SUPPORTING INFORMATION

TPDYs: Strained Macrocyclic Diynes for Bioconjugation Processes

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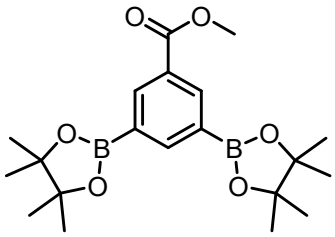
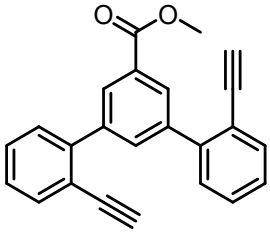
GENERAL

All reactions that were carried out under anhydrous conditions were performed under an inert argon or nitrogen atmosphere in glassware that had previously been dried overnight at 120 °C or had been flame dried and cooled under a stream of argon or nitrogen. All chemical products were obtained from Sigma-Aldrich Chemical Company, Oakwood Chemical or Alfa Aesar and were reagent quality. Technical solvents were obtained from VWR International Co. Anhydrous solvents (CH2Cl2, Et2O, THF, DMF, toluene, and n-hexane) were dried and deoxygenated using a GlassContour system (Irvine, CA). Isolated yields reflect the mass obtained following flash column silica gel chromatography. Organic compounds were purified using silica gel obtained from Silicycle Chemical division (40-63 nm; 230-240 mesh). Analytical thin-layer chromatography (TLC) was performed on glass-backed silica gel 60 coated with a fluorescence indicator (Silicycle Chemical division, 0.25 mm, F254.). Visualization of TLC plate was performed by UV (254 nm), KMnO4 or p-anisaldehyde stains. All mixed solvent eluents are reported as v/v solutions. Concentration refers to removal of volatiles at low pressure on a rotary evaporator. All reported compounds were homogeneous by thin layer chromatography (TLC) and by ^{1}H NMR. NMR spectra were taken in deuterated $CDCl_3$ using Bruker AV-400 and AV-500 instruments unless otherwise noted. Signals due to the solvent served as the internal standard ($CHCl_3$: δ 7.27 for ^{1}H, δ 77.0 for ^{13}C). The acquisition parameters are shown on all spectra. The 1H NMR chemical shifts and coupling constants were determined assuming first-order behavior. Multiplicity is indicated by one or more of the following: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), br (broad); the list of couplings constants (J) corresponds to the order of the multiplicity assignment. High resolution mass spectroscopy (HRMS) was done by the Centre régional de spectrométrie de masse at the Département de Chimie, Université de Montréal from an Agilent LC-MSD TOF system using ESI mode of ionization unless otherwise noted. X-ray structures were obtained from a shock-cooled single crystal at 150 K on a Bruker Venture Metaljet k-geometry diffractometer with a Metal Jet using a Helios MX Mirror Optics as monochromator and a Bruker CMOS Photon III detector. The diffractometer was equipped with an Oxford Cryostream 700 low temperature device and used GaK_α radiation (λ = 1.34139 Å). Computationals studies were done with a commercial computer equipped with 24 processor and 32 GB of RAM.

SYNTHESIS OF TPDYS AND ADDUCTS
Synthesis of 3,5-TPDY : Multi-Step Synthesis:

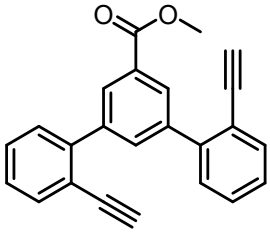


Methyl 3,5-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoate (2): In an open sealed tube was added methyl 3,5-dibromobenzoate (1.0 g, 3.4 mmol, 1 eq.), bis(pinacolato)diboron (1.99 g, 7.82 mmol, 2.3 eq.), and KOAc (2.0 g, 20.4 mmol, 6 eq.). Dry 1,4-dioxane (15 mL, [227 mM]) was added, and the mixture was purged with N_2 for 10 min. Under N_2 atomsphere, $Pd(dppf)Cl_2 \cdot CH_2Cl_2$ (124 mg, 0.170 mmol, 0.05 eq.) was added. The reaction vial was sealed with a Teflon cap and the mixture was then heated to 90 °C for 16 h. The reaction mixture was cooled to room temperature, filtered through a thin pad of Celite (eluting with 50 mL EtOAc), and concentrated. Purification by column chromatography (4 to 12% AcOEt in Hexanes) afforded the desired product as a white solid (1.21 g, 92%). **^{1}H NMR (500 MHz, $CDCl_3$):** δ 8.55 (d, *J* = 1.3 Hz, 2H), 8.45 – 8.41 (m, 1H), 3.91 (s, 3H), 1.35 (s, 24H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 167.3, 145.6, 138.7, 129.1, 84.2, 77.4, 52.1, 25.0; **HRMS (ESI)**: m/z calculated for $C_{20}H_{30}[^{11}B]_2O_6$ $[M+H]^+$, 389.2301; found: 389.2304.

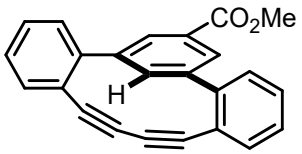


Methyl 2,2''-diethynyl-[1,1':3',1''-terphenyl]-5'-carboxylate (4): In a sealed tube vessel was added methyl 3,5-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoate (500 mg, 1.3 mmol, 1 eq.) and tripotassium phosphate (1.78 g, 7.7 mmol, 6 eq.). Toluene (26 mL [47 mM]) and H_2O (2.6 mL [47 mM]) were added, and the mixture was purged with N_2 for 10 min. Under N_2 atmosphere was added (2-bromophenylethynyl)trimethylsilane (631 µL, 3.0 mmol, 2.3 eq.), followed by SPhos (69.3 mg, 0.17 mmol, 0.13 eq.) and palladium acetate (18.8 mg, 0.084 mmol, 0.065 eq.). The vessel was sealed with a Teflon cap and the reaction mixture was then heated to 90 °C for 5 h. The reaction mixture was cooled to room temperature, filtered through a thin pad of Celite (eluting with 50 mL EtOAc), and concentrated. The crude mixture was diluted in AcOEt, washed with 10 mL of a saturated solution of K_2CO_3 and saturated brine, dried over Na_2SO_4, and concentrated *in vacuo*. The resulting solid was diluted in 5 mL of THF, and TBAF (6 mL, 1M in THF, 12 eq.) was added. The solution was stirred for 5 h. Then, 20 mL of water were added and the mixture was extracted with 3 x 10 mL of AcOEt. The combined organics were dried with $MgSO_4$ and then concentrated under reduced pressure. Purification by column chromatography (10% AcOEt in Hexanes) afforded the desired product as a brown solid (308 mg, 71 %). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.31 (d, *J* = 1.8 Hz, 2H), 7.99 (dd, *J* = 1.8, 1.8 Hz, 1H), 7.68 – 7.61 (m, 2H), 7.50 – 7.40 (m, 4H), 7.40 – 7.30 (m, 2H), 3.95 (s, 3H), 3.09 (s, 2H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 167.1, 143.4, 140.4, 134.7, 134.1, 130.0, 129.7, 129.7, 129.3, 127.7, 120.7, 83.0, 80.9, 52.4; **HRMS (ESI)**: m/z calculated for $C_{24}H_{16}O_2$ $[M+H]^+$, 337.1223; found: 337.1210.

Synthesis of 3,5-TPDY : One-Pot Synthesis:

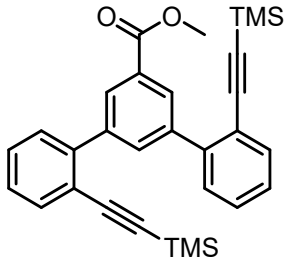


Methyl 2,2''-diethynyl-[1,1':3',1''-terphenyl]-5'-carboxylate (4): In a sealed tube vessel was added XPhos-Pd G3 (8.46 mg, 10 µmol, 0.02 eq.), XPhos (9.53 mg, 20 µmol, 0.04 eq.), tetrahydroxydiboron (269 mg, 3 mmol, 6 eq.), and KOAc (294 mg, 3 mmol, 6 eq.). The vessel was sealed and the atmosphere was flushed with N_2. Degassed EtOH (5 mL, [0.1M]) was added via syringe followed by the addition of the dibromoarene (147mg, 0.5 mmol, 1 eq.). The reaction mixture was then heated to 80 °C for 1.5 h. Then a needle outlet attached to a manifold under argon was inserted into the septum and degassed aqueous K_2CO_3 (6 eq., 1.8M, 1.67 mL, 3 mmol) and (2-bromophenylethynyl)trimethylsilane (257 mg, 1 mmol, 2 eq.) were added via syringe. The manifold needle was removed, and the reaction mixture was again heated to 80 °C for 15 h. The reaction mixture was cooled to room temperature, filtered through a thin pad of Celite (eluting with 50 mL EtOAc), and concentrated. The crude solid diluted with 20 mL of water, and the mixture was extracted with EtOAc (3 × 10 mL), and the combined organics were dried with $MgSO_4$ and then concentrated under reduced pressure. The resulting solid was diluted in 5 mL of THF, and TBAF (6 mL, 1M in THF, 12 eq.) was added. The solution was stirred for 5 h. Then, 20 mL of water was added, and the mixture was extracted with 3 x 10 mL of AcOEt. The combined organics were dried with $MgSO_4$ and then concentrated under reduced pressure. Purification by column chromatography (10% AcOEt in Hexanes) afforded the desired product as a brown solid (132 mg, 55%).

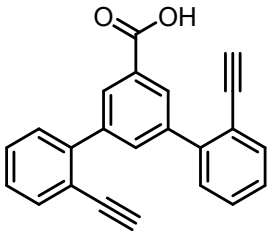


3,5-TPDY (5): To a solution of copper acetate (432 mg, 2.38 mmol, 4 eq.) in Et_2O:Pyridine 1:1 [3 mM] was slowly added over a period of 3 h a solution of methyl 2,2''-diethynyl-[1,1':3',1''-terphenyl]-5'-carboxylate (200 mg, 0.60 mmol, 1 eq.) in 20 mL of Et_2O:Pyridine 1:3. The solution was then stirred for an additional 2 h or until full consumption of the starting material observed by TLC. The solvent was removed, and the solution was diluted in CH_2Cl_2. The organic phase was then washed with 1M HCl twice, a saturated solution of NH_4OH four times and saturated brine. The organic phase was then dried over Na_2SO_4, and concentrated *in vacuo*, to give the pure product as an off-white solid (190 mg, 96%). Alternatively, the product can be purified by flash column chromatography (0→1% AcOEt in Hexanes). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.55 (dd, *J* = 1.8, 1.8 Hz, 1H), 8.02 (d, *J* = 1.8 Hz, 2H), 7.62 (dd, *J* = 7.8, 1.3 Hz, 2H), 7.51 – 7.43 (m, 2H), 7.40 – 7.31 (m, 2H), 7.31 – 7.26 (m, 2H), 3.94 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 166.9, 147.9, 142.1, 140.4, 131.5, 130.5, 130.1, 129.9, 128.1, 127.7, 121.9, 107.6, 87.0, 52.4; **HRMS (ESI)**: m/z calculated for $C_{24}H_{14}O_2$ $[M+H]^+$, 335.1067; found: 335.1069.

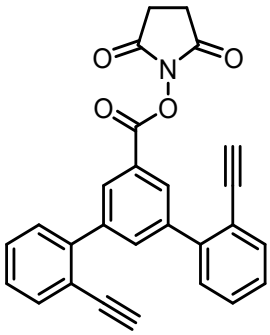
Synthesis of 3,5-TPDY-PEG-NH_3Cl



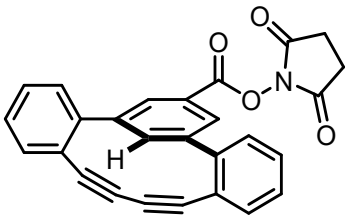
Methyl 2,2''-bis((trimethylsilyl)ethynyl)-[1,1':3',1''-terphenyl]-5'-carboxylate (S1): In a sealed tube was added methyl 3,5-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoate (500 mg, 1.3 mmol, 1 eq.) and tripotassium phosphate (1.78 g, 7.7 mmol, 6 eq.). Toluene (26 mL [47 mM]) and H_2O (2.6 mL [47 mM]) were added, and the mixture was purged with N_2 for 10 min. Under N_2 atmosphere was added (2-bromophenylethynyl)trimethylsilane (631 µL, 3.0 mmol, 2.3 eq.), followed by SPhos (69.3 mg, 0.17 mmol, 0.13 eq.) and palladium acetate (18.8 mg, 0.084 mmol, 0.065 eq.). The vessel was sealed with a Teflon cap and the reaction mixture was then heated to 90 °C for 5 h. The reaction mixture was cooled to room temperature, filtered through a thin pad of Celite (eluting with 50 mL EtOAc), and concentrated. The crude mixture was diluted in AcOEt, washed with 10 mL of a saturated solution of K_2CO_3 and saturated brine, dried over Na_2SO_4, and concentrated *in vacuo*. Purification by flash column chromatography (0→2% AcOEt in Hexanes) afforded the pure product as a orange sticky solid (450 mg, 73 %). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.35 (d, *J* = 1.8 Hz, 2H), 8.11 (dd, *J* = 1.8, 1.8 Hz, 1H), 7.60 (dd, *J* = 7.7, 1.4 Hz, 2H), 7.47 (dd, *J* = 7.8, 1.4 Hz, 2H), 7.40 (ddd, *J* = 7.6, 7.6, 1.4 Hz, 2H), 7.31 (ddd, *J* = 7.5, 7.6 1.4, Hz, 2H), 3.94 (s, 3H), 0.04 (s, 18H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 167.2, 143.0, 140.2, 135.0, 133.7, 129.7, 129.7, 129.5, 129.0, 127.5, 121.6, 104.4, 98.2, 52.2, -0.3; **HRMS (ESI)**: m/z calculated for $C_{30}H_{32}O_2Si_2$ $[M+H]^+$, 481.2014; found: 481.2007.



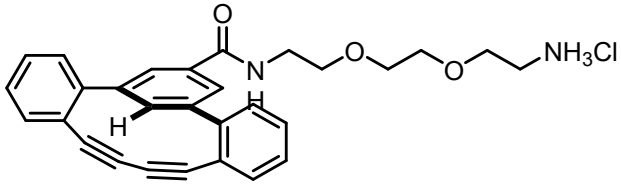
2,2''-Diethynyl-[1,1':3',1''-terphenyl]-5'-carboxylic acid (6): 2,2"-Diethynyl-[1,1':3',1"-terphenyl]-5'-carboxylate (140 mg, 0,42 mmol, 1 eq.) was dissolved in THF:H_2O 12:1 (4.4 mL, [96 mM]). Sodium methoxide (25% wt in MeOH, 2 mL, 18 eq.) was slowly added and the mixture was stirred at room temperature overnight. The solution was quenched with 1M HCl, and extracted three times with CH_2Cl_2 . The organic phases were combined, washed with saturated brine, dried over Na_2SO_4, and concentrated *in vacuo*. Purification by flash column chromatography (20→60% AcOEt in Hexanes) afforded the pure product as a orange powder (121 mg, 90%). **NMR (400 MHz, $CDCl_3$):** δ 8.43 – 8.38 (m, 2H), 8.07 – 8.02 (m, 1H), 7.69 – 7.62 (m, 2H), 7.50 – 7.42 (m, 4H), 7.41 – 7.31 (m, 2H), 3.11 (s, 2H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 143.2, 140.5, 135.5, 134.1, 130.3, 129.7, 129.3, 127.7, 120.7, 82.9, 81.0; **HRMS (ESI)**: m/z calculated for $C_{23}H_{14}O_2$ $[M+H]^+$, 323.1067; found: 323.1061.



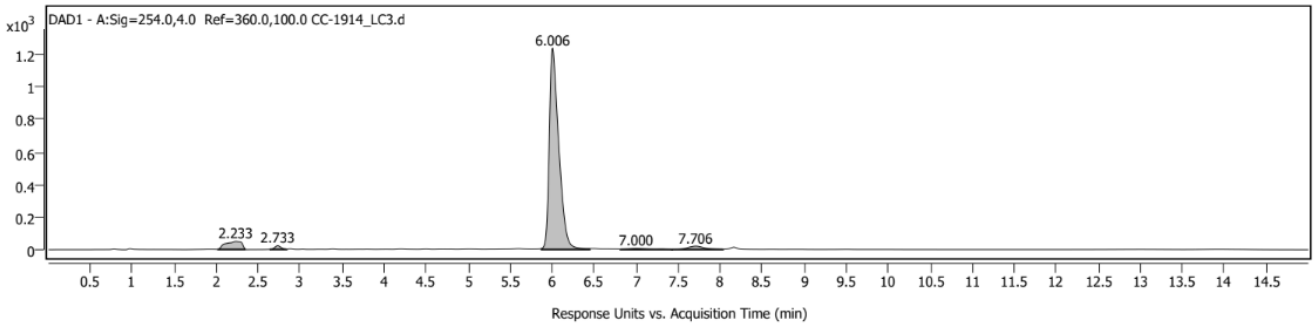
2,5-Dioxopyrrolidin-1-yl 2,2''-diethynyl-[1,1':3',1''-terphenyl]-5'-carboxylate (S2c): 2,2''-Diethynyl-[1,1':3',1''-terphenyl]-5'-carboxylic acid (150 mg, 0.47 mmol, 1 eq.) and N-hydroxysuccinimide (64 mg, 0.56 mmol, 1.2 eq.) were dissolved in dry CH_2Cl_2 (7.5 mL, [62 mM]). N-(3-Dimethylaminopropyl)-N′-ethylcarbodiimide hydrochloride (107 mg, 0.56 mmol, 1.2 eq.) was added and the mixture was stirred at room temperture overnight. The mixture was then diluted with 30 mL of CH_2Cl_2 and washed twice with 10 mL of water. The organic phase was dried over $MgSO_4$ and concentrated *in vacuo*. Purification by flash column chromatography (20→40% AcOEt in Hexanes) afforded the pure product as a off-white powder (142 mg, 73 %). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.41 (d, *J* = 1.7 Hz, 2H), 8.09 (dd, *J* = 1.7, 1.7 Hz, 1H), 7.68 – 7.61 (m, 2H), 7.49 – 7.41 (m, 4H), 7.36 (ddd, *J* = 7.6, 5.2, 3.7 Hz, 2H), 3.13 (s, 2H), 2.91 (br, 4H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 169.3, 162.0, 142.7, 140.9, 136.7, 134.1, 130.5, 129.6, 129.4, 128.0, 125.0, 120.8, 82.7, 81.3, 25.8; **HRMS (ESI)**: m/z calculated for $C_{27}H_{17}NO_4$ $[M+NH_4]^+$, 437.1496; found: 437.1507.



3,5-TPDY-OSucc (7): To a solution of copper acetate (482 mg, 2.65 mmol, 5.2 eq.) in Et_2O:Pyridine 1:1 [3 mM] was slowly added over a period of 3 h a solution of 2,5-dioxopyrrolidin-1-yl 2,2''-diethynyl-[1,1':3',1''-terphenyl]-5'-carboxylate (214 mg, 0,51 mmol, 1 eq.) in 20 mL of Et_2O:Pyridine 1:3. The solution was then stirred for an additional 2 h or until full consumption of the starting material observed by TLC. The solvent was removed, and the solution was diluted in CH_2Cl_2. The organic phase was then washed with 1M HCl twice and saturated brine. The organic phase was then dried over Na_2SO_4 and concentrated *in vacuo*. Purification by flash column chromatography (20→60% AcOEt in Hexanes) afforded the pure product as an off-white powder (170 mg, 80 %). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.63 (dd, *J* = 1.7, 1.7 Hz, 1H), 8.10 (d, *J* = 1.8 Hz, 2H), 7.62 (dd, *J* = 7.4, 1.1 Hz, 2H), 7.52 – 7.44 (m, 2H), 7.37 (dd, *J* = 7.6, 1.3 Hz, 2H), 7.31 – 7.20 (m, 2H), 2.92 (s, 4H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 169.3, 161.8, 147.2, 144.0, 141.0, 132.2, 130.4, 130.2, 128.4, 127.7, 124.9, 121.9, 107.2, 87.0, 25.8; **HRMS (ESI)**: m/z calculated for $C_{27}H_{15}NO_4$ $[M+NH_4]^+$, 435.1339; found: 435.1334.



3,5-TPDY-PEG-NH$_3$Cl (8): 3,5-TPDY-OSucc (60 mg, 0.144 mmol, 1 eq.) and tert-butyl (2-(2-(2-aminoethoxy)ethoxy)ethyl)carbamate (65 mg, 0.262 mmol, 1.8 eq.) were dissolved in CH_2Cl_2 (2 mL, [72 mM]) and the reaction was stirred at room temperature for 5 h. The solvent was then concentrated *in vacuo* and purification by by flash column chromatography (50→100% AcOEt in Hexanes) afforded 3,5-TPDY-PEG-NHBoc. The product was then directly dissolved in 1 mL of HCl 4M in dioxane. The reaction was stirred until disparition of the starting material and then 7 mL of hexanes were added. The precipitate was filtered and rinsed with hexanes, affording the desired product as an off-white solid (22 mg, 34 %)**^{1}H NMR (400 MHz, DMSO-d$_6$):** δ 8.82 (dd, *J* = 5.6, 5.6 Hz, 1H), 8.40 (dd, *J* = 1.7, 1.7 Hz, 1H), 7.97 (br, 3H), 7.84 (d, *J* = 1.8 Hz, 2H), 7.76 (dd, *J* = 7.8, 1.3 Hz, 2H), 7.66 – 7.58 (m, 2H), 7.47 (ddd, *J* = 7.6, 7.6, 1.3 Hz, 2H), 7.39 (dd, *J* = 7.7, 1.4 Hz, 2H), 3.65 – 3.52 (m, 9H), 3.50 – 3.40 (m, 2H), 2.99 – 2.87 (m, 2H); **^{13}C NMR (101 MHz, DMSO-d$_6$):** δ 165.8, 147.6, 139.5, 139.3, 134.1, 130.8, 130.6, 129.2, 128.4, 127.5, 120.4, 107.9, 86.2, 69.7, 69.5, 68.9, 66.6.



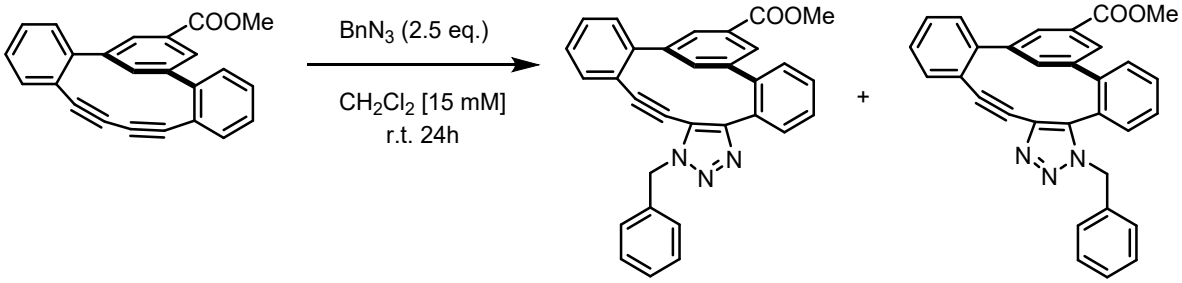
Chromatogram Peaks

RT	Area	Area Sum %
2.2	666	6.08
2.7	121	1.10
6.0	9762	89.01
7.0	123	1.12
7.7	295	2.69

Figure S1 : HPLC chromatogram of **3,5-TPDY-PEG-NH$_3$Cl**.

Strain-Promoted Alkyne-Azide Cycloadditions

General procedure



General Protocol: To a solution of 3,5-TPDY (50 mg, 0.15 mmol, 1 eq.) in CH_2Cl_2 [15 mM] was added benzyl azide (50 mg, 0.37 mmol, 2.5 eq.) and the reaction was stirred at room temperature for 24 h. The solution was then concentrated *in vacuo*. Purification by flash column chromatography (1→2% AcOEt in Hexanes) afforded the desired regioisomers as off-white solids (66 mg, 94%, 7:3).

Kinetic Measurements

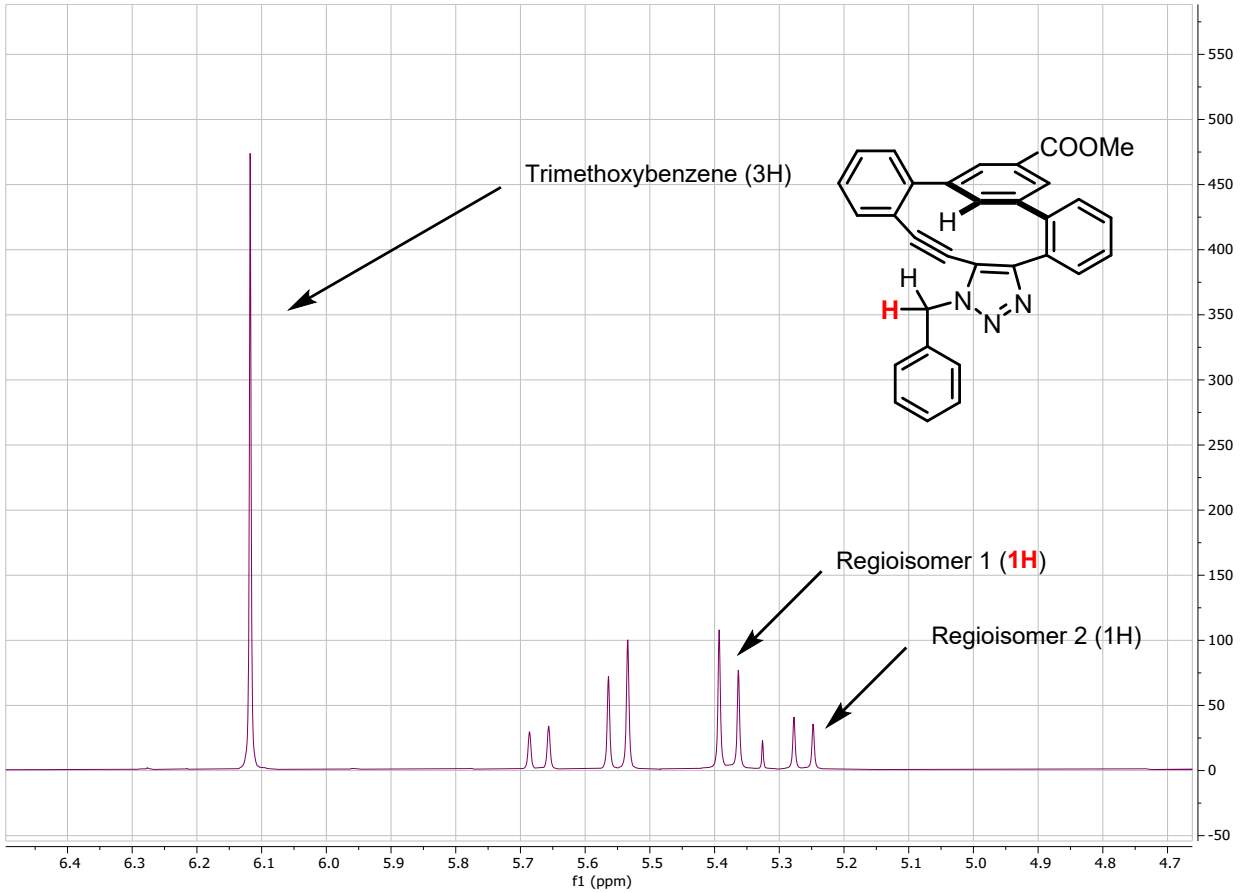
The second order rate constants were measured using ^{1}H NMR spectroscopy in $CDCl_3$ at 25 °C using 1,3,5-trimethoxybenzene as an internal standard. A solution of the diyne [22 mM] and 1,3,5-

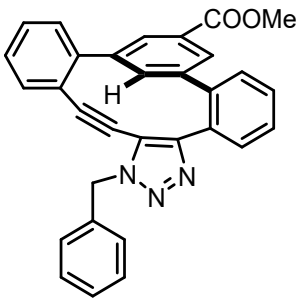
trimethoxybenzene [7mM] in 4 mL of $CDCl_3$ was prepared. In an NMR tube was added 0.5 mL of the solution. The tube was used to calibrate the NMR instrument and as a t=0 reference. Then, 0.25 mL (2.5 eq.) of a solution of benzylazide [110 mM] in $CDCl_3$ was added and the NMR tube was vigorously shaken and put into an NMR spectrometer immediately. Measurements were taken at the specified interval until 50% conversion was achieved. The experiment was repeated three times. The rate constants were estimated using the equation:

$$k = \frac{1}{t(a-b)} \times \ln \frac{b(a-x)}{a(b-x)}$$

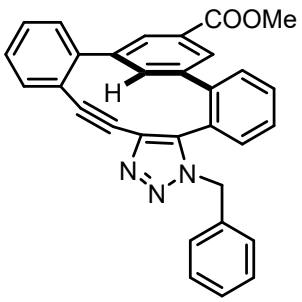
k is the rate constant in $M^{-1} \times s^{-1}$
t is the reaction time in seconds
a is the initial concentration of benzyl azide in mol/L
b is the initial concentration of the alkyne in mol/L
x is the sum of the concentrations of the regioisomer in mol/L
k is the slope of the graphic plot of $\frac{1}{(a-b)} \times \ln \frac{b(a-x)}{a(b-x)}$ versus the reaction time

3,5-TPDY





Regioisomer 5c-triazole 1: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.35 (dd, *J* = 1.7, 1.7 Hz, 1H), 7.98 – 7.91 (m, 2H), 7.76 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.71 (d, *J* = 7.6 Hz, 1H), 7.56 – 7.35 (m, 5H), 7.35 – 7.28 (m, 4H), 7.28 – 7.22 (m, 2H), 5.53 (d, *J* = 14.9 Hz, 1H), 5.36 (d, *J* = 14.8 Hz, 1H), 3.90 (s, 3H); **^{13}C NMR (176 MHz, $CDCl_3$):** δ 166.9, 149.4, 145.3, 141.9, 140.6, 140.0, 138.1, 134.7, 133.1, 131.4, 130.5, 129.9, 129.8, 129.7, 128.9, 128.8, 128.5, 128.5, 128.3, 128.2, 128.1, 128.1, 127.0, 122.3, 118.8, 103.3, 83.6, 53.1, 52.3; **HRMS (ESI)**: m/z calculated for $C_{31}H_{21}N_3O_2$ $[M+H]^+$, 468.1707; found: 468.1708.



Regioisomer 5c-triazole 2: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15 (dd, *J* = 1.8, 1.8 Hz, 1H), 7.87 (dd, *J* = 1.7, 1.7 Hz, 1H), 7.60 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.57 – 7.52 (m, 1H), 7.51 – 7.40 (m, 3H), 7.38 – 7.28 (m, 3H), 7.25 – 7.20 (m, 3H), 6.96 (dd, *J* = 1.7, 1.7 Hz, 1H), 6.68 – 6.63 (m, 2H), 5.64 (d, *J* = 14.8 Hz, 1H), 5.23 (d, *J* = 14.8 Hz, 1H), 3.91 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 166.7, 145.0, 142.9, 141.5, 138.4, 138.3, 138.0, 134.2, 131.5, 130.3, 130.3, 129.9, 129.8, 129.6, 128.9, 128.5, 128.4, 128.1, 127.6, 126.9, 123.0, 96.4, 88.2, 53.5, 52.2; **HRMS (ESI)**: m/z calculated for $C_{31}H_{21}N_3O_2$ $[M+H]^+$, 468.1707; found: 468.1708.

Note: Regioisomers configurations were confirmed by X-ray crystallography of the regioisomer **5c-triazole 1**.

Kinetics measurements were taken every 5 min for 40 minutes

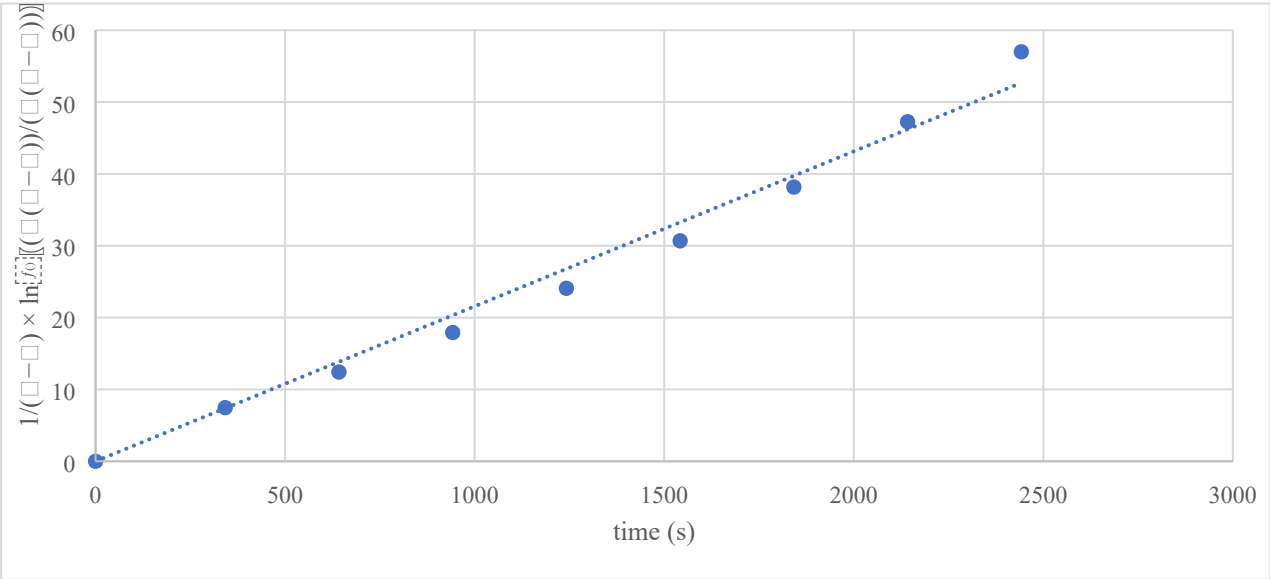


Figure S2: Plot of $\frac{1}{(a-b)} \times \ln\frac{b(a-x)}{a(b-x)}$ versus the reaction time for 3,5-TPDY Run 1

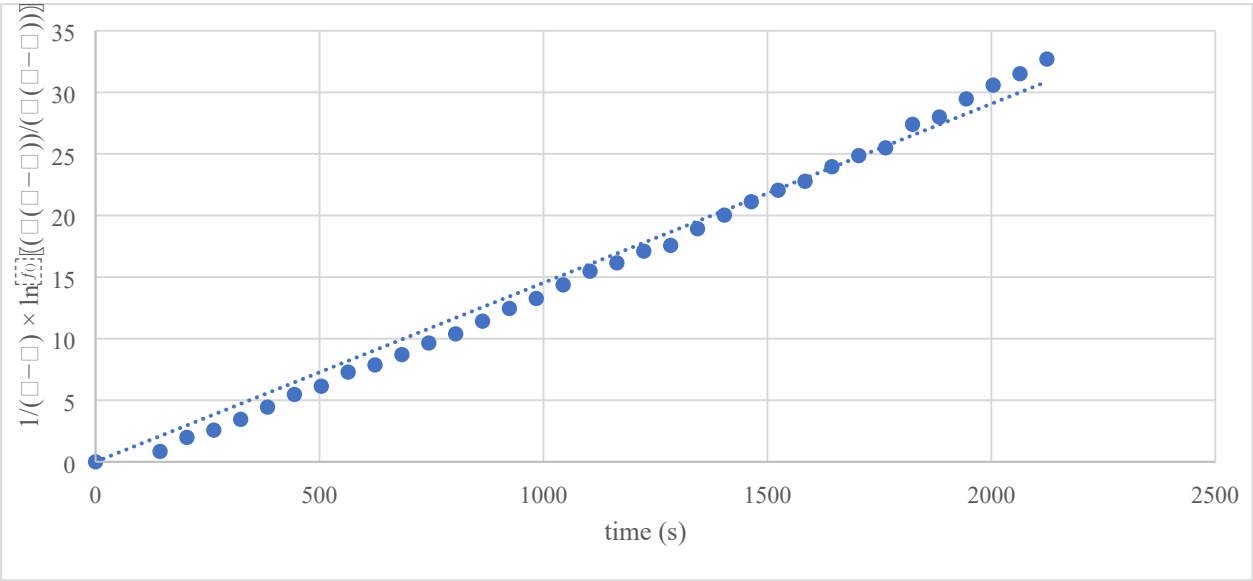


Figure S3: Plot of $\frac{1}{(a-b)} \times \ln \frac{b(a-x)}{a(b-x)}$ versus the reaction time for 3,5-TPDY Run 2

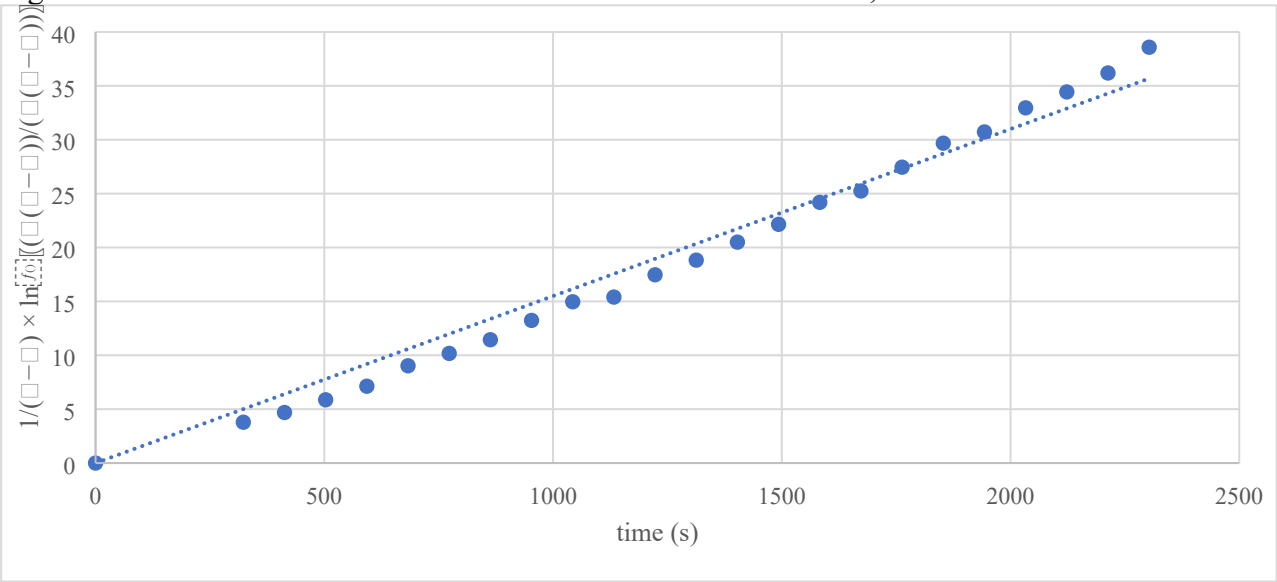
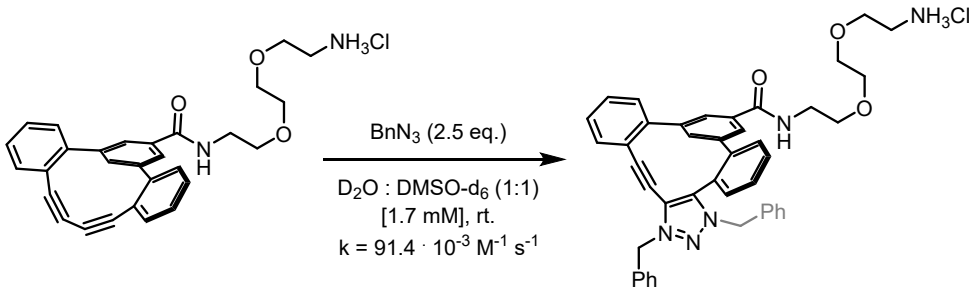


Figure S4: Plot of $\frac{1}{(a-b)} \times \ln \frac{b(a-x)}{a(b-x)}$ versus the reaction time for 3,5-TPDY Run 3

Average rate constant: $k = 1.7 \pm 1 \cdot 10^{-2}$ $M^{-1} \cdot s^{-1}$

3,5-TPDY PEG



Note: exo and endo isomers not determined due to complex spectra.

