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Photocontrol of catalysis in CuAAC reactions by air stable Cu(I) complexes of phenylazopyrazole-incorporated ligands

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S1. General methods:

Reagents and solvents: All the reagents (AR or LR grade) and solvents were purchased from commercially available sources such as Sigma Aldrich, Merck, Avra, Rankem, Spectrochem, and TCI, etc., and used without further purification. For reactions under anhydrous condition, oven dried glasswares have been used under inert atmosphere (N_2 or Ar). Dry solvents such as acetonitrile, DCE, methanol etc. were obtained from MBraun-SPS solvent purification system. HPLC or UV spectroscopic grade solvents have been used for photoswitching and kinetics studies. For column chromatography, pre-distilled solvents have been utilized.

Chromatography: Thin layer chromatography was performed on Merck Silica gel 60 F254 TLC plates, and the plates were visualized using UV chamber (λ = 254 nm). Column chromatography was performed over (100-200 mesh) silica gel .

NMR spectroscopy: ^{1}H, ^{11}B, ^{19}F, ^{31}P and ^{13}C NMR spectra were recorded either in $CDCl_3$, [D_6]DMSO or CD_3CN in Bruker Avance-III 400 MHz spectrometer with operational frequencies 400, 128.3, 376.5, 162.1, and 100 MHz, respectively. All the spectra have been recorded with 16 scans for ^{1}H NMR and 256 scans for ^{13}C NMR. Chemical shift (δ) values are reported in parts per million (ppm) and coupling constants (J) are reported in Hz. Signals of residual solvent signals of $CHCl_3$ (7.26 ppm) and [D_5]DMSO (2.50 ppm) have been used for internal calibration in ^{1}H NMR, whereas, the spectra have been calibrated using the corresponding signals of $CDCl_3$ (77.16 ppm) and [D_5]DMSO (39.52 ppm) in ^{13}C NMR. The signal multiplicities are abbreviated as singlet (s), doublet (d), triplet (t), quartet (q), doublet of doublets (dd), doublet of triplets (dt), triplet of doublets (td), doublet of doublet of doublets (ddd), multiplet (m), septet (sep) and broad (br).

HRMS: High resolution mass spectra (HRMS) have been recorded using Waters Synapt G2-Si Q-TOF mass spectrometer. The ionization for those samples has been done using electrospray ionization (ESI) method, and the detections were done in both positive and negative modes.

M. P.: Melting points were recorded on SMP20 melting point apparatus and are uncorrected.

FT-IR studies: FT-IR spectra were recorded as a neat solid or neat liquid on a Bruker Alpha ZnSe ATR spectrometer, or as a KBr pellet on a Perkin Elmer Spectrum Two FTIR spectrometer.

UV-Vis spectroscopic studies: UV-Vis spectroscopic studies in the solution state have been carried out using an Agilent Cary 5000 UV-Vis NIR spectrophotometer or Agilent Cary 60 UV-Vis spectrophotometer at 1 nm resolution using quartz cuvettes. UV-Vis spectroscopic studies in the solid state have been carried out in the Agilent Cary 5000 UV-Vis NIR spectrophotometer using a Diffuse Reflectance Accessory (DRA) in the KBr medium.

Photoswitching studies and light sources: The analysis of photoswitching, and kinetics measurements have been carried out using an Agilent Cary 5000 UV-Vis NIR spectrophotometer or Agilent Cary 60 UV-Vis spectrophotometer or Bruker Avance-III 400 MHz NMR spectrometer. For forward isomerization step, samples were irradiated (in a quartz cuvette or quartz NMR tube) at 365 nm by using an LED light source (Convoy S2+, 365 nm, 40 mW, a handheld commercial UV light source). The reverse isomerization (*ZZ* to *EE*) has been induced by using 470 nm and 490 nm SX-20 LED light sources from Applied Photophysics. PSS has been established by irradiating the sample for a prolonged time such that no further spectral changes are observed. For estimation of PSS composition, the samples have been irradiated in a quartz tube (NMR) or cuvette (UV-Vis) using the above-mentioned light sources, and then immediately transferred to the spectrometers for measurement.

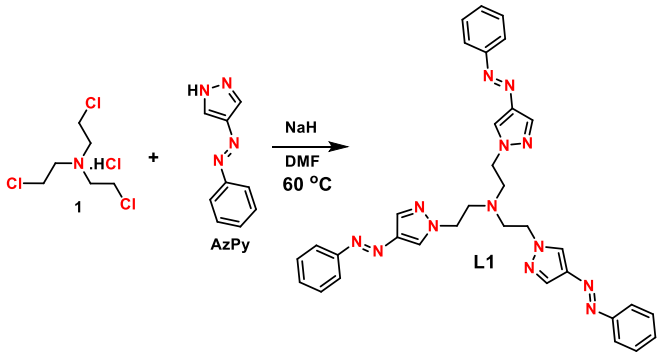
Single Crystal X-Ray Diffraction studies: Single crystal X-ray diffraction data were collected using a Rigaku XtaLAB mini diffractometer equipped with a Mercury375M CCD detector and Bruker AXS KAPPA APEX-II CCD diffractometer. (For details, see section S3).

Elemental Analysis studies: Samples for elemental analysis were analyzed using Elementar Microvario Cube with fully automated PC controlled Elemental Analyser.

S2. Synthesis:

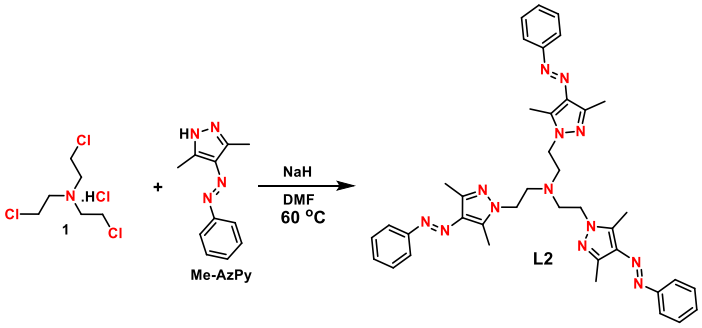
2,2',2''-Trichlorotriethylamine hydrochloride was prepared using a known procedure.[1] ***Caution*** *must be exercised while handling 2,2',2''-Trichlorotriethylamine hydrochloride since this can cause skin irritations. 2,2',2''-Trichlorotriethylamine powerful blister agent and a nitrogen mustard used for chemical warfare.*

Synthesis of tris(2-(4-((*E*)-phenyldiazenyl)-1*H*-pyrazol-1-yl)ethyl)amine (**L1**)



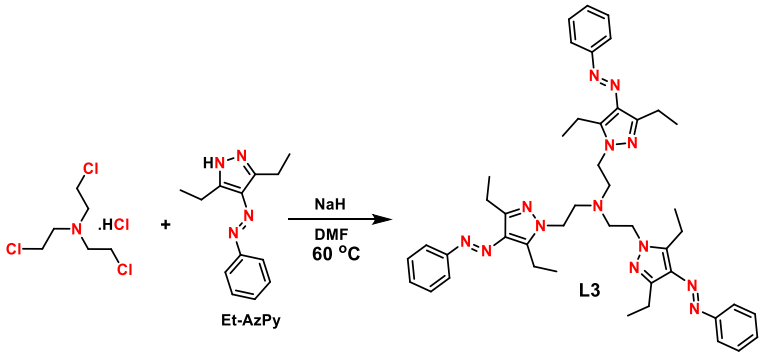
L1 was prepared according to a slightly modified version of a reported procedure.[2] A sample of phenylazopyrazole **AzPyz** (1 mmol, 172 mg) was added to 5 ml of anhydrous DMF. The mixture was stirred at rt while sodium hydride (1 mmol, 60% dispersion in mineral oil, 40 mg) was added to the mixture pinch-wise over a period of half an hour under nitrogen atmosphere. After stirring this mixture at rt for two hours, 2,2',2''-Trichlorotriethylamine hydrochloride **1** (0.25 mmole, 45 mg) was added and stirred at 60 °C for four hours. After checking TLC for completion of the reaction, the reaction mixture was quenched with water. After extracting the mixture multiple times with ethyl acetate, the combined organic layers were dried over anhydrous sodium sulfate and distilled under vacuum. The crude product was eventually purified by column chromatography over silica gel using a 2:3 mixture of hexane:ethyl acetate to give the pure product **L1**. Yellow solid, mp = 107-108 °C, Yield: 60% (91 mg), ^{1}H NMR (400 MHz, [D$_6$]DMSO): δ 3.02 (t, *J* = 5.9 Hz, 6H), 4.13 (t, *J* = 5.9 Hz, 6H), 7.42-7.44 (m, 9H), 7.63-7.66 (m, 6H), 7.98 (s, 3H), 8.25 (s ,3H) ppm; ^{13}C (100 MHz, [D$_6$]DMSO): δ 50.2, 53.0, 121.8, 128.5, 129.2, 130.2, 132.1, 140.8, 152.2 ppm; HRMS-ESI: m/z $C_{33}H_{33}N_{13}$ $[M+H]^+$ calc. 612.3060, obs. 612.3057; IR (ATR, cm^{-1}): 3130, 2942, 2828, 1537, 1432, 1392, 764, 690.

Synthesis of tris(2-(3,5-dimethyl-4-((*E*)-phenyldiazenyl)-1*H*-pyrazol-1-yl)ethyl)amine (L2)



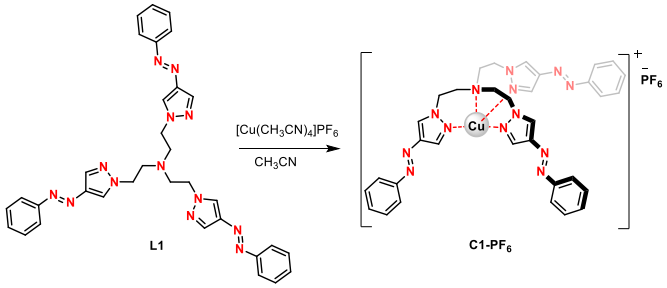
L2 was prepared in a similar procedure with phenylazo-3,5-dimethylpyrazole **Me-AzPyz.** The crude product was eventually purified by column chromatography over silica gel using a 1:1 mixture of hexane:ethyl acetate to give the pure product **L2**. Yellow sticky solid, Yield: 67% (116 mg), ^{1}H NMR (400 MHz, [D$_6$]DMSO): δ 2.37 (s, 9H), 2.50 (s, 9H; merged), 2.96 (m, 6H), 4.01 (t, 6H), 7.40-7.42 (m, 3H), 7.48 (t, *J* = 6.7 Hz ,6H), 7.68 (d, *J* =7 Hz, 6H) ppm; ^{13}C (100 MHz, [D$_6$]DMSO): δ 9.3, 14.0, 46.9, 53.2, 121.4, 129.1, 129.4, 134.4, 139.9, 140.8, 153.0 ppm; HRMS-ESI: m/z $C_{39}H_{45}N_{13}$ $[M+H]^+$ calc. 696.3999, obs. 696.4017; IR (ATR, cm^{-1}): 1539, 1469, 1355, 1161, 1026, 851.

Synthesis of tris(2-(3,5-diethyl-4-((*E*)-phenyldiazenyl)-1*H*-pyrazol-1-yl)ethyl)amine (L3)



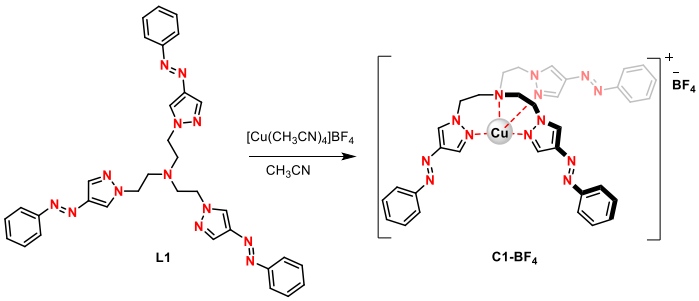
L3 was prepared in a similar procedure with phenylazo-3,5-diethylpyrazole **Et-AzPy.** The crude product was eventually purified by column chromatography over silica gel using a 3:2 mixture of hexane: ethyl acetate to give the pure product **L3**. Yellow solid, mp = 101-102 °C, Yield: 68% (132 mg), ^{1}H NMR (400 MHz, CD_3CN): δ 1.17 (t, *J* = 7.5 Hz, 18H), 2.81-2.93 (m, 12H), 3.0 (t, *J* = 6.3 Hz, 6H), 3.97 (t, *J* = 6.4 Hz, 6H), 7.39 (t, *J* = 7.2 Hz, 3H), 7.46 (t, *J* = 7.2 Hz ,6H), 7.70 (d, *J* =7.6 Hz, 6H) ppm; ^{13}C (100 MHz, [D$_6$]DMSO): δ 12.7, 13.7, 17.1, 21.1, 46. 9, 53.6, 121.3, 129.2, 129.4, 133.3, 144.4, 146.6, 153.1 ppm; HRMS-ESI: m/z $C_{45}H_{57}N_{13}$ $[M+H]^+$ calc. 780.4938, obs. 780.4927; IR (ATR, cm^{-1}): 2971, 2932, 1543, 1498, 1456, 1421, 1060, 766, 689.

Synthesis of Cu(I) complex C1-PF_6



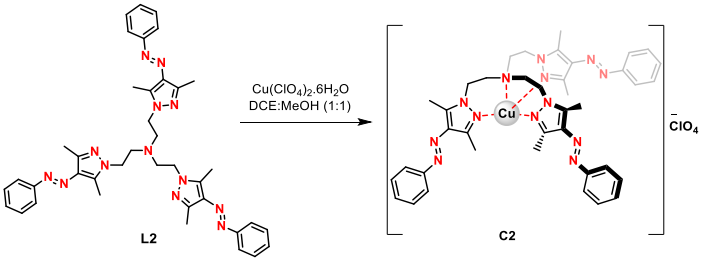
To the solution of $[Cu(CH_3CN)_4]PF_6$ (1 mmol, 373 mg) in anhydrous acetonitrile (5 ml), a solution of **L1** (1 mmol, 612 mg) in anhydrous acetonitrile was added and stirred overnight at rt. Afterwards single crystals suitable for X-ray diffraction were grown by slow evaporation of the same solution at rt. Bulk purity was verified by elemental analysis. Light orange crystals, Yield: 98% (893 mg), ^{1}H NMR (400 MHz, $[D_6]$DMSO): δ 3.15 (br, 6H), 4.38 (br, 6H), 7.54-7.56 (m, 9H), 7.76 (d, *J* =7.36 Hz ,6H), 8.29 (s , 3H), 8.75 (s, 3H) ppm; ^{13}C NMR (100 MHz, $[D_6]$DMSO): δ 48.9, 55.4, 121.9, 129.4 (2-C), 130.8, 132.5, 139.8, 152.0 ppm; ^{19}F NMR (376.5 MHz, CD_3CN) : δ −73.0 (d, *J* =706.4 Hz) ppm; ^{31}P NMR (162.1 MHz, CD_3CN) : δ −144.7 (sep, *J* = 706.8 Hz) ppm; IR (ATR, cm^{-1}): 3141, 2917, 2849, 1497, 837, 692.-ESI: *m/z* $C_{33}H_{33}CuN_{13}$ $[M\text{-}PF_6]^+$ calc. 674.2272, obs. 674.2289; Elem. Anal. Calcd. for $C_{33}H_{35}CuF_6N_{13}OP$: C, 47.28; H, 4.21; N, 21.72. Found: C, 46.93; H, 3.99; N, 21.76.

Synthesis of Cu(I) complex C1-BF_4



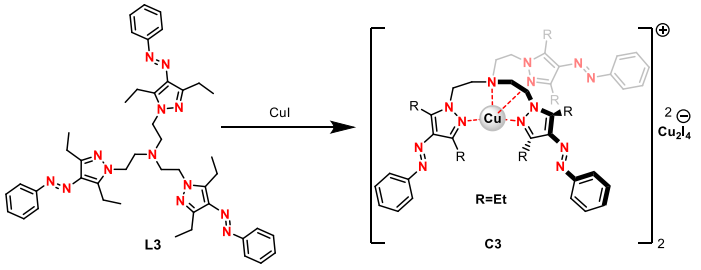
To the solution of $[Cu(CH_3CN)_4]BF_4$ (1 mmol, 315 mg) in anhydrous acetonitrile (5 ml), a solution of **L1** (1 mmol, 612 mg) in anhydrous acetonitrile was added and stirred overnight at rt. Afterwards single crystals suitable for X-ray diffraction were grown by slow evaporation of the same solution at rt. Bulk purity was verified by elemental analysis. Light orange crystals, Yield: 98% (746 mg), ^{1}H NMR (400 MHz, $[D_6]$DMSO): δ 3.14 (br, 6H), 4.38 (br, 6H), 7.51-7.57 (m, 9H), 7.76 (d, *J* = 7.12 Hz, 6H), 8.29 (s ,3H), 8.75 (s, 3H) ppm; ^{13}C NMR (100 MHz, $[D_6]$DMSO): δ 48.9, 55.5, 121.9, 129.4 (2-C), 130.9, 132.6, 139.9, 152.1 ppm; ^{19}F NMR (376.5 MHz, CD_3CN) : δ -151.8 ($^{10}BF_4^-$), -151.8 ($^{11}BF_4^-$) ppm; ^{11}B NMR (128.3 MHz, CD_3CN) : δ -1.3 ppm; IR (KBr, cm^{-1}): 3427, 1539, 1469, 1355, 1161, 1026, 851. HRMS-ESI: *m/z* $C_{33}H_{33}CuN_{13}$ $[M\text{-}BF_4]^+$ calc. 674.2272, obs. 674.2284. Elem. Anal. Calcd. for $C_{35}H_{41}BCuF_4N_{13}O_2$: C, 50.88; H, 5.0; N, 22.04. Found: C, 50.49; H, 4.69; N, 22.31.

Synthesis of Cu(I) complex C2



To the solution of $[Cu(ClO_4)_2].6H_2O$ (1 mmol, 370 mg) in anhydrous methanol (5 ml), a solution of **L2** (1 mmol, 696 mg) in anhydrous DCE was added and stirred overnight at rt. Afterwards, single crystals suitable for X-ray diffraction were grown by slow evaporation of the same solution at rt. Bulk purity was verified by elemental analysis. Light yellow crystals, Yield: 99% (850 mg), ^{1}H NMR (400 MHz, [D$_6$]DMSO): δ 2.55 (s, 9H), 2.65 (s, 9H), 3.08 (br, 6H), 4.17 (br, 6H), 7.47(t, *J* = 6.6 Hz ,3H), 7.54 (t, *J* = 5.8 Hz, 6H), 7.76 (d, *J* = 6.8 Hz, 6H) ppm; ^{13}C NMR (100 MHz, [D$_6$]DMSO): δ 9.6, 14.2, 45.2, 56.0, 121.5, 129.3, 130.2, 133.6, 140.2, 140.8, 152.7 ppm; IR (ATR, cm^{-1}): 2922, 2851, 1541, 1456, 1421, 1095. HRMS-ESI: *m/z* $C_{39}H_{45}CuN_{13}$ $[M\text{-}ClO_4]^+$ calc. 758.3217, obs. 758.3210. Elem. Anal. Calcd. for $C_{39}H_{53}ClCuN_{13}O_8$: C, 50.32; H, 5.74; N, 19.56. Found: C, 50.39; H, 5.54; N, 19.65.

Synthesis of Cu(I) complex C3



To the solution of CuI (1 mmol, 190 mg) in anhydrous acetonitrile (5 ml), a solution of **L3** (1 mmol, 780 mg) in anhydrous acetonitrile was added and stirred overnight at rt. Afterwards single crystals suitable for X-ray diffraction were grown by slow evaporation of the same solution at rt. Bulk purity was verified by elemental analysis. Light orange crystals, Yield: 41% (950 mg), ^{1}H NMR (400 MHz, CD_3CN): δ 1.04 (t, *J* = 7.24 Hz ,9H), 1.24 (t, *J* = 7.36 Hz ,9H), 3.03 (m, 12H), 3.12 (q, *J* = 7.4 Hz, 6H), 4.13 (br, 6H), 7.46 (t, *J* = 7.08 Hz, 3H), 7.53 (t, *J* = 7.04 Hz, 6H), 7.80 (d, *J* = 7.56 Hz, 6H) ppm; ^{13}C NMR (100 MHz, CD_3CN): δ 13.1, 14.0, 18.0, 22.7, 46.4, 57.6, 122.5, 130.1, 131.1, 134.0, 146.5, 147.8, 154.1 ppm; IR (ATR, cm^{-1}): 2988, 2920, 1483, 1435, 1410, 1315, 777, 680. HRMS-ESI: *m/z* $C_{45}H_{57}CuN_{13}$ $[M]^+$ calc. 842.4150, obs. 842.4127. Elem. Anal. Calcd. for $C_{94}H_{120}Cu_4I_4N_{28}$: C, 46.97; H, 5.03; N, 16.31. Found: C, 46.72; H, 4.95; N, 16.58.

S3. Crystallographic data and refinement details of complexes

Single crystal X-ray diffraction data of complexes **C1- PF_6**, **C1- BF_4** and **C2** were collected using a Rigaku XtaLAB mini diffractometer equipped with Mercury375M CCD detector. The data were collected with MoKα radiation (λ = 0.71073 Å) using omega scans. During the data collection, the detector distance was 49.9 mm (constant) and the detector was placed at 2θ = 29.85° (fixed) for all the data sets. The data collection and data reduction were done using CrysAlisPro 1.171.38.46 and all the crystal structures were solved through OLEX2[3] package using SHELXT[4] and the structures were refined using SHELXL[5]. Single crystal X-ray diffraction data of complex **C3** was collected on a Bruker *AXS KAPPA APEX-II* CCD diffractometer with MoKα radiation using omega scans. Unit cell determination and refinement and data collection were done using the Bruker APPEX-II suite[6] data reduction and integration were performed using SAINT v8.34A (Bruker, 2013)[7], and absorption corrections and scaling were done using SADABS-2014/5 (Bruker,2014/5).[8] All non-hydrogen atoms were refined anisotropically. All figures were generated using Mercury 2020.3.0.

Table S3.1.[a] Crystallographic details of complexes

Compound	**C1-PF_6**	**C1-BF_4**	**C2**	**C3**
Chemical formula	$C_{33}H_{33}CuF_6N_{13}P$	$C_{35}H_{36}BCuF_4N_{14}$	$C_{80}H_{94}Cl_4Cu_2N_{26}O_8$	$C_{45}H_{56}Cu_2I_2N_{13}$
molar mass	820.23	803.13	1816.69	1159.91
Crystal system	Trigonal	Monoclinic	Monoclinic	Monoclinic
Space group	*P*31*c*	$P2_1/n$	$P2_1/c$	*C2/c*
***T*[K]**	100.02(10)	100.10(10)	150.00(10)	296.15
***a*[Å]**	13.3299(5)	11.8020(3)	10.7720(9)	34.4407(4)
***b*[Å]**	13.3299(5)	23.0646(7)	16.1095(11)	16.5485(2)
***c*[Å]**	12.0695(4)	13.4462(5)	22.3098(16)	20.3538(3)
***α* [°]**	90	90	90.00	90
***β* [°]**	90	93.269(3)	101.158(7)	120.3538(3)
***γ* [°]**	120	90	90.00	90
***V* [$Å^3$]**	1857.26(15)	3654.2(2)	3798.3(5)	10028.3(2)
Z	2	4	4	8
***D*(calcd.) [$g \cdot cm^{-3}$]**	1.467	1.460	1.455	1.444
***μ*(Mo-K_α) [mm^{-1}]**	0 .706	0.667	0.777	1.537
Reflections collected	21255	26366	27738	38465
Independent reflections	4391	6450	6724	8861
Data/restraints/parameters	4391/1/159	6450/0/480	6724/36/492	8861/282/508
***R1, wR₂[I>2σ(I)]*[a]**	0.0509, 0.1352	0.0480, 0.1192	0.0815, 0.2162	0.0658, 0.1400
***R1, wR₂* (all data)[a]**	0.0671, 0.1487	0.0551, 0.1262	0.1113, 0.2537	0.1026, 0.1625
GOF	1.075	1.059	1.034	1.011
CCDC	2232646	2232645	2232647	2232648

[a] $R1 = \Sigma||Fo| - |Fc||/\Sigma|Fo|$. $wR2 = [\Sigma w(|Fo^2| - |Fc^2|)^2/\Sigma w|Fo^2|^2]^{1/2}$

S4. Autoreduction

The complex **C2** was prepared by adding a solution of ligand **L2** in DCE to Cu(II) precursor $Cu(ClO_4)_2.6H_2O$ in methanol in 1:1 ratio (for details see the preceding section). The green-coloured solution of $Cu(ClO_4)_2.6H_2O$ changed its colour to orange after the addition of the ligand solution signifying the change in the oxidation state. Upon leaving this solution at room temperature, yellow crystals of complex **C2** separated out. Notably, same results were achieved upon combining ligand **L2** and $Cu(ClO_4)_2.6H_2O$ in MeCN in 1:1 ratio. The ability of **L2** to carry out the spontaneous reduction has been demonstrated by UV-Vis spectroscopy (in MeCN).

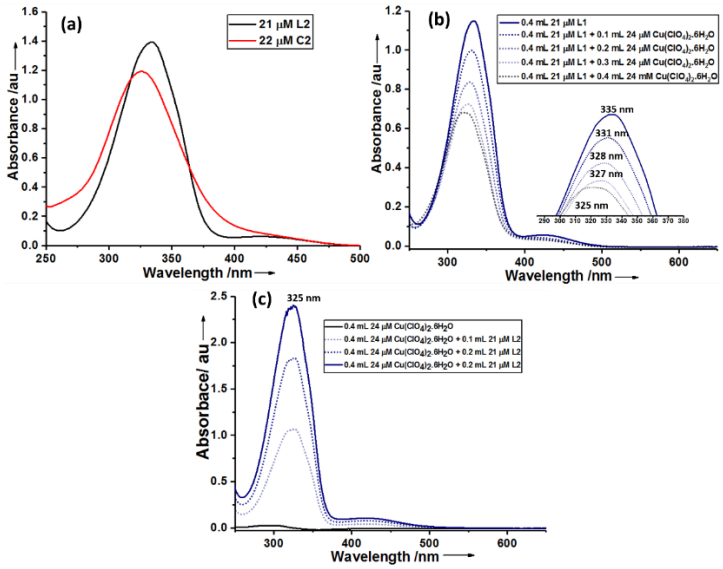
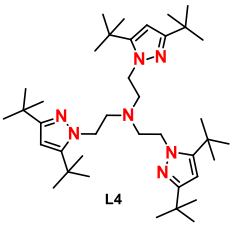


Figure S4.1. UV-Vis spectroscopic data showing (a) the difference in λ_{max} between **L2** and the Cu(I) complex **C2**; (b) Shifts observed in the λ_{max} of the ligand **L2** after gradual addition of $Cu(ClO_4)_2.6H_2O$ (a gradual addition of 24 μM solution of $Cu(ClO_4)_2.6H_2O$ to a 21 μM solution of ligand **L2** at different stoichiometric ratios showed a clear blue shift in the λ_{max} of the ligand **L2** (335 nm) towards the λ_{max} of the complex (325 nm) (c) Spectral shift due to the gradual addition of ligand **L2** to $Cu(ClO_4)_2.6H_2O$ solution (identical concentration of ligand and copper salt were used).

This phenomenon of reduction of the metal center mediated by the ligand in the absence of other external reductants is known as 'Auto-reduction'.[9] Only a limited number of ligands have been identified that facilitate the auto-reduction of Cu(II) to Cu(I) within the reaction medium, and the mechanism behind this process is still elusive.[9,12] Among the screened ligands, only **L2** has exhibited this particular phenomenon. It's worth noting that in the case of the other two ligands (**L1** and **L3**), neither the Cu(II) complex nor the Cu(I) complex could be isolated from 1:1 mixture of the ligand and $Cu(ClO_4)_2.6H_2O$ salt. One of the early reports of tris(pyrazolylethyl)amine ligands[10] by Sorrell and co-workers mentioned that their attempts at preparing Cu(II) complexes of **L4** resulted in Cu(I) complexes. However, no mechanism has been discussed for this reduction process.



To explain the reduction of Cu(II) without the presence of any external reductants, we propose two possible mechanisms based on the existing literature. According to Brotherton et al., the reduction of Cu(II) to Cu(I) can be facile in readily oxidizable alcohols (MeOH, EtOH, and iPrOH).[11] Accordingly in our case also the reduction could have been made possible by oxidation of solvent, and the resulting Cu(I) species was further stabilized by the ligand **L2**.

Alternatively, there is a possibility of *in-situ* formation of Cu(II) complex of the ligand **L2**, followed by reduction mediated by the water present in the medium. According to a recent literature,[12] the Cu(II) center coordinated to H_2O in MeCN solution that resulted in reduction to Cu(I) species. The low energy barrier required to reach the geometry of the Cu(I) complex might be a trigger for the reduction process. H_2O attached to the Cu^{2+} center was reported to undergo oxidation to $OH^{\bullet}$ radical (through a homolytic rupture of the Cu^{2+}-OH_2 bond) during this process. To detect the formation of $^{\bullet}OH$ radical species, the oxidation of ABTS (2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) to $ABTS^{+\bullet}$ was employed as an indicator. Likewise, experiments were conducted for our ligand **L2** and $Cu(ClO_4)_2.6H_2O$ salt, which behaved in a similar way; i.e. the oxidation of ABTS was followed by the appearance of bands at 415, 650 and 736 nm using UV-Vis spectroscopy, and the colour change (pale yellow to dark-green) confirmed the formation of $^{\bullet}OH$ radical (Figure S4.3).

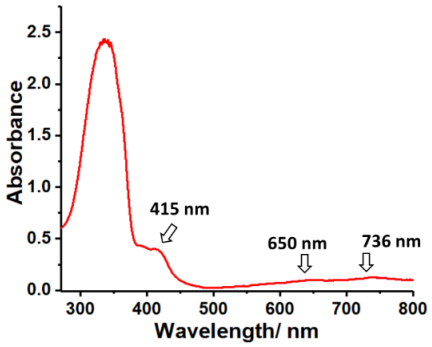


Figure S4.3. Spectral data depicting oxidation of ABTS during spontaneous reduction of Cu(II) to Cu(I) in a mixture containing 2 $x10^{-4}$ M mixture of $Cu(ClO_4)_2.6H_2O$ and **L2** in acetonitrile and 30 equivalent of H_2O.

Based on the evidences, both the literature-based mechanisms are plausible in our case. However, we are unsure of the actual mechanism of the autoreduction process; possibly, the steric constraints (containing three –N=N–Ph units) and the geometry of the ligand framework could be crucial. At this juncture, we assume the geometrical preference of symmetric tertiary amines favouring tetrahedral Cu(I) geometry could be the driving force behind the autoreduction process.

S5. Analysis of photoswitching and thermal stability aspects using UV-Vis spectroscopy in solution and solid state:

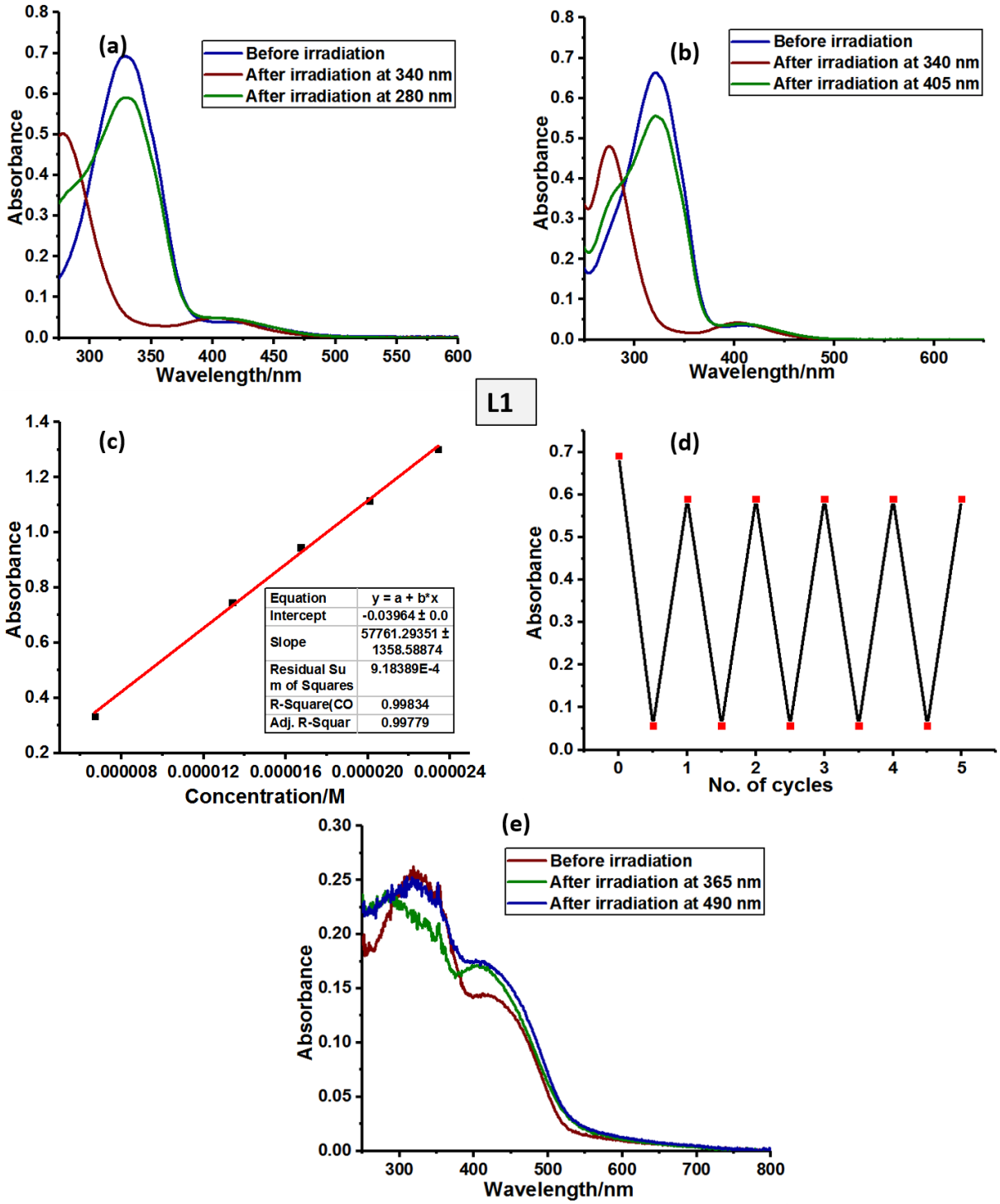


Figure S5.1. Photoswitching behaviour of **L1:** (a) Forward and reverse photoisomerization (DMSO, 12 µM) of **L1**; (b) Forward and reverse photoisomerization (MeCN, 11 µM) of **L1**; (c) Estimation of molar extinction coefficient (in DMSO) for the $\pi-\pi^*$ absorption (at λ_{max}= 330 nm); (d) Photoswitching stability test upto five cycles of **L1** in DMSO (forward isomerization step: 340 nm; reverse isomerization step: 280 nm); (e) Forward and reverse photoisomerization (in KBr medium) of **L1**.

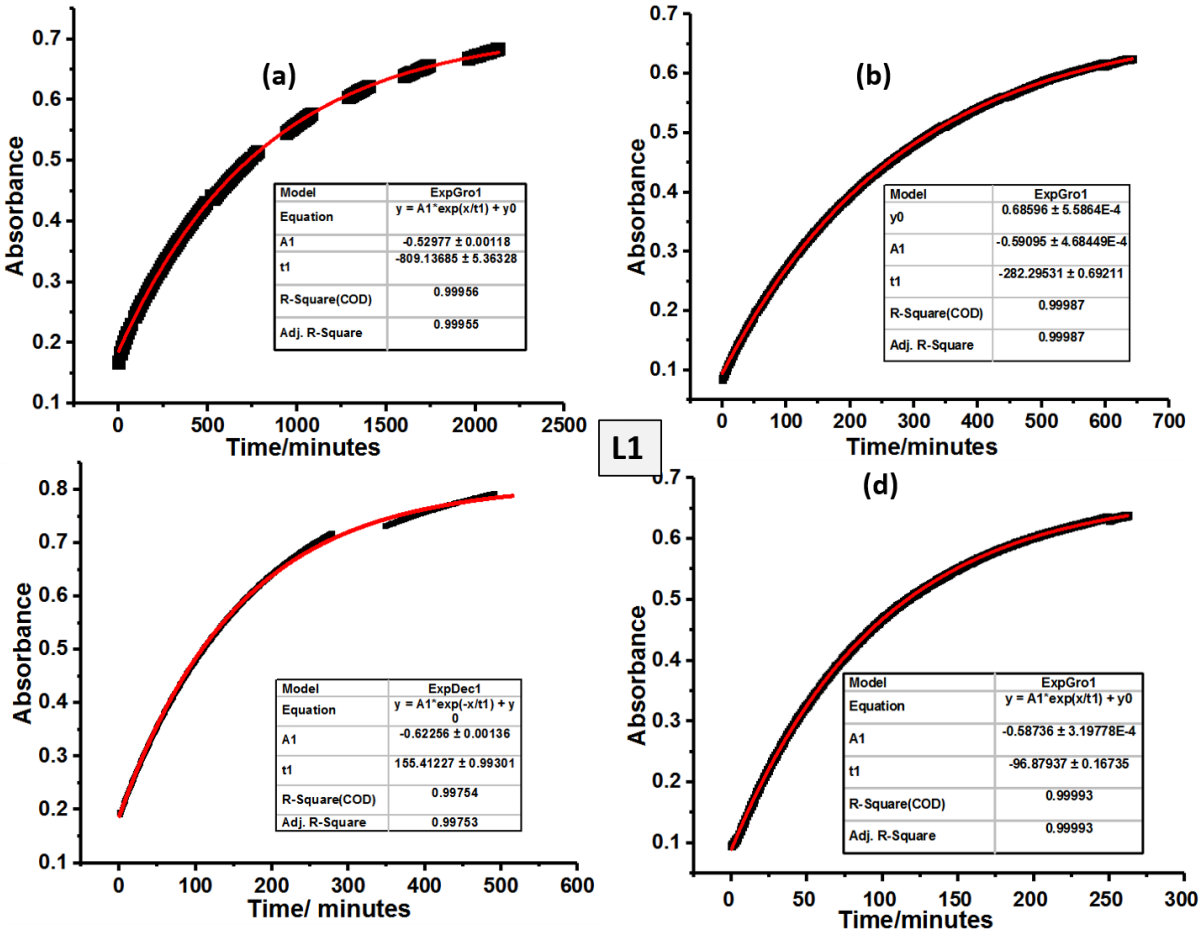


Figure S5.2. First order thermal reverse isomerization kinetics plots of **L1** at (a) 80 °C; (b) 90 °C; (c) 95 °C; (d) 100 °C.

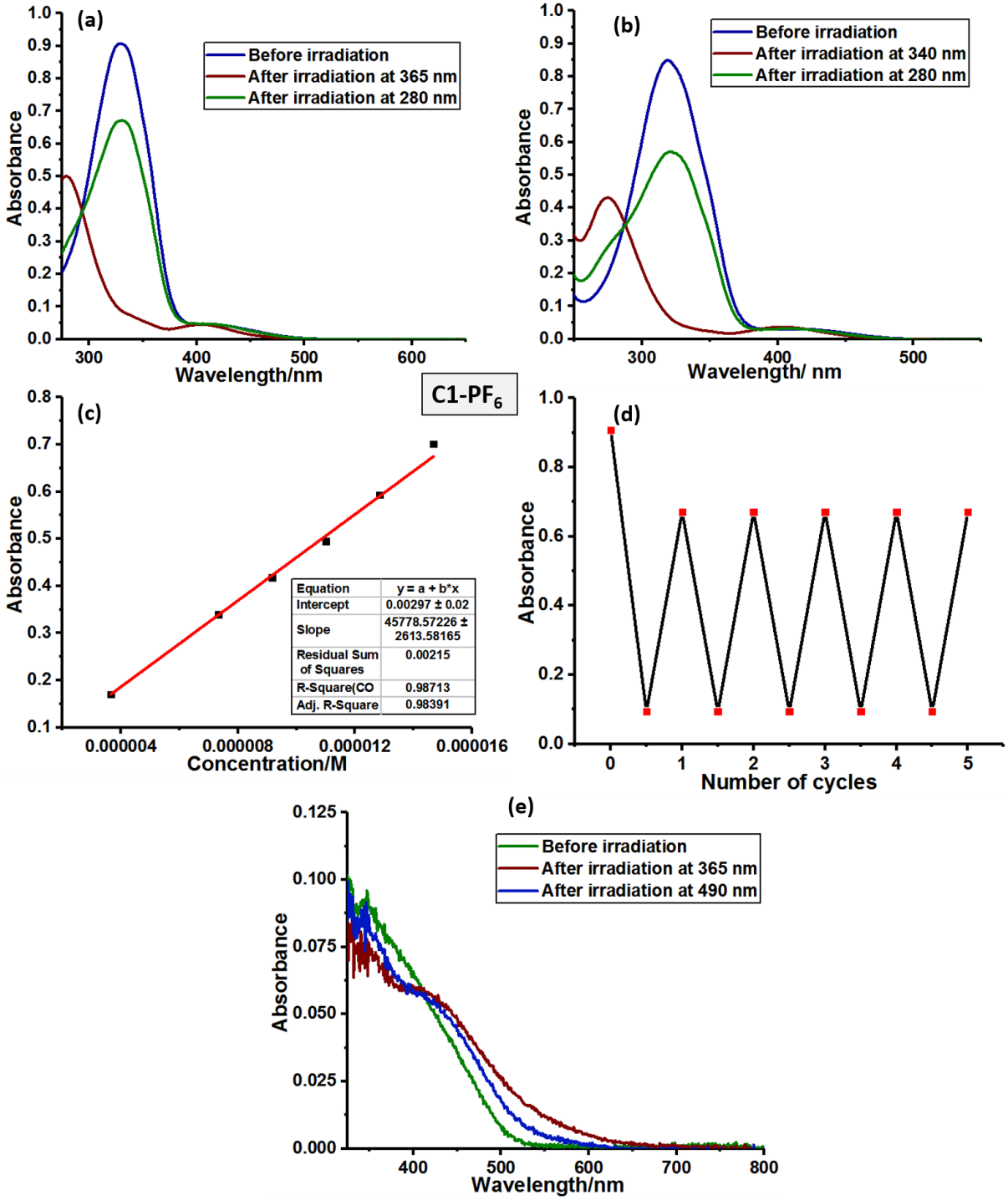


Figure S5.3. Photoswitching behaviour of **C1-PF$_6$:** (a) Forward and reverse photoisomerization (DMSO, 20 µM) of **C1-PF$_6$**; (b) Forward and reverse photoisomerization (MeCN, 18 µM) of **C1-PF$_6$**; (c) Estimation of molar extinction coefficient (in DMSO) for the $\pi-\pi^*$ absorption (λ_{max}= 328 nm); (d) Photoswitching stability test upto five cycles of **C1-PF$_6$** in DMSO (forward isomerization step: 365 nm; reverse isomerization step: 280 nm); (e) Forward and reverse photoisomerization (in KBr medium) of **C1-PF$_6$**.

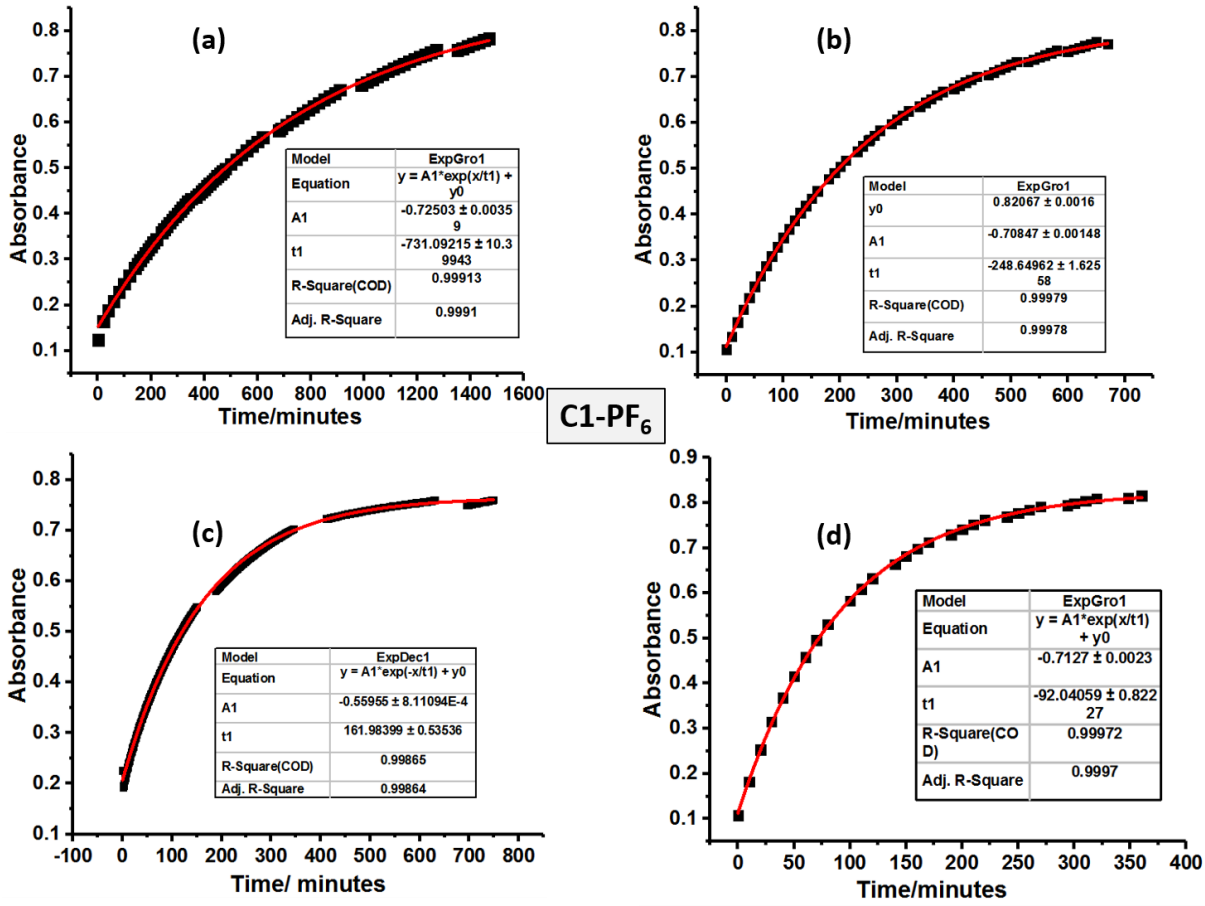


Figure S5.4. First order thermal reverse isomerization kinetics plots of **C1-PF$_6$** at (a) 80 °C; (b) 90 °C; (c) 95 °C; (d) 100 °C.

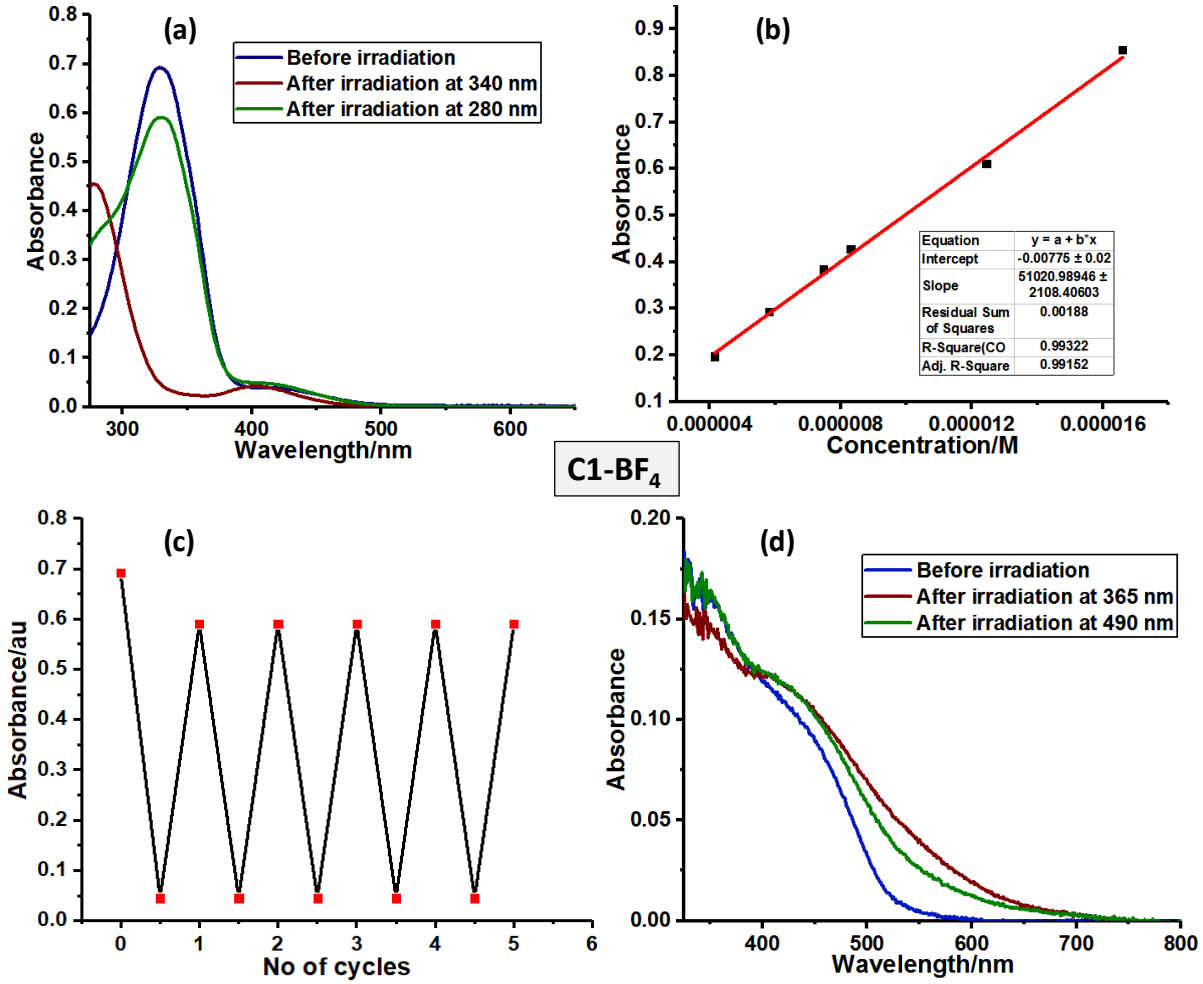


Figure S5.5. Photoswitching behaviour of **C1-BF_4:** (a) Forward and reverse photoisomerization (DMSO, 14 µM) of **C1-BF_4**; (b) Estimation of molar extinction coefficient (in DMSO) for the π–π* absorption (λ_{max}= 329 nm); (c) Photoswitching stability test upto five cycles of **C1-BF_4** in DMSO (forward isomerization step: 340 nm; reverse isomerization step: 280 nm; (d) Forward and reverse photoisomerization (in KBr medium) of **C1-BF_4.**

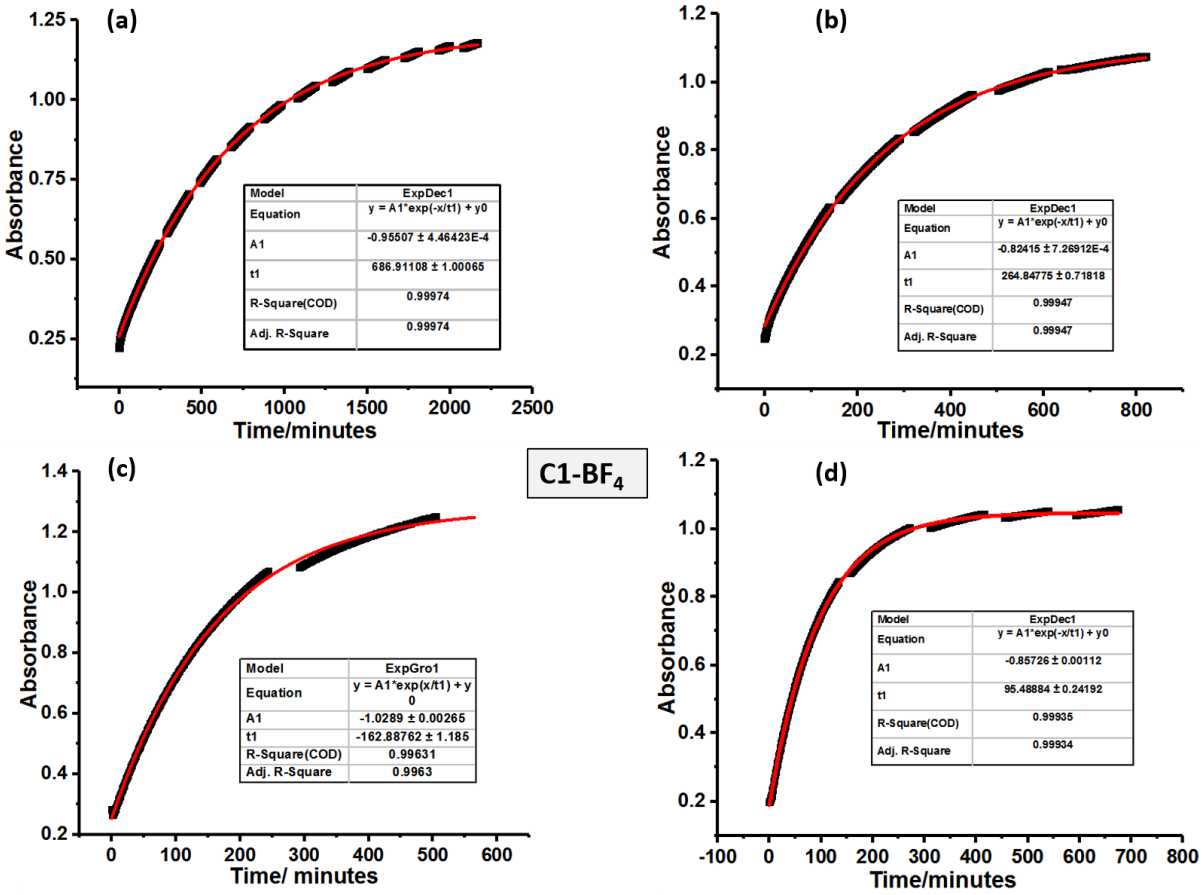


Figure S5.6. First order thermal reverse isomerization kinetics plots of **C1-BF_4** at (a) 80 °C; (b) 90 °C; (c) 95 °C; (d) 100 °C

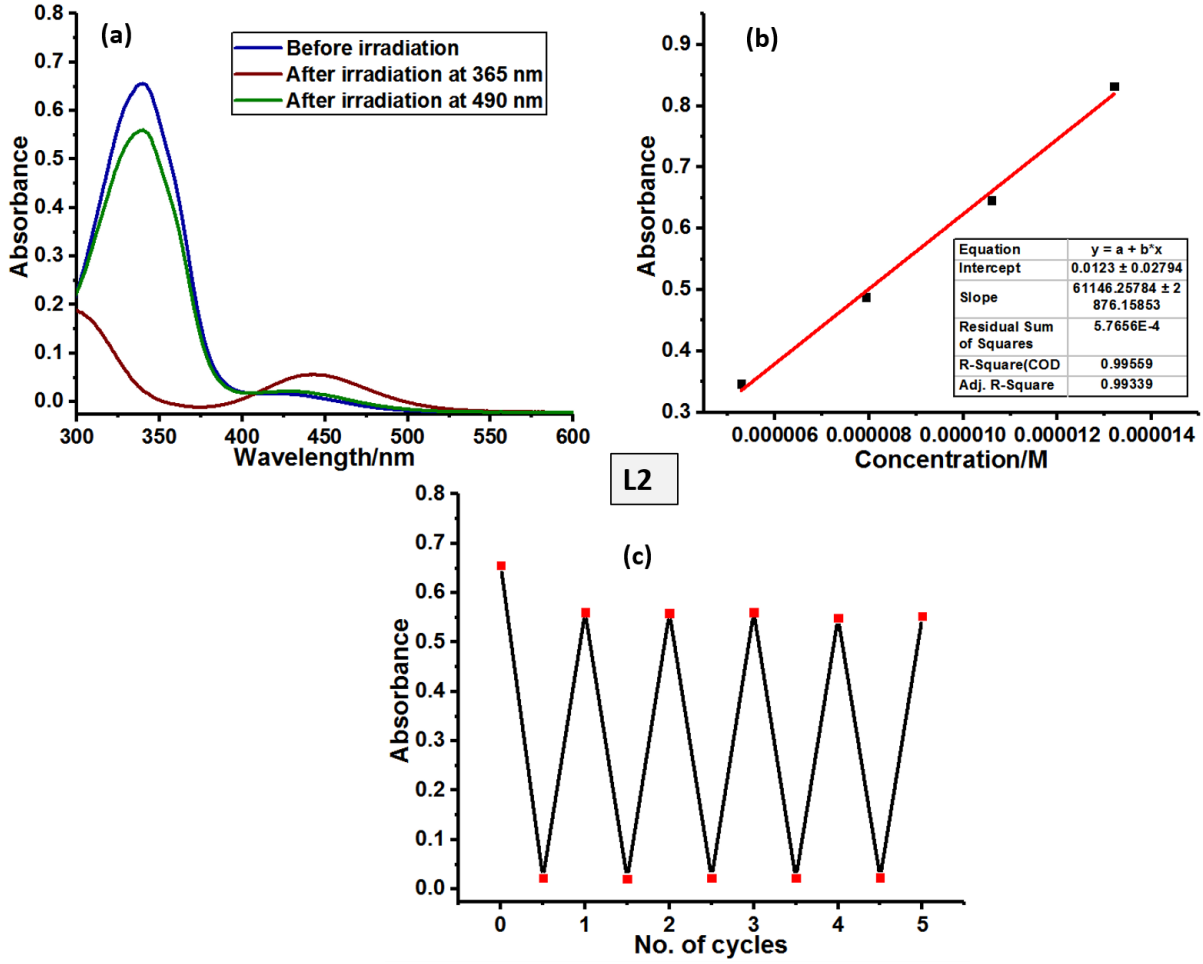


Figure S5.7. Photoswitching behaviour of **L2:** (a) Forward and reverse photoisomerization (DMSO, 11 μM) of **L2**; (b) Estimation of molar extinction coefficient (in DMSO) for the π–π* absorption (λ_{max}= 340 nm); (c) Photoswitching stability test upto five cycles of **L2** in DMSO (forward isomerization step: 365 nm; reverse isomerization step: 490 nm.

