

Supporting Information for:
Synthesis and Photophysical Characterization of Azoheteroarenes

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1. General

All reagents and solvents were purchased from commercial sources and used as supplied, unless stated otherwise. THF and toluene were distilled from sodium/benzophenone. DCM, DMF and MeCN were purchased as HPLC grade and used as received. Reactions were monitored by Thin Layer Chromatography (TLC, Merck, silica gel 60 F254) and analyzed under UV (254 nm/365 nm) or potassium permanganate solution (KMnO_4) staining. Microwave reactions were performed in a Biotage Initiator Reactor using single mode irradiation with temperature and pressure control and with fixed hold time on. Column chromatography was performed by manual flash chromatography (wet-packed silica, 0.04–0.063 mm) or by automated column chromatography on a Biotage SP-4 instrument using pre-packed silica columns.

^1H - and ^{13}C -NMR spectra were obtained at 400 and 100 MHz respectively, using a Varian 400/54 spectrometer. The HRMS data was determined by CMSI (Chalmers Mass Spectrometry Infrastructure) at Chalmers University of Technology. The photostationary distributions were determined by 500 MHz ^1H -NMR with $\text{DMSO}-d_6$ as the solvent. All reactions where azo bond were involved were carried out avoiding direct light, i.e. covering reaction vessels and columns with aluminum foil and working with the fume hood lamp turned off (ceiling lamp was left on).

UV-Vis absorption spectra were recorded using a Varian CaryBio 50 spectrophotometer. In the ns transient absorption experiments, sample excitation was provided by the third harmonic of an Nd:YAG laser (Quantel, BrilliantB) that delivered 10 ns pulses at 355 nm, or 410 nm after the OPO. Analyzing light was provided by a 150 W Xe lamp in a flash photolysis spectrometer (Applied Photophysics LKS.60) and detected by a P928 five stage photomultiplier tube (PMT). The PMT signal was digitized using an Agilent Technologies Infinium digital oscilloscope (600 MHz). All spectra were recorded in 10×10 mm quartz cuvettes. The light sources for isomerization purposes were LEDs (LED Engin) centered at around 365 nm (LZ1-10UV00, fwhm = 12 nm), 405 nm (LZ1-10UB00-00U8, Fwhm = 19 nm), 460 nm (LZ1-10B200, fwhm = 21 nm), and 523 nm (LZ1-10R200, fwhm = 40 nm).

2. Synthesis

2.1. General Procedure

General procedure A for introducing Tosyl on indole derivatives^[1]: To a solution of **1** (**1e** to **1h**, 1.0 mmol) in dry THF (4.0 ml) was added KOH (2.0 mmol) and *p*-Toluenesulfonyl chloride (1.2 mmol) at rt and the resulting mixture was allowed to stir for 3.0-5.0 h and monitored by TLC. The reaction was quenched by addition of H₂O (3.0 ml) and then extracted with DCM (5.0 ml) for 3 times, the combined organic phases were dried over Na₂SO₄, removed the solvent under reduced pressure. The residue was purified by flash silica gel column chromatography (*n*-pentane-EtOAc, 30:1 to 10:1) to give the pure product **1-2** (**1e-2** to **1h-2**) as white crystal.

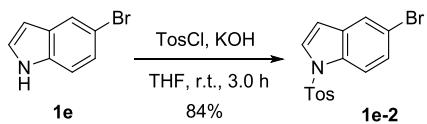
General procedure B for Buchwald-Hartwig Coupling^[2]: To a suspension of Pd(OAc)₂ (0.05 mmol), *t*-Bu₃P·HBF₄ or Xphos (0.05 mmol), Cs₂CO₃ (1.0 mmol), substrate **1** (0.5 mmol) in toluene (5.0 ml) was added **4** (0.6 mmol), the resulting mixture was stirred for 30 min at rt under N₂, followed by heating up to 110 °C and stirring overnight until completing according to TLC. The reaction mixture was filtered over celite, using DCM as the eluent. After evaporation under vacuo, the residue was then purified by automated column chromatography on silica gel (*n*-pentane-EtOAc, 10%-50% EtOAc) to give the expected product **2** (**2a** to **2h**) as yellow or brown solid.

General procedure C for oxidation^[3]: To a microwave vessel was added **2** (**2a** to **2h**, 0.5 mmol) and DMF (2.5 ml), the resulting mixture was then reacted under microwave irradiation at 160-200 °C for 0.5-2.0 h, then increasing temperature to stir for certain time until the reaction completed according to TLC. After cooling to rt, pure oxygen was exchanged into the vessel, followed by heating to 60 °C and stirring overnight. After removing DMF under vacuum, the crude product was purified by flash column chromatography on silica gel (*n*-pentane-EtOAc, 20:1 to 5:1) to give the expected azo product **3** (**3a** to **3h**) as orange or red solid.

General procedure D for deprotection of tosyl^[4]: To a solution of tosyl protected azo compound **3e-3g** (0.25 mmol) in THF/MeOH (2:1, 3.0 ml) was added Cs₂CO₃ (0.75 mmol) at 0-5 °C, the resulting mixture was allowed to stir for another 3 h at this temperature until it completed according to TLC. The reaction mixture was then quenched by water (3.0 ml), extracted by Ethyl acetate (3× 4.0 ml), the combined organic layer was dried over Na₂SO₄. After filtration, the solvent was removed under reduced pressure, and the residue was purified by flash column chromatography on silica gel (*n*-pentane-EtOAc, 10:1 to 3:1) to afford the target azo compound **5e-5g** as orange or brown solid.

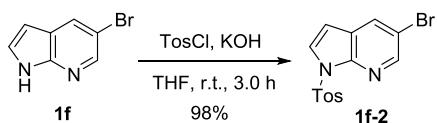
2.2. Introducing protecting group onindole derivatives

5-Bromo-1-[(4-methylphenyl)sulfonyl]-1H-indole (**1e-2**)



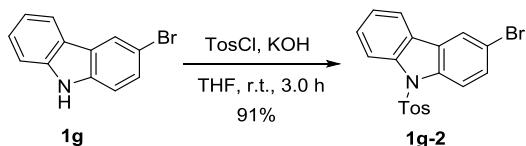
General procedure A was followed using **1e** (196.1 mg, 1.0 mmol), KOH (110.2 mg, 2.0 mmol) and *p*-Toluenesulfonyl chloride (228.1 mg, 1.2 mmol) at r.t. for 3.0 h. Purification by column chromatography (*n*-pentane-EtOAc: 20:1) gave the tosyl protected product **1e-2** (292 mg, 84% yield) as white crystals. ¹H-NMR (400 MHz, CDCl₃): δ 7.86 (1H, d, *J* = 8.8 Hz), 7.74 (2H, d, *J* = 8.4 Hz), 7.65 (1H, d, *J* = 1.9 Hz), 7.56 (1H, d, *J* = 3.6 Hz), 7.39 (1H, dd, *J* = 8.8, 1.9 Hz), 7.22 (2H, d, *J* = 8.0 Hz), 6.58 (1H, dd, *J* = 3.7, 0.8 Hz), 2.34 (3H, s); ¹³C-NMR (100 MHz, CDCl₃): δ 145.2, 134.9, 133.5, 132.4, 129.9, 127.4, 126.7, 124.0, 116.7, 114.9, 108.2, 21.5. Data is in accordance with the literature.^[5]

5-Bromo-1-tosyl-1H-pyrrolo[2,3-b]pyridine (**1f-2**)



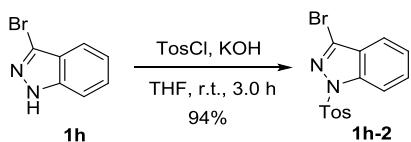
General procedure A was followed using **1f** (197.1 mg, 1.0 mmol), KOH (110.2 mg, 2.0 mmol) and *p*-Toluenesulfonyl chloride (228.1 mg, 1.2 mmol) at r.t. for 3.0 h. Purification by column chromatography (*n*-pentane-EtOAc: 30:1) gave the tosyl protected product **1f-2** (345 mg, 98% yield) as white crystals. ¹H-NMR (400 MHz, CDCl₃): δ 8.19 (1H, d, *J* = 8.6 Hz), 7.81 (2H, d, *J* = 8.5 Hz), 7.64-7.56 (2H, m), 7.38 (1H, t, *J* = 8.0 Hz), 7.25 (2H, d, *J* = 8.0 Hz), 2.36 (3H, s); ¹³C-NMR (100 MHz, CDCl₃): δ 145.8, 141.0, 134.1, 131.3, 130.4, 130.0, 127.67, 127.66, 126.0, 124.8, 120.9, 113.4, 21.7. Data is in accordance with the literature.^[6]

3-Bromo-9-tosyl-9H-carbazole (1g-2)



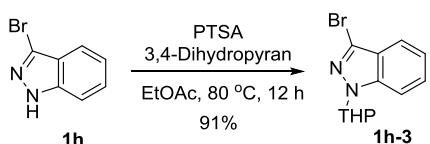
General procedure A was followed using **1g** (246.1 mg, 1.0 mmol), KOH (110.2 mg, 2.0 mmol) and *p*-Toluenesulfonyl chloride (228.1 mg, 1.2 mmol) at r.t. for 5.0 h. Purification by column chromatography (*n*-pentane-EtOAc: 30:1) gave the tosyl protected product **1g-2** (364 mg, 91% yield) as white crystals. ¹H-NMR (400 MHz, CDCl₃): δ 8.30 (1H, d, *J* = 8.4 Hz), 8.20 (1H, d, *J* = 8.9 Hz), 7.99 (1H, dd, *J* = 2.0, 0.44 Hz), 7.83 (1H, ddd, *J* = 7.8, 1.3, 0.72 Hz), 7.65 (1H, d, *J* = 8.6 Hz), 7.56 (1H, dd, *J* = 8.9, 2.0 Hz), 7.50 (1H, ddd, *J* = 8.6, 7.3, 1.32 Hz), 7.35 (1H, dt, *J* = 7.8, 0.92 Hz), 7.09 (1H, d, *J* = 8.0 Hz), 2.25 (3H, s); ¹³C-NMR (100 MHz, CDCl₃): δ 145.1, 138.7, 137.1, 134.6, 130.1, 129.7, 128.2, 128.1, 126.42, 126.41, 125.1, 124.1, 122.9, 120.1, 117.2, 116.6, 115.2, 21.5. Data is in accordance with the literature.^[7]

3-Bromo-1-tosyl-1H-indazole (1h-2)



General procedure A was followed using **1h** (197.1 mg, 1.0 mmol), KOH (110.2 mg, 2.0 mmol) and *p*-Toluenesulfonyl chloride (228.1 mg, 1.2 mmol) at r.t. for 5.0 h. Purification by column chromatography (*n*-pentane-EtOAc: 10:1) gave the tosyl protected product **1h-2** (330 mg, 94% yield) as white crystals (m.p. = 131-133 °C). ¹H-NMR (400 MHz, CDCl₃): δ 8.18 (1H, d, *J* = 8.6 Hz), 7.86 (2H, d, *J* = 8.4 Hz), 7.64-7.55 (2H, m), 7.38 (1H, ddd, *J* = 8.0, 7.2, 0.68 Hz), 7.25 (2H, d, *J* = 7.9 Hz), 2.36 (3H, s); ¹³C-NMR (100 MHz, CDCl₃): δ 145.8, 141.0, 134.1, 131.3, 130.4, 130.0, 127.7, 126.0, 124.8, 120.9, 113.4, 21.7. HRMS (ESI-TOF) *m/z* calcd for C₁₄H₁₂BrN₂O₂S⁺ [M + H]⁺: 350.9803, found: 350.9799.

3-Bromo-1-(tetrahydro-2H-pyran-2-yl)-1H-indazole (1h-3)

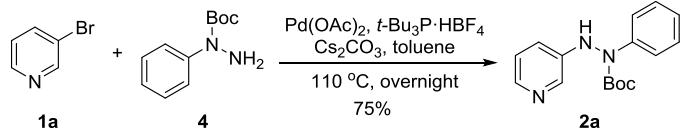


To a solution of 3-bromoindazole **1h** (197.1 mg, 1.0 mmol) dissolved in EtOAc (4 ml) were added successively a catalytic amount of PTSA (19 mg, 0.11 mmol) and 3,4-Dihydropyran (0.93 ml, 2.0 mmol). The reaction mixture was heated at 80 °C to reflux for 12 h until it was completed and then neutralized with NH₄OH. The resulting mixture was diluted by EtOAc (6 ml) and organic layer was washed with brine (3 × 4 ml), then dried over Na₂SO₄, filtered, evaporated in vacuo. The crude product was purified by flash column chromatography on silica gel (*n*-pentane-EtOAc: 50:1) to give the expected protected bromoindazoles **1h-3** (256 mg in 91% yield) as a white powder. ¹H-NMR (400 MHz, CDCl₃): δ 7.58 (2H, ddt, *J* = 14.6, 8.0,

1.0 Hz), 7.44 (1H, ddd, J = 8.0, 6.9, 1.0 Hz), 7.23 (1H, t, J = 7.8 Hz), 5.68 (1H, dd, J = 9.3, 2.9 Hz), 4.05-3.98 (1H, m), 3.77-3.68 (1H, m), 2.20-2.02 (2H, m), 1.82-1.59 (3H, m); ^{13}C -NMR (100 MHz, CDCl_3): δ 140.6, 127.7, 124.4, 122.1, 122.0, 120.4, 110.3, 85.5, 67.4, 29.3, 25.0, 22.4. Data is in accordance with the literature.^[8]

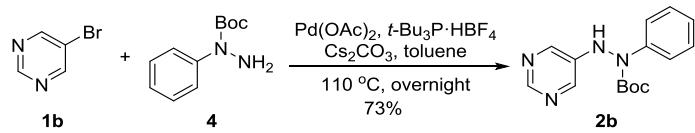
2.3. Products from Buchwald-Hartwig Coupling

tert-Butyl 1-phenyl-2-(pyridin-3-yl)hydrazine-1-carboxylate (2a)



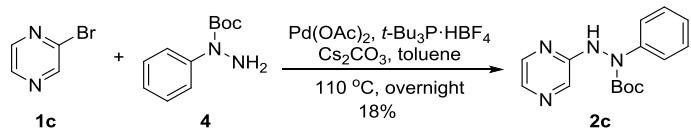
To a suspension of $\text{Pd}(\text{OAc})_2$ (33.6 mg, 0.15 mmol), $t\text{-Bu}_3\text{P}\cdot\text{HBF}_4$ (43.5 mg, 0.15 mmol), Cs_2CO_3 (975.0 mg, 3.0 mmol), **1a** (234.0 mg, 142.9 μl , 1.5 mmol) in toluene (12 ml) was added **4** (372.6 mg, 1.8 mmol) at r.t. under N_2 , the resulting mixture was stirred for 30 min at rt, followed by heating up to 110 °C and stirring overnight until completing according to TLC. The reaction mixture was filtered over celite, using DCM as the eluent. After evaporation under vacuo, the residue was then purified by automated column chromatography on silica gel (*n*-pentane-EtOAc: 2:1) gave the title product **2a** (317 mg, 75% yield) as a light yellow solid (m.p. = 104 °C). ^1H -NMR (400 MHz, CDCl_3): δ 8.25 (1H, s), 8.17 (1H, d, J = 3.8 Hz), 7.55 (2H, d, J = 7.8 Hz), 7.33 (2H, t, J = 8.5 Hz), 7.17-7.07 (3H, m), 6.66 (1H, s), 1.39 (9H, s); ^{13}C -NMR (100 MHz, CDCl_3): δ 153.6, 144.3, 142.4, 142.3, 135.9, 128.5, 124.9, 123.6, 121.8, 119.8, 82.7, 28.0. HRMS (ESI-TOF) m/z calcd for $\text{C}_{16}\text{H}_{20}\text{N}_3\text{O}_2^+$ [M + H]⁺: 286.1556, found: 286.1551.

tert-Butyl 1-phenyl-2-(pyrimidin-5-yl)hydrazine-1-carboxylate (2b)