Kinetics measurements were taken every 60 sec for 12 minutes

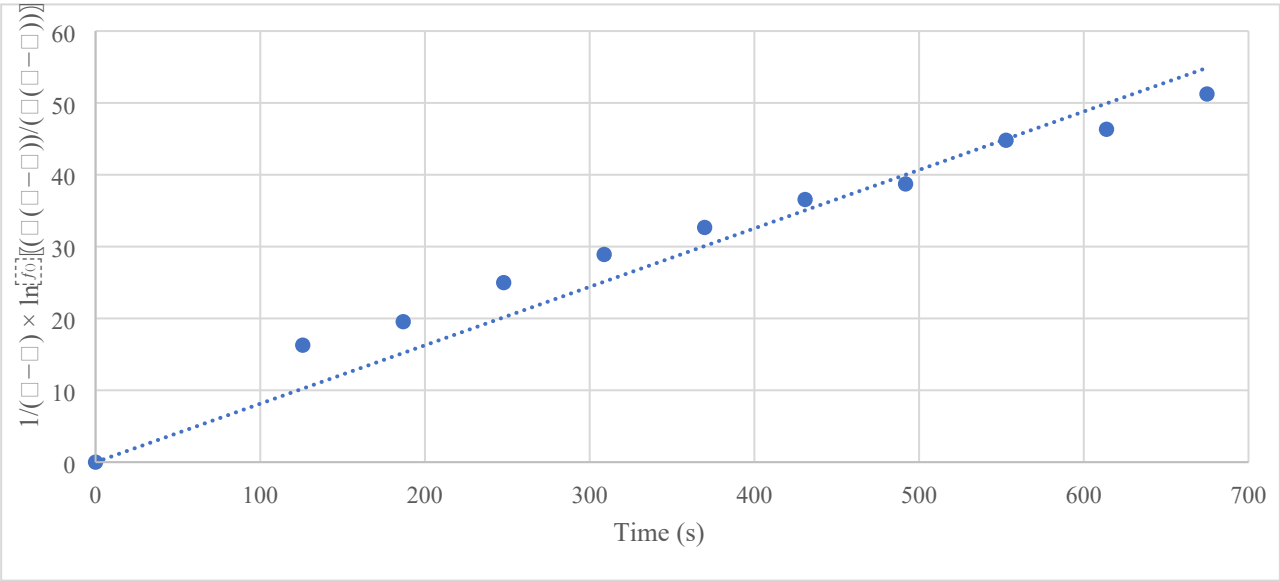


Figure S7: Plot of $\frac{1}{(a-b)} \times \ln \frac{b(a-x)}{a(b-x)}$ versus the reaction time for 3,5-TPDY PEG Run 1

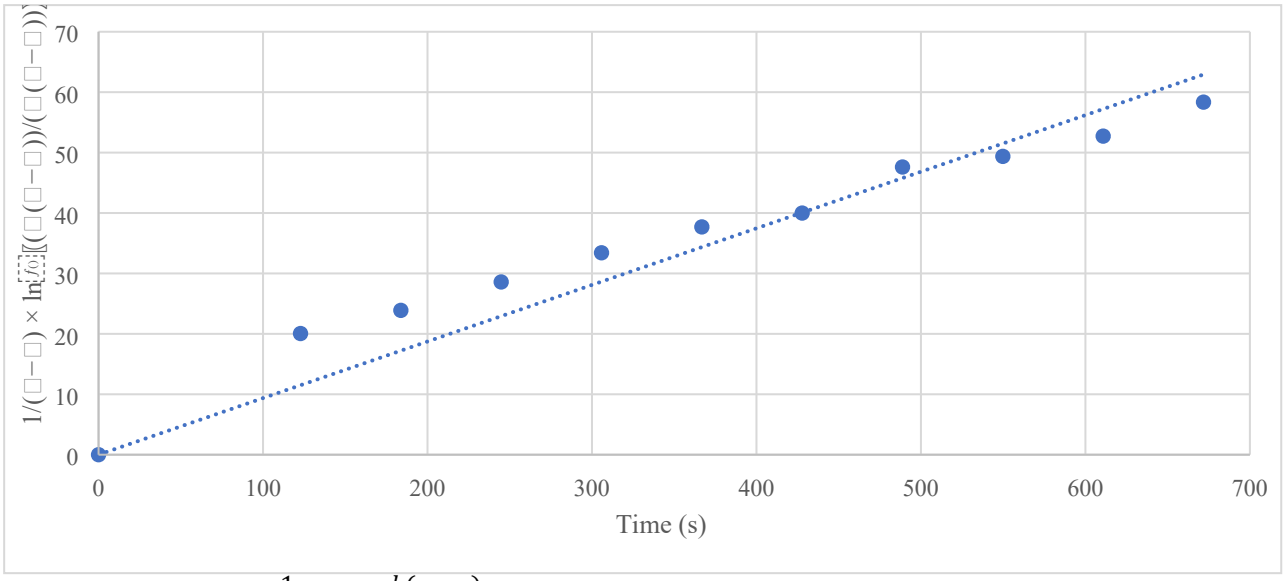


Figure S8: Plot of $\frac{1}{(a-b)} \times \ln \frac{b(a-x)}{a(b-x)}$ versus the reaction time for 3,5-TPDY PEG Run 2

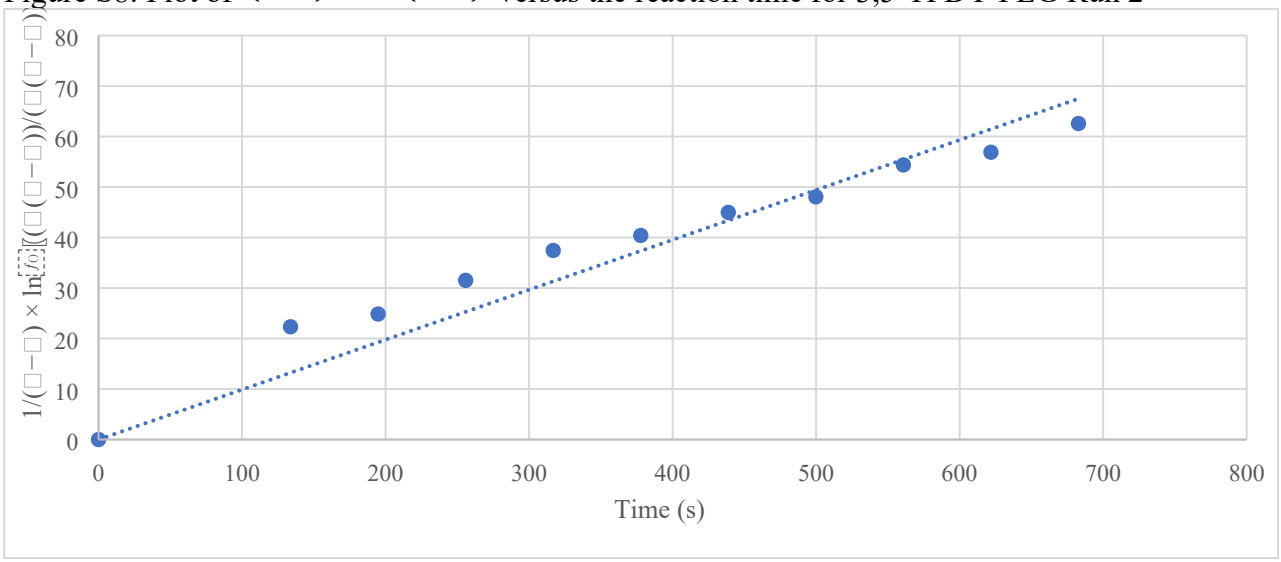
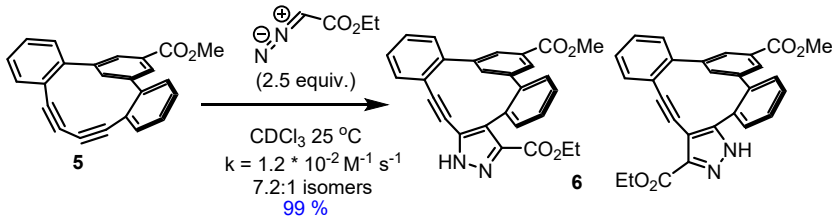


Figure S9: Plot of $\frac{1}{(a-b)} \times \ln \frac{b(a-x)}{a(b-x)}$ versus the reaction time for 3,5-TPDY PEG Run 3

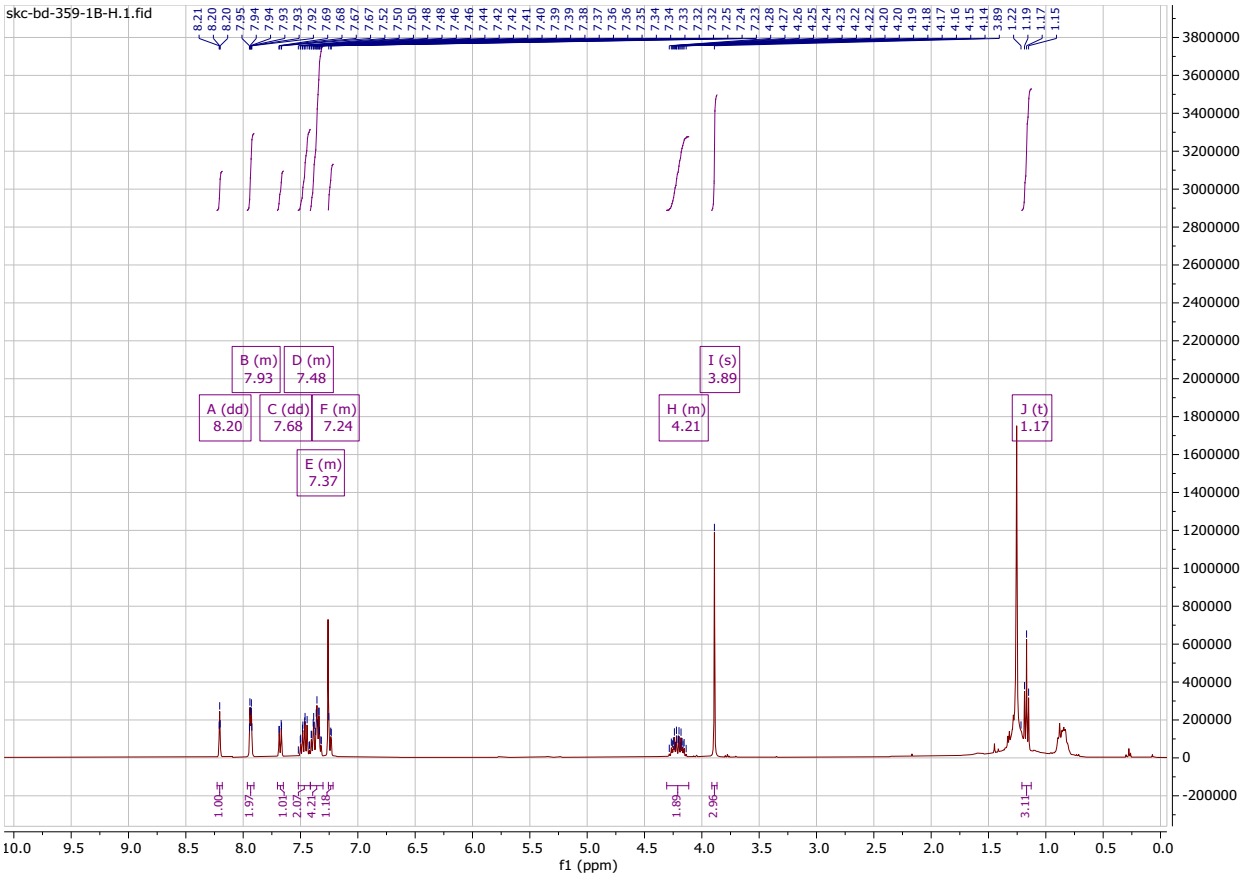
Average : k = 91.4 x 10^{-3} M^{-1} s^{-1}

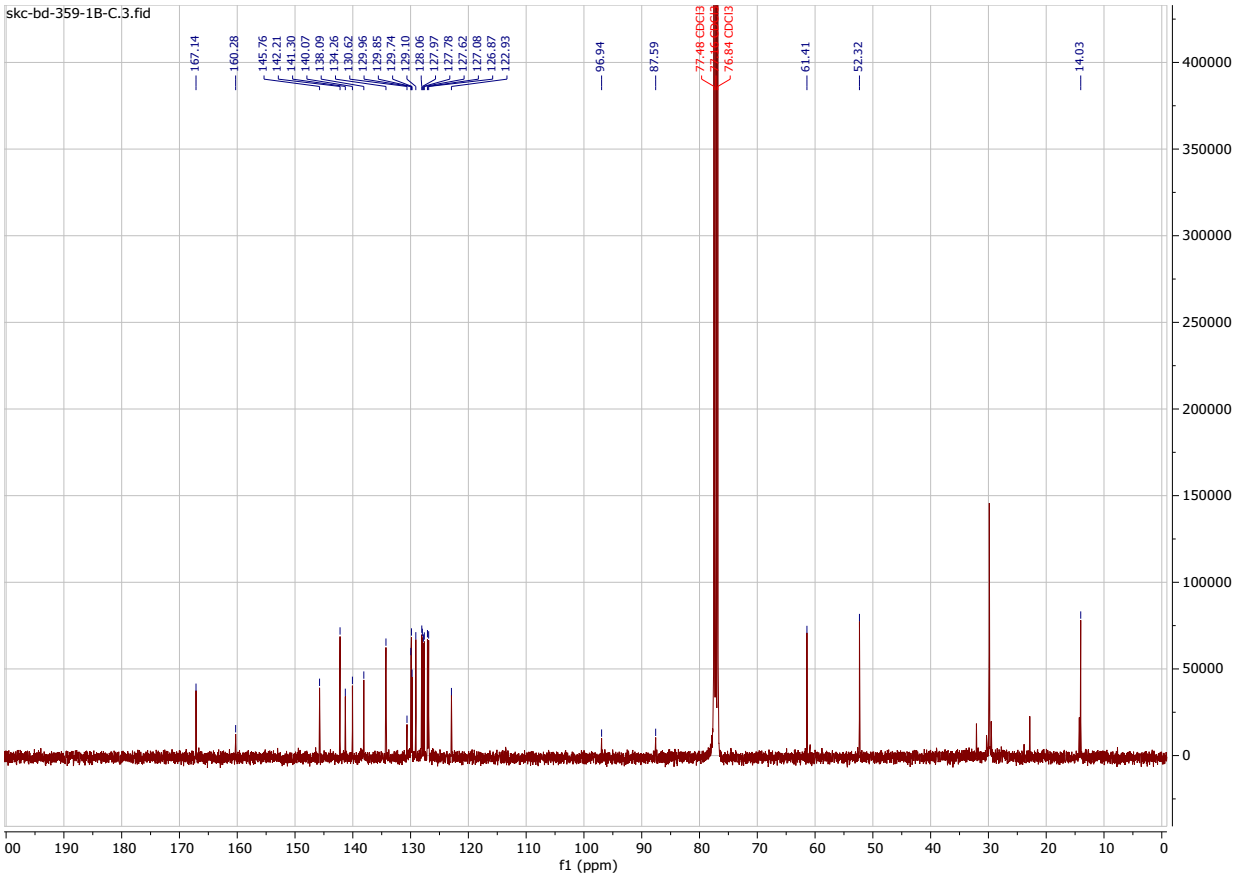
3,5-TPDY Cycloaddition with EDA



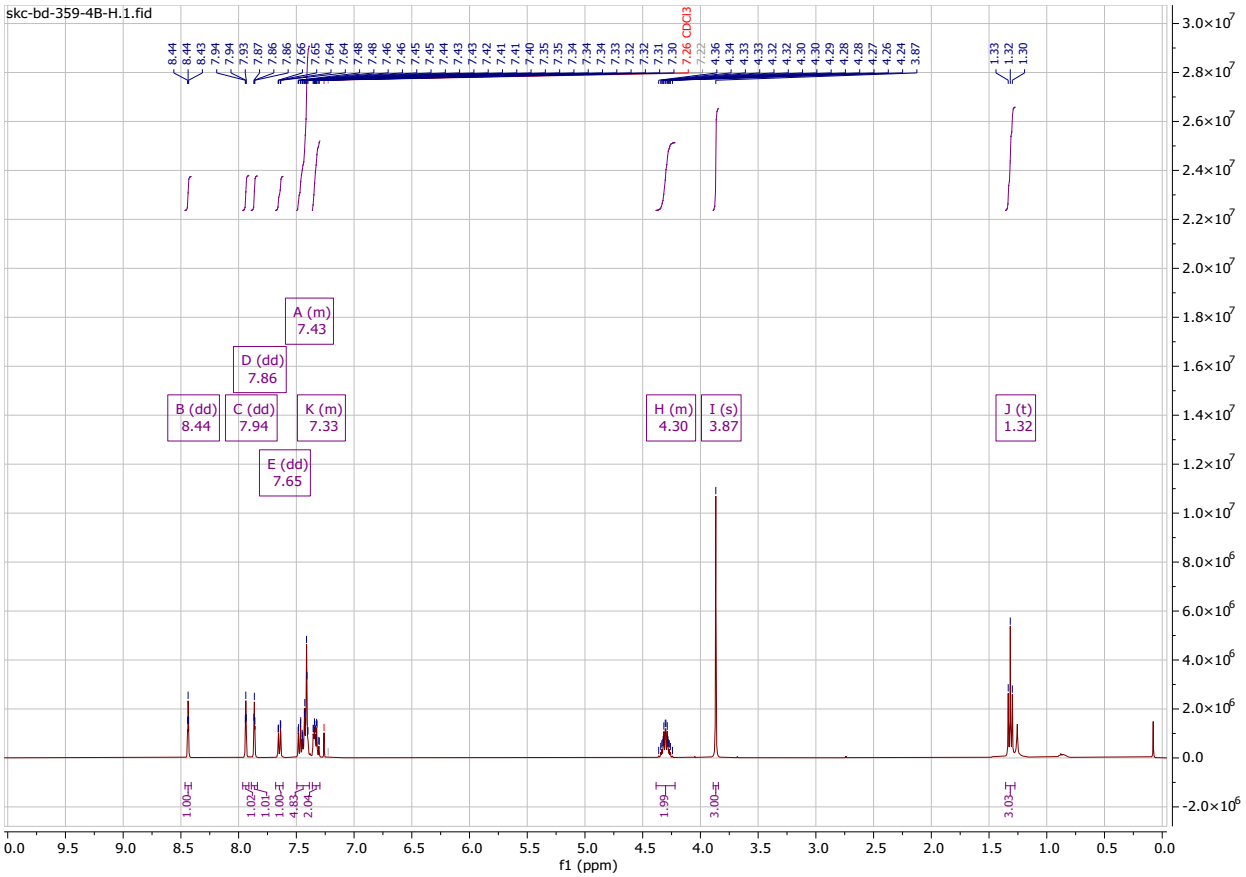
To a solution of 3,5-TPDY (30 mg, 0.0897 mmol, 1 eq.) in CH_2Cl_2 [15 mM] was added ethyl diazoacetate solution 13 % in CH_2Cl_2 (180 uL, 0.224 mmol, 2.5 eq.) and the reaction was stirred at room temperature for 3 h. The solution was then concentrated *in vacuo*. Purification by flash column chromatography (5 : 20 : 75 → 20 : 20 : 60 (AcOEt : CH_2Cl_2 : Hexanes)) afforded the desired regioisomers as a pale yellow solid (40 mg, 99%, 7.2:1). *Note: exo and endo isomers were separated and NMR spectra shown below.*

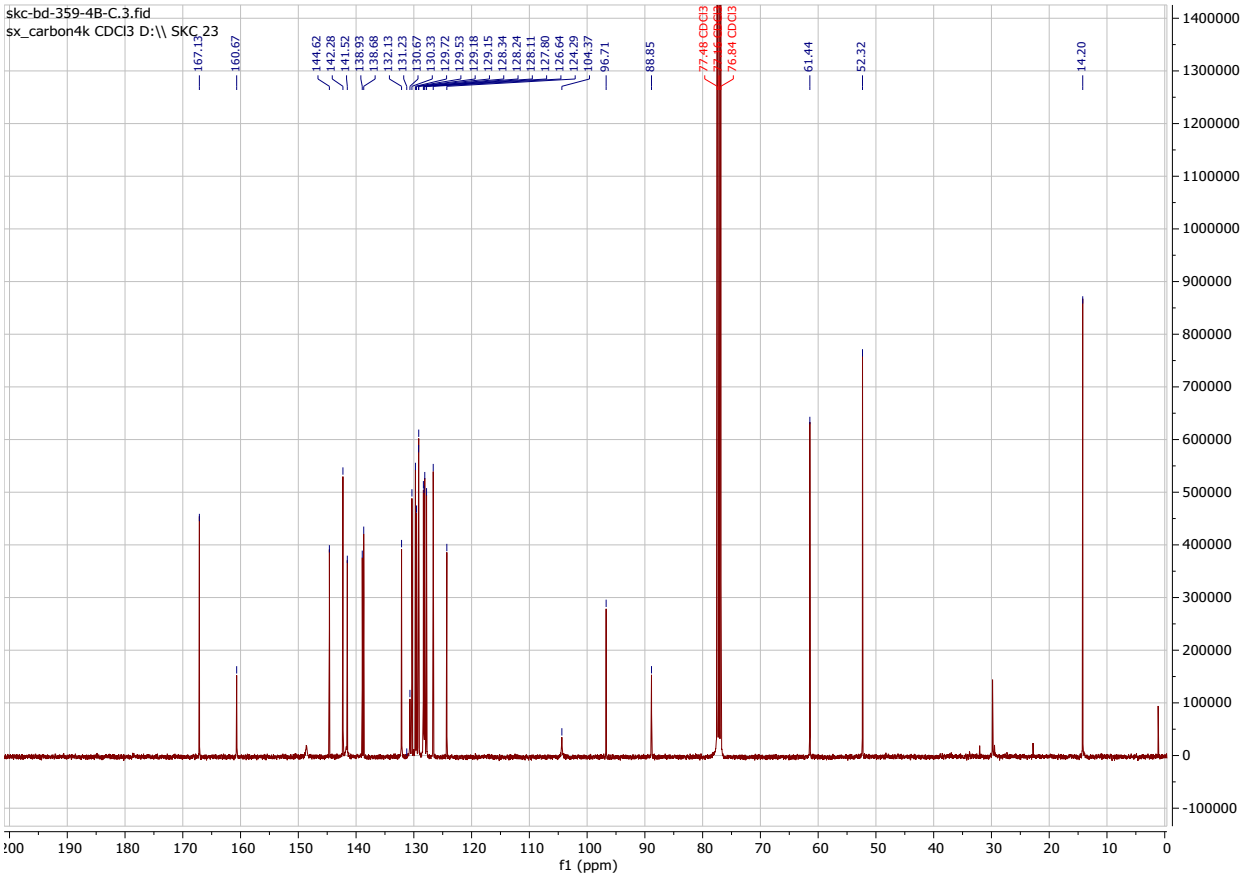
^{1}H NMR (400 MHz, Chloroform-*d*): δ 8.20 (dd, *J* = 1.7 Hz, 1H), 7.96 – 7.91 (m, 2H), 7.68 (dd, *J* = 7.7, 1.2 Hz, 1H), 7.52 – 7.41 (m, 2H), 7.41 – 7.30 (m, 4H), 7.26 – 7.22 (m, 1H), 4.31 – 4.11 (m, 2H), 3.89 (s, 3H), 1.17 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$):** 167.1, 160.3, 145.8, 142.2, 141.3, 140.1, 138.1, 134.3, 130.6, 130.0, 129.8, 129.7, 129.1, 128.1, 128.0, 127.8, 127.6, 127.1, 126.9, 122.9, 96.9, 87.6, 77.5, 77.2, 76.8, 61.4, 52.3, 14.0; **HRMS (ESI)**: m/z calculated for $C_{28}H_{20}N_2O_4$ $[M+H]^+$, 449.1515; found: 449.1496





^{1}H NMR (400 MHz, Chloroform-*d*): δ 8.44 (dd, *J* = 1.7 Hz, 1H), 7.94 (dd, *J* = 1.6 Hz, 1H), 7.86 (dd, *J* = 1.6 Hz, 1H), 7.65 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.50 – 7.39 (m, 5H), 7.36 – 7.30 (m, 2H), 4.38 – 4.22 (m, 2H), 3.87 (s, 3H), 1.32 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 167.1, 160.7, 144.6, 142.3, 141.5, 138.9, 138.7, 132.1, 131.2, 130.7, 130.3, 129.7, 129.5, 129.2, 129.2, 128.3, 128.2, 128.1, 127.8, 126.6, 124.3, 104.4, 96.7, 88.8, 61.4, 52.3, 14.2. **HRMS (ESI)**: m/z calculated for $C_{28}H_{20}N_2O_4$ $[M+H]^+$, 449.14958; found: 449.14931





Kinetics measurements were taken every 90 sec for 45 minutes

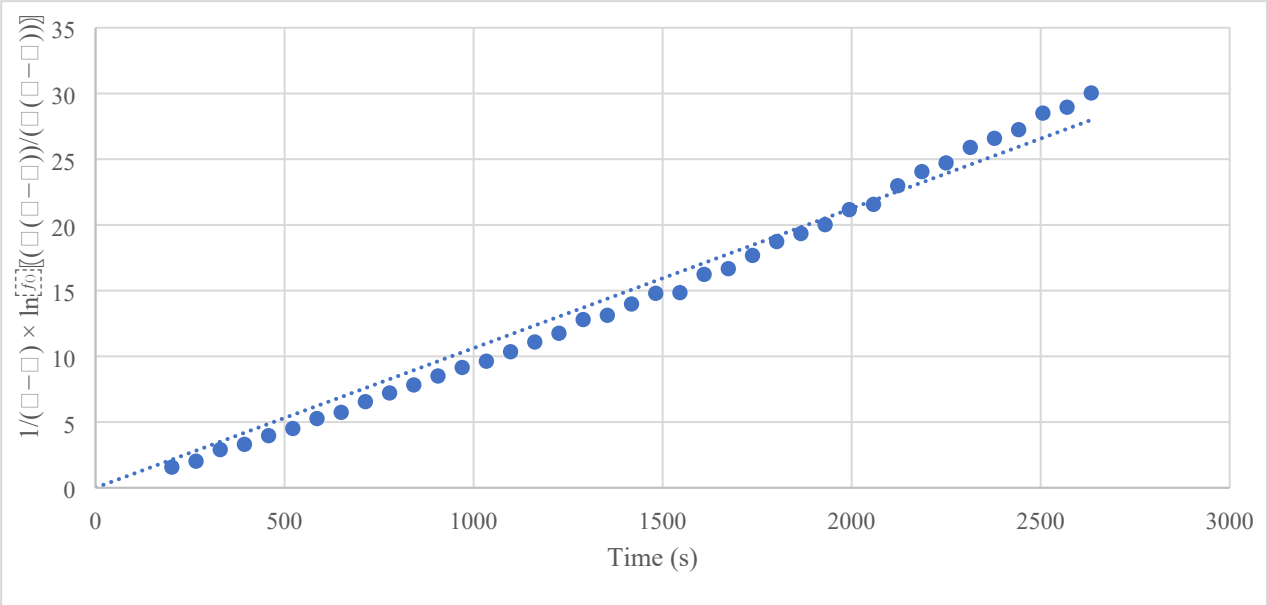


Figure 10: Plot of $\frac{1}{(a-b)} \times \ln \frac{b(a-x)}{a(b-x)}$ versus the reaction time for 3,5-TPDY cycloaddition with ethyl diazoacetate Run 1

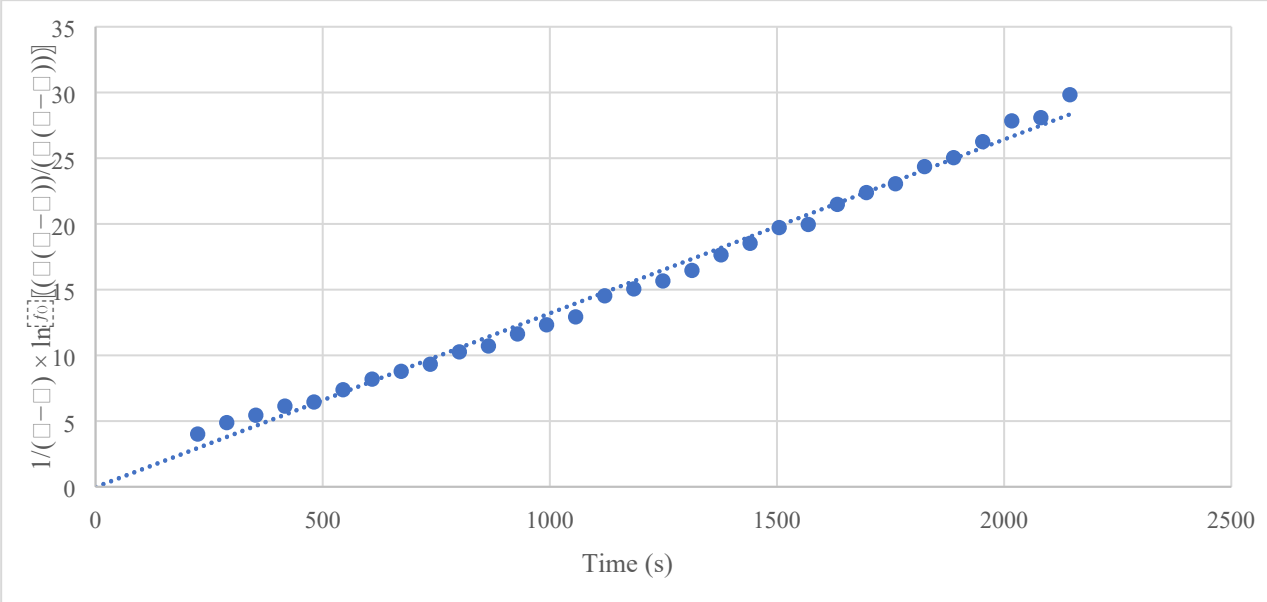


Figure 11: Plot of $\frac{1}{(a-b)} \times \ln \frac{b(a-x)}{a(b-x)}$ versus the reaction time for 3,5-TPDY cycloaddition with ethyl diazoacetate Run 2

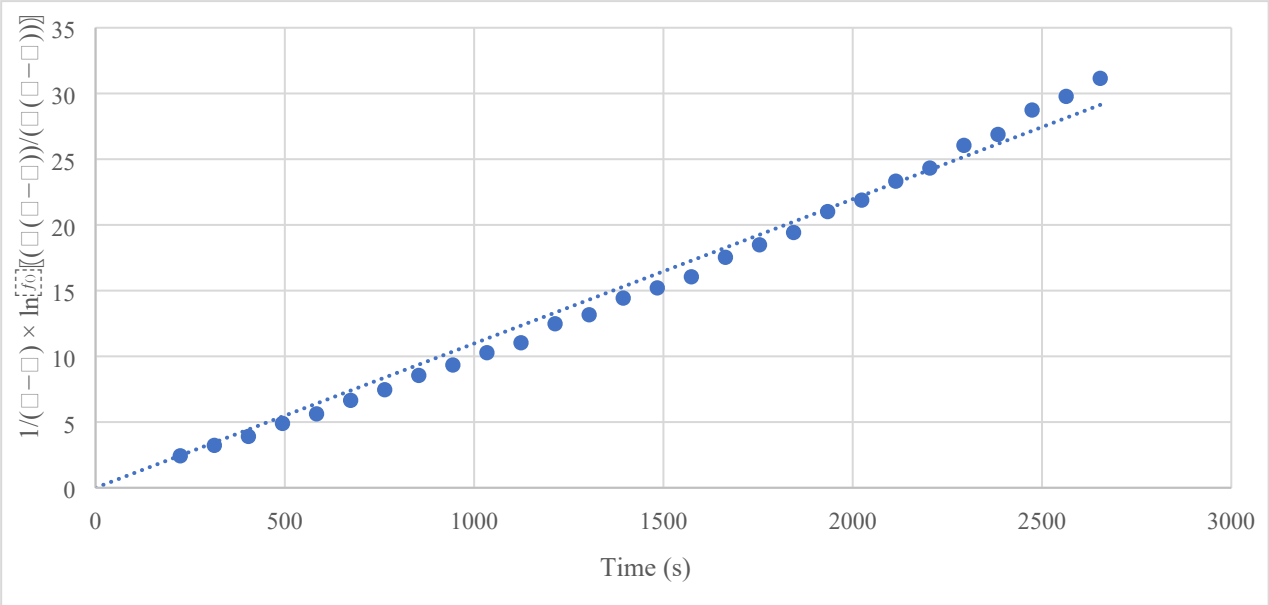
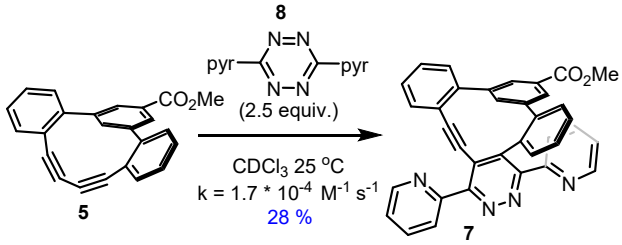


Figure 12: Plot of $\frac{1}{(a-b)} \times \ln \frac{b(a-x)}{a(b-x)}$ versus the reaction time for 3,5-TPDY cycloaddition with ethyl diazoacetate Run 3

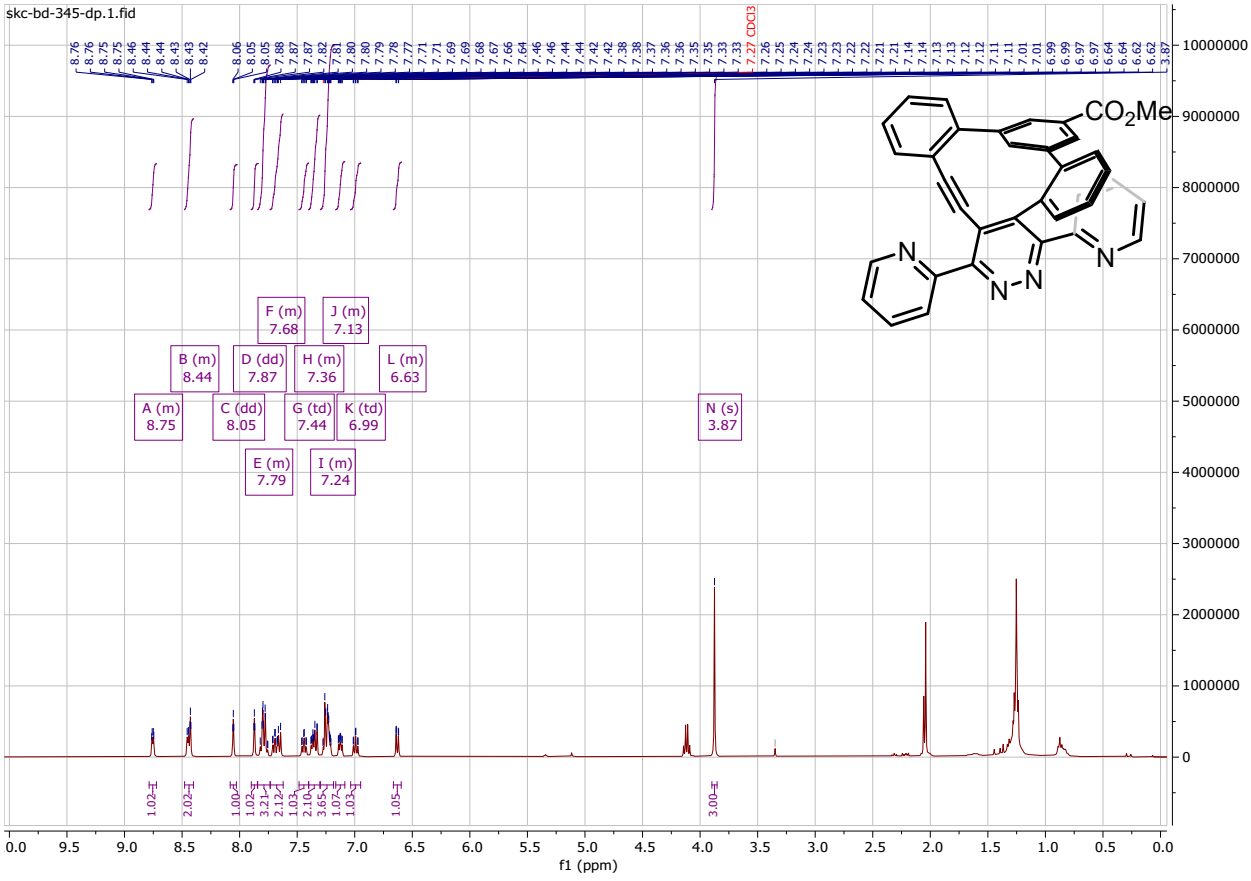
Average rate constant: k = 1.2 x 10^{-2} $M^{-1} \cdot s^{-1}$

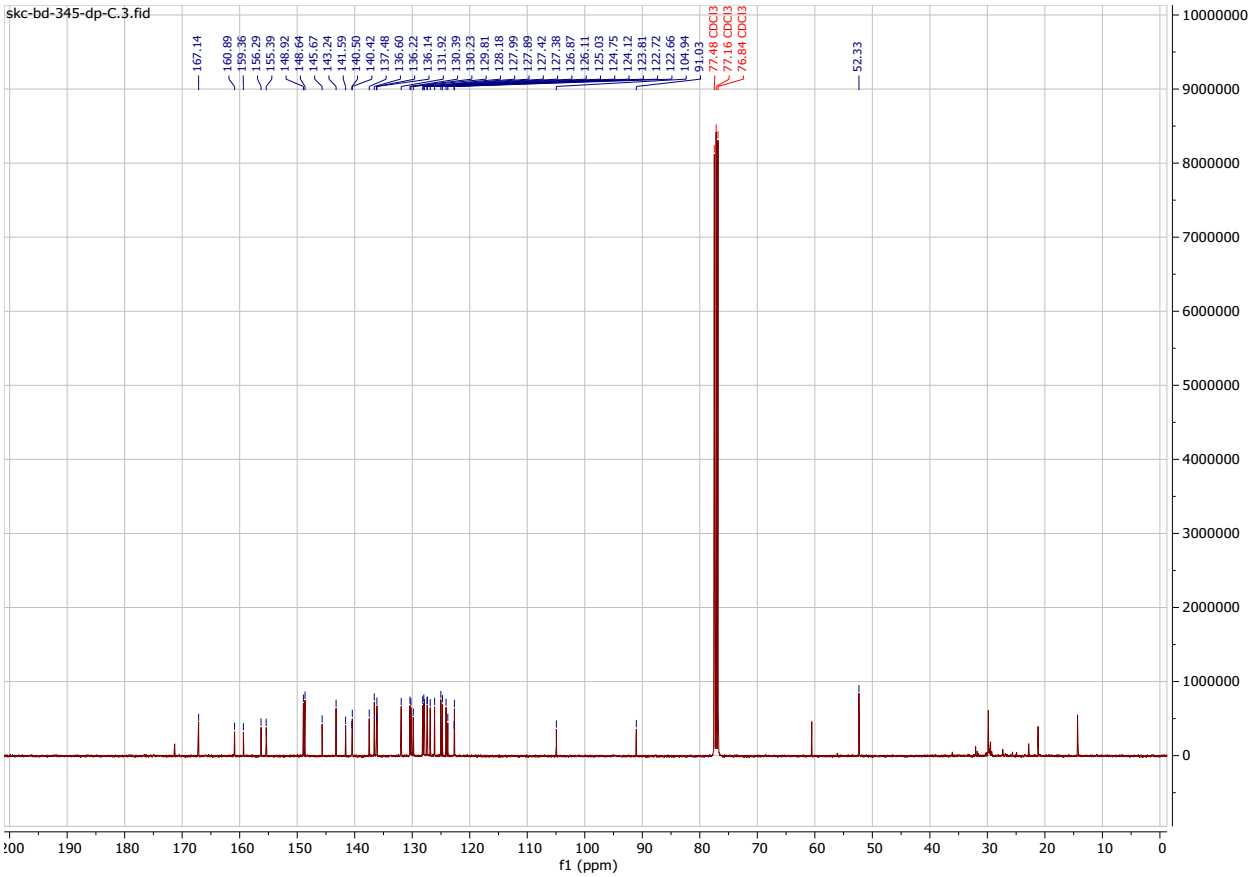
3,5-TPDY Cycloaddition with 3,6-di-2-pyridyl-1,2,4,5-tetrazine



To a solution of 3,5-TPDY (17.9 mg, 0.0535 mmol, 1 eq.) in CH_2Cl_2 [15 mM] was added 3,6-di-2-pyridyl-1,2,4,5-tetrazine (31.6 mg, 0.134 mmol, 2.5 eq.) and the reaction was stirred at room temperature for 24 h. The solution was then concentrated *in vacuo*. Purification by flash column chromatography (AcOEt in Hexanes) afforded the desired product as a dark yellow solid (8 mg, 28 %).

^{1}H NMR (400 MHz, Chloroform-*d*): δ 8.79 – 8.72 (m, 1H), 8.48 – 8.40 (m, 2H), 8.05 (dd, *J* = 1.7 Hz, 1H), 7.87 (dd, *J* = 1.7 Hz, 1H), 7.84 – 7.73 (m, 3H), 7.73 – 7.62 (m, 2H), 7.44 (td, *J* = 7.4, 1.8 Hz, 1H), 7.40 – 7.30 (m, 2H), 7.30 – 7.18 (m, 4H), 7.16 – 7.09 (m, 1H), 6.99 (td, *J* = 7.7, 1.4 Hz, 1H), 6.66 – 6.60 (m, 1H), 3.87 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 167.1, 160.9, 159.4, 156.3, 155.4, 148.9, 148.6, 145.7, 143.2, 141.6, 140.5, 140.4, 137.5, 136.6, 136.2, 136.1, 131.9, 130.4, 130.2, 129.8, 128.2, 128.0, 127.9, 127.4, 127.4, 126.9, 126.1, 125.0, 124.8, 124.1, 123.8, 122.7, 122.7, 104.9, 91.0, 52.3; **HRMS (ESI)**: m/z calculated for $C_{36}H_{22}N_4O_2$ $[M+H]^+$, 543.1816; found: 543.1817.