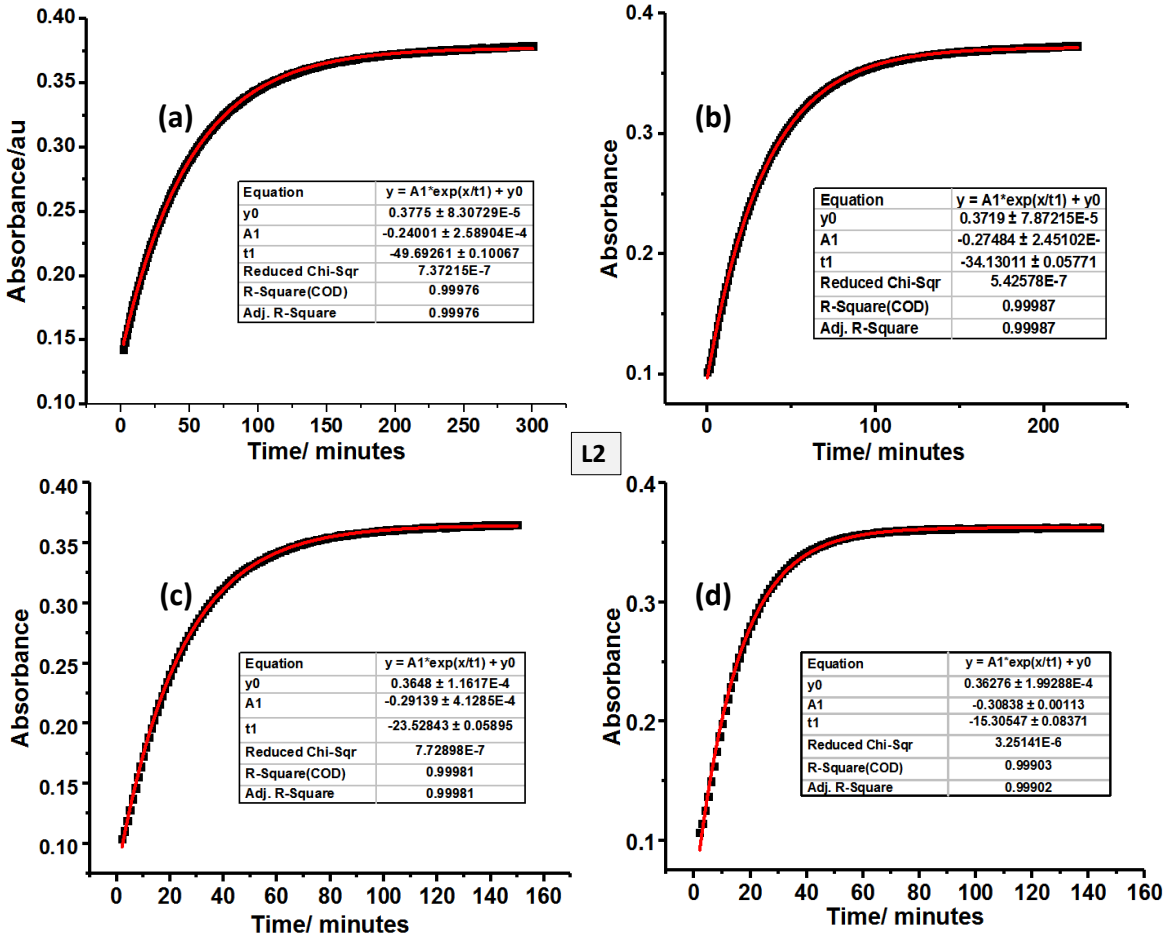


Figure S5.8. First order thermal reverse isomerization kinetics plots of **L2** (10 μM solution in DMSO) at (a) 70 °C; (b) 75 °C; (c) 80 °C; (d) 85 °C.

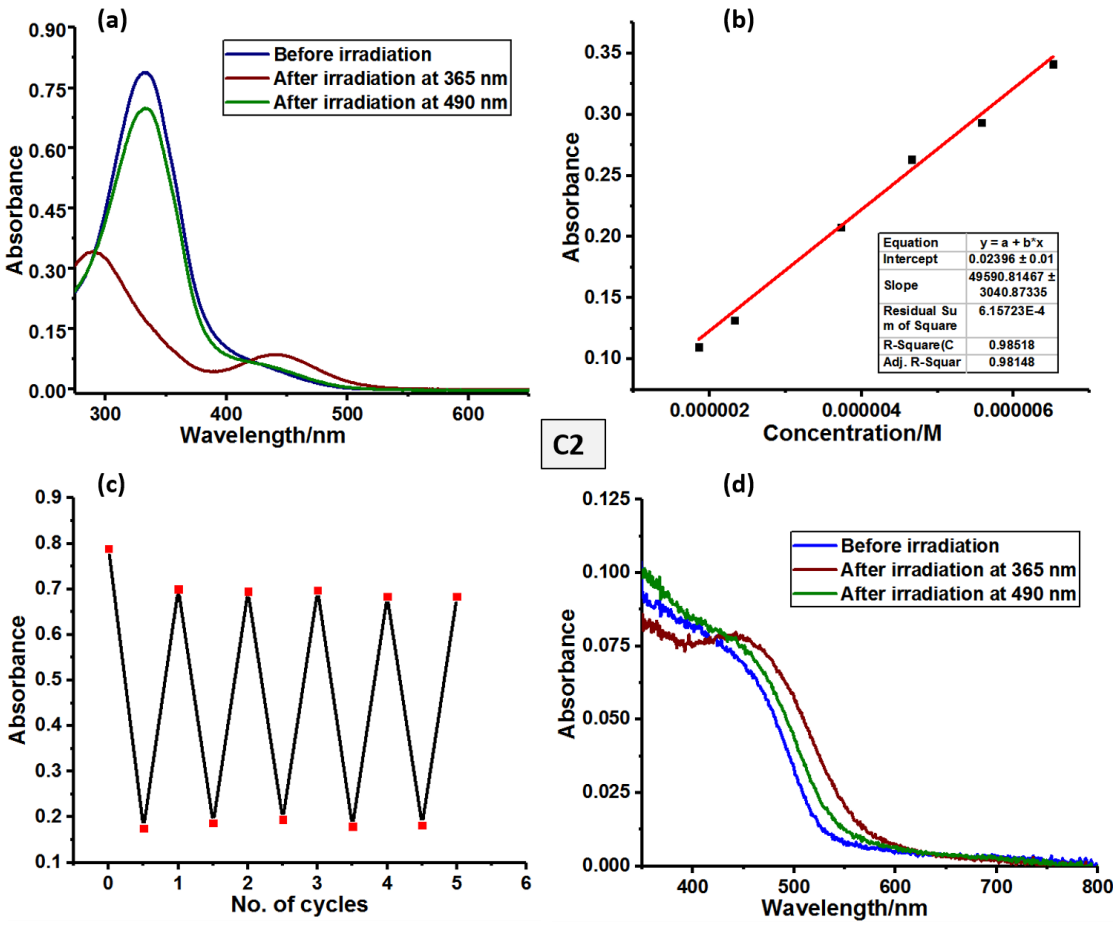


Figure S5.9. Photoswitching behaviour of **C2:** (a) Forward and reverse photoisomerization (DMSO, 16 µM) of **C2**; (b) Estimation of molar extinction coefficient (in DMSO) for the π–π* absorption (λ_{max}= 332 nm); (c) Photoswitching stability test upto five cycles of **C2** in DMSO (forward isomerization step: 365 nm; reverse isomerization step: 490 nm ; (d) Forward and reverse photoisomerization (in KBr medium) of **C2**.

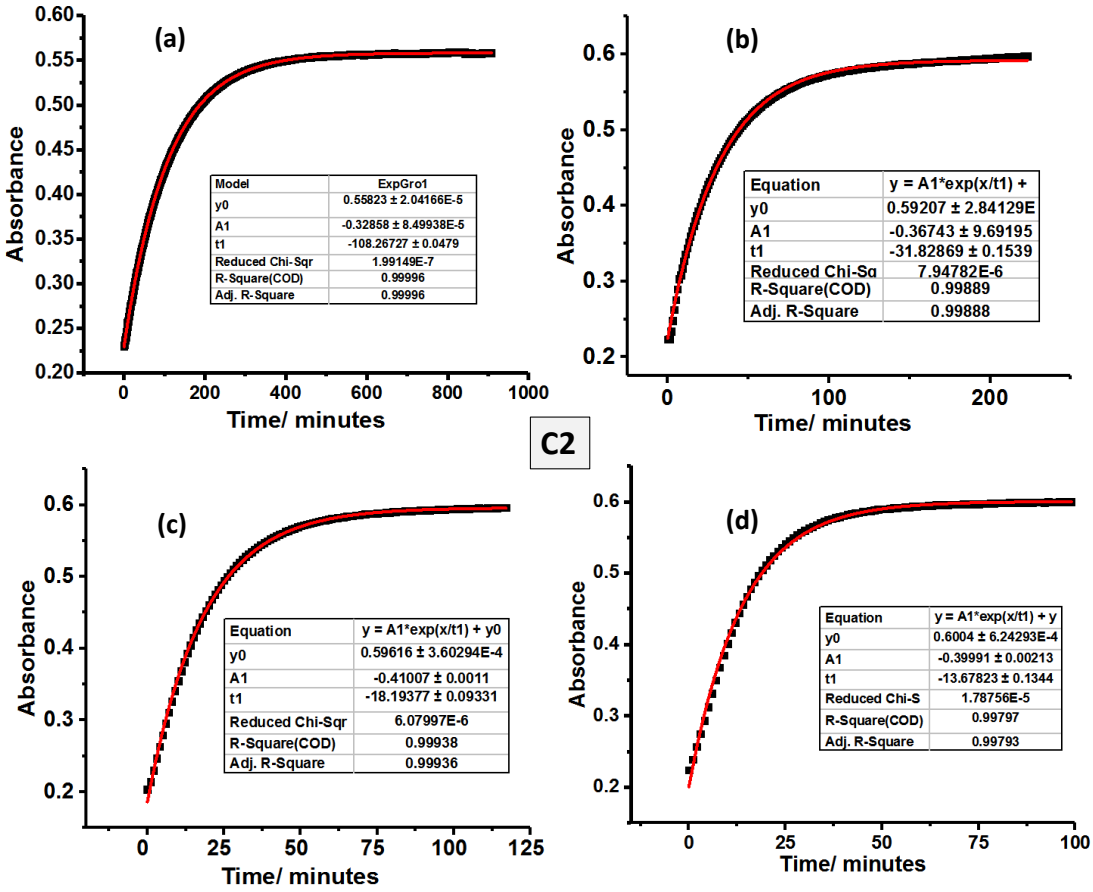


Figure S5.10. First order thermal reverse isomerization kinetics plots of **C2** at (a) 70 °C; (b) 80 °C; (c) 85 °C; (d) 88 °C.

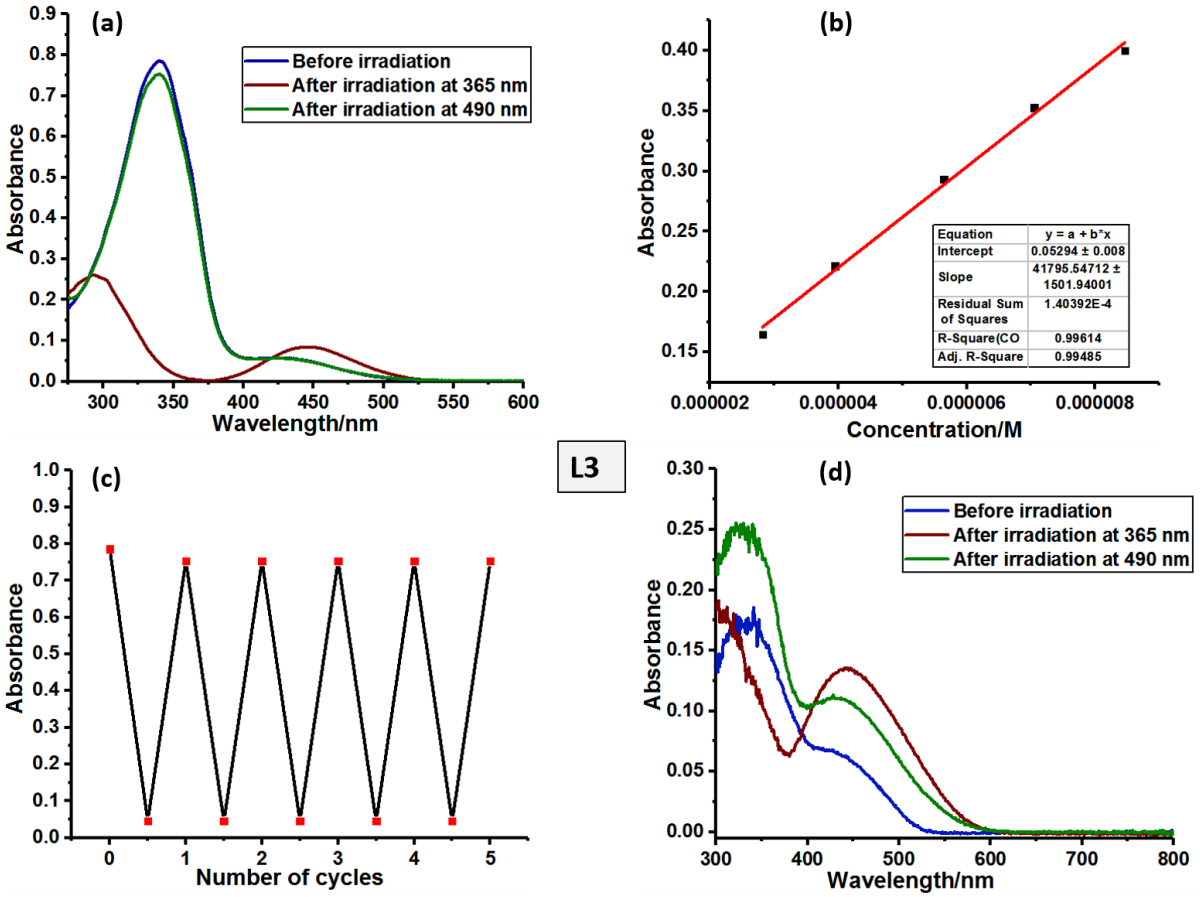


Figure S5.11. Photoswitching behaviour of **L3**: (a) Forward and reverse photoisomerization (DMSO, 19 µM) of **L3**; (b) Estimation of molar extinction coefficient (in DMSO) for the π–π* absorption (λ_{max}= 340 nm); (c) Photoswitching stability test upto five cycles of **L3** in DMSO (forward isomerization step: 365 nm; reverse isomerization step: 490 nm; (d) Forward and reverse photoisomerization (in KBr medium) of **L3**.

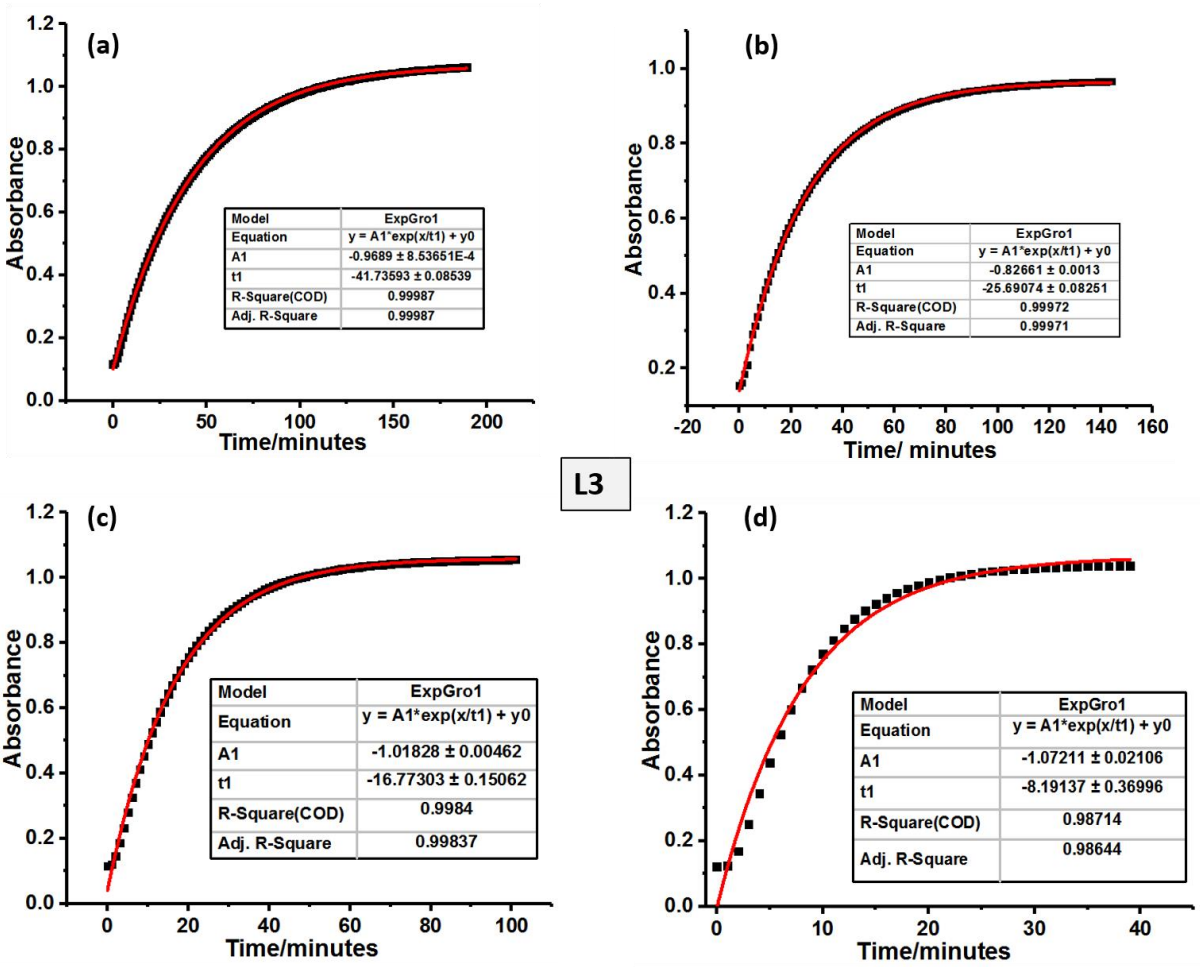


Figure S5.12. First order thermal reverse isomerization kinetics plots of **L3** at (a) 70 °C; (b) 75 °C; (c) 80 °C; (d) 90 °C.

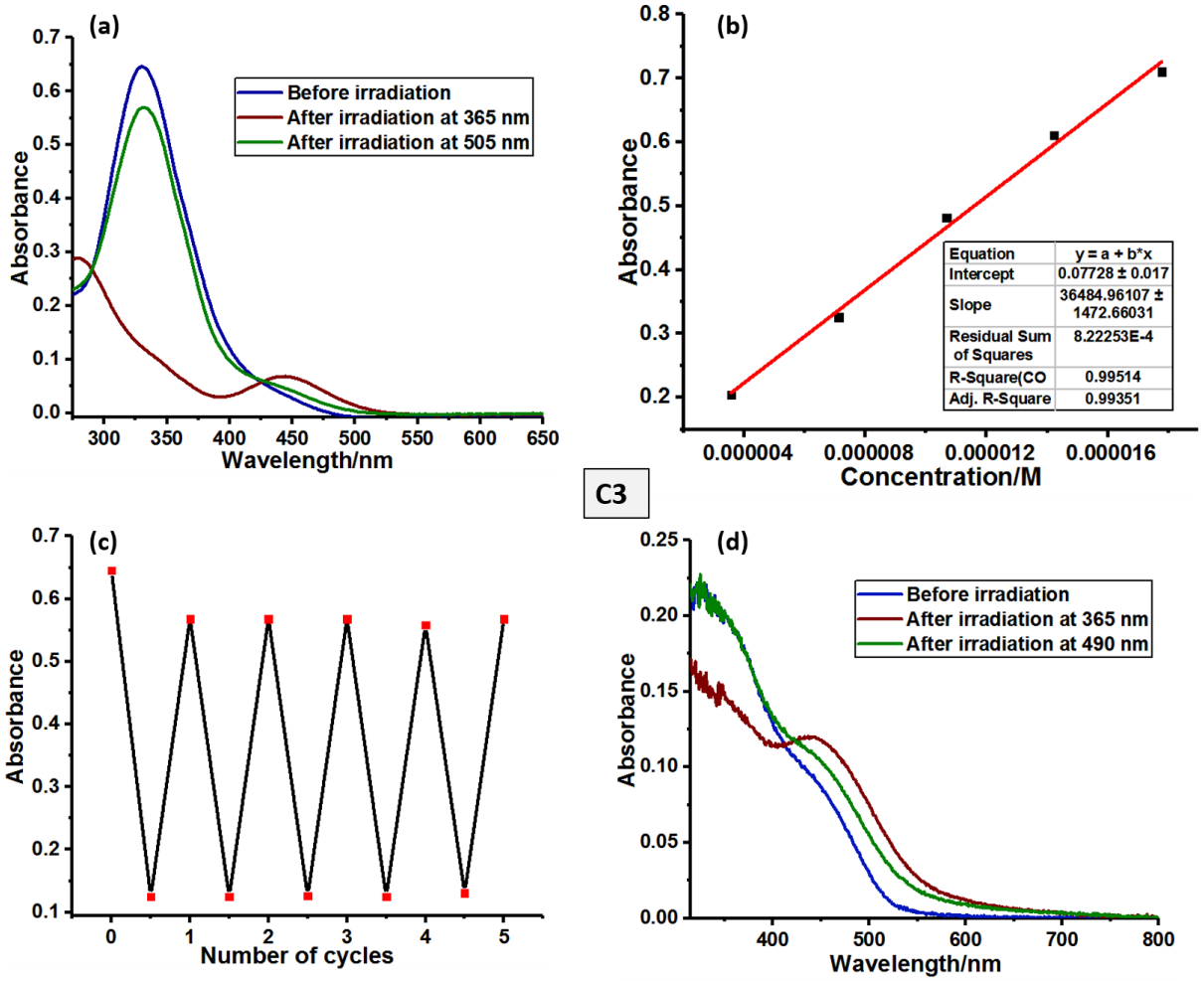


Figure S5.13. Photoswitching behaviour of **C3**: (a) Forward and reverse photoisomerization (DMSO, 18 μM) of **C3**; (b) Estimation of molar extinction coefficient (in DMSO) for the π–π* absorption (λ_{max}= 330 nm); (c) Photoswitching stability test upto five cycles of **C3** in DMSO (forward isomerization step: 365 nm; reverse isomerizarion step: 505 nm; (d) Forward and reverse photoisomerization (in KBr medium) of **C3**.

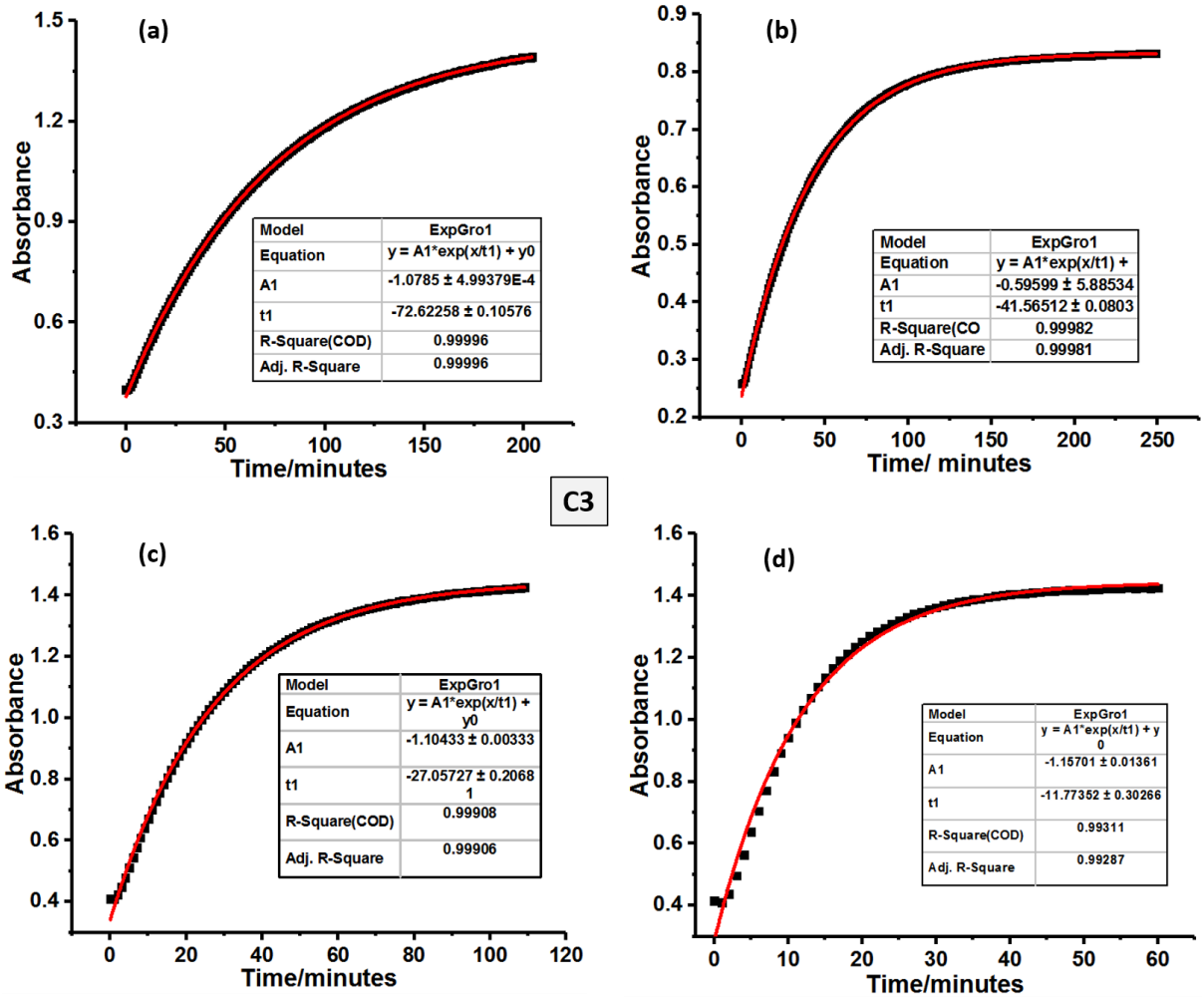


Figure S5.14. First order thermal reverse isomerization kinetics plots of **C3** (38 μM solution in DMSO) at (a) 70 °C; (b) 75 °C; (c) 80 °C; (d) 90 °C.

Table S5.1. PSS data in the forward and reverse photoisomerization in the ligands and metal complexes in the solution phase (in DMSO)

S. No.	Compound	Wavelength (nm)	PSS composition (%*EE*)[a]		
			Forward photoisomerization	Reverse photoisomerization	Concentration [μM]
1	**L1**	340 **280**	92	90	12
2	**L2**	365 **490**	97	96	11
3	**L3**	365 **490**	94	94	19
4	**C1-PF_6**	365 **280**	90	86	20
5	**C1-BF_4**	340 **280**	94	92	14
6	**C2**	365 **490**	78	75	16
7	**C3**	365 **505**	80	78	18

The λ_{max} (corresponding to $\pi-\pi^*$ transition) has been used for estimation of PSS composition. For all the forward isomerization step 365 nm LED was used; The following wavelengths of light have been used for the reverse photoisomerization: 280, 340, 365, 490 and 505 nm wavelengths of light have been used as specified.

The PSS composition has been estimated in the individual compounds using the formula given below.

$$\%\ \text{conversion of } EEE \text{ isomers} = \left(1 - \frac{A_{\pi-\pi^*}\text{absorption after irradiation at 365 nm}}{A_{\pi-\pi^*}\text{ absorption before irradiation}}\right) \mathbf{x}\ 100$$

$$\%\ \text{conversion of } ZZZ \text{ isomers (solution state)} = \left(1 - \frac{A_{\pi-\pi^*}\text{absorption after irradiation at 365 nm}}{A_{\pi-\pi^*}\text{ absorption after irradiation at 490 nm}}\right) \mathbf{x}\ 100$$

Table S5.2. PSS data in the forward and reverse photoisomerization in **L1**, **L3** and the metal complexes in solid state in KBr medium.

S. No.	Compound	PSS composition in solid state photoswitching	
		Forward *EEE-ZZZ* isomerisation (in terms of %*EEE*)	**Reverse *ZZZ-EEE* isomerisation (in terms of %*EEE*)**
1	**L1**	16	96
2	**L3**	53	81
3	**C1-PF_6**	18	95
4	**C1-BF_4**	>5%	x
5	**C2**	40	78 (94 at 455 nm)
6	**C3**	27	88

λmax (corresponding to n–π* transition) for **L1**(423 nm), **C2**(497NM), **C1-BF_4**(419 nm), **C1-PF_6** (438 nm), **L3** (442nm), **C3** (450nm) has been utilized for estimation of PSS composition. For all the forward isomerization step 365 nm LED was used; The following wavelengths of light have been used for the reverse photoisomerization: 490 nm wavelengths of light have been used as specified.

$$\%\ \text{conversion of } EE \text{ isomers (solid state)} = \left(1 - \frac{A_{n-\pi^*}\ \text{absorption before irradiation}}{A_{n-\pi^*}\ \text{absorption after irradiation at 365 nm}}\right) \mathbf{x} 100$$

$$\%\ \text{conversion of } ZZ \text{ isomers (solid state)} = \frac{A_{n-\pi^*}\text{absorption after irradiation at 490 nm}}{A_{n-\pi^*}\ \text{absorption after irradiation at 365 nm}}\ \mathbf{x}\ 100$$

Table S5.3. Thermal reverse isomerization kinetics data:

S. No.	Compound	Solvent	Temperature (°C)	Rate constant (min^{-1})	Concentration (μM)
1	**L1**	DMSO	80	$1.24 \times 10^{-3} \pm 8.19 \times 10^{-6}$	11
			90	$3.54 \times 10^{-3} \pm 8.68 \times 10^{-6}$	11
			95	$6.43 \times 10^{-3} \pm 4.11 \times 10^{-5}$	14
			100	$1.03 \times 10^{-2} \pm 1.78 \times 10^{-5}$	11
			25[a]	1.1×10^{-6}	X
2	**L2**	DMSO	70	$2.01 \times 10^{-2} \pm 4.08 \times 10^{-5}$	10
			75	$2.93 \times 10^{-2} \pm 4.95 \times 10^{-5}$	10
			80	$4.25 \times 10^{-2} \pm 1.06 \times 10^{-4}$	10
			85	$6.53 \times 10^{-2} \pm 3.57 \times 10^{-4}$	10
			25[a]	3.9×10^{-4}	X
3	**L3**	DMSO	70	$2.40 \times 10^{-2} \pm 4.90 \times 10^{-5}$	25
			75	$3.89 \times 10^{-2} \pm 1.25 \times 10^{-4}$	23
			80	$5.96 \times 10^{-2} \pm 5.35 \times 10^{-4}$	25
			90	$1.22 \times 10^{-1} \pm 5.51 \times 10^{-3}$	25
			25[a]	1.4×10^{-4}	X
4	**C1-PF_6**	DMSO	80	$1.37 \times 10^{-3} \pm 1.95 \times 10^{-5}$	17
			90	$4.02 \times 10^{-3} \pm 2.63 \times 10^{-5}$	17
			95	$6.17 \times 10^{-3} \pm 2.04 \times 10^{-5}$	17
			100	$1.09 \times 10^{-2} \pm 9.71 \times 10^{-5}$	17
			25[a]	1.0×10^{-6}	X
5	**C1-BF_4**	DMSO	80	$1.46 \times 10^{-3} \pm 2.12 \times 10^{-6}$	19
			90	$3.78 \times 10^{-3} \pm 1.02 \times 10^{-5}$	19
			95	$6.14 \times 10^{-3} \pm 4.47 \times 10^{-5}$	24
			100	$1.05 \times 10^{-2} \pm 2.65 \times 10^{-5}$	19
			25[a]	2.8×10^{-6}	X
6	**C2**	DMSO	70	$9.24 \times 10^{-3} \pm 4.09 \times 10^{-6}$	16
			80	$3.14 \times 10^{-2} \pm 1.52 \times 10^{-4}$	16
			85	$5.50 \times 10^{-2} \pm 2.82 \times 10^{-4}$	16
			88	$7.31 \times 10^{-2} \pm 7.18 \times 10^{-4}$	16
			25[a]	1.3×10^{-5}	X
7	**C3**	DMSO	70	$1.37 \times 10^{-2} \pm 2.00 \times 10^{-5}$	38
			75	$2.41 \times 10^{-2} \pm 4.65 \times 10^{-5}$	23
			80	$3.70 \times 10^{-2} \pm 2.82 \times 10^{-4}$	38
			90	$8.49 \times 10^{-2} \pm 2.18 \times 10^{-3}$	38
			25[a]	3.6×10^{-5}	X

[a]Extrapolated from Arrhenius plot

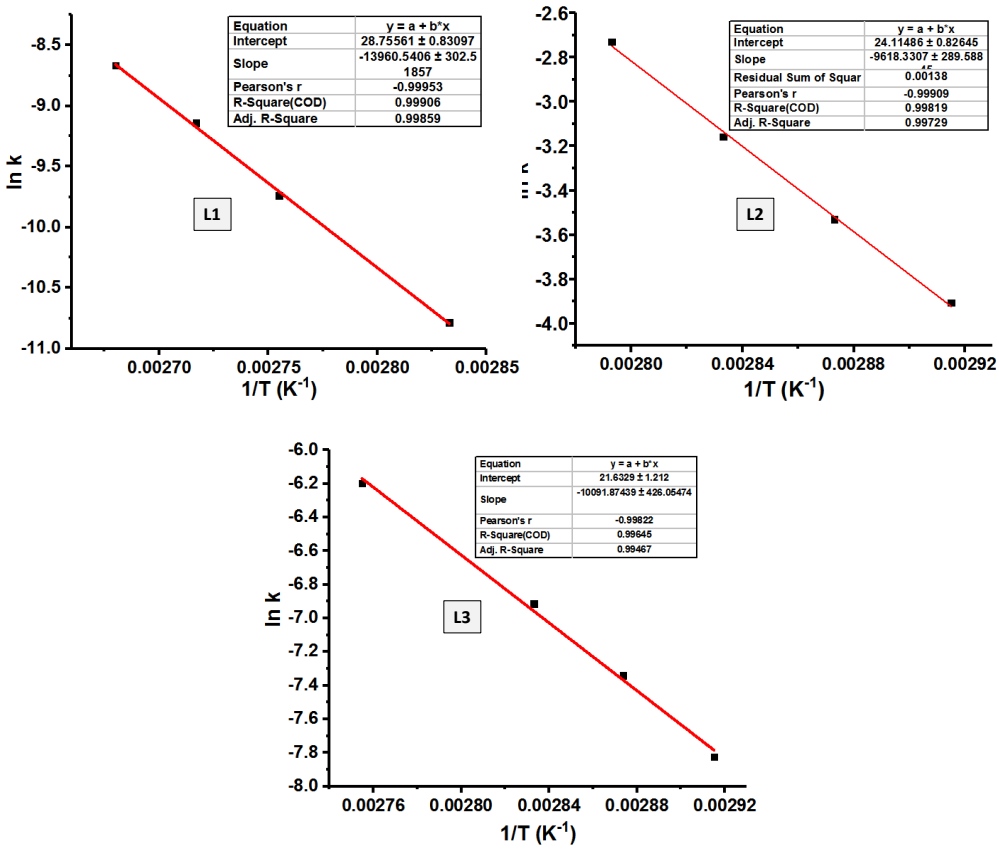


Figure S5.15. Arrhenius plots for **L1**, **L2** and **L3** (in DMSO).

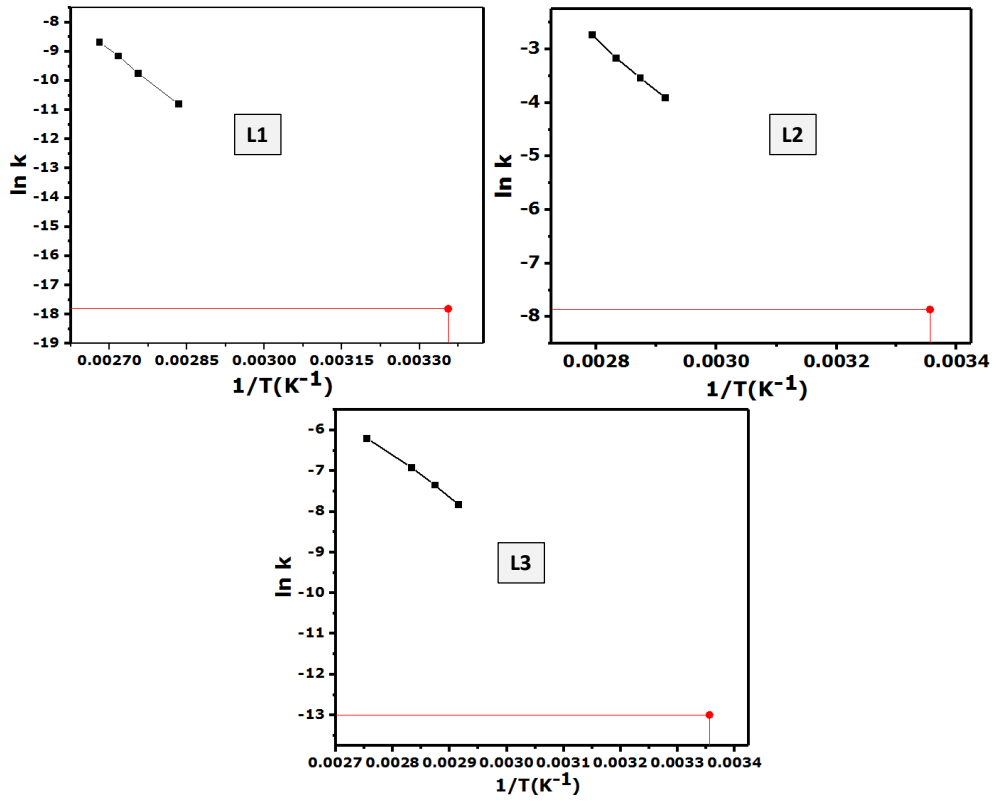


Figure S5.16. Extrapolation of Arrhenius plot for **L1**, **L2** and **L3** in DMSO to room temperature (298 K).

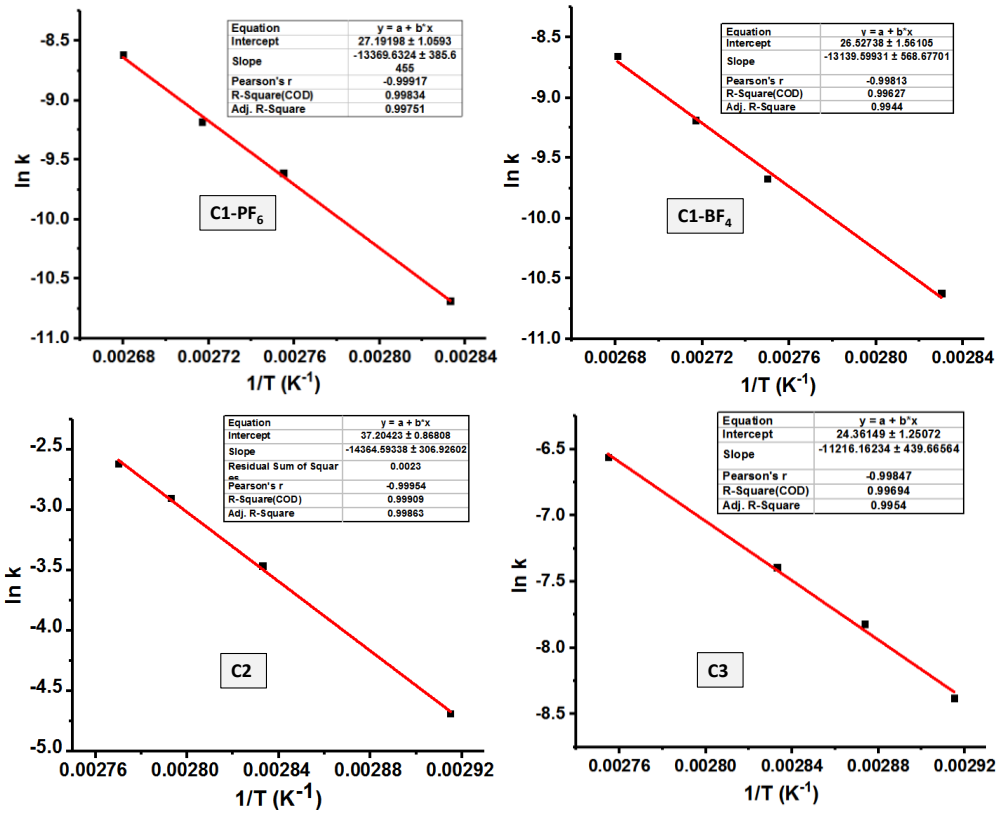


Figure S5.17. Arrhenius plots for **C1-PF$_6$**, **C1-BF$_4$**, **C2** and **C3** (in DMSO).

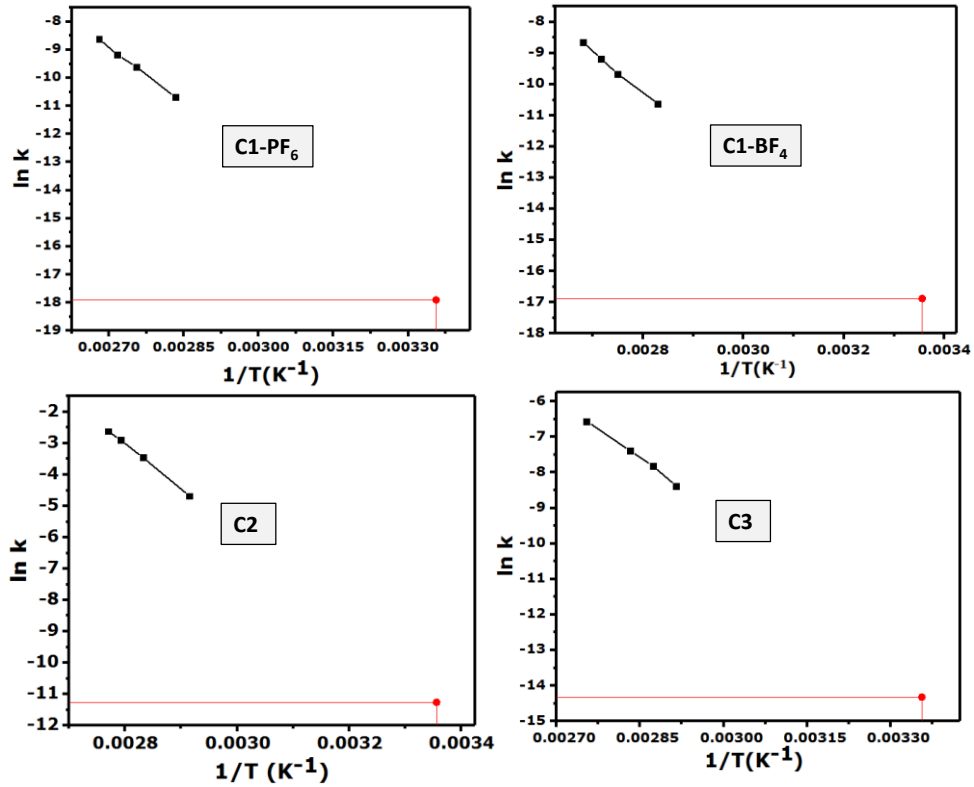


Figure S5.18. Extrapolation of Arrhenius plot for **C1-PF$_6$**, **C1-BF$_4$**, **C2,** and **C3** in DMSO to room temperature (298 K).

S6: Quantification of photoisomerization for ligands **L1**-**L3** and complexes **C1-PF$_6$**, **C1-BF$_4$**, **C2**, and **C3**

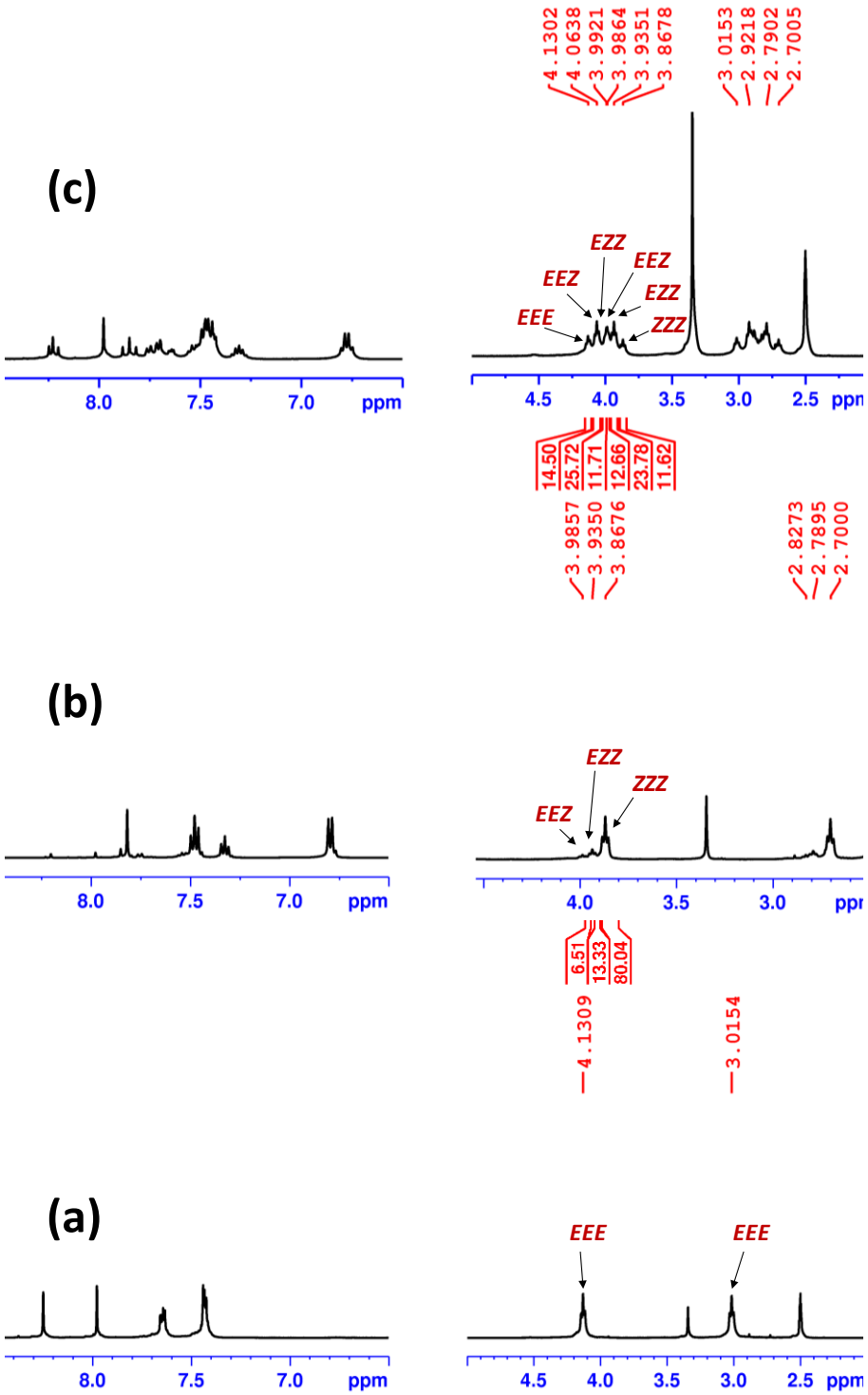


Figure S6.1. Analysis of photoswitching and estimation of PSS composition using ^{1}H-NMR spectroscopic studies of **L1** in [D$_6$]DMSO (5.0 mM) (a) before irradiation; (b) after irradiation at 340 nm [Irradiation at 365 nm also produced a similar PSS, for catalytic studies 365 nm light was used for irradiation]; (c) after irradiation at 405 nm. [Irradiation at 280 nm also produced a similar PSS] (The normalized integral values corresponding to methylene signal were used for the estimation of PSS composition.)

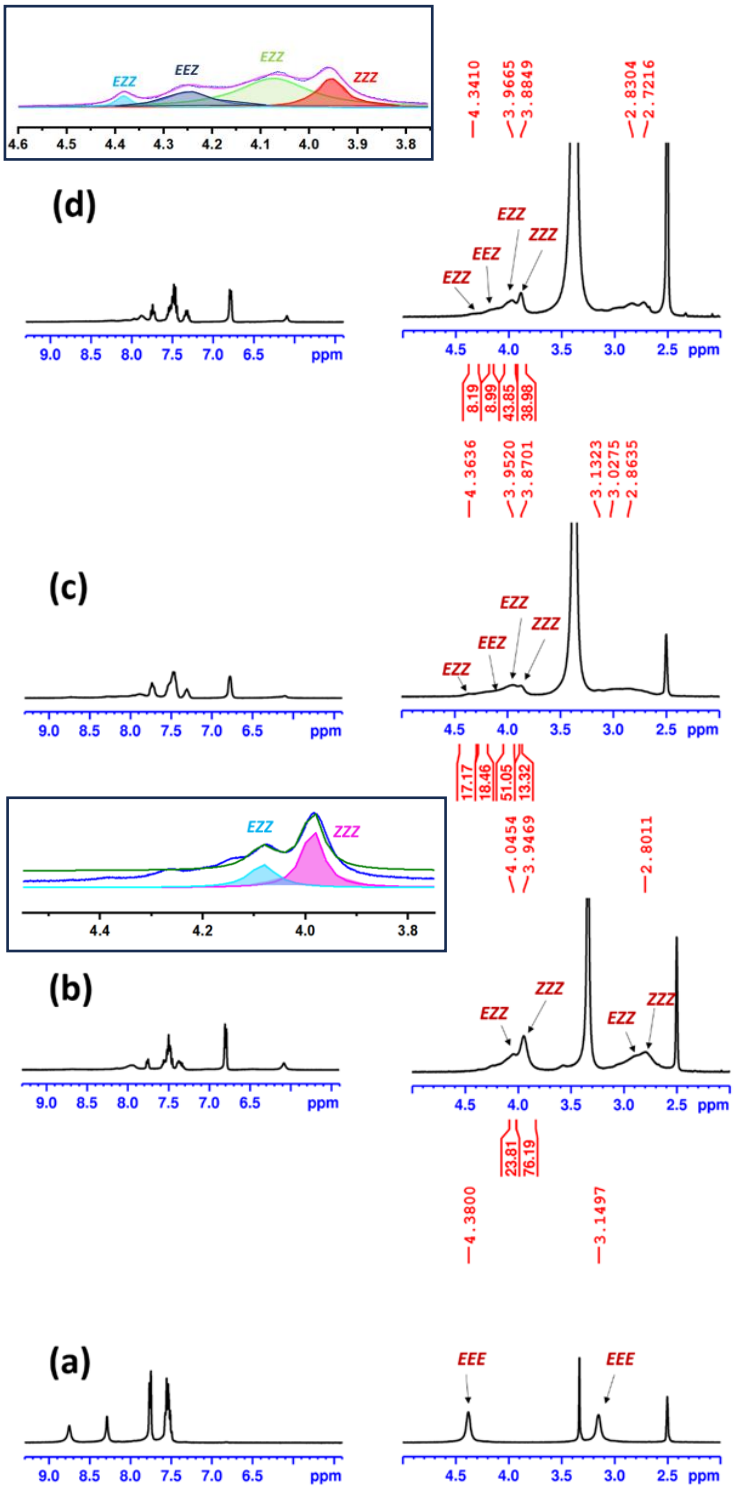


Figure S6.2a. Analysis of photoswitching and estimation of PSS composition using ^{1}H-NMR spectroscopic studies of **C1-PF$_6$** in [D$_6$]DMSO (6.5 mM) (a) before irradiation; (b) after irradiation at 340 nm [inset: deconvolution of peaks]; irradiation at 365 nm produced similar PSS(c) after irradiation at 405 nm; (c) after irradiation at 280 nm. [inset: deconvolution of peaks] (The normalized integral values corresponding to methylene signal were used for the estimation of PSS composition.)

