Electronic Supplementary Material (ESI) for Green Chemistry.

Supplementary Information

for

A molecular motor from lignocellulose

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1. Materials and methods

1.1. Reagents and solvents

The chemicals were used as received, unless otherwise specified. Solvents for purification, analysis and irradiation studies were neutralized over oven dried sodium bicarbonate.

Reagents: Dimethyl carbonate (DMC, 99%) was purchased from Alfa Aeasar. $NaHCO_3$ (99%), NaOH (98%), methanesulfonic acid (MsOH, 99%), $TiCl_4$ (99,9%) and triethylamine (Et_3N, 99%) were purchased from Sigma-Aldrich. KOH was purchased from Merck (for synthesis). P_2O_5 (98+%, ACS reagent grade) was purchased from Acros Organics. Zn powder (purum 99%) was purchased from Aldrich. (*E*)-3,4,5-Trimethoxycinnamic acid (98%, reagent grade) was purchased from TCI. 4-(3-Hydroxypropyl)-2,6-dimethoxyphenol **1** was a donation from Xianyuan Wu (PhD Barta group).

Catalysts and catalyst precursors: $Fe(NO_3)_3.9H_2O$ (99.99%-trace metal basis), Raney® Nickel (Lot #MKGB0283V), Pd@C 5wt% (Lot:#BCBQ1888V, Assey: 5% Pd basis) were purchased from Aldrich. 2,2,6,6-Tetramethylpiperidine 1-Oxyl Free Radical (TEMPO) (LOT FCB080997) was purchased from Fluorochem. KCl (99+%, for analysis) was purchased from Acros Organics.

Solvents:
Methanol anhydrous (MeOH, 99%, AR grade), ethyl acetate (EtOAc, HPLC grade), *n*-pentane (99%), diethyl ether (Et_2O, stabilized with BHT, AR grade) were purchased from Macron. Deuterated solvents: Chloroform-*d* ($CDCl_3$), DCM-d_2 (CD_2Cl_2) and DMSO-d_6 ($(CD_3)_2SO$) were purchased from Euroisotope. Dry tetrahydrofuran (THF) was obtained from an Mbraun solvent purification system (MB SPS-800). Methoxycyclopentane (CPME, stabilized with BHT, 99,5%) was purchased from TCI. UV/Vis solvents: dichloromethane (DCM, HPLC grade) and acetonitrile (ACN, HPLC grade) were purchased from Macron.

Chromatography: Reveleris X2 Flash Chromatography system or Macherey-Nagel Silicagel 60 M particle size: 0.04-0.063mm was used (TLC: silica gel 60, Merck, 0.25mm).

TLC: Merck silica gel 60, 0.25 mm. The components were visualized by UV or $KMnO_4$ staining.

1.2. Equipment and Analysis

NMR spectroscopy: ^{1}H and ^{13}C NMR spectra were recorded on a Varian Innova (^{1}H: 500 and ^{13}C: 125 MHz, respectively) and Bruker Avance NEO 600 (600 and 151 MHz, respectively) using DMSO-*d6* and basified solvents: Chloroform-*d*, DCM-d_2, Acetonitrile-d_3. Chemical shifts δ (ppm) are distinguished relative to the solvent signals of Chloroform-*d* (^{1}H: δ 7.26 ppm; ^{13}C: δ 77.0 ppm), DCM-d_2 (^{1}H: δ 5.32 ppm, ^{13}C: δ 54.00 ppm) or DMSO-*d6* (^{1}H: δ 2.5 ppm). ^{1}H and ^{13}C NMR spectra were recorded at room temperature unless otherwise stated. Data are reported as follows: chemical shifts, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, br. = broad, m = multiplet) and coupling constants (Hz).

2D NMR spectroscopy: The 2D-HSQC NMR was recorded in Chloroform-*d* using a standard pulse sequence on a Bruker Avance NEO 600 at room temperature.

UV-vis spectra: were measured on an Agilent Cary 8454 UV-Vis Diode Array System in a 1 cm quartz cuvette.

Gas chromatography-mass spectrometry (GC-MS): was performed using a Shimadzu GC-2010 plus system equipped with a GCMS QP2010 GC SE detector and a HP5 column (30 m x 0.25 mm x0.25 µm) using hydrogen as a carrier gas.

Mass spectrometry: High Resolution Mass spectra (HRMS) were recorded on an AEI-MS-902 mass spectrometer (EI$^+$) or a LTQ Orbitrap XL (ESI$^+$).

Irradiation: Thorlabs LEDs (M300F2, M340F3, M365F1) and a Spectroline TLC lamp (230V, 50Hz, 0.2 AMPS, 312 nm, 365 nm) were used.

X-ray crystal structure: was recorded on a Bruker D8 Venture diffractometer. Data collection and reduction was performed using the Bruker software suite APEX3.[1] The structures were solved by direct methods using SHELXT,[2] and refinement of the structure was performed using SHELXL.[3]

Photoisomerizaton:
UV/Vis absorption spectra of the molecular motor **7** were measured at 268-298 K in appropriate degassed solvents (Chloroform, CH_2Cl_2, DMSO or Acetonitrile [2 x 10^{-3} M, N_2]) upon irradiation with a 300 nm, 312 nm, 340 nm or 365 nm LEDs.

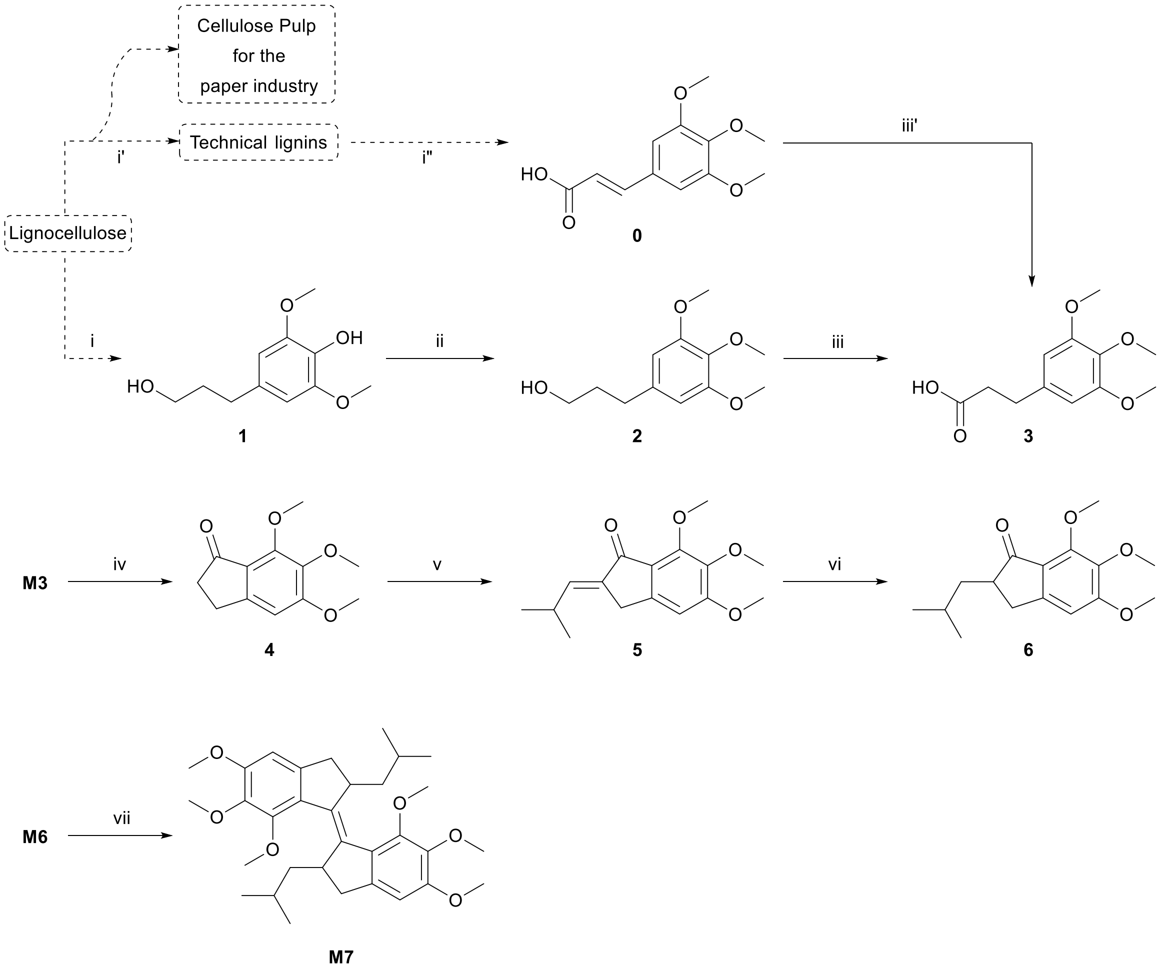
^{1}H-NMR spectra (500 MHz, 223 K) of the molecular motor **7** were measured in degassed DCM-d_2 (4.2 x 10^{-3} M). Irradiation to its PSS was performed with a Thorlab 340 nm LED coupled to a 600 µm optical fibre, which led the light into the NMR tube inside the spectrometer. Depending on the desired analysis the NMR tube was allowed to heat up to 298 K for 30 min to induce photoisomerization or thermal helix inversion.

2. Experimental procedures for synthesis of compounds (0-7):

The isolated products were confirmed by ^{1}H-NMR, ^{13}C-NMR and HRMS. Additional characterization for selected key intermediates and product with HSQC and COSY NMR, X-ray and Elemental Analysis were carried out as well. The characterization data and detailed experimental procedures are described in the ESI.

Rapid acid-induced degradation of motor **7** was observed during workup under neutral conditions, resulting in an isolated yield of merely 3%. It is likely that the double bond is activated due to the high electron density in the molecule and its electron-donating groups, and the degradation could be circumvented by workup under basic conditions. Spectroscopic analysis was carried out in acid-free solvents.

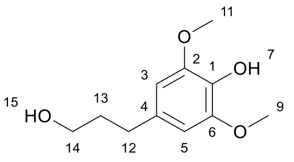
2.1. General overview of the synthesis of the molecular motor 7



Scheme S1: Synthesis of motor **7**. Dashed lines represent information from the literature. Reagents and conditions: (i) 40 bar H_2, $Cu_{20}PMO$, MeOH, 180°C, 18h.[1] (i') Various pulping conditions.[2] (i'') 1) oxidation of various technical lignins to syringaldehyde.[3,4] 2) CH_3I, K_2CO_3, DMF, rt, 6 h.[5] 3) Malonic acid, piperidine & pyridine, reflux.[6] (ii) 2 mmol (**1** 424.5 mg), 1 mol% K_2CO_3 (0.02 mmol, 2.8 mg), 5 mL dimethyl carbonate, 180 °C, 12 h, 93%. (iii) 1) 2 mmol **2** (452.5 mg), 10 mol% $Fe(NO_3)_3 \cdot 9H_2O$ (0.2 mmol, 80.8 mg), 10 mol% TEMPO (0.2 mmol, 31.6 mg), 10 mol% KCl (0.2 mmol, 14.9 mg), 10 mL EtOAc, RT, 18 h, 2) addition of 5 mL Et_3N, RT, 12h, 86.9%. (iii') 100 mmol **0** (23.82g), 2500 mg Raney Ni, 500 mL MeOH, RT, 24h, 96%. (iv) 20 mmol **3** (4805 mg), 30 g Eaton's reagent: 19 mmol P_2O_5 (2700 mg) and 284.5 mmol CH_3SO_3H (27.3 g, 100 °C, 3 min, 94%. (v) 3 mmol **4** (666 mg), 6 mmol isobutyraldehyde (432 mg), 3 mmol KOH (178 mg),4 mL H_2O, 60 °C, 18h, 83%. (vi) 1 mmol **5** (276 mg), atmospheric H_2 (balloon), 1 mol% Pd@C (21.3 mg, 5 wt% Pd loading), 5 mL EtOAc, RT, 2h, 99%. (vii) 2.16 mmol **6** (600 mg), 5.36 mmol $TiCl_4$ (1.02 g), 10.71 mmol Zn powder (0.70 g), 7 mL anhydrous THF, reflux, 7d, 16% (24% based on recovered starting material).

2.2. Synthesis and characterization of compounds (0-7)

4-(3-hydroxypropyl)-2,6-dimethoxyphenol (1)



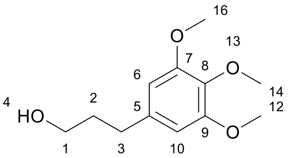
[1]

1 was a generous donation from Xianyuan Wu from the Barta group. Compound **1** can be obtained from hardwood sawdust via reductive catalytic fractionation[1] or by hydrogenolysis of hardwood lignin obtained via the propionaldehyde assisted fractionation.[7] Compound **1** can be synthetized from the corresponding carboxylic acid (3-(4-hydroxy-3,5-dimethoxyphenyl)propanoic acid) via reduction with $LiAlH_4$ in THF.[8]

Compound **1** was accessed from beech sawdust and isolated, hence its yield can be calculated on the original lignin content of beech sawdust or the theoretical maximum yield achievable from its lignin content by breaking all the ß-O-4 bonds, assuming regular ß-O-4 bond distribution. The theoretical maximum monomers yield (~34% (0.34 = 0.58 x 0.58)) is determined by the ß-O-4 content (~58%) in beech wood. The Syringil/Guacyl (S/G) ratio in beech wood is 2.8, thus the reductive catalytic fractionation (RCF) of 10 g beech wood (1.88 g lignin content) could yield a maximum of 463 mg compound **1**. As 310 mg compound **1** was accessed it corresponds to 67% of the theoretical maximum yield or 17% yield based on the lignin content. The corresponding data and discussion can be found in one of our previous study (10.26434/chemrxiv.14627745.v1).

^{1}H-NMR: δ_H (600 MHz, Chloroform-*d*) 6.42 (s, 2H, $H^{3,5}$), 5.40 (s, 1H, H^7), 3.87 (s, 6H, $H^{9,11}$), 3.68 (t, J = 6.4 Hz, 2H, H^{14}), 2.64 (t, J = 7.8 Hz, 2H, H^{12}), 1.91 – 1.83 (m, 2H, H^{13}), 1.37 (s, 1H, H^{15}). **^{13}C-NMR:** δ_C (151 MHz, Chloroform-*d*) 147.1 (2C, $C^{2,6}$), 133.1 (1C, arom. C), 133.0 (1C, arom. C), 105.2 (2C, $C^{3,5}$), 62.4 (1C, C^{14}), 56.4 (2C, $C^{9,11}$), 34.6 (1C, C^{13}), 32.4 (1C, C^{12}). **HRMS:** (ESI^+, m/z) calculated for $C_{11}H_{17}O_4$ $[M+H]^+$: 213.1121; found: 213.1121.
Spectral data are consistent with those reported in the literature.[9]

3-(3,4,5-trimethoxyphenyl)propan-1-ol (2)

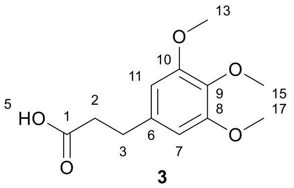


2

4-(3-Hydroxypropyl)-2,6-dimethoxyphenol (**1**, 424.5 mg, 2 mmol) was measured out to a Swagelok Stainless steel microreactor. Dimethyl carbonate (DMC) (5 mL) and K_2CO_3 (2.8 mg, 0.02 mmol, 1 mol%) were added. The microreactor was closed and heated to 180 °C for 12 h. After cooling down to rt, the product mixture was transferred with MeOH to a 50 mL round bottom flask and subsequently concentrated *in vacuo* to yield a crude mixture consisting of **2**, methyl (3-(3,4,5-trimethoxyphenyl)propyl) carbonate and bis(3-(3,4,5-trimethoxyphenyl)propyl) carbonate, as confirmed by GC-MS measurement. 9 mL MeOH, 1 mL H_2O and NaOH (40 mg, 1 mmol) were added and the solution stirred at rt for 30 min in order to hydrolyze the carbonate esters of **2**. The mixture of MeOH with water was found beneficial for the hydrolysis in contrast to pure water, because no degradation was observed after reaction. Finally, the product mixture was concentrated *in vacuo*, 5 mL water was added and the mixture was extracted with Et_2O (5 x 5mL). The organic phases were combined, dried over $MgSO_4$ then concentrated *in vacuo* to provide the product **2**. Yield: 420 mg (93%); slightly yellow oil. The material was used without further purification.

^{1}H-NMR: δ_H (600 MHz, Chloroform-*d*) 6.42 (s, 2H, $H^{6,10}$), 3.85 (s, 6H, $H^{12,16}$), 3.82 (s, 3H, H^{14}), 3.69 (t, J = 6.4 Hz, 2H, H^1), 2.66 (t, J = 7.9 Hz, 2H, H^3), 1.93 – 1.85 (m, 2H, H^2). **^{13}C-NMR:** δ_C (151 MHz, Chloroform-*d*) 153.3 (2C, $C^{7,9}$), 137.8 (1C, arom. C), 136.3 (1C, arom. C), 105.5 (2C, $C^{6,10}$), 62.3 (1C, C^1), 61.0 (1C, C^{14}), 56.2 (2C, $C^{12,16}$), 34.4 (1C, C^2), 32.7 (1C, C^3). **HRMS:** (ESI^+, m/z) calculated for $C_{12}H_{19}O_4$ $[M+H]^+$: 227.1278; found: 227.1277. Spectral data are consistent with those reported in the literature.[10]

3-(3,4,5-trimethoxyphenyl)propanoic acid (3)



3

A) Syntheses route from 2:

To a 50 mL round bottom *Schlenk* flask were added $Fe(NO_3)_3{\cdot}9H_2O$ (80.8 mg, 0.2 mmol), TEMPO (31.6 mg, 0.2 mmol), KCl (14.9 mg, 0.2 mmol), **2** (452.5 mg, 2.0 mmol), and EtOAc (10 mL) sequentially under an atmosphere of oxygen from a gas balloon. In the original report the authors used 1,2–DCE as a reaction medium for the oxidation of 3-phenylpropan-1-ol.[11] To comply with the principles of green chemistry, we aimed to avoid the use of any halogenated solvent in the synthesis and purification of all our compounds. Therefore, beforehand, the oxidation of **2** a small scope was run with 3-phenylpropan-1-ol as a model substrate applying different alternative solvents. EtOAc was identified as a competitive replacement of 1,2-DCE. The vigorously stirred orange reaction mixture turned darker after 18 h of reaction time at rt. A small sample (0.05 mL) was taken to an Eppendorf tube, 0.45 mL Et_2O and 0.5 mL H_2O were added and the organic phase was analyzed by GC-MS confirming the full conversion of the starting material. The mixture contained 83% **3**, 11% 3-(3,4,5-trimethoxyphenyl)propaneperoxoic acid and 7% self-esterification product (3-(3,4,5-trimethoxyphenyl)propyl 3-(3,4,5-trimethoxyphenyl)propanoate) based on GC-MS. The catalytic oxidative self-esterification of alcohols to the corresponding esters are known in the literature[12,13] and further optimization of this procedure is beyond the scope of this investigation. In order to reduce the percarboxylic acid to **3** in situ, 5 mL of Et_3N was added to the crude mixture and stirred overnight. Subsequently, the compound was sampled and analyzed with GC-MS to confirm the total reduction of the peroxy acid byproduct to **3**. The crude reaction mixture was concentrated under reduced pressure. To the concentrated dark red oily reaction mixture, 10 mL Et_2O and 5 mL H_2O was added and basified with a few drops of a saturated aqueous solution of NaOH to pH = ~10. The basic aqueous layer was extracted with 4 x 10 mL Et_2O in order to remove TEMPO and the ester side product. Then the leftover aqueous layer was acidified with 37wt% aq. HCl till pH = ~3 and extracted with 5 x 10 mL Et_2O. The combined organic layers were washed with 2 x 1 mL H_2O, dried over $MgSO_4$ and concentrated *in vacuo* to yield 421.7 mg crude, slightly orange, needle shaped **3**. Recrystallization did not work in our hand to remove the traces of leftover TEMPO. Therefore, the crude material was filtrated through a short column of silica gel eluted with diethyl ether (6 x 10 mL). After evaporation, **3** was obtained as an off-white powder. Yield: 417.3 mg (86.9%)

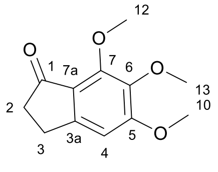
^{1}H-NMR: δ_H (600 MHz, Chloroform-*d*) 9.40 (s, 1H, H^5), 6.42 (s, 2H, $H^{7,11}$), 3.84 (s, 6H, $H^{13,17}$), 3.82 (s, 3H, H^{15}), 2.90 (t, J = 7.7 Hz, 2H, H^3), 2.68 (t, J = 7.7 Hz, 2H, H^2). **^{13}C-NMR:** δ_C (151 MHz, Chloroform-*d*) 178.8 (1C, C^1), 153.4 (2C, $C^{8,10}$), 136.6 (1C, arom. C), 136.0 (1C, arom. C), 105.3 (2C, $C^{7,11}$), 61.0 (1C, C^{15}), 56.2 (2C, $C^{13,17}$), 35.8 (1C, C^2), 31.1 (1C, C^3). **HRMS:** (ESI^-, m/z) calculated for $C_{12}H_{15}O_5$ $[M-H]^-$: 239.0914; found: 239.0933. Spectral data are consistent with those reported in the literature.[14]

B) Syntheses route from 0:

Raney® Ni (2.50 g) slurry (wetted instantly with 5 mL MeOH) and (*E*)-3-(3,4,5-trimethoxy)cinnamic acid (**0**, 23.82 g, 100 mmol) was loaded to a 500 mL Parr® reactor equipped with an overhead stirrer. An additional 495 mL MeOH was added, the reactor was purged 5 times with hydrogen and pressurized to 50 bar and stirred at rt for 24h. The pressure was then released from the reactor and the reactor was washed with 10 mL MeOH in small aliquots. The liquids were transferred to a 50 mL centrifuge tube and the catalyst was separated (6000 rpm, 10 min) in several cycles. The clean liquid phase from each cycle was filtered through an 0.2 µm PTFE filter to a 1000 mL round bottom flask. To the leftover solid catalyst, 50 mL MeOH was added, the catalyst was resuspended with intense shaking, centrifuged, filtrated to the same round bottom flask in similar fashion. The combined liquids were evaporated under reduced pressure, and the solid product was dried in high vacuum at rt. Yield: 23.11 g (96%); slightly off-white solid. The material was used without further purification.

^{1}H-NMR: δ $_{H}$ (600 MHz, Chloroform-*d*) 11.23 (s, 1H, H^{5}), 6.43 (s, 2H, $H^{7,11}$), 3.84 (s, 6H, $H^{13,17}$), 3.82 (s, 3H, H^{15}), 2.90 (t, J = 7.7 Hz, 2H, H^{3}), 2.68 (t, J = 7.7 Hz, 2H, H^{2}). **^{13}C-NMR:** δ $_{C}$ (151 MHz, Chloroform-*d*) 178.9 (1C, C^{1}), 153.6 (2C, $C^{8,10}$), 136.7 (1C, arom. C), 136.1 (1C, arom. C), 105.4 (2C, $C^{7,11}$), 61.0 (1C, C^{15}), 56.2 (2C, $C^{13,17}$), 35.8 (1C, C^{2}), 31.1 (1C, C^{3}). **HRMS:** (ESI^{+}, m/z) calculated for $C_{12}H_{17}O_5$ $[M+H]^{+}$: 241.1070; found: 241.1071. Spectral data are consistent with those reported in the literature.[14]

5,6,7-trimethoxy-2,3-dihydro-1H-inden-1-one (4)

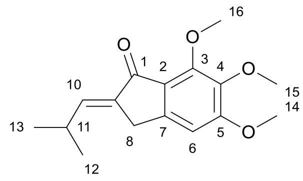


4

The procedure was adopted from literature.[15] Phosphorous pentoxide (P_2O_5, 2.70 g, 19 mmol) was added to methanesulfonic acid (MsOH, 27.3 g. 284.5 mmol, ~18.4 mL) in a 100 mL round bottom flask and the mixture was vigorously stirred at 80°C for 30 min in order to create Eaton's reagent. After reaching the desired temperature the mixture was further heated up to 100 ˚C. To a stirred colorless Eaton's reagent was added 3-(3,4,5-trimethoxyphenyl)propanoic acid (**3,** 4.805 g, 20 mmol) (as a finely grounded white crystalline powder) at 100 °C. The solid rapidly dissolved and the color of the mixture turned to slightly yellow and slowly darkened over time. The solution was stirred at the same temperature for 3 min and poured into ice-water (no exothermic reaction occurred). The mixture was extracted with EtOAc 6 times and the combined organic layers were washed with 0.5 % aq. $NaHCO_3$ solution, dried over $MgSO_4$, and evaporated to leave the solid, which was washed with small aliquots of acetone. The obtained crystals had a beige color. Average yield of two runs is: 4.182 g, (94%); the material was used without further purification.

^{1}H-NMR: δ $_{H}$ (600 MHz, Chloroform-*d*) 6.66 (s, 1H, H^{4}), 4.03 (s, 3H, H^{12}), 3.92 (s, 3H, H^{14}), 3.84 (s, 3H, H^{16}), 3.02 – 2.98 (m, 2H, H^{2}), 2.66 – 2.62 (m, 2H, H^{3}). **^{13}C-NMR:** δ $_{C}$ (151 MHz, Chloroform-*d*) 203.2 (1C, C^{1}), 159.8 (1C, arom. C), 153.3 (1C, arom. C), 151.7 (1C, arom. C), 140.8 (1C, arom. C), 123.0 (1C, arom. C), 103.9 (1C, C^{4}), 62.1 (1C, C^{14}), 61.5 (1C, C^{12}), 56.4 (1C, C^{16}), 37.3 (1C, C^{2}), 25.8 (1C, C^{3}). **HRMS:** (ESI^{+}, m/z) calculated for $C_{12}H_{15}O_4$ $[M+H]^{+}$: 223.0965; found: 223.0966. Spectral data are consistent with those reported in the literature.[16]

(*E*)-5,6,7-trimethoxy-2-(2-methylpropylidene)-2,3-dihydro-1H-inden-1-one (5)

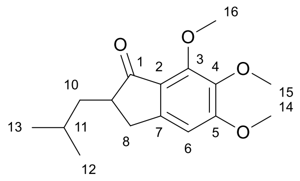


5

A 25 mL round bottom flask was charged with 5,6,7-trimethoxy-2,3-dihydro-1H-inden-1-one (**4**, 666 mg, 3 mmol). A solution of KOH (178 mg, 3 mmol) in 4 mL water was added. The reaction mixture was stirred vigorously with a magnetic stirring bar while isobutyraldehyde (432 mg, 6 mmol) was added. The mixture was vigorously stirred at 60 °C. After 5 h, all the solid starting material dissolved yielding a yellow slowly settling emulsion. After 18 h full conversion was confirmed by TLC and GC-MS. The material was extracted using 5 x 10 mL Et_2O, washed with 2 x 1 mL H_2O and concentrated *in vacuo* to yield 1.032 g crude yellow oil. The oil was redissolved in 2 mL EtOAc and the product was crashed out with pentane yielding a fine white precipitate. The precipitate was separated with centrifugation and washed with 2 x 5 mL pentane, transferred to a round bottom flask and dried under high vacuum. Yield: 689.3 mg (83%); white crystalline compound, used as such without further purification in the next step.

^{1}H-NMR: δ_H (600 MHz, Chloroform-d) 6.69 (s, 1 H, H^6), 6.60 – 6.54 (m, 1 H, H^{10}), 4.07 (s, 3 H, H^{16}), 3.94 (s, 3 H, H^{14}), 3.86 (s, 3 H, H^{15}), 3.57 (m, 2 H, H^8), 2.66 – 2.55 (m, 1H, H^{11}), 1.10 (d, 6H, J = 6.7 Hz, $H^{12,13}$). **^{13}C-NMR:** δ_C (151 MHz, Chloroform-*d*) 190.7 (1C, C^1), 159.6 (1C, arom. C), 152.6 (1C, arom. C), 147.5 (1C, arom. C), 142.3 (1C, C^{10}), 141.2 (1C, arom. C), 134.6, (1C, C^9), 125.1 (1C, arom. C), 103.8 (1C, C^6), 62.3 (1C, C^{16}), 61.6 (1C, C^{15}), 56.4 (1C, C^{14}), 29.8 (1C, C^8), 29.5 (1C, C^{11}), 22.1 (2C, $C^{12,13}$). **HRMS:** (ESI$^+$, m/z) calculated for $C_{16}H_{21}O_4$ $[M+H]^+$: 277.1434; found: 277.1437.

2-isobutyl-5,6,7-trimethoxy-2,3-dihydro-1H-inden-1-one (6)



6

Syntheses route of 6 from crude 5:

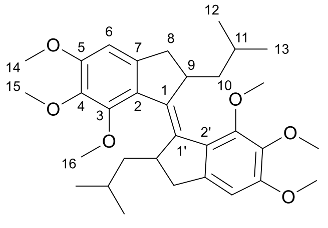
A 100 mL round bottom flask was charged with 5,6,7-trimethoxy-2,3-dihydro-1H-inden-1-one (**4**, 4.440 g, 20 mmol). A solution of KOH (1.120 g, 20 mmol) in 27 mL water was added and the mixture stirred vigorously with a magnetic stirring bar while isobutyraldehyde (2.880 g, 40 mmol) was added. The above mixture was vigorously stirred at 60 °C overnight. After 13 h, full conversion was confirmed by TLC and GC-MS. The material was extracted with EtOAc, washed with water, dried over $MgSO_4$ and concentrated *in vacuo* to yield 5.505 g crude yellow oil. (At this point of the research it was not clear, that **5** is unstable in protic environment such as MeOH.) The crude material was transferred with 40 mL MeOH to a 100 mL Parr® autoclave which was loaded with 0.50 g of Raney® Ni slurry. The resulting mixture was stirred at rt under a 45 bar H_2 atmosphere for 12 h. Subsequently, the solution was carefully poured into a 50 mL centrifuge tube, centrifuged, filtered through a PTFE syringe filter and concentrated *in vacuo*. The product was analyzed by GC-MS, which revealed the conversion was close to completion (~95%), but already a side product formed which was identified as 5,6,7-trimethoxy-2,3-dihydro-1H-inden-1-one **4**, The product was deposited on silica and purified by chromatography with increasing gradient of pentane-EtOAc-eluent mixture to yield 2-isobutyl-5,6,7-trimethoxy-2,3-dihydro-1H-inden-1-one **6** in 66% yield (3.674 g, over the two steps from **4**, without isolation of **5**).

