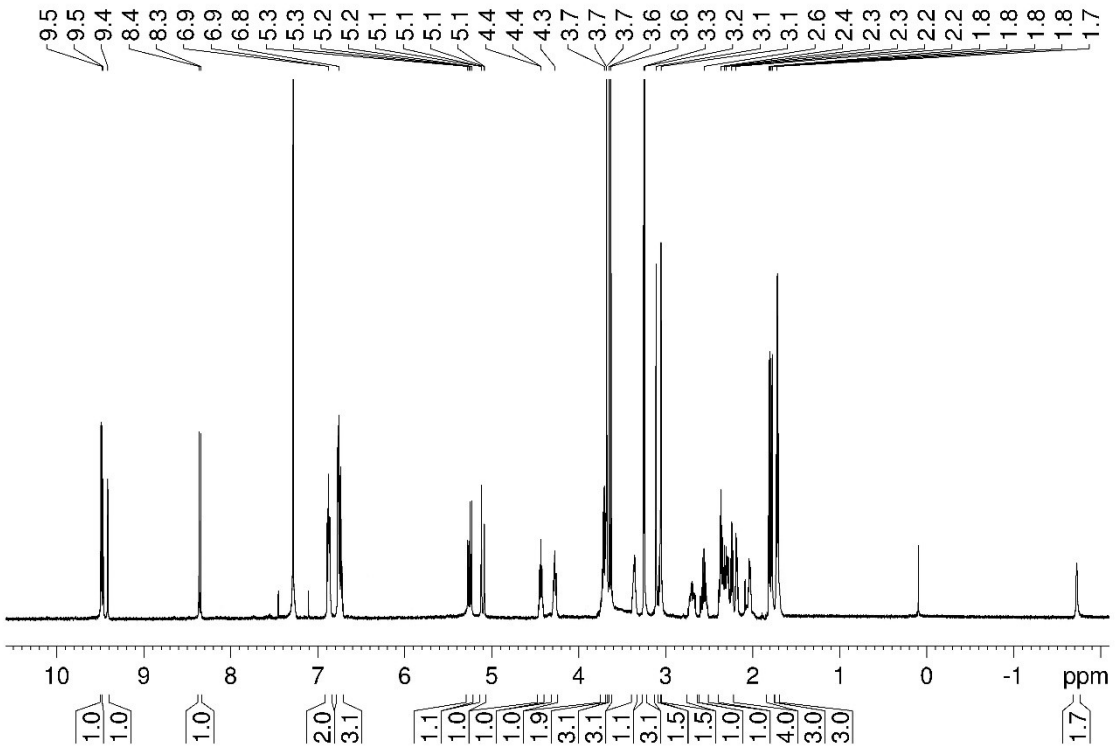

Figure S22. [1]H NMR spectrum of the cyclopropane conjugate with methyl pyropheophorbide-*d* (**9b**) in $CDCl_3$.

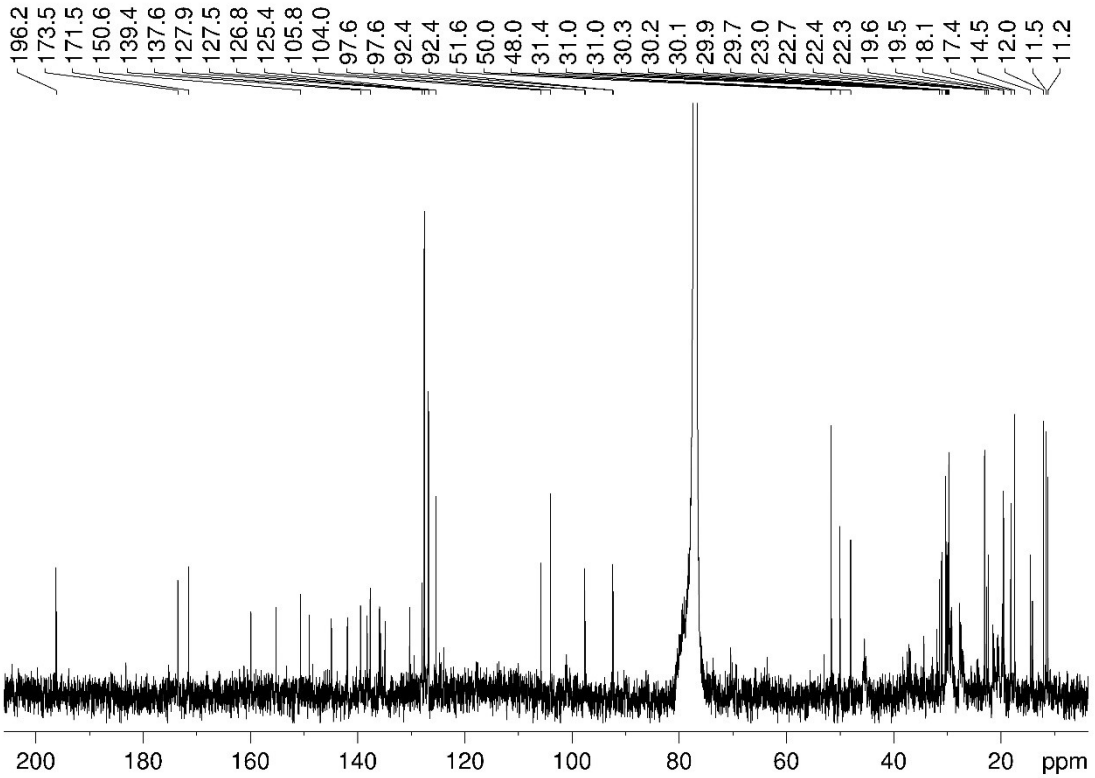

Figure S23. [13]C NMR spectrum of the cyclopropane conjugate with methyl pyropheophorbide-*d* (**9b**) in $CDCl_3$.

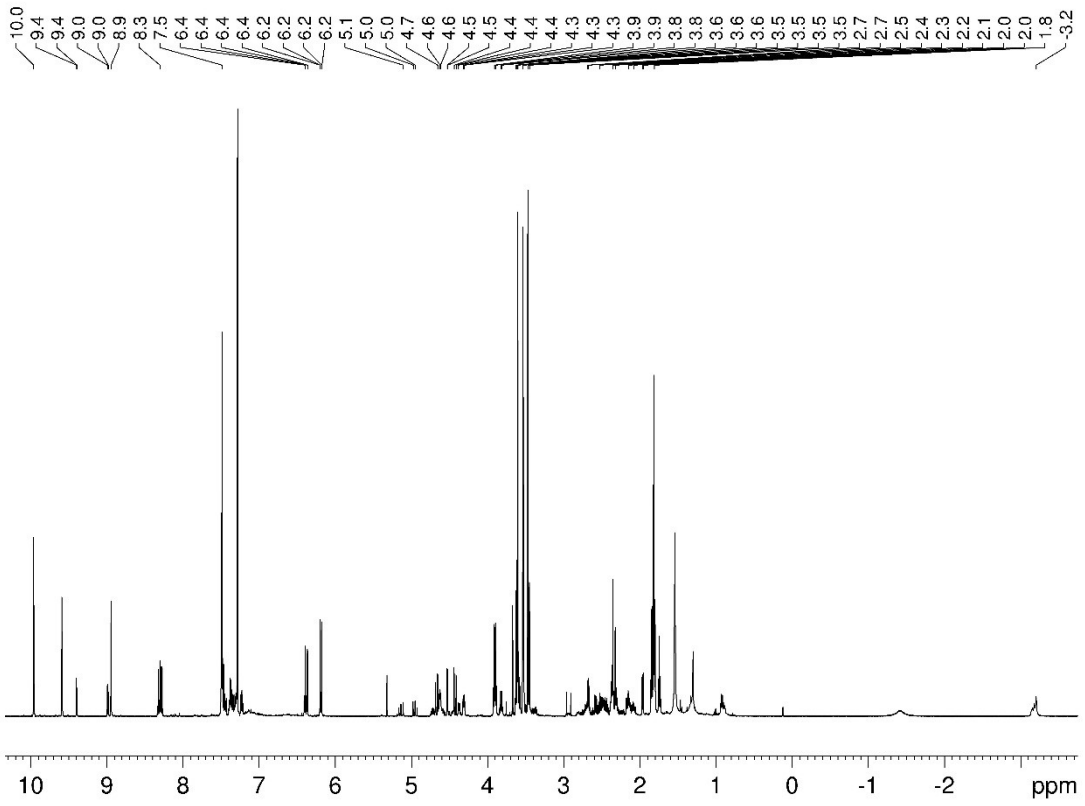

Figure S24. ^{1}H NMR spectrum of the cyclopropane conjugate with methyl pyropheophorbide-*a* (**10**) in $CDCl_3$.

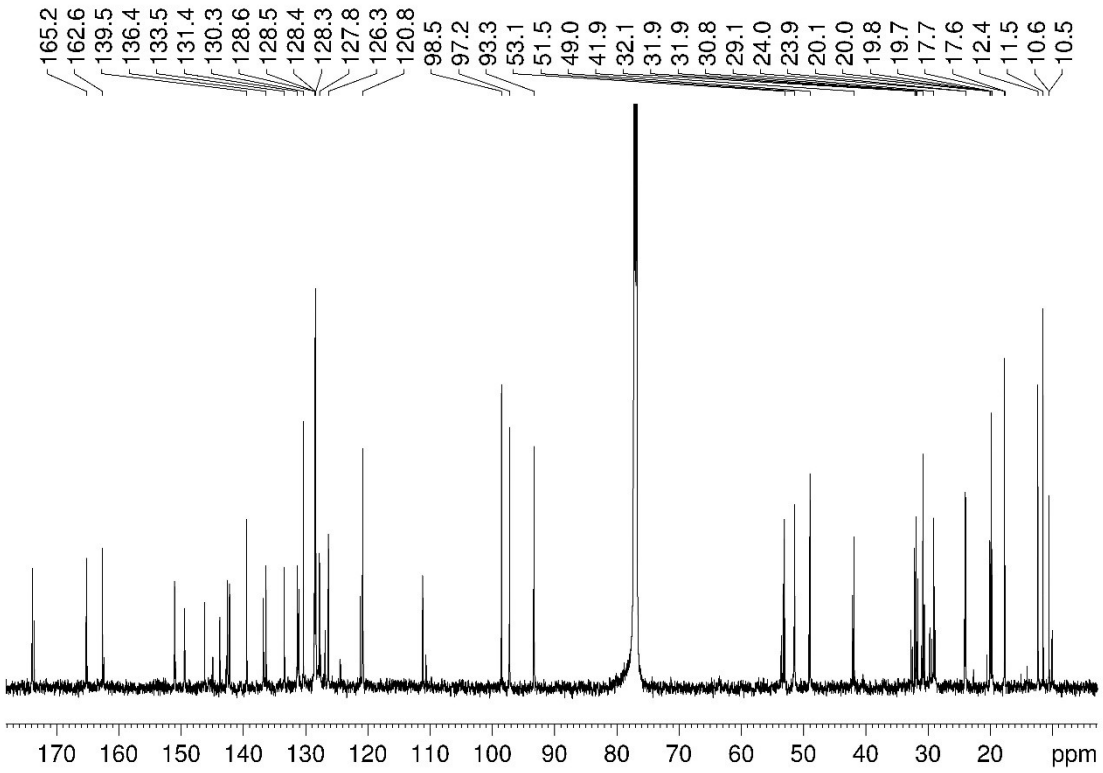

Figure S25. ^{13}C NMR spectrum of the cyclopropane conjugate with methyl pyropheophorbide-*a* (**10**) in $CDCl_3$.

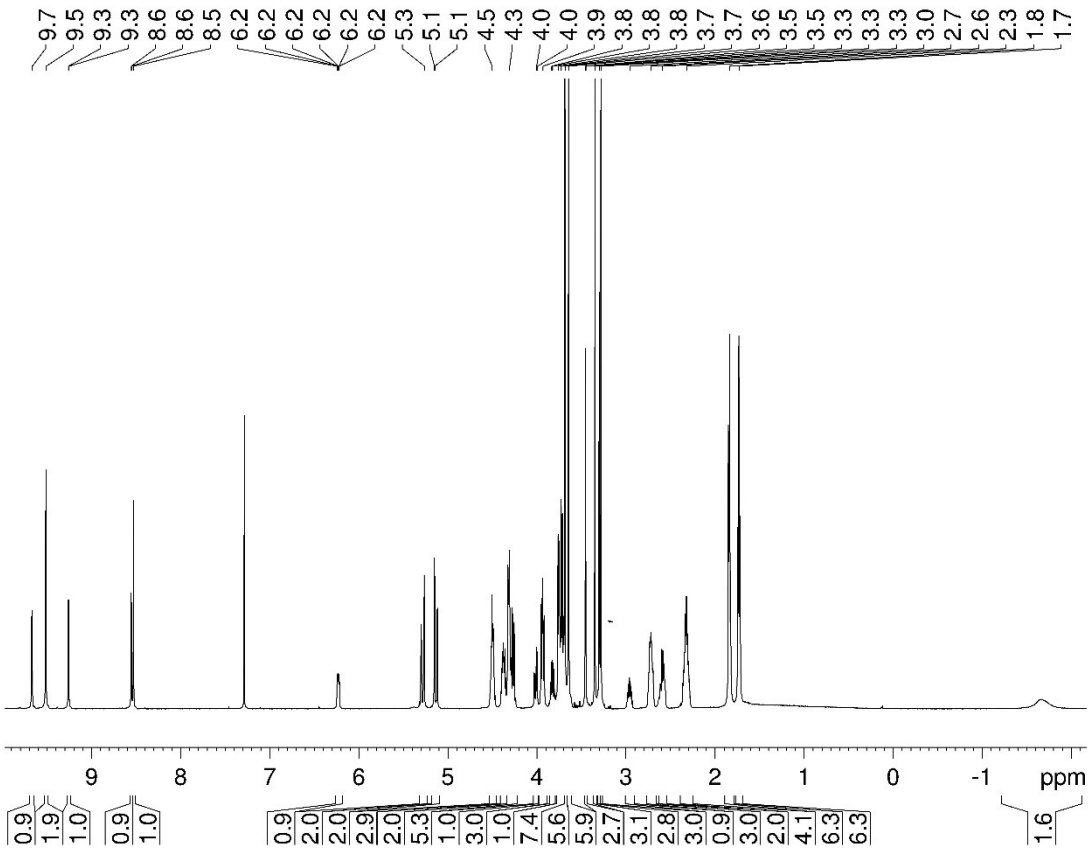

Figure S26. ^{1}H NMR spectrum of the dioxane conjugate with methyl pyropheophorbide-*d* (**11**) in $CDCl_3$.

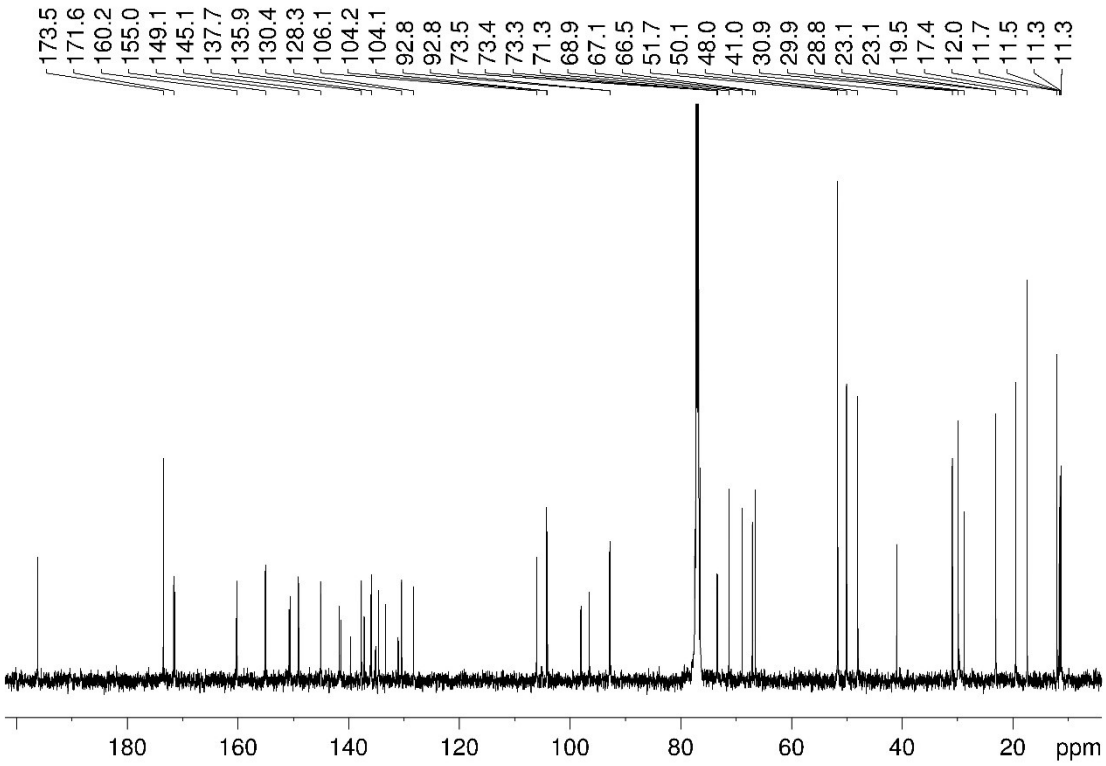

Figure S27. ^{13}C NMR spectrum of the dioxane conjugate with methyl pyropheophorbide-*d* (**11**) in $CDCl_3$.

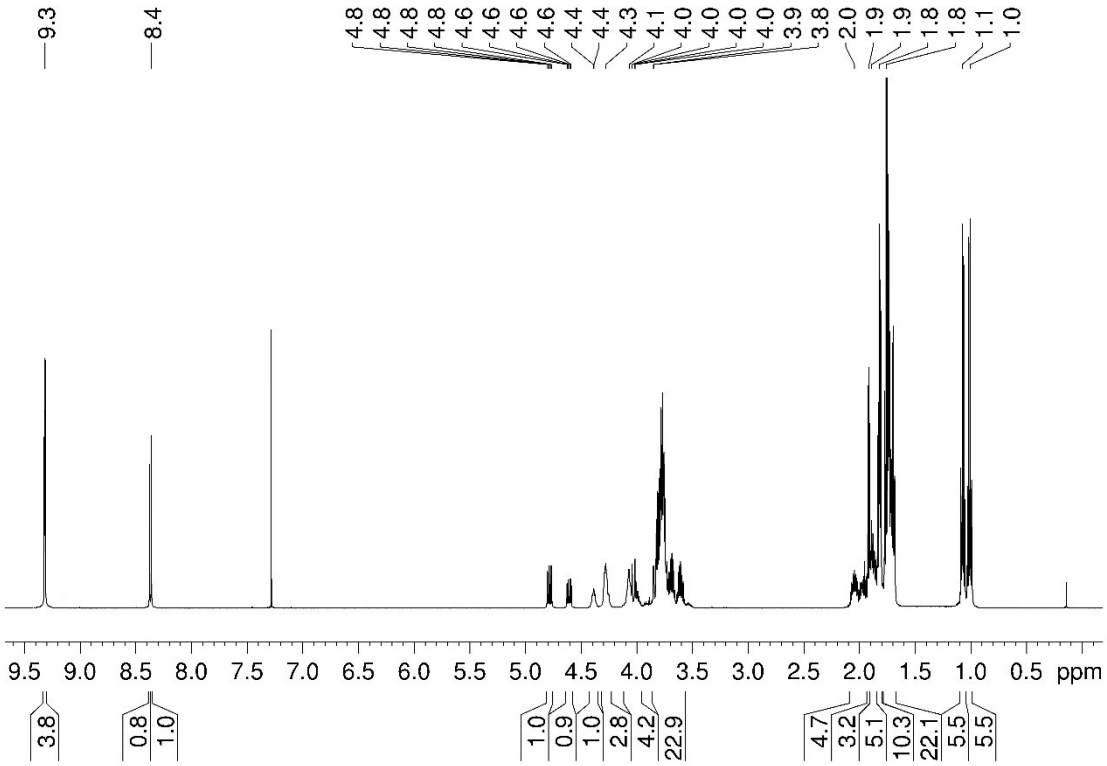

Figure S28. ^{1}H NMR spectrum of the Ni(II) 3,5-(1-methylethylene)-2,7,8,12,13,17,18-heptaethyl-17,18-*trans*-dihydroporphyrin (**13**) in $CDCl_3$.