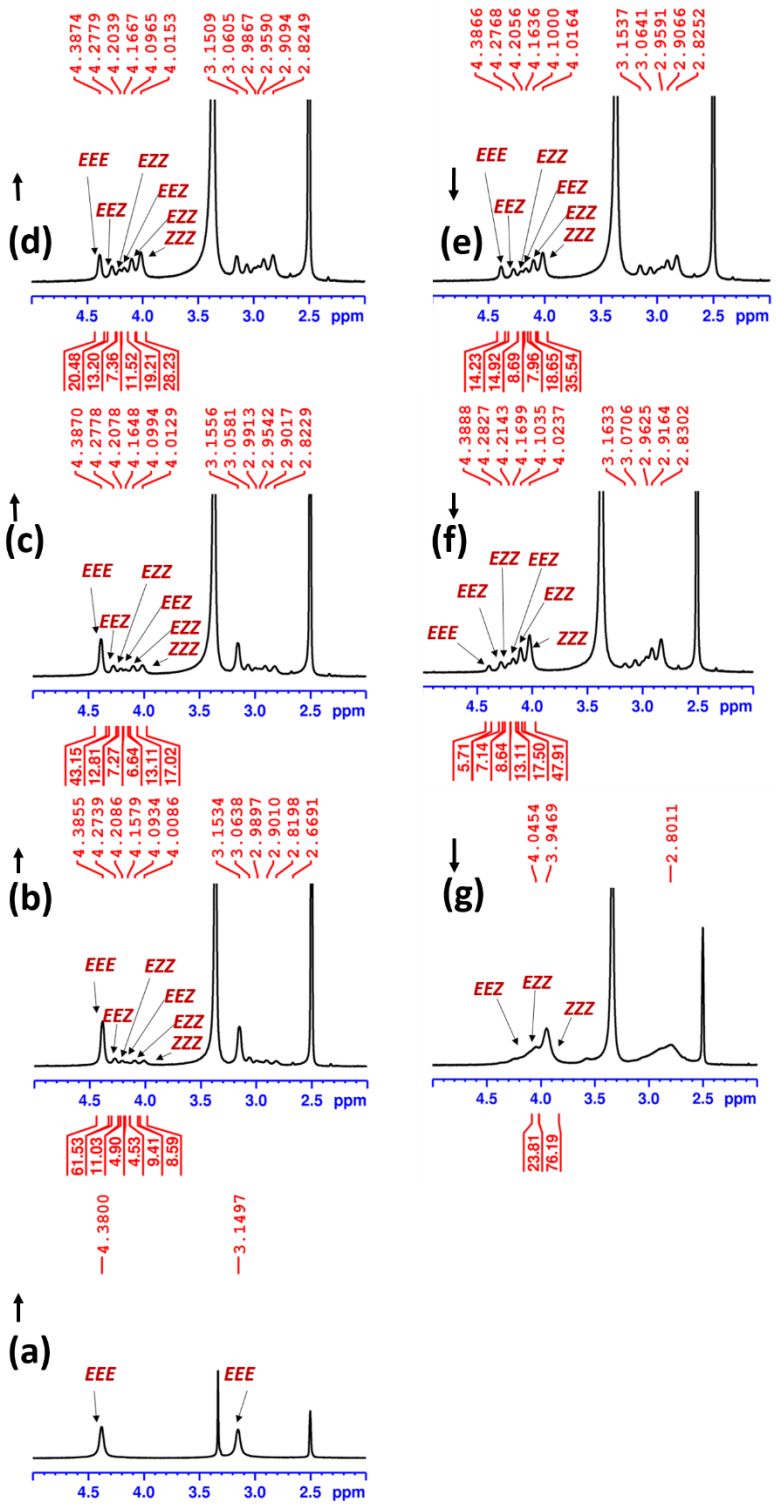


Figure S6.3. Analysis of PSS composition changes during photoisomerization steps at different intervals of irradiation times using ^{1}H-NMR spectroscopic studies of **C1-PF$_6$** in [D$_6$]DMSO (6.5 mM) (a) before irradiation; (b) after irradiation at 340 nm for 5 minutes; (c) after irradiation at 340 nm for 20 minutes; (d) after irradiation at 340 nm for 35 minutes; (e) after irradiation at 340 nm for 60 minutes; (f) after irradiation at 340 nm for 82 minutes; (g) after irradiation at 340 nm for 120 minutes (Final PSS). (The normalized integral values corresponding to methylene signal was used for the estimation of PSS composition because of lack of clarity in shifts of aromatic protons). Since the peaks are broad and almost overlapping, slight errors in the integral values may be possible.

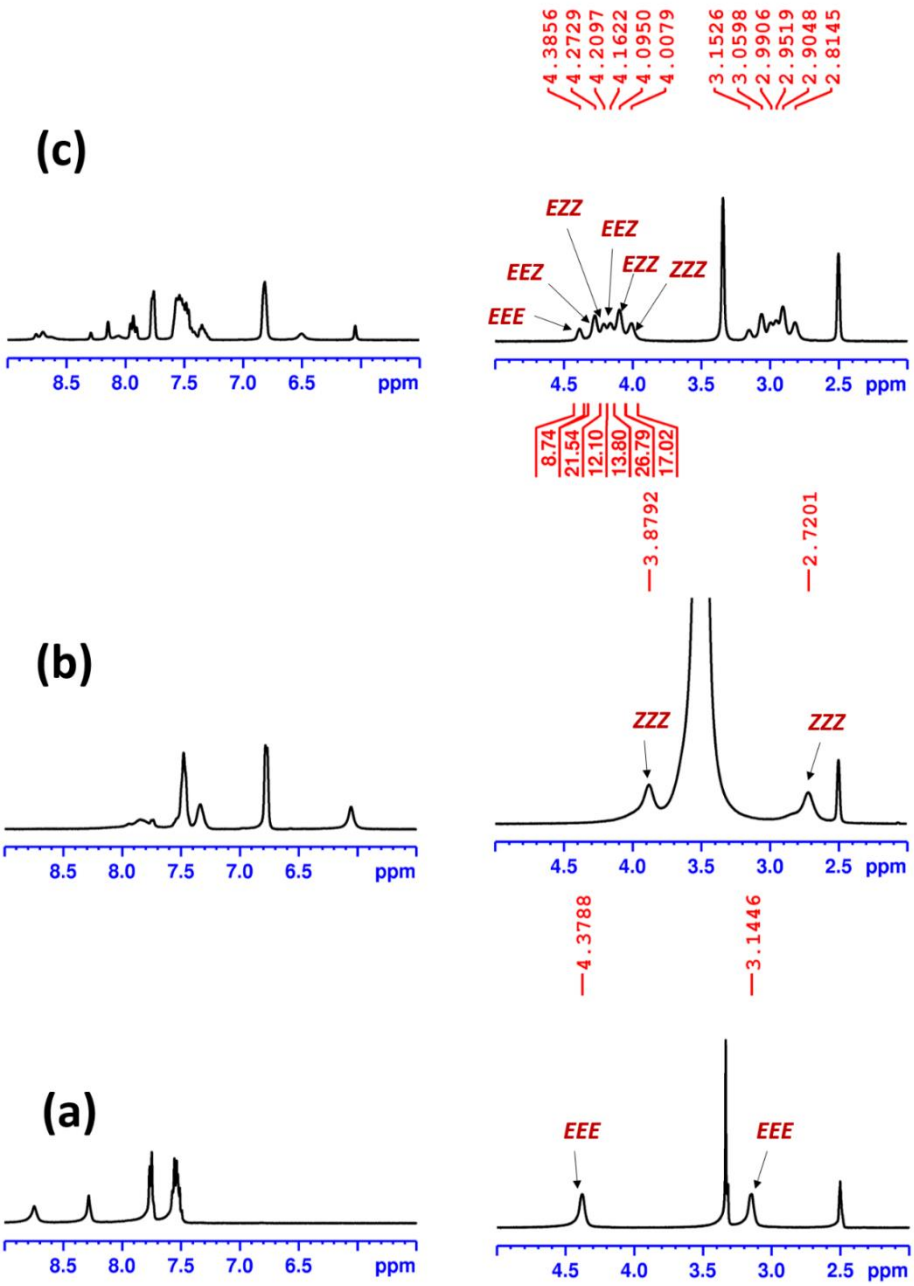


Figure S6.4. Analysis of photoswitching and estimation of PSS composition using ^{1}H-NMR spectroscopic studies of **C1-BF_4** in [D_6]DMSO (6.0 mM) (a) before irradiation; (b) after irradiation at 340 nm; (c) after irradiation at 280 nm. (The normalized integral values corresponding to methylene signal were used for the estimation of PSS composition.)

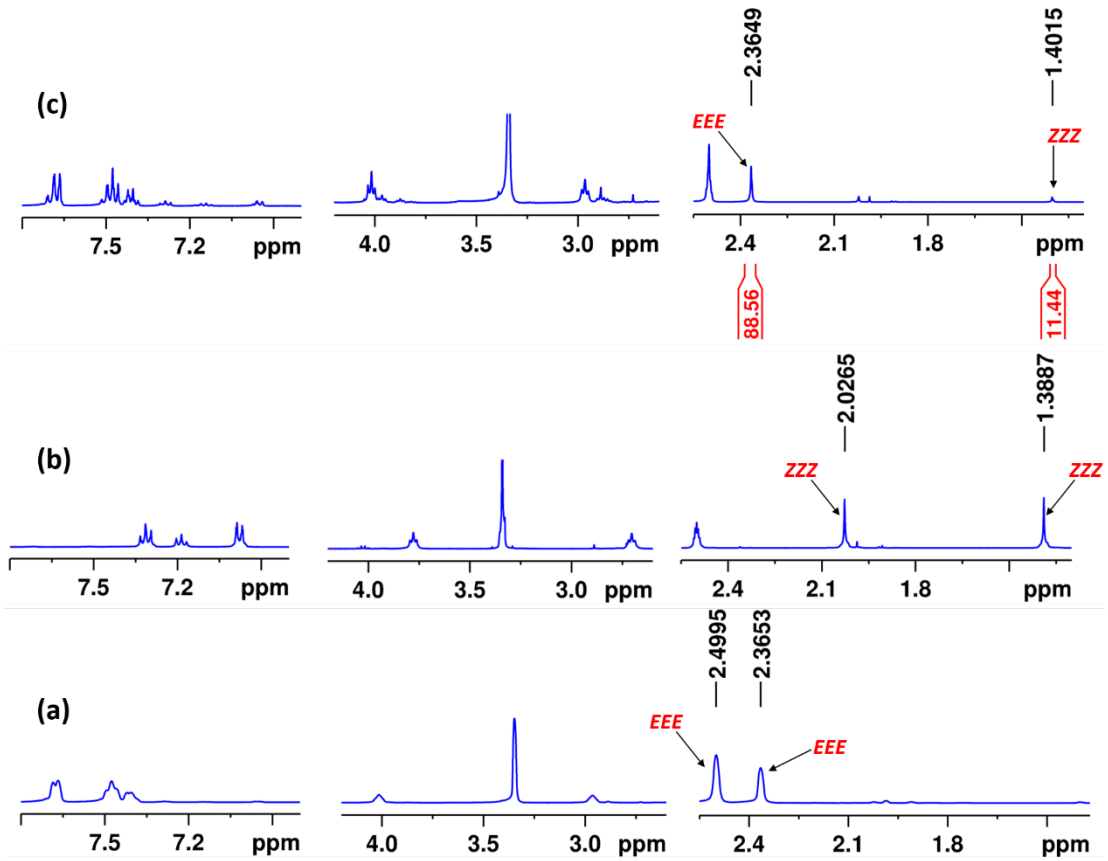


Figure S6.5. Analysis of photoswitching and estimation of PSS composition using ^{1}H-NMR spectroscopic studies of **L2** in [D_6]DMSO (5.5 mM): (a) before irradiation; (b) after irradiation at 365 nm; (c) after irradiation at 490 nm. (The normalized integral values corresponding to methyl signal was used for the estimation of PSS composition.)

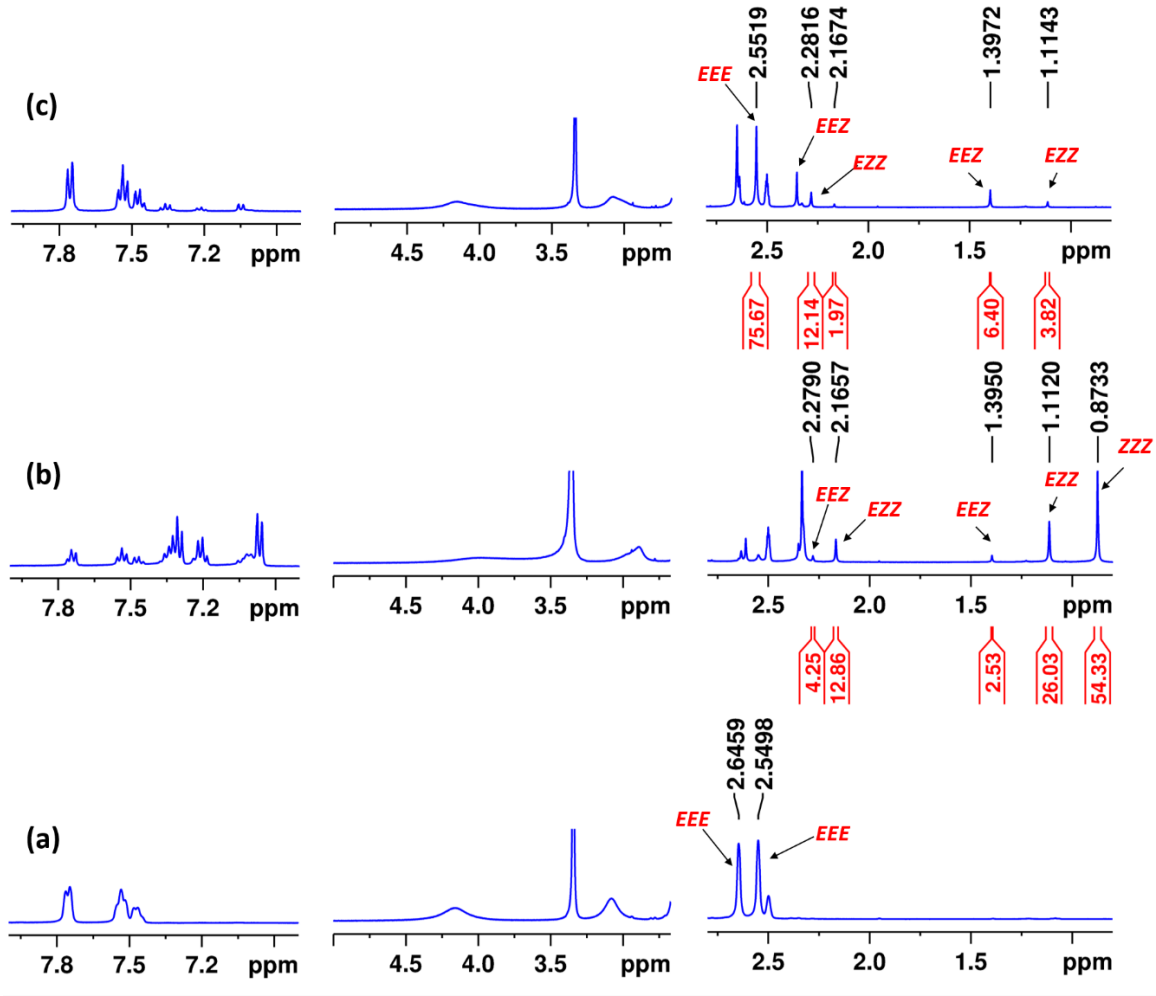


Figure S6.6. Analysis of photoswitching and estimation of PSS composition using ^{1}H-NMR spectroscopic studies of **C2** in [D_6]DMSO (7.2 mM) (a) before irradiation; (b) after irradiation at 365 nm; (c) after irradiation at 490 nm. (The normalized integral values corresponding to methyl signal were used for the estimation of PSS composition.)

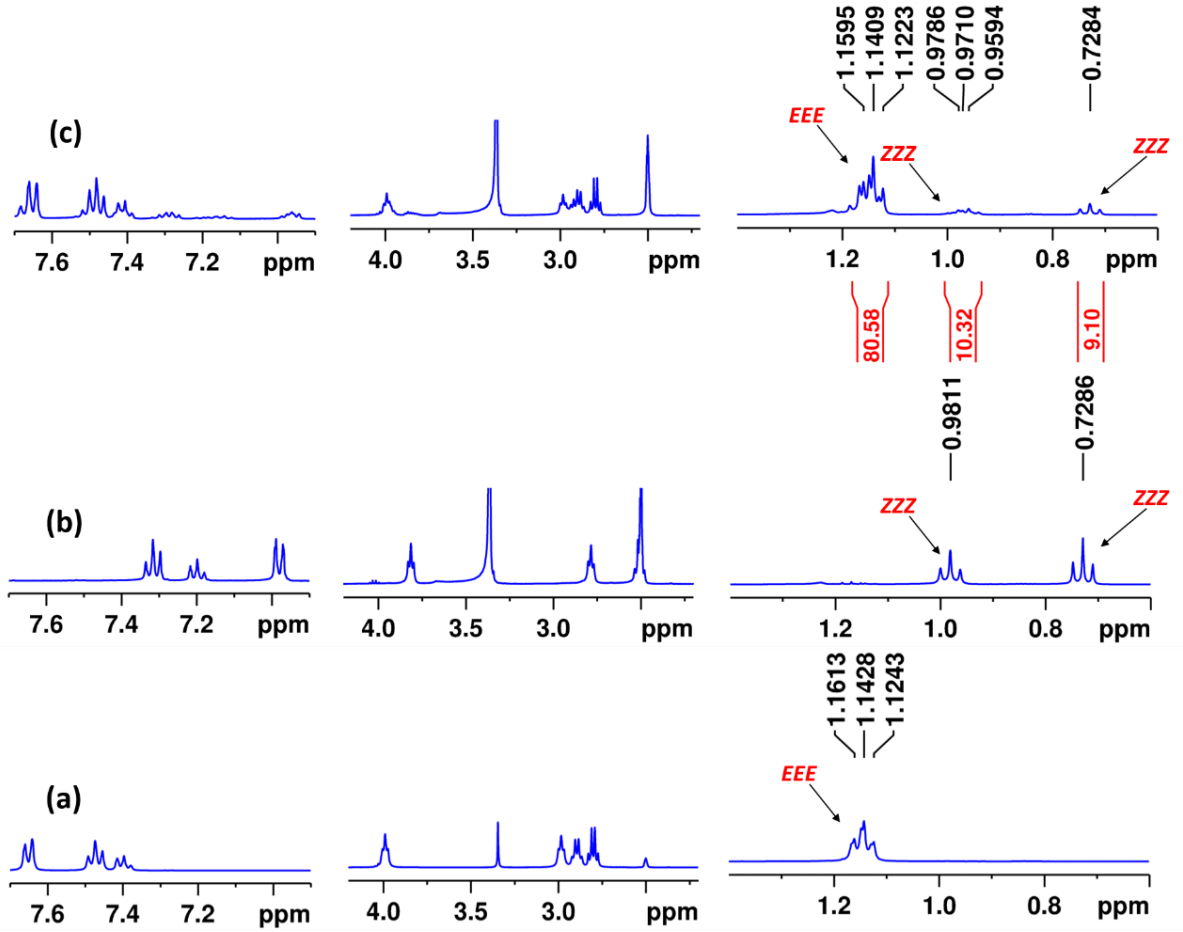


Figure S6.7. Analysis of photoswitching and estimation of PSS composition using ^{1}H-NMR spectroscopic studies of **L3** in [D_6]DMSO (6.5 mM) (a) before irradiation; (b) after irradiation at 365 nm; (c) after irradiation at 490 nm. (The normalized integral values corresponding to methyl proton signals of ethyl substituent was used for the estimation of PSS composition.)

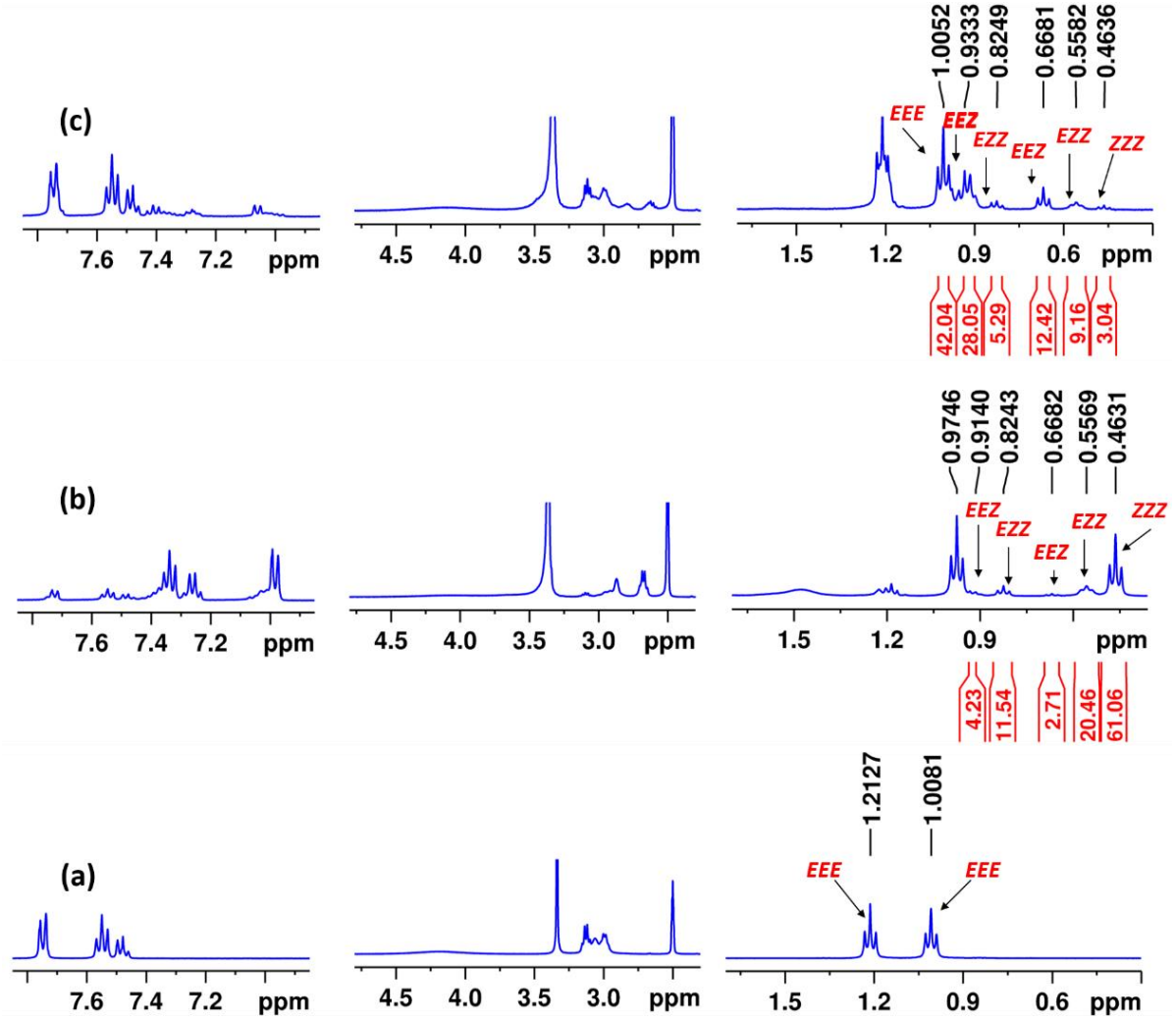


Figure S6.8. Analysis of photoswitching and estimation of PSS composition using ^{1}H-NMR spectroscopic studies of **C3** in [D_6]DMSO (7.6 mM) (a) before irradiation; (b) after irradiation at 365 nm; (c) after irradiation at 505 nm. (The normalized integral values corresponding to methyl proton signals of ethyl substituent was used for the estimation of PSS composition.)

S7: **Photocontrol of catalysis**

S7.A: Conditions for catalysis experiments with C1-PF_6:

Using *EEE*-C1-PF_6: Benzyl azide, **BzAz** 0.4 mmol and phenylacetylene, **PhAc**, 0.5 mmol were added to the reaction medium containing solid ***EEE*-C1-PF_6** (1 mol%) in 1 ml DMSO. The reaction was carried out at specified temperature for the specified time. No effort was made to perform the reaction in anaerobic conditions. For estimating percentage conversion by ^{1}H NMR spectroscopy, 10 μL aliquots were taken out of the reaction mixture under stirring, the volume was made up to 0.45 mL with [D_6]DMSO and ^{1}H NMR was recorded with that sample. The percentage conversion of triazole was estimated with respect to benzyl azide (Benzyl CH_2 protons were used for integration). For isolation of 1-benzyl-4-phenyltriazole (**Tz**), water was added to the reaction medium. The organic layer was extracted with ethyl acetate multiple times, concentrated after drying and evaporation, and purified by column chromatography using a mixture of 6:1 n-hexane:ethyl acetate as an eluent. The product **Tz** was isolated as a white solid, and the yield was calculated based on the equivalent of benzyl azide. **Tz2-Tz8** were isolated using similar procedures.

Using C1-PF_6@365 nm: A solution containing *EEE*- **C1-PF_6** (1 mol%) in 1 ml DMSO was irradiated at 365 nm for prolonged time to attain a photostationary state enriched with photoswitched isomers. Afterward, other reactants (benzyl azide, **BzAz**, 0.4 mmol; and phenylacetylene, **PhAc**, 0.5 mmol) were added to the reaction medium. The reaction was carried out at specified temperature for the specified time. No effort was made to perform the reaction in anaerobic conditions. For estimation of percentage conversion and for isolation of the product, previously mentioned procedures were adapted. **Tz2** and **Tz3** were isolated using the same procedure.

For reactions catalyzed by *EEE*-**C2, C2@365** nm and *EEE*-**C3, C3@365** nm, similar procedures were adopted. For reactions involving *in-situ* formation of Cu(I) catalyst, *EEE*-**L1** (1 mol%) and $Cu(CH_3CN)_4PF_6$ (1 mol%) were mixed in 1 mL DMSO and allowed to stir for half an hour before adding the reactants. For the reaction catalyzed by the photoswitched isomer, *EEE*-**L1** in 1 mL DMSO was subjected to irradiation at 365 nm, followed by addition of the Cu(I) salt, and the addition of other reactants.

S7.B. Control experiments and miscellaneous points:

1. The catalysis experiments with *EEE*-**C1-PF_6** and **C1-PF_6@365 nm** was carried out with the same stock solution. For example, a 2 mL of solution of **C1-PF_6** (1 mol%) was prepared**.** 1 ml of the solution (as prepared) was utilized for the reaction with ***EEE*-C1-PF_6.** The rest of the solution (1 mL) was irradiated at 365 nm to achieve PSS and then used for the catalysis with **C1-PF_6@365 nm.** Also, reproducibility of the reactions was thoroughly tested.
2. To ensure that the reactants did not decompose under heating or irradiation conditions, the mixture of reactants and products (without catalyst) was heated at 60 °C for 3-4 hours under irradiation. While no product was formed, no decomposition of reactants was observed in ^{1}H NMR spectra. We carried out a control reaction with $Cu(CH_3CN)_4PF_6$, which showed no increase in activity upon irradiation at 365 nm. The reactants (individually and as a mixture) were screened for decomposition upon prolonged irradiation at UV light. It is important to note that, performing azide-alkyne cycloaddition under UV irradiation has previously been used to reduce Cu(II) to Cu(I) within the reaction medium itself.
3. Varying the solvent did not have any pronounced effect on the yield of the reaction. However, DMSO was used to track the % conversion (by ^{1}H NMR) since we explored the

photoisomerization of **C1-PF$_6$** in DMSO and [D$_6$]DMSO (by UV-Vis and NMR spectroscopy, respectively). Similar studies carried out in CD$_3$CN also showed a similar trend of the photoswitched isomer accelerating the reaction.

4. During forward isomerization of **C1-PF$_6$**, similar PSS was obtained after irradiation at 340 nm and 365 nm. 365 nm light source was eventually selected for investigating phototriggered modulation of catalytic activity of **C1-PF$_6$** since this was more intense.
5. For **Tz1**-**Tz2**, the reaction was continued at 22 or 25 ^{o}C for 420 minutes since we evaluated the progress of the reactions with the help of ^{1}H NMR spectroscopy. For rest of the substrates, the reaction was continued under optimized conditions (60 ^{O}C, 540 minutes). The progress of the reaction for these substrates was evaluated with the help of isolated yield only.

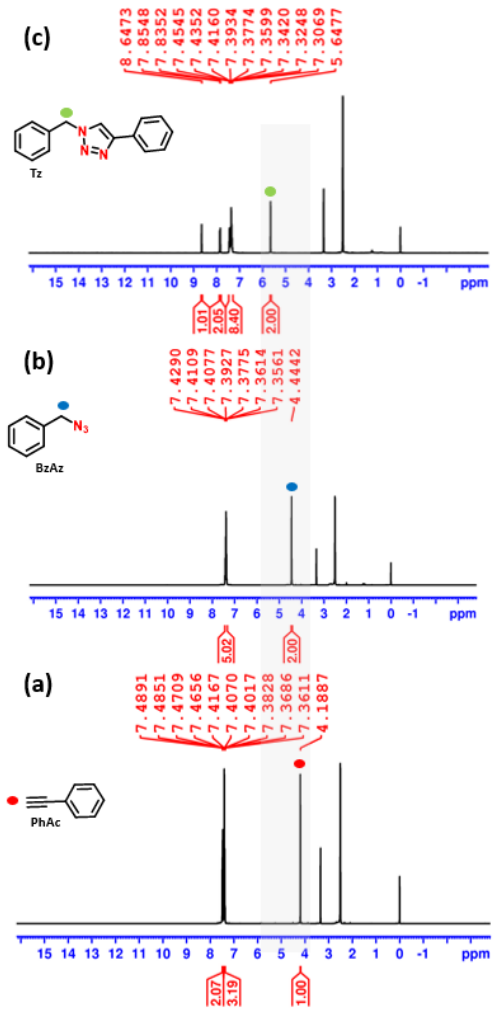


Figure S7.1. ^{1}H NMR spectra (in [D$_6$]DMSO) for (a) phenylacetylene (**PhAc**); (b) benzyl Azide (**BzAz**) and (c) 1-benzyl-4-phenyltriazole (**Tz**). For tracking the progress of CuAAC reaction, following protons have been considered: alkyne proton for (a) **PhAc** (highlighted, red dot), (b) -CH$_2$ proton for **BzAz** (highlighted, blue dot), and (c) -CH$_2$ proton for 1-benzyl-4-phenyltriazole, **Tz** (highlighted, green dot). For estimation of %conversion of product 1-benzyl-4-phenyltriazole (**Tz**), -CH$_2$ protons for **BzAz** (limiting reagent) and the product **Tz** have been integrated.

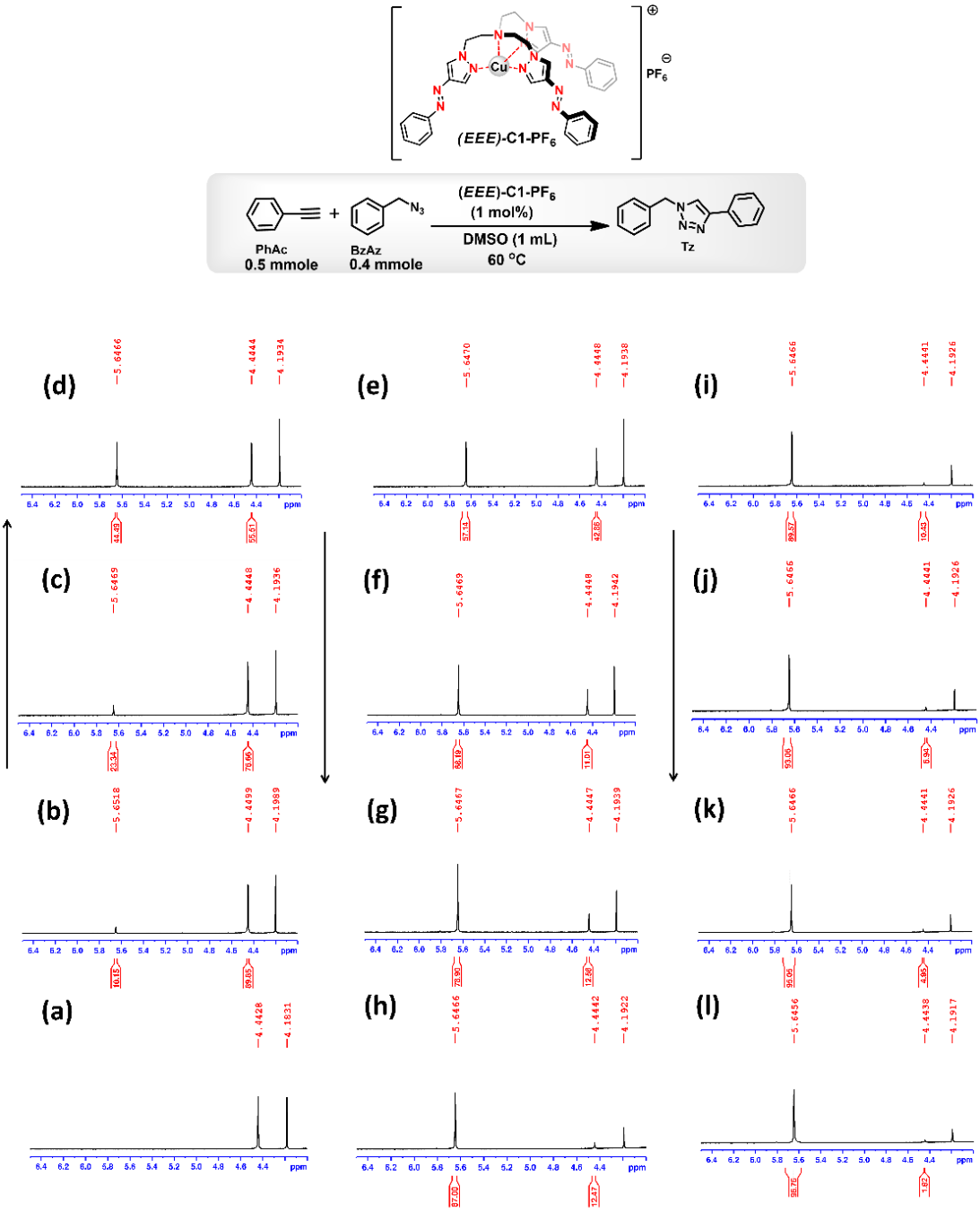


Figure S7.2. ^{1}H NMR spectra (in [D_6]DMSO) depicting the percentage conversion of product with time in CuAAC reaction catalyzed by *EEE*-**C1-PF$_6$** between **PhAc** and **BzAz** in DMSO at 60 °C; (a) 0 minutes; (b) 15 minutes; (c) 30 minutes; (d) 60 minutes; (e) 90 minutes; (f) 120 minutes; (g) 180 minutes; (h) 240 minutes; (i)300 minutes; (j) 360 minutes; (k) 420 minutes; (l) 480 minutes.

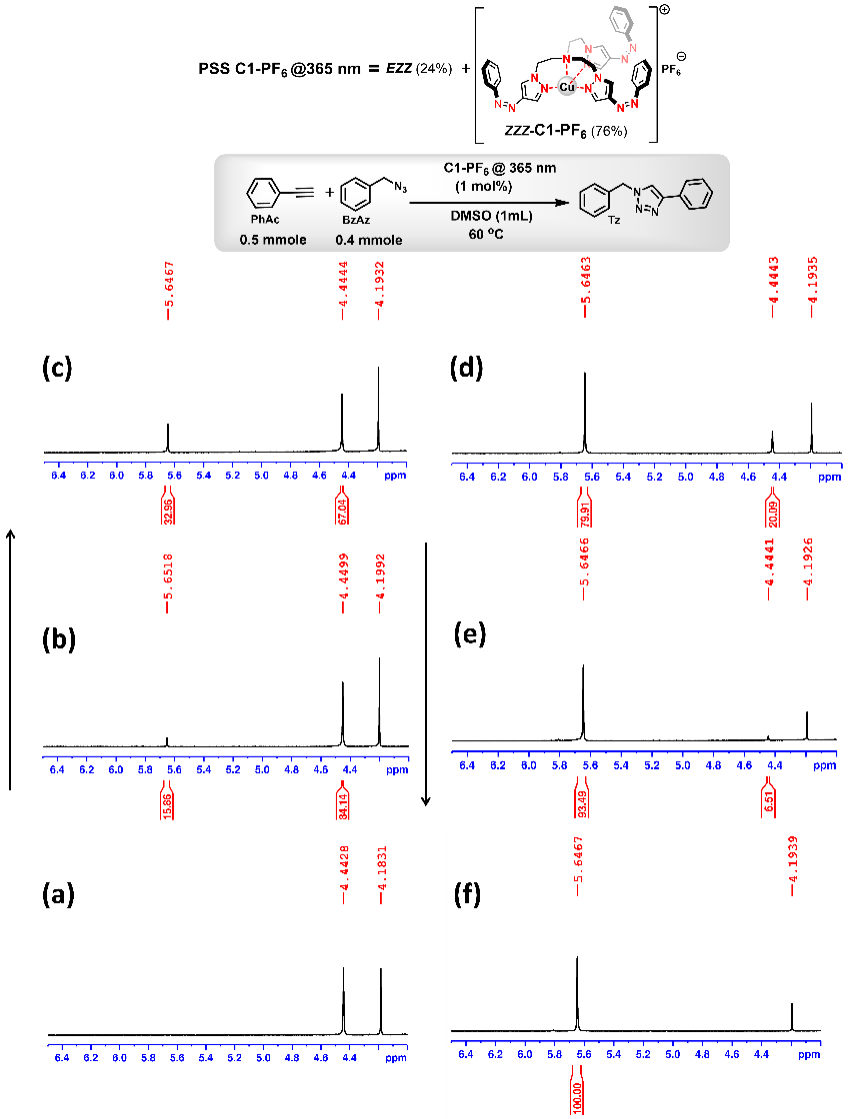


Figure S7.3. ^{1}H NMR (in [D_6]DMSO) spectra depicting the percentage conversion of product with time in CuAAC reaction catalyzed by **C1-PF$_6$** @365 nm between PhAc and BzAz in DMSO at 60 ^{o}C; (a) 0 minutes; (b) 15 minutes; (c) 30 minutes; (d) 60 minutes; (e) 90 minutes; (f) 120 minutes.

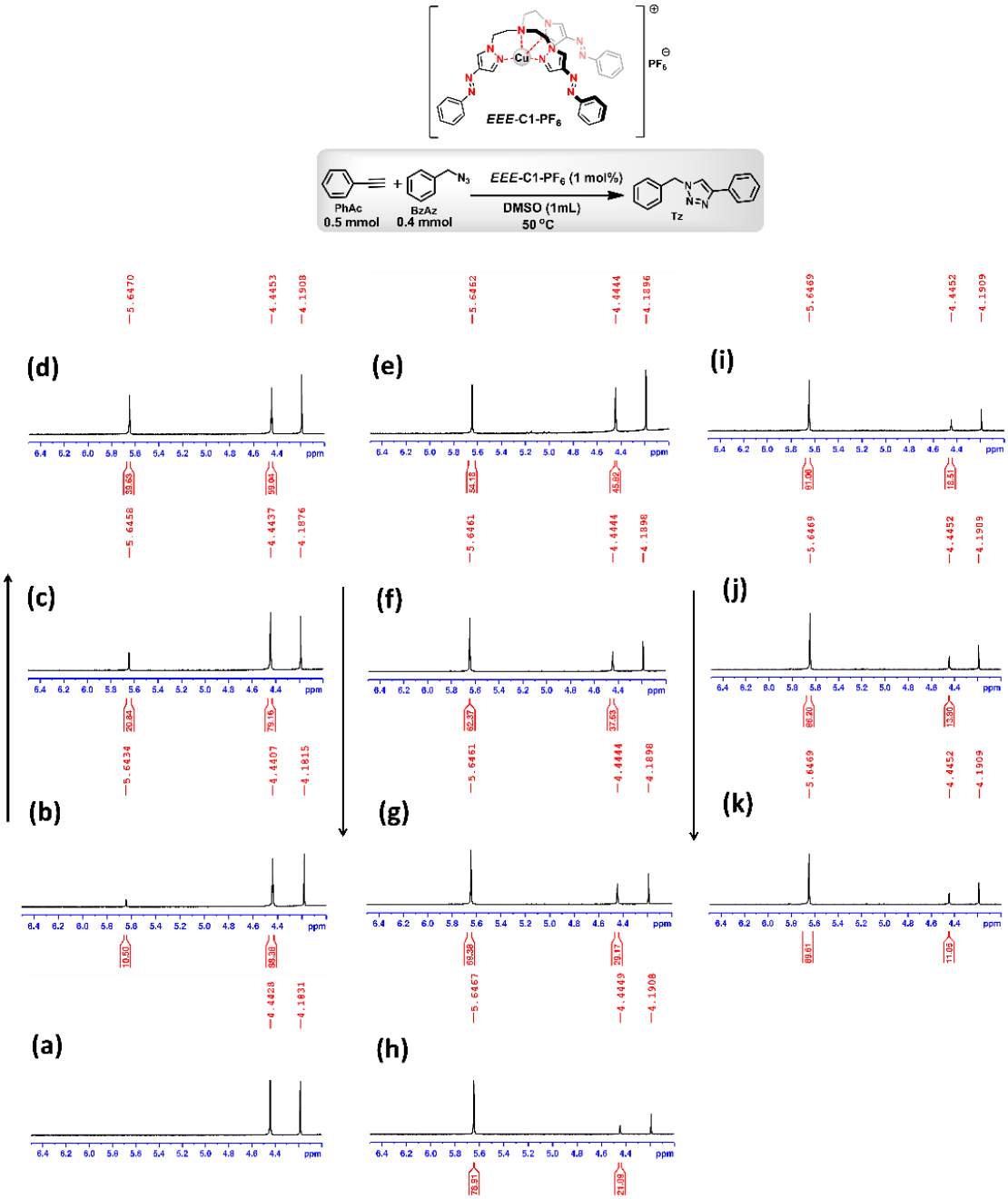


Figure S7.4. ^{1}H NMR (in [D_6]DMSO) spectra depicting the percentage conversion of product with time in CuAAC reaction catalyzed by *EEE*-**C1-PF$_6$** between **PhAc** and **BzAz** in DMSO at 50 °C; (a) 0 minutes; (b) 20 minutes; (c) 50 minutes; (d) 110 minutes; (e) 170 minutes; (f) 230 minutes; (g) 290 minutes; (h) 410 minutes; (i) 470 minutes; (j) 530 minutes; (k) 590 minutes.

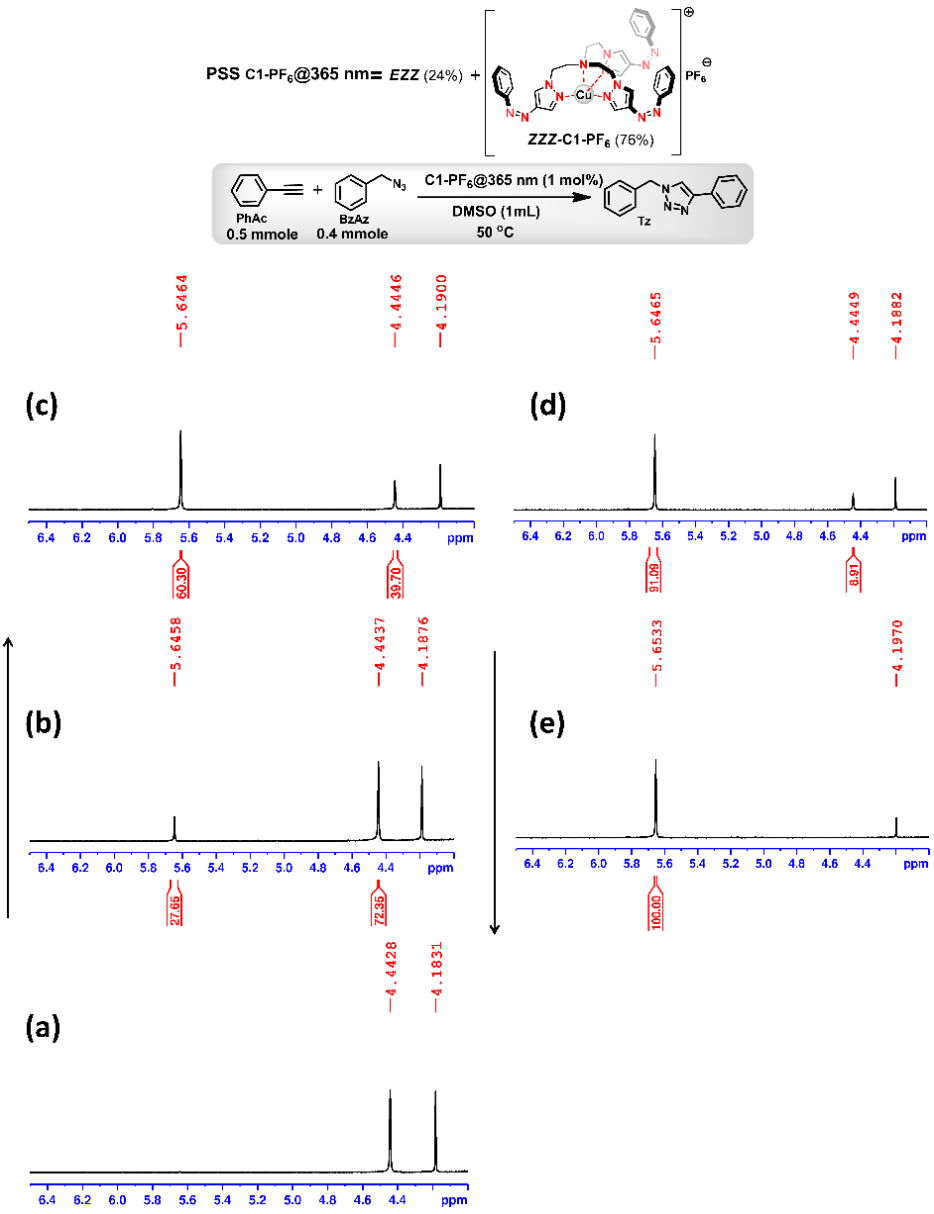


Figure S7.5a. ^{1}H NMR spectra (in [D_6]DMSO) depicting the percentage conversion of product with time in CuAAC reaction catalyzed by **C1-PF_6 @365 nm** between **PhAc** and **BzAz** in DMSO at 50 ^{o}C; (a) 0 minutes; (b) 20 minutes; (c) 50 minutes; (d) 110 minutes; (e) 170 minutes.

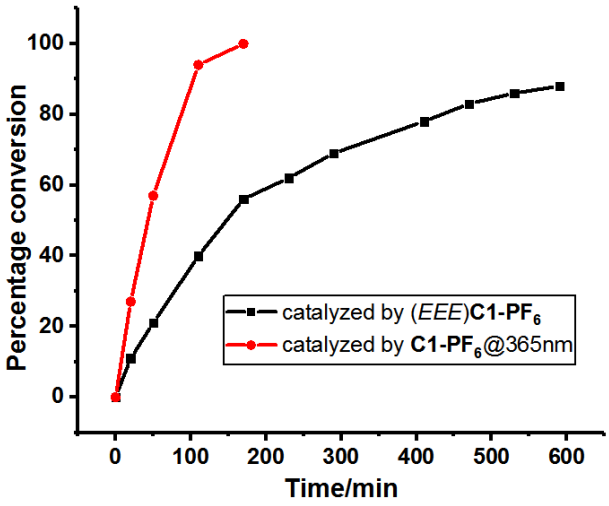


Figure S7.5b. Time evolution profiles depicting the catalytic activity of *EEE*-**C1-PF$_6$**, and *EEE*-**C1-PF$_6$**@365 nm, in CuAAC reaction in [D$_6$]DMSO at 50 °C

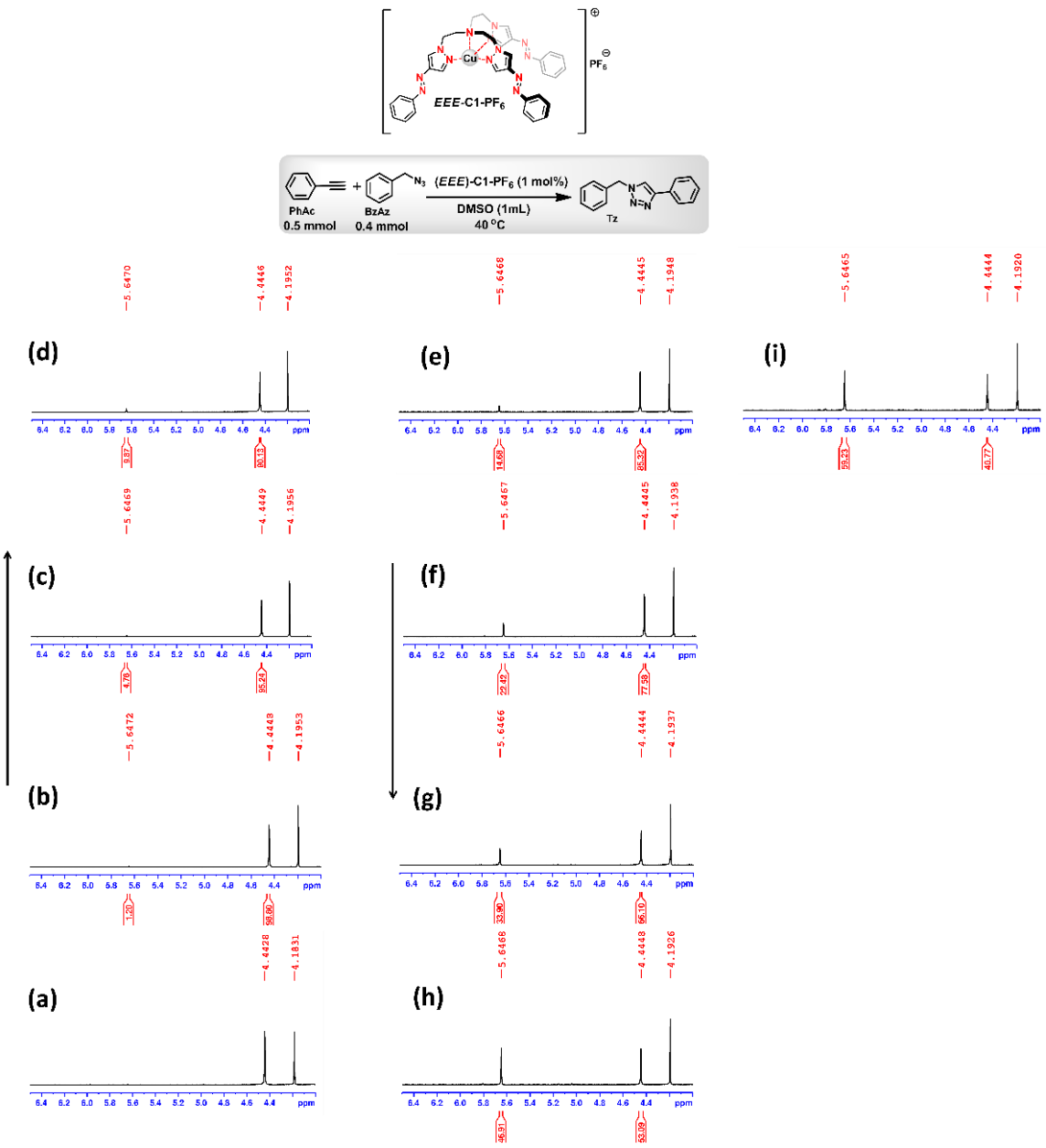


Figure S7.6. ^{1}H NMR (in [D_6]DMSO) spectra depicting the percentage conversion of product with time in CuAAC reaction catalyzed by **C1-PF$_6$** between **PhAc** and **BzAz** in DMSO at 40 °C; (a) 0 minutes; (b) 30 minutes; (c) 60 minutes; (d) 120 minutes; (e) 180 minutes; (f)300 minutes; (g) 420 minutes; (h) 540 minutes; (i) 600 minutes.

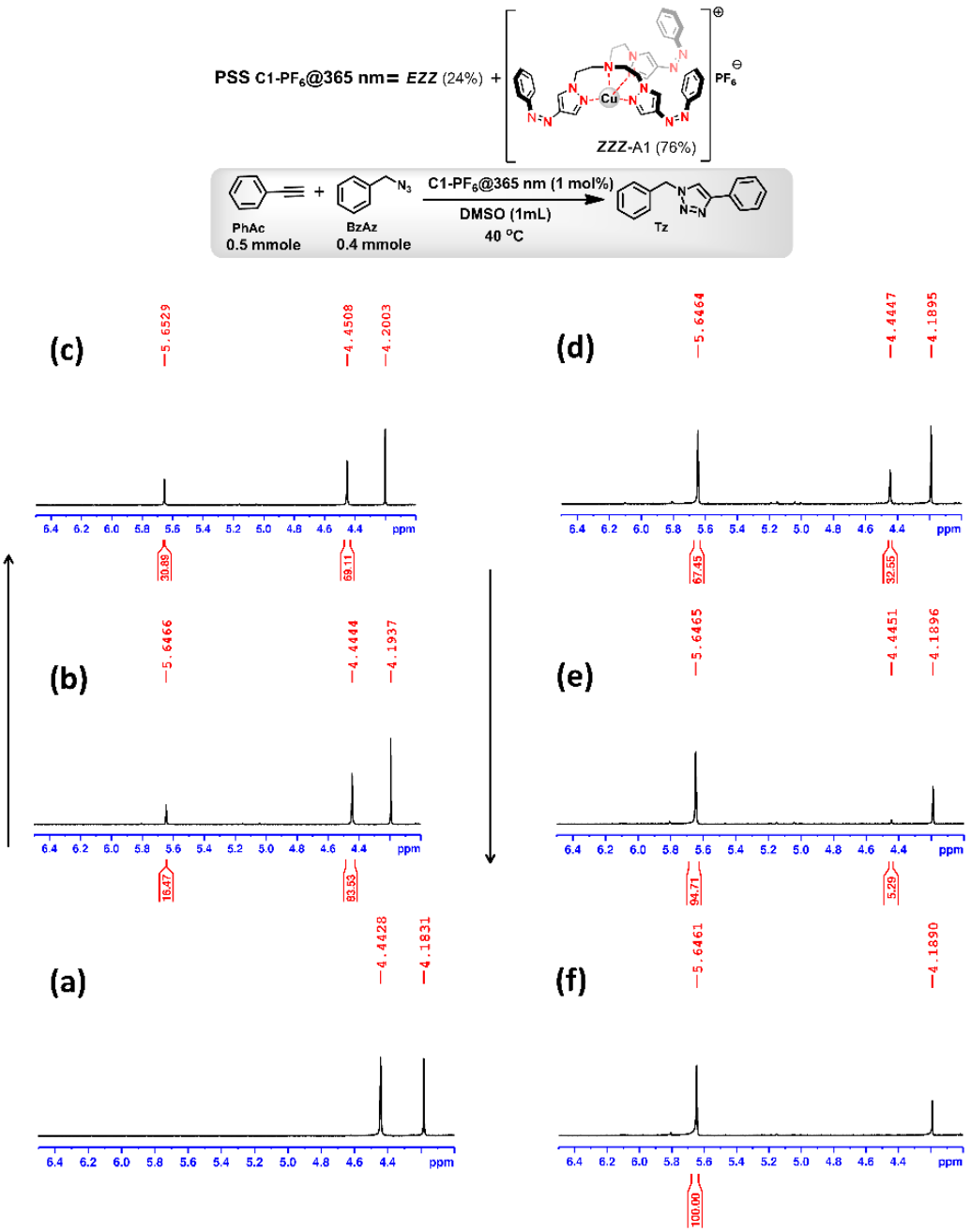


Figure S7.7. ^{1}H NMR (in [D_6]DMSO) spectra depicting the percentage conversion of product with time in CuAAC reaction catalyzed by **C1-PF_6 @365 nm** between **PhAc** and **BzAz** in DMSO at 40 °C; (a) 0 minutes; (b) 60 minutes; (c) 120 minutes; (d) 240 minutes; (e) 360 minutes; (f) 480 minutes.

