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Supporting Information

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*R. Z. Pavlović, L. Zhiquan, T. J. Finnegan, C. A. Waudby, X. Wang, V. W. L. Gunawardana, X. Zhu, C. M. Wong, T. Hamby, C. E. Moore, N. Hoefer, D. W. McComb, C. S. Sevov, J. D. Badjić**

Closed Aromatic Tubes – Capsularenes

Radoslav Z. Pavlović,[a] Lei Zhiquan,[a] Tyler J. Finnegan,[a] Christopher A. Waudby,[b] Xiuze Wang,[a] Vageesha W. Liyana Gunawardana,[a] Xingrong Zhu,[a] Curt M. Wong,[a] Taylor Hamby,[a] Curtis E. Moore,[a] Christo S. Sevov,[a] and Jovica D. Badjić*[a]

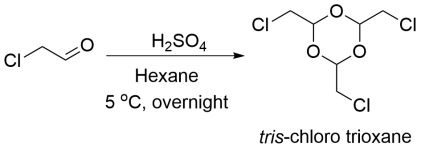
Supporting Information

Contents

General Information

All chemicals were purchased from commercial sources and used as received unless stated otherwise. All solvents were dried prior to use according to standard literature procedures. Chromatographic purifications were performed with silica gel 60 (SiO_2, Sorbent Technologies 40–75 μm, 200 × 400 mesh). Thin-layer chromatography was performed on a silica gel plate w/UV254 (200 μm). Chromatograms were visualized by UV light or stained with I_2, CAM or $KMnO_4$. All electrochemical analyses were carried out in a nitrogen-filled glovebox in solutions of acetonitrile (MeCN) with recrystallized tetrabutylammonium hexafluorophosphate ($TBAPF_6$) as supporting electrolyte. Cyclic voltammetry was performed with a Biologic VSP multichannel potentiostat/galvanostat. Cyclic voltammetry was carried out in a three-electrode electrochemical cell, consisting of a glassy carbon disk working electrode (0.07 cm^2, BASi), a Ag/Ag^+ pseudo-reference electrode (BASi) with 0.01 M $AgBF_4$ (Millipore Sigma) in 0.02 M $TBAPF_6$ in MeCN, and a platinum wire counter electrode (23 cm, ALS). All cyclic voltammetry experiments were performed at a scan rate of 100 mV/s in a MeCN electrolyte containing 0.02 M recrystallized $TBAPF_6$ unless otherwise noted. Reference electrodes were calibrated against an internal voltage reference of ferrocene (1-10 mM). All ^1H and ^{13}C NMR samples were kept in class B glass NMR tubes (Wilmad Lab Glass). NMR experiments were performed with Bruker 400 600, 700, and 850 MHz spectrometers. Chemical shifts are expressed in parts per million (δ, ppm), whereas coupling constants (*J*) are given in Hertz (Hz). Residual solvent protons were used as internal standards: ^1H NMR spectra, $CDCl_3$ = 7.26 ppm, CD_2Cl_2 = 5.32 ppm; ^{13}C NMR spectra, $CDCl_3$ = 77.16 ppm, CD_2Cl_2 = 53.84 ppm; $CDCl_3$ and CD_2Cl_2 were purchased from Cambridge Isotope Laboratories. High-resolution mass spectra (HRMS) were obtained using positive electrospray ionization (ESI) techniques recorded on a Bruker-ESI TOF instrument. All the kinetic measurements were performed on Bruker 850 MHz (5mm Tripleresonance Inverse (TCI) cryoprobe with Z-Gradients) spectrometers. Sratorius Quintix semi-micro balance was used in the preparation of standard solutions. All UV-Vis spectra were recorded on Shimadzu UV-2401 PC UV-Vis Spectrophotometer using quartz 1 cm cuvettes. Fluorescence spectra were recorded with Shimadzu RF-5301 using quartz 1 cm cuvettes.

Syntheses of Compounds

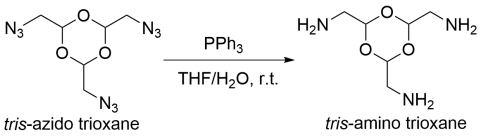


tris-chloro trioxane

***Tris*-Chloro Trioxane ((2*s*,4*s*,6*s*)-2,4,6-tris(chloromethyl)-1,3,5-trioxane).** This compound was obtained using slightly modified procedure reported by Shi et al.[1] Chloroacetaldehyde solution (~50 wt. % in H_2O) (12 g, 0.076 mol) was extracted by diethyl ether multiple times and the organic layers were combined. After evaporating diethyl ether under reduced pressure, the remained liquid was diluted by 20 ml of n-hexane and cooled to 0 °C. Maintaining the same temperature, concentrated sulfuric acid (3 ml) was added slowly with vigorous stirring continuing for 3 hours and was kept in freezer (5 °C) overnight. Then iced water (50 ml) was slowly added, the solid was extracted by CH_2Cl_2 (2 x 40 ml), washed with water (20 ml), and purified by chromatography (SiO_2, Hexanes:CH_3CO_2Et = 20:1 to 10:1). Recrystallization from *n*-hexane (5 ml) gave *tris*-chloro trioxane (2.0 g, 33%) as a colorless solid. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 5.16 (s, 3H), 3.61 (d, J = 4.7 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 99.70, 43.03.

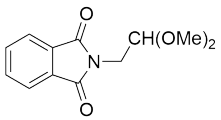
tris-chloro trioxane *tris*-azido trioxane

***Tris*-Azido Trioxane ((2*s*,4*s*,6*s*)-2,4,6-tris(azidomethyl)-1,3,5-trioxane).** To a suspension of KI (4.95g, 29.8 mmol) and NaN_3 (2.9g, 44.7 mmol) in DMSO (40 ml) *tris*-chloro trioxane (1.17 g, 4.97 mmol) was added. The mixture was heated to 90 °C for 3 days. Upon cooling down to room temperature, the reaction mixture was diluted with H_2O (30 ml), extracted with CH_2Cl_2 (2 x 40 ml), and combined organic layers washed with brine (4 x 15 ml). The organic layer was dried with Na_2SO_4 and concentrated in vacuo. The resulting residue was purified by flash column chromatography (SiO_2, Hexanes: CH_3CO_2Et = 10:1) to give *tris*-azido trioxane (963.2 mg, 76%) as a transparent oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 5.14 (t, J = 4.5 Hz, 3H), 3.41 (d, J = 4.5 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 99.04, 52.36. HRMS (ESI): m/z calcd for $C_6H_9N_9NaO_3$: 278.0721, $[M+Na]^+$; found: 278.0721, $[M+Na]^+$.



tris-azido trioxane *tris*-amino trioxane

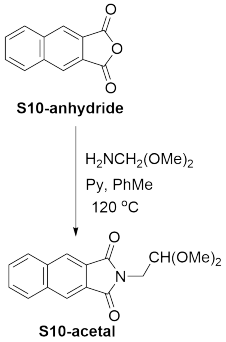
***Tris*-Amino Trioxane (((2*s*,4*s*,6*s*)-1,3,5-trioxane-2,4,6-triyl)trimethanamine).** To a solution of *tris*-azido trioxane (120 mg, 0.47 mmol) in THF/H_2O (16/1, 10 ml), PPh_3 (616.5 mg, 2.35 mmol) was added under an atmosphere of nitrogen. The mixture was stirred at 35 °C overnight, followed by removal of THF in vacuo, addition of H_2O (4 ml) and extraction with Et_2O (4 x 4 ml). The aqueous layer was lyophilized to give *tris*-amino trioxane (70.7 mg, 85%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 4.92 (t, J = 4.3 Hz, 3H), 2.87 (d, J = 4.3 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 100.99, 45.04. HRMS (ESI): *m*/*z* calcd for $C_6H_{16}N_3O_3$: 178.1186, $[M+H]^+$; found: 178.1187, $[M+H]^+$.



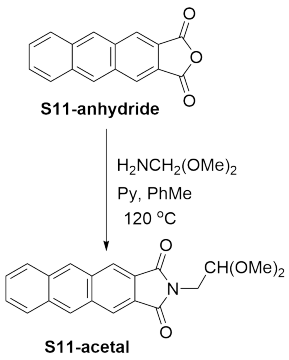
S3-acetal

2-(2,2-dimethoxyethyl)isoindoline-1,3-dione: To a suspension of phthalic anhydride (50 mg, 0.338 mmol) in anhydrous toluene (20 ml) the 2,2-dimethoxyethan-1-amine (47.81 µl, 0.439 mmol, 1.3 equiv.) and dry pyridine (168.4 µl, 2.09 mmol) were added. The mixture was purged with nitrogen (5 min), sealed, and stirred at 120 °C overnight. Upon cooling down to room temperature, the solvent was removed under reduced pressure. The residue was then purified by flash column chromatography (SiO_2, CH_2Cl_2→ CH_2Cl_2:MeOH = 100:1) to give 67 mg (84.4%) of 2-(2,2-dimethoxyethyl)isoindoline-1,3-dione as a white solid. NMR spectra of the product match the ones reported earlier (*Tetrahedron*, **2008**, *64*, 6794-6800). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.89 – 7.82 (m, 2H),

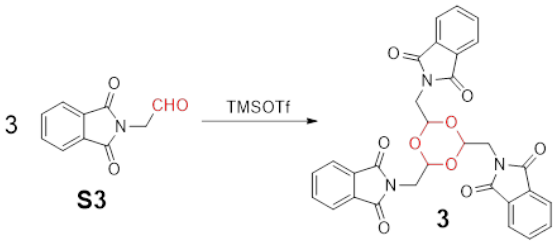
7.76 – 7.68 (m, 2H), 4.77 (t, J = 5.8 Hz, 1H), 3.83 (d, J = 5.8 Hz, 2H), 3.38 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 168.10, 134.00, 132.07, 123.37, 100.02, 53.19, 38.79.



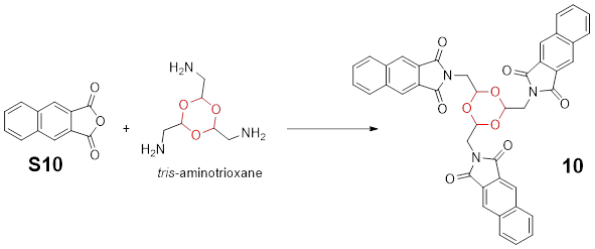
2-(2,2-dimethoxyethyl)-1*H*-benzo[*f*]isoindole-1,3(2*H*)-dione: To a suspension of naphtho[2,3-*c*]furan-1,3-dione (45 mg, 0.227 mmol) in anhydrous toluene (18 ml), 2,2-dimethoxyethan-1-amine (32.2 µl, 0.295 mmol) and dry pyridine (113.4 µl, 1.41 mmol) were added. The mixture was purged with nitrogen (5 min), sealed, and stirred at 120 °C overnight. Upon cooling down to room temperature, the solvent was removed under reduced pressure. The residue was then purified by flash column chromatography (SiO_2, CH_2Cl_2→ CH_2Cl_2:MeOH = 100:1) to give 54 mg (83%) of 2-(2,2-dimethoxyethyl)-1*H*-benzo[*f*]isoindole-1,3(2*H*)-dione as a white solid. NMR spectra of the product match the ones reported earlier (*Tetrahedron*, **2008**, *64*, 6794-6800). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.89 – 7.82 (m, 2H), 7.76 – 7.68 (m, 2H), 4.77 (t, J = 5.8 Hz, 1H), 3.83 (d, J = 5.8 Hz, 2H), 3.38 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.10, 134.00, 132.07, 123.37, 100.02, 53.19, 38.79. ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 167.82, 135.50, 130.31, 129.21, 127.75, 124.83, 100.00, 53.23, 39.07. HRMS (ESI): m/z calcd for $C_{16}H_{15}NO_4$: 308.0899, $[M+Na]^+$; found: 308.0878, $[M+Na]^+$.



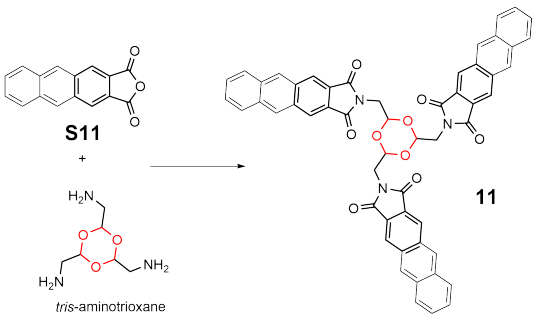
2-(2,2-dimethoxyethyl)-1*H*-naphtho[2,3-*f*]isoindole-1,3(2*H*)-dione: To a suspension of anthra[2,3-*c*]furan-1,3-dione (50 mg, 0.201 mmol) in anhydrous toluene (16 ml), 2,2-dimethoxyethan-1-amine (24 mg, 29 µL, 0.439 mmol) and dry pyridine (101 µl, 2.09 mmol) were added. The mixture was purged with nitrogen (5 min), sealed, and stirred at 120 °C overnight. Upon cooling down to room temperature, the solvent was removed under reduced pressure. The residue was then purified by flash column chromatography (SiO_2, CH_2Cl_2→ CH_2Cl_2:MeOH = 100:1) to give 56 mg (83%) of 2-(2,2-dimethoxyethyl)-1*H*-naphtho[2,3-*f*]isoindole-1,3(2*H*)-dione as a yellow solid. ^{1}H NMR (800 MHz, $CDCl_3$): δ (ppm) 8.65 (s, 2H), 8.53 (s, 2H), 8.09 (dd, J = 6.3, 3.3 Hz, 2H), 7.63 (dd, J = 6.5, 3.1 Hz, 2H), 4.86 (t, J = 5.9 Hz, 1H), 3.93 (d, J = 5.9 Hz, 2H), 3.42 (s, 6H). ^{13}C NMR (201 MHz, $CDCl_3$): δ (ppm) 167.62, 133.30, 131.98, 130.13, 128.49, 127.58, 126.56, 126.06, 99.97, 53.23, 39.15. HRMS (ESI): m/z calcd for $C_{20}H_{17}NO_4$ 358.1055, $[M+Na]^+$; found: 358.1061, $[M+Na]^+$.



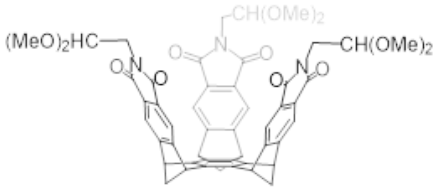
2,2',2''-(((2*s*,4*s*,6*s*)-1,3,5-trioxane-2,4,6-triyl)tris(methylene))tris(isoindoline-1,3-dione) 3. TMS triflate (2.7 µl, 0.015 mmol) was added to a stirred solution of 2-(1,3-dioxoisoindolin-2-yl)acetaldehyde (94.5 mg, 0.5 mmol) in anhydrous CH_2Cl_2 (8 ml), at a room temperature and under nitrogen atmosphere. After circa 12 h, the solvent was removed under reduced pressure and the residue was purified by flash column chromatography (SiO_2, Hexanes: CH_3CO_2Et=3:1, then CH_3OH:CH_2Cl_2 = 1:30) to give compound **3** (47.2 mg, 50%) as a white solid., ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.76 (dd, J = 5.6, 3.0 Hz, 6H), 7.67 (dd, J = 5.4, 3.1 Hz, 6H), 5.20 (t, J = 5.3 Hz, 3H), 3.90 (d, J = 5.3 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 167.52, 133.89, 131.87, 123.34, 96.72, 40.06. HRMS (ESI): m/z calcd for $C_{30}H_{21}N_3NaO_9$: 590.1170, $[M+Na]^+$; found: 590.1195, $[M+Na]^+$.



2,2',2''-(((2*s*,4*s*,6*s*)-1,3,5-trioxane-2,4,6-triyl)tris(methylene))tris(1*H*-benzo[*f*]isoindole-1,3(2*H*)-dione) 10. Naphtho[2,3-*c*]furan-1,3-dione (25 mg, 0.127 mmol), *tris*-amino trioxane (4.5 mg, 0.0254 mmol) and glacial acetic (10 ml) were added to an oven-dried vial. The vial was sealed, and the reaction mixture was stirred at 120 °C overnight. Upon cooling the reaction mixture to a room temperature, the solvent was removed under reduced pressure and the residue was purified by flash column chromatography (SiO_2, CH_2Cl_2 to CH_2Cl_2:MeOH = 100:1) to give compound **10** (10 mg, 55%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 6H), 7.86 (dd, *J* = 6.1, 3.3 Hz, 6H), 7.64 (dd, *J* = 6.2, 3.3 Hz, 6H), 5.31 (t, *J* = 5.4 Hz, 3H), 3.99 (d, *J* = 5.4 Hz, 6H).^{13}C NMR (101 MHz, $CDCl_3$) δ 167.2, 135.3, 130.2, 129.1, 127.5, 124.7, 96.7, 40.3. HRMS (ESI): m/z calcd for $C_{42}H_{27}N_3O_9$: 740.1640, $[M+Na]^+$; found: 740.1656, $[M+Na]^+$.

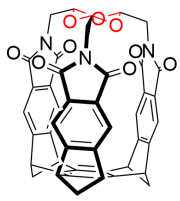


2,2',2''-(((2*s*,4*s*,6*s*)-1,3,5-trioxane-2,4,6-triyl)tris(methylene))tris(1*H*-naphtho[2,3-*f*]isoindole-1,3(2*H*)-dione) 11. Anthra[2,3-*c*]furan-1,3-dione (20 mg, 0.07521 mmol), *tris*-amino trioxane (4.5 mg, 0.0203 mmol) and glacial acetic (6.8 ml) were added to an oven-dried vial. The vial was sealed, and the reaction mixture was stirred at 120 °C overnight. Upon cooling the reaction mixture to a room temperature, the solvent was removed under reduced pressure and the residue was purified by flash column chromatography (SiO_2, CH_2Cl_2 to CH_2Cl_2:MeOH = 100:1) to give compound **10** (10.1 mg, 57%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): *δ* (ppm) 8.11 (s, 6H), 7.86 (dd, *J* = 6.1, 3.3 Hz, 6H), 7.64 (dd, *J* = 6.2, 3.3 Hz, 6H), 5.31 (t, *J* = 5.4 Hz, 3H), 3.99 (d, *J* = 5.4 Hz, 6H). HRMS (ESI): *m*/*z* calcd for $C_{54}H_{33}N_3O_9$: 890.2109, $[M+Na]^+$; found: 890.2116, $[M+Na]^+$.



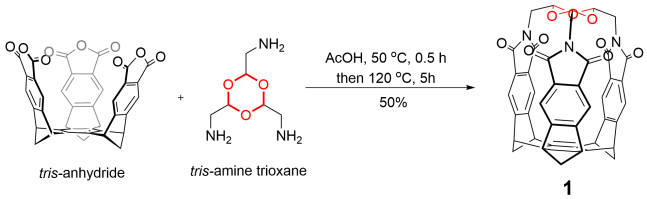
4

Compound 4. To a suspension of *tris*-anhydride[2] (15.8 mg, 0.025 mmol) in anhydrous toluene (2.00 ml) was added 2,2-dimethoxyethan-1-amine (10.5 mg, 0.1 mmol) and dry pyridine (39.5 mg, 0.5 mmol). The mixture was heated to 120 °C for 12 h. Next, the mixture was concentrated under reduced pressure to give residue which was purified by column chromatography (SiO_2, CH_3OH:CH_2Cl_2 = 1:50) to give compound **4** (13.4 mg, 60%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.54 (s, 6H), 4.62 (s, 3H), 4.52 (s, 6H), 3.64 (d, J = 5.8 Hz, 6H), 3.26 (s, 18H), 2.61 (s, 6H). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 167.87, 156.61, 137.89, 130.57, 116.16, 99.81, 65.78, 52.94, 49.12, 38.51. HRMS (ESI): *m*/*z* calcd for $C_{51}H_{45}N_3NaO_{12}$: 914.2895, $[M+Na]^+$; found: 914.2890, $[M+Na]^+$.



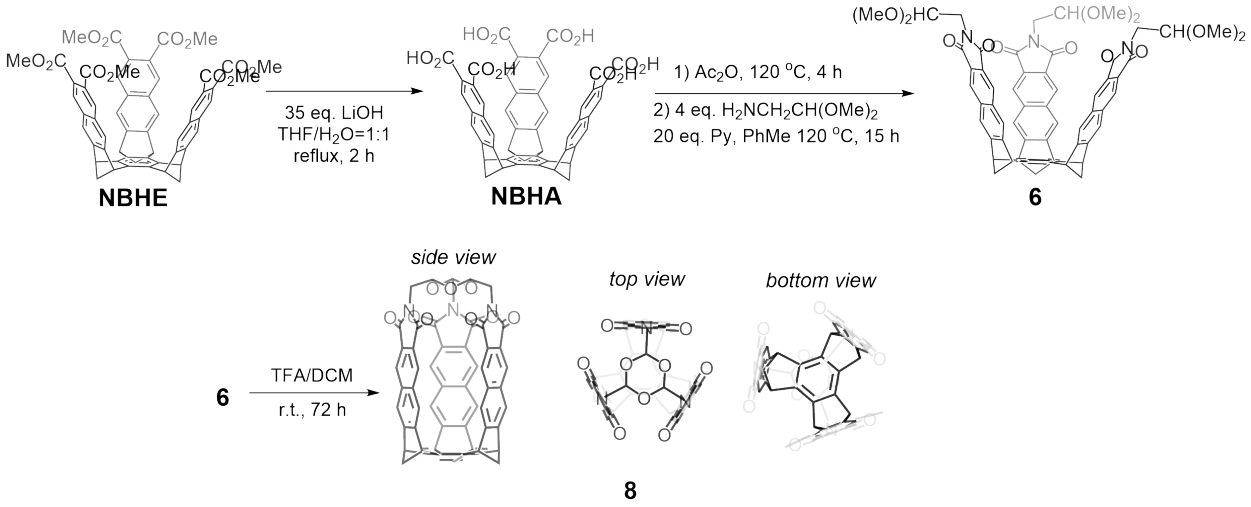
1

Capsularene 1. Compound **4** (13.4 mg, 0.015 mmol) was dissolved in 4 ml of CH_2Cl_2:TFA = 1:1, and the mixture stirred at a room temperature for 24 h. The solvent was removed under reduced pressure and the residual oil triturated with MeOH, and then 20% Et_2O in hexane to give the capsularene **1** (11.3 mg, 99%) as a white solid. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.48 (s, 6H), 5.06 (s, 3H), 4.47 (s, 6H), 3.94 (s, 6H), 2.68 (s, 6H). ^{1}H NMR (700 MHz, CD_2Cl_2) δ 7.45 (s, 6H), 5.09 (s, 3H), 4.53 (s, 6H), 3.85 (d, J = 1.4 Hz, 6H), 2.70 (dd, J = 3.1, 1.5 Hz, 6H). ^{13}C NMR (175 MHz, CD_2Cl_2): δ (ppm) 166.30, 157.14, 141.58, 129.85, 116.37, 99.83, 61.63, 49.39, 38.96. HRMS (ESI): *m*/*z* calcd for $C_{45}H_{27}N_3NaO_9$: 776.1640, $[M+Na]^+$; found: 776.1675, $[M+Na]^+$.



tris-anhydride *tris*-amine trioxane 1

Capsularene 1 via nucleophilic acyl substitution. To a suspension of *tris*-anhydride (12.6 mg, 0.02 mmol) in AcOH (2 ml) and under a nitrogen atmosphere, *tris*-amino trioxane (((2*s*,4*s*,6*s*)-1,3,5-trioxane-2,4,6-triyl)trimethanamine) (3.6 mg, 0.02 mmol) was added. The reaction mixture was stirred in a sealed vial at 50 ºC for 30 min, followed by an increase in temperature to 120 ºC for 5 h. The reaction was cooled to room temperature, the solvent removed under reduced pressure and **1** was purified by flash column chromatography (SiO_2, hexane:CH_3CO_2Et= 2:1 followed by CH_2Cl_2:CH_3OH:NH_3(aq) =100:2.5:1). The solid product was finally triturated with CH_3OH (1 ml) to give **1** as a white solid (7.5 mg, 50%).

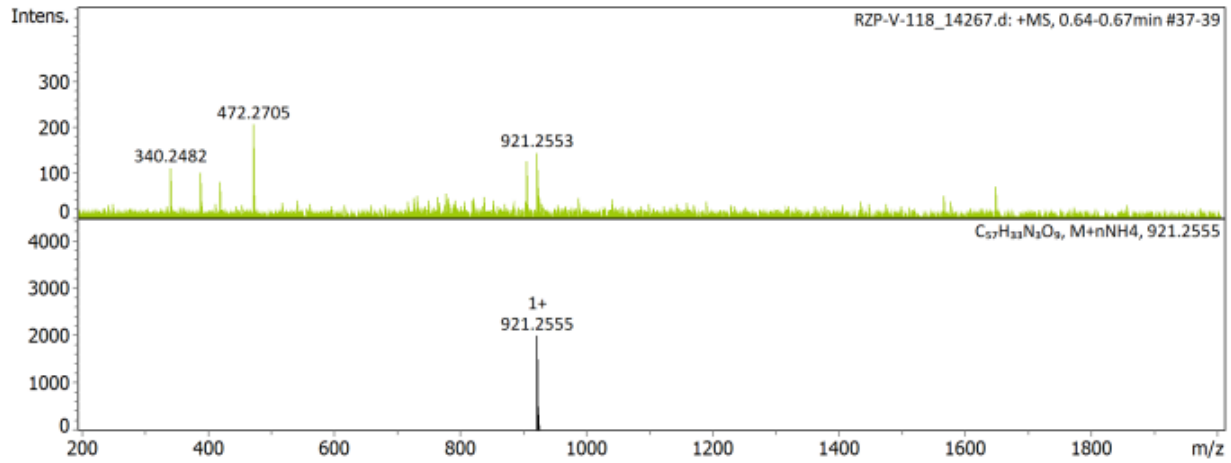


Scheme S1. Preparation of capsularene **8** from **NBHE**.[3]

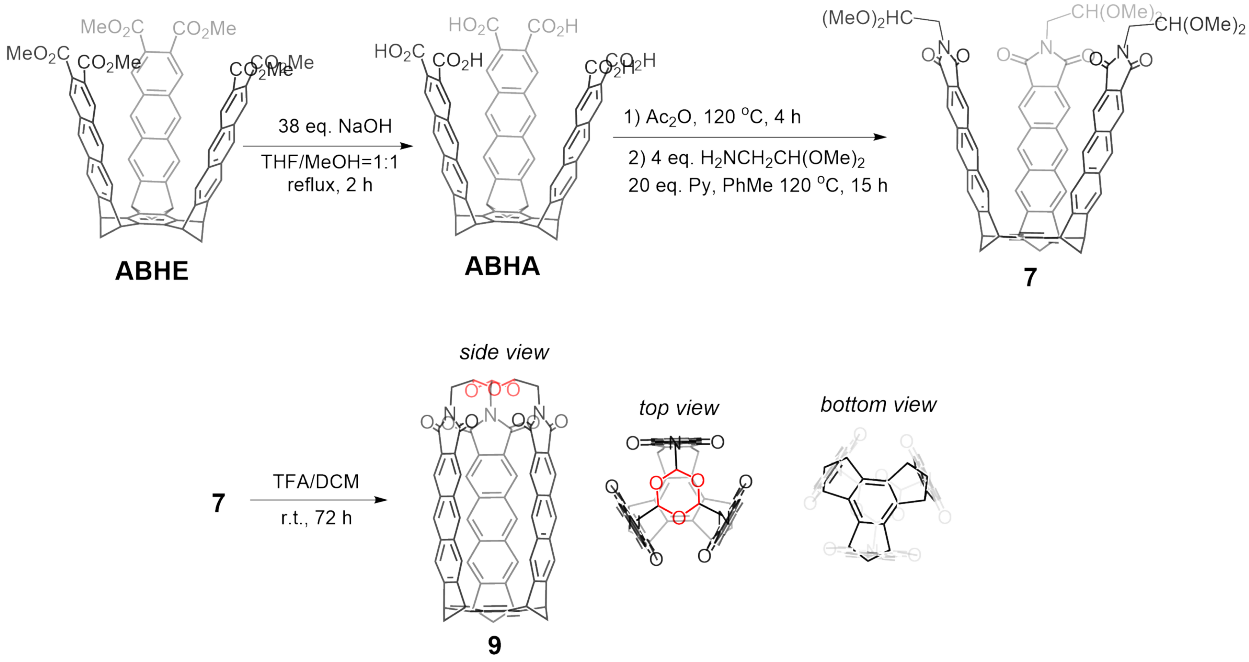
(6*R*,7*S*,14*R*,15*S*,22*R*,23*S*)-6,7,14,15,22,23-Hexahydro-6,23:7,14:15,22-trimethanoanthra[2,3-*j*]heptaphene-2,3,10,11,18,19-hexacarboxylic acid (NBHA). NBHE[3] (Hexamethyl (6*R*,7*S*,14*R*,15*S*,22*R*,23*S*)-6,7,14,15,22,23-hexahydro-6,23:7,14:15,22-trimethanoanthra[2,3-*j*]heptaphene-2,3,10,11,18,19-hexacarboxylate) (200 mg, 0.218 mmol) was dissolved in THF (12 ml) and placed in a round bottom flask to which 12 ml of aqueous 0.6 M LiOH was added. The rection mixture was refluxed for 2 h and then cooled down to room temperatur followed by the removal of THF solvent under reduced pressure. The remaining water solution was transferred to a 50 mL Felkin tube and acidified with aqueous 3 M HCl to pH=0-1, at which point a pale yellow precipitate of the product formed. The solid was isolated by centrifugation, resuspended in aqueous 0.3 M HCl, and then precipitated again using centrifugation (repeat the process three times). Finally, lyophilization of the precipitate gave pure **NBHA** (169 mg, 93%) as a white solid. ^{1}H NMR (850 MHz, DMSO-d_6): δ (ppm) 12.84 (br s, 6H), 7.97 (s, 6H), 7.77 (s, 6H), 4.77 (s, 6H), 2.52 (m, 3H), 2.44 (m, 3H). ^{13}C NMR (213 MHz, DMSO-d_6): δ (ppm) 168.6, 149.6, 137.6, 131.7, 129.1, 128.5, 119.5, 63.6, 47.9. HRMS (ESI): *m*/*z* calcd for $C_{51}H_{30}O_{12}$: 833.1505, $[M-H]^-$, found: 833.1664 $[M-H]^-$.

(6*R*,7*S*,15*R*,16*S*,24*R*,25*S*)-2,11,20-tris(2,2-dimethoxyethyl)-6,7,15,16,24,25-hexahydro-1*H*-6,25:7,15:16,24-trimethanotrinaphtho[2,3-*f*:8,9-*f*':14,15-*f*'']triisoindole-1,3,10,12,19,21(2*H*,11*H*,20*H*)-hexaone 6. NBHA (33 mg, 0.0384 mmol) was added to 4 ml of acetic anhydride in an oven-dried vial, purged with N_2 for 5 min, sealed and then heated at 120 °C for 3 h. Upon cooling the reaction mixture to room temperature, acetic anhydride was removed under reduced pressure and the solid kept under the stream of N_2 for 10 min to ensure complete removal of the solvent. Upon suspending this solid in anhydrous toluene (4 ml), 2,2-dimethoxyethan-1-amine (16.2 mg, 0.154 mmol) and dry pyridine (61 mg, 0.77 mmol) were added. The mixture was heated at 120 °C for 15 h. The solvent was removed under reduced pressure and the resulting residue purified by column chromatography (SiO_2, CH_3OH:CH_2Cl_2 = 1:50) to give **6** (29 mg, 73%) as a white solid. ^{1}H NMR (850 MHz, $CDCl_3$): δ (ppm) 8.03 (s, 6H), 7.67 (s, 6H), 4.71 (t, 3H, *J*=5.9 Hz), 4.61 (s, 6H), 3.76 (d, *J* = 5.9 Hz, 6H), 3.31 (s, 18H), 2.66 (m, 3H), 2.61 (m, 3H). ^{13}C NMR (213 MHz, $CDCl_3$): δ (ppm) 167.8, 150.4, 137.8, 134.7, 127.3, 124.0, 121.3, 100.0, 64.0, 53.2, 48.7, 38.9. HRMS (ESI): m/z calcd for $C_{63}H_{51}N_3O_{12}$: 1059.3711, $[M+NH_4]^+$; found: 1059.3811, $[M+ NH_4]^+$.

Capsularene 8. Compound **6** (15.0 mg, 0.0144 mmol) was dissolved in 4 ml of CH_2Cl_2:TFA = 1:1, and the mixture stirred at a room temperature for 72 h. The solvent was removed under reduced pressure and the residual oil triturated with MeOH, and then 20% Et_2O in hexane to give compound **8** (12.4 mg, 95%) as a white solid. ^{1}H NMR (850 MHz, $CDCl_3$): δ (ppm) 7.98 (s, 6H), 7.47 (s, 6H), 5.19 (s, 3H), 4.52 (s, 6H), 4.07 (s, 6H), 2.70 (m, 3H), 2.64 (m, 3H). ^{1}H NMR (850 MHz, 10% CF_3CO_2H in $CDCl_3$) δ 8.13 (s, 6H), 7.61 (s, 6H), 5.26 (s, 3H), 4.59 (s, 6H), 4.06 (s, 6H), 2.77 (m, 3H), 2.71 (m, 3H). ^{13}C NMR (213 MHz, 10% CF_3CO_2H in $CDCl_3$): δ (ppm) 169.01, 151.73, 141.25, 134.13, 125.11, 125.01, 122.05, 99.32, 59.67, 48.62, 39.49. HRMS (ESI): m/z calcd for $C_{57}H_{33}N_3O_9$: 921.2555, $[M+NH_4]^+$; found: 921.2553, $[M+ NH_4]^+$.



Experimental HRMS (ESI-TOF) spectrum and (bottom) simulated spectra of capsularene **8**.

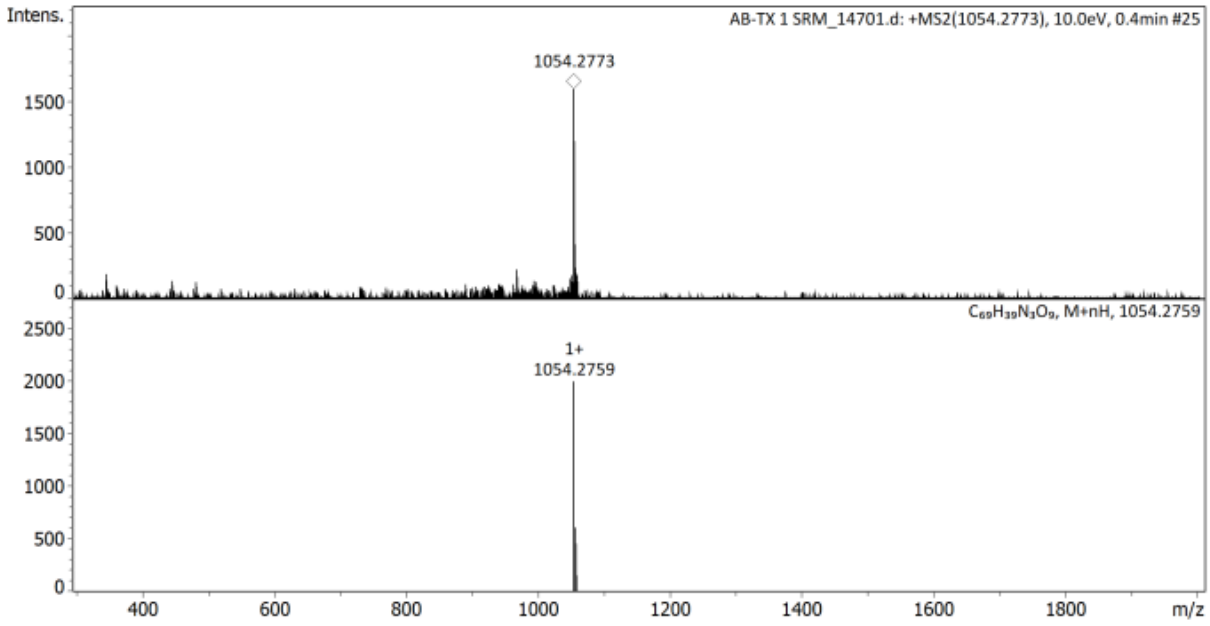


Scheme S2. Preparation of capsularene **9** from **ABHE**.[3]

(7*R*,8*S*,17*R*,18*S*,27*R*,28*S*)-7,8,17,18,27,28-hexahydro-7,28:8,17:18,27-trimethanotetraceno[2,3-*l*]nonaphene-2,3,12,13,22,23-hexacarboxylic acid (ABHA). After ABHE[3] hexamethyl (7*R*,8*S*,17*R*,18*S*,27*R*,28*S*)-7,8,17,18,27,28-hexahydro-7,28:8,17:18,27-trimethanotetraceno[2,3-*l*]nonaphene-2,3,12,13,22,23-hexacarboxylate (70 mg, 0.0655 mmol) was dissolved in THF (1 ml), methanolic NaOH (2.5 M, 1 ml) was added. The rection mixture was refluxed for 2 h. At the beginning, the reaction mixture was a homogenous solution but slowly turned into a suspension (bright yellow precipitate formed) as the reaction progressed. Upon cooling, water (4 ml) was added to render the precipitate into solution. Next, THF and MeOH were removed under reduced pressure. The remaining water solution was transferred to a 20 mL Felkin tube and acidified using aqueous 6 M HCl to pH=0-1, at which point slighty yellow precipitate of ABHA formed. The solid was isolated by centrifugation, then again resuspended in 5 ml of 0.1 M HCl, and precipitated again by centrifugation (repeat this process 3 times). Finally, lyophilization of the precipitate gave pure ABHA (61 mg, 95%) as a yellowish solid. ^{1}H NMR (850 MHz, DMSO-d_6): δ (ppm) 12.93 (br s, CO_2H), 8.37 (s, 6H), 8.23 (s, 6H), 7.83 (s, 6H), 4.80 (s, 6H), 2.56 (m, 3H), 2.46 (m, 3H). ^{13}C NMR (213 MHz, DMSO-d_6): δ (ppm) 168.54, 147.52, 137.35, 131.85, 129.65, 129.47, 128.53, 126.78, 118.57, 62.23, 47.73. HRMS (ESI): *m*/*z* calcd for $C_{63}H_{36}O_{12}$: 983.1180, $[M-H]^-$, found: 983.1134 $[M-H]^-$.

Compound 7. ABHA (16 mg, 16.84 μmol) was added to 4 ml of acetic anhydride in an oven-dried vial, purged with N_2 for 5 min, sealed and heated at 120 ºC for 3 h. Upon cooling the mixture to a room temperature, acetic anhydride was removed under reduced pressure and the remaining solid kept under a stream of N_2 for 10 min to ensure a complete removal of the solvent. Upon suspending the solid in anhydrous toluene (4 ml), 2,2-dimethoxyethan-1-amine (7 mg, 65.4 μmol) and dry pyridine (26 mg, 0.327 mmol) were added. The mixture was heated at 120 °C for 24 h. The solvent was removed under reduced pressure and the resulting residue purified by column chromatography (SiO_2, CH_3OH:CH_2Cl_2 = 1:50) to give compound **7** (14.4 mg, 74%) as a white solid. ^{1}H NMR (850 MHz, $CDCl_3$): δ (ppm) 8.27 (s, 6H), 8.24 (s, 6H), 7.68 (s, 6H), 4.74 (t, 3H, *J*=5.7 Hz), 4.64 (s, 6H), 3.81 (d, *J* = 5.7 Hz, 6H), 3.33 (s, 18H), 2.69 (m, 3H), 2.59 (m, 3H). ^{13}C NMR (213 MHz, $CDCl_3$): δ (ppm) 167.5, 148.1, 137.6, 132.8, 131.7, 129.0, 126.0, 125.4, 118.9, 99.9, 62.4, 53.1, 48.5, 39.0. HRMS (ESI): m/z calcd for $C_{75}H_{57}N_3O_{12}$: 1209.4280, $[M+NH_4]^+$; found: 1209.4272, $[M+ NH_4]^+$.

Capsularene 9. Compound **7** (10.0 mg, 8.4 μmol) was dissolved in in 4 ml of CH_2Cl_2:TFA = 1:1, and the reaction mixture stirred at a room temperature for 100 h. The solvent was removed under reduced pressure and the residue triturated with MeOH, and then 20% Et_2O in hexane to give compound **8** (8 mg, 90%) as a white solid. ^{1}H NMR (850 MHz, TFA/$CDCl_3$=3:7, 298 K): δ (ppm) 8.46 (s, 6H), 8.19 (s, 6H), 7.56 (s, 6H), 5.34 (s, 3H), 4.60 (s, 6H), 4.14 (s, 6H), 2.77 (m, 3H), 2.69 (m, 3H). ^{13}C NMR (213 MHz, TFA/$CDCl_3$=3:7, 298 K): δ (ppm) 169.13, 147.51, 140.90, 132.88, 130.99, 129.49, 127.48, 123.55, 119.66, 99.40, 58.38, 48.65, 39.88. HRMS (ESI): *m*/*z* calcd for $C_{69}H_{39}N_3O_9$: 1054.2759, $[M+H]^+$; found: 1054.2773, $[M+ H]^+$.



(Top) Experimental HRMS (ESI-TOF) spectrum and (bottom) simulated spectra of capsularene **9**.

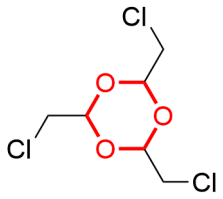
References

(1) Shi, G.; Gadhe, C. G.; Park, S. W.; Kim, K. S.; Kang, J.; Seema, H.; Singh, N. J.; Cho, S. J. *Org. Lett.* **2014**, *16* (2), 334–337. https://doi.org/10.1021/ol402819m.

(2) Border, S. E.; Pavlović, R. Z.; Zhiquan, L.; Badjić, J. D. *J. Am. Chem. Soc.* **2017**, *139* (51). https://doi.org/10.1021/jacs.7b11960.

(3) Lei, Z.; Gunther, M. J.; Liyana Gunawardana, V. W.; Pavlović, R. Z.; Xie, H.; Zhu, X.; Keenan, M.; Riggs, A.; Badjić, J. D. *Chem. Commun.* **2020**, *3*, 10243–10246. https://doi.org/10.1039/d0cc04650g.

Spectroscopic Characterizations



tris-chloro trioxane

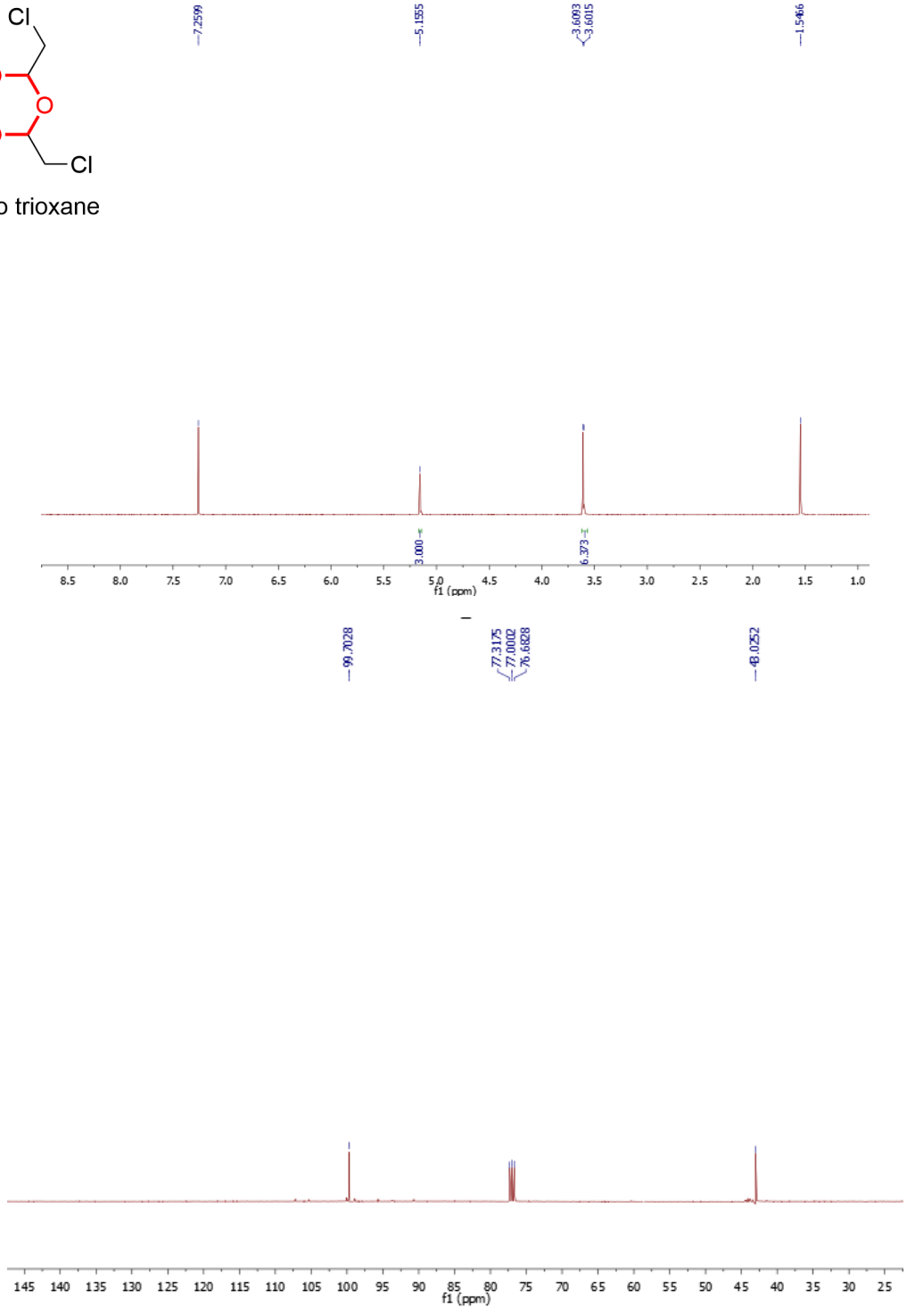
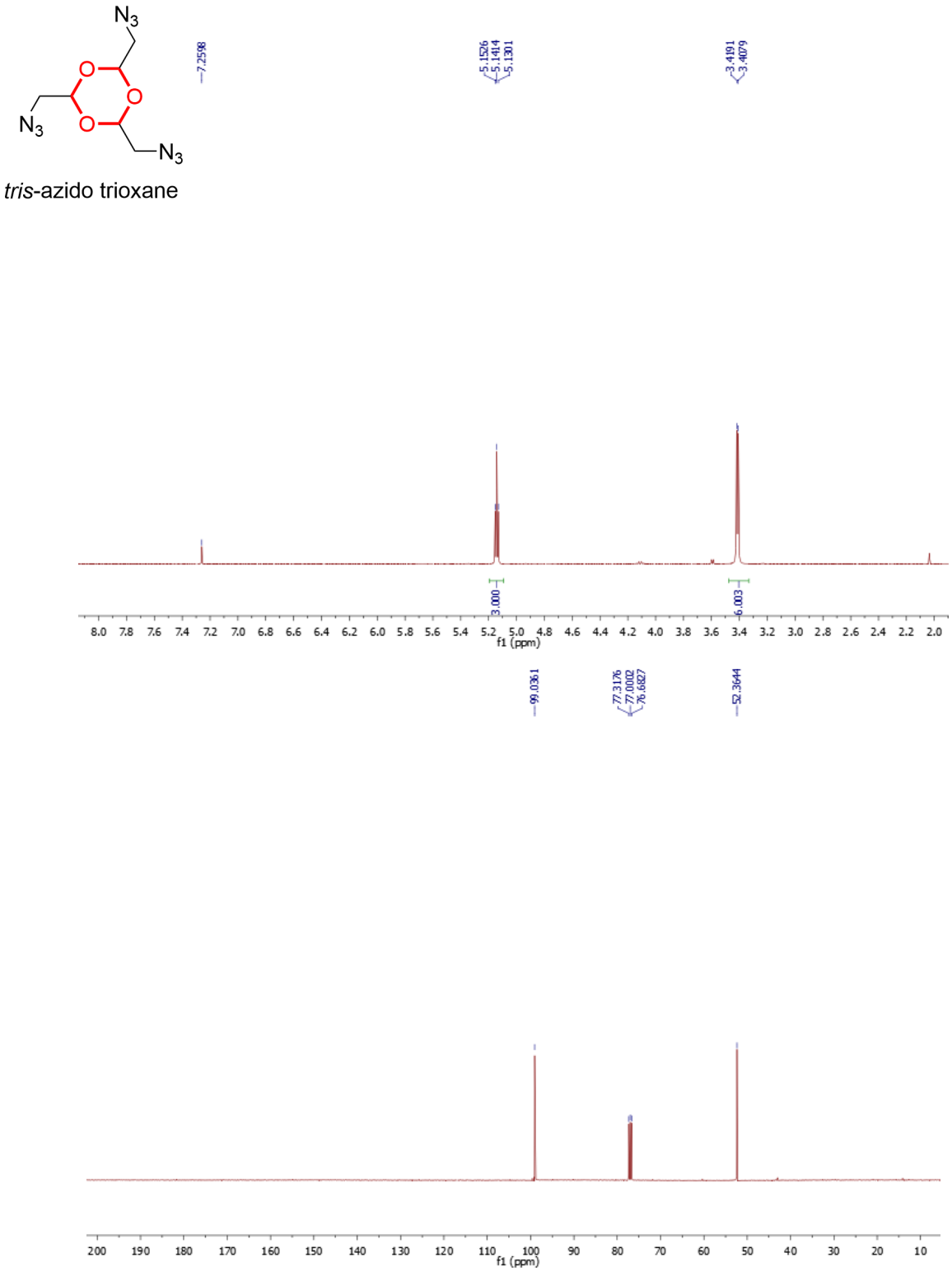


Figure S1. ^{1}H and ^{13}C NMR spectra (600/150 MHz, $CDCl_3$, 298 K) of *tris*-chloro trioxane.



tris-azido trioxane

Figure S2. ^{1}H and ^{13}C NMR spectra (400/100 MHz, $CDCl_3$, 298 K) of *tris*-azido trioxane.