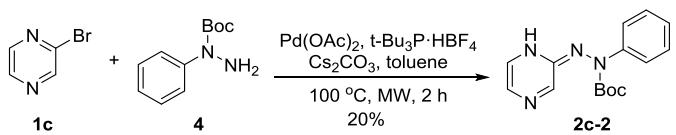
General procedure B was followed using $\text{Pd}(\text{OAc})_2$ (11.2 mg, 0.05 mmol), $t\text{-Bu}_3\text{P}\cdot\text{HBF}_4$ (14.5 mg, 0.05 mmol), Cs_2CO_3 (325 mg, 1.0 mmol), **1b** (79 mg, 0.5 mmol) and **4** (123.6 mg, 0.6 mmol) at r.t. for 30 min under N_2 , and then stirring overnight at 110 °C. Purification by automated column chromatography (*n*-pentane-EtOAc, 2:1) gave the title product **2b** (103 mg, 73% yield) as a light yellow solid (m.p. = 103 °C). ^1H -NMR (400 MHz, CDCl_3): δ 8.78 (1H, s), 8.32 (2H, s), 7.48 (2H, d, J = 8.0 Hz), 7.33 (2H, t, J = 8.4 Hz), 7.15 (1H, tt, J = 7.4, 1.0 Hz), 6.92 (1H, s), 1.40 (9H, s); ^{13}C -NMR (100 MHz, CDCl_3): δ 153.5, 151.7, 142.0, 141.9, 141.7, 128.7, 125.5, 122.3, 83.3, 28.0. HRMS (ESI-TOF) m/z calcd for $\text{C}_{15}\text{H}_{19}\text{N}_4\text{O}_2^+$ [M + H]⁺: 287.1508, found: 287.1507.

tert-Butyl 1-phenyl-2-(pyrazin-2-yl)hydrazine-1-carboxylate (2c)



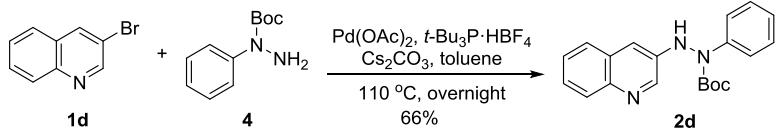
General procedure B was followed using $\text{Pd}(\text{OAc})_2$ (11.2 mg, 0.05 mmol), $t\text{-Bu}_3\text{P}\cdot\text{HBF}_4$ (14.5 mg, 0.05 mmol), Cs_2CO_3 (325 mg, 1.0 mmol), **1c** (79 mg, 0.5 mmol) and **4** (123.6 mg, 0.6 mmol) at r.t. for 30 min under N_2 , and then stirring overnight at 110 °C. Purification by automated column chromatography (*n*-pentane-EtOAc, 2:1) gave the title product **2c** (26 mg, 18 % yield) as a light yellow solid (m.p. = 154 °C). ^1H -NMR (400 MHz, CDCl_3): δ 8.14 (2H, d, J = 13.8 Hz), 8.10 (1H, s), 7.53 (2H, d, J = 7.6 Hz), 7.38 (1H, s), 7.36-7.30 (2H, m), 7.16 (1H, tt, J = 7.4, 1.1 Hz), 1.39 (9H, s); ^{13}C -NMR (100 MHz, CDCl_3): δ 155.6, 153.5, 142.0, 141.9, 136.9, 130.8, 128.6, 125.4, 122.3, 82.9, 28.0. HRMS (ESI-TOF) m/z calcd for $\text{C}_{15}\text{H}_{19}\text{N}_4\text{O}_2^+$ [M + H]⁺: 287.1508, found: 287.1506.

tert-Butyl (E)-1-phenyl-2-(pyrazin-2(1H)-ylidene)hydrazine-1-carboxylate (2c-2)



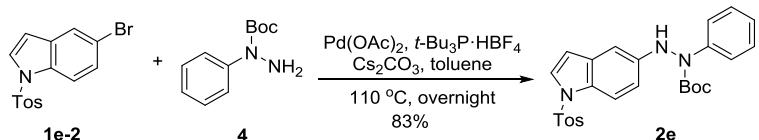
General procedure B was followed using Pd(OAc)_2 (11.2 mg, 0.05 mmol), $t\text{-Bu}_3\text{P}\cdot\text{HBF}_4$ (14.5 mg, 0.05 mmol), Cs_2CO_3 (325 mg, 1.0 mmol), **1c** (79 mg, 0.5 mmol) and **4** (123.6 mg, 0.6 mmol) at r.t. for 30 min under N_2 , and then stirring 2 h at 100°C . Purification by automated column chromatography (*n*-pentane-EtOAc, 2:1) gave the title product **2c-2** (29 mg, 20% yield) as a white solid (m.p. = 153°C). $^1\text{H-NMR}$ (400 MHz, CD_3OD): δ 8.09 (2H, d, J = 16.4 Hz), 7.95 (1H, d, J = 2.2 Hz), 7.51 (2H, d, J = 8.0 Hz), 7.31 (2H, t, J = 7.9 Hz), 7.15 (1H, t, J = 7.3 Hz), 1.37 (9H, s). $^{13}\text{C-NMR}$ (100 MHz, CD_3OD): δ 155.6, 154.1, 142.3, 142.1, 134.6, 130.7, 128.7, 125.1, 123.0, 81.9, 26.9. HRMS (ESI-TOF) m/z calcd for $\text{C}_{15}\text{H}_{19}\text{N}_4\text{O}_2^+$ [M + H] $^+$: 287.1508, found: 287.1520.

tert-Butyl 1-phenyl-2-(quinolin-3-yl)hydrazine-1-carboxylate (**2d**)



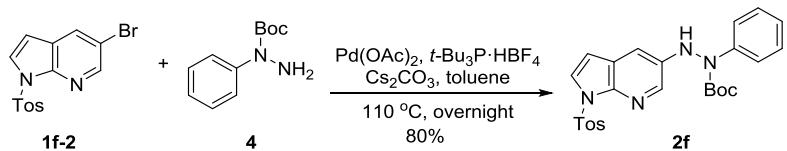
General procedure B was followed using Pd(OAc)_2 (11.2 mg, 0.05 mmol), $t\text{-Bu}_3\text{P}\cdot\text{HBF}_4$ (14.5 mg, 0.05 mmol), Cs_2CO_3 (325 mg, 1.0 mmol), **1d** (104 mg, 0.5 mmol) and **4** (123.6 mg, 0.6 mmol) at r.t. for 30 min under N_2 , and then stirring overnight at 110°C . Purification by automated column chromatography (*n*-pentane-EtOAc: 4:1) gave the title product **2d** (110 mg, 66% yield) as a brown solid (m.p. = $156\text{-}158^\circ\text{C}$). $^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 8.65 (1H, d, J = 2.8 Hz), 8.02 (1H, d, J = 8.3 Hz), 7.67-7.60 (3H, m), 7.52 (1H, ddd, J = 8.4, 6.9, 1.5 Hz), 7.46 (1H, ddd, J = 8.1, 6.9, 1.4 Hz), 7.39-7.32 (3H, m), 7.16 (1H, tt, J = 9.4, 1.1 Hz), 6.86 (1H, s), 1.38 (9H, s); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 153.7, 144.2, 142.2, 141.4, 141.0, 129.1, 128.7, 127.2, 126.63, 126.57, 125.0, 121.8, 114.2, 82.9, 28.1. HRMS (ESI-TOF) m/z calcd for $\text{C}_{20}\text{H}_{22}\text{N}_3\text{O}_2^+$ [M + H] $^+$: 336.1712, found: 336.1711.

tert-Butyl 1-phenyl-2-(1-tosyl-1*H*-indol-5-yl)hydrazine-1-carboxylate (**2e**)



General procedure B was followed using Pd(OAc)_2 (11.2 mg, 0.05 mmol), $t\text{-Bu}_3\text{P}\cdot\text{HBF}_4$ (14.5 mg, 0.05 mmol), Cs_2CO_3 (325 mg, 1.0 mmol), **1e-2** (175 mg, 0.5 mmol) and **4** (123.6 mg, 0.6 mmol) at r.t. for 30 min under N_2 , and then stirring overnight at 110°C . Purification by automated column chromatography (*n*-pentane-EtOAc: 5:1) gave the title product **2e** (199 mg, 83% yield) as a light yellow solid (m.p. = 146°C). $^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 7.85 (1H, d, J = 8.8 Hz), 7.73-7.69 (2H, m), 7.60 (2H, dd, J = 4.7, 0.56 Hz), 7.48 (1H, d, 3.6), 7.34-7.29 (2H, m), 7.19 (2H, dd, J = 8.5, 0.4 Hz), 7.11 (1H, tt, J = 7.4, 1.1 Hz), 6.89 (1H, d, J = 2.2 Hz), 6.83 (1H, dd, J = 9.1, 2.3 Hz), 6.50 (1H, dd, J = 3.6, 0.68 Hz), 6.44 (1H, s), 2.33 (3H, s), 1.32 (9H, s); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ 154.0, 144.8, 144.7, 142.8, 135.2, 131.7, 130.3, 129.7, 128.4, 127.1, 126.7, 124.5, 121.6, 114.3, 111.9, 109.1, 104.2, 82.3, 28.0, 21.5. HRMS (ESI-TOF) m/z calcd for $\text{C}_{26}\text{H}_{28}\text{N}_3\text{O}_4\text{S}^+$ [M + H] $^+$: 478.1801, found: 478.1796.

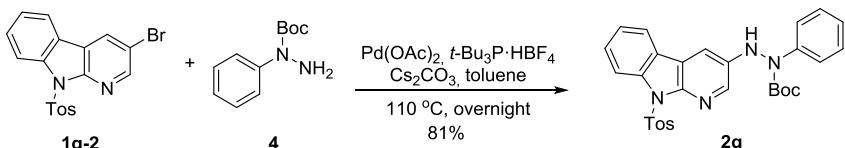
tert-Butyl 1-phenyl-2-(1-tosyl-1*H*-pyrrolo[2,3-*b*]pyridin-5-yl)hydrazine-1-carboxylate (**2f**)



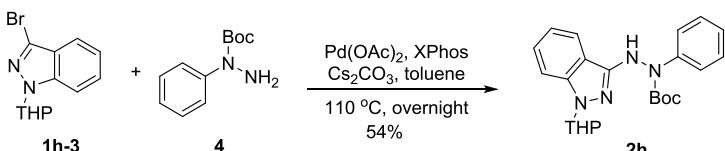
General procedure B was followed using Pd(OAc)_2 (11.2 mg, 0.05 mmol), $t\text{-Bu}_3\text{P}\cdot\text{HBF}_4$ (14.5 mg, 0.05 mmol), Cs_2CO_3

(325 mg, 1.0 mmol), **1f-2** (176 mg, 0.5 mmol) and **4** (123.6 mg, 0.6 mmol) at r.t. for 30 min under N₂, and then stirring overnight at 110 °C. Purification by automated column chromatography (*n*-pentane-EtOAc: 3:1) gave the title product **2f** (193 mg, 80 % yield) as a light yellow solid (m.p. = 154 °C). ¹H-NMR (400 MHz, CDCl₃): δ 8.10 (1H, d, *J* = 2.6 Hz), 8.01-7.97 (2H, m), 7.64 (1H, d, *J* = 4.0 Hz), 7.59-7.54 (2H, m), 7.35-7.29 (2H, m), 7.24-7.20 (3H, m), 7.13 (1H, tt, *J* = 7.4, 1.1 Hz), 6.54 (1H, s), 6.44 (1H, d, *J* = 4.0 Hz), 2.34 (3H, s), 1.37 (9H, s); ¹³C-NMR (100 MHz, CDCl₃): δ 153.8, 144.9, 143.1, 142.3, 141.1, 135.4, 133.0, 129.5, 128.5, 127.7, 127.3, 124.9, 123.1, 121.9, 113.0, 105.2, 82.7, 28.0, 21.5. HRMS (ESI-TOF) *m/z* calcd for C₂₅H₂₇N₄O₄S⁺ [M + H]⁺: 479.1753, found: 479.1769.

tert-Butyl 1-phenyl-2-(9-tosyl-9H-pyrido[2,3-b]indol-3-yl)hydrazine-1-carboxylate (2g)

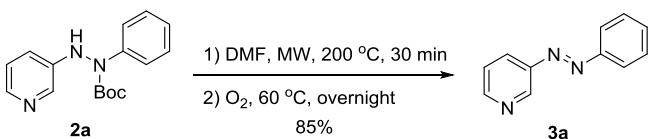


tert-Butyl 1-phenyl-2-(1-(tetrahydro-2H-pyran-2-yl)-1H-indazol-3-yl)hydrazine-1-carboxylate (2h)



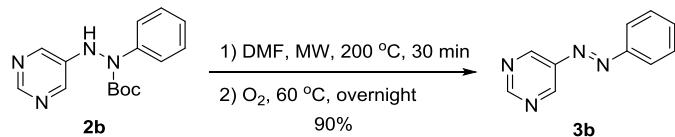
2.4. Products 3 from oxidation

(E)-3-(Phenyldiazenyl)pyridine (3a)

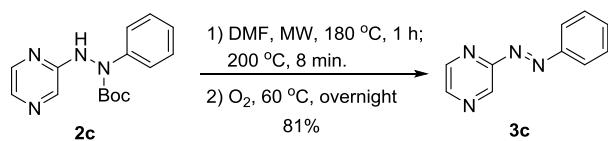


microwave irradiation at 200 °C for 30 min. After cooling to rt, pure oxygen was exchanged into the vessel, followed by heating to 60 °C and stirring overnight. After removing DMF under vacuum, the crude product was purified by flash column chromatography on silica gel (*n*-pentane-EtOAc, 10:1) to give the expected azo product **3a** (187 mg, 85% yield) as a brown solid (m.p. = 44-46 °C). ¹H-NMR (400 MHz, CDCl₃): δ 9.19 (1H, s), 8.69 (1H, d, *J* = 2.4 Hz), 8.11 (1H, d, *J* = 8.0 Hz), 7.93 (2H, d, *J* = 6.4 Hz), 7.55-7.44 (3H, m), 7.41 (1H, dd, *J* = 7.8, 4.6 Hz); ¹³C-NMR (100 MHz, CDCl₃): δ 152.4, 151.7, 147.8, 147.4, 131.7, 129.2, 126.9, 123.9, 123.1. HRMS (ESI-TOF) *m/z* calcd for C₁₁H₁₀N₃⁺ [M + H]⁺: 184.0875, found: 184.0873. Data is in accordance with the literature.^[9]

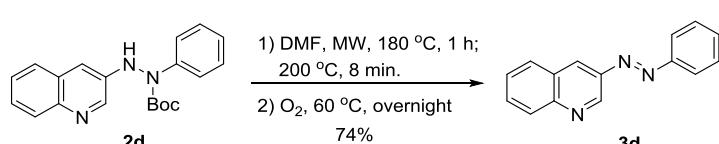
(E)-5-(Phenyldiazenyl)pyrimidine (**3b**)



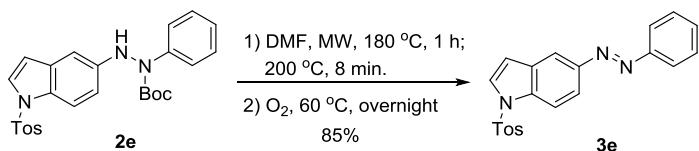
(E)-2-(Phenyldiazenyl)pyrazine (**3c**)



(E)-3-(Phenyldiazenyl)quinoline (**3d**)

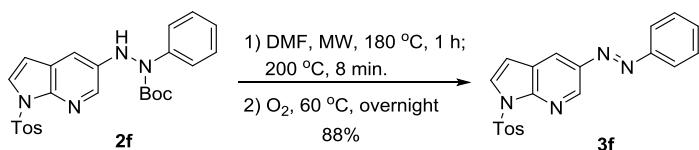


(E)-5-(Phenyldiazenyl)-1-tosyl-1H-indole (**3e**)



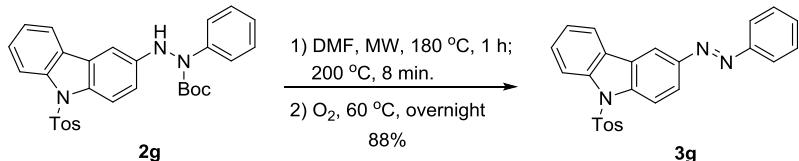
General procedure C was followed using **2e** (191.0 mg, 0.4 mmol) and DMF (2.0 ml) at 180 °C for 1 h, then 200 °C for 8 min, followed by exposing to oxygen at 60 °C and stirring overnight. Purification by flash column chromatography (*n*-pentane-EtOAc, 20:1) gave the expected azo product **3e** (128 mg, 85% yield) as a red solid (m.p. = 124-126 °C). ¹H-NMR (400 MHz, CDCl₃): δ 8.15-8.08 (2H, m), 7.99-7.88 (3H, m), 7.80 (2H, d, *J* = 8.3 Hz), 7.64 (1H, d, *J* = 3.6 Hz), 7.56-7.43 (3H, m), 7.23 (2H, d, *J* = 8.2 Hz), 6.78 (1H, d, *J* = 3.6 Hz), 2.33 (3H, s); ¹³C-NMR (100 MHz, CDCl₃): δ 152.6, 149.2, 145.3, 136.2, 135.1, 131.2, 130.8, 130.0, 129.1, 127.7, 126.8, 122.7, 118.9, 117.5, 113.9, 109.9, 21.6. HRMS (ESI-TOF) *m/z* calcd for C₂₁H₁₈N₃O₂S⁺ [M + H]⁺: 376.1120, found: 376.1120.