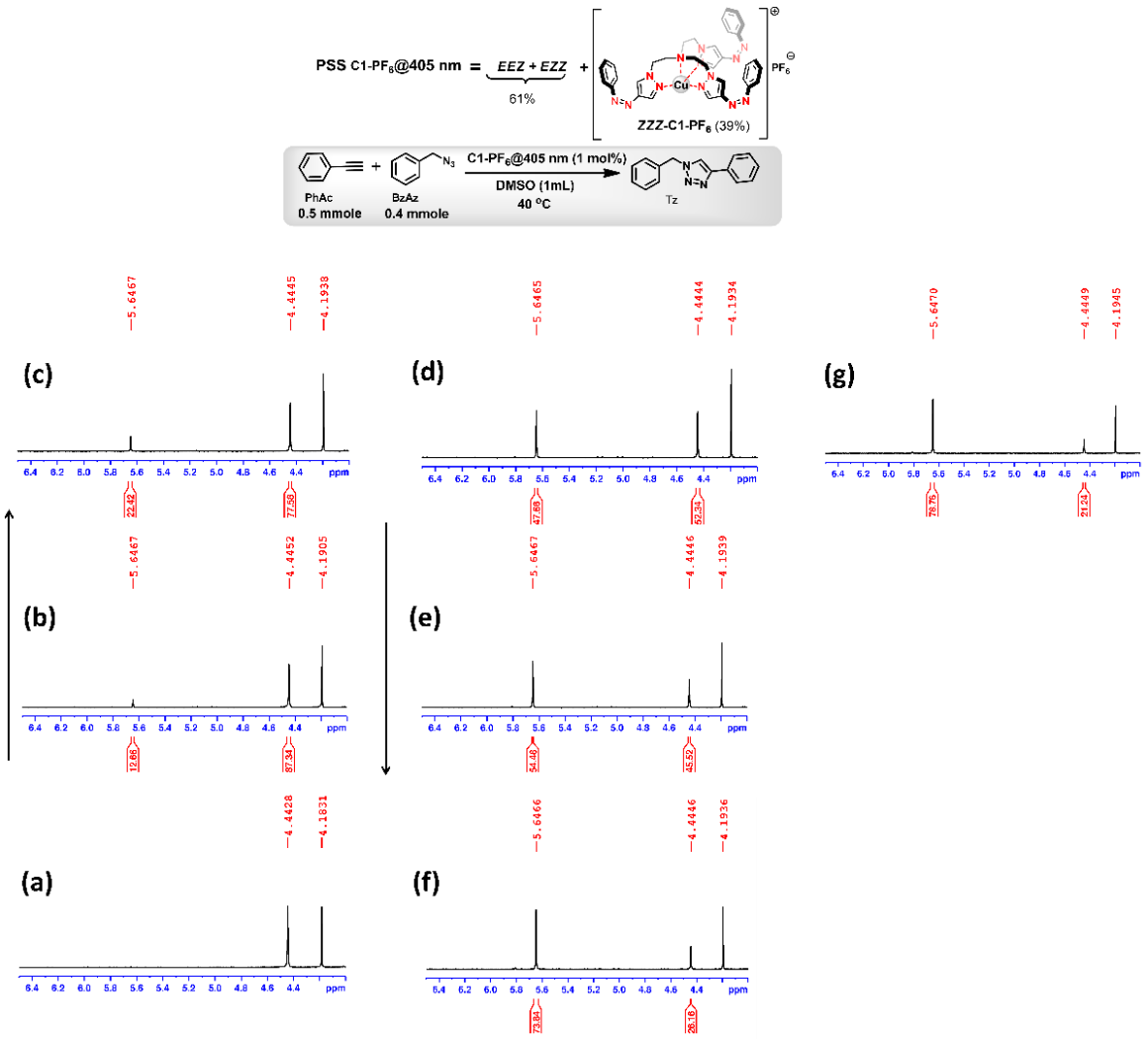


Figure S7.8. ^{1}H NMR (in $[D_6]$DMSO) spectra depicting the percentage conversion of product with time in CuAAC reaction catalyzed by **C1-PF$_6$ @405 nm** between **PhAc** and **BzAz** in DMSO at 40 °C; (a) 0 minutes; (b) 60 minutes; (c) 120 minutes; (d) 240 minutes; (e) 360 minutes; (f) 480 minutes; (g) 600 minutes.

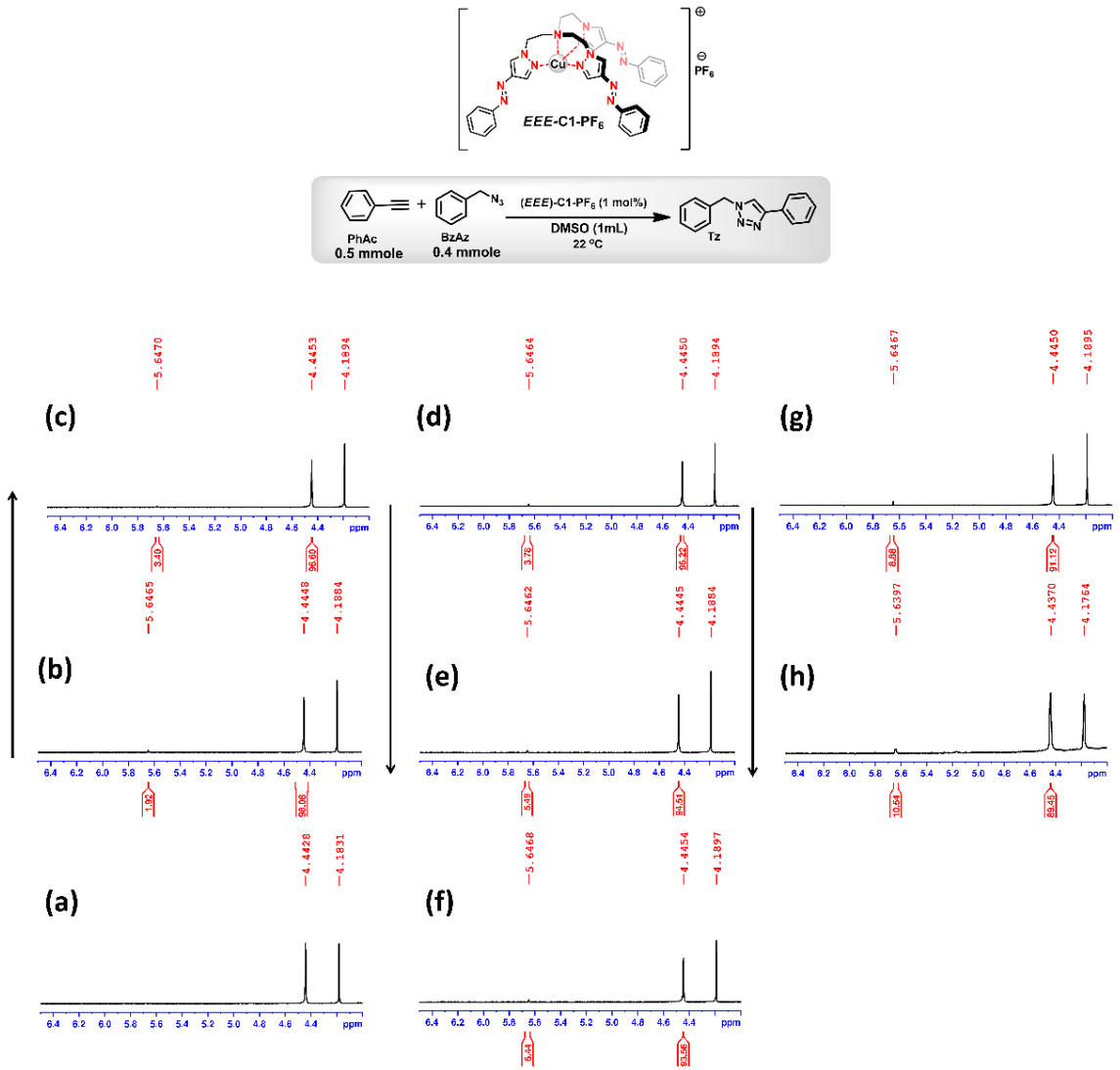


Figure S7.9. ^{1}H NMR (in [D_6]DMSO) spectra depicting the percentage conversion of product with time in CuAAC reaction catalyzed by *EEE*- **C1-PF$_6$** between **PhAc** and **BzAz** in DMSO at 22 °C; (a) 0 minutes; (b) 60 minutes; (c) 120 minutes; (d) 240 minutes; (e) 360 minutes; (f) 480 minutes; (g) 600 minutes; (h) 720 minutes.

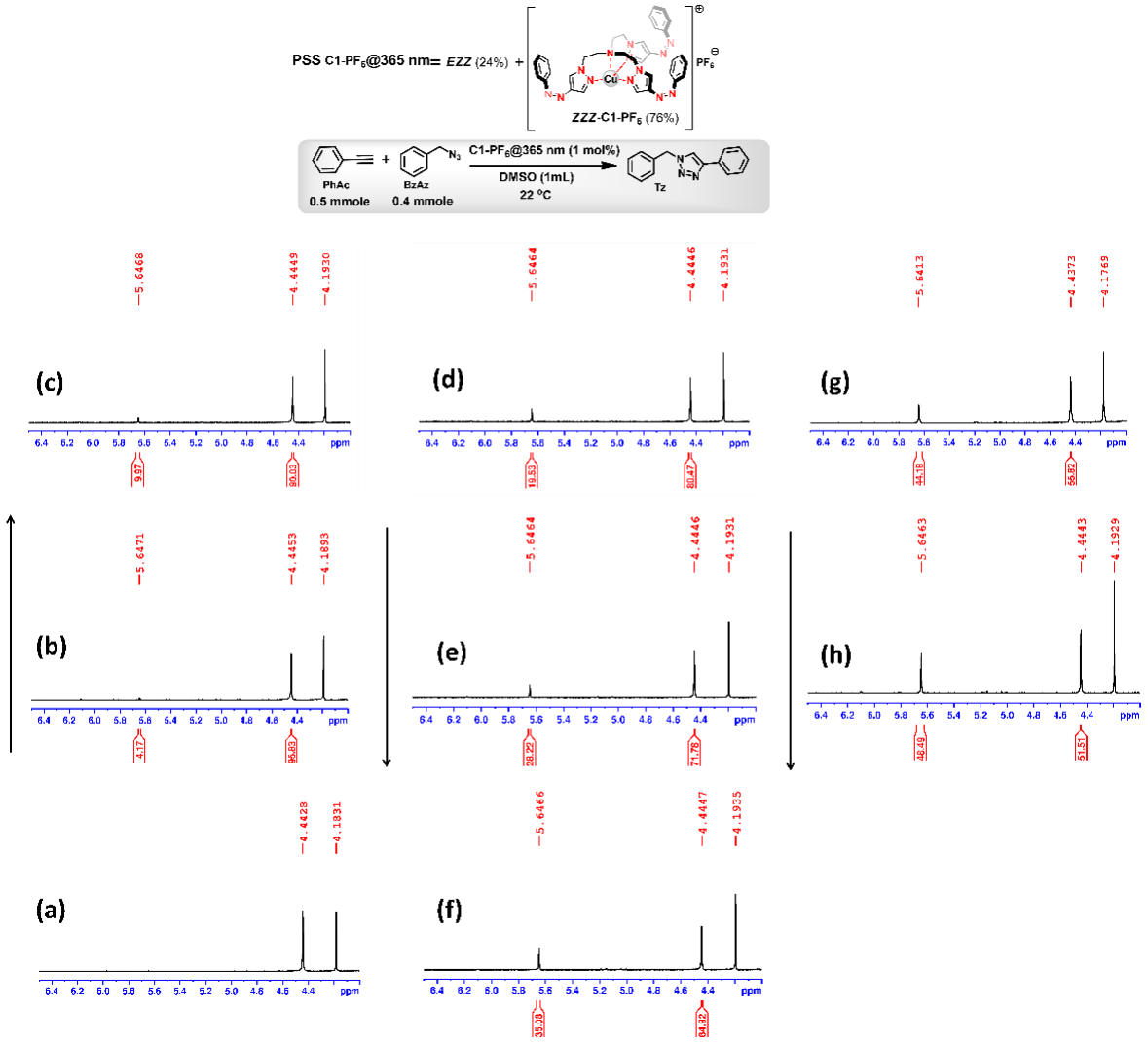


Figure S7.10a. ^{1}H NMR (in [D_6]DMSO) spectra depicting the percentage conversion of product with time in CuAAC reaction catalyzed by **C1-PF_6@365 nm** between **PhAc** and **BzAz** in DMSO at 22 °C; (a) 0 minutes; (b) 60 minutes; (c) 120 minutes; (d) 240 minutes; (e) 360 minutes; (f) 480 minutes; (g) 600 minutes; (h) 720 minutes.

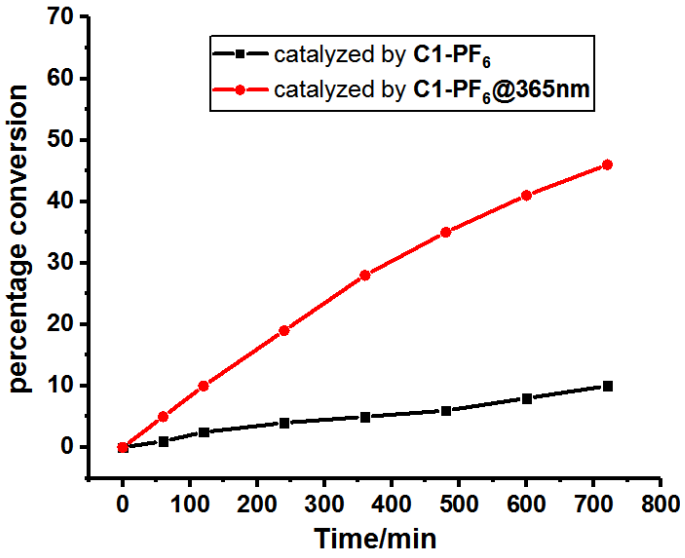


Figure S7.10b. Time evolution profiles depicting the catalytic activity of *EEE*-**C1-PF$_6$**, and *EEE*-**C1-PF$_6$**@365 nm, in CuAAC reaction in [D_6]DMSO at 22 °C

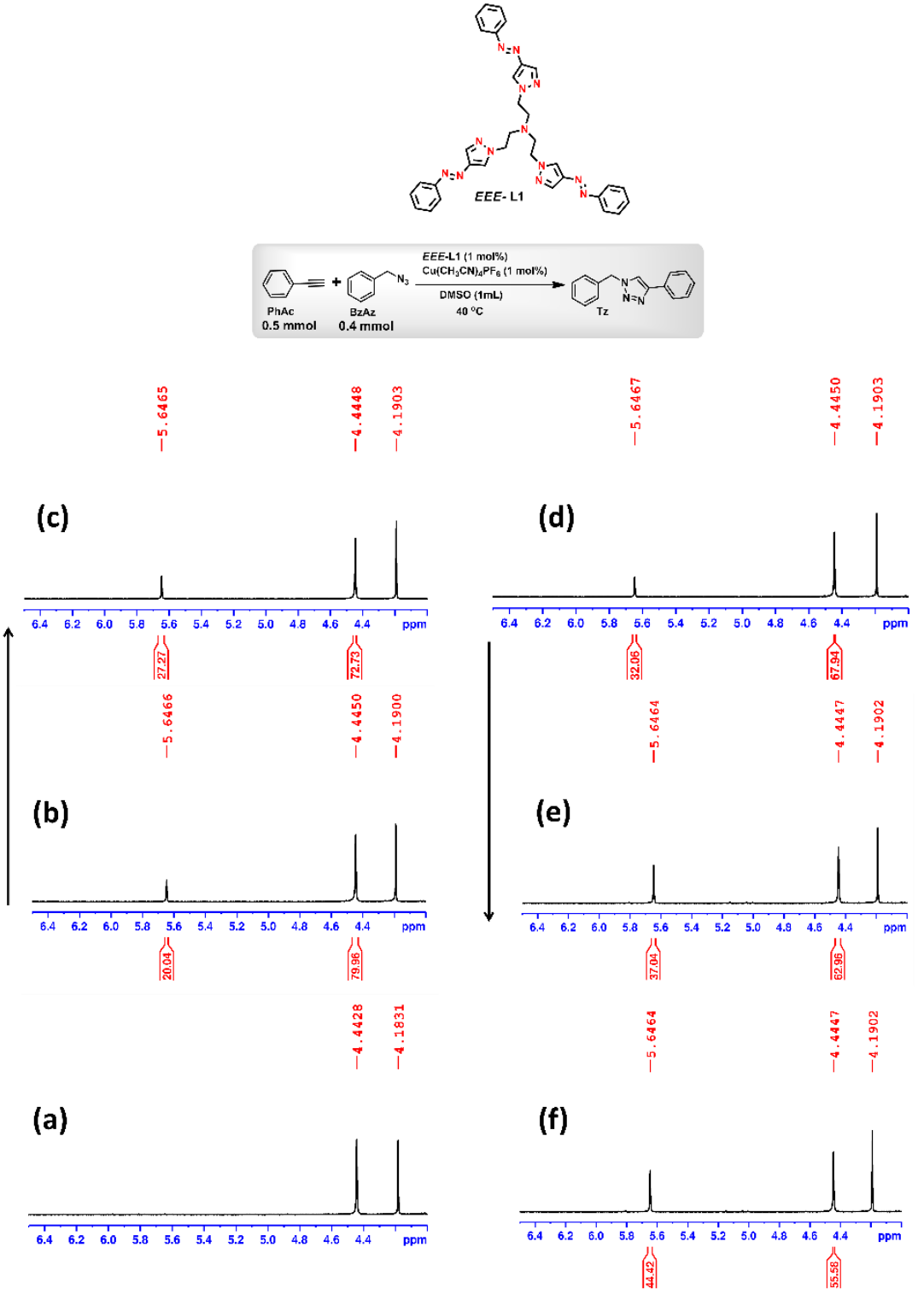


Figure S7.11. ^{1}H NMR (in [D_6]DMSO) spectra depicting the percentage conversion of product with time in CuAAC reaction catalyzed by **L1** and $Cu(CH_3CN)_4PF_6$ between **PhAc** and **BzAz** in DMSO at 40 °C; (a) 0 minutes; (b) 30 minutes; (c) 60 minutes; (d) 120 minutes; (e) 180 minutes; (f) 300 minutes.

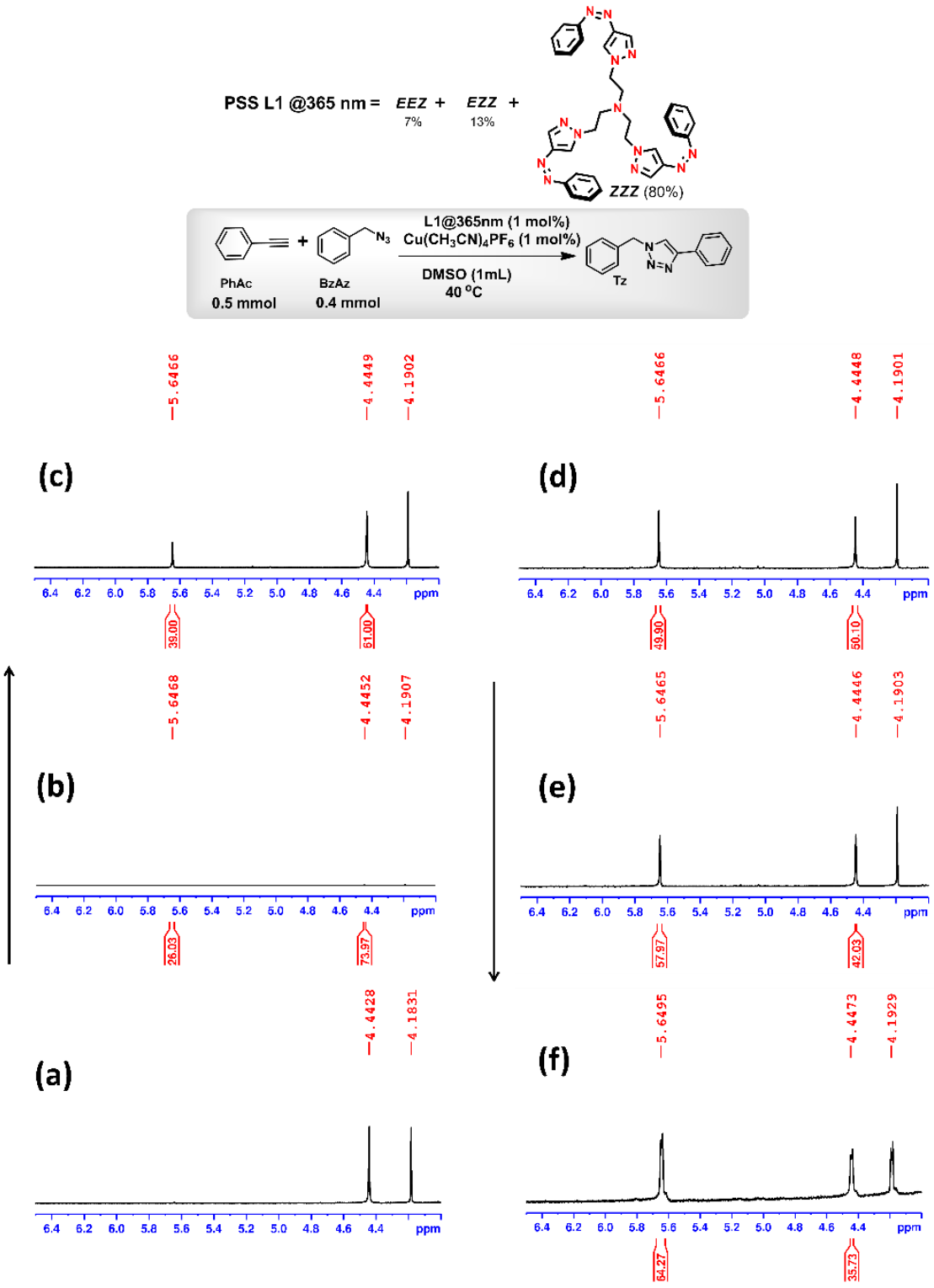


Figure S7.12a. ^{1}H NMR spectra (in [D_6]DMSO) depicting the percentage conversion of product with time in CuAAC reaction catalyzed by **L1@365 nm** and $Cu(CH_3CN)_4PF_6$ between **PhAc** and **BzAz** in DMSO at 40 °C; (a) 0 minutes; (b) 30 minutes; (c) 60 minutes; (d) 120 minutes; (e) 180 minutes; (f) 300 minutes.

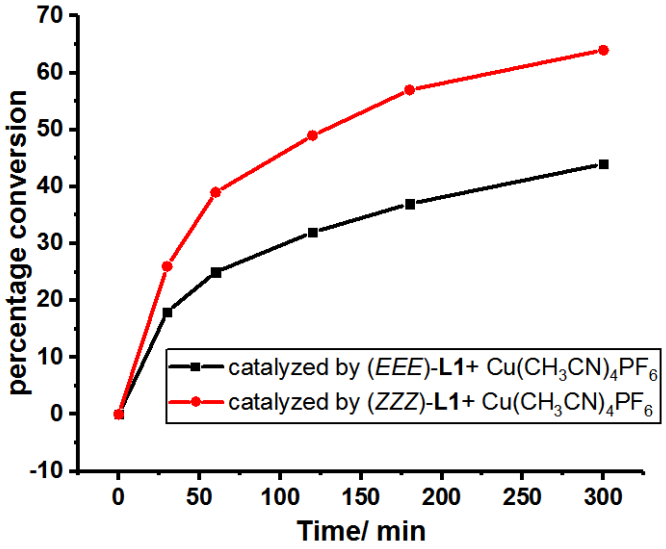


Figure S7.12b. Time evolution profiles depicting the catalytic activity of [*EEE*-**L1** + $Cu(CH_3CN)_4PF_6$], [*EEE*-**L1**@365 nm+ $Cu(CH_3CN)_4PF_6$], in Cu-catalyzed azide alkyne cycloaddition reaction between PhAc and BzAz in DMSO at 40 °C

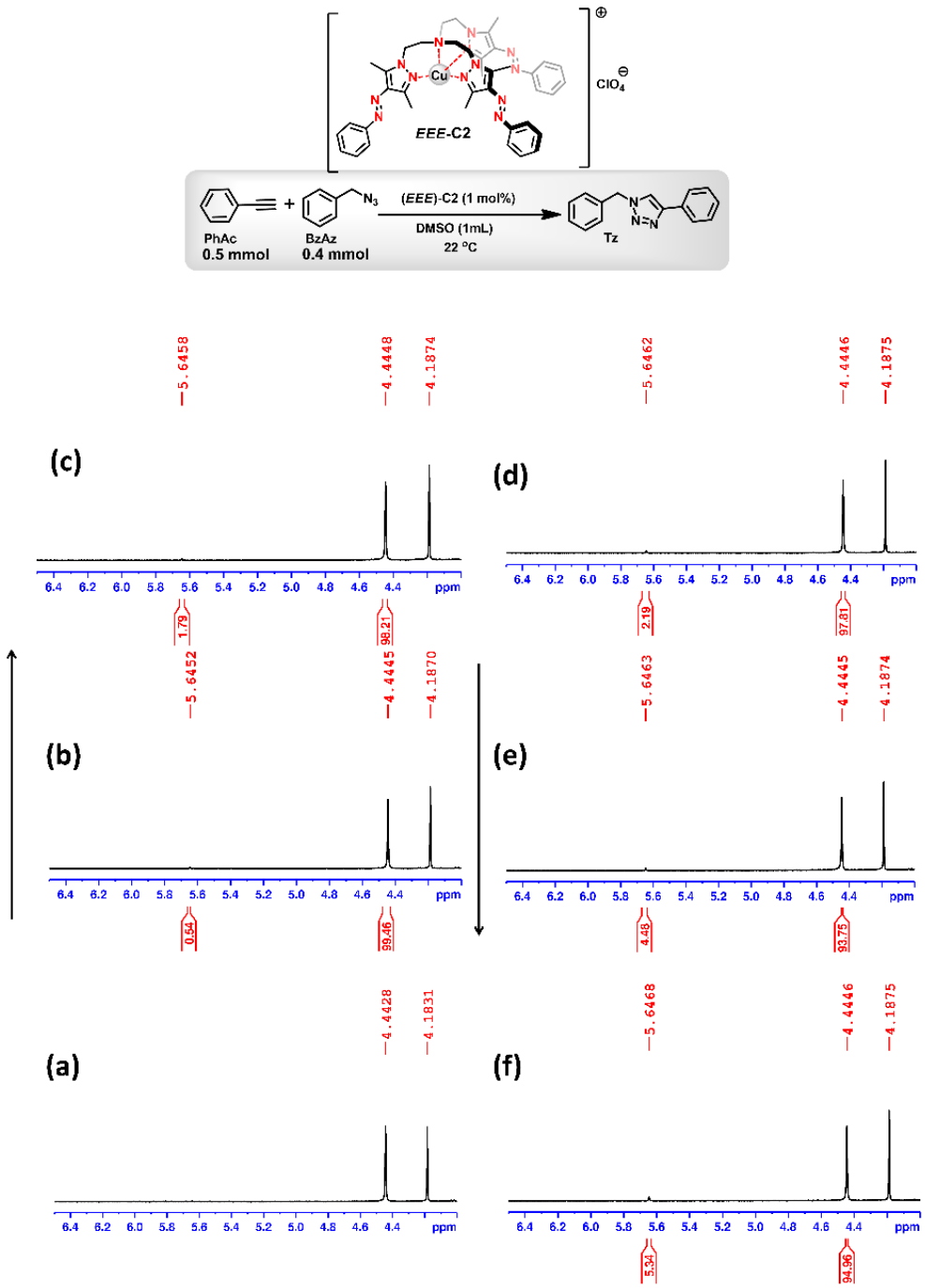


Figure S7.13. ^{1}H NMR (in [D_6]DMSO) spectra depicting the percentage conversion of product with time in CuAAC reaction catalyzed by **C2** between **PhAc** and **BzAz** in DMSO at 60 °C; (a) 0 minutes; (b) 30 minutes; (c) 60 minutes; (d) 90 minutes; (e) 120 minutes; (f) 180 minutes.

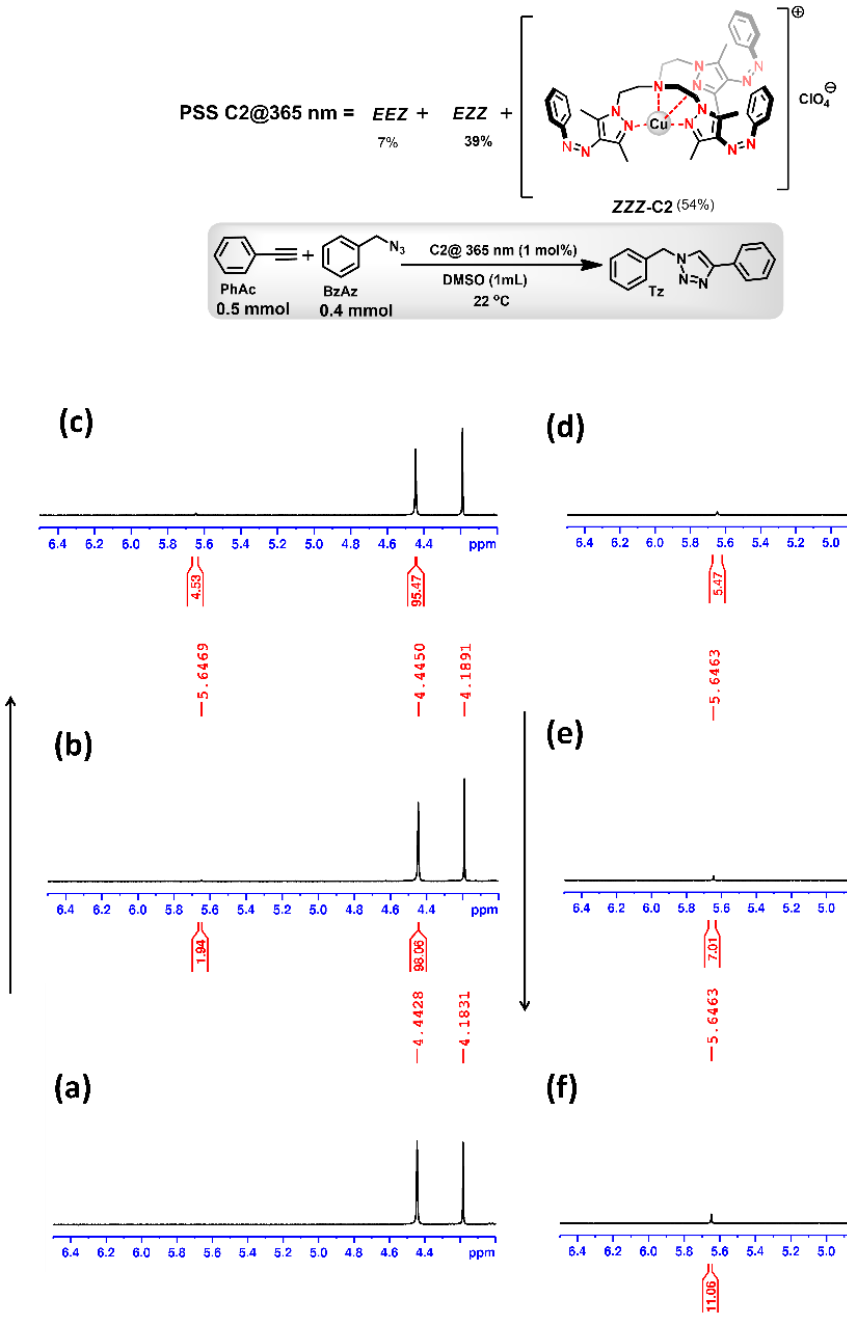


Figure S7.14a. ^{1}H NMR spectra (in [D_6]DMSO) depicting the percentage conversion of product with time in CuAAC reaction catalyzed by **C2@365 nm** between **PhAc** and **BzAz** in DMSO at 60 °C; (a) 0 minutes; (b) 30 minutes; (c) 60 minutes; (d) 90 minutes; (e) 120 minutes; (f) 180 minutes.

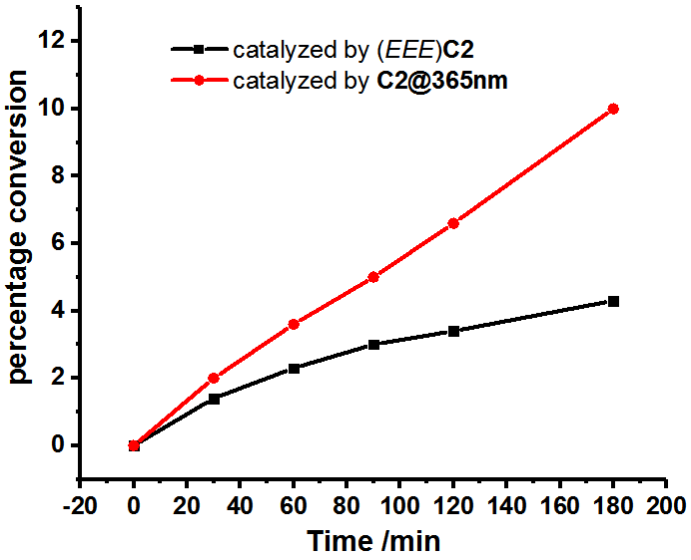


Figure S7.14b. Time evolution profiles depicting the catalytic activity of *EEE*-**C2**, *EEE*-**C2**@365 nm in Cu-catalyzed azide alkyne cycloaddition (CuAAC) reaction between **PhAc** and **BzAz** in DMSO at 60 °C

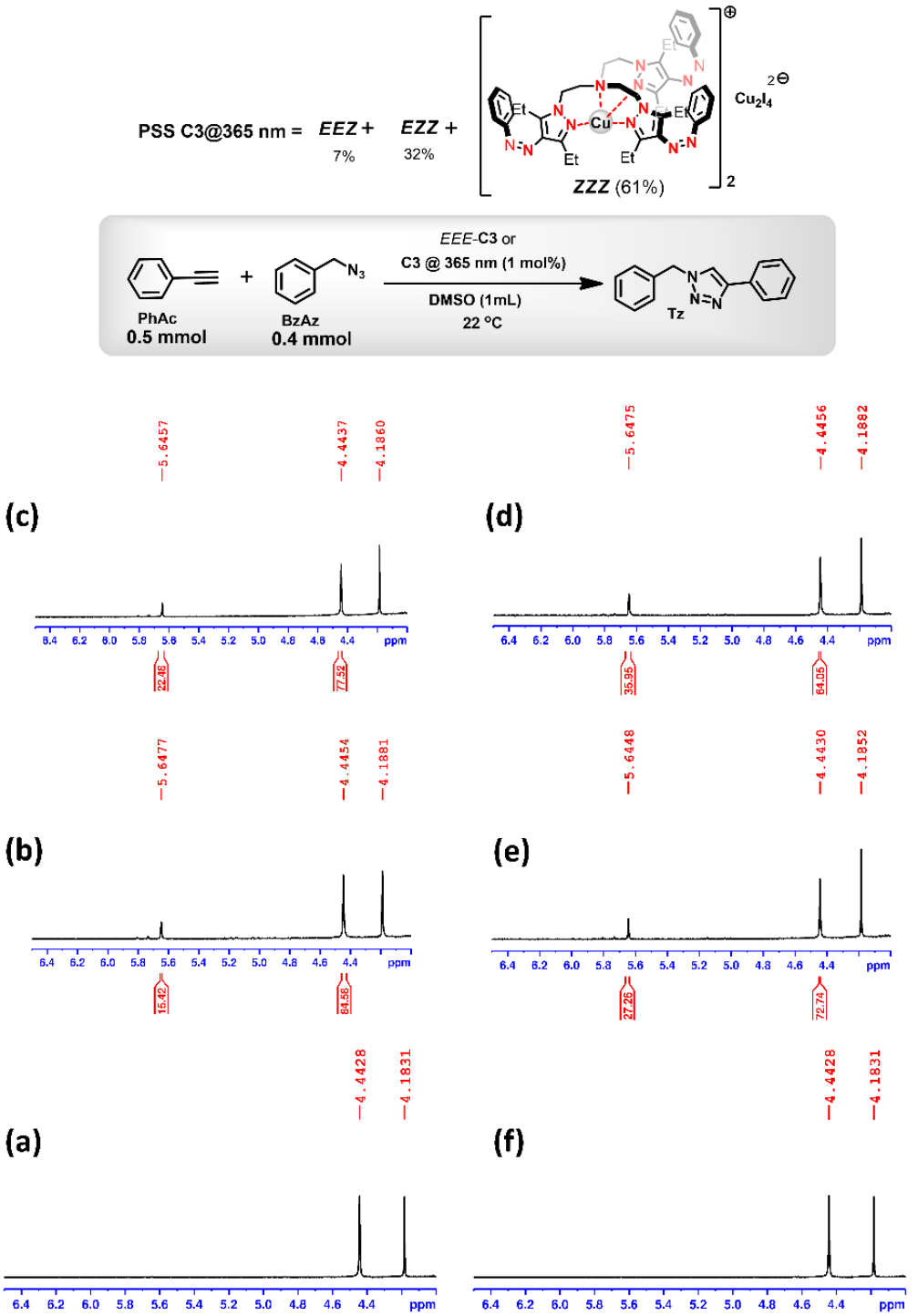


Figure S7.15a. ^{1}H NMR (in [D_6]DMSO) spectra depicting the percentage conversion of product with time in CuAAC reaction catalyzed by **C3** between **PhAc** and **BzAz** in DMSO at 25 °C; (a) 15 minutes; (b) 30 minutes; ^{1}H NMR spectra depicting the percentage conversion of product with time in CuAAC reaction catalyzed by **C3@365 nm** between **PhAc** and **BzAz** in DMSO at 25 °C; (c) 15 minutes; (d) 30 minutes.

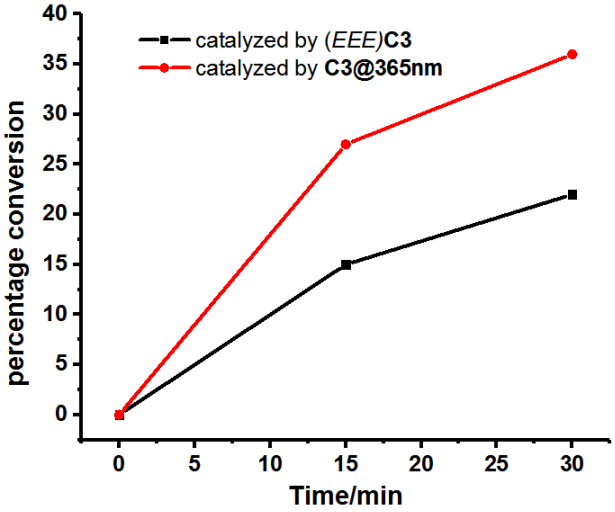


Figure S7.15b. Time evolution profiles depicting the catalytic activity of *EEE*-**C3**, *EEE*-**C3**@365 nm in Cu-catalyzed azide alkyne cycloaddition (CuAAC) reaction between **PhAc** and **BzAz** in DMSO at 25 °C

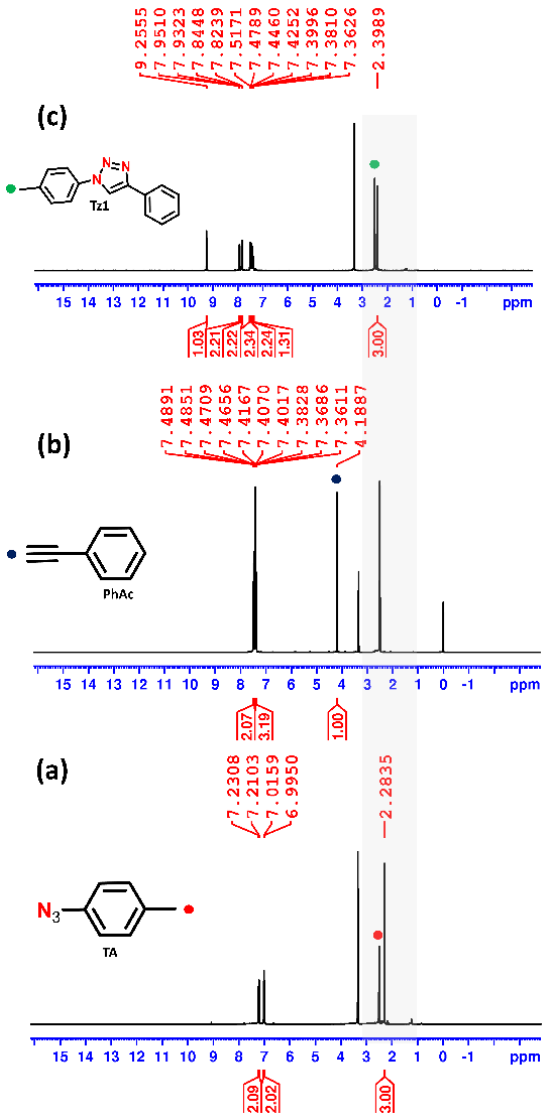


Figure S7.16. ^{1}H NMR spectra (in [D_6]DMSO) for (a) phenylacetylene (**PhAc**); (b) 4-methylphenyl azide (TA) (c) 4-phenyl-1-(*p*-tolyl)-1*H*-1,2,3-triazole (**Tz2**). For tracking the progress of CuAAC reaction, following protons have been considered, (a) -CH_3 proton for **TA** (red dot), (b) alkyne proton for **PhAc** (blue dot), and (c) -CH_2 proton for **Tz2** (highlighted, green dot). For estimation of %conversion of product **Tz2**, -CH_3 protons for **TA** and **Tz2** have been integrated.

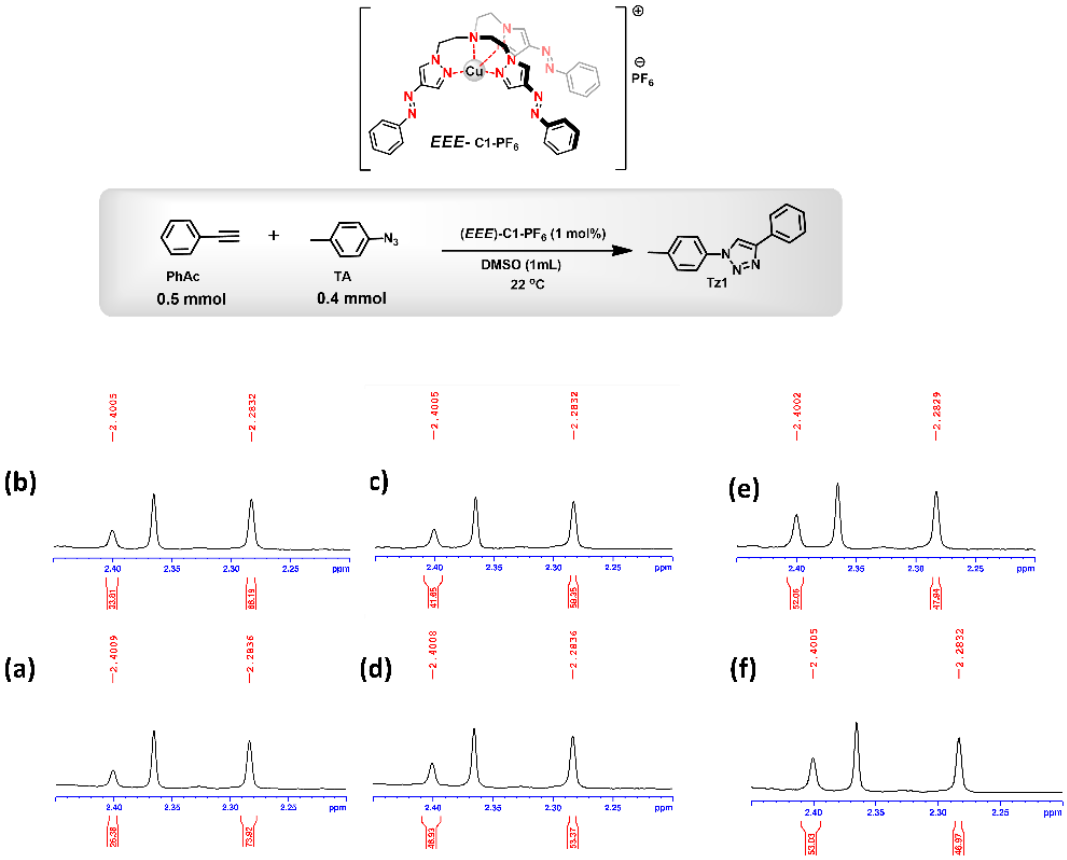


Figure S7.17. ^{1}H NMR (in [D_6]DMSO) spectra depicting the percentage conversion of product with time in CuAAC reaction catalyzed by **C1-PF$_6$** between **PhAc** and **TA** in DMSO at 22 °C; (a) 60 minutes; (b) 120 minutes; (c) 180 minutes; (d) 240 minutes; (e) 360 minutes; (f) 420 minutes. The peak at 2.3 ppm is due to an impurity present in [D_6]DMSO.

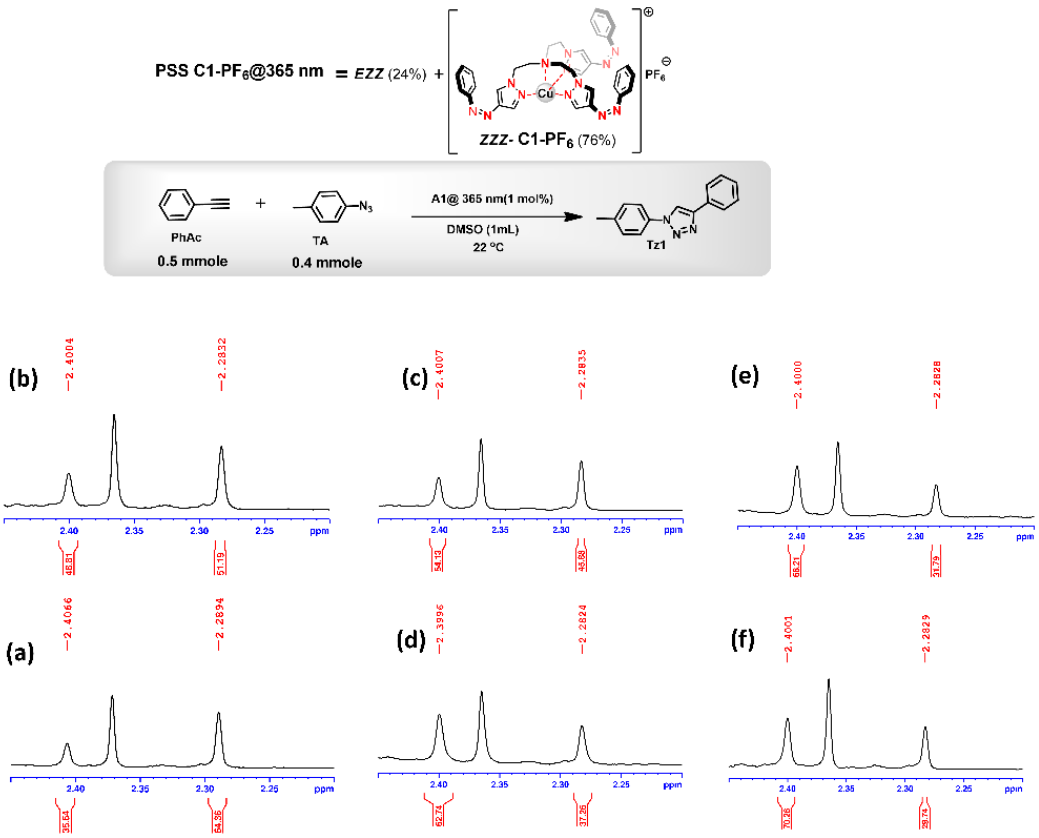


Figure S7.18. ^{1}H NMR (in [D_6]DMSO) spectra depicting the percentage conversion of product with time in CuAAC reaction catalyzed by **C1-PF_6@365 nm** between **PhAc** and **TA** in DMSO at 22 °C; (a) 60 minutes; (b) 120 minutes; (c) 180 minutes; (d) 240 minutes; (e) 360 minutes; (f) 420 minutes. The peak at 2.3 ppm is due to an impurity present in [D6]DMSO.

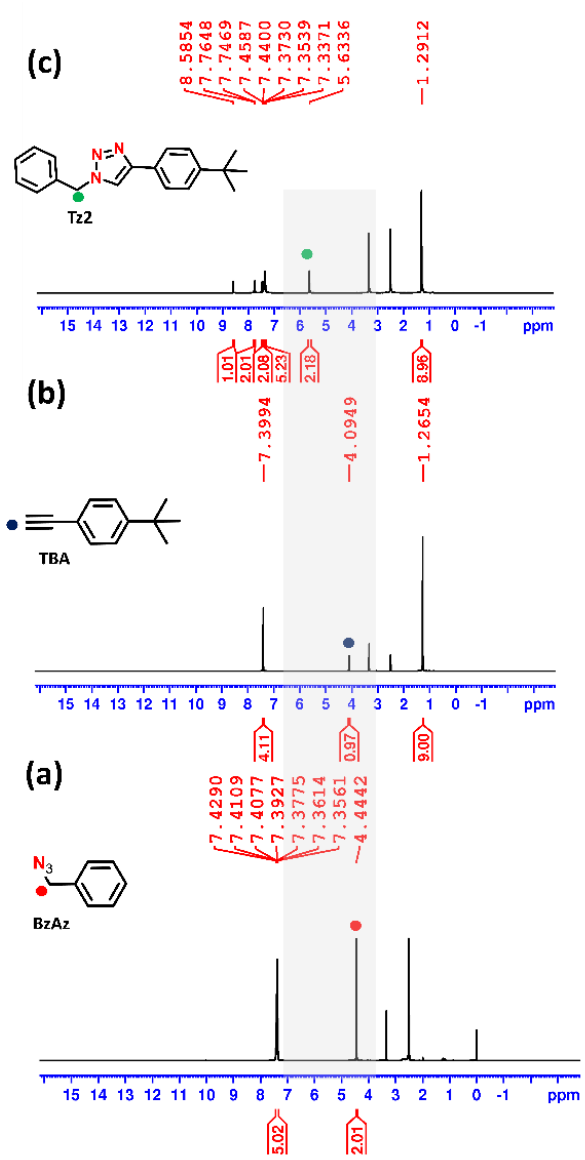


Figure S7.19. ^{1}H NMR (in [D_6]DMSO) spectra for (a) benzyl Azide (**BzAz**) and (b) 4-tert-butylphenylacetylene (**TBA**); (c) 1-benzyl-4-(4-(*tert*-butyl)phenyl)-1*H*-1,2,3-triazole (**Tz2**). For tracking the progress of CuAAC reaction, following protons have been considered, (a) -CH_2 proton for **BzAz** (highlighted, red dot), (b) alkyne proton for 4-*tert*-butylphenylacetylene (TBA) (highlighted, blue dot), and (c) -CH_2 proton for triazole (highlighted, green dot). For estimation of %conversion of product (**Tz2**), -CH_2 protons for **BzAz** (limiting reagent) and **Tz2** have been integrated.

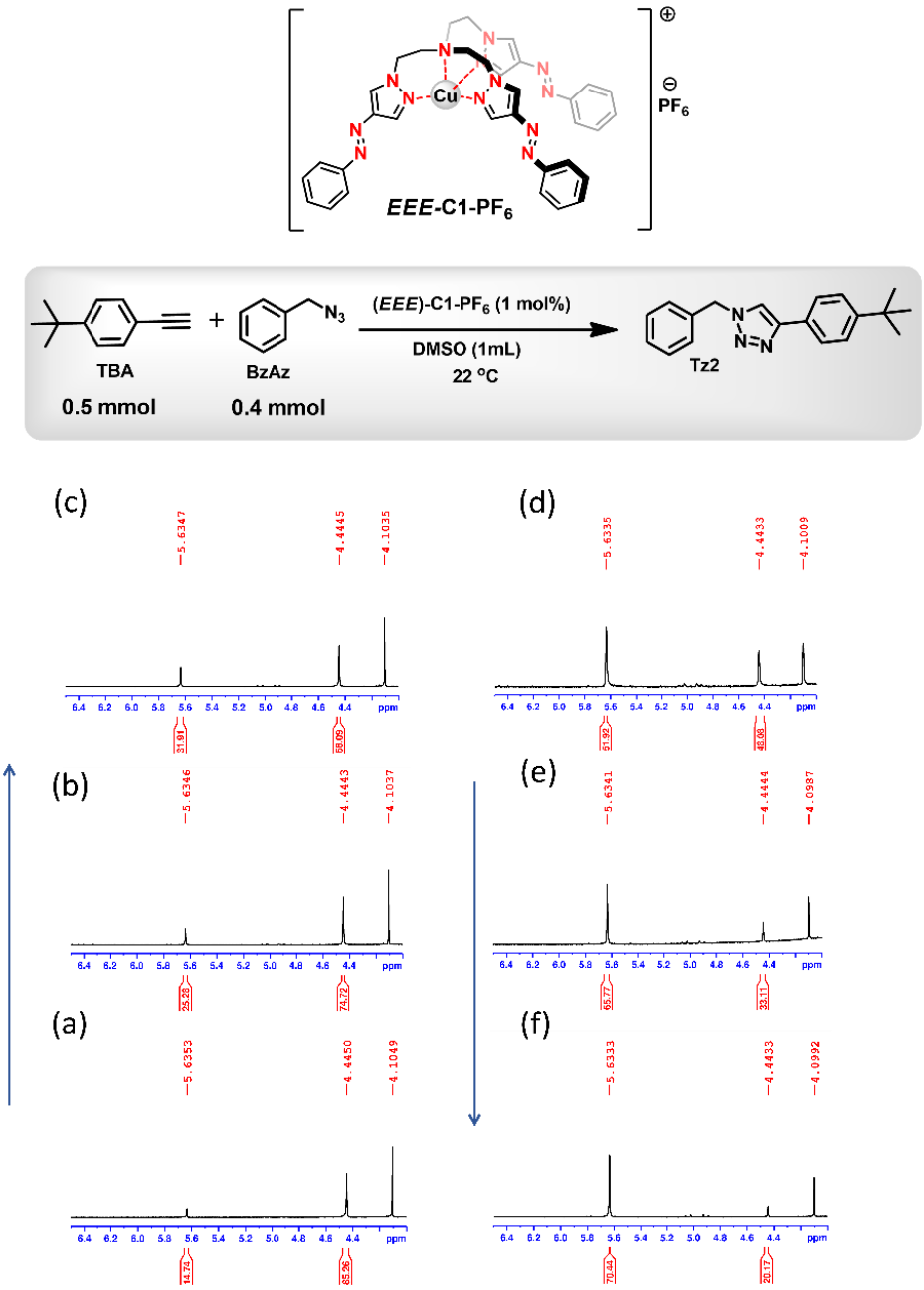


Figure S7.20. ^{1}H NMR (in [D_6]DMSO) spectra depicting the percentage conversion of product with time in CuAAC reaction catalyzed by **C1-PF$_6$** between **TBA** and **BzAz** in DMSO at 25 °C; (a) 65 minutes; (b) 134 minutes; (c) 180 minutes; (d) 305 minutes; (e) 420 minutes; (f) 540 minutes.

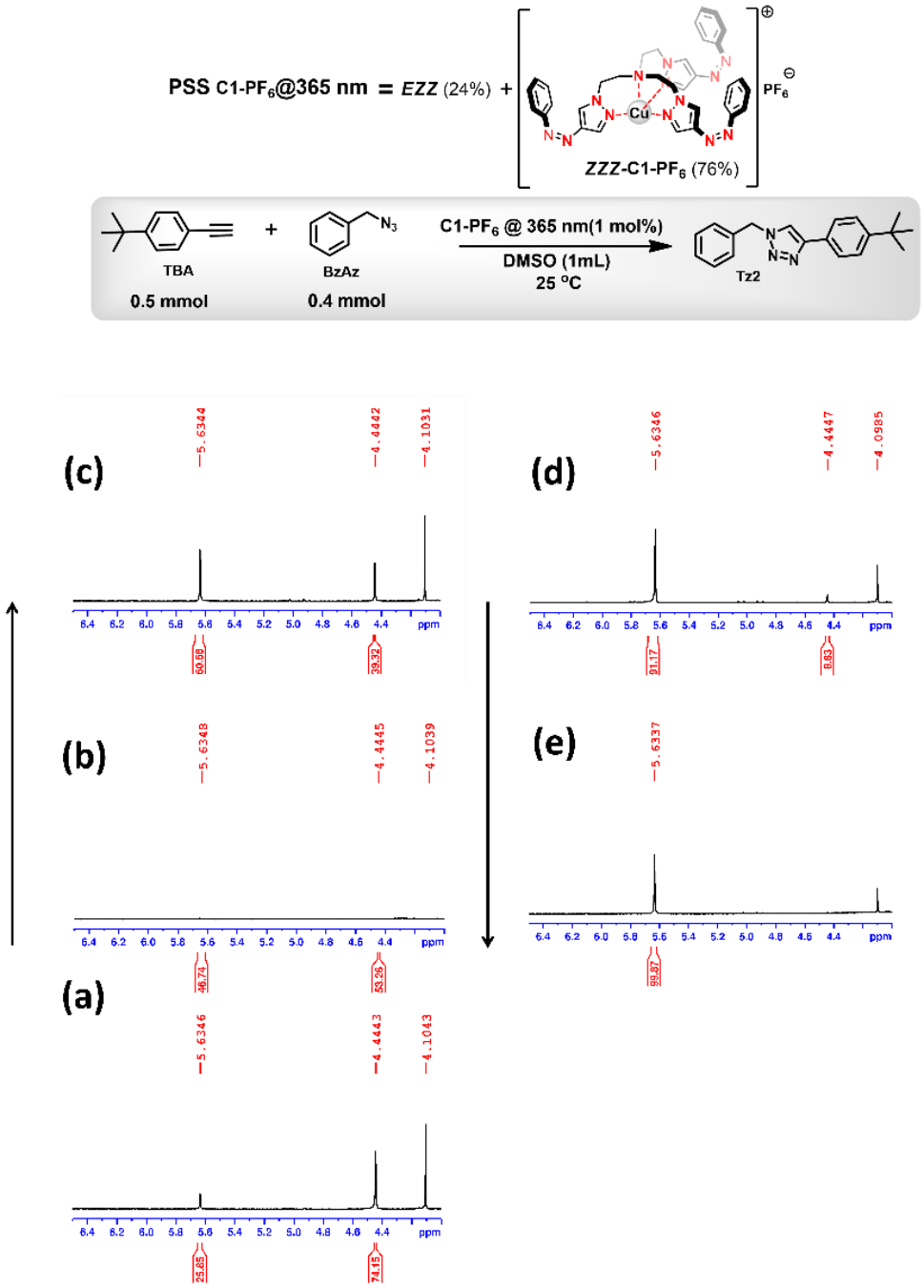


Figure S7.21. ^{1}H NMR (in [D_6]DMSO) spectra depicting the percentage conversion of product with time in CuAAC reaction catalyzed by **C1-PF$_6$ @365 nm** between TBA and BzAz in DMSO at 25 °C; (a) 65 minutes; (b) 134 minutes; (c) 180 minutes; (d) 305 minutes; (e) 420 minutes.