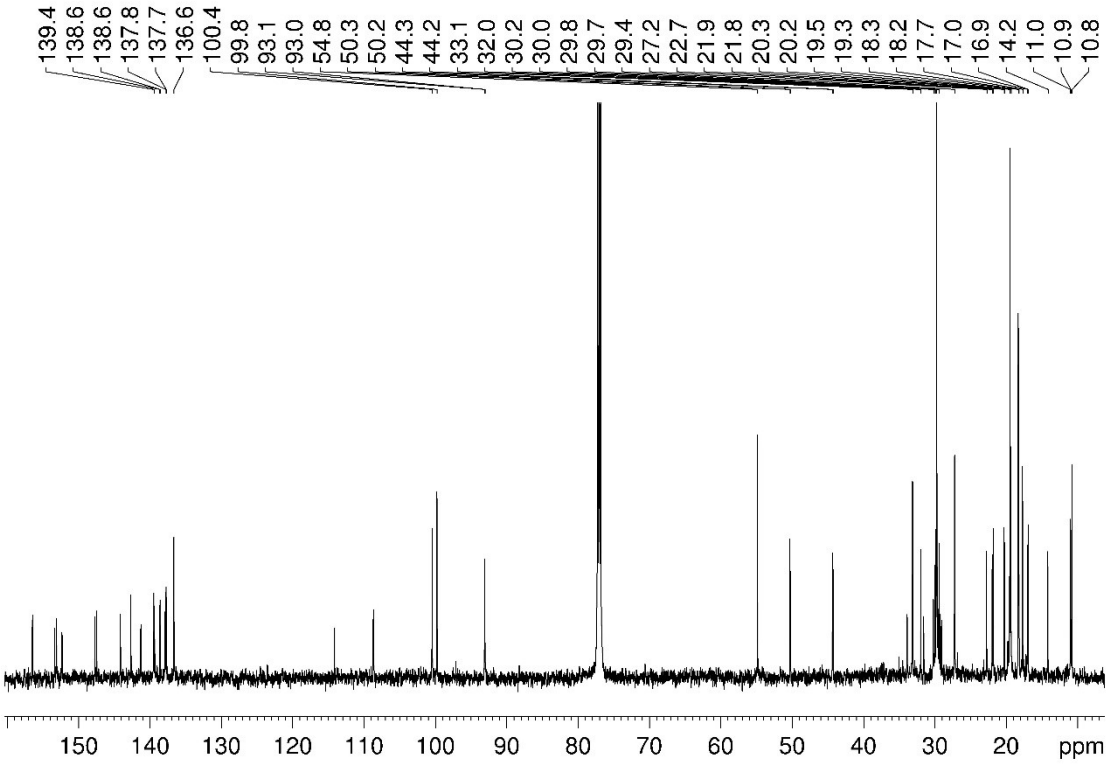

Figure S29. ^{13}C NMR spectrum of the Ni(II) 3,5-(1-methylethylene)-2,7,8,12,13,17,18-heptaethyl-17,18-*trans*-dihydroporphyrin (**13**) in $CDCl_3$.

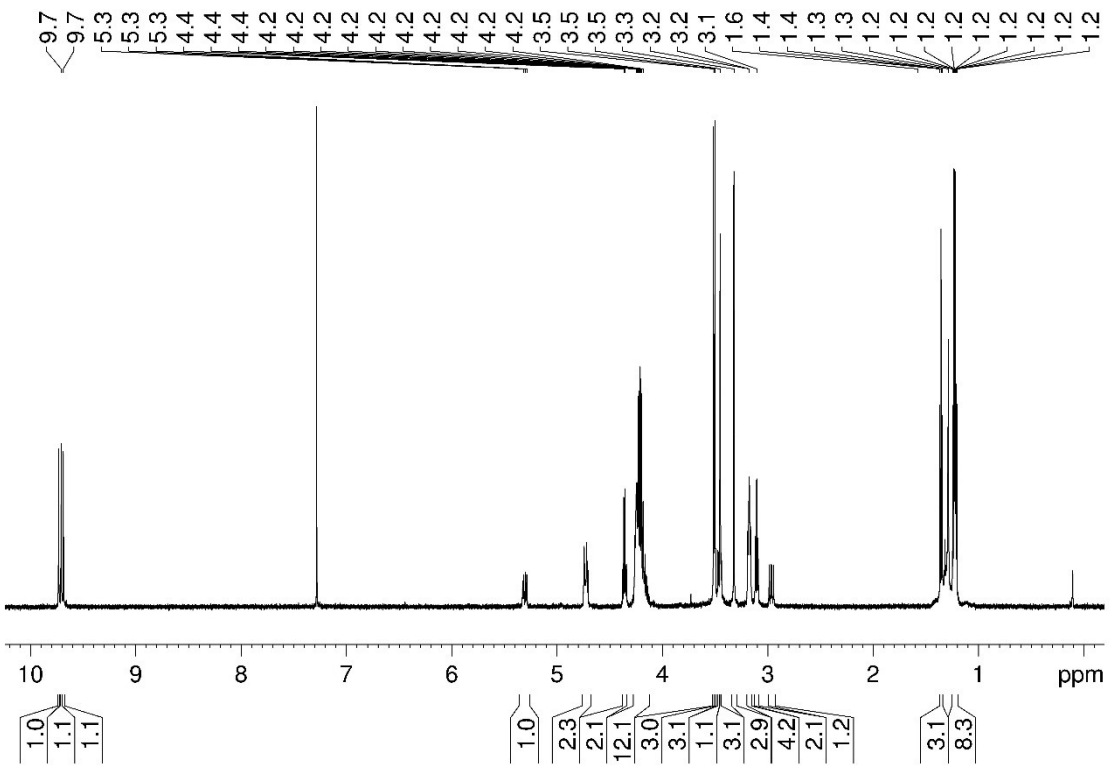

Figure S30. ^{1}H NMR spectrum of the Ni(II) 5,7-(2-((ethoxycarbonyl)methyl)ethylene)-3,8,13,18-tetramethyl-2,12,17-tri(2-(ethoxycarbonyl)ethyl)porphyrin (**14**) in $CDCl_3$.

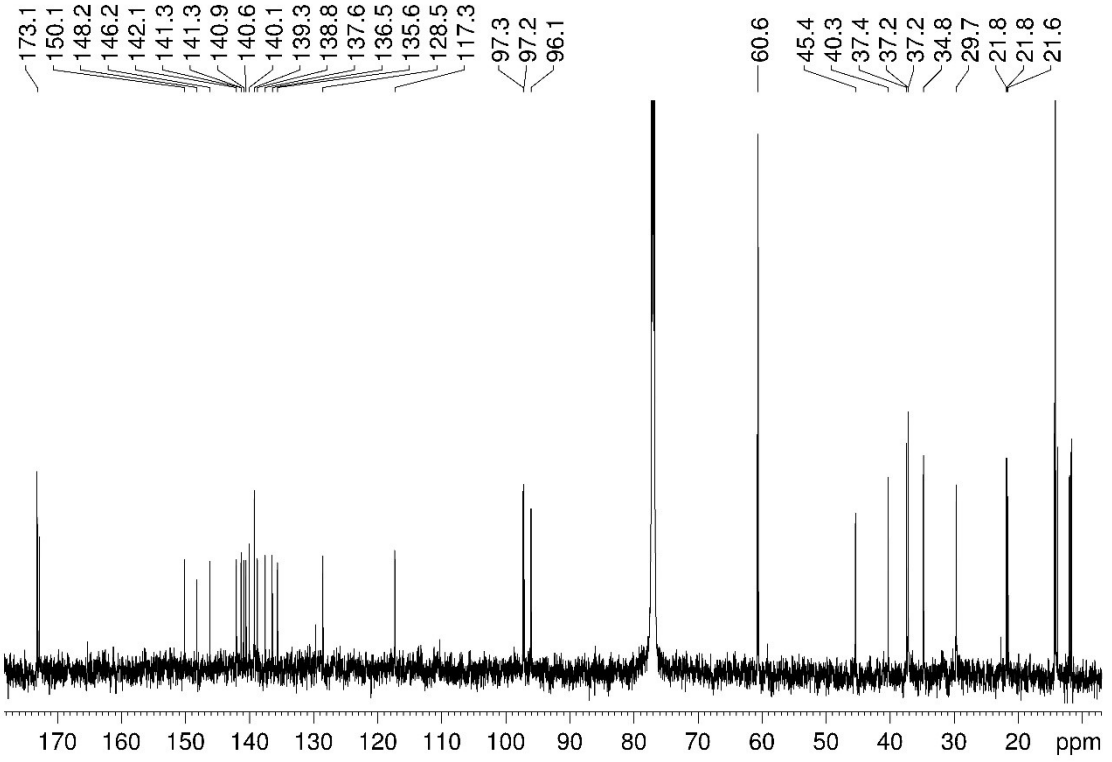

Figure S31. ^{13}C NMR spectrum of the Ni(II) 5,7-(2-((ethoxycarbonyl)methyl)ethylene)-3,8,13,18-tetramethyl-2,12,17-tri(2-(ethoxycarbonyl)ethyl)porphyrin (**14**) in $CDCl_3$.

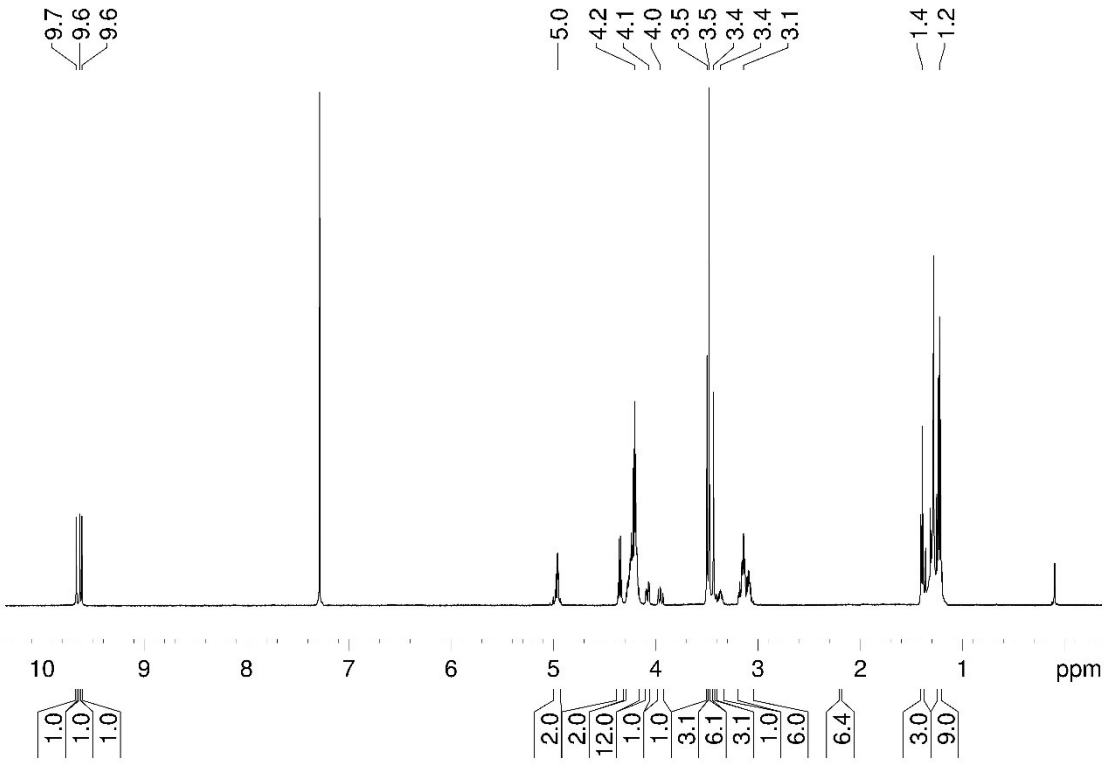

Figure S32. ^{1}H NMR spectrum of the Ni(II) 5,7-(2-(ethoxycarbonyl)-1,3-propylene)-3,8,13,18-tetramethyl-2,12,17-tri(2-(ethoxycarbonyl)ethyl)porphyrin (**15**) in $CDCl_3$.

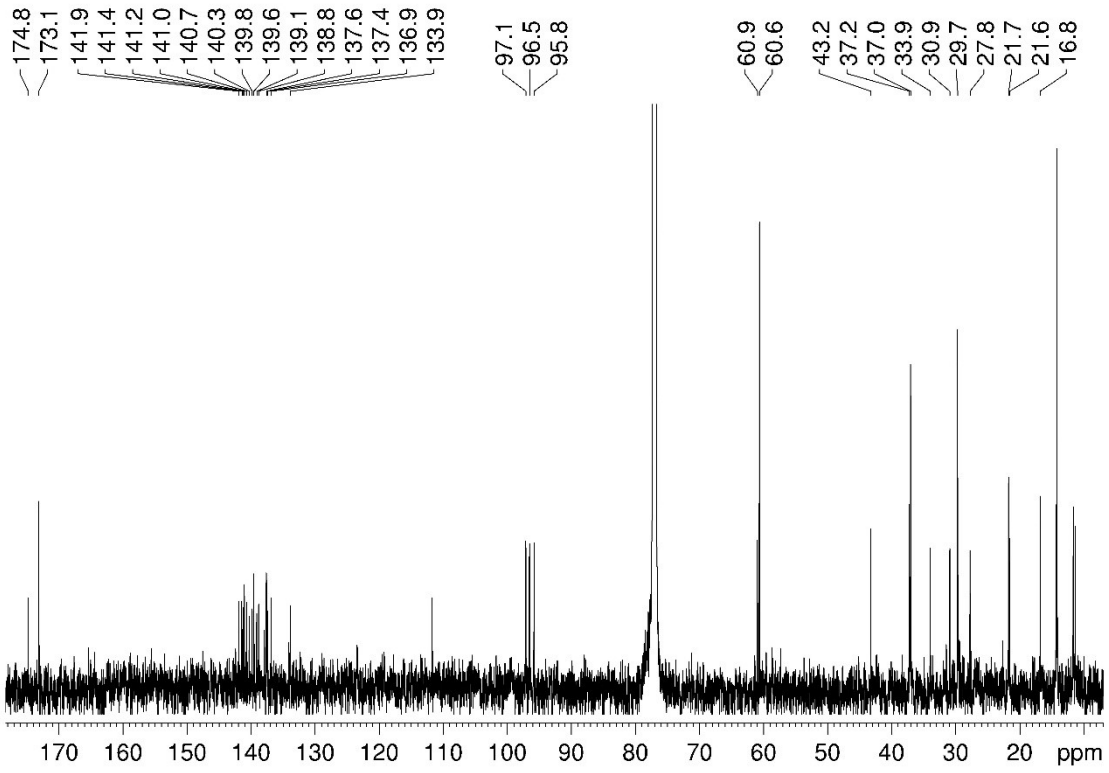

Figure S33. ^{13}C NMR spectrum of the Ni(II) 5,7-(2-(ethoxycarbonyl)-1,3-propylene)-3,8,13,18-tetramethyl-2,12,17-tri(2-(ethoxycarbonyl)ethyl)porphyrin (**15**) in $CDCl_3$.

UV-Vis absorption spectra.

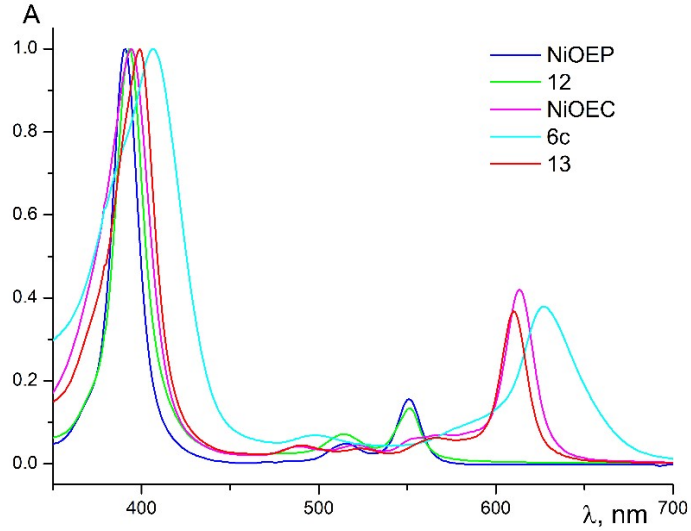

Figure S34. Normalized UV-Vis absorption spectra of nickel *β*-octaalkylporphyrin (NiOEP), nickel *β*-octaalkylchlorin (NiOEC), its tosylhydrazone **2c** and products with annulated cycles **12, 13** recorded in CH_2Cl_2 at concentration 10^{-5} M.

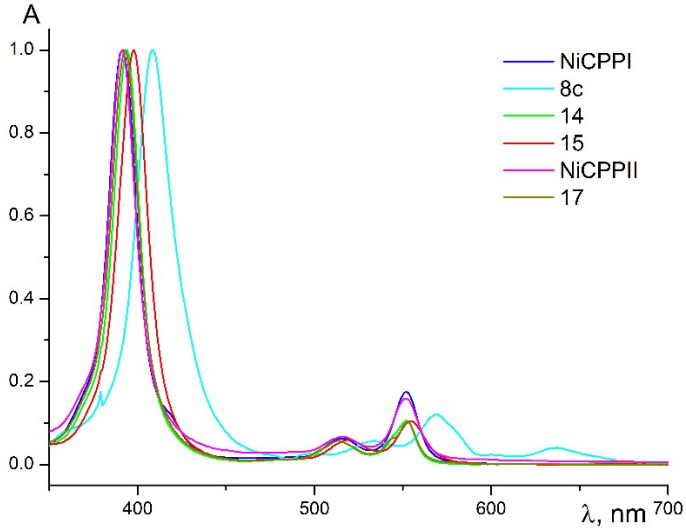

Figure S35. Normalized UV-Vis absorption spectra of the nickel coproporphyrin I (NiCPPI), nickel coproporphyrin II (NiCPPII), tosylhydrazone 4c and products with annulated cycles **14**, **15**, **17** recorded in CH_2Cl_2 at concentration 10^{-5} M.