(E)-5-(Phenyldiazenyl)-1-tosyl-1H-pyrrolo[2,3-b]pyridine (3f)



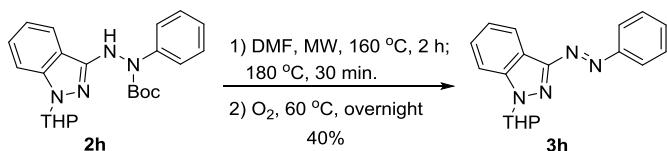
General procedure C was followed using **2f** (191.5 mg, 0.4 mmol) and DMF (2.0 ml) at 180 °C for 1 h, then 200 °C for 8 min, followed by exposing to oxygen at 60 °C and stirring overnight. Purification by flash column chromatography (*n*-pentane-EtOAc, 10:1) gave the expected azo product **3f** (133 mg, 88% yield) as a dark yellow solid (m.p. = 158-160 °C). ¹H-NMR (400 MHz, CDCl₃): δ 9.08 (1H, d, *J* = 1.7 Hz), 8.31 (1H, d, *J* = 1.7 Hz), 8.11 (2H, d, *J* = 8.2 Hz), 7.91 (2H, d, *J* = 7.0 Hz), 7.80 (1H, d, *J* = 3.9 Hz), 7.56-7.44 (3H, m), 7.33-7.22 (2H, m), 6.69 (1H, d, *J* = 3.9 Hz), 2.36 (3H, s); ¹³C-NMR (100 MHz, CDCl₃): δ 152.4, 148.1, 145.5, 145.1, 144.1, 135.1, 131.1, 129.7, 129.1, 128.2, 128.1, 123.2, 122.9, 120.2, 106.2, 21.7. HRMS (ESI-TOF) *m/z* calcd for C₂₀H₁₇N₄O₂S⁺ [M + H]⁺: 377.1072, found: 377.1078.

(E)-3-(Phenyldiazenyl)-9-tosyl-9H-carbazole (3g)



General procedure C was followed using **2g** (211.0 mg, 0.4 mmol) and DMF (2.0 ml) at 180 °C for 1 h, then 200 °C for 8 min, followed by exposing to oxygen at 60 °C and stirring overnight. Purification by flash column chromatography (*n*-pentane-EtOAc, 20:1) gave the expected azo product **3g** (151 mg, 88% yield) as an orange solid (m.p. = 167-169 °C). ¹H-NMR (400 MHz, CDCl₃): δ 8.50-8.44 (2H, m), 8.36 (1H, d, *J* = 8.4 Hz), 8.13 (1H, dd, *J* = 9.0, 1.8 Hz), 8.0 (1H, d, *J* = 7.6 Hz), 7.98-7.93 (2H, m), 7.74 (1H, d, *J* = 8.4 Hz), 7.58-7.47 (4H, m), 7.41 (1H, ddd, *J* = 8.5, 7.3, 0.52 Hz), 7.12 (1H, d, *J* = 8.2 Hz), 2.26 (3H, s); ¹³C-NMR (100 MHz, CDCl₃): δ 152.6, 149.4, 145.2, 139.9, 139.1, 134.8, 131.0, 129.8, 129.1, 128.0, 127.1, 126.5, 126.3, 124.2, 122.8, 122.6, 120.4, 115.4, 115.3, 114.6, 21.5. HRMS (ESI-TOF) *m/z* calcd for C₂₅H₂₀N₃O₂S⁺ [M + H]⁺: 426.1276, found: 426.1259.

(E)-3-(Phenyldiazenyl)-1-(tetrahydro-2H-pyran-2-yl)-1H-indazole (3h)

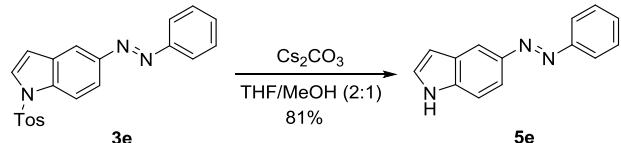


General procedure C was followed using **2h** (204.3 mg, 0.5 mmol) and DMF (2.5 ml) at 160 °C for 2 h, then 180 °C for 30 min, followed by exposing to oxygen at 60 °C and stirring overnight. Purification by flash column chromatography

(*n*-pentane-EtOAc, 30:1) gave the expected azo product **3h** (62 mg, 40% yield) as an orange solid (m.p. = 92-94 °C). ¹H-NMR (400 MHz, CDCl₃): δ 8.47 (1H, d, *J* = 8.1 Hz), 8.09-8.03 (2H, m), 7.66 (1H, d, *J* = 8.5 Hz), 7.57-7.46 (4H, m), 7.35 (1H, ddd, *J* = 7.9, 7.0, 0.68 Hz), 5.87 (1H, dd, *J* = 9.0, 2.8 Hz), 4.08-3.99 (1H, m), 3.83-3.73 (1H, m), 2.80-2.67 (1H, m), 2.28-2.14 (2H, m), 1.87-1.67 (3H, m); ¹³C-NMR (100 MHz, CDCl₃): δ 154.9, 153.1, 141.2, 131.1, 129.0, 127.7, 124.3, 123.9, 122.9, 155.5, 110.4, 85.9, 67.2, 29.1, 25.1, 22.2. HRMS (ESI-TOF) *m/z* calcd for C₁₈H₁₉N₄O⁺ [M + H]⁺: 307.1559, found: 307.1541.

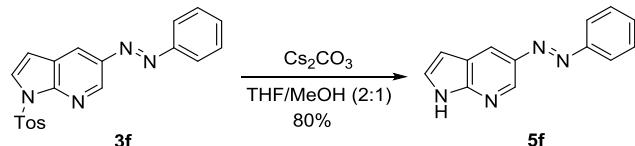
2.5. Deprotection

(E)-5-(Phenyldiazenyl)-1H-indole (**5e**)



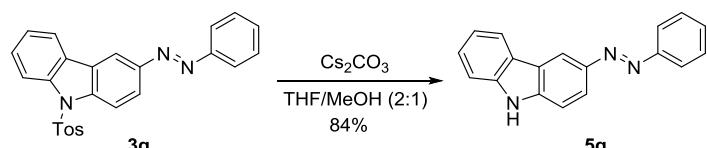
To a solution of tosyl protected azo compound **3e** (375.6 mg, 1.0 mmol) in THF/MeOH (2:1, 10 ml) was added Cs₂CO₃ (977.6 mg, 3.0 mmol) at 0-5 °C, the resulting mixture was allowed to stir for another 3 h at this temperature until it completed according to TLC. The reaction mixture was then quenched by water (10.0 ml), extracted by Ethyl acetate (3× 15.0 ml), the combined organic layer was dried over Na₂SO₄. After filtration, the solvent was removed under reduced pressure, and the residue was purified by flash column chromatography on silica gel (*n*-pentane-EtOAc, 10:1 to 3:1) to afford the target azo compound **5e** (180 mg, 81% yield) as a light brown solid (m.p. = 94-96 °C). ¹H-NMR (400 MHz, DMSO-*d*₆): δ 11.51 (1H, s), 8.22 (1H, s), 7.85 (2H, d, *J* = 7.4 Hz), 7.74 (1H, d, *J* = 8.4 Hz), 7.60-7.43 (5H, m), 6.64 (1H, s); ¹³C-NMR (100 MHz, DMSO-*d*₆): δ 152.6, 146.4, 138.2, 130.7, 129.8, 128.2, 127.7, 122.5, 119.6, 114.4, 112.6, 103.7. HRMS (ESI-TOF) *m/z* calcd for C₁₄H₁₂N₃⁺ [M + H]⁺: 222.1031, found: 222.1026.

(E)-5-(phenyldiazenyl)-1H-pyrrolo[2,3-b]pyridine (**5f**)



General procedure D was followed using **3f** (94.5 mg, 0.25 mmol) and Cs₂CO₃ (244.4 mg, 0.75 mmol) at 0-5 °C for 3 h. Purification by flash column chromatography (*n*-pentane-EtOAc, 3:1) gave the target azo compound **5f** (45 mg, 80% yield) as a brown solid (m.p. = 194-196 °C). ¹H-NMR (400 MHz, DMSO-*d*₆): δ 12.05 (1H, s), 8.88 (1H, d, *J* = 2.2 Hz), 8.43 (1H, d, *J* = 2.0 Hz), 7.90-7.86 (2H, m), 7.62-7.49 (4H, m), 6.63 (1H, dd, *J* = 3.4, 1.8 Hz); ¹³C-NMR (100 MHz, DMSO-*d*₆): δ 152.5, 150.3, 143.0, 142.1, 131.4, 129.9, 129.1, 122.7, 120.4, 119.7, 102.5. HRMS (ESI-TOF) *m/z* calcd for C₁₃H₁₁N₄⁺ [M + H]⁺: 223.0984, found: 223.0983.

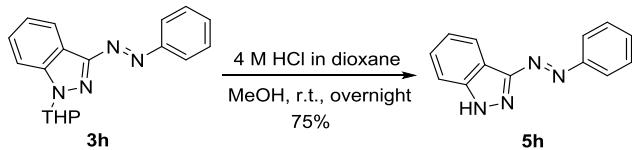
(E)-3-(phenyldiazenyl)-9H-carbazole (**5g**)



General procedure D was followed using **3g** (106.4 mg, 0.25 mmol) and Cs₂CO₃ (244.4 mg, 0.75 mmol) at 0-5 °C for 3 h. Purification by flash column chromatography (*n*-pentane-EtOAc, 10:1) gave the target azo compound **5g** (57 mg, 84% yield) as an orange solid (m.p. = 197-200 °C). ¹H-NMR (400 MHz, DMSO-*d*₆): δ 11.76 (1H, s), 8.76 (1H, d, *J* = 1.4 Hz), 8.27 (1H, d, *J* = 7.8 Hz), 8.04 (1H, dd, *J* = 8.7, 1.8 Hz), 7.90 (2H, d, *J* = 7.5 Hz), 7.63 (1H, d, *J* = 8.7 Hz), 7.60-7.53 (3H, m), 7.53-7.41 (2H, m), 7.23 (1H, t, *J* = 7.5 Hz); ¹³C-NMR (100 MHz, DMSO-*d*₆): δ 152.7, 145.9, 142.3, 141.0, 130.8, 129.8, 126.8, 123.4, 123.3, 122.6, 121.3, 120.1, 120.0, 118.1, 112.0. HRMS (ESI-TOF) *m/z* calcd for C₁₈H₁₄N₃⁺ [M + H]⁺:

272.1188, found: 272.1185. Data is in accordance with the literature.^[11]

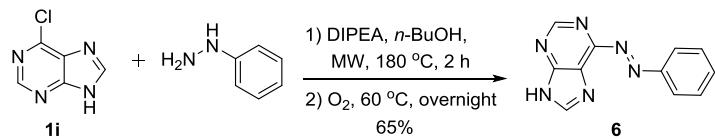
(E)-3-(Phenyldiazenyl)-1H-indazole (5h)^[12]



To a solution of **3h** (62.1 mg, 0.20 mmol) in MeOH (1.5 ml) was added 4 M HCl in dioxane (0.25 ml, 1.0 mmol). The resulting mixture was stirred at rt overnight followed by adding ethyl acetate (4.0 ml) to dilute it. The mixture was then washed with water, saturated aqueous NaHCO₃, and brine successively. The organic extracts were dried over Na₂SO₄, filtered, and concentrated under vacuum. The crude residue was purified by flash column chromatography on silica gel (*n*-pentane-EtOAc, 10:1) to provide the target azo compound **5h** (33 mg, 75% yield) as an orange solid (m.p. = 165-167 °C). ¹H-NMR (400 MHz, DMSO-*d*₆): δ 13.93 (1H, s), 8.35 (1H, d, *J* = 8.1 Hz), 7.96 (2H, d, *J* = 7.3 Hz), 7.67-7.51 (4H, s), 7.48 (1H, ddd, *J* = 8.0, 7.0, 1.0 Hz), 7.34 (1H, ddd, *J* = 7.9, 7.3, 0.84 Hz); ¹³C-NMR (100 MHz, DMSO-*d*₆): δ 155.7, 153.0, 141.9, 131.7, 129.9, 128.0, 124.5, 123.2, 122.6, 113.4, 111.2. HRMS (ESI-TOF) *m/z* calcd for C₁₃H₁₁N₄⁺ [M + H]⁺: 223.0984, found: 223.0975.

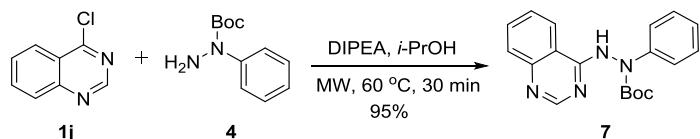
2.6. Synthesis of 6 and 8

(E)-6-(Phenyldiazenyl)-9H-purine (6)



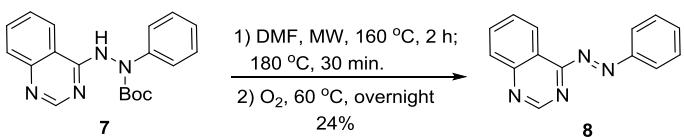
To a microwave vessel was added **1i** (155.2 mg, 1.0 mmol), phenylhydrazine (324.6 mg, 0.3 ml, 3.0 mmol), *n*-BuOH (10.0 ml), DIPEA (387.8 mg, 0.52 ml, 3.0 mmol) successively, the resulting mixture was then reacted under microwave irradiation at 180 °C for 2 h. After cooling to rt, pure oxygen was exchanged into the vessel, followed by heating to 60 °C and stirring overnight. After evaporation under vacuum, the crude residue was purified by flash column chromatography on silica gel (MeOH-CH₂Cl₂, 1:15) to give the expected azo product **6** (146 mg, 65% yield) as dark red solid (m.p. = 128-130 °C). ¹H-NMR (400 MHz, DMSO-*d*₆): δ 13.27 (1H, s), 9.13 (1H, s), 8.86 (1H, s), 8.32-8.03 (2H, m), 7.76-7.53 (3H, m); ¹³C-NMR (100 MHz, DMSO-*d*₆): δ 152.6, 152.3, 134.2, 130.1, 124.0. HRMS (ESI-TOF) *m/z* calcd for C₁₁H₉N₆⁺ [M + H]⁺: 225.0889, found: 225.0878.

tert-Butyl 1-phenyl-2-(quinazolin-4-yl)hydrazine-1-carboxylate (7)



To a microwave vessel was added **1j** (263.4 mg, 1.6 mmol), **4** (324.6 mg, 3.0 mmol), *i*-PrOH (10.0 ml), DIPEA (387.8 mg, 0.52 ml, 3.0 mmol) successively, the resulting mixture was then reacted under microwave irradiation at 60 °C for 30 min. After evaporation under vacuum, the crude residue was purified by NEt₃ neutralized flash column chromatography on silica gel (*n*-pentane-EtOAc, 3:1) to give the pure product **7** (513 mg, 95.4% yield) as light yellow oil. ¹H-NMR (400 MHz, CDCl₃): δ 8.58 (1H, s), 8.18 (1H, dd, *J* = 8.4, 0.48 Hz), 7.90-7.79 (2H, m), 7.63-7.53 (3H, m), 7.36-7.28 (2H, m), 7.16 (1H, tt, *J* = 7.4, 1.0 Hz), 1.37 (9H, s); ¹³C-NMR (100 MHz, CD₃OD): δ 160.0, 155.0, 153.1, 149.4, 142.5, 133.8, 128.8, 128.0, 127.0, 125.3, 122.9, 113.7, 81.5, 79.6, 28.1. HRMS (ESI-TOF) *m/z* calcd for C₁₉H₂₁N₄O₂⁺ [M + H]⁺: 337.1665, found: 337.1663.