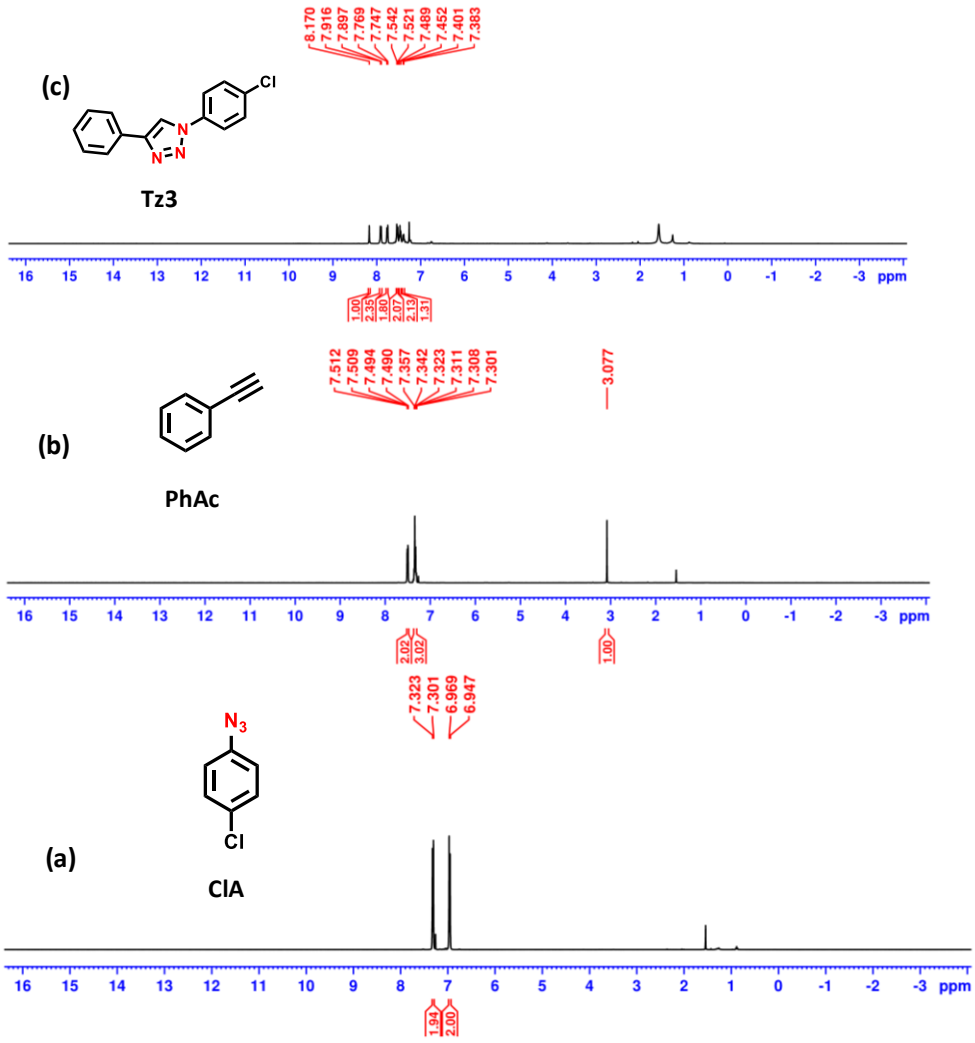


Figure S7.22. ^{1}H NMR (in $CDCl_3$) spectra depicting (a) 1-azido-4-chlorobenzene (**ClA)**; (b) **PhAc**; (c) 1-(4-chlorophenyl)-4-phenyl-1H-1,2,3-triazole (**Tz3)**.

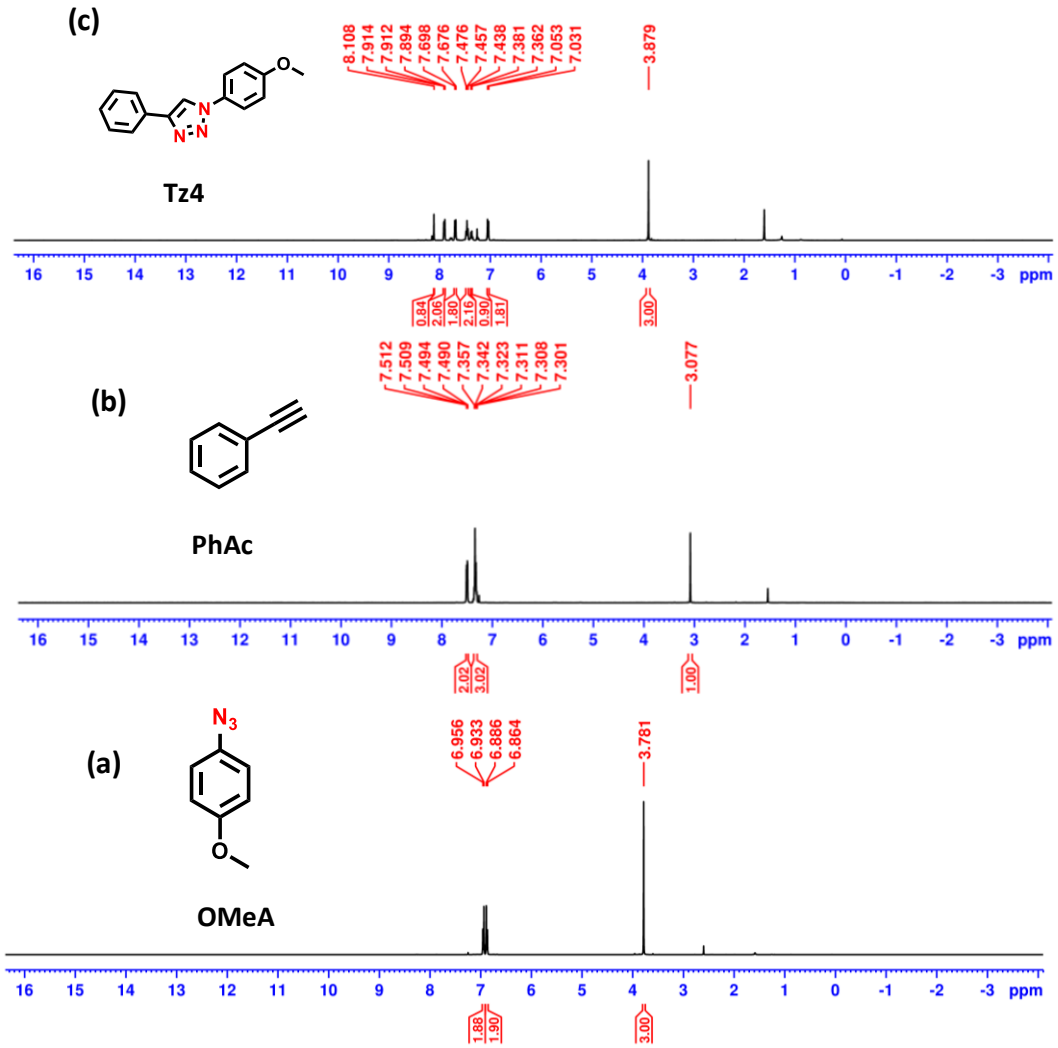


Figure S7.23. ^{1}H NMR (in $CDCl_3$) spectra depicting (a) 1-azido-4-methoxybenzene (**OMeA)**; (b) **PhAc**; (c) 1-(4-methoxyphenyl)-4-phenyl-1H-1,2,3-triazole (**Tz4)**.

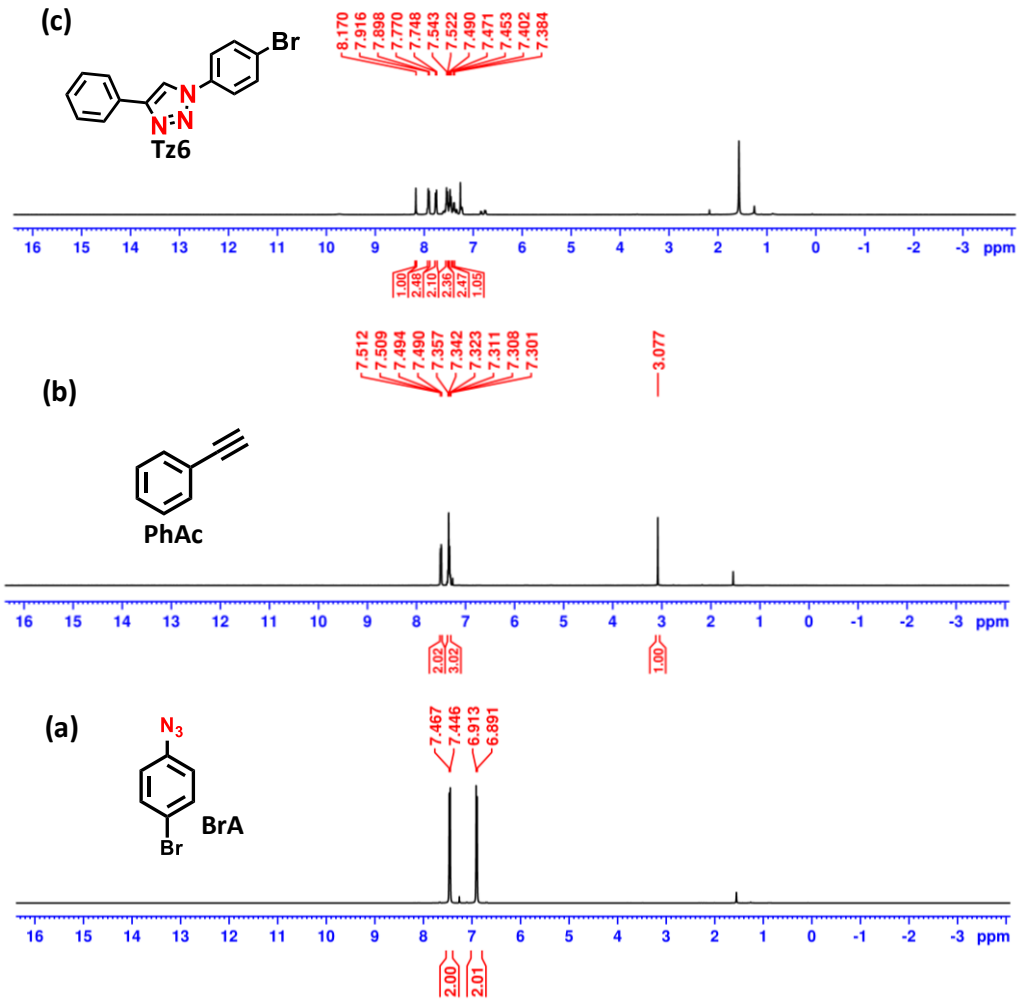


Figure S7.24. ^{1}H NMR (in $CDCl_3$) spectra depicting (a) 1-azido-4-bromobenzene (**BrA**); (b) **PhAc**; (c) 1-(4-bromophenyl)-4-phenyl-1H-1,2,3-triazole (**Tz6**)

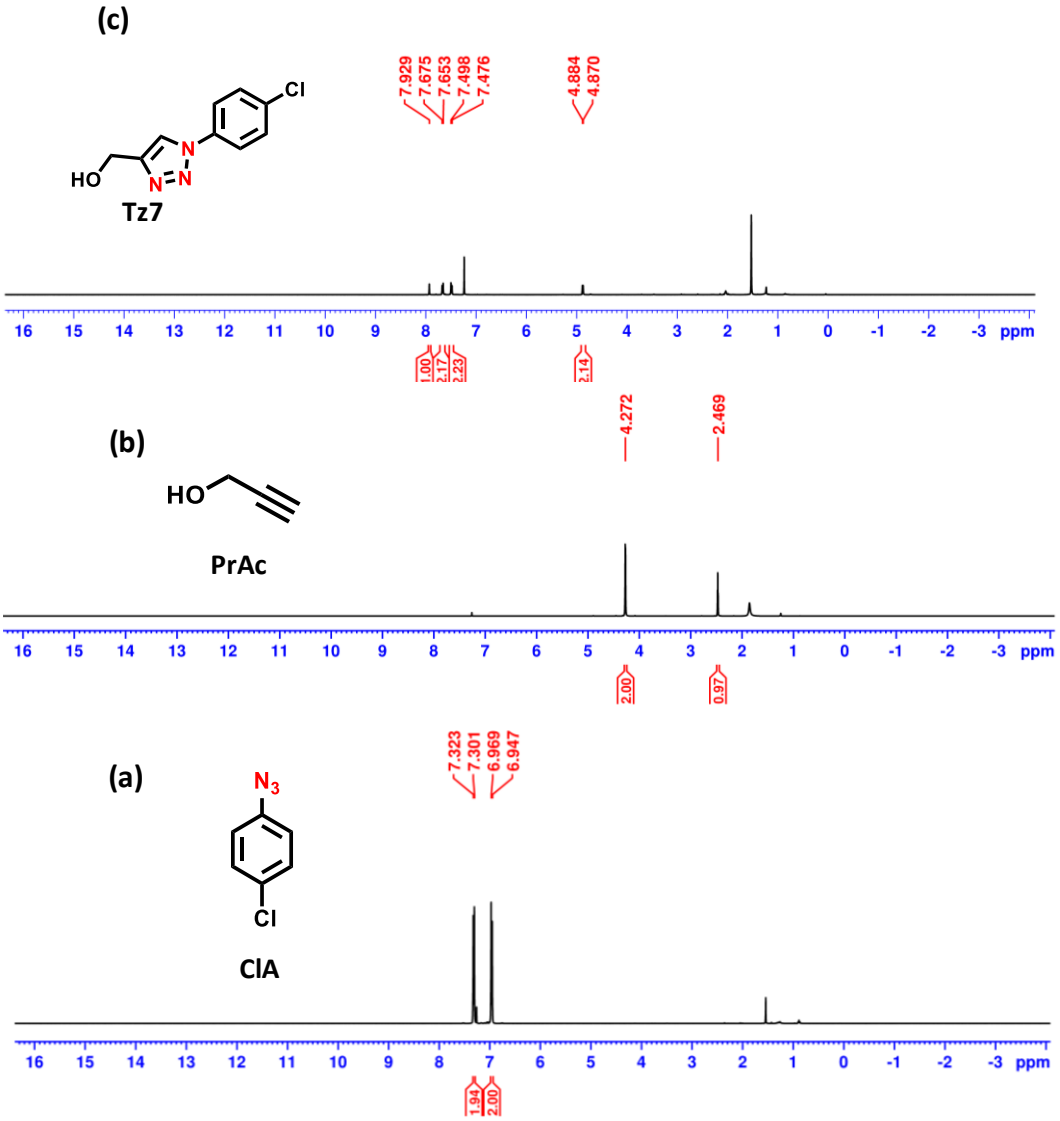


Figure S7.25. ^{1}H NMR (in $CDCl_3$) spectra depicting (a) Cl**A**; (b) Propargyl Alcohol (**PrAc)**; (c) (1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl)methanol (**Tz7).**

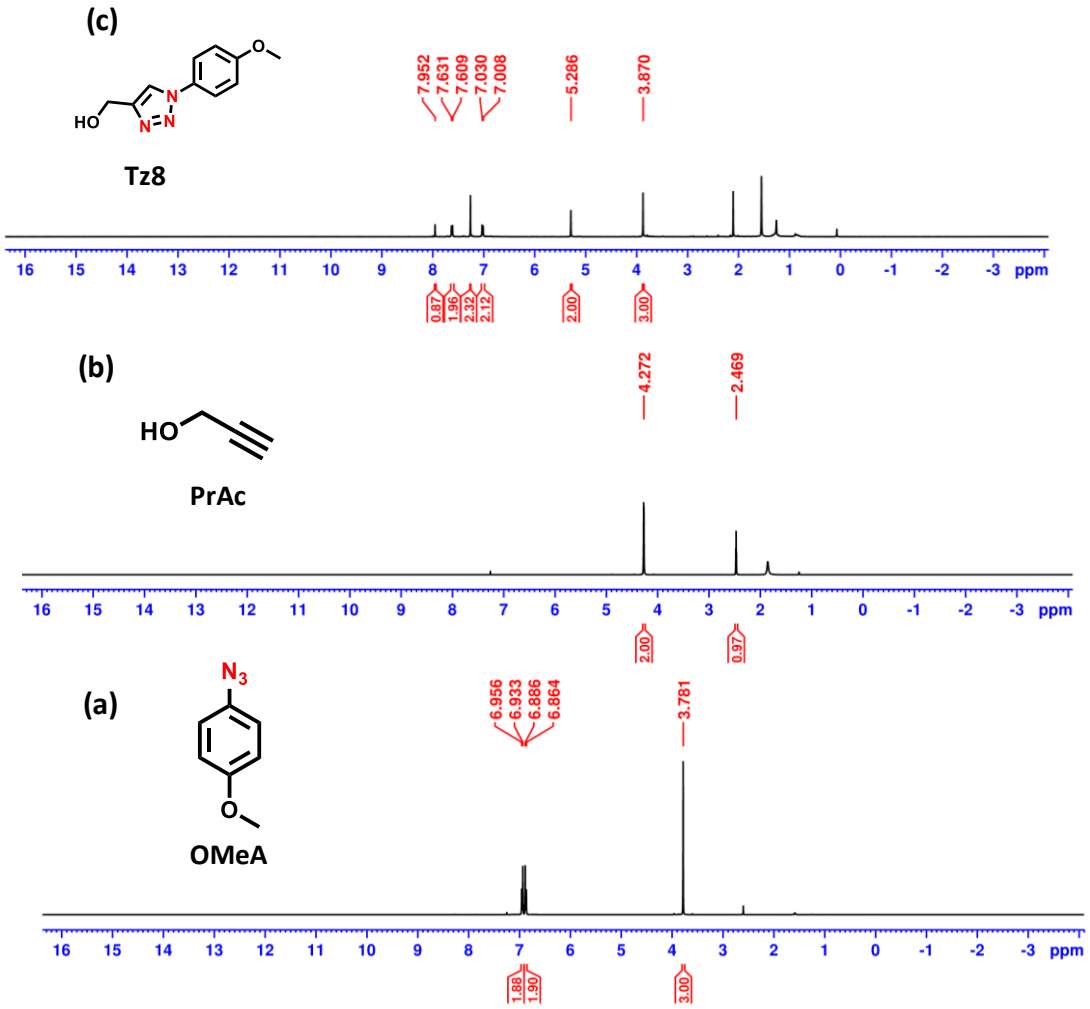


Figure S7.26. ^{1}H NMR (in $CDCl_3$) spectra depicting (a) **OMeA;** (b) **PrAc**; (c) (1-(4-methoxyphenyl)-1H-1,2,3-triazol-4-yl)methanol **(Tz8).** (acetone is present as impurity)

S8: **TD-DFT Calculations:**

In our study, we have employed the Density Functional Theory (DFT) approach to carry out geometry optimization and elucidate reaction mechanisms by using the Gaussian 09 suite.[13] For the optimization of the geometries, we have used Grimme's dispersion-corrected UB3LYP functional (UB3LYP-D3), LANL2DZ effective core potential basis set for Cu metal, and 6-31G* basis set for the rest of the atoms. The gas phase energy has been corrected by taking the solvation energy with a higher level of theory (UB3LYP-D3/def2-TZVP). We have used the polarisable continuum model (PCM) for getting the solvation energy with dimethyl sulfoxide (DMSO) as solvent. This methodology was found to yield reliable mechanistic insights based on earlier studies on Cu-mediated click reactions.[14] For the spectroscopic calculations, we have used the ORCA 4.2.1 suite.[15] Here, we have used the Time-Dependent Density Functional Theory (TD-DFT) approach to incorporate the relativistic effect via the zeroth-order regular approximation method (ZORA) as implemented in the ORCA suite.[16] The RIJCOSX approximation combined with the def2-TZVP/J auxiliary basis set was used to save computational time. Tight SCF convergence criteria with increased integration grids (Grid5, NoFinalgrid) were used.[17] The polarizable continuum model PCM was performed for solvent effects (solvent: acetonitrile), and D3 correction with Becke-Johnson damping was also used to improve the calculation efficiency.[18,19] For visualization of the optimized geometries and the electron densities, we have used Chemcraft and Gauss View software.[20]

S8.A. Analysis of experimental and theoretical absorbance results

The lowest-energy conformers of the gas-phase optimized geometries of *EEE*-, *EEZ*-, *EZZ*-, and *ZZZ* – isomers of **L1** and *EEE*-, *EEZ*-, *EZZ*-, and *ZZZ* – isomers of **C1-PF$_6$** are shown in Figures S8.1 and S8.2. The computed geometry of the *EEE*-**C1-PF$_6$** isomer is quite similar to that of the experimentally determined X-ray crystal structure of the complex (see Figure 2 in the main manuscript for crystal structure of *EEE*-**C1-PF$_6$**). The results from the calculations reveal that in *EEE*-**L1** and *EEE*-**C1-PF$_6$**, the phenylazo-3,5-dimethylpyrazole unit in the ligand adopts a nearly planar geometry with C−N=N−C dihedral angles of ∼180°.

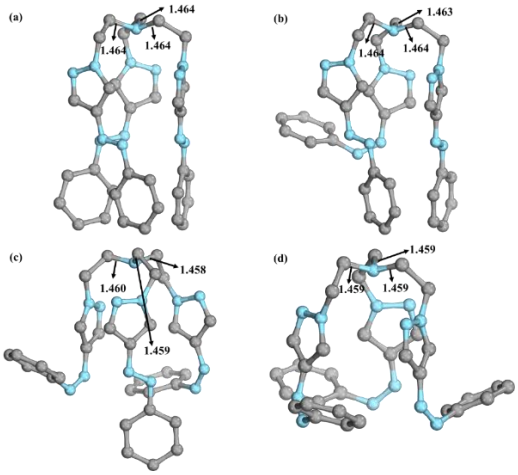


Figure S8.1. Optimised geometries of (a) *EEE*-**L1**, (b) *EEZ*-**L1**, (c) *EZZ*-**L1**, and (d) *ZZZ*-**L1**.

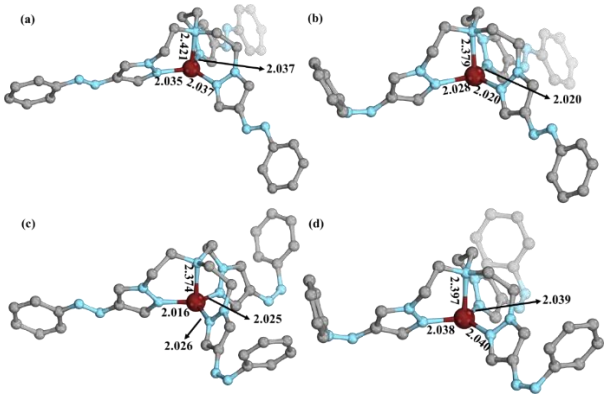


Figure S8.2. Optimised geometry of **C1-PF$_6$**. (a) Optimized geometry of *EEE*- **C1-PF$_6$**, (b) Optimised geometry of *EEZ*- **C1-PF$_6$** (c) Optimized geometry of *EZZ*- **C1-PF$_6$** (d) Optimized geometry of *EEE*- **C1-PF$_6$**.

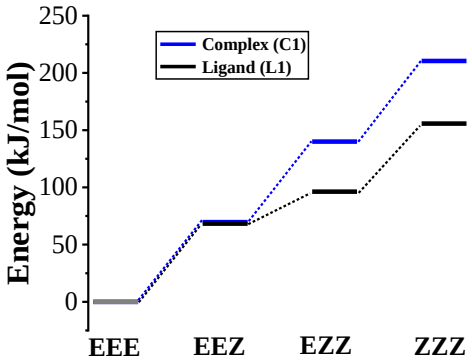


Figure S8.3. The energy profiles for *EEE*-**L1**, *EEZ*-**L1**, *EZZ*-**L1**, *ZZZ*-**L1**, and *EEE*-**C1-PF$_6$**, *EEZ*-**C1-PF$_6$**, *EZZ*-**C1-PF$_6$**, *ZZZ*-**C1-PF$_6$**

The HOMO–LUMO gap computed for the ligand **L1** and the Cu(I) complex **C1-PF$_6$** is shown in Figure S8.4. Here the *ZZZ* isomer is found to have a lower HOMO–LUMO gap compared with the *EEE* isomer. This is correlated to the fact that significant antibonding interaction of the π* orbitals of the two aromatic ends is allowed in the *EEE* isomer, while it is not allowed for the *ZZZ* isomer. So, the HOMO is more destabilized in *ZZZ* isomer compared to that of the corresponding *EEE* isomer. This trend is also retained after complexation.

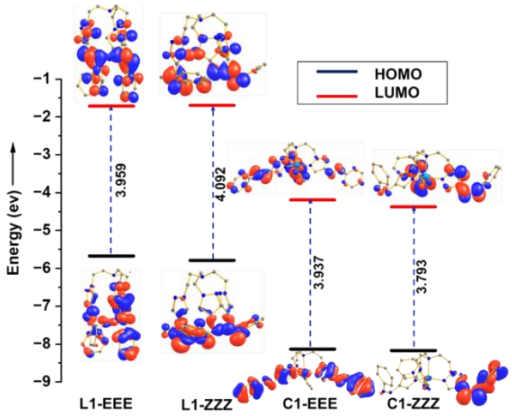


Figure S8.4. Calculated HOMO-LUMO energy gap of ligand *EEE*-**L1**, *ZZZ*-**L1**, *EEE*-**C1-PF$_6$** and *ZZZ*-**C1-PF$_6$**

Using the optimized structures, a comparative analysis of the absorption spectra of the ligands and metal complexes was performed by time-dependent TD-DFT calculations. These calculations were conducted in acetonitrile and the values were compared with the experimentally obtained absorbance poperties in acetonitrile. The computed values (absorption wavelength and oscillator strength) of the electronic transitions for the ligands **L1**-**L3** are compiled in **Table S8.1**. In agreement with the experimental results, the UV-Vis absorption data predicted from the TD-DFT calculations reveal the presence of two bands corresponding to π-π* and the n-π* transitions in all of the compounds studied However, the calculated absorption wavelengths of the ligands were significantly shifted in comparison to the experimentally observed values. For instance, the absorption spectra of ligand **L1** show the presence of an intense band (π-π* transition) centered at λ_{calcd} 322 nm, which is ascribed to (HOMO-2) → (LUMO+1), and a minor HOMO-1 → LUMO transition centered at λ_{calcd} 374 nm was also observed. This is consistent with the experimentally observed absorption feature of an intense π-π* transition at 320 nm. A weaker band (n-π* transition) centered at λ_{calcd} 534 nm, which is ascribed to a (HOMO) → (LUMO) that matches of the *EEE* isomer of ligand **L1** corresponding to n-π* transition. However, the experimentally observed n-π* band was observed at 410 nm. Whereas in the case of *ZZZ*-**L1**, calculations suggest that the π-π* transition is centered at 270 nm, which is ascribed to (HOMO-1) → (LUMO+2) transition and experimentally we observed this transition at 274 nm. The n-π* transition is computed at 457 nm, which is ascribed to the (HOMO-1) → (LUMO) transition. We observed this transition experimentally at 403 nm.

Table S8.1: Experimental and computational data of absorption spectroscopic and photoswitching characteristics of the ligands and complexes

S. No.	Compound	Solvent	Electronic spectral data (experimental)			
			Before switching		After photoswitching	
			λ_{max}/ π–π* (ε)	λ_{max}/ n-π*	λ_{max}/ π–π*	λ_{max}/ n-π*
1	**L1**	MeCN	320 **322**	410 **534**	274 **270**	403 **457**
4	**C1-PF$_6$**	MeCN	319 **322**	420 **364**	273 **292**	402 **457**

[a] The wavelengths written in normal fonts are obtained from spectroscopic experiments, while the wavelength written in bold fonts are calculated values

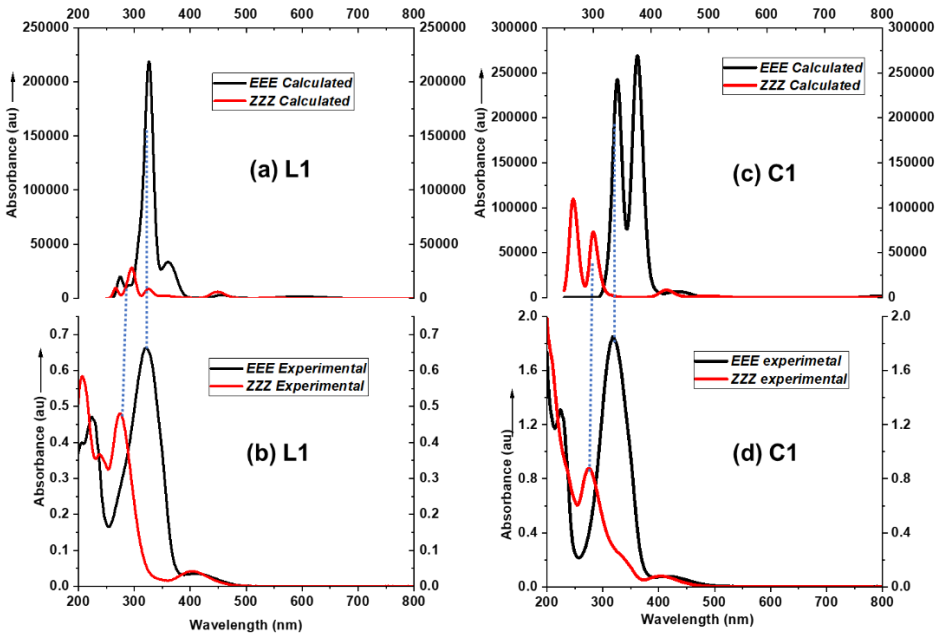


Figure S8.5. Comparison of experimental and calculated UV–Vis spectra of ligand **L1** (a and c) and the metal complex **C1-PF$_6$** (b and d) in their *EEE* and *ZZZ* photoisomeric state, respectively.

Similarly, the absorption spectra of the *EEE*-**C1-PF$_6$** complex show the presence of an intense π-π* transition centered at λ_{calcd} 322 nm, which is ascribed to (HOMO) → (LUMO) transition. A weaker n-π* transition centered at λ_{calcd} 364 nm, which is ascribed to a (HOMO-2) → (LUMO+1) transition. This matches the experimentally observed absorption feature of the *EEE* isomer of the **C1-PF$_6$** complex, which shows an intense π-π* transition at 319 nm. However, n-π* transition was observed at 420 nm experimentally. Whereas in the case of the *ZZZ*-**C1-PF$_6$**, calculations suggest that the π-π* transition is centered at 292 nm, which is ascribed to (HOMO-8) → (LUMO+1) transition, and experimentally we observed this transition at 273 nm. However, the n-π* transition is computed at 457 nm, which is ascribed to (HOMO-1) → (LUMO) transition. We observed this transition experimentally at 402 nm. All these data showed a good agreement between experiments and computations.

Mononuclear mechanism for CuAAC reaction

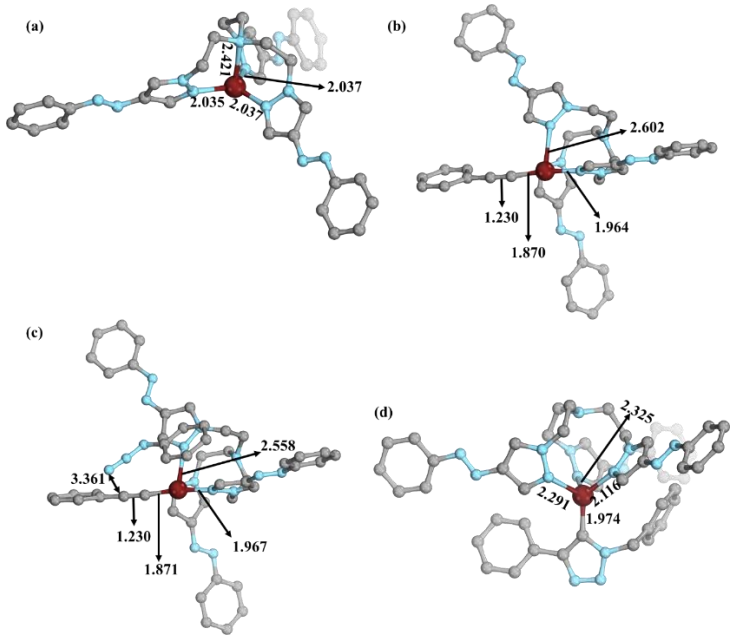


Figure S8.6. DFT optimized structures of (a) *EEE*-**C1-PF$_6$**, (b) **int1**, (c) **int2**, and (d) **int3** shown in the energy profile (for *EEE*-**C1-PF$_6$)** in mononuclear pathways.

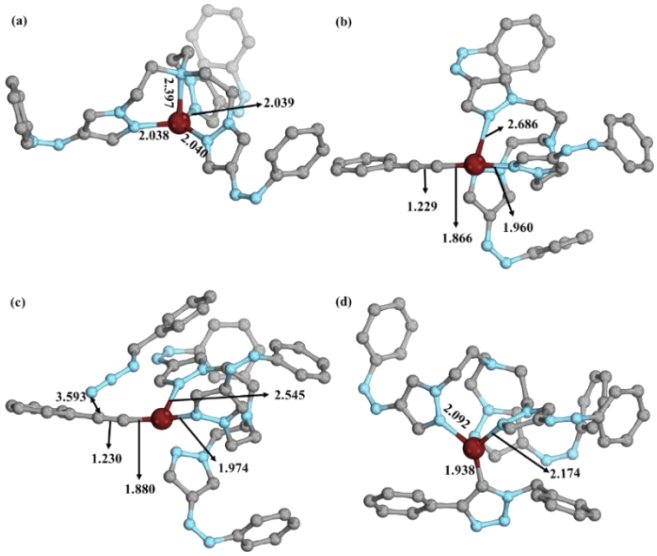


Figure S8.7. DFT optimized structures of (a) *ZZZ*-**C1-PF$_6$**, (b) **int1**, (c) **int2**, and (d) **int3** shown in the energy profile (for *ZZZ*-**C1-PF$_6$**) in mononuclear pathways.

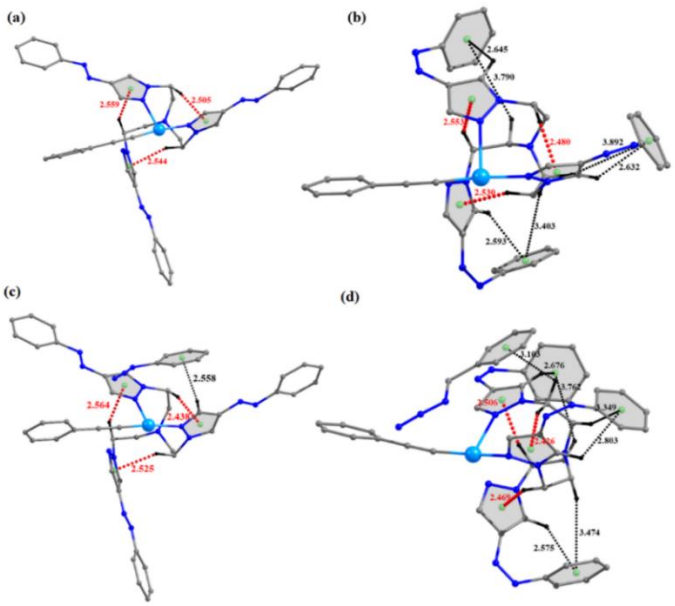


Figure S8.8. Possible C–H…π interactions in mononuclear pathways. (a) C–H…π interactions in **int1** for *EEE*-**C1-PF$_6$** (b) C–H…π interactions in **int1** for *ZZZ*-**C1-PF$_6$** (c) C–H…π interactions in **int2** for *EEE*-**C1-PF$_6$** (d) C–H…π interactions in **int2** for *ZZZ*-**C1-PF$_6$**

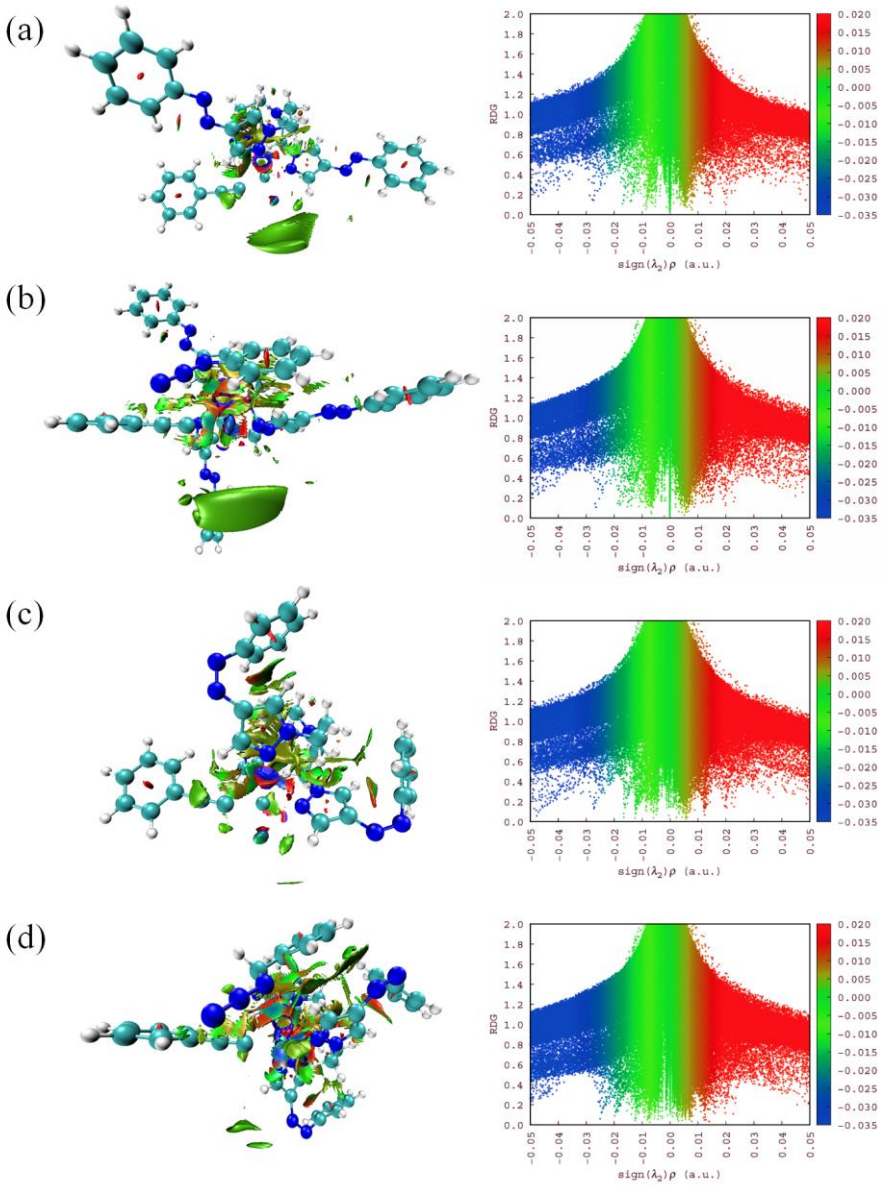


Figure S8.9. NCI plots demonstrating possible C–H…π interactions in mononuclear pathways. (a) C–H…π interactions in **int1** for *EEE*-**C1-PF$_6$** (b) C–H…π interactions in **int1** for *ZZZ*-**C1-PF$_6$** (c) C–H…π interactions in **int2** for *EEE*-**C1-PF$_6$** (d) C–H…π interactions in **int2** for *ZZZ*-**C1-PF$_6$.** In these plots, the blue-colored spike in the negative region of the scatter plot corresponds to the hydrogen bonds, the red represents the repulsive interactions, and the green-colored spikes correspond to the Vander walls interactions.

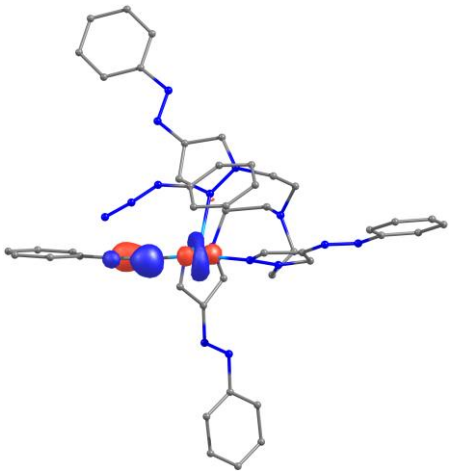


Figure S8.10. Strong σ and π-overlap of the alkyne ligand.

Dinuclear mechanism for CuAAC reaction

In the dinuclear mechanism, an alkyne is expected to coordinate first to the Cu(I) centre, leading to the formation of **int1'**, and this is followed by coordination of the second Cu(I) centre and Cu(I)–C(alkyne) bond formation at **int2'**. In the next step, phenyl azide coordination is assumed via the formation of **int3'**, followed by N…C bond formation at **int4**'. In the next step, cyclization is expected, leading to the formation of the triazole product. The computed energy level diagram for the dinuclear mechanism is shown in Figure S8.11. In this mechanism, the formation of **int1'** is found to be endothermic for both *ZZZ* and *EEE* isomers, with the former demanding significantly higher energy than the latter. The formation of the dinuclear **int2'** eases the energetics as this is exothermic, with *EEE* being more stable than the *ZZZ* isomer. Although the *EEE* isomers of the azopyrazole units exhibit less steric repulsion, the geometrical orientation of those units in coordinated state disfavours the approach of the alkyne compared to the *ZZZ* isomer (See Figures S8.12 and S8.13). The formation of **int3'** is slightly endothermic for both the isomers, and azide is found to be only weakly bound to the Cu(I), with the anchoring essentially due to the non-covalent interactions (See Figures S8.12 and S8.13). In the next step, the formation of **int4'** is assumed where the N(azide)–C(alkyne) bond formation takes place. This bond formation significantly reduces the donor ability of the alkyne, exemplified by the longer Cu(I)-C(alkyne) distances in both the isomers (2.324 Å vs. 2.284 Å in *EEE* vis-à-vis 2.296 Å vs. 2.235 Å in *ZZZ*). Due to the reduction in the donor ability of the alkyne, the formation of **int4'** is found to be significantly endothermic for both isomers (+134.4 kJ/mol vs 132.1 kJ/mol for the *EEE* and *ZZZ* isomers, respectively). Similar to the previous approach, the product formation is found to be exothermic for both isomers. The key differentiator between the two mechanisms lies in the significant energy penalty noted for the **int4'** formation. Such a large endothermic intermediate suggests that this reaction will unlikely proceed via the dinuclear mechanism, suggesting a mononuclear pathway as the favourable mechanism for this reaction. Considering no significant increase in the isolated yields upon increasing the catalytic loading, the experimental evidences also favour the mononuclear mechanism. Also, the experimental revealation on the faster reactions with ZZZ isomeric catalyst is supported by the energy requirements as predicted by the computations for the mononuclear pathway rather than the dinuclear channel. Thus, the computational mechanistic investigations support the experiments, where the *ZZZ* isomer reacted faster than the *EEE* isomer, similar to our findings in the mononuclear pathway.

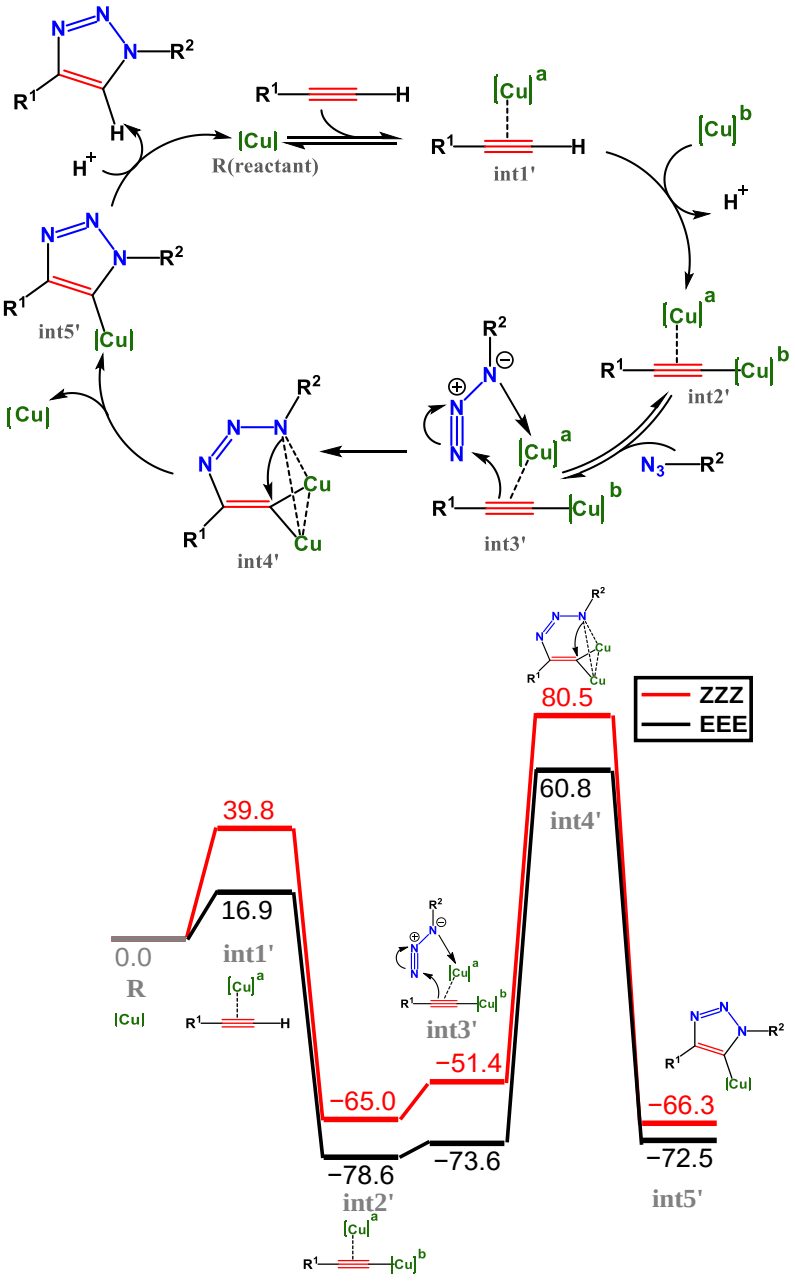


Figure S8.11. Possible reaction pathways for the dinuclear mechanism and computed energy profile for dinuclear pathways.

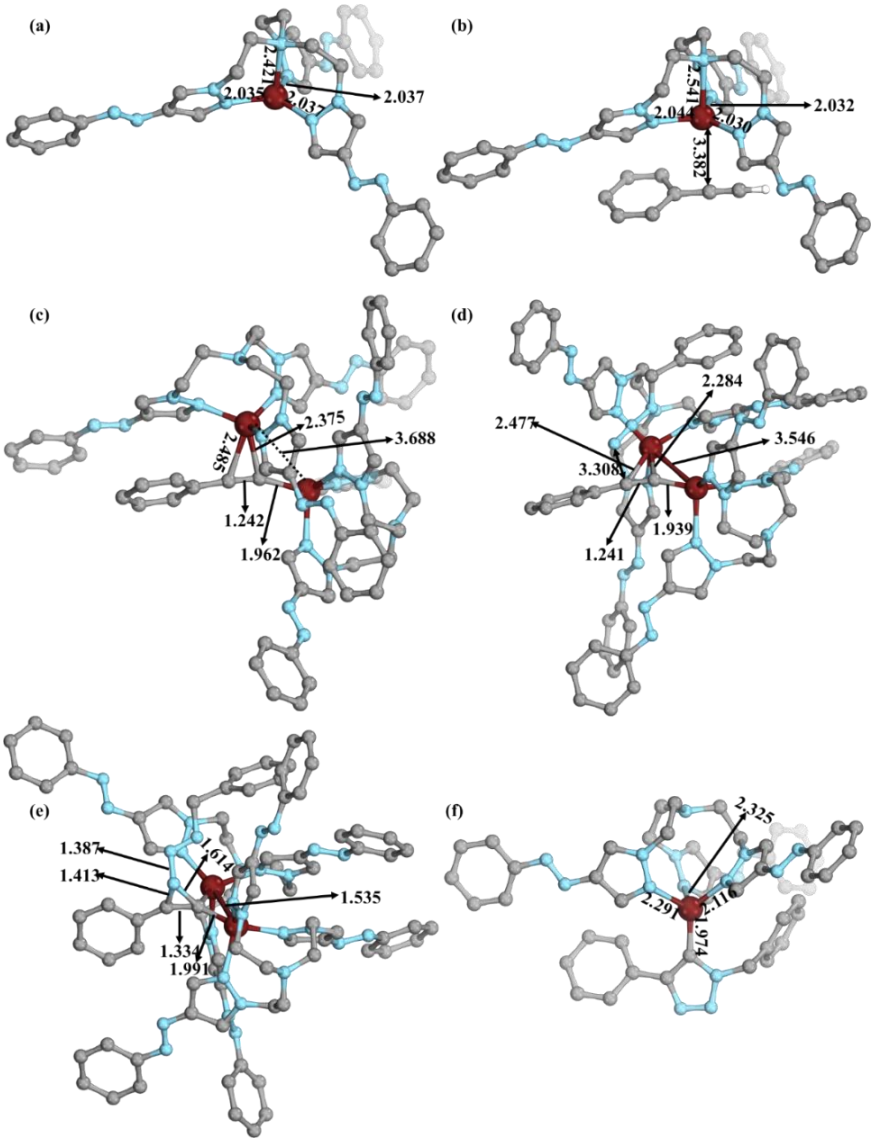


Figure S8.12. DFT optimized structures of (a) *EEE*-**C1-PF$_6$**, (b) **int1**, (c) **int2**, (d) **int3**, (e) **int4**, and (f) **int5** shown in the energy profile for *EEE*-**C1-PF$_6$** in dinuclear pathways.

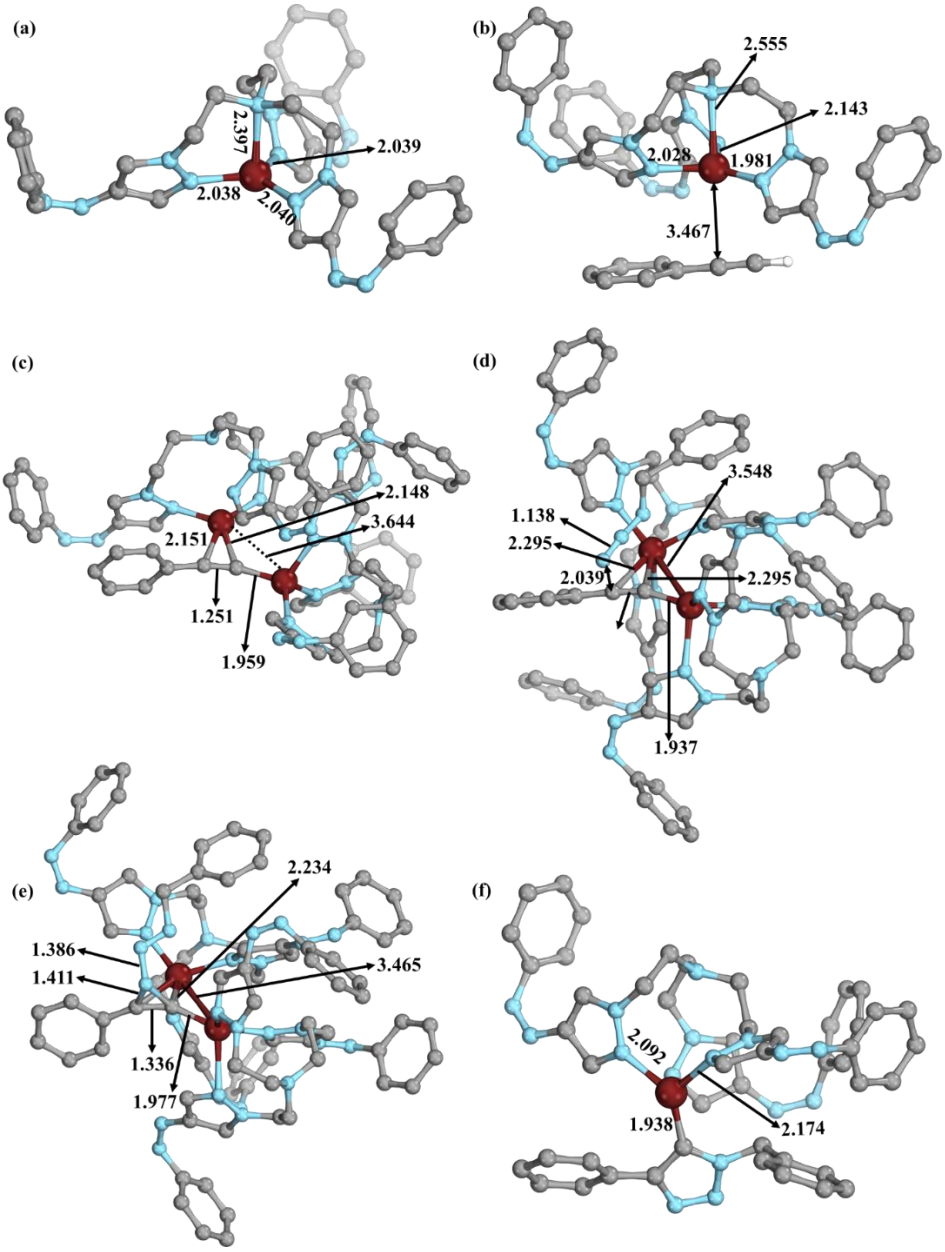


Figure S8.13. DFT optimized structures of (a) *ZZZ*-**C1-PF$_6$**, (b) **int1**, (c) **int2**, (d) **int3**, (e) **int4**, and (f) **int5** shown in the energy profile for *ZZZ*-**C1-PF$_6$** in dinuclear pathways.