Syntheses route of 6 from precipitated 5:

To a solution of (*E*)-5,6,7-trimethoxy-2-(2-methylpropylidene)-2,3-dihydro-1H-inden-1-one (**5**, 276 mg, 1 mmol) in EtOAc (5 mL) in a 25 mL round bottom flask equipped with magnetic stirring bar was added Pd@C (5wt% Pd, 21.3 mg, 1 mol%). The mixture was stirred for 2 h under an atmosphere of hydrogen from a gas balloon. (Alternatively, MeOH, and DMC were tried as well. In MeOH the same partial degradation of starting material was observed similarly to the procedure where Raney Ni was used as a catalyst. In DMC only a very small extend of degradation occurred, selectivity: 93%.) After 2 h the catalyst was filtered off with a 0.2 µm PTFE filter to a 100 mL round bottom flask and flushed with EtOAc, then concentrated on a rotary evaporator and dried in high vacuum. Yield: 275 mg (99%);

^{1}H-NMR: δ_H (600 MHz, Chloroform-*d*) 6.64 (s, 1H, H^6), 4.03 (s, 3H, H^{16}), 3.92 (s, 3H, H^{14}), 3.84 (s, 3H, H^{15}), 3.23 – 3.15 (m, 1H, H^9), 2.69 – 2.62 (m, 2H, H^{10}), 1.85 – 1.74 (m, 2H, H^8), 1.29 – 1.24 (m, 1H, H^{11}), 0.96 (t, *J* = 5.8 Hz, 6H, $H^{12,13}$). **^{13}C-NMR:** δ_C (151 MHz, Chloroform-*d*) 205.3 (1C, C^1), 159.6 (1C, arom. C), 151.6 (1C, arom. C), 151.5 (1C, arom. C), 140.7 (1C, arom. C), 122.4 (1C, arom. C), 103.6 (1C, C^6), 61.9 (1C, C^{16}), 61.4(1C, C^{15}), 56.2 (1C, C^{14}), 46.6 (1C, C^9), 41.0 (1C, C^8), 33.3 (1C, C^{10}), 26.6 (1C, C^{11}), 23.4 (1C, C^{13}), 21.7 (1C, C^{12}). **HRMS:** (ESI$^+$, m/z) calculated for $C_{16}H_{23}O_4$ $[M+H]^+$: 279.1591; found: 279.1592. **Elemental analysis:** Calc. (Found) C 69.04 (68.87), H 7.97 (7.91).

(*E*)-9,9'-diisobutyl-3,3',4,4',5,5'-hexamethoxy-8,8',9,9'-tetrahydro-1,1'-biindenylidene (7)



M7

Under a N_2 atmosphere, $TiCl_4$ (1.02 g, 5.36 mmol, 0.59 mL, 2.48 eq.) was slowly added to a vigorously stirred suspension of zinc powder (0.70 g, 10.71 mmol, 4.97 eq.) in anhydrous THF (5 mL). The suspension was stirred while heated at reflux for 2h, after which a solution of 9-isobutyl-3,4,5-trimethoxy-8,9-dihydro-1H-inden-1-one (**6**, 0.60 g, 2.16 mmol, 1.00 eq.) in anhydrous THF (2 mL) was added. The mixture was stirred at reflux for 7d. Subsequently, the black suspension was treated with a saturated aqueous $NaHCO_3$ solution (400 mL). The mixture was extracted with ethyl acetate (3x 200mL), the combined organic extracts dried over $MgSO_4$ and concentrated *in vacuo*. The brown crude was purified via column chromatography (pentane 9:1 ethyl acetate), during which 41% of starting material (205.9 mg, 0.74 mmol) could be recovered. Flash chromatography (SiO_2, pentane 4:1 diethyl ether), recrystallization from *n*-heptane and drying *in vacuo* afforded the product **7** as a white solid (90.3 mg, 0.17 mmol, yield: 16% (24% based on recovered SM)). The E^s isomer was obtained exclusively. The molecular motor **7** was still pure and stable after 2.5 years of storage in darkness under air at room temperature, without effects on the reproducibility of its photoresponsive behavior.

By following the reaction over time (12h, 24h, 48h, 72h, 7d) and repeating it several times (> 10x) an attempt for improvement was made by either reducing the reaction time or by obtaining a higher yield, but proved to be difficult as starting material was present still after 7d. Hence it was opted for recovery of the pure starting material in addition to the desired product.

^{1}H-NMR: δ_H (600 MHz, Chloroform-*d*) 6.60 (s, 2H, H$^{6,6'}$), 3.91 (s, 6H, H$^{16,16'}$), 3.87 (s, 6H, H$^{14,14'}$), 3.77 (s, 6H, H$^{15,15'}$), 2.94 (ddd, *J* = 11.8, 5.9, 2.4 Hz, 2H, H$^{9,9'}$), 2.69 (dd, *J* = 14.8, 5.9 Hz, 2H, H$^{8,8'}$), 2.48 (d, *J* = 14.7 Hz, 2H, H$^{8,8'}$), 1.74–1.64 (m, 2H, H$^{11,11'}$), 1.60–1.52 (m, 2H, H$^{10,10'}$), 1.16 (ddd, *J* = 13.1, 11.4, 4.3 Hz, 2H, H$^{10,10'}$), 0.96 (d, *J* = 6.5 Hz, 6H, H$^{12,12'}$), 0.89 (d, *J* = 6.6 Hz, 6H, H$^{13,13'}$). **^{1}H-NMR:** δ_H (600 MHz, DCM-d_2) 6.61 (s, 2H, H$^{6,6'}$), 3.84 (s, 6H, H$^{16,16'}$), 3.83 (s, 6H, H$^{14,14'}$), 3.74 (s, 6H, H$^{15,15'}$), 2.91 (ddd, *J* = 11.7, 5.9, 2.4 Hz, 2H, H$^{9,9'}$), 2.65 (dd, *J* = 14.9, 6.0 Hz, 2H, H$^{8,8'}$), 2.49 (d, *J* = 14.9 Hz, 2H, H$^{8,8'}$), 1.74–1.64 (m, 2H, H$^{11,11'}$), 1.57 (ddd, *J* = 13.4, 11.9, 2.6 Hz, 2H, H$^{10,10'}$), 1.15 (ddd, *J* = 13.7, 11.9, 4.5 Hz, 2H, H$^{10,10'}$), 0.97 (d, *J* = 6.6 Hz, 6H, $^{H12,12'}$), 0.89 (d, *J* = 6.8 Hz, 6H, H$^{13,13'}$). **^{13}C-NMR:** δ_C (151 MHz, DCM-d_2) 153.6 (2C, arom. C), 150.5 (2C, arom. C), 141.3 (2C, arom. C), 141.3 (2C, arom. C), 138.3 (2C, arom. C), 128.7 (2C, arom. C), 105.6 (s, 2C, C$^{6,6'}$), 61.6 (s, 2C, C$^{16,16'}$), 60.9 (s, 2C, C$^{15,15'}$), 56.7 (s, 2C, C$^{14,14'}$), 47.9 (s, 2C, C$^{9,9'}$), 40.8 (s, 2C, C$^{10,10'}$), 36.7 (s, 2C, C$^{8,8'}$), 26.9 (s, 2C, C$^{11,11'}$), 24.7 (s, 2C, C$^{13,13'}$), 21.4 (s, 2C, C$^{12,12'}$). **HRMS:** (ESI$^+$, m/z) calculated for $C_{32}H_{45}O_6$ $[M+H]^+$: 525.3211; found: 525.3209.

3. Photoisomerization studies of molecular motor 7

3.1. UV-VIS study of molecular motor 7

Upon irradiation of compound **7** with different wavelengths (300 nm, 340 nm, 365 nm) at 298 K in DCM, switching properties could be determined by an upcoming redshifted band while the main absorption band diminished in intensity (**Figure S1-3**). Since the absorption maximum of **7** in DCM was obtained at 325 nm, different LEDs in that range were checked for the most efficient photoisomerization. The intensity of 300 nm LED proved to be insufficient to induce switching and the 365 nm LED was able to induce switching due to its wavelength fronting. The 340 nm LED demonstrated best switching abilities and visibility of an isosbestic point, and was therefore selected for further studies, while the 365 nm LED was selected for photochemical back isomerization to irradiate the redshifted band.

Photochemical backisomerization of the unstable *Z* state (Z^u) to the stable *E* state (E^s) in DCM was attempted using all three different LEDs available, but could not be observed. Upon further heating to induce a thermal helix inversion (THI) the observed UV/Vis spectra did not change. Based on these results and our previous motor research, we hypothesized a motor with low THI barrier including no observable unstable isomers. More viscous solvents were chosen to observe photoisomerization of an unstable *Z* state at room temperature (**Figure S4, S5**). The higher the viscosity of the solvent the less flexibility is granted for the rotation of the motor and more time is needed for thermal helix inversion leading to a possibility for an observation of an unstable isomer. The change of the solvent (DMSO and ACN) led to a blueshift of the absorption maximum and a 312 nm TLC lamp was used to induce photoisomerization. However, no photochemical backisomerization of an unstable *Z* state with 365 nm could be observed.

At room temperature this molecular motor effectively performs a two consecutive isomerization processes between stable E^s and stable Z^s.[17] UV/Vis studies at lower temperature were conducted to obtain the unstable states (which would be expected at a higher wavelength band and shifting of the isosbestic point). Based on these results, we expected a motor with low THI barriers, which shows direct interconversion between stable E^s and stable Z^s at room temperature.[17]

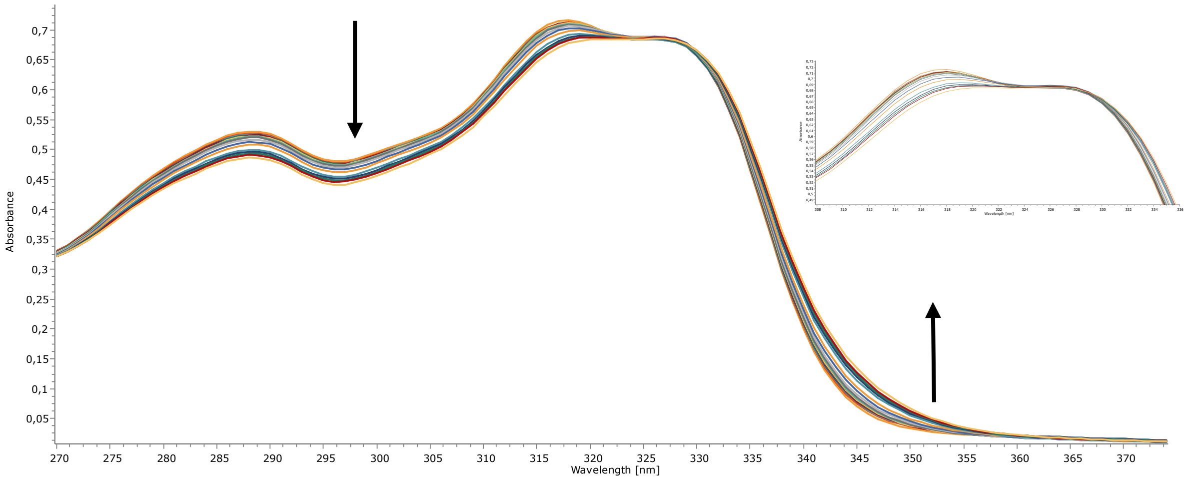


Figure S1: UV/Vis absorption spectrum of **7** measured at 298 K in degassed CH_2Cl_2 (2 x 10^{-3} M, N_2) upon irradiation with a 300 nm LED. The inset shows a close-up of the isosbestic point.

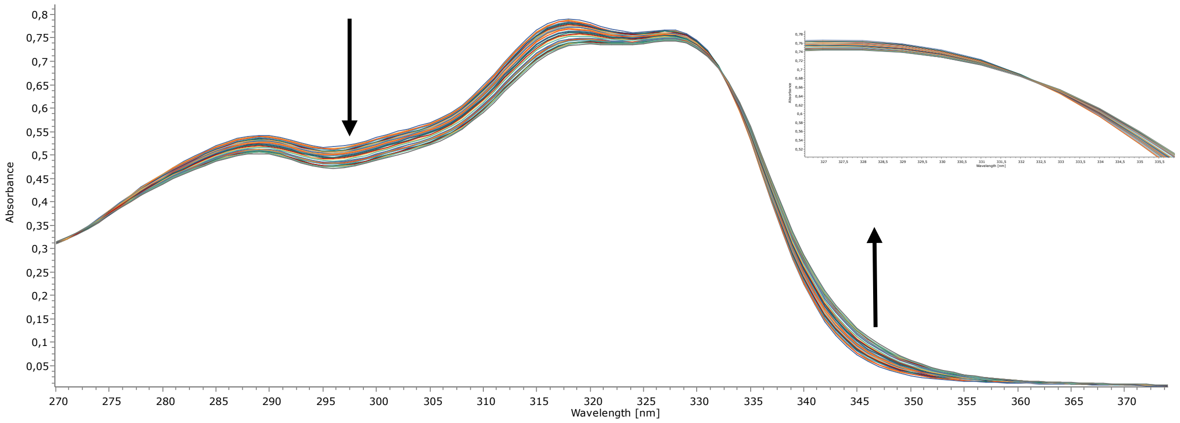


Figure S2: UV/Vis absorption spectrum of **7** measured at 298 K in degassed CH_2Cl_2 (2 x 10^{-3} M, N_2) upon irradiation with a 340 nm LED. The inset shows a close-up of the isosbestic point.

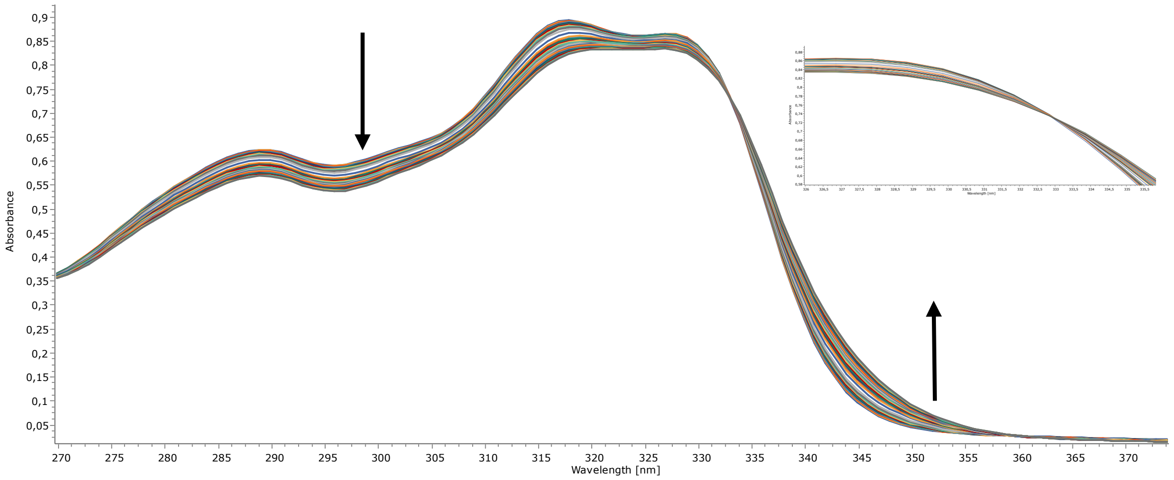


Figure S3: UV/Vis absorption spectrum of **7** measured at 298 K in degassed CH_2Cl_2 (2 x 10^{-3} M, N_2) upon irradiation with a 365 nm LED. The inset shows a close-up of the isosbestic point.

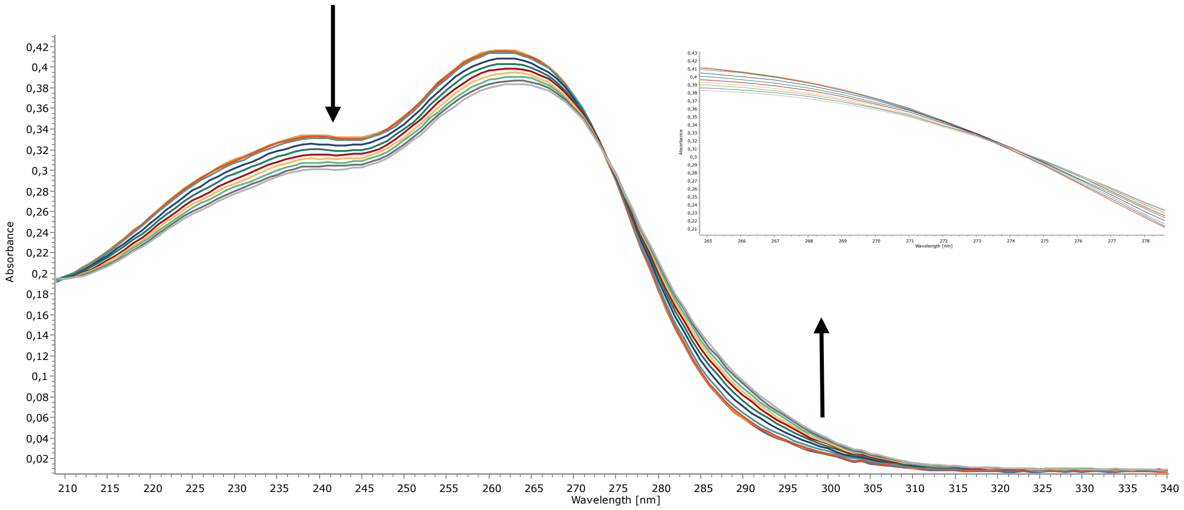


Figure S4: UV/Vis absorption spectrum of **7** measured at 298 K in degassed DMSO (2 x 10^{-5} M, N_2) upon irradiation with a 312 nm TLC lamp. The inset shows a close-up of the isosbestic point.

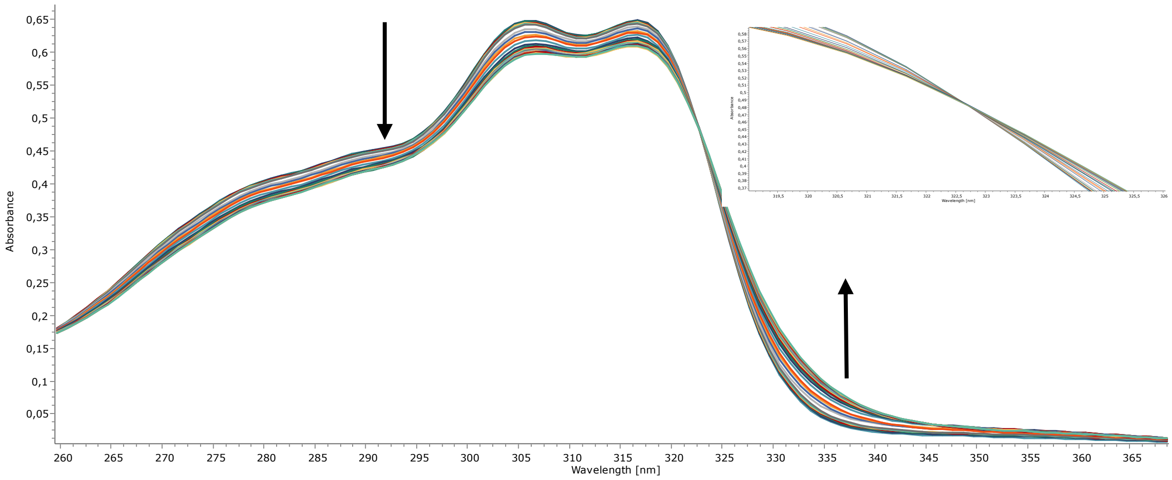


Figure S5: UV/Vis absorption spectrum of **7** measured at 298 K in degassed CH_3CN (2×10^{-5} M, N_2) upon irradiation with a 312 nm lamp. The inset shows a close-up of the isosbestic point.

3.2. ^{1}H-NMR study of molecular motor 7

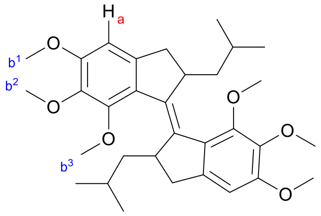


Figure S6: Depiction of protons used for integration in ^{1}H-NMR studies of compound **7.**

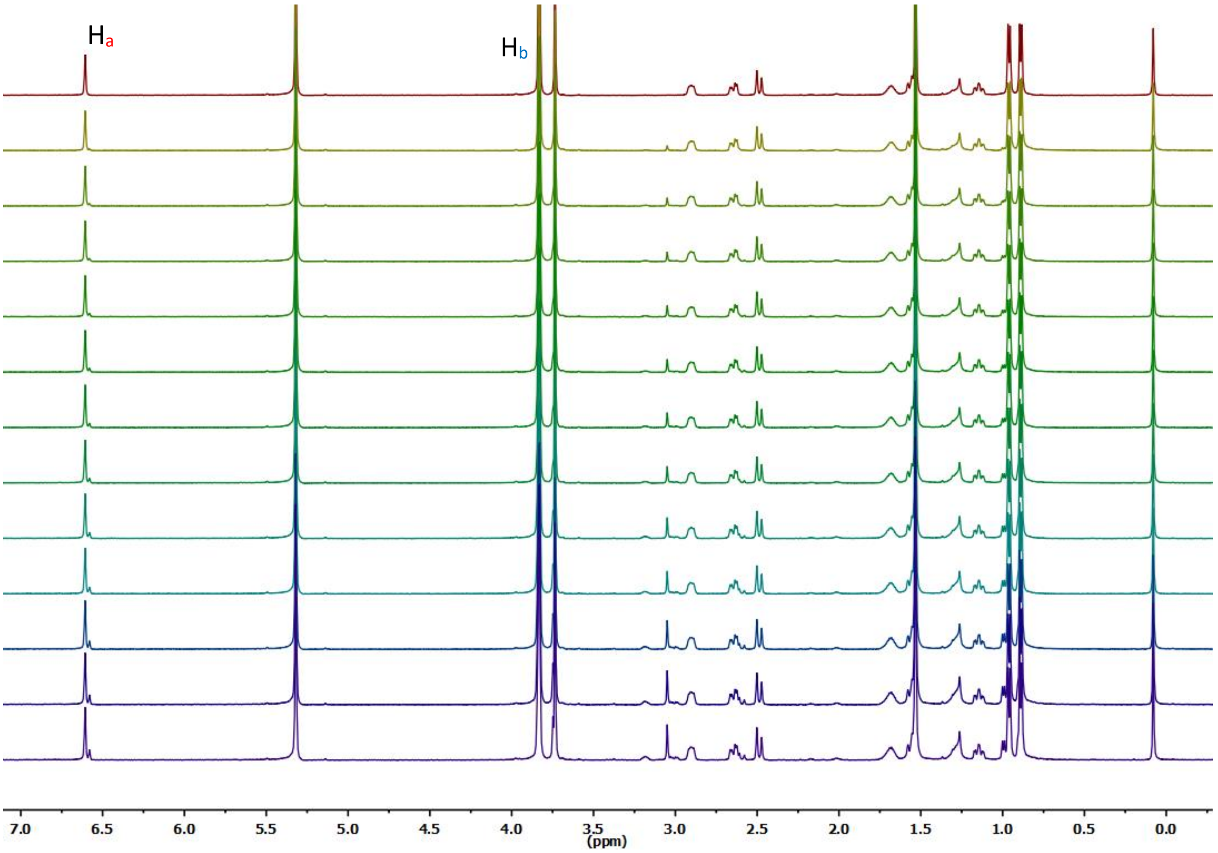


Figure S7: ^{1}H-NMR spectrum (500 MHz, 298 K) of **7** measured in degassed DCM-d_2 (4.1 x 10^{-3} M) and its spectral changes upon irradiation with a Thorlab 340 nm LED coupled to a 600 µm optical fibre, which led the light into the NMR tube inside the spectrometer. Initial state (top spectrum), PSS (bottom spectrum), PSS: 135 min, PSS$_{340}$ ratio: 85:15 (E^s:Z^s).

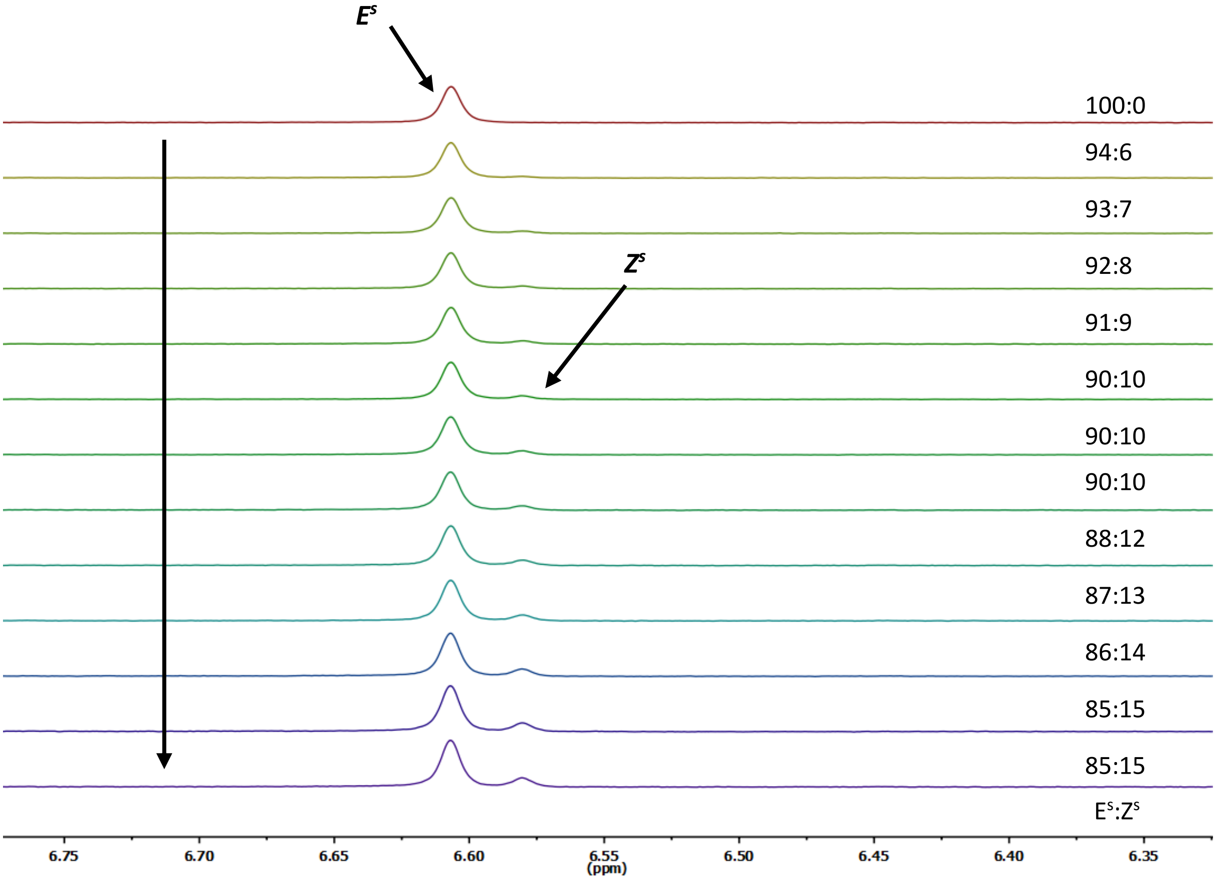


Figure S8: ^{1}H-NMR spectrum (500 MHz, 298 K) of the aromatic region H_a of **7** measured in degassed DCM-d_2 (4.1 x 10^{-3} M) and its spectral changes upon irradiation with a Thorlab 340 nm LED coupled to a 600 µm optical fibre, which led the light into the NMR tube inside the spectrometer. Initial state (top spectrum), PSS (bottom spectrum), PSS: 135 min, PSS_{340} ratio: 85:15 (E^s:Z^s).

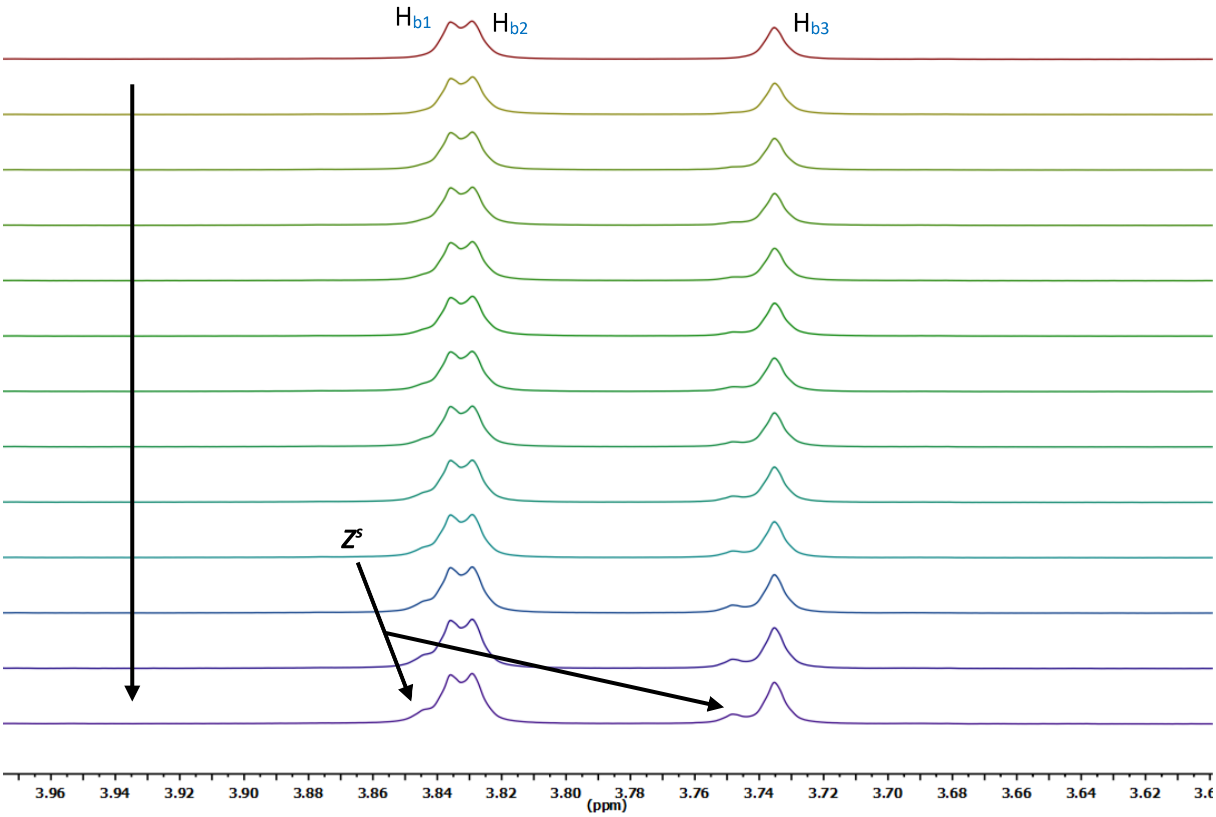


Figure S9: ^{1}H-NMR spectrum (500 MHz, 298 K) of the methoxy region H_b of **7** measured in degassed DCM-d_2 (4.1 x 10^{-3} M) and its spectral changes upon irradiation with a Thorlab 340 nm LED coupled to a 600 µm optical fibre, which led the light into the NMR tube inside the spectrometer. Initial state (top spectrum), PSS (bottom spectrum), PSS: 135 min, PSS_{340} ratio: 85:15 (E^s:Z^s).