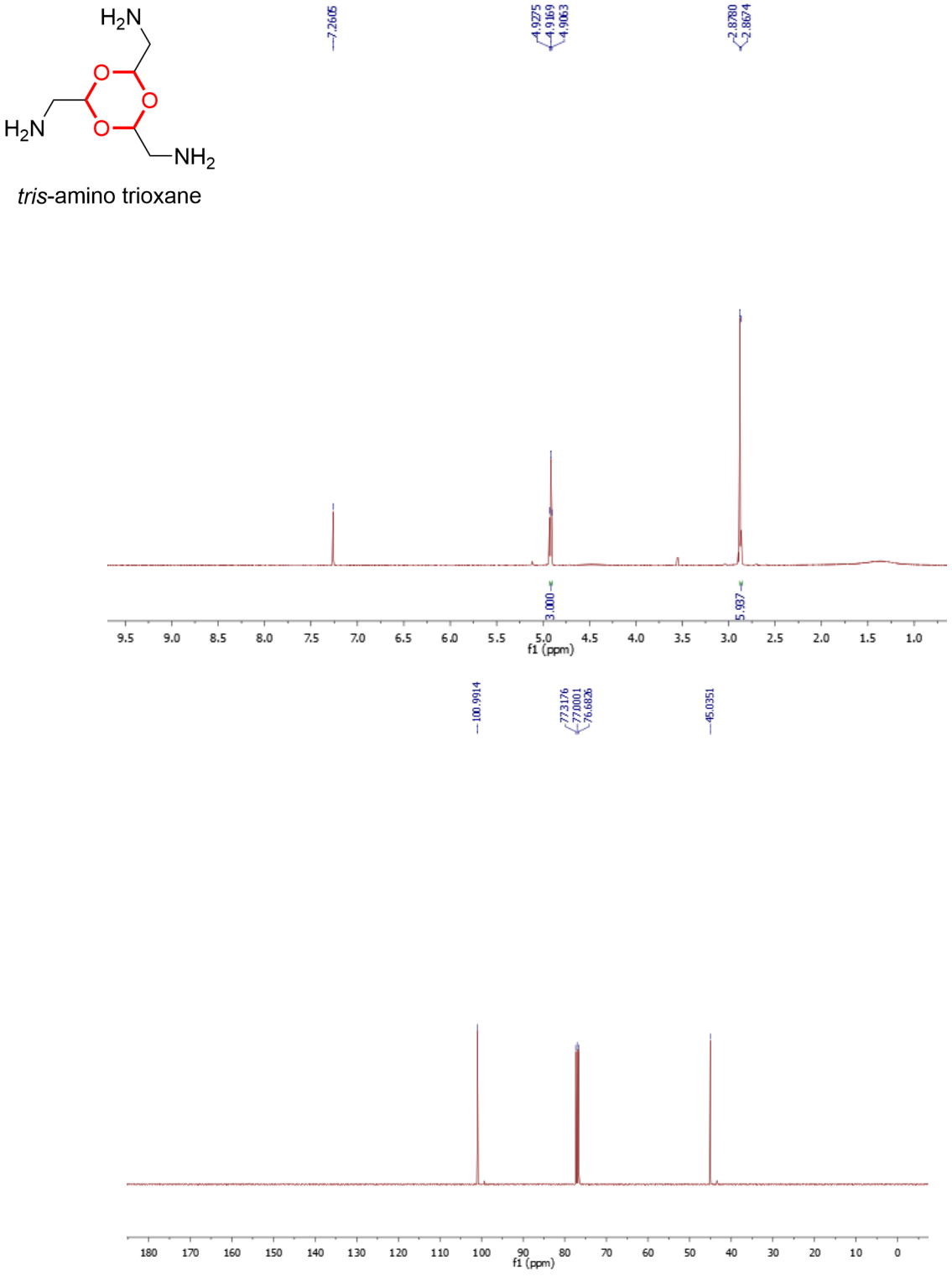


Figure S3. ^{1}H and ^{13}C NMR spectra (400/100 MHz, $CDCl_3$, 298 K) of *tris*-amino trioxane.

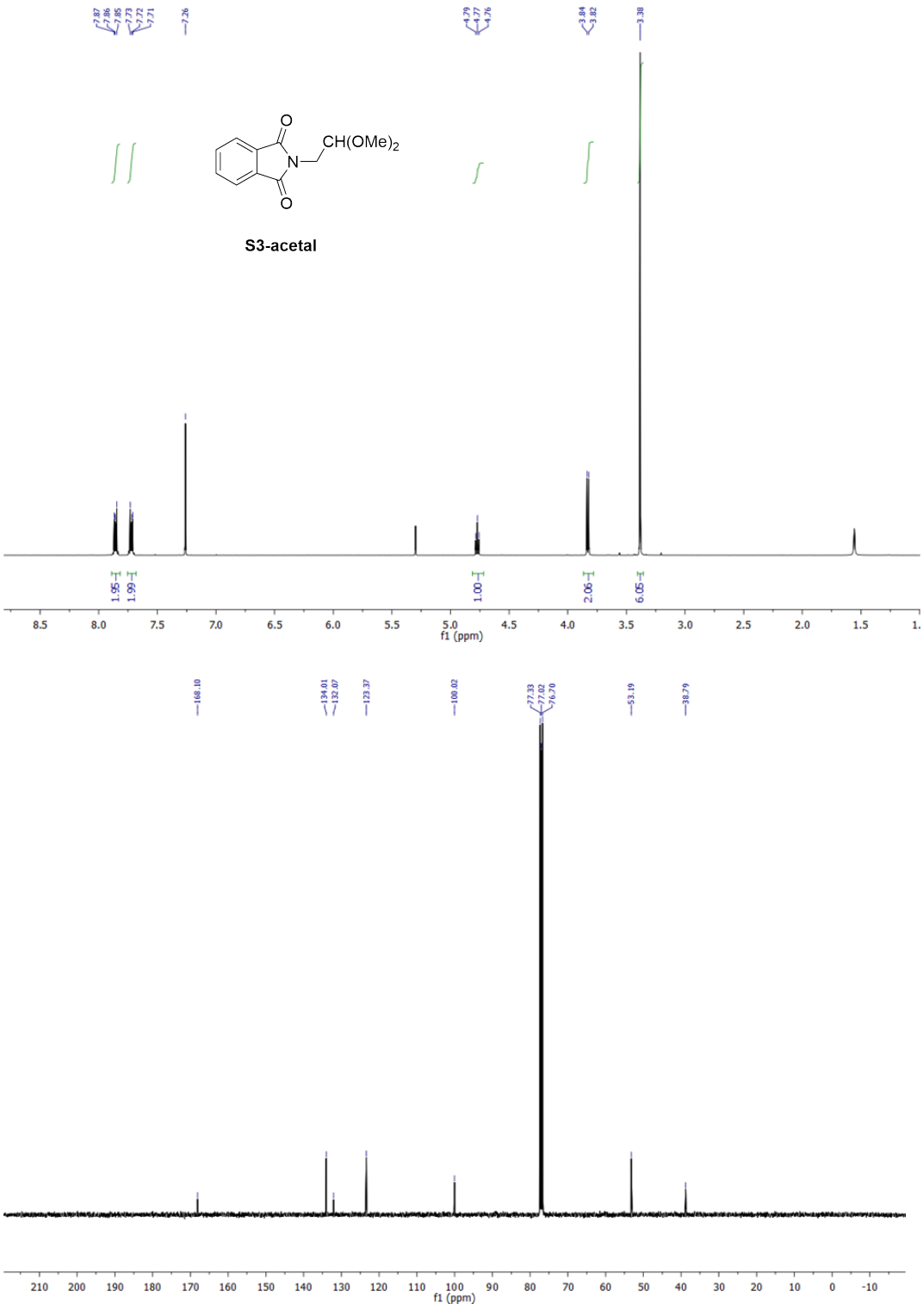


Figure S4. ^{1}H and ^{13}C NMR spectra (400/100 MHz, $CDCl_3$, 298 K) of 2-(2,2-dimethoxyethyl)isoindoline-1,3-dione.

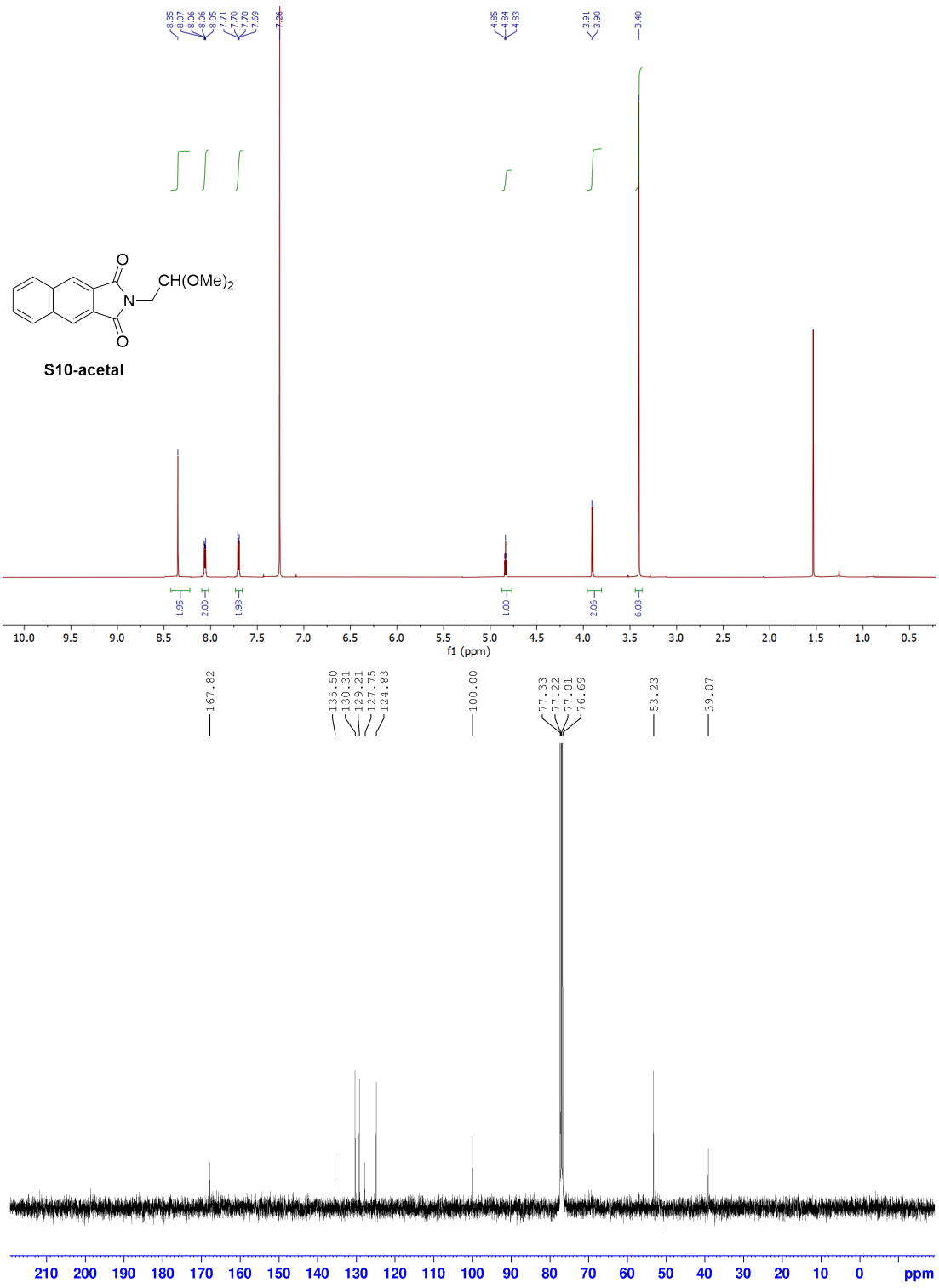


Figure S5. ^{1}H and ^{13}C NMR spectra (400/100 MHz, $CDCl_3$, 298 K) of 2-(2,2-dimethoxyethyl)-1*H*-benzo[*f*]isoindole-1,3(2*H*)-dione.

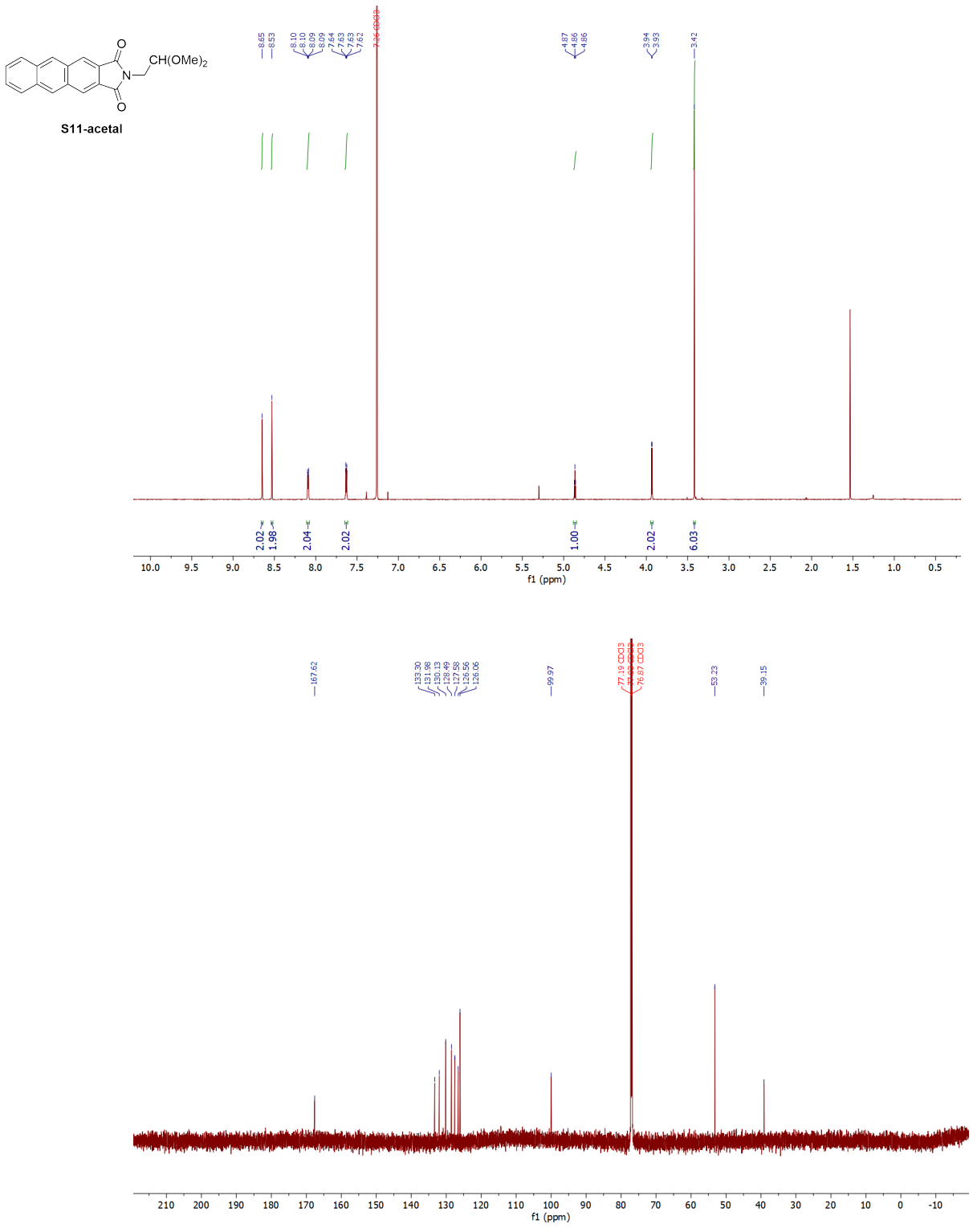


Figure S6. ^{1}H and ^{13}C NMR spectra (400/100 MHz, $CDCl_3$, 298 K) of 2-(2,2-dimethoxyethyl)-1*H*-naphtho[2,3-*f*]isoindole-1,3(2*H*)-dione.

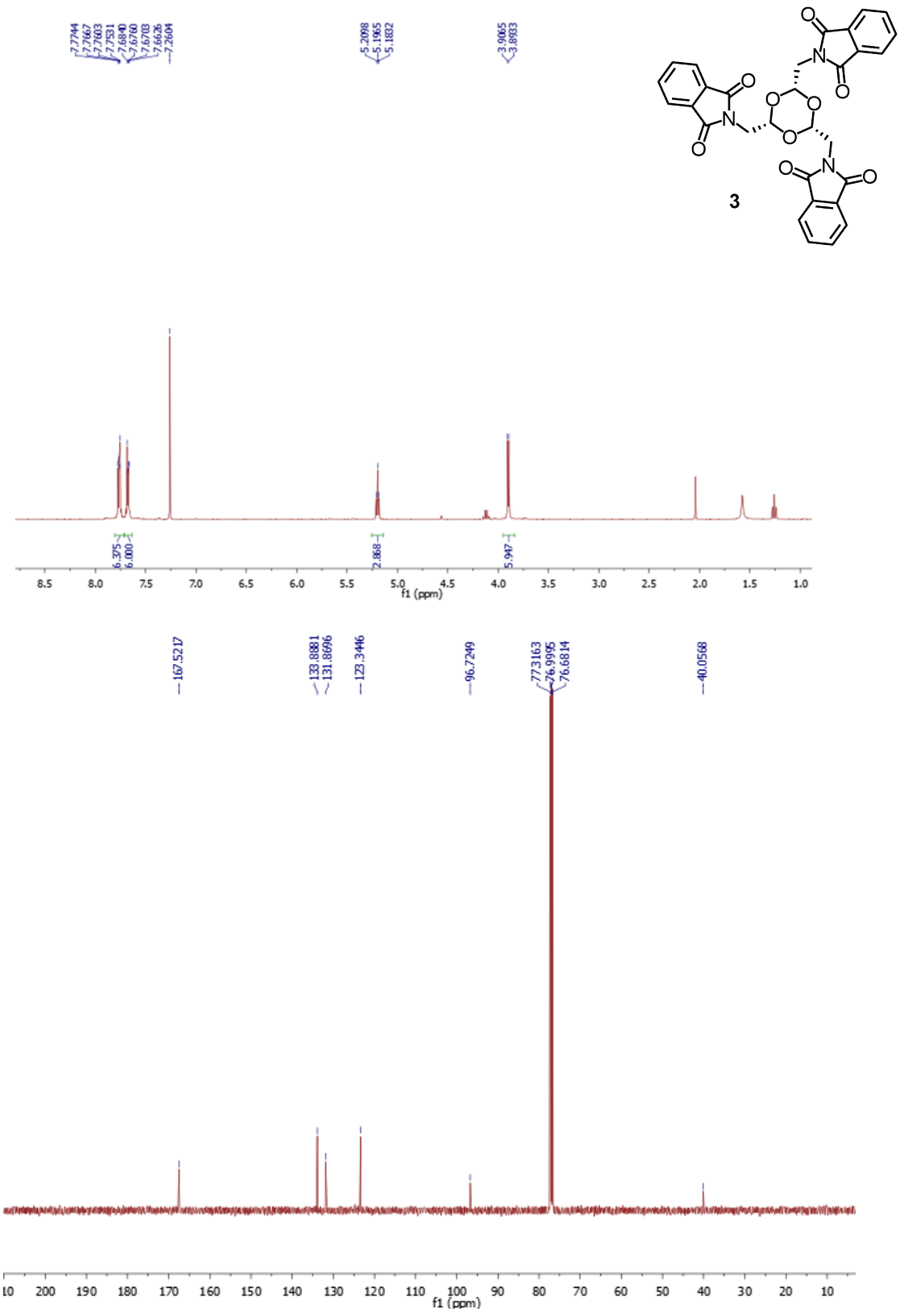


Figure S7. ^{1}H and ^{13}C NMR spectra (400/100 MHz, $CDCl_3$, 298 K) of compound **3**.

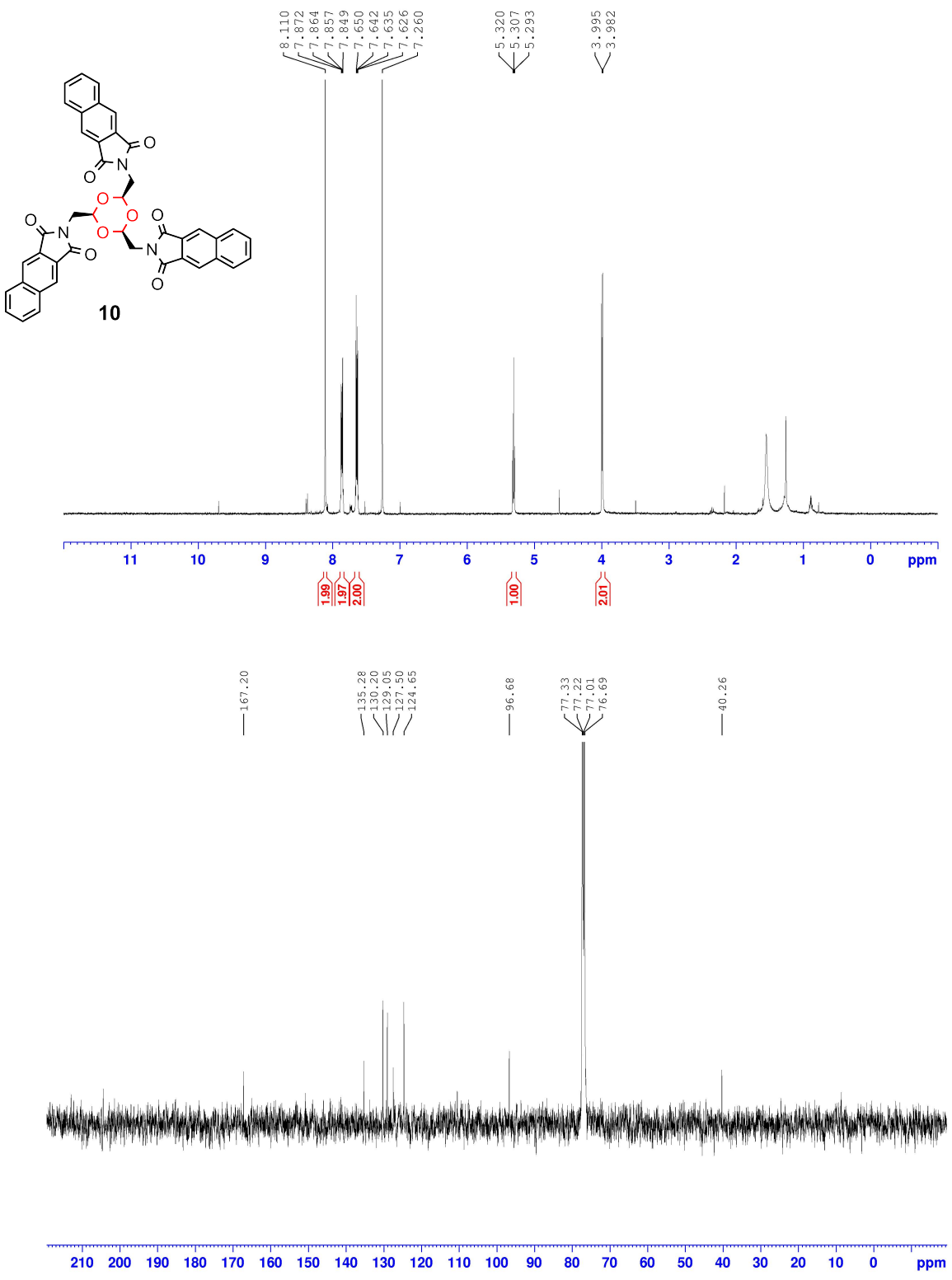


Figure S8. ^{1}H and ^{13}C NMR spectra (400/100 MHz, $CDCl_3$, 298 K) of compound **10**.

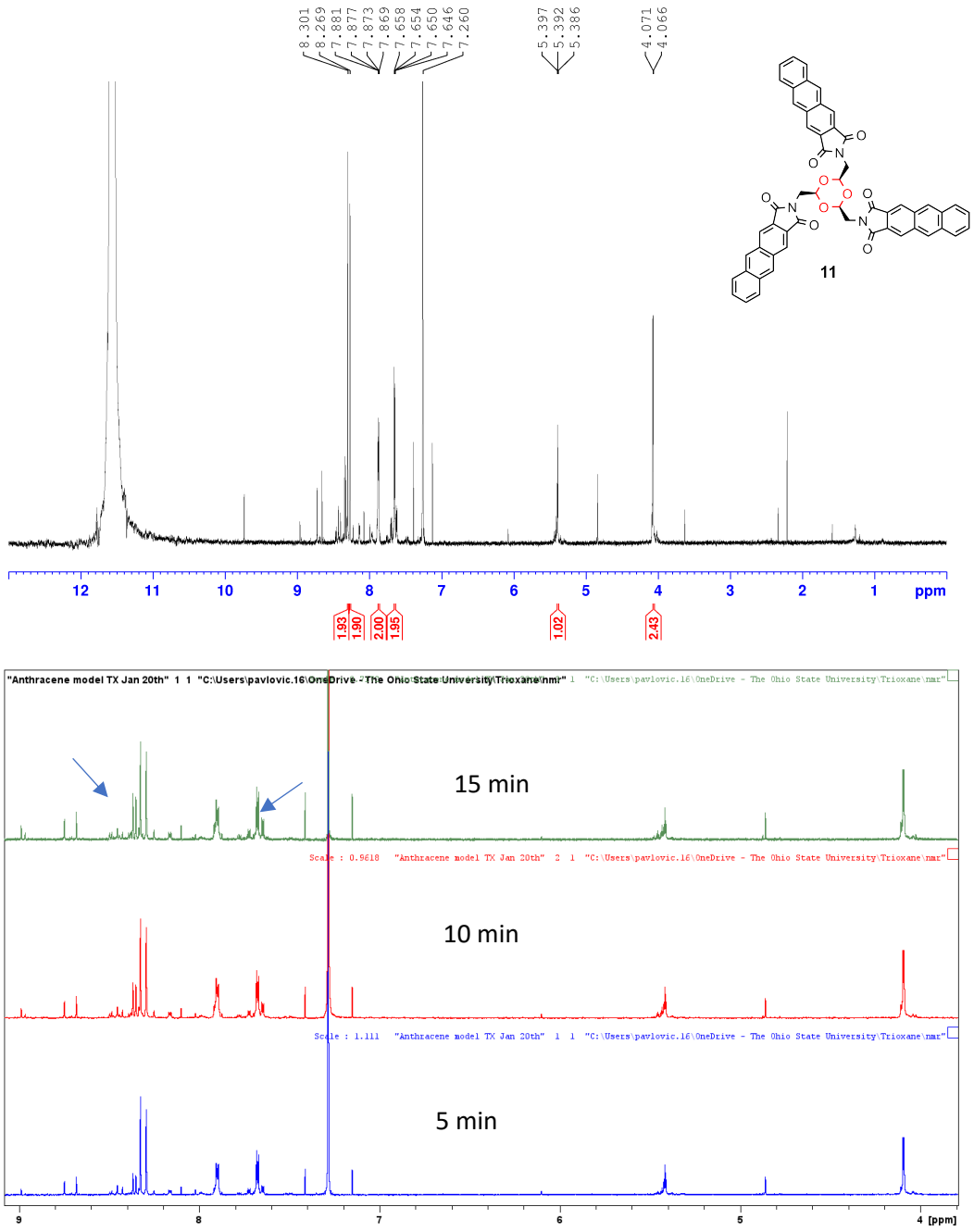


Figure S9. ^{1}H NMR spectra (800 MHz, 10% TFA in $CDCl_3$, 298 K) of compound **11**; due to poor solubility of **11** (and lability in the presence of TFA), we only collected its ^{1}H NMR spectrum.

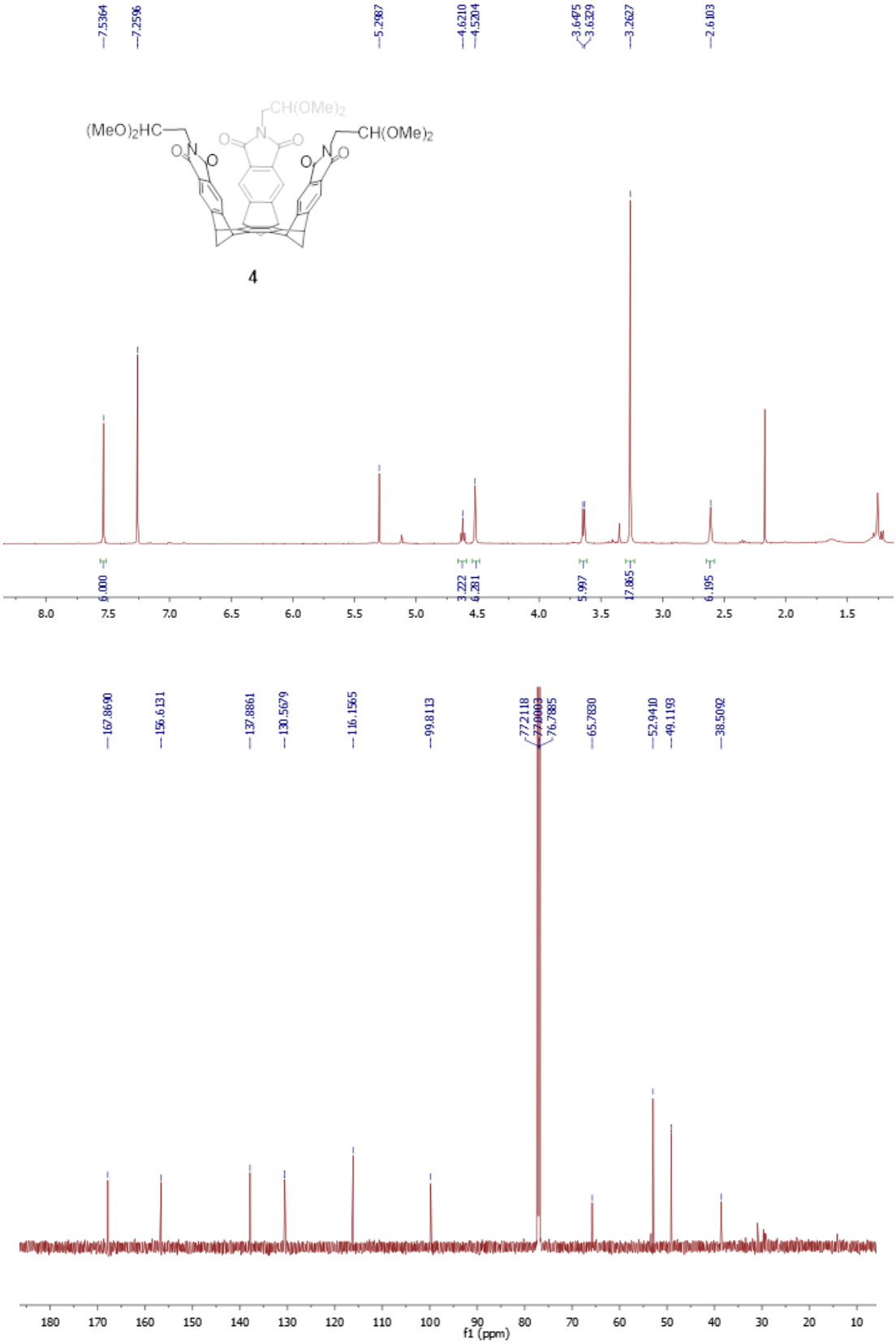
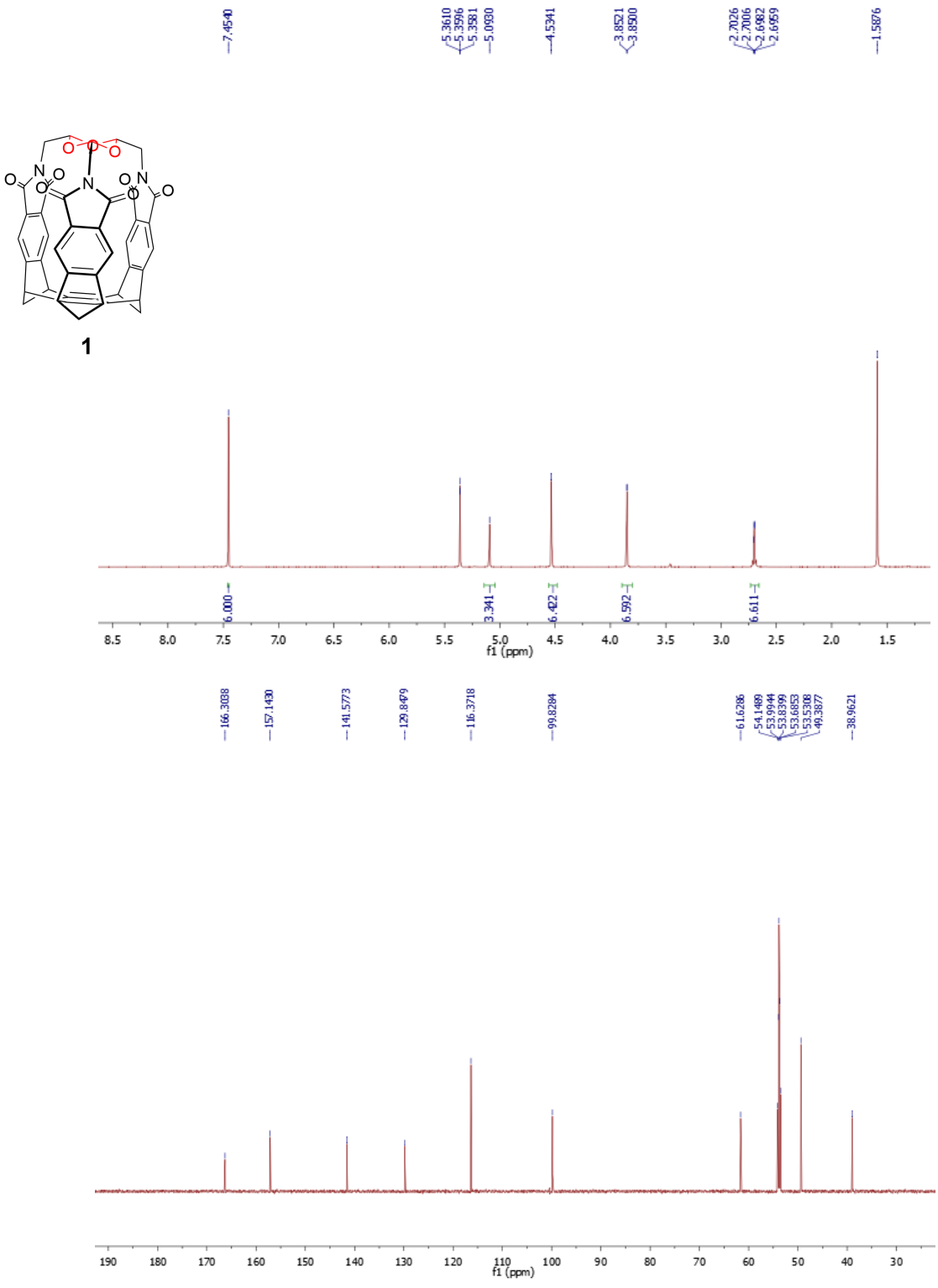


Figure S10. ^{1}H and ^{13}C NMR spectra (600/150 MHz, $CDCl_3$, 298 K) of compound **4**.



1

Figure S11. ^{1}H and ^{13}C NMR spectra (700/175 MHz, 298 K) of capsularene **1** in CD_2Cl_2.

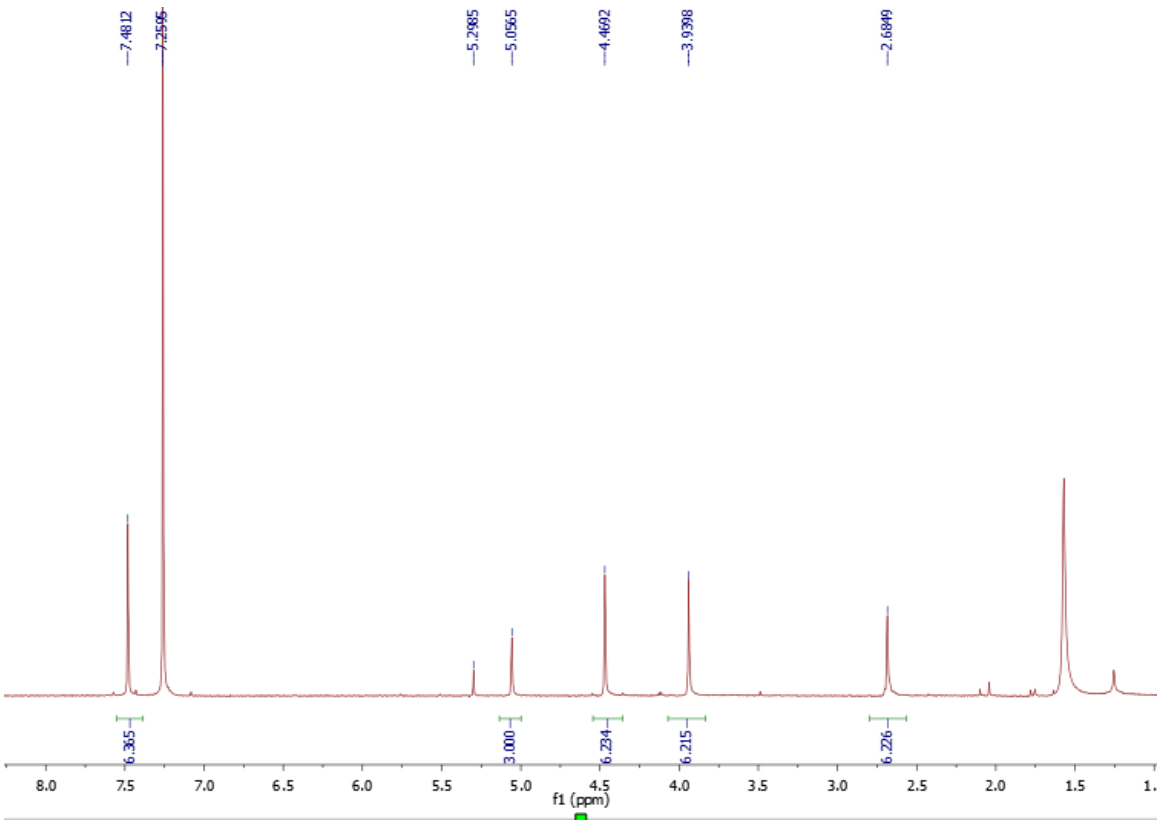


Figure S12. ^{1}H NMR spectrum (600 MHz, 298 K) of capsularene **1** in $CDCl_3$.

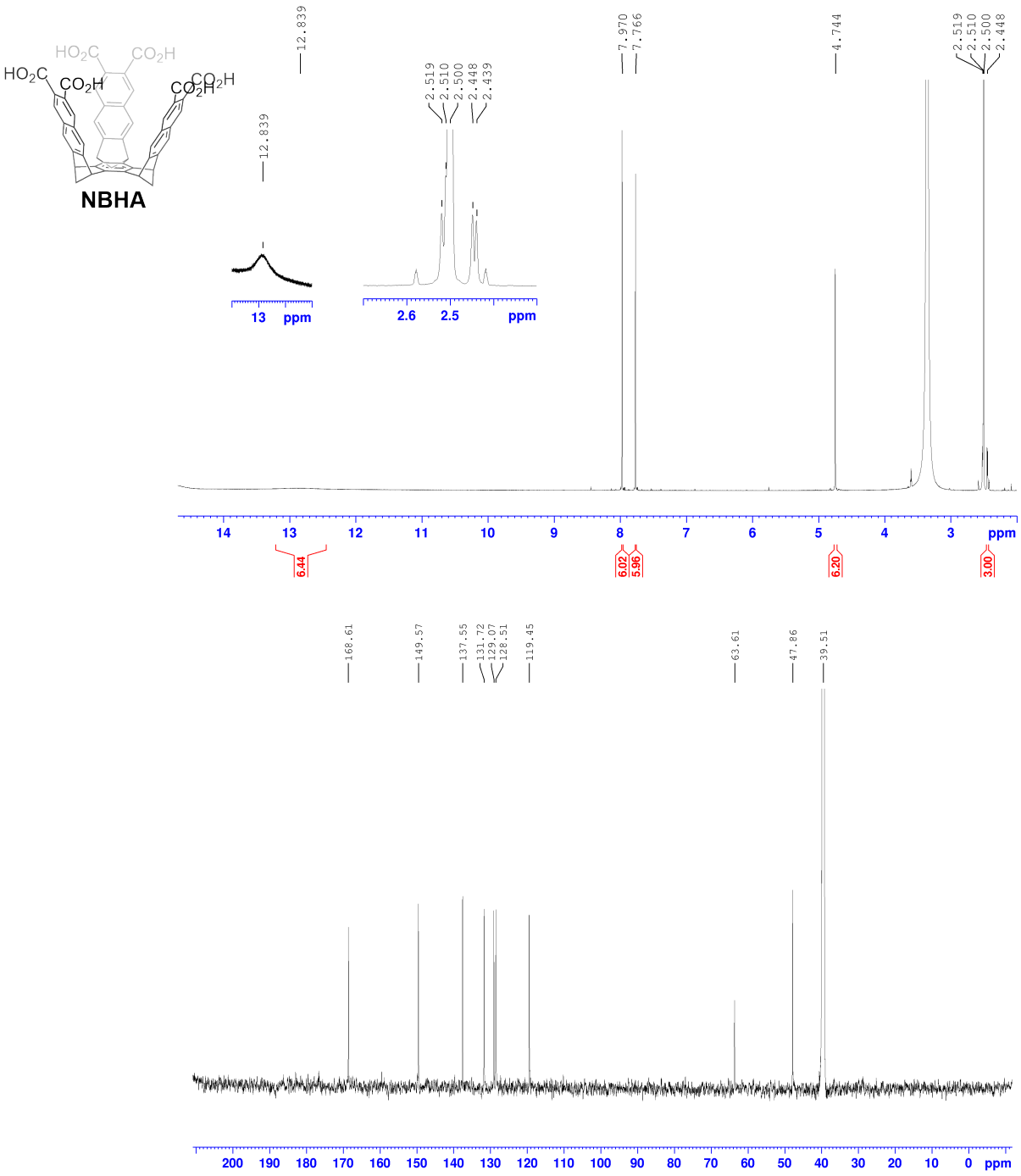


Figure S13. ^{1}H and ^{13}C NMR spectra (DMSO-d_6, 850/213 MHz, 298 K) of **NBHA**.

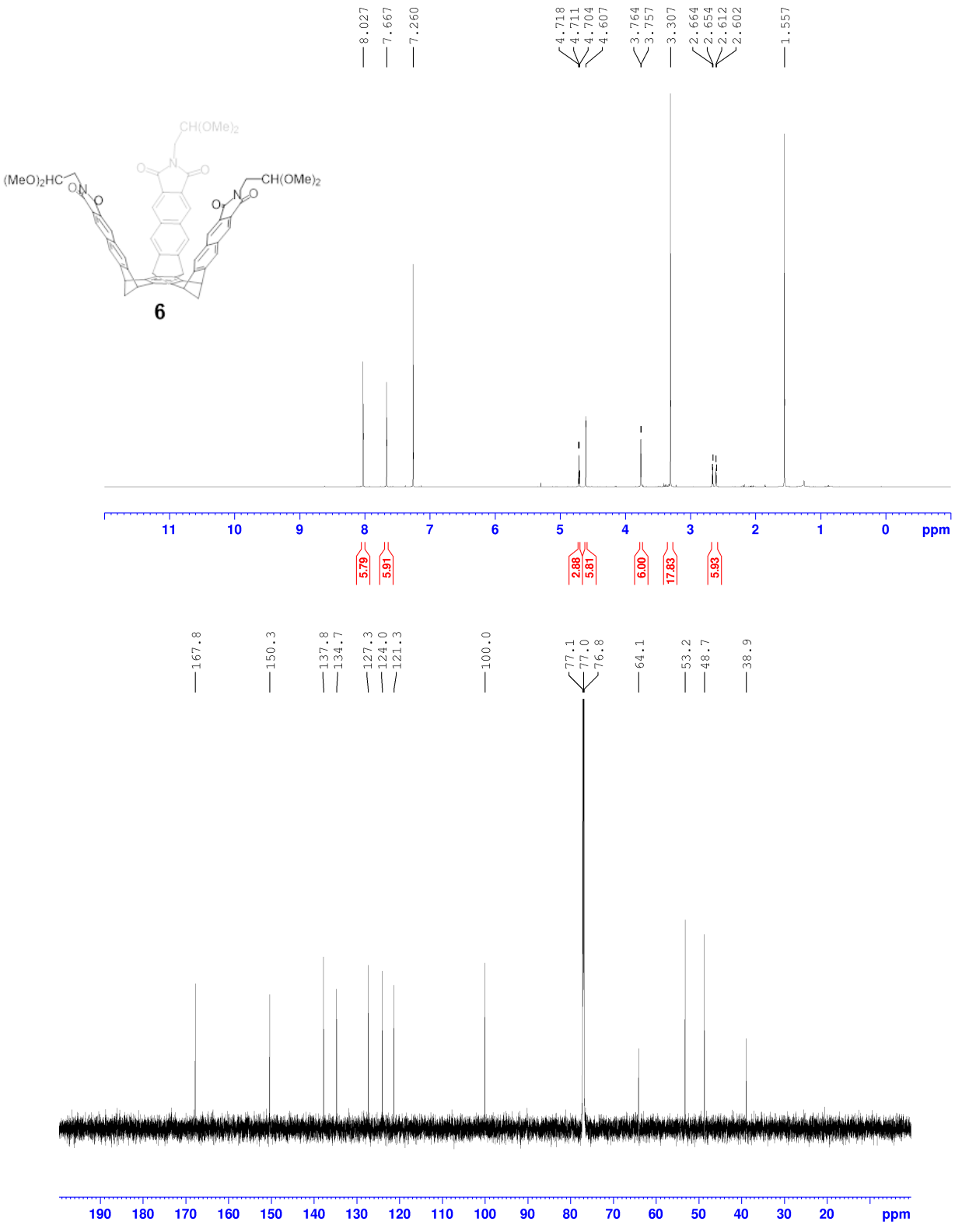


Figure S14. ^{1}H and ^{13}C NMR spectra (850/213 MHz, 298 K) of compound **6** in $CDCl_3$.

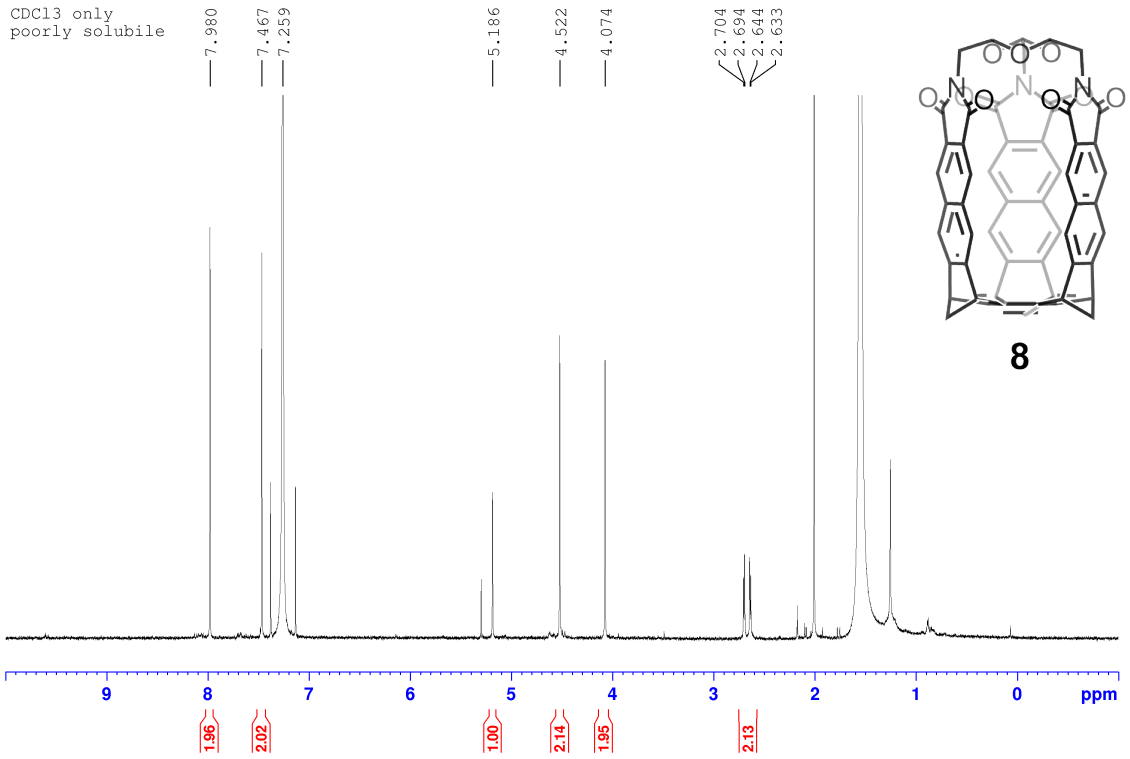


Figure S15. ^{1}H NMR spectrum (850 MHz, 298 K) of capsularene **8** in $CDCl_3$; with **8** being poorly soluble in $CDCl_3$ (and other tested solvents), we had to use TFA to increase its solubility and obtain ^{13}C NMR spectrum (see below).