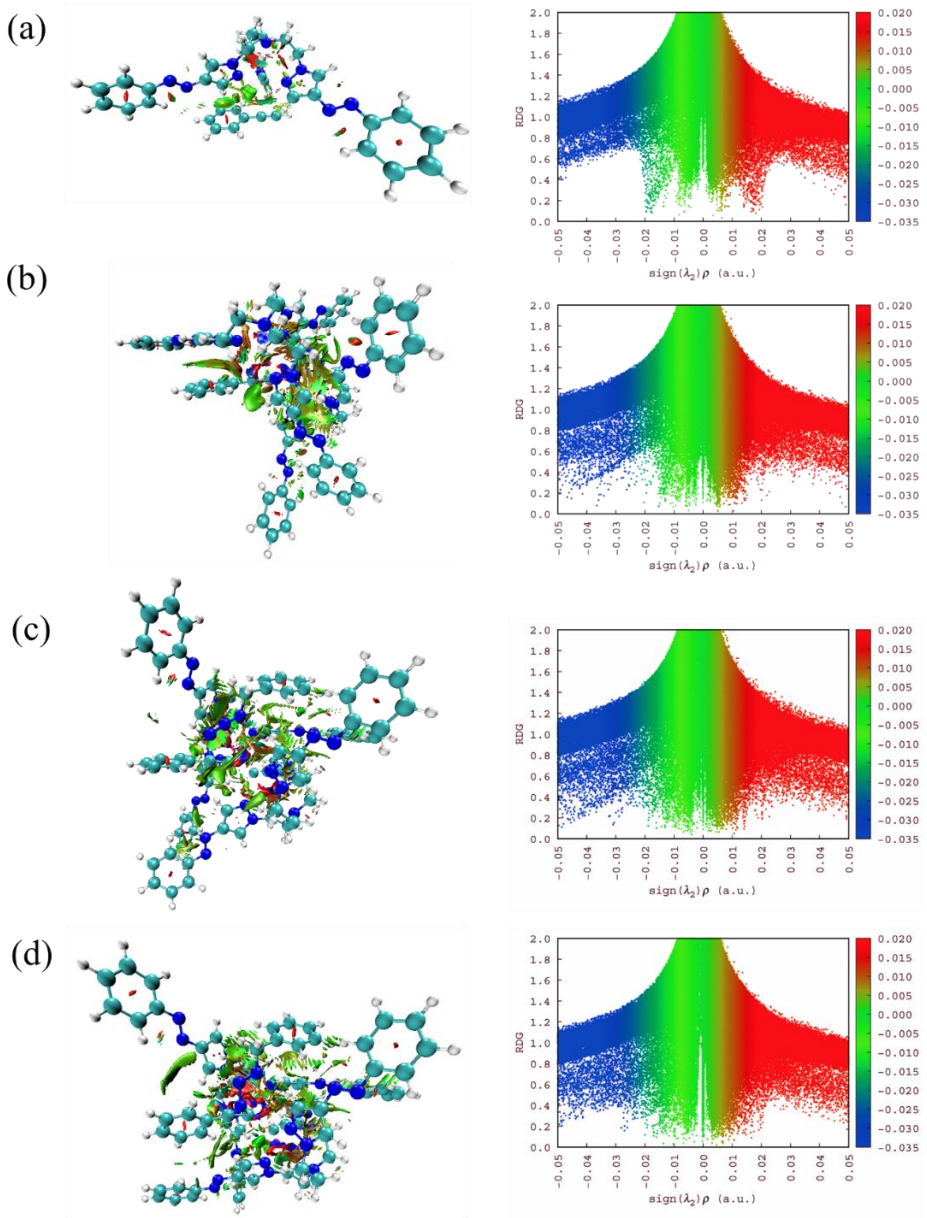


Figure S8.14. NCI plots demonstrating possible C–H…π interactions in dinuclear pathways for *EEE*-**C1-PF_6**. (a) C–H…π interactions in **int1** (b) C–H…π interactions in **int2** (c) C–H…π interactions in **int3** (d) C–H…π interactions in **int4.** In these plots, the blue-colored spike in the negative region of the scatter plot corresponds to the hydrogen bonds, the red represents the repulsive interactions, and the green-colored spikes correspond to the Vander walls interactions.

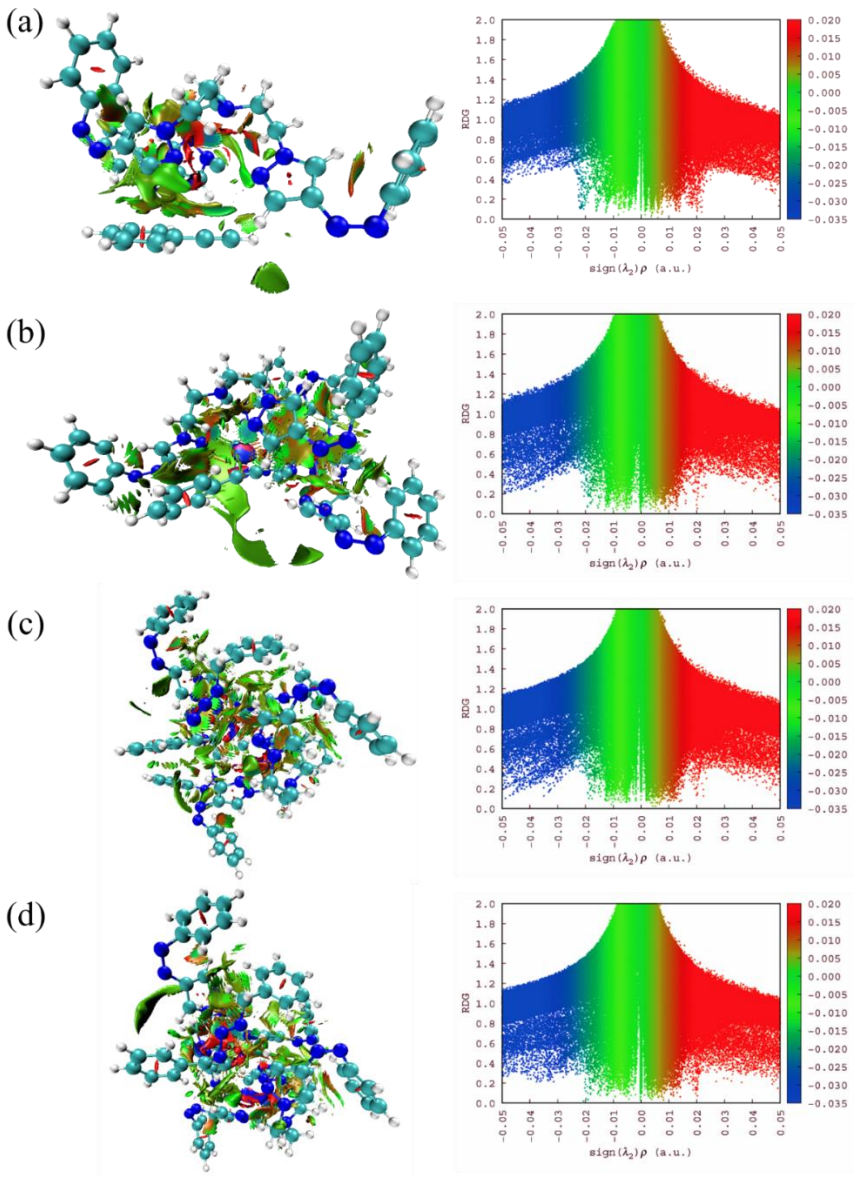


Figure S8.15. NCI plots demonstrating possible C–H…π interactions in dinuclear pathways for *ZZZ*-**C1-PF_6**. (a) C–H…π interactions in **int1** (b) C–H…π interactions in **int2** (c) C–H…π interactions in **int3** (d) C–H…π interactions in **int4.** In these plots, the blue-colored spike in the negative region of the scatter plot corresponds to the hydrogen bonds, the red represents the repulsive interactions, and the green-colored spikes correspond to the Vander walls interactions.

Table S8.1. TD-DFT data of *EEE*-**L1**

Compound	λ_{calcd} (nm)	E (eV)	f	Character	Transition
EEE-L1	326	3.5897	1.4293	π → π*	HOMO-1(α)→LUMO(α)(0.44) HOMO-1(β)→LUMO+1(β)(0.43)
	455	3.6607	0.5535	n → π*	HOMO-1(α)→LUMO(α)(0.43) HOMO(α)→LUMO+1(α)(0.48)

Table S8.2. TD-DFT data depicting the orbitals corresponding to the π–π* and n–π* transitions of *EEE*-**L1**

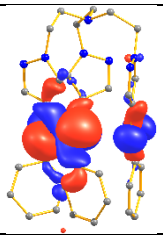
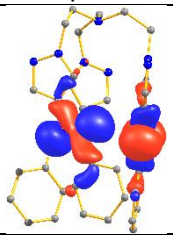
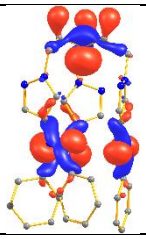
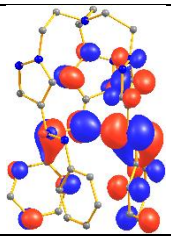
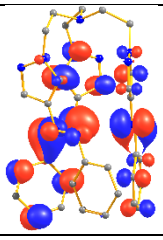
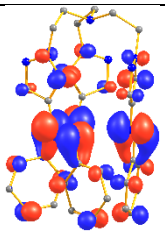
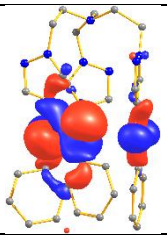
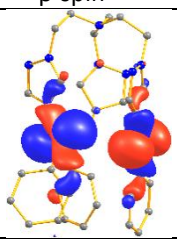
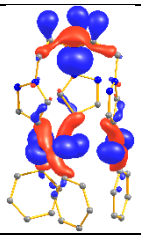
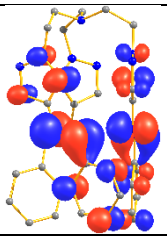
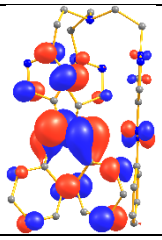
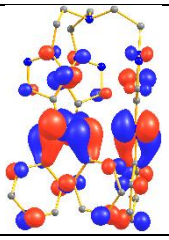
α-spin		
		
HOMO	HOMO-1	HOMO-2
		
LUMO	LUMO+1	LUMO+2
β-spin		
		
HOMO	HOMO-1	HOMO-2
		
LUMO	LUMO+1	LUMO+2

Table S8.3. TD-DFT data of *ZZZ*- **L1**

Compound	λ_{calcd} (nm)	E (eV)	f	Character	Transition
ZZZ-**L1**	292	3.5897	1.4293	π → π*	HOMO-1(α)→LUMO(α)(0.44) HOMO(α)→LUMO+1(α)(0.46)
	440	3.6607	0.5535	n → π*	HOMO-1(α)→LUMO(α)(0.43) HOMO(α)→LUMO+1(α)(0.48)

Table S8.4. TD-DFT data depicting the orbitals corresponding to the π–π* and n–π* transitions of *EEE*-**L1** in the isomeric state

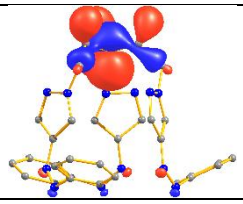
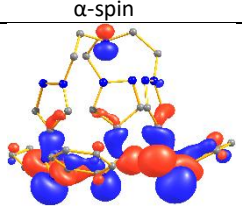
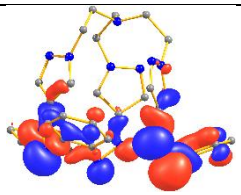
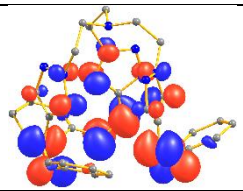
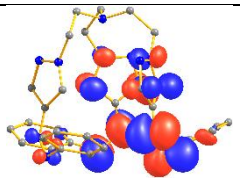
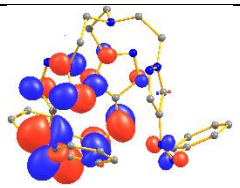
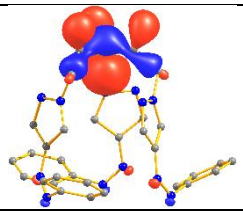
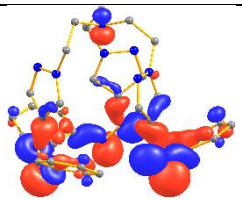
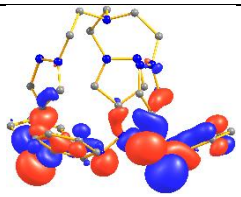
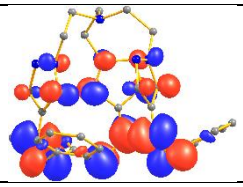
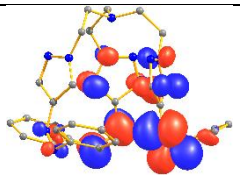
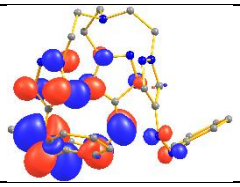
α-spin		
		
HOMO	HOMO-1	HOMO-2
		
LUMO	LUMO+1	LUMO+2
β-spin		
		
HOMO	HOMO-1	HOMO-2
		
LUMO	LUMO+1	LUMO+2

Table S8.5. TD-DFT data of **C1-PF_6** in *EEE*-isomeric state

Compound	λ_{calcd} (nm)	E (eV)	f	Character	Transition
***EEE*-C1-PF_6**	342	3.626	0.3072	π → π*	HOMO-8(α)→LUMO+2(α)(0.08) HOMO-8(β)→LUMO+3(β)(0.08)
	438	2.828	0.0127	n → π*	HOMO-11(α)→LUMO+1(α) (0.24) HOMO-11(β)→LUMO+1(β) (0.24)

Table S8.6. TD-DFT data depicting the orbitals corresponding to the π–π* and n–π* transitions of *EEE*-**C1-PF_6**

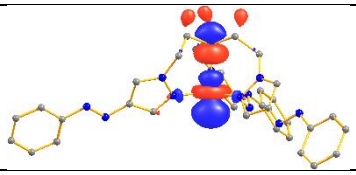
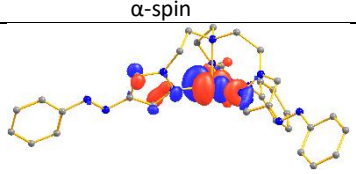
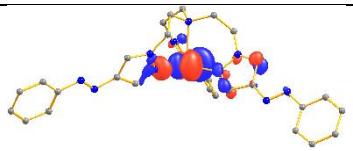
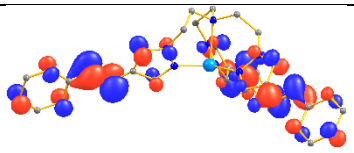
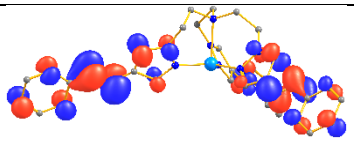
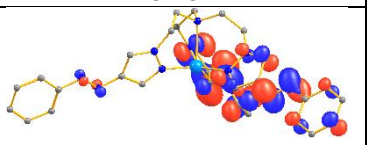
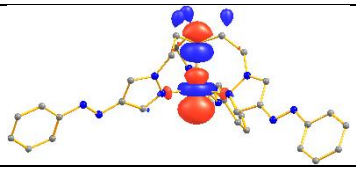
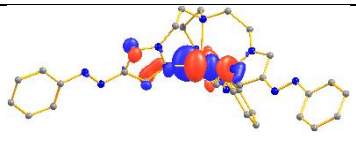
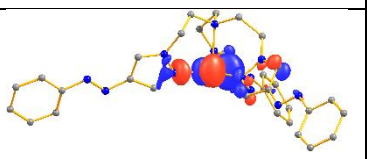
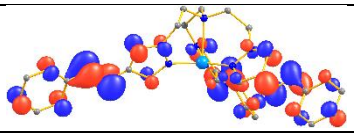
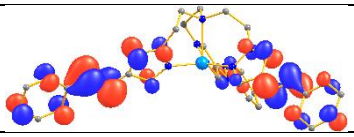
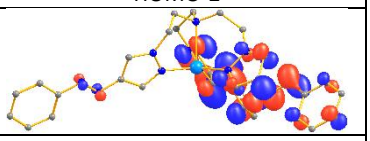
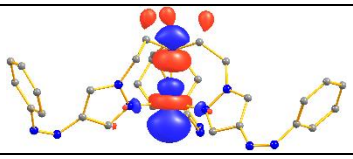
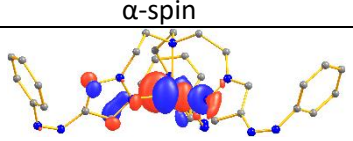
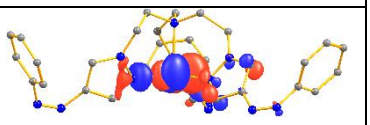
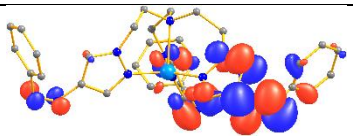
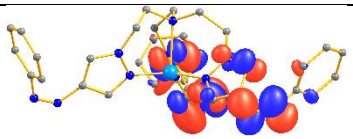
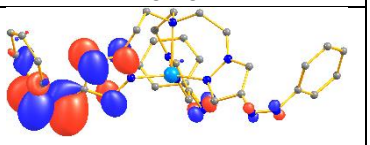
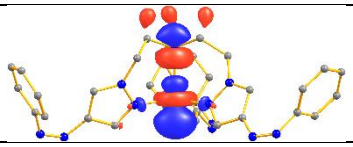
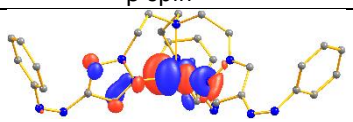
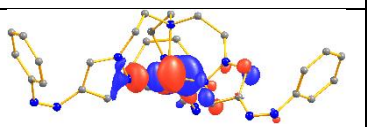
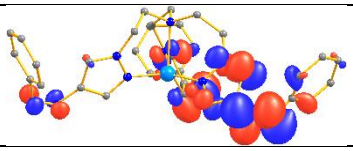
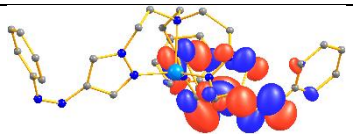
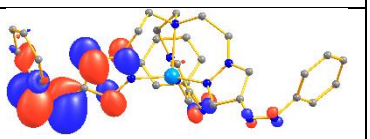
α-spin		
		
HOMO	HOMO-1	HOMO-2
		
LUMO	LUMO+1	LUMO+2
β-spin		
		
HOMO	HOMO-1	HOMO-2
		
LUMO	LUMO+1	LUMO+2

Table S8.7. TD-DFT data of *ZZZ*-**C1-PF$_6$**

Compound	λ_{calcd} (nm)	E (eV)	f	Character	Transition
C1 ZZZ	298	4.150	0.0858	π → π*	HOMO-1(α)→LUMO+3(α) (0.18) HOMO-1(β)→LUMO+3(β) (0.18)
	424	2.919	0.0232	n → π*	HOMO-4(α)→LUMO+1(α) (0.24) HOMO-4(β)→LUMO+1(β) (0.24)

Table S8.8. TD-DFT data depicting the orbitals corresponding to the π−π* and n−π* transitions of *ZZZ*-**C1-PF$_6$**

α-spin		
		
HOMO	HOMO-1	HOMO-2
		
LUMO	LUMO+1	LUMO+2
β-spin		
		
HOMO	HOMO-1	HOMO-2
		
LUMO	LUMO+1	LUMO+2

S9: ^{1}H and ^{13}C -NMR spectral data

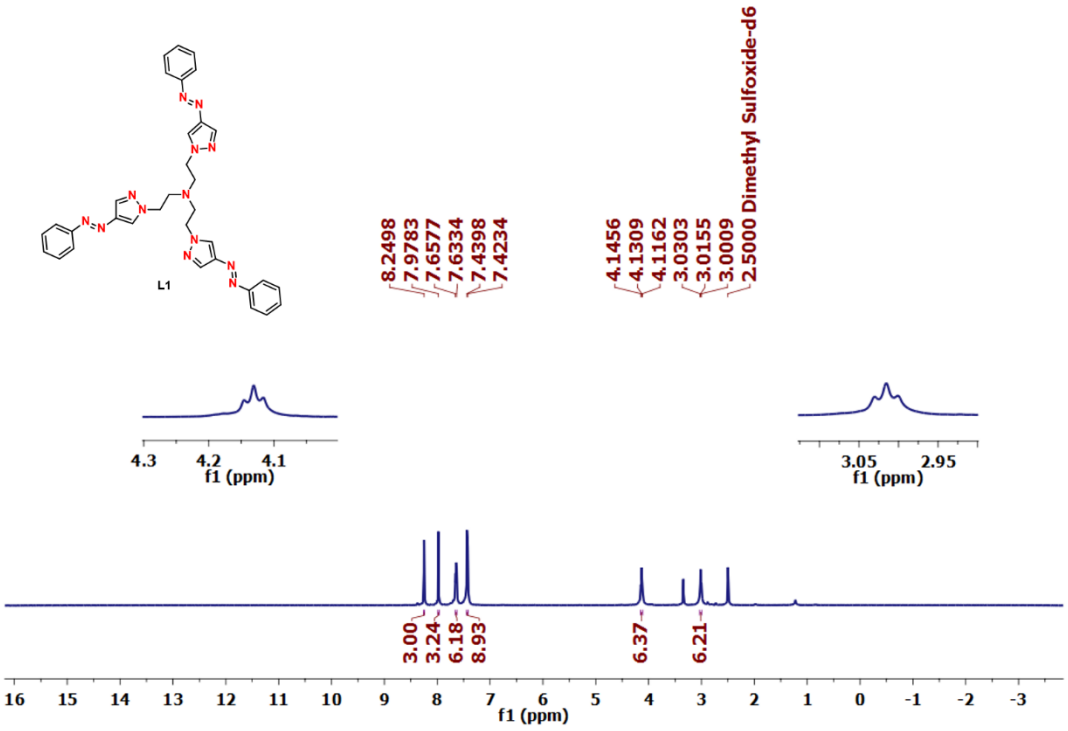


Figure S9.1. ^{1}H NMR spectrum of tris(2-(4-((*E*)-phenyldiazenyl)-1*H*-pyrazol-1-yl)ethyl)amine **L1** (400 MHz, $[D_6]$DMSO)

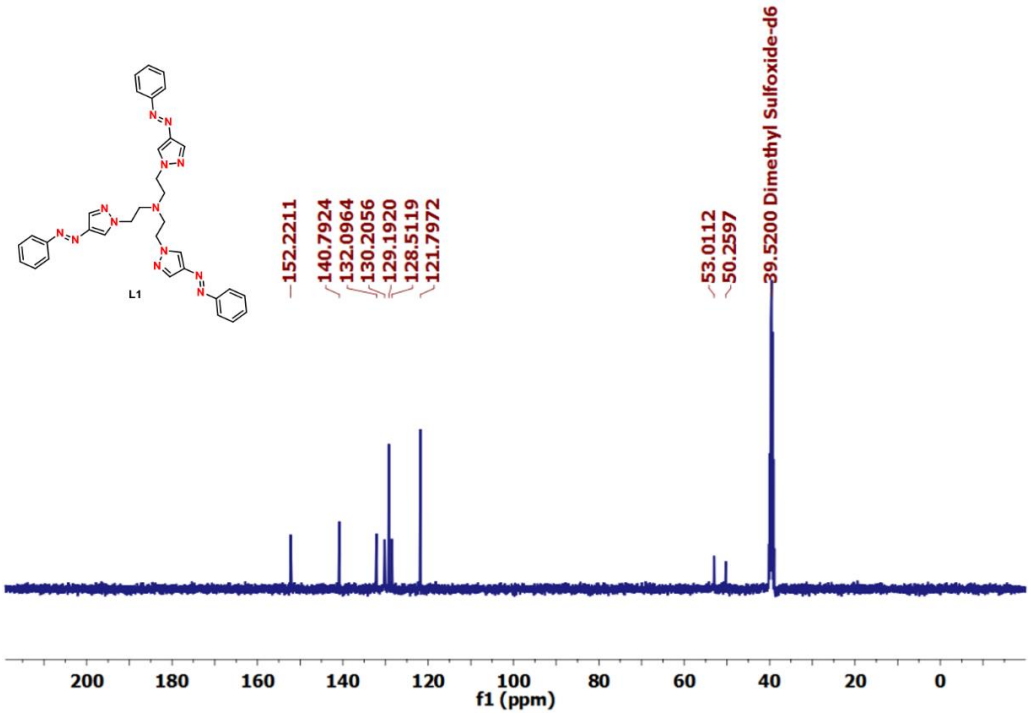


Figure S9.2. ^{13}C NMR spectrum of tris(2-(4-((*E*)-phenyldiazenyl)-1*H*-pyrazol-1-yl)ethyl)amine **L1** (100 MHz, $[D_6]$DMSO)

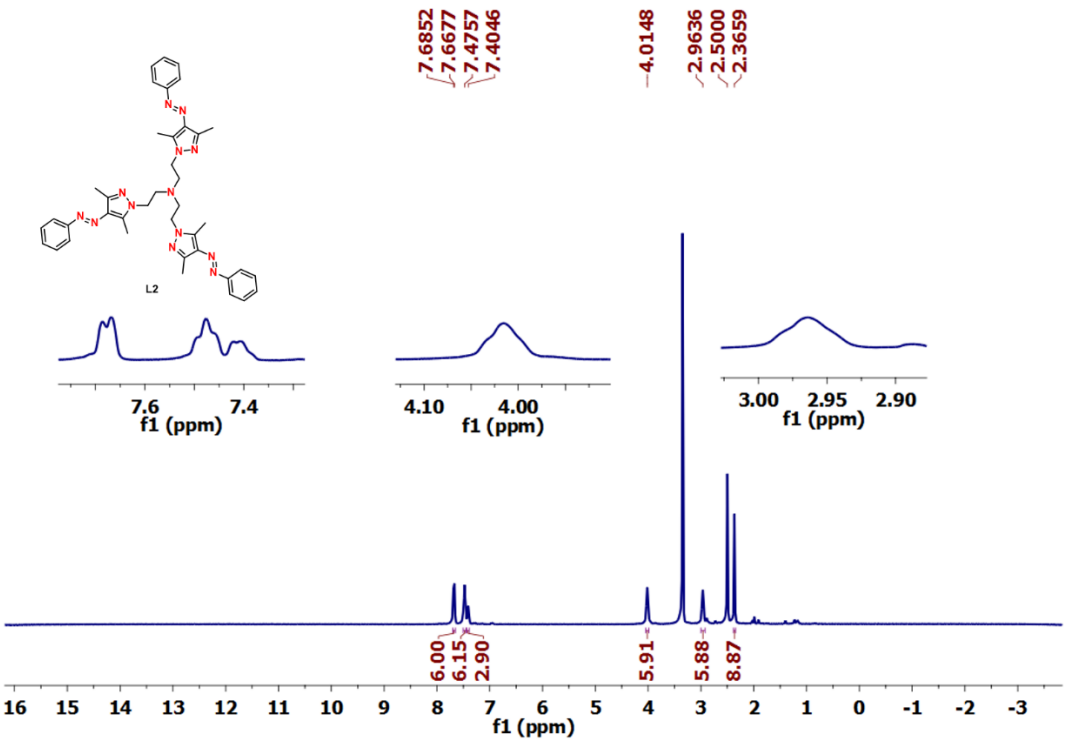


Fig S9.3. ^{1}H NMR spectrum of tris(2-(3,5-dimethyl-4-((*E*)-phenyldiazenyl)-1*H*-pyrazol-1-yl)ethyl)amine (**L2**) (400 MHz, [D_6]DMSO)

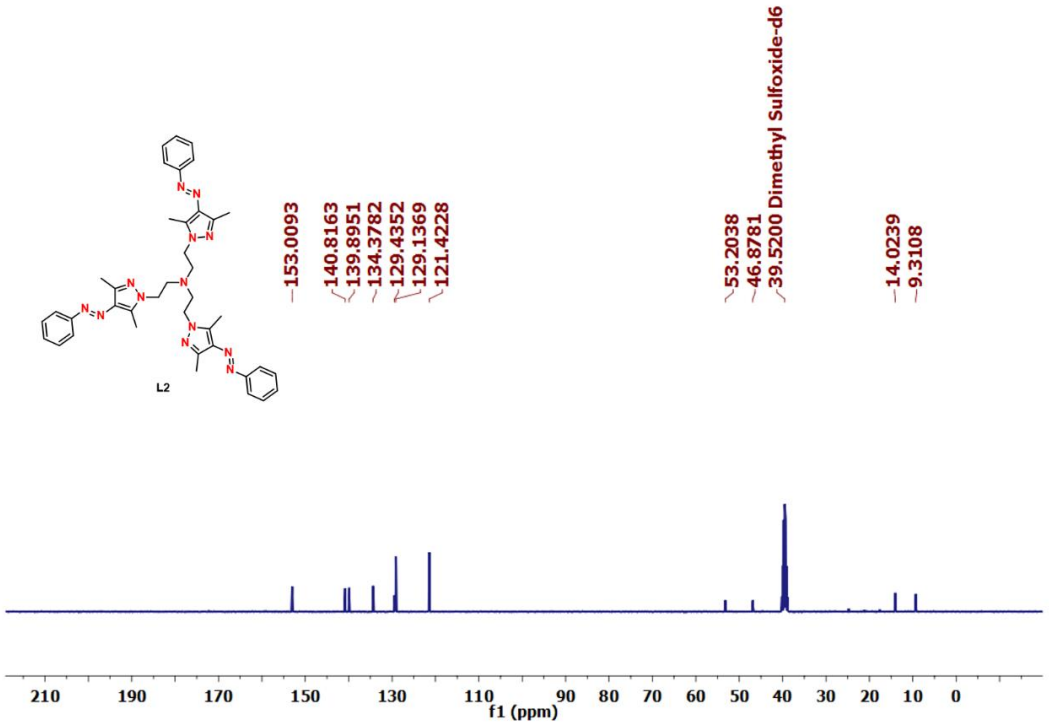


Figure S9.4. ^{13}C NMR spectrum of tris(2-(3,5-dimethyl-4-((*E*)-phenyldiazenyl)-1*H*-pyrazol-1-yl)ethyl)amine (**L2**) (100 MHz, [D_6]DMSO)

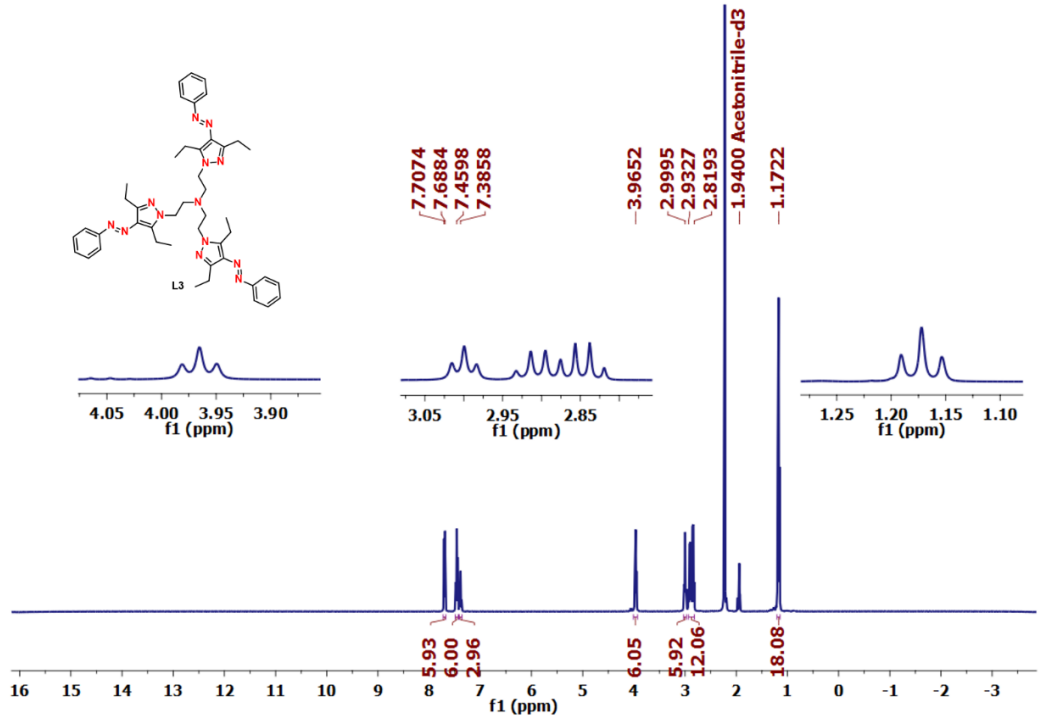


Figure S9.5: ^{1}H NMR spectrum of tris(2-(3,5-diethyl-4-((*E*)-phenyldiazenyl)-1*H*-pyrazol-1-yl)ethyl)amine (**L3**) (400 MHz, CD_3CN)

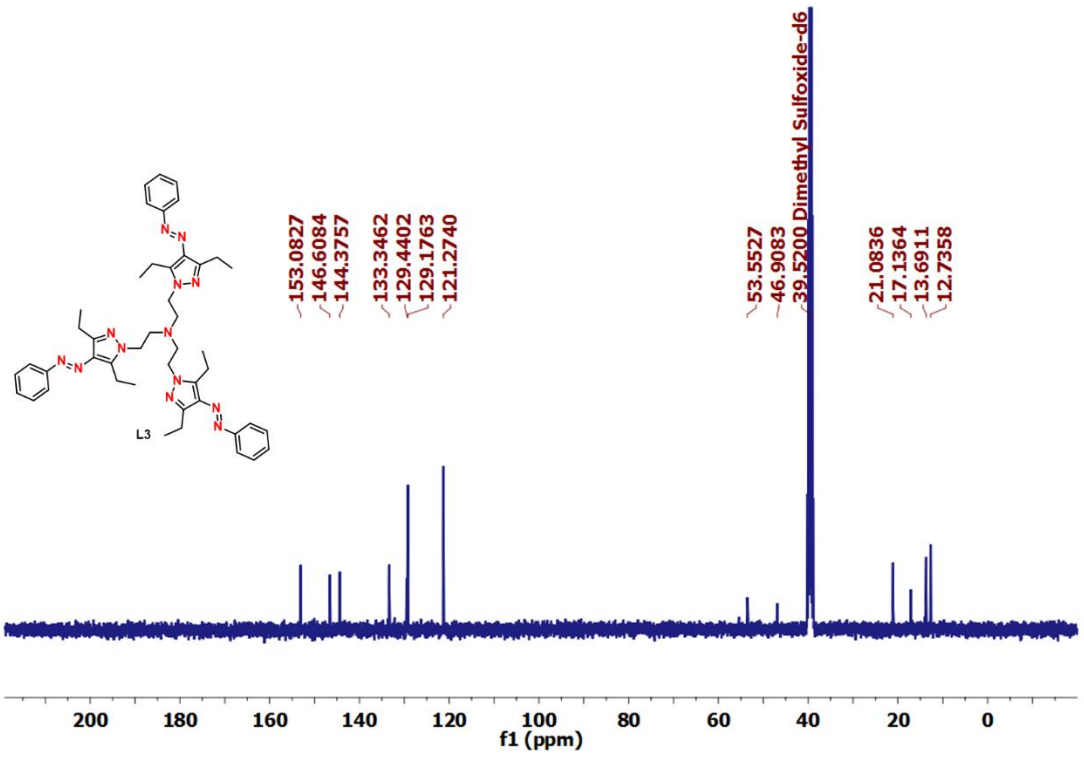


Figure S9.6. ^{1}H NMR spectrum of tris(2-(3,5-diethyl-4-((*E*)-phenyldiazenyl)-1*H*-pyrazol-1-yl)ethyl)amine (**L3**) (100 MHz, $[D_6]$DMSO)

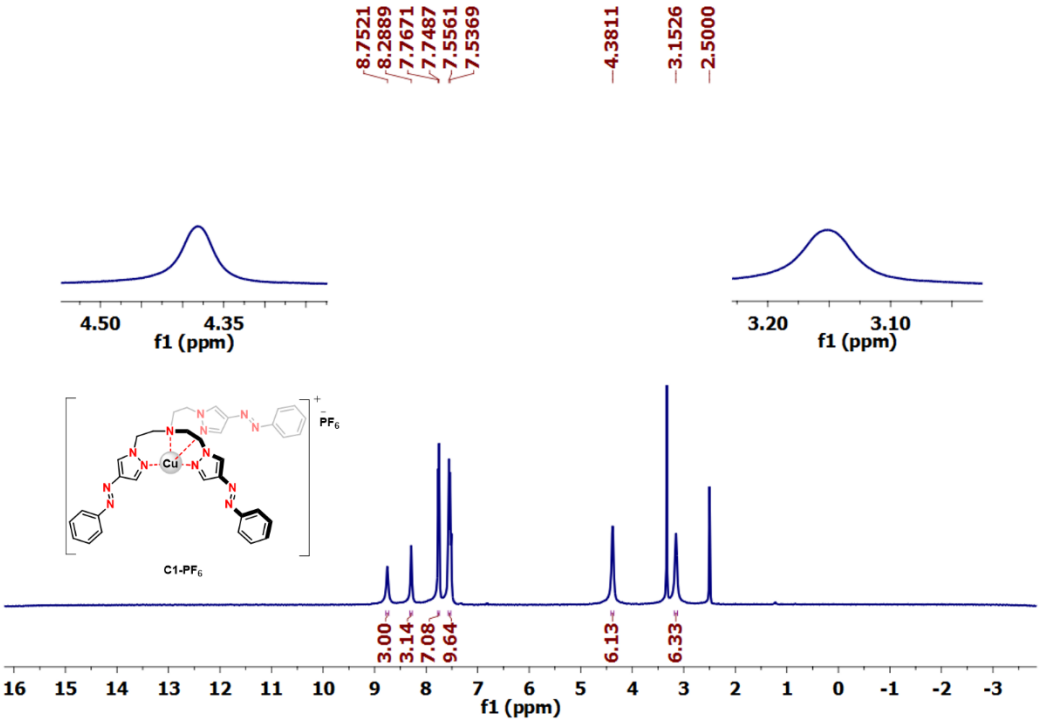


Figure S9.7. ^{1}H NMR spectrum of tris(2-(4-((*E*)-phenyldiazenyl)-1*H*-pyrazol-1-yl)ethyl)amine copper(I) hexafluorophosphate **C1-PF$_6$** (400 MHz, [D$_6$]DMSO)

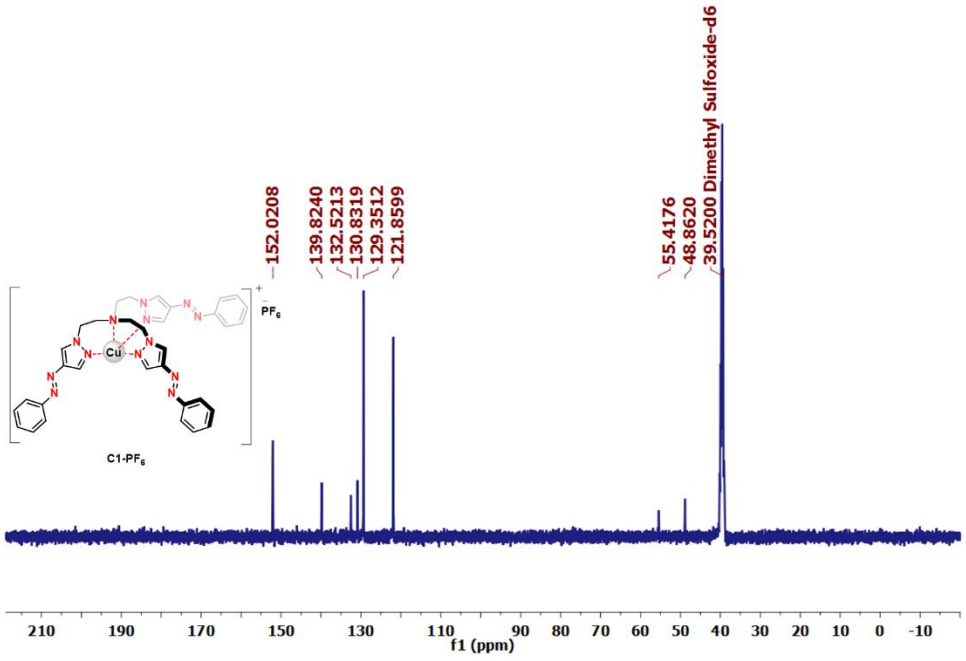


Figure S9.8. ^{13}C NMR spectrum of tris(2-(4-((*E*)-phenyldiazenyl)-1*H*-pyrazol-1-yl)ethyl)amine copper(I) hexafluorophosphate **C1-PF$_6$** (100 MHz, [D$_6$]DMSO)

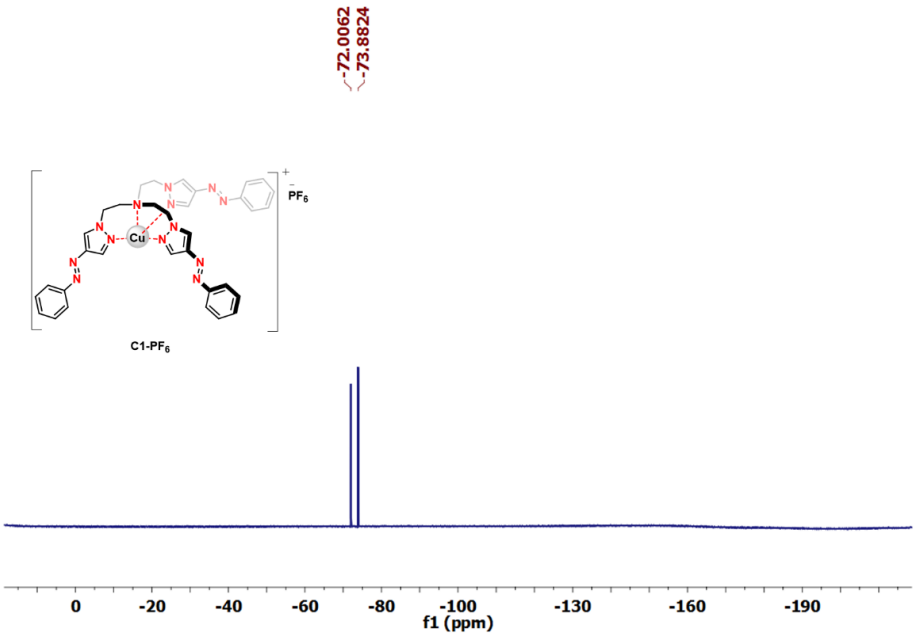


Figure S9.9: ^{19}F NMR spectrum of tris(2-(4-((*E*)-phenyldiazenyl)-1*H*-pyrazol-1-yl)ethyl)amine Copper(I) hexafluorophosphate **C1-PF$_6$** (376.5 MHz, CD_3CN)

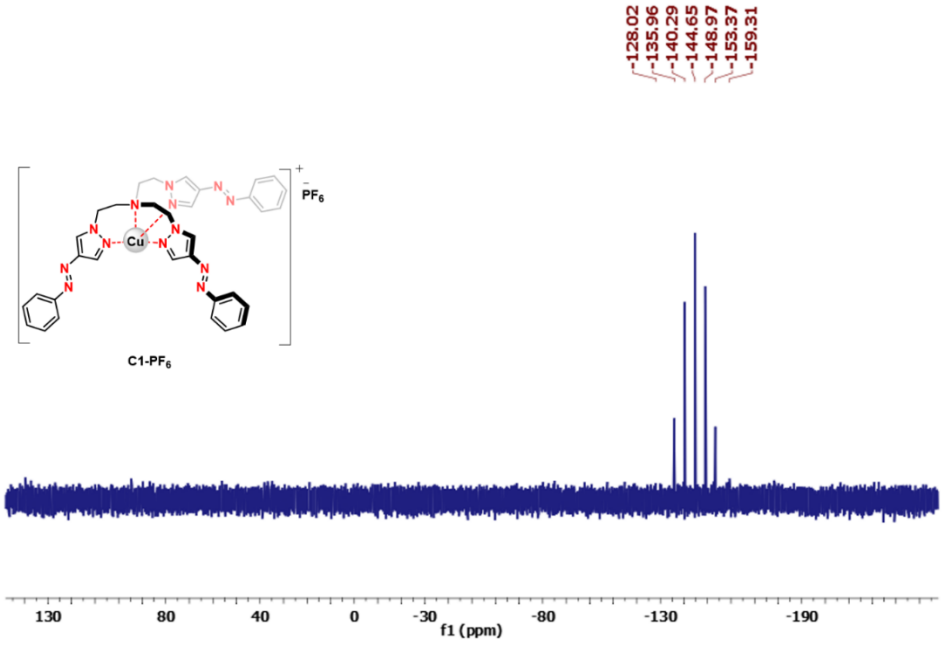


Figure S9.10. ^{31}P NMR spectrum of tris(2-(4-((*E*)-phenyldiazenyl)-1*H*-pyrazol-1-yl)ethyl)amine Copper(I) hexafluorophosphate **C1-PF$_6$** (162.1 MHz, CD_3CN)

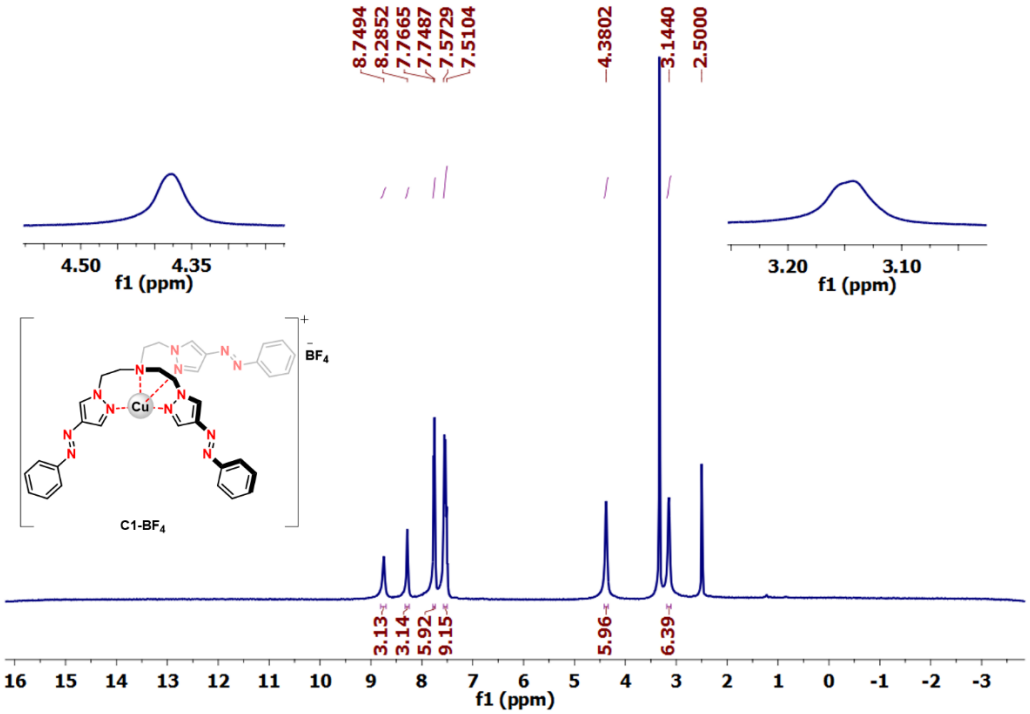


Figure S9.11. ^{1}H NMR spectrum of tris(2-(4-((*E*)-phenyldiazenyl)-1*H*-pyrazol-1-yl)ethyl)amine Copper(I) tetrafluoroborate **C1-BF$_4$** (400 MHz, [D$_6$]DMSO)

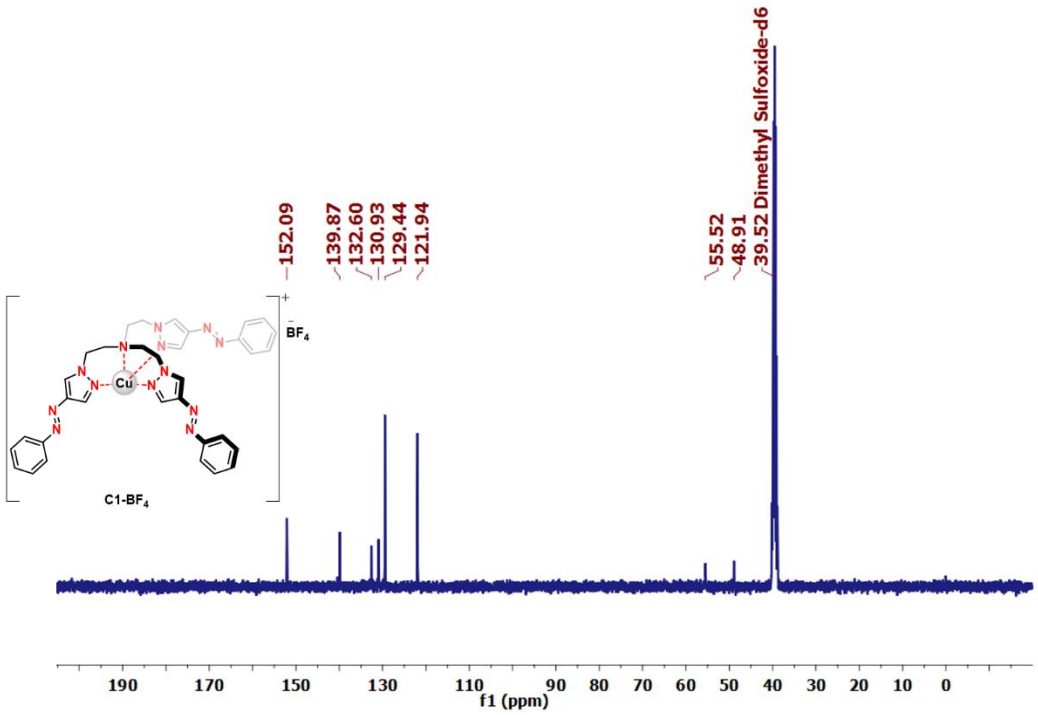


Figure S9.12. ^{13}C NMR spectrum of tris(2-(4-((*E*)-phenyldiazenyl)-1*H*-pyrazol-1-yl)ethyl)amine Copper(I) tetrafluoroborate **C1-BF$_4$** (100 MHz, [D$_6$]DMSO)

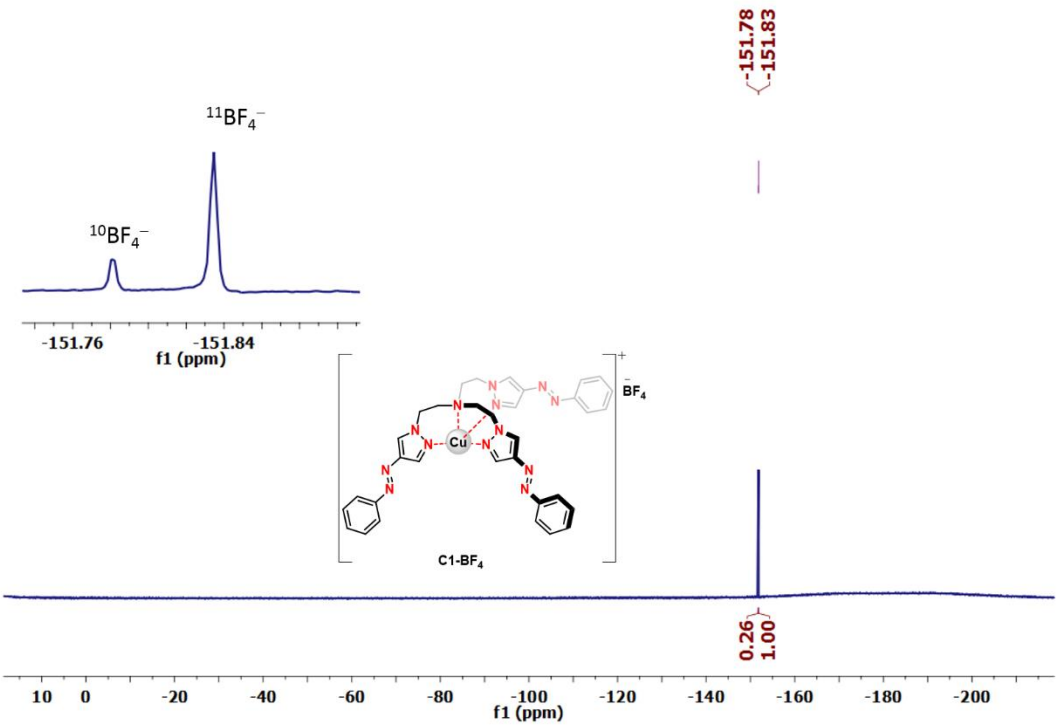


Figure S9.13. ^{19}F NMR spectrum of tris(2-(4-((*E*)-phenyldiazenyl)-1*H*-pyrazol-1-yl)ethyl)amine Copper(I) tetrafluoroborate **C1-BF$_4$** (376.5 MHz, CD_3CN)

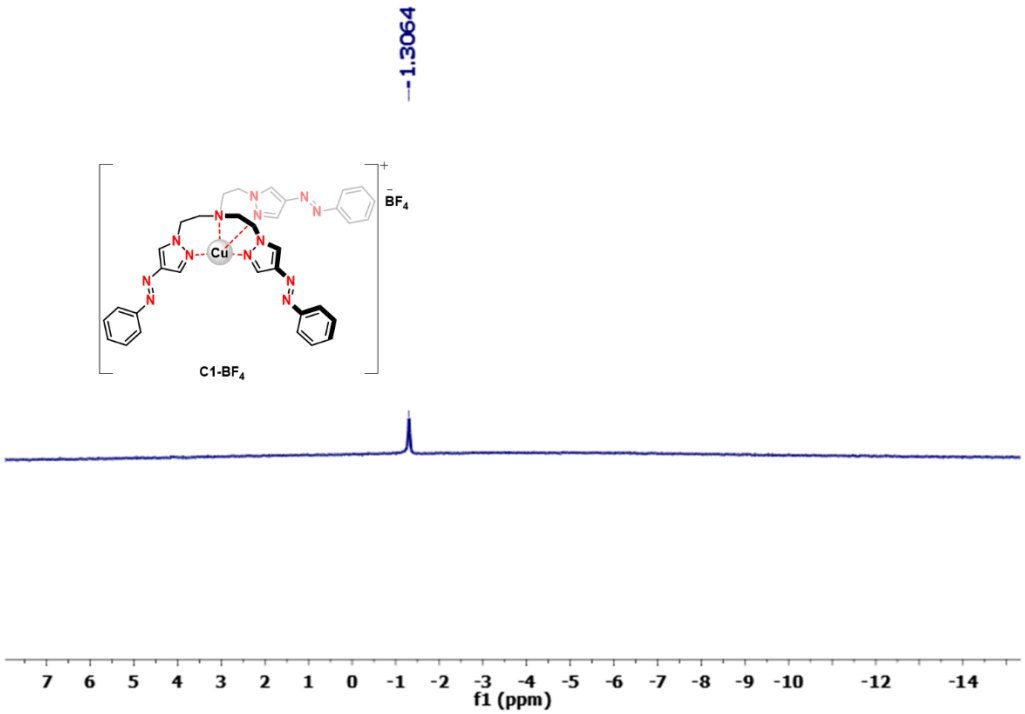


Figure S9.14. ^{11}B NMR spectrum of tris(2-(4-((E)-phenyldiazenyl)-1*H*-pyrazol-1-yl)ethyl)amine Copper(I) tetrafluoroborate **C1-BF$_4$** (128.3 MHz, CD_3CN)