(E)-4-(Phenyldiazenyl)quinazoline (8)



To a microwave vessel was added **7** (405.3 mg, 1.2 mmol) and DMF (5.0 ml), the resulting mixture was then reacted under microwave irradiation at 160 °C for 2 h, and then stirred at 180 °C for 30 min. After cooling to rt, pure oxygen was exchanged into the vessel, followed by heating to 60 °C and stirring overnight. After evaporation under vacuo, the crude product was purified by flash column chromatography on silica gel (*n*-pentane-EtOAc, 10:1) to produce the expected azo product **8** (66 mg, 24% yield) as dark red solid (m.p. = 84–86 °C). ¹H-NMR (400 MHz, CDCl₃): δ 9.40 (1H, s), 8.59 (1H, d, *J* = 8.3 Hz), 8.21–8.14 (3H, m), 7.99 (1H, ddd, *J* = 8.4, 7.0, 1.3 Hz), 7.75 (1H, ddd, *J* = 8.1, 7.3, 0.84 Hz), 7.65–7.57 (3H, m); ¹³C-NMR (100 MHz, CDCl₃): δ 165.4, 155.2, 153.1, 152.8, 134.6, 133.6, 129.4, 128.5, 128.4, 125.0, 124.3, 120.9, 110.0. HRMS (ESI-TOF) *m/z* calcd for C₁₄H₁₁N₄⁺ [M + H]⁺: 235.0984, found: 235.0979.

3. UV-Vis Absorption Spectroscopy

All compounds (3.0 μ mol) were firstly dissolved in 1.0 mL DMSO to give the 3.0 mM solutions, and then thermally adapted by heating at 50 °C for 72 h. Afterwards, 30 μ L of the solution was diluted into 3.0 mL mixed solvent (water and 0% - 100% DMSO) to give the final samples at a concentration of 30 μ M. These samples were exposed to UV-Vis characterization (absorption spectrum, thermal stability, photostability and isomerization kinetics). The samples for the measurement of PSD ($^1\text{H-NMR}$) were DMSO-*d*₆ solutions at a concentration of 0.1 mM.

3.1. UV-Vis absorption spectra

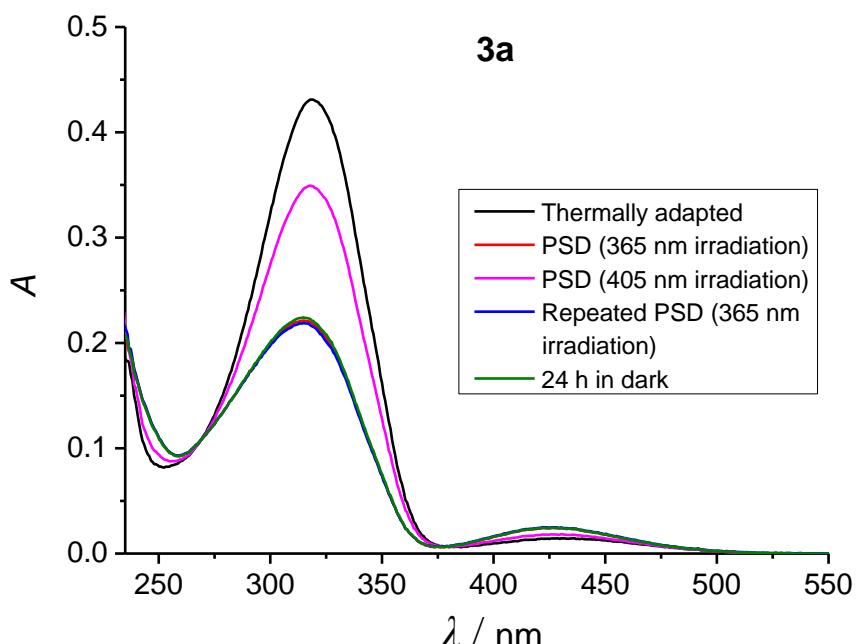


Figure S1. UV-Vis absorption spectra of **3a** (30 μ M aqueous solution with 1 vol% DMSO). Black line: After thermal adaption (at 50 °C for 72 h). Red line: After exposure to 365 nm UV to yield the PSD. Magenta line: After exposure to 405 nm light to yield the PSD. Blue line: After a second round of 365 nm UV to yield the PSD. Green line: Spectra recorded 24 h (at rt in the dark) subsequent to the second round of 365 nm UV.

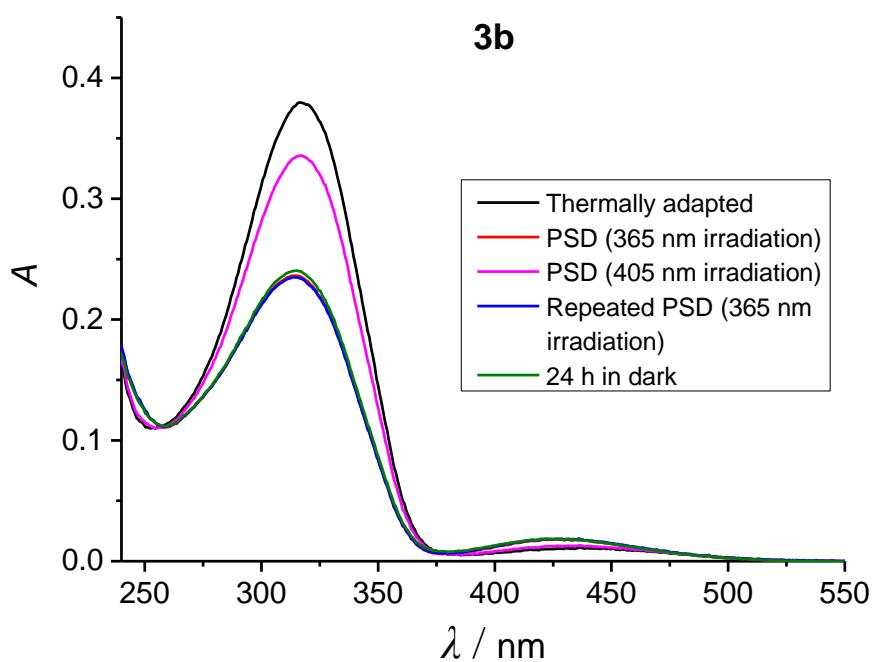


Figure S2. UV-Vis absorption spectra of **3b** (30 μM aqueous solution with 1 vol% DMSO). Black line: After thermal adaption (at 50 °C for 72 h). Red line: After exposure to 365 nm UV to yield the PSD. Magenta line: After exposure to 405 nm light to yield the PSD. Blue line: After a second round of 365 nm UV to yield the PSD. Green line: Spectra recorded 24 h (at rt in the dark) subsequent to the second round of 365 nm UV.

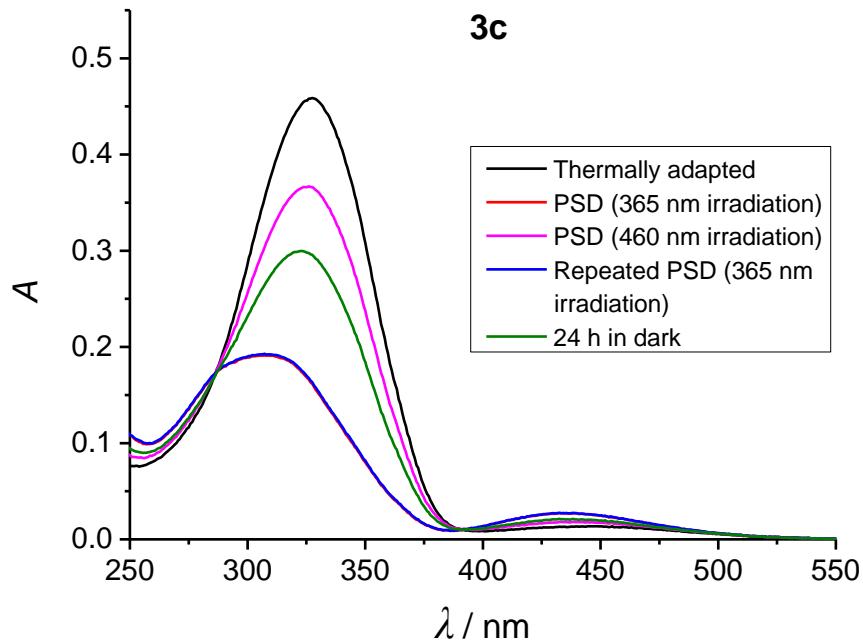


Figure S3. UV-Vis absorption spectra of **3c** (30 μM aqueous solution with 1 vol% DMSO). Black line: After thermal adaption (at 50 °C for 72 h). Red line: After exposure to 365 nm UV to yield the PSD. Magenta line: After exposure to 460 nm light to yield the PSD. Blue line: After a second round of 365 nm UV to yield the PSD. Green line: Spectra recorded 24 h (at rt in the dark) subsequent to the second round of 365 nm UV.

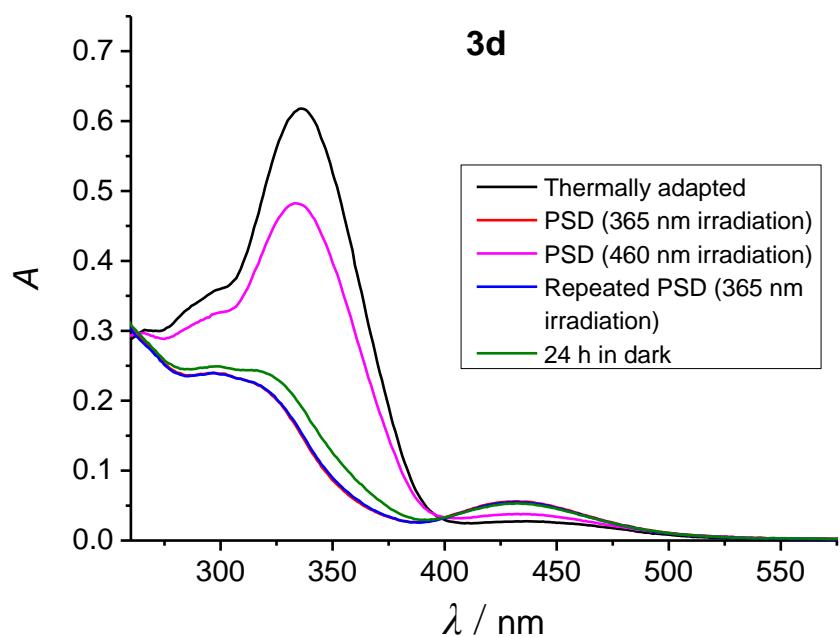


Figure S4. UV-Vis absorption spectra of **3d** (30 μM aqueous solution with 10 vol% DMSO). Black line: After thermal adaption (at 50 °C for 72 h). Red line: After exposure to 365 nm UV to yield the PSD. Magenta line: After exposure to 460 nm light to yield the PSD. Blue line: After a second round of 365 nm UV to yield the PSD. Green line: Spectra recorded 24 h (at rt in the dark) subsequent to the second round of 365 nm UV.

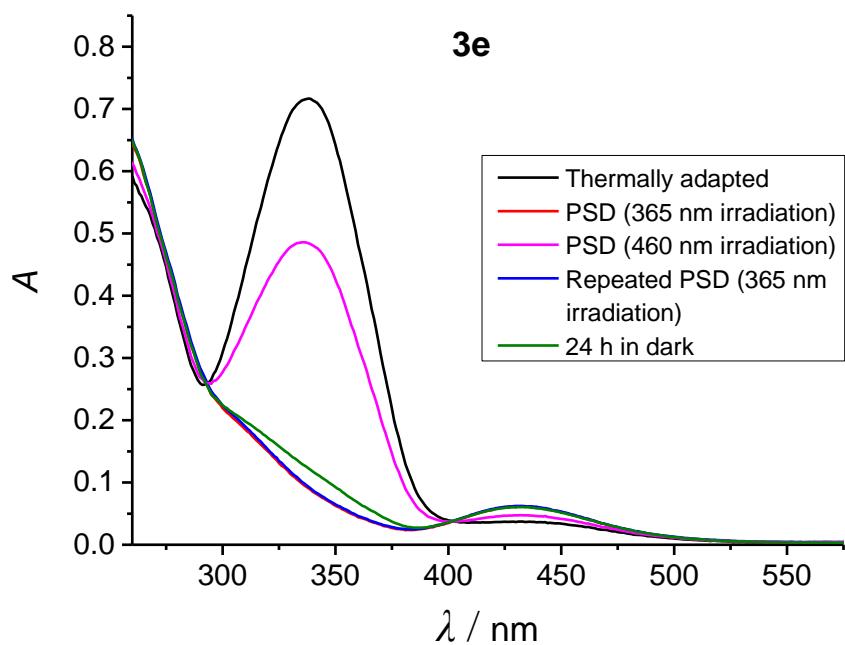


Figure S5. UV-Vis absorption spectra of **3e** (30 μM aqueous solution with 50 vol% DMSO). Black line: After thermal adaption (at 50 °C for 72 h). Red line: After exposure to 365 nm UV to yield the PSD. Magenta line: After exposure to 460 nm light to yield the PSD. Blue line: After a second round of 365 nm UV to yield the PSD. Green line: Spectra recorded 24 h (at rt in the dark) subsequent to the second round of 365 nm UV.

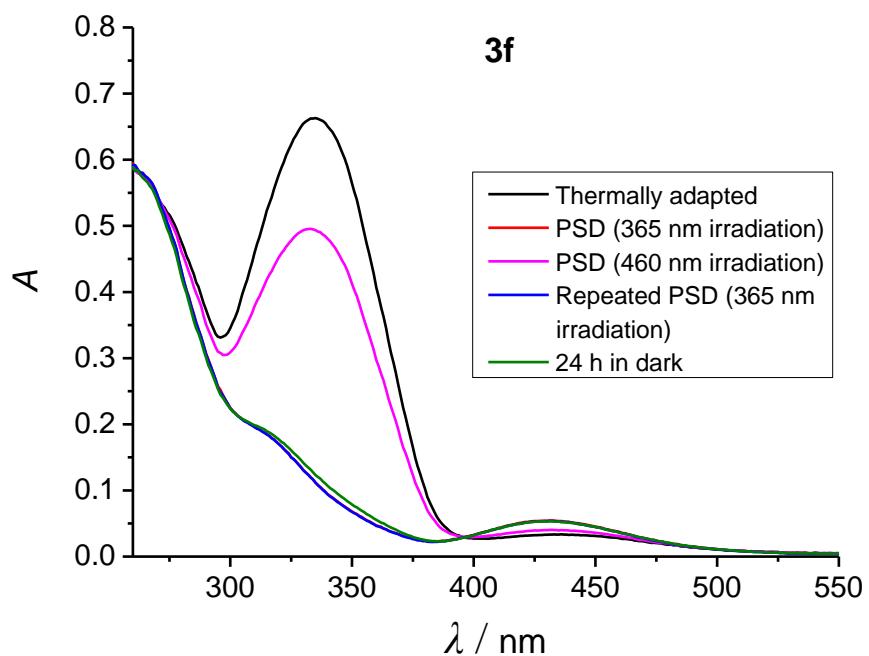


Figure S6. UV-Vis absorption spectra of **3f** (30 μM aqueous solution with 50 vol% DMSO). Black line: After thermal adaption (at 50 °C for 72 h). Red line: After exposure to 365 nm UV to yield the PSD. Magenta line: After exposure to 460 nm light to yield the PSD. Blue line: After a second round of 365 nm UV to yield the PSD. Green line: Spectra recorded 24 h (at rt in the dark) subsequent to the second round of 365 nm UV.