Kinetics measurements were taken every 40 min for 33 hours

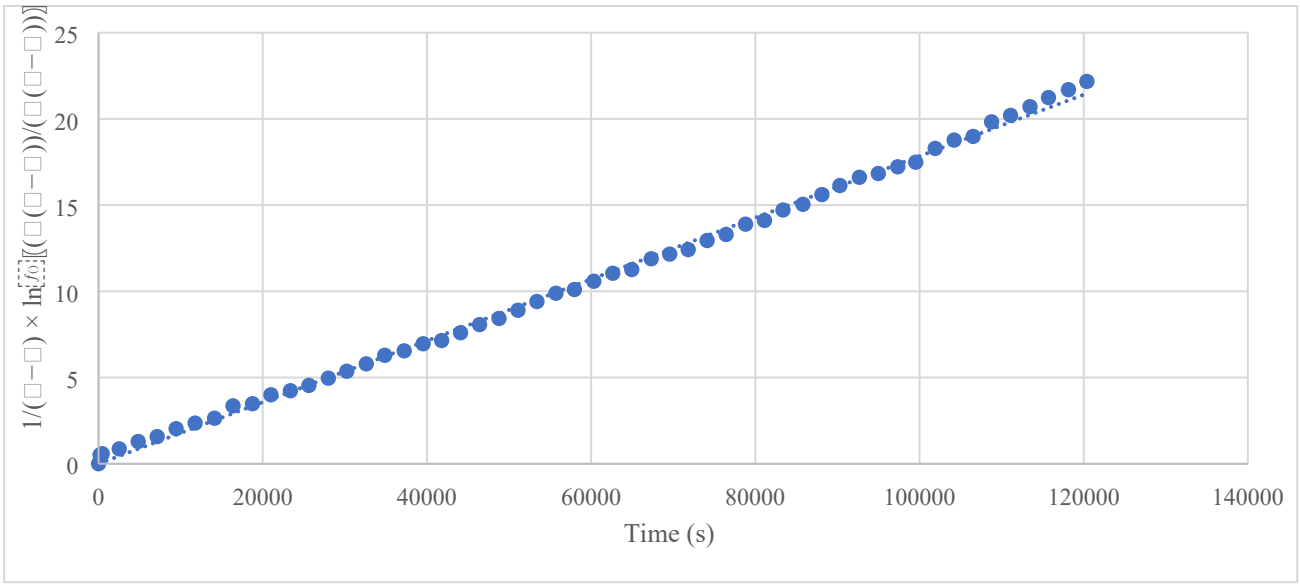


Figure 13: Plot of $\frac{1}{(a-b)} \times \ln \frac{b(a-x)}{a(b-x)}$ versus the reaction time for 3,5-TPDY cycloaddition with 3,6-di-2-pyridyl-1,2,4,5-tetrazine Run 1

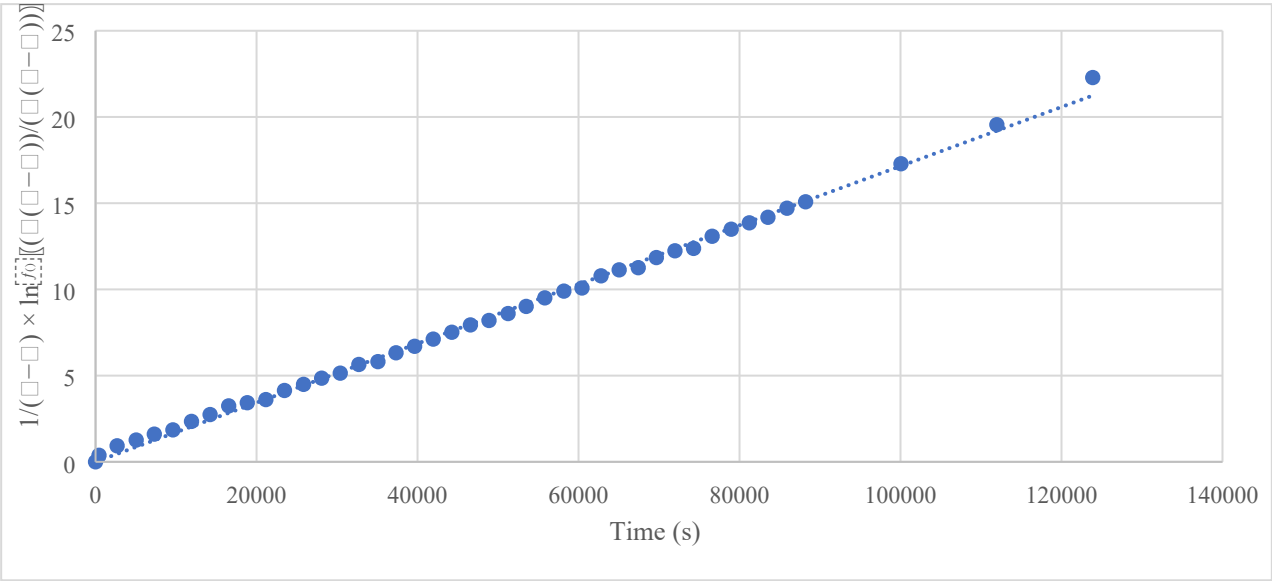


Figure 14: Plot of $\frac{1}{(a-b)} \times \ln \frac{b(a-x)}{a(b-x)}$ versus the reaction time for 3,5-TPDY cycloaddition with 3,6-di-2-pyridyl-1,2,4,5-tetrazine Run 2

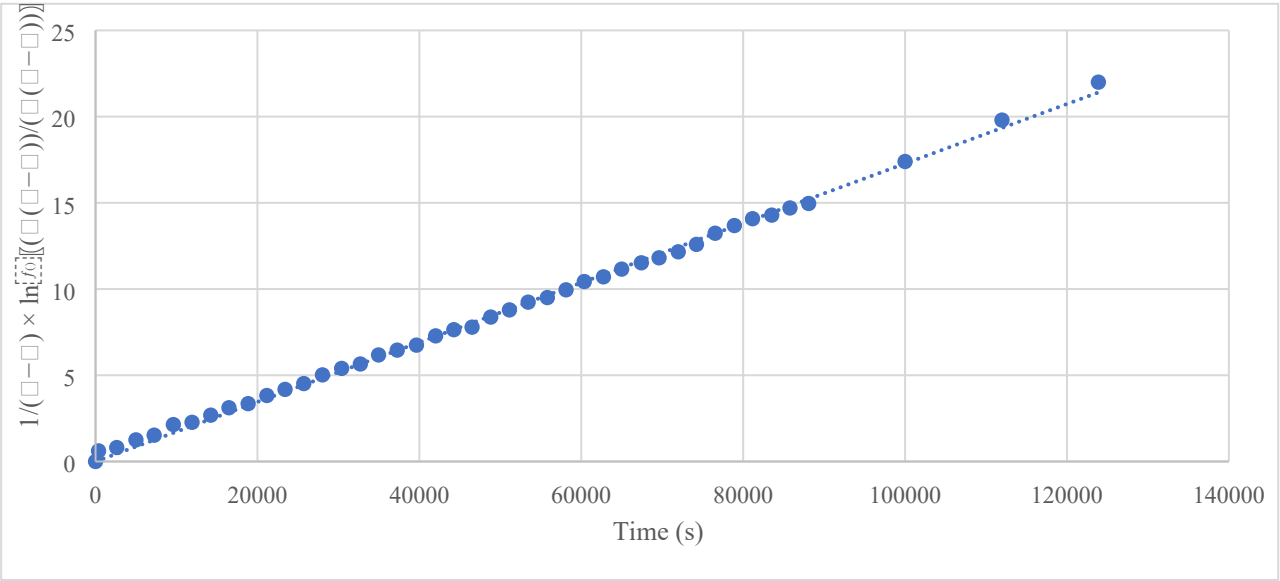


Figure 15: Plot of $\frac{1}{(a-b)} \times \ln \frac{b(a-x)}{a(b-x)}$ versus the reaction time for 3,5-TPDY cycloaddition with 3,6-di-2-pyridyl-1,2,4,5-tetrazine Run 3

Average rate constant: k = 1.7 x 10^{-4} $M^{-1} \cdot s^{-1}$

Bioligation Experiments

MTG expression and purification

mTG expression and purification and activity assay were performed as previously reported.[1] Activity greater than 20 U/mg of purified mTG was assessed, and purity was determined over 85% on 15% reducing SDS-PAGE.

hFc expression and purification

E. coli Shuffle T7 express transformed with pET-22b hFc and SOX plasmid were propagated overnight at 37 °C, 230 rpm in a 20 mL LB preculture with ampicillin (100 µg/mL) and chloramphenicol (50 µg/mL). A culture of LB media (500 mL) containing ampicillin and chloramphenicol was inoculated with an initial OD_{600} of 0.1 and propagated at 37 °C, 230 rpm. When OD_{600} reached 0.7-1.0, protein expression was induced by addition of 1 mM IPTG and the culture was incubated overnight at 22 °C, 230 rpm. Cells were pelleted at 5 500 ×g for 10 min and resuspended in 30 mL of IMAC-A buffer (50 mM Tris-HCl pH 8, 600 mM NaCl, 20 mM imidazole). The cell suspension was lysed using 3 cycles of 30 s sonication with 30 s rest on ice between cycles. The lysate was centrifuged at 50 000 ×g and filtered through 0.22 micron and applied to a 1 mL HisTrap Ni-NTA column (Cytiva) at a flow rate of 1 mL/min pre-equilibrated with IMAC-A buffer. After flow-through elution, the column was washed with 5 CV of 5% IMAC-B buffer (50 mM Tris-HCl pH 8, 600 mM NaCl, 500 mM imidazole), followed by protein elution through 10 CV of 100% IMAC-B buffer. Fractions (1 mL) were pooled according to the A_{280} peak and dialyzed overnight against PBS buffer pH 7.2 (137 mM NaCl, 2.7 mM KCl, 9.2 mM Na_2HPO_4, 1.8 mM KH_2PO_4) at 4 °C. Protein was concentrated to 5 mg/mL using a 15 mL Amicon (Millipore Sigma, MWCO 10 kDa), supplemented with 10% glycerol and stored at -72 °C. Protein concentration was measured at 280 nm using a theoretical extinction coefficient of 71680 $M^{-1}cm^{-1}$ and a molecular weight of 54 kDa. Protein purity greater than 85% and proper folding of hFc was assessed on a 15% non-reducing SDS-PAGE gel.

GB1 expression and purification

E. coli BL21 (DE3) transformed with the pET-15b Gb1 I6Q variant were propagated overnight at 37°C, 230 rpm in a 20 mL LB preculture with ampicillin (100 µg/mL). The culture of LB media (500 mL) with ampicillin was inoculated at an initial OD_{600} of 0.1 and propagated at 37°C, 230 rpm. When the OD_{600} reached 0.7-1.0, protein expression was carried out by adding 1 mM IPTG and the culture was incubated overnight at 22°C, 230 rpm. Cells were pelleted at 5,500 ×g for 10 min and resuspended in 30 mL IMAC-A buffer. The cell suspension was lysed by 3 cycles of 30 s sonication with 30 s rest on ice between cycles. The lysate was centrifuged at 50,000 ×g, filtered through 0.22 micron and applied to a 1 mL HisTrap Ni-NTA column (Cytiva) at a flow rate of 1 mL/min, pre-equilibrated with IMAC-A buffer. After flow-through elution, the column was washed with 5 CV of 5% IMAC-B buffer followed by protein elution through 10 CV of 100% IMAC-B buffer. Fractions (1 mL) were pooled according to the A280 peak, and buffer exchanged with a 5 mL HiTrap desalting column (Cytiva) to PBS buffer pH 7.2 at 4 °C. Protein was concentrated to 5 mg/mL using a 15 mL Amicon (MWCO 3 kDa, Millipore Sigma), supplemented with 10% glycerol and stored at -72 °C. Protein concentration was measured at 280 nm using a theoretical extinction coefficient of 9970 $M^{-1}cm^{-1}$ and a molecular weight of 8475 Da. Protein purity greater than 85% was assessed on a 10% reducing tricine gel.

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[1] Deweid, L.; Hadjabdelhafid-Parisien, A.; Lafontaine, K.; Rochet, L. N. C.; Kolmar, H.; Pelletier, J. N., Chapter Five - Glutamine-walking: Creating reactive substrates for transglutaminase-mediated protein labeling. In *Methods Enzymol.*, Tawfik, D. S., Ed. Academic Press: 2020; Vol. 644, pp 121-148.

SDS-PAGE analysis of conjugation reaction to proteins

Proteins (hFc or Gb1, 50 µM) were incubated in presence of 3,5-TPDY-PEG-NH_3Cl (1 mM), sulfo-Cy5 azide (2 mM, Lumiprobe) and mTG (5 µM) in PBS buffer pH 7.2, 15% (v/v) DMSO at room temperature. Control reactions were run in the absence of mTG to evaluate background fluorescence on gels and in presence N-(1R,8S,9s)-Bicyclo[6.1.0]non-4-yn-9-ylmethyloxycarbonyl-1,8-diamino-3,6-dioxaoctane (BCN-amine, 1 mM, VWR) as a reference for mTG conjugation. Reactions were stopped by adding of 4% (v/v) formic acid and aliquots (10 µL) were resolved on 16,5% reducing tricine gels (Gb1) or 15% non-reducing tris-glycine SDS-PAGE gel (hFc). Fluorescence was revealed with an iBright FL1500 imaging system (ThermoFischer) using the Cy5 filter (Ex 608-632 nm, Em 675-720 nm) with an exposure time of 500 ms prior to Coomassie staining. Fluorescence intensity was quantified using ImageJ software.

Figures for additional MTG-mediated conjugation of B domain of protein G (Gb1).

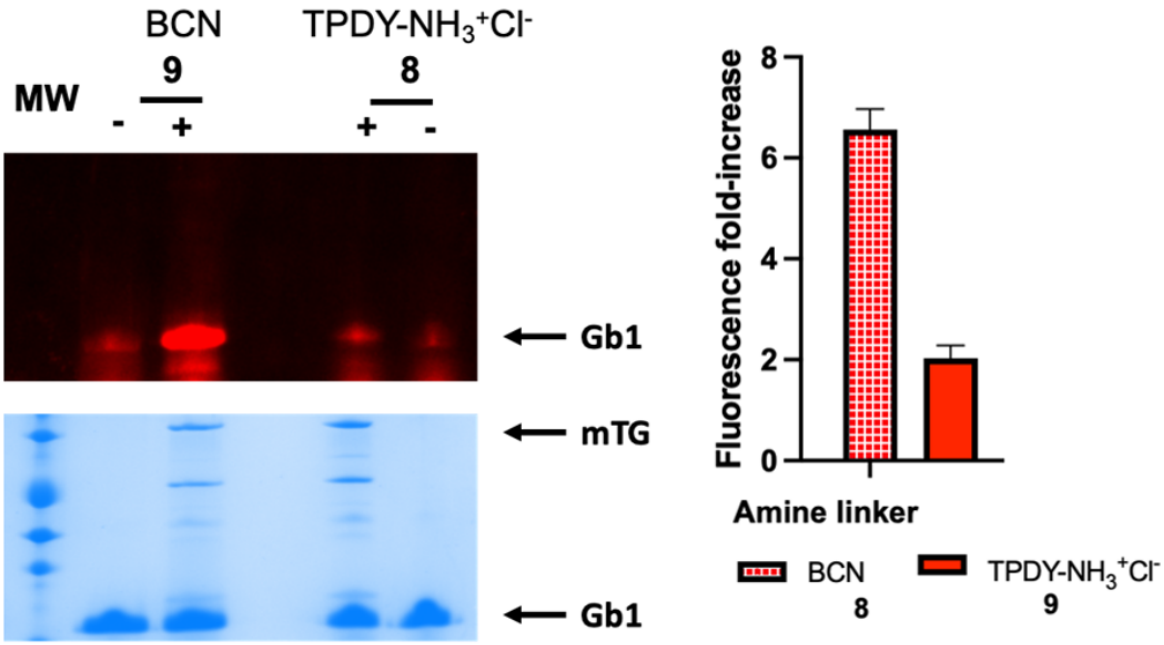
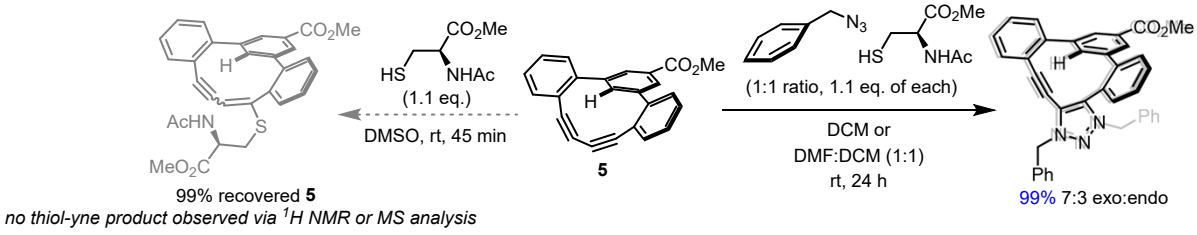
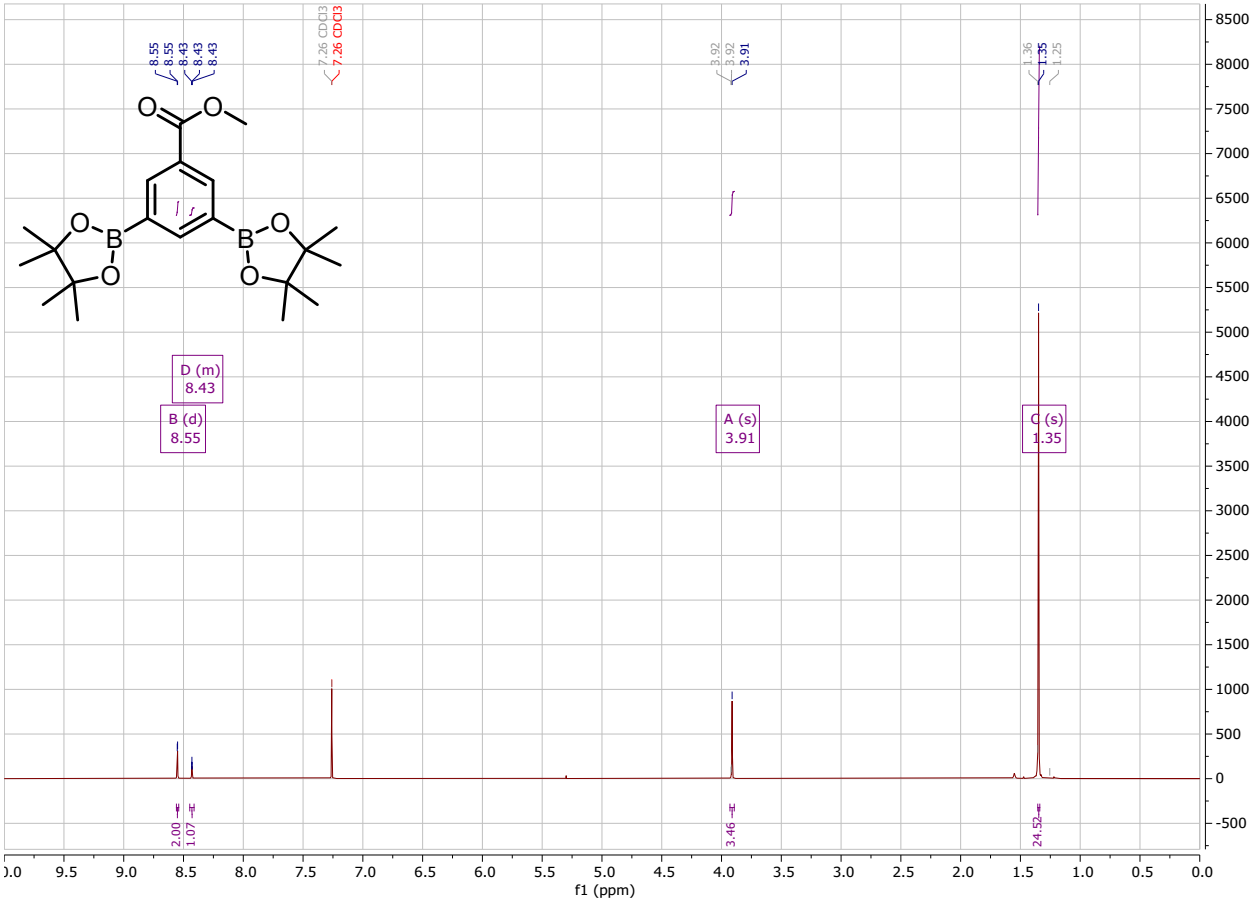


Figure S16: MTG-mediated conjugation of B domain of protein G (Gb1). Upper gel image: Fluorescence of sulfo-Cy-5 (500 ms exposure) Lower gel image: Coomassie stained to confirm equal loading of the protein. MW: molecular weight marker. The presence/absence (+ or -) of mTG is indicated. The bar graph represents fluorescence-fold increase relative to background (no mTG) for each reaction.

Thiol competition experiments.