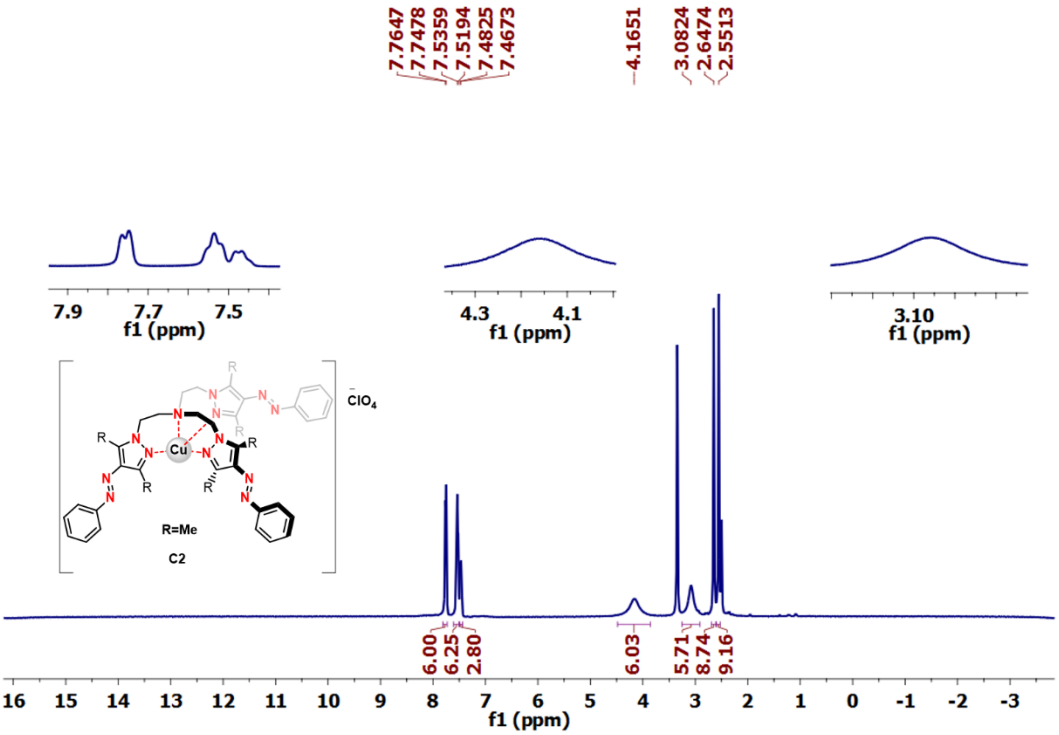


Figure S9.15. ^{1}H NMR spectrum of tris(2-(3,5-dimethyl-4-((*E*)-phenyldiazenyl)-1*H*-pyrazol-1-yl)ethyl)amine Copper(I) perchlorate **C2** (400 MHz, [D_6]DMSO)

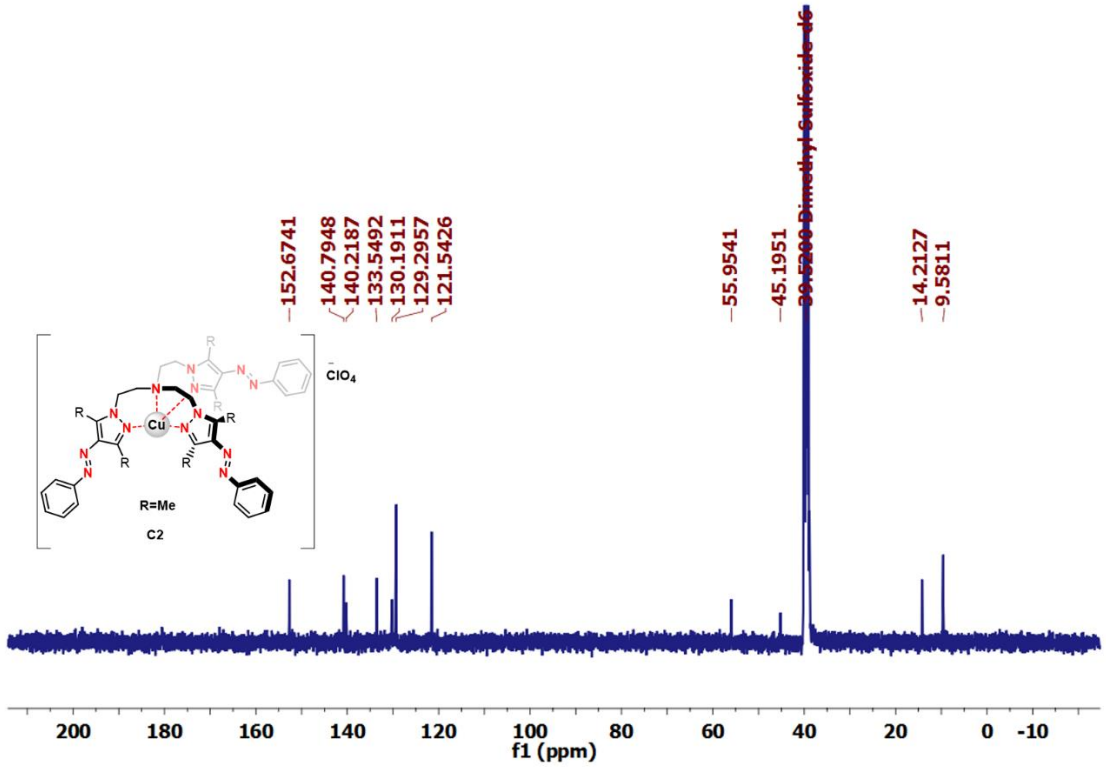


Figure S9.16. ^{13}C NMR spectrum of tris(2-(3,5-dimethyl-4-((*E*)-phenyldiazenyl)-1*H*-pyrazol-1-yl)ethyl)amine Copper(I) perchlorate **C2** (100 MHz, [D_6]DMSO)

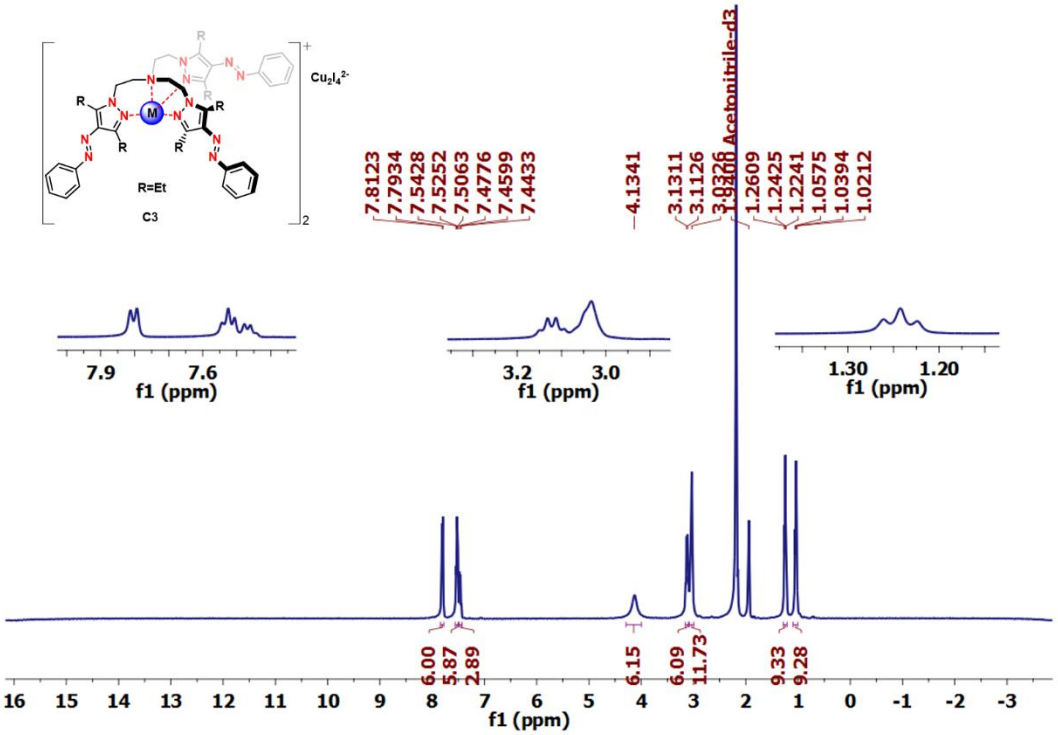


Figure S9.17. ^{1}H NMR spectrum of **C3** (400 MHz, CD_3CN)

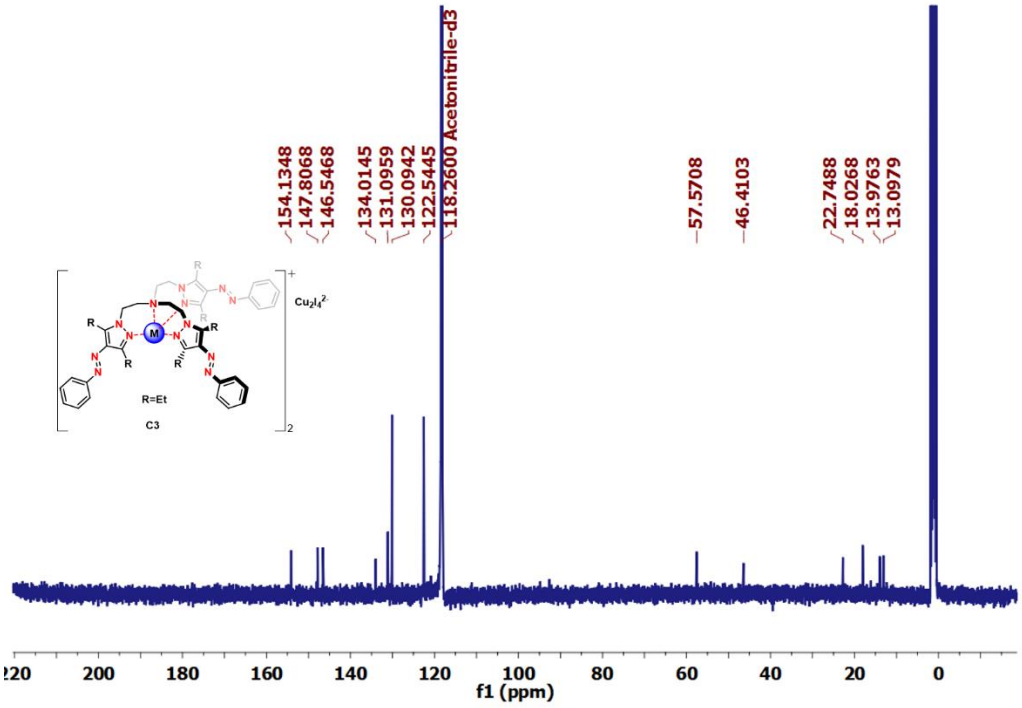


Figure S9.18. ^{13}C NMR spectrum of **C3** (100 MHz, CD_3CN)

S10. Cartesian coordinates

R(reactant) in *EEE*			
1, 1			
Cu	0.019101000	0.008173000	-0.313879000
C	-6.681570000	5.768334000	0.327313000
H	-6.230256000	6.153565000	-0.581882000
C	-7.832643000	6.339577000	0.866607000
H	-8.298834000	7.189053000	0.376506000
N	-1.530875000	2.403066000	-1.151870000
N	-1.412309000	1.451556000	-0.183057000
N	0.013734000	0.018562000	-2.734713000
C	-8.382430000	5.815176000	2.038447000
H	-9.279515000	6.257674000	2.462120000
C	-7.780109000	4.718324000	2.671922000
H	-8.213181000	4.316202000	3.583409000
C	-6.632423000	4.143709000	2.140998000
H	-6.153046000	3.296339000	2.617992000
C	-6.077316000	4.671117000	0.959427000
C	-0.605454000	2.421559000	-2.277010000
H	0.412456000	2.485802000	-1.879781000
H	-0.812487000	3.335577000	-2.838045000
C	-0.764832000	1.192691000	-3.191425000
H	-1.825357000	0.927116000	-3.213472000
H	-0.484303000	1.462084000	-4.222230000
C	-3.227448000	2.738440000	0.221298000
N	-4.918340000	4.176646000	0.323438000
N	-4.367304000	3.189992000	0.891244000
C	-2.436195000	1.653158000	0.650629000
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C	-2.610502000	3.189102000	-0.947360000
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C	-1.720796000	-8.658256000	0.319926000
H	-2.253194000	-8.461352000	-0.605546000
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H	-2.165617000	-10.764354000	0.373058000
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N	-0.530770000	-1.950414000	-0.198648000
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H	-0.931771000	-11.144993000	2.497134000
C	-0.332573000	-9.081365000	2.707512000
H	0.204179000	-9.253715000	3.636091000
C	-0.380069000	-7.803735000	2.164721000
H	0.109131000	-6.966024000	2.648798000
C	-1.078844000	-7.588336000	0.961487000
C	-1.764887000	-1.719220000	-2.296175000
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C	-0.614374000	-1.239484000	-3.200490000
H	0.144416000	-2.026456000	-3.222535000
H	-0.982005000	-1.125302000	-4.232834000
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N	-0.617094000	-5.374427000	0.883983000
C	-0.212716000	-2.941296000	0.638409000
H	0.394483000	-2.749666000	1.511439000
C	-1.457704000	-3.844907000	-0.966664000
H	-2.034452000	-4.471469000	-1.629292000
C	8.377935000	2.872281000	0.310539000
H	8.475075000	2.305766000	-0.610512000
C	9.457091000	3.565366000	0.855618000
H	10.422161000	3.547197000	0.358196000
N	2.863311000	0.145279000	-1.171830000
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C	9.291593000	4.281603000	2.043075000
H	10.130308000	4.823021000	2.471444000
C	8.045425000	4.304665000	2.686358000
H	7.924567000	4.863546000	3.609992000
C	6.965071000	3.616166000	2.149631000
H	5.994955000	3.621648000	2.633602000
C	7.130518000	2.893860000	0.952409000
C	2.407286000	-0.653824000	-2.301370000
H	1.956967000	-1.571475000	-1.910003000
H	3.297706000	-0.926957000	-2.872125000
C	1.416293000	0.106960000	-3.201559000

Int1 in *EEE* species of mononuclear pathways			
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C	-0.025725000	3.698507000	0.656094000
C	0.022112000	2.446676000	1.264478000
C	1.255610000	1.887585000	1.667627000
C	2.432486000	2.629207000	1.438266000
C	2.376283000	3.881148000	0.828321000
C	1.149655000	4.422923000	0.433996000
H	-0.984871000	4.112291000	0.353283000
H	-0.887466000	1.879249000	1.442071000
H	3.385522000	2.208096000	1.744742000
H	3.295077000	4.437892000	0.659636000
H	1.109950000	5.399945000	-0.040850000
C	1.277965000	0.602909000	2.286773000
C	1.183882000	-0.508868000	2.805339000
Cu	0.645279000	-2.165544000	3.485632000
C	-4.401677000	-1.602623000	-4.248412000
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H	-2.041981000	0.501164000	-2.983410000
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H	-3.523034000	-5.718377000	3.414505000
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C	-2.457546000	-3.497753000	-0.007235000
H	-3.198819000	-4.129450000	-0.472667000
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H	-5.355089000	1.675102000	11.373359000
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N	-2.190620000	-0.217991000	3.150704000
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H	-3.351581000	2.939811000	12.132223000
C	-2.303377000	2.706522000	10.257838000
H	-1.429666000	3.261145000	10.589950000
C	-2.337366000	2.182641000	8.970391000
H	-1.508777000	2.313907000	8.283450000
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C	-4.210857000	-1.357322000	2.437364000
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H	-5.069909000	-0.770211000	2.087338000
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H	-5.456841000	-2.527195000	3.762045000
H	-5.256687000	-3.186969000	2.145665000
C	-2.777428000	0.456623000	5.235116000
N	-3.620029000	0.883804000	7.257227000
N	-2.621139000	1.028039000	6.492879000
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H	-0.754466000	0.797102000	4.269515000
C	-3.869750000	-0.202152000	4.660997000
H	-4.856497000	-0.394164000	5.053277000
C	-0.419470000	-10.233214000	6.746631000
H	-1.406395000	-9.865263000	7.010577000
C	-0.038464000	-11.548239000	7.009365000
H	-0.735550000	-12.230243000	7.487829000

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H	1.500701000	-0.263076000	-4.235893000
C	4.017680000	1.423583000	0.210456000
N	6.113458000	2.155527000	0.309902000
N	4.987404000	2.169270000	0.885441000
C	2.684145000	1.282823000	0.646222000
H	2.214733000	1.703174000	1.524021000
C	4.087931000	0.678298000	-0.968144000
H	4.918055000	0.503867000	-1.635016000

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H	1.542639000	-13.007048000	6.861594000
C	2.138672000	-11.100368000	6.041366000
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C	1.765245000	-9.788306000	5.775361000
H	2.446956000	-9.091260000	5.301095000
C	0.476174000	-9.348848000	6.128921000
C	-1.986567000	-3.116440000	5.274316000
H	-1.703526000	-2.252008000	4.674378000
H	-1.976934000	-2.824294000	6.330528000
C	-3.395650000	-3.593213000	4.877070000
H	-3.587034000	-4.582935000	5.324315000
H	-4.087574000	-2.898891000	5.363979000
C	0.272368000	-5.973739000	5.139165000
N	-0.019587000	-8.040956000	5.912565000
N	0.783527000	-7.255801000	5.331643000
C	0.961728000	-4.935720000	4.478519000
H	1.943538000	-4.949254000	4.028913000
C	-0.948866000	-5.406680000	5.514137000
H	-1.772989000	-5.836646000	6.060003000

Int2 in *EEE* species of mononuclear pathways

0, 1

C	0.327775000	3.936938000	0.978547000
C	0.196706000	2.714435000	1.632931000
C	1.329369000	1.915547000	1.903207000
C	2.593220000	2.385363000	1.489148000
C	2.715756000	3.608920000	0.833389000
C	1.586975000	4.392040000	0.575525000
H	-0.556778000	4.537962000	0.780674000
H	-0.780292000	2.354165000	1.943365000
H	3.468291000	1.773716000	1.685532000
H	3.698707000	3.953816000	0.521069000
H	1.687203000	5.346291000	0.064631000
C	1.178635000	0.662666000	2.567782000
C	0.985785000	-0.420865000	3.117420000
Cu	0.395165000	-2.058111000	3.804647000
C	-3.760017000	-2.145648000	-4.399583000
H	-4.205767000	-3.105376000	-4.155183000
C	-3.983052000	-1.532230000	-5.631841000
H	-4.615452000	-2.015120000	-6.371820000
N	-1.934240000	-3.827158000	1.469534000
N	-1.168848000	-2.792059000	1.917973000
N	-3.870590000	-3.622508000	3.730240000
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H	-3.561589000	0.182568000	-6.870555000
C	-2.575336000	0.319122000	-4.953524000
H	-2.114633000	1.278666000	-5.173257000
C	-2.348959000	-0.286839000	-3.722858000
H	-1.719810000	0.176034000	-2.970756000
C	-2.944947000	-1.529459000	-3.439939000
C	-2.209082000	-4.946754000	2.350369000
H	-1.407598000	-4.962799000	3.085059000
H	-2.151091000	-5.874990000	1.769626000
C	-3.597991000	-4.855664000	3.018017000
H	-4.355971000	-4.989308000	2.235927000
H	-3.687599000	-5.721370000	3.694815000
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N	-2.788274000	-2.243322000	-2.225016000
N	-2.055917000	-1.666590000	-1.369485000
C	-1.138386000	-1.912662000	0.924720000
H	-0.577633000	-0.996978000	1.048414000
C	-2.401211000	-3.615904000	0.219256000
H	-3.021352000	-4.327343000	-0.304681000
C	-4.901549000	1.251285000	9.620339000
H	-5.739891000	0.670239000	9.247341000
C	-4.898395000	1.777815000	10.911458000
H	-5.747455000	1.609226000	11.568251000
N	-3.664727000	-0.589243000	3.656094000
N	-2.391828000	-0.178497000	3.398716000
C	-3.803615000	2.522244000	11.355786000
H	-3.797517000	2.935592000	12.360794000
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H	-1.862023000	3.319715000	10.850145000

Int3 in *EEE* species of mononuclear pathways

0, 1

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C	0.981506000	0.323383000	5.216782000
C	1.880854000	0.937185000	4.325241000
C	2.538522000	2.107056000	4.752117000
C	2.289897000	2.648970000	6.012008000
C	1.376480000	2.040924000	6.879568000
H	0.011795000	0.391263000	7.137173000
H	0.487478000	-0.590962000	4.908720000
H	3.247023000	2.578177000	4.078242000
H	2.808474000	3.554888000	6.317625000
H	1.182696000	2.464467000	7.862259000
C	2.145373000	0.377316000	2.992144000
C	1.315894000	-0.406234000	2.169800000
Cu	-0.507668000	-1.156420000	2.269912000
C	-4.898666000	-3.632229000	-5.056150000
H	-5.065460000	-4.568751000	-4.532507000
C	-5.384323000	-3.422819000	-6.345964000
H	-5.943858000	-4.206181000	-6.849293000
N	-2.206671000	-3.373096000	0.689608000
N	-1.649061000	-2.134921000	0.779522000
N	-3.747110000	-3.212663000	3.416473000
C	-5.148310000	-2.204874000	-6.987116000
H	-5.524626000	-2.037523000	-7.992624000
C	-4.424728000	-1.196606000	-6.335257000
H	-4.242292000	-0.250678000	-6.838012000
C	-3.936991000	-1.398721000	-5.049545000
H	-3.374125000	-0.630874000	-4.530738000
C	-4.174807000	-2.625161000	-4.402152000
C	-2.121251000	-4.314295000	1.797845000
H	-1.268776000	-4.010106000	2.397113000
H	-1.903156000	-5.301481000	1.377055000
C	-3.412180000	-4.391563000	2.635067000
H	-4.244060000	-4.637746000	1.958028000
H	-3.288590000	-5.251792000	3.307633000
C	-2.654808000	-2.385929000	-1.232084000
N	-3.733017000	-2.950165000	-3.097234000
N	-3.077300000	-2.039462000	-2.514191000
C	-1.913736000	-1.534365000	-0.381671000
H	-1.568575000	-0.526213000	-0.559237000
C	-2.818275000	-3.564264000	-0.497842000
H	-3.304495000	-4.491479000	-0.758768000
C	-4.306618000	2.429637000	9.021153000
H	-5.227748000	1.908665000	8.776857000
C	-4.144499000	3.088009000	10.239782000
H	-4.950855000	3.088326000	10.968010000
N	-3.539105000	-0.203889000	3.218745000
N	-2.277542000	0.178568000	2.851314000
C	-2.943293000	3.742267000	10.521641000
H	-2.811499000	4.252010000	11.472286000
C	-1.904458000	3.737246000	9.580589000
H	-0.968325000	4.241704000	9.805204000

C	-2.708889000	2.215605000	9.215003000
H	-1.873808000	2.374179000	8.541818000
C	-3.810224000	1.463952000	8.766361000
C	-4.364548000	-1.381683000	2.654026000
H	-3.648413000	-1.542108000	1.848552000
H	-5.210996000	-0.804968000	2.258608000
C	-4.884492000	-2.722675000	3.200841000
H	-5.646342000	-2.521418000	3.969951000
H	-5.410393000	-3.213388000	2.372757000
C	-3.034581000	0.481716000	5.471142000
N	-3.922127000	0.879469000	7.479935000
N	-2.916462000	1.056109000	6.731510000
C	-2.006271000	0.472972000	4.490485000
H	-1.004404000	0.876467000	4.540968000
C	-4.096246000	-0.210882000	4.879746000
H	-5.083079000	-0.431739000	5.256137000
C	-0.500908000	-10.273690000	6.640781000
H	-1.510886000	-9.967990000	6.896941000
C	-0.077835000	-11.592931000	6.797924000
H	-0.764657000	-12.340598000	7.184421000
N	-1.178619000	-4.063468000	5.401483000
N	-0.005287000	-3.701308000	4.804350000
C	1.229491000	-11.948265000	6.459418000
H	1.563524000	-12.974910000	6.581957000
C	2.113566000	-10.980055000	5.963385000
H	3.131168000	-11.259457000	5.703732000
C	1.698086000	-9.663359000	5.803250000
H	2.368848000	-8.899889000	5.424865000
C	0.380366000	-9.304471000	6.142052000
C	-2.247447000	-3.083973000	5.603344000
H	-1.971982000	-2.198485000	5.031322000
H	-2.273344000	-2.816957000	6.666239000
C	-3.631907000	-3.591213000	5.160405000
H	-3.814193000	-4.585209000	5.601671000
H	-4.355972000	-2.913930000	5.624805000
C	0.095422000	-5.869391000	5.412121000
N	-0.158178000	-8.000075000	6.019412000
N	0.636680000	-7.146220000	5.531768000
C	0.769052000	-4.784567000	4.812542000
H	1.750473000	-4.756594000	4.366933000
C	-1.149387000	-5.354772000	5.788406000
H	-1.972456000	-5.830323000	6.296922000
C	3.393771000	-4.360032000	2.199195000
C	3.502867000	-5.659072000	2.700049000
C	2.498844000	-6.601565000	2.463209000
C	1.380490000	-6.232609000	1.708442000
C	1.265074000	-4.944916000	1.190763000
C	2.273416000	-3.999721000	1.432504000
H	4.177261000	-3.632730000	2.393227000
H	4.376766000	-5.929088000	3.286950000
H	2.577778000	-7.603881000	2.872257000
H	0.592138000	-6.956479000	1.519006000
H	0.410926000	-4.650504000	0.592224000
N	2.081231000	-2.725882000	0.852557000
N	2.962346000	-1.870342000	1.019708000
N	3.695053000	-1.002737000	1.086151000

C	-2.059865000	3.088635000	8.360781000
H	-1.263328000	3.066696000	7.624741000
C	-3.271882000	2.431632000	8.076210000
C	-4.339338000	-1.015768000	2.312448000
H	-3.711769000	-1.193257000	1.443545000
H	-5.216053000	-0.437317000	1.993823000
C	-4.806759000	-2.343730000	2.931568000
H	-5.505317000	-2.123532000	3.751498000
H	-5.393258000	-2.860127000	2.158417000
C	-2.829830000	1.107884000	4.842477000
N	-3.532199000	1.720766000	6.876719000
N	-2.621275000	1.835570000	6.008038000
C	-1.856221000	0.986048000	3.823332000
H	-0.864393000	1.410303000	3.788182000
C	-3.907940000	0.333630000	4.401590000
H	-4.876489000	0.161128000	4.845640000
C	1.424929000	-9.216731000	5.133623000
H	0.444868000	-9.238761000	5.600872000
C	2.204251000	-10.367911000	5.022382000
H	1.834230000	-11.312972000	5.410095000
N	-1.056281000	-3.332330000	4.855563000
N	-0.216171000	-2.654290000	4.024752000
C	3.458763000	-10.302174000	4.412540000
H	4.068750000	-11.197024000	4.323914000
C	3.933541000	-9.080233000	3.916533000
H	4.911840000	-9.030699000	3.445861000
C	3.162583000	-7.928508000	4.025567000
H	3.515293000	-6.972962000	3.653891000
C	1.895990000	-7.994555000	4.635663000
C	-2.240152000	-2.659740000	5.367077000
H	-2.153888000	-1.619949000	5.053614000
H	-2.222016000	-2.694041000	6.463120000
C	-3.547400000	-3.283186000	4.855326000
H	-3.590420000	-4.331270000	5.190475000
H	-4.365856000	-2.759634000	5.365337000
C	0.587524000	-4.730894000	4.414854000
N	1.015323000	-6.892823000	4.784015000
N	1.452837000	-5.813121000	4.292993000
C	0.791452000	-3.487097000	3.771217000
H	1.591092000	-3.178456000	3.115251000
C	-0.616936000	-4.583293000	5.112276000
H	-1.140829000	-5.267851000	5.761902000
C	3.220593000	-4.716959000	1.387817000
C	3.127046000	-3.373780000	1.023734000
C	2.026974000	-2.913140000	0.285754000
C	1.039998000	-3.825339000	-0.099372000
C	1.133570000	-5.171938000	0.265750000
C	2.218994000	-5.620807000	1.019174000
H	4.069581000	-5.057916000	1.974396000
H	3.890679000	-2.662150000	1.327346000
H	0.192026000	-3.479697000	-0.683917000
H	0.355626000	-5.868999000	-0.038309000
H	2.284764000	-6.660931000	1.325854000
C	1.912808000	-1.438760000	-0.062327000
H	2.661984000	-1.155998000	-0.808984000
H	0.920144000	-1.225277000	-0.468004000
N	2.139082000	-0.584126000	1.089816000
N	3.363395000	0.012458000	1.224081000
N	3.354266000	0.607896000	2.377850000

R in *ZZZ* species of mononuclear pathways

1, 1

Cu	0.047585000	-0.015233000	0.804377000
C	5.406283000	-4.849945000	0.942964000
H	4.983760000	-5.131770000	1.902685000
C	5.379169000	-5.727328000	-0.141748000
H	4.934231000	-6.711335000	-0.023540000
N	2.165211000	-1.924322000	-0.052261000
N	1.798920000	-1.050638000	0.929874000
N	0.039368000	0.003167000	-1.593458000
C	5.925994000	-5.348021000	-1.371762000
H	5.906667000	-6.036380000	-2.211477000
C	6.526252000	-4.092487000	-1.508122000
H	6.975341000	-3.803326000	-2.454239000
C	6.565187000	-3.208079000	-0.428586000
H	7.033655000	-2.232553000	-0.518551000

Int1 in *ZZZ* species of mononuclear pathways

0, 1

C	0.721191000	3.240186000	-0.386851000
C	0.637954000	2.163425000	0.492354000
C	1.764488000	1.754989000	1.239964000
C	2.971338000	2.464307000	1.073731000
C	3.046764000	3.540775000	0.191889000
C	1.924734000	3.934652000	-0.542540000
H	-0.156391000	3.538939000	-0.955283000
H	-0.294616000	1.620295000	0.618756000
H	3.842862000	2.157482000	1.644468000
H	3.986502000	4.075545000	0.076540000
H	1.987579000	4.774356000	-1.229849000
C	1.656994000	0.648601000	2.134068000
C	1.471113000	-0.312216000	2.879030000
Cu	0.852602000	-1.775079000	3.859125000

C	5.980341000	-3.583057000	0.785698000
C	1.284031000	-2.158081000	-1.189732000
H	0.321026000	-2.509677000	-0.806386000
H	1.734016000	-2.964405000	-1.773230000
C	1.107839000	-0.906857000	-2.069508000
H	2.057217000	-0.364401000	-2.074851000
H	0.912866000	-1.214855000	-3.109149000
C	3.871284000	-1.867019000	1.354312000
N	6.019560000	-2.676913000	1.895586000
N	5.051181000	-1.921886000	2.139012000
C	2.826122000	-1.013820000	1.775251000
H	2.799099000	-0.391266000	2.658309000
C	3.397441000	-2.434070000	0.160291000
H	3.828391000	-3.139224000	-0.531907000
C	1.467337000	7.055260000	1.016407000
H	1.918207000	6.820769000	1.975967000
C	2.244465000	7.492592000	-0.056859000
H	3.317254000	7.607259000	0.070442000
N	0.621752000	2.789353000	-0.020991000
N	0.055054000	2.019117000	0.952698000
C	1.648543000	7.788693000	-1.286927000
H	2.257071000	8.133215000	-2.117786000
C	0.263042000	7.670796000	-1.434201000
H	-0.207719000	7.924558000	-2.379946000
C	-0.526211000	7.240786000	-0.365812000
H	-1.604031000	7.152310000	-0.464299000
C	0.085369000	6.909105000	0.847891000
C	1.277453000	2.162369000	-1.162324000
H	2.066250000	1.505303000	-0.782447000
H	1.747823000	2.966190000	-1.733054000
C	0.293120000	1.387787000	-2.057243000
H	-0.652951000	1.935873000	-2.068069000
H	0.667261000	1.381480000	-3.093306000
C	-0.311122000	4.213255000	1.391288000
N	-0.723390000	6.468488000	1.946189000
N	-0.875789000	5.248054000	2.179361000
C	-0.508278000	2.875273000	1.801489000
H	-1.032907000	2.525453000	2.679258000
C	0.424435000	4.106912000	0.200071000
H	0.811311000	4.844513000	-0.484400000
C	-6.833514000	-2.130072000	1.036661000
H	-6.828006000	-1.620591000	1.995517000
C	-7.594457000	-1.649912000	-0.029828000
H	-8.196912000	-0.755546000	0.101965000
N	-2.681891000	-0.873114000	-0.031961000
N	-1.732655000	-1.002714000	0.939748000
C	-7.588438000	-2.316679000	-1.259183000
H	-8.185980000	-1.941600000	-2.084771000
C	-6.836429000	-3.485502000	-1.412449000
H	-6.848964000	-4.021171000	-2.357602000
C	-6.076425000	-3.979883000	-0.350697000
H	-5.493366000	-4.890167000	-0.453522000
C	-6.058852000	-3.282854000	0.862140000
C	-2.450806000	0.007755000	-1.170618000
H	-2.269740000	1.017249000	-0.788213000
H	-3.378655000	0.022767000	-1.746831000
C	-1.286911000	-0.465361000	-2.060019000
H	-1.292753000	-1.558685000	-2.067716000
H	-1.463733000	-0.140519000	-3.097748000
C	-3.489163000	-2.364770000	1.387553000
N	-5.281034000	-3.790134000	1.954070000
N	-4.130741000	-3.350677000	2.179443000
C	-2.216267000	-1.902928000	1.792299000
H	-1.656826000	-2.196565000	2.669161000
C	-3.747942000	-1.670252000	0.195138000
H	-4.582385000	-1.682532000	-0.487266000

C	-4.307533000	-2.728902000	-1.348237000
H	-4.233977000	-1.699396000	-1.012366000
C	-5.428408000	-3.504734000	-1.054391000
H	-6.248169000	-3.071260000	-0.486493000
N	-1.308574000	-4.019155000	1.570387000
N	-0.429028000	-3.016584000	1.851297000
N	-3.471077000	-3.362072000	3.474466000
C	-5.504705000	-4.830615000	-1.494153000
H	-6.378539000	-5.433516000	-1.264135000
C	-4.463922000	-5.364948000	-2.259512000
H	-4.526205000	-6.387077000	-2.623482000
C	-3.342827000	-4.591438000	-2.568550000
H	-2.528419000	-4.996769000	-3.161721000
C	-3.250409000	-3.282282000	-2.083755000
C	-1.703408000	-4.949793000	2.613358000
H	-0.992596000	-4.812232000	3.425168000
H	-1.599353000	-5.976735000	2.241703000
C	-3.157167000	-4.722671000	3.081745000
H	-3.825694000	-5.020567000	2.264546000
H	-3.341889000	-5.420715000	3.913204000
C	-1.180292000	-2.833776000	-0.282427000
N	-2.113545000	-2.474490000	-2.410649000
N	-1.208378000	-2.257719000	-1.565876000
C	-0.330583000	-2.311911000	0.733602000
H	0.306086000	-1.437483000	0.708513000
C	-1.796554000	-3.945777000	0.316551000
H	-2.500441000	-4.674564000	-0.051351000
C	-4.618156000	-0.087837000	7.043539000
H	-3.667286000	-0.395882000	7.468939000
C	-5.733838000	-0.924172000	7.091118000
H	-5.653045000	-1.902023000	7.559505000
N	-3.201018000	-0.406204000	2.833811000
N	-1.899037000	-0.048073000	2.646312000
C	-6.952227000	-0.507406000	6.545288000
H	-7.819770000	-1.159928000	6.583121000
C	-7.054939000	0.766735000	5.978647000
H	-8.004091000	1.105936000	5.572349000
C	-5.945703000	1.613483000	5.934261000
H	-6.014016000	2.603477000	5.493201000
C	-4.717013000	1.172601000	6.438982000
C	-3.801897000	-1.381896000	1.935149000
H	-3.004990000	-1.691511000	1.260840000
H	-4.587705000	-0.893200000	1.344356000
C	-4.404687000	-2.598119000	2.660008000
H	-5.257369000	-2.265357000	3.272833000
H	-4.818655000	-3.242441000	1.875485000
C	-2.776581000	1.037516000	4.443292000
N	-3.577961000	2.038806000	6.418232000
N	-2.706354000	1.941241000	5.517205000
C	-1.643462000	0.832072000	3.604269000
H	-0.654003000	1.259726000	3.688830000
C	-3.770432000	0.210436000	3.889269000
H	-4.802387000	0.039298000	4.146479000
C	-1.933423000	-7.677562000	5.630863000
H	-1.301873000	-7.843056000	4.762935000
C	-3.323760000	-7.724289000	5.528474000
H	-3.784029000	-7.942395000	4.568367000
N	-0.991197000	-3.438488000	5.516437000
N	0.273907000	-3.217244000	5.053977000
C	-4.123717000	-7.494900000	6.652712000
H	-5.205967000	-7.527957000	6.568138000
C	-3.523193000	-7.251147000	7.891283000
H	-4.138422000	-7.091852000	8.772580000
C	-2.131820000	-7.222853000	8.009210000
H	-1.653773000	-7.041439000	8.967232000
C	-1.339881000	-7.406047000	6.870783000
C	-2.045683000	-2.432786000	5.349064000
H	-1.680128000	-1.714688000	4.615735000
H	-2.177149000	-1.915880000	6.305995000
C	-3.389187000	-3.022839000	4.882395000
H	-3.646423000	-3.896538000	5.503418000
H	-4.139260000	-2.259877000	5.111812000
C	0.187908000	-5.215745000	6.110196000
N	0.088639000	-7.393284000	6.991303000
N	0.760187000	-6.403951000	6.611524000

C	0.990181000	-4.276179000	5.423956000
H	2.038140000	-4.346608000	5.172074000
C	-1.081652000	-4.618481000	6.156944000
H	-2.005907000	-4.937096000	6.607421000

Int2 in *ZZZ* species of mononuclear pathways

0, 1

C	2.036784000	3.276078000	-0.206563000
C	1.426577000	2.300987000	0.579435000
C	2.168879000	1.576395000	1.536010000
C	3.543352000	1.866364000	1.674813000
C	4.146946000	2.842132000	0.884671000
C	3.399137000	3.552242000	-0.059238000
H	1.446745000	3.822964000	-0.938073000
H	0.367483000	2.087229000	0.465324000
H	4.122332000	1.313640000	2.408382000
H	5.207164000	3.050720000	1.006743000
H	3.873031000	4.313498000	-0.673557000
C	1.555098000	0.564353000	2.333208000
C	1.055983000	-0.330196000	3.015383000
Cu	0.331523000	-1.848527000	3.856604000
C	-4.619133000	-3.555795000	-2.269184000
H	-3.940846000	-3.760174000	-3.092410000
C	-5.625082000	-4.460538000	-1.921872000
H	-5.735108000	-5.382174000	-2.487114000
N	-1.850487000	-3.652681000	1.491065000
N	-1.027496000	-2.634191000	1.852967000
N	-3.663096000	-3.843471000	3.857313000
C	-6.493173000	-4.182228000	-0.862184000
H	-7.280767000	-4.883904000	-0.602929000
C	-6.361457000	-2.980250000	-0.158349000
H	-7.052219000	-2.742170000	0.646861000
C	-5.349734000	-2.079070000	-0.487022000
H	-5.230559000	-1.147026000	0.056671000
C	-4.461195000	-2.379681000	-1.528757000
C	-1.931241000	-4.850365000	2.309146000
H	-1.098756000	-4.793855000	3.004935000
H	-1.766120000	-5.723613000	1.670015000
C	-3.287150000	-4.975799000	3.027989000
H	-4.061508000	-5.134746000	2.265471000
H	-3.245339000	-5.893940000	3.630541000
C	-2.124597000	-2.113326000	-0.061061000
N	-3.439939000	-1.440472000	-1.887374000
N	-2.408960000	-1.308502000	-1.180628000
C	-1.171970000	-1.708628000	0.913422000
H	-0.614152000	-0.784836000	0.991149000
C	-2.534753000	-3.389948000	0.362380000
H	-3.217537000	-4.110950000	-0.056846000
C	-6.021984000	0.135462000	7.848347000
H	-6.181121000	1.199921000	7.703981000
C	-7.086159000	-0.766567000	7.791048000
H	-8.091672000	-0.397528000	7.607389000
N	-3.655233000	-0.824885000	4.014744000
N	-2.412646000	-0.326096000	3.768537000
C	-6.865705000	-2.135336000	7.972489000
H	-7.697698000	-2.832473000	7.932821000
C	-5.572115000	-2.597845000	8.235763000
H	-5.396875000	-3.657101000	8.406810000
C	-4.501623000	-1.704592000	8.286475000
H	-3.492439000	-2.048727000	8.493026000
C	-4.723584000	-0.338941000	8.065752000
C	-4.338301000	-1.575276000	2.969169000
H	-3.643536000	-1.616229000	2.132251000
H	-5.231145000	-1.021097000	2.651417000
C	-4.752206000	-2.990039000	3.410145000
H	-5.514126000	-2.907445000	4.200255000
H	-5.250087000	-3.446692000	2.545729000
C	-3.072796000	0.184084000	5.886045000
N	-3.627089000	0.578310000	8.140518000
N	-2.885875000	0.780185000	7.145373000
C	-2.063050000	0.293876000	4.887293000
H	-1.093767000	0.768385000	4.959653000
C	-4.096040000	-0.550977000	5.259791000
H	-5.071394000	-0.868180000	5.589450000
C	-1.123786000	-8.828320000	6.096260000
H	-0.573441000	-8.973325000	7.021270000

Int3 in *ZZZ* species of mononuclear pathways

0, 1

C	-4.313931000	0.870850000	-1.077346000
H	-4.411348000	0.142778000	-0.276252000
C	-4.602189000	0.519328000	-2.397524000
H	-4.923928000	-0.494003000	-2.620229000
N	0.481810000	2.447723000	-0.728727000
N	0.898548000	2.163296000	0.538831000
N	0.840351000	0.622714000	-3.201079000
C	-4.491173000	1.465187000	-3.421617000
H	-4.726238000	1.190434000	-4.445995000
C	-4.110648000	2.774951000	-3.113721000
H	-4.050759000	3.524146000	-3.898994000
C	-3.816272000	3.133439000	-1.796691000
H	-3.534812000	4.152892000	-1.547125000
C	-3.884197000	2.172405000	-0.779027000
C	1.497870000	2.605546000	-1.762437000
H	2.383442000	2.098587000	-1.381887000
H	1.739380000	3.672382000	-1.868050000
C	1.110761000	2.048855000	-3.141145000
H	0.241568000	2.602942000	-3.525476000
H	1.948580000	2.295691000	-3.806528000
C	-1.343977000	2.542370000	0.505758000
N	-3.711865000	2.525919000	0.597909000
N	-2.591437000	2.682799000	1.139144000
C	-0.190864000	2.238173000	1.287048000
H	-0.158938000	2.027363000	2.347510000
C	-0.848405000	2.683372000	-0.799319000
H	-1.330807000	2.944987000	-1.725351000
C	-4.786647000	-4.210629000	-3.836224000
H	-4.400765000	-4.685014000	-4.733793000
C	-5.836296000	-3.291173000	-3.900708000
H	-6.271075000	-3.040065000	-4.864491000
N	-1.079976000	-1.796237000	-1.735294000
N	-0.065214000	-2.442173000	-1.093665000
C	-6.340654000	-2.712251000	-2.732073000
H	-7.168099000	-2.010140000	-2.784345000
C	-5.783493000	-3.050875000	-1.493244000
H	-6.166934000	-2.613781000	-0.575606000
C	-4.722489000	-3.950134000	-1.420325000
H	-4.280434000	-4.204551000	-0.464158000
C	-4.217389000	-4.521659000	-2.596759000
C	-1.091534000	-0.344365000	-1.855293000
H	-0.509843000	0.053700000	-1.024101000
H	-2.125342000	-0.027517000	-1.726114000
C	-0.545420000	0.196472000	-3.199168000
H	-0.704138000	-0.571482000	-3.970662000
H	-1.179867000	1.048255000	-3.475921000
C	-1.570371000	-3.944141000	-1.884843000
N	-3.191686000	-5.520703000	-2.533146000
N	-2.025189000	-5.251142000	-2.157558000
C	-0.351138000	-3.739022000	-1.197549000
H	0.293822000	-4.485212000	-0.755412000
C	-2.003328000	-2.651531000	-2.213597000
H	-2.870556000	-2.289146000	-2.740808000
C	6.833567000	2.010022000	-3.102196000
H	7.689421000	1.403481000	-2.821020000
C	6.531598000	2.253604000	-4.443999000
H	7.164995000	1.833293000	-5.220506000
N	3.191935000	-0.556963000	-1.710083000
N	2.755725000	-0.610926000	-0.415165000
C	5.429462000	3.040965000	-4.790314000
H	5.205786000	3.237138000	-5.834949000
C	4.636631000	3.602043000	-3.783482000
H	3.798880000	4.244040000	-4.044371000
C	4.918809000	3.349275000	-2.441523000
H	4.308652000	3.772688000	-1.649922000
C	6.004607000	2.530434000	-2.102888000
C	2.482845000	-1.244116000	-2.779921000
H	1.729452000	-1.866206000	-2.297968000
H	3.188712000	-1.894443000	-3.310559000

C	-2.483238000	-9.136896000	6.010541000	C	1.832743000	-0.262348000	-3.775113000
H	-3.000929000	-9.523874000	6.884023000	H	2.623660000	0.339718000	-4.239965000
N	-0.943994000	-4.145606000	5.409912000	H	1.388163000	-0.872764000	-4.577867000
N	0.151163000	-3.532049000	4.873362000	C	4.584271000	0.715927000	-0.561326000
C	-3.171868000	-8.967386000	4.806088000	N	6.315037000	2.295041000	-0.723292000
H	-4.225014000	-9.224433000	4.738713000	N	5.629444000	1.502554000	-0.032435000
C	-2.491297000	-8.488541000	3.681871000	C	3.604683000	0.140088000	0.283280000
H	-3.015543000	-8.375024000	2.736294000	H	3.478035000	0.266462000	1.347608000
C	-1.140600000	-8.150302000	3.762341000	C	4.273146000	0.232981000	-1.841158000
H	-0.606393000	-7.761701000	2.900525000	H	4.744006000	0.373528000	-2.800614000
C	-0.461997000	-8.310968000	4.977944000	Cu	1.000983000	-1.348833000	0.454473000
C	-2.115670000	-3.362457000	5.797290000	C	0.979497000	-0.558520000	3.354999000
H	-1.959447000	-2.362777000	5.394653000	C	2.424084000	-0.678877000	3.578788000
H	-2.138925000	-3.294849000	6.891413000	C	3.142838000	-1.769110000	3.054326000
C	-3.441894000	-3.949162000	5.286871000	C	3.134775000	0.316420000	4.272463000
H	-3.520838000	-5.000279000	5.610286000	C	4.530135000	-1.840891000	3.180652000
H	-4.230216000	-3.405475000	5.818746000	H	2.596129000	-2.553760000	2.537924000
C	0.572959000	-5.733806000	5.144855000	C	4.521087000	0.239744000	4.404524000
N	0.947112000	-8.050280000	5.046331000	H	2.583487000	1.154123000	4.688495000
N	1.393415000	-6.879144000	5.084842000	C	5.227528000	-0.832831000	3.851083000
C	1.078224000	-4.478315000	4.741762000	H	5.066995000	-2.687928000	2.759915000
H	2.037119000	-4.235198000	4.307897000	H	5.055354000	1.026873000	4.930657000
C	-0.731480000	-5.465335000	5.585582000	H	6.308925000	-0.883079000	3.945353000
H	-1.484623000	-6.102420000	6.019131000	C	-2.212700000	-0.649744000	1.766946000
C	2.139525000	-5.603975000	1.720072000	H	-2.874893000	0.152683000	2.099556000
C	1.529350000	-6.822214000	1.405183000	H	-1.943244000	-0.449780000	0.726201000
C	0.575249000	-6.889020000	0.387699000	C	-2.912046000	-1.991925000	1.876296000
C	0.232769000	-5.725216000	-0.309976000	C	-4.297099000	-2.046526000	2.069398000
C	0.831228000	-4.509339000	0.017689000	C	-2.192331000	-3.189509000	1.771293000
C	1.794056000	-4.434456000	1.034469000	C	-4.954909000	-3.275886000	2.170931000
H	2.890180000	-5.565160000	2.501552000	H	-4.859728000	-1.120553000	2.170176000
H	1.809967000	-7.716208000	1.955906000	C	-2.846083000	-4.417800000	1.873839000
H	0.111618000	-7.838804000	0.132366000	H	-1.116045000	-3.143448000	1.634599000
H	-0.506160000	-5.761683000	-1.106720000	C	-4.229120000	-4.465802000	2.079423000
H	0.540432000	-3.605672000	-0.511952000	H	-6.028301000	-3.303097000	2.340310000
C	2.440999000	-3.095967000	1.320342000	H	-2.276241000	-5.340271000	1.797731000
H	3.145523000	-2.847936000	0.512351000	H	-4.735786000	-5.423157000	2.166695000
H	1.685162000	-2.302660000	1.356737000	N	0.139225000	0.018474000	4.272890000
N	3.829932000	-2.132372000	2.885325000	N	-1.070544000	0.020148000	3.789761000
N	4.501645000	-1.284461000	3.242021000	N	-0.994130000	-0.545479000	2.547337000
N	3.158619000	-3.135259000	2.614277000	C	0.274426000	-0.921535000	2.200239000
Int1 in *EEE* species of dinuclear pathways				**Int2 in *EEE* species of dinuclear pathways**			
1, 1				1, 1			
Cu	-0.170415000	-0.400841000	-0.356036000	Cu	0.449907000	0.271822000	-0.269322000
C	-6.203895000	5.980091000	0.811851000	C	-7.429378000	3.683383000	1.997342000
H	-5.727610000	6.388786000	-0.074088000	H	-7.594986000	3.845553000	0.936516000
C	-7.270063000	6.630722000	1.430208000	C	-8.444306000	3.889020000	2.931048000
H	-7.642340000	7.567830000	1.027141000	H	-9.425051000	4.219092000	2.600853000
N	-1.500332000	2.176109000	-1.073236000	N	-1.860882000	2.342567000	-0.961395000
N	-1.495887000	1.131432000	-0.198046000	N	-1.301333000	1.428311000	-0.115944000
N	-0.077209000	-0.160026000	-2.884297000	N	0.111917000	0.919323000	-3.196266000
C	-7.855914000	6.072949000	2.568642000	C	-8.193492000	3.683048000	4.290238000
H	-8.686976000	6.577018000	3.053769000	H	-8.979651000	3.858692000	5.019425000
C	-7.374527000	4.862846000	3.089129000	C	-6.923565000	3.271697000	4.716370000
H	-7.834864000	4.434699000	3.975104000	H	-6.712673000	3.136700000	5.772669000
C	-6.312466000	4.208234000	2.478367000	C	-5.910854000	3.051916000	3.789451000
H	-5.927974000	3.271991000	2.867019000	H	-4.919288000	2.755468000	4.108555000
C	-5.721096000	4.769260000	1.330473000	C	-6.166441000	3.244854000	2.419337000
C	-0.554555000	2.214603000	-2.182561000	C	-1.139954000	2.821937000	-2.139628000
H	0.455864000	2.157327000	-1.766430000	H	-0.142769000	3.121686000	-1.808325000
H	-0.675836000	3.190010000	-2.658803000	H	-1.675634000	3.712595000	-2.477162000
C	-0.789975000	1.091423000	-3.211031000	C	-1.047136000	1.809943000	-3.295397000
H	-1.863860000	0.886507000	-3.245055000	H	-1.962388000	1.210720000	-3.296850000
H	-0.504326000	1.449548000	-4.214000000	H	-1.041088000	2.367497000	-4.250285000
C	-3.136572000	2.584707000	0.352226000	C	-3.219179000	2.223121000	0.778267000
N	-4.640248000	4.201020000	0.621286000	N	-5.201253000	3.058774000	1.400107000
N	-4.204684000	3.107866000	1.084667000	N	-4.210648000	2.355712000	1.748848000
C	-2.484131000	1.374551000	0.666348000	C	-2.112188000	1.365221000	0.937401000
H	-2.672975000	0.687755000	1.478233000	H	-1.870632000	0.713323000	1.762303000
C	-2.473474000	3.065960000	-0.779018000	C	-3.014062000	2.842273000	-0.457512000
H	-2.637274000	3.962322000	-1.356898000	H	-3.588407000	3.600324000	-0.967999000
C	-1.679607000	-9.097864000	-0.985483000	C	-1.394458000	-8.142745000	-0.468180000
H	-2.203620000	-8.788271000	-1.884539000	H	-1.990637000	-7.889874000	-1.340279000
C	-1.592731000	-10.439805000	-0.619746000	C	-1.535147000	-9.369413000	0.179242000
H	-2.054734000	-11.203015000	-1.238807000	H	-2.253223000	-10.097703000	-0.186628000

N	-1.432278000	-2.804478000	-1.603413000
N	-0.692134000	-2.353157000	-0.552171000
C	-0.910560000	-10.797425000	0.545248000
H	-0.841087000	-11.842279000	0.834285000
C	-0.314604000	-9.811629000	1.345341000
H	0.213602000	-10.097247000	2.250633000
C	-0.396414000	-8.472010000	0.987305000
H	0.057574000	-7.696467000	1.593838000
C	-1.083380000	-8.110155000	-0.187175000
C	-1.901352000	-1.875764000	-2.623379000
H	-2.436398000	-1.063540000	-2.121517000
H	-2.612518000	-2.424560000	-3.245160000
C	-0.751947000	-1.327256000	-3.487362000
H	-0.021596000	-2.130943000	-3.619074000
H	-1.133029000	-1.080705000	-4.491919000
C	-0.872391000	-4.604395000	-0.453130000
N	-1.235411000	-6.787609000	-0.657108000
N	-0.692191000	-5.893715000	0.053844000
C	-0.354122000	-3.438626000	0.148433000
H	0.221288000	-3.341831000	1.057046000
C	-1.556349000	-4.149819000	-1.582915000
H	-2.108959000	-4.695507000	-2.331992000
C	8.251111000	2.196404000	0.687068000
H	8.396349000	1.653814000	-0.242035000
C	9.312091000	2.827009000	1.334936000
H	10.310942000	2.782710000	0.911215000
N	2.708858000	-0.256831000	-1.226560000
N	1.800936000	0.136657000	-0.286802000
C	9.085392000	3.513708000	2.529526000
H	9.909771000	4.005743000	3.037827000
C	7.795272000	3.569915000	3.076839000
H	7.626393000	4.105588000	4.006855000
C	6.733018000	2.944599000	2.436490000
H	5.728312000	2.976330000	2.843386000
C	6.960098000	2.252181000	1.231995000
C	2.260670000	-0.966089000	-2.417217000
H	1.747493000	-1.879378000	-2.100368000
H	3.158277000	-1.249702000	-2.971513000
C	1.340266000	-0.097524000	-3.296624000
H	1.687989000	0.936774000	-3.225074000
H	1.451570000	-0.393802000	-4.352206000
C	3.841809000	0.952913000	0.232077000
N	5.963587000	1.576165000	0.492322000
N	4.799632000	1.637287000	0.982127000
C	2.481988000	0.869620000	0.594915000
H	1.985378000	1.303373000	1.447051000
C	3.942958000	0.221590000	-0.953986000
H	4.796316000	0.022777000	-1.583873000
C	1.119456000	2.440767000	3.675752000
C	0.108802000	1.550726000	3.313378000
C	0.345952000	0.162364000	3.344870000
C	1.609570000	-0.311385000	3.748447000
C	2.613961000	0.585849000	4.105604000
C	2.373408000	1.962431000	4.069514000
H	0.927692000	3.509572000	3.650201000
H	-0.863634000	1.920057000	3.004213000
H	1.791845000	-1.381154000	3.776307000
H	3.587811000	0.211681000	4.406300000
H	3.159899000	2.658776000	4.344456000
C	-0.680672000	-0.759140000	2.968400000
C	-1.545598000	-1.545200000	2.649001000
H	-2.305999000	-2.244300000	2.383339000