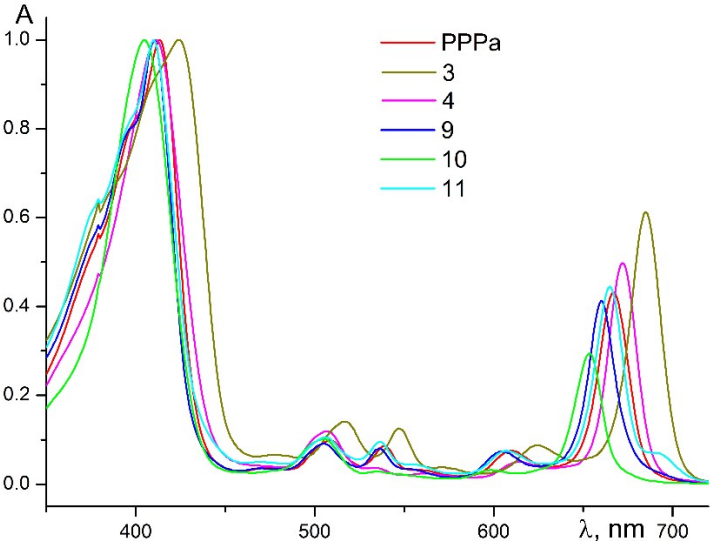

Figure S36. Normalized UV-Vis absorption spectra of the pyropheophorbide-*a* (PPPa), tosylhydrazones **6**, **8** and conjugates **9-11** recorded in CH_2Cl_2 at concentration 10^{-5} M.

DFT calculations of the reaction intermediates

Computed geometry and energy data of **5d**.
Electronic energy E = -1934.315154 a.u. Free Energy G = -1933.648384 a.u. Entropy S = 259.257 kcal/mol•K
Table S5. Atom coordinates of **5d**.

N	-1.45439	1.183635	0.069856
N	-1.124	-1.5846	0.015137
C	-1.48481	2.505001	-0.34175
C	-2.73568	0.871298	0.41078
C	-0.77566	-2.89892	-0.4476
C	-2.41389	-1.58377	0.264474
C	-0.33157	3.273971	-0.54623
C	-2.82022	2.996696	-0.32078
C	-3.07505	-0.45246	0.919069
C	-3.61791	1.962407	0.175047
C	0.571708	-3.30776	-0.55398
C	-1.90303	-3.67952	-0.58647
C	-3.02574	-2.86604	-0.16021
C	0.953467	2.851466	-0.29621
H	-0.4722	4.312537	-0.82744
C	-3.25641	4.392212	-0.68074
C	-3.88776	-0.67793	1.974806
C	-5.12257	1.985536	0.287091
C	1.661202	-2.54541	-0.21939
H	0.7434	-4.34894	-0.80023
C	-1.96313	-5.10934	-1.03898
C	-4.33578	-3.2225	-0.29482
C	2.12245	3.701295	-0.25214
N	1.301558	1.547901	0.044515
C	-3.23975	5.367736	0.513334
H	-4.27011	4.363941	-1.09935
H	-2.61778	4.791973	-1.47868
C	-5.83208	1.677773	-1.0467
H	-5.46813	1.271056	1.039672
H	-5.44765	2.972137	0.642027
C	3.018421	-3.07813	-0.08931
N	1.653944	-1.19278	0.078102
C	-2.04171	-6.12313	0.120652
H	-2.82863	-5.25447	-1.70045
H	-1.08514	-5.33448	-1.65521
C	-5.6109	-2.4801	-0.06352
H	-4.48964	-4.22611	-0.69232
C	2.138079	5.180854	-0.52588
C	3.169239	2.909584	0.154145
C	2.639517	1.568117	0.29796
H	-2.23224	5.45343	0.935713
H	-3.90344	5.020225	1.313081
H	-3.56883	6.368428	0.20802
H	-6.92227	1.717526	-0.93126
H	-5.56358	0.679213	-1.41038
H	-5.54632	2.396144	-1.82302

C	3.40771	-4.51546	-0.3015
C	3.808948	-2.04358	0.31152
C	2.954375	-0.85652	0.365949
H	-2.92825	-5.94838	0.740466
H	-2.09115	-7.14945	-0.2615
H	-1.16248	-6.04139	0.769093
H	-6.27294	-2.63113	-0.9263
H	-6.14615	-2.89519	0.803149
H	-5.47399	-1.4133	0.106551
C	1.772519	6.034529	0.704852
H	3.133842	5.47379	-0.87987
H	1.447738	5.417037	-1.3456
C	4.608611	3.304552	0.347906
C	3.418584	0.428104	0.553106
C	3.122342	-5.41463	0.918139
H	2.883015	-4.91837	-1.17754
H	4.47585	-4.56953	-0.54239
C	5.290052	-2.0536	0.573843
H	1.796705	7.102893	0.459637
H	0.768843	5.789486	1.069096
H	2.475083	5.856892	1.526664
C	5.483198	3.077611	-0.90119
H	5.03758	2.75055	1.193042
H	4.660123	4.363203	0.630255
H	4.471235	0.569594	0.76476
H	2.058159	-5.40245	1.177046
H	3.41347	-6.45162	0.713799
H	3.680706	-5.07002	1.795604
C	6.133329	-1.68406	-0.66303
H	5.589725	-3.0481	0.925398
H	5.526141	-1.36179	1.392176
H	5.473991	2.024354	-1.2027
H	6.522852	3.369395	-0.71023
H	5.113744	3.666232	-1.74845
H	7.202538	-1.69156	-0.42119
H	5.873504	-0.68687	-1.03396
H	5.962681	-2.39549	-1.47864
H	-4.31192	0.140731	2.545522
Ni	0.112922	-5.5E-05	0.080625
H	-4.11041	-1.68511	2.311567

Computed geometry and energy data of **5e**.
Electronic energy E = -1824.762293 a.u. Free Energy G = -1824.107852 a.u. Entropy S = 253.178 kcal/mol•K
Table S6. Atom coordinates of **5e**.

N	-1.3124	-1.38939	-0.1375
N	-1.30686	1.393535	-0.06538
C	-1.16072	-2.70434	0.281655
C	-2.64328	-1.21203	-0.31977
C	-1.13824	2.72392	0.306166
C	-2.60194	1.283586	-0.43473

C	0.065758	-3.33677	0.405516
C	-2.44718	-3.32849	0.427586
C	-3.18126	0.02607	-0.88383
C	-3.38857	-2.39082	0.039496
C	0.092383	3.313172	0.532836
C	-2.39177	3.426839	0.216496
C	-3.30917	2.523464	-0.28564
C	1.295051	-2.7466	0.127298
H	0.063068	-4.38976	0.665238
C	-2.68863	-4.74849	0.863314
C	-4.09014	-0.06066	-1.86914
C	-4.8847	-2.54689	0.156209
C	1.326753	2.702504	0.3257
H	0.098277	4.365636	0.795501
C	-2.61088	4.882854	0.525315
C	-4.76873	2.748819	-0.57186
C	2.548824	-3.4608	0.007814
N	1.475685	-1.40401	-0.09923
C	-2.6808	-5.75381	-0.30625
H	-3.65352	-4.81274	1.379968
H	-1.93441	-5.04836	1.60149
C	-5.40362	-2.22716	1.57244
H	-5.40386	-1.90079	-0.55506
H	-5.16567	-3.57448	-0.10628
C	2.595403	3.392871	0.320939
N	1.492017	1.376073	-0.0012
C	-2.36247	5.810898	-0.68092
H	-3.63974	5.025751	0.87749
H	-1.96497	5.191168	1.356979
C	-5.69407	2.336286	0.588753
H	-5.05253	2.18898	-1.47297
H	-4.9341	3.807992	-0.80457
C	2.726551	-4.94725	0.159089
C	3.497972	-2.52522	-0.3239
C	2.818013	-1.24492	-0.34778
H	-1.71835	-5.74247	-0.82983
H	-3.45801	-5.50868	-1.03854
H	-2.86119	-6.77305	0.054945
H	-6.49	-2.36477	1.62931
H	-5.17703	-1.18999	1.844314
H	-4.93805	-2.87507	2.323393
C	2.802027	4.856965	0.602173
C	3.539999	2.465288	-0.05407
C	2.836477	1.212444	-0.22032
H	-3.0284	5.558179	-1.51322
H	-2.53812	6.858209	-0.40864
H	-1.3324	5.720083	-1.04305
H	-5.46041	2.901842	1.498005
H	-6.74491	2.518597	0.334242
H	-5.58079	1.271492	0.820083

C	2.369055	-5.74004	-1.11381
H	3.766325	-5.16119	0.433164
H	2.116727	-5.31417	0.99496
C	4.971164	-2.73823	-0.54406
C	3.451125	-0.01467	-0.46814
C	2.601382	5.753229	-0.63611
H	2.123428	5.185753	1.399452
H	3.815115	5.010413	0.992704
C	5.024916	2.663977	-0.19593
H	2.512753	-6.81526	-0.9559
H	1.325445	-5.5735	-1.40257
H	2.998418	-5.43141	-1.95588
C	5.81526	-2.56282	0.734229
H	5.337034	-2.04925	-1.31584
H	5.134908	-3.74633	-0.94335
H	4.518646	-0.01312	-0.65564
H	1.587637	5.649733	-1.03866
H	2.762927	6.807787	-0.38402
H	3.302143	5.481576	-1.4333
C	5.815273	2.330612	1.08513
H	5.225144	3.704899	-0.47694
H	5.407058	2.053916	-1.02446
H	5.698581	-1.55587	1.149884
H	6.878881	-2.7242	0.523589
H	5.508111	-3.27658	1.506638
H	6.889466	2.487778	0.932647
H	5.66183	1.287669	1.383772
H	5.492811	2.963556	1.919344
H	-4.66781	-0.90231	-2.23565
Ni	0.092757	-0.00407	-0.10111

Computed geometry and energy data of **5f**.
Electronic energy E = -1824.767137 a.u. Free Energy G = -1824.112562 a.u. Entropy S = 254.066 kcal/mol•K
Table S7. Atom coordinates of **5f**.

N	0	0	0
N	0	0	2.766031
C	0.425479	0	-1.31862
C	-0.81496	-1.08316	0.125409
C	0.38728	0.006415	4.097659
C	-0.84032	-1.05941	2.632671
C	1.095923	1.049567	-1.92998
C	-0.08358	-1.15271	-2.00756
C	-1.47358	-1.42543	1.378039
C	-0.8926	-1.82437	-1.11043
C	1.078194	1.039645	4.710682
C	-0.18438	-1.1176	4.789024
C	-0.98806	-1.77133	3.87772
C	1.385985	2.267842	-1.33356
H	1.325724	0.944213	-2.98436
C	0.181791	-1.49236	-3.44984

C	-2.65555	-2.08366	1.398395
C	-1.60437	-3.1245	-1.39422
C	1.39918	2.250405	4.111969
H	1.295635	0.932956	5.767675
C	0.007121	-1.4447	6.245519
C	-1.77608	-3.02939	4.133968
C	1.849876	3.444146	-2.03795
N	1.210607	2.536394	0.003865
C	-0.85183	-0.89107	-4.42294
H	0.195872	-2.5819	-3.57335
H	1.184964	-1.15139	-3.73331
C	-0.97935	-4.34753	-0.69753
H	-2.66738	-3.06167	-1.13608
H	-1.58575	-3.29414	-2.4767
C	1.885781	3.416553	4.81756
N	1.218318	2.52686	2.776952
C	-1.01084	-0.74725	7.170317
H	-0.06956	-2.52939	6.386765
H	1.023294	-1.17519	6.559335
C	-0.98613	-4.31621	3.829258
H	-2.69718	-3.02459	3.539305
H	-2.09388	-3.04432	5.183906
C	2.118878	3.53128	-3.5159
C	1.924975	4.448777	-1.10498
C	1.55798	3.854579	0.165115
H	-0.87161	0.202092	-4.35011
H	-1.86038	-1.2551	-4.19783
H	-0.61496	-1.16044	-5.45891
H	-1.515	-5.26455	-0.97008
H	-1.01389	-4.24619	0.391492
H	0.069775	-4.46528	-0.99074
C	2.170813	3.493927	6.293172
C	1.96415	4.425331	3.889175
C	1.576345	3.843338	2.619898
H	-2.03601	-1.03544	6.912962
H	-0.83334	-1.01665	8.218084
H	-0.94245	0.342658	7.081631
H	-0.07813	-4.37444	4.440258
H	-1.59355	-5.20546	4.035517
H	-0.68054	-4.34952	2.778004
C	0.851932	3.790087	-4.35542
H	2.842247	4.333183	-3.70529
H	2.599824	2.608185	-3.86428
C	2.371402	5.871201	-1.30981
C	1.662633	4.495033	1.394958
C	0.921077	3.795374	7.144101
H	2.623796	2.55537	6.637238
H	2.922329	4.271221	6.475871
C	2.431832	5.840387	4.097073
H	1.096609	3.846318	-5.42253

H	0.115399	2.991153	-4.21543
H	0.375984	4.732969	-4.06403
C	3.878676	6.084226	-1.06537
H	1.80111	6.540344	-0.65301
H	2.129518	6.182108	-2.33326
H	1.942496	5.541995	1.397762
H	0.155679	3.023139	7.009406
H	1.176781	3.841063	8.209133
H	0.475835	4.754868	6.858498
C	3.937525	6.035352	3.828806
H	2.21109	6.146805	5.126601
H	1.859544	6.521775	3.454706
H	4.15613	5.808439	-0.04201
H	4.154526	7.133464	-1.22298
H	4.476097	5.468311	-1.7467
H	4.23015	7.079561	3.989521
H	4.19367	5.763569	2.798828
H	4.537935	5.406141	4.495221
H	-3.3829	-2.43636	0.683729
Ni	0.591868	1.277881	1.387237

Computed geometry and energy data of **5g**.
Electronic energy E = -1824.801792 a.u. Free Energy G = -1824.147322 a.u. Entropy S = 253.158 kcal/mol•K
Table S8. Atom coordinates of **5g**.

N	-1.49293	1.129879	0.061553
N	-1.05936	-1.60237	-0.007
C	-1.55128	2.458966	-0.33918
C	-2.76342	0.779153	0.371884
C	-0.67516	-2.87555	-0.41781
C	-2.38854	-1.66603	0.247289
C	-0.43813	3.26262	-0.51139
C	-2.91648	2.909195	-0.3514
C	-3.08892	-0.55222	0.869324
C	-3.68398	1.856176	0.114957
C	0.646832	-3.28036	-0.54295
C	-1.8093	-3.7346	-0.5045
C	-2.93438	-2.97309	-0.08977
C	0.873618	2.87211	-0.25027
H	-0.6065	4.301195	-0.77461
C	-3.38112	4.290769	-0.7249
C	-3.94535	-0.74723	1.906716
C	-5.19095	1.824659	0.179752
C	1.758089	-2.4991	-0.24626
H	0.825156	-4.31794	-0.80277
C	-1.80359	-5.17392	-0.92768
C	-4.26242	-3.44092	-0.13434
C	2.003073	3.771507	-0.17197
N	1.254673	1.584638	0.04159
C	-3.39768	5.271321	0.465536
H	-4.38983	4.233825	-1.1507

H	-2.74404	4.699079	-1.51934
C	-5.84059	1.499292	-1.18039
H	-5.5342	1.090806	0.912765
H	-5.56069	2.797475	0.528095
C	3.111985	-2.99348	-0.13826
N	1.706417	-1.15454	0.03805
C	-1.78126	-6.16148	0.257768
H	-2.69116	-5.37413	-1.54205
H	-0.94243	-5.37144	-1.57692
C	-5.53857	-2.66411	-0.03282
H	-4.37637	-4.49886	-0.358
C	1.957487	5.258563	-0.39894
C	3.081235	3.00814	0.208903
C	2.602978	1.644968	0.303338
H	-2.39756	5.38213	0.899081
H	-4.06371	4.913739	1.258532
H	-3.74478	6.261921	0.149129
H	-6.93406	1.492696	-1.0985
H	-5.52012	0.515441	-1.54086
H	-5.56074	2.235665	-1.9419
C	3.543707	-4.42005	-0.34551
C	3.886071	-1.92374	0.24642
C	2.998531	-0.78298	0.31595
H	-2.65001	-6.01334	0.908169
H	-1.79357	-7.19791	-0.09928
H	-0.88192	-6.02025	0.867628
H	-6.31808	-3.15199	-0.63011
H	-5.92677	-2.60034	0.996687
H	-5.43011	-1.63494	-0.38759
C	1.523093	6.055933	0.846982
H	2.947251	5.606592	-0.71763
H	1.278961	5.49046	-1.22995
C	4.503971	3.453556	0.413359
C	3.411394	0.533259	0.511348
C	3.347165	-5.30709	0.900106
H	2.996364	-4.85866	-1.18985
H	4.601228	-4.43997	-0.6344
C	5.372698	-1.89309	0.478106
H	1.504251	7.131253	0.634507
H	0.523048	5.755847	1.179156
H	2.213129	5.884651	1.680636
C	5.374612	3.328624	-0.85295
H	4.963843	2.876365	1.225694
H	4.511667	4.497476	0.749178
H	4.459917	0.705318	0.725776
H	2.294282	-5.33659	1.201636
H	3.675083	-6.33437	0.702587
H	3.923315	-4.92199	1.748759
C	6.182749	-1.50945	-0.77633
H	5.70466	-2.87775	0.828674

H	5.610562	-1.19308	1.289229
H	5.413187	2.291758	-1.20485
H	6.400475	3.660779	-0.65518
H	4.969355	3.93878	-1.66778
H	7.25714	-1.49804	-0.55854
H	5.898043	-0.51663	-1.14194
H	6.006663	-2.22323	-1.58874
H	-4.41632	0.083274	2.419826
Ni	0.109248	-0.01099	0.059946
H	-4.14404	-1.74261	2.287145

Computed geometry and energy data of **5h**.
Electronic energy E = -1824.811496 a.u. Free Energy G = - 1824.153198 a.u. Entropy S = 249.489 kcal/mol•K
Table S9. Atom coordinates of **5h**.