NMR SPECTRA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7.26 CDCl3
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3.92
3.91
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1.35
1.25
D (m)
8.43
B (d)
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A (s)
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C (s)
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1.07
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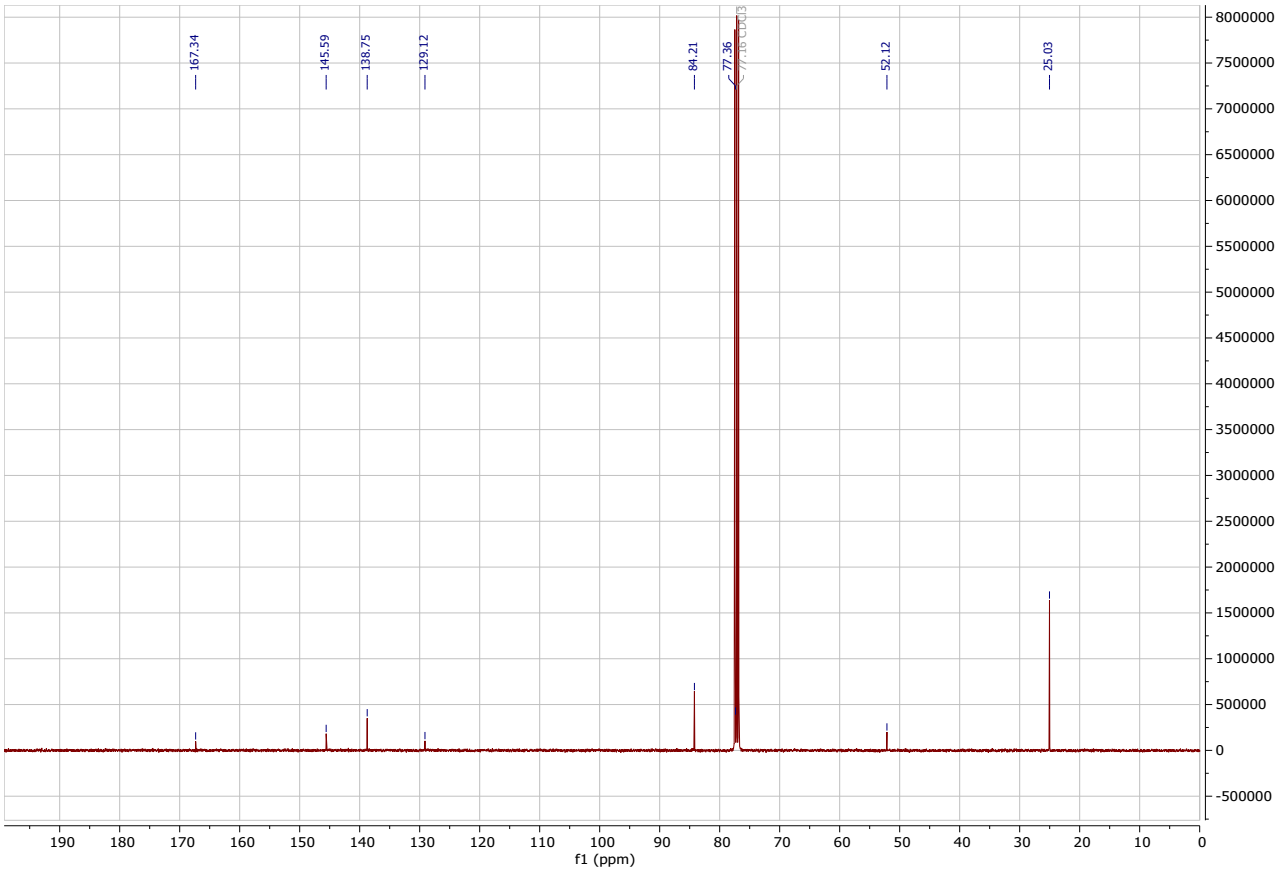
f1 (ppm)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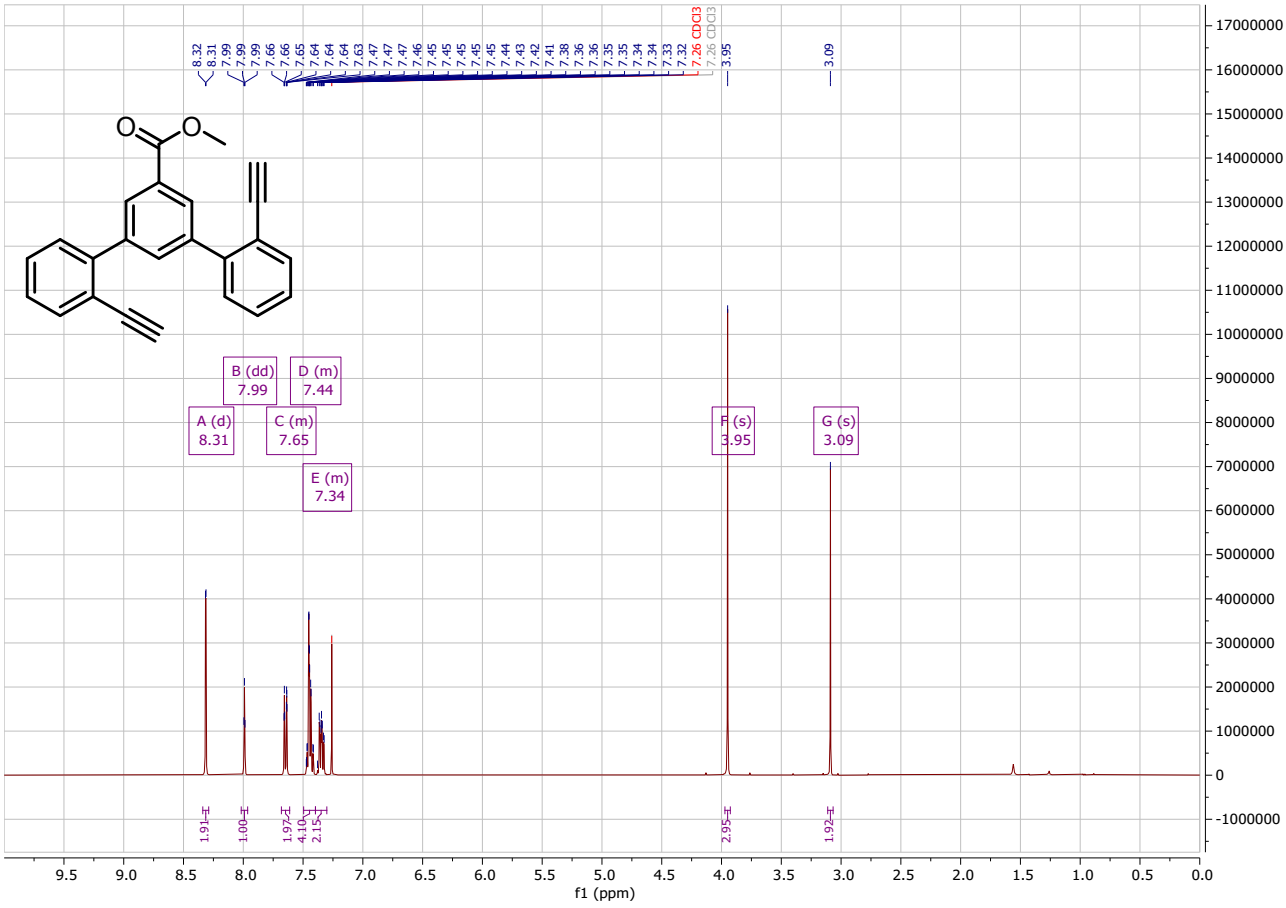
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E (m)
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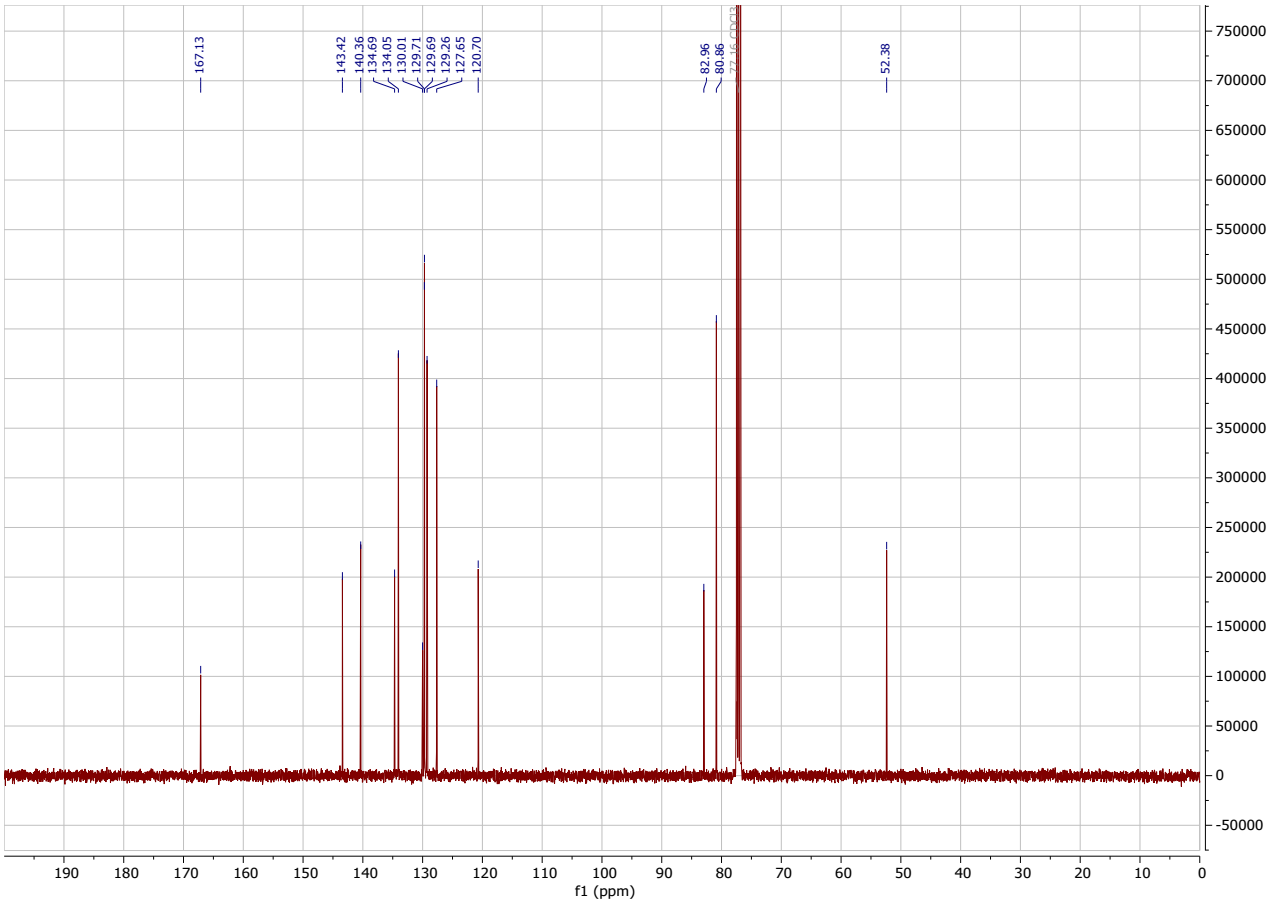
f1 (ppm)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700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
-50000
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180
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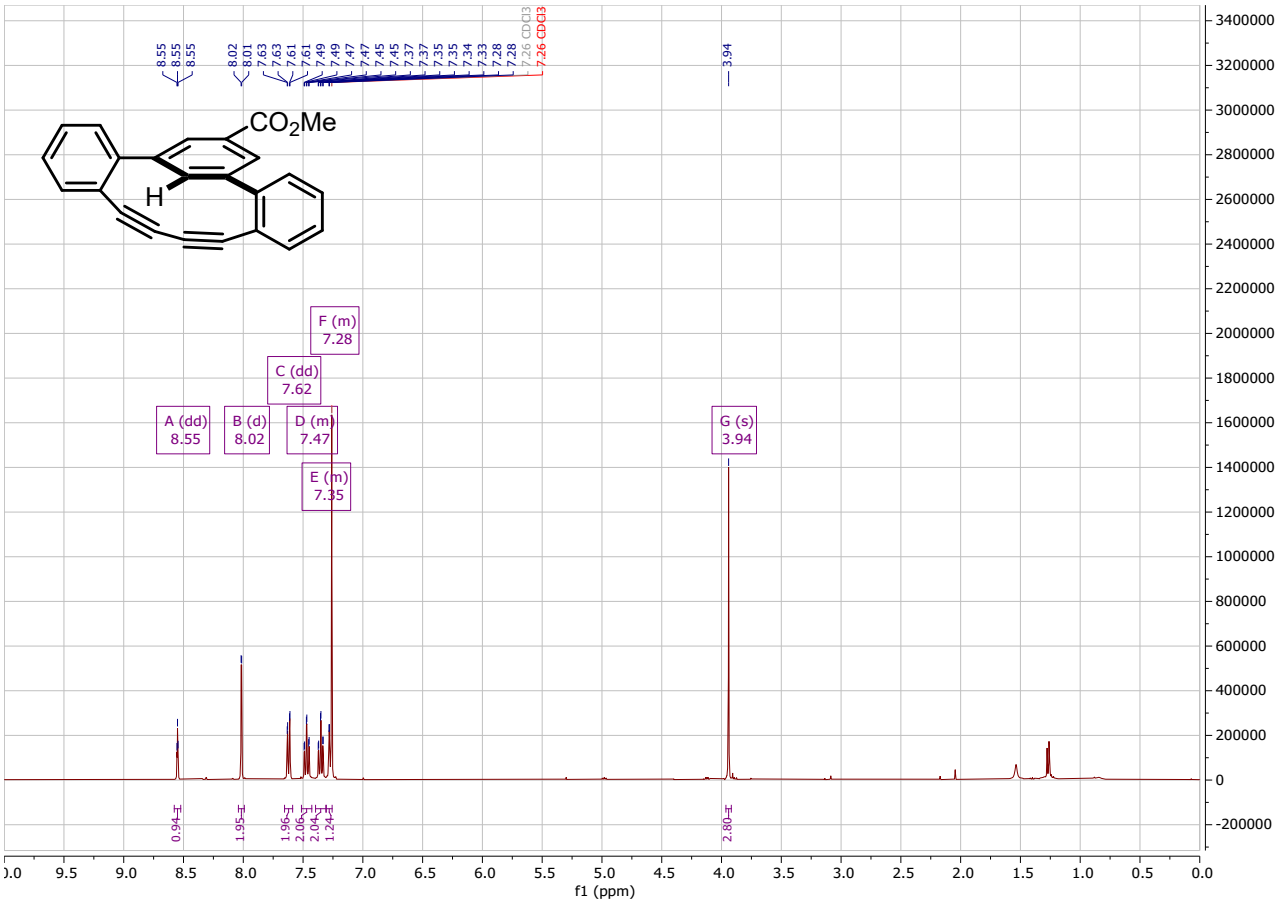
f1 (ppm)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7.45
7.45
7.37
7.37
7.35
7.35
7.34
7.33
7.28
7.28
7.26 CDCl3
7.26 CDCl3
3.94
CO2Me
H
F (m)
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C (dd)
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A (dd)
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B (d)
8.02
D (m)
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E (m)
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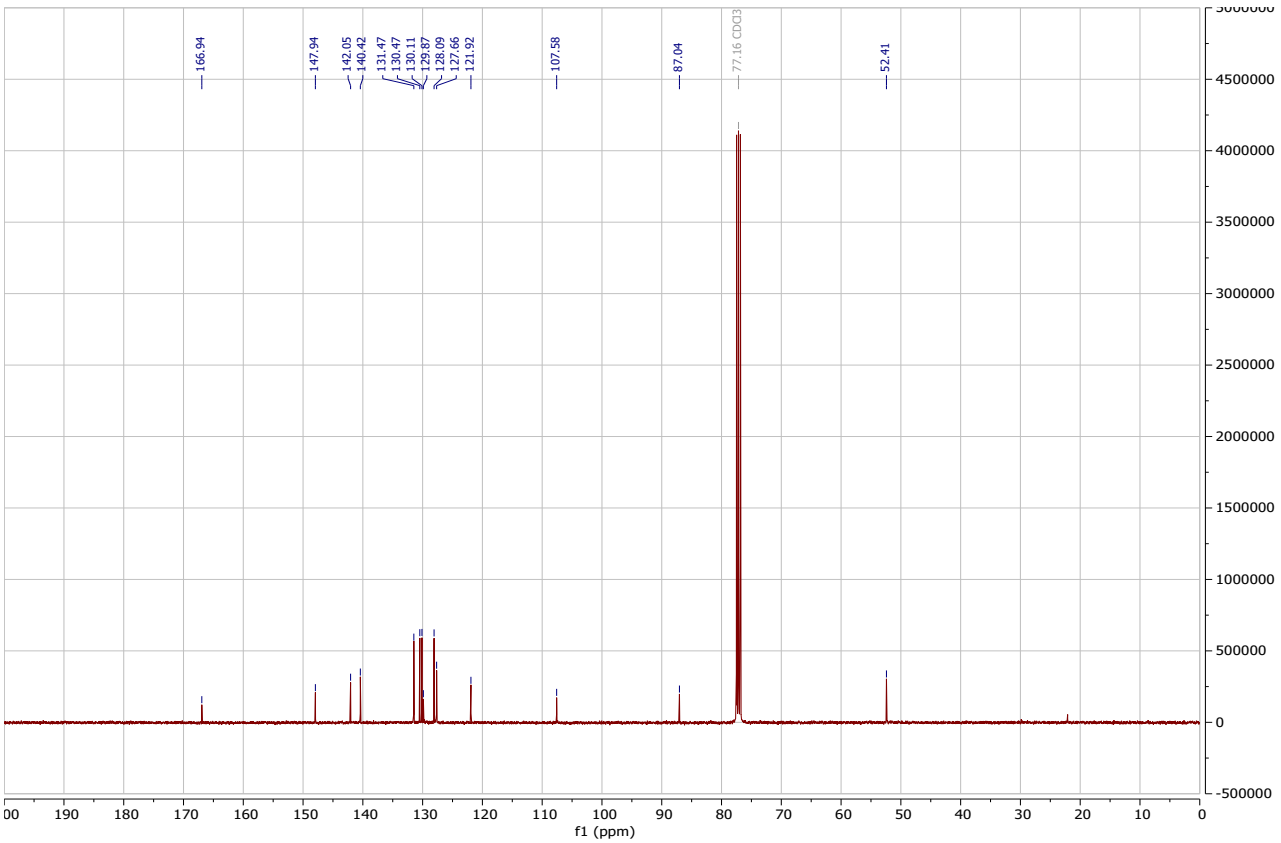
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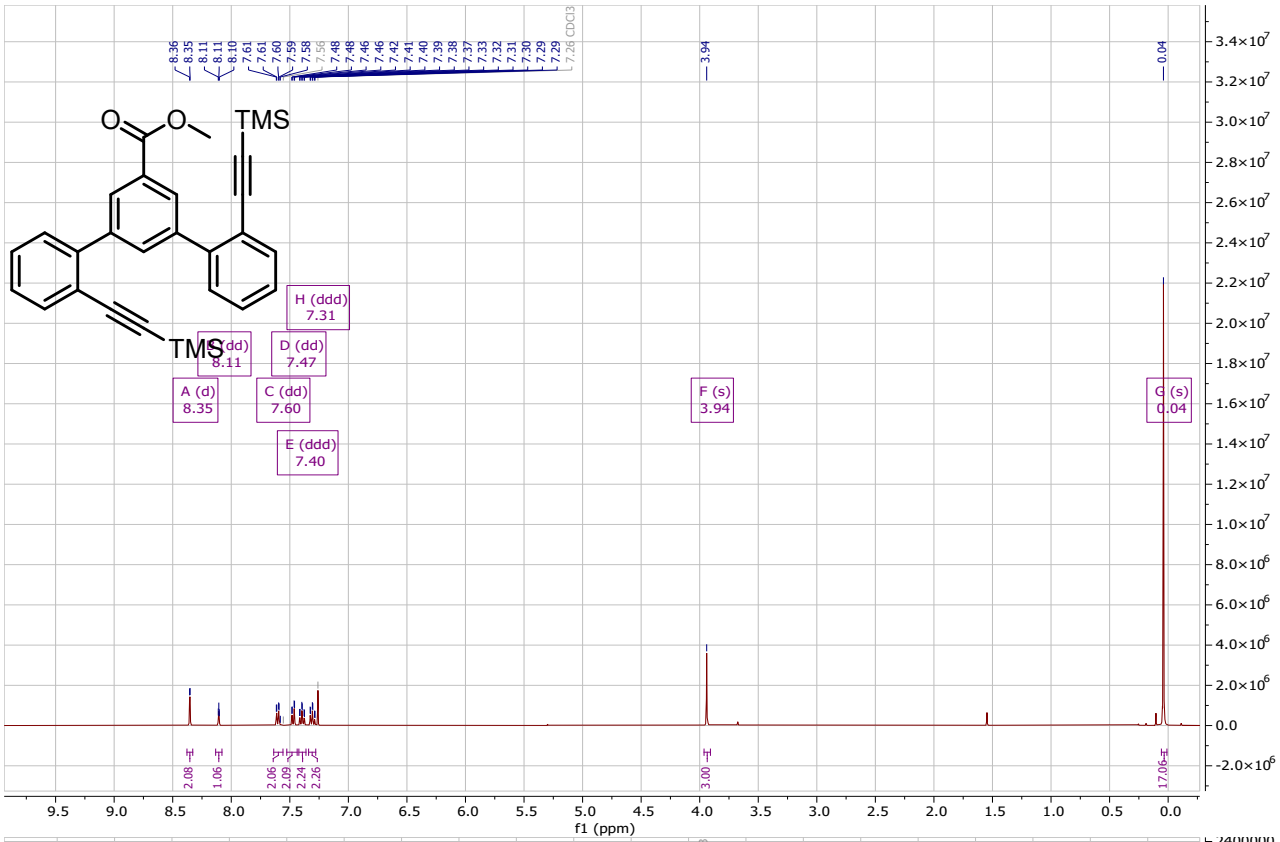
f1 (ppm)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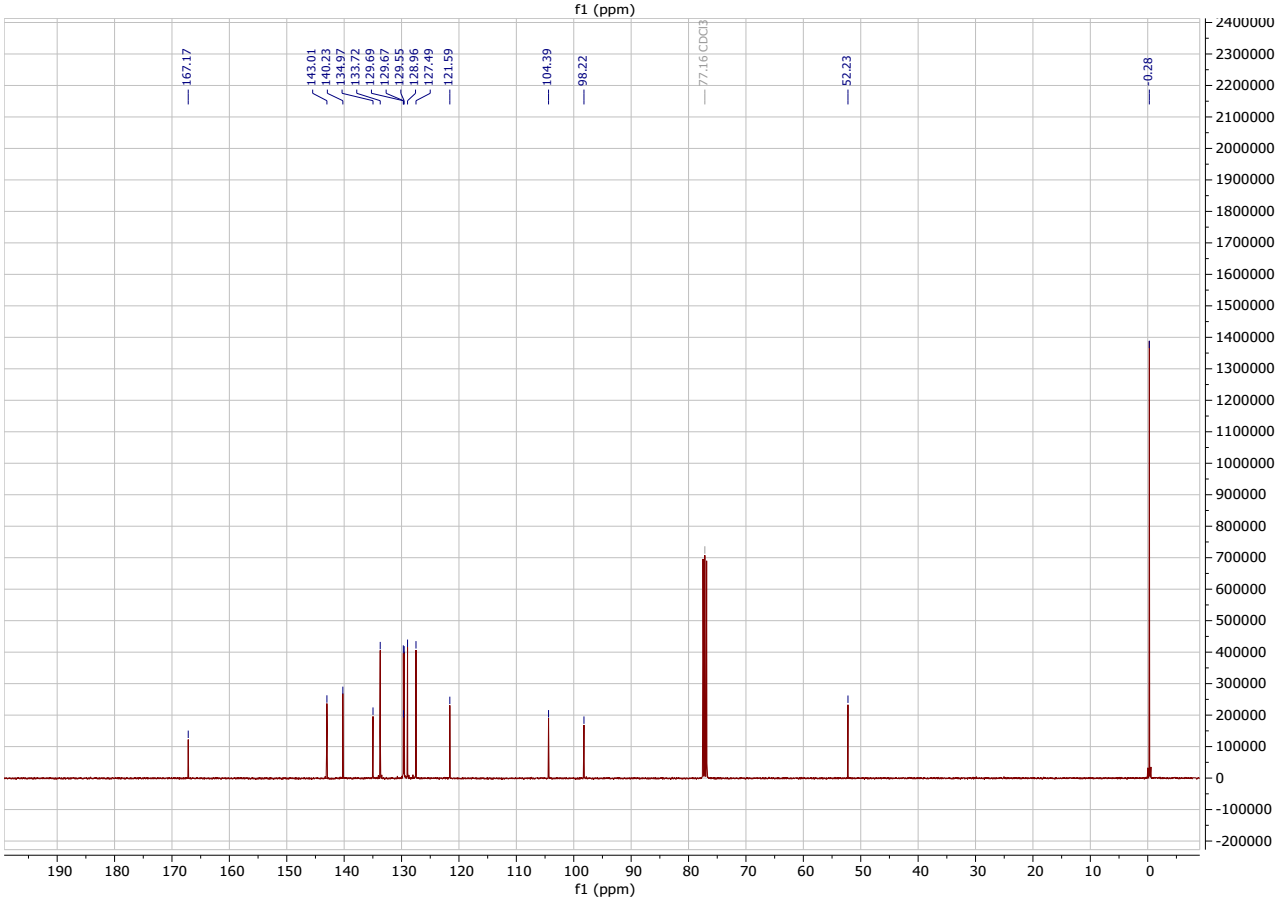
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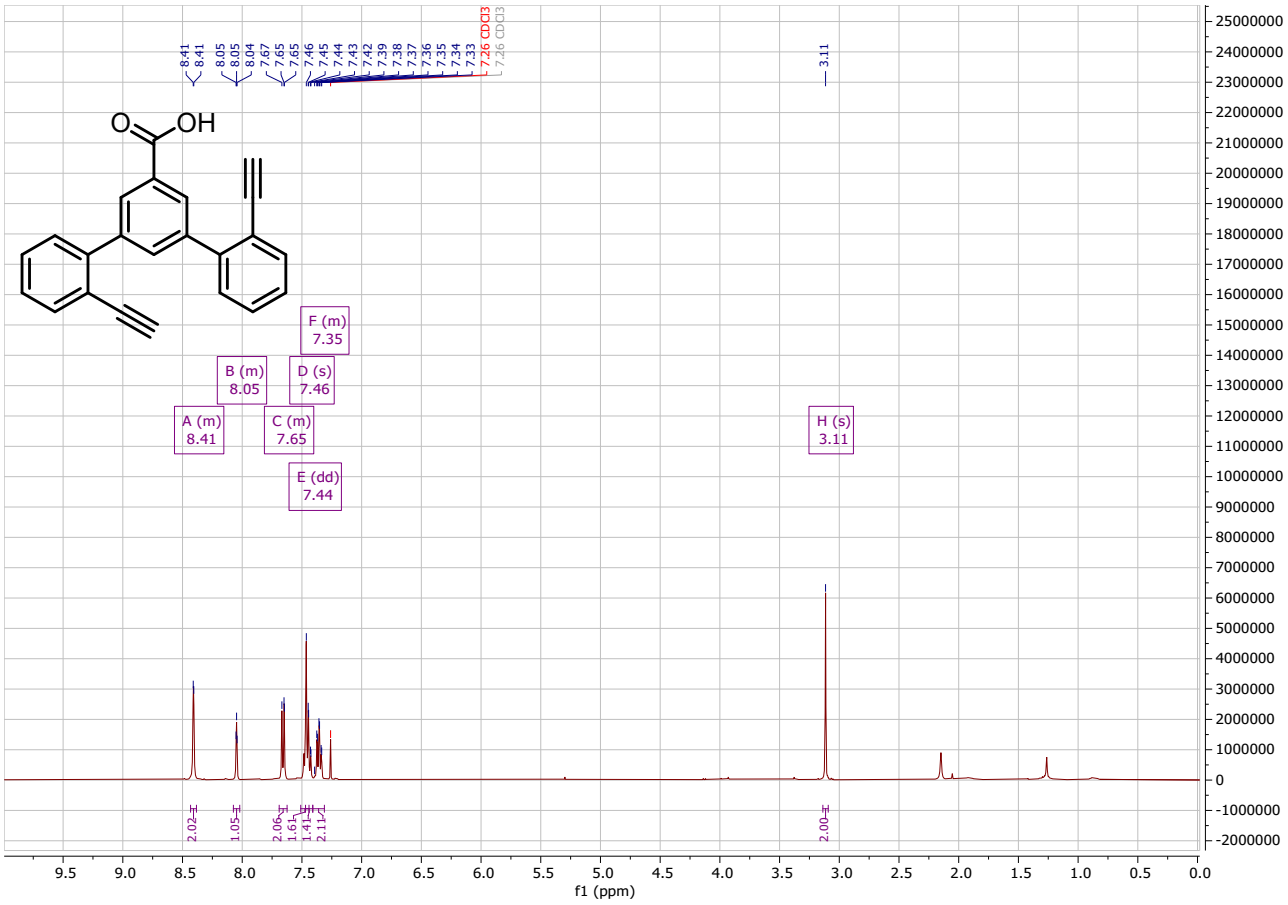
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7.37
7.36
7.35
7.34
7.33
7.26 CDCl3
7.26 CDCl3
3.11
O
OH
F (m)
7.35
B (m)
8.05
D (s)
7.46
A (m)
8.41
C (m)
7.65
E (dd)
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2.11
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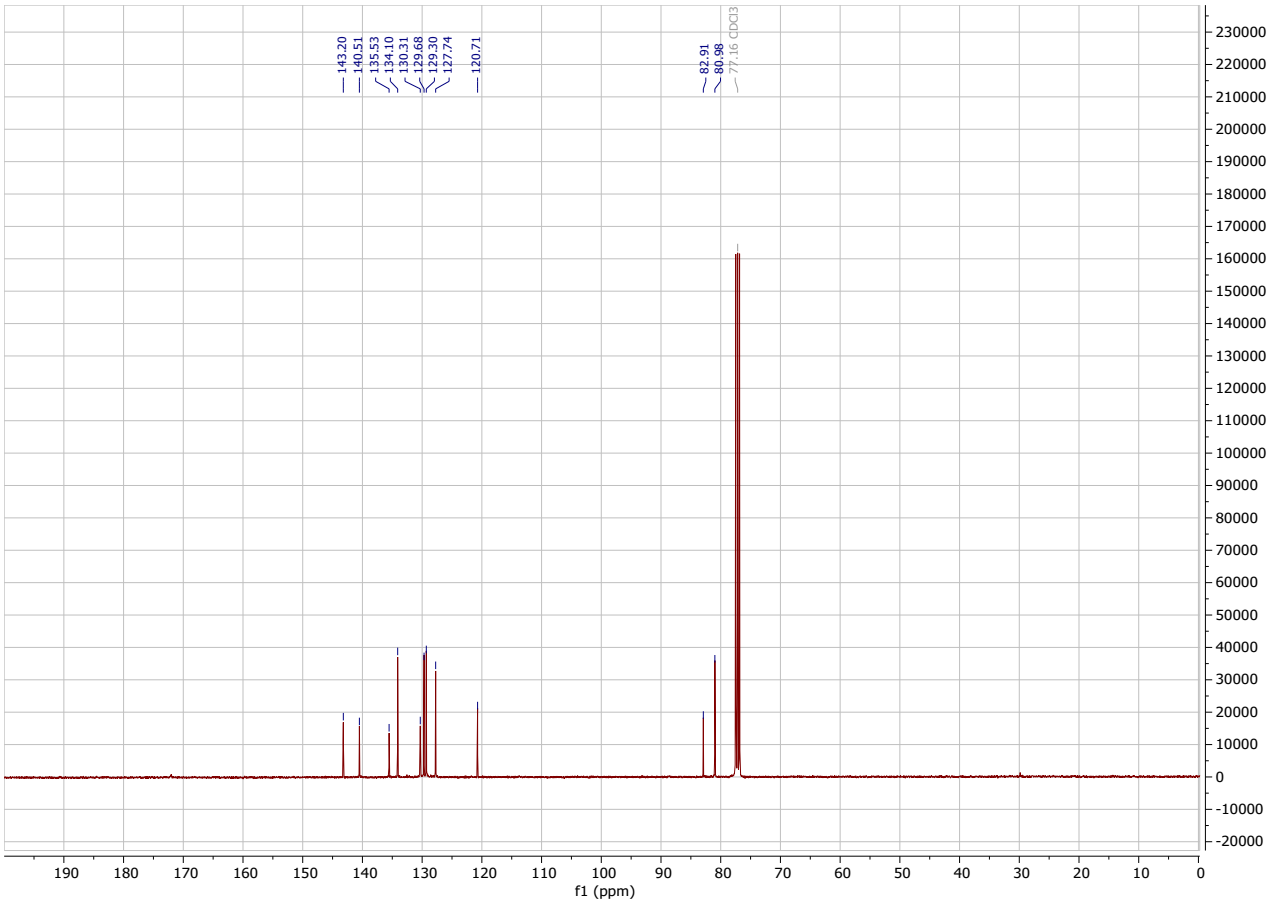
f1 (ppm)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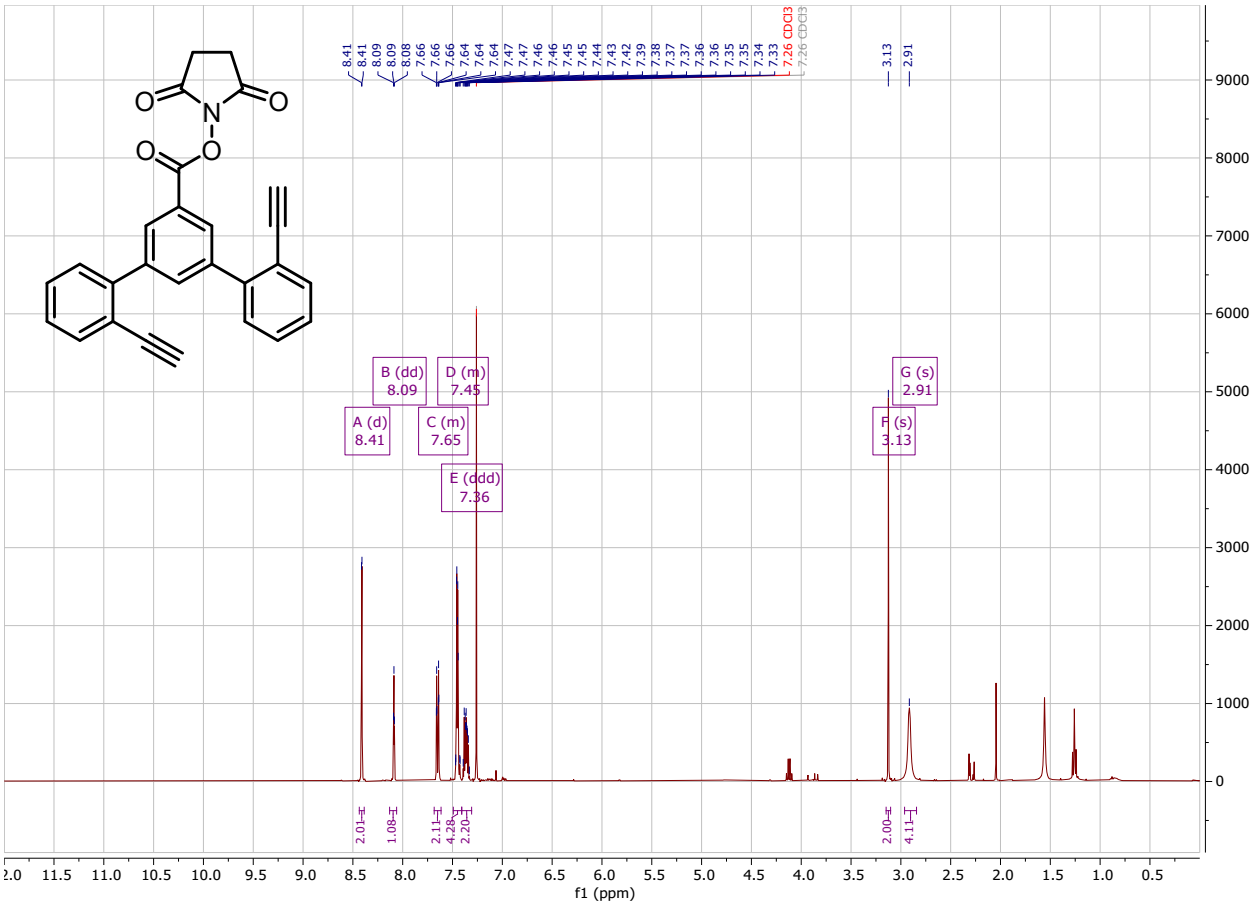
f1 (ppm)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B (dd)
8.09
C (m)
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D (m)
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E (ddd)
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F (s)
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G (s)
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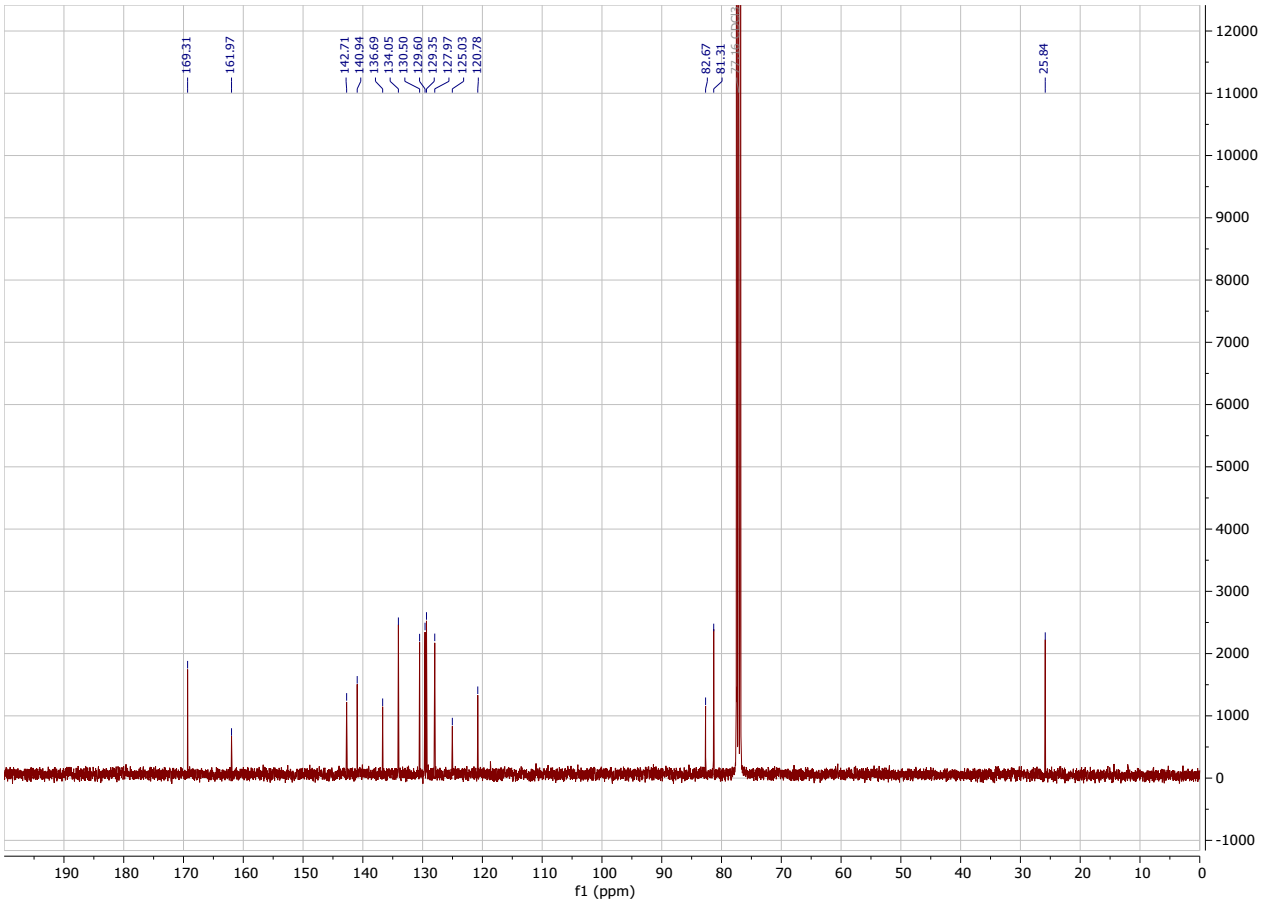
f1 (ppm)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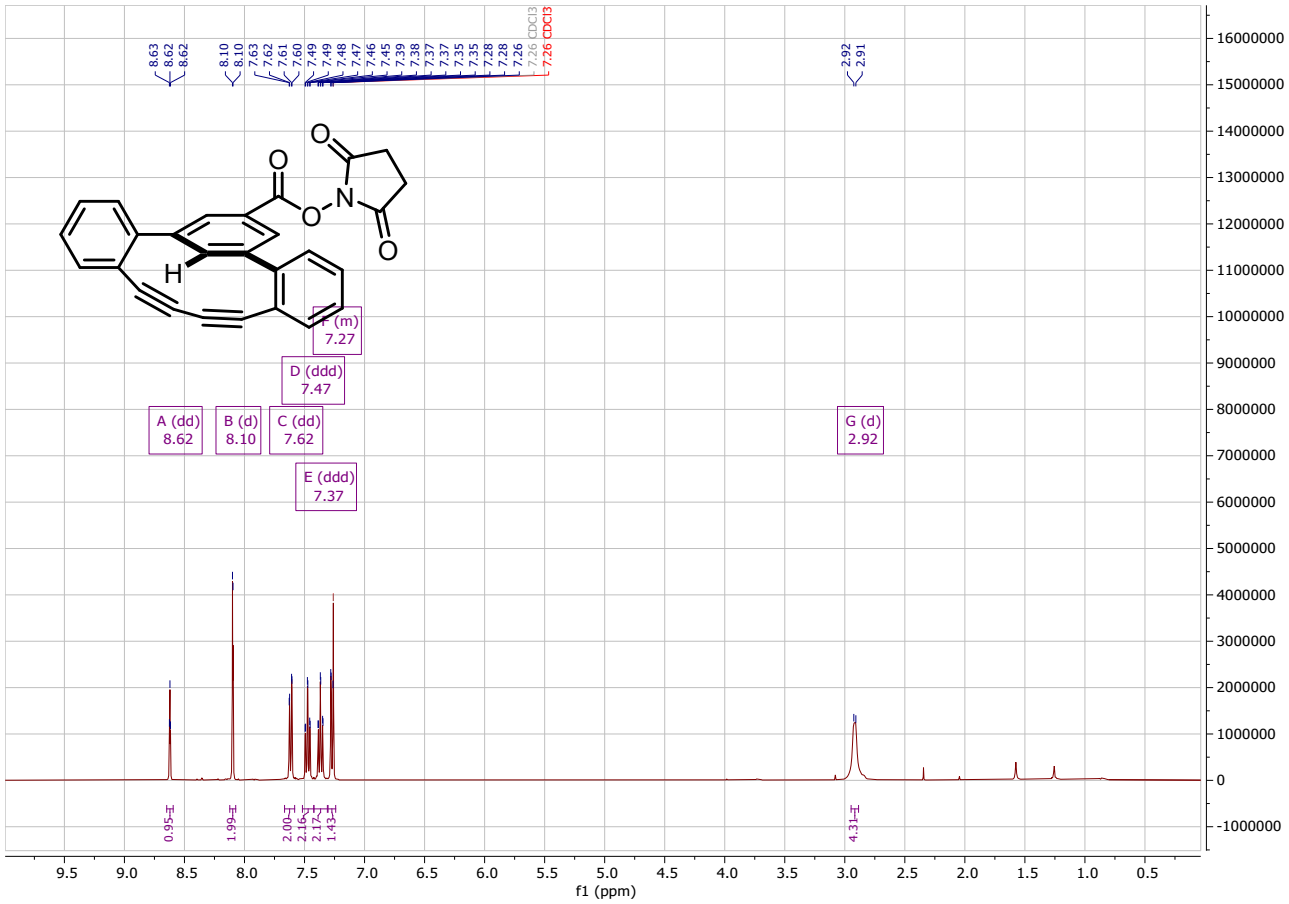
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7.37
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7.28
7.26
CDCl3
7.26
7.26 CDCl3
2.92
2.91
O
O
N
O
O
H
F (m)
7.27
D (ddd)
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A (dd)
8.62
B (d)
8.10
C (dd)
7.62
E (ddd)
7.37
G (d)
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1.99
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2.16
2.17
1.43
4.31
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13000000
12000000
11000000
10000000
9000000
8000000
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6000000
5000000
4000000
3000000
2000000
1000000
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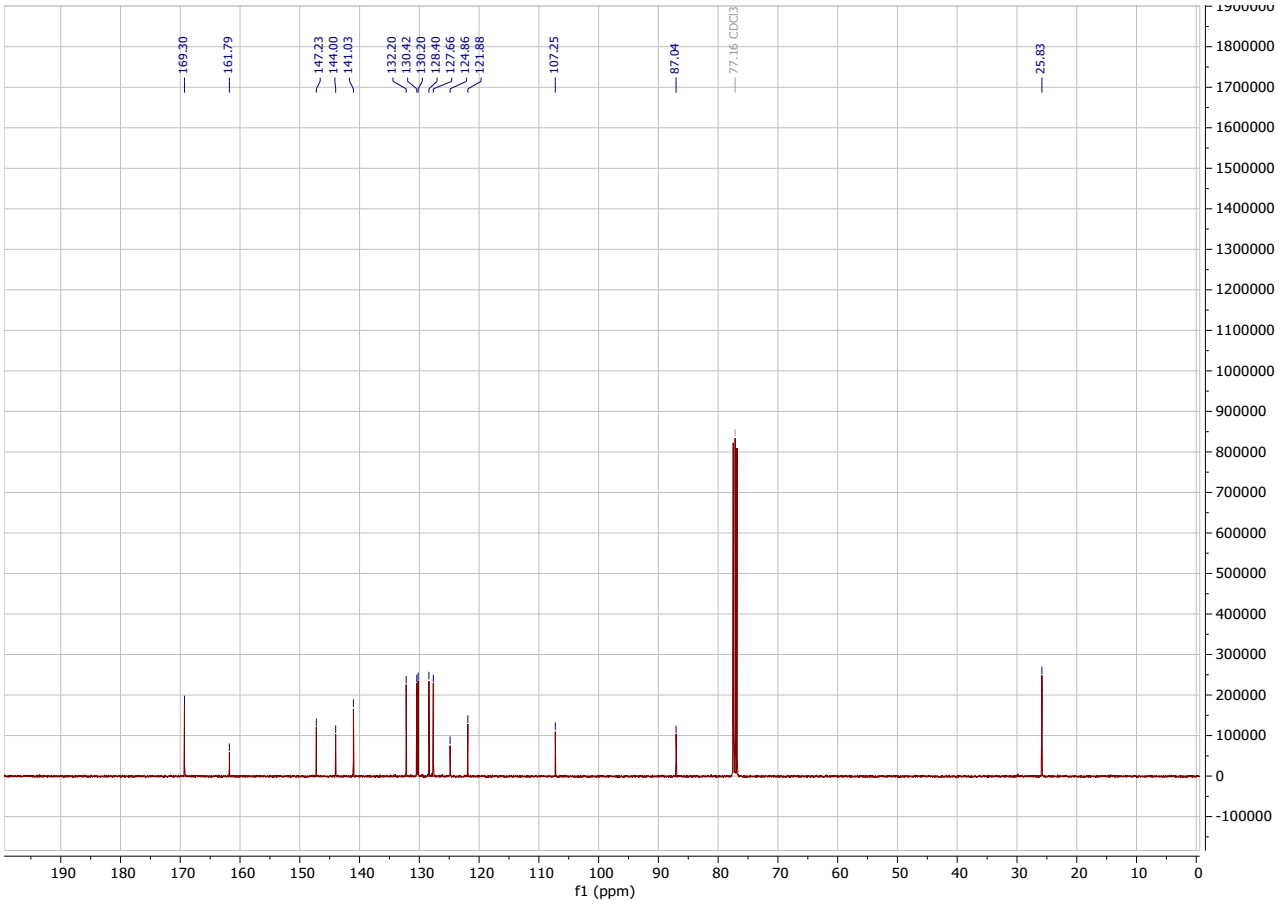
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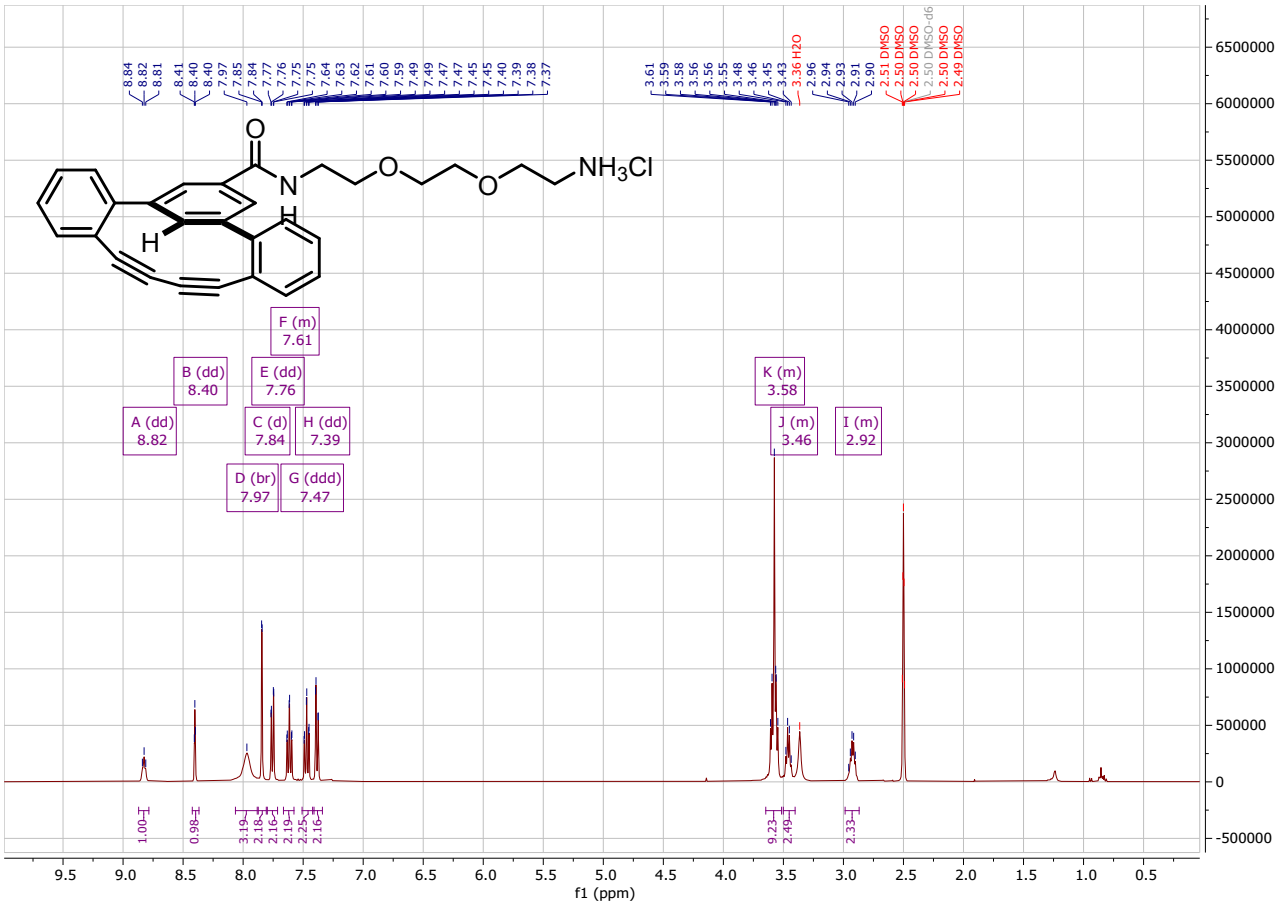
f1 (ppm)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H
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O
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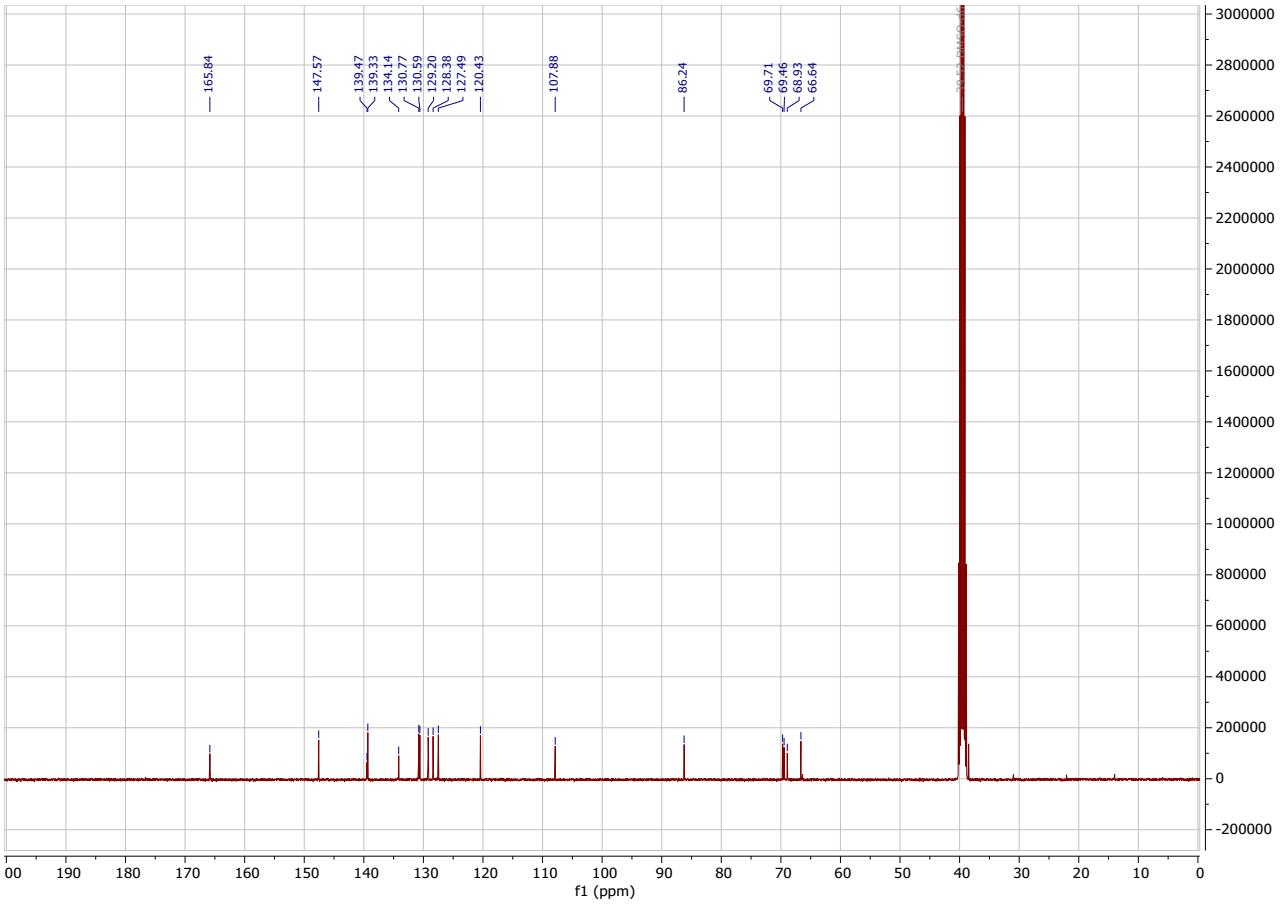
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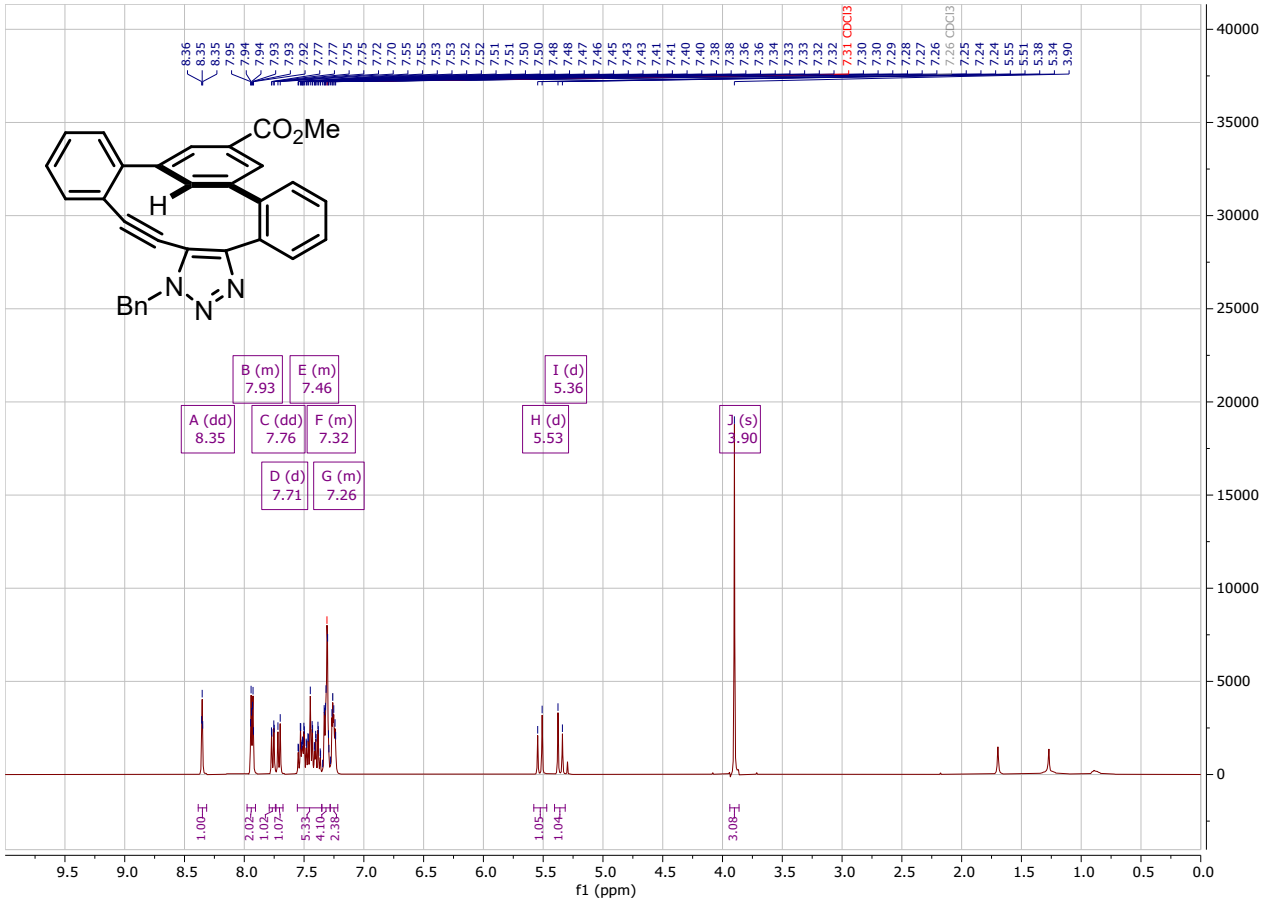
f1 (ppm)