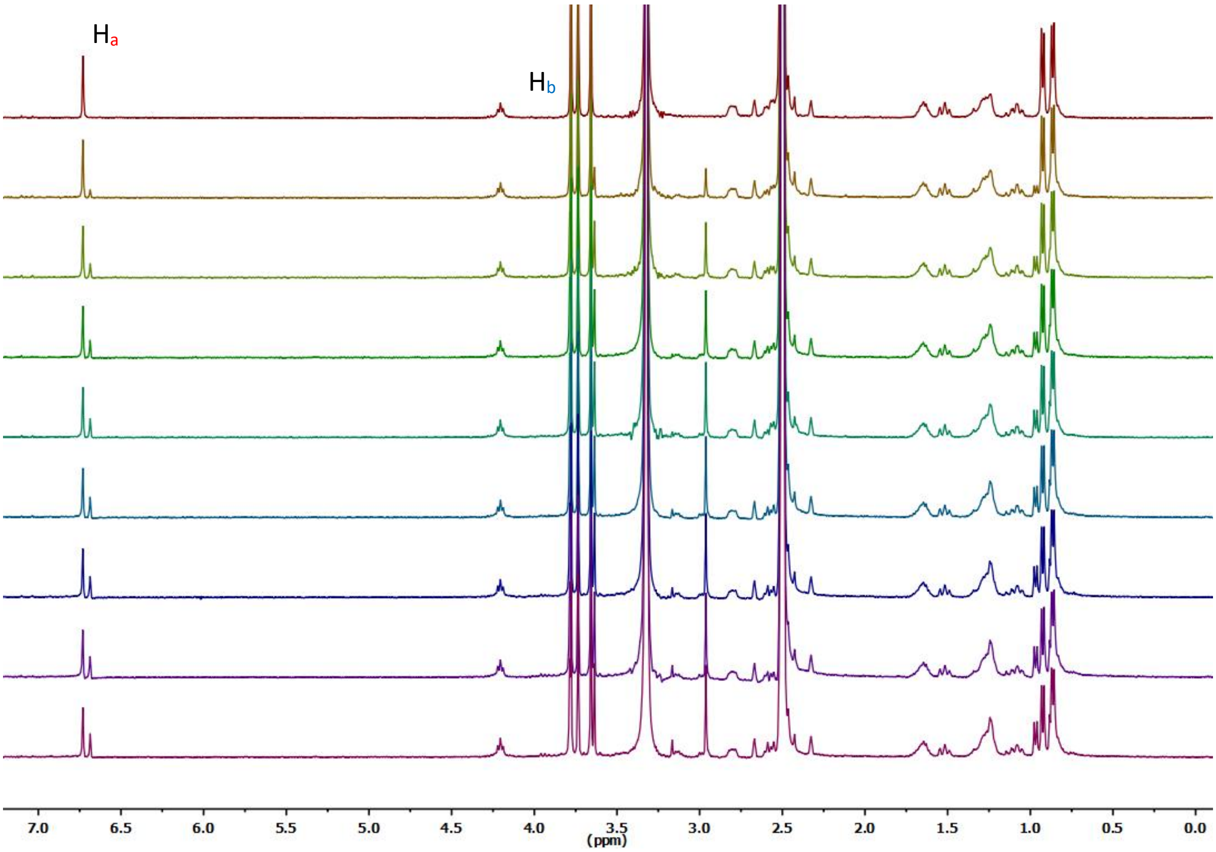


Figure S10: ^{1}H-NMR spectrum (400 MHz, 298 K) of **7** measured in degassed DMSO-d_6 (2 x 10^{-3} M) and its spectral changes upon irradiation with a 312 nm TLC lamp, Initial state (top spectrum), PSS (bottom spectrum), PSS: 120 min, PSS$_{312}$ ratio: 69:31 (E^s:Z^s).

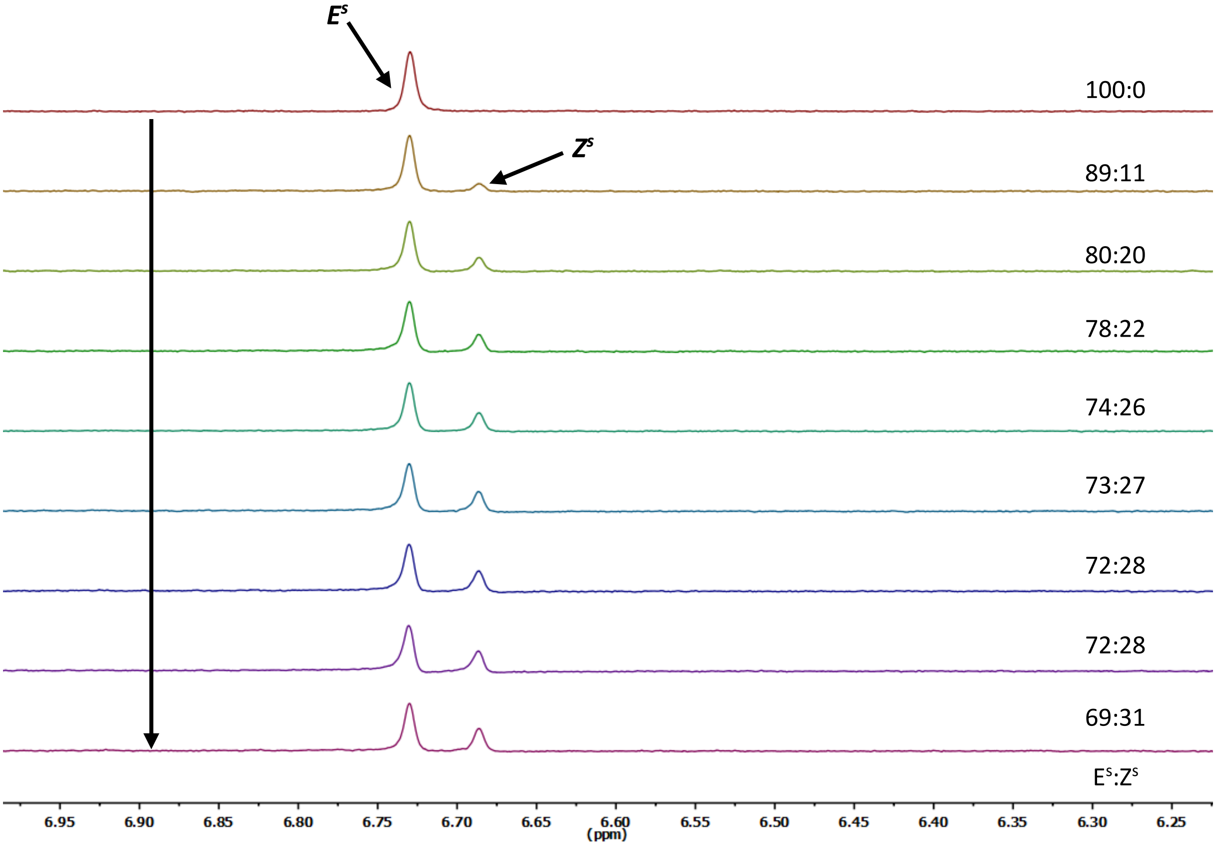


Figure S11: ^{1}H-NMR spectrum (400 MHz, 298 K) of the aromatic region H_a of **7** measured in degassed DMSO-d_6 (2×10^{-3} M) and its spectral changes upon irradiation with a 312 nm TLC lamp, Initial state (top spectrum), PSS (bottom spectrum), PSS: 120 min, PSS_{312} ratio: 69:31 (E^s:Z^s).

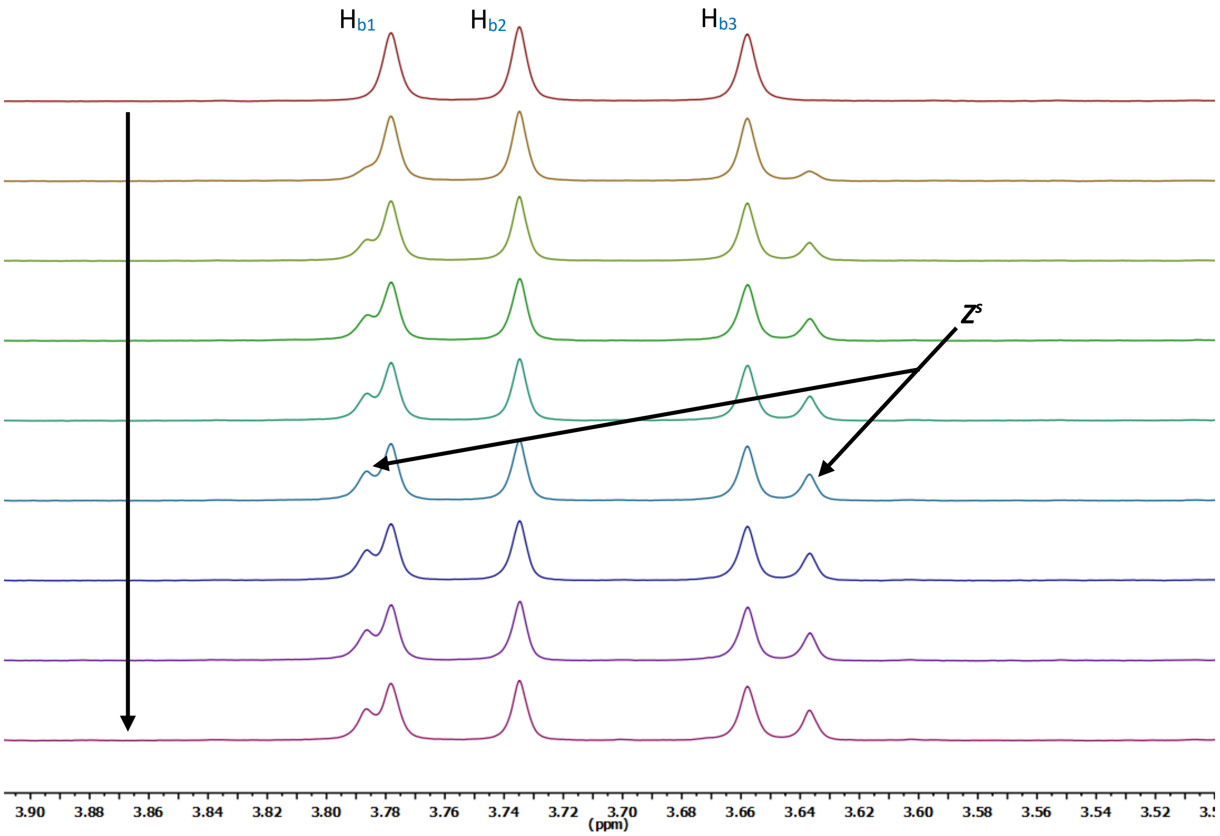


Figure S12: ^{1}H-NMR spectrum (400 MHz, 298 K) of the methoxy region H$_b$ of **7** measured in degassed DMSO-d_6 (2 x 10^{-3} M) and its spectral changes upon irradiation with a 312 nm TLC lamp, Initial state (top spectrum), PSS (bottom spectrum), PSS: 120 min, PSS$_{312}$ ratio: 69:31 (E^s:Z^s).

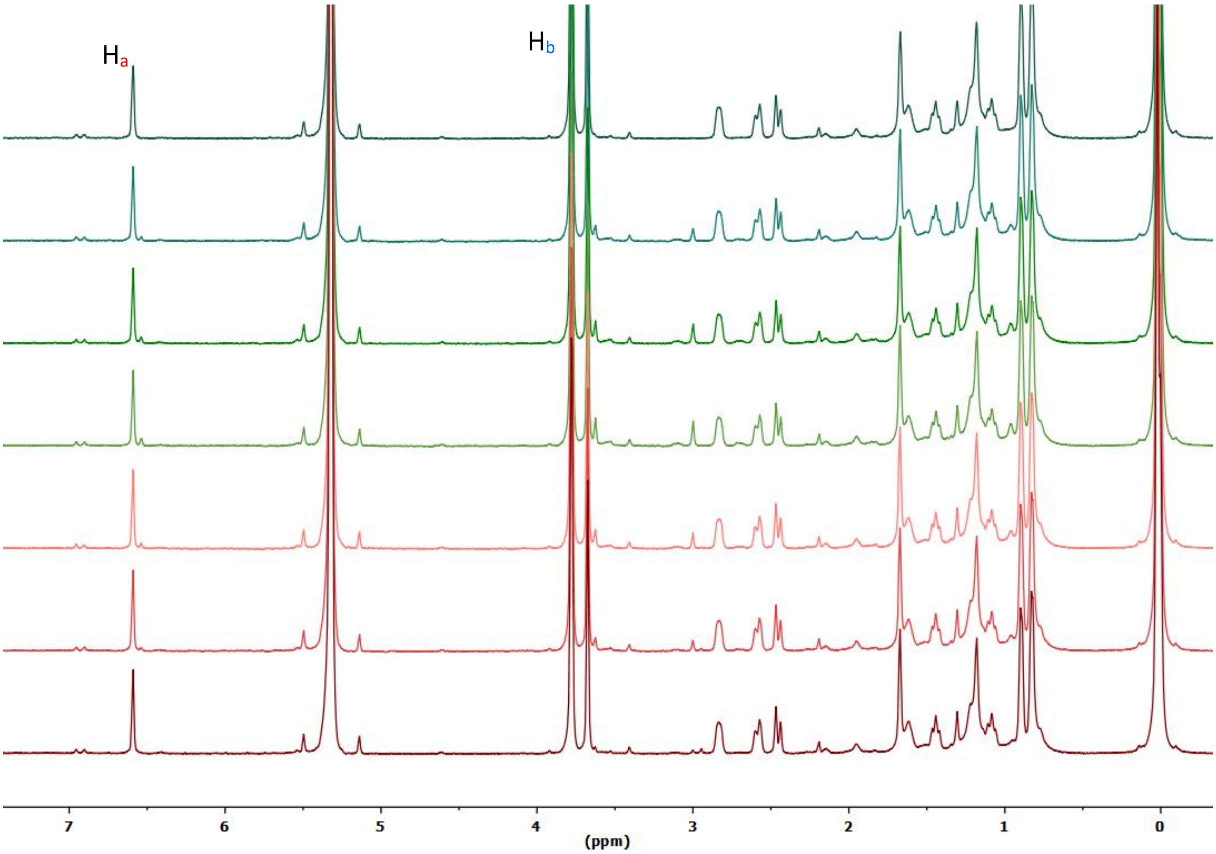


Figure S13: ^{1}H-NMR spectrum (500 MHz, 223 K) of **7** measured in degassed DCM-d_2 (1.8 x 10^{-3} M). First irradiation to its PSS with a Thorlab 340 nm LED coupled to a 600 µm optical fibre, which led the light into the NMR tube inside the spectrometer, was carried out, PSS: 120 min, PSS$_{340}$ ratio: 92:8 (E^{s}:Z^{u}). Then Spectral changes upon irradiation with a Thorlab 365 nm LED coupled to a 600 µm optical fibre are displayed. Initial state (top spectrum, ratio: 99:1 (E^{s}:Z^{u})), Photoisomerization to unstable state, PSS$_{340}$ (middle spectrum 4, ratio$_{340}$: 92:8 (E^{s}:Z^{u})), Photoisomerization of unstable state (bottom spectrum, 50 min, ratio$_{365}$: 97:3 (E^{s}:Z^{u})).

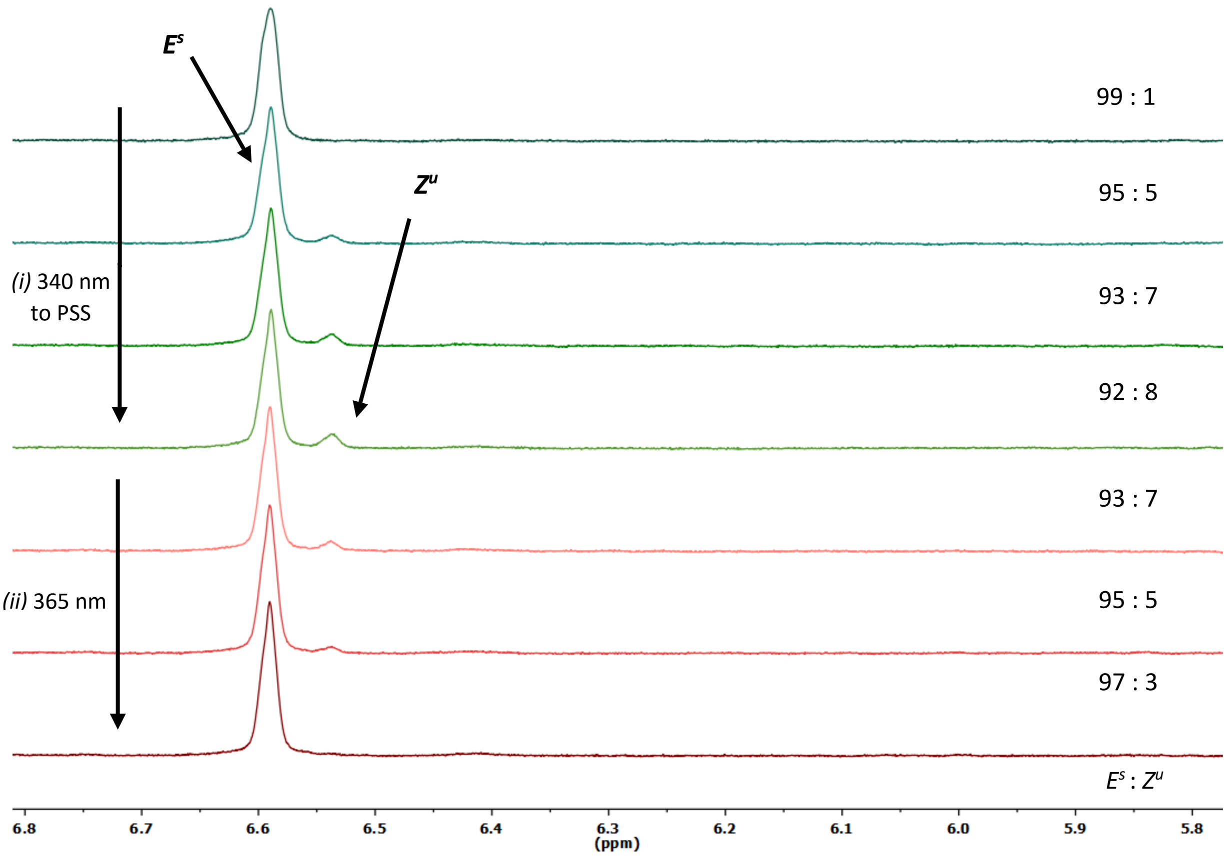


Figure S14: ^{1}H-NMR spectrum (500 MHz, 223 K) of the aromatic region H_a of **7** measured in degassed DCM-d_2 (1.8 x 10^{-3} M). First irradiation to its PSS with a Thorlab 340 nm LED coupled to a 600 µm optical fibre, which led the light into the NMR tube inside the spectrometer, was carried out, PSS: 120 min, PSS_{340} ratio: 92:8 (E^s:Z^u). Then Spectral changes upon irradiation with a Thorlab 365 nm LED coupled to a 600 µm optical fibre are displayed. Initial state (top spectrum, ratio: 99:1 (E^s:Z^u)), Photoisomerization to unstable state, PSS_{340} (middle spectrum 4, $ratio_{340}$: 92:8 (E^s:Z^u)), Photoisomerization of unstable state (bottom spectrum, 50 min, $ratio_{365}$: 97:3 (E^s:Z^u)).

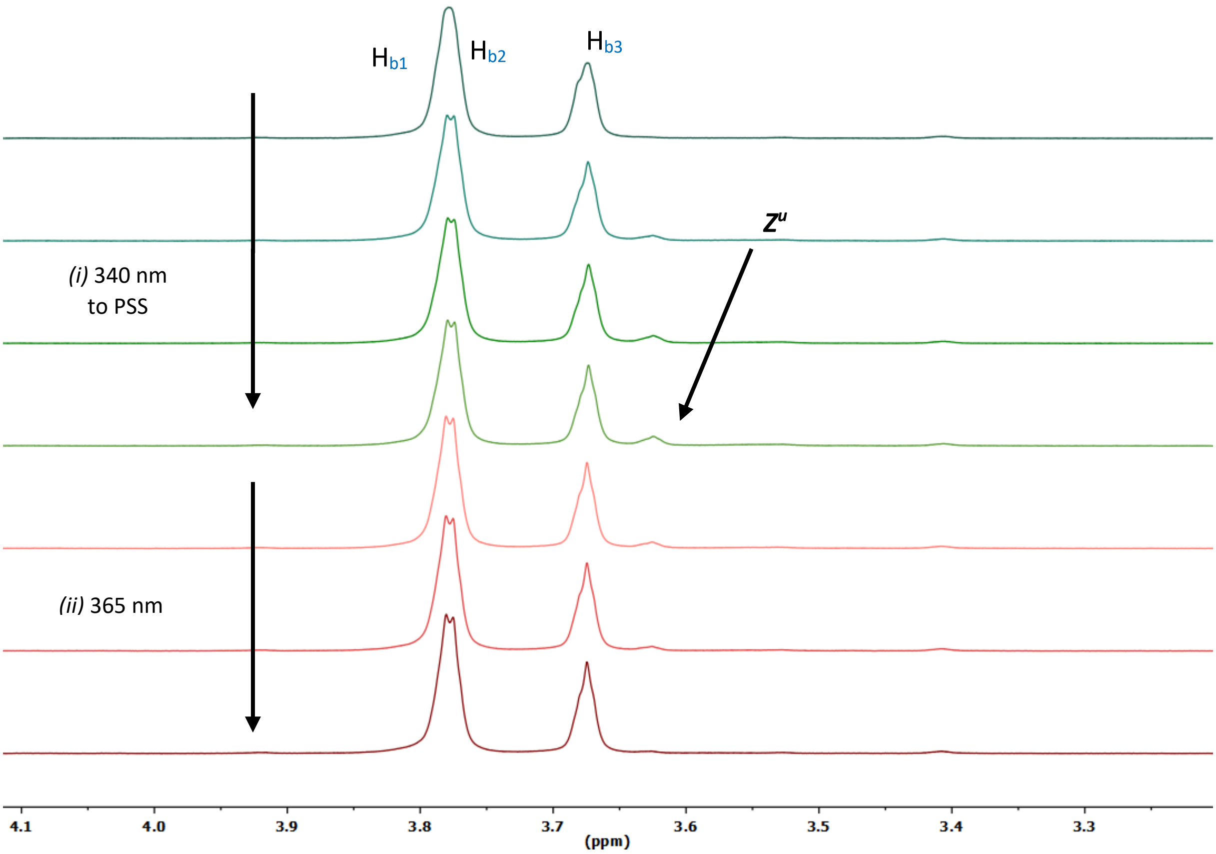


Figure S15: ^{1}H-NMR spectrum (500 MHz, 223 K) of the methoxy region H_b of **7** measured in degassed DCM-d_2 (1.8 x 10^{-3} M). First irradiation to its PSS with a Thorlab 340 nm LED coupled to a 600 µm optical fibre, which led the light into the NMR tube inside the spectrometer, was carried out, PSS: 120 min, PSS_{340} ratio: 92:8 (E^s:Z^u). Then Spectral changes upon irradiation with a Thorlab 365 nm LED coupled to a 600 µm optical fibre are displayed. Initial state (top spectrum, ratio: 99:1 (E^s:Z^u)), Photoisomerization to unstable state, PSS_{340} (middle spectrum 4, $ratio_{340}$: 92:8 (E^s:Z^u)), Photoisomerization of unstable state (bottom spectrum, 50 min, $ratio_{365}$: 97:3 (E^s:Z^u)).

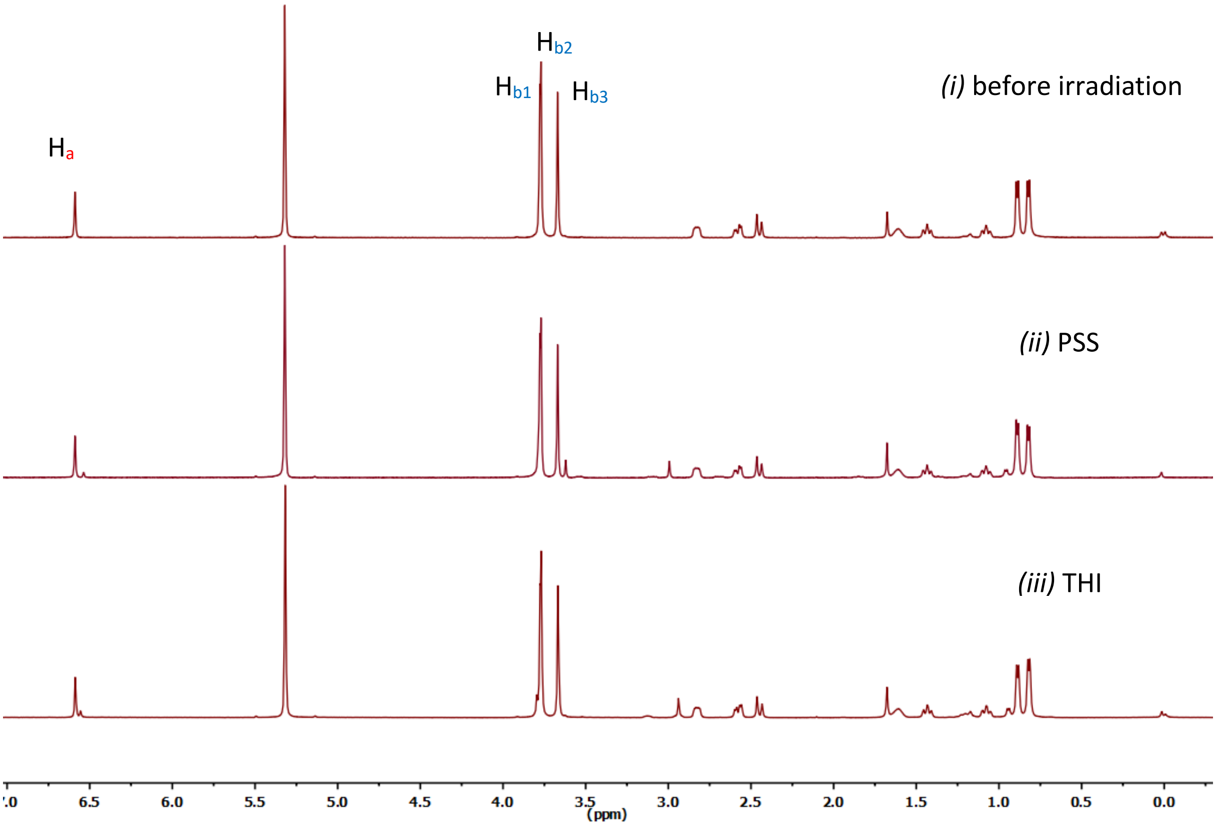


Figure S16: ^{1}H-NMR spectrum (500 MHz, 223 K) of **7** measured in degassed DCM-d_2 (4.2 x 10^{-3} M). First irradiation to its PSS with a Thorlab 340 nm LED coupled to a 600 µm optical fibre, which led the light into the NMR tube inside the spectrometer, PSS: 169 min, PSS$_{340}$ ratio: 88:12 (E^s:Z^u). The NMR tube was allowed to heat up to 298 K for 30 min to induce thermal helix inversion and measured again. *i)* Initial state (E^s), *ii)* Photoisomerization to unstable state (PSS ratio$_{340}$: 88:12 (E^s:Z^u)) and *iii)* thermal helix inversion (ratio$_{\mathrm{THI}}$: 88:12 (E^s:Z^s)).

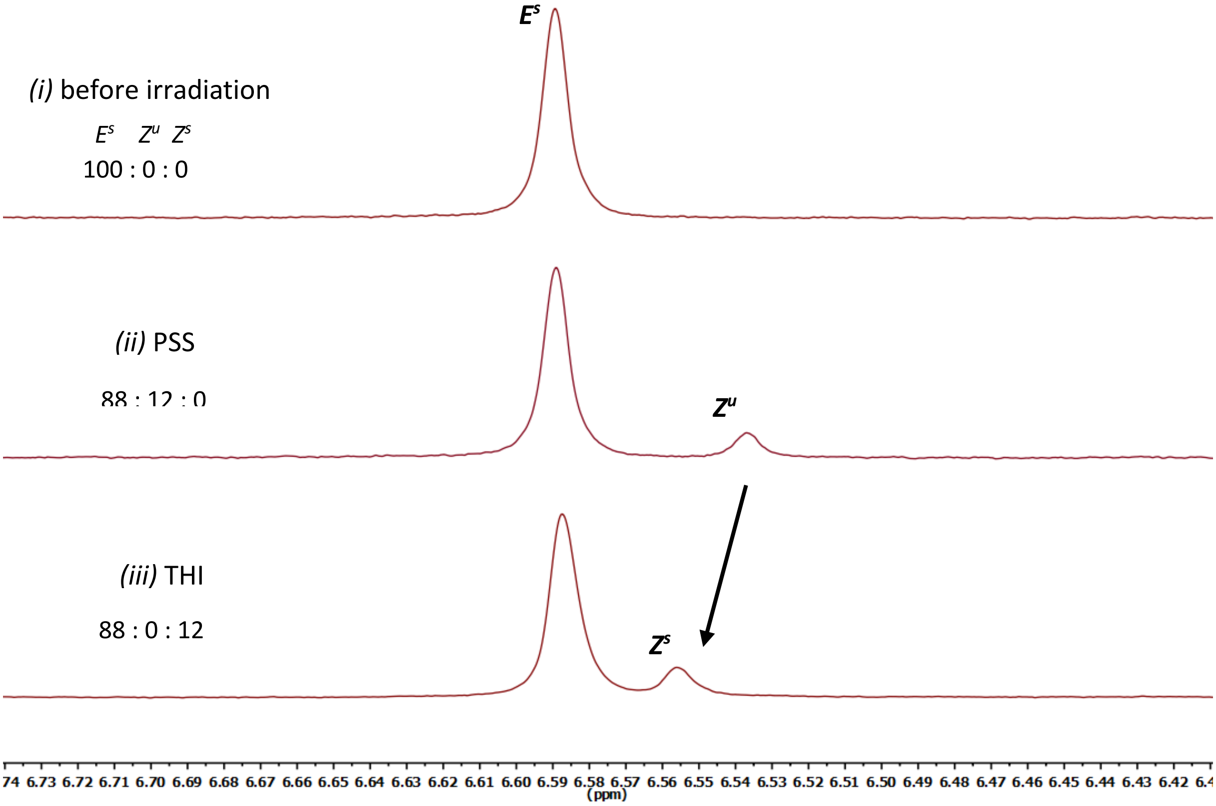


Figure S17: ^{1}H-NMR spectrum (500 MHz, 223 K) of the aromatic region H$_a$ of **7** measured in degassed DCM-d$_2$ (4.2 x 10^{-3} M). First irradiation to its PSS with a Thorlab 340 nm LED coupled to a 600 µm optical fibre, which led the light into the NMR tube inside the spectrometer, PSS: 169 min, PSS$_{340}$ ratio: 88:12 (E^s:Z^u). The NMR tube was allowed to heat up to 298 K for 30 min to induce thermal helix inversion and measured again. *i)* Initial state (E^s), *ii)* Photoisomerization to unstable state (PSS ratio$_{340}$: 88:12 (E^s:Z^u)) and *iii)* thermal helix inversion (ratio$_{THI}$: 88:12 (E^s:Z^s)).