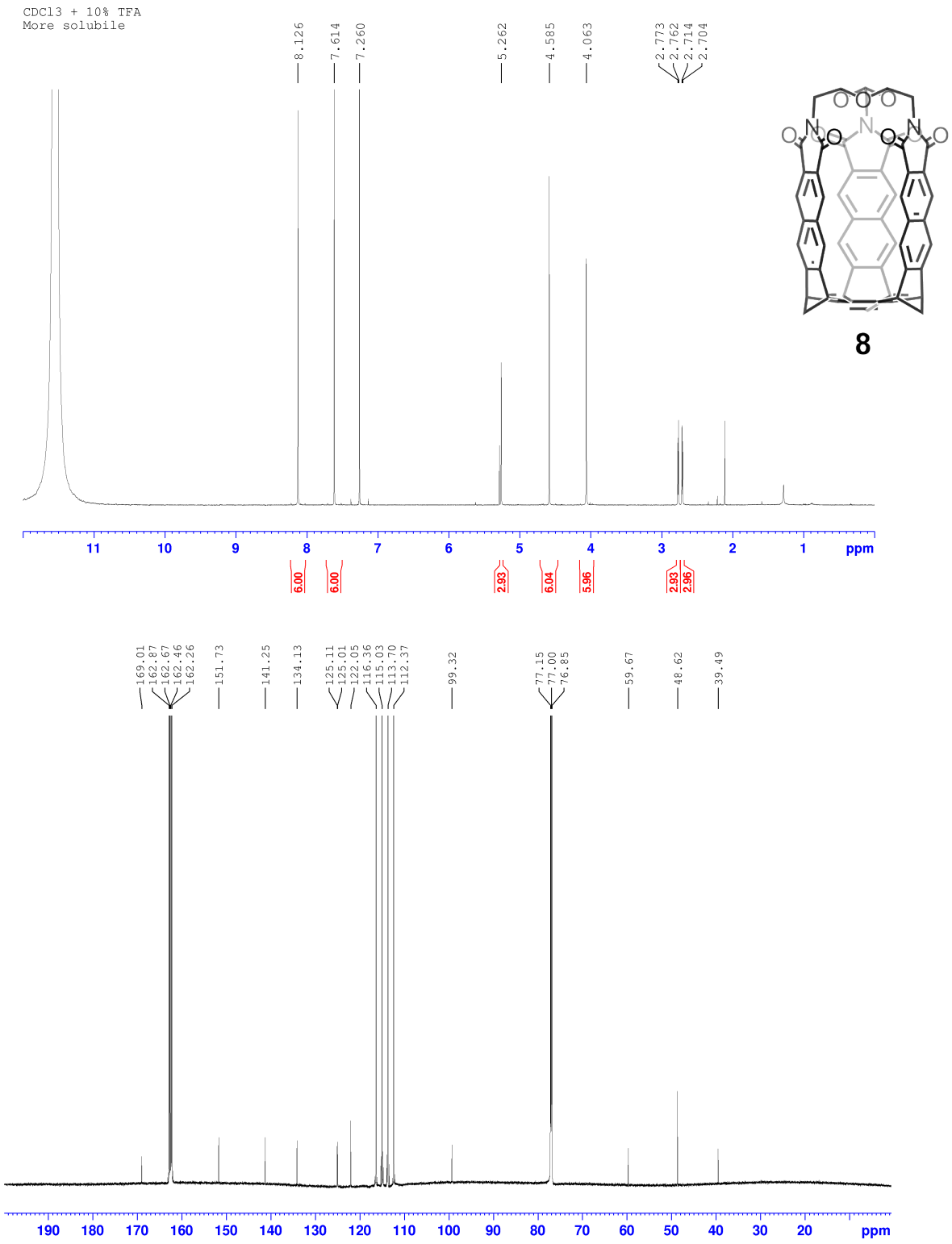


Figure S16. ^{1}H and ^{13}C NMR spectra (850/213 MHz, 298 K) of capsularene **8** in $CDCl_3$: TFA = 9:1.

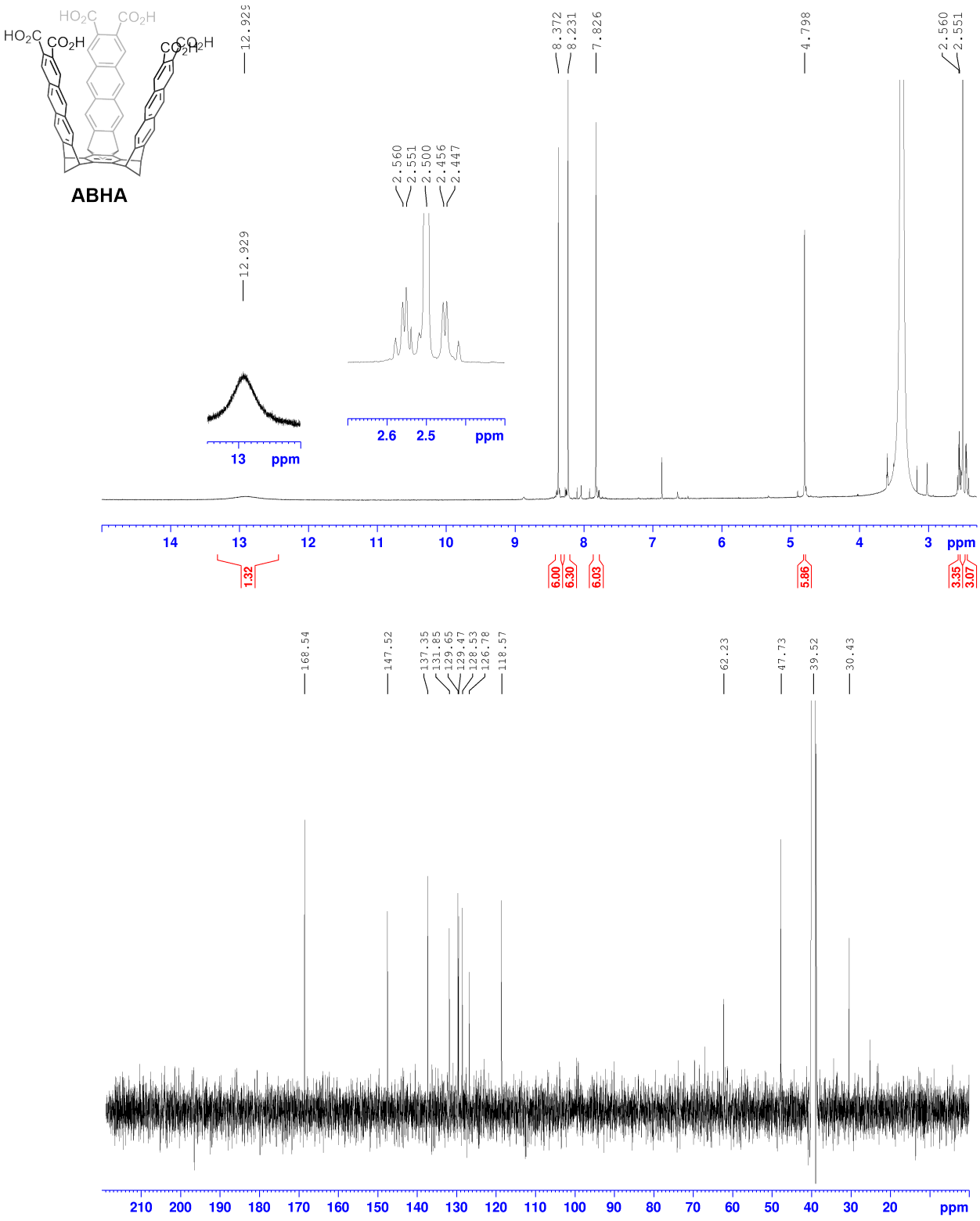


Figure S17. ^{1}H and ^{13}C NMR spectra (850/213 MHz, 298 K) of **ABHA** in DMSO-d_6.

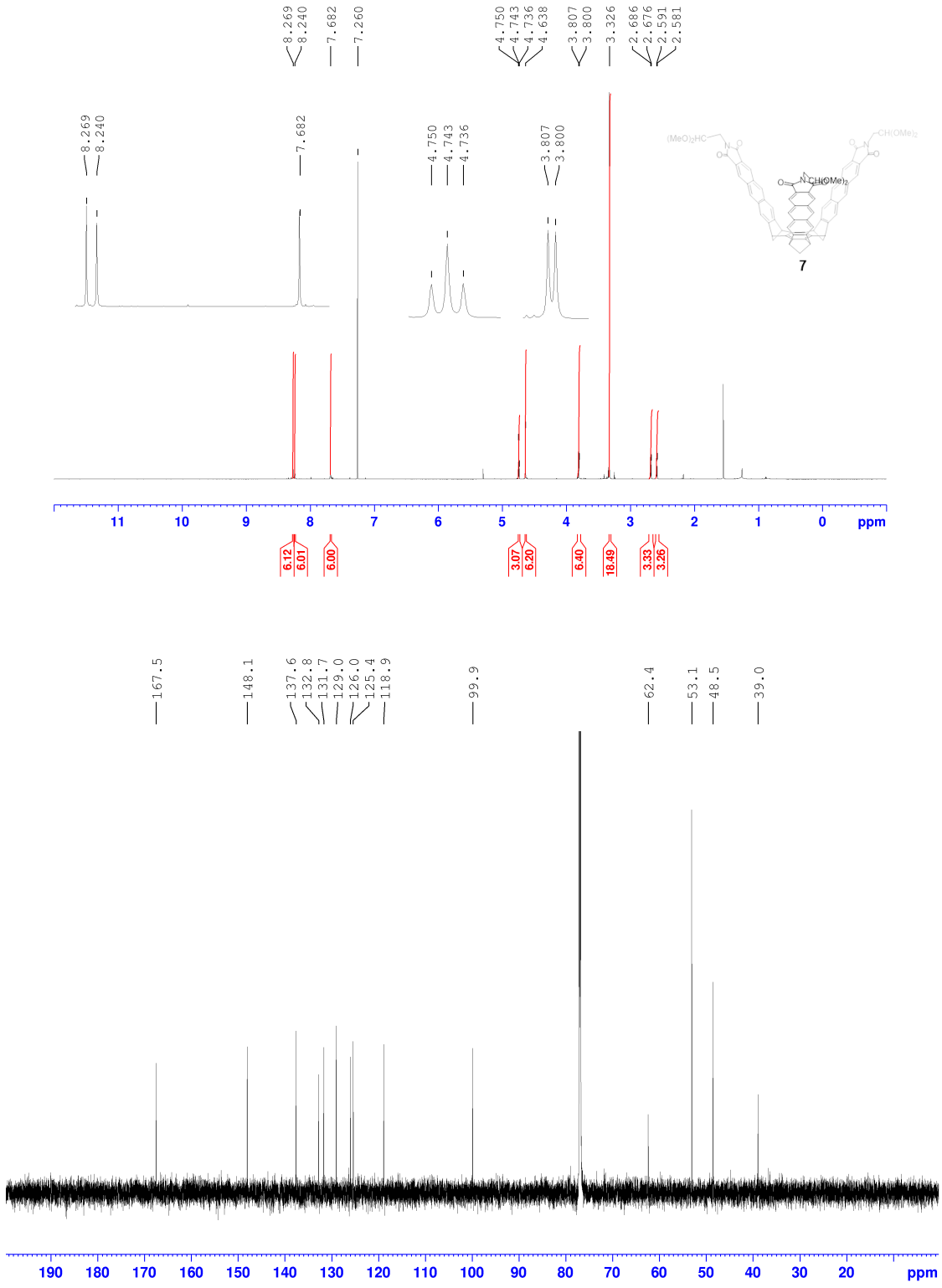


Figure S18. ^{1}H and ^{13}C NMR spectra (850/213 MHz, 298 K) of compound **7** in $CDCl_3$.

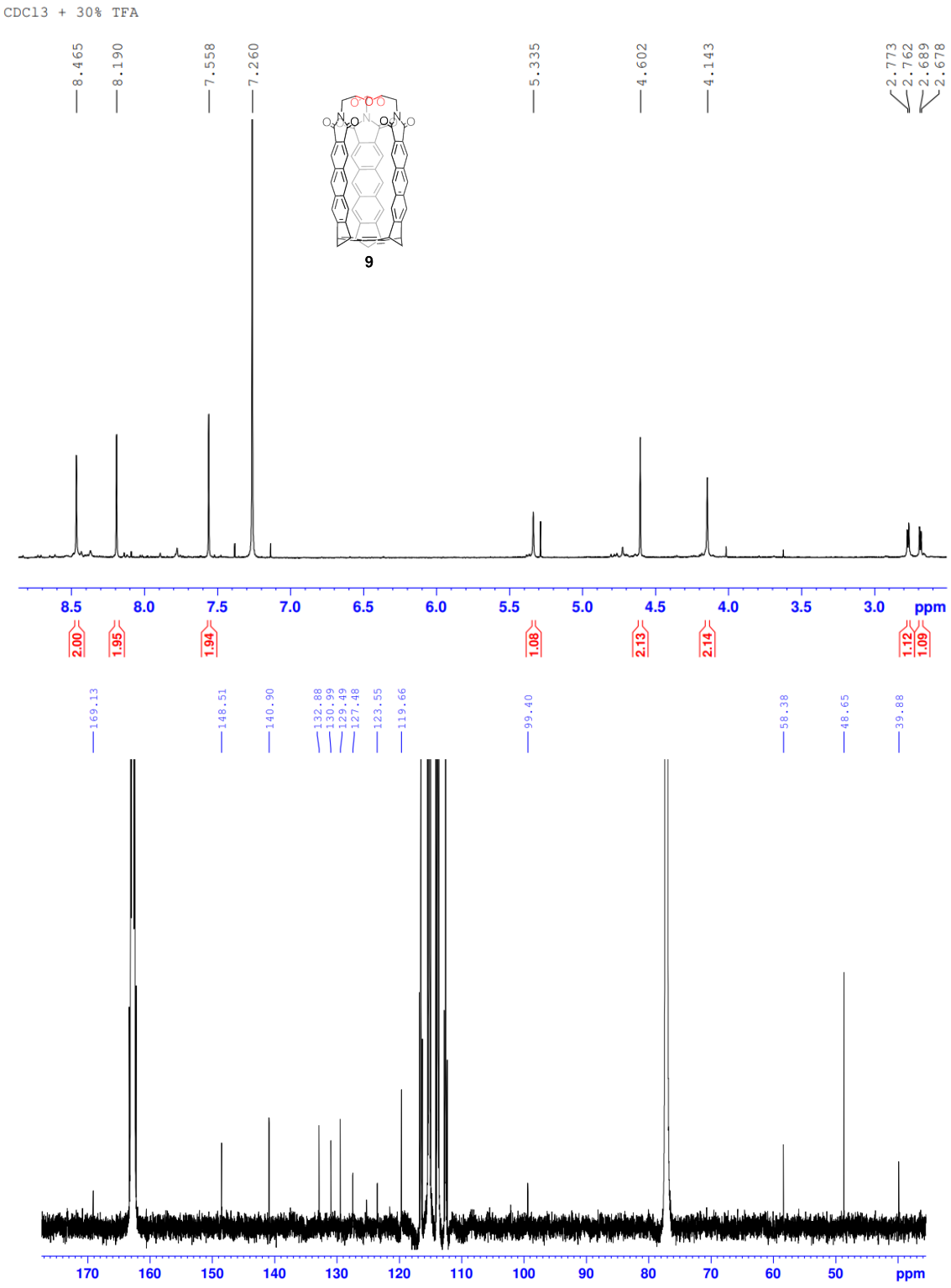
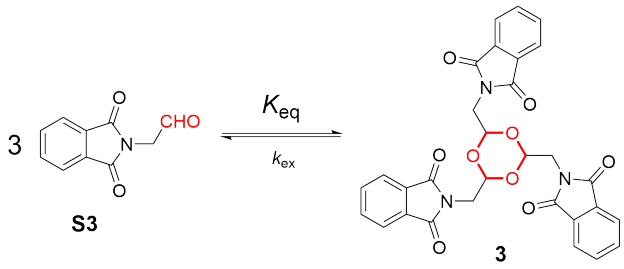


Figure S19. ^{1}H and ^{13}C NMR spectra (850/213 MHz, 298 K) of capsularene **9** in TFA : $CDCl_3$ = 3:7.

Mechanistic Studies

Dynamic exchange of 2-(1,3-dioxoisoindolin-2-yl)acetaldehyde and trioxane 3: The equilibrium between 2-(1,3-dioxoisoindolin-2-yl)acetaldehyde and trioxane **3** (see below; see also Figure 2A in the main text) was inspected using ^{1}H NMR spectroscopy. We have found that the reaction is slow on the chemical shift time scale ($k_{ex}<\Delta\omega$; $\Delta\omega$ = 2860 Hz, Figure S20) below 298 K, but fast enough to allow quantifying the process with ^{1}H/^{1}H EXSY (Figure S21). After obtaining equilibrium constants corresponding to the chemical exchange at different temperatures (Figure S22), we extracted thermodynamic $\Delta H°$ and $\Delta S°$ parameters from the Van't Hoff analysis.



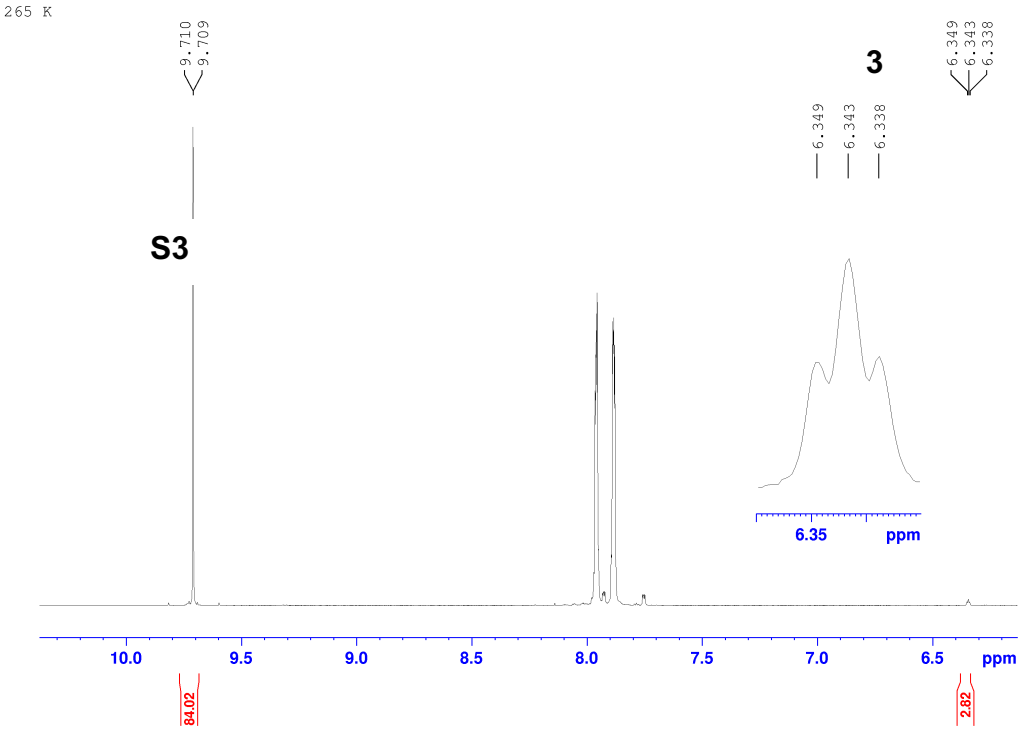


Figure S20. A segment of ^{1}H NMR spectrum (850 MHz, 265 K, C_{tot}=35.2 mM) of diluted 2-(1,3-dioxoisoindolin-2-yl)acetaldehyde in 33%$_{vol}$ TFA in CD_2Cl_2 revealing the formation of trioxane **3** (see a triplet at 6.343 ppm, 1.2%).

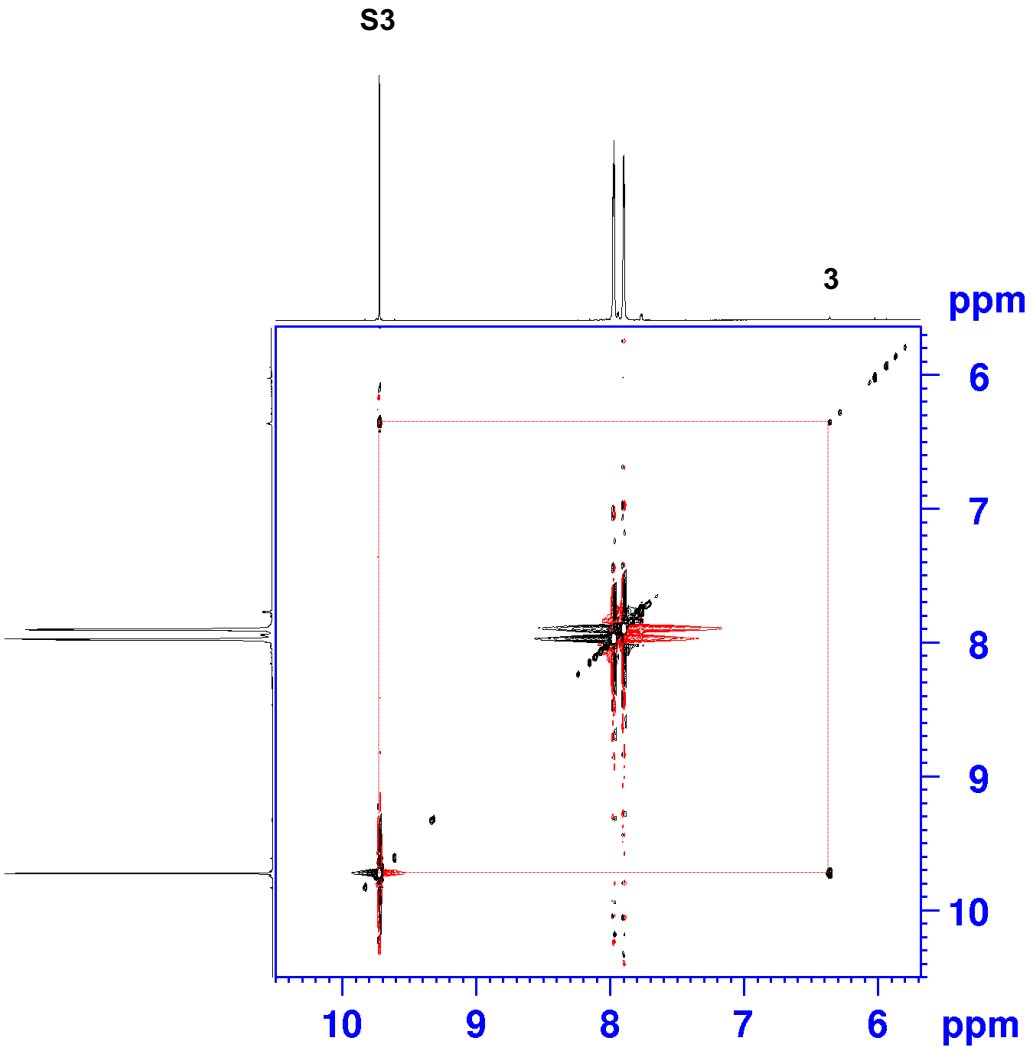


Figure S21. Partial ^{1}H-^{1}H EXSY NMR spectrum (850 MHz, 265 K, 33%$_{vol}$ TFA in CD_2Cl_2, C_{tot}=35.2 mM, t_{mix} = 1 s) showing the exchange signal between 2-(1,3-dioxoisoindolin-2-yl)acetaldehyde and trioxane **3**. The same observation was made after acquiring the EXSY spectrum with t_{mix}=40 ms, which together with $\Delta\omega$ and populations suggests that k_{ex} is between 25 and 1800 s^{-1}.

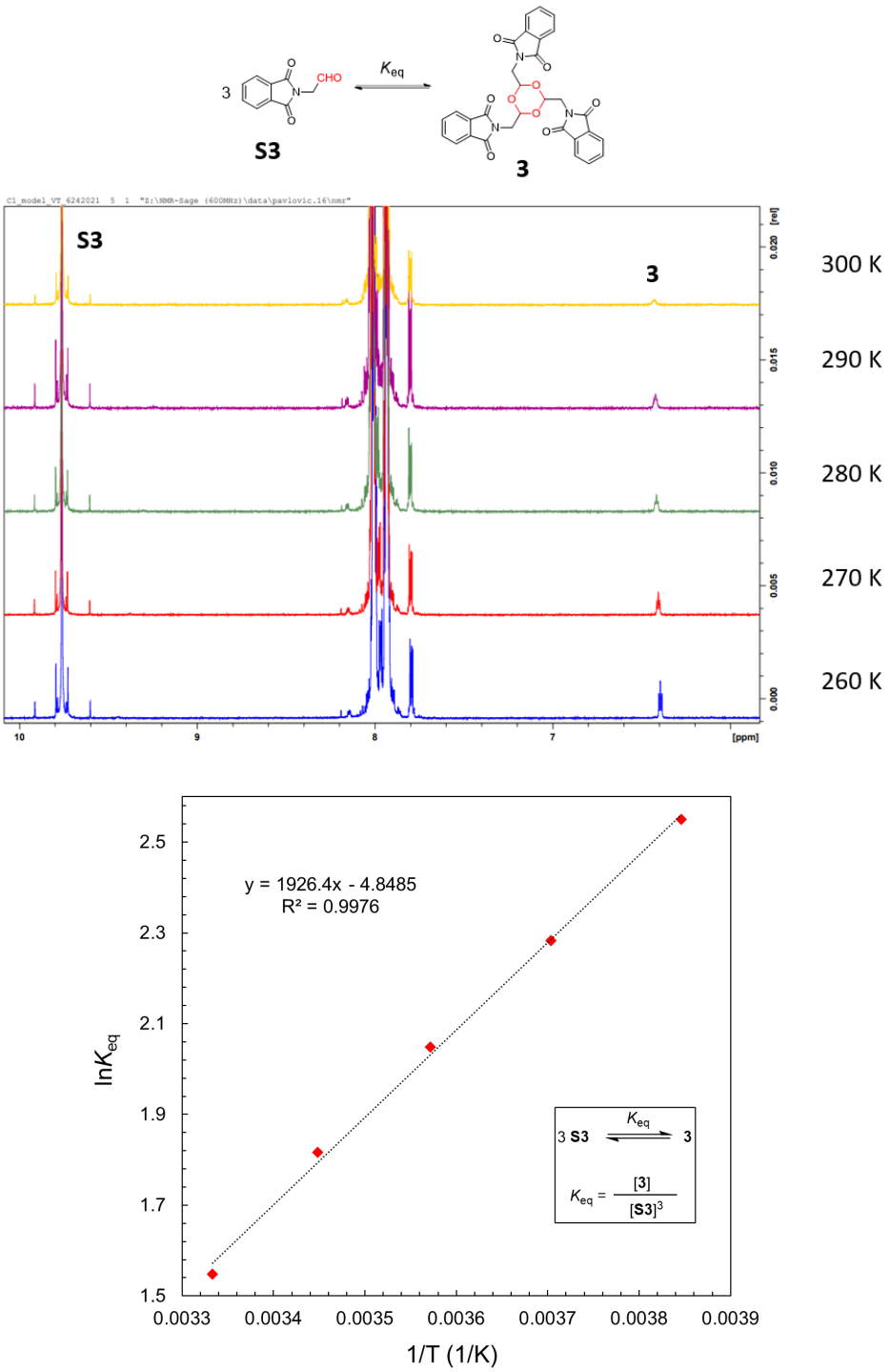
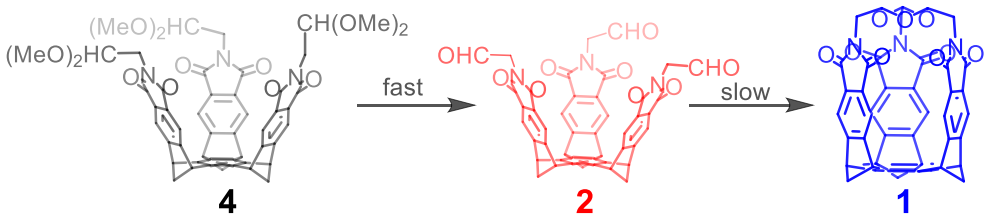


Figure S22. (Top) A segment of variable temperature ^{1}H NMR spectra (600 MHz, 33%$_{vol}$ TFA in CD_2Cl_2) of a solution of 2-(1,3-dioxoisoindolin-2-yl)acetaldehyde (35.2 mM). The integration of the aldehyde resonance from 2-(1,3-dioxoisoindolin-2-yl)acetaldehyde and the triplet resonance (6.343 ppm) from **3** gave the values of K_{eq} at each temperature (shown on the right). (Bottom) A plot showing the experimental dependence of lnK_{eq} and 1/T that was fit to a linear function. From the fitted curve, the slow was 1926.4 and the intercept −4.85 so that using the van't Hoff equation we have ΔH^o = 3.83 kcal/mol and ΔS^o = −9.64 cal/molK.

The Reaction's Rate Law and other Mechanistic Studies Pertaining the Formation Capsularene 1: The formation of capsularene **1** (Scheme S3) was monitored with ^{1}H NMR spectroscopy, in which capsularene **1** and *tris*-aldehyde **2** showed sets of well separated proton resonances (i.e., H_A, H_C and H_E; Figure S23). Under the established experimental conditions (TFA/CD_2Cl_2), compound **4** underwent a rapid cleavage to produce *tris*-aldehyde **2**, which then slowly converted into capsularene **1** (Scheme S3). Accordingly, in the analysis of the kinetic data we considered *tris*-acetal **4** (Scheme S3) as the reactant; note that *tris*-aldehyde **2** was difficult to isolate. The real time NMR data were measured using Bruker 850 MHz (5mm Tripleresonance Inverse (TCI) cryoprobe with Z-Gradients), at T=298 K using 5 mm NMR cuvettes. Upon acquisition, the spectra were processed in Topspin (Furrier transformation; phase correction; baseline correction), and then the peak intensities were determined using Kinetic Analysis feature within Bruker Dynamic Center (Topspin). In particular, the intensities of aromatic H_C protons from **1** and **2** were used for quantification.



Scheme S3. *Tris*-acetal **4** undergoes an acetal cleavage reaction (TFA/CD_2Cl_2) to give **2** which after intramolecular cyclotrimerization turns into capsularene **1**.

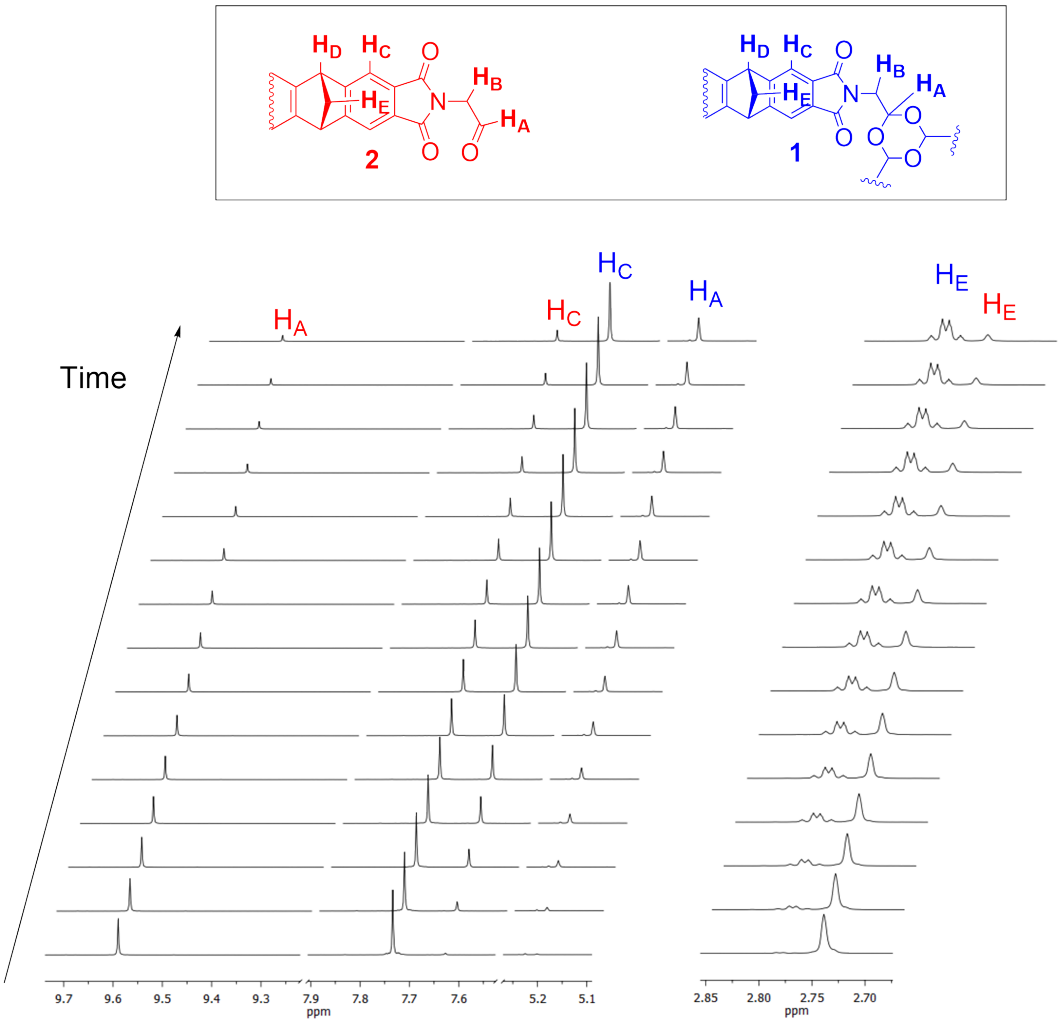


Figure S23. (A) An example of reaction progress kinetic analysis done by ^{1}H NMR spectroscopy (CD_2Cl_2, 850 MHz, T=298 K) using $[\mathbf{3}]_0$ = 2 mM and $[TFA]_0$ = 6.54 M. Three well separated proton resonances (H_A, H_C and H_E) from *tris*-aldehyde **2** and capsularene **1** were used in the analysis.

The order of the reaction in trifluoracetic acid (TFA): To determine the reaction order in TFA, variable time normalization analysis (VTNA) was performed (Figure S24). For this purpose, we monitored the reaction's progress in the samples where *tris*-acetal **4** initial concentration was kept constant ($[\mathbf{4}]_0$ = 0.25 mM), while the total TFA concertation was varied ($[TFA]_0$ = 0.654 - 6.54 M). To prepare the samples, 65 µL of stock solution of [**4**] = 2.50 mM was transferred to a 2 mL drum vial using volumetric syringe; for preparing stock solution of **4**, 2.3 mg of **4** was weighted in a 2 mL drum vial and dissolved in 1025.0 µL of dry CD_2Cl_2 to give 2.52 mM solution. Then, the samples were diluted with the corresponding amount of CD_2Cl_2 followed by addition of the required amount of TFA (Table S1) to obtain V_{tot}=650 µL and match the desired $[TFA]_{tot}$ concentration. The vial was closed and shaken 3 times. This was considered t = 0 s for the kinetic time course. Next, the solution was transferred to the NMR tube via Pasteur pipette, capped, and heavily wrapped with parafilm film to minimize evaporation (TFA is also corrosive and can damage the NMR probe!). The NMR tube was then inserted in Bruker 850 and series of ^{1}H NMR spectra over time

were recorded at T=298 K. The data were processed according to explanation given at the beginning of the section.

Table S1. Reaction mixtures used for determining the reaction's order in TFA.

$[TFA]_0$, M	$[\mathbf{4}]_0$, mM	V(2.55 mM **4**), µL	V(CD_2Cl_2), µL	V(TFA), µL
6.54	0.252	65.0	260.0	325.0
3.92	0.252	65.0	390.0	195.0
0.98	0.252	65.0	536.0	49.0

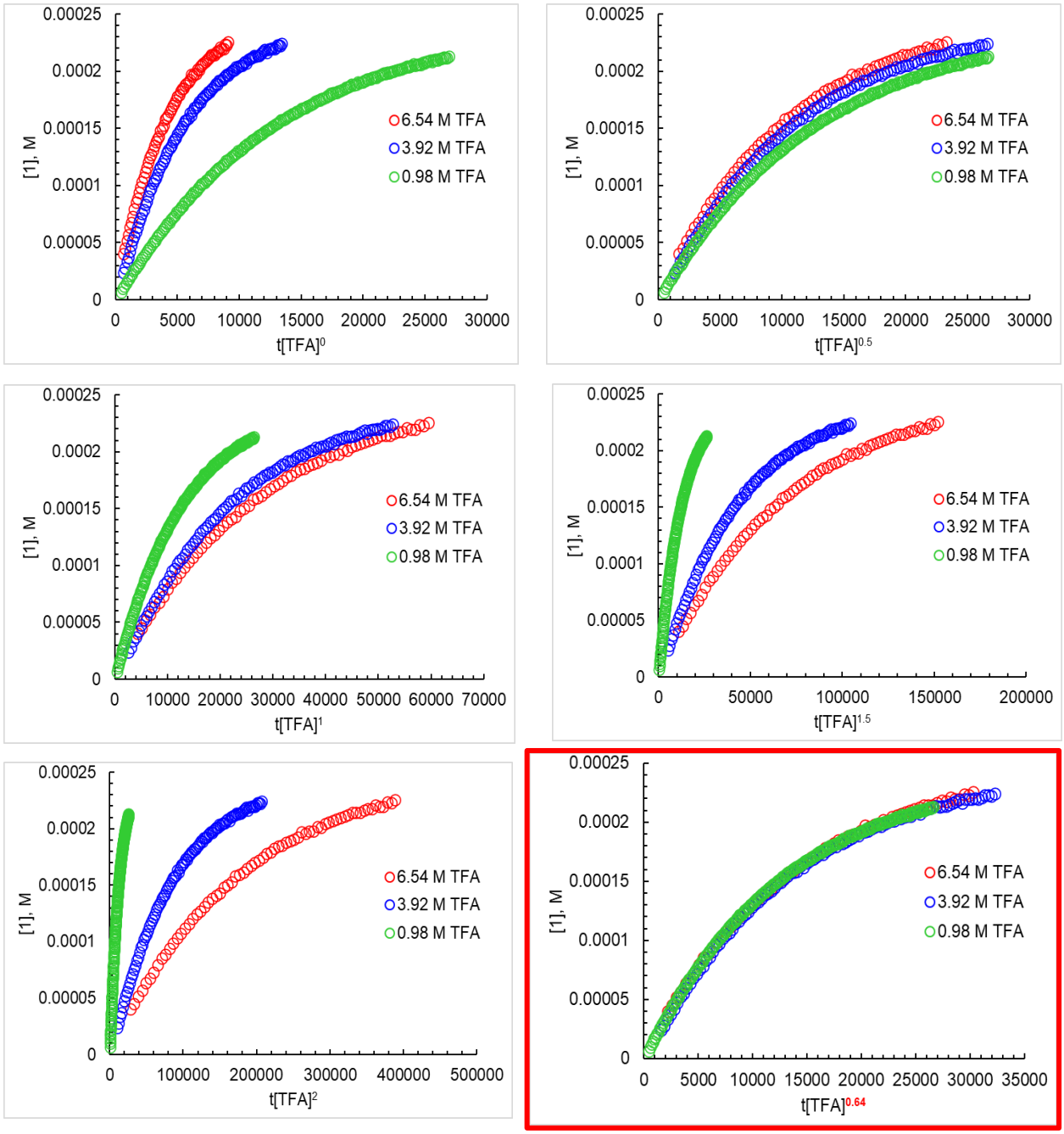


Figure S24. Change in the concentration of capsularene **1** as a function of time multiplied by modified concentration of TFA ($[TFA]^n$) allowed us to determine the reaction's order in TFA. The plot circled by a red square shows that the three curves overlap when n = 0.64. The time/concentration data (obtained from real time ^{1}H NMR measurements) used for this analysis are given in Tables S2-S4.

Table S2. Concentration of capsularene **1** as a function of time (from real time ^{1}H NMR measurement, Figure S25) in the experiment where [**4**]$_0$=0.25 mM, [**TFA**]$_0$=6.54 M.

t,s	[1], M
660	4.01E-05
784	4.5E-05
908	5.17E-05
1032	5.68E-05
1157	6.34E-05
1281	6.74E-05
1405	7.3E-05
1529	7.95E-05
1653	8.52E-05
1777	8.86E-05
1901	9.43E-05
2025	9.88E-05
2150	0.000103
2274	0.000107
2398	0.000112
2522	0.000116
2646	0.00012
2770	0.000124
2894	0.000127
3019	0.000131
3143	0.000135
3267	0.000139
3391	0.000141
3515	0.000143
3639	0.000148
3763	0.00015
3887	0.000153
4011	0.000158
4136	0.000159
4260	0.000161
4384	0.000165
4508	0.000167
4632	0.00017
4756	0.000172
4880	0.000174
5004	0.000178
5128	0.00018
5252	0.000182
5376	0.000185
5501	0.000185
5625	0.000188
5749	0.000189
5873	0.00019
5997	0.000192
6121	0.000197
6245	0.000196
6369	0.000198
6494	0.000198
6618	0.000202
6742	0.000201
6866	0.000205
6990	0.000206
7114	0.000207
7238	0.000208
7362	0.00021
7486	0.000211
7610	0.000213
7734	0.000214
7859	0.000215
7983	0.000214
8107	0.000216
8231	0.000218
8355	0.000218
8479	0.000221
8603	0.00022
8727	0.00022
8852	0.000224
8976	0.000223
9100	0.000226
9224	0.000225
9348	0.000224
9472	0.000227
9596	0.000227
9721	0.000227
9845	0.000228
9969	0.00023
10093	0.00023
10217	0.000231
10341	0.000232
10465	0.000232
10590	0.000232
10714	0.000233
10838	0.000233
10962	0.000234
11086	0.000232
11210	0.000234
11334	0.000234
11458	0.000235
11582	0.000236
11707	0.000237
11831	0.000236
11955	0.000235
12079	0.000239
12203	0.000238
12327	0.000238
12451	0.000239
12575	0.00024
12699	0.000238
12824	0.00024
12948	0.00024
13072	0.000239
13196	0.000242
13320	0.00024
13444	0.00024
13568	0.000241
13693	0.000242
13817	0.000242
13941	0.000242
14065	0.000242
14189	0.000242
14313	0.000244
14438	0.000244
14562	0.000243
14686	0.000245
14810	0.000243
14934	0.000243
15058	0.000245
15182	0.000244
15307	0.000245
15431	0.000241
15555	0.000244
15679	0.000245
15803	0.000243
15928	0.000246
16052	0.000246
16176	0.000246
16300	0.000246
16424	0.000245
16548	0.000245
16672	0.000247
16796	0.000246
16920	0.000246
17044	0.000245
17169	0.000245
17293	0.000246
17417	0.000247
17541	0.000246
17665	0.000248
17789	0.000247
17913	0.000248
18037	0.000247
18161	0.000246
18286	0.000249
18410	0.000248
18534	0.000246
18658	0.000248
18782	0.000247
18906	0.000246

Table S3. Concentration of capsularene **1** as a function of time (from real time ^{1}H NMR measurement, Figure S25) in the experiment where [**4**]$_0$=0.25 mM, [**TFA**]$_0$=3.92 M.

time [s]:	[1], M
660	2.42E-05
784	2.77E-05
908	3.37E-05
1032	3.74E-05
1157	4.23E-05
1281	4.74E-05
1405	5.26E-05
1529	5.54E-05
1653	5.95E-05
1777	6.36E-05
1902	6.8E-05
2026	7.14E-05
2150	7.55E-05
2274	7.84E-05
2398	8.35E-05
2522	8.62E-05
2646	9.09E-05
2770	9.52E-05
2895	9.74E-05
3019	0.000102
3143	0.000104
3267	0.000106
3391	0.00011
3515	0.000114
3639	0.000116
3764	0.000119
3888	0.000122
4012	0.000124
4136	0.000128
4260	0.000131
4384	0.000133
4508	0.000135
4633	0.000138
4757	0.00014
4881	0.000142
5005	0.000145
5129	0.000148
5253	0.00015
5377	0.000152
5502	0.000154
5626	0.000157
5750	0.000158
5874	0.000159
5998	0.000163
6122	0.000162
6247	0.000166
6371	0.000168
6495	0.000169
6619	0.000171
6743	0.000173
6867	0.000173
6992	0.000176
7116	0.000178
7240	0.000179
7364	0.00018
7488	0.000182
7612	0.000182
7736	0.000184
7861	0.000185
7985	0.000187
8109	0.000189
8233	0.000189
8357	0.000192
8482	0.000192
8606	0.000193
8730	0.000195
8854	0.000196
8978	0.000197
9102	0.000197
9226	0.000198
9350	0.0002
9475	0.000201
9599	0.000201
9723	0.000203
9847	0.000203
9971	0.000205
10095	0.000205
10219	0.000205
10343	0.000207
10468	0.000208
10592	0.000207
10716	0.00021
10840	0.000211
10964	0.000212
11088	0.000213
11212	0.000214
11336	0.000213
11460	0.000214
11584	0.000214
11708	0.000215
11833	0.000216
11957	0.000217
12081	0.000219
12205	0.000216
12329	0.000219
12453	0.00022
12577	0.00022
12701	0.00022
12826	0.00022
12950	0.000221
13074	0.000223
13198	0.000223
13322	0.000222
13446	0.000224
13570	0.000224
13695	0.000224
13819	0.000225
13943	0.000225
14067	0.000228
14191	0.000226
14315	0.000227
14439	0.000227
14563	0.000228
14687	0.000228
14812	0.000229
14936	0.000228
15060	0.000228
15185	0.000229
15309	0.00023
15433	0.00023
15557	0.000231
15681	0.000232
15805	0.000234
15929	0.00023
16053	0.000231
16177	0.000232
16301	0.000233
16425	0.000232
16550	0.000233
16674	0.000235
16798	0.000233
16922	0.000231
17046	0.000231
17170	0.000235
17294	0.000234
17418	0.000235
17542	0.000235
17667	0.000235
17791	0.000235
17915	0.000236
18039	0.000238
18163	0.000236
18287	0.000237
18411	0.000238
18535	0.000238
18660	0.000237
18784	0.000238
18908	0.000236
19032	0.000238
19156	0.000237
19280	0.000239
19404	0.000238
19528	0.000241

19652	0.000239
19777	0.00024
19901	0.000239
20025	0.000239
20149	0.000239
20273	0.000238
20397	0.000238
20521	0.000238
20645	0.000239
20769	0.000241
20894	0.00024
21018	0.000239
21142	0.000238
21266	0.00024
21390	0.00024
21515	0.00024
21639	0.000239
21763	0.00024

21887	0.000242
22011	0.000243
22135	0.000241
22259	0.000242
22383	0.000242
22508	0.000242
22632	0.00024
22756	0.000242
22880	0.000241
23004	0.000242
23128	0.000241
23252	0.000241
23376	0.000243
23501	0.000244
23625	0.000243
23749	0.000243
23873	0.000244
23997	0.000242

24121	0.000242
24245	0.000241
24369	0.000242
24493	0.000242
24618	0.000244
24742	0.000243
24866	0.000244
24990	0.000243
25114	0.000242
25238	0.000243
25362	0.000243
25486	0.000244
25610	0.000245
25734	0.000245
25858	0.000243
25983	0.000243
26107	0.000243
26231	0.000243

26355	0.000244
26479	0.000244
26603	0.000244
26727	0.000243
26851	0.000245
26976	0.000246
27100	0.000244
27224	0.000243
27348	0.000244
27472	0.000244
27596	0.000244
27720	0.000244
27844	0.000245
27969	0.000247
28093	0.000244
28217	0.000245
28341	0.000244
28465	0.000244

28589	0.000247
28713	0.000246
28837	0.000245
28962	0.000243
29086	0.000245
29210	0.000244
29334	0.000243
29458	0.000244
29582	0.000245
29707	0.000246
29831	0.000246
29955	0.000244
30079	0.000243
30203	0.000244
30327	0.000245

Table S4. Concentration of capsularene **1** as a function of time (real time ^{1}H NMR measurement, Figure S25) in the experiment where $[\mathbf{4}]_0$=0.25 mM, $[\mathbf{TFA}]_0$=0.98 M.

time [s]:	[1], M
480	6.67E-06
604	9.73E-06
728	1.21E-05
852	1.43E-05
976	1.71E-05
1100	1.83E-05
1224	2.09E-05
1348	2.24E-05
1472	2.57E-05
1596	2.7E-05
1720	2.92E-05
1844	3.08E-05
1968	3.26E-05
2092	3.49E-05
2216	3.72E-05
2340	3.92E-05
2464	4.07E-05
2589	4.29E-05
2713	4.52E-05
2837	4.66E-05
2961	4.88E-05
3085	5.09E-05
3209	5.19E-05
3334	5.45E-05
3458	5.63E-05
3582	5.78E-05
3706	5.99E-05
3830	6.16E-05
3954	6.27E-05
4078	6.49E-05
4203	6.71E-05
4327	6.77E-05
4451	6.99E-05
4575	7.13E-05
4699	7.29E-05
4823	7.44E-05
4947	7.64E-05
5072	7.83E-05
5195	7.92E-05
5320	8.13E-05
5444	8.2E-05
5568	8.44E-05
5692	8.6E-05
5816	8.75E-05
5940	8.9E-05
6064	9.04E-05
6189	9.17E-05
6313	9.39E-05
6437	9.49E-05
6561	9.59E-05
6685	9.77E-05
6809	9.91E-05
6933	0.000101
7057	0.000102
7182	0.000103
7306	0.000104
7430	0.000105
7554	0.000107
7678	0.000108
7802	0.000109
7926	0.000111
8050	0.000113
8174	0.000114
8298	0.000115
8422	0.000116
8547	0.000117
8671	0.000118
8795	0.000119
8919	0.000121
9043	0.000122
9167	0.000123
9291	0.000124
9415	0.000126
9539	0.000126
9663	0.000128
9788	0.000128
9912	0.00013
10036	0.000131
10160	0.000132
10284	0.000133
10408	0.000134
10532	0.000135
10656	0.000136
10780	0.000137
10904	0.000138
11029	0.000139
11153	0.00014
11277	0.000141
11401	0.000142
11525	0.000143
11649	0.000144
11773	0.000145
11897	0.000146
12021	0.000147
12145	0.000148
12270	0.000149
12394	0.00015
12518	0.00015
12642	0.000151
12766	0.000152
12890	0.000153
13015	0.000154
13139	0.000155
13263	0.000156
13387	0.000157
13511	0.000158
13636	0.000158
13760	0.000159
13884	0.00016
14008	0.000161
14132	0.000162
14256	0.000162
14380	0.000163
14504	0.000164
14629	0.000164
14753	0.000165
14877	0.000166
15001	0.000167
15125	0.000168
15249	0.000168
15373	0.000168
15498	0.000169
15622	0.00017
15746	0.000171
15870	0.000172
15994	0.000172
16118	0.000174
16243	0.000174
16367	0.000175
16491	0.000174
16615	0.000176
16739	0.000176
16863	0.000177
16988	0.000178
17112	0.000179
17236	0.000179
17360	0.00018
17482	0.00018
17605	0.000181
17730	0.000181
17854	0.000182
17978	0.000182
18102	0.000182
18226	0.000184
18350	0.000184
18475	0.000184
18599	0.000186
18723	0.000186
18847	0.000186
18971	0.000188
19095	0.000188
19219	0.000188
19344	0.000188

19468	0.000188	**21082**	0.000195	**22696**	0.000201	**24309**	0.000206	**25923**	0.00021
19592	0.00019	**21206**	0.000196	**22820**	0.000201	**24433**	0.000206	**26047**	0.00021
19716	0.00019	**21330**	0.000197	**22944**	0.000202	**24557**	0.000207	**26171**	0.000211
19840	0.00019	**21454**	0.000197	**23068**	0.000202	**24682**	0.000206	**26295**	0.000211
19965	0.00019	**21578**	0.000198	**23192**	0.000203	**24806**	0.000207	**26419**	0.000212
20089	0.000192	**21702**	0.000198	**23316**	0.000203	**24930**	0.000207	**26543**	0.000212
20213	0.000192	**21826**	0.000198	**23440**	0.000204	**25054**	0.000208	**26668**	0.000212
20337	0.000193	**21951**	0.000199	**23565**	0.000205	**25178**	0.000208	**26792**	0.000212
20461	0.000193	**22075**	0.000199	**23689**	0.000204	**25302**	0.000209	**26914**	0.000213
20585	0.000193	**22199**	0.000199	**23813**	0.000204	**25426**	0.00021		
20709	0.000195	**22323**	0.0002	**23937**	0.000205	**25550**	0.000209		
20834	0.000195	**22447**	0.0002	**24061**	0.000206	**25674**	0.00021		
20958	0.000195	**22571**	0.000201	**24185**	0.000205	**25799**	0.00021		

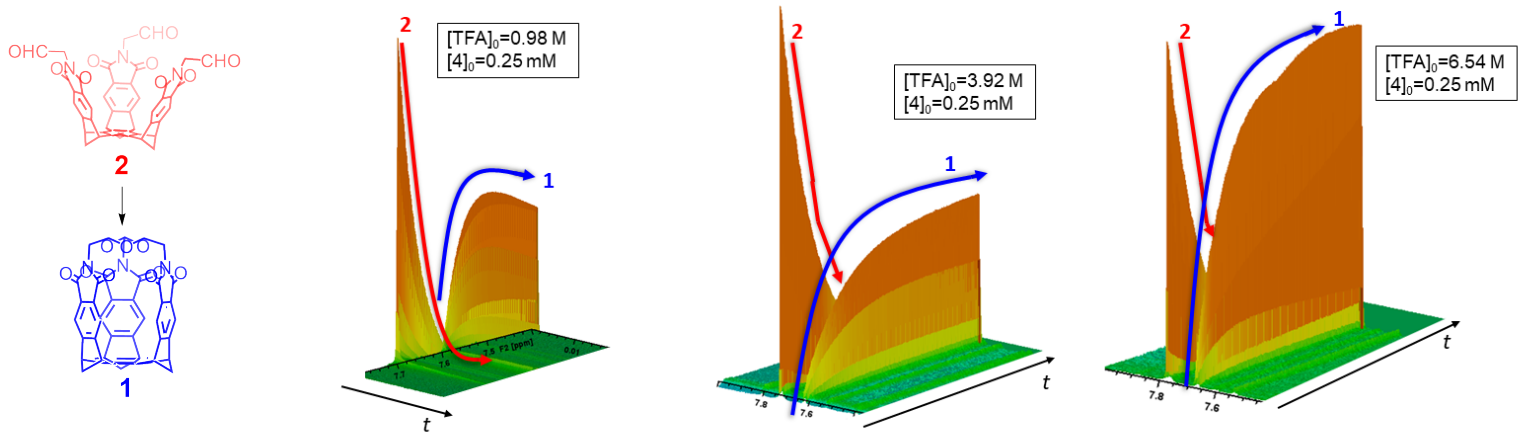


Figure S25. Using the intensity of aromatic $\mathbf{H}_C$ resonances in **2** and **1** (left), we monitored a change in the concentration of these two compounds (right) over time for three different reaction conditions (real time ^{1}H NMR spectroscopy).