CO2Me
H
Bn
N
N
N
A (dd) 8.35
B (m) 7.93
C (dd) 7.76
D (d) 7.71
E (m) 7.46
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I (d) 5.36
J (s) 3.90
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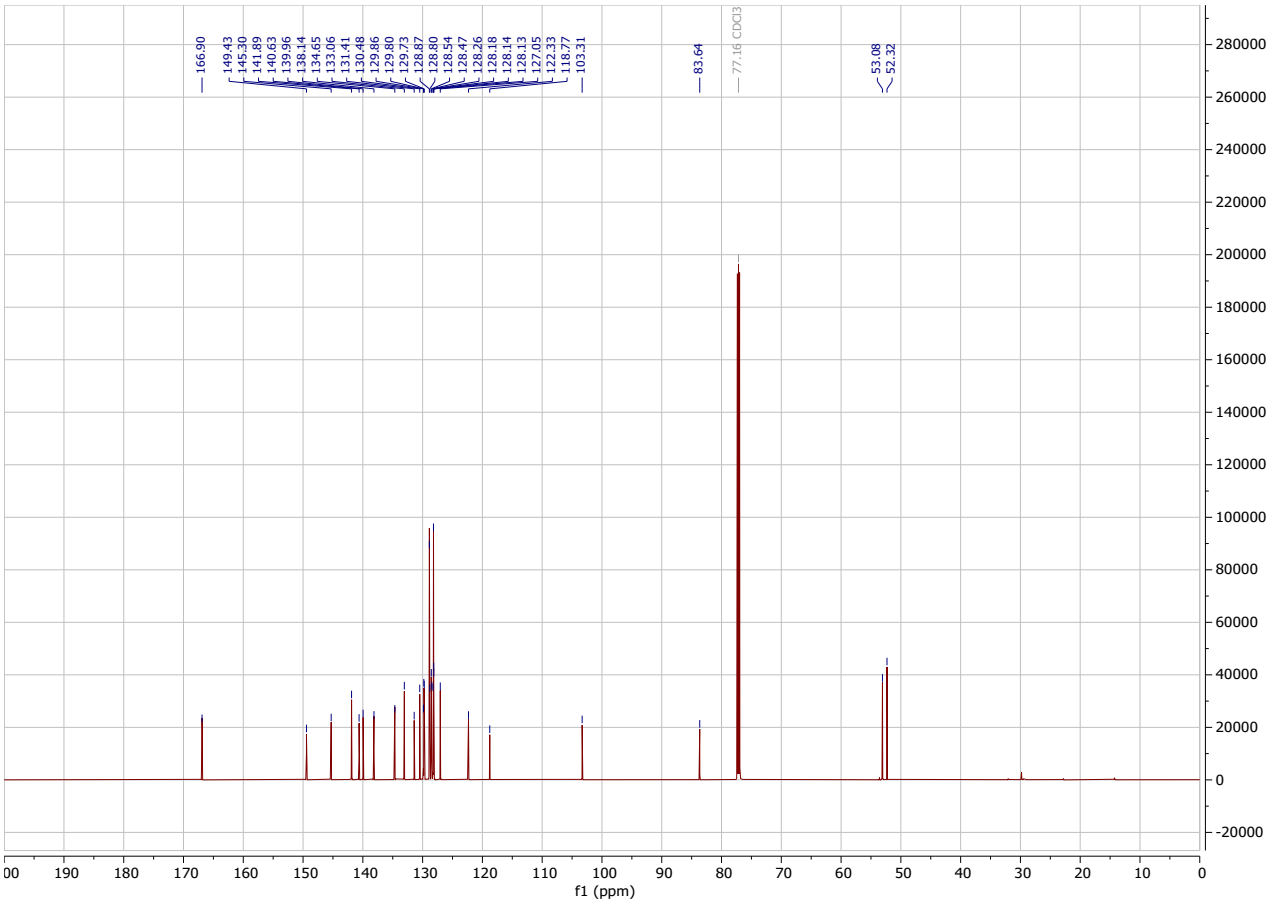
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118.77
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220000
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180000
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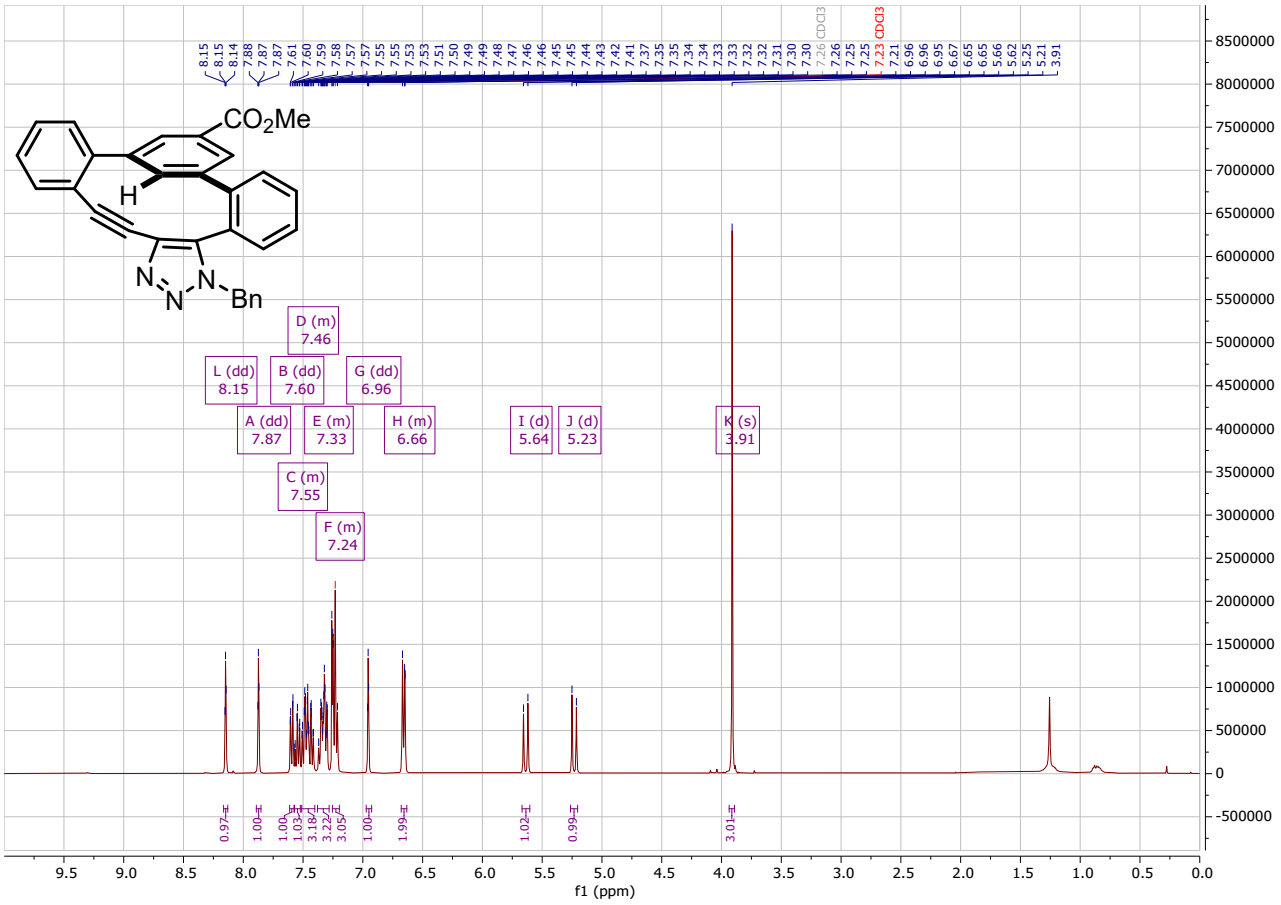
f1 (ppm)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Bn
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G (dd) 6.96
A (dd) 7.87
E (m) 7.33
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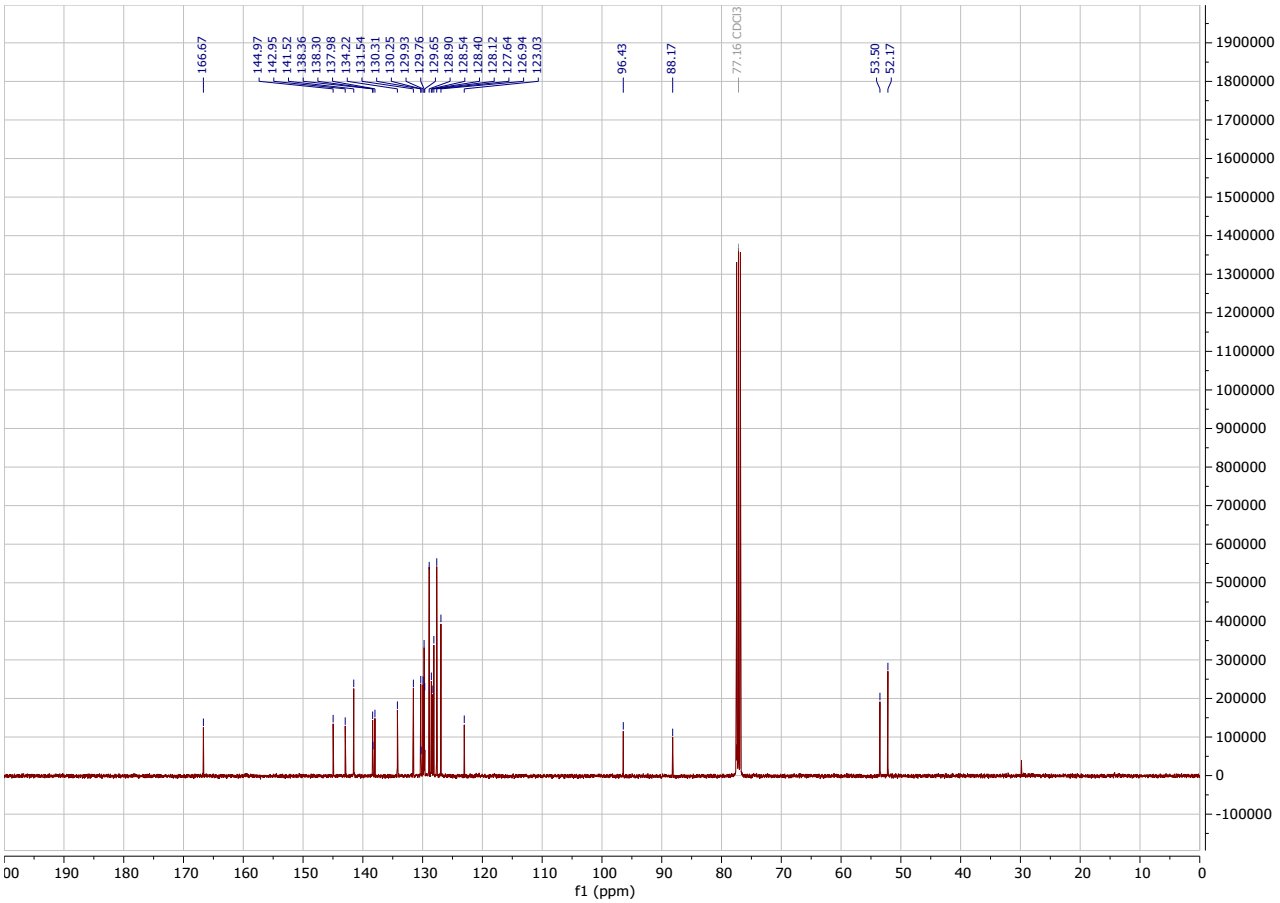
f1 (ppm)



COMPUTATIONAL STRUCTURES

The reaction energy profiles of each SPAAC reaction were examined using density functional theory (DFT) calculations using Gaussian16c.01.[2] All geometries were optimized using B3LYP functional with Grimme's dispersion correction (D3BJ) with the Popel triple zeta basis set (6-311+G(d,p)) in a continuum solvation model (SMD) with a dielectric constant for dichloromethane. Frequency calculations were performed in conjunction with all optimizations to confirm each structure as either a minimum (zero imaginary frequencies) or transition state structure (one imaginary frequency). Single point calculations were performed on the optimized and transition state structures using SMD(DCM)HF/STO-3G for a more accurate energy and molecular orbital depiction. NBO orbitals were calculated using single points from SMD(DCM)HF/STO-3G.[3] VESTA was used to visualize

[2] Gaussian 16, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A., Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Rendell, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma K.; Farkas, O.; Foresman, J. B.; Fox, D. J.; Gaussian, Inc., Wallingford CT, 2016.

[3] NBO Version 3.1, E. D. Glendening, A. E. Reed, J. E. Carpenter, and F. Weinhold

all molecular orbitals (isovalue = 0.3).[4] NCI plots were calculated using NCIPlot.[5] NBO orbitals and NCI plots were visualized using VMD.

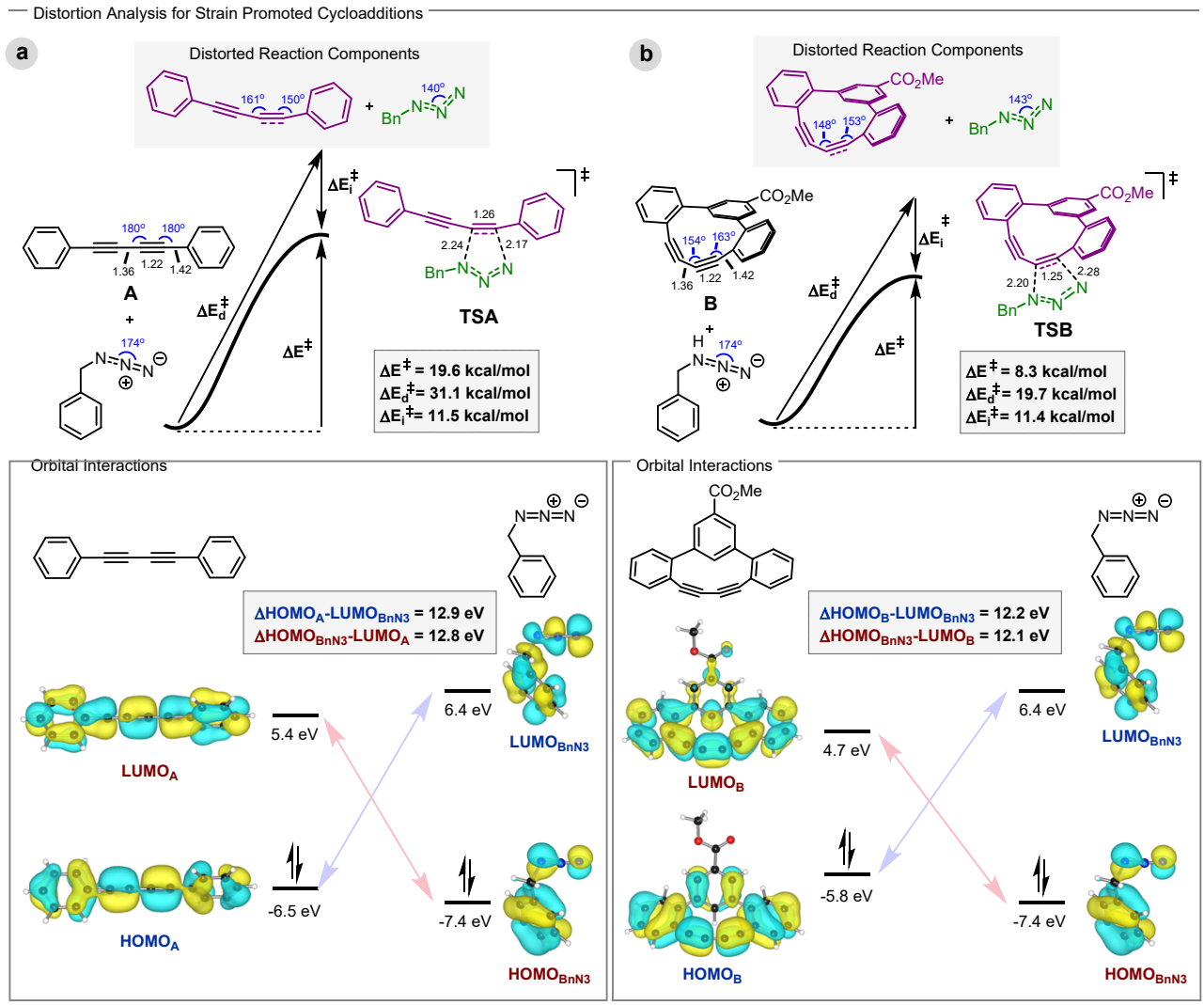
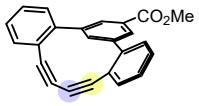


Figure S17: *top*: Distortion/interaction analysis for the cycloadditions between benzyl azide, a: A (1,4-diphenylbutadiyne) and b: B (3,5-TPDY 5). *bottom*: Orbital interaction diagrams for the respective cycloadditions (isovalue = 0.3). All bond lengths are reported in Angstroms.

Table S1. Experimental and computational parameters for cycloadditions.

[4] Momma, K.; Izumi, F. *J. Appl. Crystallogr.* **2011**, *44*, 1272
[5] VMD: Humphrey, W.; Dalke, A.; Schulten, K. *J. Molec. Graphics* **1996**, *14*, 33



Entry	diyne	Reagent	k_{obs} ($M^{-1}s^{-1}$)	$\Delta HOMO_X$-$LUMO_{diyne}$ (eV)	$\Delta HOMO_{diyne}$-$LUMO_X$ (eV)	$\Delta G^{\ddagger}$ (kcal·mol^{-1})	$\Delta E^{\ddagger}$ (kcal·mol^{-1})	$\Delta E_d^{\ddagger}$ (kcal·mol^{-1})	(∠🟡)	(∠🔵)
1	A	BnN_3	--	12.8	12.9	30.2	19.6	31.1		
2	B	BnN_3	$1.7\cdot10^{-2}$	12.1	12.2	22.3	8.3	19.7	10	6
3	B	N_2CO_2Et	$1.2\cdot10^{-2}$	11.6	12.0	22.5	9.7	22.1	8	9
4	B	**8**	$1.7\cdot10^{-4}$	12.1	9.5	23.7	11.9	29.5	9	16

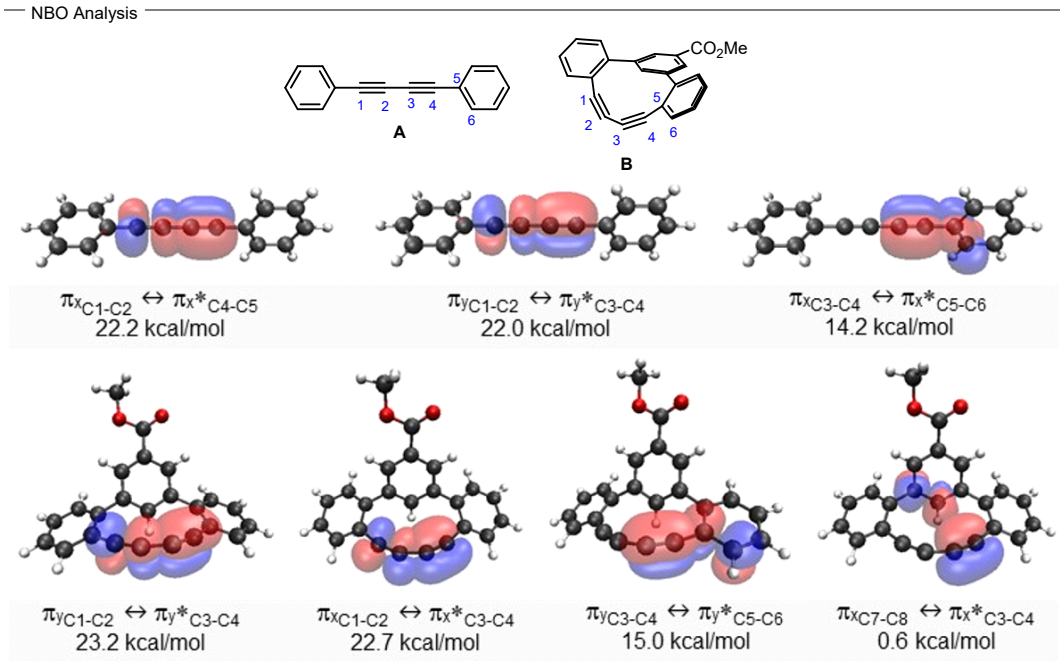


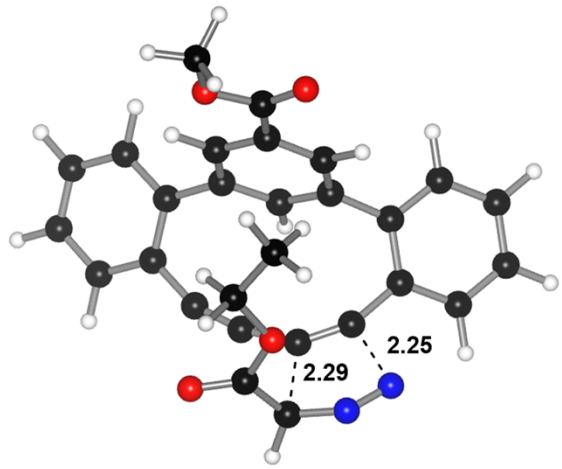
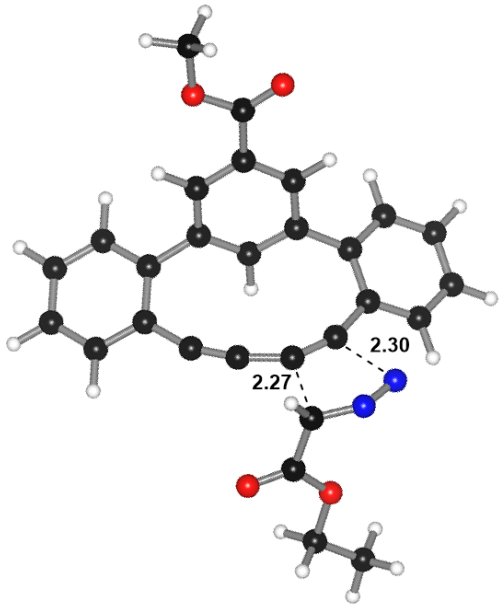
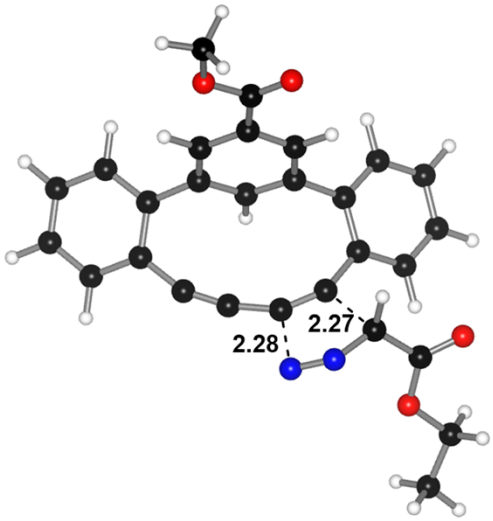
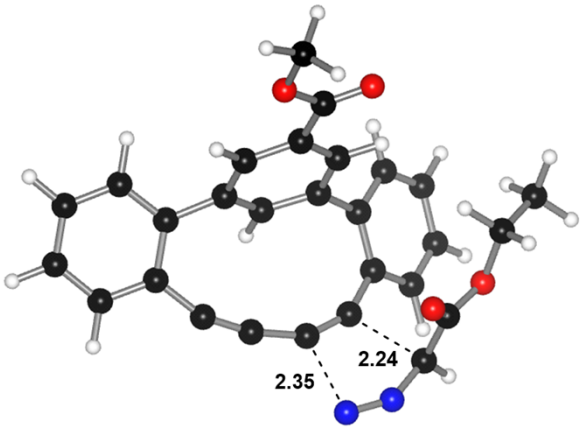
Figure S18: NBO analysis of orbital interactions in 1,4-diphenyl-1,3-butadiyne (A) and 3,5-TPDY 5 (B) (isovalue = 0.3).

Ball and Stick Models of Transition States.

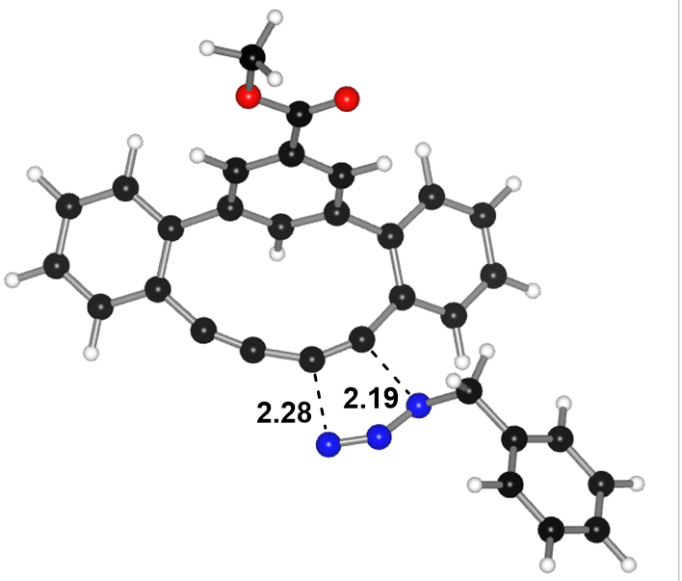
The lowest energy transition state for 3,5-TPDY and N_2CO_2Et was chosen for modeling of the reaction. Experimentally, a mixture of regioisomers was observed, and the pseudo-endo R transition state structure (**TSC**) was computationally determined to be equal in energy to the pseudo-endo S transition state structure ($\mathbf{TSC_{EndoS}}$). Experimentally, the enantiomers of both regioisomers were not identified, but due to the computationally determined small energy barrier difference it is likely that both are present with a slight preference for the lower barrier enantiomer.

Table S2. Transition States for enantiomers of both regio-isomers of 3,5-TPDY and N_2CO_2Et.

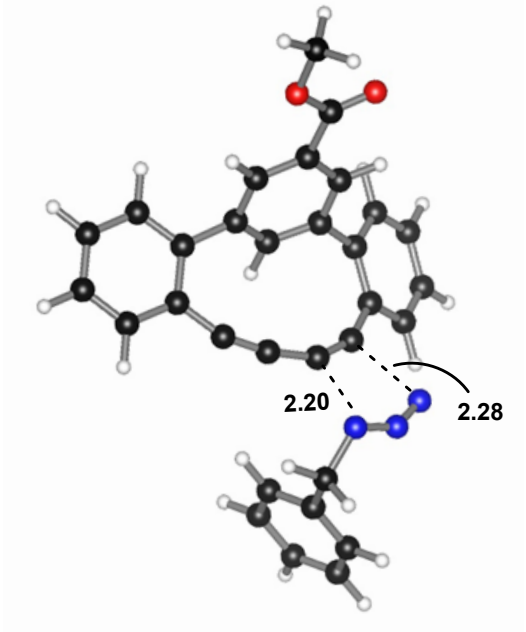
TSC	$\mathbf{TSC_{EndoS}}$

	
[0.0] kcal/mol	**0.2 kcal/mol**
TSC_{ExoR}	**TSC_{ExoS}**
	
2.5 kcal/mol	**1.1 kcal/mol**

TSB-Pseudo Exo	**TSC**



0.1 kcal/mol



[0.0]

Table S3. Transition States of both regio-isomers of 3,5-TPDY and BnN_3

As both regioisomers are equal The pseudo-endo conformer (**TSB**) was chosen as a model for the reaction as it was shown to be experimentally preferred.

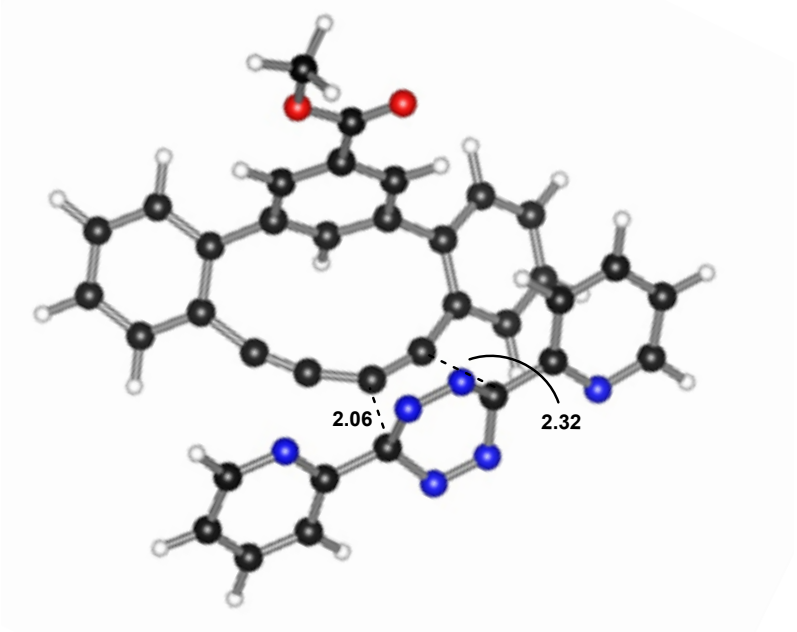
TSD

23.7 kcal/mol

Table S4. Transition state of tetrazine with 3,5-TPDY, energy is relative to starting material

NCI Plot

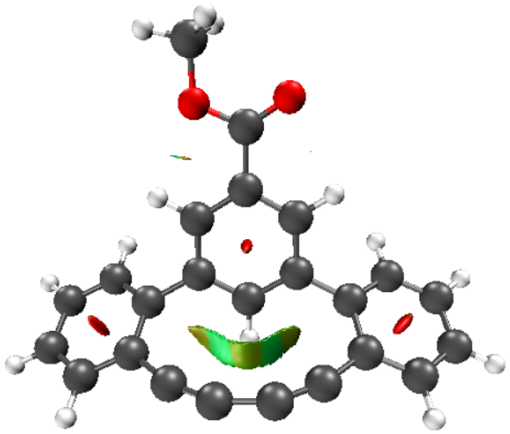


Figure S19. NCI plot of B.

Molecular Orbitals of Other Systems

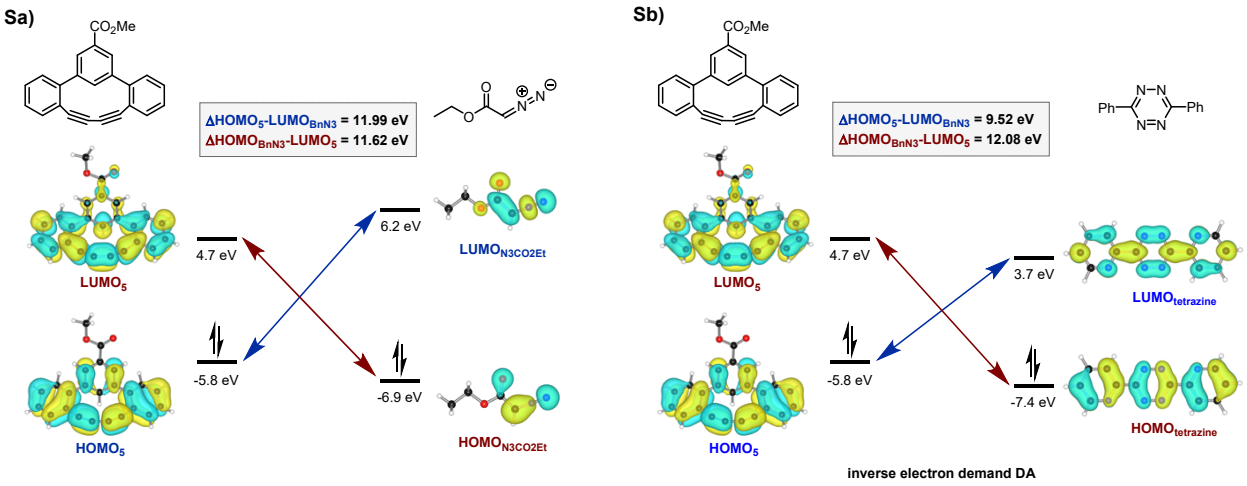


FIGURE S20. ORBITAL INTERACTION DIAGRAMS FOR THE RESPECTIVE CYCLOADDITIONS (ISOVALUE = 0.3)

NBO Orbitals

1,4-diphenyl-1,3-butadiyne (A)

NATURAL POPULATIONS: Natural atomic orbital occupancies
NAO Atom No lang Type(AO) Occupancy Energy
---
1 C 1 S Cor(1S) 1.99995 -10.96225
2 C 1 S Val(2S) 1.08053 -0.19337
3 C 1 px Val(2p) 0.97593 0.14653
4 C 1 py Val(2p) 0.99372 0.06901
5 C 1 pz Val(2p) 0.99377 0.06850
6 C 2 S Cor(1S) 1.99994 -10.96985
7 C 2 S Val(2S) 1.08423 -0.19988
8 C 2 px Val(2p) 0.97549 0.14283
9 C 2 py Val(2p) 0.97862 0.06866
10 C 2 pz Val(2p) 0.97865 0.06815
11 C 3 S Cor(1S) 1.99990 -10.99407
12 C 3 S Val(2S) 1.06054 -0.19180
13 C 3 px Val(2p) 0.93617 0.15325
14 C 3 py Val(2p) 1.01260 0.05963
15 C 3 pz Val(2p) 1.01279 0.05912
16 C 4 S Cor(1S) 1.99994 -10.96985
17 C 4 S Val(2S) 1.08423 -0.19988
18 C 4 px Val(2p) 0.97550 0.14283
19 C 4 py Val(2p) 0.97863 0.06865
20 C 4 pz Val(2p) 0.97865 0.06816

21 C 5 S Cor(1S) 1.99995 -10.96225
22 C 5 S Val(2S) 1.08053 -0.19337
23 C 5 px Val(2p) 0.97593 0.14653
24 C 5 py Val(2p) 0.99372 0.06900
25 C 5 pz Val(2p) 0.99377 0.06851
26 C 6 S Cor(1S) 1.99995 -10.96565
27 C 6 S Val(2S) 1.08323 -0.19611
28 C 6 px Val(2p) 0.99001 0.13856
29 C 6 py Val(2p) 0.97553 0.07462
30 C 6 pz Val(2p) 0.97555 0.07412
31 H 7 S Val(1S) 0.95341 0.07095
32 H 8 S Val(1S) 0.95104 0.06876
33 H 9 S Val(1S) 0.95104 0.06876
34 H 10 S Val(1S) 0.95341 0.07095
35 H 11 S Val(1S) 0.95365 0.06934
36 C 12 S Cor(1S) 1.99943 -10.92543
37 C 12 S Val(2S) 1.07461 -0.19514
38 C 12 px Val(2p) 0.96376 0.28678
39 C 12 py Val(2p) 0.97689 0.03292
40 C 12 pz Val(2p) 0.97692 0.03290
41 C 13 S Cor(1S) 1.99946 -10.92294
42 C 13 S Val(2S) 1.03741 -0.17034
43 C 13 px Val(2p) 0.97283 0.29025
44 C 13 py Val(2p) 1.03410 0.02128
45 C 13 pz Val(2p) 1.03408 0.02128
46 C 14 S Cor(1S) 1.99946 -10.92294
47 C 14 S Val(2S) 1.03742 -0.17034
48 C 14 px Val(2p) 0.97283 0.29025
49 C 14 py Val(2p) 1.03409 0.02128
50 C 14 pz Val(2p) 1.03409 0.02128
51 C 15 S Cor(1S) 1.99943 -10.92544
52 C 15 S Val(2S) 1.07463 -0.19515
53 C 15 px Val(2p) 0.96375 0.28678
54 C 15 py Val(2p) 0.97690 0.03291
55 C 15 pz Val(2p) 0.97691 0.03291
56 C 16 S Cor(1S) 1.99990 -10.99408
57 C 16 S Val(2S) 1.06055 -0.19182
58 C 16 px Val(2p) 0.93615 0.15325
59 C 16 py Val(2p) 1.01266 0.05947
60 C 16 pz Val(2p) 1.01273 0.05928
61 C 17 S Cor(1S) 1.99994 -10.96985
62 C 17 S Val(2S) 1.08424 -0.19988
63 C 17 px Val(2p) 0.97549 0.14283
64 C 17 py Val(2p) 0.97863 0.06849
65 C 17 pz Val(2p) 0.97864 0.06831
66 C 18 S Cor(1S) 1.99994 -10.96985
67 C 18 S Val(2S) 1.08423 -0.19988

68 C 18 px Val(2p) 0.97550 0.14283
69 C 18 py Val(2p) 0.97863 0.06850
70 C 18 pz Val(2p) 0.97864 0.06831
71 C 19 S Cor(1S) 1.99995 -10.96225
72 C 19 S Val(2S) 1.08053 -0.19337
73 C 19 px Val(2p) 0.97593 0.14653
74 C 19 py Val(2p) 0.99374 0.06884
75 C 19 pz Val(2p) 0.99375 0.06866
76 H 20 S Val(1S) 0.95104 0.06876
77 C 21 S Cor(1S) 1.99995 -10.96225
78 C 21 S Val(2S) 1.08053 -0.19337
79 C 21 px Val(2p) 0.97593 0.14653
80 C 21 py Val(2p) 0.99374 0.06884
81 C 21 pz Val(2p) 0.99376 0.06866
82 H 22 S Val(1S) 0.95104 0.06876
83 C 23 S Cor(1S) 1.99995 -10.96565
84 C 23 S Val(2S) 1.08323 -0.19611
85 C 23 px Val(2p) 0.99001 0.13856
86 C 23 py Val(2p) 0.97553 0.07447
87 C 23 pz Val(2p) 0.97555 0.07427
88 H 24 S Val(1S) 0.95341 0.07095
89 H 25 S Val(1S) 0.95341 0.07095
90 H 26 S Val(1S) 0.95365 0.06934

Natural Bond Orbitals (Summary):

Principal Delocalizations
NBO Occupancy Energy (geminal,vicinal,remote)
==========
==========
Molecular unit 1 (C16H10)
1. BD (1) C 1 - C 2 1.98883 -0.79394 68(v),62(v),66(v),61(v),60(g),57(g)
2. BD (1) C 1 - C 6 1.98918 -0.78832 67(v),60(v),58(v),63(v),68(g),57(g)
3. BD (2) C 1 - C 6 1.65082 -0.25066 59(v),64(v)
4. BD (1) C 1 - H 7 1.98902 -0.65747 58(v),66(v),60(v),68(v),55(g),54(g)
5. BD (1) C 2 - C 3 1.98028 -0.78563 70(v),57(v),65(v),55(v),63(v),60(g),62(g)
6. BD (2) C 2 - C 3 1.64421 -0.25181 64(v),56(v),71(v)
7. BD (1) C 2 - H 8 1.98924 -0.66221 55(v),61(v),62(v),58(g),57(v),54(g)
8. BD (1) C 3 - C 4 1.98028 -0.78562 70(v),67(v),60(v),66(v),54(v),65(g),62(g)
9. BD (1) C 3 - C 12 1.99020 -0.81353 54(v),63(v),69(g),61(g),58(g),72(v),60(v),65(v)
10. BD (1) C 4 - C 5 1.98883 -0.79395 68(v),62(v),55(v),58(v),65(g),67(g)
11. BD (2) C 4 - C 5 1.66846 -0.25669 56(v),59(v)
12. BD (1) C 4 - H 9 1.98924 -0.66221 66(v),58(v),62(v),61(g),67(v),63(g)
13. BD (1) C 5 - C 6 1.98918 -0.78831 57(v),65(v),61(v),54(v),68(g),67(g)
14. BD (1) C 5 - H 10 1.98902 -0.65747 61(v),55(v),65(v),68(v)66(g),63(g)
15. BD (1) C 6 - H 11 1.98939 -0.65931 54(v),63(v),57(v),67(v),55(g),66(g)
16. BD (1) C 12 - C 13 1.99743 -0.99143 62(g)

17. BD (2) C 12 - C 13 1.93866 -0.33778 75(v),58(v),61(v)
18. BD (3) C 12 - C 13 1.91479 -0.33391 74(v),59(v)
19. BD (1) C 13 - C 14 1.99786 -0.88789 62(v),76(v)
20. BD (1) C 14 - C 15 1.99743 -0.99143 76(g)
21. BD (2) C 14 - C 15 1.93866 -0.33778 71(v),77(v),78(v)
22. BD (3) C 14 - C 15 1.91480 -0.33392 70(v),79(v)
23. BD (1) C 15 - C 16 1.99020 -0.81350 80(v),83(v),73(g),78(g),77(g),72(v),82(v),84(v)
24. BD (1) C 16 - C 17 1.98028 -0.78562 74(v),86(v),84(v),85(v),83(v),82(g),76(g)
25. BD (1) C 16 - C 18 1.98028 -0.78563 74(v),89(v),82(v),87(v),80(v),84(g),76(g)
26. BD (2) C 16 - C 18 1.64422 -0.25182 81(v),88(v),75(v)
27. BD (1) C 17 - C 19 1.98883 -0.79394 90(v),76(v),87(v),78(v),82(g),86(g)
28. BD (2) C 17 - C 19 1.66846 -0.25668 88(v),79(v)
29. BD (1) C 17 - H 20 1.98924 -0.66221 85(v),78(v),76(v),77(g),86(v),80(g)
30. BD (1) C 18 - C 21 1.98883 -0.79395 90(v),76(v),85(v),77(v),84(g),89(g)
31. BD (1) C 18 - H 22 1.98924 -0.66221 87(v),77(v),76(v),78(g),89(v),83(g)
32. BD (1) C 19 - C 23 1.98918 -0.78831 89(v),82(v),77(v),83(v),90(g),86(g)
33. BD (1) C 19 - H 24 1.98902 -0.65747 77(v),87(v),82(v),90(v),85(g),80(g)
34. BD (1) C 21 - C 23 1.98918 -0.78832 86(v),84(v),78(v),80(v),90(g),89(g)
35. BD (2) C 21 - C 23 1.65082 -0.25066 79(v),81(v)
36. BD (1) C 21 - H 25 1.98902 -0.65747 78(v),85(v),84(v),90(v),87(g),83(g)
37. BD (1) C 23 - H 26 1.98939 -0.65931 83(v),80(v),86(v),89(v),85(g),87(g)
38. CR (1) C 1 1.99995 -10.96222
39. CR (1) C 2 1.99994 -10.96976
40. CR (1) C 3 1.99990 -10.99413
41. CR (1) C 4 1.99994 -10.96976
42. CR (1) C 5 1.99995 -10.96223
43. CR (1) C 6 1.99995 -10.96563
44. CR (1) C 12 1.99943 -10.92550 72(v),62(g),69(g)
45. CR (1) C 13 1.99946 -10.92314 62(v),72(g),73(v),69(g)
46. CR (1) C 14 1.99946 -10.92314 76(v),72(g),69(v),73(g)
47. CR (1) C 15 1.99943 -10.92551 72(v),76(g),73(g)
48. CR (1) C 16 1.99990 -10.99413
49. CR (1) C 17 1.99994 -10.96976
50. CR (1) C 18 1.99994 -10.96976
51. CR (1) C 19 1.99995 -10.96223
52. CR (1) C 21 1.99995 -10.96222
53. CR (1) C 23 1.99995 -10.96563
54. BD*(1) C 1 - C 2 0.01039 0.87924
55. BD*(1) C 1 - C 6 0.01097 0.87285
56. BD*(2) C 1 - C 6 0.32947 0.24728 64(v),59(v)
57. BD*(1) C 1 - H 7 0.01011 0.73607
58. BD*(1) C 2 - C 3 0.01677 0.85131
59. BD*(2) C 2 - C 3 0.37802 0.23253 56(v),64(v),71(v)
60. BD*(1) C 2 - H 8 0.00999 0.73284
61. BD*(1) C 3 - C 4 0.01677 0.85129
62. BD*(1) C 3 - C 12 0.01245 0.82695
63. BD*(1) C 4 - C 5 0.01039 0.87925