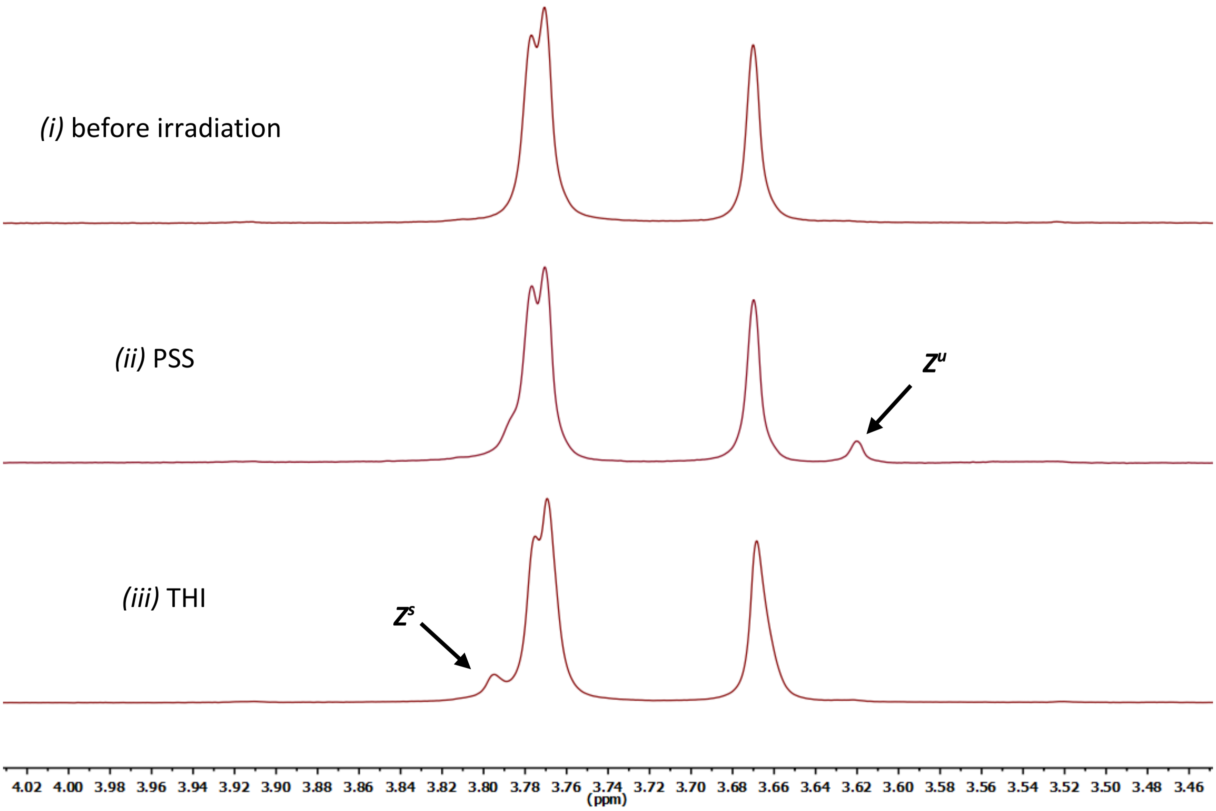


Figure S18: ^{1}H-NMR spectrum (500 MHz, 223 K) of the methoxy region H_b of **7** measured in degassed DCM-d_2 (4.2 x 10^{-3} M). First irradiation to its PSS with a Thorlab 340 nm LED coupled to a 600 µm optical fibre, which led the light into the NMR tube inside the spectrometer, PSS: 169 min, PSS_{340} ratio: 88:12 (E^s:Z^u). The NMR tube was allowed to heat up to 298 K for 30 min to induce thermal helix inversion and measured again. *i)* Initial state (E^s), *ii)* Photoisomerization to unstable state (PSS $ratio_{340}$: 88:12 (E^s:Z^u)) and *iii)* thermal helix inversion ($ratio_{THI}$: 88:12 (E^s:Z^s)).

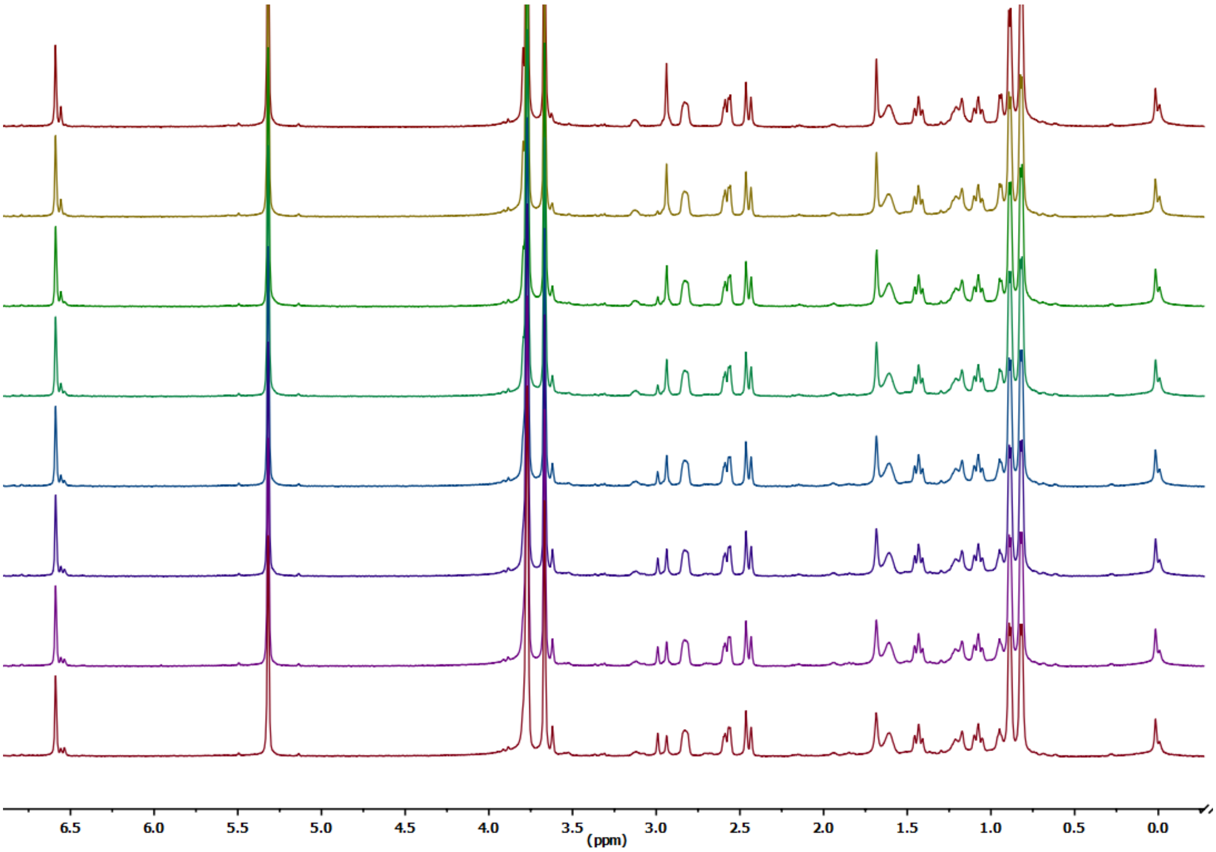


Figure S19: ^{1}H-NMR spectrum (500 MHz, 223 K) of **7** measured in degassed DCM-d_2 (4.1 x 10^{-3} M). First irradiation to its PSS at 298 K with a Thorlab 340 nm LED coupled to a 600 µm optical fibre, which led the light into the NMR tube inside the spectrometer, PSS: 135 min, PSS$_{340}$ ratio: 85:15 (E^s:Z^s). The NMR tube was cooled down to 223 K and irradiated with 340 nm again. Initial state (top spectrum, PSS$_{340}$ ratio: 81:0:19 (E^s:Z^u:Z^s)), Photoisomerization to unstable state (bottom spectrum, 3h, ratio$_{340}$: 83:9:8 (E^s:Z^u:Z^s)), E^u could not be observed since the thermal helix inversion barrier is too low.

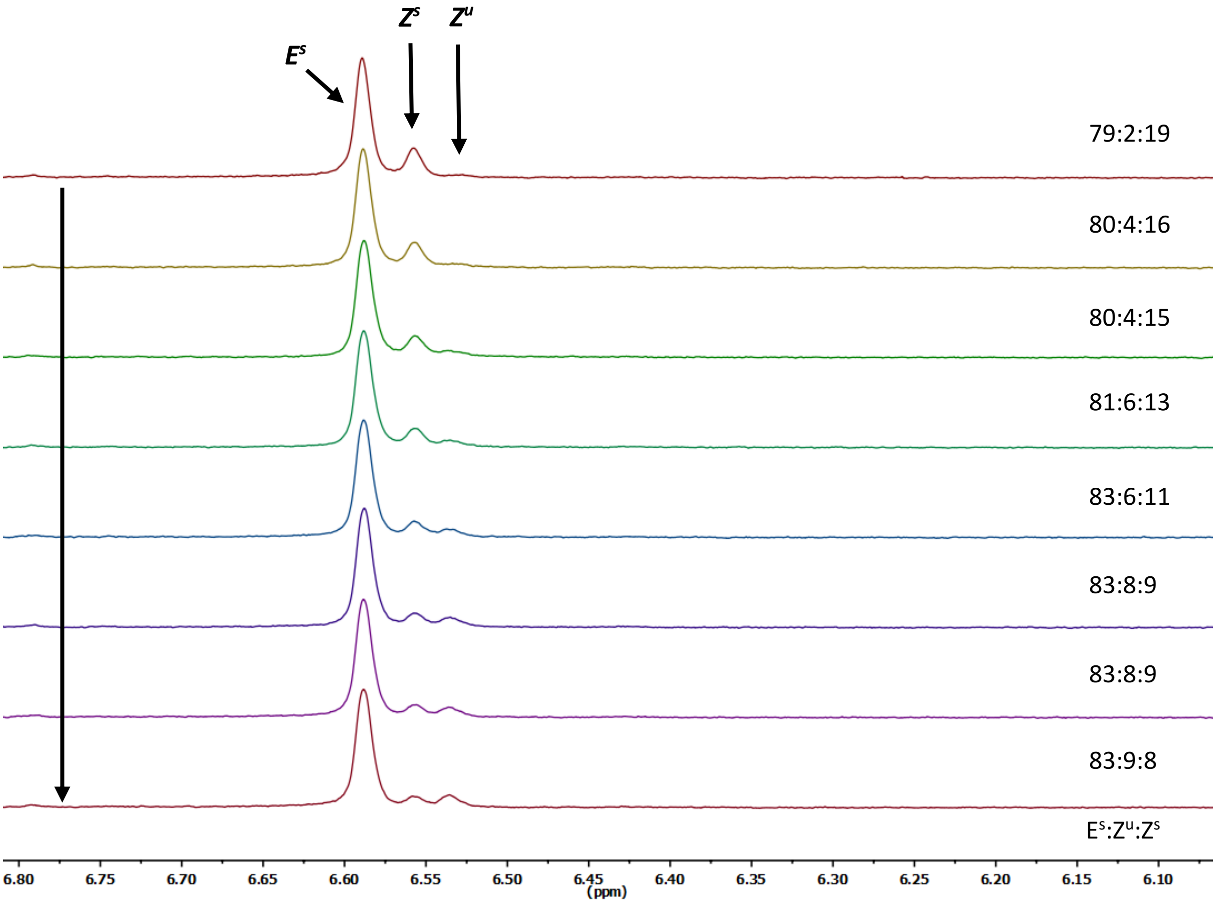


Figure S20: ^{1}H-NMR spectrum (500 MHz, 223 K) of the aromatic region H_a of **7** measured in degassed DCM-d_2 (4.1 x 10^{-3} M). First irradiation to its PSS at 298 K with a Thorlab 340 nm LED coupled to a 600 µm optical fibre, which led the light into the NMR tube inside the spectrometer, PSS: 135 min, PSS_{340} ratio: 85:15 (E^s:Z^s). The NMR tube was cooled down to 223 K and irradiated with 340 nm again. Initial state (top spectrum, PSS_{340} ratio: 79:2:19 (E^s:Z^u:Z^s)), Photoisomerization to unstable state (bottom spectrum, 3h, $ratio_{340}$: 83:9:8 (E^s:Z^u:Z^s)), E^u could not be observed since the thermal helix inversion barrier is too low.

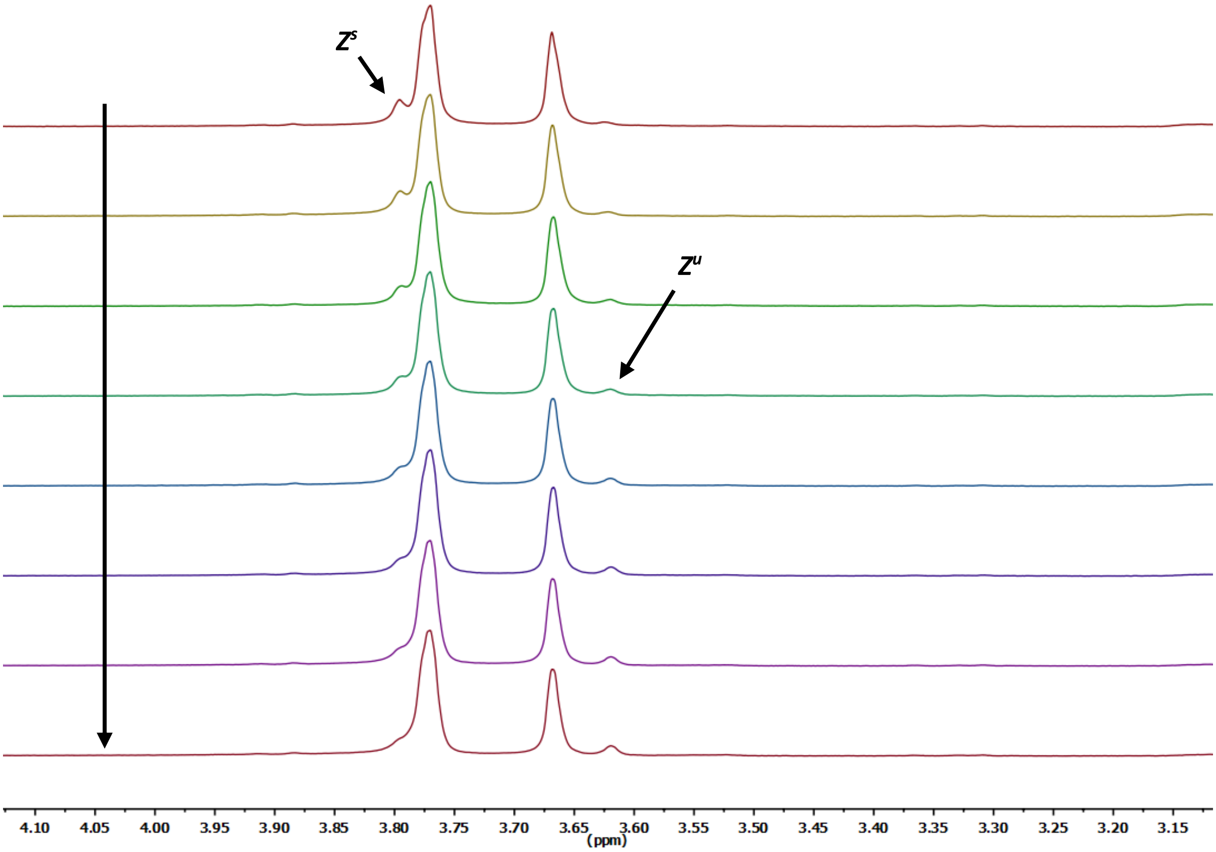


Figure S21: ^{1}H-NMR spectrum (500 MHz, 223 K) of the methoxy region H_b of **7** measured in degassed DCM-d_2 (4.1 x 10^{-3} M). First irradiation to its PSS at 298 K with a Thorlab 340 nm LED coupled to a 600 µm optical fibre, which led the light into the NMR tube inside the spectrometer, PSS: 135 min, PSS_{340} ratio: 85:15 (E^s:Z^s). The NMR tube was cooled down to 223 K and irradiated with 340 nm again. Initial state (top spectrum, PSS_{340} ratio: 81:0:19 (E^s:Z^u:Z^s)), Photoisomerization to unstable state (bottom spectrum, 3h, $ratio_{340}$: 83:9:8 (E^s:Z^u:Z^s)), E^u could not be observed since the thermal helix inversion barrier is too low.

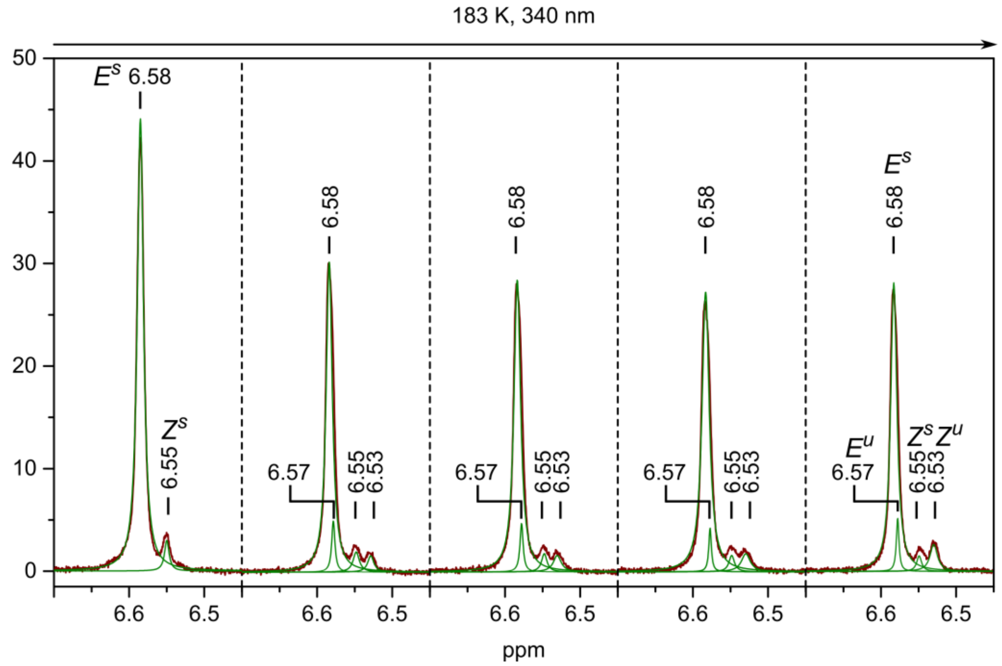


Figure S22: ^{1}H-NMR spectrum (500 MHz, 183 K) of the aromatic region H_a of **7** measured in degassed DCM-d_2 (1.8×10^{-3} M). First irradiation to its PSS at 298 K with a Thorlab 340 nm LED coupled to a 600 µm optical fibre, which led the light into the NMR tube inside the spectrometer, PSS: 45 min, PSS_{340} ratio: 91:9 (E^s:Z^s). The NMR tube was cooled down to 183 K and irradiated with 340 nm again. Initial state (left spectrum, PSS_{340} ratio: 94:0:6:0 (E^s:Z^u:Z^s:E^u)), Photoisomerization to unstable states (right spectrum, 85 min, $ratio_{340}$: 81:9:3:6 (E^s:Z^u:Z^s:E^u)), Z^u could be observed similarly to previous experiments, E^u could be observed as a shoulder of E^s and was identified via deconvolution via Lorentzian fit. The integrals are based on the deconvolution area and not on the peak area.

3.3. HRMS Spectra of molecular motor 7

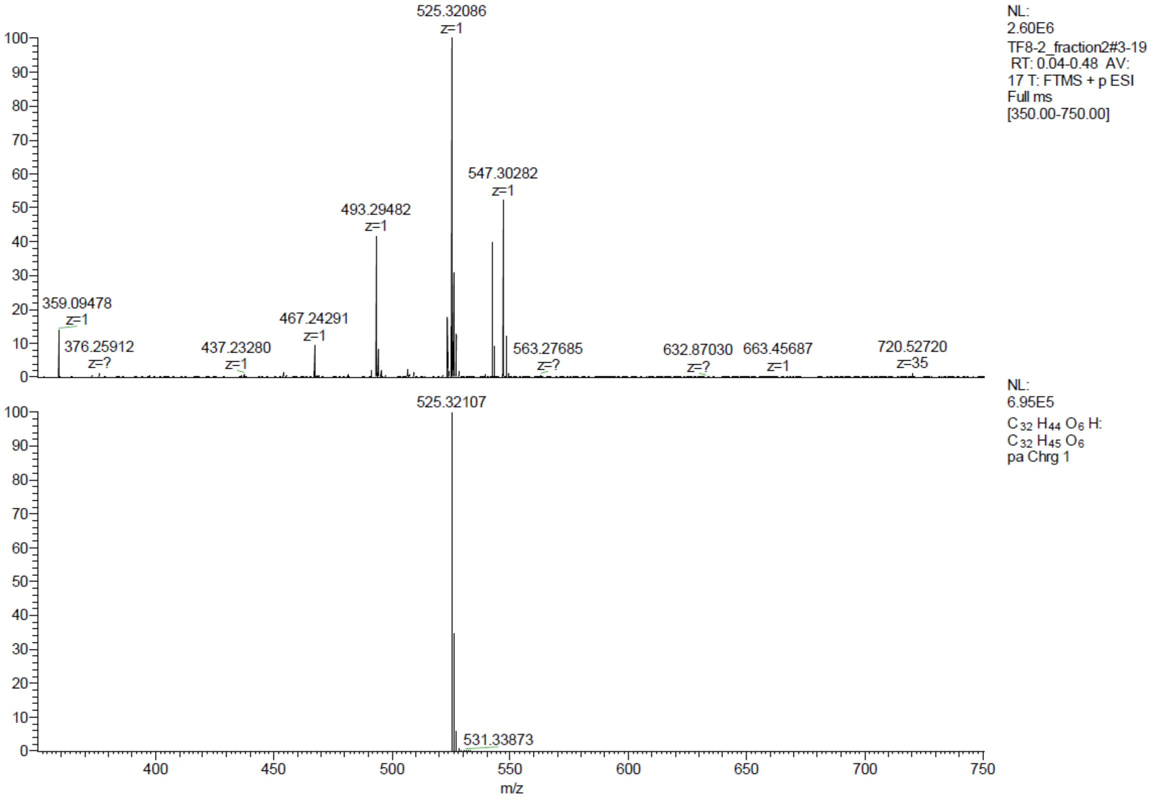


Figure S23: HRMS of **7** (top: measured, bottom: calculated), LTQ Orbitrap XL (ESI$^+$).

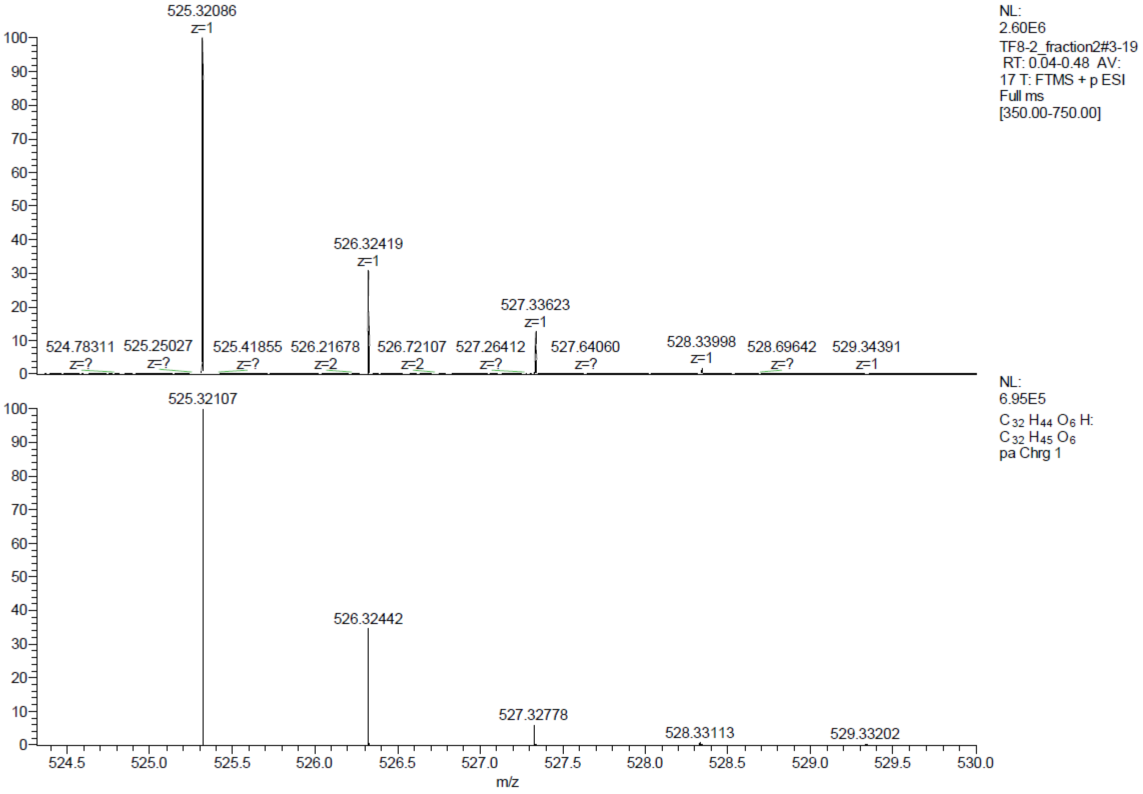


Figure S24: HRMS (zoomed in) of **7** (top: measured, bottom: calculated), LTQ Orbitrap XL (ESI$^+$).

3.4. X-ray structure of 5

A suitable crystal of compound **5** was mounted on top of a cryoloop and transferred into the cold (100 K) nitrogen stream of a Bruker D8 Venture diffractometer. Data collection and reduction was done using the Bruker software suite APEX3.[1] The final unit cell was obtained from the xyz centroids of 1535 reflections after integration. A multiscan absorption correction was applied, based on the intensities of symmetry-related reflections measured at different angular settings (*SADABS*).[1] The structures were solved by dual-space methods using *SHELXT,*[2] and refinement of the structure was performed using *SHELXL*.[3] The hydrogen atoms were generated by geometrical considerations, constrained to idealized geometries and allowed to ride on their carrier atoms with an isotropic displacement parameter related to the equivalent displacement parameter of their carrier atoms. One reflection was omitted from refinement because it was affected by the beam stop. **5** was observed with *E*-configuration as major component. Crystal data and details on data collection and refinement are presented in**.**

Table S1.

Table S1: Crystallographic data for compound **5**.

chem formula	$C_{16}H_{20}O_4$
M_r	276.32
cryst syst	triclinic
color, habit	colorless, block
size (mm)	0.473 x 0.296 x 0.142
space group	P_{-1}
a (Å)	11.0534(16)
b (Å)	11.5940(17)
c (Å)	12.4153(18)
α (°)	75.979(5)
β (°)	86.095(5)
γ (°)	73.276(4)
V (Å^3)	1478.4(4)
Z	4
ρ_{calc}, g.cm^{-3}	1.241
Radiation [Å]	Mo K_{α} 0.71073
μ(Mo K_{α}), mm^{-1}	0.088
F(000)	592
temp (K)	100(2)
θ range (°)	2.571 – 26.083
data collected (h,k,l)	-13:13; -14:14; -15:14
no. of rflns collected	19212
no. of indpndt reflns	5834
observed reflns $F_o \geq 2.0\ \sigma (F_o)$	3476
R(F) (%)	6.66
wR(F^2) (%)	17.7
GooF	1.029
weighting a,b	0.0247, 0.0453
params refined	371
min, max resid dens	-0.306, 0.377

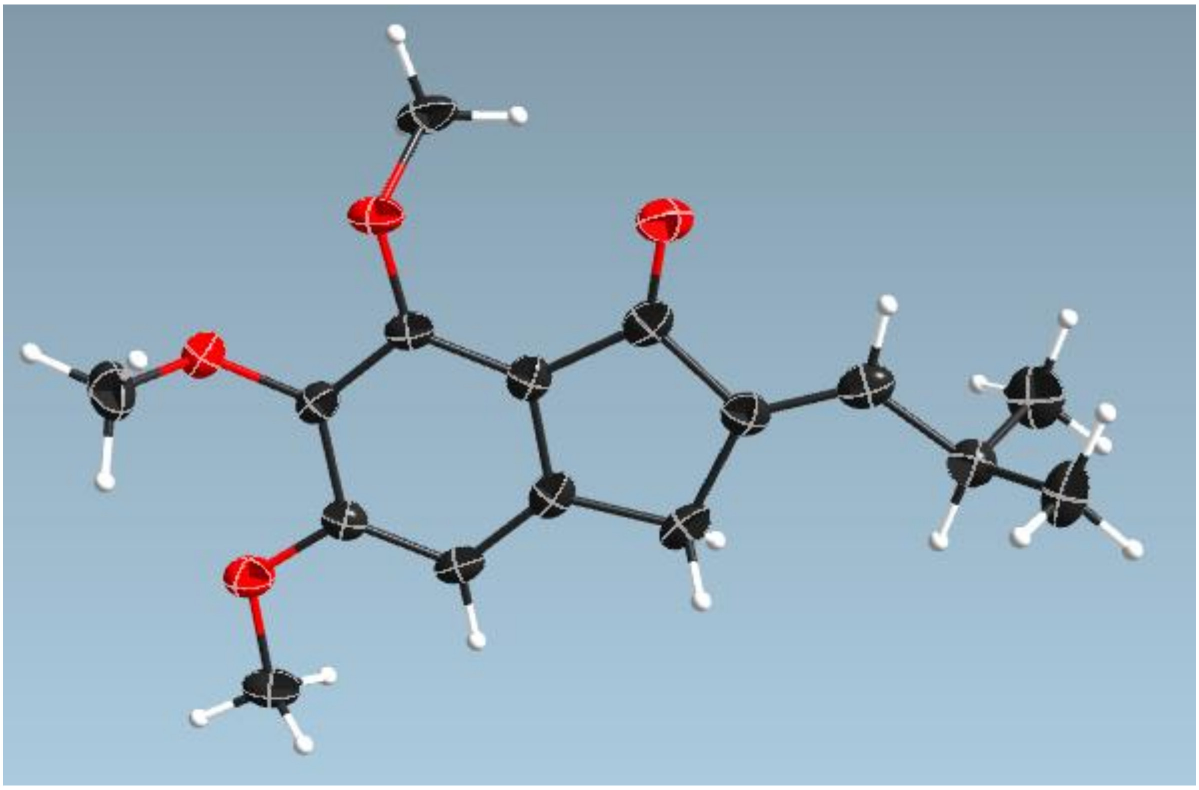


Figure S25: Molecular structure of compound **5** (50% probability ellipsoids).

3.5. X-ray structure of the molecular motor 7

A suitable crystal of compound **7** was mounted on top of a cryoloop and transferred into the cold (100 K) nitrogen stream of a Bruker D8 Venture diffractometer. Data collection and reduction was done using the Bruker software suite APEX3.[18] The final unit cell was obtained from the xyz centroids of 8100 reflections after integration. A multiscan absorption correction was applied, based on the intensities of symmetry-related reflections measured at different angular settings (*SADABS*).[1] The structure was solved by dual space methods using *SHELXT,*[19] and refinement of the structure was performed using *SHELXL*.[20] The hydrogen atoms were generated by geometrical considerations, constrained to idealized geometries and allowed to ride on their carrier atoms with an isotropic displacement parameter related to the equivalent displacement parameter of their carrier atoms. The Flack parameter refined to 0.07(9) with the major component being the R,R-configuration. Crystal data and details on data collection and refinement are presented in **Table S2**.