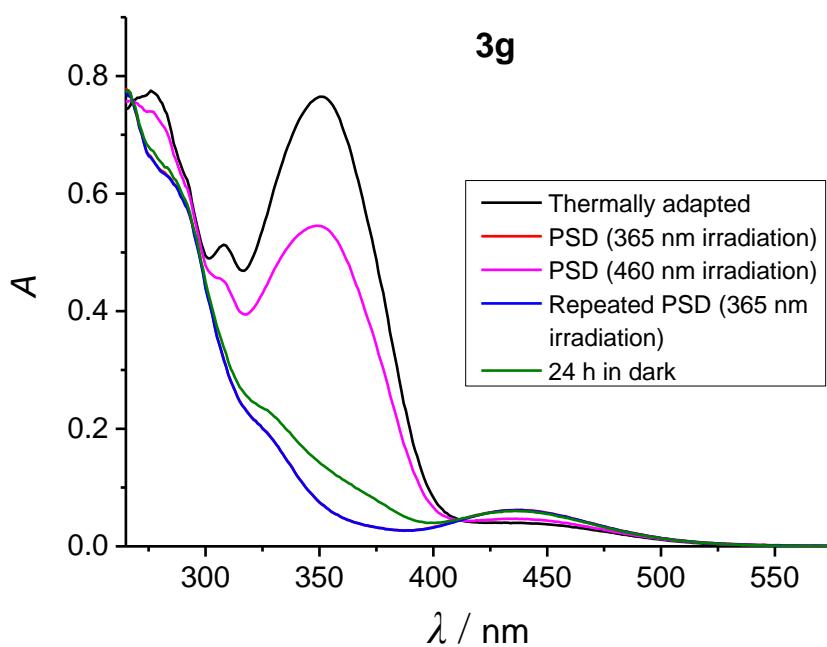


Figure S7. UV-Vis absorption spectra of **3g** (30 μM in DMSO). Black line: After thermal adaption (at 50 °C for 72 h). Red line: After exposure to 365 nm UV to yield the PSD. Magenta line: After exposure to 460 nm light to yield the PSD. Blue line: After a second round of 365 nm UV to yield the PSD. Green line: Spectra recorded 24 h (at rt in the dark) subsequent to the second round of 365 nm UV.

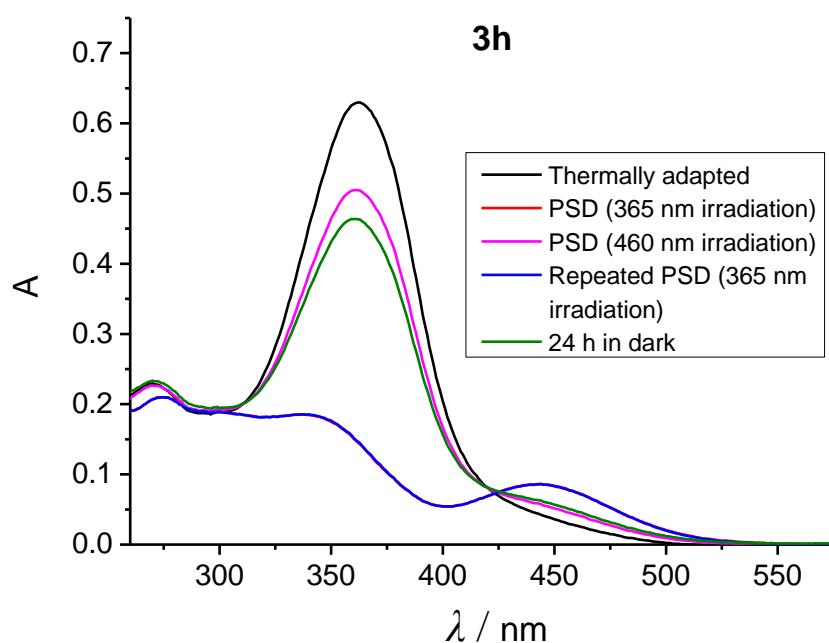


Figure S8. UV-Vis absorption spectra of **3h** (30 μM aqueous solution with 20 vol% DMSO). Black line: After thermal adaption (at 50 °C for 72 h). Red line: After exposure to 365 nm UV to yield the PSD. Magenta line: After exposure to 460 nm light to yield the PSD. Blue line: After a second round of 365 nm UV to yield the PSD. Green line: Spectra recorded 24 h (at rt in the dark) subsequent to the second round of 365 nm UV.

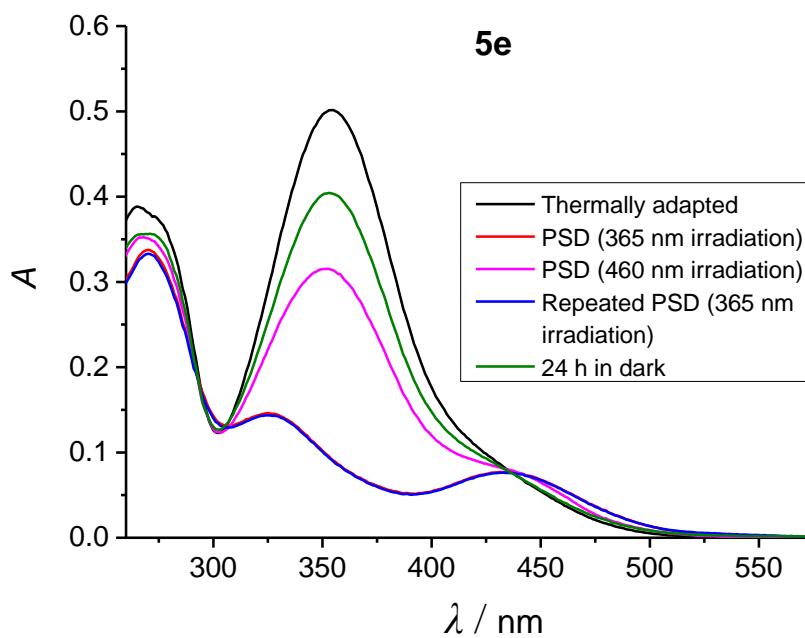


Figure S9. UV-Vis absorption spectra of **5e** (30 μM aqueous solution with 5 vol% DMSO). Black line: After thermal adaption (at 50 °C for 72 h). Red line: After exposure to 365 nm UV to yield the PSD. Magenta line: After exposure to 460 nm light to yield the PSD. Blue line: After a second round of 365 nm UV to yield the PSD. Green line: Spectra recorded 24 h (at rt in the dark) subsequent to the second round of 365 nm UV.

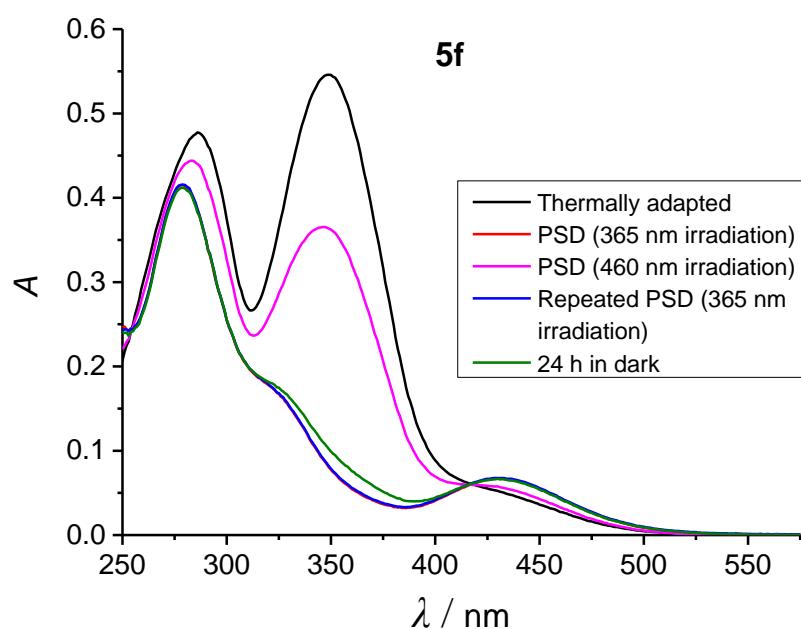


Figure S10. UV-Vis absorption spectra of **5f** (30 μM aqueous solution with 7.5 vol% DMSO). Black line: After thermal adaption (at 50 °C for 72 h). Red line: After exposure to 365 nm UV to yield the PSD. Magenta line: After exposure to 460 nm light to yield the PSD. Blue line: After a second round of 365 nm UV to yield the PSD. Green line: Spectra recorded 24 h (at rt in the dark) subsequent to the second round of 365 nm UV.

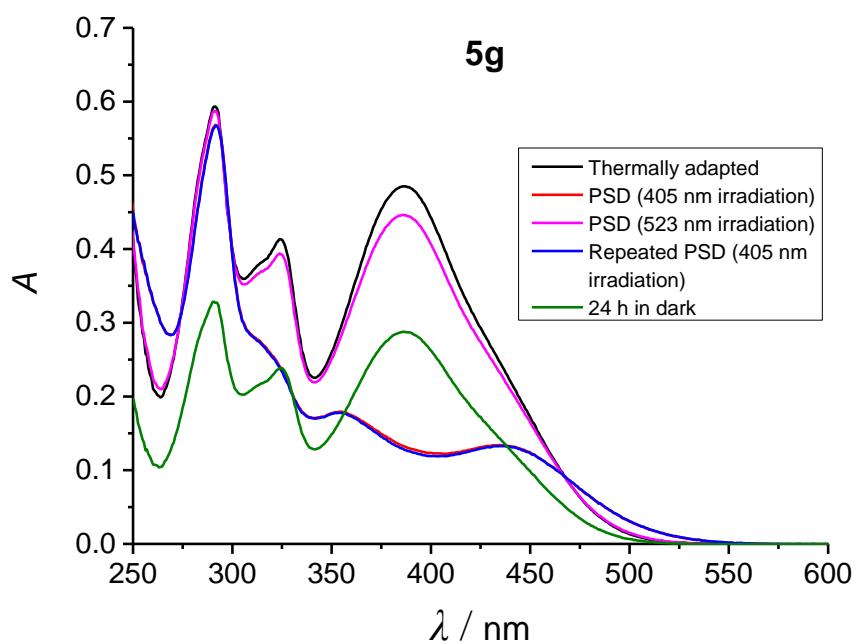


Figure S11. UV-Vis absorption spectra of **5g** (30 μM aqueous solution with 33.3 vol% DMSO). Black line: After thermal adaption (at 50 °C for 72 h). Red line: After exposure to 405 nm UV to yield the PSD. Magenta line: After exposure to 523 nm light to yield the PSD. Blue line: After a second round of 405 nm UV to yield the PSD. Green line: Spectra recorded 24 h (at rt in the dark) subsequent to the second round of 405 nm UV.

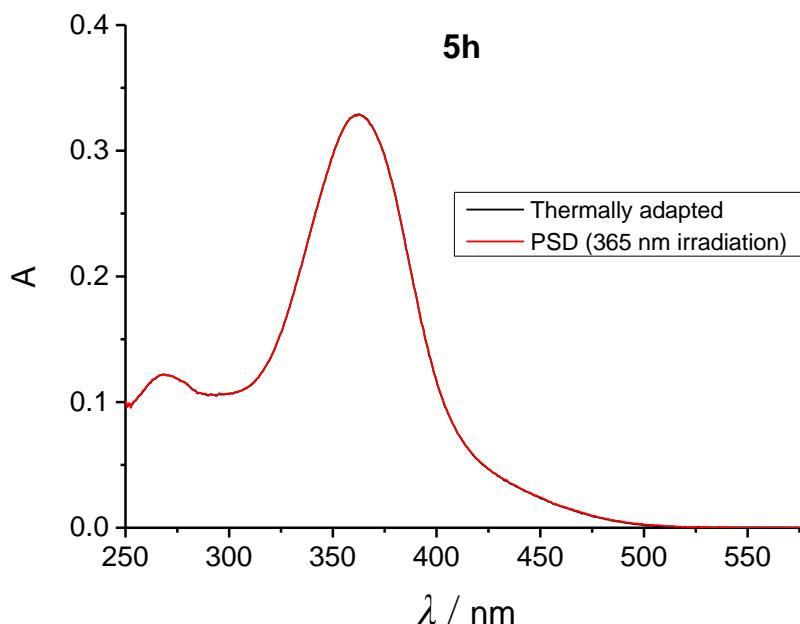


Figure S12. UV-Vis absorption spectra of **5h** (30 μ M aqueous solution with 5 vol% DMSO). Black line: After thermal adaption (at 50 °C for 72 h). Red line: After exposure to 365 nm UV to yield the PSD.

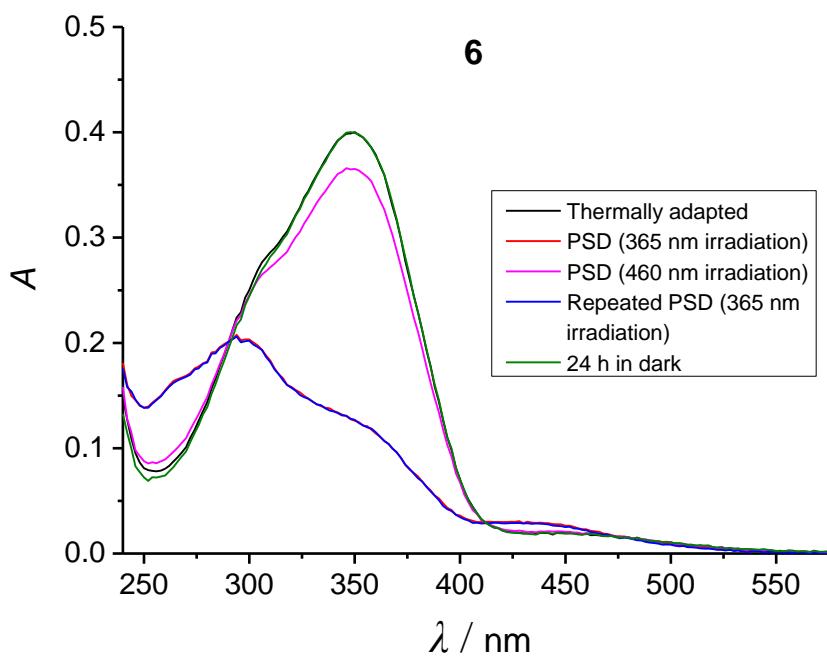


Figure S13. UV-Vis absorption spectra of **6** (30 μ M aqueous solution with 1 vol% DMSO). Black line: After thermal adaption (at 50 °C for 72 h). Red line: After exposure to 365 nm UV to yield the PSD. Magenta line: After exposure to 460 nm light to yield the PSD. Blue line: After a second round of 365 nm UV to yield the PSD. Green line: Spectra recorded 24 h (at rt in the dark) subsequent to the second round of 365 nm UV.

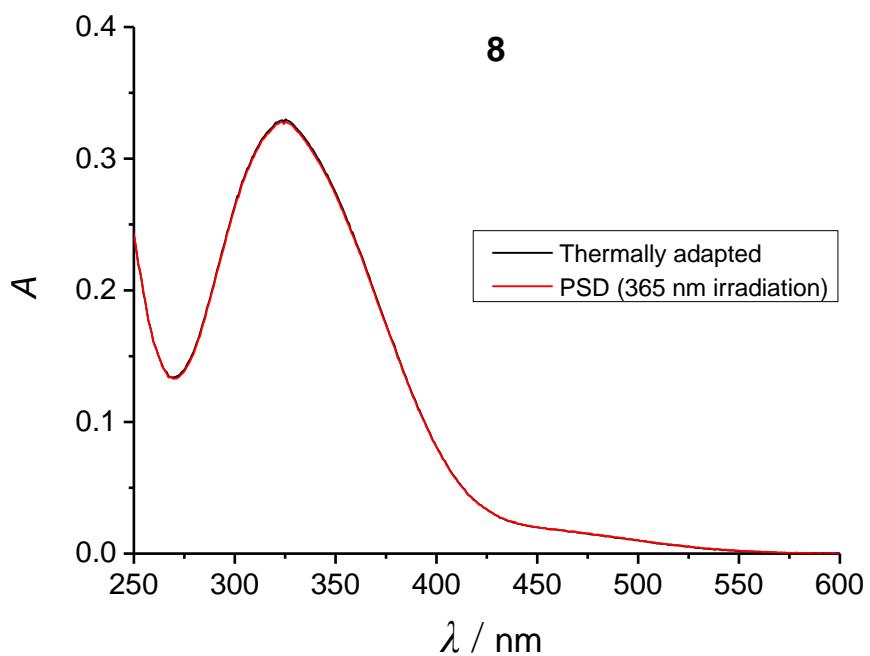


Figure S14. UV-Vis absorption spectra of **8** (30 μ M aqueous solution with 1 vol% DMSO). Black line: After thermal adaption (at 50 °C for 72 h). Red line: After exposure to 365 nm UV to yield the PSD.