64. BD*(2) C 4 - C 5 0.31489 0.24955 56(v),59(v)
65. BD*(1) C 4 - H 9 0.00999 0.73284
66. BD*(1) C 5 - C 6 0.01097 0.87284
67. BD*(1) C 5 - H 10 0.01011 0.73607
68. BD*(1) C 6 - H 11 0.01008 0.73442
69. BD*(1) C 12 - C 13 0.00395 1.21535
70. BD*(2) C 12 - C 13 0.06878 0.39362
71. BD*(3) C 12 - C 13 0.09976 0.38645
72. BD*(1) C 13 - C 14 0.00334 0.92893
73. BD*(1) C 14 - C 15 0.00395 1.21536
74. BD*(2) C 14 - C 15 0.06877 0.39362
75. BD*(3) C 14 - C 15 0.09975 0.38646
76. BD*(1) C 15 - C 16 0.01245 0.82689
77. BD*(1) C 16 - C 17 0.01677 0.85128
78. BD*(1) C 16 - C 18 0.01677 0.85130
79. BD*(2) C 16 - C 18 0.37802 0.23253 88(v),81(v),75(v)
80. BD*(1) C 17 - C 19 0.01039 0.87924
81. BD*(2) C 17 - C 19 0.31490 0.24955 88(v),79(v)
82. BD*(1) C 17 - H 20 0.00999 0.73284
83. BD*(1) C 18 - C 21 0.01039 0.87924
84. BD*(1) C 18 - H 22 0.00999 0.73284
85. BD*(1) C 19 - C 23 0.01097 0.87284
86. BD*(1) C 19 - H 24 0.01011 0.73607
87. BD*(1) C 21 - C 23 0.01097 0.87285
88. BD*(2) C 21 - C 23 0.32948 0.24728 81(v),79(v)
89. BD*(1) C 21 - H 25 0.01011 0.73607
90. BD*(1) C 23 - H 26 0.01008 0.73442

Total Lewis 103.32902 (97.4802%)
Valence non-Lewis 2.67098 (2.5198%)
Rydberg non-Lewis 0.00000 (0.0000%)

Total unit 1 106.00000 (100.0000%)
Charge unit 1 0.00000
Sorting of NBOs: 48 40 49 50 41 39 53 43 51 42
Sorting of NBOs: 52 38 47 44 46 45 20 16 19 9
Sorting of NBOs: 23 10 30 27 1 2 34 13 32 25
Sorting of NBOs: 5 8 24 12 7 31 29 37 15 33
Sorting of NBOs: 14 4 36 21 17 22 18 11 28 26
Sorting of NBOs: 6 35 3 79 59 88 56 81 64 71
Sorting of NBOs: 75 70 74 60 84 82 65 68 90 89
Sorting of NBOs: 67 57 86 76 62 77 61 78 58 85
Sorting of NBOs: 66 55 87 80 54 83 63 72 69 73
Reordering of NBOs for storage: 48 40 49 50 41 39 53 43 51 42
Reordering of NBOs for storage: 52 38 47 44 46 45 20 16 19 9
Reordering of NBOs for storage: 23 10 30 27 1 2 34 13 32 25
Reordering of NBOs for storage: 5 8 24 12 7 31 29 37 15 33

Reordering of NBOs for storage: 14 4 36 21 17 22 18 11 28 26
Reordering of NBOs for storage: 6 35 3 79 59 88 56 81 64 71
Reordering of NBOs for storage: 75 70 74 60 84 82 65 68 90 89
Reordering of NBOs for storage: 67 57 86 76 62 77 61 78 58 85
Reordering of NBOs for storage: 66 55 87 80 54 83 63 72 69 73

3,5-TPDY 5 (B)

Natural Bond Orbitals (Summary):

NBO	Occupancy	Energy	Principal Delocalizations (geminal,vicinal,remote)
Molecular unit 1 (C24H14O2)			
1. BD (1) C 1 - C 2	1.98386	-0.78853	96(v),102(v),105(v),93(g) 94(v),99(v),91(g),104(v) 90(g)
2. BD (2) C 1 - C 2	1.63731	-0.24533	95(v),100(v),105(v),103(v) 104(v)
3. BD (1) C 1 - C 6	1.98373	-0.78810	101(v),93(v),119(v),102(g) 97(v),92(v),91(g),118(v) 88(g)
4. BD (1) C 1 - H 7	1.98851	-0.65921	92(v),99(v),93(v),102(v) 90(g),88(g)
5. BD (1) C 2 - C 3	1.98245	-0.78865	98(v),91(v),105(v),90(v) 97(v),93(g),96(g),103(v)
6. BD (1) C 2 - C 10	1.97871	-0.72297	109(v),94(v),90(v),106(v) 103(g),88(g),92(g),110(v) 104(g),108(v),96(v),91(v)
7. BD (1) C 3 - C 4	1.98565	-0.79397	101(v),93(v),138(v),98(g) 140(v),99(v),88(v),96(g)
8. BD (2) C 3 - C 4	1.65310	-0.25469	100(v),89(v),139(v)
9. BD (1) C 3 - H 8	1.98805	-0.66123	97(v),88(v),98(v),93(v) 92(g),94(g)
10. BD (1) C 4 - C 5	1.98459	-0.79188	96(v),102(v),140(v),138(v) 92(v),98(g),90(v),101(g)
11. BD (1) C 4 - C 34	1.97836	-0.76283	141(v),140(g),99(v),138(g) 92(v),94(g),97(g),101(v) 96(v)
12. BD (1) C 5 - C 6	1.98279	-0.78988	91(v),98(v),119(v),88(v) 94(v),102(g),101(g),117(v)
13. BD (2) C 5 - C 6	1.64593	-0.24958	89(v),95(v),119(v),117(v) 118(v)
14. BD (1) C 5 - H 9	1.98813	-0.66120	94(v),90(v),98(v),102(v) 99(g),97(g)
15. BD (1) C 6 - C 20	1.97874	-0.72305	123(v),97(v),88(v),120(v)

117(g),90(g),99(g),124(v)
101(v),122(v),118(g),91(v)
16. BD (1) C 10 - C 11 1.97157 -0.77439 136(v),110(v),112(v),89(v)
93(g),109(v),111(v),104(g)
106(g)
17. BD (1) C 10 - C 12 1.98317 -0.78980 115(v),108(v),89(v),113(v)
93(g),106(v),88(v),110(g)
103(g)
18. BD (2) C 10 - C 12 1.65599 -0.25154 114(v),107(v),89(v),88(v)
92(v)
19. BD (1) C 11 - C 13 1.98287 -0.79009 136(v),116(v),93(v),113(v)
104(v),112(g),108(g),103(g)
20. BD (2) C 11 - C 13 1.65440 -0.25531 114(v),105(v),137(v)
21. BD (1) C 11 - C 32 1.98914 -0.81047 111(v),104(v),135(g),103(g)
93(v),112(v)
22. BD (1) C 12 - C 14 1.98914 -0.79056 116(v),93(v),111(v),103(v)
115(g),110(g)
23. BD (1) C 12 - H 15 1.98830 -0.65677 113(v),103(v),93(v),115(v)
104(g),109(g)
24. BD (1) C 13 - C 16 1.98918 -0.79477 115(v),108(v),109(v),103(v)
116(g),112(g)
25. BD (1) C 13 - H 17 1.98878 -0.66178 103(v),113(v),108(v),116(v)
106(g),111(g)
26. BD (1) C 14 - C 16 1.98918 -0.78938 112(v),110(v),106(v),104(v)
115(g),116(g)
27. BD (2) C 14 - C 16 1.65162 -0.25132 107(v),105(v)
28. BD (1) C 14 - H 18 1.98915 -0.65923 104(v),111(v),110(v),116(v)
113(g),109(g)
29. BD (1) C 16 - H 19 1.98916 -0.65829 106(v),109(v),112(v),115(v)
113(g),111(g)
30. BD (1) C 20 - C 21 1.97156 -0.77431 132(v),124(v),126(v),100(v)
102(g),123(v),125(v),118(g)
120(g)
31. BD (1) C 20 - C 22 1.98318 -0.78968 129(v),122(v),100(v),127(v)
102(g),120(v),90(v),124(g)
117(g)
32. BD (2) C 20 - C 22 1.65584 -0.25137 128(v),121(v),100(v),90(v)
99(v)
33. BD (1) C 21 - C 23 1.98286 -0.78996 132(v),130(v),102(v),127(v)
118(v),126(g),122(g),117(g)
34. BD (2) C 21 - C 23 1.65440 -0.25520 128(v),119(v),133(v)
35. BD (1) C 21 - C 30 1.98915 -0.81053 125(v),118(v),131(g),117(g)
102(v),126(v)
36. BD (1) C 22 - C 24 1.98914 -0.79040 130(v),102(v),125(v),117(v)
129(g),124(g)
37. BD (1) C 22 - H 25 1.98830 -0.65657 127(v),117(v),102(v),129(v)
118(g),123(g)

38. BD (1) C 23 - C 26	1.98918	-0.79465	129(v),122(v),123(v),117(v) 130(g),126(g)
39. BD (1) C 23 - H 27	1.98878	-0.66167	117(v),127(v),122(v),130(v) 120(g),125(g)
40. BD (1) C 24 - C 26	1.98918	-0.78922	126(v),124(v),120(v),118(v) 129(g),130(g)
41. BD (2) C 24 - C 26	1.65150	-0.25113	121(v),119(v)
42. BD (1) C 24 - H 28	1.98915	-0.65904	118(v),125(v),124(v),130(v) 127(g),123(g)
43. BD (1) C 26 - H 29	1.98916	-0.65814	120(v),123(v),126(v),129(v) 127(g),125(g)
44. BD (1) C 30 - C 31	1.99651	-0.96546	122(g)
45. BD (2) C 30 - C 31	1.93941	-0.34876	136(v),120(v),117(v),134(g),89(r)
46. BD (3) C 30 - C 31	1.90505	-0.33171	137(v),121(v)
47. BD (1) C 31 - C 33	1.99629	-0.87234	
48. BD (1) C 32 - C 33	1.99652	-0.96553	108(g)
49. BD (2) C 32 - C 33	1.93953	-0.34878	132(v),106(v),103(v),134(g)
50. BD (3) C 32 - C 33	1.90506	-0.33173	133(v),107(v)
51. BD (1) C 34 - O 35	1.99314	-1.05945	140(g),98(g),94(v)
52. BD (2) C 34 - O 35	1.98327	-0.42790	95(v),139(g)
53. BD (1) C 34 - O 36	1.98405	-0.94029	141(g),98(g),138(g),142(v),97(v)
54. BD (1) O 36 - C 37	1.98196	-0.80241	138(v),98(v),140(g),144(g),143(g),142(g)
55. BD (1) C 37 - H 38	1.99626	-0.66101	140(v),141(g)
56. BD (1) C 37 - H 39	1.99708	-0.66139	141(g)
57. BD (1) C 37 - H 40	1.99707	-0.66146	141(g)
58. CR (1) C 1	1.99994	-10.97029	
59. CR (1) C 2	1.99990	-10.98063	
60. CR (1) C 3	1.99994	-10.96745	
61. CR (1) C 4	1.99990	-10.97593	
62. CR (1) C 5	1.99994	-10.96669	
63. CR (1) C 6	1.99990	-10.98056	
64. CR (1) C 10	1.99990	-10.98953	
65. CR (1) C 11	1.99989	-10.99625	
66. CR (1) C 12	1.99994	-10.96111	
67. CR (1) C 13	1.99994	-10.96877	
68. CR (1) C 14	1.99995	-10.96498	
69. CR (1) C 16	1.99994	-10.96182	
70. CR (1) C 20	1.99990	-10.98939	
71. CR (1) C 21	1.99989	-10.99613	
72. CR (1) C 22	1.99994	-10.96094	
73. CR (1) C 23	1.99994	-10.96868	
74. CR (1) C 24	1.99995	-10.96483	
75. CR (1) C 26	1.99994	-10.96168	
76. CR (1) C 30	1.99941	-10.92295	134(v),122(g),132(g)
77. CR (1) C 31	1.99935	-10.92422	122(v),132(g),134(g),135(v)
78. CR (1) C 32	1.99941	-10.92283	134(v),108(g),136(g)
79. CR (1) C 33	1.99935	-10.92428	108(v),136(g),134(g),131(v)

80. CR (1) C 34 1.99991 -11.11154 140(g)
81. CR (1) O 35 1.99999 -20.08615
82. CR (1) O 36 1.99999 -20.20865
83. CR (1) C 37 1.99982 -11.03993 141(g)
84. LP (1) O 35 1.99814 -0.94744
85. LP (2) O 35 1.89080 -0.33197 140(v),98(v),141(r)
86. LP (1) O 36 1.98319 -0.80782 138(v),98(v),142(v),144(v),143(v),96(r)
87. LP (2) O 36 1.84520 -0.36932 139(v),143(v),144(v)
88. BD*(1) C 1 - C 2 0.01569 0.86233
89. BD*(2) C 1 - C 2 0.33698 0.24717 100(v),95(v),105(v),103(v), 128(r),104(v)
90. BD*(1) C 1 - C 6 0.01576 0.86170
91. BD*(1) C 1 - H 7 0.01165 0.73908
92. BD*(1) C 2 - C 3 0.01494 0.86922
93. BD*(1) C 2 - C 10 0.02237 0.74418
94. BD*(1) C 3 - C 4 0.01398 0.87231
95. BD*(2) C 3 - C 4 0.36089 0.24075 89(v),100(v),139(v)
96. BD*(1) C 3 - H 8 0.01249 0.73735
97. BD*(1) C 4 - C 5 0.01334 0.87430
98. BD*(1) C 4 - C 34 0.06541 0.70848
99. BD*(1) C 5 - C 6 0.01465 0.87098
100. BD*(2) C 5 - C 6 0.33585 0.24790 89(v),95(v),119(v),117(v), 118(v)
101. BD*(1) C 5 - H 9 0.01293 0.73561
102. BD*(1) C 6 - C 20 0.02239 0.74453
103. BD*(1) C 10 - C 11 0.02356 0.82514
104. BD*(1) C 10 - C 12 0.01455 0.87058
105. BD*(2) C 10 - C 12 0.32610 0.24930 114(v),89(v),107(v),92(v),88(v),119(r)
106. BD*(1) C 11 - C 13 0.01680 0.85666
107. BD*(2) C 11 - C 13 0.37355 0.23395 114(v),105(v),137(v)
108. BD*(1) C 11 - C 32 0.01344 0.82522
109. BD*(1) C 12 - C 14 0.01105 0.87597
110. BD*(1) C 12 - H 15 0.01101 0.73654
111. BD*(1) C 13 - C 16 0.01036 0.88087
112. BD*(1) C 13 - H 17 0.00985 0.73310
113. BD*(1) C 14 - C 16 0.01090 0.87528
114. BD*(2) C 14 - C 16 0.33002 0.24766 105(v),107(v)
115. BD*(1) C 14 - H 18 0.01009 0.73466
116. BD*(1) C 16 - H 19 0.01017 0.73621
117. BD*(1) C 20 - C 21 0.02354 0.82534
118. BD*(1) C 20 - C 22 0.01454 0.87086
119. BD*(2) C 20 - C 22 0.32609 0.24950 128(v),100(v),121(v),99(v)
90(v),105(r)
120. BD*(1) C 21 - C 23 0.01680 0.85673
121. BD*(2) C 21 - C 23 0.37368 0.23402 128(v),119(v),133(v)
122. BD*(1) C 21 - C 30 0.01343 0.82535
123. BD*(1) C 22 - C 24 0.01105 0.87619
124. BD*(1) C 22 - H 25 0.01101 0.73682
125. BD*(1) C 23 - C 26 0.01035 0.88102

126. BD*(1) C 23 - H 27	0.00985	0.73315		
127. BD*(1) C 24 - C 26	0.01090	0.87543		
128. BD*(2) C 24 - C 26	0.33000	0.24783	119(v),121(v),89(r)	
129. BD*(1) C 24 - H 28	0.01008	0.73487		
130. BD*(1) C 26 - H 29	0.01016	0.73638		
131. BD*(1) C 30 - C 31	0.00553	1.15687		
132. BD*(2) C 30 - C 31	0.06538	0.42971		
133. BD*(3) C 30 - C 31	0.10656	0.38987	137(v),121(v)	
134. BD*(1) C 31 - C 33	0.00569	0.89994		
135. BD*(1) C 32 - C 33	0.00551	1.15708		
136. BD*(2) C 32 - C 33	0.06545	0.42970		
137. BD*(3) C 32 - C 33	0.10652	0.38993	133(v),107(v)	
138. BD*(1) C 34 - O 35	0.02023	0.92853		
139. BD*(2) C 34 - O 35	0.18471	0.26436	95(v)	
140. BD*(1) C 34 - O 36	0.08446	0.69442		
141. BD*(1) O 36 - C 37	0.01712	0.58847		
142. BD*(1) C 37 - H 38	0.00705	0.69989		
143. BD*(1) C 37 - H 39	0.01310	0.69316		
144. BD*(1) C 37 - H 40	0.01313	0.69298		

Total Lewis	169.68730	(97.5214%)
Valence non-Lewis	4.31270	(2.4786%)
Rydberg non-Lewis	0.00000	(0.0000%)

Total unit 1	174.00000	(100.0000%)
Charge unit 1	0.00000	

NATURAL POPULATIONS: Natural atomic orbital occupancies

NAO	Atom	No	lang	Type(AO)	Occupancy	Energy
1	C	1	S	Cor(1S)	1.99994	-10.97039
2	C	1	S	Val(2S)	1.09019	-0.20368
3	C	1	px	Val(2p)	0.96388	0.14744
4	C	1	py	Val(2p)	0.99018	0.12398
5	C	1	pz	Val(2p)	0.96855	0.01184
6	C	2	S	Cor(1S)	1.99990	-10.98068
7	C	2	S	Val(2S)	1.07951	-0.20361
8	C	2	px	Val(2p)	0.95421	0.15162
9	C	2	py	Val(2p)	0.96269	0.14136
10	C	2	pz	Val(2p)	1.00806	0.00481
11	C	3	S	Cor(1S)	1.99994	-10.96756
12	C	3	S	Val(2S)	1.08760	-0.20034
13	C	3	px	Val(2p)	0.99001	0.13555
14	C	3	py	Val(2p)	0.96939	0.13801
15	C	3	pz	Val(2p)	0.97394	0.00570
16	C	4	S	Cor(1S)	1.99990	-10.97597

17	C	4	S	Val(2S)	1.08685	-0.20983
18	C	4	px	Val(2p)	0.97942	0.14817
19	C	4	py	Val(2p)	0.96044	0.12848
20	C	4	pz	Val(2p)	1.03717	-0.00765
21	C	5	S	Cor(1S)	1.99994	-10.96681
22	C	5	S	Val(2S)	1.08765	-0.20015
23	C	5	px	Val(2p)	0.98301	0.13789
24	C	5	py	Val(2p)	0.97702	0.13518
25	C	5	pz	Val(2p)	0.97283	0.00603
26	C	6	S	Cor(1S)	1.99990	-10.98062
27	C	6	S	Val(2S)	1.07916	-0.20323
28	C	6	px	Val(2p)	0.94870	0.15062
29	C	6	py	Val(2p)	0.96870	0.14227
30	C	6	pz	Val(2p)	1.00809	0.00499
31	H	7	S	Val(1S)	0.94951	0.07408
32	H	8	S	Val(1S)	0.94670	0.07444
33	H	9	S	Val(1S)	0.94825	0.07281
34	C	10	S	Cor(1S)	1.99990	-10.98966
35	C	10	S	Val(2S)	1.08694	-0.21266
36	C	10	px	Val(2p)	0.95928	0.12260
37	C	10	py	Val(2p)	0.94934	0.11449
38	C	10	pz	Val(2p)	0.96904	0.06318
39	C	11	S	Cor(1S)	1.99989	-10.99620
40	C	11	S	Val(2S)	1.06621	-0.19775
41	C	11	px	Val(2p)	0.96529	0.12679
42	C	11	py	Val(2p)	0.99174	0.09301
43	C	11	pz	Val(2p)	0.99739	0.05026
44	C	12	S	Cor(1S)	1.99994	-10.96118
45	C	12	S	Val(2S)	1.08456	-0.19656
46	C	12	px	Val(2p)	0.97135	0.13011
47	C	12	py	Val(2p)	0.99418	0.09654
48	C	12	pz	Val(2p)	0.99864	0.05451
49	C	13	S	Cor(1S)	1.99994	-10.96885
50	C	13	S	Val(2S)	1.08324	-0.19861
51	C	13	px	Val(2p)	0.96616	0.12740
52	C	13	py	Val(2p)	0.98573	0.09597
53	C	13	pz	Val(2p)	0.98643	0.05541
54	C	14	S	Cor(1S)	1.99995	-10.96500
55	C	14	S	Val(2S)	1.08239	-0.19501
56	C	14	px	Val(2p)	0.98428	0.12180
57	C	14	py	Val(2p)	0.97680	0.10564
58	C	14	pz	Val(2p)	0.98313	0.05940
59	H	15	S	Val(1S)	0.95468	0.07076
60	C	16	S	Cor(1S)	1.99994	-10.96184
61	C	16	S	Val(2S)	1.07948	-0.19219
62	C	16	px	Val(2p)	0.98887	0.12178
63	C	16	py	Val(2p)	0.98622	0.10262

64	C	16	pz	Val(2p)	0.98911	0.05973
65	H	17	S	Val(1S)	0.95078	0.06884
66	H	18	S	Val(1S)	0.95322	0.06961
67	H	19	S	Val(1S)	0.95288	0.07108
68	C	20	S	Cor(1S)	1.99990	-10.98952
69	C	20	S	Val(2S)	1.08681	-0.21241
70	C	20	px	Val(2p)	0.95179	0.13926
71	C	20	py	Val(2p)	0.95679	0.09919
72	C	20	pz	Val(2p)	0.96914	0.06224
73	C	21	S	Cor(1S)	1.99989	-10.99609
74	C	21	S	Val(2S)	1.06617	-0.19762
75	C	21	px	Val(2p)	0.96667	0.13923
76	C	21	py	Val(2p)	0.98945	0.08193
77	C	21	pz	Val(2p)	0.99850	0.04914
78	C	22	S	Cor(1S)	1.99994	-10.96101
79	C	22	S	Val(2S)	1.08454	-0.19633
80	C	22	px	Val(2p)	0.97193	0.14431
81	C	22	py	Val(2p)	0.99327	0.08389
82	C	22	pz	Val(2p)	0.99886	0.05356
83	C	23	S	Cor(1S)	1.99994	-10.96876
84	C	23	S	Val(2S)	1.08323	-0.19850
85	C	23	px	Val(2p)	0.96329	0.14193
86	C	23	py	Val(2p)	0.98848	0.08271
87	C	23	pz	Val(2p)	0.98647	0.05452
88	C	24	S	Cor(1S)	1.99995	-10.96485
89	C	24	S	Val(2S)	1.08239	-0.19483
90	C	24	px	Val(2p)	0.98062	0.13880
91	C	24	py	Val(2p)	0.98057	0.08998
92	C	24	pz	Val(2p)	0.98290	0.05862
93	H	25	S	Val(1S)	0.95455	0.07109
94	C	26	S	Cor(1S)	1.99994	-10.96170
95	C	26	S	Val(2S)	1.07946	-0.19204
96	C	26	px	Val(2p)	0.99042	0.13522
97	C	26	py	Val(2p)	0.98449	0.09054
98	C	26	pz	Val(2p)	0.98930	0.05881
99	H	27	S	Val(1S)	0.95078	0.06892
100	H	28	S	Val(1S)	0.95316	0.06985
101	H	29	S	Val(1S)	0.95288	0.07123
102	C	30	S	Cor(1S)	1.99940	-10.92292
103	C	30	S	Val(2S)	1.07841	-0.19556
104	C	30	px	Val(2p)	0.99840	0.17128
105	C	30	py	Val(2p)	0.96754	0.08554
106	C	30	pz	Val(2p)	0.95338	0.09202
107	C	31	S	Cor(1S)	1.99936	-10.92404
108	C	31	S	Val(2S)	1.04685	-0.16736
109	C	31	px	Val(2p)	0.96426	0.24735
110	C	31	py	Val(2p)	1.02702	0.04236

111	C	31	pz	Val(2p)	1.03275	0.03602
112	C	32	S	Cor(1S)	1.99940	-10.92280
113	C	32	S	Val(2S)	1.07837	-0.19543
114	C	32	px	Val(2p)	0.99343	0.20776
115	C	32	py	Val(2p)	0.97297	0.04685
116	C	32	pz	Val(2p)	0.95359	0.09414
117	C	33	S	Cor(1S)	1.99936	-10.92410
118	C	33	S	Val(2S)	1.04672	-0.16741
119	C	33	px	Val(2p)	0.96547	0.26183
120	C	33	py	Val(2p)	1.02591	0.02703
121	C	33	pz	Val(2p)	1.03225	0.03700
122	C	34	S	Cor(1S)	1.99991	-11.11157
123	C	34	S	Val(2S)	1.04005	-0.24435
124	C	34	px	Val(2p)	0.77164	0.19051
125	C	34	py	Val(2p)	0.90848	0.11267
126	C	34	pz	Val(2p)	0.88592	-0.02257
127	O	35	S	Cor(1S)	1.99999	-20.08609
128	O	35	S	Val(2S)	1.80496	-1.05119
129	O	35	px	Val(2p)	1.57870	-0.20216
130	O	35	py	Val(2p)	1.63878	-0.22835
131	O	35	pz	Val(2p)	1.30071	-0.14039
132	O	36	S	Cor(1S)	1.99999	-20.20865
133	O	36	S	Val(2S)	1.72298	-1.02190
134	O	36	px	Val(2p)	1.40498	-0.17741
135	O	36	py	Val(2p)	1.32689	-0.14636
136	O	36	pz	Val(2p)	1.82064	-0.35870
137	C	37	S	Cor(1S)	1.99982	-11.03995
138	C	37	S	Val(2S)	1.08273	-0.22552
139	C	37	px	Val(2p)	1.03959	0.04007
140	C	37	py	Val(2p)	0.80790	0.09375
141	C	37	pz	Val(2p)	1.03538	0.04469
142	H	38	S	Val(1S)	0.94645	0.06172
143	H	39	S	Val(1S)	0.95197	0.05906
144	H	40	S	Val(1S)	0.95214	0.05883

NBO Key

Sorting of NBOs:	82 81 80 83 65 71 64 70 59 63
Sorting of NBOs:	61 58 67 73 60 62 68 74 69 75
Sorting of NBOs:	66 72 79 77 76 78 51 48 44 84
Sorting of NBOs:	53 47 35 21 86 54 24 38 7 10
Sorting of NBOs:	22 36 19 33 12 17 31 26 40 5
Sorting of NBOs:	1 3 16 30 11 15 6 25 39 57
Sorting of NBOs:	56 9 14 55 28 4 42 29 43 23
Sorting of NBOs:	37 52 87 49 45 85 50 46 20 34
Sorting of NBOs:	8 18 32 27 41 13 2 107 121 95
Sorting of NBOs:	89 114 128 100 105 119 139 133 137 136

Sorting of NBOs: 132 141 144 143 140 142 98 112 126 115
Sorting of NBOs: 129 101 116 130 110 124 96 91 93 102
Sorting of NBOs: 103 108 117 122 106 120 90 88 92 104
Sorting of NBOs: 118 99 94 97 113 127 109 123 111 125
Sorting of NBOs: 134 138 131 135
Reordering of NBOs for storage: 82 81 80 83 65 71 64 70 59 63
Reordering of NBOs for storage: 61 58 67 73 60 62 68 74 69 75
Reordering of NBOs for storage: 66 72 79 77 76 78 51 48 44 84
Reordering of NBOs for storage: 53 47 35 21 86 54 24 38 7 10
Reordering of NBOs for storage: 22 36 19 33 12 17 31 26 40 5
Reordering of NBOs for storage: 1 3 16 30 11 15 6 25 39 57
Reordering of NBOs for storage: 56 9 14 55 28 4 42 29 43 23
Reordering of NBOs for storage: 37 52 87 49 45 85 50 46 20 34
Reordering of NBOs for storage: 8 18 32 27 41 13 2 107 121 95
Reordering of NBOs for storage: 89 114 128 100 105 119 139 133 137 136
Reordering of NBOs for storage: 132 141 144 143 140 142 98 112 126 115
Reordering of NBOs for storage: 129 101 116 130 110 124 96 91 93 102
Reordering of NBOs for storage: 103 108 117 122 106 120 90 88 92 104
Reordering of NBOs for storage: 118 99 94 97 113 127 109 123 111 125
Reordering of NBOs for storage: 134 138 131 135

Coordinates

3,5-TPDY

HF = -1073.4528074 hartrees
Zero-point correction= 0.303750 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.254542
Sum of electronic and zero-point Energies= -1073.149057
Sum of electronic and thermal Enthalpies= -1073.127577
Sum of electronic and thermal Free Energies= -1073.198266

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.164626	-0.631977	-0.564570
2	6	0	-1.149909	-0.163931	-0.384627
3	6	0	-1.342473	1.194859	-0.094136
4	6	0	-0.245429	2.056233	0.034849
5	6	0	1.057110	1.556298	-0.081136
6	6	0	1.280548	0.203112	-0.369472
7	1	0	0.322162	-1.664218	-0.852086
8	1	0	-2.345751	1.576084	0.055178
9	1	0	1.894276	2.226936	0.078924
10	6	0	-2.351011	-1.056077	-0.449589
11	6	0	-2.465397	-2.252508	0.327659
12	6	0	-3.449755	-0.677761	-1.233430
13	6	0	-3.653480	-3.007184	0.289416
14	6	0	-4.621814	-1.438449	-1.269227
15	1	0	-3.379214	0.225512	-1.832387
16	6	0	-4.725577	-2.603804	-0.503719
17	1	0	-3.721588	-3.908874	0.889949
18	1	0	-5.450036	-1.120085	-1.895546
19	1	0	-5.635266	-3.196331	-0.525325
20	6	0	2.692400	-0.293480	-0.417369
21	6	0	3.145504	-1.405094	0.362059
22	6	0	3.639928	0.395976	-1.186391
23	6	0	4.504190	-1.774062	0.340635
24	6	0	4.985011	0.016574	-1.205575
25	1	0	3.312874	1.240253	-1.786214
26	6	0	5.419028	-1.068515	-0.438081
27	1	0	4.828338	-2.616933	0.943048
28	1	0	5.690128	0.568427	-1.820245
29	1	0	6.463623	-1.364805	-0.446793
30	6	0	2.184755	-2.127744	1.123155
31	6	0	1.137579	-2.588211	1.561006
32	6	0	-1.343892	-2.659991	1.102825

33	6	0	-0.212171	-2.791233	1.552465
34	6	0	-0.414020	3.507025	0.337269
35	8	0	0.512570	4.293126	0.471609
36	8	0	-1.704697	3.871301	0.444579
37	6	0	-1.958273	5.264123	0.738348
38	1	0	-3.043467	5.355495	0.783631
39	1	0	-1.510851	5.538034	1.697293
40	1	0	-1.553091	5.900018	-0.053111

N_2CO_2Et

HF = -415.985719 hartrees

Zero-point correction= 0.104481 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.070578
Sum of electronic and zero-point Energies= -415.881238
Sum of electronic and thermal Enthalpies= -415.871758
Sum of electronic and thermal Free Energies= -415.915141

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.226226	0.186871	0.000267
2	8	0	-0.385511	1.402863	0.000161
3	8	0	0.974056	-0.425173	0.000142
4	6	0	-1.294324	-0.801563	0.000206
5	7	0	-2.523723	-0.360542	-0.000249
6	7	0	-3.586841	0.039781	-0.000248
7	1	0	-1.150481	-1.873596	0.000963
8	6	0	2.147825	0.438635	-0.000086
9	1	0	2.109267	1.076827	-0.888240
10	1	0	2.109535	1.076917	0.888016
11	6	0	3.365939	-0.460385	-0.000211
12	1	0	3.383824	-1.097688	-0.890349
13	1	0	4.270159	0.157706	-0.000288
14	1	0	3.383997	-1.097718	0.889903

BnN_3

HF = -435.1939152 hartrees

Zero-point correction= 0.132001 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.096325
Sum of electronic and zero-point Energies= -435.061915
Sum of electronic and thermal Enthalpies= -435.052481
Sum of electronic and thermal Free Energies= -435.097590

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.707467	-1.405230	-0.812934
2	7	0	2.429421	-0.355624	-0.454129

3	7	0	2.206220	0.815777	-0.149184
4	6	0	1.154370	1.016434	0.905977
5	1	0	1.494777	0.543591	1.833964
6	1	0	1.128299	2.096105	1.053751
7	6	0	-0.194747	0.484463	0.486054
8	6	0	-1.046132	1.259038	-0.316764
9	6	0	-0.592379	-0.809303	0.853773
10	6	0	-2.275601	0.749938	-0.741515
11	1	0	-0.742477	2.261810	-0.607191
12	6	0	-1.823315	-1.320633	0.429349
13	1	0	0.059722	-1.414553	1.478747
14	6	0	-2.666611	-0.541907	-0.369047
15	1	0	-2.929100	1.359903	-1.359078
16	1	0	-2.122443	-2.322702	0.723911
17	1	0	-3.624035	-0.936801	-0.697339

N_2CO_2Et Pseudo-Endo S

HF = -1489.4230025 hartrees
Zero-point correction= 0.409244 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.345768
Sum of electronic and zero-point Energies= -1489.013759
Sum of electronic and thermal Enthalpies= -1488.982989
Sum of electronic and thermal Free Energies= -1489.077235

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.194297	-0.036866	-1.087507
2	6	0	2.116805	0.939535	-0.673396
3	6	0	3.238377	0.532459	0.061204
4	6	0	3.414658	-0.817814	0.397050
5	6	0	2.448743	-1.764148	0.032716
6	6	0	1.321501	-1.379715	-0.704984
7	1	0	0.354251	0.252297	-1.707339
8	1	0	3.959714	1.269120	0.394923
9	1	0	2.576225	-2.797079	0.338355
10	6	0	1.897011	2.393913	-0.931980
11	6	0	0.671520	3.038095	-0.572083
12	6	0	2.928123	3.180029	-1.462434
13	6	0	0.531469	4.426062	-0.758377
14	6	0	2.772131	4.556349	-1.652560

15	1	0	3.862806	2.701098	-1.740044
16	6	0	1.572050	5.180423	-1.298691
17	1	0	-0.401573	4.901836	-0.472554
18	1	0	3.586188	5.136740	-2.076999
19	1	0	1.446644	6.249673	-1.441528
20	6	0	0.297065	-2.398560	-1.082628
21	6	0	-1.076519	-2.294959	-0.704531
22	6	0	0.708586	-3.520878	-1.816367
23	6	0	-1.972540	-3.306662	-1.111069
24	6	0	-0.193234	-4.510432	-2.212838
25	1	0	1.755433	-3.604454	-2.094289
26	6	0	-1.542330	-4.395174	-1.865698
27	1	0	-3.014765	-3.229223	-0.821685
28	1	0	0.155955	-5.360670	-2.791448
29	1	0	-2.255826	-5.154886	-2.171221
30	6	0	-1.555866	-1.185890	0.076935
31	6	0	-1.593728	0.014790	0.451462
32	6	0	-0.381115	2.241074	-0.032343
33	6	0	-1.044837	1.262085	0.278844
34	6	0	4.597071	-1.288016	1.173909
35	8	0	4.786653	-2.450579	1.501900
36	8	0	5.450175	-0.293236	1.480742
37	6	0	6.625530	-0.664081	2.236208
38	1	0	7.175334	0.264858	2.387768
39	1	0	6.339044	-1.099748	3.196951
40	1	0	7.230400	-1.379278	1.672651
41	7	0	-3.114341	-2.106628	1.499517
42	7	0	-3.381513	-1.124282	2.040702
43	6	0	-3.143149	0.193432	2.096639
44	6	0	-4.147453	1.113483	1.521598
45	8	0	-4.071607	2.323374	1.665122
46	8	0	-5.067461	0.477805	0.784467
47	6	0	-6.041218	1.308519	0.080814
48	1	0	-5.495747	1.987793	-0.580878
49	1	0	-6.585590	1.901608	0.821662
50	6	0	-6.952364	0.374244	-0.685036
51	1	0	-7.699387	0.964586	-1.226196
52	1	0	-6.386189	-0.216788	-1.412121
53	1	0	-7.475860	-0.307167	-0.006667
54	1	0	-2.581671	0.529366	2.962148

TSC

HF = -1489.4251436 hartrees
Zero-point correction= 0.409310 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.347612
Sum of electronic and zero-point Energies= -1489.015833
Sum of electronic and thermal Enthalpies= -1488.985223
Sum of electronic and thermal Free Energies= -1489.077532

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.317070	-0.377615	-1.683264
2	6	0	-1.634080	-0.220686	-1.219795
3	6	0	-2.021574	1.025122	-0.709345
4	6	0	-1.103110	2.083731	-0.650733
5	6	0	0.219404	1.891372	-1.070413
6	6	0	0.628639	0.651194	-1.574873
7	1	0	-0.011803	-1.325811	-2.110291
8	1	0	-3.028604	1.162097	-0.332765
9	1	0	0.931323	2.704055	-0.974008
10	6	0	-2.594178	-1.364421	-1.183266
11	6	0	-2.261815	-2.590924	-0.526785
12	6	0	-3.876786	-1.229222	-1.728658
13	6	0	-3.214989	-3.622860	-0.451923
14	6	0	-4.812263	-2.266126	-1.655369
15	1	0	-4.139328	-0.300438	-2.227312
16	6	0	-4.480278	-3.464526	-1.016425
17	1	0	-2.952059	-4.544816	0.057435
18	1	0	-5.795829	-2.136140	-2.097423
19	1	0	-5.204099	-4.271801	-0.954243
20	6	0	2.057437	0.435373	-1.954628
21	6	0	2.883878	-0.502442	-1.267916
22	6	0	2.624013	1.206125	-2.978815
23	6	0	4.234417	-0.636755	-1.648007
24	6	0	3.960294	1.050565	-3.355659
25	1	0	1.997542	1.929820	-3.492836
26	6	0	4.765035	0.120152	-2.690289
27	1	0	4.862845	-1.337285	-1.107153
28	1	0	4.368849	1.653467	-4.161375
29	1	0	5.806264	-0.006065	-2.972434
30	6	0	2.356164	-1.274758	-0.176210
31	6	0	1.478214	-1.958370	0.410668
32	6	0	-0.960543	-2.715352	0.045368
33	6	0	0.207727	-2.470232	0.311435

34	6	0	-1.472045	3.416949	-0.095908
35	8	0	-0.736116	4.393056	-0.103105
36	8	0	-2.712852	3.440163	0.425608
37	6	0	-3.153972	4.700423	0.978921
38	1	0	-4.166881	4.518576	1.338220
39	1	0	-2.504378	5.002860	1.804395
40	1	0	-3.155056	5.475679	0.208215
41	7	0	3.820221	-0.872915	1.490227
42	7	0	3.213755	-1.372714	2.336376
43	6	0	2.073918	-2.016254	2.621832
44	6	0	0.939098	-1.231799	3.157820
45	8	0	-0.061598	-1.771937	3.601327
46	8	0	1.102226	0.086997	3.000642
47	6	0	-0.055602	0.933985	3.278624
48	1	0	-0.308658	0.836365	4.338522
49	1	0	-0.894172	0.566035	2.680491
50	6	0	0.329519	2.349017	2.906655
51	1	0	-0.525143	3.011336	3.079730
52	1	0	1.168901	2.701870	3.514472
53	1	0	0.605563	2.411970	1.850536
54	1	0	2.176892	-3.048603	2.937575

N_2CO_2Et Pseudo-Exo R

HF = -1489.4195728 hartrees
Zero-point correction= 0.409269 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.346066
Sum of electronic and zero-point Energies= -1489.010304
Sum of electronic and thermal Enthalpies= -1488.979568
Sum of electronic and thermal Free Energies= -1489.073507

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.406822	0.182642	-1.161944
2	6	0	2.618927	0.515709	-0.535141
3	6	0	3.285614	-0.474541	0.198548
4	6	0	2.731816	-1.757498	0.324784
5	6	0	1.486904	-2.047196	-0.250433
6	6	0	0.807426	-1.072698	-0.990147
7	1	0	0.905008	0.919739	-1.777496
8	1	0	4.220636	-0.239896	0.693846
9	1	0	1.050342	-3.029946	-0.107323
10	6	0	3.162469	1.906336	-0.574193
11	6	0	2.362043	3.029457	-0.190657