The order of the reaction in *tris*-aldehyde 2: To determine the reaction order in *tris*-aldehyde **2**, we completed VTNA analysis (Figure S26). For this purpose, we monitored the reaction's progress by varying the initial concentration of *tris*-acetal **4** (i.e. *tris*-aldehyde **2**) while keeping the total TFA concentration constant (all the reactions are performed in dry CD_2Cl_2 if not stated otherwise). To prepare reaction mixtures, the appropriate amount of the corresponding stock solution of **4** (see below) was transferred to a 2 mL drum vial with a volumetric syringe (Table S5). Then, the samples were diluted with the corresponding amount of CD_2Cl_2 followed by the addition of TFA (Table S5) to obtain V_{tot}=650 µL. The vial was closed and shaken 3 times. This was considered t = 0 s for the course of the reaction. Next, the solution was transferred to an NMR tube via Pasteur pipette, capped, and heavily wrapped with parafilm to minimize evaporation (TFA is corrosive and can damage the probe!). The NMR tube was then inserted in Bruker 850 and series of ^{1}H NMR spectra were recorded at T=298 K. The data were processed according to explanation given at the beginning of the section.

*Stock solutions tris-acetal **4***: 2.3 mg of **4** was weighted out in a 2 mL drum vial and dissolved in 1025.0 µL of dry CD_2Cl_2 to give 2.52 mM stock solution; 6.0 mg of **4** was weighted out in a 2 mL drum vial and dissolved in 341.7 µL of dry CD_2Cl_2 to give 19.69 mM stock solution.

Table S5. Reaction mixtures used for determining order of the reaction in *tris*-aldehyde **2**.

$[TFA]_0$, M	$[\mathbf{4}]_0$, mM	V(2.55 mM **4**), µL	V(CD_2Cl_2), µL	V(TFA), µL
6.54	0.20	51.0	274.0	325
6.54	0.30	76.5	248.5	325
6.54	0.50	127.5	197.5	325
$[TFA]_0$, M	$[\mathbf{4}]_0$, mM	V(19.69 mM **4**), µL	V(CD_2Cl_2), µL	V(TFA), µL
6.54	0.99	32.7	292.3	325
6.54	1.92	63.4	261.7	325
6.54	3.83	126.4	198.6	325

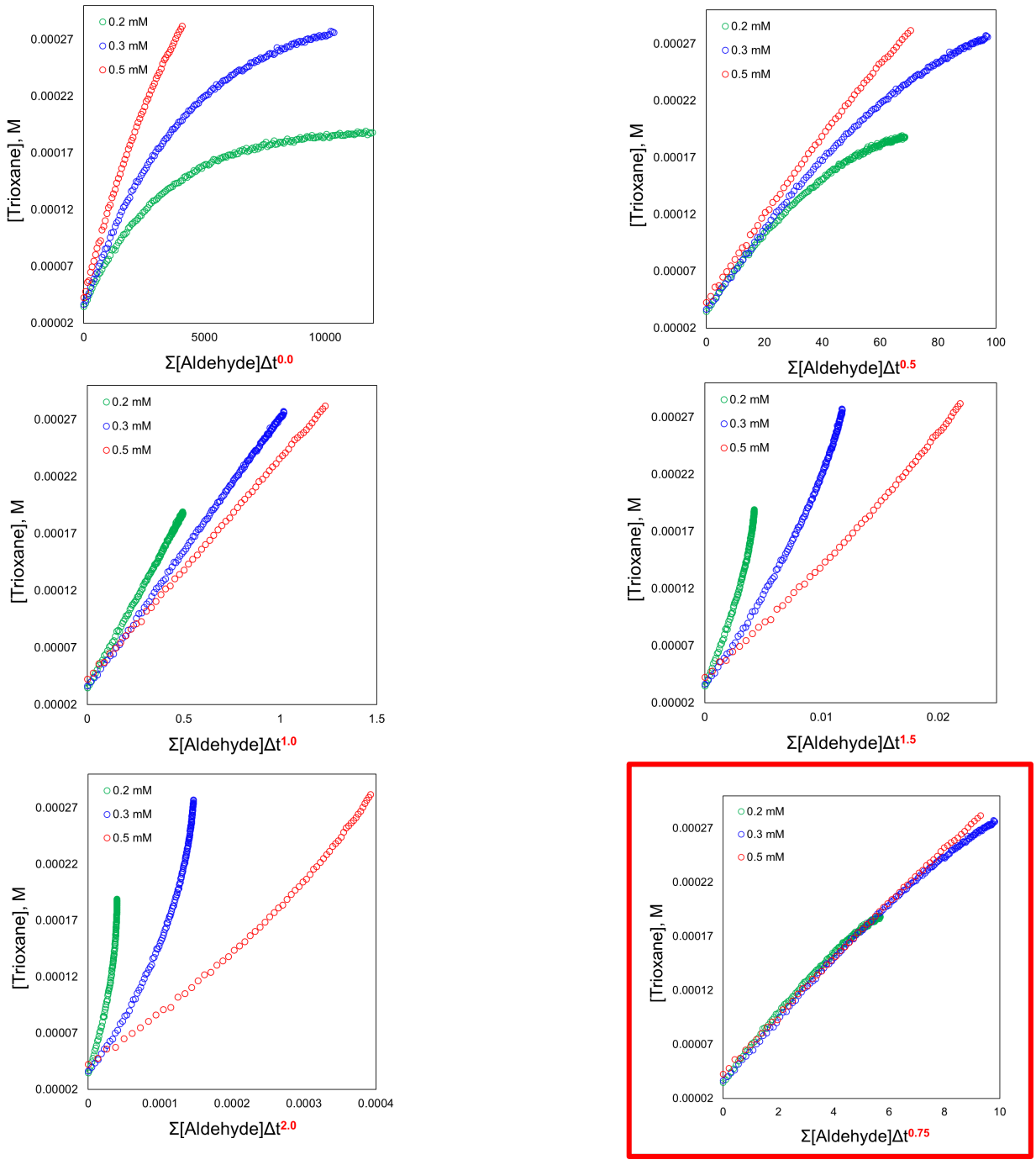


Figure S26. Change in the concentration of capsularene **1** as a function of time (Δt^n) multiplied by modified concentration of *tris*-aldehyde **2** (Σ[**2**]) allowed us to determine the reaction's order in **2**. The plot circled by a red square shows that the three curves overlap when n = 0.75. The time/concentration data (obtained from real time ^{1}H NMR measurements) used for this analysis are given in Tables S6-S8.

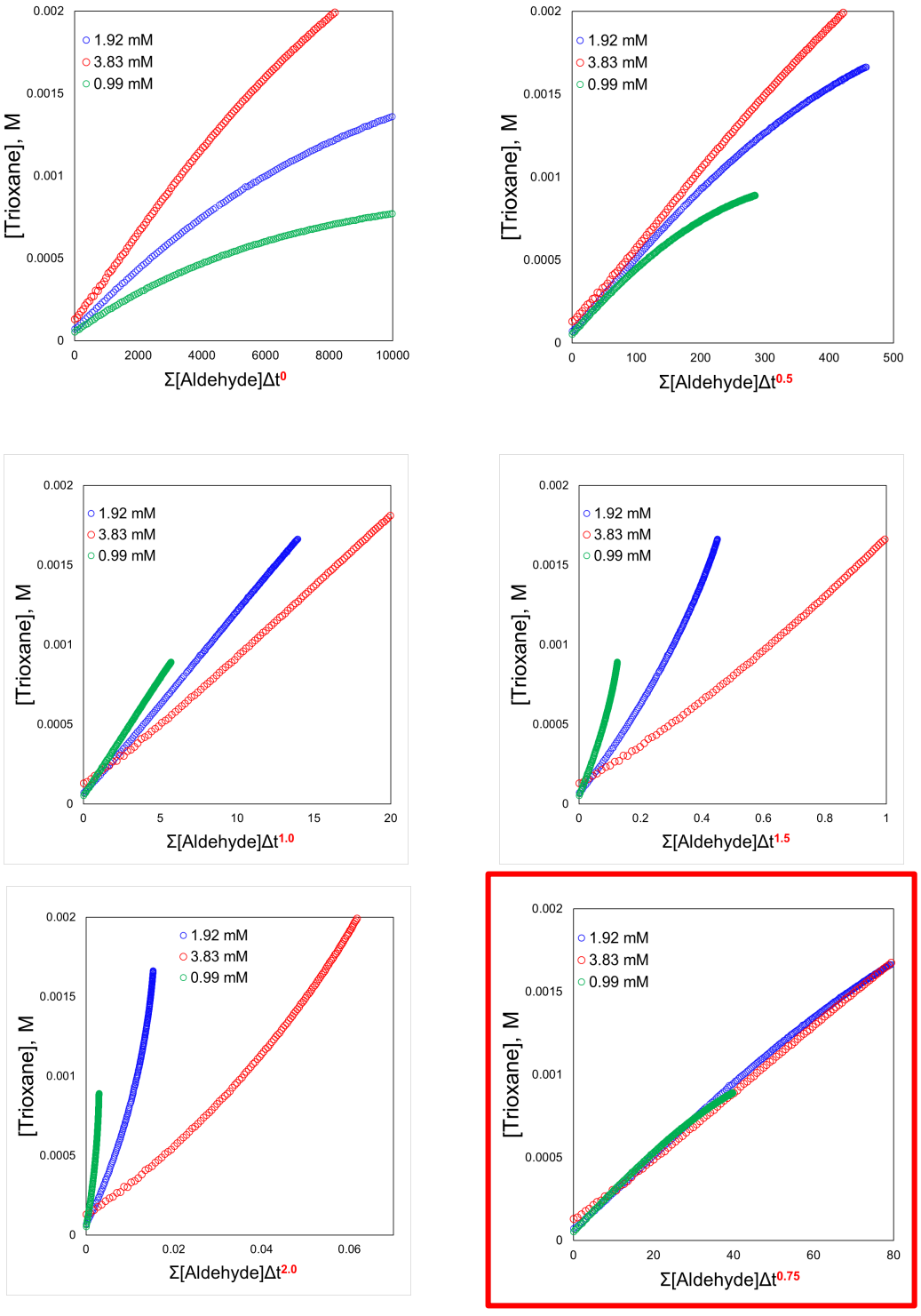


Figure S27. Change in the concentration of capsularene **1** as a function of time (Δt^n) multiplied by modified concentration of *tris*-aldehyde **2** (Σ[**2**]) allowed us to determine the reaction's order in **2**. The plot circled by a red square shows that the three curves overlap when n = 0.75. The time/concentration data (obtained from real time ^{1}H NMR measurements) used for this analysis are given in Tables S9-S11.

Table S6. Concentration of **1** and **2** as a function of time (real time ^{1}H NMR measurement, Figure S28) in the experiment where [**4**]$_0$=0.20 mM, [**TFA**]$_0$=6.54 M.

time [s]:	[1], M	[2], M
660	3.48E-05	0.000157
728	3.74E-05	0.000155
796	4.07E-05	0.000151
864	4.46E-05	0.000147
932	4.77E-05	0.000144
1000	5.08E-05	0.000141
1067	5.45E-05	0.000138
1135	5.7E-05	0.000135
1203	5.92E-05	0.000133
1271	6.33E-05	0.000129
1339	6.46E-05	0.000127
1407	6.74E-05	0.000125
1475	7.09E-05	0.000121
1543	7.22E-05	0.00012
1611	7.49E-05	0.000117
1678	7.64E-05	0.000116
1746	8E-05	0.000112
1814	8.45E-05	0.000108
1882	8.55E-05	0.000107
1950	8.46E-05	0.000107
2018	8.85E-05	0.000103
2086	9.14E-05	0.000101
2154	9.32E-05	9.88E-05
2222	9.54E-05	9.66E-05
2290	9.82E-05	9.38E-05
2358	9.84E-05	9.36E-05
2426	1E-04	9.2E-05
2494	0.000104	8.82E-05
2562	0.000105	8.67E-05
2630	0.000107	8.46E-05
2698	0.000108	8.36E-05
2765	0.00011	8.22E-05
2834	0.000111	8.11E-05
2901	0.000112	7.96E-05
2969	0.000115	7.73E-05
3037	0.000115	7.69E-05
3105	0.000118	7.43E-05
3173	0.000119	7.3E-05
3241	0.000121	7.13E-05
3309	0.000122	7.02E-05
3377	0.000125	6.72E-05
3445	0.000126	6.61E-05
3512	0.000128	6.42E-05
3580	0.000128	6.37E-05
3648	0.000129	6.29E-05
3716	0.00013	6.16E-05
3784	0.000132	5.96E-05
3852	0.000134	5.85E-05
3920	0.000134	5.76E-05
3988	0.000136	5.63E-05
4056	0.000137	5.52E-05
4124	0.000138	5.38E-05
4192	0.000139	5.29E-05
4260	0.00014	5.21E-05
4328	0.00014	5.16E-05
4396	0.000143	4.92E-05
4464	0.000143	4.85E-05
4531	0.000144	4.83E-05
4599	0.000144	4.79E-05
4667	0.000146	4.65E-05
4735	0.000146	4.61E-05
4803	0.000149	4.33E-05
4871	0.00015	4.25E-05
4939	0.000149	4.32E-05
5007	0.000151	4.11E-05
5075	0.000151	4.11E-05
5143	0.000152	3.97E-05
5211	0.000155	3.74E-05
5279	0.000154	3.84E-05
5346	0.000155	3.71E-05
5414	0.000157	3.5E-05
5482	0.000158	3.41E-05
5550	0.000157	3.55E-05
5618	0.000159	3.28E-05
5686	0.00016	3.19E-05
5754	0.00016	3.19E-05
5822	0.000159	3.27E-05
5890	0.00016	3.15E-05
5958	0.000162	2.97E-05
6026	0.000164	2.77E-05
6094	0.000164	2.78E-05
6162	0.000164	2.85E-05
6230	0.000163	2.87E-05
6298	0.000166	2.65E-05
6366	0.000165	2.65E-05
6433	0.000167	2.52E-05
6501	0.000167	2.5E-05
6569	0.000166	2.57E-05
6637	0.000168	2.37E-05
6705	0.000168	2.35E-05
6773	0.000168	2.36E-05
6841	0.000168	2.37E-05
6909	0.00017	2.16E-05
6977	0.000169	2.29E-05
7045	0.000169	2.26E-05
7113	0.000172	1.99E-05
7181	0.000172	2.03E-05
7249	0.000173	1.9E-05
7317	0.000172	1.98E-05
7385	0.000174	1.78E-05
7452	0.000172	2.05E-05
7520	0.000172	1.96E-05
7588	0.000174	1.84E-05
7656	0.000175	1.73E-05
7724	0.000173	1.89E-05
7792	0.000175	1.66E-05
7860	0.000174	1.82E-05
7928	0.000175	1.65E-05
7996	0.000175	1.68E-05
8064	0.000177	1.45E-05
8132	0.000178	1.44E-05
8200	0.00018	1.22E-05
8268	0.000176	1.61E-05
8336	0.000177	1.48E-05
8404	0.000177	1.46E-05
8472	0.000179	1.35E-05
8540	0.000181	1.11E-05
8608	0.000178	1.44E-05
8675	0.000178	1.4E-05
8743	0.00018	1.22E-05
8811	0.00018	1.24E-05
8879	0.00018	1.23E-05
8947	0.000179	1.33E-05
9015	0.000181	1.13E-05
9083	0.000182	9.58E-06
9151	0.000181	1.14E-05
9219	0.00018	1.21E-05

9287	0.000181	1.07E-05
9355	0.00018	1.23E-05
9423	0.000181	1.06E-05
9491	0.000182	9.94E-06
9559	0.000182	9.97E-06
9627	0.000184	8.42E-06
9695	0.000182	9.97E-06
9762	0.000182	9.66E-06
9830	0.000183	8.81E-06
9898	0.000185	7.25E-06
9966	0.000184	8E-06
10034	0.000184	8.27E-06
10102	0.000186	6.29E-06
10170	0.000183	8.61E-06
10238	0.000183	8.56E-06
10306	0.000184	7.54E-06
10374	0.000184	7.87E-06
10442	0.000185	6.82E-06
10510	0.000184	7.78E-06
10578	0.000184	8.44E-06
10646	0.000185	7.45E-06
10714	0.000187	5.28E-06
10782	0.000184	7.75E-06
10850	0.000184	8.26E-06
10918	0.000185	6.58E-06
10986	0.000186	6.44E-06
11053	0.000186	6.3E-06
11121	0.000186	6.12E-06
11189	0.000186	5.84E-06
11257	0.000188	4.4E-06
11325	0.000186	6.33E-06
11393	0.000186	6.36E-06
11461	0.000186	6.43E-06
11529	0.000186	5.63E-06
11597	0.000187	4.82E-06
11665	0.000187	5.31E-06
11733	0.000187	5.07E-06
11801	0.000187	5.03E-06
11869	0.000186	5.89E-06
11936	0.000187	4.77E-06
12005	0.000189	3.08E-06
12072	0.000187	4.55E-06
12140	0.000188	3.81E-06
12208	0.000187	4.75E-06
12276	0.000188	4.27E-06
12344	0.000189	2.67E-06
12412	0.000186	5.59E-06
12480	0.000188	3.8E-06
12548	0.000188	4.37E-06
12616	0.000188	3.99E-06
12684	0.000188	3.9E-06
12752	0.000188	4.36E-06
12820	0.000188	4E-06

Table S7. Concentration of **1** and **2** as a function of time (real time ^{1}H NMR measurement, Figure S28) in the experiment where [**4**]$_0$=0.30 mM, [**TFA**]$_0$=6.54 M.

time [s]:	[1], M	[2], M
420	3.65E-05	0.000263
487	4E-05	0.00026
555	4.36E-05	0.000256
623	4.64E-05	0.000254
691	5.17E-05	0.000248
758	5.6E-05	0.000244
826	5.91E-05	0.000241
894	6.3E-05	0.000237
962	6.48E-05	0.000235
1029	7.03E-05	0.00023
1097	7.28E-05	0.000227
1165	7.83E-05	0.000222
1233	8.05E-05	0.00022
1300	8.54E-05	0.000215
1368	8.63E-05	0.000214
1436	9E-05	0.00021
1503	9.58E-05	0.000204
1571	9.98E-05	0.0002
1639	0.000101	0.000199
1707	0.000105	0.000195
1775	0.000109	0.000191
1842	0.000111	0.000189
1910	0.000115	0.000185
1978	0.000118	0.000182
2046	0.000122	0.000178
2113	0.000124	0.000176
2181	0.000127	0.000173
2249	0.000129	0.000171
2317	0.000131	0.000169
2385	0.000136	0.000164
2452	0.000137	0.000163
2520	0.000141	0.000159
2588	0.000145	0.000155
2656	0.000145	0.000155
2724	0.000147	0.000153
2791	0.00015	0.00015
2859	0.000153	0.000147
2927	0.000155	0.000145
2995	0.000157	0.000143
3063	0.00016	0.00014
3130	0.000163	0.000137
3198	0.000164	0.000136
3266	0.000168	0.000132
3334	0.000168	0.000132
3401	0.000171	0.000129
3469	0.000174	0.000126
3537	0.000174	0.000126
3605	0.000176	0.000124
3673	0.000178	0.000122
3741	0.000181	0.000119
3808	0.000183	0.000117
3876	0.000183	0.000117
3944	0.000186	0.000114
4012	0.000188	0.000112
4079	0.000191	0.000109
4147	0.000191	0.000109
4215	0.000193	0.000107
4283	0.000195	0.000105
4350	0.000197	0.000103
4418	0.000198	0.000102
4486	0.000199	0.000101
4554	0.000202	9.8E-05
4621	0.000203	9.68E-05
4689	0.000204	9.59E-05
4757	0.000207	9.26E-05
4825	0.000207	9.26E-05
4892	0.000209	9.09E-05
4960	0.000211	8.88E-05
5028	0.000213	8.73E-05
5095	0.000213	8.71E-05
5163	0.000214	8.58E-05
5231	0.000217	8.32E-05
5299	0.000218	8.18E-05
5367	0.000219	8.07E-05
5434	0.00022	7.96E-05
5502	0.000221	7.86E-05
5570	0.000222	7.85E-05
5638	0.000224	7.57E-05
5705	0.000226	7.44E-05
5773	0.000227	7.27E-05
5841	0.000226	7.36E-05
5909	0.00023	6.96E-05
5976	0.000228	7.15E-05
6044	0.00023	6.95E-05
6112	0.000232	6.82E-05
6179	0.000234	6.63E-05
6247	0.000234	6.56E-05
6315	0.000234	6.57E-05
6383	0.000235	6.45E-05
6451	0.000237	6.34E-05
6519	0.000239	6.12E-05
6587	0.000239	6.09E-05
6654	0.00024	6E-05
6722	0.000241	5.86E-05
6790	0.000242	5.76E-05
6857	0.000243	5.66E-05
6925	0.000243	5.69E-05
6993	0.000242	5.75E-05
7061	0.000244	5.58E-05
7129	0.000245	5.48E-05
7197	0.000246	5.38E-05
7265	0.000247	5.34E-05
7332	0.00025	5.04E-05
7400	0.00025	5.01E-05
7468	0.00025	5.01E-05
7536	0.000252	4.84E-05
7604	0.000251	4.9E-05
7671	0.000253	4.73E-05
7739	0.000254	4.59E-05
7807	0.000253	4.71E-05
7875	0.000254	4.62E-05
7942	0.000255	4.53E-05
8010	0.000256	4.45E-05
8078	0.000257	4.26E-05
8146	0.000258	4.21E-05
8214	0.000258	4.25E-05
8281	0.000257	4.31E-05
8349	0.000258	4.18E-05
8417	0.000263	3.72E-05
8485	0.000261	3.94E-05
8553	0.00026	4E-05
8620	0.000262	3.78E-05
8688	0.000262	3.83E-05
8756	0.000262	3.8E-05
8824	0.000264	3.6E-05
8892	0.000264	3.62E-05
8960	0.000264	3.62E-05

9028	0.000266	3.38E-05
9095	0.000266	3.4E-05
9163	0.000267	3.29E-05
9231	0.000266	3.41E-05
9299	0.000268	3.21E-05
9366	0.000269	3.13E-05
9434	0.000268	3.23E-05
9502	0.000269	3.14E-05
9570	0.000268	3.23E-05
9638	0.00027	2.97E-05
9706	0.000271	2.91E-05
9773	0.00027	2.96E-05
9841	0.00027	2.96E-05
9909	0.000272	2.81E-05
9977	0.000272	2.77E-05
10045	0.000272	2.84E-05
10112	0.000273	2.73E-05
10180	0.000274	2.64E-05
10248	0.000272	2.76E-05
10316	0.000273	2.69E-05
10383	0.000274	2.59E-05
10451	0.000273	2.68E-05
10519	0.000274	2.61E-05
10587	0.000275	2.54E-05
10655	0.000277	2.26E-05
10723	0.000277	2.32E-05
10790	0.000276	2.39E-05
10858	0.000278	2.21E-05
10926	0.000277	2.34E-05
10994	0.000277	2.29E-05
11061	0.000277	2.28E-05
11129	0.000279	2.13E-05
11197	0.000278	2.2E-05
11264	0.000279	2.08E-05
11332	0.00028	1.98E-05
11400	0.000279	2.08E-05
11468	0.000279	2.15E-05
11536	0.000282	1.77E-05
11603	0.00028	2E-05
11671	0.000281	1.91E-05
11739	0.00028	2E-05
11807	0.00028	1.96E-05
11875	0.000281	1.85E-05
11942	0.000282	1.75E-05
12010	0.000282	1.82E-05
12078	0.000283	1.71E-05
12146	0.000282	1.78E-05
12213	0.000282	1.75E-05
12281	0.000281	1.89E-05
12349	0.000282	1.77E-05
12417	0.000284	1.62E-05
12484	0.000283	1.67E-05
12552	0.000283	1.65E-05

Table S8. Concentration of **1** and **2** as a function of the reaction time in the experiment where $[\mathbf{4}]_0$=0.50 mM, $[\mathbf{TFA}]_0$=6.54 M.

480	**4.25576E-05**	**0.000437**	**2722**	0.000197081	0.000283	**4963**	0.000297803	0.000182	**7205**	0.000362224	0.000118
549	4.7873E-05	0.000432	**2790**	0.00020035	0.00028	**5031**	0.000298945	0.000181	**7273**	0.000363031	0.000117
617	5.60841E-05	0.000424	**2858**	0.000204318	0.000276	**5099**	0.000302111	0.000178	**7341**	0.000364507	0.000115
685	5.74664E-05	0.000423	**2926**	0.000206839	0.000273	**5167**	0.000302917	0.000177	**7409**	0.000365885	0.000114
752	6.50421E-05	0.000415	**2993**	0.000210934	0.000269	**5235**	0.000305754	0.000174	**7476**	0.000368348	0.000112
820	6.97627E-05	0.00041	**3061**	0.000215759	0.000264	**5303**	0.000308692	0.000171	**7544**	0.000368921	0.000111
888	7.48103E-05	0.000405	**3129**	0.00021789	0.000262	**5371**	0.000310932	0.000169	**7612**	0.000369525	0.00011
956	8.0565E-05	0.000399	**3197**	0.000221746	0.000258	**5439**	0.000312466	0.000168	**7680**	0.000372527	0.000107
1024	8.62788E-05	0.000394	**3265**	0.000225272	0.000255	**5506**	0.000316263	0.000164	**7748**	0.000373372	0.000107
1092	9.10604E-05	0.000389	**3333**	0.000228755	0.000251	**5574**	0.000316329	0.000164	**7816**	0.000375826	0.000104
1160	9.29663E-05	0.000387	**3401**	0.000231436	0.000249	**5642**	0.000320245	0.00016	**7884**	0.000377174	0.000103
1228	0.000102156	0.000378	**3469**	0.00023577	0.000244	**5710**	0.000322175	0.000158	**7952**	0.000376695	0.000103
1296	0.000105347	0.000375	**3537**	0.000238495	0.000242	**5778**	0.000323426	0.000157	**8020**	0.000379113	0.000101
1363	0.000110599	0.000369	**3605**	0.000241048	0.000239	**5846**	0.000326074	0.000154	**8088**	0.00037943	0.000101
1431	0.000116715	0.000363	**3673**	0.000244261	0.000236	**5914**	0.00033027	0.00015	**8156**	0.000381372	9.86E-05
1499	0.000121833	0.000358	**3740**	0.000248668	0.000231	**5982**	0.000329268	0.000151	**8224**	0.000381387	9.86E-05
1567	0.00012424	0.000356	**3808**	0.000252332	0.000228	**6050**	0.000331035	0.000149	**8292**	0.000384355	9.56E-05
1635	0.000130555	0.000349	**3876**	0.000254236	0.000226	**6118**	0.000333953	0.000146	**8360**	0.000383845	9.62E-05
1703	0.000134285	0.000346	**3944**	0.000256822	0.000223	**6186**	0.000337738	0.000142	**8428**	0.00038757	9.24E-05
1771	0.000138103	0.000342	**4012**	0.000258849	0.000221	**6254**	0.000338626	0.000141	**8496**	0.000386938	9.31E-05
1839	0.000143608	0.000336	**4080**	0.000261336	0.000219	**6321**	0.000339636	0.00014	**8564**	0.000389078	9.09E-05
1907	0.000147619	0.000332	**4148**	0.000264543	0.000215	**6389**	0.000341261	0.000139	**8632**	0.000389866	9.01E-05
1975	0.000151396	0.000329	**4216**	0.000267294	0.000213	**6457**	0.000342774	0.000137	**8700**	0.000391422	8.86E-05
2043	0.000156574	0.000323	**4284**	0.000270715	0.000209	**6525**	0.000345056	0.000135	**8767**	0.00039223	8.78E-05
2111	0.000160448	0.00032	**4351**	0.000274136	0.000206	**6593**	0.000344514	0.000135	**8835**	0.000391824	8.82E-05
2178	0.000164386	0.000316	**4419**	0.000276982	0.000203	**6661**	0.00034781	0.000132	**8903**	0.000395446	8.46E-05
2246	0.000168694	0.000311	**4487**	0.000279519	0.0002	**6729**	0.000351691	0.000128	**8971**	0.000395482	8.45E-05
2314	0.00017354	0.000306	**4555**	0.000281991	0.000198	**6797**	0.000350817	0.000129	**9039**	0.000395454	8.45E-05
2382	0.000177214	0.000303	**4623**	0.000285507	0.000194	**6865**	0.000354083	0.000126	**9107**	0.000397238	8.28E-05
2450	0.000181226	0.000299	**4691**	0.00028701	0.000193	**6933**	0.000355059	0.000125	**9175**	0.000397375	8.26E-05
2518	0.00018377	0.000296	**4759**	0.000289081	0.000191	**7001**	0.000358237	0.000122	**9243**	0.000400353	7.96E-05
2586	0.000188827	0.000291	**4827**	0.000291882	0.000188	**7069**	0.000359582	0.00012	**9311**	0.000400104	7.99E-05
2654	0.000193182	0.000287	**4895**	0.00029467	0.000185	**7137**	0.000360514	0.000119	**9379**	0.000403395	7.66E-05

9447	0.000403998	7.6E-05
9515	0.000405574	7.44E-05
9583	0.000406334	7.37E-05
9651	0.000404996	7.5E-05
9719	0.000406772	7.32E-05
9787	0.000408137	7.19E-05
9855	0.000408853	7.11E-05
9923	0.000409622	7.04E-05
9991	0.000409179	7.08E-05
10059	0.000412261	6.77E-05
10127	0.000410831	6.92E-05
10195	0.000410797	6.92E-05
10263	0.00041448	6.55E-05
10330	0.000416021	6.4E-05
10399	0.000415332	6.47E-05
10466	0.000417357	6.26E-05
10534	0.000416352	6.36E-05
10602	0.000417245	6.28E-05
10670	0.000418743	6.13E-05
10738	0.000420267	5.97E-05
10806	0.000420164	5.98E-05
10874	0.00042306	5.69E-05
10942	0.000422809	5.72E-05
11010	0.000422802	5.72E-05
11078	0.000421692	5.83E-05
11146	0.000425409	5.46E-05
11214	0.000423865	5.61E-05
11282	0.000427427	5.26E-05
11349	0.000425457	5.45E-05
11417	0.00042814	5.19E-05
11485	0.000428586	5.14E-05
11553	0.000427746	5.23E-05
11621	0.000429524	5.05E-05
11689	0.00042768	5.23E-05
11757	0.000432458	4.75E-05
11825	0.000432301	4.77E-05
11893	0.000432156	4.78E-05
11961	0.000433292	4.67E-05
12029	0.000432875	4.71E-05
12097	0.000434536	4.55E-05
12165	0.000432828	4.72E-05
12233	0.000434205	4.58E-05
12301	0.000434811	4.52E-05
12369	0.000433702	4.63E-05
12437	0.000436346	4.37E-05
12505	0.000436805	4.32E-05
12573	0.00043964	4.04E-05
12640	0.000438159	4.18E-05
12708	0.000438007	4.2E-05
12776	0.000439836	4.02E-05
12844	0.000439633	4.04E-05
12912	0.00044064	3.94E-05
12980	0.000440208	3.98E-05
13048	0.000438963	4.1E-05
13116	0.00044286	3.71E-05
13184	0.000441152	3.88E-05
13252	0.000441902	3.81E-05
13320	0.000442519	3.75E-05
13388	0.000441586	3.84E-05
13456	0.00044287	3.71E-05
13524	0.000443728	3.63E-05
13592	0.000445095	3.49E-05
13660	0.000447088	3.29E-05
13727	0.000445236	3.48E-05
13795	0.000446934	3.31E-05
13863	0.000445077	3.49E-05
13931	0.000447444	3.26E-05
13999	0.000444635	3.54E-05
14067	0.000446288	3.37E-05
14135	0.000447847	3.22E-05
14203	0.000446763	3.32E-05
14271	0.000447081	3.29E-05
14338	0.000447595	3.24E-05
14406	0.000447556	3.24E-05
14474	0.000450943	2.91E-05
14542	0.000449958	3E-05
14610	0.000449933	3.01E-05
14678	0.000448561	3.14E-05
14746	0.000449319	3.07E-05
14814	0.000449894	3.01E-05
14882	0.000454312	2.57E-05
14950	0.000453038	2.7E-05
15018	0.000453453	2.65E-05
15086	0.000452047	2.8E-05
15154	0.000453096	2.69E-05
15222	0.000454223	2.58E-05
15290	0.00045314	2.69E-05
15357	0.000452356	2.76E-05
15425	0.000452738	2.73E-05
15493	0.000454938	2.51E-05
15561	0.000454574	2.54E-05
15629	0.000455347	2.47E-05
15697	0.000454937	2.51E-05
15765	0.00045363	2.64E-05
15833	0.000455703	2.43E-05
15901	0.000456033	2.4E-05
15969	0.000456052	2.39E-05
16037	0.000459543	2.05E-05
16105	0.000456094	2.39E-05
16173	0.000456359	2.36E-05
16241	0.000458504	2.15E-05
16308	0.00045833	2.17E-05
16376	0.000458493	2.15E-05
16444	0.000457688	2.23E-05
16512	0.000459215	2.08E-05
16580	0.000456582	2.34E-05
16648	0.000460092	1.99E-05
16716	0.000457423	2.26E-05
16784	0.000458413	2.16E-05
16852	0.000460455	1.95E-05
16920	0.000459167	2.08E-05
16988	0.000460131	1.99E-05
17056	0.000461701	1.83E-05
17124	0.000463477	1.65E-05
17192	0.00046211	1.79E-05
17259	0.00046062	1.94E-05
17327	0.000462626	1.74E-05
17395	0.000462931	1.71E-05
17463	0.000462296	1.77E-05
17531	0.000462254	1.77E-05
17599	0.000463219	1.68E-05
17667	0.000464005	1.6E-05
17735	0.000464044	1.6E-05
17803	0.000460548	1.95E-05
17871	0.000462479	1.75E-05
17939	0.000464763	1.52E-05
18007	0.000463043	1.7E-05
18075	0.000460469	1.95E-05
18142	0.000462328	1.77E-05
18210	0.000463242	1.68E-05
18278	0.000463014	1.7E-05
18346	0.000465042	1.5E-05
18414	0.000463549	1.65E-05
18482	0.000461159	1.88E-05
18550	0.000466792	1.32E-05
18618	0.000463552	1.64E-05
18686	0.000463383	1.66E-05
18754	0.000468457	1.15E-05
18822	0.000462858	1.71E-05
18889	0.00046492	1.51E-05
18957	0.000468276	1.17E-05
19025	0.000466104	1.39E-05
19093	0.000467496	1.25E-05
19161	0.000468203	1.18E-05
19229	0.000465168	1.48E-05
19297	0.000467606	1.24E-05
19365	0.000469267	1.07E-05
19433	0.000468346	1.17E-05
19501	0.00046701	1.3E-05
19568	0.000466273	1.37E-05
19636	0.000469671	1.03E-05
19704	0.000466729	1.33E-05

Table S9. Concentration of **1** and **2** as a function of time (real time ^{1}H NMR measurement, Figure S28) in the experiment where [**4**]$_0$=0.99 mM, [**TFA**]$_0$=6.54 M.

time [s]:	[1], M	[2], M
420	5.49E-05	0.00093
488	6.46E-05	0.00092
556	6.96E-05	0.000915
623	8.16E-05	0.000903
691	8.98E-05	0.000895
759	9.95E-05	0.000886
827	0.000103	0.000882
895	0.000114	0.000871
962	0.000123	0.000862
1030	0.000131	0.000854
1098	0.000142	0.000843
1166	0.00015	0.000835
1233	0.000156	0.000829
1301	0.000165	0.00082
1369	0.000174	0.000811
1437	0.000186	0.000799
1505	0.000191	0.000794
1573	0.000198	0.000787
1641	0.000206	0.000779
1709	0.000213	0.000772
1777	0.000219	0.000766
1845	0.00023	0.000755
1913	0.000237	0.000748
1980	0.000243	0.000742
2048	0.000251	0.000734
2116	0.000259	0.000726
2184	0.000264	0.000721
2252	0.000273	0.000712
2320	0.000279	0.000706
2388	0.000287	0.000698
2455	0.000294	0.000691
2523	0.000302	0.000683
2591	0.000306	0.000679
2659	0.000316	0.000669
2727	0.000323	0.000662
2795	0.000328	0.000657
2863	0.000337	0.000648
2931	0.000341	0.000644
2999	0.000349	0.000636
3067	0.000355	0.00063
3135	0.000362	0.000623
3202	0.000366	0.000619
3270	0.000374	0.000611
3338	0.00038	0.000605
3406	0.000385	0.0006
3474	0.000392	0.000593
3542	0.000398	0.000587
3610	0.000402	0.000583
3678	0.000411	0.000574
3746	0.000415	0.00057
3814	0.00042	0.000565
3881	0.000425	0.00056
3949	0.000432	0.000553
4017	0.000439	0.000546
4085	0.000443	0.000542
4153	0.000447	0.000538
4221	0.000454	0.000531
4288	0.000459	0.000526
4356	0.000464	0.000521
4424	0.000469	0.000516
4492	0.000477	0.000508
4559	0.00048	0.000505
4627	0.000485	0.0005
4695	0.000491	0.000494
4763	0.000495	0.00049
4831	0.0005	0.000485
4899	0.000505	0.00048
4967	0.00051	0.000475
5035	0.000517	0.000468
5103	0.00052	0.000465
5170	0.000525	0.00046
5238	0.000528	0.000457
5306	0.000533	0.000452
5374	0.000539	0.000446
5442	0.000543	0.000442
5509	0.000546	0.000439
5577	0.000552	0.000433
5645	0.000556	0.000429
5713	0.000561	0.000424
5780	0.000566	0.000419
5848	0.00057	0.000415
5916	0.000575	0.00041
5984	0.000577	0.000408
6052	0.000584	0.000401
6120	0.000586	0.000399
6188	0.000589	0.000396
6256	0.000593	0.000392
6323	0.000598	0.000387
6391	0.000602	0.000383
6459	0.000604	0.000381
6527	0.00061	0.000375
6595	0.000613	0.000372
6663	0.000616	0.000369
6731	0.000621	0.000364
6799	0.000624	0.000361
6866	0.000629	0.000356
6934	0.000631	0.000354
7002	0.000636	0.000349
7070	0.000638	0.000347
7137	0.000643	0.000342
7205	0.000645	0.00034
7273	0.000649	0.000336
7341	0.000652	0.000333
7409	0.000656	0.000329
7476	0.000659	0.000326
7544	0.000662	0.000323
7612	0.000664	0.000321
7680	0.000667	0.000318
7748	0.000672	0.000313
7816	0.000676	0.000309
7884	0.000677	0.000308
7952	0.000681	0.000304
8020	0.000684	0.000301
8088	0.000687	0.000298
8156	0.00069	0.000295
8223	0.000692	0.000293
8292	0.000695	0.00029
8360	0.000699	0.000286
8428	0.000702	0.000283
8496	0.000704	0.000281
8563	0.000708	0.000277
8631	0.000711	0.000274
8699	0.000712	0.000273
8767	0.000715	0.00027
8835	0.000717	0.000268
8902	0.000721	0.000264
8970	0.000724	0.000261

9038	0.000725	0.00026
9106	0.000728	0.000257
9174	0.000732	0.000253
9242	0.000732	0.000253
9310	0.000735	0.00025
9377	0.000739	0.000246
9445	0.00074	0.000245
9513	0.000744	0.000241
9581	0.000746	0.000239
9648	0.000749	0.000236
9716	0.000749	0.000236
9784	0.000753	0.000232
9852	0.000755	0.00023
9920	0.000756	0.000229
9988	0.000759	0.000226
10055	0.000761	0.000224
10123	0.000765	0.00022
10191	0.000765	0.00022
10259	0.000768	0.000217
10327	0.00077	0.000215
10395	0.000773	0.000212
10463	0.000774	0.000211
10531	0.000776	0.000209
10599	0.000778	0.000207
10666	0.000781	0.000204
10734	0.000782	0.000203
10802	0.000784	0.000201
10870	0.000787	0.000198
10937	0.000788	0.000197
11005	0.000791	0.000194
11073	0.000791	0.000194
11141	0.000795	0.00019
11209	0.000795	0.00019
11277	0.000797	0.000188
11345	0.0008	0.000185
11412	0.000801	0.000184
11480	0.000803	0.000182
11548	0.000805	0.00018
11616	0.000807	0.000178
11684	0.000811	0.000174
11752	0.000811	0.000174
11819	0.000811	0.000174
11887	0.000814	0.000171
11955	0.000815	0.00017
12023	0.000816	0.000169
12090	0.000818	0.000167
12158	0.00082	0.000165
12226	0.000823	0.000162
12294	0.000823	0.000162
12362	0.000824	0.000161
12430	0.000827	0.000158
12498	0.000826	0.000159
12565	0.000831	0.000154
12633	0.00083	0.000155
12701	0.000832	0.000153
12769	0.000835	0.00015
12837	0.000834	0.000151
12905	0.000837	0.000148
12973	0.000839	0.000146
13040	0.000839	0.000146
13108	0.000841	0.000144
13176	0.000842	0.000143
13244	0.000844	0.000141
13312	0.000845	0.00014
13380	0.000846	0.000139
13448	0.000847	0.000138
13516	0.000847	0.000138
13584	0.000851	0.000134
13652	0.000852	0.000133
13720	0.000853	0.000132
13788	0.000855	0.00013
13856	0.000856	0.000129
13923	0.000856	0.000129
13991	0.000857	0.000128
14059	0.000859	0.000126
14127	0.00086	0.000125
14195	0.00086	0.000125
14263	0.000862	0.000123
14331	0.000864	0.000121
14399	0.000864	0.000121
14467	0.000866	0.000119
14534	0.000867	0.000118
14602	0.000869	0.000116
14670	0.000871	0.000114
14738	0.000871	0.000114
14806	0.000872	0.000113
14874	0.000873	0.000112
14942	0.000873	0.000112
15010	0.000875	0.00011
15078	0.000875	0.00011
15146	0.000877	0.000108
15213	0.000876	0.000109
15281	0.000877	0.000108
15349	0.00088	0.000105
15417	0.00088	0.000105
15485	0.000882	0.000103
15552	0.000881	0.000104
15620	0.000881	0.000104
15688	0.000885	9.96E-05
15756	0.000886	9.95E-05
15824	0.000886	9.88E-05
15892	0.000888	9.69E-05
15960	0.000889	9.65E-05
16028	0.000888	9.66E-05
16096	0.00089	9.52E-05
16164	0.000892	9.26E-05
16232	0.000891	9.44E-05

Table S10. Concentration of **1** and **2** as a function of time (real time ^{1}H NMR measurement, Figure S28) in the experiment where [**4**]$_0$=1.92 mM, [**TFA**]$_0$=6.54 M.