Table S2: Crystallographic data for compound **7**

chem formula	$C_{32}H_{44}O_6$
M_r	524.67
cryst syst	monoclinic
color, habit	colorless, block
size (mm)	0.465 x 0.291 x 0.109
space group	C2
a (Å)	23.8610(8)
b (Å)	6.1612(2)
c (Å)	10.0136(3)
α (°)	90
β (°)	95.846(2)
γ (°)	90
V (Å^3)	1464.47(8)
Z	2
ρ_{calc}, g.cm^{-3}	1.190
Radiation [Å]	Cu K_α 1.54178
μ(Cu K_α), mm^{-1}	0.646
F(000)	568
temp (K)	100(2)
θ range (°)	3.724 – 72.360
data collected (h,k,l)	-29:29; -7:7; -12:12
no. of rflns collected	11160
no. of indpndt reflns	2820
observed reflns $F_o \geq 2.0\ \sigma(F_o)$	2661
R(F) (%)	3.53
wR(F^2) (%)	8.42
GooF	1.160
weighting a,b	0.0299, 0.7920
params refined	177
min, max resid dens	-0.226, 0.181
Flack x	0.07(9)

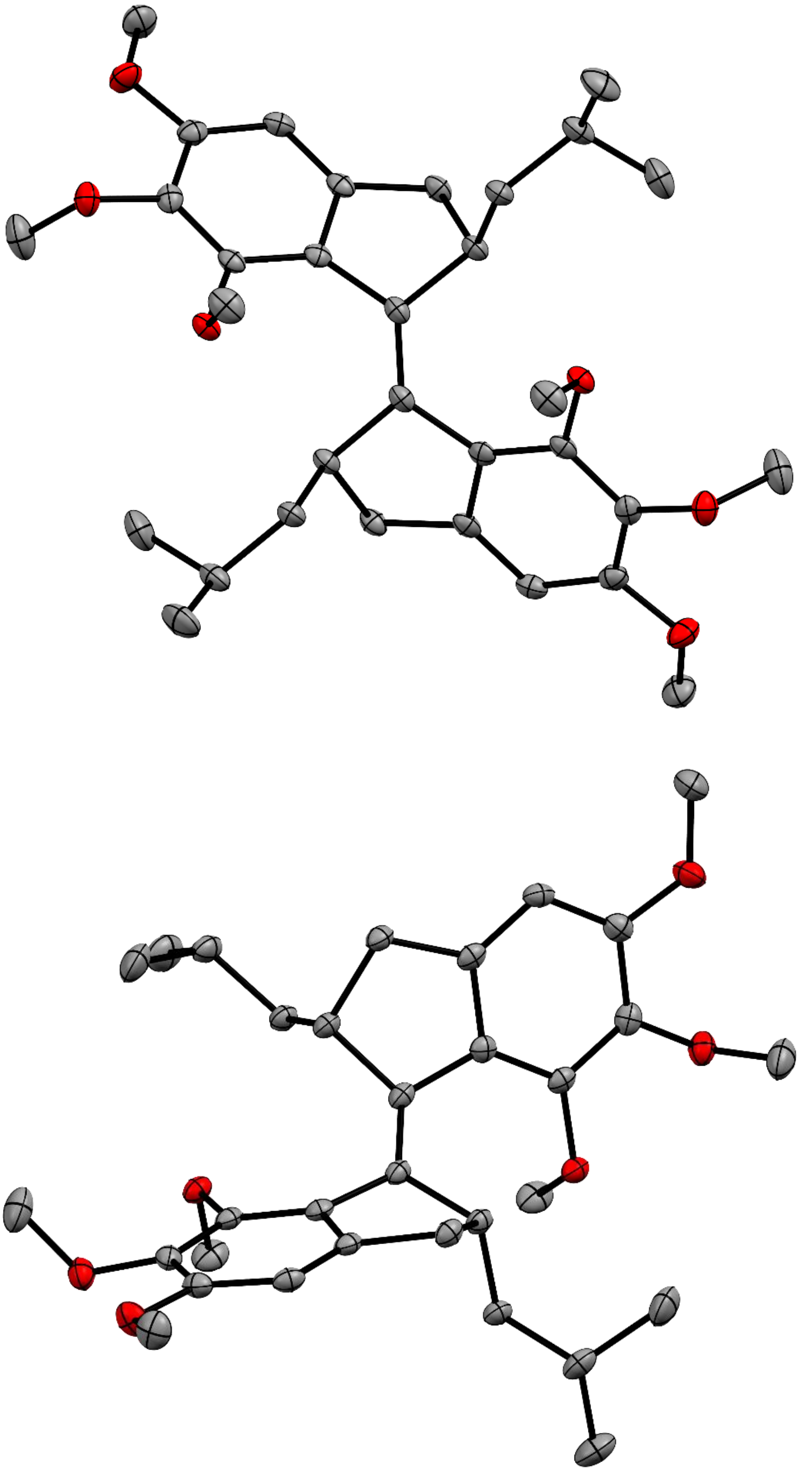


Figure S26: Molecular structure of compound **7** (50% probability ellipsoids). Hydrogen atoms are omitted for clarity.

4. NMR spectra of compounds (1-7)

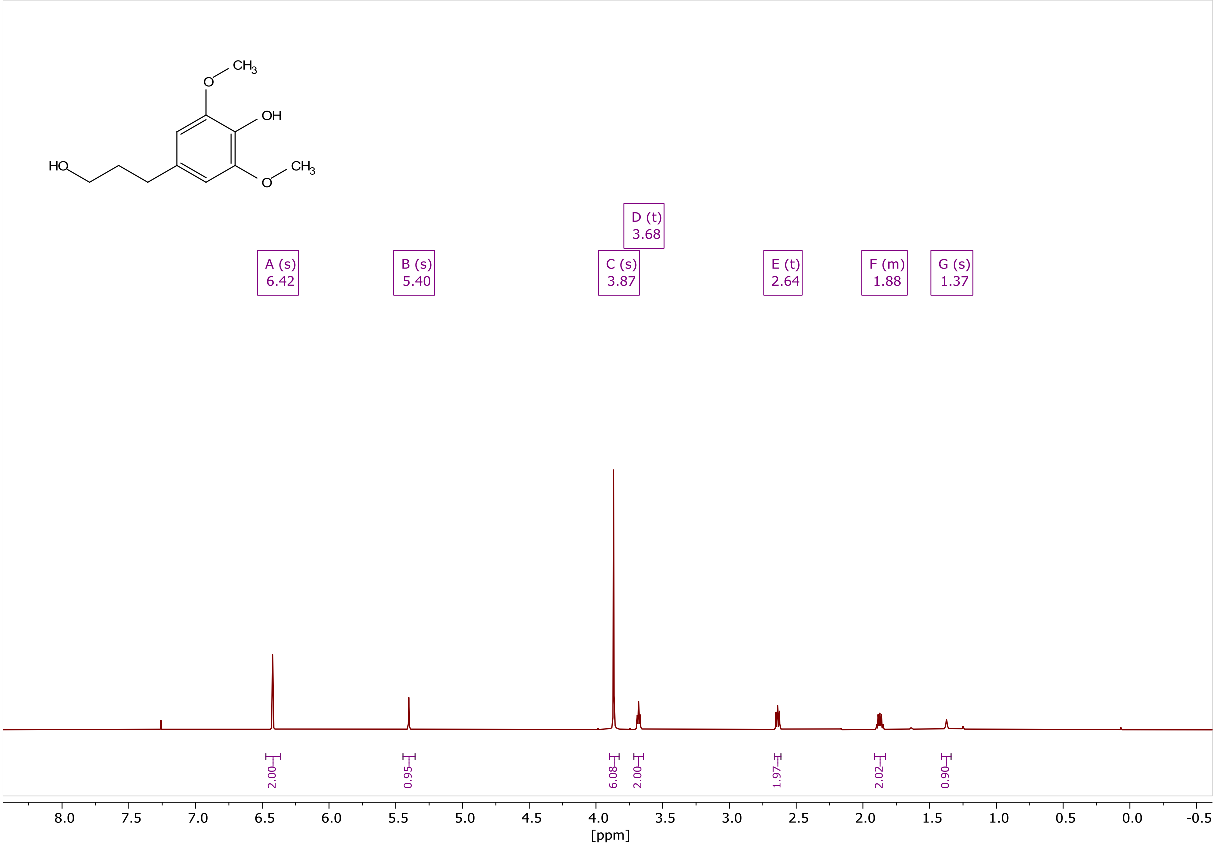


Figure S27: ^{1}H-NMR (Chloroform-*d*, 600 MHz): **1**

^{1}H NMR: δ_H (600 MHz, Chloroform-*d*) 6.42 (s, 2H, $H^{3,5}$), 5.40 (s, 1H, H^7), 3.87 (s, 6H, $H^{9,11}$), 3.68 (t, J = 6.4 Hz, 2H, H^{14}), 2.64 (t, J = 7.8 Hz, 2H, H^{12}), 1.91 – 1.83 (m, 2H, H^{13}), 1.37 (s, 1H, H^{15}). Spectral data are consistent with those reported in the literature.[9]

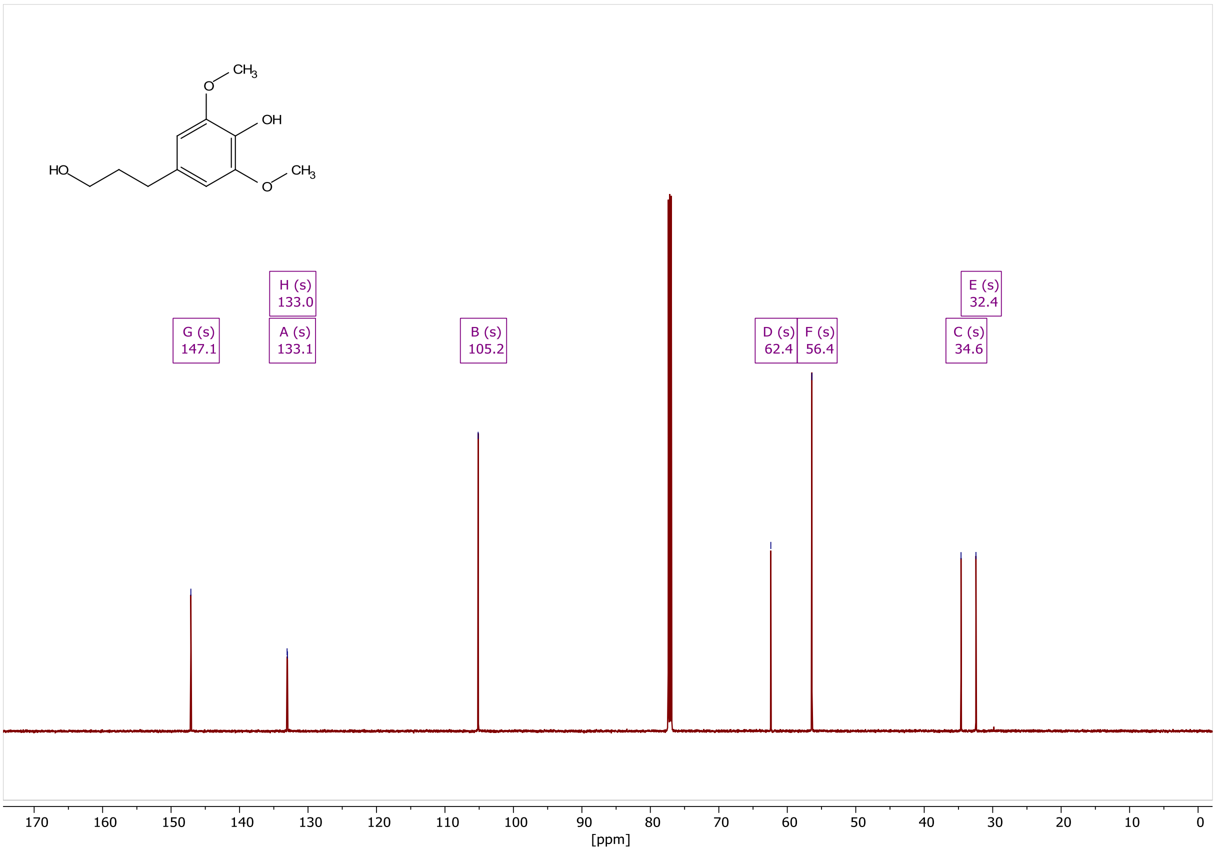


Figure S28: ^{13}C-NMR (Chloroform-*d*, 151 MHz): **1**

^{13}C-NMR: δ $_C$ (151 MHz, Chloroform-*d*) 147.1 (2C, $C^{2,6}$), 133.1 (1C, arom. C), 133.0 (1C, arom. C), 105.2 (2C, $C^{3,5}$), 62.4 (1C, C^{14}), 56.4 (2C, $C^{9,11}$), 34.6 (1C, C^{13}), 32.4 (1C, C^{12}). Spectral data are consistent with those reported in the literature.[9]

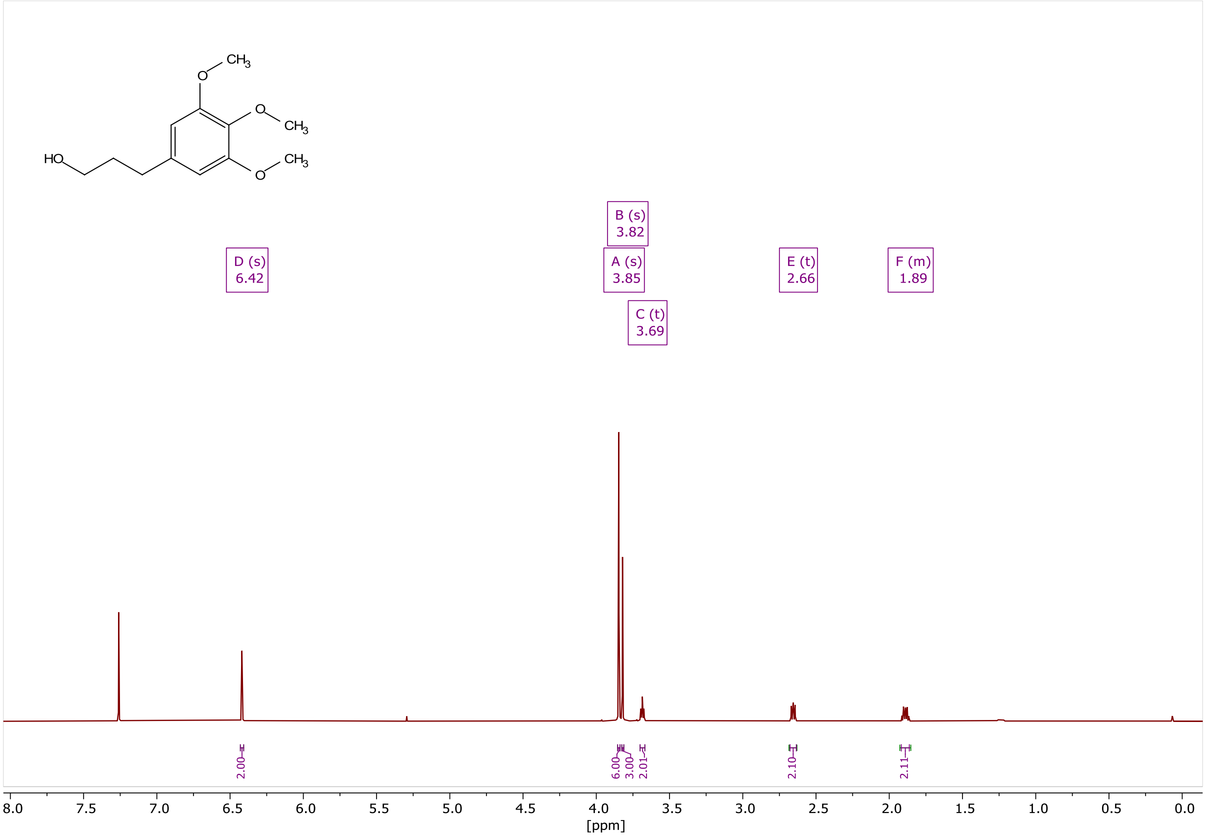


Figure S29: ^{1}H-NMR (Chloroform-*d*, 600 MHz): **2**

^{1}H-NMR: δ_H (600 MHz, Chloroform-*d*) 6.42 (s, 2H, $H^{6,10}$), 3.85 (s, 6H, $H^{12,16}$), 3.82 (s, 3H, H^{14}), 3.69 (t, J = 6.4 Hz, 2H, H^1), 2.66 (t, J = 7.9 Hz, 2H, H^3), 1.93 – 1.85 (m, 2H, H^2). Spectral data are consistent with those reported in the literature.[10]

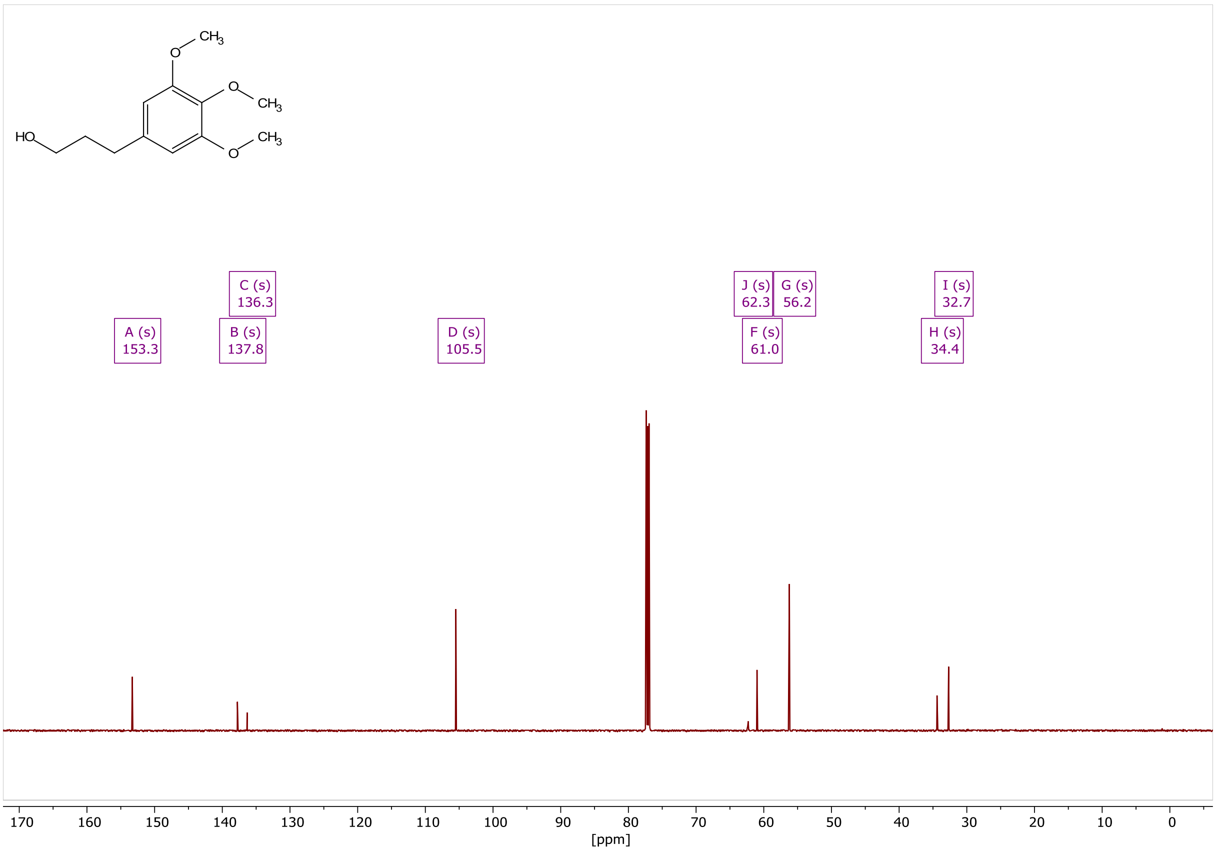


Figure S30: ^{13}C-NMR (Chloroform-*d*, 151 MHz): **2**

^{13}C-NMR: δ_{C} (151 MHz, Chloroform-*d*) 153.3 (2C, $C^{7,9}$), 137.8 (1C, arom. C), 136.3 (1C, arom. C), 105.5 (2C, $C^{6,10}$), 62.3 (1C, C^{1}), 61.0 (1C, C^{14}), 56.2 (2C, $C^{12,16}$), 34.4 (1C, C^{2}), 32.7 (1C, C^{3}). Spectral data are consistent with those reported in the literature.[10]

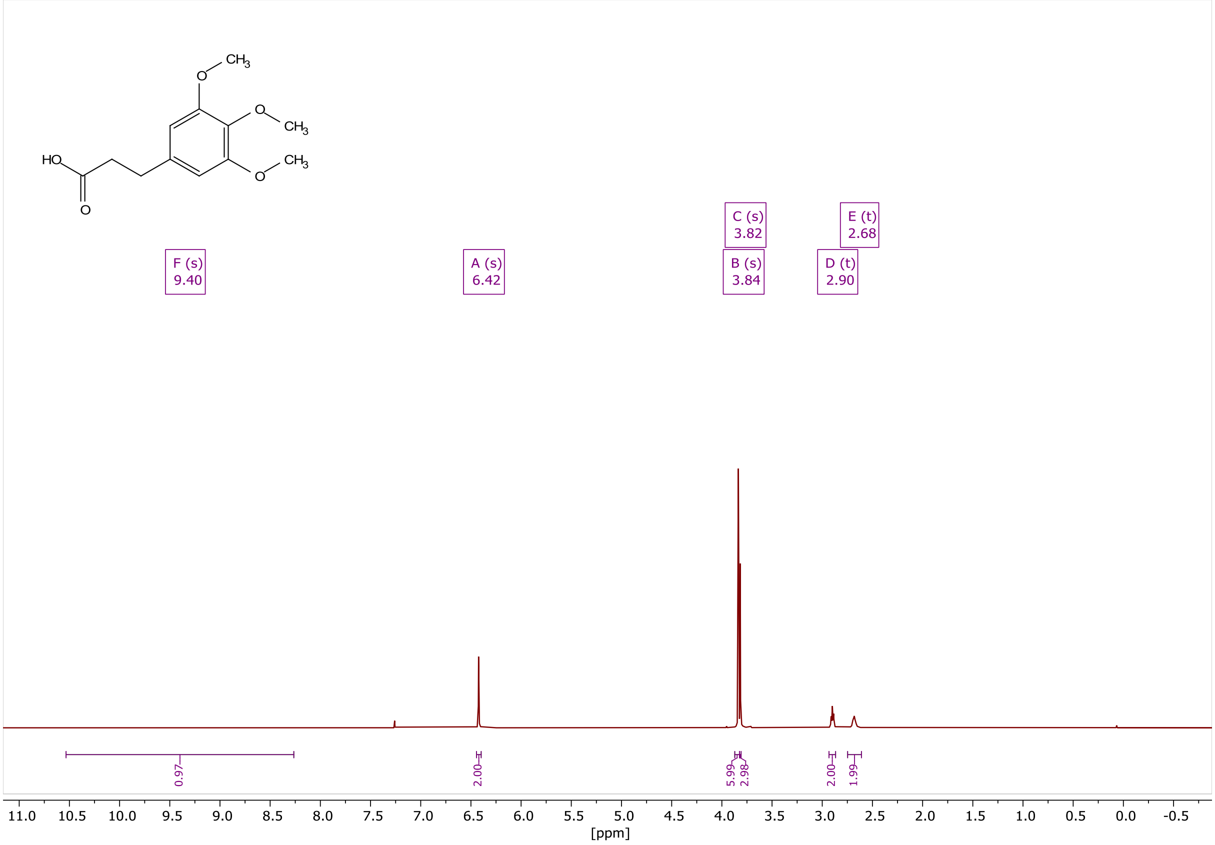


Figure S31: ^{1}H-NMR (Chloroform-*d*, 600 MHz): **3**

^{1}H-NMR: δ_H (600 MHz, Chloroform-*d*) 9.40 (s, 1H, H^5), 6.42 (s, 2H, $H^{7,11}$), 3.84 (s, 6H, $H^{13,17}$), 3.82 (s, 3H, H^{15}), 2.90 (t, J = 7.7 Hz, 2H, H^3), 2.68 (t, J = 7.7 Hz, 2H, H^2). Spectral data are consistent with those reported in the literature.[14]

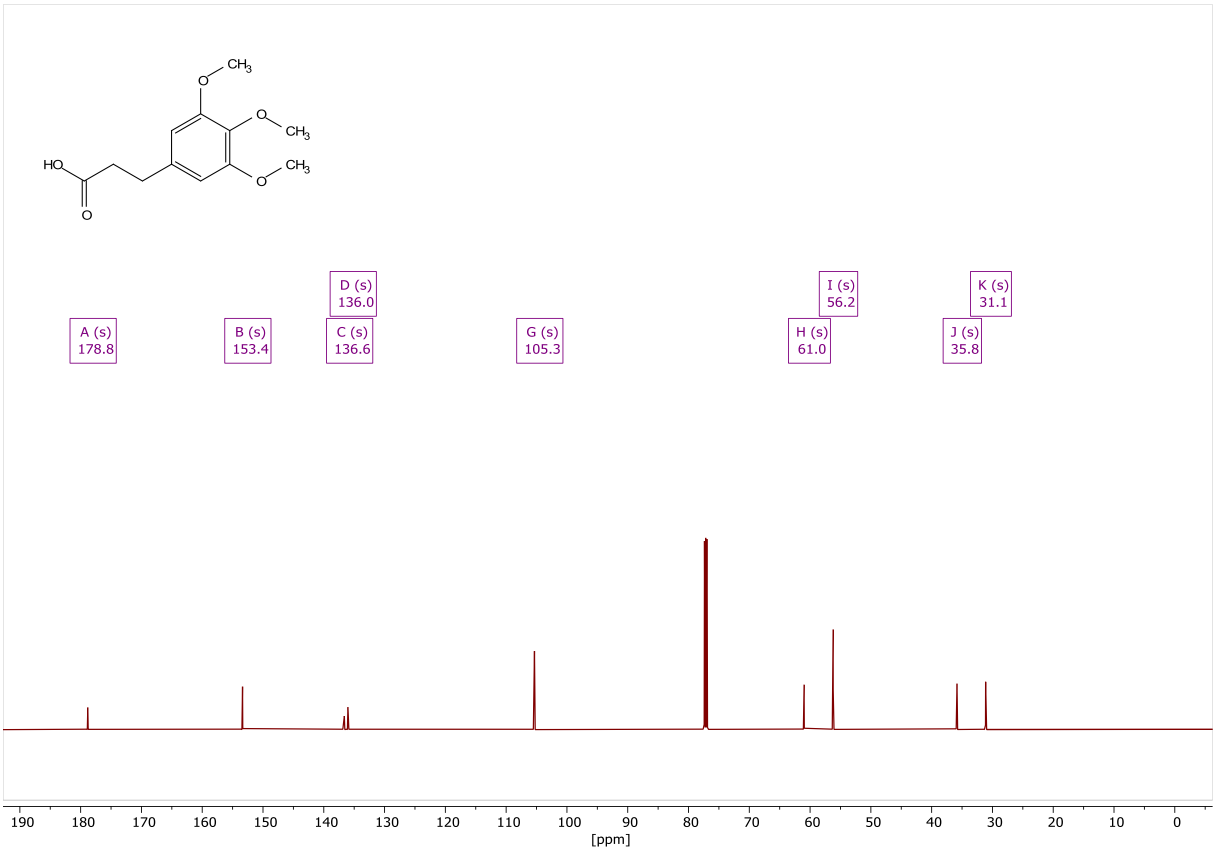


Figure S32: ^{13}C-NMR (Chloroform-*d*, 151 MHz): **3**

^{13}C-NMR: δ $_C$ (151 MHz, Chloroform-*d*) 178.8 (1C, C^1), 153.4 (2C, $C^{8,10}$), 136.6 (1C, arom. C), 136.0 (1C, arom. C), 105.3 (2C, $C^{7,11}$), 61.0 (1C, C^{15}), 56.2 (2C, $C^{13,17}$), 35.8 (1C, C^2), 31.1 (1C, C^3). Spectral data are consistent with those reported in the literature.[14]

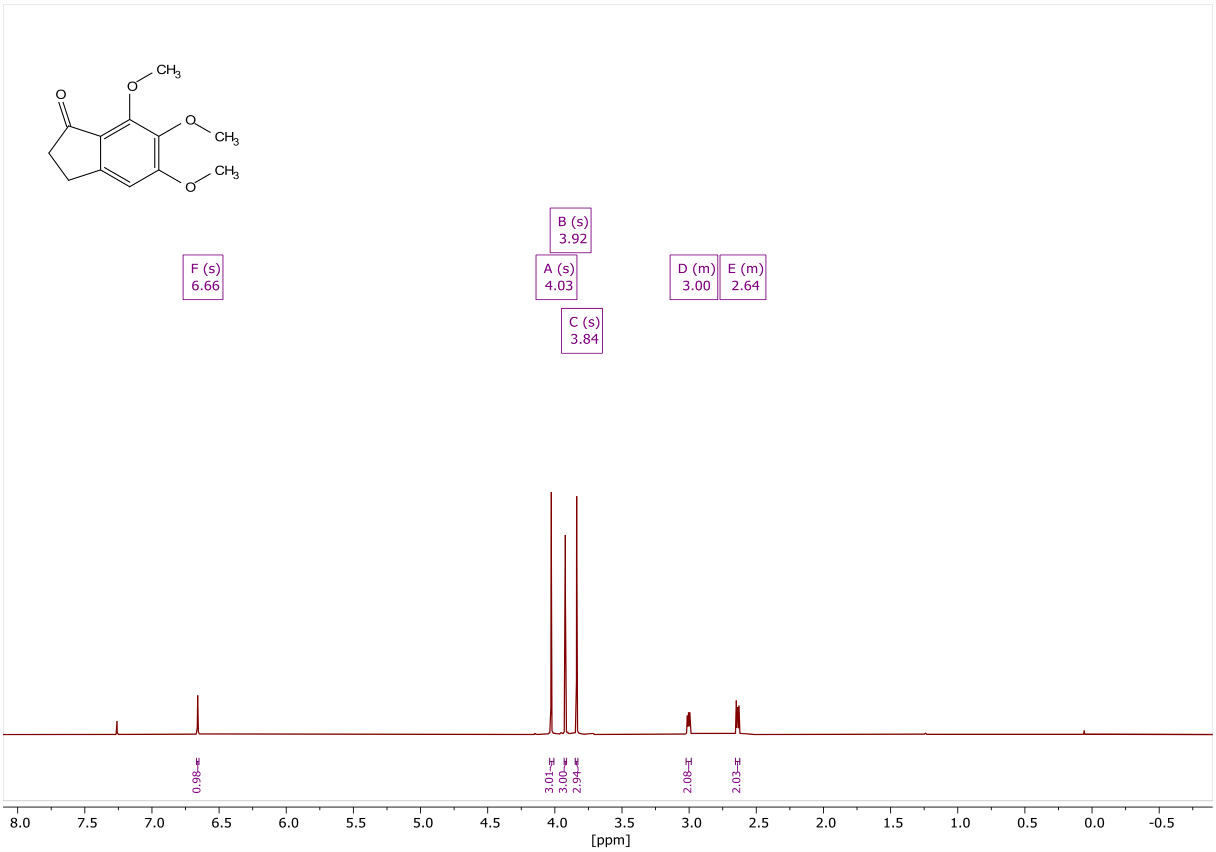


Figure S33: ^{1}H-NMR (Chloroform-d, 600 MHz): **4**

^{1}H-NMR: δ_H (600 MHz, Chloroform-*d*) 6.66 (s, 1H, H^4), 4.03 (s, 3H, H^{12}), 3.92 (s, 3H, H^{14}), 3.84 (s, 3H, H^{16}), 3.02 – 2.98 (m, 2H, H^2), 2.66 – 2.62 (m, 2H, H^3). Spectral data are consistent with those reported in the literature.[16]