12	6	0	4.500348	2.132467	-0.921300
13	6	0	2.928912	4.317577	-0.180562
14	6	0	5.048248	3.418930	-0.915837
15	1	0	5.116209	1.286024	-1.211955
16	6	0	4.260284	4.512992	-0.545911
17	1	0	2.313005	5.159457	0.120366
18	1	0	6.086170	3.563514	-1.201294
19	1	0	4.680777	5.514273	-0.537967
20	6	0	-0.526880	-1.364493	-1.596722
21	6	0	-1.708406	-0.666340	-1.210574
22	6	0	-0.621467	-2.352000	-2.587121
23	6	0	-2.916563	-0.950410	-1.875351
24	6	0	-1.831181	-2.632235	-3.227039
25	1	0	0.278137	-2.891287	-2.870590
26	6	0	-2.978658	-1.914610	-2.879546
27	1	0	-3.811120	-0.404269	-1.600729
28	1	0	-1.872004	-3.396153	-3.998032
29	1	0	-3.922677	-2.110163	-3.379710
30	6	0	-1.667323	0.323207	-0.151314
31	6	0	-1.113404	1.342363	0.339297
32	6	0	1.004965	2.796840	0.183562
33	6	0	-0.069116	2.223131	0.316012
34	6	0	3.412625	-2.835839	1.096860
35	8	0	2.957322	-3.959358	1.257046
36	8	0	4.596247	-2.447150	1.606229
37	6	0	5.321395	-3.434205	2.374154
38	1	0	6.233814	-2.933352	2.697888
39	1	0	4.732546	-3.752080	3.238580
40	1	0	5.560638	-4.300599	1.751919
41	7	0	-2.733317	0.626784	2.292675
42	7	0	-2.086495	1.575569	2.385243
43	6	0	-3.056076	-0.404693	1.490943
44	6	0	-4.461664	-0.497394	1.030270
45	8	0	-4.935483	-1.528942	0.582395
46	8	0	-5.102973	0.676352	1.104834
47	6	0	-6.481505	0.709567	0.622795
48	1	0	-6.484281	0.404882	-0.427854
49	1	0	-7.063702	-0.015812	1.198911
50	6	0	-6.985072	2.124269	0.808423
51	1	0	-6.380208	2.834187	0.235181
52	1	0	-8.019488	2.186382	0.454176
53	1	0	-6.963311	2.413408	1.864047
54	1	0	-2.571610	-1.339999	1.757438

N_2CO_2Et Pseudo-Exo S

HF = -1489.4239634 hartrees

Zero-point correction= 0.409637 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.348111
Sum of electronic and zero-point Energies= -1489.014326
Sum of electronic and thermal Enthalpies= -1488.983783
Sum of electronic and thermal Free Energies= -1489.075852

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.144030	-0.389125	1.199616
2	6	0	2.325687	0.100665	0.618220
3	6	0	2.332263	1.410067	0.118512
4	6	0	1.172335	2.197035	0.175149
5	6	0	-0.013563	1.664639	0.697152
6	6	0	-0.040196	0.360221	1.203191
7	1	0	1.136036	-1.379838	1.637890
8	1	0	3.230761	1.806953	-0.339566
9	1	0	-0.915298	2.267634	0.691201
10	6	0	3.537869	-0.758140	0.461163
11	6	0	3.468428	-2.044225	-0.164208
12	6	0	4.792994	-0.283283	0.862679
13	6	0	4.646135	-2.792415	-0.350501
14	6	0	5.953549	-1.041552	0.680328
15	1	0	4.856745	0.692165	1.336499
16	6	0	5.879251	-2.298860	0.073318
17	1	0	4.579770	-3.761862	-0.834601
18	1	0	6.910411	-0.650078	1.013199
19	1	0	6.777652	-2.891069	-0.073772
20	6	0	-1.316566	-0.210719	1.728893
21	6	0	-1.954460	-1.331534	1.124655
22	6	0	-1.931168	0.398991	2.832214
23	6	0	-3.162407	-1.806694	1.670633
24	6	0	-3.126134	-0.088177	3.365828
25	1	0	-1.450652	1.262851	3.282848
26	6	0	-3.738038	-1.203245	2.786115
27	1	0	-3.651688	-2.655510	1.204080
28	1	0	-3.573246	0.399216	4.227266
29	1	0	-4.666565	-1.594102	3.191803
30	6	0	-1.381412	-1.969698	-0.044413
31	6	0	-0.376592	-2.448806	-0.630510
32	6	0	2.194512	-2.524055	-0.590509
33	6	0	0.976220	-2.607413	-0.693925
34	6	0	1.139360	3.593384	-0.345159
35	8	0	0.145731	4.306316	-0.337416
36	8	0	2.327847	4.000967	-0.826913

37	6	0	2.380690	5.346100	-1.353739
38	1	0	3.407190	5.481742	-1.694487
39	1	0	1.683099	5.455776	-2.188072
40	1	0	2.138045	6.070684	-0.571993
41	7	0	-2.296553	-2.659544	-2.470052
42	7	0	-1.265598	-3.114161	-2.702941
43	6	0	-3.010016	-1.952959	-1.579065
44	1	0	-3.862719	-2.463557	-1.145288
45	6	0	-3.067962	-0.495778	-1.861854
46	8	0	-2.390770	0.075522	-2.700884
47	8	0	-3.902263	0.099160	-1.003501
48	6	0	-3.906546	1.561031	-1.001405
49	1	0	-2.872088	1.904988	-0.913825
50	1	0	-4.308828	1.902342	-1.959858
51	6	0	-4.755847	2.003859	0.169621
52	1	0	-4.336105	1.643912	1.113822
53	1	0	-4.784512	3.098396	0.196895
54	1	0	-5.781825	1.633687	0.074620

TSA

HF = -1050.8598628 hartrees

Zero-point correction= 0.334021 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.275747

Sum of electronic and zero-point Energies= -1050.525842

Sum of electronic and thermal Enthalpies= -1050.502670

Sum of electronic and thermal Free Energies= -1050.584116

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.932712	4.440809	0.737110
2	6	0	-0.281355	3.207582	0.784672
3	6	0	-0.728674	2.136867	-0.017503
4	6	0	-1.839131	2.331503	-0.862679
5	6	0	-2.479649	3.569677	-0.908692
6	6	0	-2.032345	4.627332	-0.108226
7	1	0	-0.580574	5.256685	1.362011
8	1	0	0.571794	3.062099	1.440233
9	1	0	-2.187292	1.509354	-1.479197
10	1	0	-3.330687	3.708263	-1.569491
11	1	0	-2.536813	5.588629	-0.142642
12	6	0	-0.017582	0.883878	0.026168
13	6	0	1.032857	0.193938	0.035432
14	6	0	2.377268	-0.054249	-0.016985
15	6	0	3.575645	-0.296868	-0.055471

16	6	0	4.973402	-0.567586	-0.103721
17	6	0	5.439006	-1.889259	-0.281182
18	6	0	5.912299	0.479650	0.025554
19	6	0	6.807943	-2.150527	-0.328529
20	1	0	4.720952	-2.697445	-0.380700
21	6	0	7.278952	0.206625	-0.020769
22	1	0	5.559437	1.497443	0.160740
23	6	0	7.731364	-1.106354	-0.198138
24	1	0	7.155019	-3.170623	-0.466162
25	1	0	7.992431	1.019501	0.080355
26	1	0	8.796859	-1.314527	-0.234598
27	7	0	-0.888738	-1.575887	0.250564
28	7	0	-1.593507	-0.541137	0.135567
29	7	0	0.227008	-1.914826	0.177705
30	6	0	-2.797220	-0.392809	0.987646
31	1	0	-3.008212	0.677735	0.970244
32	1	0	-2.559750	-0.683727	2.016378
33	6	0	-3.975241	-1.175368	0.450706
34	6	0	-4.188392	-2.498663	0.861067
35	6	0	-4.845340	-0.600236	-0.486046
36	6	0	-5.255352	-3.238152	0.341951
37	1	0	-3.516871	-2.949295	1.588004
38	6	0	-5.912891	-1.337594	-1.006396
39	1	0	-4.686135	0.426660	-0.805415
40	6	0	-6.119138	-2.658847	-0.594075
41	1	0	-5.412927	-4.262312	0.668695
42	1	0	-6.583450	-0.881520	-1.729533
43	1	0	-6.949413	-3.232049	-0.997146

TSB-Pseudo Exo

HF = -1508.6327564 hartrees
Zero-point correction= 0.436674 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.372246
Sum of electronic and zero-point Energies= -1508.196082
Sum of electronic and thermal Enthalpies= -1508.165427
Sum of electronic and thermal Free Energies= -1508.260510

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.993064	-0.187600	1.124206
2	6	0	3.171032	-0.301659	0.366020
3	6	0	3.594698	0.804846	-0.382368
4	6	0	2.839040	1.986402	-0.392695
5	6	0	1.632904	2.055352	0.315979
6	6	0	1.192325	0.962564	1.072924
7	1	0	1.683272	-1.011986	1.755070
8	1	0	4.497898	0.737635	-0.977533
9	1	0	1.036673	2.959956	0.262511
10	6	0	3.939736	-1.580167	0.285790
11	6	0	3.306494	-2.814977	-0.063626
12	6	0	5.327610	-1.578121	0.476475
13	6	0	4.081753	-3.981520	-0.201831
14	6	0	6.084195	-2.746716	0.346761
15	1	0	5.818981	-0.646452	0.742158
16	6	0	5.459890	-3.950527	0.006498
17	1	0	3.588200	-4.908988	-0.475379
18	1	0	7.157028	-2.714557	0.513133
19	1	0	6.042852	-4.860763	-0.098327
20	6	0	-0.102657	1.043443	1.813661
21	6	0	-1.184558	0.144375	1.576725
22	6	0	-0.274958	2.061653	2.762977
23	6	0	-2.368961	0.283257	2.328865
24	6	0	-1.456700	2.189799	3.495677
25	1	0	0.544098	2.753989	2.935907
26	6	0	-2.503849	1.288353	3.283284
27	1	0	-3.184714	-0.407605	2.145431
28	1	0	-1.554161	2.983411	4.230691
29	1	0	-3.425293	1.370585	3.852264
30	6	0	-1.068299	-0.897385	0.587096
31	6	0	-0.461194	-1.808822	-0.026860
32	6	0	1.893665	-2.822736	-0.261684
33	6	0	0.726763	-2.454464	-0.230050

34	6	0	3.259757	3.184127	-1.174675
35	8	0	2.623881	4.227124	-1.230138
36	8	0	4.426574	3.003825	-1.820230
37	6	0	4.906292	4.118989	-2.605198
38	1	0	5.846892	3.781065	-3.040145
39	1	0	4.188696	4.367502	-3.391470
40	1	0	5.071410	4.990990	-1.967007
41	7	0	-3.037108	-0.912240	-0.378270
42	7	0	-2.774495	-1.794182	-1.227338
43	7	0	-1.982892	-2.593935	-1.528865
44	6	0	-3.733973	0.321407	-0.821815
45	1	0	-3.485962	1.058610	-0.056533
46	1	0	-3.316772	0.656939	-1.776731
47	6	0	-5.231429	0.128554	-0.908386
48	6	0	-5.814258	-0.346620	-2.091493
49	6	0	-6.048319	0.391577	0.199827
50	6	0	-7.194016	-0.558383	-2.165695
51	1	0	-5.185593	-0.550801	-2.955048
52	6	0	-7.428623	0.181304	0.127873
53	1	0	-5.601580	0.763503	1.118470
54	6	0	-8.003833	-0.295719	-1.055008
55	1	0	-7.635963	-0.924690	-3.088153
56	1	0	-8.053216	0.391816	0.991664
57	1	0	-9.076459	-0.458773	-1.112258

TSB

HF = -1508.6335045 hartrees

Zero-point correction= 0.436586 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.373202

Sum of electronic and zero-point Energies= -1508.196919

Sum of electronic and thermal Enthalpies= -1508.166291

Sum of electronic and thermal Free Energies= -1508.260303

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.441537	-0.008798	-1.061301
2	6	0	-2.349106	-0.994500	-0.635705
3	6	0	-3.500751	-0.592728	0.053821
4	6	0	-3.722108	0.763177	0.334994
5	6	0	-2.771898	1.721709	-0.038286
6	6	0	-1.614508	1.343030	-0.731027
7	1	0	-0.576979	-0.297560	-1.646924
8	1	0	-4.210552	-1.336868	0.395491
9	1	0	-2.934348	2.760791	0.227183
10	6	0	-2.085513	-2.451870	-0.830782
11	6	0	-0.859683	-3.052678	-0.402946
12	6	0	-3.077758	-3.283105	-1.366279
13	6	0	-0.680204	-4.442685	-0.529767
14	6	0	-2.883289	-4.661593	-1.495945
15	1	0	-4.012627	-2.838437	-1.695171
16	6	0	-1.683058	-5.242633	-1.075590
17	1	0	0.252761	-4.884300	-0.193368
18	1	0	-3.668046	-5.277486	-1.925488
19	1	0	-1.528273	-6.313218	-1.171530
20	6	0	-0.608342	2.380586	-1.110295
21	6	0	0.751517	2.343204	-0.674579
22	6	0	-1.030419	3.462319	-1.897118
23	6	0	1.624185	3.376763	-1.073243
24	6	0	-0.151162	4.474790	-2.286557
25	1	0	-2.067040	3.496469	-2.219947
26	6	0	1.184358	4.425248	-1.877739
27	1	0	2.654391	3.347037	-0.737698
28	1	0	-0.507736	5.292279	-2.906438
29	1	0	1.880126	5.204276	-2.175416
30	6	0	1.236477	1.267898	0.152450
31	6	0	1.267436	0.075666	0.540972
32	6	0	0.153024	-2.207903	0.139546
33	6	0	0.774598	-1.198049	0.440387
34	6	0	-4.936775	1.228340	1.063762

35	8	0	-5.172792	2.397811	1.331150
36	8	0	-5.762007	0.219999	1.401386
37	6	0	-6.964803	0.585246	2.115223
38	1	0	-7.485560	-0.354074	2.301629
39	1	0	-6.713309	1.076745	3.058695
40	1	0	-7.582063	1.250581	1.505864
41	7	0	2.802545	2.203936	1.515482
42	7	0	3.078951	1.205222	2.047243
43	7	0	2.724549	0.012106	2.189389
44	6	0	3.760300	-1.049683	2.234031
45	1	0	4.251202	-1.014791	3.212019
46	1	0	3.185834	-1.976884	2.178989
47	6	0	4.760525	-0.947982	1.105599
48	6	0	4.455692	-1.466039	-0.161600
49	6	0	5.978080	-0.280090	1.296874
50	6	0	5.356255	-1.322663	-1.220105
51	1	0	3.509426	-1.976900	-0.316819
52	6	0	6.881055	-0.135510	0.238419
53	1	0	6.219813	0.125888	2.276234
54	6	0	6.571193	-0.656251	-1.022106
55	1	0	5.110836	-1.729969	-2.197044
56	1	0	7.823339	0.381107	0.398780
57	1	0	7.272187	-0.545313	-1.844775

TSD

HF = -1864.0352728 hartrees

Zero-point correction= 0.492933 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.424285

Sum of electronic and zero-point Energies= -1863.542340

Sum of electronic and thermal Enthalpies= -1863.506944

Sum of electronic and thermal Free Energies= -1863.610988

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.977053	-1.411899	-1.471278
2	6	0	2.206409	-1.721142	-0.869113
3	6	0	2.215700	-2.623066	0.202688
4	6	0	1.015534	-3.178735	0.672324
5	6	0	-0.207748	-2.806434	0.098827
6	6	0	-0.234815	-1.905582	-0.970736
7	1	0	0.954821	-0.758128	-2.335082
8	1	0	3.151325	-2.871335	0.689987
9	1	0	-1.130453	-3.209799	0.501864
10	6	0	3.467714	-1.050503	-1.301777
11	6	0	3.548688	0.373160	-1.412218
12	6	0	4.625149	-1.799100	-1.547443
13	6	0	4.765709	0.982748	-1.766306
14	6	0	5.827921	-1.182606	-1.906147
15	1	0	4.577848	-2.881180	-1.465476
16	6	0	5.898466	0.209352	-2.016526
17	1	0	4.810932	2.065112	-1.835656
18	1	0	6.706488	-1.790800	-2.100630
19	1	0	6.831519	0.691365	-2.292556
20	6	0	-1.518849	-1.462723	-1.587059
21	6	0	-1.918761	-0.094560	-1.573491
22	6	0	-2.336684	-2.389473	-2.243832
23	6	0	-3.085079	0.298721	-2.260688
24	6	0	-3.502118	-1.990477	-2.903552
25	1	0	-2.037942	-3.433656	-2.253741
26	6	0	-3.866159	-0.640412	-2.927069
27	1	0	-3.380285	1.341858	-2.238047
28	1	0	-4.116059	-2.731049	-3.407635
29	1	0	-4.764144	-0.321863	-3.447263
30	6	0	-1.157721	0.873557	-0.838614
31	6	0	-0.105864	1.510114	-0.542970
32	6	0	2.380239	1.137521	-1.126183
33	6	0	1.239654	1.473714	-0.853626
34	6	0	0.987006	-4.141725	1.810862

35	8	0	-0.034457	-4.635736	2.266304
36	8	0	2.212396	-4.419519	2.291038
37	6	0	2.273660	-5.337564	3.406328
38	1	0	3.333149	-5.429453	3.645353
39	1	0	1.722628	-4.934973	4.260213
40	1	0	1.859070	-6.308686	3.123445
41	6	0	-0.370808	2.803652	1.041330
42	6	0	-2.574002	1.581289	0.862433
43	6	0	-3.808282	0.775765	0.697503
44	6	0	-3.814124	-0.566045	1.104282
45	6	0	-4.973098	-1.315634	0.913951
46	1	0	-2.928410	-1.005212	1.548733
47	6	0	-5.978032	0.642217	-0.041824
48	6	0	-6.081697	-0.702054	0.329659
49	1	0	-5.005155	-2.359567	1.210379
50	1	0	-6.821304	1.152335	-0.501649
51	1	0	-7.005056	-1.246142	0.158507
52	6	0	0.930112	3.534005	1.130964
53	6	0	1.116872	4.738230	0.440981
54	6	0	2.363598	5.359084	0.515753
55	1	0	0.307701	5.170465	-0.135822
56	6	0	3.087879	3.551022	1.915143
57	6	0	3.372813	4.757272	1.268059
58	1	0	2.541696	6.293692	-0.007658
59	1	0	3.850761	3.047612	2.504460
60	1	0	4.359203	5.202346	1.351554
61	7	0	-1.750936	1.235576	1.925240
62	7	0	-0.644283	1.865764	2.041496
63	7	0	-2.573909	2.909012	0.476893
64	7	0	-1.465043	3.542091	0.590831
65	7	0	-4.869326	1.371721	0.126071
66	7	0	1.897802	2.942832	1.848637

Pseudo-Endo S

HF = -1489.5165663 hartrees
Zero-point correction= 0.414052 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.351188
Sum of electronic and zero-point Energies= -1489.102514
Sum of electronic and thermal Enthalpies= -1489.072876
Sum of electronic and thermal Free Energies= -1489.165378

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.245217	-0.051405	-1.370931
2	6	0	2.151801	0.888171	-0.860699
3	6	0	3.131484	0.459445	0.039951
4	6	0	3.159091	-0.881224	0.460442
5	6	0	2.172146	-1.778009	0.024870
6	6	0	1.200007	-1.359903	-0.889646
7	1	0	0.512402	0.261548	-2.105861
8	1	0	3.839918	1.171077	0.448425
9	1	0	2.167383	-2.793064	0.407654
10	6	0	1.912151	2.332536	-1.124950
11	6	0	0.625763	2.878660	-0.820096
12	6	0	2.912249	3.191303	-1.588919
13	6	0	0.388144	4.252099	-1.005231
14	6	0	2.660760	4.554663	-1.776862
15	1	0	3.893494	2.783172	-1.813696
16	6	0	1.398854	5.083515	-1.488232
17	1	0	-0.588897	4.657779	-0.762050
18	1	0	3.450260	5.200960	-2.149175
19	1	0	1.203036	6.141725	-1.632884
20	6	0	0.106108	-2.258549	-1.365088
21	6	0	-1.206257	-2.218437	-0.831991
22	6	0	0.394935	-3.158944	-2.402043
23	6	0	-2.178123	-3.087975	-1.372207
24	6	0	-0.580541	-4.005799	-2.929026
25	1	0	1.406271	-3.185861	-2.797507
26	6	0	-1.878158	-3.963084	-2.413509
27	1	0	-3.183934	-3.070238	-0.964902
28	1	0	-0.328272	-4.690269	-3.733736
29	1	0	-2.652620	-4.611338	-2.812803
30	6	0	-1.658390	-1.402240	0.321186
31	6	0	-1.612592	-0.083045	0.697824
32	6	0	-0.369146	2.005024	-0.282717
33	6	0	-0.984297	1.041112	0.144395

34	6	0	4.186335	-1.384033	1.416524
35	8	0	4.233840	-2.532084	1.834272
36	8	0	5.071341	-0.436668	1.778273
37	6	0	6.101865	-0.841530	2.707903
38	1	0	6.701452	0.052304	2.880029
39	1	0	5.655679	-1.188814	3.643368
40	1	0	6.714735	-1.636042	2.274126
41	7	0	-2.447973	-2.113648	1.291163
42	7	0	-2.874801	-1.366997	2.209515
43	6	0	-2.404490	0.009928	1.977388
44	6	0	-3.602105	0.969373	1.919170
45	8	0	-3.783896	1.870129	2.713326
46	8	0	-4.395191	0.671967	0.891929
47	6	0	-5.590618	1.496191	0.706793
48	1	0	-5.269495	2.533893	0.578118
49	1	0	-6.196659	1.424032	1.614468
50	6	0	-6.313070	0.963455	-0.510795
51	1	0	-7.215590	1.559768	-0.681657
52	1	0	-5.681118	1.029632	-1.402227
53	1	0	-6.610752	-0.079812	-0.364822
54	1	0	-1.781365	0.309527	2.826953

C (Pseudo-Endo R)

HF = -1489.5195017 hartrees
Zero-point correction= 0.414524 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.354936
Sum of electronic and zero-point Energies= -1489.104978
Sum of electronic and thermal Enthalpies= -1489.075701
Sum of electronic and thermal Free Energies= -1489.164565

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.168025	-1.432903	-1.361060
2	6	0	-1.511779	-1.105050	-1.133586
3	6	0	-1.929186	0.212912	-1.338985
4	6	0	-0.996882	1.190724	-1.725996
5	6	0	0.362373	0.864539	-1.841202
6	6	0	0.784956	-0.453652	-1.642296
7	1	0	0.158706	-2.457565	-1.221552
8	1	0	-2.961441	0.488905	-1.155751
9	1	0	1.081362	1.645530	-2.064605
10	6	0	-2.381438	-2.103283	-0.453169
11	6	0	-1.949627	-2.626265	0.806148

12	6	0	-3.623601	-2.499065	-0.954865
13	6	0	-2.765403	-3.535133	1.501619
14	6	0	-4.423662	-3.409949	-0.255912
15	1	0	-3.960208	-2.096738	-1.906046
16	6	0	-3.992824	-3.930119	0.968311
17	1	0	-2.432821	-3.919280	2.460809
18	1	0	-5.381384	-3.712430	-0.669318
19	1	0	-4.613596	-4.636662	1.511032
20	6	0	2.227330	-0.843684	-1.647028
21	6	0	2.998367	-0.860062	-0.458907
22	6	0	2.828121	-1.223851	-2.855690
23	6	0	4.352884	-1.242144	-0.533797
24	6	0	4.166824	-1.615632	-2.910761
25	1	0	2.230460	-1.206309	-3.762577
26	6	0	4.932087	-1.626326	-1.741598
27	1	0	4.951135	-1.239091	0.372169
28	1	0	4.607966	-1.905883	-3.859948
29	1	0	5.975331	-1.926792	-1.768631
30	6	0	2.514107	-0.414569	0.867790
31	6	0	1.455877	-0.719872	1.683713
32	6	0	-0.712872	-2.147081	1.341062
33	6	0	0.336161	-1.546853	1.513152
34	6	0	-1.395676	2.607401	-1.959101
35	8	0	-0.656434	3.461420	-2.426761
36	8	0	-2.665985	2.859450	-1.592670
37	6	0	-3.137553	4.210952	-1.794991
38	1	0	-4.167438	4.212756	-1.437884
39	1	0	-2.532063	4.915921	-1.220024
40	1	0	-3.100045	4.472263	-2.855759
41	7	0	3.350591	0.534605	1.550104
42	7	0	2.881921	0.866060	2.671410
43	6	0	1.626844	0.144536	2.912462
44	6	0	0.426570	1.092864	3.070241
45	8	0	-0.467484	0.900777	3.869620
46	8	0	0.476382	2.082411	2.183126
47	6	0	-0.670957	2.989680	2.120596
48	1	0	-0.887834	3.343265	3.131998
49	1	0	-1.526894	2.414144	1.754783
50	6	0	-0.295194	4.118390	1.186566
51	1	0	-1.148438	4.797111	1.083890
52	1	0	0.552709	4.686528	1.582087
53	1	0	-0.032538	3.741759	0.194681
54	1	0	1.720669	-0.433593	3.837237

TSC Pseudo-Exo R

HF = -1489.5116077 hartrees

Zero-point correction= 0.414168 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.352369

Sum of electronic and zero-point Energies= -1489.097440

Sum of electronic and thermal Enthalpies= -1489.067869

Sum of electronic and thermal Free Energies= -1489.159239

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.428831	0.364938	1.299651
2	6	0	-2.640962	0.517400	0.614028
3	6	0	-3.209696	-0.601603	-0.001883
4	6	0	-2.535744	-1.834963	0.024397
5	6	0	-1.266107	-1.935706	0.614344
6	6	0	-0.702503	-0.825678	1.249432
7	1	0	-0.999146	1.217024	1.814203
8	1	0	-4.145300	-0.505674	-0.540971
9	1	0	-0.728330	-2.876652	0.565636
10	6	0	-3.158674	1.894265	0.388679
11	6	0	-2.286012	2.863087	-0.198958
12	6	0	-4.475249	2.263539	0.677561
13	6	0	-2.756892	4.162407	-0.452665
14	6	0	-4.931286	3.561168	0.421744
15	1	0	-5.143918	1.528509	1.116468
16	6	0	-4.071327	4.510471	-0.138459
17	1	0	-2.088806	4.888586	-0.905048
18	1	0	-5.955956	3.828785	0.662751
19	1	0	-4.423541	5.518419	-0.336313
20	6	0	0.666079	-0.820688	1.848693
21	6	0	1.794658	-0.341026	1.135971
22	6	0	0.819807	-1.230451	3.180827
23	6	0	3.030462	-0.264872	1.810598
24	6	0	2.053750	-1.158458	3.828744
25	1	0	-0.051397	-1.601373	3.713185
26	6	0	3.160819	-0.656848	3.141769
27	1	0	3.896932	0.133931	1.296091
28	1	0	2.144768	-1.480844	4.861832
29	1	0	4.124996	-0.573054	3.634240
30	6	0	1.778141	-0.004761	-0.310099
31	6	0	1.090307	0.896523	-1.075089
32	6	0	-0.965678	2.447125	-0.566477
33	6	0	0.044806	1.801756	-0.783843
34	6	0	-3.104261	-3.053992	-0.618223

35	8	0	-2.533616	-4.134238	-0.669620
36	8	0	-4.327222	-2.846924	-1.140132
37	6	0	-4.951512	-3.979988	-1.785566
38	1	0	-5.915237	-3.614357	-2.139967
39	1	0	-4.341267	-4.324659	-2.624395
40	1	0	-5.090903	-4.795481	-1.071118
41	7	0	2.337652	-0.137821	-2.607581
42	7	0	1.488052	0.774278	-2.458529
43	6	0	2.625830	-0.763331	-1.302832
44	6	0	4.146924	-0.772521	-1.094425
45	8	0	4.810458	-1.785157	-1.006374
46	8	0	4.623675	0.471007	-1.043618
47	6	0	6.067618	0.627734	-0.860830
48	1	0	6.353031	0.102189	0.055254
49	1	0	6.569264	0.153411	-1.709146
50	6	0	6.346224	2.112310	-0.782326
51	1	0	5.819792	2.565539	0.063768
52	1	0	7.421388	2.268528	-0.644819
53	1	0	6.037990	2.618462	-1.702566
54	1	0	2.305197	-1.811016	-1.356931

TSC Pseudo-Exo S

HF = -1489.5145255 hartrees
Zero-point correction= 0.414206 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.352782
Sum of electronic and zero-point Energies= -1489.100320
Sum of electronic and thermal Enthalpies= -1489.070813
Sum of electronic and thermal Free Energies= -1489.161743

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.273848	-0.513186	1.262641
2	6	0	2.392884	0.174754	0.774808
3	6	0	2.252720	1.519510	0.417420
4	6	0	0.994525	2.140455	0.499686
5	6	0	-0.134386	1.400808	0.882084
6	6	0	0.002757	0.061545	1.257329
7	1	0	1.379483	-1.545242	1.577517
8	1	0	3.104503	2.068214	0.032077
9	1	0	-1.110511	1.873809	0.871135
10	6	0	3.623046	-0.601022	0.459135
11	6	0	3.510627	-1.746730	-0.389383
12	6	0	4.889831	-0.222811	0.912679
13	6	0	4.662231	-2.475901	-0.732290
14	6	0	6.028030	-0.958751	0.566154
15	1	0	4.980461	0.651071	1.551517
16	6	0	5.913306	-2.086337	-0.252489
17	1	0	4.567506	-3.339363	-1.383296
18	1	0	7.001274	-0.651414	0.937644
19	1	0	6.795913	-2.658612	-0.522087
20	6	0	-1.161930	-0.806099	1.602109
21	6	0	-1.769710	-1.649315	0.639845
22	6	0	-1.645509	-0.810353	2.918151
23	6	0	-2.841863	-2.471783	1.043799
24	6	0	-2.701213	-1.638227	3.303359
25	1	0	-1.177551	-0.153740	3.646040
26	6	0	-3.295271	-2.481111	2.360713
27	1	0	-3.317342	-3.116768	0.311527
28	1	0	-3.054451	-1.624900	4.330271
29	1	0	-4.114753	-3.134834	2.644113
30	6	0	-1.439078	-1.662653	-0.802699
31	6	0	-0.320790	-1.909377	-1.550504
32	6	0	2.219743	-2.077551	-0.912147
33	6	0	1.038278	-2.085797	-1.210996

34	6	0	0.795798	3.570813	0.130122
35	8	0	-0.277601	4.153254	0.191257
36	8	0	1.930171	4.167372	-0.279667
37	6	0	1.822878	5.556217	-0.666487
38	1	0	2.828702	5.849599	-0.967126
39	1	0	1.126693	5.665377	-1.502089
40	1	0	1.484010	6.161978	0.178090
41	7	0	-1.875336	-1.621546	-3.128114
42	7	0	-0.661797	-1.898818	-2.957216
43	6	0	-2.518627	-1.407767	-1.832176
44	1	0	-3.377028	-2.084815	-1.747062
45	6	0	-3.015433	0.044451	-1.703870
46	8	0	-2.547066	0.984202	-2.311314
47	8	0	-3.976064	0.115411	-0.784211
48	6	0	-4.431004	1.453615	-0.399342
49	1	0	-3.549962	2.057995	-0.166112
50	1	0	-4.944495	1.896791	-1.257393
51	6	0	-5.342394	1.284258	0.795970
52	1	0	-4.805900	0.825833	1.632614
53	1	0	-5.704285	2.268119	1.112851
54	1	0	-6.207622	0.661611	0.546830

B (BnN_3 pseudo-Endo)

HF = -1508.7686577 hartrees

Zero-point correction= 0.442549 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.380803

Sum of electronic and zero-point Energies= -1508.326109

Sum of electronic and thermal Enthalpies= -1508.296816

Sum of electronic and thermal Free Energies= -1508.387855

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.507984	-0.039415	-1.389417
2	6	0	-1.936044	-1.287358	-0.914477
3	6	0	-2.911473	-1.327817	0.086303
4	6	0	-3.401892	-0.131465	0.637001
5	6	0	-2.878146	1.103091	0.224462
6	6	0	-1.916889	1.152687	-0.790384
7	1	0	-0.787720	0.003298	-2.198650
8	1	0	-3.255079	-2.282267	0.468449
9	1	0	-3.221310	2.014314	0.702799
10	6	0	-1.200541	-2.508878	-1.339662
11	6	0	0.221025	-2.536072	-1.192496
12	6	0	-1.846743	-3.652085	-1.818755
13	6	0	0.939332	-3.691716	-1.544552
14	6	0	-1.121140	-4.796296	-2.167188
15	1	0	-2.927390	-3.639122	-1.928192
16	6	0	0.270684	-4.814812	-2.032842
17	1	0	2.018153	-3.701234	-1.424149
18	1	0	-1.643549	-5.669994	-2.545882
19	1	0	0.834550	-5.702188	-2.304521
20	6	0	-1.300726	2.431728	-1.255994
21	6	0	-0.025330	2.870302	-0.822804
22	6	0	-2.009530	3.204760	-2.189058
23	6	0	0.489912	4.068456	-1.358520
24	6	0	-1.485140	4.389669	-2.706557
25	1	0	-2.988630	2.860783	-2.510343
26	6	0	-0.222755	4.819617	-2.291351
27	1	0	1.466065	4.409357	-1.029029
28	1	0	-2.055686	4.966480	-3.428825
29	1	0	0.206418	5.735263	-2.687752
30	6	0	0.798357	2.237153	0.240626
31	6	0	1.300820	0.945693	0.481146
32	6	0	0.864116	-1.385688	-0.637708
33	6	0	1.122104	-0.310195	-0.128603
34	6	0	-4.441722	-0.127477	1.704975

35	8	0	-4.868227	0.882039	2.246896
36	8	0	-4.874623	-1.363568	2.016907
37	6	0	-5.884580	-1.449851	3.047567
38	1	0	-6.099742	-2.513436	3.151314
39	1	0	-5.504498	-1.042767	3.988166
40	1	0	-6.783333	-0.905217	2.746636
41	7	0	1.313017	3.049758	1.214032
42	7	0	2.075459	2.359809	2.023542
43	7	0	2.076797	1.090947	1.601184
44	6	0	2.867329	0.067560	2.291077
45	1	0	3.147762	0.514460	3.247846
46	1	0	2.215286	-0.786956	2.485985
47	6	0	4.089397	-0.353282	1.498095
48	6	0	4.338420	-1.709068	1.255156
49	6	0	4.986513	0.608719	1.012118
50	6	0	5.474548	-2.102801	0.539899
51	1	0	3.638414	-2.456899	1.618802
52	6	0	6.117141	0.217346	0.291439
53	1	0	4.795339	1.663553	1.192770
54	6	0	6.364950	-1.140352	0.054961
55	1	0	5.657317	-3.157860	0.355660
56	1	0	6.804922	0.970099	-0.083689
57	1	0	7.244523	-1.443935	-0.505869

BnN3 Pseudo-exo

HF = -1508.7673096 hartrees

Zero-point correction= 0.442683 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.381461

Sum of electronic and zero-point Energies= -1508.324627

Sum of electronic and thermal Enthalpies= -1508.295375

Sum of electronic and thermal Free Energies= -1508.385848

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.776789	-0.410669	1.242513
2	6	0	3.018205	-0.318057	0.600146
3	6	0	3.411803	0.918159	0.078049
4	6	0	2.544191	2.021482	0.154295
5	6	0	1.260719	1.877484	0.704128
6	6	0	0.869389	0.650441	1.245554
7	1	0	1.477415	-1.353924	1.685041
8	1	0	4.366127	1.013275	-0.427169
9	1	0	0.578664	2.721051	0.694354
10	6	0	3.775391	-1.570959	0.332491

11	6	0	3.107157	-2.650837	-0.324888
12	6	0	5.127091	-1.714526	0.659606
13	6	0	3.811272	-3.834034	-0.606742
14	6	0	5.816287	-2.897300	0.371726
15	1	0	5.638622	-0.893599	1.154107
16	6	0	5.156907	-3.957490	-0.257332
17	1	0	3.298103	-4.647053	-1.110818
18	1	0	6.864214	-2.989634	0.641984
19	1	0	5.689112	-4.877467	-0.480461
20	6	0	-0.494939	0.375684	1.787749
21	6	0	-1.486171	-0.259786	1.001494
22	6	0	-0.769827	0.654802	3.133774
23	6	0	-2.701236	-0.631715	1.605305
24	6	0	-1.990590	0.303058	3.713789
25	1	0	-0.005538	1.143359	3.731295
26	6	0	-2.954059	-0.357904	2.949015
27	1	0	-3.453621	-1.138689	1.011433
28	1	0	-2.178972	0.530645	4.759008
29	1	0	-3.900362	-0.656511	3.390001
30	6	0	-1.351669	-0.489630	-0.459694
31	6	0	-0.528440	-1.270238	-1.287338
32	6	0	1.745752	-2.462917	-0.731666
33	6	0	0.652031	-1.994224	-0.991903
34	6	0	2.920100	3.354812	-0.396030
35	8	0	2.183196	4.330803	-0.397651
36	8	0	4.169114	3.380468	-0.896176
37	6	0	4.609623	4.635410	-1.462676
38	1	0	5.628517	4.454788	-1.805216
39	1	0	3.969018	4.919620	-2.301647
40	1	0	4.594969	5.422189	-0.703943
41	7	0	-2.223182	0.082706	-1.342889
42	7	0	-1.972903	-0.309933	-2.608390
43	7	0	-0.959001	-1.125888	-2.583799
44	6	0	-3.293601	1.056939	-1.104575
45	1	0	-2.988476	1.684906	-0.266033
46	1	0	-3.324599	1.681857	-2.001345
47	6	0	-4.651808	0.433167	-0.839589
48	6	0	-5.073159	-0.724355	-1.506939
49	6	0	-5.513081	1.045006	0.080336
50	6	0	-6.337598	-1.264007	-1.252233
51	1	0	-4.414240	-1.210190	-2.220425
52	6	0	-6.780831	0.510991	0.328967
53	1	0	-5.185976	1.934247	0.613344
54	6	0	-7.195673	-0.648169	-0.334897
55	1	0	-6.651113	-2.165050	-1.772125
56	1	0	-7.437480	0.993551	1.047608
57	1	0	-8.177402	-1.069431	-0.137457

D

HF = -1864.095677 hartrees
Zero-point correction= 0.495567 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.428617
Sum of electronic and zero-point Energies= -1863.600110
Sum of electronic and thermal Enthalpies= -1863.565360
Sum of electronic and thermal Free Energies= -1863.667060

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.925522	-1.821887	-1.553779
2	6	0	2.122450	-1.936848	-0.836212
3	6	0	2.069318	-2.353909	0.497176
4	6	0	0.825208	-2.591613	1.107243
5	6	0	-0.365567	-2.343243	0.407250
6	6	0	-0.317573	-1.943697	-0.930104
7	1	0	0.959153	-1.507169	-2.591144
8	1	0	2.981452	-2.432905	1.077457
9	1	0	-1.314458	-2.441807	0.922776
10	6	0	3.351618	-1.351834	-1.439371
11	6	0	3.308944	0.019407	-1.848249
12	6	0	4.548213	-2.059168	-1.577926
13	6	0	4.455921	0.616693	-2.397468
14	6	0	5.682990	-1.451659	-2.127310
15	1	0	4.586281	-3.097406	-1.260652
16	6	0	5.634661	-0.117154	-2.540926
17	1	0	4.417530	1.659472	-2.696772
18	1	0	6.601058	-2.022273	-2.233366
19	1	0	6.514237	0.354892	-2.968470
20	6	0	-1.503947	-1.480571	-1.710203
21	6	0	-1.942615	-0.138209	-1.616927
22	6	0	-2.119576	-2.339303	-2.631584
23	6	0	-2.978296	0.300288	-2.461057
24	6	0	-3.155202	-1.893511	-3.454957
25	1	0	-1.772890	-3.366497	-2.701174
26	6	0	-3.577473	-0.563794	-3.376930
27	1	0	-3.318256	1.328062	-2.387009
28	1	0	-3.621822	-2.578063	-4.157473
29	1	0	-4.373208	-0.199659	-4.020123
30	6	0	-1.413262	0.818634	-0.604166
31	6	0	-0.176999	1.371357	-0.473593
32	6	0	2.108583	0.760802	-1.598247
33	6	0	1.008888	1.094270	-1.189435