N	-1.49293	1.129879	0.061553
N	-1.05936	-1.60237	-0.007
C	-1.55128	2.458966	-0.33918
C	-2.76342	0.779153	0.371884
C	-0.67516	-2.87555	-0.41781
C	-2.38854	-1.66603	0.247289
C	-0.43813	3.26262	-0.51139
C	-2.91648	2.909195	-0.3514
C	-3.08892	-0.55222	0.869324
C	-3.68398	1.856176	0.114957
C	0.646832	-3.28036	-0.54295
C	-1.8093	-3.7346	-0.5045
C	-2.93438	-2.97309	-0.08977
C	0.873618	2.87211	-0.25027
H	-0.6065	4.301195	-0.77461
C	-3.38112	4.290769	-0.7249
C	-3.94535	-0.74723	1.906716
C	-5.19095	1.824659	0.179752
C	1.758089	-2.4991	-0.24626
H	0.825156	-4.31794	-0.80277
C	-1.80359	-5.17392	-0.92768
C	-4.26242	-3.44092	-0.13434
C	2.003073	3.771507	-0.17197
N	1.254673	1.584638	0.04159
C	-3.39768	5.271321	0.465536
H	-4.38983	4.233825	-1.1507
H	-2.74404	4.699079	-1.51934
C	-5.84059	1.499292	-1.18039
H	-5.5342	1.090806	0.912765
H	-5.56069	2.797475	0.528095
C	3.111985	-2.99348	-0.13826
N	1.706417	-1.15454	0.03805
C	-1.78126	-6.16148	0.257768
H	-2.69116	-5.37413	-1.54205
H	-0.94243	-5.37144	-1.57692
C	-5.53857	-2.66411	-0.03282

H	-4.37637	-4.49886	-0.358
C	1.957487	5.258563	-0.39894
C	3.081235	3.00814	0.208903
C	2.602978	1.644968	0.303338
H	-2.39756	5.38213	0.899081
H	-4.06371	4.913739	1.258532
H	-3.74478	6.261921	0.149129
H	-6.93406	1.492696	-1.0985
H	-5.52012	0.515441	-1.54086
H	-5.56074	2.235665	-1.9419
C	3.543707	-4.42005	-0.34551
C	3.886071	-1.92374	0.24642
C	2.998531	-0.78298	0.31595
H	-2.65001	-6.01334	0.908169
H	-1.79357	-7.19791	-0.09928
H	-0.88192	-6.02025	0.867628
H	-6.31808	-3.15199	-0.63011
H	-5.92677	-2.60034	0.996687
H	-5.43011	-1.63494	-0.38759
C	1.523093	6.055933	0.846982
H	2.947251	5.606592	-0.71763
H	1.278961	5.49046	-1.22995
C	4.503971	3.453556	0.413359
C	3.411394	0.533259	0.511348
C	3.347165	-5.30709	0.900106
H	2.996364	-4.85866	-1.18985
H	4.601228	-4.43997	-0.6344
C	5.372698	-1.89309	0.478106
H	1.504251	7.131253	0.634507
H	0.523048	5.755847	1.179156
H	2.213129	5.884651	1.680636
C	5.374612	3.328624	-0.85295
H	4.963843	2.876365	1.225694
H	4.511667	4.497476	0.749178
H	4.459917	0.705318	0.725776
H	2.294282	-5.33659	1.201636
H	3.675083	-6.33437	0.702587
H	3.923315	-4.92199	1.748759
C	6.182749	-1.50945	-0.77633
H	5.70466	-2.87775	0.828674
H	5.610562	-1.19308	1.289229
H	5.413187	2.291758	-1.20485
H	6.400475	3.660779	-0.65518
H	4.969355	3.93878	-1.66778
H	7.25714	-1.49804	-0.55854
H	5.898043	-0.51663	-1.14194
H	6.006663	-2.22323	-1.58874
H	-4.41632	0.083274	2.419826
Ni	0.109248	-0.01099	0.059946
H	-4.14404	-1.74261	2.287145

Computed geometry and energy data of **12**.
Electronic energy E = -1824.890182 a.u. Free Energy G = -1824.227729 a.u. Entropy S = 246.812 kcal/mol•K
Table S10. Atom coordinates of **12**.

N	-1.63589	1.032525	-0.00544
N	-0.86649	-1.667	-0.00919
C	-1.74317	2.400233	0.00404
C	-2.94598	0.56434	-0.02205
C	-0.45222	-2.9866	-0.00695
C	-2.21561	-1.74319	-0.01525
C	-0.67948	3.294997	0.016879
C	-3.12933	2.816284	-0.00981
C	-3.22827	-0.79971	-0.01865
C	-3.88295	1.669845	-0.02736
C	0.885314	-3.35069	-0.01121
C	-1.59312	-3.90002	-0.01141
C	-2.69617	-3.08455	-0.0184
C	0.662462	2.961645	0.020683
H	-0.92539	4.350322	0.018629
C	-3.61746	4.239536	0.030953
C	-4.55659	-1.55204	0.004634
C	-5.38625	1.596676	-0.09593
C	1.936101	-2.44434	-0.01023
H	1.127396	-4.40721	-0.01908
C	-1.50734	-5.40117	0.037014
C	-4.20331	-3.0902	-0.04577
C	1.742503	3.932096	0.027827
N	1.157806	1.677679	0.007093
C	-3.65785	4.832516	1.453532
H	-4.62166	4.292171	-0.40534
H	-2.9851	4.871826	-0.60518
C	-5.9271	1.532502	-1.5382
H	-5.75758	0.737038	0.469807
H	-5.8077	2.4807	0.397399
C	3.335864	-2.8284	-0.01689
N	1.80748	-1.07065	-0.00837
C	-1.29199	-5.95553	1.459223
H	-2.42991	-5.82627	-0.3759
H	-0.69529	-5.75303	-0.61296
C	-4.80303	-3.78956	-1.27783
C	1.57396	5.426272	0.079925
C	2.907853	3.21324	0.01964
C	2.525682	1.812734	0.005131
H	-2.66362	4.824499	1.913654
H	-4.32551	4.251765	2.099722
H	-4.01696	5.868157	1.434154
H	-7.02201	1.47631	-1.5422
H	-5.53895	0.658048	-2.07196
H	-5.62898	2.421291	-2.10541
C	3.852146	-4.24142	0.015173

C	4.058962	-1.66527	-0.01588
C	3.092638	-0.58259	-0.01165
H	-2.11548	-5.66362	2.120358
H	-1.23563	-7.05033	1.446673
H	-0.36389	-5.57125	1.896637
H	-4.52991	-4.85024	-1.30429
H	-5.89748	-3.72415	-1.26797
H	-4.44048	-3.32517	-2.20231
C	1.329056	5.965189	1.503422
H	2.468326	5.906236	-0.33435
H	0.74393	5.732762	-0.5695
C	4.319525	3.732791	-0.01388
C	3.429985	0.761589	-0.00251
C	3.882603	-4.85029	1.431183
H	3.242237	-4.87825	-0.63837
H	4.864105	-4.26655	-0.40569
C	5.554015	-1.50077	-0.05643
H	1.208796	7.054781	1.49211
H	0.426288	5.526578	1.942522
H	2.169459	5.721139	2.162691
C	4.925155	3.769158	-1.43113
H	4.959133	3.121964	0.63617
H	4.343616	4.743392	0.410316
H	4.484391	1.011317	0.003651
H	2.881777	-4.8669	1.876422
H	4.261875	-5.87853	1.404942
H	4.529462	-4.26447	2.093653
C	6.104334	-1.25092	-1.47467
H	6.028518	-2.39822	0.357511
H	5.857865	-0.67442	0.598966
H	4.942348	2.769939	-1.88001
H	5.952867	4.149933	-1.40599
H	4.33675	4.417396	-2.08996
H	7.194164	-1.13387	-1.45471
H	5.671705	-0.34484	-1.91289
H	5.862784	-2.08753	-2.13967
Ni	0.126031	-0.00267	-0.00383
H	-4.6053	-3.58015	0.85139
H	-5.12757	-1.32272	0.912808
H	-5.19844	-1.27922	-0.84117

Computed geometry and energy data of methyl ester analog of **7d**.
Electronic energy E = -2688.533325 a.u. Free Energy G = -2687.874316 a.u. Entropy S = 384.519 kcal/mol•K
Table S11. Atom coordinates of methyl ester analog of **7d**.

C	2.916747	-2.69292	0.23832
C	3.513558	-1.54446	0.699346
C	2.471563	-0.52558	0.723494
N	1.290336	-1.04485	0.25283
C	1.528925	-2.37949	0.014521
C	-3.0441	-3.36788	-0.16817

C	-1.85796	-4.04858	-0.24303
C	-0.81119	-3.04517	-0.25316
N	-1.34523	-1.77917	-0.21264
C	-2.70742	-1.95439	-0.19199
C	0.54315	-3.32351	-0.24251
C	-3.45962	2.488161	-1.41702
C	-4.21045	1.394428	-1.07584
C	-3.27601	0.378703	-0.63025
N	-1.98858	0.856645	-0.65001
C	-2.08059	2.143808	-1.12369
C	-3.62941	-0.92903	-0.33327
C	2.196382	3.257165	0.353114
C	1.212301	3.810307	-0.42934
C	0.245403	2.771676	-0.67151
N	0.668277	1.57764	-0.13887
C	1.86218	1.845234	0.499124
C	2.660255	0.831273	1.07824
C	-1.01409	3.020267	-1.2029
C	-1.62336	-5.52941	-0.27791
C	-5.69706	1.214353	-1.15984
C	1.08502	5.221012	-0.92586
C	4.984686	-1.39023	0.971981
C	-4.43615	-3.92398	-0.07135
C	-4.96696	-3.92463	1.374039
C	-6.38704	-4.46027	1.46377
C	-3.93113	3.821237	-1.92648
C	-4.18152	4.831422	-0.79117
C	-4.61881	6.189813	-1.31624
C	3.407433	3.991853	0.858612
C	4.694083	3.698919	0.045855
C	5.944289	4.022802	0.837324
C	3.557416	-4.02613	-0.02979
C	3.896547	-4.23608	-1.51679
C	4.451938	-5.61872	-1.79846
O	4.411769	-6.56379	-1.03674
O	4.993908	-5.68098	-3.03298
O	-7.02903	-4.82163	0.502238
O	-6.96827	-4.53368	2.68847
O	-4.72272	6.451102	-2.49431
O	-4.90276	7.164789	-0.41482
O	6.852918	4.696404	0.11264
O	6.119995	3.692072	1.996746
H	0.846115	-4.36063	-0.3299
H	-4.68313	-1.18298	-0.3407
H	-1.20145	4.013917	-1.59345
H	-0.98121	-5.81659	-1.11958
H	-1.13165	-5.88505	0.636908
H	-2.56362	-6.07881	-0.38048
H	-6.18041	2.096343	-1.59005
H	-5.96603	0.354444	-1.78575

H	-6.1427	1.04335	-0.17117
H	0.919421	5.2502	-2.00955
H	0.240443	5.743366	-0.45738
H	1.984311	5.806983	-0.71886
H	5.355734	-0.40997	0.659274
H	5.233264	-1.51194	2.033797
H	5.550845	-2.14834	0.422332
H	-5.12927	-3.35579	-0.70093
H	-4.46304	-4.94819	-0.45573
H	-4.30973	-4.52413	2.017038
H	-4.93783	-2.90942	1.791202
H	-3.20639	4.248554	-2.6271
H	-4.85632	3.701054	-2.49915
H	-4.94245	4.444108	-0.10167
H	-3.27395	4.955088	-0.18564
H	3.213508	5.068461	0.813549
H	3.587036	3.776982	1.914751
H	4.746941	2.630635	-0.20011
H	4.691265	4.241116	-0.90288
H	4.471361	-4.13029	0.563683
H	2.903408	-4.84191	0.296902
H	2.999706	-4.10428	-2.13689
H	4.613323	-3.48729	-1.87204
C	5.517966	-6.96366	-3.42009
H	4.727312	-7.71862	-3.41693
H	5.911391	-6.82679	-4.42745
H	6.312274	-7.27551	-2.73699
C	8.090874	5.001619	0.78453
H	8.696287	5.533446	0.050947
H	7.904713	5.630077	1.658866
H	8.589224	4.082321	1.10189
C	-4.80996	6.930343	0.995454
H	-5.07349	7.878628	1.465586
H	-5.51459	6.158867	1.322722
H	-3.79412	6.651206	1.293359
C	-6.27055	-4.12876	3.872596
H	-5.37771	-4.73908	4.042667
H	-5.99152	-3.07076	3.835265
H	-6.97331	-4.28566	4.691868
Ni	-0.35104	-0.09601	-0.17273
C	3.70304	1.141789	2.053324
H	4.338567	2.016167	2.076581
N	3.871772	0.367142	3.090906
N	4.048816	-0.29442	4.008599

Computed geometry and energy data of **7e**.
Electronic energy E = -2578.999345 a.u. Free Energy G = -2578.358383 a.u. Entropy S = 388.036 kcal/mol•K
Table S12. Atom coordinates of **7e**.

N	-1.78613	0.580176	0.182539
N	-0.45729	-1.85794	0.03464

C	-2.28135	1.829567	-0.16334
C	-2.87533	-0.20243	0.387954
C	0.327891	-2.93177	-0.37431
C	-1.65716	-2.38922	0.354621
C	-1.49867	2.966392	-0.29555
C	-3.71586	1.794232	-0.22848
C	-2.77552	-1.58951	0.832302
C	-4.0957	0.515121	0.136441
C	1.696227	-2.86803	-0.56236
C	-0.44466	-4.14567	-0.36419
C	-1.69055	-3.80911	0.126405
C	-0.13012	3.021198	-0.06399
H	-2.00309	3.900571	-0.51811
C	-4.6088	2.950369	-0.58001
C	-3.6729	-2.05604	1.718595
C	-5.50081	-0.01392	0.182722
C	2.491122	-1.75518	-0.30433
H	2.199639	-3.78746	-0.8422
C	0.059158	-5.49637	-0.77856
C	-2.87257	-4.71141	0.342749
C	0.637282	4.243663	0.039063
N	0.668538	1.92334	0.150217
C	-5.09367	3.724695	0.658931
H	-5.48429	2.591619	-1.13364
H	-4.09939	3.644855	-1.25576
H	-5.54028	-1.07806	-0.07036
H	-5.96586	0.101938	1.171231
C	3.936636	-1.76485	-0.26317
N	2.00197	-0.51335	0.025301
H	-0.69461	-6.27028	-0.60843
H	0.323496	-5.52188	-1.84354
C	-3.85919	-4.69638	-0.83724
H	-3.40593	-4.4172	1.255231
H	-2.53641	-5.74009	0.508697
C	0.085422	5.62579	-0.14956
C	1.920541	3.87012	0.350588
C	1.926943	2.419695	0.383447
H	-4.24162	4.094407	1.244065
H	-5.65447	3.072278	1.338618
C	4.810367	-2.95694	-0.53812
C	4.320767	-0.50446	0.128234
C	3.104743	0.26529	0.272471
H	-3.35256	-4.98292	-1.76837
H	-4.25099	-3.6879	-1.01236
H	0.841579	6.387129	0.062947
H	-0.26326	5.787007	-1.17793
C	3.122751	4.749201	0.552909
C	3.067332	1.636447	0.512717
C	5.036883	-3.82763	0.710758
H	4.381498	-3.57859	-1.33138

H	5.782957	-2.6276	-0.91945
C	5.706958	0.025709	0.346136
C	3.918515	4.978052	-0.74457
H	3.790715	4.322213	1.308878
H	2.812824	5.720969	0.951841
H	4.009312	2.137668	0.704601
H	4.080451	-4.16914	1.127194
H	5.514129	-3.25037	1.511532
H	6.462837	-0.72533	0.098474
H	5.869333	0.32348	1.390216
H	4.239252	4.023885	-1.18136
H	3.292641	5.453513	-1.50956
H	-4.6146	-1.66105	2.079577
Ni	0.111454	0.033925	0.120539
H	-6.13614	0.521752	-0.53155
C	-5.02875	-5.63985	-0.63641
O	-5.13994	-6.44949	0.261622
O	-5.95298	-5.47713	-1.60833
C	5.888401	-5.04957	0.425494
O	6.28239	-5.39632	-0.66958
O	6.156535	-5.72658	1.561906
C	5.148962	5.838487	-0.5317
O	5.52659	6.280249	0.534469
O	5.792289	6.056866	-1.69814
C	-5.96824	4.911126	0.302124
O	-6.20103	5.304604	-0.82278
O	-6.46315	5.497361	1.412905
H	-0.76785	5.816159	0.513106
H	0.956908	-5.78617	-0.21787
H	5.906972	0.908457	-0.27427
C	-7.29701	6.648594	1.19186
H	-7.59716	6.986984	2.183704
H	-6.74014	7.432453	0.671771
H	-8.17382	6.379045	0.597302
C	6.983314	6.859242	-1.61344
H	7.362196	6.928574	-2.63323
H	6.749775	7.853174	-1.22299
H	7.721384	6.383867	-0.96205
C	6.947477	-6.91812	1.406672
H	7.923132	-6.67795	0.976154
H	7.062635	-7.32547	2.411205
H	6.437837	-7.63583	0.75843
C	-7.09773	-6.34411	-1.53086
H	-7.72524	-6.07718	-2.38145
H	-6.79187	-7.39175	-1.59459
H	-7.63656	-6.18635	-0.59286

Computed geometry and energy data of **7f**.
Electronic energy E = -2579.004906 a.u. Free Energy G = -2578.364214 a.u. Entropy S = 389.403 kcal/mol•K
Table S13. Atom coordinates of **7f**.