3.2. Extended Photocycling

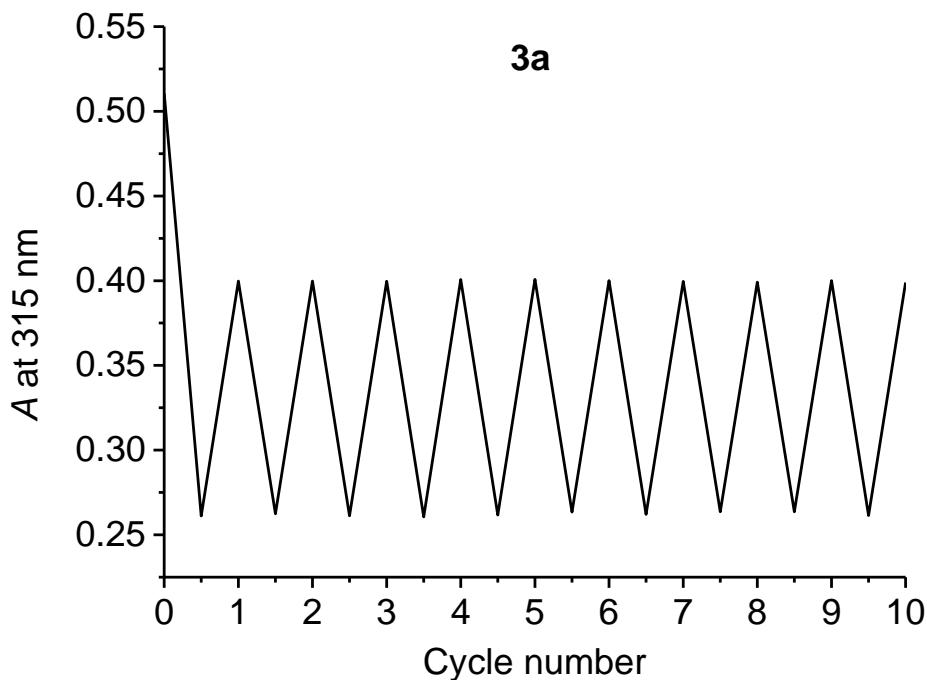


Figure S15. Extended photocycling for **3a** in aqueous solution with 1% DMSO. Ten cycles of 365 nm/405 nm light irradiation performed without significant photodecomposition.

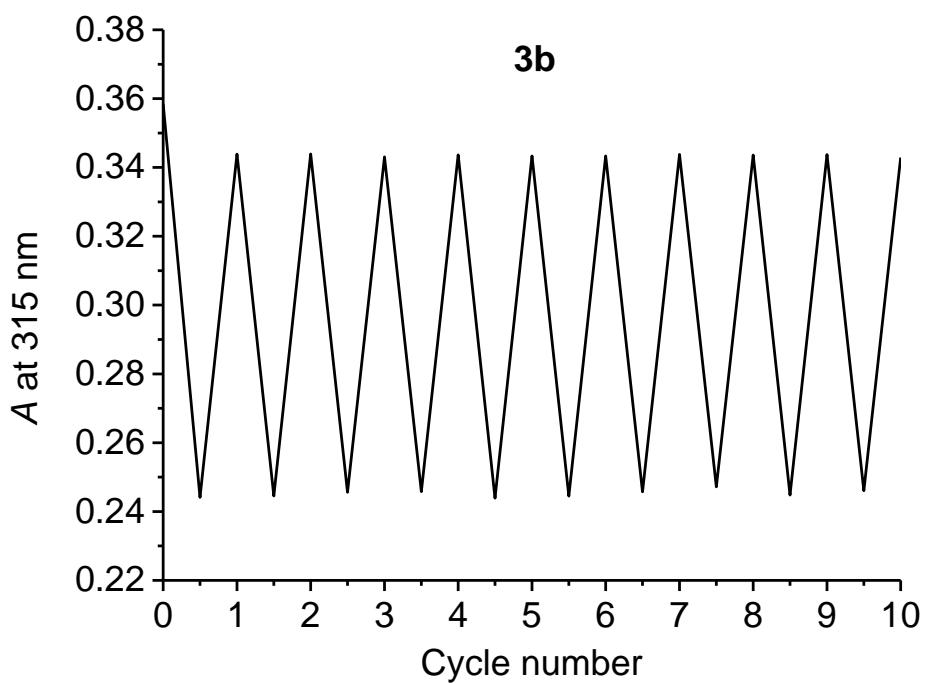


Figure S16. Extended photocycling for **3b** in aqueous solution with 1% DMSO. Ten cycles of 365 nm/405 nm light irradiation performed without significant photodecomposition.

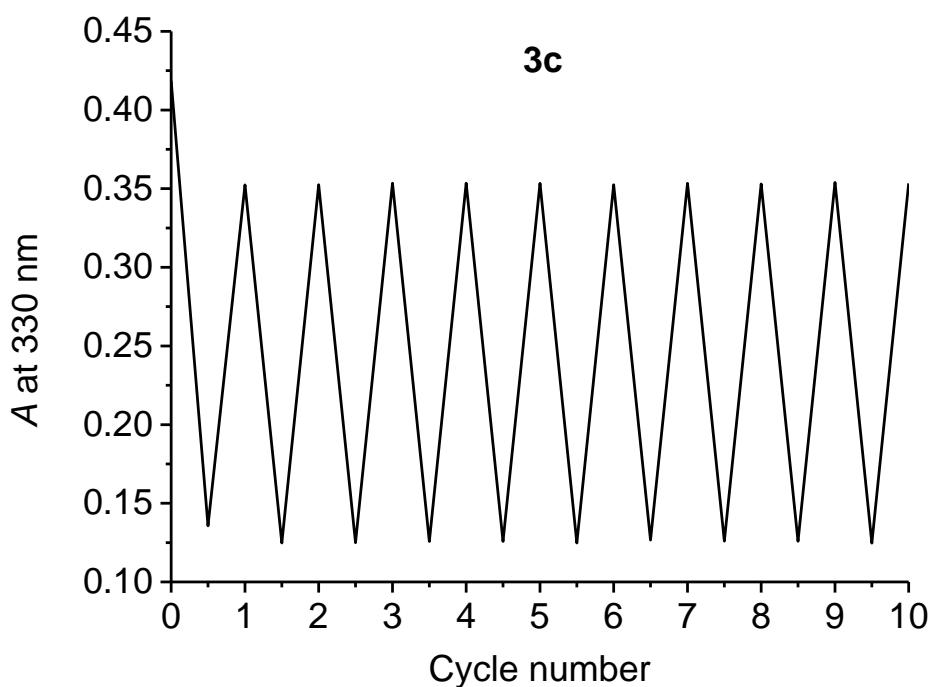


Figure S17. Extended photocycling for **3c** in aqueous solution with 1% DMSO. Ten cycles of 365 nm/460 nm light irradiation performed without significant photodecomposition.

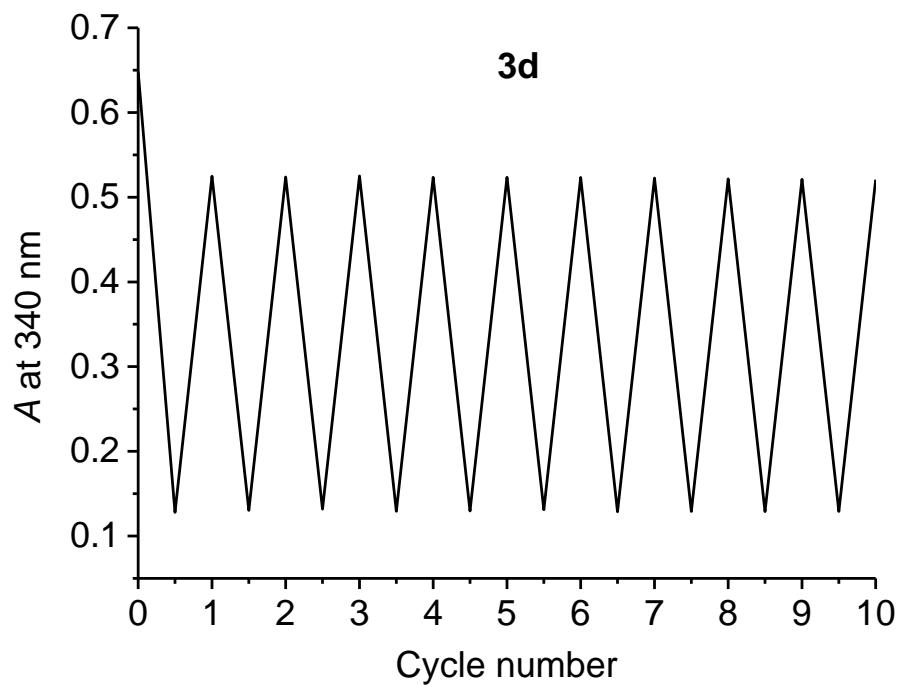


Figure S18. Extended photocycling for **3d** in aqueous solution with 10% DMSO. Ten cycles of 365 nm/460 nm light irradiation performed without significant photodecomposition.

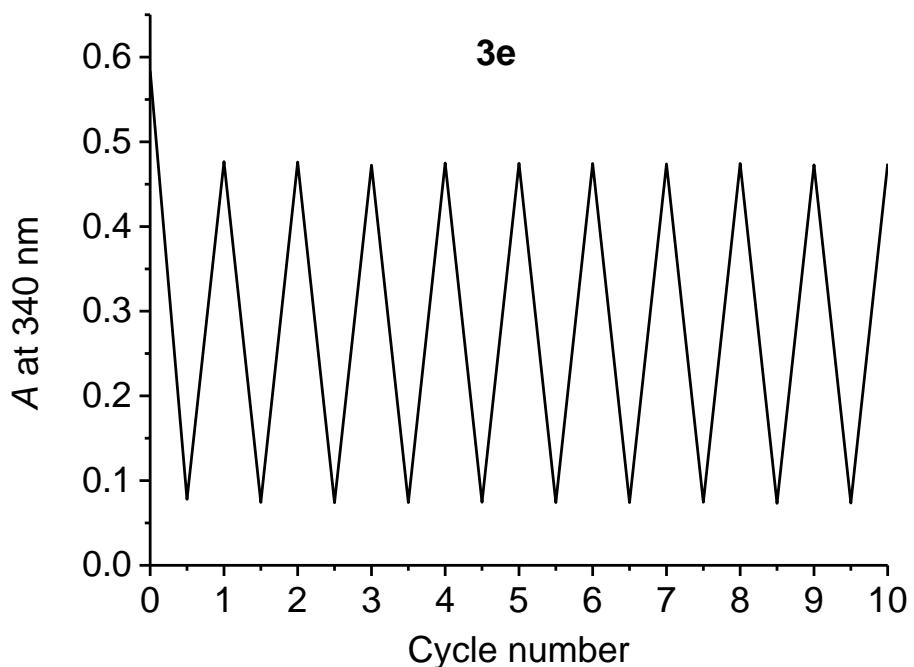


Figure S19. Extended photocycling for **3e** in aqueous solution with 50% DMSO. Ten cycles of 365 nm/460 nm light irradiation performed without significant photodecomposition.

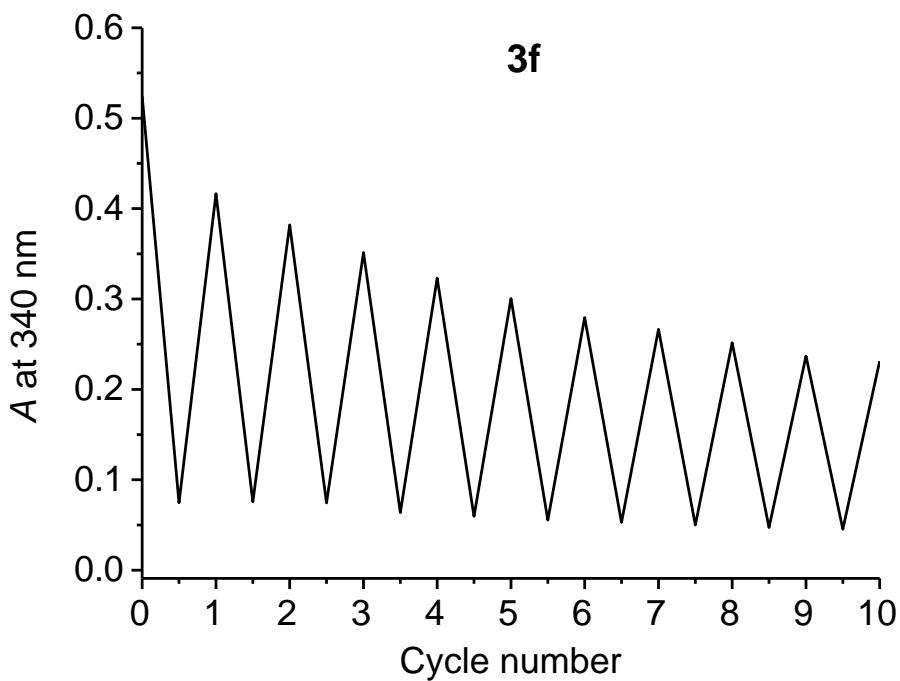


Figure S20. Extended photocycling for **3f** in aqueous solution with 50% DMSO. Ten cycles of 365 nm/460 nm light irradiation was performed. Substantial photodecomposition was observed.

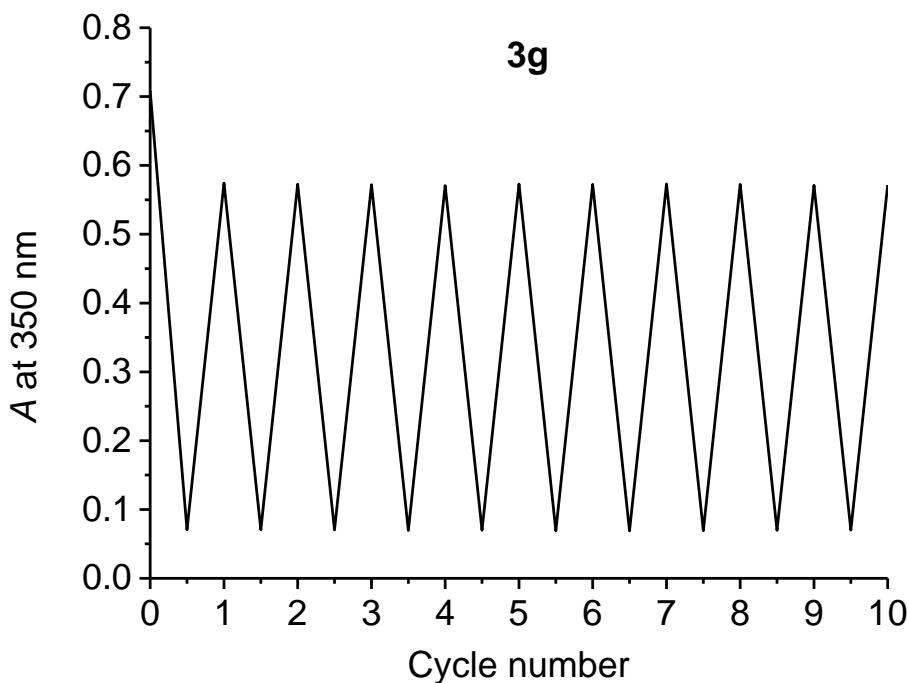


Figure S21. Extended photocycling for **3g** in aqueous solution with 100% DMSO. Ten cycles of 365 nm/460 nm light irradiation performed without significant photodecomposition.