34	6	0	0.716250	-3.022087	2.529591
35	8	0	-0.342790	-3.210831	3.111471
36	8	0	1.914503	-3.187259	3.119468
37	6	0	1.897551	-3.586814	4.508373
38	1	0	2.945425	-3.660463	4.799469
39	1	0	1.384503	-2.835129	5.113835
40	1	0	1.400370	-4.553890	4.621041
41	6	0	-0.079022	2.301024	0.727757
42	6	0	-2.342302	1.302135	0.496798
43	6	0	-3.747746	0.750008	0.530691
44	6	0	-3.980995	-0.514992	1.080255
45	6	0	-5.277441	-1.027333	1.045093
46	1	0	-3.167419	-1.083400	1.516240
47	6	0	-5.955921	0.996989	-0.045010
48	6	0	-6.289822	-0.257025	0.471131
49	1	0	-5.489641	-2.009244	1.457258
50	1	0	-6.716253	1.626984	-0.500779
51	1	0	-7.313377	-0.614366	0.420518
52	6	0	1.259573	2.945694	0.980275
53	6	0	1.518304	4.266575	0.606650
54	6	0	2.804395	4.771266	0.811606
55	1	0	0.739677	4.877333	0.164809
56	6	0	3.410864	2.636324	1.720060
57	6	0	3.772728	3.942648	1.377935
58	1	0	3.042037	5.792807	0.530261
59	1	0	4.137173	1.958648	2.162562
60	1	0	4.785478	4.292265	1.551653
61	7	0	-1.619631	0.958024	1.827443
62	7	0	-0.510068	1.451541	1.939766
63	7	0	-2.316759	2.809469	0.482604
64	7	0	-1.191600	3.301440	0.594917
65	7	0	-4.711788	1.496524	-0.024419
66	7	0	2.182693	2.140111	1.526113

1,4-diphenyl-1,3-butadiyne (A) and 3,5-TPDY 5 (B)

HF = -1050.9990446 hartrees

Zero-point correction= 0.340369 (Hartree/Particle)

Thermal correction to Gibbs Free Energy= 0.285981

Sum of electronic and zero-point Energies= -1050.658676

Sum of electronic and thermal Enthalpies= -1050.636987

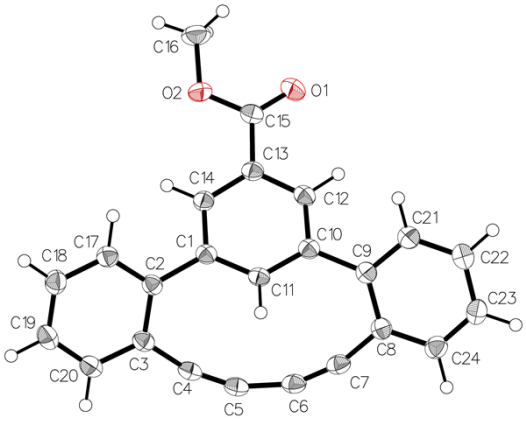
Sum of electronic and thermal Free Energies= -1050.713064

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.605460	3.265950	-0.873722
2	6	0	-0.528644	1.893173	-1.112264
3	6	0	0.525378	1.135671	-0.568470
4	6	0	1.493979	1.777577	0.223343
5	6	0	1.412834	3.151722	0.456662
6	6	0	0.365381	3.899765	-0.090453
7	1	0	-1.421013	3.840283	-1.303616
8	1	0	-1.278287	1.405916	-1.727260
9	1	0	2.295812	1.202788	0.672810
10	1	0	2.165361	3.634649	1.073322
11	1	0	0.304387	4.968477	0.094171
12	6	0	0.567020	-0.310990	-0.817683
13	6	0	-0.453635	-1.268319	-0.766441
14	6	0	-1.810075	-1.084806	-0.415846
15	6	0	-2.970532	-0.885218	-0.108146
16	6	0	-4.324264	-0.616887	0.250660
17	6	0	-5.278996	-1.654695	0.293272
18	6	0	-4.721680	0.700421	0.566203
19	6	0	-6.599944	-1.375436	0.643539
20	1	0	-4.976650	-2.668991	0.051647
21	6	0	-6.045319	0.967269	0.914831
22	1	0	-3.988034	1.500367	0.536275
23	6	0	-6.987999	-0.066991	0.954876
24	1	0	-7.327809	-2.181246	0.673937
25	1	0	-6.341376	1.984141	1.156441
26	1	0	-8.017863	0.145159	1.227307
27	7	0	1.348422	-2.337526	-1.356368
28	7	0	1.660957	-1.032022	-1.188613
29	7	0	0.078945	-2.487815	-1.100320
30	6	0	3.032208	-0.591481	-1.443082
31	1	0	2.983077	0.416290	-1.860943
32	1	0	3.421615	-1.258998	-2.216856
33	6	0	3.927784	-0.617273	-0.216416
34	6	0	3.719910	-1.514754	0.838270

35	6	0	5.009138	0.272761	-0.155087
36	6	0	4.581570	-1.519236	1.940238
37	1	0	2.885116	-2.208285	0.807480
38	6	0	5.874377	0.263350	0.942169
39	1	0	5.167772	0.982045	-0.964072
40	6	0	5.661486	-0.632807	1.995467
41	1	0	4.406715	-2.217126	2.754326
42	1	0	6.706995	0.960485	0.977914
43	1	0	6.328810	-0.637020	2.852702

X-RAY CRYSTALLOGRAPHY
3,5-TPDY



The data for **3,5-TPDY** crystalised from DCM/Et_2O, were collected from a shock-cooled single crystal at 150 K on a Bruker Venture Metaljet k-geometry diffractometer with a Metal Jet using Helios MX Mirror Optics as monochromator and a Bruker CMOS Photon III detector. The diffractometer was equipped with an Oxford Cryostream 700 low temperature device and used Ga K_α radiation ($\lambda = 1.34139$ Å). All data were integrated with *SAINT* (2020) and a multi-scan absorption correction using *SADABS* 2016/2 was applied. [6,7]The structure was solved by dual methods with *XT* and refined by full-matrix least-squares methods against F^2 using *XL*.[8,9] Structure solution and refinement cycles were performed within the graphical user interface of *OLEX2*. All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were located from difference Fourier map and refined isotropically.[10] This report and the CIF file were generated using FinalCif.[11]

Table S5. Crystal data and structure refinement for 3,5-TPDY

Empirical formula	$C_{24}H_{14}O_2$
Formula weight	334.35
Temperature [K]	150
Crystal system	monoclinic
Space group (number)	$P2_1/c$ (14)
a [Å]	3.8764(2)
b [Å]	38.1644(16)
c [Å]	10.9214(6)
α [°]	90
β [°]	99.461(2)
γ [°]	90

[6] Bruker, SAINT, (2020), Bruker AXS Inc., Madison, Wisconsin, USA.
[7] L. Krause, R. Herbst-Irmer, G. M. Sheldrick, D. Stalke, J. Appl. Cryst. 2015, 48, 3–10, doi:10.1107/S1600576714022985.
[8] G. M. Sheldrick, Acta Cryst. 2015, A71, 3–8, doi:10.1107/S2053273314026370.
[9] G. M. Sheldrick, Acta Cryst. 2015, C71, 3–8, doi:10.1107/S2053229614024218.
[10] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard & H. Puschmann, J. Appl. Cryst. 2009, 42, 339-341, doi:10.1107/S0021889808042726
[11] D. Kratzert, FinalCif, V84, https://www.xs3.uni-freiburg.de/research/finalcif.

Volume [Å^3]	1593.74(14)
Z	4
ρ_{calc} [gcm^{-3}]	1.393
μ [mm^{-1}]	0.443
F(000)	696
Crystal size [mm^3]	0.02×0.02×0.3
Crystal colour	clear light colourless
Crystal shape	Needle
Radiation	Ga K_α (λ=1.34139 Å)
2Θ range [°]	4.03 to 113.91 (0.80 Å)
Index ranges	-4 ≤ h ≤ 4 -45 ≤ k ≤ 47 -13 ≤ l ≤ 13
Reflections collected	14884
Independent reflections	3171 R_{int} = 0.0525 R_{sigma} = 0.0457
Completeness to θ = 53.594°	100.0 %
Data / Restraints / Parameters	3171 / 0 / 292
Goodness-of-fit on F^2	1.054
Final R indexes [I≥2σ(I)]	R_1 = 0.0452 wR_2 = 0.1017
Final R indexes [all data]	R_1 = 0.0737 wR_2 = 0.1134
Largest peak/hole [eÅ^{-3}]	0.25/−0.18
Extinction coefficient	0.0034(5)

Table S6. Atomic coordinates and Ueq [Å^2] for 3,5-TPDY

Atom	***x***	***y***	***z***	U_{eq}
O1	−0.0166(4)	0.72812(3)	0.62060(13)	0.0414(4)
O2	0.1030(4)	0.69897(3)	0.80075(11)	0.0342(4)
C1	0.4569(5)	0.61153(4)	0.63393(16)	0.0239(4)
C2	0.5315(5)	0.57862(4)	0.70878(16)	0.0242(4)
C3	0.4162(5)	0.54509(4)	0.66197(17)	0.0262(4)
C4	0.2508(5)	0.54262(4)	0.53539(18)	0.0278(4)
C5	0.1553(5)	0.54790(4)	0.42597(18)	0.0279(4)
C6	0.1468(5)	0.56668(5)	0.31805(17)	0.0287(4)
C7	0.2256(5)	0.59050(5)	0.25602(17)	0.0282(4)
C8	0.3617(5)	0.62283(5)	0.21693(16)	0.0261(4)
C9	0.4584(5)	0.64908(5)	0.30824(16)	0.0253(4)
C10	0.4211(5)	0.64508(4)	0.44125(16)	0.0244(4)
C11	0.5165(5)	0.61480(4)	0.51158(16)	0.0225(4)
H11	0.630(5)	0.5956(5)	0.4759(16)	0.022(5)
C12	0.2838(5)	0.67308(5)	0.49973(17)	0.0257(4)
H12	0.215(5)	0.6949(5)	0.4551(17)	0.031(5)
C13	0.2381(5)	0.67109(4)	0.62301(17)	0.0253(4)
C14	0.3186(5)	0.64009(5)	0.68907(17)	0.0252(4)
H14	0.276(5)	0.6377(4)	0.7740(17)	0.019(4)
C15	0.0928(5)	0.70227(5)	0.67809(17)	0.0283(4)
C16	−0.0152(7)	0.72892(6)	0.8629(2)	0.0415(6)
H16A	0.113(7)	0.7501(7)	0.842(2)	0.059(7)
H16B	0.055(7)	0.7247(6)	0.951(3)	0.066(8)

H16C	−0.263(9)	0.7338(7)	0.835(2)	0.071(9)
C17	0.6996(5)	0.58073(5)	0.83099(17)	0.0279(4)
H17	0.778(5)	0.6047(5)	0.8661(17)	0.031(5)
C18	0.7591(6)	0.55124(5)	0.90602(19)	0.0323(5)
H18	0.873(5)	0.5536(5)	0.9929(19)	0.033(5)
C19	0.6471(5)	0.51871(5)	0.85939(19)	0.0321(5)
H19	0.679(6)	0.4976(6)	0.9111(19)	0.041(6)
C20	0.4750(5)	0.51561(5)	0.73876(18)	0.0302(5)
H20	0.391(5)	0.4928(5)	0.7053(17)	0.026(5)
C21	0.5814(5)	0.68089(5)	0.26850(18)	0.0289(4)
H21	0.646(5)	0.6993(5)	0.3325(18)	0.034(5)
C22	0.6182(5)	0.68662(5)	0.14621(18)	0.0326(5)
H22	0.712(6)	0.7098(5)	0.1210(18)	0.036(5)
C23	0.5305(6)	0.66033(5)	0.05875(18)	0.0337(5)
H23	0.562(5)	0.6647(5)	−0.0282(19)	0.032(5)
C24	0.4019(5)	0.62883(5)	0.09401(18)	0.0312(5)
H24	0.338(6)	0.6100(5)	0.0298(19)	0.041(6)

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table S7 Bond lengths and angles for 3,5-TPDY

Atom–Atom	Length [Å]	Atom–Atom–Atom	Angle [°]
O1–C15	1.208(2)	C21–C9–C10	118.91(16)
O2–C15	1.340(2)	C11–C10–C9	123.94(16)
O2–C16	1.442(2)	C12–C10–C9	118.26(16)
C1–C2	1.501(2)	C12–C10–C11	117.81(16)
C1–C11	1.398(2)	C1–C11–C10	121.75(16)
C1–C14	1.394(2)	C1–C11–H11	118.3(10)
C2–C3	1.422(2)	C10–C11–H11	120.0(10)
C2–C17	1.388(3)	C10–C12–H12	121.2(11)
C3–C4	1.428(3)	C13–C12–C10	121.43(17)
C3–C20	1.400(3)	C13–C12–H12	117.4(11)
C4–C5	1.208(3)	C12–C13–C14	119.65(17)
C5–C6	1.375(3)	C12–C13–C15	117.78(16)
C6–C7	1.203(3)	C14–C13–C15	122.54(16)
C7–C8	1.434(3)	C1–C14–H14	118.4(10)
C8–C9	1.419(2)	C13–C14–C1	120.60(17)
C8–C24	1.396(3)	C13–C14–H14	121.0(10)
C9–C10	1.491(2)	O1–C15–O2	123.14(17)
C9–C21	1.399(3)	O1–C15–C13	124.60(17)
C10–C11	1.403(2)	O2–C15–C13	112.25(15)
C10–C12	1.394(2)	O2–C16–H16A	109.2(15)
C11–H11	0.970(18)	O2–C16–H16B	106.0(16)
C12–H12	0.98(2)	O2–C16–H16C	112.2(16)
C12–C13	1.389(3)	H16A–C16–H16B	107(2)
C13–C14	1.394(2)	H16A–C16–H16C	106(2)
C13–C15	1.486(2)	H16B–C16–H16C	116(2)
C14–H14	0.972(18)	C2–C17–H17	118.5(11)
C16–H16A	0.99(3)	C2–C17–C18	121.78(18)
C16–H16B	0.97(3)	C18–C17–H17	119.7(11)
C16–H16C	0.98(3)	C17–C18–H18	120.1(11)
C17–H17	1.02(2)	C19–C18–C17	119.86(19)
C17–C18	1.389(3)	C19–C18–H18	120.0(11)
C18–H18	0.98(2)	C18–C19–H19	121.5(12)
C18–C19	1.384(3)	C20–C19–C18	120.08(18)
C19–H19	0.98(2)	C20–C19–H19	118.3(12)
C19–C20	1.380(3)	C3–C20–H20	118.7(11)
C20–H20	0.978(19)	C19–C20–C3	120.56(18)
C21–H21	0.99(2)	C19–C20–H20	120.8(11)
C21–C22	1.384(3)	C9–C21–H21	117.1(11)
C22–H22	1.01(2)	C22–C21–C9	122.07(18)
C22–C23	1.388(3)	C22–C21–H21	120.9(11)
C23–H23	0.99(2)	C21–C22–H22	120.0(11)

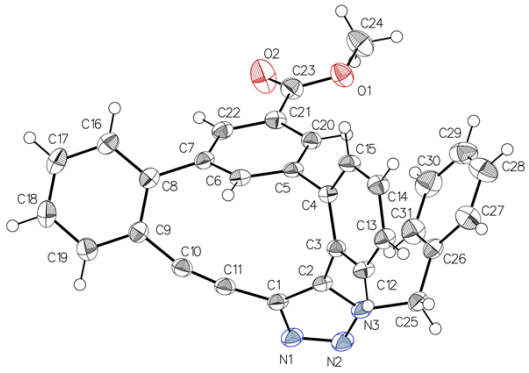
C23–C24	1.380(3)	C21–C22–C23	119.83(18)
C24–H24	1.01(2)	C23–C22–H22	120.2(11)
		C22–C23–H23	118.9(11)
Atom–Atom–Atom	**Angle [°]**	C24–C23–C22	119.75(18)
C15–O2–C16	115.89(16)	C24–C23–H23	121.3(11)
C11–C1–C2	123.21(16)	C8–C24–H24	120.0(12)
C14–C1–C2	118.18(16)	C23–C24–C8	120.91(18)
C14–C1–C11	118.60(16)	C23–C24–H24	119.1(12)
C3–C2–C1	122.43(16)		
C17–C2–C1	119.55(16)		
C17–C2–C3	117.89(16)		
C2–C3–C4	118.15(16)		
C20–C3–C2	119.82(17)		
C20–C3–C4	122.00(17)		
C5–C4–C3	164.18(19)		
C4–C5–C6	153.46(19)		
C7–C6–C5	154.71(19)		
C6–C7–C8	163.29(19)		
C9–C8–C7	117.73(16)		
C24–C8–C7	122.14(17)		
C24–C8–C9	120.13(17)		
C8–C9–C10	123.76(16)		
C21–C9–C8	117.28(17)		

Table S8. Torsion angles for 3,5-TPDY

Atom–Atom–Atom–Atom	**Torsion Angle [°]**
C1–C2–C3–C4	5.6(3)
C1–C2–C3–C20	−176.09(17)
C1–C2–C17–C18	176.77(17)
C2–C1–C11–C10	175.43(17)
C2–C1–C14–C13	−178.76(17)
C2–C3–C4–C5	23.0(8)
C2–C3–C20–C19	−0.6(3)
C2–C17–C18–C19	−0.5(3)
C3–C2–C17–C18	0.7(3)
C3–C4–C5–C6	−0.3(11)
C4–C3–C20–C19	177.61(18)
C4–C5–C6–C7	0.4(8)
C5–C6–C7–C8	−10.9(11)
C6–C7–C8–C9	−14.9(8)
C6–C7–C8–C24	164.8(6)
C7–C8–C9–C10	−1.0(3)
C7–C8–C9–C21	−178.21(17)
C7–C8–C24–C23	179.38(19)

C8–C9–C10–C11	44.6(3)
C8–C9–C10–C12	−135.56(19)
C8–C9–C21–C22	−1.8(3)
C9–C8–C24–C23	−0.9(3)
C9–C10–C11–C1	−176.08(17)
C9–C10–C12–C13	179.29(17)
C9–C21–C22–C23	0.2(3)
C10–C9–C21–C22	−179.13(18)
C10–C12–C13–C14	−2.4(3)
C10–C12–C13–C15	179.52(17)
C11–C1–C2–C3	−48.8(3)
C11–C1–C2–C17	135.40(19)
C11–C1–C14–C13	0.7(3)
C11–C10–C12–C13	−0.8(3)
C12–C10–C11–C1	4.0(3)
C12–C13–C14–C1	2.4(3)
C12–C13–C15–O1	6.7(3)
C12–C13–C15–O2	−171.90(16)
C14–C1–C2–C3	130.66(19)
C14–C1–C2–C17	−45.2(2)
C14–C1–C11–C10	−4.0(3)
C14–C13–C15–O1	−171.34(19)
C14–C13–C15–O2	10.0(3)
C15–C13–C14–C1	−179.54(17)
C16–O2–C15–O1	−2.0(3)
C16–O2–C15–C13	176.67(18)
C17–C2–C3–C4	−178.47(17)
C17–C2–C3–C20	−0.2(3)
C17–C18–C19–C20	−0.3(3)
C18–C19–C20–C3	0.9(3)
C20–C3–C4–C5	−155.2(7)
C21–C9–C10–C11	−138.25(19)
C21–C9–C10–C12	41.6(3)
C21–C22–C23–C24	1.0(3)
C22–C23–C24–C8	−0.7(3)
C24–C8–C9–C10	179.32(18)
C24–C8–C9–C21	2.1(3)

3,5-Triazole-Reg2



The data for 3,5-Triazole-Reg2, crystallised from DCM/Et_2O, were collected from a shock-cooled single crystal at 150 K on a Bruker Venture Metaljet k-geometry diffractometer with a Metal Jet using Helios MX Mirror Optics as monochromator and a Bruker CMOS Photon III detector. The diffractometer was equipped with an Oxford Cryostream 700 low temperature device and used Ga K_α radiation (λ = 1.34139 Å). All data were integrated with *SAINT* (2020) and a multi-scan absorption correction using *SADABS* 2016/2 was applied.[12,13]The structure was solved by dual methods with *XT* and refined by full-matrix least-squares methods against F^2 using *XL*.[1415] Structure solution and refinement cycles were performed within the graphical user interface of *OLEX2*. All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were located from difference Fourier map and refined isotropically.[16] This report and the CIF file were generated using FinalCif.[17]

Table S9. Crystal data and structure refinement for 3,5-Triazole-Reg2

Empirical formula	$C_{31}H_{21}N_3O_2$
Formula weight	467.51
Temperature [K]	150
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	9.1237(13)
b [Å]	10.4155(15)
c [Å]	12.6877(19)
α [°]	100.575(6)
β [°]	91.287(6)
γ [°]	93.604(6)
Volume [Å^3]	1182.2(3)
Z	2
ρ_{calc} [gcm^{-3}]	1.313
μ [mm^{-1}]	0.423

[12] Bruker, SAINT, (2020), Bruker AXS Inc., Madison, Wisconsin, USA.
[13] L. Krause, R. Herbst-Irmer, G. M. Sheldrick, D. Stalke, J. Appl. Cryst. 2015, 48, 3–10, doi:10.1107/S1600576714022985.
[14] G. M. Sheldrick, Acta Cryst. 2015, A71, 3–8, doi:10.1107/S2053273314026370.
[15] G. M. Sheldrick, Acta Cryst. 2015, C71, 3–8, doi:10.1107/S2053229614024218.
[16] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard & H. Puschmann, J. Appl. Cryst. 2009, 42, 339-341, doi:10.1107/S0021889808042726
[17] D. Kratzert, FinalCif, V84, https://www.xs3.uni-freiburg.de/research/finalcif.

$F(000)$	488
Crystal size [mm^3]	0.11×0.15×0.16
Crystal colour	clear light colourless
Crystal shape	Block
Radiation	Ga K_α (λ=1.34139 Å)
2θ range [°]	6.17 to 114.03 (0.80 Å)
Index ranges	−11 ≤ h ≤ 11 −12 ≤ k ≤ 12 −15 ≤ l ≤ 15
Reflections collected	45392
Independent reflections	4777 R_{int} = 0.0292 R_{sigma} = 0.0169
Completeness to θ = 53.594°	99.1 %
Data / Restraints / Parameters	4777 / 0 / 327
Goodness-of-fit on F^2	1.032
Final R indexes [I≥2σ(I)]	R_1 = 0.0350 wR_2 = 0.0907
Final R indexes [all data]	R_1 = 0.0385 wR_2 = 0.0930
Largest peak/hole [eÅ^{-3}]	0.25/−0.18
Extinction coefficient	0.0117(12)

Table S10. Atomic coordinates and Ueq [Å^2] for 3,5-Triazole-Reg2

Atom	***x***	***y***	***z***	U_{eq}
O1	0.15694(10)	0.53286(8)	0.95431(6)	0.0365(2)
C1	0.48365(11)	0.11700(10)	0.60471(9)	0.0260(2)
N1	0.62407(10)	0.11664(9)	0.64530(8)	0.0318(2)
O2	0.24689(14)	0.68273(9)	0.86332(8)	0.0591(3)
N2	0.62080(10)	0.05520(10)	0.72614(8)	0.0319(2)
C2	0.38860(11)	0.05039(10)	0.66364(8)	0.0235(2)
N3	0.48000(9)	0.01395(9)	0.73754(7)	0.0259(2)
C3	0.22969(11)	0.00773(10)	0.66190(8)	0.0228(2)
C4	0.11832(11)	0.09576(10)	0.68387(8)	0.0227(2)
C5	0.14799(10)	0.23858(10)	0.68437(8)	0.0232(2)
C6	0.16732(11)	0.27584(10)	0.58577(9)	0.0245(2)
H6	0.153167	0.211467	0.522211	0.029
C7	0.20701(11)	0.40531(10)	0.57716(9)	0.0255(2)
C8	0.25406(12)	0.43658(10)	0.47281(9)	0.0269(2)
C9	0.36228(12)	0.36261(10)	0.41537(9)	0.0276(2)
C10	0.42259(12)	0.26020(11)	0.46197(9)	0.0281(2)
C11	0.45392(11)	0.18791(10)	0.52139(9)	0.0273(2)
C12	0.19244(12)	−0.12662(10)	0.64908(9)	0.0269(2)
H12	0.266148	−0.186636	0.631066	0.032
C13	0.04983(12)	−0.17377(10)	0.66220(9)	0.0285(2)
H13	0.026376	−0.265338	0.653680	0.034

C14	−0.05859(11)	−0.08663(11)	0.68784(9)	0.0288(2)
H14	−0.155940	−0.118192	0.698903	0.035
C15	−0.02423(11)	0.04678(10)	0.69724(9)	0.0272(2)
H15	−0.099397	0.105802	0.713096	0.033
C16	0.20093(13)	0.54102(11)	0.43259(9)	0.0317(3)
H16	0.128221	0.590631	0.470283	0.038
C17	0.25266(15)	0.57380(11)	0.33813(10)	0.0371(3)
H17	0.215664	0.645538	0.311760	0.045
C18	0.35832(15)	0.50162(12)	0.28249(10)	0.0377(3)
H18	0.394084	0.524466	0.218175	0.045
C19	0.41235(13)	0.39599(12)	0.32016(9)	0.0333(3)
H19	0.483718	0.346281	0.280904	0.040
C20	0.15774(11)	0.33393(10)	0.77723(9)	0.0255(2)
H20	0.143731	0.310201	0.845294	0.031
C21	0.18837(11)	0.46514(10)	0.76933(9)	0.0271(2)
C22	0.21486(11)	0.49996(10)	0.66995(9)	0.0271(2)
H22	0.238401	0.589031	0.665874	0.033
C23	0.20122(13)	0.57203(11)	0.86499(10)	0.0328(3)
C24	0.16333(16)	0.63285(14)	1.04978(10)	0.0440(3)
H24A	0.098735	0.701572	1.039519	0.066
H24B	0.264491	0.670770	1.063779	0.066
H24C	0.131113	0.594138	1.110899	0.066
C25	0.44281(12)	−0.04244(11)	0.83198(9)	0.0280(2)
H25A	0.533745	−0.066436	0.865436	0.034
H25B	0.378098	−0.123238	0.809482	0.034
C26	0.36589(12)	0.05306(11)	0.91354(9)	0.0279(2)
C27	0.24242(13)	0.01146(13)	0.96249(10)	0.0374(3)
H27	0.203640	−0.076779	0.943186	0.045
C28	0.17464(15)	0.09837(15)	1.03997(11)	0.0464(3)
H28	0.090309	0.068927	1.073697	0.056
C29	0.22922(15)	0.22682(14)	1.06797(11)	0.0458(3)
H29	0.182487	0.286088	1.120540	0.055
C30	0.35220(17)	0.26875(13)	1.01914(11)	0.0469(3)
H30	0.390438	0.357165	1.038322	0.056
C31	0.42023(15)	0.18247(12)	0.94222(11)	0.0400(3)
H31	0.504758	0.212224	0.908874	0.048

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table S11. Anisotropic displacement parameters (Å^2) for 3,5-Triazole-Reg2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.0447(5)	0.0311(4)	0.0306(4)	−0.0013(3)	0.0073(4)	−0.0026(4)
C1	0.0197(5)	0.0239(5)	0.0353(6)	0.0066(4)	0.0035(4)	0.0049(4)
N1	0.0203(4)	0.0329(5)	0.0454(6)	0.0145(4)	0.0028(4)	0.0047(4)
O2	0.0997(9)	0.0281(5)	0.0439(5)	−0.0028(4)	0.0162(5)	−0.0166(5)
N2	0.0189(4)	0.0346(5)	0.0451(6)	0.0144(4)	0.0010(4)	0.0031(4)
C2	0.0201(5)	0.0210(5)	0.0297(5)	0.0042(4)	0.0014(4)	0.0056(4)
N3	0.0181(4)	0.0268(4)	0.0343(5)	0.0088(4)	0.0010(3)	0.0038(3)
C3	0.0196(5)	0.0233(5)	0.0257(5)	0.0049(4)	0.0013(4)	0.0023(4)
C4	0.0208(5)	0.0229(5)	0.0242(5)	0.0034(4)	0.0005(4)	0.0028(4)

C5	0.0155(4)	0.0227(5)	0.0318(5)	0.0050(4)	0.0017(4)	0.0040(4)
C6	0.0202(5)	0.0236(5)	0.0293(5)	0.0026(4)	−0.0002(4)	0.0044(4)
C7	0.0212(5)	0.0254(5)	0.0309(5)	0.0068(4)	0.0000(4)	0.0048(4)
C8	0.0270(5)	0.0237(5)	0.0296(5)	0.0050(4)	−0.0030(4)	−0.0001(4)
C9	0.0282(5)	0.0251(5)	0.0294(5)	0.0059(4)	−0.0016(4)	0.0000(4)
C10	0.0243(5)	0.0286(5)	0.0318(6)	0.0058(4)	0.0055(4)	0.0035(4)
C11	0.0212(5)	0.0269(5)	0.0346(6)	0.0064(4)	0.0061(4)	0.0040(4)
C12	0.0244(5)	0.0234(5)	0.0331(6)	0.0040(4)	0.0012(4)	0.0055(4)
C13	0.0278(5)	0.0216(5)	0.0354(6)	0.0048(4)	−0.0009(4)	−0.0012(4)
C14	0.0203(5)	0.0294(6)	0.0362(6)	0.0061(5)	0.0009(4)	−0.0021(4)
C15	0.0198(5)	0.0272(5)	0.0348(6)	0.0050(4)	0.0027(4)	0.0040(4)
C16	0.0352(6)	0.0251(5)	0.0347(6)	0.0054(5)	−0.0035(5)	0.0038(4)
C17	0.0490(7)	0.0272(6)	0.0366(6)	0.0113(5)	−0.0081(5)	0.0013(5)
C18	0.0496(7)	0.0348(6)	0.0302(6)	0.0116(5)	0.0001(5)	−0.0026(5)
C19	0.0363(6)	0.0326(6)	0.0312(6)	0.0066(5)	0.0026(5)	0.0003(5)
C20	0.0213(5)	0.0258(5)	0.0297(5)	0.0051(4)	0.0032(4)	0.0036(4)
C21	0.0245(5)	0.0241(5)	0.0319(6)	0.0021(4)	0.0028(4)	0.0030(4)
C22	0.0252(5)	0.0210(5)	0.0355(6)	0.0056(4)	0.0018(4)	0.0036(4)
C23	0.0351(6)	0.0268(6)	0.0352(6)	0.0025(5)	0.0044(5)	0.0003(5)
C24	0.0483(8)	0.0443(7)	0.0330(7)	−0.0073(5)	0.0060(5)	−0.0061(6)
C25	0.0255(5)	0.0275(5)	0.0332(6)	0.0107(4)	−0.0007(4)	0.0039(4)
C26	0.0254(5)	0.0295(5)	0.0293(5)	0.0072(4)	−0.0048(4)	0.0030(4)
C27	0.0317(6)	0.0392(7)	0.0383(6)	0.0013(5)	0.0017(5)	−0.0038(5)
C28	0.0331(6)	0.0602(9)	0.0409(7)	−0.0033(6)	0.0047(5)	0.0001(6)
C29	0.0462(8)	0.0492(8)	0.0379(7)	−0.0064(6)	−0.0050(6)	0.0167(6)
C30	0.0603(9)	0.0311(6)	0.0460(8)	−0.0003(5)	−0.0040(6)	0.0025(6)
C31	0.0429(7)	0.0332(6)	0.0425(7)	0.0057(5)	0.0013(5)	−0.0036(5)

Table S12. Bond lengths and angles for 3,5-Triazole-Reg2

Atom–Atom	**Length [Å]**	**Atom–Atom–Atom**	**Angle [°]**
O1–C23	1.3355(14)	C23–O1–C24	115.71(9)
O1–C24	1.4428(14)	N1–C1–C2	108.75(9)
C1–N1	1.3705(14)	N1–C1–C11	120.46(9)
C1–C2	1.3915(15)	C2–C1–C11	130.57(10)
C1–C11	1.4268(15)	N2–N1–C1	108.79(9)
N1–N2	1.3047(14)	N1–N2–N3	107.77(8)
O2–C23	1.2051(15)	C1–C2–C3	138.21(10)
N2–N3	1.3482(12)	N3–C2–C1	103.20(9)
C2–N3	1.3616(13)	N3–C2–C3	118.50(9)
C2–C3	1.4880(14)	N2–N3–C2	111.48(9)
N3–C25	1.4654(14)	N2–N3–C25	118.77(9)
C3–C4	1.4096(14)	C2–N3–C25	128.99(9)
C3–C12	1.3979(15)	C4–C3–C2	123.24(9)
C4–C5	1.4939(14)	C12–C3–C2	117.38(9)
C4–C15	1.3924(14)	C12–C3–C4	119.01(9)
C5–C6	1.3879(15)	C3–C4–C5	121.21(9)
C5–C20	1.3918(15)	C15–C4–C3	119.05(9)
C6–H6	0.9500	C15–C4–C5	119.56(9)

C6–C7	1.3986(15)	C6–C5–C4	117.05(9)
C7–C8	1.4864(15)	C6–C5–C20	119.26(9)
C7–C22	1.3873(15)	C20–C5–C4	123.70(9)
C8–C9	1.4218(15)	C5–C6–H6	119.0
C8–C16	1.3920(15)	C5–C6–C7	121.98(10)
C9–C10	1.4425(15)	C7–C6–H6	119.0
C9–C19	1.3956(16)	C6–C7–C8	120.06(9)
C10–C11	1.2011(16)	C22–C7–C6	118.21(10)
C12–H12	0.9500	C22–C7–C8	121.43(10)
C12–C13	1.3862(15)	C9–C8–C7	119.20(9)
C13–H13	0.9500	C16–C8–C7	121.72(10)
C13–C14	1.3882(15)	C16–C8–C9	118.98(10)
C14–H14	0.9500	C8–C9–C10	118.03(10)
C14–C15	1.3877(15)	C19–C9–C8	119.40(10)
C15–H15	0.9500	C19–C9–C10	122.46(10)
C16–H16	0.9500	C11–C10–C9	164.25(11)
C16–C17	1.3896(17)	C10–C11–C1	171.22(11)
C17–H17	0.9500	C3–C12–H12	119.4
C17–C18	1.3856(19)	C13–C12–C3	121.14(9)
C18–H18	0.9500	C13–C12–H12	119.4
C18–C19	1.3901(17)	C12–C13–H13	120.1
C19–H19	0.9500	C12–C13–C14	119.72(10)
C20–H20	0.9500	C14–C13–H13	120.1
C20–C21	1.3997(15)	C13–C14–H14	120.1
C21–C22	1.3965(16)	C15–C14–C13	119.75(10)
C21–C23	1.4858(16)	C15–C14–H14	120.1
C22–H22	0.9500	C4–C15–H15	119.4
C24–H24A	0.9800	C14–C15–C4	121.25(9)
C24–H24B	0.9800	C14–C15–H15	119.4
C24–H24C	0.9800	C8–C16–H16	119.5
C25–H25A	0.9900	C17–C16–C8	120.99(11)
C25–H25B	0.9900	C17–C16–H16	119.5
C25–C26	1.5151(15)	C16–C17–H17	120.1
C26–C27	1.3825(16)	C18–C17–C16	119.84(11)
C26–C31	1.3867(17)	C18–C17–H17	120.1
C27–H27	0.9500	C17–C18–H18	119.8
C27–C28	1.3925(18)	C17–C18–C19	120.44(11)
C28–H28	0.9500	C19–C18–H18	119.8
C28–C29	1.378(2)	C9–C19–H19	119.8
C29–H29	0.9500	C18–C19–C9	120.33(11)
C29–C30	1.379(2)	C18–C19–H19	119.8
C30–H30	0.9500	C5–C20–H20	120.3
C30–C31	1.3859(19)	C5–C20–C21	119.34(10)
C31–H31	0.9500	C21–C20–H20	120.3
		C20–C21–C23	122.31(10)

		C22–C21–C20	120.56(10)
		C22–C21–C23	117.07(10)
		C7–C22–C21	120.42(10)
		C7–C22–H22	119.8
		C21–C22–H22	119.8
		O1–C23–C21	112.91(10)
		O2–C23–O1	122.93(11)
		O2–C23–C21	124.16(11)
		O1–C24–H24A	109.5
		O1–C24–H24B	109.5
		O1–C24–H24C	109.5
		H24A–C24–H24B	109.5
		H24A–C24–H24C	109.5
		H24B–C24–H24C	109.5
		N3–C25–H25A	109.4
		N3–C25–H25B	109.4
		N3–C25–C26	111.37(9)
		H25A–C25–H25B	108.0
		C26–C25–H25A	109.4
		C26–C25–H25B	109.4
		C27–C26–C25	120.36(10)
		C27–C26–C31	119.02(11)
		C31–C26–C25	120.60(10)
		C26–C27–H27	119.9
		C26–C27–C28	120.28(12)
		C28–C27–H27	119.9
		C27–C28–H28	119.8
		C29–C28–C27	120.36(13)
		C29–C28–H28	119.8
		C28–C29–H29	120.2
		C28–C29–C30	119.53(12)
		C30–C29–H29	120.2
		C29–C30–H30	119.9
		C29–C30–C31	120.29(13)
		C31–C30–H30	119.9
		C26–C31–H31	119.7
		C30–C31–C26	120.52(12)
		C30–C31–H31	119.7

Table S13. Torsion angles for 3,5-Triazole-Reg2

Atom–Atom–Atom–Atom	**Torsion Angle [°]**	**Atom–Atom–Atom–Atom**	**Torsion Angle [°]**
C1–N1–N2–N3	0.88(12)	C11–C1–C2–C3	9.6(2)

C1–C2–N3–N2	0.36(11)	C12–C3–C4–C5	−172.05(10)
C1–C2–N3–C25	170.10(10)	C12–C3–C4–C15	3.03(15)
C1–C2–C3–C4	−67.96(17)	C12–C13–C14–C15	1.76(17)
C1–C2–C3–C12	119.09(14)	C13–C14–C15–C4	−1.51(17)
N1–C1–C2–N3	0.18(11)	C15–C4–C5–C6	−102.93(11)
N1–C1–C2–C3	−175.92(11)	C15–C4–C5–C20	77.42(13)
N1–N2–N3–C2	−0.79(12)	C16–C8–C9–C10	176.11(10)
N1–N2–N3–C25	−171.71(9)	C16–C8–C9–C19	−0.17(16)
N2–N3–C25–C26	104.40(11)	C16–C17–C18–C19	0.41(19)
C2–C1–N1–N2	−0.67(12)	C17–C18–C19–C9	−0.94(18)
C2–N3–C25–C26	−64.71(14)	C19–C9–C10–C11	168.0(4)
C2–C3–C4–C5	15.10(15)	C20–C5–C6–C7	4.78(15)
C2–C3–C4–C15	−169.82(10)	C20–C21–C22–C7	1.86(16)
C2–C3–C12–C13	170.45(10)	C20–C21–C23–O1	−10.47(16)
N3–C2–C3–C4	116.36(11)	C20–C21–C23–O2	169.37(12)
N3–C2–C3–C12	−56.59(13)	C22–C7–C8–C9	124.37(11)
N3–C25–C26–C27	135.15(11)	C22–C7–C8–C16	−52.04(15)
N3–C25–C26–C31	−46.48(14)	C22–C21–C23–O1	172.36(10)
C3–C2–N3–N2	177.41(9)	C22–C21–C23–O2	−7.80(18)
C3–C2–N3–C25	−12.85(16)	C23–C21–C22–C7	179.08(10)
C3–C4–C5–C6	72.12(13)	C24–O1–C23–O2	1.56(18)
C3–C4–C5–C20	−107.53(12)	C24–O1–C23–C21	−178.59(10)
C3–C4–C15–C14	−0.91(16)	C25–C26–C27–C28	177.92(11)
C3–C12–C13–C14	0.42(17)	C25–C26–C31–C30	−178.10(11)
C4–C3–C12–C13	−2.82(16)	C26–C27–C28–C29	0.5(2)
C4–C5–C6–C7	−174.88(9)	C27–C26–C31–C30	0.28(19)
C4–C5–C20–C21	178.96(9)	C27–C28–C29–C30	−0.4(2)
C5–C4–C15–C14	174.25(10)	C28–C29–C30–C31	0.2(2)
C5–C6–C7–C8	168.36(9)	C29–C30–C31–C26	−0.1(2)
C5–C6–C7–C22	−5.46(15)	C31–C26–C27–C28	−0.47(18)
C5–C20–C21–C22	−2.58(15)		
C5–C20–C21–C23	−179.65(10)		
C6–C5–C20–C21	−0.69(15)		
C6–C7–C8–C9	−49.24(14)		
C6–C7–C8–C16	134.35(11)		
C6–C7–C22–C21	2.08(15)		
C7–C8–C9–C10	−0.41(15)		
C7–C8–C9–C19	−176.68(10)		
C7–C8–C16–C17	176.08(10)		
C8–C7–C22–C21	−171.65(10)		
C8–C9–C10–C11	−8.1(5)		
C8–C9–C19–C18	0.81(17)		
C8–C16–C17–C18	0.23(18)		
C9–C8–C16–C17	−0.35(16)		
C10–C9–C19–C18	−175.30(11)		

C11–C1–N1–N2	174.51(10)		
C11–C1–C2–N3	−174.35(11)		

Table S14. Hydrogen bonds for 3,5-Triazole-Reg2

D–H···A [Å]	**d(D–H) [Å]**	**d(H···A) [Å]**	**d(D···A) [Å]**	**<(DHA) [°]**
C25–H25B···O2$^{\#1}$	0.99	2.49	3.3696(15)	147.2

Symmetry transformations used to generate equivalent atoms:
#1: +X, -1+Y, +Z;