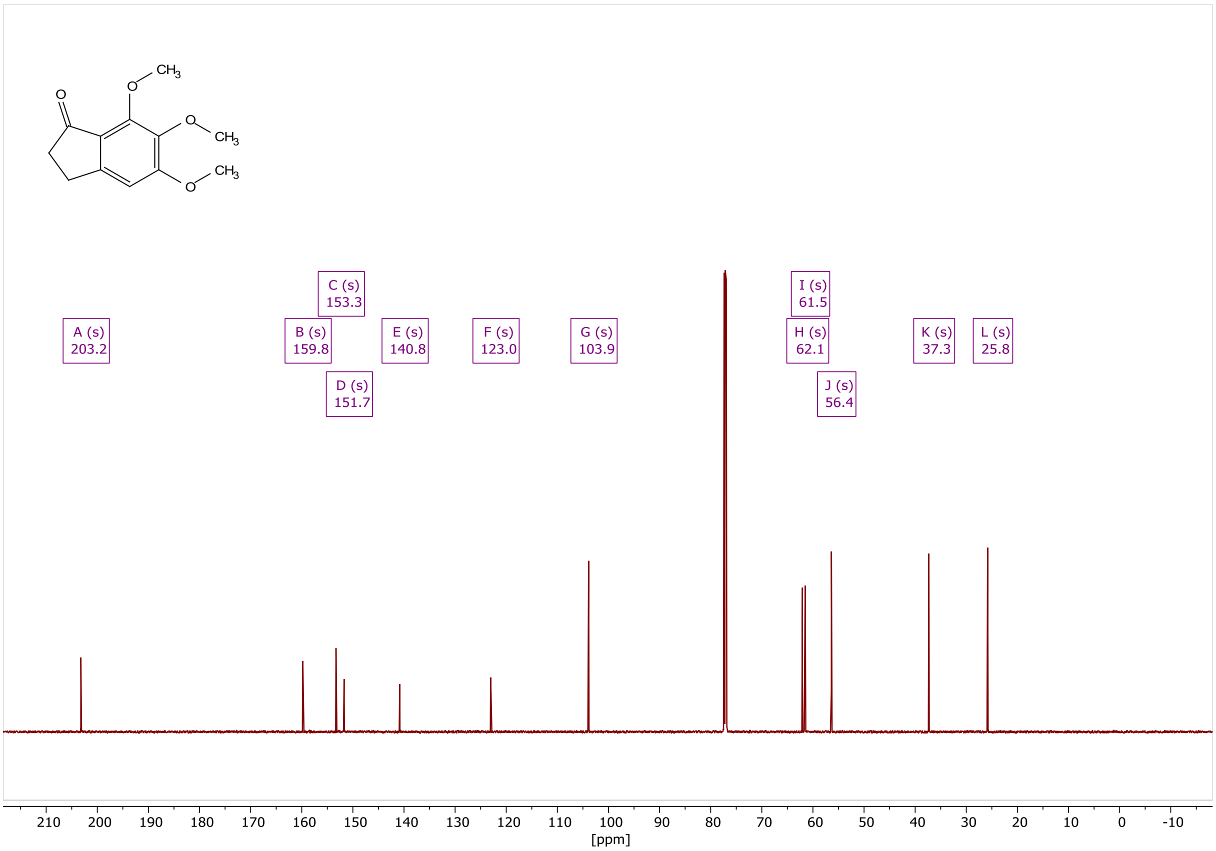


Figure S34: ^{13}C-NMR (Chloroform-*d*, 151 MHz): **4**

^{13}C-NMR: δ $_{C}$ (151 MHz, Chloroform-*d*) 203.2 (1C, C^{1}), 159.8 (1C, arom. C), 153.3 (1C, arom. C), 151.7 (1C, arom. C), 140.8 (1C, arom. C), 123.0 (1C, arom. C), 103.9 (1C, C^{4}), 62.1 (1C, C^{14}), 61.5 (1C, C^{12}), 56.4 (1C, C^{16}), 37.3 (1C, C^{2}), 25.8 (1C, C^{3}). Spectral data are consistent with those reported in the literature.[16]

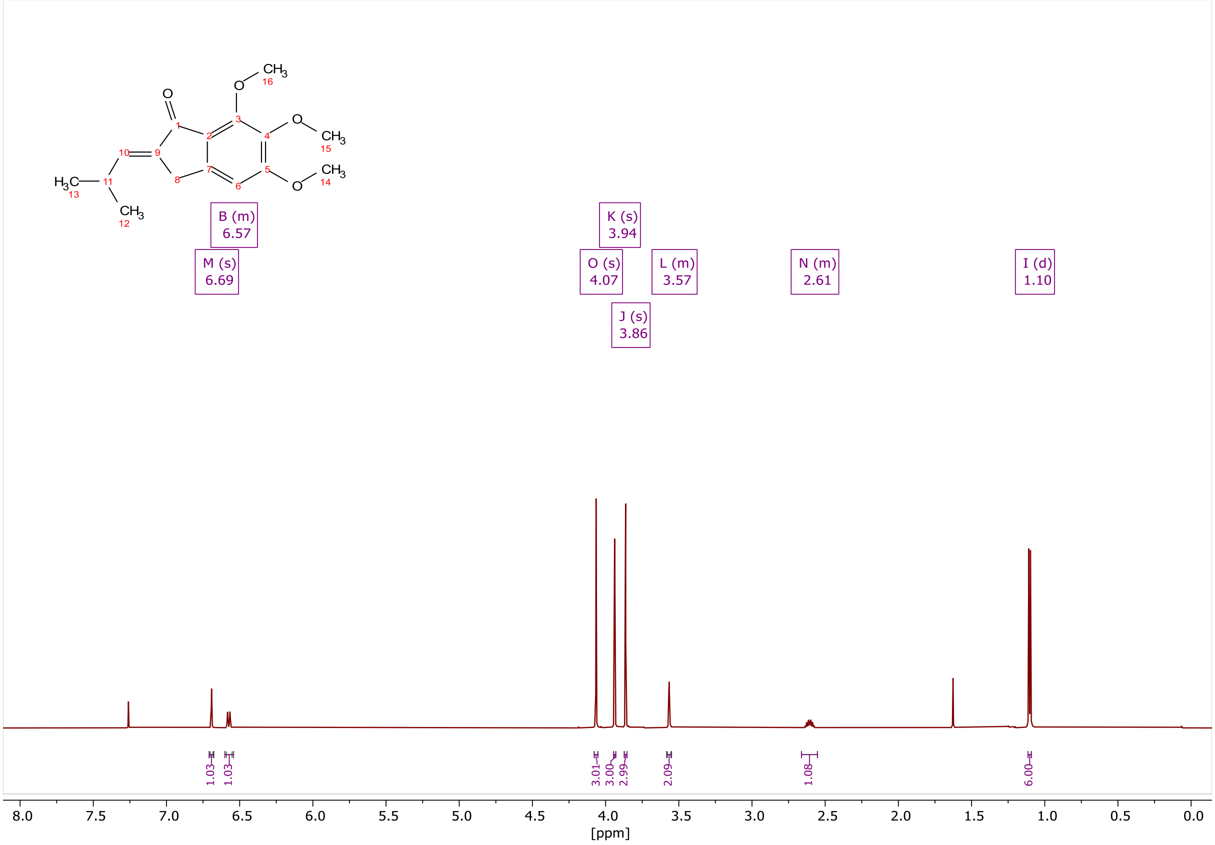


Figure S35: ^{1}H-NMR (Chloroform-*d*, 600 MHz): **5**

^{1}H-NMR: δ $_{H}$ (600 MHz, Chloroform-*d*) 6.69 (s, 1 H, H^{6}), 6.60 – 6.54 (m, 1 H, H^{10}), 4.07 (s, 3 H, H^{16}), 3.94 (s, 3 H, H^{14}), 3.86 (s, 3 H, H^{15}), 3.57 (m, 2 H, H^{8}), 2.66 – 2.55 (m, 1H, H^{11}), 1.10 (d, 6H, J = 6.7 Hz, H^{12,13}).

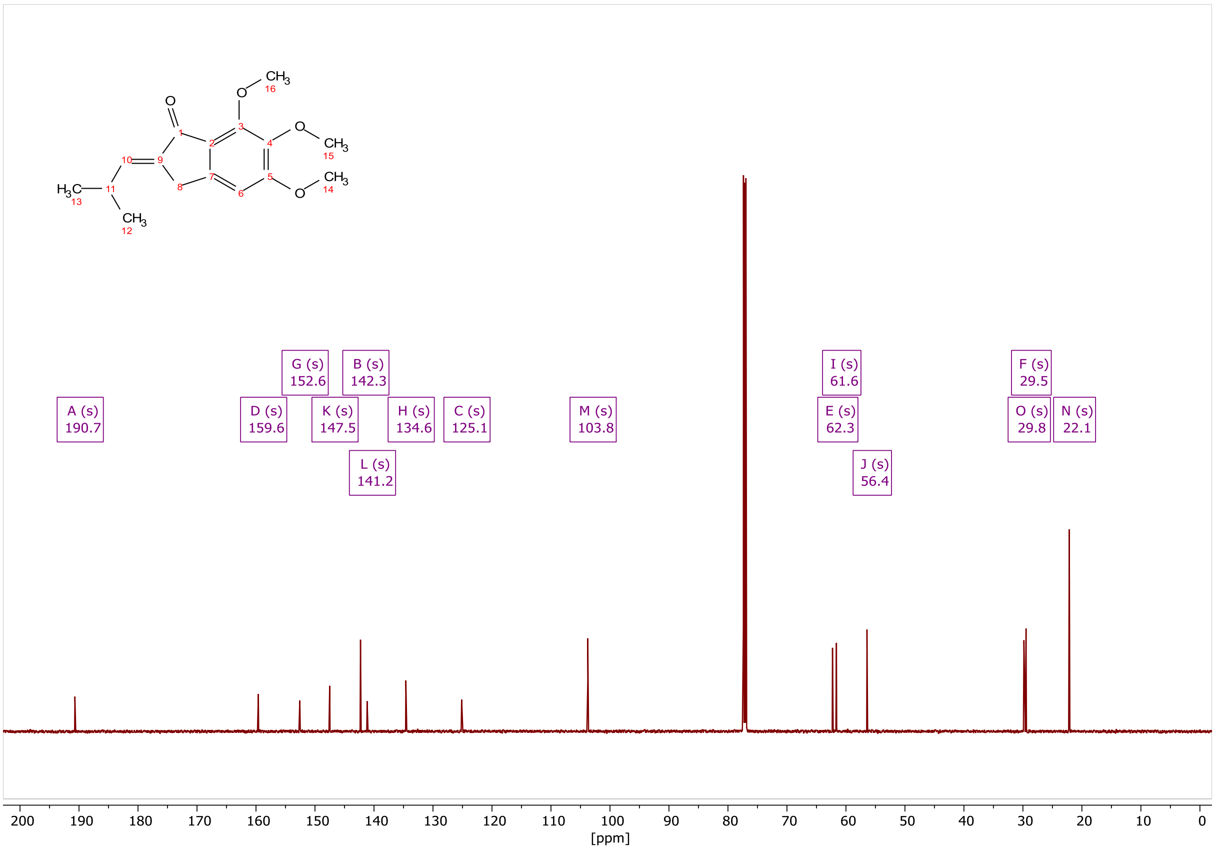


Figure S*36:* ^{13}C-NMR (Chloroform-d, 151 MHz): **5**

^{13}C-NMR: δ $_{C}$ (151 MHz, Chloroform-*d*) 190.7 (1C, C^{1}), 159.6 (1C, arom. C), 152.6 (1C, arom. C), 147.5 (1C, arom. C), 142.3 (1C, C^{10}), 141.2 (1C, arom. C), 134.6, (1C, C^{9}), 125.1 (1C, arom. C), 103.8 (1C, C^{6}), 62.3 (1C, C^{16}), 61.6 (1C, C^{15}), 56.4 (1C, C^{14}), 29.8 (1C, C^{8}), 29.5 (1C, C^{11}), 22.1 (2C, C^{12,13}).

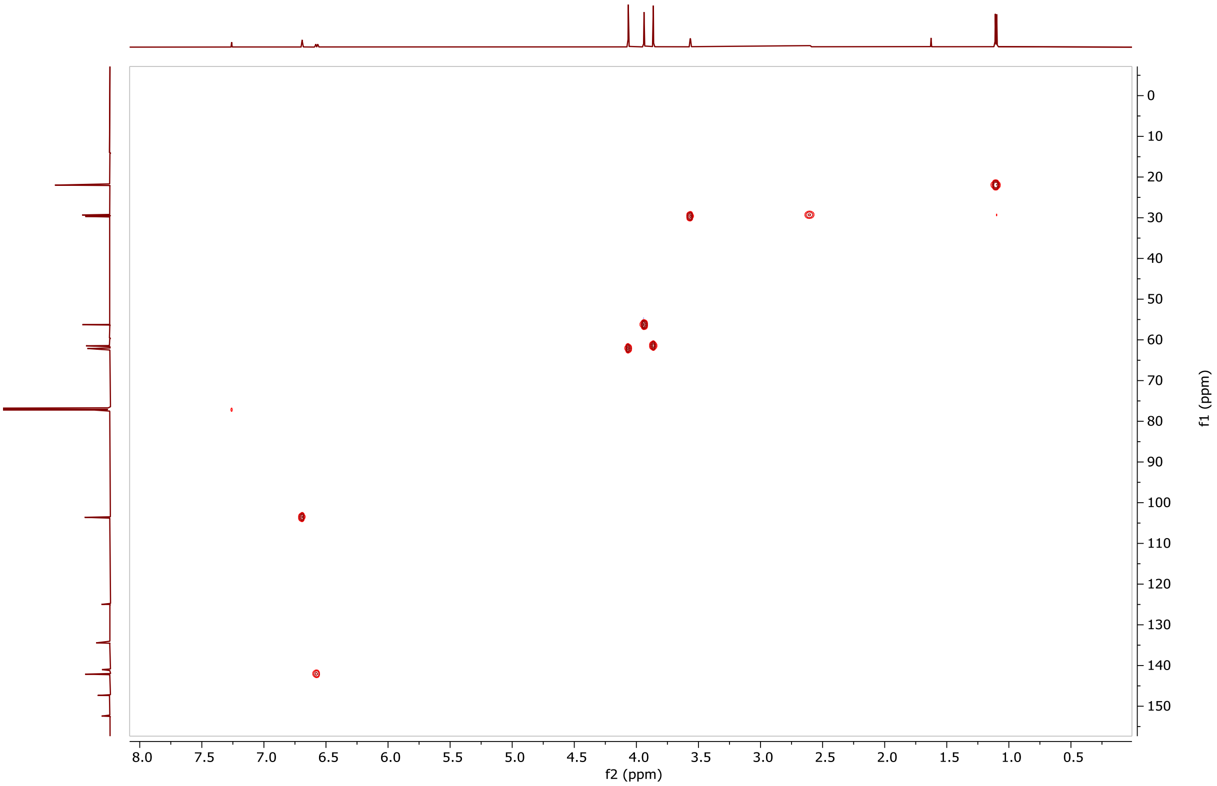


Figure S37: {^{1}H-^{13}C} HSQC NMR (Chloroform-*d*, 600 MHz): **5**

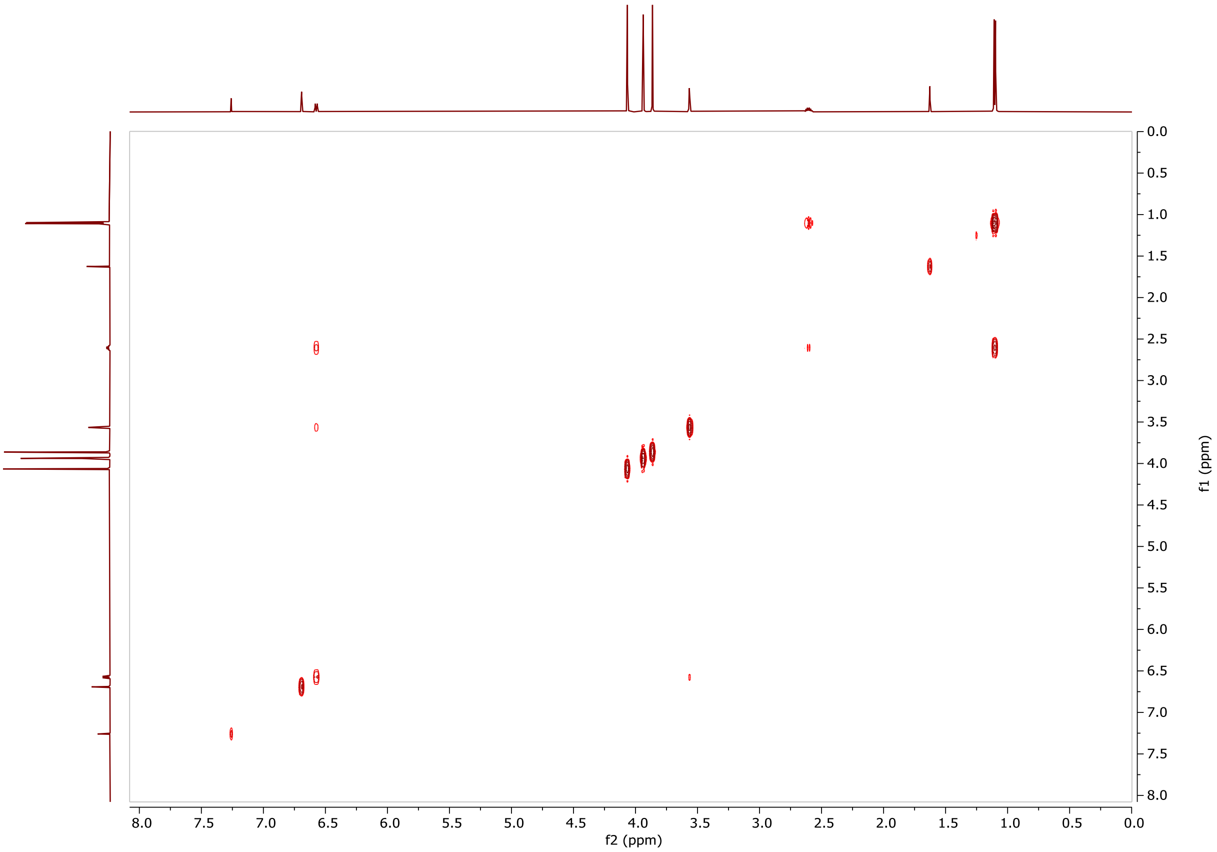


Figure S38: {^{1}H-^{1}H} COSY NMR (Chloroform-*d*, 600 MHz): **5**

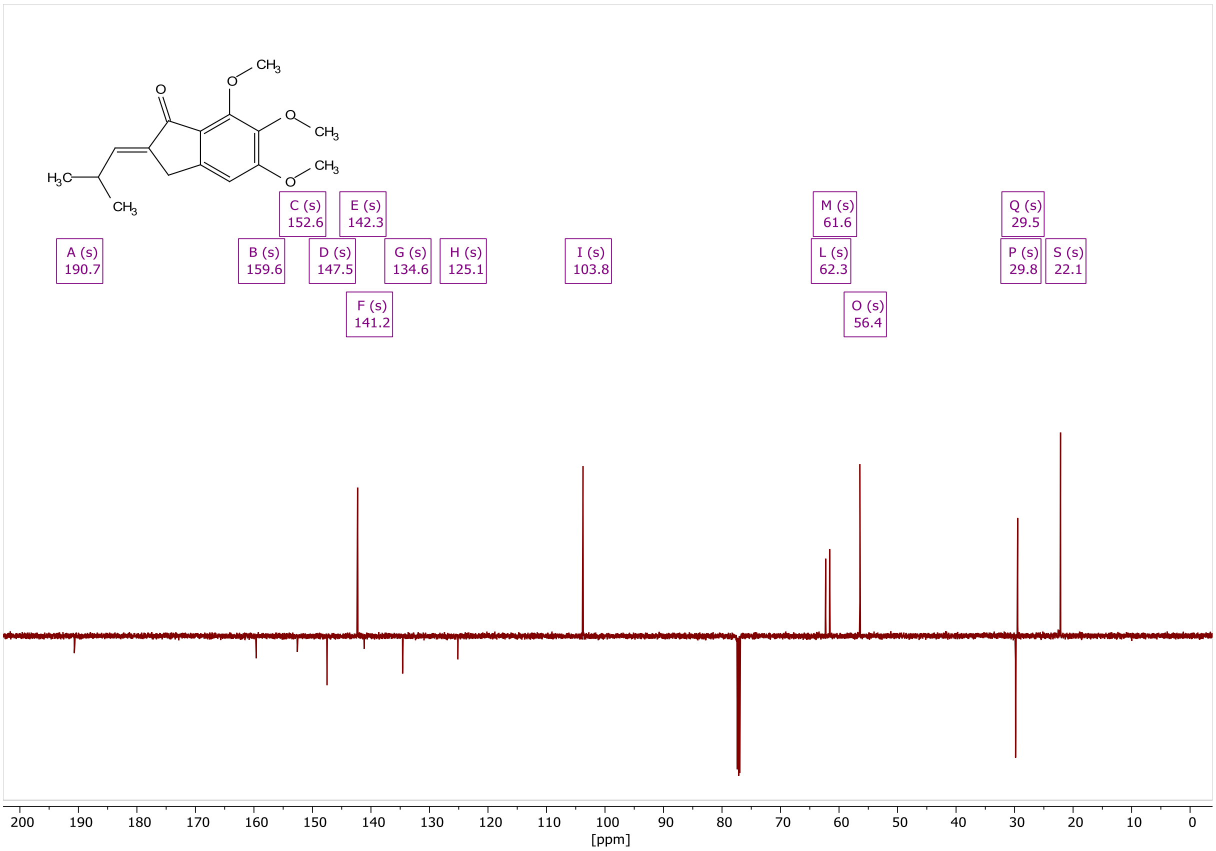


Figure S39: ^{13}C-APT NMR (Chloroform-*d*, 151 MHz): **5**

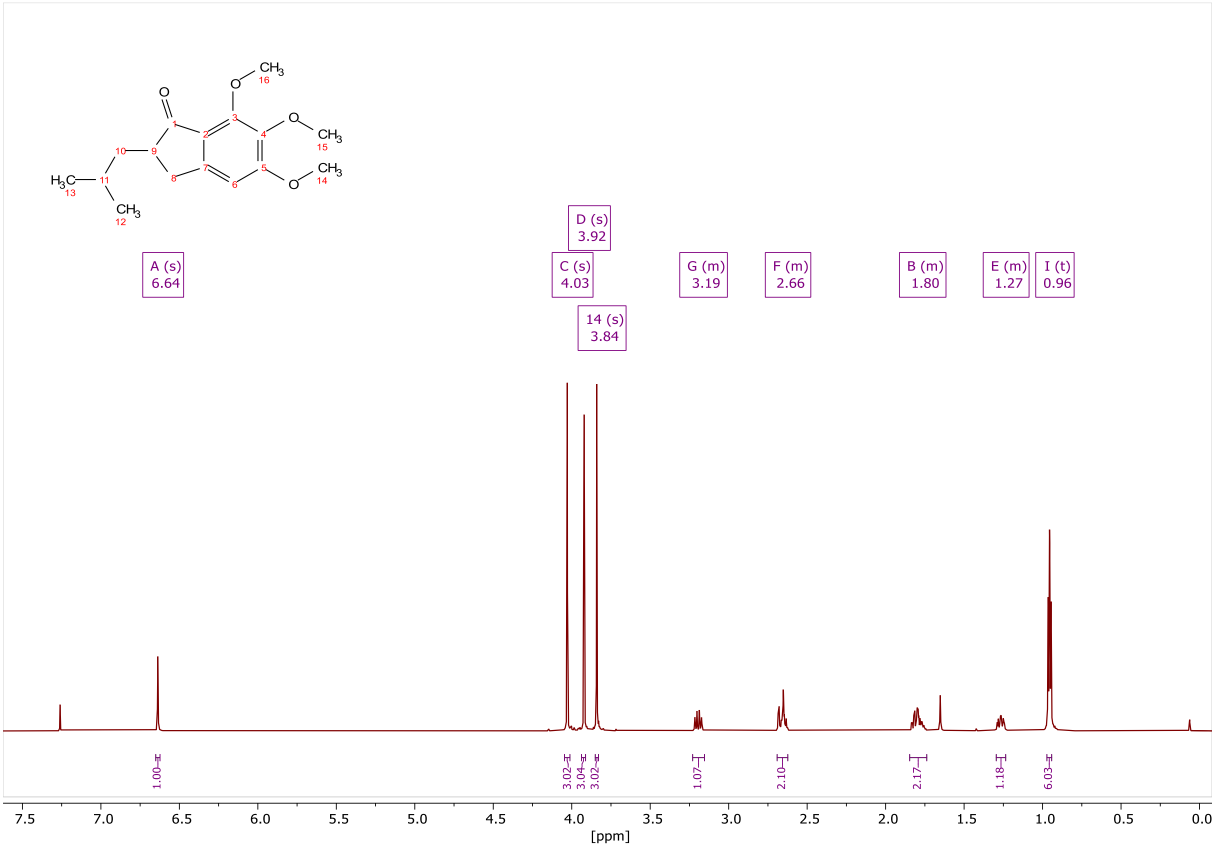


Figure S40: ^{1}H-NMR (*Chloroform*-d, 600 MHz): **6**

^{1}H-NMR: δ_H (600 MHz, Chloroform-*d*) 6.64 (s, 1H, H^6), 4.03 (s, 3H, H^{16}), 3.92 (s, 3H, H^{14}), 3.84 (s, 3H, H^{15}), 3.23 – 3.15 (m, 1H, H^9), 2.69 – 2.62 (m, 2H, H^{10}), 1.85 – 1.74 (m, 2H, H^8), 1.29 – 1.24 (m, 1H, H^{11}), 0.96 (t, *J* = 5.8 Hz, 6H, $H^{12,13}$).

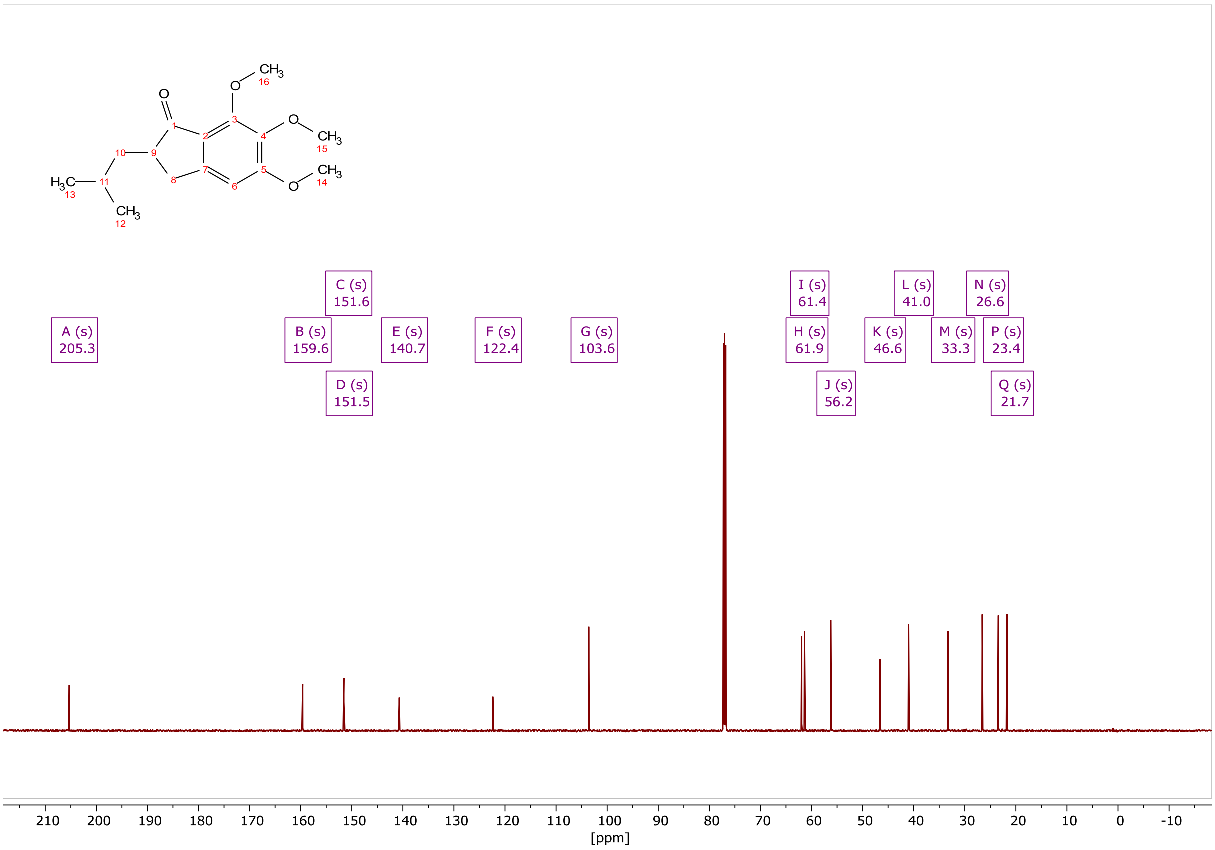


Figure S41: ^{13}C-NMR (Chloroform-*d*, 151 MHz): **6**

^{13}C-NMR: δ $_{C}$ (151 MHz, Chloroform-*d*) 205.3 (1C, C^{1}), 159.6 (1C, arom. C), 151.6 (1C, arom. C), 151.5 (1C, arom. C), 140.7 (1C, arom. C), 122.4 (1C, arom. C), 103.6 (1C, C^{6}), 61.9 (1C, C^{16}), 61.4(1C, C^{15}), 56.2 (1C, C^{14}), 46.6 (1C, C^{9}), 41.0 (1C, C^{8}), 33.3 (1C, C^{10}), 26.6 (1C, C^{11}), 23.4 (1C, C^{13}), 21.7 (1C, C^{12}).