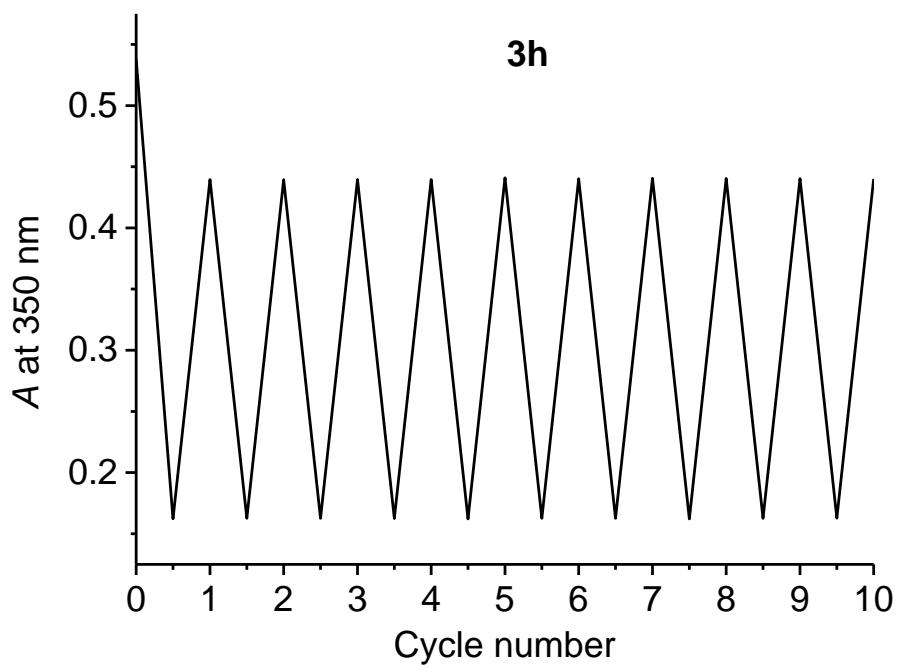


Figure S22. Extended photocycling for **3h** in aqueous solution with 20% DMSO. Ten cycles of 365 nm/460 nm light irradiation performed without significant photodecomposition.

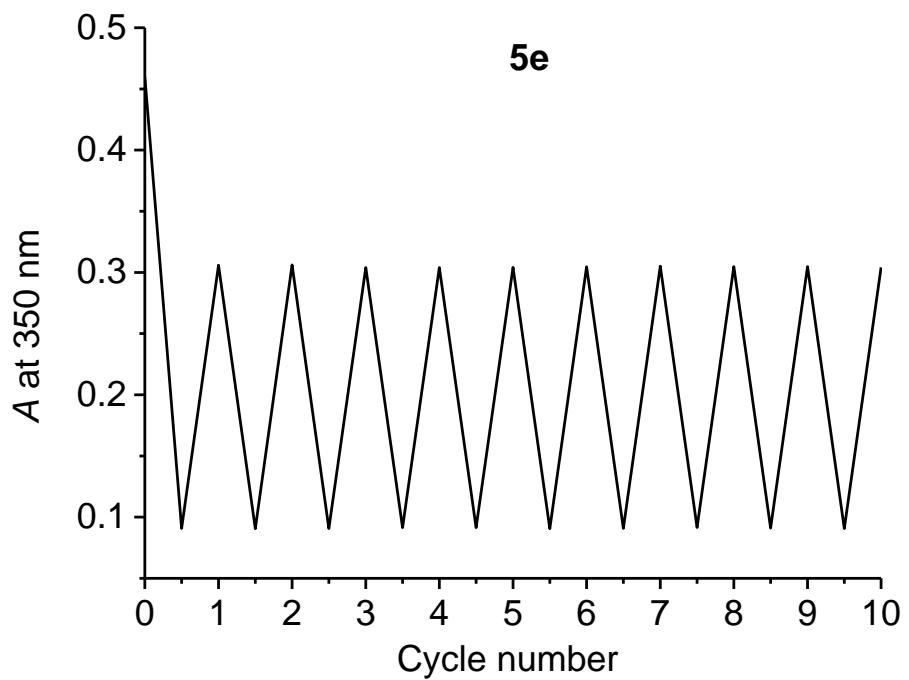


Figure S23. Extended photocycling for **5e** in aqueous solution with 5% DMSO. Ten cycles of 365 nm/460 nm light irradiation performed without significant photodecomposition.

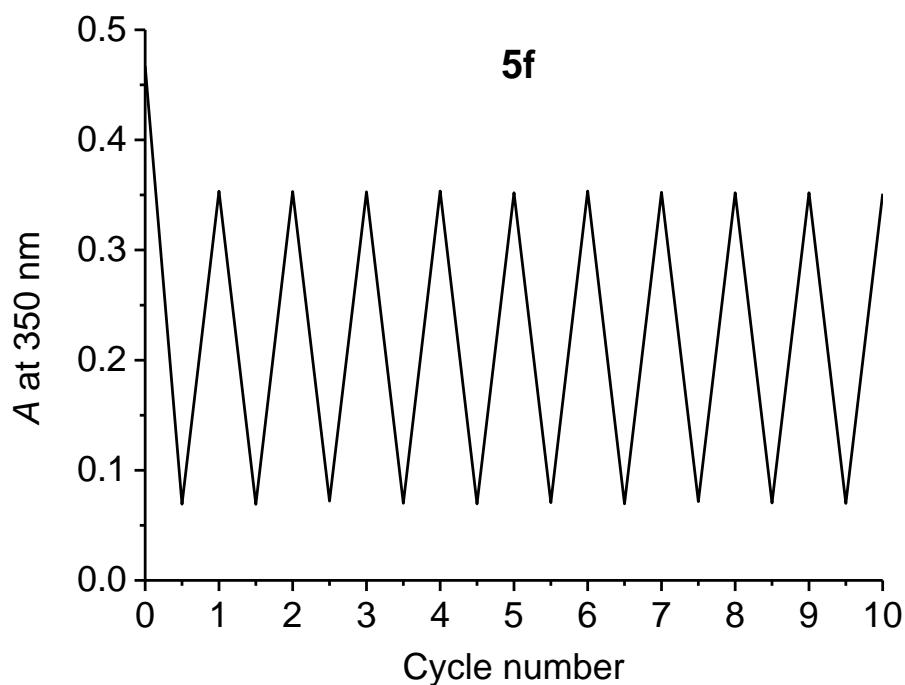


Figure S24. Extended photocycling for **5f** in aqueous solution with 7.5% DMSO. Ten cycles of 365 nm/460 nm light irradiation performed without significant photodecomposition.

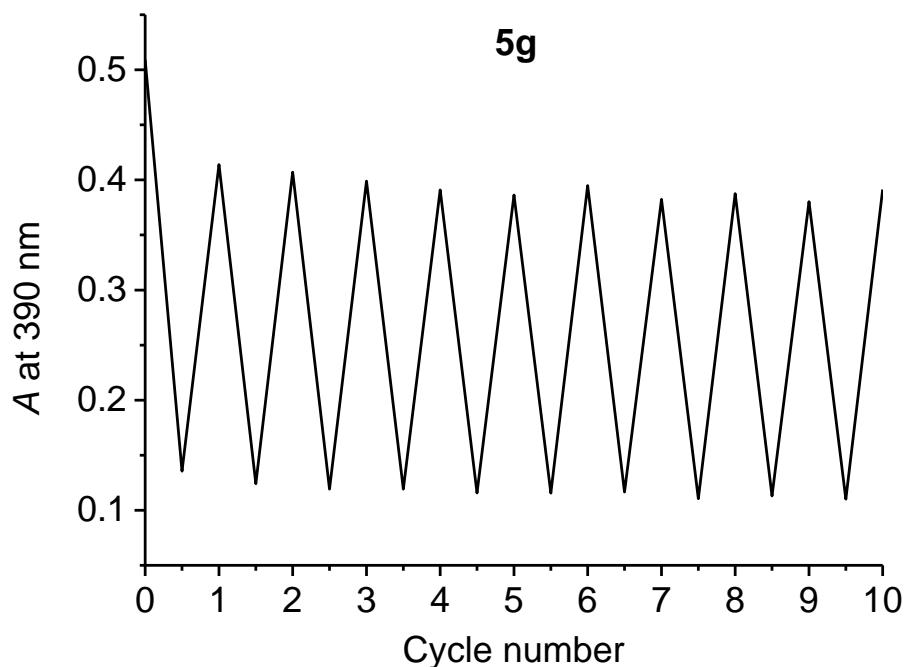


Figure S25. Extended photocycling for **5g** in aqueous solution with 33.3% DMSO. Ten cycles of 405 nm/523 nm light irradiation performed without significant photodecomposition.

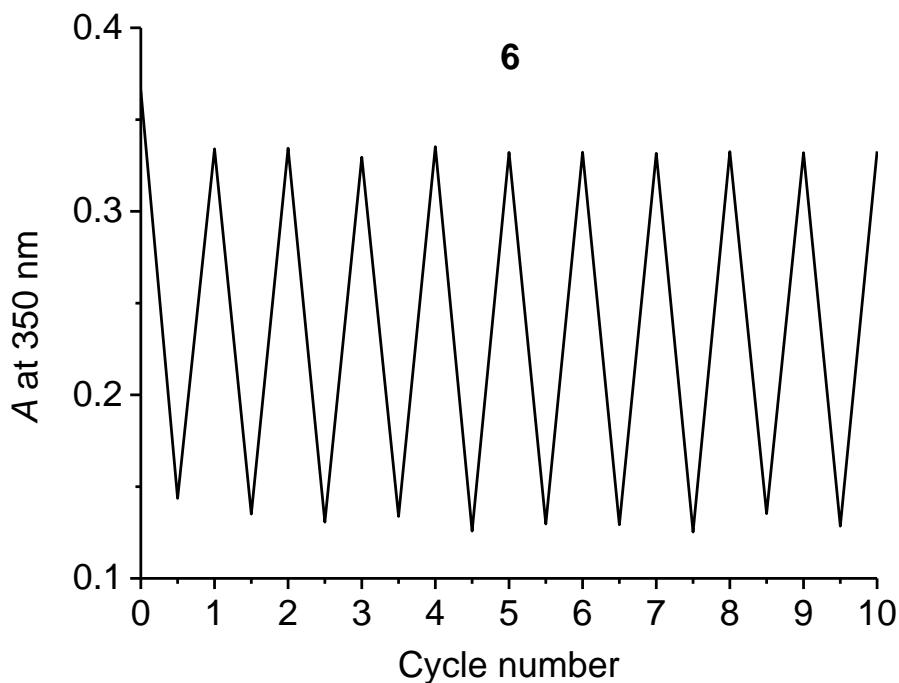
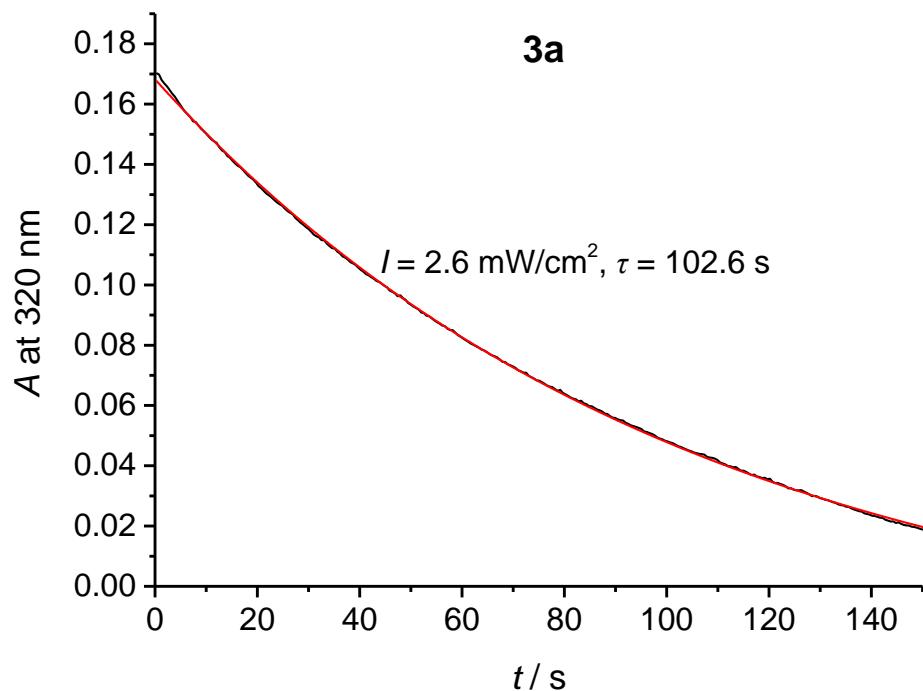


Figure S26. Extended photocycling for **6** in aqueous solution with 1% DMSO. Ten cycles of 365 nm/460 nm light irradiation performed without significant photodecomposition.

3.3. Isomerization kinetics



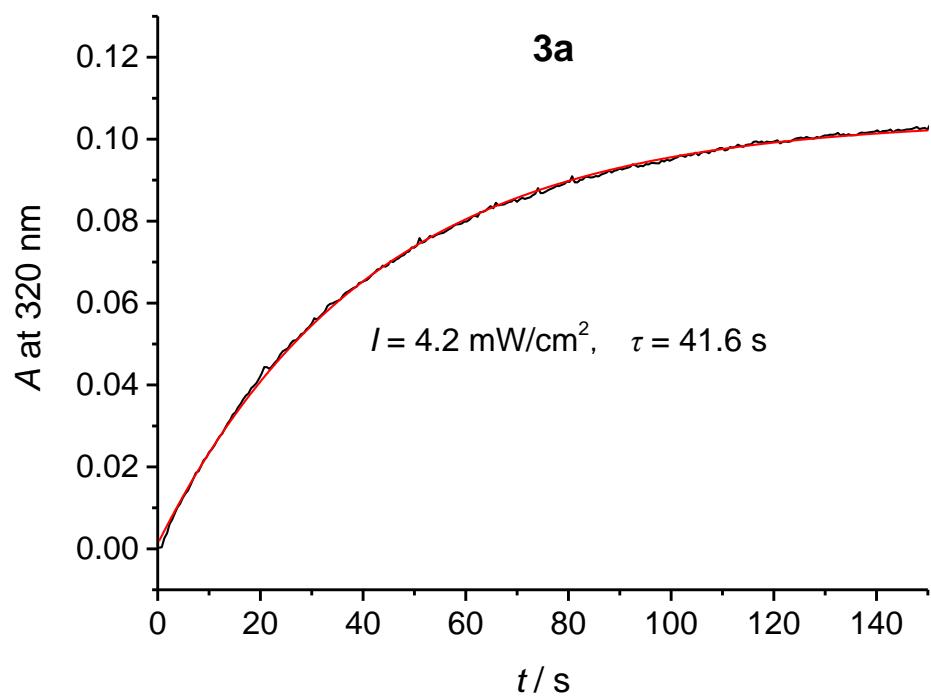
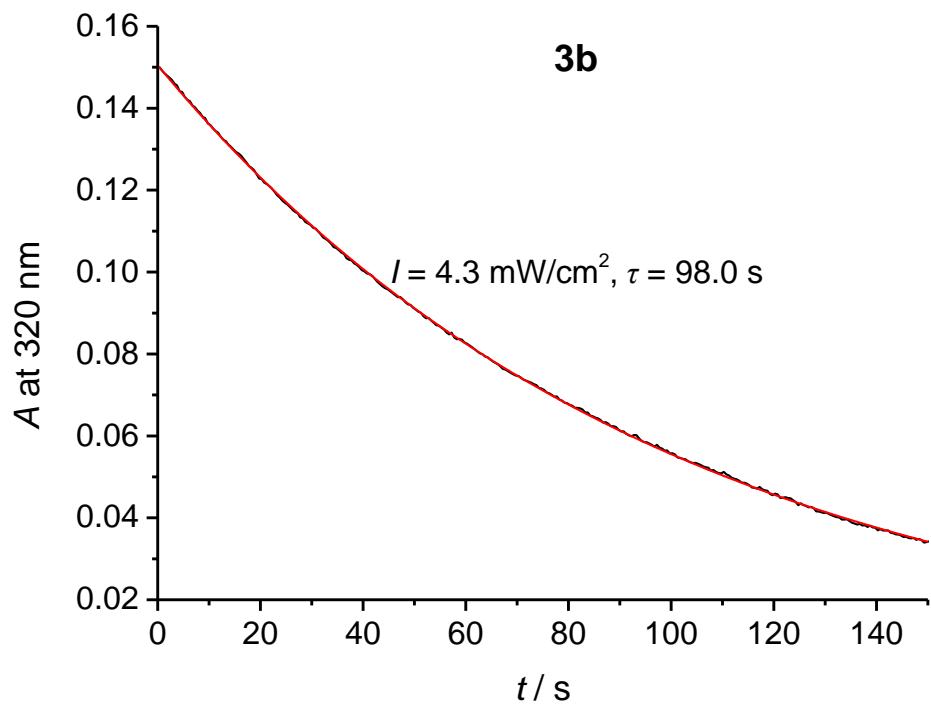


Figure S27. Isomerization kinetics of **3a** in aqueous solution with 1% DMSO. Sample exposed to 365 nm irradiation (top), and subsequently to 405 nm irradiation (bottom) while the absorption changes were monitored at 320 nm. Black lines are the experimental data, red lines are the fitting to mono-exponential kinetics.