N	-0.286952000	-2.173801000	-2.220538000
N	0.499143000	-1.649023000	-1.228196000
C	-0.745107000	-9.657978000	1.294157000
H	-0.847591000	-10.613912000	1.800250000
C	0.185044000	-8.718669000	1.760937000
H	0.799694000	-8.950113000	2.624497000
C	0.331363000	-7.491916000	1.121986000
H	1.044892000	-6.758154000	1.480419000
C	-0.465602000	-7.199522000	-0.001842000
C	-0.997694000	-1.323439000	-3.168300000
H	-1.793651000	-0.802556000	-2.629184000
H	-1.484908000	-1.997192000	-3.876066000
C	-0.095681000	-0.340897000	-3.916289000
H	0.874305000	-0.821064000	-4.074817000
H	-0.523659000	-0.159124000	-4.919613000
C	0.264580000	-3.881958000	-0.939346000
N	-0.448670000	-5.978705000	-0.717988000
N	0.327547000	-5.093308000	-0.255443000
C	0.852120000	-2.689363000	-0.472125000
H	1.442854000	-2.523619000	0.414075000
C	-0.453874000	-3.503915000	-2.077157000
H	-1.088040000	-4.080044000	-2.733081000
C	7.739172000	4.993675000	0.781731000
H	7.976761000	4.700270000	-0.236374000
C	8.670345000	5.648567000	1.586557000
H	9.657828000	5.878713000	1.197095000
N	2.817944000	1.800245000	-1.643204000
N	1.836391000	1.872308000	-0.700274000
C	8.331177000	6.002439000	2.894321000
H	9.056236000	6.507715000	3.526236000
C	7.057225000	5.701099000	3.395642000
H	6.799609000	5.973328000	4.415622000
C	6.121739000	5.053941000	2.596871000
H	5.132420000	4.809630000	2.967299000
C	6.461352000	4.699810000	1.277996000
C	2.586078000	1.045084000	-2.864763000
H	2.452575000	-0.008532000	-2.598462000
H	3.490363000	1.141853000	-3.470564000
C	1.356938000	1.565374000	-3.631800000
H	1.288073000	2.643981000	-3.466037000
H	1.513563000	1.428016000	-4.716006000
C	3.627373000	3.094282000	-0.054372000
N	5.605103000	4.014727000	0.384233000
N	4.426072000	3.843500000	0.805893000
C	2.321304000	2.664429000	0.256936000
H	1.745545000	2.843857000	1.152973000
C	3.905872000	2.515276000	-1.295621000
H	4.793467000	2.564062000	-1.906614000
C	5.209380000	1.072909000	2.484400000
C	3.858513000	0.761341000	2.622956000
C	3.189225000	0.008281000	1.636711000
C	3.923944000	-0.432442000	0.517018000
C	5.275558000	-0.119734000	0.385547000
C	5.923210000	0.638647000	1.364956000
H	5.703849000	1.674323000	3.242172000
H	3.299046000	1.110765000	3.485463000
H	3.411351000	-1.002687000	-0.253138000
H	5.825301000	-0.463705000	-0.487140000
H	6.971103000	0.900199000	1.251579000
C	1.789884000	-0.276920000	1.750895000
C	0.598989000	-0.571958000	1.946388000
Cu	-0.962114000	-1.564201000	2.601600000
C	-4.400038000	-4.261733000	-5.062711000
H	-4.206233000	-5.266802000	-4.700438000
C	-4.753292000	-4.021805000	-6.389952000
H	-4.842486000	-4.850808000	-7.085724000
N	-2.535740000	-3.927284000	1.025508000
N	-2.129087000	-2.632530000	1.148404000
N	-3.597174000	-3.819747000	3.985917000
C	-4.995759000	-2.715275000	-6.819732000
H	-5.276198000	-2.525873000	-7.851923000
C	-4.886530000	-1.647100000	-5.918221000
H	-5.088463000	-0.633735000	-6.254573000
C	-4.532405000	-1.877919000	-4.593933000
H	-4.457263000	-1.065553000	-3.879264000

C	-4.281098000	-3.194117000	-4.161214000
C	-2.277901000	-4.893041000	2.084847000
H	-1.329552000	-4.617583000	2.538360000
H	-2.153074000	-5.868983000	1.608323000
C	-3.406441000	-4.982232000	3.127585000
H	-4.341347000	-5.208280000	2.595211000
H	-3.176828000	-5.861941000	3.745170000
C	-3.205311000	-2.920278000	-0.815486000
N	-3.883823000	-3.550218000	-2.849831000
N	-3.644064000	-2.569628000	-2.086784000
C	-2.541262000	-2.017437000	0.042384000
H	-2.297630000	-0.978664000	-0.118251000
C	-3.172758000	-4.146167000	-0.141714000
H	-3.519210000	-5.124166000	-0.436397000
C	-5.551925000	3.383574000	8.456637000
H	-6.375638000	2.712496000	8.231032000
C	-5.683127000	4.399863000	9.401590000
H	-6.626092000	4.539355000	9.922051000
N	-3.787583000	-0.693545000	3.934928000
N	-2.440369000	-0.533925000	3.790397000
C	-4.599033000	5.236762000	9.674563000
H	-4.698353000	6.033447000	10.406384000
C	-3.382155000	5.053430000	9.002863000
H	-2.543110000	5.709801000	9.216395000
C	-3.242434000	4.039465000	8.062790000
H	-2.310172000	3.885391000	7.531165000
C	-4.334080000	3.196141000	7.786037000
C	-4.529348000	-1.627646000	3.098484000
H	-3.963381000	-1.739050000	2.177778000
H	-5.491499000	-1.159156000	2.865583000
C	-4.778223000	-2.999279000	3.752274000
H	-5.314189000	-2.837646000	4.698401000
H	-5.472429000	-3.533022000	3.088248000
C	-3.222000000	0.877642000	5.376742000
N	-4.319953000	2.143630000	6.841871000
N	-3.191237000	1.898113000	6.325531000
C	-2.096033000	0.419730000	4.658199000
H	-1.065783000	0.739875000	4.723741000
C	-4.291526000	0.131979000	4.872429000
H	-5.345845000	0.181439000	5.095927000
C	2.550610000	-9.280512000	5.048659000
H	1.779027000	-9.297495000	5.812444000
C	3.374102000	-10.382260000	4.820772000
H	3.252533000	-11.283080000	5.415155000
N	-0.673081000	-3.804592000	4.918751000
N	-0.092446000	-3.064752000	3.933329000
C	4.355375000	-10.321687000	3.828888000
H	4.999415000	-11.177780000	3.648772000
C	4.513141000	-9.156336000	3.065595000
H	5.279787000	-9.113455000	2.296988000
C	3.695325000	-8.054461000	3.285448000
H	3.803092000	-7.146214000	2.703435000
C	2.703996000	-8.115371000	4.282746000
C	-1.793940000	-3.254445000	5.670484000
H	-1.834852000	-2.197276000	5.414697000
H	-1.573379000	-3.352159000	6.739814000
C	-3.133963000	-3.941288000	5.361318000
H	-3.054364000	-5.003499000	5.637764000
H	-3.872587000	-3.496995000	6.041328000
C	0.975049000	-5.047159000	4.142853000
N	1.792465000	-7.074502000	4.580520000
N	1.899713000	-6.047484000	3.850915000
C	0.910686000	-3.807841000	3.466768000
H	1.533214000	-3.429331000	2.670291000
C	-0.063629000	-4.997959000	5.078755000
H	-0.368558000	-5.715103000	5.825480000

Int3 in *EEE* species of dinuclear pathways

1, 1

Cu	0.222975000	0.553356000	-0.006823000
C	-6.653242000	5.634979000	2.193342000
H	-6.498825000	6.083627000	1.216667000
C	-7.621292000	6.118614000	3.070969000
H	-8.243780000	6.960935000	2.783031000
N	-1.828660000	2.805406000	-0.759529000
N	-1.611703000	1.636257000	-0.092474000

Int4 in *EEE* species of dinuclear pathways

1, 1

Cu	0.387343000	0.332147000	1.392182000
C	-8.059744000	2.551462000	2.595241000
H	-7.962038000	2.869386000	1.561612000
C	-9.305697000	2.472357000	3.215312000
H	-10.203775000	2.730482000	2.661702000
N	-1.856623000	2.494872000	1.108621000
N	-1.393343000	1.389430000	1.752512000

N	-0.152677000	1.153342000	-3.042923000	N	-0.212504000	1.564229000	-1.510519000
C	-7.778709000	5.522143000	4.324083000	C	-9.395066000	2.075344000	4.552207000
H	-8.523029000	5.903237000	5.017926000	H	-10.364142000	2.028613000	5.041039000
C	-6.969477000	4.440874000	4.697160000	C	-8.233370000	1.759676000	5.268944000
H	-7.081775000	3.996348000	5.680397000	H	-8.301819000	1.481000000	6.317417000
C	-6.008727000	3.944974000	3.822539000	C	-6.986288000	1.816661000	4.653295000
H	-5.367438000	3.117751000	4.104563000	H	-6.075841000	1.627586000	5.212433000
C	-5.851149000	4.542972000	2.558415000	C	-6.900870000	2.201189000	3.302642000
C	-0.948146000	3.208628000	-1.850514000	C	-1.008659000	3.233832000	0.177806000
H	0.077853000	3.213061000	-1.468559000	H	0.015428000	3.169789000	0.553903000
H	-1.228608000	4.233287000	-2.106582000	H	-1.333677000	4.277511000	0.216289000
C	-1.061433000	2.300000000	-3.086607000	C	-1.097856000	2.701599000	-1.265087000
H	-2.091489000	1.934619000	-3.140047000	H	-2.134401000	2.398915000	-1.448144000
H	-0.895842000	2.906397000	-3.995522000	H	-0.891362000	3.532382000	-1.961627000
C	-3.300819000	2.779402000	0.885540000	C	-3.527623000	1.801605000	2.374697000
N	-4.895371000	4.155688000	1.592302000	N	-5.685786000	2.307191000	2.588230000
N	-4.281451000	3.077332000	1.834928000	N	-4.731923000	1.624057000	3.059539000
C	-2.500855000	1.618388000	0.904713000	C	-2.392562000	0.978102000	2.535161000
H	-2.485212000	0.814430000	1.626748000	H	-2.247551000	0.123352000	3.179346000
C	-2.831545000	3.519426000	-0.203285000	C	-3.136341000	2.769353000	1.445515000
H	-3.136989000	4.484698000	-0.576373000	H	-3.672569000	3.618518000	1.050211000
C	-0.367153000	-8.116121000	-1.164204000	C	-1.128387000	-7.905633000	-0.970681000
H	-0.993645000	-7.905958000	-2.026069000	H	-1.893077000	-7.517687000	-1.637594000
C	-0.190309000	-9.416776000	-0.692917000	C	-1.014911000	-9.270855000	-0.709231000
H	-0.684657000	-10.245795000	-1.191163000	H	-1.701958000	-9.971538000	-1.175064000
N	-0.636330000	-1.798251000	-1.966749000	N	-0.799750000	-1.538229000	-0.950031000
N	0.214952000	-1.295072000	-1.020438000	N	0.118624000	-1.263653000	0.028383000
C	0.624362000	-9.649258000	0.417609000	C	-0.012103000	-9.732631000	0.146264000
H	0.765096000	-10.661411000	0.786468000	H	0.082981000	-10.796000000	0.347821000
C	1.263132000	-8.578040000	1.057491000	C	0.876770000	-8.827137000	0.742535000
H	1.896723000	-8.760950000	1.919538000	H	1.659483000	-9.188294000	1.402137000
C	1.093259000	-7.278404000	0.592242000	C	0.768631000	-7.464040000	0.489397000
H	1.583484000	-6.443027000	1.076559000	H	1.445872000	-6.753909000	0.949571000
C	0.273426000	-7.042182000	-0.528929000	C	-0.241060000	-6.997408000	-0.374626000
C	-1.496834000	-0.917186000	-2.747535000	C	-1.625381000	-0.489010000	-1.531495000
H	-2.073400000	-0.301621000	-2.051636000	H	-2.161506000	0.015993000	-0.722204000
H	-2.195059000	-1.559960000	-3.287680000	H	-2.367403000	-0.988020000	-2.158237000
C	-0.706213000	-0.026464000	-3.713766000	C	-0.811579000	0.523232000	-2.347278000
H	0.103380000	-0.621948000	-4.146715000	H	-0.018945000	-0.021862000	-2.869275000
H	-1.359532000	0.257625000	-4.555804000	H	-1.457369000	0.955780000	-3.130656000
C	0.294128000	-3.550405000	-1.001373000	C	0.047784000	-3.486011000	-0.355388000
N	0.009301000	-5.764878000	-1.081413000	N	-0.465709000	-5.634500000	-0.691953000
N	0.597342000	-4.809058000	-0.497066000	N	0.298986000	-4.826422000	-0.090641000
C	0.788997000	-2.349303000	-0.448447000	C	0.642486000	-2.435555000	0.373601000
H	1.502990000	-2.190667000	0.344641000	H	1.396282000	-2.460251000	1.144349000
C	-0.610748000	-3.146594000	-1.988946000	C	-0.864477000	-2.861035000	-1.211143000
H	-1.249312000	-3.725743000	-2.637455000	H	-1.561029000	-3.274406000	-1.923949000
C	8.834515000	0.874035000	0.481143000	C	8.447712000	4.042207000	1.148144000
H	8.783589000	0.374980000	-0.481941000	H	8.437673000	3.724641000	0.109885000
C	10.032764000	0.973300000	1.186697000	C	9.569476000	4.646793000	1.713251000
H	10.942665000	0.546838000	0.774555000	H	10.459310000	4.809838000	1.112222000
N	2.869761000	1.016057000	-1.672760000	N	2.830684000	1.418605000	-0.225161000
N	2.114945000	1.423097000	-0.608579000	N	2.108154000	1.472224000	0.932280000
C	10.058273000	1.623123000	2.422572000	C	9.544664000	5.039885000	3.052981000
H	10.990268000	1.703255000	2.975094000	H	10.417209000	5.510438000	3.497492000
C	8.882832000	2.173837000	2.952653000	C	8.395297000	4.827423000	3.827403000
H	8.908314000	2.678330000	3.914594000	H	8.382060000	5.133903000	4.869780000
C	7.684637000	2.080084000	2.255006000	C	7.273100000	4.226139000	3.270710000
H	6.765464000	2.498855000	2.649253000	H	6.375871000	4.052394000	3.854131000
C	7.658495000	1.425445000	1.009498000	C	7.296801000	3.829977000	1.920543000
C	2.264490000	0.533081000	-2.908739000	C	2.217116000	0.972789000	-1.468078000
H	1.838740000	-0.454545000	-2.714206000	H	1.810037000	-0.027260000	-1.305007000
H	3.087872000	0.418775000	-3.618246000	H	3.024795000	0.903230000	-2.200407000
C	1.201400000	1.485895000	-3.483568000	C	1.126898000	1.951318000	-1.952231000
H	1.441912000	2.501252000	-3.155847000	H	1.360627000	2.941566000	-1.549903000
H	1.276593000	1.485547000	-4.586445000	H	1.175783000	2.040443000	-3.051892000
C	4.318036000	1.555557000	-0.100772000	C	4.144132000	2.410640000	1.244723000
N	6.501862000	1.259857000	0.211832000	N	6.222190000	3.207619000	1.243440000
N	5.441472000	1.748312000	0.699689000	N	5.182041000	3.030410000	1.939888000
C	2.995109000	1.769806000	0.334329000	C	2.902661000	2.071997000	1.821267000
H	2.659327000	2.120216000	1.296822000	H	2.577502000	2.220919000	2.838078000
C	4.190798000	1.078572000	-1.406832000	C	4.050033000	1.979759000	-0.080569000
H	4.943385000	0.807570000	-2.131185000	H	4.759595000	2.042392000	-0.891107000
C	0.617392000	4.906235000	2.406562000	C	-0.073609000	3.616017000	5.503191000
C	0.321310000	3.606493000	2.003784000	C	-0.119094000	2.372159000	4.880032000

C	0.720921000	2.501402000	2.783965000	C	1.040512000	1.575125000	4.808763000
C	1.430975000	2.745279000	3.978902000	C	2.235928000	2.041648000	5.390564000
C	1.721028000	4.049042000	4.376153000	C	2.272597000	3.289345000	6.010586000
C	1.317401000	5.134983000	3.594399000	C	1.121343000	4.080753000	6.065719000
H	0.298112000	5.745072000	1.793213000	H	-0.975700000	4.217778000	5.565776000
H	-0.218373000	3.425824000	1.082662000	H	-1.047913000	2.006762000	4.460289000
H	1.758402000	1.900670000	4.575825000	H	3.122553000	1.416269000	5.338246000
H	2.269606000	4.217626000	5.298929000	H	3.199345000	3.644080000	6.452810000
H	1.548139000	6.149569000	3.906634000	H	1.151798000	5.053103000	6.549624000
C	0.423648000	1.158269000	2.386952000	C	1.034721000	0.286766000	4.162341000
C	0.139267000	-0.035325000	2.198862000	C	0.453206000	-0.697912000	3.474224000
Cu	-0.606756000	-1.797675000	2.515162000	Cu	-0.799875000	-2.245276000	3.500877000
C	-5.586801000	-4.223476000	-4.351447000	C	-5.468181000	-3.575326000	-3.828244000
H	-5.326626000	-5.243161000	-4.084189000	H	-5.155214000	-4.609623000	-3.722815000
C	-6.274830000	-3.932635000	-5.528551000	C	-6.105642000	-3.121680000	-4.982124000
H	-6.563779000	-4.735299000	-6.200604000	H	-6.300817000	-3.808968000	-5.799968000
N	-2.228060000	-4.164861000	1.057310000	N	-2.422503000	-4.276621000	1.715195000
N	-1.920062000	-2.851052000	1.240436000	N	-2.138814000	-2.997289000	2.093685000
N	-2.813996000	-4.507055000	4.105248000	N	-2.897719000	-4.971272000	4.802419000
C	-6.594525000	-2.608747000	-5.837606000	C	-6.495627000	-1.784257000	-5.080390000
H	-7.134970000	-2.379324000	-6.751573000	H	-6.997518000	-1.428980000	-5.975874000
C	-6.225872000	-1.574548000	-4.965610000	C	-6.247873000	-0.899778000	-4.021035000
H	-6.486746000	-0.547286000	-5.205298000	H	-6.563545000	0.137117000	-4.098258000
C	-5.537750000	-1.856354000	-3.791306000	C	-5.609785000	-1.343520000	-2.868680000
H	-5.256443000	-1.070184000	-3.099185000	H	-5.421228000	-0.676367000	-2.034600000
C	-5.210804000	-3.190231000	-3.481002000	C	-5.211826000	-2.690554000	-2.770887000
C	-1.664125000	-5.187654000	1.928787000	C	-1.946883000	-5.417394000	2.486240000
H	-0.693204000	-4.819357000	2.247951000	H	-0.960521000	-5.162637000	2.868499000
H	-1.500144000	-6.081805000	1.321505000	H	-1.834544000	-6.248442000	1.784600000
C	-2.562100000	-5.554018000	3.125703000	C	-2.915526000	-5.818722000	3.617488000
H	-3.519678000	-5.919431000	2.728582000	H	-3.930160000	-5.844076000	3.197578000
H	-2.076132000	-6.412527000	3.612795000	H	-2.665242000	-6.855519000	3.889579000
C	-3.365971000	-3.067133000	-0.479727000	C	-3.523778000	-2.985208000	0.308647000
N	-4.503699000	-3.600009000	-2.325938000	N	-4.543071000	-3.254478000	-1.658972000
N	-4.087337000	-2.653899000	-1.595477000	N	-4.209103000	-2.424019000	-0.764029000
C	-2.615124000	-2.182071000	0.324350000	C	-2.812758000	-2.215581000	1.251907000
H	-2.514506000	-1.110279000	0.247260000	H	-2.728562000	-1.143711000	1.318629000
C	-3.086394000	-4.339756000	0.032050000	C	-3.242734000	-4.312983000	0.647003000
H	-3.410610000	-5.316750000	-0.290908000	H	-3.537268000	-5.238665000	0.178519000
C	-6.124712000	2.923285000	8.006568000	C	-5.297849000	4.040941000	7.115267000
H	-6.714817000	2.016970000	8.104457000	H	-6.191966000	3.586787000	6.700407000
C	-6.466260000	4.091438000	8.686784000	C	-5.315112000	5.348929000	7.599235000
H	-7.335920000	4.106476000	9.337406000	H	-6.236064000	5.924057000	7.569541000
N	-3.789243000	-1.463864000	4.044811000	N	-3.651612000	-1.809036000	5.025871000
N	-2.493030000	-1.095235000	3.816341000	N	-2.291551000	-1.824505000	5.163336000
C	-5.691280000	5.242302000	8.522458000	C	-4.150391000	5.914925000	8.121256000
H	-5.961144000	6.157641000	9.041686000	H	-4.162943000	6.932579000	8.501449000
C	-4.570029000	5.220403000	7.682337000	C	-2.964580000	5.168103000	8.160142000
H	-3.976366000	6.120498000	7.549340000	H	-2.060895000	5.607703000	8.573783000
C	-4.218420000	4.057351000	7.006898000	C	-2.937457000	3.864256000	7.679109000
H	-3.363595000	4.026230000	6.340741000	H	-2.028946000	3.273604000	7.701753000
C	-4.999454000	2.899266000	7.169334000	C	-4.110473000	3.295786000	7.147232000
C	-4.382738000	-2.632995000	3.406346000	C	-4.370989000	-2.932854000	4.430005000
H	-3.996384000	-2.689531000	2.391825000	H	-4.106481000	-3.000626000	3.375612000
H	-5.459418000	-2.441923000	3.348764000	H	-5.432014000	-2.675717000	4.496115000
C	-4.162840000	-3.959128000	4.152911000	C	-4.141878000	-4.283486000	5.132763000
H	-4.464159000	-3.812526000	5.197624000	H	-4.177730000	-4.109071000	6.212482000
H	-4.874606000	-4.678947000	3.719865000	H	-5.012314000	-4.915103000	4.884585000
C	-3.516866000	0.428389000	5.145943000	C	-3.141404000	0.097185000	6.016223000
N	-4.776903000	1.679652000	6.487564000	N	-4.189967000	1.983776000	6.617075000
N	-3.672844000	1.605314000	5.875268000	N	-3.085451000	1.372482000	6.566200000
C	-2.330517000	0.051867000	4.476047000	C	-1.988075000	-0.678940000	5.777791000
H	-1.384163000	0.570692000	4.419334000	H	-0.956267000	-0.425268000	5.970903000
C	-4.432254000	-0.579119000	4.838136000	C	-4.196940000	-0.675745000	5.517043000
H	-5.473630000	-0.682939000	5.102148000	H	-5.256356000	-0.481157000	5.467444000
C	4.037461000	-9.127715000	4.152473000	C	3.981454000	-9.521173000	3.043660000
H	3.341165000	-9.264480000	4.974242000	H	3.355898000	-9.907189000	3.842955000
C	4.955523000	-10.117814000	3.804908000	C	4.874535000	-10.342989000	2.357182000
H	4.985811000	-11.049346000	4.362374000	H	4.956919000	-11.393567000	2.620100000
N	0.226257000	-4.049091000	4.568215000	N	0.175230000	-4.836027000	5.130244000
N	0.579294000	-3.255104000	3.517248000	N	0.487179000	-3.770262000	4.340054000
C	5.834544000	-9.906827000	2.740662000	C	5.662448000	-9.810811000	1.334276000
H	6.550791000	-10.676057000	2.466300000	H	6.358754000	-10.448193000	0.796723000
C	5.795035000	-8.701832000	2.025044000	C	5.558001000	-8.453058000	1.001876000
H	6.481099000	-8.540623000	1.198208000	H	6.174983000	-8.040656000	0.208343000

C	4.883509000	-7.709946000	2.365778000	C	4.670415000	-7.627140000	1.681513000
H	4.846822000	-6.776223000	1.817871000	H	4.585994000	-6.575828000	1.433089000
C	3.994650000	-7.921688000	3.437052000	C	3.870679000	-8.163428000	2.708373000
C	-0.859891000	-3.651430000	5.456568000	C	-0.816478000	-4.680068000	6.187612000
H	-1.132768000	-2.633790000	5.175041000	H	-1.032923000	-3.613537000	6.243221000
H	-0.477381000	-3.649569000	6.483909000	H	-0.366459000	-5.009790000	7.131166000
C	-2.082202000	-4.577877000	5.360810000	C	-2.109337000	-5.464273000	5.927214000
H	-1.757472000	-5.612079000	5.555340000	H	-1.857512000	-6.523113000	5.772264000
H	-2.746108000	-4.300161000	6.188568000	H	-2.698349000	-5.422316000	6.853054000
C	1.927403000	-5.067252000	3.603589000	C	1.809674000	-5.524536000	3.819675000
N	2.999361000	-7.009303000	3.860762000	N	2.904487000	-7.438341000	3.446973000
N	2.938267000	-5.935284000	3.196185000	N	2.787189000	-6.223453000	3.117613000
C	1.616113000	-3.860751000	2.937662000	C	1.484161000	-4.175184000	3.556817000
H	2.094816000	-3.423726000	2.076381000	H	1.937721000	-3.478460000	2.867562000
C	1.006866000	-5.145812000	4.653871000	C	0.945666000	-5.909498000	4.852015000
H	0.891491000	-5.884184000	5.432394000	H	0.865345000	-6.840643000	5.392012000
C	3.804093000	-5.286685000	-0.652770000	C	3.897475000	-2.673468000	-2.012579000
C	4.150546000	-4.310575000	0.282671000	C	4.171078000	-1.892718000	-0.885381000
C	4.342422000	-2.982129000	-0.113948000	C	4.133123000	-2.448602000	0.396511000
C	4.176673000	-2.644684000	-1.462008000	C	3.828910000	-3.811107000	0.532279000
C	3.827153000	-3.617965000	-2.399740000	C	3.544989000	-4.591594000	-0.587880000
C	3.640583000	-4.942160000	-1.996159000	C	3.575380000	-4.023624000	-1.865170000
H	3.649314000	-6.311898000	-0.330322000	H	3.938384000	-2.228200000	-3.003784000
H	4.247645000	-4.582571000	1.330390000	H	4.422212000	-0.841142000	-0.998001000
H	4.322601000	-1.613721000	-1.771650000	H	3.786443000	-4.262568000	1.520258000
H	3.705125000	-3.345207000	-3.444900000	H	3.289807000	-5.639902000	-0.462876000
H	3.362112000	-5.700870000	-2.722016000	H	3.352484000	-4.631298000	-2.737859000
C	4.657094000	-1.919857000	0.909493000	N	1.933714000	-0.802682000	4.109509000
H	5.241261000	-2.342167000	1.737160000	N	3.067975000	-0.717331000	3.314534000
H	5.237047000	-1.101787000	0.466972000	N	3.044615000	-1.521952000	2.359066000
N	3.361015000	-1.386993000	1.427207000	C	4.329461000	-1.593819000	1.627320000
N	3.445800000	-0.645824000	2.414409000	H	5.077966000	-2.042598000	2.294254000
N	3.396528000	0.044453000	3.319534000	H	4.679759000	-0.586582000	1.370117000
Int1 in *ZZZ* species of dinuclear pathways				**Int2 in *ZZZ* species of dinuclear pathways**			
1, 1				1, 1			
Cu	-0.620127000	-1.035133000	-0.190843000	Cu	0.947652000	0.751665000	0.748272000
C	-0.487704000	6.252643000	-0.278977000	C	-6.052490000	1.103495000	-1.487889000
H	-1.496476000	6.551151000	-0.548055000	H	-6.020113000	0.018918000	-1.504679000
C	0.618091000	6.730515000	-0.984675000	C	-6.288137000	1.829053000	-2.657610000
H	0.468330000	7.413512000	-1.816193000	H	-6.473223000	1.296133000	-3.586034000
N	-0.500226000	1.751812000	-1.391751000	N	-1.575214000	1.864904000	-0.724155000
N	-1.367922000	0.880750000	-0.794786000	N	-0.973254000	1.393347000	0.408774000
N	0.305140000	-1.187580000	-2.568117000	N	0.585341000	0.382522000	-2.579773000
C	1.910677000	6.346302000	-0.614748000	C	-6.291116000	3.226929000	-2.638894000
H	2.769975000	6.729150000	-1.157402000	H	-6.484731000	3.783946000	-3.550829000
C	2.097300000	5.488830000	0.474192000	C	-6.059350000	3.906316000	-1.438851000
H	3.098164000	5.201392000	0.780083000	H	-6.071520000	4.992324000	-1.414618000
C	0.998720000	4.988492000	1.175683000	C	-5.809124000	3.193824000	-0.266099000
H	1.139342000	4.302593000	2.005710000	H	-5.605203000	3.711007000	0.666092000
C	-0.292115000	5.363492000	0.783604000	C	-5.795067000	1.794002000	-0.299251000
C	0.427130000	1.335915000	-2.446719000	C	-0.798032000	2.339678000	-1.867674000
H	1.417251000	1.192749000	-2.002486000	H	0.136692000	2.738629000	-1.469494000
H	0.504336000	2.176744000	-3.142236000	H	-1.364711000	3.162034000	-2.313437000
C	-0.019968000	0.095418000	-3.224642000	C	-0.542069000	1.251035000	-2.923723000
H	-1.101519000	0.151406000	-3.366881000	H	-1.450158000	0.646405000	-3.012066000
H	0.438040000	0.139987000	-4.226952000	H	-0.397948000	1.741085000	-3.904236000
C	-1.466150000	2.908461000	0.225113000	C	-3.223787000	1.326377000	0.650374000
N	-1.433368000	4.883787000	1.509045000	N	-5.553516000	1.061398000	0.911453000
N	-1.951250000	3.777506000	1.230656000	N	-4.381047000	0.908986000	1.335329000
C	-1.966580000	1.588610000	0.164282000	C	-1.962286000	1.082373000	1.237767000
H	-2.698951000	1.123030000	0.807751000	H	-1.733735000	0.648077000	2.196129000
C	-0.520933000	2.967963000	-0.810899000	C	-2.917448000	1.842701000	-0.622211000
H	0.097547000	3.769537000	-1.181921000	H	-3.535604000	2.185619000	-1.435801000
C	-2.783818000	-7.627292000	-1.950559000	C	-2.451019000	-6.652598000	-0.361725000
H	-1.825078000	-7.933173000	-1.542476000	H	-2.988320000	-6.364363000	0.535419000
C	-3.068270000	-7.771876000	-3.309235000	C	-3.144520000	-7.004040000	-1.521003000
H	-2.321074000	-8.201951000	-3.970465000	H	-4.230673000	-6.979262000	-1.522560000
N	-2.096775000	-3.187308000	-1.531622000	N	0.097040000	-2.721498000	-1.544064000
N	-1.625846000	-2.736853000	-0.333571000	N	1.044029000	-2.206971000	-0.705654000
C	-4.309116000	-7.375301000	-3.817613000	C	-2.447403000	-7.406790000	-2.662691000
H	-4.528025000	-7.494604000	-4.874576000	H	-2.988116000	-7.693962000	-3.559564000
C	-5.278876000	-6.853945000	-2.955548000	C	-1.049583000	-7.465660000	-2.636343000
H	-6.253024000	-6.566938000	-3.341391000	H	-0.503335000	-7.803108000	-3.512644000
C	-5.007981000	-6.708267000	-1.593920000	C	-0.348746000	-7.096192000	-1.489386000
H	-5.753815000	-6.308594000	-0.913468000	H	0.736070000	-7.131310000	-1.461535000

C	-3.749748000	-7.073192000	-1.102663000
C	-1.923939000	-2.383088000	-2.735881000
H	-2.341950000	-1.391858000	-2.538041000
H	-2.524031000	-2.858672000	-3.514864000
C	-0.452858000	-2.294859000	-3.188336000
H	0.032276000	-3.237874000	-2.921354000
H	-0.421948000	-2.215465000	-4.288226000
C	-2.540556000	-4.791894000	-0.074532000
N	-3.467437000	-6.929433000	0.295292000
N	-2.916052000	-5.894508000	0.733620000
C	-1.892993000	-3.700139000	0.545476000
H	-1.637337000	-3.581736000	1.588069000
C	-2.647852000	-4.414558000	-1.423913000
H	-3.070195000	-4.905063000	-2.285863000
C	3.781793000	3.037142000	-1.630608000
H	2.803999000	3.447751000	-1.397885000
C	4.180836000	2.815160000	-2.947626000
H	3.502595000	3.053361000	-3.763210000
N	2.317742000	-0.701731000	-0.273918000
N	1.190602000	-0.343556000	0.407667000
C	5.453740000	2.303864000	-3.222963000
H	5.761803000	2.131742000	-4.249924000
C	6.341557000	2.049100000	-2.173919000
H	7.339571000	1.675806000	-2.384509000
C	5.961878000	2.291430000	-0.851308000
H	6.648420000	2.114473000	-0.028829000
C	4.669980000	2.751696000	-0.583465000
C	2.299725000	-1.841865000	-1.180176000
H	1.684188000	-2.619357000	-0.719315000
H	3.325344000	-2.212469000	-1.264484000
C	1.760011000	-1.466767000	-2.570223000
H	2.312852000	-0.590895000	-2.925917000
H	1.999729000	-2.280457000	-3.267613000
C	2.797230000	1.211026000	0.721233000
N	4.282283000	3.019930000	0.772291000
N	3.384881000	2.346800000	1.330602000
C	1.486180000	0.794000000	1.035689000
H	0.755978000	1.287766000	1.656987000
C	3.296653000	0.217511000	-0.127828000
H	4.258113000	0.096947000	-0.602311000
C	-0.043134000	2.435050000	4.009931000
C	-1.098351000	1.658012000	3.532386000
C	-0.969912000	0.256321000	3.466285000
C	0.222057000	-0.349041000	3.909454000
C	1.268563000	0.436283000	4.388946000
C	1.143690000	1.828694000	4.433590000
H	-0.156618000	3.514413000	4.053046000
H	-2.013352000	2.134584000	3.198271000
H	0.318637000	-1.429482000	3.865719000
H	2.186419000	-0.037479000	4.724131000
H	1.966857000	2.436704000	4.795807000
C	-2.036178000	-0.533681000	2.934308000
C	-2.949317000	-1.173092000	2.458433000
H	-3.769020000	-1.746871000	2.088930000

C	-1.052331000	-6.666000000	-0.355838000
C	-0.508875000	-1.891818000	-2.586193000
H	-1.363821000	-1.359885000	-2.154118000
H	-0.903852000	-2.580960000	-3.337987000
C	0.491538000	-0.931354000	-3.235539000
H	1.478013000	-1.400862000	-3.205474000
H	0.229440000	-0.813201000	-4.302500000
C	0.414013000	-4.286540000	-0.023992000
N	-0.355792000	-6.337800000	0.851734000
N	0.342973000	-5.295824000	0.947329000
C	1.233737000	-3.148590000	0.206719000
H	1.908548000	-2.978573000	1.031236000
C	-0.309004000	-3.954757000	-1.182904000
H	-1.075858000	-4.471445000	-1.736124000
C	6.435410000	4.673315000	-2.079684000
H	5.727595000	5.469177000	-2.291736000
C	7.137342000	4.041281000	-3.106789000
H	6.979949000	4.354343000	-4.135337000
N	3.268251000	1.699512000	-0.983159000
N	2.282922000	2.118321000	-0.139915000
C	8.041764000	3.014688000	-2.817556000
H	8.586867000	2.526281000	-3.619922000
C	8.262484000	2.639004000	-1.489233000
H	8.979501000	1.856337000	-1.256698000
C	7.572130000	3.270153000	-0.453765000
H	7.733247000	2.988298000	0.581152000
C	6.638424000	4.266691000	-0.755422000
C	2.993447000	0.614010000	-1.918134000
H	2.692369000	-0.268661000	-1.348172000
H	3.935631000	0.399328000	-2.426589000
C	1.875428000	1.010838000	-2.908509000
H	1.765937000	2.097910000	-2.879335000
H	2.178367000	0.764309000	-3.940047000
C	4.085029000	3.484907000	0.030688000
N	5.935125000	4.919762000	0.308704000
N	4.778237000	4.558527000	0.630325000
C	2.778567000	3.188410000	0.479379000
H	2.209301000	3.700927000	1.242316000
C	4.356341000	2.487424000	-0.923805000
H	5.219175000	2.278170000	-1.533559000
C	5.845364000	1.065600000	2.002567000
C	4.496633000	0.888024000	2.304690000
C	3.754597000	-0.135112000	1.685439000
C	4.402814000	-0.974616000	0.757417000
C	5.750880000	-0.789878000	0.456434000
C	6.476457000	0.231871000	1.075746000
H	6.401235000	1.862301000	2.489110000
H	4.002320000	1.539851000	3.018046000
H	3.837103000	-1.765454000	0.274383000
H	6.238800000	-1.448882000	-0.256970000
H	7.526912000	0.373445000	0.839756000
C	2.355843000	-0.311239000	1.978737000
C	1.212107000	-0.617615000	2.383220000
Cu	-0.235230000	-1.591947000	3.275771000
C	-5.786858000	-4.302278000	-1.002704000
H	-5.256120000	-4.645926000	-1.885398000
C	-6.594710000	-5.168739000	-0.262961000
H	-6.713900000	-6.199808000	-0.584977000
N	-2.399870000	-3.656664000	2.023610000
N	-1.470282000	-2.671945000	1.868973000
N	-3.195680000	-3.317730000	5.004934000
C	-7.255343000	-4.711749000	0.881570000
H	-7.887466000	-5.387037000	1.450532000
C	-7.124882000	-3.375020000	1.273077000
H	-7.660788000	-3.009015000	2.144688000
C	-6.313403000	-2.500770000	0.549016000
H	-6.197515000	-1.463103000	0.850413000
C	-5.626440000	-2.981809000	-0.573090000
C	-2.243433000	-4.655679000	3.077305000
H	-1.227169000	-4.547550000	3.443565000
H	-2.317093000	-5.644948000	2.618953000
C	-3.277447000	-4.530102000	4.204966000
H	-4.282867000	-4.614211000	3.765621000
H	-3.136697000	-5.415802000	4.839311000
C	-3.045501000	-2.503340000	0.252357000

N	-4.761421000	-2.103621000	-1.308269000
N	-3.592756000	-1.896731000	-0.893294000
C	-1.838776000	-1.997988000	0.788642000
H	-1.227785000	-1.185286000	0.433767000
C	-3.367075000	-3.590482000	1.089765000
H	-4.174257000	-4.303599000	1.079119000
C	-4.960703000	3.480141000	6.154224000
H	-4.479009000	3.428488000	7.125999000
C	-6.320676000	3.205027000	6.008652000
H	-6.911229000	2.942077000	6.881924000
N	-3.055663000	-0.168176000	4.229925000
N	-1.700657000	-0.326088000	4.337130000
C	-6.921957000	3.266449000	4.748172000
H	-7.979959000	3.048840000	4.636549000
C	-6.161378000	3.631287000	3.633630000
H	-6.633954000	3.690692000	2.657831000
C	-4.801675000	3.916479000	3.768123000
H	-4.196050000	4.189236000	2.908254000
C	-4.199355000	3.811585000	5.027642000
C	-3.935463000	-1.232744000	3.759523000
H	-3.495412000	-1.655072000	2.861571000
H	-4.862811000	-0.740111000	3.459608000
C	-4.238861000	-2.325484000	4.797767000
H	-4.477476000	-1.836789000	5.749757000
H	-5.163398000	-2.819691000	4.456825000
C	-2.282729000	1.815631000	4.833783000
N	-2.801120000	4.087915000	5.182722000
N	-1.957500000	3.161797000	5.113071000
C	-1.239930000	0.867576000	4.712580000
H	-0.177471000	1.024693000	4.834271000
C	-3.443318000	1.089002000	4.515008000
H	-4.481169000	1.364577000	4.439889000
C	-0.800621000	-7.730541000	4.045369000
H	-0.513115000	-7.390769000	3.053424000
C	-2.122154000	-8.073613000	4.333503000
H	-2.873159000	-8.008569000	3.549273000
N	-0.226747000	-3.696003000	5.629560000
N	0.460865000	-3.103421000	4.614207000
C	-2.484064000	-8.511162000	5.612042000
H	-3.514953000	-8.776193000	5.828830000
C	-1.503962000	-8.641861000	6.600399000
H	-1.772373000	-9.003827000	7.589040000
C	-0.172027000	-8.329918000	6.318797000
H	0.601904000	-8.447190000	7.071889000
C	0.167427000	-7.841939000	5.052901000
C	-1.163126000	-2.920712000	6.435022000
H	-1.098688000	-1.896788000	6.067704000
H	-0.832321000	-2.949364000	7.480174000
C	-2.608420000	-3.432713000	6.330855000
H	-2.642279000	-4.479499000	6.666643000
H	-3.199768000	-2.856789000	7.054517000
C	1.117007000	-5.259031000	4.833392000
N	1.541802000	-7.560407000	4.744934000
N	1.942499000	-6.384180000	4.591859000
C	1.296481000	-4.034097000	4.153623000
H	1.957604000	-3.815212000	3.329889000
C	0.128617000	-4.989717000	5.785808000
H	-0.305368000	-5.606903000	6.556633000

Int3 in *ZZZ* species of dinuclear pathways

1, 1

Cu	0.119395000	0.526736000	-0.381256000
C	-4.203991000	4.502393000	1.758598000
H	-3.636323000	3.849956000	2.414571000
C	-3.839198000	5.835211000	1.577706000
H	-2.964866000	6.217552000	2.095194000
N	-2.422970000	2.111812000	-1.317971000
N	-1.925321000	1.110458000	-0.544257000
N	-0.356557000	0.673425000	-3.387695000
C	-4.587896000	6.669655000	0.741523000
H	-4.294606000	7.706342000	0.602655000
C	-5.730887000	6.175935000	0.106170000
H	-6.325836000	6.825615000	-0.529696000
C	-6.129122000	4.852975000	0.306693000
H	-7.031838000	4.462294000	-0.154196000
C	-5.345479000	4.014890000	1.106127000

Int4 in *ZZZ* species of dinuclear pathways

1, 1

Cu	0.392019000	0.793461000	1.842234000
C	-6.602126000	2.998479000	0.693007000
H	-6.963137000	3.582931000	1.534210000
C	-6.664224000	3.497014000	-0.610861000
H	-7.088127000	4.481328000	-0.788519000
N	-1.980743000	2.734761000	1.260886000
N	-1.390567000	1.906497000	2.166824000
N	-0.626768000	1.873971000	-1.388167000
C	-6.196215000	2.731270000	-1.682837000
H	-6.258813000	3.118744000	-2.695556000
C	-5.680426000	1.451659000	-1.449313000
H	-5.352449000	0.835616000	-2.282956000
C	-5.594748000	0.949013000	-0.151316000
H	-5.190983000	-0.040553000	0.042646000
C	-6.034634000	1.741324000	0.917648000

C	-1.662600000	2.604692000	-2.459848000	C	-1.167889000	3.579469000	0.390381000
H	-0.683026000	2.930013000	-2.095008000	H	-0.145347000	3.500799000	0.758576000
H	-2.198120000	3.480798000	-2.833819000	H	-1.510236000	4.614375000	0.501782000
C	-1.513465000	1.554246000	-3.573976000	C	-1.246838000	3.159879000	-1.086953000
H	-2.423872000	0.947392000	-3.583627000	H	-2.302726000	3.141273000	-1.389079000
H	-1.468121000	2.069124000	-4.550715000	H	-0.773034000	3.962478000	-1.669539000
C	-3.924905000	1.787163000	0.268453000	C	-3.642268000	1.708121000	2.294171000
N	-5.799635000	2.677526000	1.354051000	N	-5.944400000	1.232994000	2.256969000
N	-5.107707000	1.680522000	1.045676000	N	-4.835713000	1.196023000	2.846018000
C	-2.838490000	0.900920000	0.406404000	C	-2.388205000	1.311754000	2.813653000
H	-2.644729000	0.192639000	1.197335000	H	-2.168899000	0.600894000	3.595053000
C	-3.613507000	2.558857000	-0.853443000	C	-3.324499000	2.643031000	1.293500000
H	-4.146525000	3.365689000	-1.332521000	H	-3.940867000	3.245829000	0.645855000
C	-0.375109000	-7.194423000	-1.333620000	C	-1.548638000	-5.843877000	-1.984766000
H	-0.891907000	-7.375259000	-0.395616000	H	-2.071345000	-6.396256000	-1.209892000
C	-0.829277000	-7.770128000	-2.521414000	C	-2.072008000	-5.749826000	-3.276146000
H	-1.713333000	-8.399960000	-2.507843000	H	-3.013790000	-6.237460000	-3.512852000
N	-0.220053000	-2.209899000	-2.012977000	N	-0.958481000	-1.154819000	-0.323420000
N	0.501066000	-1.424269000	-1.156091000	N	0.015077000	-0.854246000	0.585925000
C	-0.136643000	-7.560853000	-3.716217000	C	-1.376636000	-5.056587000	-4.269742000
H	-0.483205000	-8.024001000	-4.635203000	H	-1.777834000	-5.002014000	-5.277347000
C	1.020502000	-6.773697000	-3.719349000	C	-0.149063000	-4.455083000	-3.968945000
H	1.575558000	-6.627415000	-4.641814000	H	0.406027000	-3.935386000	-4.744989000
C	1.470913000	-6.179894000	-2.542579000	C	0.371041000	-4.522075000	-2.678710000
H	2.361164000	-5.559385000	-2.531115000	H	1.318560000	-4.053160000	-2.430132000
C	0.759593000	-6.376590000	-1.349498000	C	-0.341926000	-5.206195000	-1.682198000
C	-1.206380000	-1.623879000	-2.918712000	C	-1.963981000	-0.168215000	-0.704229000
H	-1.956830000	-1.104633000	-2.317685000	H	-2.240904000	0.379412000	0.195392000
H	-1.704104000	-2.458203000	-3.416514000	H	-2.843840000	-0.728560000	-1.030370000
C	-0.585387000	-0.666337000	-3.942550000	C	-1.525938000	0.805103000	-1.809769000
H	0.362077000	-1.093063000	-4.284944000	H	-1.055298000	0.223336000	-2.612034000
H	-1.238587000	-0.626101000	-4.830135000	H	-2.451404000	1.230381000	-2.227933000
C	0.951002000	-3.608049000	-0.759246000	C	0.121658000	-3.047762000	0.057593000
N	1.251761000	-5.862215000	-0.109603000	N	0.208404000	-5.366094000	-0.371184000
N	1.404771000	-4.631095000	0.090895000	N	0.490275000	-4.375033000	0.347684000
C	1.209638000	-2.260306000	-0.409029000	C	0.661238000	-1.988673000	0.821090000
H	1.845234000	-1.862114000	0.367104000	H	1.483455000	-1.988897000	1.518393000
C	0.026479000	-3.520496000	-1.815496000	C	-0.918452000	-2.457403000	-0.677180000
H	-0.486239000	-4.272713000	-2.391867000	H	-1.640344000	-2.870010000	-1.363747000
C	7.088905000	1.031023000	-1.530255000	C	6.698335000	2.152612000	0.212059000
H	7.055644000	0.359067000	-0.678479000	H	6.594370000	1.782320000	1.227285000
C	7.498457000	0.573122000	-2.783100000	C	7.181562000	1.331763000	-0.806456000
H	7.785990000	-0.467699000	-2.903317000	H	7.457100000	0.305077000	-0.582980000
N	2.659071000	1.348322000	-2.092348000	N	2.429486000	1.909832000	-0.246938000
N	1.897319000	1.559485000	-0.976625000	N	1.839777000	2.052589000	0.975158000
C	7.540569000	1.446980000	-3.873698000	C	7.299592000	1.822180000	-2.111075000
H	7.865733000	1.089918000	-4.846504000	H	7.672137000	1.178510000	-2.902460000
C	7.190871000	2.790254000	-3.700590000	C	6.964348000	3.151232000	-2.386596000
H	7.245308000	3.479186000	-4.539038000	H	7.077796000	3.543839000	-3.393343000
C	6.771756000	3.256269000	-2.453346000	C	6.495276000	3.986929000	-1.370149000
H	6.487781000	4.294299000	-2.308789000	H	6.237733000	5.023052000	-1.568708000
C	6.695372000	2.365645000	-1.376676000	C	6.331960000	3.473073000	-0.079940000
C	2.140593000	0.637592000	-3.254750000	C	1.802183000	1.145688000	-1.318830000
H	1.943288000	-0.392748000	-2.948405000	H	1.440422000	0.210426000	-0.893563000
H	2.953775000	0.629738000	-3.984397000	H	2.596271000	0.907800000	-2.029818000
C	0.884511000	1.281270000	-3.869044000	C	0.676782000	1.907098000	-2.043533000
H	0.882826000	2.343428000	-3.608218000	H	0.996761000	2.948002000	-2.166549000
H	0.954146000	1.228933000	-4.971335000	H	0.604092000	1.481628000	-3.057231000
C	4.026715000	2.266759000	-0.620117000	C	3.749095000	3.270286000	0.894472000
N	6.255582000	2.830663000	-0.094324000	N	5.847482000	4.329218000	0.963803000
N	5.040095000	2.782290000	0.216831000	N	4.686773000	4.192114000	1.417778000
C	2.720207000	2.123955000	-0.097218000	C	2.622827000	2.888041000	1.656685000
H	2.373455000	2.402127000	0.885003000	H	2.385548000	3.158442000	2.675193000
C	3.933159000	1.755480000	-1.924787000	C	3.575432000	2.616675000	-0.333812000
H	4.649978000	1.655306000	-2.723317000	H	4.162009000	2.613365000	-1.238574000
C	-0.383824000	5.140293000	1.334408000	C	-0.163324000	4.132382000	5.724462000
C	-0.483811000	3.758816000	1.189386000	C	-0.132936000	2.840198000	5.207942000
C	0.202531000	2.891567000	2.063891000	C	1.104480000	2.218479000	4.953501000
C	0.981126000	3.456198000	3.096633000	C	2.302039000	2.899770000	5.243530000
C	1.069636000	4.839772000	3.239910000	C	2.260139000	4.197762000	5.749866000
C	0.393072000	5.688426000	2.359420000	C	1.029370000	4.817640000	5.986328000
H	-0.922862000	5.790318000	0.650657000	H	-1.121047000	4.600796000	5.933617000
H	-1.094137000	3.332985000	0.403436000	H	-1.061083000	2.308765000	5.030749000
H	1.519263000	2.797040000	3.770083000	H	3.249689000	2.401288000	5.060630000
H	1.675317000	5.257035000	4.039545000	H	3.186094000	4.723742000	5.963589000

H	0.471188000	6.766222000	2.470592000	H	0.998896000	5.827710000	6.385270000
C	0.128989000	1.469594000	1.907798000	C	1.173958000	0.888478000	4.399781000
C	0.050673000	0.231834000	1.894375000	C	0.629474000	-0.192670000	3.833635000
Cu	-0.353407000	-1.585970000	2.429965000	Cu	-0.437963000	-1.855723000	3.916917000
C	-4.152389000	-6.662323000	-1.871193000	C	-4.947872000	-5.198735000	-1.186623000
H	-3.518512000	-6.617237000	-2.750895000	H	-4.453186000	-4.767573000	-2.050546000
C	-4.397138000	-7.872971000	-1.219622000	C	-5.048256000	-6.582883000	-1.031132000
H	-3.964203000	-8.790887000	-1.608105000	H	-4.638472000	-7.240290000	-1.793253000
N	-1.650862000	-4.341346000	1.342645000	N	-2.057313000	-4.065058000	2.321573000
N	-1.437678000	-2.997980000	1.266396000	N	-1.861104000	-2.768981000	2.699766000
N	-2.260198000	-4.298970000	4.401941000	N	-2.115084000	-5.093566000	5.308127000
C	-5.209997000	-7.913204000	-0.083260000	C	-5.683409000	-7.123683000	0.090385000
H	-5.406816000	-8.859165000	0.412320000	H	-5.769197000	-8.200422000	0.201190000
C	-5.792748000	-6.735083000	0.395476000	C	-6.233245000	-6.272837000	1.055192000
H	-6.446938000	-6.765061000	1.262489000	H	-6.751695000	-6.688300000	1.914776000
C	-5.541768000	-5.518237000	-0.237164000	C	-6.122455000	-4.889296000	0.919704000
H	-5.980006000	-4.594819000	0.129825000	H	-6.536102000	-4.217732000	1.666190000
C	-4.702031000	-5.483933000	-1.358120000	C	-5.458947000	-4.358612000	-0.193781000
C	-1.005926000	-5.156613000	2.364693000	C	-1.303043000	-5.166559000	2.909857000
H	-0.092502000	-4.642512000	2.643346000	H	-0.341444000	-4.767357000	3.219475000
H	-0.716269000	-6.099154000	1.894123000	H	-1.116765000	-5.887569000	2.110850000
C	-1.909400000	-5.445315000	3.576016000	C	-2.053257000	-5.851293000	4.069325000
H	-2.827468000	-5.924658000	3.206036000	H	-3.070467000	-6.088460000	3.724336000
H	-1.378527000	-6.200474000	4.173840000	H	-1.544704000	-6.812992000	4.230168000
C	-2.909384000	-3.639433000	-0.332996000	C	-3.567457000	-2.892906000	1.212879000
N	-4.437549000	-4.241897000	-2.022573000	N	-5.335246000	-2.939854000	-0.351364000
N	-3.652704000	-3.406448000	-1.509380000	N	-4.494691000	-2.303119000	0.330527000
C	-2.182445000	-2.576406000	0.252008000	C	-2.762708000	-2.062391000	2.026122000
H	-2.157614000	-1.540440000	-0.040414000	H	-2.810433000	-0.991772000	2.127678000
C	-2.529003000	-4.767826000	0.414315000	C	-3.066826000	-4.186735000	1.440430000
H	-2.791830000	-5.810168000	0.340925000	H	-3.331437000	-5.151349000	1.039367000
C	-7.344780000	1.488056000	4.064746000	C	-6.761156000	1.412139000	5.621562000
H	-7.324438000	1.981877000	3.098361000	H	-6.685402000	1.894192000	4.654687000
C	-8.402277000	0.659126000	4.444917000	C	-7.945617000	0.789970000	6.019772000
H	-9.237886000	0.515110000	3.765120000	H	-8.804673000	0.805226000	5.354794000
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H	-7.330201000	-0.240186000	7.549013000	H	-6.993854000	-0.308133000	9.098440000
C	-6.257337000	1.040198000	6.195253000	C	-5.729544000	0.751605000	7.721195000
H	-5.418304000	1.202831000	6.865460000	H	-4.861243000	0.748072000	8.373350000
C	-6.262061000	1.652804000	4.935428000	C	-5.645367000	1.365564000	6.463373000
C	-4.060293000	-2.855989000	3.331884000	C	-4.024361000	-3.449521000	5.031501000
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H	-4.308807000	-4.770262000	4.231599000	H	-4.172829000	-5.475983000	5.655864000
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C	0.539177000	-8.801150000	4.730165000	C	0.626095000	-9.343270000	3.661499000
H	-0.282684000	-9.451838000	5.014631000	H	-0.110428000	-10.096672000	3.925617000
C	1.572381000	-8.540867000	5.634861000	C	1.848237000	-9.289967000	4.338572000
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C	2.645597000	-7.726966000	5.264946000	C	2.806822000	-8.335296000	3.990694000
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C	-0.397295000	-3.100376000	5.597392000	C	-0.044479000	-4.470960000	6.556648000
H	-0.785229000	-2.154687000	5.217945000	H	-0.462137000	-3.471382000	6.672103000
H	0.014661000	-2.946342000	6.601798000	H	0.546322000	-4.728509000	7.443992000
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C	1.555805000	-4.512849000	4.828661000	C	1.620132000	-5.384599000	4.892671000
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C	4.639321000	-2.657398000	-2.201403000	C	3.804564000	-3.726467000	-0.574520000
C	4.610879000	-4.010577000	-1.851081000	C	3.925374000	-3.205743000	-1.867705000
H	4.604047000	-5.427736000	-0.220679000	H	4.350414000	-1.445291000	-3.042152000
H	4.724521000	-3.706118000	1.533928000	H	4.649920000	0.022673000	-1.064473000
H	4.734416000	-0.631138000	-1.475406000	H	3.903904000	-3.325524000	1.527807000
H	4.635824000	-2.363449000	-3.248219000	H	3.592991000	-4.780838000	-0.420257000
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C	4.756970000	-0.982090000	1.219084000	N	2.186043000	-0.088712000	4.284125000
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H	5.271522000	-0.078229000	0.871652000	N	3.196773000	-0.726913000	2.435241000
N	3.345759000	-0.630010000	1.552911000	C	4.400403000	-0.635539000	1.578200000
N	3.188787000	-0.016856000	2.616632000	H	5.263490000	-0.955030000	2.179173000
N	2.915770000	0.535567000	3.574504000	H	4.575744000	0.405282000	1.283265000

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