time [s]:	[1]], M	[2], M
480	7.21E-05	0.001851
548	8.02E-05	0.001843
616	9.3E-05	0.001831
684	0.000109	0.001816
752	0.00012	0.001805
820	0.000132	0.001793
887	0.000146	0.00178
955	0.000159	0.001768
1023	0.000171	0.001756
1091	0.000181	0.001747
1159	0.000198	0.00173
1227	0.000208	0.00172
1295	0.000222	0.001707
1363	0.000236	0.001694
1430	0.000245	0.001685
1498	0.00026	0.00167
1566	0.000273	0.001658
1634	0.000285	0.001647
1702	0.000296	0.001636
1770	0.000312	0.001621
1838	0.000322	0.001611
1906	0.000333	0.0016
1973	0.000347	0.001587
2041	0.000356	0.001579
2109	0.000371	0.001563
2177	0.000383	0.001552
2245	0.000394	0.001542
2313	0.000405	0.001531
2381	0.000416	0.00152
2448	0.00043	0.001507
2517	0.000441	0.001496
2584	0.000455	0.001483
2652	0.000464	0.001474
2720	0.000476	0.001463
2788	0.000487	0.001453
2856	0.000501	0.001439
2924	0.000511	0.001429
2992	0.000521	0.001419
3060	0.000531	0.00141
3127	0.000542	0.0014
3195	0.000555	0.001387
3263	0.000565	0.001377
3331	0.000574	0.001369
3399	0.000587	0.001357
3467	0.000597	0.001347
3535	0.000606	0.001338
3602	0.000618	0.001327
3671	0.000629	0.001316
3738	0.000637	0.001308
3806	0.00065	0.001296
3874	0.000661	0.001285
3942	0.000669	0.001278
4010	0.00068	0.001267
4077	0.000691	0.001256
4145	0.000698	0.00125
4213	0.00071	0.001238
4281	0.00072	0.001229
4349	0.00073	0.001219
4417	0.00074	0.00121
4485	0.000748	0.001202
4553	0.000759	0.001192
4621	0.000767	0.001184
4689	0.000778	0.001173
4756	0.000788	0.001164
4824	0.000797	0.001154
4892	0.000805	0.001147
5028	0.000824	0.001129
5096	0.000834	0.001119
5164	0.00084	0.001113
5232	0.000849	0.001105
5300	0.00086	0.001095
5368	0.000869	0.001086
5436	0.000878	0.001077
5503	0.000886	0.001069
5571	0.000894	0.001062
5639	0.0009	0.001056
5707	0.000912	0.001045
5775	0.00092	0.001036
5843	0.000935	0.001022
5911	0.000934	0.001023
5979	0.000944	0.001014
6047	0.000951	0.001007
6114	0.000962	0.000997
6182	0.000965	0.000993
6250	0.000975	0.000984
6318	0.000984	0.000975
6386	0.000992	0.000967
6454	0.000999	0.000961
6522	0.001004	0.000956
6590	0.001013	0.000948
6658	0.001022	0.000939
6726	0.001029	0.000933
6794	0.001037	0.000924
6861	0.001044	0.000918
6929	0.001052	0.00091
6997	0.001059	0.000903
7065	0.001065	0.000897
7133	0.001072	0.000891
7201	0.00108	0.000884
7269	0.001088	0.000876
7337	0.001094	0.00087
7405	0.001101	0.000863
7472	0.001107	0.000857
7540	0.001114	0.00085
7609	0.001121	0.000844
7676	0.001128	0.000837
7744	0.001134	0.000831
7812	0.00114	0.000825
7880	0.00115	0.000816
7948	0.001155	0.000812
8016	0.001161	0.000806
8084	0.001167	0.000799
8152	0.001174	0.000793
8220	0.001182	0.000786
8288	0.001189	0.000779
8356	0.001193	0.000774
8424	0.001198	0.00077
8492	0.001207	0.000761
8560	0.00121	0.000759
8627	0.001216	0.000753
8695	0.001224	0.000745
8763	0.001228	0.000741
8831	0.001235	0.000734
8899	0.001243	0.000727
8967	0.001246	0.000724
9035	0.001253	0.000718
9103	0.001259	0.000711

9171	0.001264	0.000707
9238	0.001268	0.000703
9306	0.001274	0.000697
9374	0.001278	0.000693
9442	0.001285	0.000687
9510	0.00129	0.000682
9578	0.001299	0.000673
9646	0.001301	0.000671
9714	0.001305	0.000667
9781	0.00131	0.000662
9849	0.001317	0.000656
9917	0.001319	0.000653
9985	0.001328	0.000645
10053	0.001334	0.000639
10121	0.001337	0.000636
10189	0.001341	0.000633
10257	0.001348	0.000626
10325	0.001352	0.000622
10392	0.001357	0.000618
10460	0.001362	0.000613
10528	0.001366	0.000609
10596	0.001372	0.000603
10664	0.001374	0.000601
10732	0.001381	0.000594
10800	0.001384	0.000591
10868	0.001391	0.000585
10936	0.001394	0.000582
11004	0.001399	0.000577
11072	0.001403	0.000573
11139	0.001409	0.000568
11207	0.001411	0.000565
11275	0.001416	0.000561
11343	0.001421	0.000556
11411	0.001425	0.000552
11479	0.001431	0.000546
11547	0.001433	0.000545
11615	0.001439	0.000538
11683	0.001443	0.000535
11751	0.001448	0.00053
11819	0.001448	0.00053
11887	0.001455	0.000523
11954	0.001459	0.00052
12022	0.001466	0.000512
12090	0.001468	0.000511
12158	0.001473	0.000506
12226	0.001476	0.000503
12294	0.00148	0.0005
12362	0.001483	0.000497
12430	0.001487	0.000493
12498	0.001493	0.000487
12565	0.001493	0.000487
12633	0.001496	0.000483
12701	0.0015	0.00048
12769	0.001504	0.000476
12837	0.001508	0.000473
12905	0.001513	0.000467
12973	0.001514	0.000466
13041	0.001518	0.000463
13109	0.001523	0.000458
13177	0.001526	0.000455
13245	0.001532	0.00045
13312	0.001533	0.000448
13380	0.001538	0.000443
13448	0.001538	0.000444
13516	0.001543	0.000439
13584	0.001546	0.000436
13652	0.001549	0.000433
13720	0.001554	0.000428
13788	0.001557	0.000425
13856	0.001562	0.00042
13924	0.001564	0.000418
13992	0.001566	0.000416
14059	0.001569	0.000414
14127	0.001572	0.000411
14195	0.001576	0.000407
14263	0.00158	0.000403
14331	0.001583	0.0004
14399	0.001588	0.000395
14466	0.001584	0.0004
14534	0.001593	0.000391
14602	0.001595	0.000389
14670	0.001597	0.000387
14738	0.001599	0.000385
14806	0.001602	0.000382
14874	0.001607	0.000377
14942	0.00161	0.000374
15010	0.001613	0.000372
15078	0.001614	0.000371
15146	0.001616	0.000369
15213	0.001621	0.000364
15281	0.001622	0.000363
15349	0.001629	0.000357
15417	0.001627	0.000358
15485	0.00163	0.000355
15553	0.001632	0.000354
15621	0.001638	0.000347
15689	0.001639	0.000347
15756	0.00164	0.000345
15824	0.001646	0.00034
15892	0.001648	0.000338
15960	0.001648	0.000338
16028	0.001652	0.000334
16096	0.001655	0.000331
16164	0.001655	0.000331
16232	0.00166	0.000326
16300	0.00166	0.000326
16368	0.001664	0.000323
16436	0.001664	0.000322

Table S11. Concentration of **1** and **2** as a function of time (real time ^{1}H NMR measurement, Figure S28) in the experiment where $[\mathbf{4}]_0$=3.83 mM, $[TFA]_0$=6.54 M.

time [s]:	[1], M	[2], M
600	0.000131	0.003699
666	0.000139	0.003691
732	0.000157	0.003673
798	0.000178	0.003652
863	0.000192	0.003638
929	0.000214	0.003616
995	0.000232	0.003598
1061	0.000242	0.003588
1127	0.000266	0.003564
1193	0.000271	0.003559
1259	0.000305	0.003525
1325	0.000303	0.003527
1391	0.000333	0.003497
1457	0.000341	0.003489
1523	0.000358	0.003472
1588	0.000381	0.003449
1654	0.000409	0.003421
1720	0.00042	0.00341
1786	0.000433	0.003397
1852	0.000457	0.003373
1918	0.000472	0.003358
1984	0.000489	0.003341
2050	0.000511	0.003319
2116	0.000525	0.003305
2181	0.000538	0.003292
2247	0.00056	0.00327
2313	0.000579	0.003251
2379	0.000599	0.003231
2445	0.000615	0.003215
2511	0.000632	0.003198
2577	0.000651	0.003179
2643	0.000671	0.003159
2709	0.000683	0.003147
2774	0.000703	0.003127
2840	0.00072	0.00311
2906	0.00074	0.00309
2972	0.000755	0.003075
3038	0.000772	0.003058
3104	0.000788	0.003042
3170	0.000808	0.003022
3236	0.000825	0.003005
3302	0.000845	0.002985
3368	0.00086	0.00297
3434	0.000876	0.002954
3500	0.00089	0.00294
3565	0.000906	0.002924
3631	0.000927	0.002903
3697	0.000946	0.002884
3763	0.00096	0.00287
3829	0.000978	0.002852
3895	0.000992	0.002838
3961	0.001012	0.002818
4027	0.001028	0.002802
4092	0.001043	0.002787
4158	0.00106	0.00277
4224	0.001079	0.002751
4290	0.001088	0.002742
4356	0.001109	0.002721
4422	0.001122	0.002708
4488	0.00114	0.00269
4553	0.001154	0.002676
4619	0.001172	0.002658
4685	0.001183	0.002647
4751	0.001198	0.002632
4817	0.001215	0.002615
4882	0.001232	0.002598
4948	0.001248	0.002582
5014	0.001262	0.002568
5080	0.001273	0.002557
5146	0.001291	0.002539
5212	0.001307	0.002523
5278	0.001319	0.002511
5344	0.001333	0.002497
5410	0.001351	0.002479
5476	0.001366	0.002464
5542	0.001379	0.002451
5607	0.001395	0.002435
5673	0.001409	0.002421
5739	0.001422	0.002408
5805	0.001436	0.002394
5871	0.001454	0.002376
5937	0.001465	0.002365
6003	0.001476	0.002354
6069	0.001493	0.002337
6135	0.001507	0.002323
6201	0.00152	0.00231
6267	0.001532	0.002298
6332	0.001544	0.002286
6398	0.001561	0.002269
6464	0.001571	0.002259
6530	0.001586	0.002244
6596	0.001601	0.002229
6662	0.001612	0.002218
6728	0.001627	0.002203
6794	0.001639	0.002191
6860	0.001651	0.002179
6926	0.001662	0.002168
6992	0.001676	0.002154
7058	0.001691	0.002139
7124	0.001702	0.002128
7189	0.001716	0.002114
7255	0.001727	0.002103
7321	0.001739	0.002091
7387	0.00175	0.00208
7453	0.001766	0.002064
7519	0.001772	0.002058
7585	0.001788	0.002042
7651	0.001798	0.002032
7717	0.001812	0.002018
7783	0.001824	0.002006
7849	0.001834	0.001996
7915	0.001846	0.001984
7981	0.001859	0.001971
8046	0.001869	0.001961
8112	0.001883	0.001947
8178	0.001892	0.001938
8244	0.001905	0.001925
8310	0.001917	0.001913
8376	0.001925	0.001905
8442	0.001938	0.001892
8507	0.001948	0.001882
8573	0.001961	0.001869
8639	0.001972	0.001858
8705	0.001982	0.001848
8771	0.001994	0.001836
8837	0.002004	0.001826
8902	0.002013	0.001817

8968	0.002026	0.001804
9034	0.002035	0.001795
9100	0.002043	0.001787
9166	0.002055	0.001775
9232	0.002068	0.001762
9298	0.002076	0.001754
9364	0.002087	0.001743
9430	0.002095	0.001735
9496	0.002107	0.001723
9562	0.002117	0.001713
9628	0.002126	0.001704
9694	0.002137	0.001693
9760	0.002146	0.001684
9826	0.002158	0.001672
9892	0.002167	0.001663
9958	0.002176	0.001654
10024	0.002186	0.001644
10089	0.002191	0.001639
10155	0.002206	0.001624
10221	0.002212	0.001618
10287	0.002223	0.001607
10353	0.002237	0.001593
10419	0.002241	0.001589
10485	0.002249	0.001581
10551	0.00226	0.00157
10617	0.002266	0.001564
10683	0.002278	0.001552
10749	0.002285	0.001545
10815	0.002297	0.001533
10880	0.002303	0.001527
10946	0.002313	0.001517
11012	0.002321	0.001509
11078	0.002329	0.001501
11144	0.002335	0.001495
11210	0.002347	0.001483
11276	0.002353	0.001477
11342	0.002364	0.001466
11407	0.002373	0.001457
11473	0.002379	0.001451
11539	0.002387	0.001443
11605	0.002394	0.001436
11671	0.002406	0.001424
11737	0.002412	0.001418
11803	0.002422	0.001408
11869	0.00243	0.0014
11935	0.002435	0.001395
12001	0.002441	0.001389
12066	0.002453	0.001377
12133	0.002462	0.001368
12198	0.002468	0.001362
12264	0.002475	0.001355
12330	0.002483	0.001347
12396	0.00249	0.00134

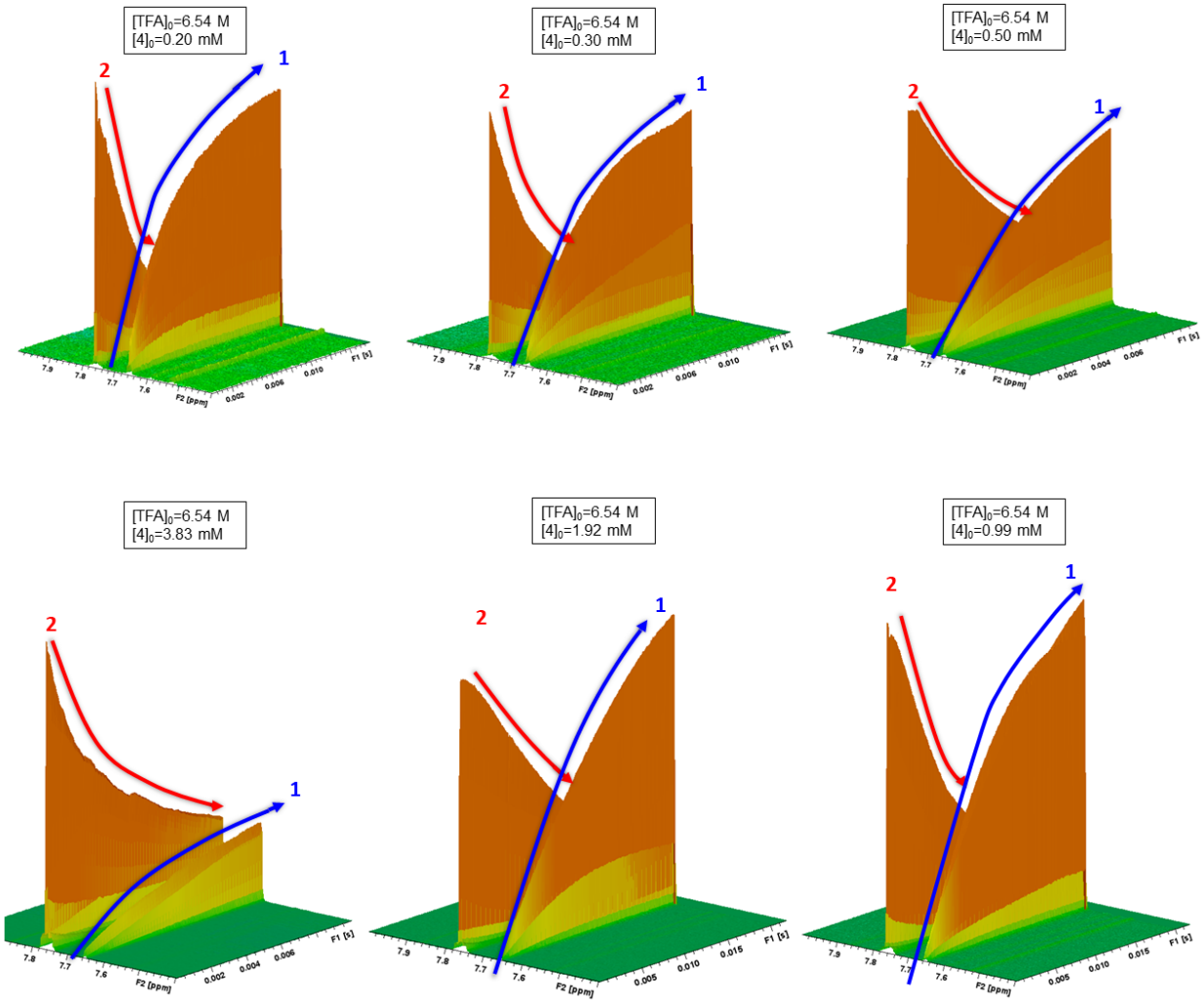


Figure S28. Using the intensity of aromatic $\mathbf{H}_C$ resonances in **2** and **1**, we monitored a change in the concentration of these two compounds (right) over time for six different reaction conditions (real time ^{1}H NMR spectroscopy).

Product inhibition: Using the concertation/time data obtained in experiments with different starting concentrations of *tris*-aldehyde $[\mathbf{2}]_0$ = 1, 0.5 mM, 0.3 mM, 0.25 mM and the same concertation of TFA catalyst (6.54 M), the "time normalized plot" was constructed to evaluate if the product inhibition was taking place (Figure S29). That is to say, for each experiment we identified a point in time at which the aldehyde concentration dropped to 0.25 mM ([**2**] = 0.25 mM) followed by setting the time scale to, at this point, be 0. In this way, the concentration of starting *tris*-aldehyde **2** was in these four experiments set to be identical at the beginning of the conversion (Figure S29) while the amount of capsularene **1** different (Table S12). If there was no product inhibition, one would expect that four curves overlay. However, if the product inhibition was taking place, one would expect an increase in the rate reduction for reactions with larger quantity of **1**.

Table S12. Concentrations of capsularene **1** and *tris*-aldehyde **2** at normalized time 0 s in the four experiments used to evaluate the product inhibition.

Concentration at actual time 0 s	Original data with actual times	Concentrations at normalized time 0 s	
$[\mathbf{2}]_{tot}$, mM		$[\mathbf{2}]_{initial}$, mM	$[\mathbf{1}]_{initial}$, mM
1.00	Table S9	0.25	0.75
0.50	Table S8	0.25	0.25
0.30	Table S7	0.25	0.05
0.25	Table S13	0.25	0.00

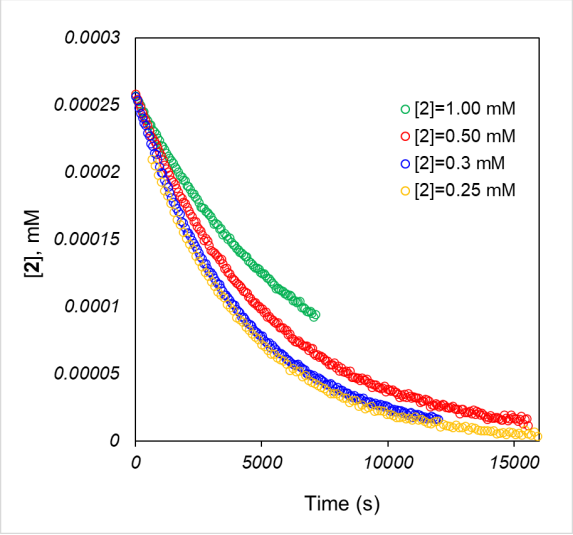


Figure S29. Four curves depicting the reaction progress for the conversion of 0.25 mM of [**2**] when increasingly greater amounts of capsularene **1** were present at the beginning. It is apparent that the reaction with the lowest starting concentration of capsularene **1** (yellow) proceeded at a higher rate that the one with the highest concentration of **1** (green).

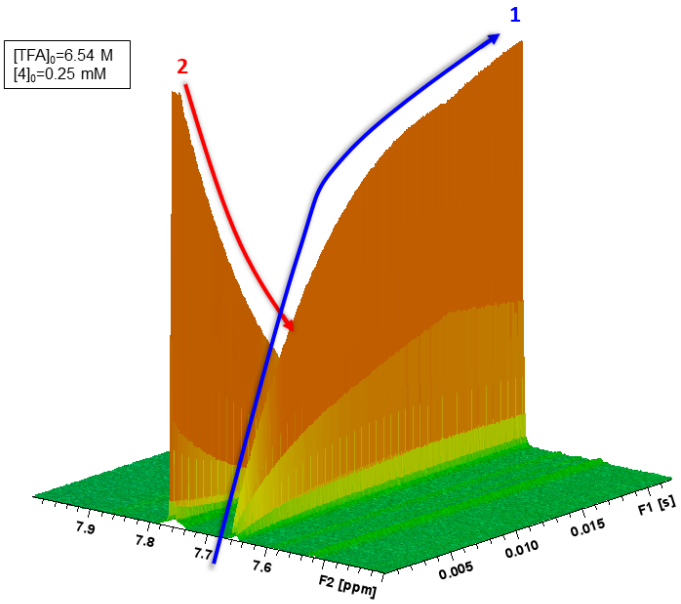


Figure S30. Real time ^{1}H NMR experiments were used for evaluating the product inhibition with $[\mathbf{2}]_0$ = 0.25 mM at the beginning of the reaction (no capsularene **1** present); all other experiments used for this analysis are shown in Figure S28.

Table S13. Concentration of *tris*-aldehyde **2** as a function of time in the experiment where $[\mathbf{4}]_0$=0.25 mM and $[TFA]_0$=6.54 M.

t(s)	[2] (M)						
660	0.00021	**2522**	0.000134	**4508**	8.26E-05	**6494**	5.23E-05
784	0.000205	**2646**	0.00013	**4632**	8E-05	**6618**	4.8E-05
908	0.000198	**2770**	0.000126	**4756**	7.77E-05	**6742**	4.89E-05
1032	0.000193	**2894**	0.000123	**4880**	7.55E-05	**6866**	4.53E-05
1157	0.000187	**3019**	0.000119	**5004**	7.21E-05	**6990**	4.4E-05
1281	0.000183	**3143**	0.000115	**5128**	7.05E-05	**7114**	4.32E-05
1405	0.000177	**3267**	0.000111	**5252**	6.77E-05	**7238**	4.16E-05
1529	0.000171	**3391**	0.000109	**5376**	6.51E-05	**7362**	4.04E-05
1653	0.000165	**3515**	0.000107	**5501**	6.48E-05	**7486**	3.91E-05
1777	0.000161	**3639**	0.000102	**5625**	6.2E-05	**7610**	3.75E-05
1901	0.000156	**3763**	9.95E-05	**5749**	6.06E-05	**7734**	3.57E-05
2025	0.000151	**3887**	9.7E-05	**5873**	5.98E-05	**7859**	3.54E-05
2150	0.000147	**4011**	9.22E-05	**5997**	5.77E-05	**7983**	3.56E-05
2274	0.000143	**4136**	9.07E-05	**6121**	5.3E-05	**8107**	3.38E-05
2398	0.000138	**4260**	8.86E-05	**6245**	5.42E-05	**8231**	3.21E-05
		4384	8.51E-05	**6369**	5.2E-05	**8355**	3.25E-05

8479	2.89E-05
8603	3.03E-05
8727	3.02E-05
8852	2.63E-05
8976	2.73E-05
9100	2.43E-05
9224	2.52E-05
9348	2.6E-05
9472	2.27E-05
9596	2.29E-05
9721	2.3E-05
9845	2.23E-05
9969	2.01E-05
10093	2.03E-05
10217	1.94E-05
10341	1.79E-05
10465	1.77E-05
10590	1.8E-05
10714	1.69E-05
10838	1.72E-05
10962	1.58E-05
11086	1.81E-05
11210	1.59E-05
11334	1.62E-05
11458	1.49E-05
11582	1.37E-05
11707	1.29E-05
11831	1.44E-05
11955	1.49E-05
12079	1.06E-05
12203	1.24E-05
12327	1.18E-05
12451	1.12E-05
12575	1.04E-05

12699	1.23E-05
12824	1.03E-05
12948	1.04E-05
13072	1.1E-05
13196	8.44E-06
13320	1.04E-05
13444	9.67E-06
13568	8.65E-06
13693	7.82E-06
13817	7.98E-06
13941	8.09E-06
14065	7.64E-06
14189	8.13E-06
14313	5.65E-06
14438	5.92E-06
14562	6.51E-06
14686	4.99E-06
14810	6.82E-06
14934	6.64E-06
15058	5.16E-06
15182	6.06E-06
15307	4.64E-06
15431	8.52E-06
15555	5.56E-06
15679	4.56E-06
15803	7.08E-06
15928	3.88E-06
16052	3.94E-06
16176	3.63E-06
16300	4.07E-06
16424	4.52E-06
16548	5.37E-06
16672	3.18E-06
16796	3.9E-06

16920	4.43E-06
17044	5.27E-06
17169	5.25E-06
17293	4.23E-06
17417	2.9E-06
17541	4.24E-06
17665	1.99E-06
17789	2.51E-06
17913	2.07E-06
18037	2.9E-06
18161	4.02E-06
18286	1.38E-06
18410	1.74E-06
18534	3.78E-06
18658	2.31E-06
18782	2.88E-06
18906	3.51E-06
19030	2.48E-06
19154	1.34E-06
19278	1.88E-06
19402	3.08E-06
19527	1.69E-06
19651	9.56E-07
19775	5.56E-07
19899	-5.5E-07
20023	2.61E-06
20147	2.2E-06
20272	-4.9E-07
20396	2.25E-06
20520	1.5E-06
20644	-5.1E-07
20768	1.66E-06
20892	2.4E-06
21016	8.2E-07

21140	1.78E-06
21265	3.88E-07
21389	-8.3E-07
21513	-6.6E-07
21637	1.59E-06
21761	1.7E-06
21885	8.94E-07
22009	-9.6E-07
22133	2.66E-06
22257	2.03E-06
22381	-7.7E-07
22506	1.38E-06
22630	5.6E-07
22754	1.23E-06
22878	1.03E-06
23002	-1E-06
23126	8.79E-07
23250	3.91E-07
23374	1.06E-06
23498	-2.2E-06
23622	8.57E-07
23747	1.69E-06
23871	1.83E-06
23995	-5.6E-07
24119	-2.2E-07
24243	1.21E-06
24367	-9.1E-07
24491	-1.9E-06
24615	6.17E-07
24739	-8E-07
24864	-7.9E-07
24988	-1.3E-06
25112	2.24E-06
25236	-1.3E-07

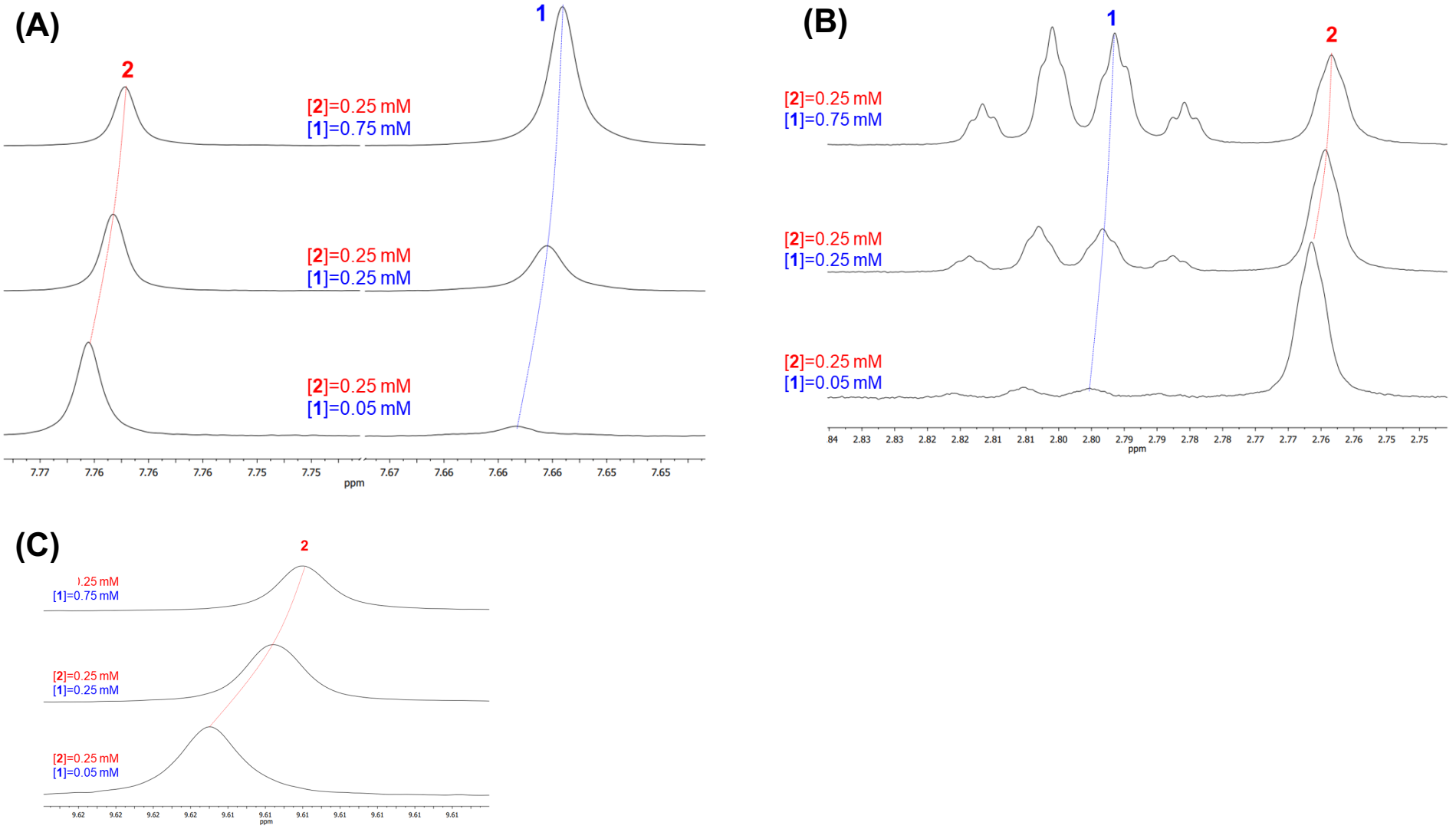


Figure S31. Partial ^{1}H NMR spectra measured at [**2**] = 0.25 mM, [**TFA**] = 6.54 M and [**1**] = 0.05 to 0.75 mM. Observed upfield shifts of (A) $\mathbf{H}_{C}$, (B) $\mathbf{H}_{E}$ and (C) C**H**O resonances from **2** and **1** were, we posit, caused by noncovalent interaction of capsularene **1** and *tris*-aldehyde **2** (**1** + **2** ↔ **1**⊂**2**).

Fitting procedure (Figure 4C in the main text): Concentrations of tris-aldehyde basket **2** (substrate, S) were determined as a function of time by NMR integration for reactions with initial total concentrations of 0.25, 0.3, 0.5 and 1.0 mM of *tris*-acetal basket **4**. For each series, results with the concentration of **2** (S) starting at 0.25 mM were extracted in order to obtain comparable time series with distinct concentrations of capsularene **1** (product, P) These data were then fitted directly in Julia 1.7 (https://epubs.siam.org/doi/10.1137/141000671) using DifferentialEquations.jl (Rackauckas, Christopher and Nie, Qing, A Performant and Feature-Rich Ecosystem for Solving Differential Equations in Julia, The Journal of Open Research Software, doi = 10.5334/jors.151) to a kinetic model with first order reaction rate k, and product inhibition, i.e. rapidly reversible formation of the complex [**1**⊂**2**] with dissociation constant K_d.

$$\frac{d[\mathrm{S}]}{dt} = -k[\mathrm{S}]_{\mathrm{free}}$$

$$[\mathrm{S}]_{\mathrm{free}} = \frac{[\mathrm{S}]_0 - [\mathrm{P}]_0 - K_d + \sqrt{([\mathrm{S}]_0 + [\mathrm{P}]_0 + K_d)^2 - 4[\mathrm{S}]_0[\mathrm{P}]_0}}{2}$$

Solvent Effect

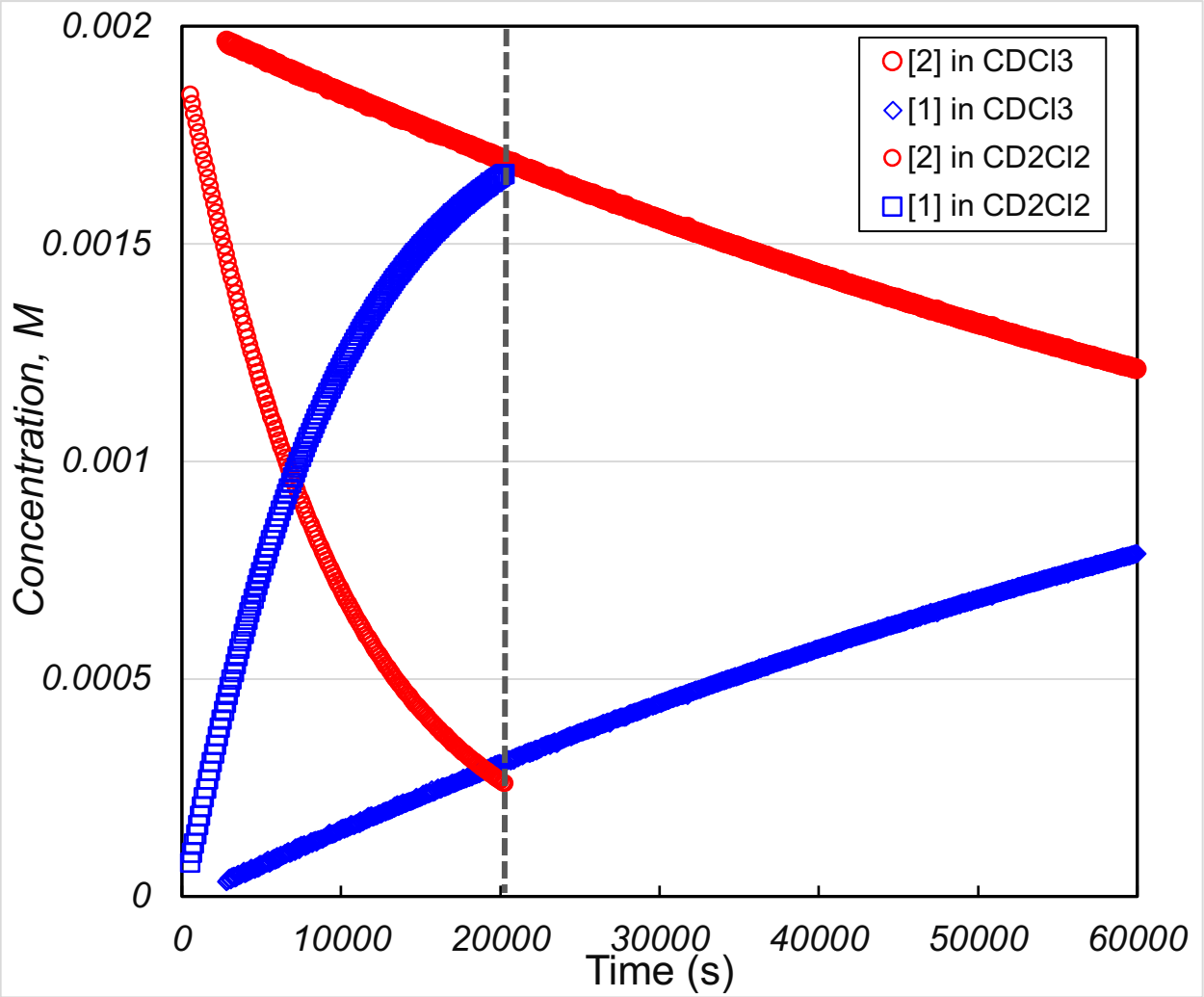


Figure S32. A plot showing the reaction progress for the formation of capsularene **1** and disappearance of *tris*-aldehyde **2** in CD_2Cl_2 and $CDCl_3$; note that for both reactions, $[\mathbf{2}]_0 = 2.00$ mM and $[\mathbf{TFA}]_0 = 3.27$ M. For convenience, we compared the ratio R=[**2**]/[**1**] at t=20.000 s and find that $R(CD_2Cl_2)$=0.18 while $R(CDCl_3)$=5.66. Apparently, the reaction was much slower in $CDCl_3$ than CD_2Cl_2.

Electrochemical Measurements

Bulk Electrolysis: Bulk electrolysis experiments were carried out with a BioLogic VSP galvanostat in a custom glass H-cell and reticulated vitreous carbon electrodes (100 ppi). A porous glass frit (P5, Adams and Chittenden) was used as the separator. A quasi-reference electrode (BASi) with 0.01 M $AgBF_4$ (Millipore Sigma) in 0.02 M recrystallized $TBAPF_6$ in MeCN was used on the working side of the H-cell. The electrolyte solution in the working chamber of the H-cell contained the corresponding sample and 0.02 M recrystallized $TBAPF_6$ in MeCN. The counter electrolyte contained the same solution. The working chamber of the H-cell was loaded with 5.5 mL of the electrolyte solution and stirred continuously during cycling at a rate of 0.5 mA with a voltaic cutoff. The counter chamber of the H-cell was also loaded with 5.5 mL of the electrolyte solution.

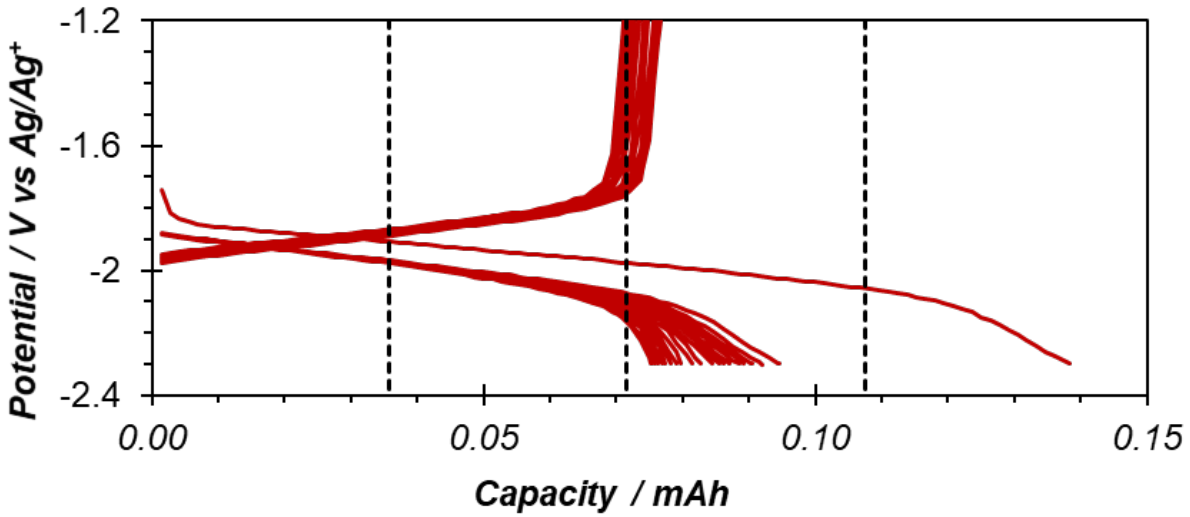


Figure S33. A plot showing bulk electrolysis data for *tris*-acetal basket **4** (0.243 mM). The cell was cycled at 0.5 mA in 0.02 M $TBAPF_6$ acetonitrile solution. Dashed lines show theoretical capacities for one-electron processes. The experimental data are in line with a 3-electron process, although a complete 3-electron reduction was limited by low solubility of **4**.

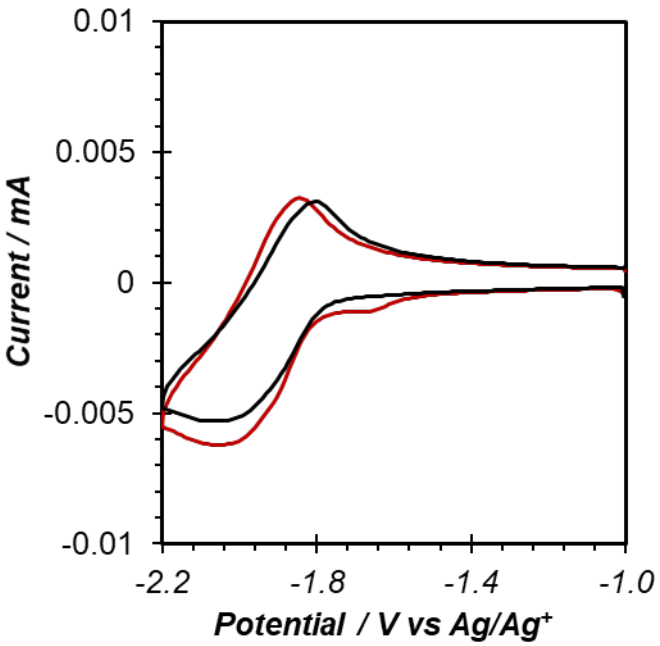


Figure 34. Cyclic voltammograms recorded before (red trace) and after (black trace) bulk electrolysis of *tris*-acetal basket **4** (0.243 mM). The cell was cycled at 0.5 mA in 0.02 M $TBAPF_6$ acetonitrile solution. No significant attenuation of the signal was observed after bulk electrolysis, which suggests that **4** is stable to bulk electrolysis.

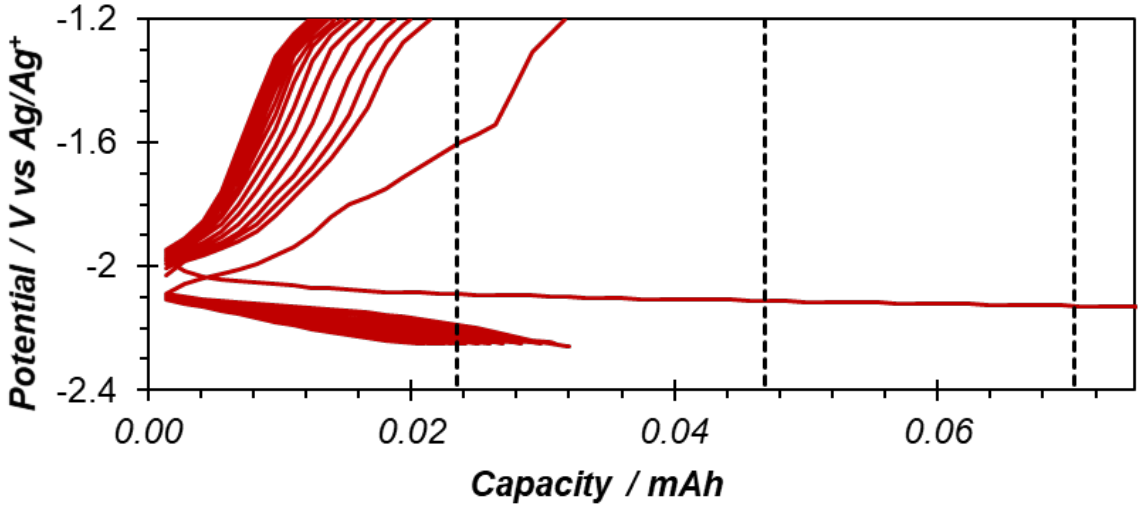


Figure 35. A plot showing bulk electrolysis data for capsularene **1** (0.175 mM). The cell was cycled at 0.5 mA in 0.02 M $TBAPF_6$ acetonitrile solution. Dashed lines show theoretical capacities for 1-electron processes. Capacity decay was observed with each cycle which suggests degradation of **1** during bulk electrolysis.

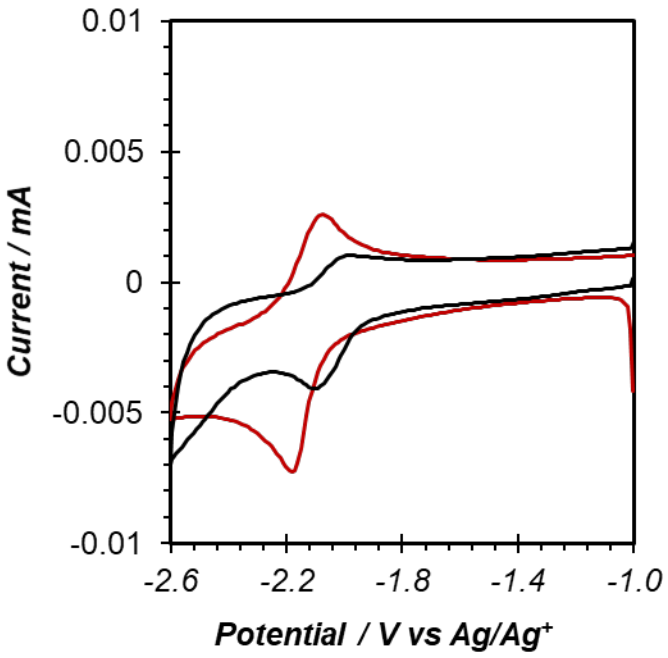


Figure 36. Cyclic voltammograms of 0.175 mM solution of capsularene **1** in acetonitrile, recorded before (red trace) and after bulk electrolysis (black trace). The cell was cycled at 0.5 mA in 0.02 M $TBAPF_6$ acetonitrile. Attenuation of the black trace suggests decay of **1** during bulk electrolysis.

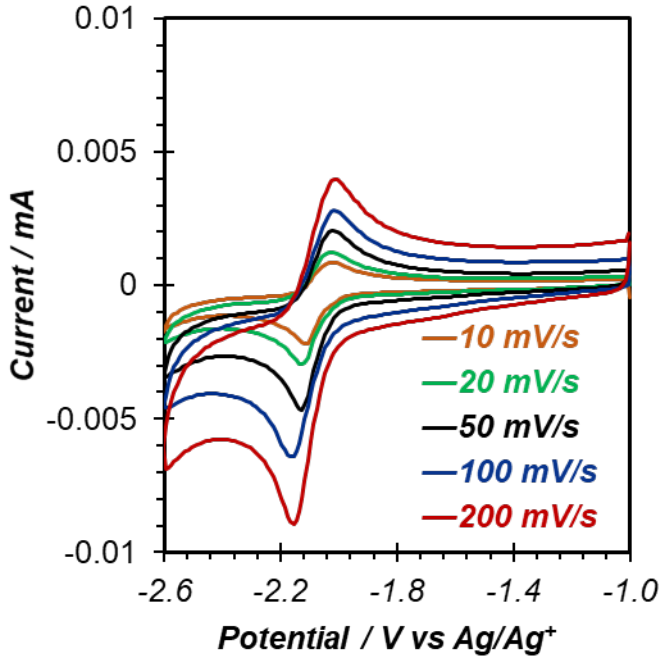


Figure 37. Cyclic voltammograms of *tris*-acetal basket **4** (0.175 mM) in 0.02 M $TBAPF_6$ acetonitrile solution obtained by varying the scan rate.

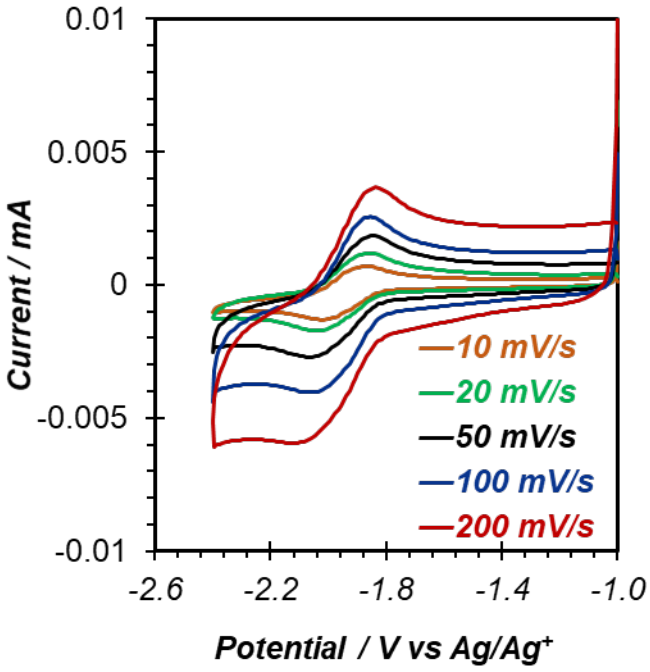
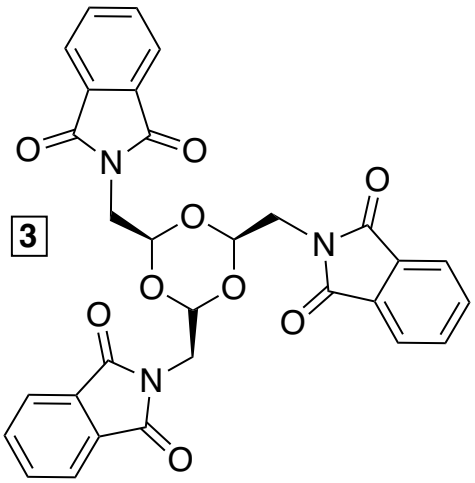


Figure 38. Cyclic voltammograms of capsularene **1** (0.175 mM) in 0.02 M $TBAPF_6$ in acetonitrile obtained by varying scan rates.