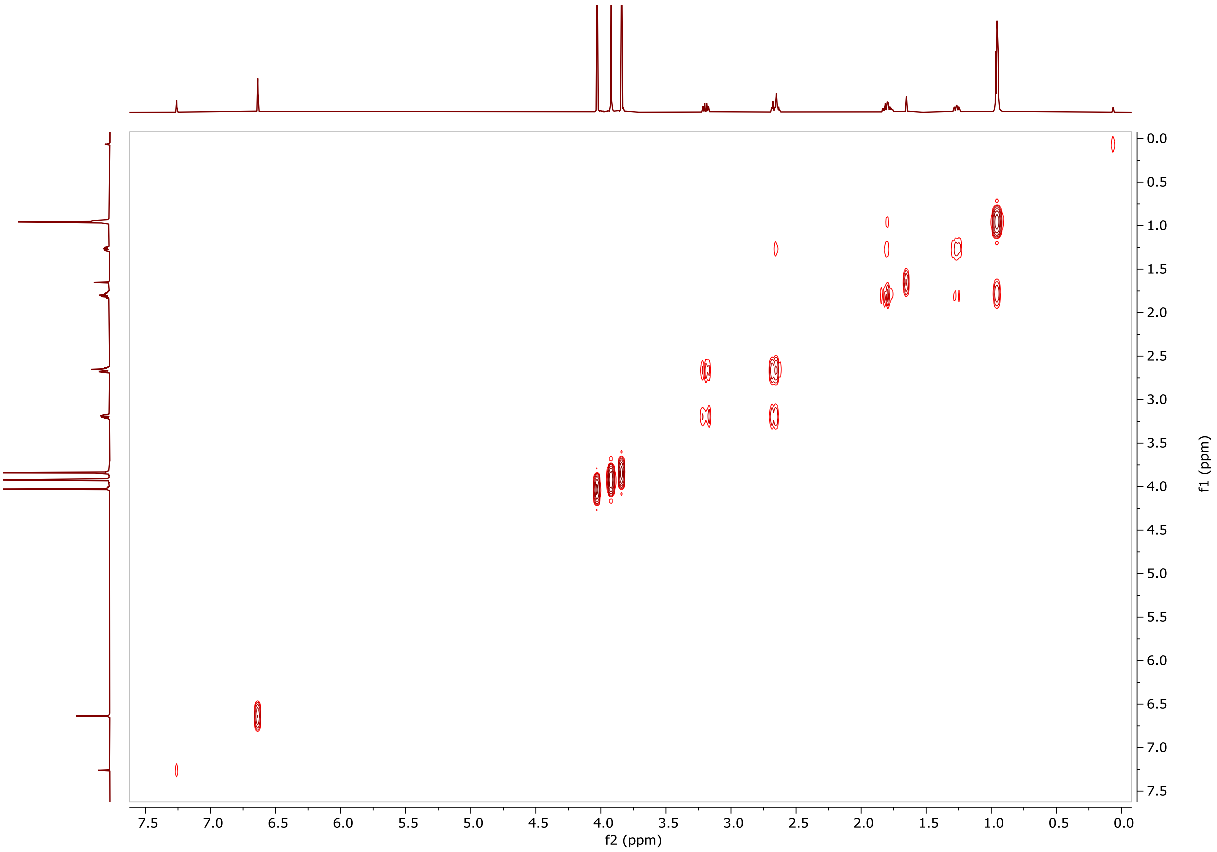


Figure S42: {^{1}H-^{1}H} COSY NMR (Chloroform-*d*, 600 MHz): **6**

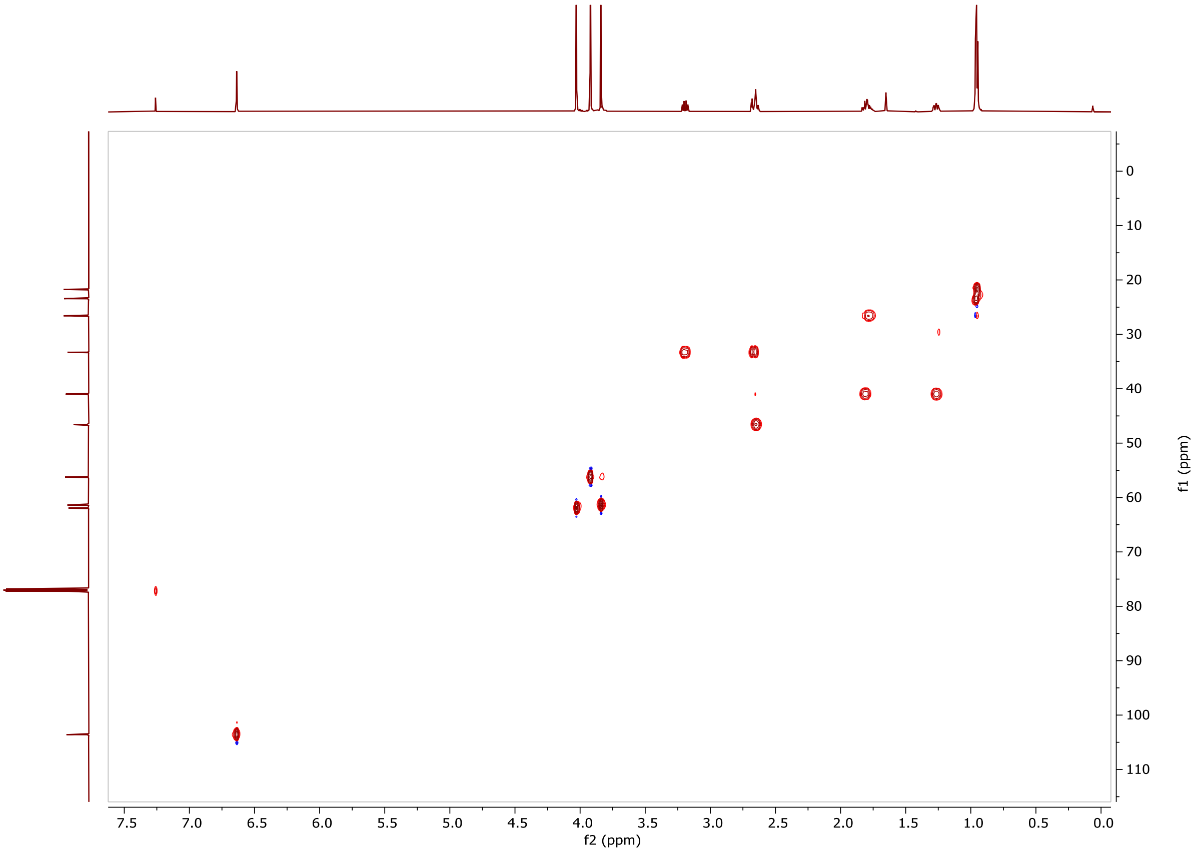


Figure S43: {^{1}H-^{13}C} HSQC NMR (Chloroform-*d*, 600 MHz): **6**

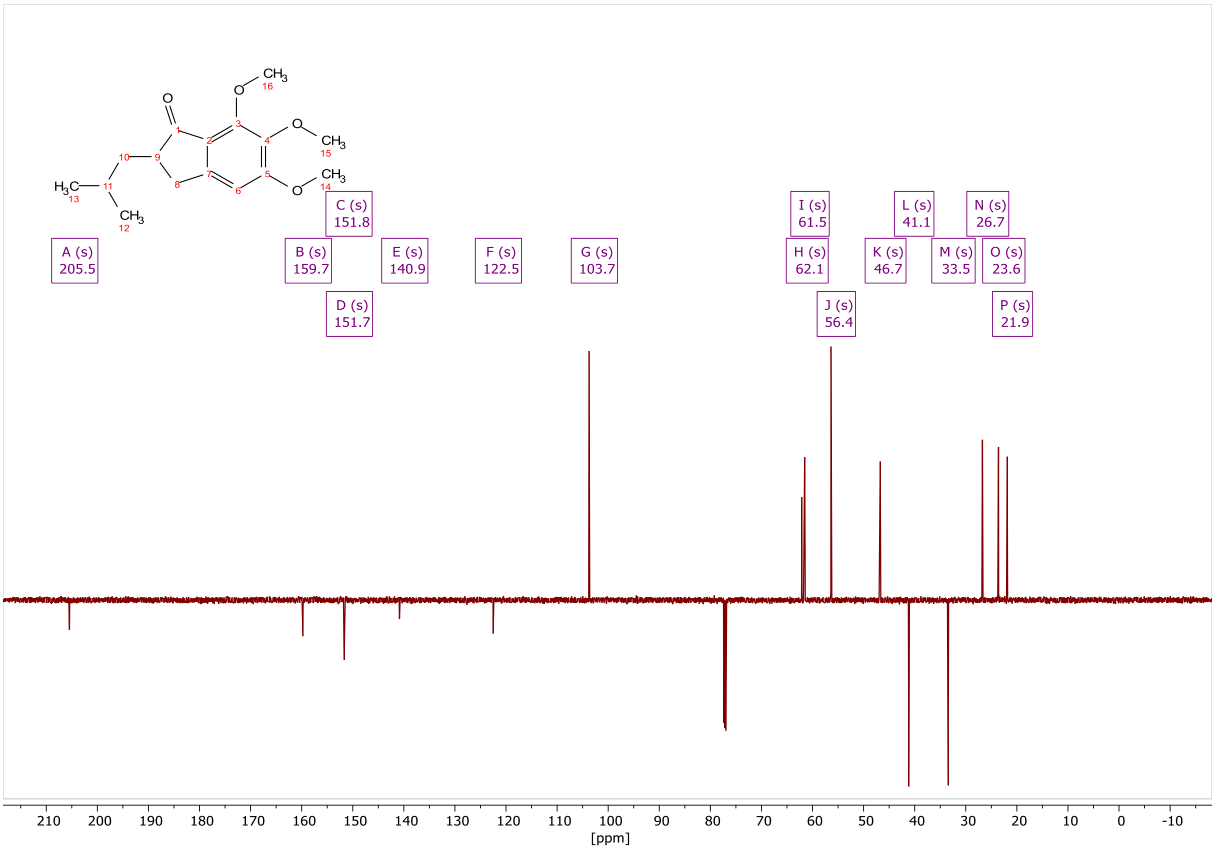


Figure S44*:* ^{13}C-APT NMR (Chloroform-*d*, 151 MHz): **6**

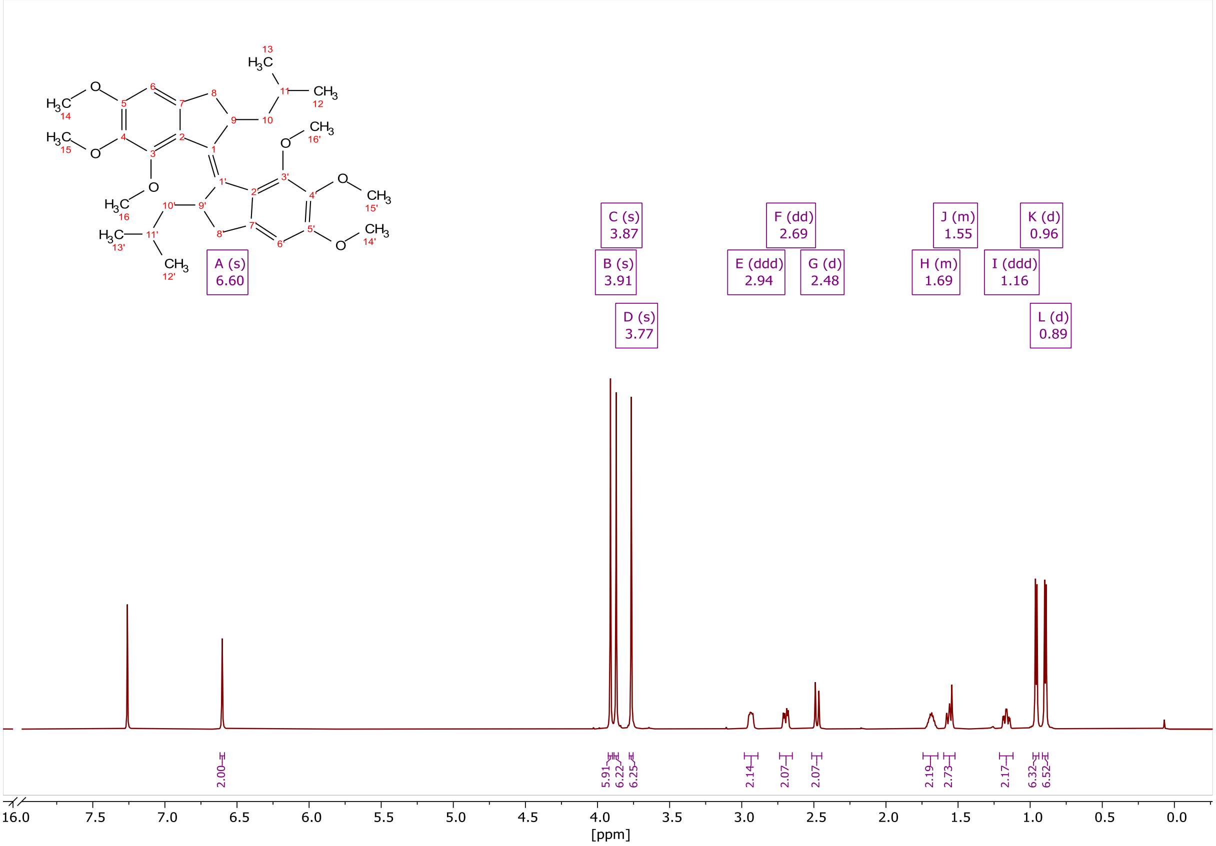


Figure S45: ^{1}H-NMR (Chloroform-*d*, 600 MHz): **7**

^{1}H-NMR: δ_H (600 MHz, Chloroform-*d*) 6.60 (s, 2H, $H^{6,6'}$), 3.91 (s, 6H, $H^{16,16'}$), 3.87 (s, 6H, $H^{14,14'}$), 3.77 (s, 6H, $H^{15,15'}$), 2.94 (ddd, *J* = 11.8, 5.9, 2.4 Hz, 2H, $H^{9,9'}$), 2.69 (dd, *J* = 14.8, 5.9 Hz, 2H, $H^{8,8'}$), 2.48 (d, *J* = 14.7 Hz, 2H, $H^{8,8'}$), 1.74–1.64 (m, 2H, $H^{11,11'}$), 1.60–1.52 (m, 2H, $H^{10,10'}$), 1.16 (ddd, *J* = 13.1, 11.4, 4.3 Hz, 2H, $H^{10,10'}$), 0.96 (d, *J* = 6.5 Hz, 6H, $H^{12,12'}$), 0.89 (d, *J* = 6.6 Hz, 6H, $H^{13,13'}$).

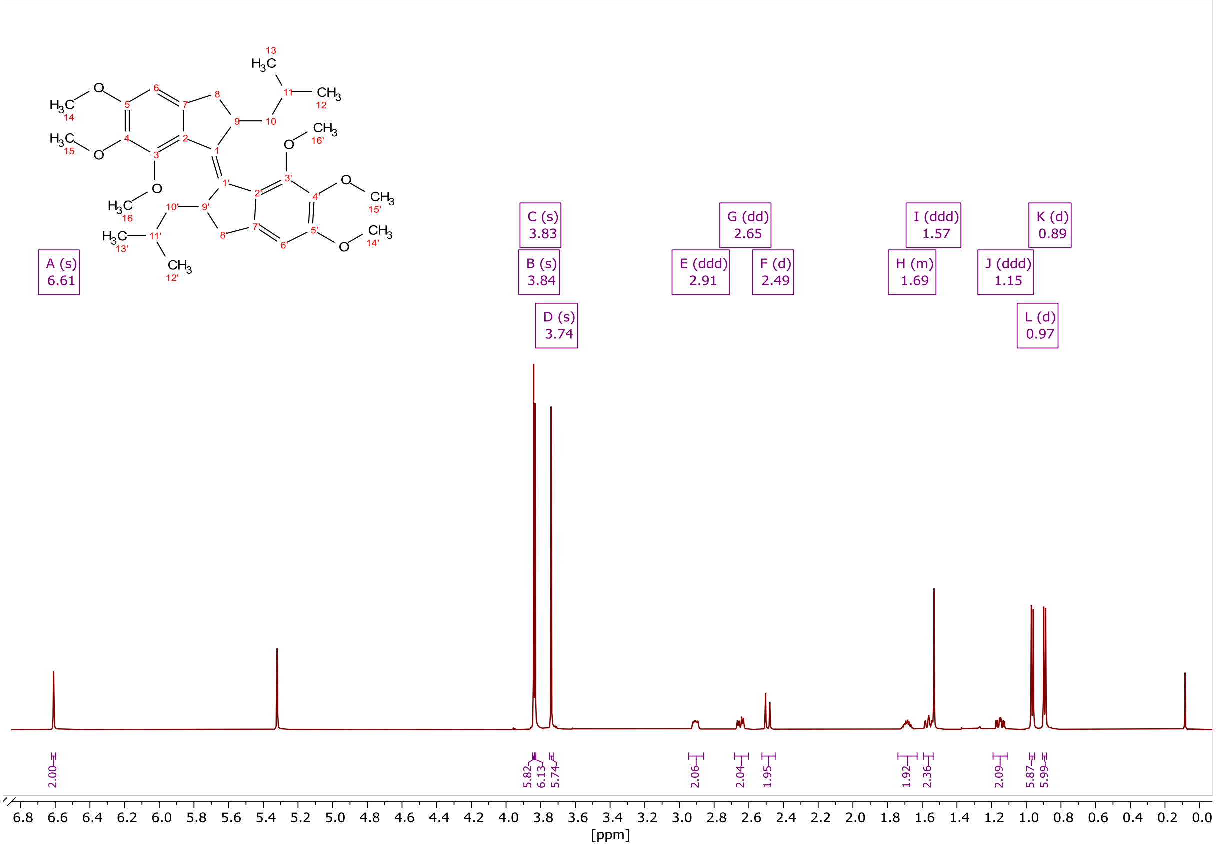


Figure S46: ^{1}H-NMR (DCM-d_2, 600 MHz): **7**

^{1}H-NMR: δ $_{\mathrm{H}}$ (600 MHz, DCM-d_2) 6.61 (s, 2H, H$^{6, 6'}$), 3.84 (s, 6H, H$^{16, 16'}$), 3.83 (s, 6H, H$^{14, 14'}$), 3.74 (s, 6H, H$^{15, 15'}$), 2.91 (ddd, *J* = 11.7, 5.9, 2.4 Hz, 2H, H$^{9, 9'}$), 2.65 (dd, *J* = 14.9, 6.0 Hz, 2H, H$^{8, 8'}$), 2.49 (d, *J* = 14.9 Hz, 2H, H$^{8, 8'}$), 1.74–1.64 (m, 2H, H$^{11, 11'}$), 1.57 (ddd, *J* = 13.4, 11.9, 2.6 Hz, 2H, H$^{10, 10'}$), 1.15 (ddd, *J* = 13.7, 11.9, 4.5 Hz, 2H, H$^{10, 10'}$), 0.97 (d, *J* = 6.6 Hz, 6H, $^{\mathrm{H}12, 12'}$), 0.89 (d, *J* = 6.8 Hz, 6H, H$^{13, 13'}$).

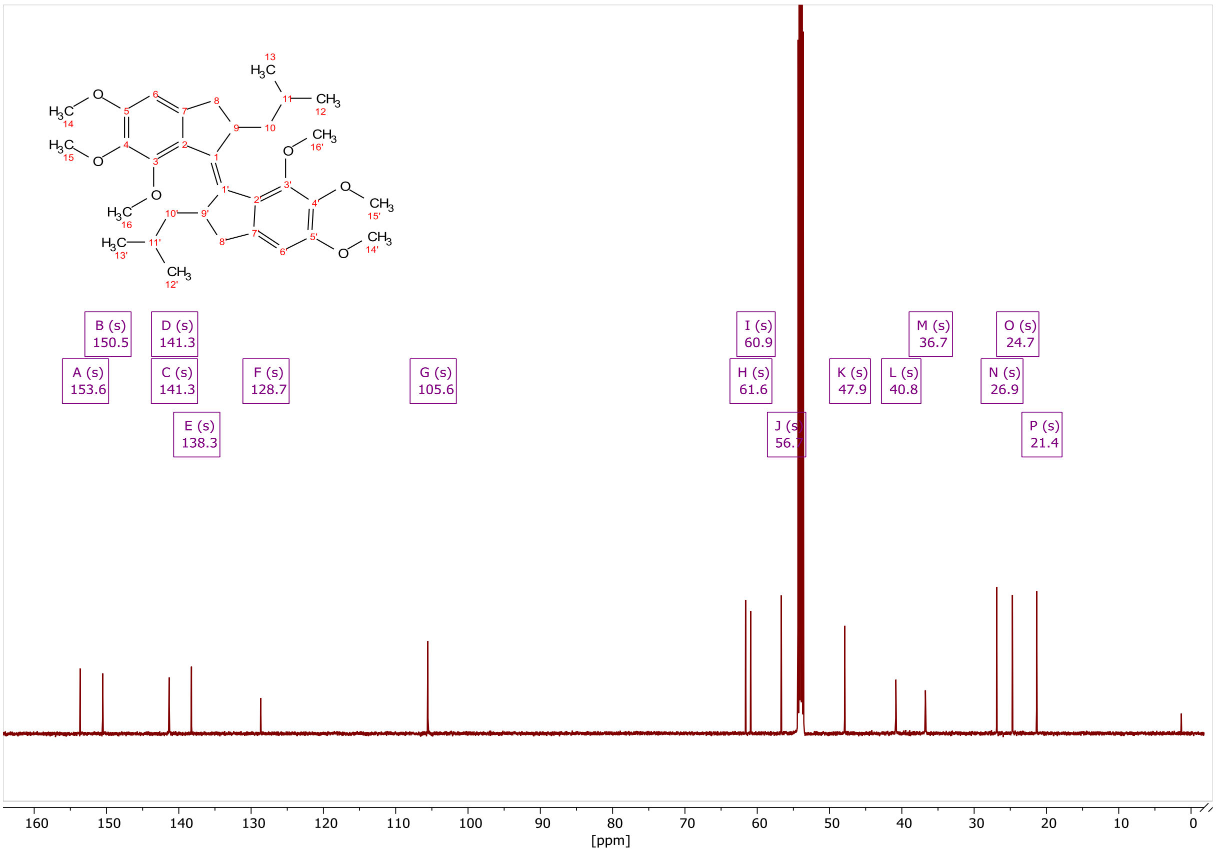


Figure S47*:* ^{13}C-NMR (DCM-*d*$_2$, 151 MHz): **7**

^{13}C-NMR: δ $_{C}$ (151 MHz, DCM-*d*$_2$) 153.6 (2C, arom. C), 150.5 (2C, arom. C), 141.3 (2C, arom. C), 141.3 (2C, arom. C), 138.3 (2C, arom. C), 128.7 (2C, arom. C), 105.6 (s, 2C, $C^{6, 6'}$), 61.6 (s, 2C, $C^{16, 16'}$), 60.9 (s, 2C, $C^{15, 15'}$), 56.7 (s, 2C, $C^{14, 14'}$), 47.9 (s, 2C, $C^{9, 9'}$), 40.8 (s, 2C, $C^{10, 10'}$), 36.7 (s, 2C, $C^{8, 8'}$), 26.9 (s, 2C, $C^{11, 11'}$), 24.7 (s, 2C, $C^{13, 13'}$), 21.4 (s, 2C, $C^{12, 12'}$).

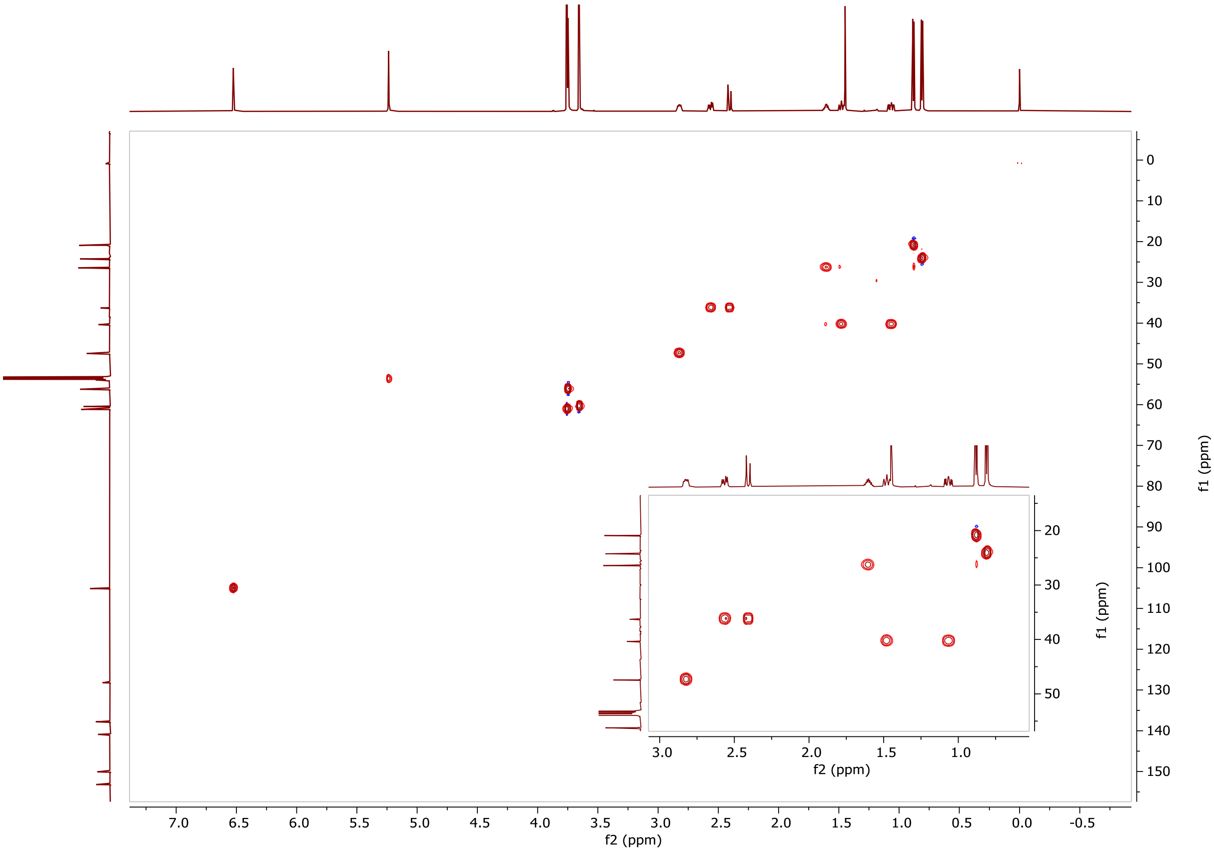


Figure S48: {^{1}H-^{13}C} HSQC NMR (DCM-*d*$_2$, 600 MHz, insert: zoomed in {^{1}H-^{13}C} HSQC NMR {1.0-3.0 ppm and 15-55 ppm}): **7**

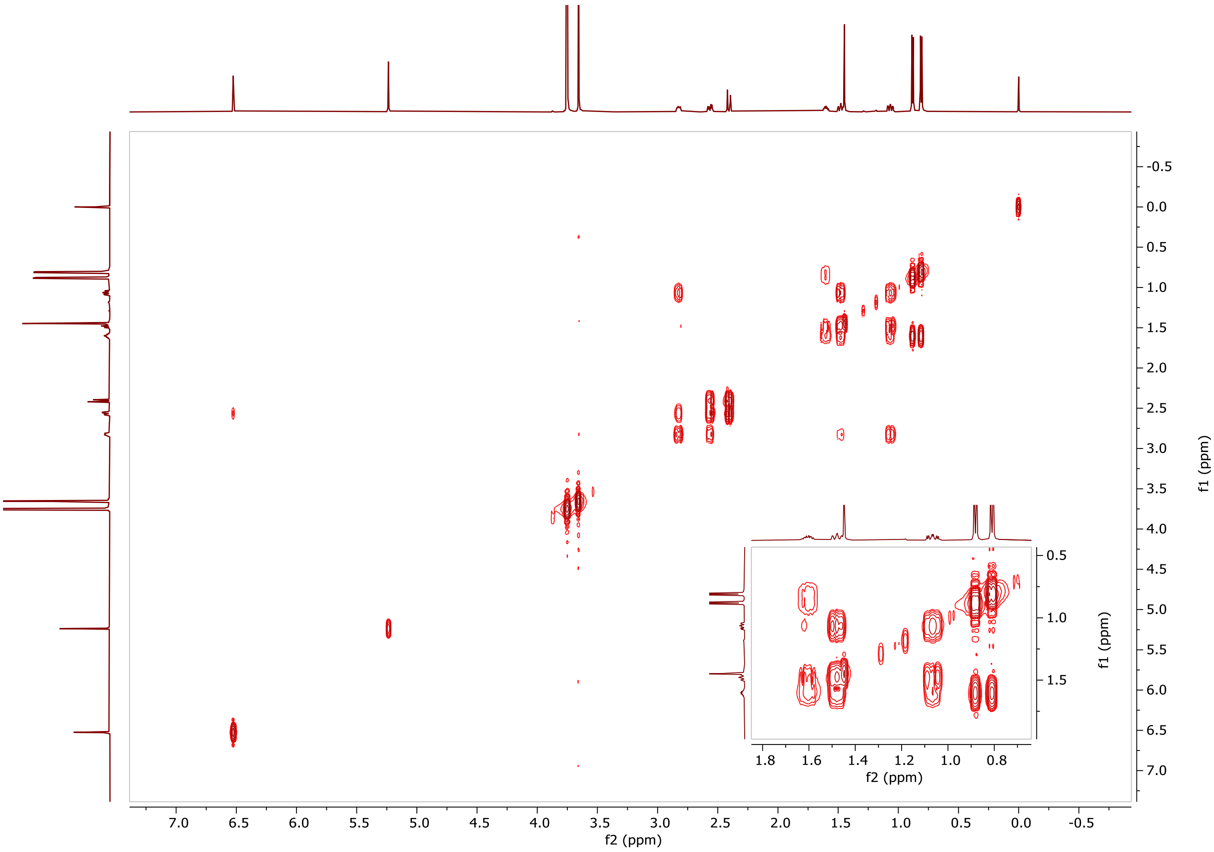


Figure S49: {^{1}H-^{1}H} COSY NMR (DCM-d_2, 600 MHz, insert: zoomed in {^{1}H-^{1}H} COSY NMR {0.7-1.8 ppm and 0.5-1.75 ppm}): **7**

5. Computational analysis

Computational analysis was employed to optimize the structures of isomeric species involved in the rotational cycle of motor **7**, namely *E*^{s}-, *Z*^{u}-, *Z*^{s}- and *E*^{u}-**7**. The minimum energy structure of compound *E*^{s}-**7** was obtained via a pre-screen using the CREST driver of the xTB software, at the GFN2 xTB level. In this way, the most stable conformer of *E*^{s}-**7** was picked via the default series of metadynamics and dynamics runs implemented in CREST. The structures of the other isomeric forms were constructed on the basis of the most stable form of *E*^{s}-**7**. All the minima and transition state geometries were then optimized at the r^{2}SCAN-3c level of theory as implemented in the ORCA 5.0.1 software. The nature of the stationary point was confirmed by means of frequency calculations. The electronic energy was then refined at the ωB97X-D3BJ/def2-TZVP level. Energy and cartesian coordinates of the optimized geometries follow.