N	1.791416	0.605055	-0.13779
N	0.512088	-1.84881	-0.04056
C	2.256807	1.87043	0.180439
C	2.900021	-0.13621	-0.41079
C	-0.25805	-2.93605	0.344378
C	1.739981	-2.35338	-0.32595
C	1.45008	2.988799	0.337303
C	3.692801	1.893748	0.165783
C	2.8525	-1.54049	-0.77624
C	4.102124	0.635469	-0.23164
C	-1.63214	-2.9084	0.51485
C	0.537618	-4.13476	0.357438
C	1.789328	-3.77817	-0.09757
C	0.07967	3.017624	0.132741
H	1.940303	3.932711	0.549451
C	4.553792	3.0876	0.468658
C	3.843229	-2.10097	-1.51267
C	5.522929	0.1712	-0.37276
C	-2.44556	-1.81271	0.258613
H	-2.11647	-3.84253	0.777834
C	0.042267	-5.49011	0.767743
C	2.981132	-4.68287	-0.2539
C	-0.71471	4.225155	0.063841
N	-0.69663	1.906718	-0.10533
C	4.907061	3.899755	-0.7902
H	5.484012	2.767099	0.951298
H	4.062633	3.747277	1.1914
H	5.654216	-0.8543	-0.01043
H	5.873411	0.193524	-1.41388
C	-3.89208	-1.85461	0.191921
N	-1.97926	-0.55378	-0.03424
H	0.812962	-6.25437	0.635538
H	-0.26168	-5.5084	1.822186
C	3.949109	-4.60685	0.938698
H	3.53102	-4.44357	-1.17052
H	2.646331	-5.71876	-0.37028
C	-0.19205	5.613871	0.284576
C	-1.99003	3.831148	-0.25344
C	-1.96427	2.382365	-0.32428
H	3.998405	4.240823	-1.30248
H	5.43959	3.280031	-1.52175
C	-4.73938	-3.07406	0.425519
C	-4.29806	-0.59653	-0.1764
C	-3.09659	0.206014	-0.28087
H	3.432555	-4.84978	1.87612
H	4.334229	-3.58855	1.067146
H	-0.96616	6.363738	0.097427
H	0.161182	5.755862	1.314166
C	-3.21218	4.687571	-0.43232
C	-3.08906	1.580297	-0.48292

C	-4.90019	-3.93681	-0.83893
H	-4.31742	-3.69237	1.225187
H	-5.7327	-2.77729	0.778874
C	-5.69135	-0.09151	-0.40697
C	-4.0194	4.854879	0.867419
H	-3.86679	4.270048	-1.20505
H	-2.92383	5.678978	-0.79779
H	-4.03957	2.067081	-0.66936
H	-3.92127	-4.24339	-1.22941
H	-5.37121	-3.36543	-1.64762
H	-6.4346	-0.86656	-0.19838
H	-5.83862	0.235088	-1.44457
H	-4.31828	3.879152	1.271095
H	-3.40967	5.320531	1.651094
H	4.727213	-1.76679	-2.03373
Ni	-0.09696	0.028824	-0.09736
H	6.196475	0.814764	0.203076
C	5.1292	-5.54731	0.794631
O	5.300584	-6.33599	-0.11269
O	5.989622	-5.40443	1.826353
C	-5.7209	-5.18795	-0.59273
O	-6.14035	-5.55722	0.485394
O	-5.92825	-5.86284	-1.74314
C	-5.27057	5.689739	0.674727
O	-5.66353	6.140626	-0.3821
O	-5.91416	5.872332	1.847259
C	5.760669	5.114952	-0.48324
O	6.108027	5.473794	0.623537
O	6.09305	5.769483	-1.61629
H	0.651741	5.840398	-0.37903
H	-0.82932	-5.80005	0.177186
H	-5.9237	0.767122	0.23571
C	6.898678	6.948442	-1.44213
H	7.065285	7.339707	-2.44587
H	6.374963	7.684219	-0.82616
H	7.850033	6.696608	-0.96622
C	-7.12537	6.645572	1.780627
H	-7.50144	6.688457	2.802913
H	-6.91871	7.651425	1.405827
H	-7.85412	6.162559	1.124359
C	-6.68493	-7.08054	-1.62485
H	-7.68239	-6.87577	-1.22729
H	-6.75156	-7.48267	-2.63587
H	-6.17524	-7.78707	-0.96448
C	7.144531	-6.26079	1.797632
H	7.714387	-6.01382	2.69363
H	6.844599	-7.31195	1.812258
H	7.740714	-6.0726	0.90078

Computed geometry and energy data of triplet **7g**.

Electronic energy E = -2579.033576 a.u. Free Energy G = -2578.389897 a.u. Entropy S = 384.137 kcal/mol•K

Table S14. Atom coordinates of **7g**.

N	-1.78088	0.055935	0.036141
N	0.011964	-2.03614	-0.12161
C	-2.51661	1.186208	-0.28806
C	-2.68934	-0.92084	0.283328
C	0.989455	-2.89009	-0.61405
C	-1.07847	-2.80656	0.102464
C	-1.97862	2.460241	-0.38889
C	-3.91805	0.871378	-0.31638
C	-2.3064	-2.26851	0.670832
C	-4.03275	-0.45287	0.067937
C	2.328323	-2.5523	-0.73399
C	0.454164	-4.2119	-0.7803
C	-0.84531	-4.16856	-0.30707
C	-0.65633	2.789415	-0.11751
H	-2.65976	3.276722	-0.60423
C	-5.0269	1.830751	-0.64441
C	-3.06493	-2.99606	1.536453
C	-5.30587	-1.24544	0.159161
C	2.877322	-1.33296	-0.35348
H	3.009828	-3.32984	-1.06248
C	1.220211	-5.3817	-1.32387
C	-1.83465	-5.31044	-0.30344
C	-0.15529	4.138095	0.02504
N	0.338494	1.872042	0.129844
C	-5.61218	2.513449	0.604765
H	-5.83514	1.30526	-1.16544
H	-4.68023	2.600176	-1.34228
H	-5.16796	-2.28035	-0.17074
H	-5.70859	-1.28231	1.180872
C	4.293738	-1.06067	-0.22742
N	2.137552	-0.23176	0.005897
H	0.557594	-6.20945	-1.59323
H	1.786796	-5.11103	-2.22211
C	-3.14445	-4.98734	-0.94138
H	-2.02055	-5.70755	0.701613
H	-1.38042	-6.14851	-0.85681
C	-0.96271	5.385064	-0.18481
C	1.16181	4.025141	0.398197
C	1.458171	2.606232	0.426461
H	-4.83722	3.067982	1.1487
H	-5.99236	1.769404	1.315569
C	5.396825	-2.04259	-0.5077
C	4.400758	0.225775	0.241917
C	3.049484	0.736507	0.344749
H	-3.17534	-4.40932	-1.85934
H	-0.38167	6.279369	0.058563
H	-1.29563	5.482952	-1.22624
C	2.151899	5.125436	0.660048

C	2.7267	2.063107	0.611506
C	5.707571	-2.94755	0.697806
H	5.145144	-2.6723	-1.3681
H	6.309662	-1.50881	-0.79276
C	5.641241	1.004573	0.564605
C	2.944555	5.524159	-0.59766
H	2.856232	4.832602	1.446328
H	1.634377	6.010399	1.045713
H	3.537193	2.737528	0.863769
H	4.811333	-3.49578	1.015321
H	6.010125	-2.35285	1.568005
H	6.542758	0.429547	0.333776
H	5.686329	1.274923	1.627581
H	3.4737	4.658748	-1.01661
H	2.271846	5.867759	-1.39267
H	-3.96144	-2.58587	1.984327
Ni	0.180933	-0.08174	0.038197
H	-6.08145	-0.79653	-0.47099
C	-4.39155	-5.4556	-0.37562
O	-4.49668	-6.13593	0.640364
O	-5.46524	-5.04604	-1.10677
C	6.798708	-3.95895	0.404317
O	7.330832	-4.13207	-0.6734
O	7.111051	-4.6662	1.510833
C	3.963287	6.614508	-0.32791
O	4.211781	7.097387	0.75819
O	4.580655	6.99049	-1.4681
C	-6.73994	3.471863	0.274055
O	-7.16547	3.706288	-0.83876
O	-7.22679	4.048303	1.393718
H	-1.86228	5.397273	0.443174
H	1.939753	-5.77176	-0.5911
H	5.693829	1.940021	-0.00673
C	-8.30585	4.979097	1.197557
H	-8.56302	5.342594	2.192596
H	-7.98819	5.806434	0.557566
H	-9.16378	4.481245	0.738021
C	5.578546	8.016995	-1.32749
H	5.963196	8.190596	-2.3326
H	5.134992	8.930815	-0.9236
H	6.380212	7.685122	-0.66246
C	8.129819	-5.66811	1.344232
H	9.068942	-5.21088	1.021845
H	8.246937	-6.13162	2.323904
H	7.821233	-6.41047	0.603501
C	-6.74154	-5.48187	-0.61864
H	-7.4768	-5.07049	-1.31085
H	-6.7978	-6.57413	-0.60633
H	-6.91815	-5.1075	0.393725
H	-2.78057	-3.9922	1.850974

Computed geometry and energy data of triplet **7h**.
Electronic energy E = -2579.038703 a.u. Free Energy G = -2578.398289 a.u. Entropy S = 388.842 kcal/mol•K
Table S15. Atom coordinates of **7h**.

N	-1.79508	0.389358	0.152025
N	-0.28863	-1.93082	0.007783
C	-2.39626	1.598407	-0.16857
C	-2.8036	-0.44213	0.512177
C	0.570605	-2.93294	-0.43855
C	-1.48959	-2.52143	0.217622
C	-1.70468	2.778863	-0.37857
C	-3.82645	1.481008	-0.06767
C	-2.57653	-1.827	0.885482
C	-4.08486	0.203504	0.392294
C	1.946921	-2.77672	-0.53589
C	-0.13632	-4.15944	-0.59904
C	-1.47792	-3.9121	-0.20881
C	-0.33454	2.940968	-0.19696
H	-2.2844	3.667878	-0.60259
C	-4.81764	2.573719	-0.35133
C	-3.31646	-2.44521	1.849625
C	-5.4367	-0.39866	0.647184
C	2.647265	-1.62024	-0.21608
H	2.52852	-3.65084	-0.80616
C	0.400864	-5.45418	-1.12047
C	-2.51664	-4.84596	-0.37055
C	0.341803	4.218493	-0.16646
N	0.541159	1.917807	0.07696
C	-5.19109	3.380363	0.90551
H	-5.73229	2.145992	-0.7783
H	-4.43217	3.26062	-1.11152
H	-5.46578	-1.46008	0.380722
H	-5.73755	-0.3248	1.701487
C	4.087002	-1.52852	-0.09739
N	2.058798	-0.40856	0.05838
H	0.27337	-6.26567	-0.39161
H	-0.12975	-5.76304	-2.03105
C	-3.99004	-4.59397	-0.35285
H	-2.23186	-5.84736	-0.67742
C	-0.30616	5.544342	-0.43693
C	1.647553	3.957523	0.170612
C	1.758211	2.517609	0.290997
H	-4.29422	3.813838	1.367282
H	-5.63427	2.73579	1.673358
C	5.050592	-2.66467	-0.29699
C	4.363576	-0.23507	0.274071
C	3.091869	0.453189	0.330243
H	-4.25338	-3.6394	-0.82722
H	-4.40604	-4.50878	0.665281
H	0.391502	6.369112	-0.26474

H	-0.65666	5.621514	-1.47433
C	2.781283	4.93226	0.324712
C	2.947371	1.827668	0.496267
C	5.218141	-3.53067	0.964281
H	4.729167	-3.30493	-1.12587
H	6.031272	-2.27624	-0.59142
C	5.6963	0.39711	0.546268
C	3.581937	5.125984	-0.9755
H	3.464592	4.608257	1.117353
H	2.396709	5.904918	0.649718
H	3.843359	2.406487	0.690266
H	4.251343	-3.9333	1.292626
H	5.586815	-2.93219	1.805916
H	6.514069	-0.30725	0.368187
H	5.778554	0.740819	1.585552
H	3.980433	4.169005	-1.33573
H	2.937399	5.495962	-1.78199
H	-4.10052	-1.9271	2.388286
Ni	0.135353	-0.00603	0.097589
H	-6.20544	0.115	0.059714
C	-4.77371	-5.70208	-1.03956
O	-4.33881	-6.78133	-1.38437
O	-6.06264	-5.33524	-1.19966
C	6.165015	-4.69587	0.751718
O	6.684674	-5.00106	-0.30252
O	6.360939	-5.37422	1.902133
C	4.742318	6.088155	-0.81032
O	5.079708	6.616989	0.229442
O	5.374452	6.287921	-1.98622
C	-6.1561	4.512011	0.608643
O	-6.50308	4.873165	-0.49754
O	-6.58522	5.09202	1.749631
H	-1.17671	5.711258	0.209653
H	1.464014	-5.39466	-1.36797
H	5.870953	1.270245	-0.09519
C	-7.49039	6.197938	1.584996
H	-7.72486	6.536632	2.594277
H	-7.01736	6.99974	1.011938
H	-8.3983	5.876997	1.067707
C	6.501665	7.180682	-1.94496
H	6.882159	7.218533	-2.9658
H	6.191528	8.175479	-1.61454
H	7.268092	6.800986	-1.26418
C	7.234949	-6.51332	1.813702
H	8.232859	-6.20719	1.489022
H	7.272093	-6.93211	2.819464
H	6.839015	-7.24765	1.107307
C	-6.91884	-6.31692	-1.80967
H	-7.90353	-5.85238	-1.8643
H	-6.55893	-6.5712	-2.80988

H	-6.95661	-7.22468	-1.20164
H	-3.09536	-3.46214	2.152945

Computed geometry and energy data of triplet **7i**.
Electronic energy E = -2579.038282 a.u. Free Energy G = -2578.396461 a.u. Entropy S = 387.024 kcal/mol•K
Table S16. Atom coordinates of **7i**.

N	1.783047	0.425523	-0.19505
N	0.297404	-1.8932	-0.10555
C	2.369596	1.631878	0.180861
C	2.793928	-0.4092	-0.53144
C	-0.53013	-2.89431	0.386215
C	1.46784	-2.49618	-0.4175
C	1.659367	2.812297	0.366484
C	3.789002	1.523392	0.160562
C	2.577697	-1.76161	-1.00847
C	4.090439	0.21933	-0.31095
C	-1.89322	-2.75235	0.569314
C	0.192944	-4.13632	0.467408
C	1.447634	-3.89726	-0.0593
C	0.298723	2.968974	0.139717
H	2.228111	3.702759	0.611807
C	4.777165	2.597468	0.500549
C	3.374464	-2.31384	-1.96873
C	5.36456	-0.33554	-0.45166
C	-2.61964	-1.60371	0.259214
H	-2.44831	-3.6285	0.88706
C	-0.37452	-5.41406	1.011264
C	2.588639	-4.87978	-0.12056
C	-0.38703	4.239508	0.078268
N	-0.56729	1.935057	-0.13621
C	5.305232	3.331781	-0.74665
H	5.627527	2.162543	1.03949
H	4.338563	3.329757	1.185629
H	5.519557	-1.36406	-0.7502
C	-4.06365	-1.5278	0.183887
N	-2.05183	-0.4	-0.07206
H	0.346316	-6.23366	0.953121
H	-0.67061	-5.30917	2.062631
C	3.701753	-4.5664	0.893869
H	3.031024	-4.93785	-1.11837
H	2.208457	-5.88579	0.081503
C	0.245284	5.574987	0.337962
C	-1.6861	3.962386	-0.27465
C	-1.78376	2.520321	-0.3713
H	4.478218	3.78761	-1.30639
H	5.78156	2.631863	-1.44284
C	-5.00904	-2.66465	0.454419
C	-4.36374	-0.25201	-0.22786
C	-3.10092	0.446926	-0.34446
H	3.306163	-4.54363	1.916368

H	4.124814	-3.57026	0.715618
H	-0.45456	6.391037	0.135671
H	0.57249	5.673823	1.381187
C	-2.82526	4.925521	-0.45997
C	-2.97162	1.813048	-0.55486
C	-5.22395	-3.56554	-0.77501
H	-4.64766	-3.28034	1.285259
H	-5.97922	-2.27445	0.780329
C	-5.71023	0.35741	-0.48276
C	-3.63557	5.145676	0.830067
H	-3.50103	4.577847	-1.24903
H	-2.4449	5.892548	-0.80622
H	-3.87387	2.379713	-0.75567
H	-4.26679	-3.96264	-1.13755
H	-5.64112	-2.9961	-1.6137
H	-6.51518	-0.34787	-0.25659
H	-5.82539	0.66358	-1.53057
H	-4.02921	4.195135	1.212052
H	-2.99871	5.540495	1.630889
H	4.16834	-1.7438	-2.43556
Ni	-0.14045	0.021578	-0.15262
H	6.245056	0.241349	-0.18949
C	4.835913	-5.57028	0.838999
O	4.943686	-6.47355	0.03412
O	5.740856	-5.33162	1.812443
C	-6.13768	-4.74069	-0.48564
O	-6.55637	-5.05703	0.609494
O	-6.42876	-5.41605	-1.61738
C	-4.80203	6.094714	0.634475
O	-5.13527	6.597673	-0.41931
O	-5.44497	6.315438	1.800781
C	6.298005	4.425113	-0.40302
O	6.58927	4.788132	0.718534
O	6.825633	4.966537	-1.52135
H	1.128294	5.736366	-0.29274
H	-1.26817	-5.7273	0.456021
H	-5.87495	1.250914	0.132644
C	7.771665	6.030119	-1.31327
H	8.085633	6.341155	-2.30978
H	7.303283	6.862696	-0.78175
H	8.628451	5.674123	-0.73522
C	-6.57849	7.198409	1.730984
H	-6.9666	7.256928	2.747976
H	-6.27345	8.187599	1.379738
H	-7.33715	6.797207	1.053836
C	-7.27405	-6.5689	-1.45612
H	-8.2402	-6.28048	-1.03392
H	-7.40177	-6.98012	-2.45755
H	-6.8014	-7.30282	-0.79808
C	6.872231	-6.21881	1.84292

H	7.485225	-5.88255	2.679358
H	6.547247	-7.2512	1.996762
H	7.434364	-6.15755	0.907252
H	3.193342	-3.30925	-2.35384

Computed geometry and energy data of singlet **7g**.
Electronic energy E = -2579.033671 a.u.
Table S17. Atom coordinates of singlet **7g**.