Thermal Gravimetric Analysis (TGA)



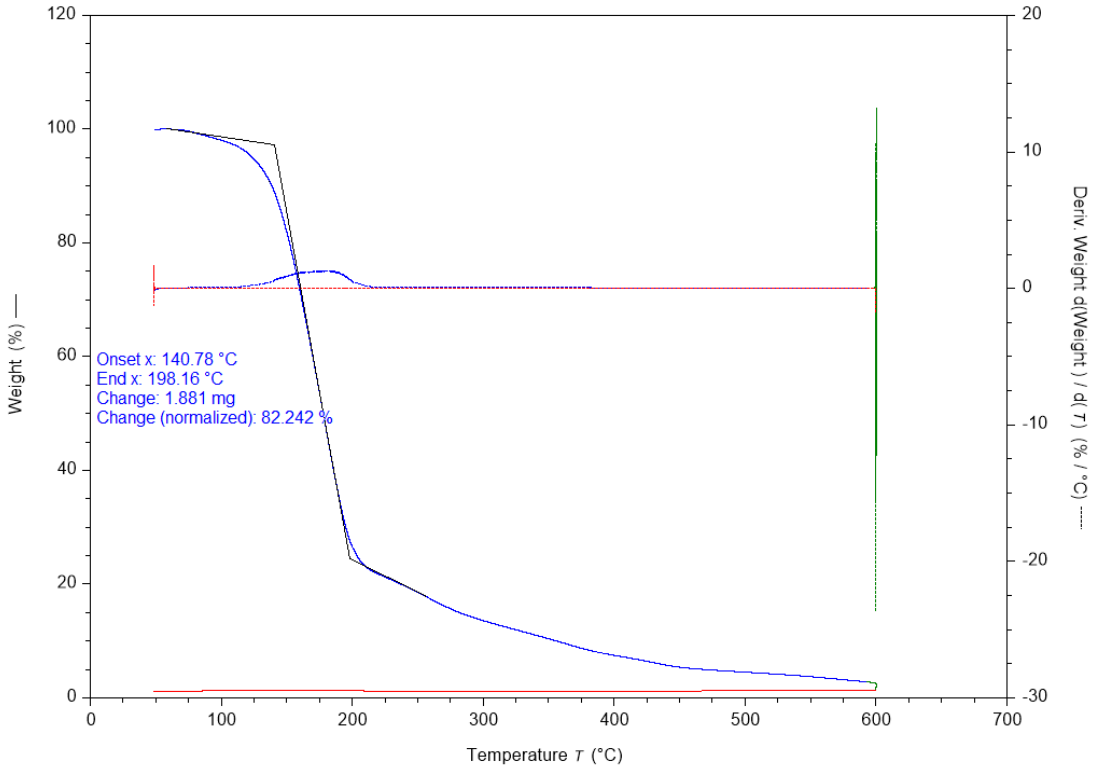


Figure S39. TGA plot obtained from 2.30 mg of compound **3**.

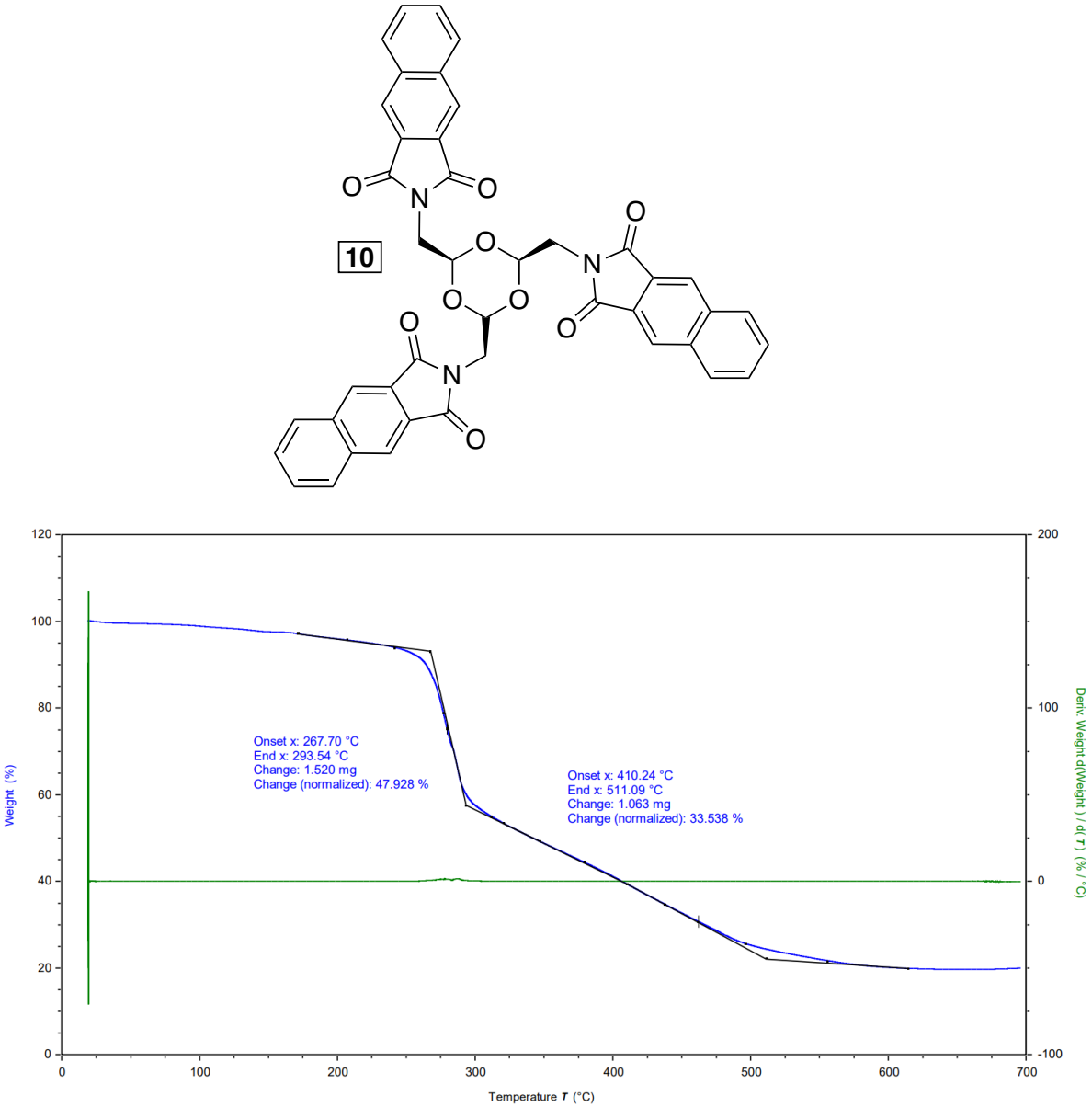


Figure S40. TGA plot obtained from 1.85 mg of compound **10**.

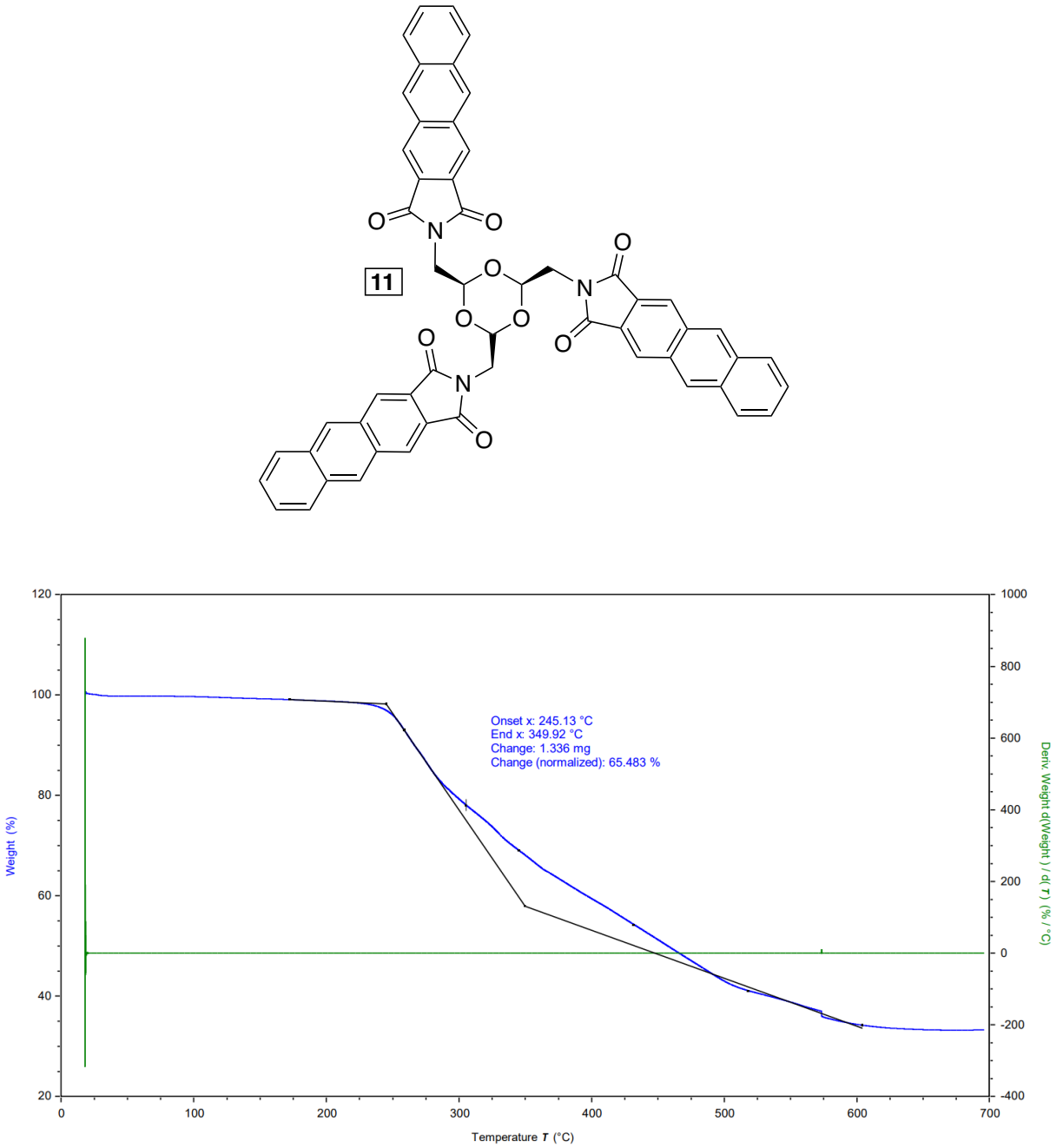


Figure S41. TGA plot obtained from 2.04 mg of compound **11**.

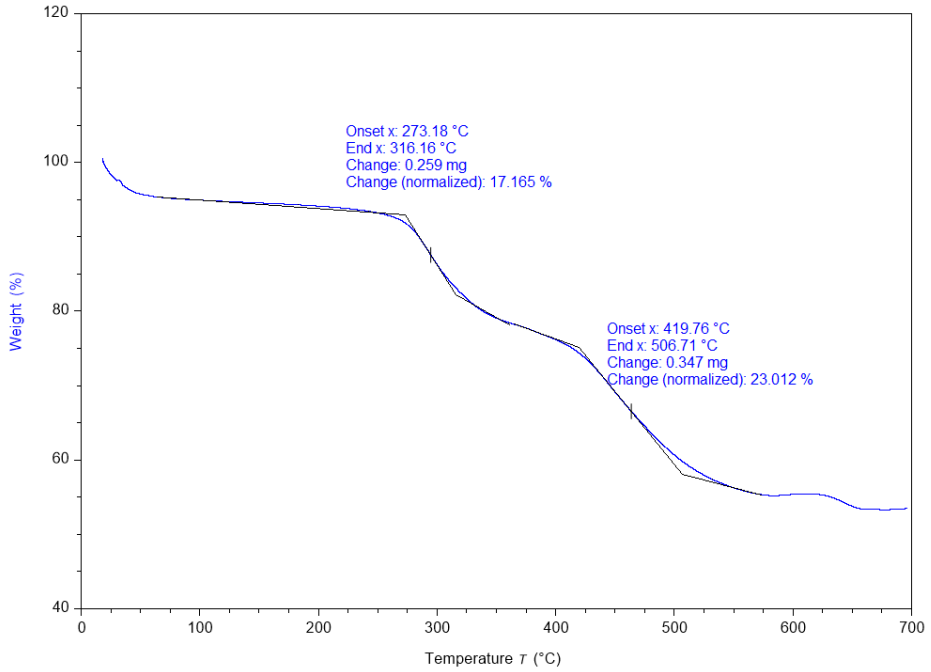


Figure S42. TGA plot obtained from 1.51 mg of capsularene **1**.

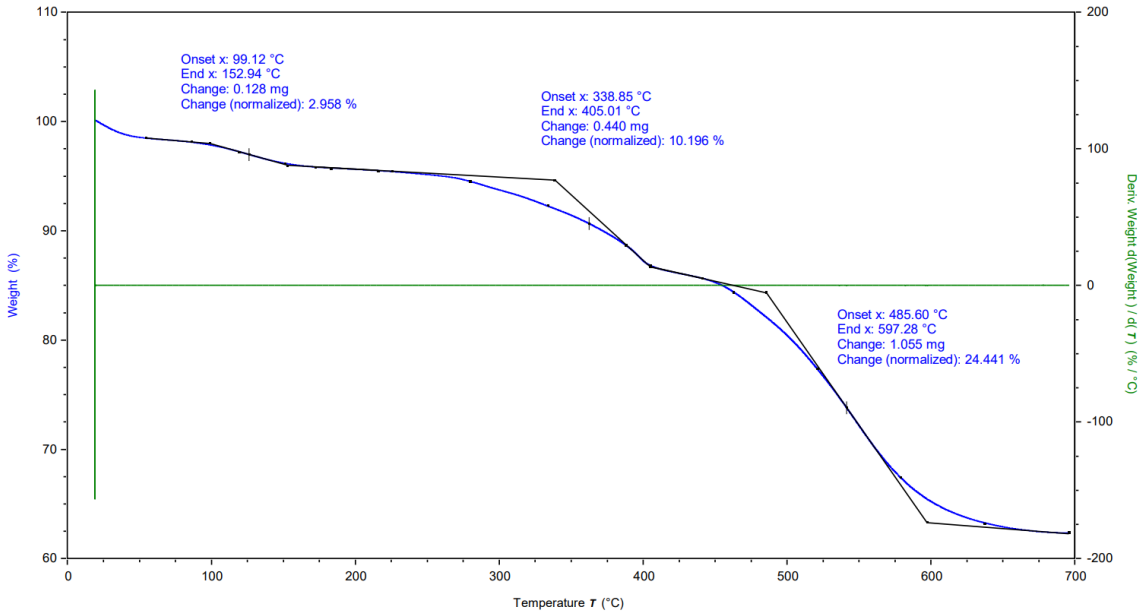


Figure S43. TGA plot obtained from 4.32 mg of capsularene **8**.

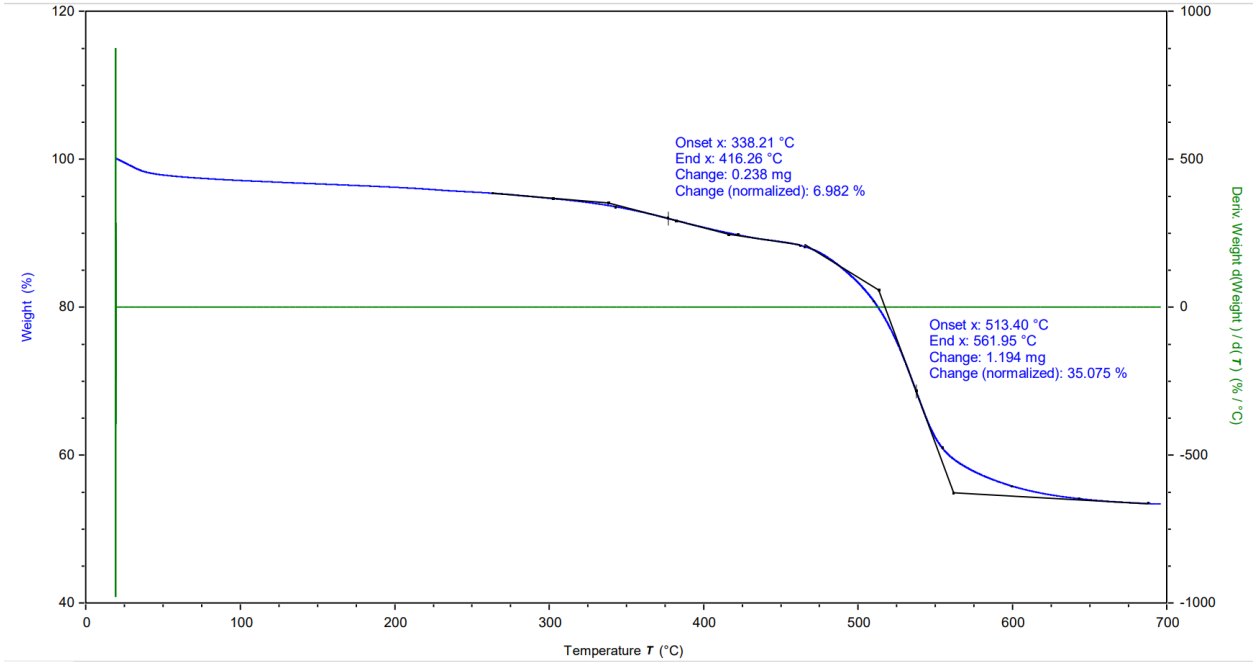


Figure S44. TGA plot obtained from 3.40 mg of capsularene **9**.

Computational Studies

Thermochemical Calculations with Capsularenes and Model Compounds: To inspect the thermodynamics of trioxane ring formation, density functional theory (DFT) calculations were carried out using Gaussian 16.[1] The specific reactions inspected are shown below (Figure S45).

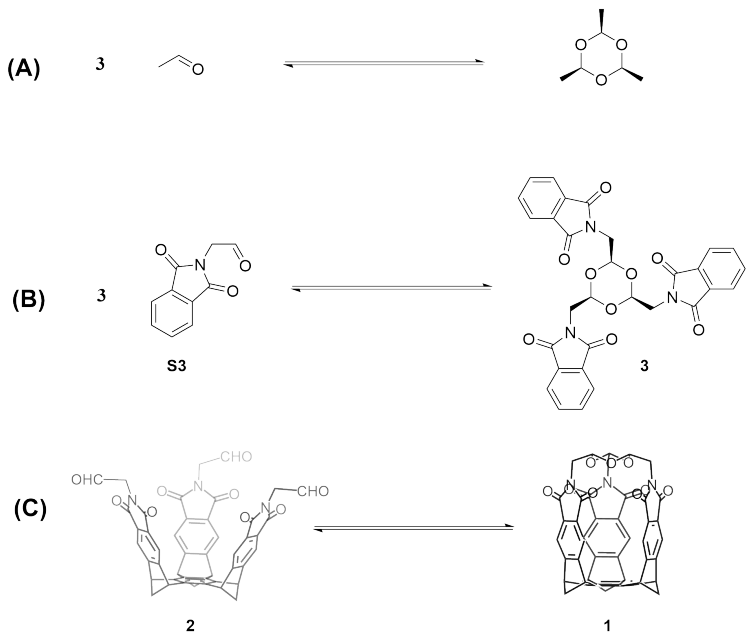


Figure S45. Thermodynamics of three chemical transformations (**A)**, (**B)** and (**C)** were studied using DFT.

To complete thermochemistry calculations, the following steps were taken. First, for 2-(2,2-dimethoxyethyl)isoindoline-1,3-dione, compound **3**, and *tris*-aldehyde **2**, a conformational search was completed in Macromodel.[2] Next, the optimization of the 10 lowest energy conformers (or fewer, if fewer were found in the search) was carried out at the B3LYP/6-31+G* level of theory[3] with the SMD[4] dichloromethane solvation model. A frequency calculation was carried out to compare thermodynamic stabilities and ensure that geometries were stable minima on the potential energy surface (PES). The thermodynamic quantities were then retrieved at 298 K, and the reaction free energies, enthalpies and entropies were compared. A table summarizing the values found for the free energy (*G*) and the enthalpy (*H*) for all conformers inspected is given below (Table S14). Then, a table summarizing the reactions' enthalpies and free energies is given (Table S15). Last, the coordinates of the lowest energy conformer of each molecule are given at the end of the computational section of the SI.

Table S14. Computed thermodynamic parameters (298 K) for conformers of reactants and products in Figure S45.

Reaction	Molecule	Conformer	Enthalpy (Hartree)	Free Energy (Hartree)
Figure S45 – (A)	Acetaldehyde	1	-153.778533	-153.807094
	Trioxane	1	-461.363856	-461.407542
Figure S45 – (B)	Aldehyde	1	-665.603172	-665.654776
	Aldehyde	2	-665.60314	-665.654379
	Aldehyde	3	-665.604515	-665.655101
	Aldehyde	4	-665.603105	-665.654436
	Trioxane **3**	1	N/A	N/A
	Trioxane **3**	2	-1996.822719	-1996.924989
	Trioxane **3**	3	-1996.826213	-1996.93273
	Trioxane **3**	4	N/A	N/A
	Trioxane **3**	5	-1996.826256	-1996.930192
	Trioxane **3**	6	-1996.825226	-1996.927997
	Trioxane **3**	7	-1996.825219	-1996.927735
	Trioxane **3**	8	-1996.822047	-1996.924127
	Trioxane **3**	9	-1996.827647	-1996.933128
	Trioxane **3**	10	-1996.818571	-1996.91936
Figure S45 – (C)	Aldehyde **2**	1	-2571.846089	-2571.973259
	Aldehyde **2**	2	-2571.845989	-2571.972815
	Aldehyde **2**	3	-2571.84504	-2571.972025
	Aldehyde **2**	4	-2571.843284	-2571.970203
	Aldehyde **2**	5	-2571.844618	-2571.971966
	Aldehyde **2**	6	-2571.844464	-2571.971379
	Aldehyde **2**	7	-2571.844447	-2571.971753
	Aldehyde **2**	8	N/A	N/A
	Aldehyde **2**	9	-2571.844531	-2571.97139
	Aldehyde **2**	10	-2571.841403	-2571.968588
	Trioxane **1**	1	-2571.838525	-2571.941255

*For entries marked N/A the calculation did not finish in the allocated wall time.

Table S15. The Boltzmann weighted thermodynamic parameters (298 K) for three reactions shown in Figure S45.

Reaction	Reaction Enthalpy $\Delta H°$ (kcal/mol)	Reaction Free Energy $\Delta G°$ (kcal/mol)
Figure S45 – (A)	-17.7312675	8.62185
Figure S45 – (B)	-8.849005	20.1898125
Figure S45 – (C)	4.74641	20.08251

Calculation of Strain Energy for 1: The strain energy of **1** was computed by considering two transformations below (A and B, Figure S46) comprising an isodesmic (B-minus-A) reaction. The enthalpy of the bonds forming in the absence of the bicyclic base (**S3** to **3**, ΔH_A) was subtracted from the energy of the bond forming reaction in the presence of the bicyclic base (**2** to **1**, ΔH_B). This $\Delta H_B - \Delta H_A$ was then taken as the strain energy (Table S16).

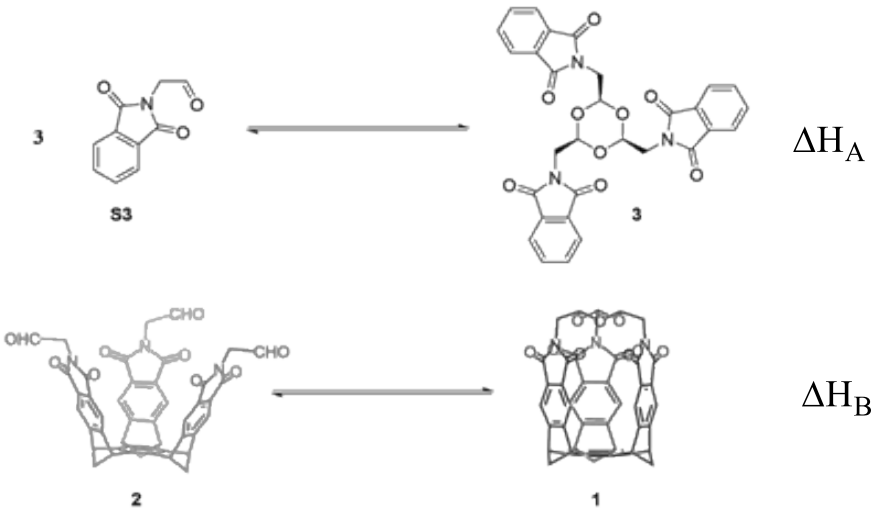


Figure S46. Chemical transformations (**A)** and (**B)** were used to compute the strain of capsularene **1**.

Table S16. The Boltzmann weighted thermodynamic parameters (298 K) for strain calculation represented in figure S46.

Reaction	Reaction Enthalpy $\Delta H°$ (kcal/mol)
Figure S46 – (ΔH_A)	-8.849
Figure S46 – (ΔH_B)	4.746
Strain Energy	13.595

Calculation of UV-vis spectra with time dependent DFT (TD-DFT): In addition to reaction thermodynamics, the optical characteristics of capsularenes **1**, **8**, and **9** were studied using the TD-DFT method described in previous publications.[5,6] In brief, capsularenes were first optimized at the B3LYP/6-31+G* level of theory with SMD dichloromethane solvation and frequency calculations were run to ensure the structures were minima on the PES. These optimized structures were then put through a TD-DFT calculation at the CAM-B3LYP[7]/def2svpd level of theory. Since the def2svpd basis set is not implemented in Gaussian 16, the basis set was obtained from the basis set exchange website.[8] For **1** and **8**, the calculation of 20 states was sufficient to reproduce the observed UV transitions. For **9**, 30 states were calculated to reproduce the experimentally observed UV-Vis transitions. The calculated UV-Vis spectra were in Figures S46-S48 plotted against the experimental data.

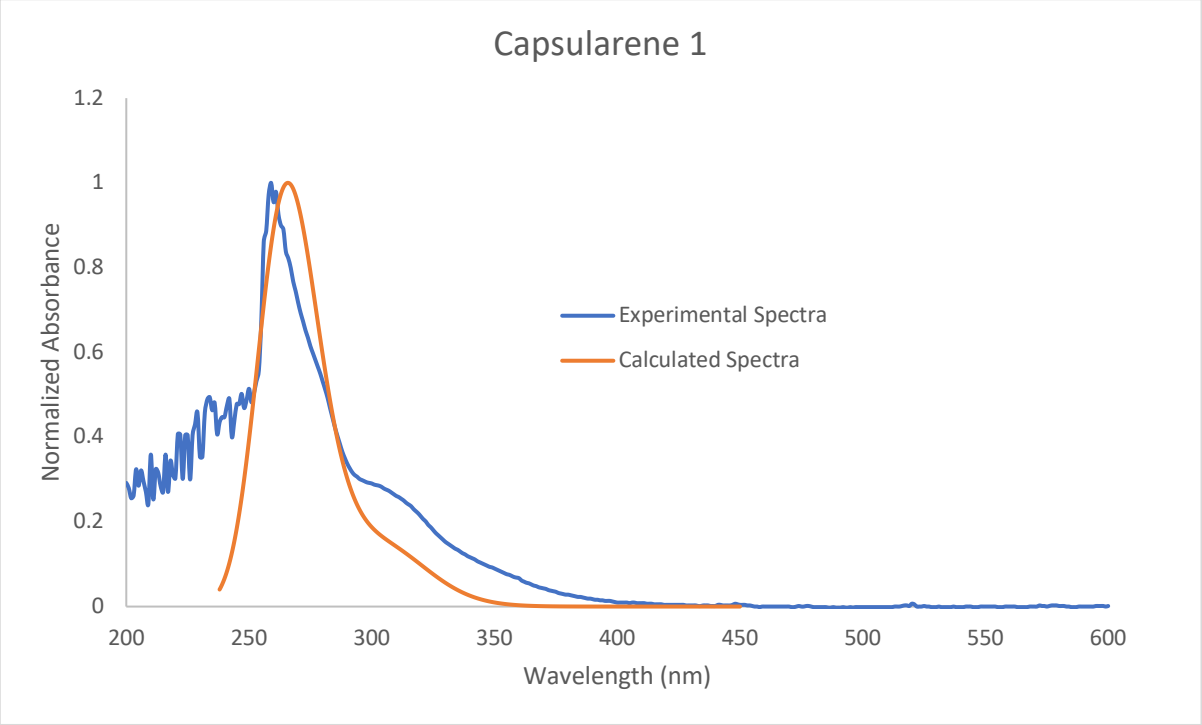


Figure S47. Computed (red) and experimental (blue) UV-vis spectra of capsularene **1**. GaussView 6.0 was used to apply gaussian line broadening of the computed transitions, with no shift applied to the spectrum.

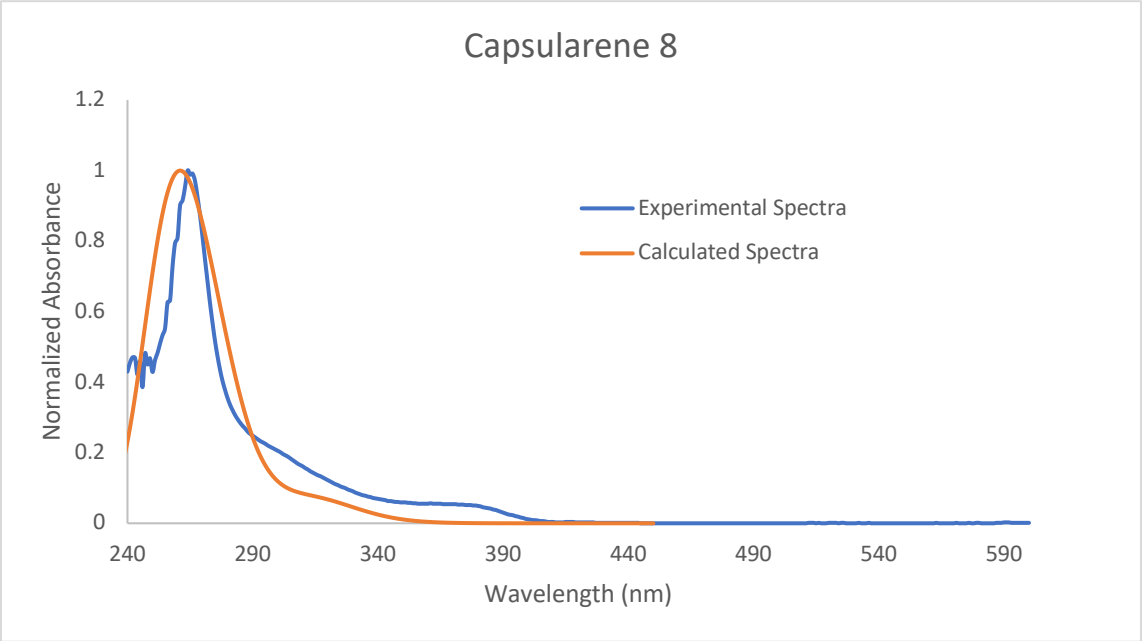


Figure S48. Computed (red) and experimental (blue) UV-vis spectra for capsularene **8**. GaussView 6.0 was used to apply gaussian line broadening of the computed transitions, with no shift applied to the spectrum.

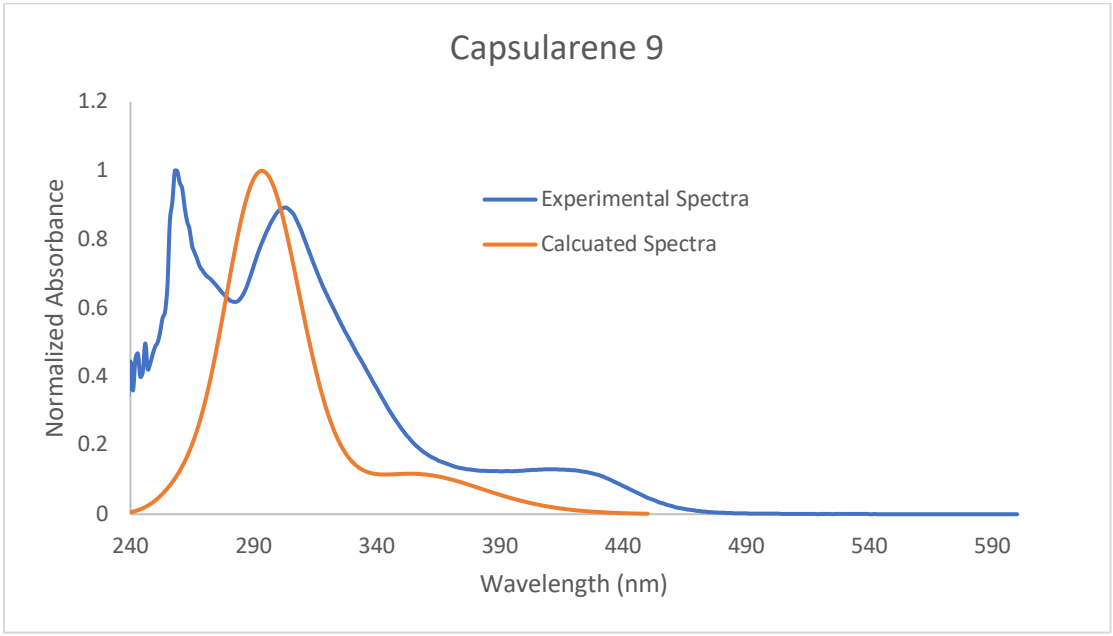


Figure S49. Computed (red) and experimental (blue) UV-vis spectra for capsularene **8**. GaussView 6.0 was used to apply gaussian line broadening of the computed transitions, with no shift applied to the spectrum.

Orbital analysis of electronic transitions: Following the calculation of UV-vis spectra via a TD-DFT methodology, a natural transition orbital (NTO) calculation was carried out at the same level of theory to inspect the type of orbital transition giving rise to the lowest energy UV-vis band. Visualizations of these lowest energy NTOs are given below (Figures S49-S51). Note that only one NTO is shown to identify the type of transition and that other NTOs, which are comprised of linear combinations of very similar orbitals localized on the independent arms, are not shown here.

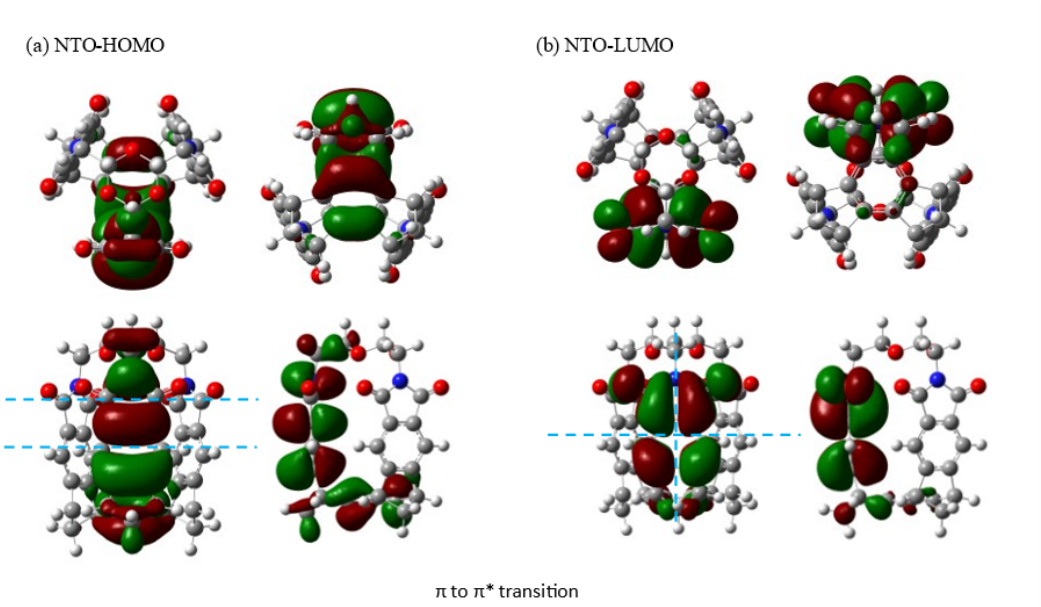


Figure S50. NTOs for the lowest energy electronic transition of **1**. (a) HOMO orbital for the first transition. (b) LUMO orbital for the first transition. To visualize the orbitals, we used GaussView 6.0.

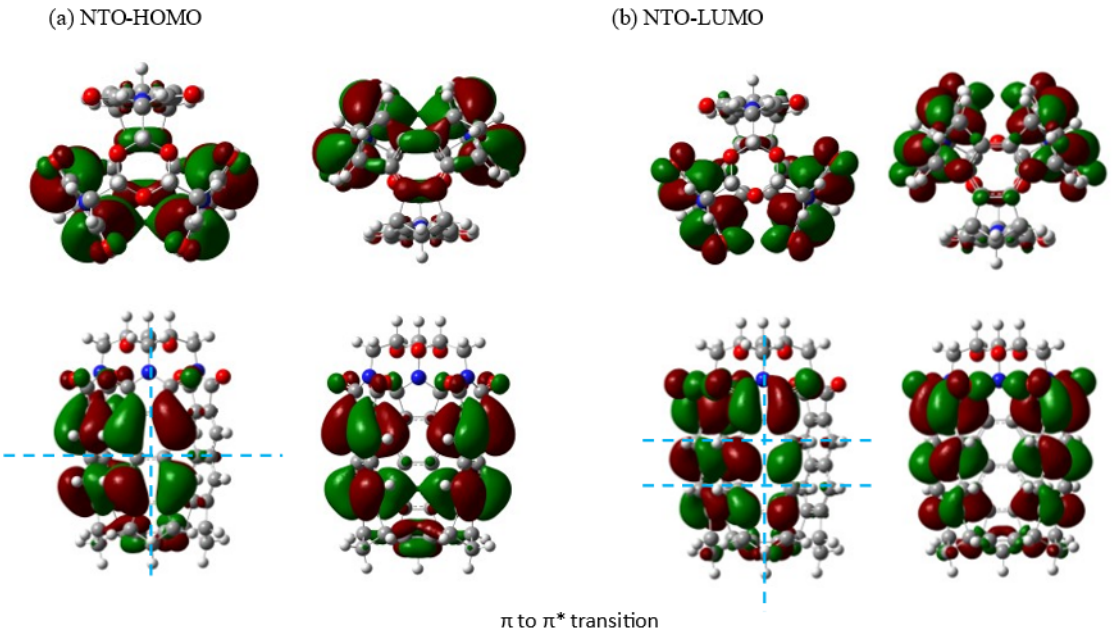


Figure S51. NTOs for the lowest energy UV transition of **8**. (a) HOMO orbital for the first transition. (b) LUMO orbital for the first transition. To visualize the orbitals, we used GaussView 6.0.

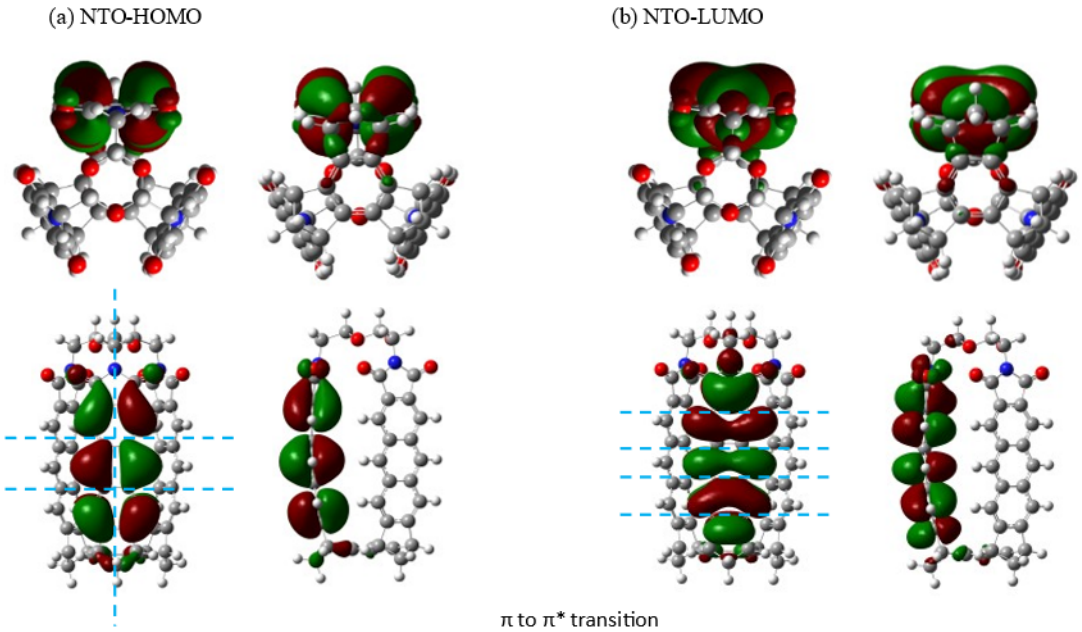


Figure S52. NTOs for the lowest energy UV transition of **8**. (a) HOMO orbital for the first transition. (b) LUMO orbital for the first transition. To visualize the orbitals, we used GaussView 6.0.

Molecular coordinates for computed structures (B3LYP/6-31+G*)

Acetaldehyde
E(RB3LYP) = 153.838116
Number of imaginary frequencies: 0

Cartesian Coordinates:

C	0.07645200	-0.93507300	0.00002400
H	0.60788100	-1.91174900	0.00252300
C	-1.43530300	-0.98471300	0.00001300
H	-1.81056900	-2.01246400	0.00154300
H	-1.81784500	-0.45641400	0.88180400
H	-1.81778600	-0.45897400	-0.88332500
O	0.71416900	0.09738800	-0.00258200

Methyl Trioxane
E(RB3LYP) = -461.556155
Number of imaginary frequencies: 0

Cartesian Coordinates:

C	0.46883600	-1.67076600	0.06212700
C	0.47014500	0.40777700	1.15054100
C	-1.46825100	-0.91397500	1.14807500
H	0.80737600	-2.16925700	0.98994900
H	0.80872600	-0.07122000	2.08856800
H	-1.14737300	-1.40534500	2.08590900
O	0.97551800	-0.34469300	0.05800600
O	-0.95064200	-1.65771900	0.05535000
O	-0.94936600	0.40728800	1.13676000
C	-2.97334500	-0.85264200	1.03278300
H	-3.38901100	-1.86489500	1.04358100
H	-3.38798700	-0.28468500	1.87126400
H	-3.25150100	-0.36154900	0.09554100
C	0.96299400	1.83139300	1.03750800
H	0.58423100	2.42405400	1.87587100
H	2.05711200	1.84855700	1.05032800
H	0.60915400	2.27059700	0.10003500
C	0.96024400	-2.38924400	-1.17264900
H	2.05433400	-2.41079200	-1.18004800
H	0.58030200	-3.41545700	-1.18209900
H	0.60650400	-1.86842600	-2.06740100

Phthalimide Aldehyde **S3**
E(RB3LYP) = -665.770102
Number of imaginary frequencies: 0

Cartesian Coordinates:

C	5.76429500	-3.83366700	0.16423200
C	4.36805100	-3.86169700	0.07566600
C	3.62612300	-2.69710400	-0.06800700
C	4.33212100	-1.48523100	-0.12227400
C	5.73063700	-1.45723200	-0.03319100
C	6.47164800	-2.64020600	0.11280400
C	6.24759300	-5.23502300	0.30978600
C	3.92688400	-5.28179400	0.16334000
H	2.54257600	-2.72204800	-0.13804900
H	3.78589500	-0.55292600	-0.23651500
H	6.24957900	-0.50374900	-0.07922700
H	7.55548400	-2.62188600	0.18096000
N	5.09783600	-6.03981600	0.31920700

O	2.79964500	-5.74614600	0.12630000
O	7.38841900	-5.65368200	0.41436800
C	5.12328700	-7.48162200	0.38007100
H	5.98054000	-7.80751300	0.98188000
H	4.21711300	-7.84368000	0.88101700
C	5.21528000	-8.14851200	-0.97911500
O	5.26543500	-7.55492000	-2.03648400
H	5.23406000	-9.25554900	-0.93996900

Phthalimide Trioxane (**3**)
E(RB3LYP) = -1997.334723
Number of imaginary frequencies: 0

Cartesian Coordinates:

C	-13.17061900	-5.81893100	-13.82195800
C	-13.64561500	-4.67650000	-13.16987400
C	-14.68129400	-4.74433800	-12.24768700
C	-15.23882600	-6.00753700	-11.99614200
C	-14.76345000	-7.15251000	-12.65057400
C	-13.71380800	-7.07350500	-13.57882100
C	-12.06353900	-5.40530900	-14.72894600
C	-12.85171100	-3.50690700	-13.64287600
H	-15.04617100	-3.85538600	-11.74136800
H	-16.05195000	-6.10042900	-11.28126400
H	-15.21481700	-8.11700400	-12.43421900
H	-13.34120000	-7.95888200	-14.08588000
N	-11.94301900	-4.01618500	-14.58981300
O	-12.92351800	-2.34176700	-13.29643700
O	-11.36838200	-6.09376300	-15.45983600
C	-10.94600300	-3.21346200	-15.27758000
H	-10.91595900	-2.23455900	-14.79420200
H	-9.96679600	-3.69197400	-15.18424100
C	-11.25614100	-3.03549600	-16.75964200
H	-11.31657300	-3.99957300	-17.28637900
C	-12.74192900	-2.06960900	-18.27351700
C	-10.44434600	-1.98211600	-18.68028800
H	-12.82683400	-3.01906500	-18.82351200
H	-10.48380200	-2.92564400	-19.24541000
O	-12.48579500	-2.34584200	-16.90589700
O	-11.68172600	-1.30373000	-18.82348200
O	-10.19581000	-2.26923800	-17.31320900
C	-9.31559300	-1.07569600	-19.15877200
N	-9.43660200	-0.73022800	-20.56484600
H	-8.36445500	-1.58961500	-18.99376500
H	-9.32880400	-0.14772200	-18.58309200
C	-9.11531300	-1.60171600	-21.61519800
C	-9.82761900	0.53519600	-21.03976100
C	-9.35176300	-0.84022800	-22.87311000
O	-8.71885700	-2.74745400	-21.47070500
C	-9.78252700	0.44462100	-22.52702600
O	-10.11621500	1.48887000	-20.33870400
C	-9.20304500	-1.22471100	-24.19898800
C	-10.08015100	1.39558700	-23.49390600
C	-9.50394800	-0.27154600	-25.18413000
H	-8.86747100	-2.22322100	-24.46384900
C	-9.93509500	1.01646600	-24.83743900
H	-10.41256600	2.39329300	-23.22225800
H	-9.40088100	-0.53548000	-26.23314300
H	-10.16007700	1.73302500	-25.62261700
C	-14.00466800	-1.22364700	-18.39220100
N	-15.18085800	-1.89334000	-17.86355900

H	-14.16438000	-0.98631600	-19.44801900
H	-13.87056000	-0.29584700	-17.83189800
C	-15.83217900	-2.95710500	-18.50140400
C	-15.84997000	-1.50251300	-16.68821500
C	-17.00154200	-3.30193000	-17.64487700
O	-15.47294900	-3.46183700	-19.55403300
C	-17.01058400	-2.42814500	-16.55287000
O	-15.52168400	-0.57559100	-15.97018200
C	-17.97523300	-4.27952400	-17.80133300
C	-17.99431700	-2.49670200	-15.57557300
C	-18.97292100	-4.35893100	-16.81747600
H	-17.96664700	-4.95537200	-18.65167800
C	-18.98228100	-3.48250600	-15.72340300
H	-17.99915000	-1.81477700	-14.73014800
H	-19.75218700	-5.11115600	-16.90550800
H	-19.76887400	-3.56754100	-14.97846100

Basket Aldehyde (**2**)
E(RB3LYP) = -2572.517622
Number of imaginary frequencies: 0

Cartesian Coordinates:

O	15.18208900	48.70030000	24.05947100
O	6.13397200	50.54701600	22.71631500
O	12.63278700	55.41251700	18.07581900
O	16.66582500	51.90442500	21.11560900
O	9.15223600	47.91674700	24.97619100
O	8.12358200	54.83673100	18.76357900
N	16.03713700	50.49430700	22.85356400
N	7.57017300	49.40163400	24.14053500
N	10.36608900	55.42564200	18.59324800
C	12.55095700	48.22406200	17.50952700
C	10.74006900	47.05637000	18.63037000
C	10.24505600	48.82975700	17.04618100
C	12.08933300	47.22885100	18.42484600
C	9.80059000	47.87200900	17.92790400
C	11.64635300	49.00916400	16.83301300
C	13.34299700	46.55143300	18.99145700
C	8.40969000	47.41971700	18.38813000
C	11.78366900	50.13967900	15.80621500
H	13.19730000	45.58530700	19.47592000
H	7.56917700	47.71490300	17.75905400
H	12.74658800	50.22446200	15.30137800
C	14.05257200	47.61747500	19.82874600
C	8.30838600	47.81094400	19.86385700
C	11.28390000	51.40510400	16.50599500
C	14.51017500	48.60472200	18.92139300
C	9.23984400	47.00194200	20.56050700
C	9.89434200	51.22731100	16.71793900
C	14.08233100	48.14605800	17.52582500
C	9.91434900	46.11326800	19.51363700
C	9.53900200	49.85244600	16.14809500
H	14.60212400	48.61663400	16.69053400
H	10.42874500	45.23192400	19.89829600
H	8.48056600	49.67828200	15.95128500
C	14.24818600	46.60365900	17.71805100
C	8.69286400	45.89234000	18.56340000
C	10.52312400	49.83417700	14.93356800
H	15.28341200	46.30586100	17.91642600
H	7.86769000	45.35655800	19.04474300
H	10.31105100	50.61850500	14.19904100