E^s-**7**

Electronic Energy (ωB97X-D3BJ/def2-TZVP): -1698.560312 Ha

Gibbs Free Energy correction (r^{2}SCAN-3c): 0.63497668 Ha

C	4.26639031841194	-1.69403919379705	-1.36116613962770
C	3.31314253067442	-2.53359158988330	-0.75884300228681
C	2.10074404909069	-2.01263976166051	-0.29549677492736
C	1.81970194747135	-0.65078317529388	-0.44054396966825
C	2.81361624494798	0.17566761004196	-0.98674432459593
C	4.02016899148736	-0.31942196950713	-1.45432659208853
C	0.66310465535061	0.18092085513964	-0.06710191089930
C	1.23461458271063	1.58343533153068	0.12221356454548
C	2.35087553628645	1.60864516082969	-0.95571984781564
O	5.39864220497744	-2.31248101597597	-1.79694776988308
O	3.60644039902875	-3.86137437289340	-0.56673649223789
O	1.21569438638186	-2.86707261265017	0.31808783266601
C	6.40117395318640	-1.49415599737155	-2.38775111945569
C	3.03377251633976	-4.71313176571123	-1.56906172157020
C	1.55246437091979	-3.12452353570754	1.69010235811339
C	1.82863897166324	1.76017998908110	1.53149604345372
C	-4.21210978539742	2.18441047717228	-0.47733089595198
C	-3.29259977002539	2.58462363289240	0.50890388858585
C	-2.10353933554617	1.87085036774861	0.70573420843293
C	-1.79653675954452	0.79010743616418	-0.13170843174162
C	-2.75281722635409	0.38393759694737	-1.07299499947722
C	-3.94958256565908	1.05648935327654	-1.26111750868554
C	-0.64740090192424	-0.12771158277785	-0.19499956619885
C	-1.20337334634880	-1.41336806971576	-0.79933274377244
C	-2.27493791670829	-0.85958136400814	-1.77498534020499
O	-5.32656913951551	2.95985270385071	-0.58129076774457
O	-3.60066127509648	3.66605895545919	1.30154472047153
O	-1.22965212933557	2.20896736837244	1.70176846026660
C	-6.28962944782265	2.58569002767042	-1.55937215172505
C	-2.89085778942458	4.85350604658555	0.92349753281571

C	-1.76712576095262	2.34521499156456	3.02789631591967
C	-1.85139705601966	-2.30195488782691	0.27723909952944
C	2.43811724868254	3.13499057564527	1.84582649882848
C	1.43455678951041	4.27868318647137	1.68574053391940
C	3.00948850236349	3.12711259014451	3.26630989062413
C	-2.45616253456112	-3.62769737673247	-0.20938848101873
C	-1.44148635968578	-4.50656879652888	-0.94428194578952
C	-3.04863028293805	-4.38415762721717	0.98277629711580
H	4.75513641875020	0.35694965268101	-1.87716896126097
H	0.47077718521388	2.34184598178687	-0.06589438576306
H	3.16112509219321	2.31093464830915	-0.73396271891653
H	1.92401424562038	1.89044760870376	-1.92893628074303
H	6.02443448887414	-0.98099348074277	-3.28314495149167
H	7.20881317728315	-2.17146594042594	-2.67054588437710
H	6.78312449031827	-0.75085509919365	-1.67488525356418
H	3.43670948991197	-4.46602363279426	-2.56006170898157
H	1.93989480724020	-4.62238560180125	-1.57752973826177
H	3.31618675764716	-5.73491008473072	-1.30470747613664
H	1.50291748493079	-2.19529695907302	2.27388643717154
H	2.55231926954004	-3.56636182492201	1.76956226588477
H	0.80686535609368	-3.83148751422229	2.06349978842653
H	2.60570027623747	0.99386610926429	1.67108119448652
H	1.04061034247284	1.54687773348759	2.26300216830564
H	-4.65909517378100	0.70549059654945	-2.00215341383058
H	-0.41980046136613	-1.96581620539609	-1.32372964779039
H	-3.08397938561328	-1.56776333684756	-1.98090871363644
H	-1.80921433941705	-0.59735367582420	-2.73578737534150
H	-5.86256330012841	2.60457842621536	-2.57137736722136
H	-7.08782519736321	3.32653559957409	-1.48832063136472
H	-6.70048986415184	1.58775431584079	-1.35528018893885
H	-3.21941074517820	5.64117513452369	1.60608018094680
H	-3.13628741987593	5.13726401545629	-0.10806746025176
H	-1.80516811926516	4.71141307309666	1.01608713983823
H	-0.95329134235172	2.07904633116207	3.70892922961632
H	-2.60950400226559	1.66061743833394	3.17548571338516
H	-2.10012042548394	3.36852242915945	3.22571439527315
H	-2.63964682880432	-1.71708583880242	0.77388035175432
H	-1.09458158139146	-2.52172987740067	1.03836230138169
H	3.27406888031190	3.31606932992959	1.15382806755650
H	1.89397030048712	5.23775396311283	1.95062875869458
H	0.56912355680344	4.12232264840606	2.34025735685417
H	1.06219080858628	4.35878289115626	0.65945325031415
H	3.49849716047645	4.07800795225904	3.50520982755466
H	3.74385301134537	2.32464040369143	3.39679372968379
H	2.20843690871824	2.97002662010339	3.99987844402777
H	-3.28161583129840	-3.40693778667633	-0.90296036708149
H	-1.89201783561154	-5.46517700848435	-1.22577632287471

H	-0.57329938782224	-4.70762322166385	-0.30629653229296
H	-1.07322540215031	-4.03085868489073	-1.85908516867672
H	-3.53770936116391	-5.31102086691527	0.66333050803425
H	-3.78769570761879	-3.77510680807966	1.51505947006644
H	-2.25915225357888	-4.65173915824559	1.69660189861980

E^u-**7**

Electronic Energy (ωB97X-D3BJ/def2-TZVP): -1698.549309 Ha

Gibbs Free Energy correction (r^2SCAN-3c): 0.63510909 Ha

C	4.22116998092045	-3.79669578234919	-1.04126017614283
C	3.19155082703902	-3.58570320553837	-1.98062152773850
C	2.07908680354303	-2.80401677884921	-1.63757983905212
C	1.95947065520352	-2.28922794897769	-0.33053121922360
C	3.03978376317386	-2.45127613902095	0.54390634793763
C	4.16292642329826	-3.19340550871161	0.21635626748223
C	0.95774844476755	-1.39192234996820	0.24472146716699
C	1.64027259464674	-0.70910028561890	1.44162525122550
C	2.78299323941182	-1.69437255609430	1.81053305023816
O	5.23083431874666	-4.61846853223218	-1.45350497680868
O	3.20367680764015	-4.21594105493285	-3.20260769318902
O	1.06735465520951	-2.54847170774345	-2.51282219874739
C	6.26583695194438	-4.90340743606869	-0.51943438391576
C	4.26231722241068	-3.84729078270285	-4.09907131441444
C	1.38913590617936	-2.15803780405842	-3.85115296279862
C	0.73360362812385	-0.43677815493472	2.64170864908612
C	-3.35098734954247	1.70804737519360	0.40459571721110
C	-2.01420612055736	2.15040309200261	0.47238949415274
C	-0.96429899578263	1.23509451545245	0.30995123126430
C	-1.24703889396807	-0.13662286298302	0.14907002528011
C	-2.58445595869688	-0.52163130837396	0.00358759728175
C	-3.63758481231904	0.36979067875535	0.12935875468637
C	-0.35207468219497	-1.26196987438053	-0.11855853637705
C	-1.21953927565182	-2.34389189364463	-0.78294238128571
C	-2.65813468913348	-1.98158745212029	-0.32180326967115
O	-4.29813870959193	2.66467115690610	0.63443831643493
O	-1.70997663824146	3.45127395023914	0.79791455771903
O	0.34429418528462	1.61255262901781	0.34383385750592
C	-5.66011657124734	2.25293671728280	0.62427275528578
C	-2.12552192491400	4.45645134219816	-0.13857197491788
C	0.75129928982107	2.76394289597214	-0.40185106281450
C	-0.86499174462445	-3.78341730985960	-0.41005983748948
C	1.43398830471189	0.20071157913725	3.85046732474253
C	2.01657507844509	1.57616306868904	3.51524310824646

C	0.44611184597463	0.31517028334193	5.01439569508643
C	-1.76646987010541	-4.85404035112679	-1.04235374819687
C	-1.66702289156719	-4.85553245096177	-2.57012566096011
C	-1.39363057408465	-6.23177735434342	-0.48900384993260
H	4.96927145545387	-3.30297541840700	0.93291253846899
H	2.09741968754849	0.22936873618490	1.10355358414965
H	2.43642882765418	-2.38159286159378	2.59804445525556
H	3.67861846160985	-1.19058839953803	2.19151926899272
H	6.81797147883286	-3.99552035518818	-0.24164666250351
H	6.94028764372187	-5.59640478780028	-1.02563266738968
H	5.86534875632924	-5.37892002897930	0.38564465665471
H	4.33169092464688	-2.75516890088744	-4.19168781401750
H	4.00015516090770	-4.27822619468477	-5.06881763092221
H	5.22516066293401	-4.24549136539838	-3.76665913196713
H	1.53804273449611	-3.02493088835682	-4.50073376490893
H	2.28530156197117	-1.52538182427172	-3.86576452103914
H	0.53267322288579	-1.57404504005557	-4.20033412675185
H	0.28498205570436	-1.39429774750889	2.94674661059053
H	-0.09919637792823	0.21407383906815	2.35974547200823
H	-4.65902594511341	0.02176077556625	0.02353125632438
H	-1.17079919362835	-2.22217274137948	-1.87214320896530
H	-2.91059654783961	-2.55746076103525	0.58217487845327
H	-3.42096576851742	-2.20974063569431	-1.07472750165600
H	-5.95801951624793	1.87340411934749	-0.36238342053033
H	-6.24221399230174	3.14580364334563	0.85941847734017
H	-5.84917582583042	1.48317661616621	1.38419968109864
H	-3.21181398618144	4.58270281160258	-0.13515263616718
H	-1.79049500801287	4.20482386191248	-1.15368274026466
H	-1.64559535593337	5.38434348755403	0.18296430379544
H	1.80925181519448	2.60710590050053	-0.63134004080321
H	0.62842886431517	3.68379091214586	0.17660461407841
H	0.18707875027560	2.83732237440452	-1.33972459144920
H	-0.91654516057346	-3.86687576450783	0.68597134401194
H	0.16808458320855	-4.01508890106934	-0.68488815059569
H	2.25824482110852	-0.45452196277710	4.17271051082581
H	2.46002893909185	2.03902023739235	4.40419372519569
H	1.22902952061316	2.24122130710128	3.13984236755374
H	2.79425612906687	1.51828296851128	2.74686358373871
H	0.92590875941151	0.73819648288496	5.90409891799966
H	0.03292909084763	-0.66316627051116	5.28400386619937
H	-0.39194074302602	0.96906950979898	4.74229641403071
H	-2.81193190779970	-4.65034032625190	-0.76364288062245
H	-2.27419925645430	-5.66048467531370	-2.99982093622643
H	-0.62661257113448	-5.00815148153020	-2.88289191280914
H	-2.00837227498366	-3.91166834130723	-3.00733255276087
H	-2.03860221846435	-7.01519742890000	-0.90247408762195
H	-1.48156622043604	-6.26021722983548	0.60277313677244

H	-0.35655726169449	-6.47952964930047	-0.74801553792837

Z^{s}-**7**

Electronic Energy (ωB97X-D3BJ/def2-TZVP): -1698.559648 Ha

Gibbs Free Energy correction (r^2SCAN-3c): 0.63411499 Ha

C	4.60231270089069	-2.39025672206393	-1.47906605505226
C	3.43831402026456	-2.66401793724596	-2.22161849699041
C	2.17281702628861	-2.39550333738697	-1.68873817675852
C	2.07883285204189	-1.75798465078426	-0.44026612067229
C	3.24771406807665	-1.55449888924522	0.30169138814243
C	4.50859812441766	-1.85678765494615	-0.19103536530235
C	0.91717386953111	-1.37801717645852	0.35888349851083
C	1.39832649582547	-1.40883401565816	1.80964603812635
C	2.89552173262574	-1.03018564548462	1.67012119197214
O	5.77270816017436	-2.69185875303870	-2.11158155931627
O	3.55852860646496	-3.21348018415354	-3.48032944064751
O	1.01946386944569	-2.72888650314791	-2.32740603400544
C	6.97849050533466	-2.43471181403314	-1.40294178890511
C	3.69638860832944	-2.20883202471124	-4.49313722249086
C	0.92822753315173	-4.01274949660140	-2.95946526418724
C	1.23656508528277	-2.82044412807458	2.40624848309623
C	-2.61437332243037	-0.35022418304268	-3.51079422411682
C	-1.22935293859039	-0.12364885442480	-3.61344924744729
C	-0.39487496478168	-0.28621518106096	-2.50243926583014
C	-0.94155564240330	-0.76397025829234	-1.30057907021042
C	-2.32974443525373	-0.91665491845207	-1.20725494032227
C	-3.17827617018084	-0.72052833842690	-2.28659865811520
C	-0.33304251499482	-1.00192634304008	0.00550739824679
C	-1.46322451624747	-0.80715009236339	1.01751035874405
C	-2.70715478379586	-1.26083352642593	0.21064959429663
O	-3.31519091027101	-0.17352302516400	-4.66718962259050
O	-0.70432350060818	0.27051004522363	-4.82527851210202
O	0.93489903701014	0.00300023852039	-2.53964864316141
C	-4.71866451029479	-0.39646592334154	-4.61538278284544
C	-0.24024858680972	-0.84620238640384	-5.59415139700682
C	1.34794035254188	1.23180949759311	-3.15319084394082
C	-1.56806866935951	0.67394587326538	1.42829066288171
C	1.53341560986596	-2.94443505899946	3.90679932610169
C	0.47877989976925	-2.22889541112694	4.75340690493553
C	1.62204988748999	-4.41968586778501	4.30474844446644
C	-2.61374674537133	1.00680636258128	2.50143349132390
C	-2.28329791942443	0.35773710010953	3.84655199898936
C	-2.73059584934579	2.52502058142014	2.65899510082312

H	5.38883560723708	-1.68557469327533	0.41841592459462
H	0.85881074947658	-0.67915345015858	2.42303144497432
H	3.52594765844482	-1.45910832616064	2.45705931236891
H	3.01593575687637	0.06183045903380	1.70792409917793
H	7.07696093703672	-1.36989536699130	-1.15072733453749
H	7.78702230242015	-2.72494425977595	-2.07627463114208
H	7.03905382416192	-3.03349843373101	-0.48403346129060
H	2.85313980033756	-1.50456855099457	-4.45773979089100
H	3.70522392876493	-2.73119724334159	-5.45364728448426
H	4.63676778757508	-1.65675982486576	-4.36759962001615
H	1.52210632598093	-4.75817986788765	-2.41921447398832
H	1.26623263480816	-3.97629962464057	-3.99931315348371
H	-0.13118783333413	-4.28159036203831	-2.91909396275550
H	1.89559887987231	-3.49599321438158	1.84188593729091
H	0.21100188573469	-3.17253768249875	2.22295212343624
H	-4.24859155341423	-0.84933921782602	-2.17030540786303
H	-1.31271793937769	-1.43121912137576	1.90453911522976
H	-3.63523151540463	-0.77279646456243	0.52729563689145
H	-2.85072019771575	-2.34548283766492	0.31790659730610
H	-4.95023482820364	-1.42614504190469	-4.31002314935761
H	-5.08462919774728	-0.22669086148333	-5.62957046225682
H	-5.21145895659870	0.30594205260044	-3.92945199626992
H	-1.07778723707836	-1.49890747741398	-5.87380204152188
H	0.49963369223012	-1.42810478154584	-5.02644826034333
H	0.22044629866365	-0.43636379130004	-6.49707641188351
H	2.27041462664018	1.51787040355358	-2.63997490552693
H	0.58968608217368	2.01091988635952	-3.01689225609540
H	1.53797332103872	1.10629619856209	-4.22346242311103
H	-1.77849779495666	1.25749443212857	0.52029970645463
H	-0.58372739947619	1.01122551473289	1.78495788688274
H	2.50988993767466	-2.48032827071967	4.11275149927943
H	0.70102821633323	-2.32197464486953	5.82221021061471
H	-0.51228637471595	-2.66718269811960	4.57908737630343
H	0.41595027820040	-1.16189542747965	4.51990761382974
H	1.83952998960355	-4.53206959694192	5.37275235665235
H	2.40561907605775	-4.93771677378242	3.74126656025263
H	0.67179973909366	-4.92989848749169	4.10273978491549
H	-3.59223407174163	0.62841478076158	2.17012150429504
H	-3.02763128011382	0.62500806520279	4.60476106054414
H	-1.30431393970176	0.70002623691538	4.20597403676303
H	-2.25187779100914	-0.73421763020215	3.78386074272401
H	-3.48450649882100	2.79064751536350	3.40830086700743
H	-3.00768346050619	3.00318668008798	1.71321838542875
H	-1.77327098816086	2.95298333789134	2.98211580988031

Z^{u}-**7**

Electronic Energy (ωB97X-D3BJ/def2-TZVP): -1698.542137 Ha

Gibbs Free Energy correction (r^{2}SCAN-3c): 0.63494401 Ha

C	4.05083303269510	-3.53813627474006	-2.04882321476132
C	2.79193220034367	-3.49849956832219	-2.68408954275984
C	1.70257007548777	-2.87762829346500	-2.06737914718242
C	1.87209362347143	-2.31132074818891	-0.77765569960202
C	3.16604517798138	-2.24830362456539	-0.24605782386170
C	4.25194983677496	-2.87786215323813	-0.83761827950020
C	0.94634192523433	-1.54665988103669	0.03391806366557
C	1.74396960675833	-0.91596765454372	1.18673254579482
C	3.21366179323678	-1.34041307755221	0.94998522227522
O	5.02463813777870	-4.19273280414308	-2.74535806684630
O	2.67009886160063	-4.05477272057304	-3.93986578766936
O	0.51594252166530	-2.65559516879224	-2.68306498891811
C	6.32515507114374	-4.22208719912327	-2.17168142650751
C	3.12819569283456	-3.18158764274949	-4.97929498935476
C	-0.03930513084654	-3.61833873505754	-3.59449992281115
C	1.23051097861182	-1.47662361086726	2.52829529517240
C	-3.77737139151822	-3.65482705624275	-1.25929376768723
C	-2.55021150501636	-4.34390798588249	-1.17230274217045
C	-1.39178279167287	-3.66345453087688	-0.77680243214799
C	-1.43854258265314	-2.27219691929094	-0.54185465787183
C	-2.69646919098004	-1.65659652387536	-0.50457459927392
C	-3.85955131099398	-2.31629664143581	-0.87153385657175
C	-0.40930749131120	-1.38152171309686	-0.05309400824266
C	-1.08879409029725	-0.07138829243629	0.37661391919294
C	-2.59887876696620	-0.27962820868130	0.08941156010031
O	-4.83121480243771	-4.38610175960532	-1.73056259962991
O	-2.43550766474015	-5.65363164263066	-1.57575971528671
O	-0.19545162834406	-4.29321875907344	-0.62383231703567
C	-6.07883649791042	-3.71760195724870	-1.87172623176611
C	-3.17521038056654	-6.61912639266164	-0.81347733357260
C	-0.15014997999720	-5.50422291535127	0.13506769308350
C	-0.53350818251948	1.10036030177865	-0.45726339100898
C	1.81946040557948	-0.81864802776457	3.78388271210284
C	1.30525847964328	0.61106324632883	3.96347437934814
C	1.49228410337456	-1.65838470006134	5.02082534461778
C	-1.02523818367870	2.49482590527704	-0.04489332318267
C	-0.46457164921143	2.91558830423634	1.31516374836686
C	-0.64358665015013	3.52121152014798	-1.11460918569257
H	5.23247509968407	-2.81926323330988	-0.37832854835196
H	1.65432038682082	0.17752249952766	1.19648576370247
H	3.62923034734687	-1.84377092855762	1.83267889519328

H	3.86975244556946	-0.48504716766587	0.74197358075622
H	6.74495861465307	-3.21129490951895	-2.07443219910535
H	6.94063375725175	-4.80525365569160	-2.85908299656364
H	6.31706509514656	-4.70849154165272	-1.18690336504147
H	2.54324124551125	-2.25093467948433	-4.99133393174512
H	2.98549235607555	-3.71814906751677	-5.92101204709394
H	4.19152257599438	-2.94347382525122	-4.85247831238307
H	0.14845538418937	-4.63791882631257	-3.24728994008957
H	0.36028225204213	-3.49312543840233	-4.60468895635771
H	-1.11514482189091	-3.42406985542054	-3.59251390414260
H	1.45200566218635	-2.55432099168141	2.53701343848812
H	0.13620347932807	-1.39623054628742	2.56962212001928
H	-4.81064926647245	-1.79589914861250	-0.84381349236079
H	-0.92889032650495	0.13824308548652	1.44248955136244
H	-2.97880678272943	0.48731455294976	-0.59830354019227
H	-3.21233259868915	-0.21526326707400	0.99721461032703
H	-6.46923923109227	-3.38442368606943	-0.90046007569898
H	-6.76234253315871	-4.45116405023203	-2.30321269642176
H	-5.99437575161320	-2.85512318036947	-2.54617545006297
H	-4.25130396218252	-6.52627953930211	-0.98569837182899
H	-2.96575838222133	-6.50944507099067	0.25895952861332
H	-2.83059895670987	-7.59921191291797	-1.15287555336254
H	0.87590391056666	-5.57608141915889	0.50673812339159
H	-0.38355572109179	-6.37735914031195	-0.48136833870155
H	-0.84230418671302	-5.45434974215975	0.98525650699657
H	-0.80245532540406	0.90974150571087	-1.50637343948991
H	0.56392639322846	1.09213030735312	-0.42581847430021
H	2.91473697767528	-0.77738493045405	3.68131845404834
H	1.74832981909531	1.08198006034680	4.84793369285464
H	0.21574188568052	0.61012417188601	4.09734411583421
H	1.53392531717927	1.24406885592436	3.10066205474549
H	1.89693914717624	-1.20221599108449	5.93117763758292
H	1.90305393952994	-2.67041897255016	4.93626631726746
H	0.40596908549191	-1.74816954456341	5.14708320166203
H	-2.12345753198228	2.47525579820018	0.02951141014915
H	-0.82289382949441	3.91168286920484	1.59757430876838
H	0.63186304653228	2.95373233389403	1.27977655622884
H	-0.74859528976015	2.22284615007583	2.11334151632273
H	-0.98428836351364	4.52645259305705	-0.84274915080255
H	-1.07981702926661	3.26488177711265	-2.08613806993522
H	0.44606721513100	3.55934658327999	-1.23771054408686

E^{u}-E^{s}-**7** TS

Electronic Energy (ωB97X-D3BJ/def2-TZVP): -1698.532207 Ha

Gibbs Free Energy correction (r^2SCAN-3c): 0.63740875 Ha

C	4.59228923933525	-1.95610127708998	-1.24371172360362
C	3.45005901874895	-2.32162332413786	-1.96869513120581
C	2.19013165011443	-1.77519590120885	-1.68739208007585
C	2.02707034505428	-0.79475861716829	-0.67032139109965
C	3.22407545235155	-0.42899985932349	-0.01238776239697
C	4.46696676934937	-0.99316670546894	-0.25009543126448
C	0.92152233823027	0.08600450764085	-0.17395402293761
C	1.50270025312013	0.83062138575940	1.03448077798750
C	3.01842495796898	0.72338908258858	0.91399067127779
O	5.75219295443342	-2.56385878136777	-1.61288556380797
O	3.58117168933474	-3.24583113214278	-2.97991949775528
O	1.16958980596737	-2.18824302321043	-2.50901593013217
C	6.92911946962348	-2.19477062181037	-0.90197779273893
C	3.90834272396103	-2.64360653812487	-4.24002127558204
C	0.77302614636381	-3.56061698262231	-2.32334418216894
C	0.94739531452886	0.12640910136405	2.29367240261488
C	-3.77119576760567	2.90970476996869	-0.32872420823044
C	-2.70011977055932	3.21708978969512	0.52210408191249
C	-1.52610925420609	2.44125694498632	0.52356771956318
C	-1.41183509203695	1.28442401992904	-0.28885405585996
C	-2.50831134131316	1.05343209524699	-1.15033495681642
C	-3.65374400268377	1.82819744142203	-1.19481737984195
C	-0.38915182045718	0.21056239075003	-0.54445697905078
C	-1.18482659617400	-0.88375310934307	-1.26190275798971
C	-2.25713931559647	-0.12518014937684	-2.03495101416725
O	-4.88008667326524	3.69498028533105	-0.20824100537551
O	-2.79844533979005	4.21272908660879	1.46151966999240
O	-0.54453330747160	2.80141655001467	1.40104628200817
C	-6.00064614512943	3.36767035826033	-1.02322759109733
C	-3.06938736559762	5.53817409240479	0.98178587837107
C	-0.04814477682668	4.14484972830708	1.32347599090935
C	-1.77212758809449	-1.77936525318484	-0.13520436788625
C	1.52615420659523	0.54937261238866	3.65194615816047
C	1.48696599490018	2.06195197347362	3.86995568295566
C	0.76866240144363	-0.17175835278136	4.77070667801269
C	-2.98396599542695	-2.65637548077787	-0.48084425884466
C	-2.74766542382960	-3.58315363115619	-1.67293848108319
C	-3.39524341572428	-3.46903841142627	0.75026025182697
H	5.32242832329646	-0.64319050455254	0.31745503822066
H	1.18389592037029	1.86504541975308	1.04701101735771
H	3.52371330978483	0.58560876913624	1.87569367118401
H	3.44319772177166	1.63044723546838	0.45949111434536
H	7.15746085400655	-1.12798922904039	-1.03070249568030
H	7.73518079627388	-2.79272966398868	-1.33046516119245
H	6.83622633874085	-2.42156292681088	0.16848854542504
H	4.87566409537016	-2.12793994194859	-4.18374675830903

H	3.12577761624190	-1.93689999952269	-4.54430860644525
H	3.97200344655976	-3.45854130733413	-4.96519492903342
H	1.60078072884559	-4.24195065327376	-2.53410025715883
H	-0.04359635116086	-3.73669163805165	-3.02636705728612
H	0.41138330630085	-3.71244338197489	-1.29852973028769
H	1.09284339169183	-0.95813072926258	2.17630509301434
H	-0.13838382865148	0.29157838501353	2.30667186640489
H	-4.44532524073550	1.56435952580522	-1.88714754914496
H	-0.55762825271712	-1.47134434706680	-1.91975906679701
H	-3.16262223831579	-0.70161231316171	-2.24492059658438
H	-1.85148308817288	0.21224362641877	-3.00035386951972
H	-5.76100352191600	3.46070379550388	-2.09091157214698
H	-6.77849937949838	4.08744626842735	-0.76243410128444
H	-6.35934540302137	2.35086591627875	-0.81596366620886
H	-4.14534413194091	5.72248628587279	0.91666791391615
H	-2.61642517466060	5.69967259110139	-0.00464193959301
H	-2.62001356779310	6.22529924022902	1.70507933131223
H	1.04461538779922	4.08482586204933	1.39023014512292
H	-0.43363238481296	4.74602697614130	2.15148691566319
H	-0.32128243598693	4.60982793430668	0.36992002251948
H	-2.06494810698710	-1.13416663423585	0.70460750599828
H	-0.95631654997736	-2.41061225824254	0.24675165435090
H	2.57562871184623	0.22316931998095	3.70543830746952
H	1.87396202537497	2.32166869997062	4.86196660779595
H	0.45903092972087	2.43311207498702	3.79271410458341
H	2.09245775088969	2.59284811140189	3.12714729410955
H	1.20110639720834	0.05285979823450	5.75218785671998
H	0.79022167534515	-1.25829439517379	4.63061190491075
H	-0.28182253999425	0.14342617316201	4.78632029231979
H	-3.82312316092472	-1.98853250698426	-0.72543850388502
H	-3.65940934865365	-4.13753895726980	-1.92257268886730
H	-1.96813005156732	-4.31719068066322	-1.43798742448688
H	-2.43339838596409	-3.03186959901781	-2.56560927262544
H	-4.29600003671059	-4.06106211772917	0.55282738622310
H	-3.59757939510616	-2.81757866721613	1.60727614055072
H	-2.59544789180641	-4.16248862113856	1.03851211243928

Z^u-Z^s-**7** TS

Electronic Energy (ωB97X-D3BJ/def2-TZVP): -1698.512514 Ha

Gibbs Free Energy correction (r^2SCAN-3c): 0.63588881 Ha

C	3.13161020722234	-2.99349786678230	-3.23851021276452
C	2.66758505975581	-1.69368786520183	-3.49546378569951
C	1.99203756643381	-0.96683239427219	-2.49321707467457

C	1.65433356126540	-1.59976355703233	-1.28902704468897
C	2.28188797345999	-2.82587905879460	-1.01182885288704
C	3.00144361281945	-3.53605805284315	-1.95800501856283
C	0.87524613606418	-1.23496596868375	-0.06198401386739
C	1.83106457193357	-1.73385604764237	1.04097074257788
C	2.16758939604013	-3.13291697801531	0.45960211486390
O	3.72078761517507	-3.63712346256947	-4.29148796603535
O	2.79585765046096	-1.10303854446102	-4.72931133365757
O	1.72307137145305	0.35782079895397	-2.66039141344188
C	4.19939692545220	-4.95676798928798	-4.06166079634055
C	4.12079117258282	-0.98691211881774	-5.26910404727684
C	2.80254248974081	1.18467169866887	-3.10500308123891
C	1.52155273596308	-1.71699413104680	2.53676747112109
C	-3.62024171496475	-1.57302852560882	-2.77357208471528
C	-2.63713015715668	-0.63020662041160	-3.13202332133967
C	-1.61120277665961	-0.29943148994152	-2.22823691449653
C	-1.49086038077451	-1.04842710231860	-1.04097252432437
C	-2.54705650116128	-1.88230808903475	-0.67087106887237
C	-3.61129108098233	-2.16933938609255	-1.51284744961173
C	-0.46770885451199	-1.07927595890062	0.03356551695692
C	-1.28767965282005	-1.37153338299062	1.29436298807513
C	-2.35868283618932	-2.34824554724253	0.74573231917441
O	-4.57313125990114	-1.79442689380010	-3.72513661896009
O	-2.75213682829226	0.00273974447056	-4.35335300447585
O	-0.77515963020471	0.74862547013220	-2.32321864850312
C	-5.61562667228228	-2.70499427729539	-3.40004530245298
C	-2.21162208384128	-0.77287221872257	-5.43117073273726
C	-0.78014104761253	1.65877333702793	-3.42315664840854
C	-1.90275730117948	-0.08807794633838	1.87477945958195
C	2.78887490533063	-1.73586913149476	3.41244901607505
C	3.48848693637997	-0.37462868348744	3.42333407703473
C	2.42914326549924	-2.15335498034318	4.83990669654139
C	-2.65736139650395	-0.25262926424054	3.20140958265910
C	-1.73313291465392	-0.68949159478502	4.34139193906735
C	-3.36064776441450	1.05796034419213	3.56434525643252
H	3.45358598962022	-4.48588592053798	-1.69535062417998
H	2.74198194495521	-1.13094824143424	0.90190691763650
H	1.33496150109723	-3.81955027668206	0.67746929985086
H	3.08954128971320	-3.57089402873974	0.85965247590907
H	5.00663955426311	-4.96829338276242	-3.31679691938733
H	4.58849573139005	-5.30391377325091	-5.02066815683164
H	3.39014947995796	-5.62242146821688	-3.73290177949328
H	4.84688082639475	-0.75747587424733	-4.47850794542445
H	4.08767051634325	-0.15935729088333	-5.98366482448401
H	4.42388812343940	-1.90447685268618	-5.78066630812773
H	2.80015863362199	1.29702617009631	-4.19382687886977
H	3.76945374293927	0.77764871061933	-2.78246264151114

H	2.65064529479341	2.15966380498830	-2.63187846614585
H	0.90969758439626	-2.58776938250435	2.80659642952581
H	0.94386545103875	-0.82188451621778	2.80286010923127
H	-4.40524450432780	-2.83033961300593	-1.18523934630019
H	-0.69886407839047	-1.86854289113735	2.05651962983274
H	-3.29656654932139	-2.32957776579172	1.31242132968953
H	-1.97424685496226	-3.37823488411449	0.77572295909094
H	-5.22014072188592	-3.70551858910279	-3.17761368300460
H	-6.25382157093879	-2.75442593243937	-4.28426643218660
H	-6.20689563796215	-2.34876673875054	-2.54562355796549
H	-2.74539071479387	-1.72522168979566	-5.53498791898968
H	-1.14159975536100	-0.97010293535311	-5.27207498237952
H	-2.34592137135147	-0.17761368860201	-6.33832041285754
H	-0.04588240099183	2.41957495605545	-3.14830404171980
H	-1.76275590094743	2.11881721509771	-3.55929025967453
H	-0.46423030548865	1.17569647800192	-4.35296843190772
H	-2.57611339271391	0.34572997815929	1.12188931198068
H	-1.09700930020362	0.64648386106101	2.02310937567520
H	3.48613783736471	-2.48222120917890	3.00146426561599
H	4.41634901325045	-0.41420972875363	4.00433804583011
H	2.83821532318258	0.38086524395673	3.88212643978855
H	3.74234292215186	-0.02828819120213	2.41649330793486
H	3.30952989376730	-2.15206972011393	5.49195082369859
H	1.99067808321960	-3.15708846431879	4.86303744963706
H	1.69462219882924	-1.45855504454007	5.26711563980794
H	-3.43213708135590	-1.02384994597344	3.07537901056440
H	-2.28470735204267	-0.76669077426647	5.28491581640534
H	-0.92890685751768	0.04404546836375	4.48356569286697
H	-1.26691388904771	-1.66166902509027	4.15108292597451
H	-3.92773844433800	0.96090062015779	4.49677222122308
H	-4.05363018231428	1.36839223100539	2.77500460317405
H	-2.62731234739896	1.86264114918529	3.70121902336929

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