N	-1.78088	0.055935	0.036425
N	0.011945	-2.03614	-0.12164
C	-2.51665	1.186211	-0.28764
C	-2.6893	-0.92084	0.283748
C	0.989357	-2.89009	-0.61423
C	-1.07845	-2.80656	0.102608
C	-1.97868	2.460245	-0.38855
C	-3.9181	0.871381	-0.31574
C	-2.30629	-2.26851	0.671177
C	-4.03274	-0.45287	0.068576
C	2.328206	-2.5523	-0.73438
C	0.45404	-4.2119	-0.78042
C	-0.84536	-4.16856	-0.30698
C	-0.65635	2.789416	-0.11738
H	-2.65986	3.276728	-0.60377
C	-5.027	1.830757	-0.64359
C	-3.06468	-2.99608	1.536912
C	-5.30584	-1.24544	0.159995
C	2.877266	-1.33296	-0.35396
H	3.009659	-3.32983	-1.06299
C	1.22	-5.38169	-1.32412
C	-1.8347	-5.31043	-0.3032
C	-0.15528	4.138095	0.025106
N	0.338515	1.872041	0.129809
C	-5.61208	2.513443	0.605685
H	-5.83533	1.305271	-1.1645
H	-4.68045	2.600189	-1.3415
H	-5.16798	-2.28035	-0.16994
H	-5.70841	-1.28232	1.18177
C	4.293702	-1.06067	-0.22812
N	2.137553	-0.23176	0.005554
H	0.55734	-6.20943	-1.59338
H	1.786442	-5.11101	-2.22244
C	-3.1446	-4.98733	-0.94093
H	-2.02044	-5.70755	0.701879
H	-1.38056	-6.1485	-0.85665
C	-0.96274	5.385066	-0.1846
C	1.161873	4.025137	0.398052
C	1.458239	2.606228	0.426254
H	-4.83703	3.067971	1.149502
H	-5.99215	1.769391	1.316542
C	5.396744	-2.04258	-0.50858

C	4.400797	0.225773	0.241217
C	3.049539	0.736504	0.34427
H	-3.17563	-4.4093	-1.85888
H	-0.38167	6.279368	0.058686
H	-1.29582	5.482964	-1.22598
C	2.152004	5.125429	0.659756
C	2.726797	2.063101	0.611092
C	5.707682	-2.94756	0.696867
H	5.144926	-2.67229	-1.36894
H	6.309536	-1.5088	-0.79378
C	5.641331	1.004567	0.563715
C	2.94446	5.524165	-0.59807
H	2.856463	4.832588	1.44592
H	1.634544	6.010389	1.045512
H	3.537331	2.737519	0.863232
H	4.811495	-3.49579	1.014519
H	6.010375	-2.35286	1.567023
H	6.542811	0.429544	0.332737
H	5.686588	1.274907	1.626687
H	3.473538	4.658758	-1.01711
H	2.271624	5.867773	-1.39298
H	-3.96113	-2.58589	1.984933
Ni	0.180939	-0.08174	0.038167
H	-6.08152	-0.79653	-0.47003
C	-4.39161	-5.4556	-0.37498
O	-4.49658	-6.13594	0.64102
O	-5.46542	-5.04603	-1.10595
C	6.798772	-3.95896	0.403194
O	7.330725	-4.13206	-0.67461
O	7.111292	-4.66622	1.509653
C	3.963235	6.614511	-0.32847
O	4.211902	7.09738	0.757589
O	4.580421	6.990505	-1.46876
C	-6.7399	3.47186	0.275164
O	-7.1656	3.706296	-0.83758
O	-7.22657	4.048289	1.39491
H	-1.86221	5.397269	0.443524
H	1.939659	-5.77175	-0.59146
H	5.693828	1.940021	-0.00762
C	-8.30566	4.979085	1.198931
H	-8.56267	5.342572	2.194014
H	-7.9881	5.806428	0.558897
H	-9.16367	4.481238	0.739526
C	5.578334	8.017008	-1.3283
H	5.962824	8.190619	-2.33347
H	5.134845	8.930824	-0.92433
H	6.380106	7.685129	-0.6634
C	8.130033	-5.66812	1.34288
H	9.069105	-5.21089	1.020347
H	8.247308	-6.13164	2.322528

H	7.821329	-6.41048	0.60219
C	-6.74164	-5.48187	-0.61762
H	-7.47701	-5.07048	-1.30971
H	-6.7979	-6.57412	-0.60531
H	-6.91809	-5.1075	0.394778
H	-2.78028	-3.99222	1.851378

Computed geometry and energy data of singlet **7h**.
Electronic energy E = -2579.047378 a.u. Free Energy G = -2578.399843 a.u. Entropy S = 380.249 kcal/mol•K
Table S18. Atom coordinates of singlet **7h**.

N	1.831723	0.169832	-0.18697
N	0.077132	-1.99599	-0.0751
C	2.574373	1.286611	0.149582
C	2.736166	-0.76901	-0.58892
C	-0.91106	-2.92082	0.414783
C	1.174024	-2.6793	-0.30633
C	2.010812	2.54372	0.410358
C	3.965102	1.016795	0.00919
C	2.332199	-2.1051	-0.98994
C	4.069364	-0.2838	-0.48543
C	-2.27202	-2.55607	0.504489
C	-0.35802	-4.16924	0.595446
C	1.025394	-4.07472	0.177811
C	0.684404	2.861342	0.248143
H	2.691034	3.351292	0.661205
C	5.08642	1.981548	0.277202
C	2.938418	-2.81858	-1.96851
C	5.341343	-1.02169	-0.79218
C	-2.79081	-1.33344	0.166808
H	-2.96917	-3.34569	0.758626
C	-1.01612	-5.40209	1.12967
C	1.949514	-5.05382	0.386158
C	0.140015	4.20102	0.26835
N	-0.31274	1.947212	-0.08109
C	5.518471	2.756816	-0.98028
H	5.957484	1.446762	0.674197
H	4.804803	2.69831	1.055988
H	5.255358	-2.09328	-0.57994
H	5.640202	-0.93076	-1.84622
C	-4.22489	-1.06446	0.035003
N	-2.06708	-0.18705	-0.11508
H	-0.97864	-6.22951	0.408308
H	-0.52532	-5.75581	2.04673
C	3.429689	-5.08746	0.17455
H	1.57189	-5.96398	0.848313
C	0.916568	5.440096	0.603071
C	-1.17946	4.093638	-0.09387
C	-1.44291	2.678329	-0.27868
H	4.672226	3.313994	-1.40231
H	5.840254	2.071203	-1.77372

C	-5.31188	-2.08306	0.230827
C	-4.34534	0.238524	-0.34127
C	-2.99162	0.791744	-0.38317
H	3.883	-4.09716	0.108569
H	3.670076	-5.58641	-0.77814
H	0.312838	6.340235	0.454916
H	1.25276	5.43701	1.64802
C	-2.2044	5.185708	-0.22254
C	-2.71082	2.13292	-0.53172
C	-5.53255	-2.96124	-1.01377
H	-5.08551	-2.7294	1.086131
H	-6.25291	-1.58273	0.481859
C	-5.5877	1.025011	-0.62917
C	-3.03496	5.378053	1.058949
H	-2.88409	4.980032	-1.05712
H	-1.7147	6.133614	-0.47062
H	-3.53315	2.812761	-0.71874
H	-4.60397	-3.46989	-1.30194
H	-5.81267	-2.34978	-1.87993
H	-6.48705	0.416661	-0.49762
H	-5.59171	1.407314	-1.658
H	-3.53171	4.442177	1.345066
H	-2.39121	5.638126	1.907952
H	3.744913	-2.39904	-2.55858
Ni	-0.12726	0.002845	-0.14081
H	6.171529	-0.63202	-0.19235
C	4.124395	-5.91	1.256349
O	3.590989	-6.74017	1.962002
O	5.433972	-5.61257	1.298941
C	-6.60239	-4.015	-0.80507
O	-7.18718	-4.23373	0.236457
O	-6.82938	-4.70337	-1.94431
C	-4.09673	6.450702	0.91727
O	-4.35365	7.063868	-0.09905
O	-4.74532	6.645902	2.086059
C	6.64359	3.737425	-0.71451
O	7.148266	3.962135	0.366942
O	7.027463	4.353229	-1.85444
H	1.812748	5.538584	-0.02195
H	-2.06632	-5.22525	1.375694
H	-5.67528	1.894475	0.034734
C	8.086521	5.315944	-1.71591
H	8.261823	5.704949	-2.71917
H	7.78822	6.121584	-1.03976
H	8.990324	4.840056	-1.32626
C	-5.78594	7.638153	2.063256
H	-6.19339	7.658267	3.074233
H	-5.37848	8.616545	1.795142
H	-6.5619	7.365436	1.34303
C	-7.82228	-5.74046	-1.8589

H	-8.79203	-5.32148	-1.57786
H	-7.87088	-6.18162	-2.8546
H	-7.53061	-6.49215	-1.12066
C	6.214877	-6.35913	2.253116
H	7.234334	-5.98937	2.146495
H	5.845687	-6.18365	3.266355
H	6.167211	-7.42816	2.031498
H	2.60208	-3.81605	-2.22951

Computed geometry and energy data of singlet **7i**.
Electronic energy E = -2579.047473 a.u. Free Energy G = -2578.399753 a.u. Entropy S = 380.509 kcal/mol•K
Table S19. Atom coordinates of singlet **7i**.

N	1.864695	0.517869	-0.24491
N	0.351194	-1.8257	-0.20813
C	2.484738	1.750025	0.17538
C	2.830404	-0.30757	-0.56332
C	-0.46261	-2.85205	0.245075
C	1.528641	-2.41345	-0.55466
C	1.72302	2.919211	0.358743
C	3.860472	1.62011	0.208584
C	2.614099	-1.6335	-1.1346
C	4.152856	0.284555	-0.24512
C	-1.83602	-2.70303	0.46536
C	0.253053	-4.08357	0.247092
C	1.518483	-3.80884	-0.2724
C	0.374515	3.031936	0.119249
H	2.269267	3.826788	0.589024
C	4.869471	2.664444	0.582602
C	3.37467	-2.04299	-2.17735
C	5.330769	-0.38656	-0.27743
C	-2.5575	-1.55432	0.228218
H	-2.38808	-3.58908	0.761392
C	-0.26821	-5.41353	0.708657
C	2.660906	-4.78353	-0.39029
C	-0.32792	4.314387	0.068557
N	-0.50254	1.999901	-0.15702
C	5.431055	3.417067	-0.63823
H	5.703904	2.207063	1.127445
H	4.429467	3.387903	1.277168
H	5.38588	-1.4283	-0.56948
C	-4.00023	-1.45531	0.214865
N	-1.99494	-0.32819	-0.1052
H	0.266481	-6.23785	0.223893
H	-0.15772	-5.54906	1.793652
C	3.264383	-5.15581	0.976774
H	3.462516	-4.38238	-1.01213
H	2.326741	-5.70294	-0.88962
C	0.313011	5.64374	0.330252
C	-1.61809	4.041504	-0.27178
C	-1.72774	2.584891	-0.37022

H	4.631632	3.932719	-1.18343
H	5.873591	2.716406	-1.35808
C	-4.9512	-2.58507	0.495181
C	-4.30175	-0.16778	-0.15826
C	-3.03813	0.520126	-0.31741
H	2.529979	-5.63643	1.630982
H	3.584675	-4.24648	1.504144
H	-0.39492	6.463861	0.180005
H	0.688634	5.71516	1.359285
C	-2.76172	5.000623	-0.44383
C	-2.91283	1.90241	-0.53412
C	-5.25883	-3.42544	-0.7571
H	-4.55193	-3.24378	1.273706
H	-5.89163	-2.19191	0.896669
C	-5.64985	0.463042	-0.34486
C	-3.58589	5.177436	0.844195
H	-3.42565	4.664822	-1.24788
H	-2.38588	5.979413	-0.75969
H	-3.81925	2.471099	-0.7033
H	-4.33287	-3.82083	-1.19446
H	-5.7149	-2.81148	-1.54251
H	-6.45401	-0.23824	-0.10253
H	-5.80533	0.79618	-1.37952
H	-3.97335	4.213375	1.196285
H	-2.95983	5.557104	1.660811
H	4.156248	-1.41441	-2.58894
Ni	-0.09262	0.093956	-0.20518
H	6.259614	0.095626	0.013172
C	4.47591	-6.05877	0.852232
O	5.140853	-6.21469	-0.15247
O	4.751509	-6.66936	2.025082
C	-6.17607	-4.59702	-0.46573
O	-6.53767	-4.95563	0.636701
O	-6.54446	-5.21728	-1.60715
C	-4.75789	6.122083	0.662525
O	-5.07565	6.663427	-0.3769
O	-5.42471	6.291423	1.82409
C	6.492491	4.432705	-0.26212
O	6.955952	4.591043	0.849025
O	6.875372	5.152233	-1.33811
H	1.167453	5.81778	-0.33594
H	-1.33247	-5.53883	0.479609
H	-5.7789	1.343963	0.297342
C	7.894699	6.138879	-1.09844
H	8.075652	6.612584	-2.0634
H	7.551146	6.875972	-0.36801
H	8.807285	5.66585	-0.72642
C	-6.5642	7.167451	1.767369
H	-6.9724	7.181979	2.778069
H	-6.26115	8.172452	1.462109

H	-7.30614	6.787802	1.059968
C	-7.40073	-6.36163	-1.44637
H	-8.33709	-6.0754	-0.96025
H	-7.59059	-6.72896	-2.45505
H	-6.90703	-7.12999	-0.84552
C	5.91398	-7.51616	2.028833
H	5.981988	-7.91547	3.040962
H	5.800854	-8.32657	1.303964
H	6.810354	-6.94046	1.783207
H	3.187333	-2.98844	-2.67367

Computed geometry and energy data of **14**.
Electronic energy E = -2579.125385 a.u. Free Energy G = -2578.472309 a.u. Entropy S = 375.556 kcal/mol•K
Table S20. Atom coordinates of **14**.

N	-1.21478	-1.77707	-0.10904
N	1.507862	-1.09149	-0.08674
C	-2.58442	-1.85244	-0.07926
C	-0.77935	-3.09453	-0.16512
C	2.837339	-0.71702	-0.03724
C	1.548922	-2.43768	-0.18041
C	-3.44901	-0.76437	-0.05408
C	-3.0324	-3.23	-0.10489
C	0.573338	-3.4165	-0.21487
C	-1.90347	-4.00702	-0.16059
C	3.240648	0.605365	0.058647
C	3.720529	-1.87971	-0.09986
C	2.877388	-2.95801	-0.20477
C	-3.07297	0.566145	-0.04383
H	-4.51251	-0.97432	-0.05756
C	-4.46568	-3.67946	-0.04211
C	1.27511	-4.76699	-0.2781
C	-1.83085	-5.50558	-0.20451
C	2.36365	1.680495	0.094227
H	4.304193	0.812478	0.092812
C	5.218383	-1.81049	-0.04017
C	2.825635	-4.46519	-0.31687
C	-4.01295	1.671409	-0.04727
N	-1.77604	1.026062	-0.02895
C	-5.00125	-3.75403	1.398924
H	-4.57203	-4.66426	-0.50899
H	-5.10861	-3.01089	-0.62452
H	-1.30207	-5.86538	-1.09504
H	-1.30746	-5.91701	0.667381
C	2.783964	3.06864	0.171808
N	0.988384	1.591694	0.038809
H	5.649862	-2.80659	0.079999
H	5.642782	-1.36698	-0.95137
C	3.46744	-5.04123	-1.59468
H	3.319612	-4.93992	0.53832
C	-5.50556	1.526878	-0.06967

C	-3.26367	2.816703	-0.03275
C	-1.87307	2.396589	-0.01554
H	-4.90215	-2.78332	1.901855
H	-4.41379	-4.4568	2.001541
C	4.207022	3.538263	0.286891
C	1.641522	3.822861	0.153659
C	0.535498	2.888945	0.070984
H	3.138897	-4.4976	-2.48614
H	3.139296	-6.08271	-1.72446
H	-6.0004	2.498374	0.018824
H	-5.85484	1.063476	-1.00149
C	-3.73864	4.242208	-0.06355
C	-0.79653	3.269143	0.033903
C	4.723208	3.514312	1.736768
H	4.869811	2.927139	-0.335
H	4.296865	4.557875	-0.10281
C	1.500735	5.314901	0.213201
C	-3.73171	4.839411	-1.48206
H	-3.12225	4.870612	0.58872
H	-4.75403	4.307235	0.341319
H	-1.01093	4.331362	0.061923
H	4.63444	2.507094	2.164377
H	4.116813	4.160987	2.381625
H	2.47681	5.807751	0.182124
H	0.997859	5.639314	1.133545
H	-2.72975	4.781143	-1.92617
H	-4.38251	4.265354	-2.15247
H	0.969235	-5.34075	-1.16126
Ni	-0.12732	-0.05234	-0.04698
H	-2.83235	-5.94507	-0.22032
C	4.982059	-5.08681	-1.55586
O	5.657081	-5.17818	-0.54855
O	5.503008	-5.06124	-2.7978
C	6.173408	3.942816	1.848686
O	6.924881	4.145563	0.916526
O	6.541855	4.065751	3.141584
C	-4.17418	6.289457	-1.50848
O	-4.43014	6.968551	-0.53484
O	-4.24546	6.749451	-2.77573
C	-6.45884	-4.16716	1.461283
O	-7.19443	-4.31176	0.505901
O	-6.85389	-4.35175	2.738949
H	-5.8641	0.898769	0.755327
H	5.556167	-1.19317	0.801524
H	0.910953	5.700158	-0.6279
C	-8.23011	-4.72989	2.918062
H	-8.36774	-4.83146	3.994674
H	-8.89551	-3.96046	2.517729
H	-8.4364	-5.67779	2.414179
C	-4.64478	8.12393	-2.91867

H	-4.64544	8.31822	-3.99133
H	-5.64276	8.279332	-2.50047
H	-3.93769	8.784537	-2.41004
C	7.909977	4.448495	3.36682
H	8.115556	5.422412	2.914919
H	8.025372	4.497601	4.449703
H	8.591634	3.706758	2.94227
C	6.935994	-5.17351	-2.87801
H	7.171331	-5.14636	-3.94189
H	7.41429	-4.33977	-2.35788
H	7.272483	-6.11364	-2.43348
H	1.030597	-5.38998	0.59054

Computed geometry and energy data of **15**.
Electronic energy E = -2579.131747 a.u. Free Energy G = -2578.476933 a.u. Entropy S = 373.881 kcal/mol•K
Table S21. Atom coordinates of **15**.

N	-1.78749	0.367618	-0.06166
N	-0.36304	-1.98228	-0.1971
C	-2.28705	1.609096	0.249636
C	-2.89405	-0.43475	-0.2893
C	0.459487	-3.07786	-0.0603
C	-1.60367	-2.49484	-0.49595
C	-1.53952	2.768767	0.398203
C	-3.72897	1.594677	0.280342
C	-2.80452	-1.79638	-0.61114
C	-4.11917	0.329561	-0.0764
C	1.829072	-3.02631	0.14432
C	-0.27188	-4.30961	-0.26041
C	-1.55022	-3.93928	-0.56766
C	-0.17608	2.859999	0.205853
H	-2.076	3.68887	0.59723
C	-4.59442	2.764913	0.659153
C	-4.03519	-2.59811	-1.01581
C	-5.55021	-0.12949	-0.14877
C	2.575687	-1.86401	0.099799
H	2.355235	-3.96784	0.250892
C	0.302455	-5.69162	-0.16898
C	-2.74718	-4.76773	-0.91534
C	0.555927	4.110511	0.162611
N	0.655917	1.789428	-0.02022
C	-4.74108	2.924789	2.182861
H	-5.58948	2.661648	0.215613
H	-4.19084	3.694829	0.245073
H	-5.87533	-0.34864	-1.17282
H	-5.73199	-1.02911	0.447914
C	4.027135	-1.82476	0.108381
N	2.048399	-0.60449	-0.06946
H	-0.44186	-6.44391	-0.44662
H	1.166896	-5.81967	-0.8324
C	-3.69955	-3.91275	-1.75559

H	-3.2767	-5.10752	-0.01409
H	-2.4586	-5.6751	-1.45769
C	-0.05217	5.466235	0.36582
C	1.855516	3.784886	-0.11669
C	1.904639	2.335615	-0.19702
H	-3.75643	3.017129	2.659543
H	-5.20127	2.036432	2.631117
C	4.925242	-3.00984	0.323802
C	4.376812	-0.51883	-0.1028
C	3.136515	0.227082	-0.19335
H	-3.21497	-3.64932	-2.70481
H	0.714871	6.24558	0.393471
H	-0.75264	5.722576	-0.43962
C	3.026203	4.704735	-0.31909
C	3.074011	1.603594	-0.31709
C	5.087023	-3.36803	1.81175
H	4.546237	-3.88702	-0.21233
H	5.914862	-2.8118	-0.10068
C	5.746266	0.084744	-0.20021
C	3.334521	4.952821	-1.80625
H	3.923187	4.304632	0.166791
H	2.834546	5.66721	0.166178
H	4.007506	2.14394	-0.42229
H	4.112631	-3.56859	2.275193
H	5.51062	-2.52679	2.373528
H	6.520946	-0.68743	-0.20831
H	5.957091	0.75318	0.644755
H	3.530235	4.008766	-2.33026
H	2.470473	5.396276	-2.316
H	-4.67527	-1.99839	-1.66318
Ni	0.13982	-0.10666	-0.09237
H	-6.21437	0.649095	0.235936
C	-4.97938	-4.66189	-2.09079
O	-5.34298	-5.70275	-1.58189
O	-5.68925	-4.01098	-3.03719
C	5.969786	-4.58186	2.027143
O	6.45437	-5.26796	1.150182
O	6.153271	-4.81787	3.343523
C	4.529278	5.863712	-2.01085
O	5.221192	6.331005	-1.12905
O	4.739205	6.096812	-3.32379
C	-5.56125	4.141016	2.566851
O	-5.94823	5.002316	1.803117
O	-5.80695	4.158624	3.893988
H	-0.61155	5.521639	1.307883
H	0.640103	-5.92533	0.849171
H	5.862745	0.67742	-1.11597
C	-6.55976	5.286507	4.374078
H	-6.65789	5.136255	5.449305
H	-6.03001	6.219471	4.164361

H	-7.54434	5.320553	3.900334
C	5.855896	6.948276	-3.63543
H	5.871957	7.023141	-4.72285
H	5.723293	7.93557	-3.18527
H	6.787598	6.510266	-3.26778
C	6.969989	-5.95754	3.66494
H	7.973261	-5.84117	3.246816
H	7.010982	-5.99009	4.753794
H	6.522968	-6.87409	3.270955
C	-6.93513	-4.62283	-3.41633
H	-7.36529	-3.96597	-4.17242
H	-6.76123	-5.62001	-3.82879
H	-7.60142	-4.70392	-2.55359
H	-4.63334	-2.85116	-0.1278

Computed geometry and energy data of **16**.
Electronic energy E = -2579.123979 a.u. Free Energy G = -2578.472455 a.u. Entropy S = 379.125 kcal/mol•K
Table S22. Atom coordinates of **16**.