H	13.84338400	46.02338900	16.88248500
H	8.96565700	45.39815500	17.62522400
H	10.57254600	48.85869700	14.43882600
C	14.26387700	47.72589800	21.20022800
C	7.51916700	48.75222900	20.51851900
C	11.94787800	52.55784300	16.91534100
H	13.91926200	46.97421300	21.90526300
H	6.79896500	49.37598000	19.99576700
H	13.01239500	52.70659200	16.75525600
C	14.96200500	48.85920500	21.62373200
C	7.69437700	48.84166900	21.90142400
C	11.15982500	53.52958600	17.53640200
C	15.41357100	49.83347600	20.72837600
C	8.61306700	48.04283600	22.58883600
C	9.78862500	53.35424000	17.74559000
C	15.19607000	49.73676700	19.35199500
C	9.41606400	47.10385300	21.93734700
C	9.11752600	52.19577900	17.34727300
H	15.55415200	50.49888400	18.66505100
H	10.12487500	46.48633700	22.48248200
H	8.05067300	52.07176400	17.51269100
C	15.36979200	49.26755800	22.99539500
C	7.00622700	49.71206800	22.89306900
C	11.54109700	54.86712200	18.06585700
C	16.11971700	50.88613200	21.50816000
C	8.53132900	48.38388700	24.03511200
C	9.26309700	54.57597300	18.41313800
C	7.12740200	49.97130500	25.38988300
H	6.82932000	51.01520300	25.23316100
H	7.95883200	49.97419300	26.10549400
C	10.27776400	56.75796200	19.13988700
H	9.49688300	56.78807300	19.90987500
H	11.22521500	57.01780800	19.62769100
C	16.65991300	51.20625500	23.94294200
H	16.09067900	51.03380200	24.86464800
H	16.63419100	52.28406500	23.74060300
C	18.10078700	50.80450100	24.19343700
H	18.58487600	51.35153100	25.02662300
C	9.96666200	57.82364300	18.10660300
H	9.89722800	58.84939100	18.51997600
C	5.96159200	49.23360800	26.02006900
H	5.61187600	49.67186800	26.97580600
O	9.80111500	57.60984200	16.92327800
O	18.70332300	49.96303800	23.55925800
O	5.43308700	48.24753300	25.54926300

Benzene Capsularene (**1**)
E(RB3LYP) = -2572.516041
Number of imaginary frequencies: 0

Cartesian Coordinates:

O	-4.98436600	-8.08800700	-11.14010500
O	-5.15770700	-9.47642800	-9.28396800
O	-5.58869200	-7.20096700	-9.07762800
O	-4.57864200	-6.12107600	-6.10229700
O	-2.83571300	-11.86162200	-9.44725700
O	-2.52071400	-9.11100500	-13.09953100
O	-4.33427700	-4.14805800	-8.74942800
O	-3.69266300	-10.59961000	-6.51295600
N	-3.07562000	-10.34781300	-11.20380000
N	-4.41876900	-8.38627000	-6.62750300

N	-4.04587700	-5.30293600	-10.75326900
C	-2.20481000	-9.63109700	-12.04461100
C	-2.20010400	-8.71488400	-6.06326000
C	0.15473300	-4.26831600	-9.15267000
C	-2.12492100	-4.51339400	-9.73432800
C	-0.86751600	-9.68247800	-11.38759300
C	-0.90906900	-9.23327500	-5.94042700
H	-0.71288400	-10.29634500	-6.04858500
C	0.10304000	-10.71402200	-9.39448700
H	0.01082600	-11.36029100	-8.52610400
C	-0.96482900	-10.51903900	-10.27352800
C	1.35911900	-9.14092600	-10.79823000
C	2.39061800	-8.33402600	-8.32214400
C	-3.91757800	-7.13761800	-6.21640600
C	2.23435200	-6.13330700	-9.34111600
C	2.49288700	-7.48066800	-9.46319900
C	-3.60812100	-4.59881700	-9.61691600
C	1.86031000	-5.58977500	-8.07412200
C	-2.46853600	-7.35001700	-5.93858500
C	-1.75812500	-5.04206400	-10.97371000
C	-1.46219800	-6.41508200	-5.68449100
H	-1.68279400	-5.35466700	-5.59965100
C	-5.33683700	-9.38740400	-10.68960600
H	-6.39990400	-9.56820700	-10.92477800
C	-2.36531500	-11.02312600	-10.19482800
C	-4.50793400	-10.45190200	-11.40782300
H	-4.71179600	-10.37394600	-12.47898200
H	-4.83722700	-11.43256100	-11.05444600
C	1.44601200	-4.13433200	-8.33768600
H	1.40288900	-3.47228300	-7.47207300
C	1.63110000	-8.44637400	-5.76099500
H	2.02438700	-9.44231600	-5.55426100
C	0.10551200	-8.30259000	-5.73449600
C	-5.77256400	-7.10675800	-10.48310800
H	-6.83576000	-7.29121000	-10.71532300
C	-2.99876900	-5.47524500	-11.67704600
C	2.69807200	-8.40467900	-10.67292300
H	3.08059300	-7.94251200	-11.58365000
C	1.75977300	-6.41269000	-6.97425400
C	-5.77050700	-8.60565000	-7.10511200
H	-6.08763300	-9.60629200	-6.79981200
H	-6.42661200	-7.86761000	-6.63629500
C	3.54962700	-9.52594000	-10.00478600
H	4.52273500	-9.16927200	-9.65169600
H	3.68156800	-10.40225400	-10.64831900
C	0.30502100	-8.98809900	-11.69511100
H	0.36462300	-8.33347000	-12.56009800
C	2.03179000	-7.80945200	-7.10007100
C	1.25928100	-9.98794700	-9.66715200
C	2.04610800	-5.00368700	-10.36502100
C	-0.42205700	-5.18181100	-11.35630000
C	0.52676800	-4.80624500	-10.40929600
C	2.53591000	-9.77051300	-8.84677400
H	2.77197600	-10.54014100	-8.11105400
C	-0.16592300	-6.91783900	-5.60968500
C	1.19389600	-6.21146000	-5.56027900
H	1.19316100	-5.19204200	-5.17280900
C	-5.41988200	-5.70654500	-10.98436300
H	-6.07892200	-4.99206300	-10.48405200
H	-5.61364500	-5.67431900	-12.05971500
C	-3.47042200	-9.40541500	-6.42454500
C	2.44158800	-3.78121800	-9.48328500

H	3.48795800	-3.80750400	-9.16207400
C	-5.94299200	-8.49782000	-8.61999300
H	-7.00705700	-8.67859100	-8.85188800
C	-1.17945200	-4.08846100	-8.79797700
H	-1.47828200	-3.68759600	-7.83347800
C	2.01819100	-7.28836300	-4.79267100
H	3.09280600	-7.07863000	-4.78645600
H	1.66113400	-7.44999400	-3.76999000
H	-0.15020600	-5.60478000	-12.31938200
H	2.21915500	-2.82114500	-9.96107700
O	-3.12921600	-5.87688700	-12.81934900
H	2.54432200	-5.12610900	-11.32735100

Naphthalene Capsularene (**8**)
E(RB3LYP) = -3033.489751
Number of imaginary frequencies: 0

Cartesian Coordinates:

O	1.16243400	0.66405300	-5.05243300
O	0.00000000	-1.34978300	-5.06871000
O	-1.16243400	0.66405300	-5.05243300
O	-4.01344900	0.32668400	-3.32386000
O	1.70646800	-3.63630800	-3.31499600
O	4.01344700	0.32668600	-3.32385900
O	-2.29270800	3.28198100	-3.30227100
O	-1.70646800	-3.63630800	-3.31499600
N	2.61019900	-1.51009900	-3.63506900
N	-2.61019900	-1.51009900	-3.63506900
N	0.00000000	2.99856800	-3.61717500
C	3.36355300	-0.59900300	-2.86875800
C	-0.71558000	3.00979600	3.36535300
C	-2.03429200	-2.81634900	2.18974700
H	-1.48523100	-3.75528000	2.17910000
C	2.03429300	-2.81634900	2.18974700
H	1.48523100	-3.75528000	2.17910100
C	2.49275600	-2.26978000	0.95149700
C	2.95654400	-0.87640300	3.34904100
C	0.68968300	-1.21904900	4.96423000
C	-3.36355300	-0.59900400	-2.86875800
C	0.71383400	1.21189100	4.97164300
C	1.40342300	0.01747200	4.96574400
C	-1.16444500	3.19284200	-2.84960400
C	-0.71383400	1.21189100	4.97164300
C	-3.21527900	-1.02023200	0.95043700
C	0.72173300	3.30018300	0.96685500
C	-3.45953100	-0.34838500	2.18822000
H	-3.99947500	0.59575100	2.17666300
C	1.16583400	-0.67631300	-5.52231800
H	1.16241300	-0.66461100	-6.62588400
C	2.19277200	-2.61293500	-2.86497800
C	2.42983400	-1.40780300	-5.07185400
H	3.29007300	-0.87841700	-5.48956400
H	2.40063500	-2.41767900	-5.48899500
C	-1.14520900	2.67408300	4.79620300
H	-2.17557500	2.91568300	5.05935500
C	-1.74032300	-2.32278600	4.78169900
H	-1.43636100	-3.33681500	5.04386500
C	-2.24119400	-2.11602000	3.34957500
C	0.00000000	1.33947300	-5.51082500
H	0.00000000	1.33491900	-6.61429000
C	1.16444600	3.19284100	-2.84960400

C	2.88469700	-0.33882200	4.78155400
H	3.60978000	0.43247900	5.04353200
C	-1.40342300	0.01747200	4.96574400
C	-2.42983400	-1.40780300	-5.07185400
H	-2.40063500	-2.41767900	-5.48899500
H	-3.29007300	-0.87841700	-5.48956400
C	2.92882600	-1.68625000	5.56509700
H	2.71831200	-1.56461800	6.63276900
H	3.87016400	-2.22933500	5.42767100
C	3.45953000	-0.34838500	2.18822000
H	3.99947400	0.59575100	2.17666300
C	-0.68968300	-1.21904900	4.96423000
C	2.24119400	-2.11602000	3.34957500
C	1.14520900	2.67408300	4.79620300
C	1.42501600	3.17926400	2.20500800
C	0.71558000	3.00979600	3.36535300
C	1.74032300	-2.32278600	4.78169900
H	1.43636100	-3.33681500	5.04386600
C	-2.95654400	-0.87640300	3.34904000
C	-2.88469700	-0.33882200	4.78155400
H	-3.60978000	0.43247900	5.04353200
C	0.00000000	2.79720400	-5.05454700
H	-0.88896600	3.27911900	-5.46954900
H	0.88896600	3.27911900	-5.46954900
C	-2.19277200	-2.61293600	-2.86497800
C	0.00000000	3.38178000	5.58280800
H	0.00000000	3.13421900	6.64943000
C	-1.16583400	-0.67631300	-5.52231800
H	-1.16241400	-0.66461100	-6.62588400
C	-1.42501600	3.17926400	2.20500800
H	-2.51276000	3.17252000	2.19408700
C	-2.92882600	-1.68624900	5.56509700
H	-2.71831200	-1.56461800	6.63276900
H	-3.87016400	-2.22933500	5.42767000
H	2.51276000	3.17251900	2.19408700
H	0.00000000	4.46912700	5.45008600
O	2.29270800	3.28197900	-3.30227100
H	2.17557500	2.91568300	5.05935500
C	-2.49275500	-2.26978000	0.95149700
C	-2.16968700	-2.89922600	-0.28562900
C	-2.50715500	-2.26398900	-1.45477900
H	-1.62086100	-3.83741100	-0.28678300
C	-3.60041100	-0.42914100	-0.28817600
C	-3.21681800	-1.04000100	-1.45639600
H	-4.14200900	0.51330800	-0.29098400
C	3.21527900	-1.02023200	0.95043700
C	3.60041100	-0.42914100	-0.28817600
C	3.21681800	-1.04000100	-1.45639600
H	4.14200800	0.51330900	-0.29098400
C	2.16968700	-2.89922600	-0.28562900
C	2.50715500	-2.26398900	-1.45477900
H	1.62086200	-3.83741100	-0.28678300
C	-0.72173300	3.30018400	0.96685500
C	-1.42741900	3.33021400	-0.27109400
C	-0.70732300	3.29674600	-1.43924700
H	-2.51446700	3.32623700	-0.27307200
C	1.42741900	3.33021400	-0.27109400
C	0.70732300	3.29674500	-1.43924700
H	2.51446800	3.32623600	-0.27307200

Anthracene Capsularene (**9**)

E(RB3LYP) = -3494.436446
Number of imaginary frequencies: 0

Cartesian Coordinates:

O	0.99009900	1.37728900	-7.99471200
O	0.13968800	-0.78502200	-8.07204700
O	-1.30813900	1.03204900	-7.99977400
O	-4.06591700	0.21224800	-6.30014300
O	2.18007500	-2.88050900	-6.45990400
O	3.88043900	1.37742200	-6.25384900
O	-2.80930600	3.38745400	-6.16843900
O	-1.23811700	-3.39693200	-6.46996900
N	2.75595000	-0.62859200	-6.65320400
N	-2.42335300	-1.39952000	-6.67747900
N	-0.50004900	3.46868100	-6.48748600
C	3.39067800	0.33700700	-5.84661600
C	-1.14627700	2.93064000	2.91467400
C	-1.67164600	-3.01922800	1.51700900
H	-0.99808500	-3.87208800	1.46563500
C	2.46205700	-2.43265700	1.53375100
H	2.05416900	-3.43970200	1.47714000
C	2.87319400	-1.78141700	0.31853100
C	3.07695900	-0.41490000	2.77327100
C	0.85627400	-1.13681900	4.33193800
C	-3.30926400	-0.64742500	-5.88053500
C	0.53840900	1.27166800	4.43136000
C	1.38922100	0.18604000	4.38796400
C	-1.67907600	3.46398800	-5.71616700
C	-0.87456800	1.07093300	4.42856800
C	-3.13685500	-1.37321300	0.35271300
C	0.21612800	3.60657000	0.54304400
C	-3.43781400	-0.77196900	1.62438400
H	-4.10745400	0.08501400	1.65417100
C	1.19032500	0.06718300	-8.50497500
H	1.17774700	0.11156200	-9.60757700
C	2.52610200	-1.82805800	-5.94962000
C	2.55189800	-0.48240000	-8.08331700
H	3.31962200	0.19160700	-8.47214500
H	2.67491500	-1.46380000	-8.54881000
C	-1.50884400	2.46325600	4.32612000
H	-2.56069700	2.54323300	4.60313100
C	-1.39532800	-2.56427800	4.11297000
H	-0.94642600	-3.53275200	4.33666700
C	-1.94260300	-2.38613600	2.69455200
C	-0.26078500	1.88722700	-8.43345700
H	-0.26277600	1.91782100	-9.53654500
C	0.62736600	3.82221800	-5.72002300
C	2.90747000	0.04747300	4.22181500
H	3.51297100	0.90150300	4.52764400
C	-1.38993500	-0.20808100	4.37750800
C	-2.25585600	-1.20210900	-8.10571700
H	-2.08089900	-2.17684600	-8.56852100
H	-3.18263000	-0.78221300	-8.50527000
C	3.12943000	-1.31062100	4.95539400
H	2.89032000	-1.26157000	6.02292400
H	4.13946100	-1.71124900	4.81556400
C	3.52885000	0.21867800	1.65333600
H	3.93190500	1.22864300	1.68809600
C	-0.50987700	-1.33037200	4.32581500
C	2.53843800	-1.75164200	2.71338600
C	0.75985300	2.78605200	4.32684400
C	0.94652300	3.48939500	1.77723800

C	0.28161200	3.13471300	2.91452000
C	2.05161300	-2.07614300	4.12814700
H	1.88794100	-3.13136100	4.35003600
C	-2.83286700	-1.25258200	2.74856100
C	-2.80874000	-0.76262400	4.19838000
H	-3.63022300	-0.11135500	4.49926900
C	-0.47686800	3.31314600	-7.93067500
H	-1.43019400	3.66832400	-8.33031100
H	0.32817600	3.93542500	-8.33002900
C	-1.87027900	-2.48281700	-5.96709500
C	-0.46895900	3.28657200	5.14650500
H	-0.42682800	2.98943600	6.19965800
C	-1.11124200	-0.27702900	-8.51348200
H	-1.10294500	-0.22638400	-9.61556600
C	-1.88437900	3.08064300	1.77756200
H	-2.96088800	2.92349700	1.76700100
C	-2.65000200	-2.13014200	4.93115200
H	-2.44218300	-2.01798000	6.00047800
H	-3.50746600	-2.79590300	4.78382600
H	2.02335700	3.64446800	1.76638400
H	-0.62313100	4.36835900	5.06804700
O	1.72454800	4.09506300	-6.17818500
H	1.74737500	3.15621200	4.60488400
C	-2.24262000	-2.51110600	0.29830200
C	-1.89595100	-3.04545600	-0.95102500
H	-1.21887100	-3.89629900	-0.99275300
C	-3.63055700	-0.83696700	-0.84533600
C	-3.23657100	-1.33223900	-2.09700800
H	-4.29652700	0.02261000	-0.80508300
C	3.41243800	-0.43865100	0.37954700
C	3.73842700	0.21972000	-0.81459100
H	4.13607100	1.23155500	-0.76955500
C	2.69354000	-2.38654900	-0.93386900
C	2.96177200	-1.70627000	-2.13085700
H	2.28357600	-3.39338900	-0.98108300
C	-1.21687100	3.39690700	0.54323200
C	-1.91123700	3.43641100	-0.67432100
H	-2.98644700	3.26916900	-0.67538000
C	0.86824900	3.84876200	-0.67491900
C	0.18327900	3.83308300	-1.89909000
H	1.94543100	4.00269600	-0.67648000
C	-2.34071700	-2.47236800	-2.15138200
C	-1.87651300	-2.94795900	-3.42226300
C	-2.25905100	-2.27767600	-4.54947800
H	-1.20301900	-3.80022200	-3.46540700
C	-3.64650500	-0.69492800	-3.31487800
C	-3.13904300	-1.15665700	-4.49633300
H	-4.31505000	0.16144500	-3.27603900
C	3.50070600	-0.36051100	-2.06878200
C	3.71710100	0.37289600	-3.28174200
C	3.36230100	-0.20693400	-4.46645600
H	4.11807400	1.38231500	-3.23682600
C	2.65291100	-2.28681700	-3.40563300
C	2.83355500	-1.52967100	-4.52847700
H	2.24832900	-3.29461400	-3.45497100
C	-1.25162700	3.61765700	-1.89852500
C	-1.95539300	3.52984800	-3.14503900
C	-1.23968700	3.60971700	-4.30585400
H	-3.02964200	3.36307500	-3.14661500
C	0.87916800	3.96084800	-3.14710500
C	0.17001500	3.82627900	-4.30730800
H	1.95425900	4.12226500	-3.15023300

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X-ray Crystallographic Data

Compound 4: The single crystal X-ray diffraction studies were carried out on a Nonius Kappa diffractometer equipped with a Bruker APEX-II CCD and Mo K_α radiation (λ = 0.71073 Å). A 0.384 x 0.363 x 0.257 mm piece of a colorless block was mounted on a MiTeGen Micromount with CHRISTO-LUBE MCG 1024 oil. Data were collected in a nitrogen gas stream at 100(2) K using ϕ and ϖ scans. Crystal-to-detector distance was 40 mm and exposure time was 5 seconds per frame using a scan width of 1.0°. Data collection was 100% complete to 25.00° in θ. A total of 31039 reflections were collected covering the indices, -20<=h<=20, -20<=k<=20, -39<=l<=39. 3361 reflections were found to be symmetry independent, with a R_{int} of 0.0349. Indexing and unit cell refinement indicated a trigonal, rhombohedral lattice. The space group was found to be *R*-3. The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by direct methods (SHELXT) produced a complete phasing model for refinement.

All nonhydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014. Crystallographic data are summarized in Table 1.

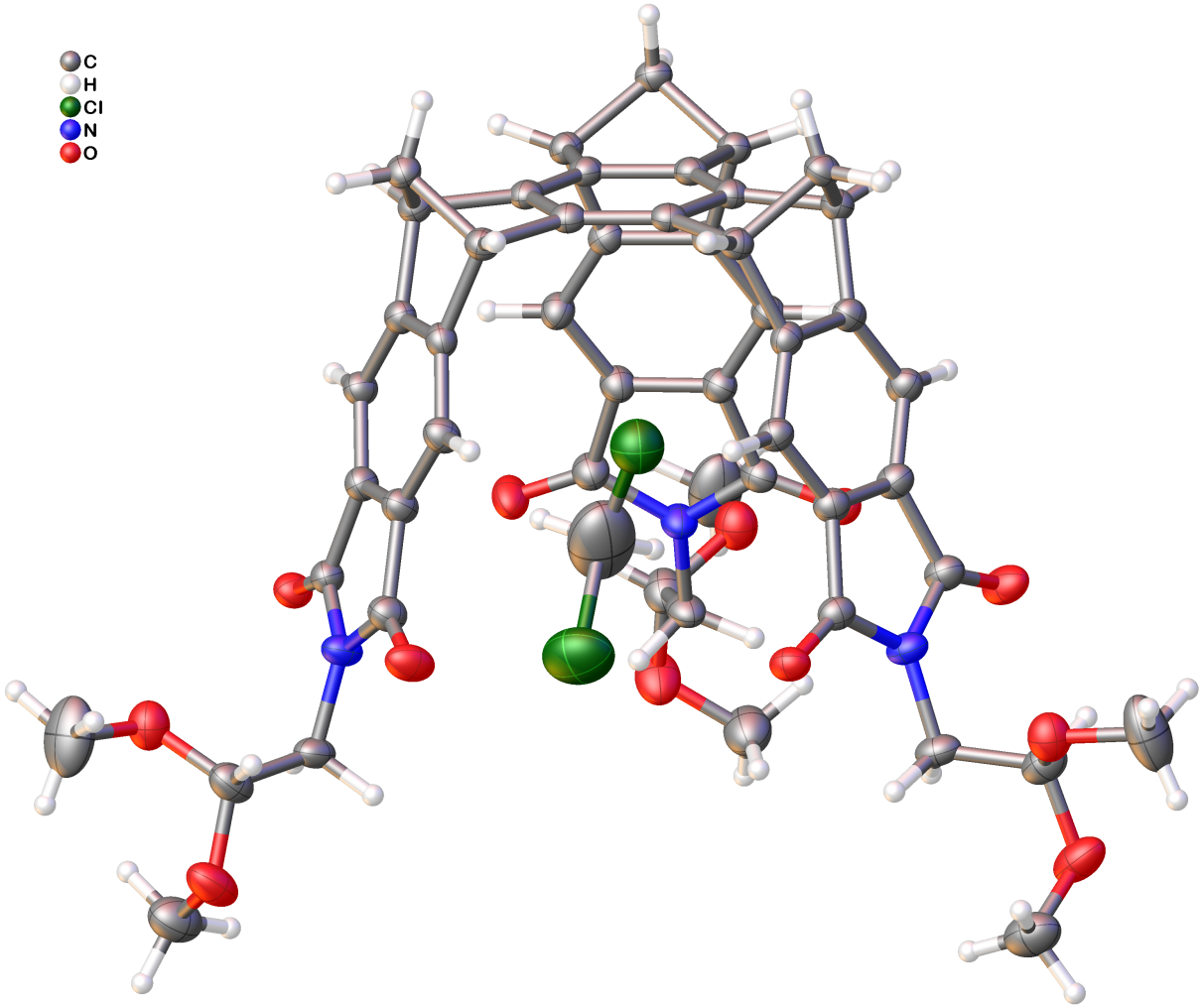
C
H
Cl
N
O

Table 1. Crystal data and structure refinement for Compound 4.

Report date	2021-06-03	
Identification code	Trisacetal	
Empirical formula	C52.50 H48 Cl3 N3 O12	
Molecular formula	C51 H45 N3 O12, 1.5(C1 H2 Cl2)	
Formula weight	1019.29	
Temperature	100.0 K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	R -3	
Unit cell dimensions	a = 16.2785(5) Å	α= 90°.
	b = 16.2785(5) Å	β= 90°.
	c = 31.9470(10) Å	γ = 120°.
Volume	7331.4(5) $Å^3$	
Z	6	
Density (calculated)	1.385 Mg/m^3	
Absorption coefficient	0.255 mm^{-1}	
F(000)	3186	
Crystal size	0.384 x 0.363 x 0.257 mm^3	
Crystal color, habit	Colorless Block	
Theta range for data collection	1.579 to 26.434°.	
Index ranges	-20<=h<=20, -20<=k<=20, -39<=l<=39	
Reflections collected	31039	
Independent reflections	3361 [R(int) = 0.0349, R(sigma) = 0.0226]	
Completeness to theta = 25.000°	100.0 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.0932 and 0.0665
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3361 / 15 / 241
Goodness-of-fit on F^2	1.085
Final R indices [I>2sigma(I)]	R1 = 0.0559, wR2 = 0.1503
R indices (all data)	R1 = 0.0703, wR2 = 0.1612
Extinction coefficient	n/a
Largest diff. peak and hole	0.603 and -0.472 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	6790(1)	9031(1)	4330(1)	37(1)
O(2)	5756(1)	5857(1)	4306(1)	28(1)
O(3)	8128(1)	7644(1)	3974(1)	40(1)
O(4)	8069(1)	8324(1)	3338(1)	48(1)
N(1)	6374(1)	7468(1)	4220(1)	28(1)
C(1)	4019(1)	6395(1)	6030(1)	22(1)
C(2)	4288(1)	7370(1)	6031(1)	22(1)
C(3)	5370(1)	7933(1)	6010(1)	23(1)
C(4)	5585(1)	7258(1)	6274(1)	25(1)
C(5)	4937(1)	6361(1)	6008(1)	23(1)
C(6)	5335(1)	6750(1)	5576(1)	23(1)
C(7)	5606(1)	7716(1)	5577(1)	23(1)
C(8)	5981(2)	8280(2)	5227(1)	27(1)
C(9)	6073(2)	7832(2)	4877(1)	27(1)
C(10)	5784(2)	6871(1)	4872(1)	25(1)
C(11)	5409(1)	6302(1)	5222(1)	24(1)
C(12)	6458(2)	8227(2)	4457(1)	29(1)
C(13)	5947(2)	6625(2)	4446(1)	25(1)
C(14)	6687(2)	7552(2)	3790(1)	31(1)
C(15)	7759(2)	8133(2)	3755(1)	37(1)

C(16)	9133(2)	8181(2)	4014(2)	76(1)
C(17)	7884(2)	7517(2)	3100(1)	52(1)
Cl(1B)	4071(9)	7647(10)	4479(6)	110(4)
Cl(1S)	3333	6667	4923(1)	58(1)
Cl(2S)	2869(2)	5961(2)	4054(1)	81(1)
C(1S)	2803(9)	6680(10)	4461(4)	110(4)
Cl(3S)	9665(6)	8541(6)	5072(2)	94(2)
Cl(4S)	8709(5)	9630(8)	4954(2)	94(2)
C(2S)	8574(16)	8509(15)	4917(9)	94(2)

Table 3. Bond lengths [Å] and angles [°] for compound **4**.

O(1)-C(12)	1.210(3)	C(8)-H(8)	0.9500
O(2)-C(13)	1.212(3)	C(8)-C(9)	1.384(3)
O(3)-C(15)	1.401(3)	C(9)-C(10)	1.391(3)
O(3)-C(16)	1.423(4)	C(9)-C(12)	1.484(3)
O(4)-C(15)	1.402(3)	C(10)-C(11)	1.384(3)
O(4)-C(17)	1.414(3)	C(10)-C(13)	1.480(3)
N(1)-C(12)	1.397(3)	C(11)-H(11)	0.9500
N(1)-C(13)	1.392(3)	C(14)-H(14A)	0.9900
N(1)-C(14)	1.445(3)	C(14)-H(14B)	0.9900
C(1)-C(2)	1.421(3)	C(14)-C(15)	1.517(3)
C(1)-C(2)#1	1.366(3)	C(15)-H(15)	1.0000
C(1)-C(5)	1.524(3)	C(16)-H(16A)	0.9800
C(2)-C(3)	1.528(3)	C(16)-H(16B)	0.9800
C(3)-H(3)	1.0000	C(16)-H(16C)	0.9800
C(3)-C(4)	1.557(3)	C(17)-H(17A)	0.9800
C(3)-C(7)	1.523(3)	C(17)-H(17B)	0.9800
C(4)-H(4A)	0.9900	C(17)-H(17C)	0.9800
C(4)-H(4B)	0.9900	Cl(1B)-Cl(2S)#1	1.938(17)
C(4)-C(5)	1.556(3)	Cl(1B)-Cl(2S)#2	1.798(14)
C(5)-H(5)	1.0000	Cl(1B)-C(1S)#2	2.15(2)
C(5)-C(6)	1.523(3)	Cl(1B)-C(1S)#1	0.64(2)
C(6)-C(7)	1.406(3)	Cl(1B)-C(1S)	1.869(16)
C(6)-C(11)	1.383(3)	Cl(1S)-C(1S)	1.716(12)
C(7)-C(8)	1.380(3)	Cl(1S)-C(1S)#1	1.716(12)

Cl(1S)-C(1S)#2	1.716(12)	C(2)-C(3)-C(4)	98.77(15)
Cl(2S)-Cl(2S)#1	1.752(6)	C(4)-C(3)-H(3)	117.2
Cl(2S)-Cl(2S)#2	1.752(6)	C(7)-C(3)-C(2)	104.37(16)
Cl(2S)-C(1S)	1.791(12)	C(7)-C(3)-H(3)	117.2
Cl(2S)-C(1S)#2	1.453(14)	C(7)-C(3)-C(4)	98.94(15)
C(1S)-H(1SC)	0.9900	C(3)-C(4)-H(4A)	112.8
C(1S)-H(1SD)	0.9900	C(3)-C(4)-H(4B)	112.8
C(1S)-H(1SA)	0.9900	H(4A)-C(4)-H(4B)	110.2
C(1S)-H(1SB)	0.9900	C(5)-C(4)-C(3)	94.68(15)
Cl(3S)-C(2S)	1.819(18)	C(5)-C(4)-H(4A)	112.8
Cl(4S)-C(2S)	1.730(18)	C(5)-C(4)-H(4B)	112.8
C(2S)-H(2SA)	0.9900	C(1)-C(5)-C(4)	99.12(15)
C(2S)-H(2SB)	0.9900	C(1)-C(5)-H(5)	117.1
		C(4)-C(5)-H(5)	117.1
C(15)-O(3)-C(16)	112.5(2)	C(6)-C(5)-C(1)	104.35(15)
C(15)-O(4)-C(17)	114.7(2)	C(6)-C(5)-C(4)	98.98(16)
C(12)-N(1)-C(14)	123.86(18)	C(6)-C(5)-H(5)	117.1
C(13)-N(1)-C(12)	111.70(17)	C(7)-C(6)-C(5)	106.98(17)
C(13)-N(1)-C(14)	124.44(18)	C(11)-C(6)-C(5)	130.77(19)
C(2)#1-C(1)-C(2)	120.25(19)	C(11)-C(6)-C(7)	122.18(18)
C(2)-C(1)-C(5)	106.34(17)	C(6)-C(7)-C(3)	106.75(17)
C(2)#1-C(1)-C(5)	133.35(18)	C(8)-C(7)-C(3)	131.40(18)
C(1)#2-C(2)-C(1)	119.75(19)	C(8)-C(7)-C(6)	121.83(18)
C(1)-C(2)-C(3)	106.75(16)	C(7)-C(8)-H(8)	122.1
C(1)#2-C(2)-C(3)	133.43(18)	C(7)-C(8)-C(9)	115.79(19)
C(2)-C(3)-H(3)	117.2	C(9)-C(8)-H(8)	122.1

C(8)-C(9)-C(10)	122.37(19)	C(14)-C(15)-H(15)	108.0
C(8)-C(9)-C(12)	129.61(19)	O(3)-C(16)-H(16A)	109.5
C(10)-C(9)-C(12)	108.02(18)	O(3)-C(16)-H(16B)	109.5
C(9)-C(10)-C(13)	107.98(17)	O(3)-C(16)-H(16C)	109.5
C(11)-C(10)-C(9)	122.20(19)	H(16A)-C(16)-H(16B)	109.5
C(11)-C(10)-C(13)	129.81(19)	H(16A)-C(16)-H(16C)	109.5
C(6)-C(11)-C(10)	115.60(19)	H(16B)-C(16)-H(16C)	109.5
C(6)-C(11)-H(11)	122.2	O(4)-C(17)-H(17A)	109.5
C(10)-C(11)-H(11)	122.2	O(4)-C(17)-H(17B)	109.5
O(1)-C(12)-N(1)	124.64(19)	O(4)-C(17)-H(17C)	109.5
O(1)-C(12)-C(9)	129.4(2)	H(17A)-C(17)-H(17B)	109.5
N(1)-C(12)-C(9)	105.95(17)	H(17A)-C(17)-H(17C)	109.5
O(2)-C(13)-N(1)	124.72(19)	H(17B)-C(17)-H(17C)	109.5
O(2)-C(13)-C(10)	129.02(19)	Cl(2S)#2-Cl(1B)-Cl(2S)#1	55.8(5)
N(1)-C(13)-C(10)	106.26(17)	Cl(2S)#2-Cl(1B)-C(1S)#2	53.0(4)
N(1)-C(14)-H(14A)	109.3	Cl(2S)#1-Cl(1B)-C(1S)#2	67.1(6)
N(1)-C(14)-H(14B)	109.3	Cl(2S)#2-Cl(1B)-C(1S)	76.3(6)
N(1)-C(14)-C(15)	111.80(19)	Cl(2S)#1-Cl(1B)-H(1SC)#1	103.8(13)
H(14A)-C(14)-H(14B)	107.9	Cl(2S)#2-Cl(1B)-H(1SC)#1	123.2(14)
C(15)-C(14)-H(14A)	109.3	Cl(2S)#2-Cl(1B)-H(1SD)#1	55.2(12)
C(15)-C(14)-H(14B)	109.3	Cl(2S)#1-Cl(1B)-H(1SD)#1	108.1(17)
O(3)-C(15)-O(4)	113.04(19)	C(1S)#1-Cl(1B)-Cl(2S)#2	48.3(18)
O(3)-C(15)-C(14)	107.16(18)	C(1S)-Cl(1B)-Cl(2S)#1	44.8(5)
O(3)-C(15)-H(15)	108.0	C(1S)#1-Cl(1B)-Cl(2S)#1	67(2)
O(4)-C(15)-C(14)	112.5(2)	C(1S)#1-Cl(1B)-C(1S)	48(2)
O(4)-C(15)-H(15)	108.0	C(1S)#1-Cl(1B)-C(1S)#2	5.4(18)

C(1S)-Cl(1B)-C(1S)#2	43.6(5)	C(1S)#2-Cl(2S)-Cl(1B)#2	65.1(6)
C(1S)-Cl(1B)-H(1SC)#1	60.4(10)	C(1S)#2-Cl(2S)-Cl(1B)#1	19.2(8)
C(1S)#1-Cl(1B)-H(1SC)#1	75(2)	C(1S)#2-Cl(2S)-Cl(2S)#1	89.5(5)
C(1S)#2-Cl(1B)-H(1SC)#1	70.1(13)	C(1S)#2-Cl(2S)-Cl(2S)#2	67.2(6)
C(1S)-Cl(1B)-H(1SD)#1	127.1(16)	C(1S)#2-Cl(2S)-C(1S)	54.5(8)
C(1S)#2-Cl(1B)-H(1SD)#1	87.0(12)	C(1S)-Cl(2S)-H(1SA)#2	53.1(10)
C(1S)#1-Cl(1B)-H(1SD)#1	82(2)	C(1S)#2-Cl(2S)-H(1SA)#2	42.9(5)
H(1SC)#1-Cl(1B)-H(1SD)#1	129.1	Cl(1B)-C(1S)-H(1SC)	111.8
C(1S)-Cl(1S)-C(1S)#1	52.4(7)	Cl(1B)-C(1S)-H(1SD)	111.8
C(1S)#1-Cl(1S)-C(1S)#2	52.4(7)	Cl(1S)-C(1S)-Cl(2S)	115.0(8)
C(1S)-Cl(1S)-C(1S)#2	52.4(7)	Cl(1S)-C(1S)-H(1SA)	108.5
C(1S)-Cl(1S)-H(1SC)#1	64.9(8)	Cl(1S)-C(1S)-H(1SA)#2	90.1(6)
C(1S)#1-Cl(1S)-H(1SC)#1	34.4(3)	Cl(1S)-C(1S)-H(1SB)	108.5
C(1S)#2-Cl(1S)-H(1SC)#1	86.2(9)	Cl(2S)-C(1S)-Cl(1B)	99.8(7)
Cl(1B)#1-Cl(2S)-Cl(1B)#2	83.7(11)	Cl(2S)-C(1S)-H(1SC)	111.8
Cl(2S)#1-Cl(2S)-Cl(1B)#2	58.1(4)	Cl(2S)-C(1S)-H(1SD)	111.8
Cl(2S)#2-Cl(2S)-Cl(1B)#2	98.6(5)	Cl(2S)-C(1S)-H(1SA)#2	35.3(3)
Cl(2S)#2-Cl(2S)-Cl(1B)#1	66.2(6)	Cl(2S)-C(1S)-H(1SA)	108.5
Cl(2S)#1-Cl(2S)-Cl(1B)#1	104.1(4)	Cl(2S)-C(1S)-H(1SB)	108.5
Cl(2S)#2-Cl(2S)-Cl(2S)#1	60.002(1)	H(1SC)-C(1S)-H(1SD)	109.5
Cl(2S)#2-Cl(2S)-C(1S)	79.6(4)	H(1SA)-C(1S)-H(1SA)#2	143.2
Cl(2S)#1-Cl(2S)-C(1S)	48.4(5)	H(1SA)-C(1S)-H(1SB)	107.5
Cl(2S)#2-Cl(2S)-H(1SA)#2	108.8(9)	H(1SB)-C(1S)-H(1SA)#2	95.4
Cl(2S)#1-Cl(2S)-H(1SA)#2	101.5(7)	Cl(3S)-C(2S)-H(2SA)	109.6
C(1S)-Cl(2S)-Cl(1B)#1	73.6(7)	Cl(3S)-C(2S)-H(2SB)	109.6
C(1S)-Cl(2S)-Cl(1B)#2	19.2(7)	Cl(4S)-C(2S)-Cl(3S)	110.1(12)

Cl(4S)-C(2S)-H(2SA)	109.6
Cl(4S)-C(2S)-H(2SB)	109.6
H(2SA)-C(2S)-H(2SB)	108.1

Symmetry transformations used to generate equivalent atoms:

#1 -x+y,-x+1,z #2 -y+1,x-y+1,z

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	51(1)	29(1)	32(1)	7(1)	11(1)	20(1)
O(2)	34(1)	28(1)	25(1)	-1(1)	2(1)	18(1)
O(3)	36(1)	37(1)	49(1)	-1(1)	-1(1)	20(1)
O(4)	57(1)	44(1)	46(1)	10(1)	23(1)	28(1)
N(1)	37(1)	29(1)	22(1)	3(1)	6(1)	18(1)
C(1)	26(1)	25(1)	16(1)	-1(1)	-1(1)	14(1)
C(2)	25(1)	24(1)	18(1)	-1(1)	-1(1)	11(1)
C(3)	24(1)	23(1)	21(1)	-1(1)	0(1)	11(1)
C(4)	25(1)	28(1)	22(1)	-2(1)	-2(1)	14(1)
C(5)	24(1)	24(1)	21(1)	-1(1)	-1(1)	12(1)
C(6)	20(1)	25(1)	24(1)	2(1)	1(1)	11(1)
C(7)	22(1)	26(1)	24(1)	-2(1)	-1(1)	13(1)
C(8)	29(1)	24(1)	27(1)	0(1)	3(1)	14(1)
C(9)	29(1)	26(1)	26(1)	2(1)	4(1)	15(1)
C(10)	26(1)	27(1)	24(1)	0(1)	1(1)	15(1)
C(11)	26(1)	24(1)	24(1)	1(1)	1(1)	14(1)
C(12)	34(1)	30(1)	27(1)	1(1)	4(1)	17(1)
C(13)	26(1)	29(1)	23(1)	2(1)	1(1)	16(1)
C(14)	42(1)	35(1)	21(1)	4(1)	6(1)	23(1)
C(15)	44(1)	35(1)	36(1)	4(1)	12(1)	22(1)

C(16)	46(2)	55(2)	123(3)	-21(2)	-27(2)	22(2)
C(17)	68(2)	51(2)	44(2)	2(1)	12(1)	34(2)
Cl(1B)	84(8)	101(9)	150(9)	-24(7)	24(6)	49(7)
Cl(1S)	57(1)	57(1)	60(1)	0	0	28(1)
Cl(2S)	107(2)	75(2)	74(2)	-8(1)	10(2)	56(2)
C(1S)	84(8)	101(9)	150(9)	-24(7)	24(6)	49(7)
Cl(3S)	70(3)	130(5)	63(2)	37(3)	-6(2)	36(2)
Cl(4S)	70(3)	130(5)	63(2)	37(3)	-6(2)	36(2)
C(2S)	70(3)	130(5)	63(2)	37(3)	-6(2)	36(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **4**.

	x	y	z	U(eq)
H(3)	5689	8614	6097	27
H(4A)	6262	7434	6263	30
H(4B)	5372	7201	6568	30
H(5)	4905	5754	6093	27
H(8)	6165	8933	5227	32
H(11)	5215	5646	5220	29
H(14A)	6402	7856	3622	37
H(14B)	6465	6911	3674	37
H(15)	7975	8752	3899	45
H(16A)	9425	8286	3737	114
H(16B)	9351	7834	4190	114
H(16C)	9314	8794	4144	114
H(17A)	8304	7714	2856	78
H(17B)	7222	7190	3007	78
H(17C)	7997	7086	3273	78
H(1SC)	2596	6333	4730	132
H(1SD)	2375	6925	4386	132
H(1SA)	3102	7343	4360	132
H(1SB)	2126	6463	4517	132

H(2SA)	8413	8278	4625	113
H(2SB)	8048	8066	5100	113

Compound 5: The single crystal X-ray diffraction studies were carried out on a Bruker Kappa Photon II CPAD diffractometer equipped with Mo K_α radiation (λ = 0.71073 Å). A 0.243 x 0.226 x 0.118 mm piece of a colorless block was mounted on a MiTeGen Micromount with CHRISTO-LUBE MCG 1024 oil. Data were collected in a nitrogen gas stream at 100(2) K using ϕ and ϖ scans. Crystal-to-detector distance was 60 mm using variable exposure time (2s-10s) depending on θ with a scan width of 1.0°. Data collection was 99.8% complete to 25.00° in θ. A total of 21428 reflections were collected covering the indices, -12<=h<=12, -18<=k<=18, -15<=l<=15. 3728 reflections were found to be symmetry independent, with a R_{int} of 0.0305. Indexing and unit cell refinement indicated a primitive, monoclinic lattice. The space group was found to be $P2_1/m$. The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by direct methods (SHELXT) produced a complete phasing model for refinement.

All nonhydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All carbon bonded hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014. All other nitrogen bonded hydrogen atoms were located in the difference map. Their relative positions were restrained using DFIX commands and their thermals freely refined. Crystallographic data are summarized in Table 1.

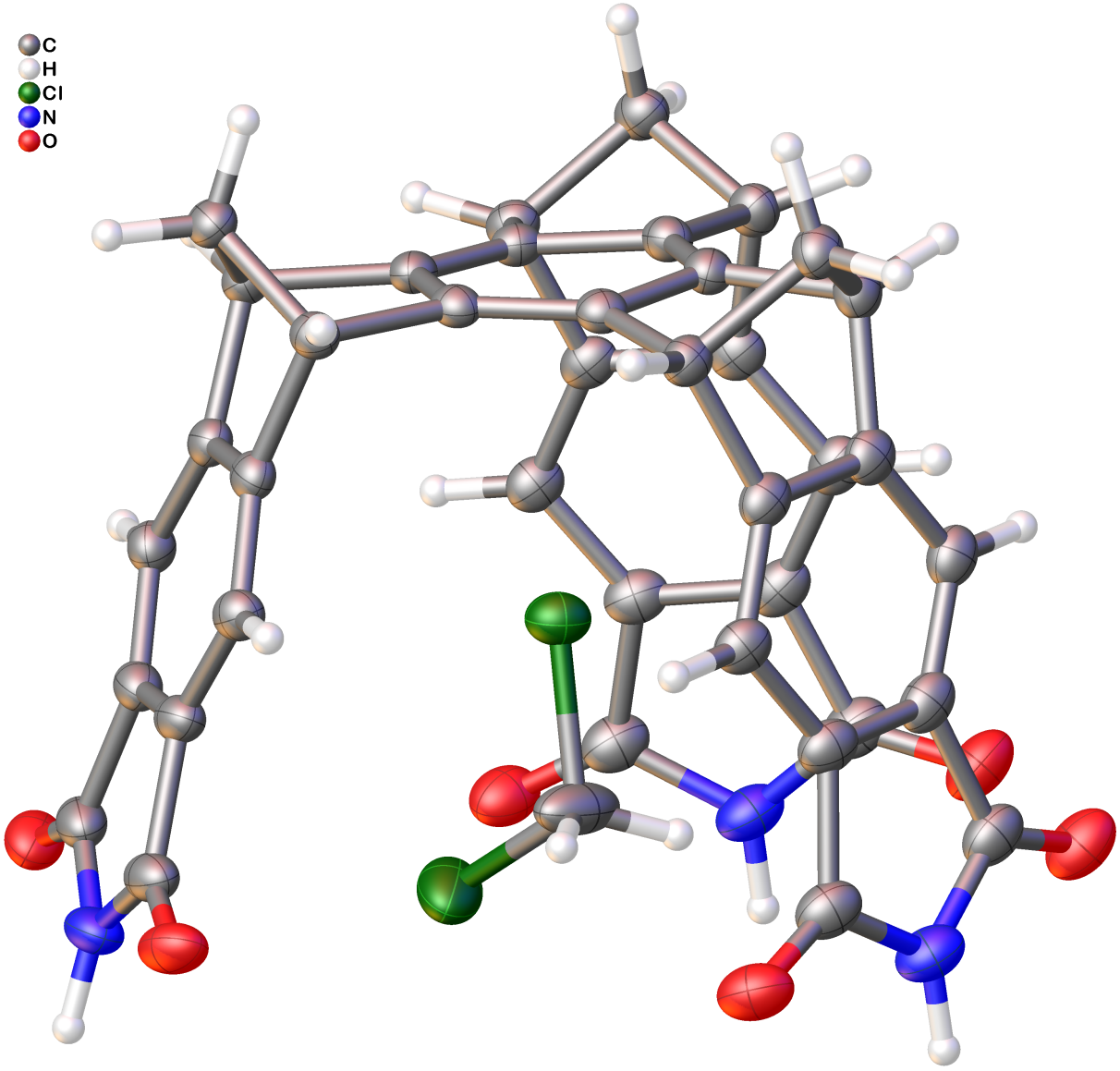
C
H
Cl
N
O

Table 1. Crystal data and structure refinement for compound **5**.

Report date	2021-06-03	
Identification code	TrisNH	
Empirical formula	C41 H25 Cl4 N3 O6	
Molecular formula	C39 H21 N3 O6, 2(C H2 Cl2)	
Formula weight	797.44	
Temperature	100.0 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/m 1	
Unit cell dimensions	a = 9.8486(7) Å	α= 90°.
	b = 14.6173(10) Å	β= 102.991(3)°.
	c = 12.4874(9) Å	γ = 90°.
Volume	1751.7(2) $Å^3$	
Z	2	
Density (calculated)	1.512 Mg/m^3	
Absorption coefficient	0.394 mm^{-1}	
F(000)	816	
Crystal size	0.243 x 0.226 x 0.118 mm^3	
Crystal color, habit	Colorless Block	
Theta range for data collection	2.984 to 26.374°.	
Index ranges	-12<=h<=12, -18<=k<=18, -15<=l<=15	
Reflections collected	21428	
Independent reflections	3728 [R(int) = 0.0305, R(sigma) = 0.0209]	
Completeness to theta = 25.000°	99.8 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.0452 and 0.0251
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3728 / 2 / 285
Goodness-of-fit on F^2	1.027
Final R indices [I>2sigma(I)]	R1 = 0.0421, wR2 = 0.1094
R indices (all data)	R1 = 0.0525, wR2 = 0.1172
Extinction coefficient	n/a
Largest diff. peak and hole	0.534 and -0.574 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	5488(2)	4664(1)	8628(1)	40(1)
O(2)	8357(2)	6358(1)	11286(1)	40(1)
O(3)	2631(2)	5932(1)	4766(1)	38(1)
N(1)	6712(2)	5464(1)	10133(1)	35(1)
N(2)	2294(2)	7500	4808(2)	34(1)
C(1)	10800(2)	7034(1)	7062(1)	23(1)
C(2)	9923(2)	6541(1)	6189(1)	22(1)
C(3)	10029(2)	5533(1)	6535(1)	24(1)
C(4)	11592(2)	5510(1)	7145(2)	26(1)
C(5)	11472(2)	6327(1)	7913(2)	26(1)
C(6)	10256(2)	6001(1)	8378(2)	26(1)
C(7)	9360(2)	5505(1)	7532(2)	25(1)
C(8)	8108(2)	5152(1)	7669(2)	27(1)
C(9)	7781(2)	5332(1)	8683(2)	29(1)
C(10)	8649(2)	5841(1)	9492(2)	29(1)
C(11)	9917(2)	6187(1)	9372(2)	28(1)
C(12)	6514(2)	5089(1)	9092(2)	33(1)
C(13)	7962(2)	5947(1)	10435(2)	33(1)
C(14)	9159(2)	7012(1)	5310(1)	22(1)
C(15)	8171(2)	6719(1)	4237(1)	22(1)
C(16)	8467(3)	7500	3472(2)	24(1)

C(17)	6729(2)	7016(1)	4349(1)	22(1)
C(18)	5577(2)	6515(1)	4463(1)	25(1)
C(19)	4431(2)	7026(1)	4574(1)	27(1)
C(20)	3046(2)	6707(2)	4722(2)	31(1)
Cl(3S)	7250(1)	7500	7241(1)	33(1)
Cl(4S)	4520(3)	6969(2)	7523(2)	54(1)
C(2S)	5874(8)	7776(6)	7850(8)	54(3)
Cl(1S)	7439(1)	2500	8226(1)	65(1)
Cl(2S)	5587(1)	2500	9764(1)	61(1)
C(1S)	5685(4)	2500	8366(3)	54(1)
Cl(3B)	5013(2)	6511(1)	7300(2)	44(1)
C(2SB)	6035(9)	7500	7297(8)	40(2)

Table 3. Bond lengths [Å] and angles [°] for compound **5**.

O(1)-C(12)	1.217(3)	C(6)-C(11)	1.383(3)
O(2)-C(13)	1.206(3)	C(7)-C(8)	1.383(3)
O(3)-C(20)	1.211(3)	C(8)-H(8)	0.9500
N(1)-H(1)	0.915(17)	C(8)-C(9)	1.400(3)
N(1)-C(12)	1.384(3)	C(9)-C(10)	1.384(3)
N(1)-C(13)	1.395(3)	C(9)-C(12)	1.494(3)
N(2)-H(2)	0.927(19)	C(10)-C(11)	1.386(3)
N(2)-C(20)	1.392(3)	C(10)-C(13)	1.492(3)
N(2)-C(20)#1	1.392(3)	C(11)-H(11)	0.9500
C(1)-C(1)#1	1.361(4)	C(14)-C(14)#1	1.428(4)
C(1)-C(2)	1.425(2)	C(14)-C(15)	1.529(2)
C(1)-C(5)	1.523(2)	C(15)-H(15)	1.0000
C(2)-C(3)	1.533(2)	C(15)-C(16)	1.558(2)
C(2)-C(14)	1.369(2)	C(15)-C(17)	1.521(2)
C(3)-H(3)	1.0000	C(16)-H(16A)	0.9900
C(3)-C(4)	1.558(3)	C(16)-H(16B)	0.9900
C(3)-C(7)	1.534(2)	C(17)-C(17)#1	1.416(4)
C(4)-H(4A)	0.9900	C(17)-C(18)	1.384(3)
C(4)-H(4B)	0.9900	C(18)-H(18)	0.9500
C(4)-C(5)	1.553(3)	C(18)-C(19)	1.386(3)
C(5)-H(5)	1.0000	C(19)-C(19)#1	1.385(4)
C(5)-C(6)	1.520(3)	C(19)-C(20)	1.491(3)
C(6)-C(7)	1.414(3)	Cl(3S)-C(2S)#1	1.744(8)

Cl(3S)-C(2S)	1.744(8)	C(14)-C(2)-C(1)	119.24(17)
Cl(4S)-Cl(4S)#1	1.551(7)	C(14)-C(2)-C(3)	134.38(17)
Cl(4S)-C(2S)#1	1.356(9)	C(2)-C(3)-H(3)	117.3
Cl(4S)-C(2S)	1.758(8)	C(2)-C(3)-C(4)	98.95(15)
Cl(4S)-H(2SA)#1	1.092(8)	C(2)-C(3)-C(7)	103.82(14)
C(2S)-H(2SA)	0.9900	C(4)-C(3)-H(3)	117.3
C(2S)-H(2SB)	0.9900	C(7)-C(3)-H(3)	117.3
Cl(1S)-C(1S)	1.775(5)	C(7)-C(3)-C(4)	99.16(14)
Cl(2S)-C(1S)	1.769(4)	C(3)-C(4)-H(4A)	112.8
C(1S)-H(1SA)	0.9900	C(3)-C(4)-H(4B)	112.8
C(1S)-H(1SB)	0.9900	H(4A)-C(4)-H(4B)	110.2
Cl(3B)-C(2SB)	1.763(6)	C(5)-C(4)-C(3)	94.68(14)
C(2SB)-H(2SC)	0.9900	C(5)-C(4)-H(4A)	112.8
C(2SB)-H(2SD)	0.9900	C(5)-C(4)-H(4B)	112.8
		C(1)-C(5)-C(4)	99.94(14)
C(12)-N(1)-H(1)	122.5(19)	C(1)-C(5)-H(5)	117.1
C(12)-N(1)-C(13)	112.60(17)	C(4)-C(5)-H(5)	117.1
C(13)-N(1)-H(1)	124.5(19)	C(6)-C(5)-C(1)	102.90(14)
C(20)#1-N(2)-H(2)	123.67(12)	C(6)-C(5)-C(4)	99.79(15)
C(20)-N(2)-H(2)	123.67(12)	C(6)-C(5)-H(5)	117.1
C(20)-N(2)-C(20)#1	112.6(2)	C(7)-C(6)-C(5)	106.76(16)
C(1)#1-C(1)-C(2)	120.41(10)	C(11)-C(6)-C(5)	130.56(18)
C(1)#1-C(1)-C(5)	132.73(10)	C(11)-C(6)-C(7)	122.40(18)
C(2)-C(1)-C(5)	106.49(15)	C(6)-C(7)-C(3)	106.49(16)
C(1)-C(2)-C(3)	106.29(15)	C(8)-C(7)-C(3)	131.85(17)

C(8)-C(7)-C(6)	121.52(17)	C(17)-C(15)-C(14)	105.28(14)
C(7)-C(8)-H(8)	122.1	C(17)-C(15)-H(15)	116.8
C(7)-C(8)-C(9)	115.75(18)	C(17)-C(15)-C(16)	98.89(15)
C(9)-C(8)-H(8)	122.1	C(15)#1-C(16)-C(15)	94.24(19)
C(8)-C(9)-C(12)	130.09(19)	C(15)#1-C(16)-H(16A)	112.9
C(10)-C(9)-C(8)	122.09(18)	C(15)-C(16)-H(16A)	112.9
C(10)-C(9)-C(12)	107.77(17)	C(15)#1-C(16)-H(16B)	112.9
C(9)-C(10)-C(11)	122.76(18)	C(15)-C(16)-H(16B)	112.9
C(9)-C(10)-C(13)	108.45(18)	H(16A)-C(16)-H(16B)	110.3
C(11)-C(10)-C(13)	128.78(18)	C(17)#1-C(17)-C(15)	106.58(10)
C(6)-C(11)-C(10)	115.45(18)	C(18)-C(17)-C(15)	131.49(17)
C(6)-C(11)-H(11)	122.3	C(18)-C(17)-C(17)#1	121.91(11)
C(10)-C(11)-H(11)	122.3	C(17)-C(18)-H(18)	122.3
O(1)-C(12)-N(1)	125.25(19)	C(17)-C(18)-C(19)	115.48(18)
O(1)-C(12)-C(9)	128.84(19)	C(19)-C(18)-H(18)	122.3
N(1)-C(12)-C(9)	105.90(18)	C(18)-C(19)-C(20)	129.17(19)
O(2)-C(13)-N(1)	125.44(19)	C(19)#1-C(19)-C(18)	122.61(11)
O(2)-C(13)-C(10)	129.3(2)	C(19)#1-C(19)-C(20)	108.22(12)
N(1)-C(13)-C(10)	105.25(17)	O(3)-C(20)-N(2)	125.79(18)
C(2)-C(14)-C(14)#1	120.17(11)	O(3)-C(20)-C(19)	128.8(2)
C(2)-C(14)-C(15)	133.53(17)	N(2)-C(20)-C(19)	105.46(18)
C(14)#1-C(14)-C(15)	106.26(10)	C(2S)#1-Cl(3S)-C(2S)	26.7(5)
C(14)-C(15)-H(15)	116.8	Cl(4S)#1-Cl(4S)-C(2S)	47.9(3)
C(14)-C(15)-C(16)	99.33(15)	Cl(4S)#1-Cl(4S)-H(2SA)#1	118.6(5)
C(16)-C(15)-H(15)	116.8	C(2S)#1-Cl(4S)-Cl(4S)#1	74.0(4)

C(2S)#1-Cl(4S)-C(2S)	26.2(6)
C(2S)-Cl(4S)-H(2SA)#1	71.6(8)
C(2S)#1-Cl(4S)-H(2SA)#1	46.2(3)
Cl(3S)-C(2S)-Cl(4S)	111.5(5)
Cl(3S)-C(2S)-H(2SA)	109.3
Cl(3S)-C(2S)-H(2SB)	109.3
Cl(4S)-C(2S)-H(2SA)	109.3
Cl(4S)-C(2S)-H(2SB)	109.3
H(2SA)-C(2S)-H(2SB)	108.0
Cl(1S)-C(1S)-H(1SA)	109.3
Cl(1S)-C(1S)-H(1SB)	109.3
Cl(2S)-C(1S)-Cl(1S)	111.56(19)
Cl(2S)-C(1S)-H(1SA)	109.3
Cl(2S)-C(1S)-H(1SB)	109.3
H(1SA)-C(1S)-H(1SB)	108.0
Cl(3B)#1-C(2SB)-Cl(3B)	110.2(5)
Cl(3B)#1-C(2SB)-H(2SC)	109.6
Cl(3B)-C(2SB)-H(2SC)	109.6
Cl(3B)#1-C(2SB)-H(2SD)	109.6
Cl(3B)-C(2SB)-H(2SD)	109.6
H(2SC)-C(2SB)-H(2SD)	108.1

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+3/2,z

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	43(1)	38(1)	43(1)	-5(1)	20(1)	-8(1)
O(2)	60(1)	33(1)	31(1)	-3(1)	18(1)	-1(1)
O(3)	31(1)	49(1)	35(1)	-7(1)	12(1)	-14(1)
N(1)	43(1)	35(1)	33(1)	-1(1)	19(1)	-1(1)
N(2)	20(1)	52(2)	32(1)	0	8(1)	0
C(1)	20(1)	27(1)	22(1)	1(1)	6(1)	2(1)
C(2)	20(1)	23(1)	23(1)	-1(1)	8(1)	1(1)
C(3)	26(1)	23(1)	23(1)	1(1)	7(1)	3(1)
C(4)	27(1)	28(1)	24(1)	2(1)	6(1)	5(1)
C(5)	26(1)	27(1)	24(1)	1(1)	3(1)	4(1)
C(6)	29(1)	21(1)	26(1)	4(1)	6(1)	5(1)
C(7)	31(1)	21(1)	24(1)	3(1)	8(1)	5(1)
C(8)	33(1)	21(1)	28(1)	1(1)	9(1)	0(1)
C(9)	35(1)	24(1)	31(1)	4(1)	13(1)	3(1)
C(10)	40(1)	22(1)	26(1)	3(1)	10(1)	5(1)
C(11)	35(1)	24(1)	24(1)	2(1)	6(1)	5(1)
C(12)	41(1)	27(1)	35(1)	2(1)	16(1)	1(1)
C(13)	45(1)	26(1)	30(1)	5(1)	14(1)	4(1)
C(14)	19(1)	26(1)	22(1)	-2(1)	7(1)	0(1)
C(15)	21(1)	24(1)	21(1)	-2(1)	5(1)	0(1)
C(16)	24(1)	30(1)	21(1)	0	6(1)	0

C(17)	22(1)	27(1)	18(1)	-1(1)	4(1)	1(1)
C(18)	24(1)	28(1)	23(1)	-2(1)	5(1)	-4(1)
C(19)	22(1)	37(1)	22(1)	-1(1)	5(1)	-3(1)
C(20)	24(1)	47(1)	23(1)	-2(1)	6(1)	-5(1)
Cl(3S)	30(1)	34(1)	38(1)	0	13(1)	0
Cl(4S)	38(1)	83(2)	43(1)	-10(1)	15(1)	-24(1)
C(2S)	41(4)	53(6)	79(6)	-30(4)	36(4)	-16(3)
Cl(1S)	72(1)	66(1)	45(1)	0	-12(1)	0
Cl(2S)	77(1)	53(1)	42(1)	0	-10(1)	0
C(1S)	71(3)	36(2)	42(2)	0	-16(2)	0
Cl(3B)	40(1)	48(1)	41(1)	11(1)	6(1)	-2(1)
C(2SB)	32(5)	50(6)	35(5)	0	2(4)	0

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **5.**

	x	y	z	U(eq)
H(1)	6040(20)	5450(20)	10530(20)	64(9)
H(2)	1400(20)	7500	4920(30)	55(11)
H(3)	9709	5067	5946	29
H(4A)	11858	4932	7552	32
H(4B)	12230	5636	6653	32
H(5)	12339	6515	8453	31
H(8)	7507	4810	7110	32
H(11)	10512	6530	9935	34
H(15)	8266	6077	3986	26
H(16A)	9441	7500	3382	29
H(16B)	7810	7500	2745	29
H(18)	5572	5865	4465	30
H(2SA)	5510	8388	7596	65
H(2SB)	6219	7801	8658	65
H(1SA)	5202	3048	7998	65
H(1SB)	5202	1952	7998	65
H(2SC)	6815	7500	7954	48
H(2SD)	6435	7500	6637	48

Table 6. Hydrogen bonds for Badjic_TrisNH [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(1)#2	0.915(17)	2.025(18)	2.938(2)	176(3)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+3/2,z #2 -x+1,-y+1,-z+2

Capsularene 1: The single crystal X-ray diffraction studies were carried out on a Bruker Kappa Photon II CPAD diffractometer equipped with Mo K_α radiation (λ = 0.71073 Å). A 0.273 x 0.256 x 0.189 mm piece of a colorless plate was mounted on a MiTeGen Micromount with CHRISTO-LUBE MCG 1024 oil. Data were collected in a nitrogen gas stream at 100(2) K using ϕ and ϖ scans. Crystal-to-detector distance was 60 mm using variable exposure time (2s-10s) depending on θ with a scan width of 0.75°. Data collection was 99.7% complete to 25.00° in θ. A total of 104884 reflections were collected covering the indices, -16<=h<=16, -18<=k<=18, -34<=l<=34. 10576 reflections were found to be symmetry independent, with a R_{int} of 0.0304. Indexing and unit cell refinement indicated a primitive, monoclinic lattice. The space group was found to be $P2_1/c$. The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by direct methods (SHELXT) produced a complete phasing model consistent with the proposed structure.

All nonhydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014. Crystallographic data are summarized in Table 1.

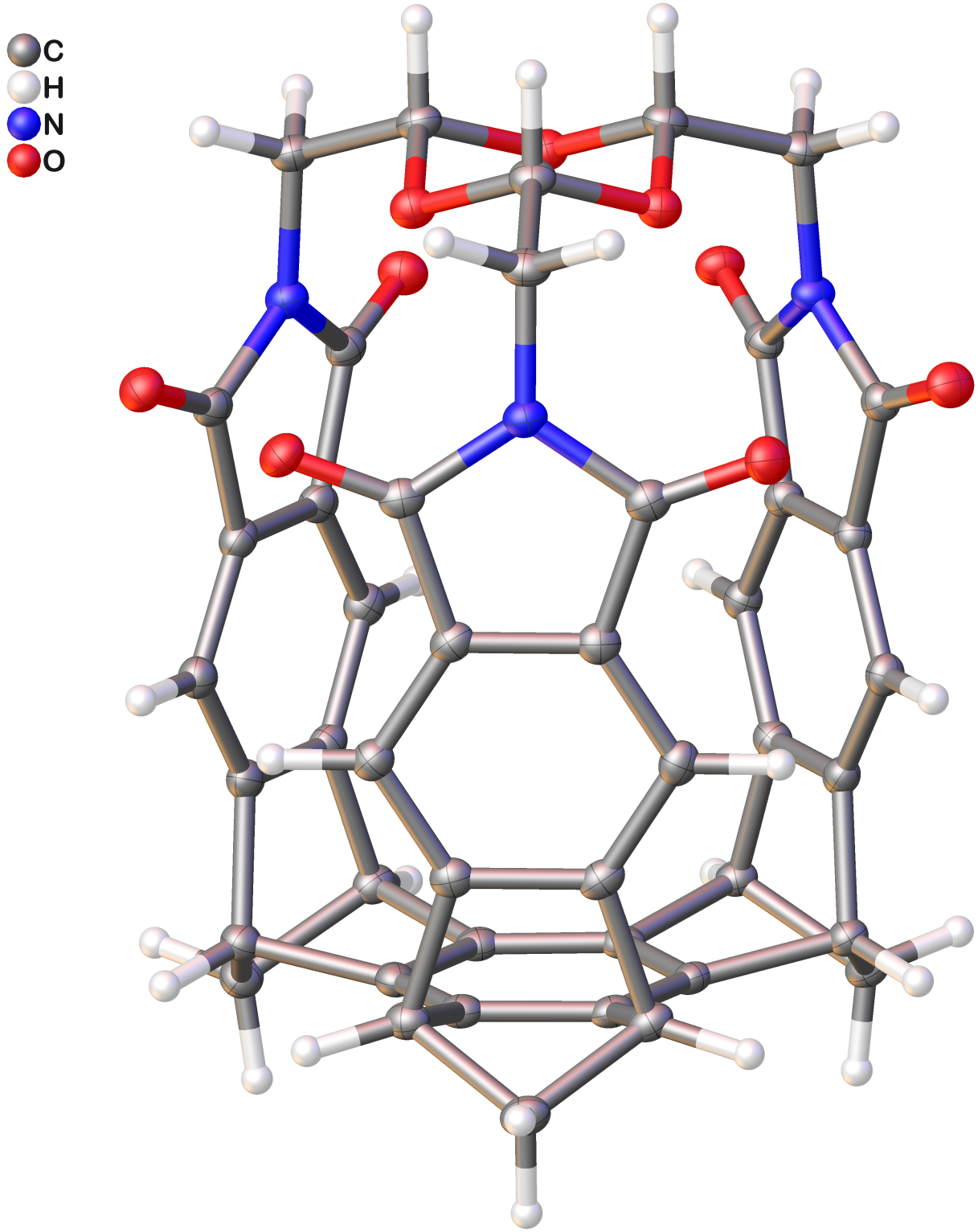
C
H
N
O

Table 1. Crystal data and structure refinement for capsularene **1**.

Report date	2019-08-07	
Identification code	LZQ-8-38	
Empirical formula	C48 H33 Cl6 N3 O9	
Molecular formula	C45 H27 N3 O9, 3(C H2 Cl2)	
Formula weight	1008.47	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 12.1863(9) Å	α= 90°.
	b = 13.6712(9) Å	β= 90.471(3)°.
	c = 25.6177(18) Å	γ = 90°.
Volume	4267.8(5) $Å^3$	
Z	4	
Density (calculated)	1.570 Mg/m^3	
Absorption coefficient	0.468 mm^{-1}	
F(000)	2064	
Crystal size	0.273 x 0.256 x 0.189 mm^3	
Crystal color, habit	Colorless Block	
Theta range for data collection	2.902 to 28.285°.	
Index ranges	-16<=h<=16, -18<=k<=18, -34<=l<=34	
Reflections collected	104884	
Independent reflections	10576 [R(int) = 0.0304, R(sigma) = 0.0154]	

Completeness to theta = 25.000°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.0962 and 0.0679
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10576 / 27 / 642
Goodness-of-fit on F^2	1.061
Final R indices [I>2sigma(I)]	R1 = 0.0363, wR2 = 0.0858
R indices (all data)	R1 = 0.0403, wR2 = 0.0887
Extinction coefficient	n/a
Largest diff. peak and hole	0.393 and -0.265 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for capsularene **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	1627(1)	2323(1)	5836(1)	17(1)
O(2)	1679(1)	1532(1)	6639(1)	16(1)
O(3)	1610(1)	3223(1)	6605(1)	16(1)
O(4)	3027(1)	5200(1)	6490(1)	20(1)
O(5)	3077(1)	3411(1)	4982(1)	19(1)
O(6)	3088(1)	1233(1)	5007(1)	19(1)
O(7)	3239(1)	-309(1)	6591(1)	21(1)
O(8)	3228(1)	860(1)	7625(1)	20(1)
O(9)	3040(1)	4189(1)	7525(1)	18(1)
N(1)	2778(1)	4190(1)	5771(1)	17(1)
N(2)	2875(1)	540(1)	5826(1)	17(1)
N(3)	2849(1)	2501(1)	7485(1)	16(1)
C(1)	1597(1)	4081(1)	5789(1)	18(1)
C(2)	1223(1)	3179(1)	6082(1)	17(1)
C(3)	1691(1)	570(1)	5856(1)	18(1)
C(4)	1276(1)	1490(1)	6119(1)	17(1)
C(5)	1666(1)	2439(1)	7443(1)	16(1)
C(6)	1263(1)	2379(1)	6882(1)	16(1)
C(7)	3400(1)	4728(1)	6134(1)	16(1)
C(8)	4564(1)	4607(1)	5972(1)	16(1)

C(9)	4580(1)	4067(1)	5513(1)	16(1)
C(10)	3428(1)	3818(1)	5366(1)	16(1)
C(11)	5524(1)	4920(1)	6222(1)	16(1)
C(12)	6493(1)	4641(1)	5985(1)	16(1)
C(13)	6505(1)	4097(1)	5516(1)	16(1)
C(14)	5547(1)	3805(1)	5266(1)	17(1)
C(15)	7685(1)	4717(1)	6174(1)	16(1)
C(16)	8271(1)	4768(1)	5638(1)	18(1)
C(17)	7706(1)	3837(1)	5413(1)	16(1)
C(18)	7955(1)	3661(1)	6325(1)	15(1)
C(19)	7965(1)	3111(1)	5852(1)	15(1)
C(20)	3479(1)	922(1)	5409(1)	16(1)
C(21)	4653(1)	834(1)	5571(1)	16(1)
C(22)	4695(1)	362(1)	6050(1)	16(1)
C(23)	3555(1)	137(1)	6214(1)	17(1)
C(24)	5591(1)	1164(1)	5317(1)	16(1)
C(25)	6573(1)	1003(1)	5580(1)	16(1)
C(26)	6615(1)	518(1)	6068(1)	16(1)
C(27)	5684(1)	181(1)	6312(1)	16(1)
C(28)	7748(1)	1319(1)	5459(1)	16(1)
C(29)	8373(1)	441(1)	5707(1)	18(1)
C(30)	7812(1)	535(1)	6249(1)	16(1)
C(31)	7984(1)	2109(1)	5870(1)	15(1)
C(32)	8018(1)	1619(1)	6361(1)	15(1)
C(33)	3535(1)	1687(1)	7545(1)	15(1)

C(34)	4675(1)	2072(1)	7509(1)	15(1)
C(35)	4618(1)	3088(1)	7484(1)	14(1)
C(36)	3439(1)	3382(1)	7496(1)	15(1)
C(37)	5664(1)	1564(1)	7495(1)	16(1)
C(38)	6591(1)	2142(1)	7447(1)	15(1)
C(39)	6539(1)	3173(1)	7426(1)	14(1)
C(40)	5551(1)	3672(1)	7447(1)	15(1)
C(41)	7793(1)	1862(1)	7382(1)	15(1)
C(42)	8336(1)	2742(1)	7671(1)	17(1)
C(43)	7711(1)	3537(1)	7350(1)	14(1)
C(44)	8014(1)	2148(1)	6815(1)	14(1)
C(45)	7971(1)	3190(1)	6797(1)	15(1)
Cl(5B)	9148(11)	8134(10)	6218(4)	57(3)
Cl(5C)	8400(14)	7874(10)	6209(5)	72(3)
Cl(5S)	9325(3)	8245(3)	6199(1)	35(1)
Cl(6B)	10043(5)	7540(5)	5218(3)	56(2)
Cl(6C)	10070(7)	8183(8)	5369(6)	65(3)
Cl(6S)	10031(2)	7152(1)	5283(1)	44(1)
C(3S)	8891(2)	7554(2)	5638(1)	31(1)
Cl(1S)	9847(1)	4062(1)	3312(1)	27(1)
Cl(2S)	10014(1)	4889(1)	2260(1)	27(1)
C(1S)	9583(2)	5092(1)	2910(1)	26(1)
Cl(3B)	3196(14)	2384(12)	3666(6)	31(1)
Cl(4B)	5542(17)	2469(15)	3883(8)	33(1)
C(2SB)	4350(20)	1770(30)	3920(20)	25(1)

Cl(3S)	4688(1)	2433(1)	4030(1)	31(1)
Cl(4S)	7080(1)	2411(1)	4163(1)	33(1)
C(2S)	5969(2)	2535(1)	3715(1)	25(1)

Table 3. Bond lengths [Å] and angles [°] for capsularene **1.**

O(1)-C(2)	1.4179(18)	C(1)-C(2)	1.515(2)
O(1)-C(4)	1.4191(19)	C(2)-H(2)	1.0000
O(2)-C(4)	1.4162(19)	C(3)-H(3A)	0.9900
O(2)-C(6)	1.4120(18)	C(3)-H(3B)	0.9900
O(3)-C(2)	1.4182(18)	C(3)-C(4)	1.516(2)
O(3)-C(6)	1.4213(19)	C(4)-H(4)	1.0000
O(4)-C(7)	1.209(2)	C(5)-H(5A)	0.9900
O(5)-C(10)	1.2053(19)	C(5)-H(5B)	0.9900
O(6)-C(20)	1.2086(19)	C(5)-C(6)	1.518(2)
O(7)-C(23)	1.208(2)	C(6)-H(6)	1.0000
O(8)-C(33)	1.2082(19)	C(7)-C(8)	1.490(2)
O(9)-C(36)	1.2080(19)	C(8)-C(9)	1.388(2)
N(1)-C(1)	1.448(2)	C(8)-C(11)	1.397(2)
N(1)-C(7)	1.404(2)	C(9)-C(10)	1.490(2)
N(1)-C(10)	1.406(2)	C(9)-C(14)	1.389(2)
N(2)-C(3)	1.446(2)	C(11)-H(11)	0.9500
N(2)-C(20)	1.402(2)	C(11)-C(12)	1.386(2)
N(2)-C(23)	1.403(2)	C(12)-C(13)	1.414(2)
N(3)-C(5)	1.4470(19)	C(12)-C(15)	1.530(2)
N(3)-C(33)	1.401(2)	C(13)-C(14)	1.387(2)
N(3)-C(36)	1.4027(19)	C(13)-C(17)	1.531(2)
C(1)-H(1A)	0.9900	C(14)-H(14)	0.9500
C(1)-H(1B)	0.9900	C(15)-H(15)	1.0000

C(15)-C(16)	1.554(2)	C(29)-H(29A)	0.9900
C(15)-C(18)	1.530(2)	C(29)-H(29B)	0.9900
C(16)-H(16A)	0.9900	C(29)-C(30)	1.556(2)
C(16)-H(16B)	0.9900	C(30)-H(30)	1.0000
C(16)-C(17)	1.555(2)	C(30)-C(32)	1.531(2)
C(17)-H(17)	1.0000	C(31)-C(32)	1.426(2)
C(17)-C(19)	1.531(2)	C(32)-C(44)	1.369(2)
C(18)-C(19)	1.428(2)	C(33)-C(34)	1.489(2)
C(18)-C(45)	1.369(2)	C(34)-C(35)	1.392(2)
C(19)-C(31)	1.370(2)	C(34)-C(37)	1.391(2)
C(20)-C(21)	1.490(2)	C(35)-C(36)	1.493(2)
C(21)-C(22)	1.388(2)	C(35)-C(40)	1.393(2)
C(21)-C(24)	1.395(2)	C(37)-H(37)	0.9500
C(22)-C(23)	1.487(2)	C(37)-C(38)	1.385(2)
C(22)-C(27)	1.398(2)	C(38)-C(39)	1.412(2)
C(24)-H(24)	0.9500	C(38)-C(41)	1.524(2)
C(24)-C(25)	1.386(2)	C(39)-C(40)	1.386(2)
C(25)-C(26)	1.414(2)	C(39)-C(43)	1.526(2)
C(25)-C(28)	1.530(2)	C(40)-H(40)	0.9500
C(26)-C(27)	1.379(2)	C(41)-H(41)	1.0000
C(26)-C(30)	1.527(2)	C(41)-C(42)	1.558(2)
C(27)-H(27)	0.9500	C(41)-C(44)	1.531(2)
C(28)-H(28)	1.0000	C(42)-H(42A)	0.9900
C(28)-C(29)	1.555(2)	C(42)-H(42B)	0.9900
C(28)-C(31)	1.533(2)	C(42)-C(43)	1.557(2)

C(43)-H(43)	1.0000	C(2S)-H(2SC)	0.9900
C(43)-C(45)	1.531(2)	C(2S)-H(2SD)	0.9900
C(44)-C(45)	1.426(2)		
Cl(5B)-C(3S)	1.710(9)	C(2)-O(1)-C(4)	109.19(12)
Cl(5C)-C(3S)	1.643(11)	C(6)-O(2)-C(4)	108.93(12)
Cl(5S)-C(3S)	1.796(4)	C(2)-O(3)-C(6)	109.81(12)
Cl(6B)-C(3S)	1.775(6)	C(7)-N(1)-C(1)	124.37(13)
Cl(6C)-C(3S)	1.815(9)	C(7)-N(1)-C(10)	111.99(13)
Cl(6S)-C(3S)	1.755(3)	C(10)-N(1)-C(1)	123.52(13)
C(3S)-H(3SA)	0.9900	C(20)-N(2)-C(3)	124.16(13)
C(3S)-H(3SB)	0.9900	C(20)-N(2)-C(23)	112.05(13)
C(3S)-H(3SC)	0.9900	C(23)-N(2)-C(3)	123.79(14)
C(3S)-H(3SD)	0.9900	C(33)-N(3)-C(5)	123.71(13)
C(3S)-H(3SE)	0.9900	C(33)-N(3)-C(36)	111.97(13)
C(3S)-H(3SF)	0.9900	C(36)-N(3)-C(5)	124.25(13)
Cl(1S)-C(1S)	1.773(2)	N(1)-C(1)-H(1A)	108.8
Cl(2S)-C(1S)	1.7721(19)	N(1)-C(1)-H(1B)	108.8
C(1S)-H(1SA)	0.9900	N(1)-C(1)-C(2)	113.74(13)
C(1S)-H(1SB)	0.9900	H(1A)-C(1)-H(1B)	107.7
Cl(3B)-C(2SB)	1.75(2)	C(2)-C(1)-H(1A)	108.8
Cl(4B)-C(2SB)	1.75(2)	C(2)-C(1)-H(1B)	108.8
C(2SB)-H(2SA)	0.9900	O(1)-C(2)-O(3)	109.88(12)
C(2SB)-H(2SB)	0.9900	O(1)-C(2)-C(1)	110.19(13)
Cl(3S)-C(2S)	1.769(2)	O(1)-C(2)-H(2)	109.1
Cl(4S)-C(2S)	1.776(2)	O(3)-C(2)-C(1)	109.47(13)

O(3)-C(2)-H(2)	109.1	C(5)-C(6)-H(6)	109.1
C(1)-C(2)-H(2)	109.1	O(4)-C(7)-N(1)	125.11(15)
N(2)-C(3)-H(3A)	109.1	O(4)-C(7)-C(8)	129.41(15)
N(2)-C(3)-H(3B)	109.1	N(1)-C(7)-C(8)	105.45(13)
N(2)-C(3)-C(4)	112.62(13)	C(9)-C(8)-C(7)	108.42(13)
H(3A)-C(3)-H(3B)	107.8	C(9)-C(8)-C(11)	122.24(14)
C(4)-C(3)-H(3A)	109.1	C(11)-C(8)-C(7)	129.29(14)
C(4)-C(3)-H(3B)	109.1	C(8)-C(9)-C(10)	108.37(13)
O(1)-C(4)-C(3)	109.63(13)	C(8)-C(9)-C(14)	122.78(14)
O(1)-C(4)-H(4)	109.1	C(14)-C(9)-C(10)	128.81(14)
O(2)-C(4)-O(1)	110.10(12)	O(5)-C(10)-N(1)	124.82(14)
O(2)-C(4)-C(3)	109.67(13)	O(5)-C(10)-C(9)	129.72(15)
O(2)-C(4)-H(4)	109.1	N(1)-C(10)-C(9)	105.44(13)
C(3)-C(4)-H(4)	109.1	C(8)-C(11)-H(11)	122.3
N(3)-C(5)-H(5A)	109.0	C(12)-C(11)-C(8)	115.40(14)
N(3)-C(5)-H(5B)	109.0	C(12)-C(11)-H(11)	122.3
N(3)-C(5)-C(6)	112.81(13)	C(11)-C(12)-C(13)	122.10(14)
H(5A)-C(5)-H(5B)	107.8	C(11)-C(12)-C(15)	130.81(14)
C(6)-C(5)-H(5A)	109.0	C(13)-C(12)-C(15)	106.73(13)
C(6)-C(5)-H(5B)	109.0	C(12)-C(13)-C(17)	106.56(13)
O(2)-C(6)-O(3)	109.66(12)	C(14)-C(13)-C(12)	122.04(14)
O(2)-C(6)-C(5)	110.30(13)	C(14)-C(13)-C(17)	131.01(14)
O(2)-C(6)-H(6)	109.1	C(9)-C(14)-H(14)	122.3
O(3)-C(6)-C(5)	109.53(12)	C(13)-C(14)-C(9)	115.40(14)
O(3)-C(6)-H(6)	109.1	C(13)-C(14)-H(14)	122.3

C(12)-C(15)-H(15)	117.3	O(6)-C(20)-C(21)	129.51(15)
C(12)-C(15)-C(16)	99.57(12)	N(2)-C(20)-C(21)	105.50(13)
C(12)-C(15)-C(18)	102.59(12)	C(22)-C(21)-C(20)	108.19(14)
C(16)-C(15)-H(15)	117.3	C(22)-C(21)-C(24)	122.55(14)
C(18)-C(15)-H(15)	117.3	C(24)-C(21)-C(20)	129.25(14)
C(18)-C(15)-C(16)	99.60(12)	C(21)-C(22)-C(23)	108.54(13)
C(15)-C(16)-H(16A)	112.8	C(21)-C(22)-C(27)	122.26(14)
C(15)-C(16)-H(16B)	112.8	C(27)-C(22)-C(23)	129.19(14)
C(15)-C(16)-C(17)	94.86(12)	O(7)-C(23)-N(2)	125.13(15)
H(16A)-C(16)-H(16B)	110.2	O(7)-C(23)-C(22)	129.41(15)
C(17)-C(16)-H(16A)	112.8	N(2)-C(23)-C(22)	105.44(13)
C(17)-C(16)-H(16B)	112.8	C(21)-C(24)-H(24)	122.3
C(13)-C(17)-C(16)	99.61(12)	C(25)-C(24)-C(21)	115.43(14)
C(13)-C(17)-H(17)	117.3	C(25)-C(24)-H(24)	122.3
C(16)-C(17)-H(17)	117.3	C(24)-C(25)-C(26)	121.89(14)
C(19)-C(17)-C(13)	102.46(12)	C(24)-C(25)-C(28)	131.46(14)
C(19)-C(17)-C(16)	99.88(12)	C(26)-C(25)-C(28)	106.55(13)
C(19)-C(17)-H(17)	117.3	C(25)-C(26)-C(30)	106.74(13)
C(19)-C(18)-C(15)	106.56(13)	C(27)-C(26)-C(25)	122.33(14)
C(45)-C(18)-C(15)	132.02(14)	C(27)-C(26)-C(30)	130.79(14)
C(45)-C(18)-C(19)	120.08(14)	C(22)-C(27)-H(27)	122.2
C(18)-C(19)-C(17)	106.17(13)	C(26)-C(27)-C(22)	115.52(14)
C(31)-C(19)-C(17)	132.55(14)	C(26)-C(27)-H(27)	122.2
C(31)-C(19)-C(18)	119.91(14)	C(25)-C(28)-H(28)	117.2
O(6)-C(20)-N(2)	124.98(14)	C(25)-C(28)-C(29)	98.91(12)

C(25)-C(28)-C(31)	103.35(12)	C(35)-C(34)-C(33)	108.07(13)
C(29)-C(28)-H(28)	117.2	C(37)-C(34)-C(33)	129.31(14)
C(31)-C(28)-H(28)	117.2	C(37)-C(34)-C(35)	122.62(14)
C(31)-C(28)-C(29)	100.08(12)	C(34)-C(35)-C(36)	108.36(13)
C(28)-C(29)-H(29A)	112.8	C(34)-C(35)-C(40)	122.38(14)
C(28)-C(29)-H(29B)	112.8	C(40)-C(35)-C(36)	129.26(14)
C(28)-C(29)-C(30)	94.79(12)	O(9)-C(36)-N(3)	125.32(14)
H(29A)-C(29)-H(29B)	110.2	O(9)-C(36)-C(35)	129.44(14)
C(30)-C(29)-H(29A)	112.8	N(3)-C(36)-C(35)	105.20(13)
C(30)-C(29)-H(29B)	112.8	C(34)-C(37)-H(37)	122.4
C(26)-C(30)-C(29)	98.84(12)	C(38)-C(37)-C(34)	115.19(14)
C(26)-C(30)-H(30)	117.3	C(38)-C(37)-H(37)	122.4
C(26)-C(30)-C(32)	103.10(12)	C(37)-C(38)-C(39)	122.42(14)
C(29)-C(30)-H(30)	117.3	C(37)-C(38)-C(41)	130.71(14)
C(32)-C(30)-C(29)	100.07(12)	C(39)-C(38)-C(41)	106.80(13)
C(32)-C(30)-H(30)	117.3	C(38)-C(39)-C(43)	106.80(13)
C(19)-C(31)-C(28)	132.70(14)	C(40)-C(39)-C(38)	121.94(14)
C(19)-C(31)-C(32)	119.95(14)	C(40)-C(39)-C(43)	131.19(14)
C(32)-C(31)-C(28)	106.16(13)	C(35)-C(40)-H(40)	122.3
C(31)-C(32)-C(30)	106.58(13)	C(39)-C(40)-C(35)	115.43(14)
C(44)-C(32)-C(30)	132.02(14)	C(39)-C(40)-H(40)	122.3
C(44)-C(32)-C(31)	120.09(14)	C(38)-C(41)-H(41)	117.3
O(8)-C(33)-N(3)	125.20(14)	C(38)-C(41)-C(42)	99.16(12)
O(8)-C(33)-C(34)	129.18(14)	C(38)-C(41)-C(44)	102.53(12)
N(3)-C(33)-C(34)	105.58(13)	C(42)-C(41)-H(41)	117.3

C(44)-C(41)-H(41)	117.3	Cl(5C)-C(3S)-H(3SF)	107.2
C(44)-C(41)-C(42)	100.12(12)	Cl(5S)-C(3S)-H(3SA)	109.5
C(41)-C(42)-H(42A)	112.8	Cl(5S)-C(3S)-H(3SB)	109.5
C(41)-C(42)-H(42B)	112.8	Cl(6B)-C(3S)-H(3SC)	109.0
H(42A)-C(42)-H(42B)	110.2	Cl(6B)-C(3S)-H(3SD)	109.0
C(43)-C(42)-C(41)	94.84(11)	Cl(6C)-C(3S)-H(3SE)	107.2
C(43)-C(42)-H(42A)	112.8	Cl(6C)-C(3S)-H(3SF)	107.2
C(43)-C(42)-H(42B)	112.8	Cl(6S)-C(3S)-Cl(5S)	110.56(17)
C(39)-C(43)-C(42)	99.19(12)	Cl(6S)-C(3S)-H(3SA)	109.5
C(39)-C(43)-H(43)	117.4	Cl(6S)-C(3S)-H(3SB)	109.5
C(39)-C(43)-C(45)	102.52(12)	H(3SA)-C(3S)-H(3SB)	108.1
C(42)-C(43)-H(43)	117.4	H(3SC)-C(3S)-H(3SD)	107.8
C(45)-C(43)-C(42)	99.70(12)	H(3SE)-C(3S)-H(3SF)	106.8
C(45)-C(43)-H(43)	117.4	Cl(1S)-C(1S)-H(1SA)	109.3
C(32)-C(44)-C(41)	132.30(14)	Cl(1S)-C(1S)-H(1SB)	109.3
C(32)-C(44)-C(45)	119.99(14)	Cl(2S)-C(1S)-Cl(1S)	111.55(9)
C(45)-C(44)-C(41)	106.23(13)	Cl(2S)-C(1S)-H(1SA)	109.3
C(18)-C(45)-C(43)	132.06(14)	Cl(2S)-C(1S)-H(1SB)	109.3
C(18)-C(45)-C(44)	119.96(14)	H(1SA)-C(1S)-H(1SB)	108.0
C(44)-C(45)-C(43)	106.68(13)	Cl(3B)-C(2SB)-H(2SA)	109.1
Cl(5B)-C(3S)-Cl(6B)	113.1(6)	Cl(3B)-C(2SB)-H(2SB)	109.1
Cl(5B)-C(3S)-H(3SC)	109.0	Cl(4B)-C(2SB)-Cl(3B)	112.6(19)
Cl(5B)-C(3S)-H(3SD)	109.0	Cl(4B)-C(2SB)-H(2SA)	109.1
Cl(5C)-C(3S)-Cl(6C)	120.5(8)	Cl(4B)-C(2SB)-H(2SB)	109.1
Cl(5C)-C(3S)-H(3SE)	107.2	H(2SA)-C(2SB)-H(2SB)	107.8

Cl(3S)-C(2S)-Cl(4S)	111.67(11)
Cl(3S)-C(2S)-H(2SC)	109.3
Cl(3S)-C(2S)-H(2SD)	109.3
Cl(4S)-C(2S)-H(2SC)	109.3
Cl(4S)-C(2S)-H(2SD)	109.3
H(2SC)-C(2S)-H(2SD)	107.9

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for capsularene **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	17(1)	16(1)	19(1)	-2(1)	0(1)	1(1)
O(2)	16(1)	15(1)	19(1)	-2(1)	0(1)	0(1)
O(3)	16(1)	16(1)	17(1)	-1(1)	0(1)	-1(1)
O(4)	20(1)	20(1)	22(1)	-3(1)	2(1)	1(1)
O(5)	19(1)	20(1)	18(1)	-1(1)	-2(1)	0(1)
O(6)	18(1)	20(1)	18(1)	-1(1)	-4(1)	1(1)
O(7)	22(1)	18(1)	22(1)	3(1)	1(1)	-1(1)
O(8)	19(1)	16(1)	25(1)	2(1)	1(1)	-2(1)
O(9)	16(1)	16(1)	24(1)	-1(1)	0(1)	2(1)
N(1)	15(1)	17(1)	18(1)	-1(1)	-1(1)	1(1)
N(2)	14(1)	17(1)	19(1)	-1(1)	-1(1)	0(1)
N(3)	12(1)	15(1)	20(1)	1(1)	1(1)	-1(1)
C(1)	14(1)	18(1)	20(1)	-1(1)	-1(1)	2(1)
C(2)	14(1)	18(1)	18(1)	-2(1)	-1(1)	2(1)
C(3)	14(1)	19(1)	22(1)	-4(1)	0(1)	-2(1)
C(4)	14(1)	17(1)	21(1)	-2(1)	-1(1)	-2(1)
C(5)	12(1)	18(1)	19(1)	0(1)	2(1)	-1(1)
C(6)	13(1)	17(1)	20(1)	-1(1)	2(1)	0(1)
C(7)	16(1)	14(1)	18(1)	2(1)	-1(1)	0(1)
C(8)	16(1)	14(1)	18(1)	2(1)	0(1)	2(1)

C(9)	16(1)	15(1)	17(1)	2(1)	-3(1)	-1(1)
C(10)	15(1)	14(1)	18(1)	2(1)	0(1)	2(1)
C(11)	18(1)	13(1)	18(1)	0(1)	-1(1)	0(1)
C(12)	16(1)	13(1)	18(1)	2(1)	-3(1)	0(1)
C(13)	16(1)	15(1)	16(1)	2(1)	1(1)	1(1)
C(14)	18(1)	16(1)	16(1)	1(1)	0(1)	0(1)
C(15)	14(1)	14(1)	19(1)	1(1)	-2(1)	-1(1)
C(16)	17(1)	18(1)	20(1)	2(1)	0(1)	-3(1)
C(17)	14(1)	17(1)	18(1)	1(1)	1(1)	-1(1)
C(18)	10(1)	14(1)	20(1)	-1(1)	-1(1)	-1(1)
C(19)	11(1)	19(1)	16(1)	0(1)	1(1)	-1(1)
C(20)	16(1)	12(1)	19(1)	-4(1)	-1(1)	-1(1)
C(21)	16(1)	14(1)	17(1)	-3(1)	-3(1)	1(1)
C(22)	17(1)	13(1)	18(1)	-2(1)	0(1)	-1(1)
C(23)	18(1)	14(1)	20(1)	-2(1)	-1(1)	0(1)
C(24)	17(1)	16(1)	16(1)	-2(1)	-1(1)	1(1)
C(25)	16(1)	14(1)	17(1)	-3(1)	0(1)	0(1)
C(26)	16(1)	13(1)	19(1)	-4(1)	-4(1)	2(1)
C(27)	20(1)	13(1)	17(1)	0(1)	-2(1)	1(1)
C(28)	14(1)	18(1)	18(1)	-3(1)	-1(1)	0(1)
C(29)	16(1)	17(1)	22(1)	-5(1)	-1(1)	2(1)
C(30)	15(1)	14(1)	19(1)	-2(1)	-4(1)	1(1)
C(31)	11(1)	17(1)	18(1)	-2(1)	0(1)	1(1)
C(32)	10(1)	15(1)	19(1)	-2(1)	-2(1)	1(1)
C(33)	16(1)	16(1)	14(1)	-1(1)	0(1)	1(1)

C(34)	16(1)	14(1)	14(1)	0(1)	0(1)	-1(1)
C(35)	14(1)	14(1)	14(1)	-1(1)	0(1)	1(1)
C(36)	15(1)	17(1)	14(1)	-1(1)	0(1)	-2(1)
C(37)	18(1)	13(1)	15(1)	1(1)	-1(1)	0(1)
C(38)	15(1)	15(1)	14(1)	0(1)	-1(1)	2(1)
C(39)	14(1)	15(1)	14(1)	-2(1)	0(1)	-2(1)
C(40)	17(1)	13(1)	15(1)	-1(1)	-1(1)	1(1)
C(41)	14(1)	16(1)	16(1)	0(1)	-1(1)	1(1)
C(42)	14(1)	18(1)	18(1)	-1(1)	-2(1)	1(1)
C(43)	12(1)	14(1)	16(1)	-1(1)	-1(1)	0(1)
C(44)	10(1)	15(1)	17(1)	1(1)	-1(1)	2(1)
C(45)	10(1)	16(1)	18(1)	-3(1)	-1(1)	-1(1)
Cl(5B)	115(8)	31(3)	24(2)	-3(2)	-14(3)	15(4)
Cl(5C)	92(8)	61(7)	63(5)	1(4)	14(5)	13(7)
Cl(5S)	51(1)	22(1)	32(1)	-4(1)	-13(1)	7(1)
Cl(6B)	28(2)	102(6)	38(2)	0(3)	-2(1)	4(3)
Cl(6C)	37(4)	46(5)	112(8)	3(5)	10(4)	-7(4)
Cl(6S)	26(1)	65(1)	41(1)	-19(1)	-3(1)	2(1)
C(3S)	28(1)	30(1)	35(1)	-7(1)	-4(1)	2(1)
Cl(1S)	23(1)	30(1)	29(1)	-7(1)	-4(1)	4(1)
Cl(2S)	22(1)	25(1)	34(1)	-4(1)	0(1)	-2(1)
C(1S)	21(1)	21(1)	36(1)	-11(1)	-2(1)	2(1)
Cl(3B)	34(1)	32(1)	26(1)	-2(1)	0(1)	0(1)
Cl(4B)	36(1)	43(1)	21(1)	-2(1)	-4(1)	2(1)
C(2SB)	35(1)	24(1)	15(1)	0(1)	-1(1)	1(1)

Cl(3S)	34(1)	32(1)	26(1)	-2(1)	0(1)	0(1)
Cl(4S)	36(1)	43(1)	21(1)	-2(1)	-4(1)	2(1)
C(2S)	35(1)	24(1)	15(1)	0(1)	-1(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for capsularene **1**.

	x	y	z	U(eq)
H(1A)	1306	4051	5428	21
H(1B)	1280	4667	5958	21
H(2)	403	3158	6081	20
H(3A)	1433	-8	6053	22
H(3B)	1377	531	5499	22
H(4)	455	1476	6124	20
H(5A)	1338	3021	7611	20
H(5B)	1412	1853	7635	20
H(6)	443	2352	6878	20
H(11)	5513	5299	6533	20
H(14)	5551	3450	4947	20
H(15)	7862	5239	6434	19
H(16A)	9077	4698	5669	22
H(16B)	8084	5367	5438	22
H(17)	7901	3639	5050	20
H(24)	5560	1476	4986	20
H(27)	5714	-152	6638	20
H(28)	7917	1482	5088	20
H(29A)	9176	547	5726	22

H(29B)	8208	-188	5532	22
H(30)	8034	56	6525	19
H(37)	5700	871	7516	19
H(40)	5512	4366	7437	18
H(41)	8016	1190	7495	18
H(42A)	8160	2760	8047	20
H(42B)	9141	2770	7622	20
H(43)	7867	4237	7436	17
H(3SA)	8455	6983	5752	37
H(3SB)	8419	7967	5412	37
H(3SC)	8273	7887	5458	37
H(3SD)	8664	6872	5709	37
H(3SE)	8285	7615	5380	37
H(3SF)	9081	6851	5659	37
H(1SA)	8787	5237	2911	31
H(1SB)	9974	5668	3055	31
H(2SA)	4210	1589	4284	30
H(2SB)	4452	1155	3716	30
H(2SC)	6016	3179	3540	30
H(2SD)	6025	2022	3444	30