N	-0.74616	-1.73355	-0.02473
N	-1.68225	0.895532	-0.00586
C	-0.2485	-3.02523	-0.04227
C	-2.08773	-1.90022	-0.02961
C	-1.88062	2.253525	-0.00594
C	-2.96111	0.347045	0.024694
C	1.107442	-3.30407	-0.01828
C	-1.32582	-4.00997	-0.06373
C	-3.1615	-1.02918	-0.0046
C	-2.47853	-3.27003	-0.0543
C	-0.88542	3.219857	-0.04748
C	-3.28774	2.581327	0.038056
C	-3.96617	1.390619	0.061581
C	2.088599	-2.32718	0.011984
H	1.422684	-4.34132	-0.01199
C	-1.15011	-5.50133	-0.11803
C	-4.44067	-1.86396	-0.04731
C	-3.97701	-3.36705	-0.04051
C	0.472359	2.970332	-0.06875
H	-1.2047	4.255546	-0.05269
C	-3.84417	3.97453	0.062199
C	-5.45561	1.207991	0.165376
C	3.507293	-2.62176	0.054914
N	1.868645	-0.96419	0.002429
C	-0.9174	-6.01948	-1.54872
H	-2.03999	-5.98881	0.295639
H	-0.31343	-5.82033	0.513563
H	-4.37636	-3.90654	-0.90759
C	1.488448	4.007433	-0.10483
N	1.045699	1.719264	-0.03465
H	-4.9368	3.968462	0.013512
H	-3.56004	4.510328	0.977172

C	-5.93531	1.095683	1.625213
H	-5.79233	0.327047	-0.38388
H	-5.96223	2.059399	-0.3033
C	4.093281	-4.00216	0.08366
C	4.154513	-1.41648	0.06806
C	3.121334	-0.39773	0.030016
H	-0.0435	-5.53195	-2.00048
H	-1.76236	-5.76976	-2.2009
C	1.220023	5.483733	-0.18814
C	2.695429	3.364251	-0.08326
C	2.401907	1.944971	-0.03744
H	-5.74198	2.019263	2.180449
H	-5.37621	0.310088	2.151933
H	5.185701	-3.97053	0.039328
H	3.81658	-4.54183	0.998581
C	5.631787	-1.15146	0.14621
C	3.375937	0.962375	0.003182
C	0.949537	5.956469	-1.62761
H	0.367826	5.76003	0.442483
H	2.073078	6.041905	0.211453
C	4.074775	3.95262	-0.10591
C	6.108671	-0.87476	1.583134
H	5.90855	-0.30317	-0.48948
H	6.186845	-2.0079	-0.25048
H	4.410805	1.284141	0.003652
H	0.102921	5.41313	-2.06609
H	1.80496	5.738828	-2.27846
H	4.041158	5.045193	-0.06628
H	4.62078	3.673036	-1.01623
H	5.568655	-0.02436	2.018429
H	5.890108	-1.72616	2.23893
H	-5.10331	-1.6566	0.799864
Ni	0.131479	-0.01755	-0.01685
H	-4.34972	-3.88948	0.849323
C	-7.40789	0.748648	1.72944
O	-8.07186	0.228597	0.855159
O	-7.89894	1.068875	2.944629
C	0.650774	7.44072	-1.70968
O	0.557756	8.196905	-0.76406
O	0.491338	7.830315	-2.99236
C	7.593881	-0.57958	1.66059
O	8.348319	-0.49302	0.712965
O	7.98658	-0.41519	2.941707
C	-0.69251	-7.51814	-1.59981
O	-0.54606	-8.24435	-0.63762
O	-0.66251	-7.9589	-2.87561
H	3.747151	-4.60718	-0.76361
H	-3.48231	4.570844	-0.78469
H	4.67517	3.611037	0.74656
C	-0.43013	-9.36852	-3.04317

H	-0.44058	-9.54068	-4.11956
H	0.536997	-9.65178	-2.61939
H	-1.21761	-9.94824	-2.55456
C	9.380986	-0.1191	3.133745
H	9.513084	-0.01946	4.211232
H	10.00289	-0.92965	2.744846
H	9.649506	0.811623	2.627106
C	0.192756	9.22361	-3.18864
H	0.999997	9.848263	-2.7973
H	0.097761	9.353255	-4.26684
H	-0.74092	9.490935	-2.68681
C	-9.27968	0.731357	3.168322
H	-9.49901	1.057053	4.185206
H	-9.92191	1.25033	2.452163
H	-9.4324	-0.34659	3.069608
H	-5.02213	-1.64949	-0.95168

Computed geometry and energy data of **3a**.
Electronic energy E = -1832.161079 a.u. Free Energy G = - -1831.650903 a.u. Entropy S = 284.861 kcal/mol•K
Table S23. Atom coordinates of **3a**.

N	1.043711	0.677634	-0.11822
C	1.35416	1.982603	-0.17994
C	2.191855	-0.05455	-0.13464
C	2.854366	2.224429	-0.35712
C	0.431142	3.030921	-0.13074
C	3.4392	0.819101	-0.06154
C	2.17648	-1.43756	-0.19469
C	3.185579	2.738984	-1.76937
H	3.206344	2.964766	0.372708
C	-0.96225	2.949373	-0.03288
H	0.840957	4.034465	-0.18001
C	4.112663	0.721872	1.328127
H	4.168286	0.514995	-0.82069
C	3.357087	-2.40203	-0.29754
C	1.018575	-2.23888	-0.20977
H	4.266791	2.87765	-1.88593
H	2.850461	2.027113	-2.53242
H	2.69739	3.699306	-1.9686
N	-1.69283	1.787909	-0.00165
C	-1.89291	4.043038	0.058111
C	5.461378	1.443154	1.417203
H	3.434008	1.142088	2.080751
H	4.26186	-0.32952	1.590331
C	2.727085	-3.82528	-0.3631
H	3.970601	-2.23519	-1.19231
H	4.04769	-2.35383	0.55291
N	-0.31227	-2.05888	-0.15501
C	1.275445	-3.63092	-0.29964
C	-3.04377	2.049676	0.073995
H	-1.28426	0.863672	-0.0537

C	-1.51873	5.494597	0.115085
C	-3.16831	3.496432	0.120565
C	6.561565	0.756749	0.627929
H	5.395475	2.4854	1.082859
H	5.797598	1.491198	2.461625
O	3.360869	-4.86593	-0.44942
C	-0.95082	-3.29621	-0.20501
H	-0.85121	-1.19909	-0.08722
C	0.058362	-4.31281	-0.29845
C	-4.06968	1.119056	0.079626
H	-0.49261	5.627353	0.46951
H	-1.59178	5.986292	-0.86435
H	-2.17026	6.041965	0.804143
C	-4.45	4.157345	0.22582
O	7.672037	1.521648	0.584382
O	6.484641	-0.33947	0.110179
C	-2.34408	-3.40007	-0.16427
C	-0.16683	-5.79138	-0.37762
C	-3.99332	-0.28867	0.028361
H	-5.07255	1.53212	0.113307
H	-5.34167	3.651594	0.574993
C	8.797091	0.951089	-0.11
C	-3.23433	-2.32318	-0.07807
H	-2.75982	-4.40193	-0.20548
H	-0.767	-6.06119	-1.25555
H	0.790411	-6.31364	-0.44494
H	-0.69972	-6.16576	0.505454
C	-5.17056	-1.16029	0.030406
N	-2.84635	-1.00598	-0.03518
H	9.1015	0.012323	0.359477
H	8.545349	0.762705	-1.15674
H	9.592548	1.692546	-0.0352
C	-4.69255	-2.44202	-0.03639
C	-6.59498	-0.69488	0.097085
C	-5.46621	-3.73117	-0.0265
H	-6.82674	0.022241	-0.701
H	-7.29347	-1.53111	-0.00271
H	-6.81747	-0.19695	1.050383
C	-5.57502	-4.36973	1.372234
H	-5.00162	-4.44994	-0.71414
H	-6.47582	-3.55614	-0.41736
H	-4.58397	-4.5828	1.787728
H	-6.08802	-3.69762	2.068868
H	-6.13634	-5.31037	1.328978
N	-4.64586	5.396658	-0.12798
N	-4.84632	6.481598	-0.43776

Computed geometry and energy data of **3b**.
Electronic energy E = -1722.594395 a.u. Free Energy G = -1722.090671 a.u. Entropy S = 270.491 kcal/mol•K
Table S24. Atom coordinates of **3b**.

N	0.963161	0.848248	-0.17219
C	1.501185	2.088894	-0.2311
C	1.959657	-0.06433	-0.1687
C	3.021025	2.056336	-0.39757
C	0.769612	3.267883	-0.18964
C	3.341056	0.573295	-0.07717
C	1.707633	-1.43418	-0.22304
C	3.446519	2.47974	-1.81474
H	3.497318	2.73116	0.324665
C	-0.62728	3.416988	-0.09693
H	1.332347	4.195436	-0.23353
C	3.9532	0.376246	1.33101
H	4.020388	0.133692	-0.81604
C	2.720474	-2.57471	-0.31647
C	0.439899	-2.03023	-0.2366
H	4.535626	2.421365	-1.92468
H	2.99326	1.82757	-2.57008
H	3.137768	3.508423	-2.03044
N	-1.54417	2.378094	-0.05987
C	-1.36045	4.629513	-0.03198
C	5.413275	0.826719	1.439466
H	3.351941	0.934575	2.059098
H	3.892666	-0.67831	1.615232
C	1.871172	-3.87803	-0.36507
H	3.346762	-2.51701	-1.21624
H	3.416436	-2.62377	0.529115
N	-0.84745	-1.63826	-0.18615
C	0.466994	-3.4505	-0.31068
C	-2.82301	2.839773	0.018183
H	-1.26933	1.403325	-0.0975
C	-0.76185	5.998072	-0.04298
C	-2.74366	4.299206	0.043277
C	6.373861	-0.08071	0.691973
H	5.557516	1.853698	1.083648
H	5.730305	0.832733	2.490967
O	2.324806	-5.00851	-0.43458
C	-1.67493	-2.75499	-0.22068
H	-1.25016	-0.70493	-0.12711
C	-0.83775	-3.92734	-0.30322
C	-4.00294	2.099463	0.057565
H	-0.07111	6.14071	0.797496
H	-0.19219	6.179589	-0.96318
H	-1.5402	6.762314	0.026778
C	-3.89226	5.104569	0.123775
O	7.604851	0.465674	0.630153
O	6.099014	-1.16611	0.219993
C	-3.06364	-2.63709	-0.16984
C	-1.30107	-5.349	-0.36557
C	-4.16973	0.71151	0.019875
H	-4.89025	2.722642	0.117653

H	-3.64186	6.180381	0.136836
C	8.61123	-0.33101	-0.02328
C	-3.76167	-1.42139	-0.08272
H	-3.63861	-3.55681	-0.19772
H	-1.92776	-5.52832	-1.24808
H	-0.44188	-6.02193	-0.41341
H	-1.89897	-5.61546	0.514841
C	-5.47912	0.046038	0.050035
N	-3.1581	-0.1964	-0.05793
H	8.740242	-1.28472	0.494434
H	8.332566	-0.52227	-1.06259
H	9.526662	0.258509	0.025609
C	-5.22357	-1.29494	-0.01631
C	-6.79979	0.749204	0.13892
C	-6.19833	-2.43886	0.012385
H	-6.9158	1.493301	-0.65878
H	-7.63381	0.045568	0.060054
H	-6.90914	1.284468	1.091038
C	-6.37582	-3.05769	1.413066
H	-5.87608	-3.22053	-0.68819
H	-7.17407	-2.09618	-0.35181
H	-5.42453	-3.43597	1.80337
H	-6.75205	-2.31303	2.12288
H	-7.08712	-3.89108	1.382513

Computed geometry and energy data of **3c**.
Electronic energy E = -1722.597605 a.u. Free Energy G = -1722.096893 a.u. Entropy S = 275.093 kcal/mol•K
Table S25. Atom coordinates of **3c**.

N	0.960789	0.830903	-0.16066
C	1.497272	2.064484	-0.22759
C	1.962564	-0.08881	-0.15988
C	3.017918	2.034679	-0.39564
C	0.773835	3.254991	-0.19166
C	3.342303	0.553637	-0.07232
C	1.711374	-1.45052	-0.21365
C	3.440372	2.456234	-1.81428
H	3.492594	2.713453	0.324285
C	-0.6188	3.420152	-0.10084
H	1.351198	4.172857	-0.23604
C	3.959525	0.36181	1.333941
H	4.021336	0.114931	-0.81214
C	2.715303	-2.59875	-0.30124
C	0.435954	-2.04845	-0.23082
H	4.529651	2.402167	-1.92528
H	2.989282	1.79949	-2.56698
H	3.126977	3.482814	-2.03347
N	-1.53797	2.385713	-0.05848
C	-1.33712	4.642666	-0.0446
C	5.416348	0.823713	1.439702
H	3.355611	0.914901	2.063912

H	3.907869	-0.69346	1.617064
C	1.857407	-3.89797	-0.35492
H	3.348459	-2.54584	-1.19654
H	3.404732	-2.65333	0.549576
N	-0.84755	-1.65029	-0.18355
C	0.45907	-3.46384	-0.30519
C	-2.82669	2.848297	0.019132
H	-1.27148	1.409263	-0.0955
C	-0.76375	6.023916	-0.04303
C	-2.7281	4.31804	0.040397
C	6.382603	-0.07538	0.689634
H	5.552038	1.852197	1.085095
H	5.735973	0.830198	2.490574
O	2.30968	-5.03092	-0.42418
C	-1.68051	-2.76552	-0.22094
H	-1.24223	-0.71395	-0.12429
C	-0.85589	-3.93491	-0.30141
C	-3.99531	2.114889	0.057756
H	-0.66889	6.424931	0.975826
H	0.229576	6.053594	-0.50025
H	-1.4053	6.714118	-0.60232
C	-3.7851	5.175215	0.123853
O	7.604238	0.490778	0.607084
O	6.121212	-1.1703	0.232802
C	-3.0752	-2.63336	-0.17214
C	-1.32078	-5.35733	-0.36579
C	-4.1629	0.712098	0.018566
H	-4.90035	2.711705	0.117959
H	-3.92936	6.245859	0.165724
C	8.615192	-0.29736	-0.04903
C	-3.76711	-1.42382	-0.08576
H	-3.65421	-3.55105	-0.20135
H	-1.94648	-5.53788	-1.24886
H	-0.46112	-6.02988	-0.41424
H	-1.918	-5.62736	0.51414
C	-5.47369	0.054458	0.046235
N	-3.15868	-0.18794	-0.05805
H	8.765728	-1.24289	0.477882
H	8.327405	-0.5055	-1.08263
H	9.521757	0.307006	-0.01818
C	-5.22432	-1.2896	-0.02171
C	-6.79388	0.760307	0.133807
C	-6.20743	-2.42673	0.005259
H	-6.9128	1.500561	-0.66779
H	-7.62883	0.057215	0.058024
H	-6.90515	1.298764	1.084419
C	-6.40285	-3.03536	1.407972
H	-5.88374	-3.21556	-0.68643
H	-7.17772	-2.08076	-0.37091
H	-5.45759	-3.41775	1.808535

H	-6.77965	-2.28348	2.109995
H	-7.12012	-3.86378	1.376676

Computed geometry and energy data of **3d**.
Electronic energy E = -2032.313158 a.u. Free Energy G = -2031.691362 a.u. Entropy S = 322.476 kcal/mol•K
Table S26. Atom coordinates of **3d**.

C	-4.52513	-1.60187	-1.13567
C	-5.38346	-2.83401	-1.32851
C	-6.856	-2.57127	-1.17057
C	-7.50822	-2.33743	0.06426
C	-6.81782	-2.31854	1.312055
C	-8.91655	-2.11235	0.096492
C	-7.49688	-2.09239	2.501461
C	-9.58407	-1.88845	1.290367
C	-8.8816	-1.87687	2.504516
H	-5.05469	-0.65742	-1.22084
H	-5.0636	-3.62191	-0.63294
H	-5.21113	-3.24492	-2.3352
H	-5.74336	-2.47315	1.330781
H	-9.46721	-2.12098	-0.84131
H	-6.94618	-2.08098	3.438585
H	-10.6581	-1.72108	1.283967
H	-9.40627	-1.70074	3.439166
H	-7.46443	-2.55007	-2.07156
N	1.81394	-0.77753	-0.0175
C	1.546514	-2.09594	-0.07259
C	3.151927	-0.60413	0.159637
C	2.783532	-2.9572	0.195005
C	0.292024	-2.65565	-0.30524
C	3.925224	-1.91538	0.080596
C	3.708747	0.647023	0.366796
C	2.71485	-3.63635	1.574351
H	2.875755	-3.73681	-0.57192
C	-0.93643	-2.00203	-0.50818
H	0.253165	-3.73951	-0.3287
C	4.712399	-2.02085	-1.2476
H	4.63509	-1.99666	0.911408
C	5.163767	1.009627	0.657951
C	2.997036	1.862426	0.381553
H	3.619866	-4.22645	1.760463
H	2.626102	-2.89015	2.372289
H	1.851523	-4.30708	1.644684
N	-1.1173	-0.63133	-0.47129
C	-2.19656	-2.60042	-0.77494
C	5.652362	-3.22851	-1.31791
H	3.998415	-2.07564	-2.07871
H	5.301923	-1.11178	-1.39793
C	5.180613	2.559063	0.82476
H	5.546317	0.542633	1.574834
H	5.861955	0.723164	-0.13759

N	1.727294	2.267848	0.207902
C	3.797815	3.003288	0.63602
C	-2.42635	-0.28436	-0.68448
H	-0.36804	0.025552	-0.28875
C	-2.42658	-4.07568	-0.91652
C	-3.16022	-1.55129	-0.88827
C	6.854334	-3.10395	-0.39909
H	5.136712	-4.1686	-1.08877
H	6.040675	-3.34764	-2.33842
O	6.177572	3.223973	1.06475
C	1.661717	3.652639	0.33813
H	0.890309	1.724851	0.007302
C	2.981058	4.137238	0.614519
C	-2.95009	0.993878	-0.68799
H	-3.04891	-4.30565	-1.7871
H	-1.48482	-4.61581	-1.04397
H	-2.92823	-4.50352	-0.03777
O	7.530584	-4.26932	-0.32826
O	7.194513	-2.09745	0.189924
C	0.447242	4.338163	0.193609
C	3.386363	5.562873	0.83204
C	-2.29455	2.229491	-0.47833
H	-4.01735	1.060532	-0.86701
C	8.717262	-4.25442	0.487183
C	-0.78521	3.745303	-0.083
H	0.479254	5.417309	0.30562
H	2.860226	6.006629	1.68653
H	4.460191	5.620729	1.025592
H	3.162648	6.185086	-0.04366
C	-2.99699	3.517916	-0.49387
N	-0.97615	2.387745	-0.2338
H	9.435691	-3.52463	0.105463
H	8.467965	-4.00396	1.521387
H	9.126358	-5.26286	0.425308
C	-2.04726	4.470547	-0.24322
C	-4.46479	3.701526	-0.74097
C	-2.21282	5.963605	-0.18044
H	-5.07218	3.110814	-0.04309
H	-4.76099	4.748733	-0.62753
H	-4.7495	3.390127	-1.75495
C	-1.86804	6.675144	-1.5037
H	-1.58625	6.374721	0.621946
H	-3.24622	6.206144	0.095167
H	-0.83187	6.478618	-1.80017
H	-2.5162	6.325194	-2.31464
H	-1.99569	7.759714	-1.40778

Computed geometry and energy data of **3e**.
Electronic energy E = -2032.2845701 a.u.
Table S27. Atom coordinates of **3e**.

C	-4.52513	-1.60187	-1.13567
C	-5.38346	-2.83401	-1.32851
C	-6.856	-2.57127	-1.17057
C	-7.50822	-2.33743	0.06426
C	-6.81782	-2.31854	1.312055
C	-8.91655	-2.11235	0.096492
C	-7.49688	-2.09239	2.501461
C	-9.58407	-1.88845	1.290367
C	-8.8816	-1.87687	2.504516
H	-5.05469	-0.65742	-1.22084
H	-5.0636	-3.62191	-0.63294
H	-5.21113	-3.24492	-2.3352
H	-5.74336	-2.47315	1.330781
H	-9.46721	-2.12098	-0.84131
H	-6.94618	-2.08098	3.438585
H	-10.6581	-1.72108	1.283967
H	-9.40627	-1.70074	3.439166
H	-7.46443	-2.55007	-2.07156
N	1.81394	-0.77753	-0.0175
C	1.546514	-2.09594	-0.07259
C	3.151927	-0.60413	0.159637
C	2.783532	-2.9572	0.195005
C	0.292024	-2.65565	-0.30524
C	3.925224	-1.91538	0.080596
C	3.708747	0.647023	0.366796
C	2.71485	-3.63635	1.574351
H	2.875755	-3.73681	-0.57192
C	-0.93643	-2.00203	-0.50818
H	0.253165	-3.73951	-0.3287
C	4.712399	-2.02085	-1.2476
H	4.63509	-1.99666	0.911408
C	5.163767	1.009627	0.657951
C	2.997036	1.862426	0.381553
H	3.619866	-4.22645	1.760463
H	2.626102	-2.89015	2.372289
H	1.851523	-4.30708	1.644684
N	-1.1173	-0.63133	-0.47129
C	-2.19656	-2.60042	-0.77494
C	5.652362	-3.22851	-1.31791
H	3.998415	-2.07564	-2.07871
H	5.301923	-1.11178	-1.39793
C	5.180613	2.559063	0.82476
H	5.546317	0.542633	1.574834
H	5.861955	0.723164	-0.13759
N	1.727294	2.267848	0.207902
C	3.797815	3.003288	0.63602
C	-2.42635	-0.28436	-0.68448
H	-0.36804	0.025552	-0.28875
C	-2.42658	-4.07568	-0.91652
C	-3.16022	-1.55129	-0.88827

C	6.854334	-3.10395	-0.39909
H	5.136712	-4.1686	-1.08877
H	6.040675	-3.34764	-2.33842
O	6.177572	3.223973	1.06475
C	1.661717	3.652639	0.33813
H	0.890309	1.724851	0.007302
C	2.981058	4.137238	0.614519
C	-2.95009	0.993878	-0.68799
H	-3.04891	-4.30565	-1.7871
H	-1.48482	-4.61581	-1.04397
H	-2.92823	-4.50352	-0.03777
O	7.530584	-4.26932	-0.32826
O	7.194513	-2.09745	0.189924
C	0.447242	4.338163	0.193609
C	3.386363	5.562873	0.83204
C	-2.29455	2.229491	-0.47833
H	-4.01735	1.060532	-0.86701
C	8.717262	-4.25442	0.487183
C	-0.78521	3.745303	-0.083
H	0.479254	5.417309	0.30562
H	2.860226	6.006629	1.68653
H	4.460191	5.620729	1.025592
H	3.162648	6.185086	-0.04366
C	-2.99699	3.517916	-0.49387
N	-0.97615	2.387745	-0.2338
H	9.435691	-3.52463	0.105463
H	8.467965	-4.00396	1.521387
H	9.126358	-5.26286	0.425308
C	-2.04726	4.470547	-0.24322
C	-4.46479	3.701526	-0.74097
C	-2.21282	5.963605	-0.18044
H	-5.07218	3.110814	-0.04309
H	-4.76099	4.748733	-0.62753
H	-4.7495	3.390127	-1.75495
C	-1.86804	6.675144	-1.5037
H	-1.58625	6.374721	0.621946
H	-3.24622	6.206144	0.095167
H	-0.83187	6.478618	-1.80017
H	-2.5162	6.325194	-2.31464
H	-1.99569	7.759714	-1.40778

Computed geometry and energy data of **3f**.
Electronic energy E = -1723.282429 a.u. Free Energy G = -1722.768201 a.u. Entropy S = 274.448 kcal/mol•K
Table S28. Atom coordinates of **3f**.

N	0.965579	0.82103	-0.17018
C	1.485621	2.062316	-0.24025
C	1.979746	-0.08422	-0.17058
C	3.006055	2.050699	-0.41748
C	0.74927	3.243427	-0.20157
C	3.350398	0.577022	-0.08406

C	1.747645	-1.44956	-0.22175
C	3.411755	2.46458	-1.84324
H	3.477841	2.741496	0.292886
C	-0.64513	3.4	-0.10249
H	1.318993	4.165538	-0.25398
C	3.961655	0.402193	1.327182
H	4.038934	0.142412	-0.81747
C	2.765629	-2.58509	-0.30931
C	0.480129	-2.06315	-0.23495
H	4.500713	2.424166	-1.96305
H	2.963064	1.795088	-2.58608
H	3.082238	3.484742	-2.06869
N	-1.55776	2.356841	-0.05745
C	-1.37471	4.612041	-0.0391
C	5.414338	0.875433	1.437892
H	3.349626	0.957299	2.048866
H	3.915284	-0.65094	1.619444
C	1.923286	-3.89512	-0.35853
H	3.39554	-2.52622	-1.20656
H	3.458484	-2.62804	0.539385
N	-0.80746	-1.67915	-0.18624
C	0.519814	-3.47791	-0.30682
C	-2.85041	2.810513	0.023898
H	-1.28611	1.382	-0.0968
C	-0.82369	6.002144	-0.05237
C	-2.76128	4.281334	0.045853
C	6.391946	-0.02225	0.701037
H	5.545019	1.902208	1.076111
H	5.727504	0.892657	2.490586
O	2.389161	-5.02262	-0.42705
C	-1.62744	-2.80362	-0.22062
H	-1.21091	-0.74655	-0.1278
C	-0.79018	-3.96371	-0.30033
C	-4.0036	2.05318	0.063564
H	-1.08614	6.543953	0.866119
H	0.265434	6.01466	-0.14045
H	-1.22958	6.58282	-0.89123
C	-3.81607	5.163254	0.131646
O	7.611158	0.550378	0.625876
O	6.140969	-1.12106	0.247805
C	-3.02386	-2.68618	-0.17027
C	-1.23901	-5.39149	-0.36075
C	-4.14897	0.646645	0.022951
H	-4.92664	2.620419	0.12492
H	-3.64765	6.234577	0.139099
C	8.631858	-0.23532	-0.01787
C	-3.72849	-1.48477	-0.08377
H	-3.59271	-3.61024	-0.19821
H	-1.8764	-5.57802	-1.23412
H	-0.37193	-6.05325	-0.42367

H	-1.81877	-5.67075	0.528019
C	-5.45206	-0.0273	0.05125
N	-3.13468	-0.24058	-0.05551
H	8.781904	-1.17835	0.51367
H	8.354761	-0.44852	-1.05339
H	9.535284	0.373385	0.01928
C	-5.1869	-1.36795	-0.0189
C	-6.7815	0.660948	0.140284
C	-6.15684	-2.51641	0.004173
H	-6.91776	1.389362	-0.66959
H	-7.60657	-0.05517	0.079539
H	-6.89413	1.208832	1.085402
C	-6.34951	-3.12945	1.405359
H	-5.82199	-3.30035	-0.68772
H	-7.12988	-2.18094	-0.37457
H	-5.40139	-3.50279	1.807713
H	-6.73577	-2.3827	2.107758
H	-7.05818	-3.96509	1.37081
H	-4.84512	4.828104	0.195813

Computed geometry and energy data of **9**.
Electronic energy E = -2032.36544 a.u. Free Energy G = -2031.734115 a.u. Entropy S = 312.114 kcal/mol•K
Table S29. Atom coordinates of **9**.

O	-5.46135	4.130095	-0.59067
O	-7.51861	-0.94099	0.100832
O	-8.23068	-3.04198	0.521986
N	1.442287	1.782926	0.056173
N	0.942922	-1.19132	0.097564
H	0.33769	-0.38339	0.029874
N	-1.25801	2.232176	-0.16166
H	-0.53793	1.520398	-0.06349
N	-1.96746	-0.74409	-0.09077
C	2.718119	1.344759	0.184248
C	3.664858	2.462519	0.233952
C	2.912119	3.601123	0.121941
C	1.522555	3.153756	0.012256
C	0.416307	3.999438	-0.12837
H	0.596416	5.06905	-0.17035
C	-0.91571	3.581725	-0.21543
C	-2.12528	4.34095	-0.35377
C	-3.15589	3.400016	-0.37331
C	-2.59327	2.104066	-0.25153
C	-4.61145	3.260708	-0.47055
C	-4.90604	1.733332	-0.39003
H	-5.4421	1.419858	-1.29527
H	-5.58971	1.540825	0.445372
C	-3.54151	1.061755	-0.24218
C	-3.24997	-0.28736	-0.14535
C	-4.27056	-1.41744	-0.06367
H	-5.03793	-1.30335	-0.83774

C	-3.37997	-2.66175	-0.31633
H	-3.57344	-3.44814	0.424443
C	-1.97659	-2.08534	-0.12126
C	-0.83781	-2.89323	-0.029
H	-0.9999	-3.96658	-0.04933
C	0.493457	-2.48498	0.081846
C	1.656322	-3.33773	0.19407
C	2.769059	-2.52277	0.254006
C	2.317438	-1.14676	0.200828
C	3.10877	-0.00906	0.24545
H	4.173564	-0.19854	0.33175
C	5.150869	2.336215	0.392839
H	5.649208	3.301723	0.261644
H	5.584892	1.638655	-0.33413
H	5.422544	1.962059	1.389009
C	3.371676	5.032453	0.148346
H	4.412919	5.088824	-0.19158
H	2.790685	5.62407	-0.57142
C	3.264389	5.686203	1.540158
H	2.23112	5.673805	1.904137
H	3.602434	6.728601	1.508539
H	3.879152	5.149767	2.271227
C	-2.24018	5.831055	-0.45263
H	-1.69042	6.221213	-1.31826
H	-1.83384	6.326699	0.437994
H	-3.28868	6.120686	-0.55549
C	-4.96812	-1.44265	1.317588
H	-5.35269	-0.44601	1.552597
H	-4.22288	-1.6835	2.085763
C	-6.12311	-2.4448	1.412509
H	-5.82433	-3.45297	1.102248
H	-6.45293	-2.54396	2.455558
C	-7.33907	-2.0326	0.602599
C	-9.44692	-2.74592	-0.18971
H	-9.98329	-1.92493	0.29276
H	-10.0365	-3.66201	-0.15335
H	-9.22792	-2.47102	-1.22455
C	-3.55575	-3.26394	-1.72188
H	-3.37423	-2.50862	-2.49512
H	-4.57442	-3.64691	-1.85373
H	-2.8576	-4.09128	-1.89017
C	1.591023	-4.83484	0.257043
H	2.561256	-5.26032	0.520734
H	1.280933	-5.27127	-0.70179
H	0.865834	-5.16669	1.009637
C	4.198392	-2.91443	0.382103
H	4.614521	-2.79646	1.383101
C	5.193689	-2.59216	-0.73734
H	4.736988	-2.17842	-1.63325
C	6.550459	-2.04403	-0.45073

C	7.325409	-2.46988	0.640507
H	6.944659	-3.23413	1.313751
C	8.587716	-1.92691	0.878419
H	9.168295	-2.27316	1.729624
C	9.106859	-0.94596	0.030006
H	10.09102	-0.52495	0.216195
C	8.349315	-0.51443	-1.05971
H	8.740917	0.24563	-1.73079
C	7.085424	-1.05834	-1.29536
H	6.50483	-0.71987	-2.15062
C	4.807206	-4.02295	-0.4364
H	4.184209	-4.52897	-1.168
H	5.54813	-4.66042	0.038996

Computed geometry and energy data of **11**.
Electronic energy E = -2030.390044 a.u. Free Energy G = -2029.768864 a.u. Entropy S = 306.376 kcal/mol•K
Table S30. Atom coordinates of **11**.

C	4.766251	-2.24988	-1.12065
C	5.522793	-2.2703	0.216974
O	6.913465	-2.3673	-0.10721
C	5.128926	-3.4331	1.129852
C	7.72653	-2.39734	1.064174
C	7.318674	-3.55591	1.964957
O	5.93796	-3.4576	2.301844
H	4.932399	-3.20879	-1.62396
H	5.245394	-1.48926	-1.74824
H	5.346194	-1.32959	0.764091
H	5.23567	-4.38189	0.576641
H	4.093766	-3.33406	1.467564
H	7.629093	-1.44812	1.61519
H	8.761755	-2.50374	0.724538
H	7.875411	-3.5388	2.907157
H	7.516153	-4.51171	1.452354
N	-1.57243	-0.66333	-0.40187
C	-1.47542	-1.97849	-0.64755
C	-2.88074	-0.34354	-0.19532
C	-2.83896	-2.66707	-0.72613
C	-0.27368	-2.66542	-0.85325
C	-3.77772	-1.57541	-0.14959
C	-3.29548	0.966476	-0.03306
C	-3.18731	-3.07308	-2.16937
H	-2.84467	-3.56915	-0.10095
C	1.020922	-2.14167	-0.86288
H	-0.34874	-3.73506	-1.02348
C	-4.24264	-1.87671	1.295345
H	-4.66521	-1.43093	-0.77607
C	-4.71693	1.503598	0.127642
C	-2.45083	2.09397	-0.02106
H	-4.17721	-3.54222	-2.21088
H	-3.19848	-2.19765	-2.82878

H	-2.45707	-3.78516	-2.5692
N	1.363029	-0.82588	-0.69888
C	2.252404	-2.87607	-1.05249
C	-5.2842	-2.99608	1.390787
H	-3.36839	-2.1501	1.898975
H	-4.66359	-0.97113	1.741609
C	-4.56682	3.050036	0.239715
H	-5.36438	1.263765	-0.7258
H	-5.23828	1.125204	1.01499
N	-1.13412	2.348098	-0.11401
C	-3.1309	3.327777	0.140199
C	2.729499	-0.65594	-0.78035
H	0.692659	-0.08077	-0.56068
C	2.313691	-4.35886	-1.26922
C	3.294266	-1.97255	-0.99529
C	-6.64033	-2.59729	0.837253
H	-4.95703	-3.91141	0.88382
H	-5.43853	-3.28044	2.440494
O	-5.49365	3.833057	0.381206
C	-0.91782	3.720889	-0.01682
H	-0.35267	1.708251	-0.23365
C	-2.19239	4.360413	0.145152
C	3.415314	0.546995	-0.7001
H	2.007001	-4.91225	-0.37226
H	1.649193	-4.67133	-2.08369
H	3.324861	-4.68532	-1.52596
O	-7.44777	-3.67121	0.716616
O	-6.98389	-1.46747	0.552111
C	0.370249	4.261771	-0.07738
C	-2.44441	5.829743	0.288533
C	2.905372	1.849349	-0.51858
H	4.493095	0.471555	-0.8029
C	-8.77916	-3.40122	0.239033
C	1.550773	3.527312	-0.23833
H	0.451328	5.34069	0.008837
H	-2.08523	6.38754	-0.58536
H	-3.51524	6.017494	0.396444
H	-1.93392	6.242617	1.167629
C	3.748333	3.046764	-0.47068
N	1.594674	2.161093	-0.37531
H	-9.29935	-2.72132	0.918345
H	-8.74492	-2.9543	-0.75772
H	-9.27975	-4.36896	0.208025
C	2.89539	4.103635	-0.29552
C	5.243346	3.060333	-0.59175
C	3.230329	5.561828	-0.14623
H	5.581926	2.563173	-1.50982
H	5.633407	4.082443	-0.60997
H	5.725094	2.542417	0.248321
C	3.312132	6.025838	1.321457

H	2.48531	6.171377	-0.67436
H	4.187744	5.76983	-0.63894
H	2.362946	5.859613	1.842669
H	4.087731	5.472697	1.862426
H	3.550623	7.094245	1.379646

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