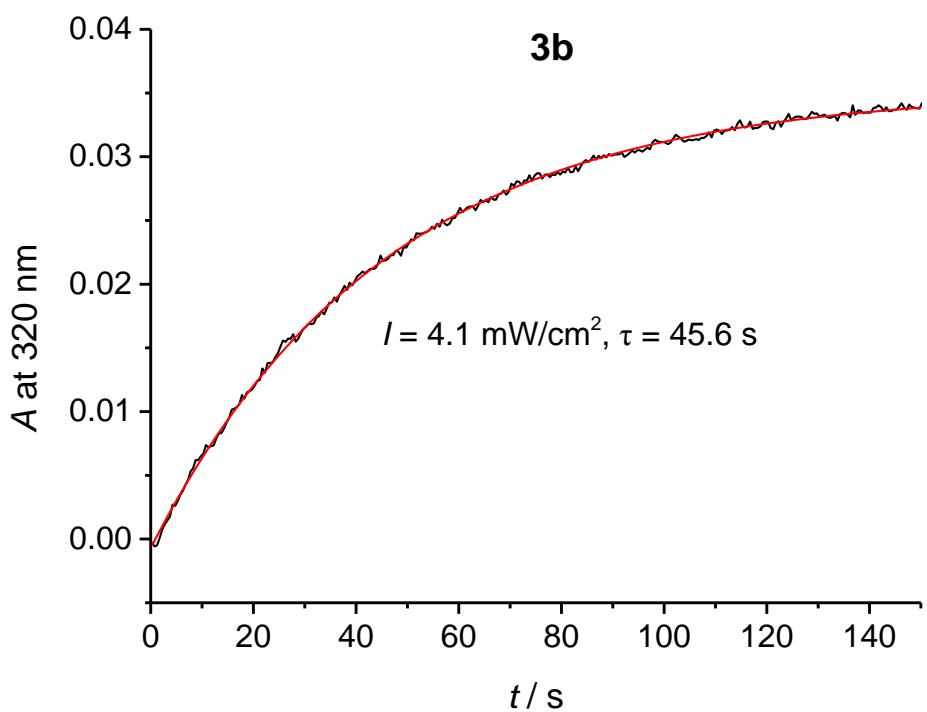
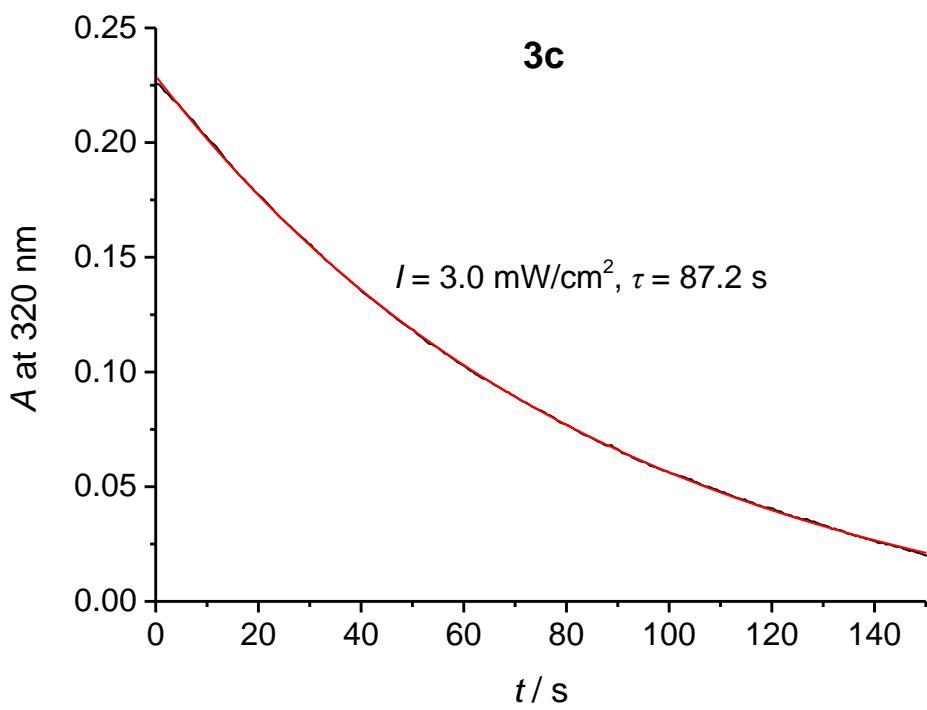


Figure S28. Isomerization kinetics of **3b** in aqueous solution with 1% DMSO. Sample exposed to 365 nm irradiation (top), and subsequently to 405 nm irradiation (bottom) while the absorption changes were monitored at 320 nm. Black lines are the experimental data, red lines are the fitting to mono-exponential kinetics.



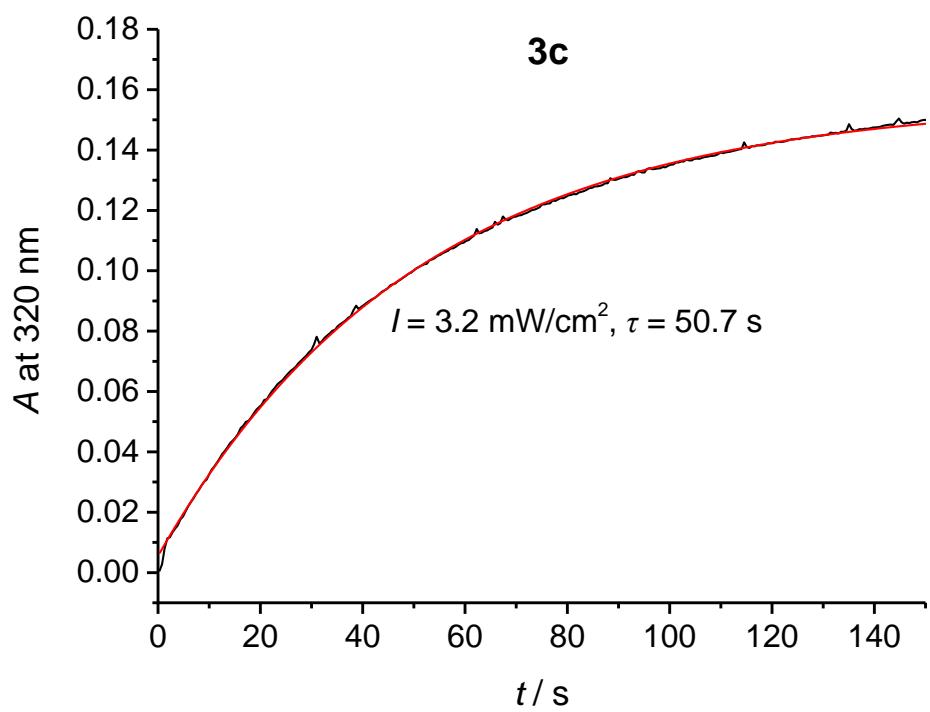
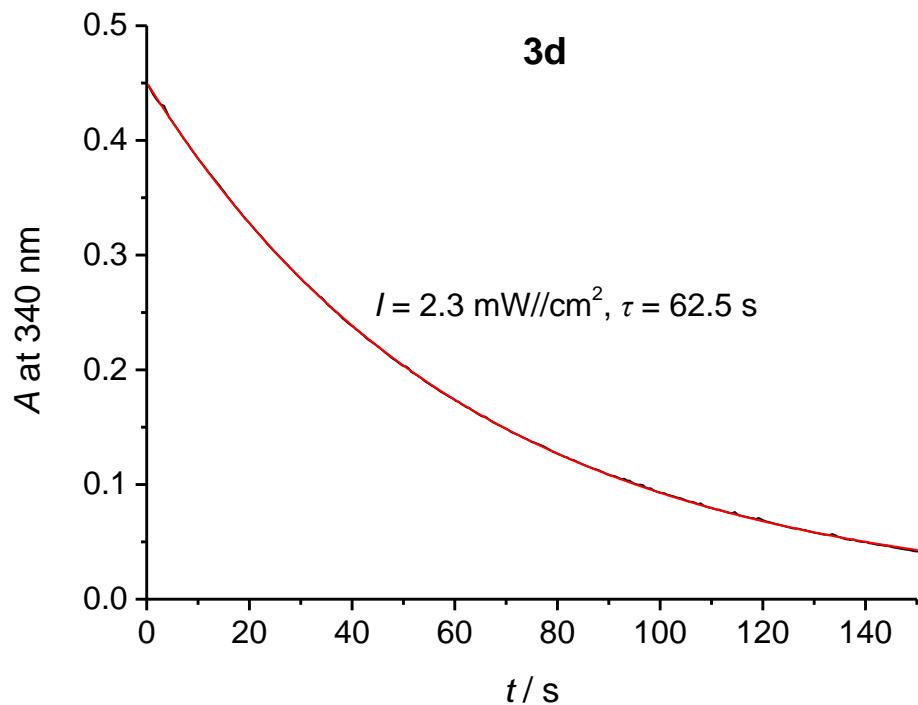


Figure S29. Isomerization kinetics of **3c** in aqueous solution with 1% DMSO. Sample exposed to 365 nm irradiation (top), and subsequently to 460 nm irradiation (bottom) while the absorption changes were monitored at 320 nm. Black lines are the experimental data, red lines are the fitting to mono-exponential kinetics.



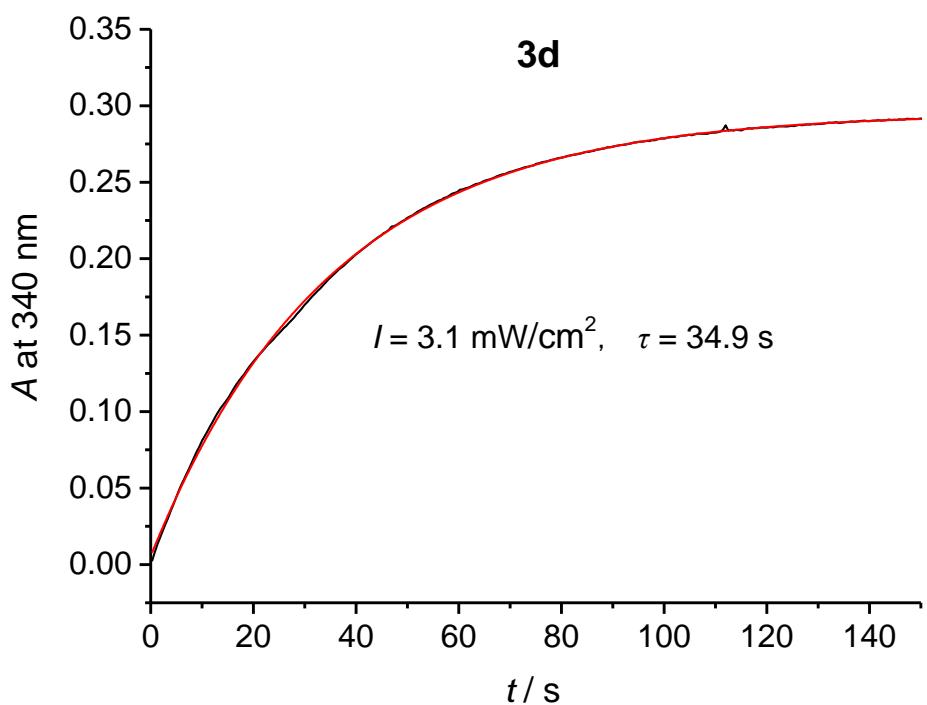
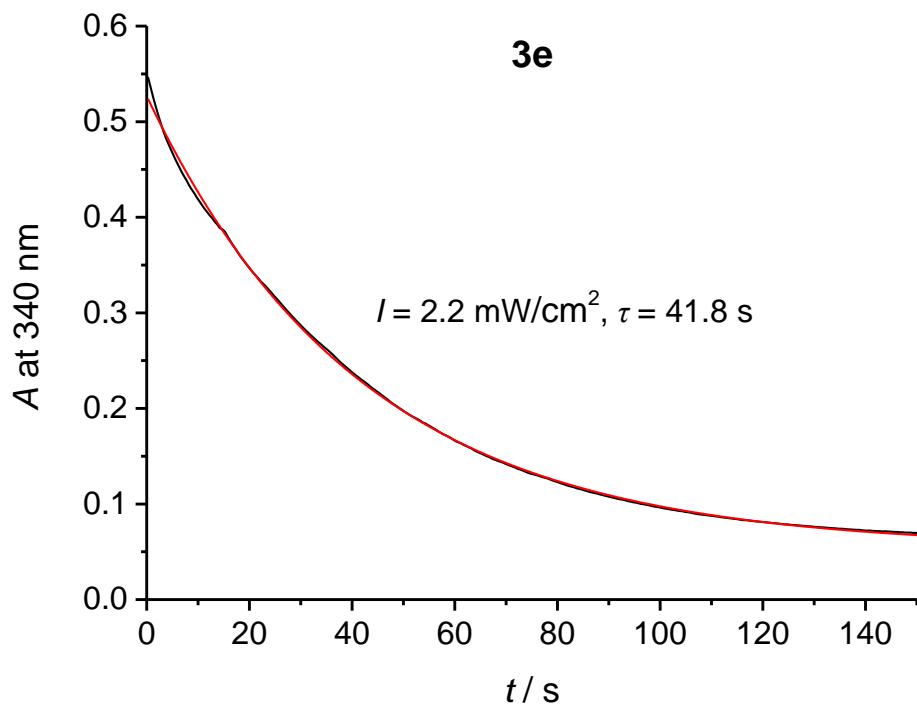


Figure S30. Isomerization kinetics of **3d** in aqueous solution with 10% DMSO. Sample exposed to 365 nm irradiation (top), and subsequently to 460 nm irradiation (bottom) while the absorption changes were monitored at 340 nm. Black lines are the experimental data, red lines are the fitting to mono-exponential kinetics.



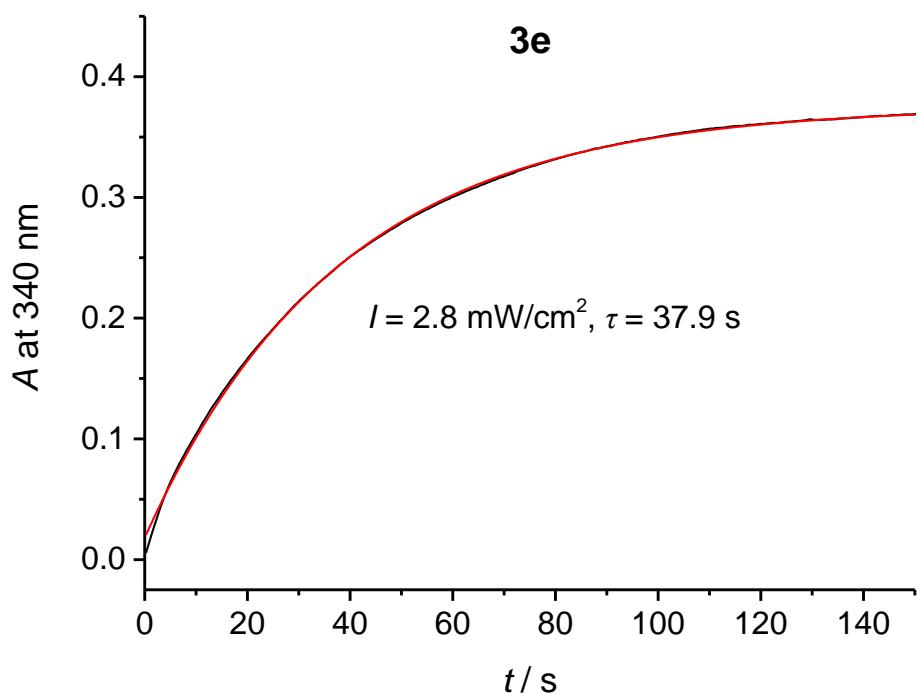
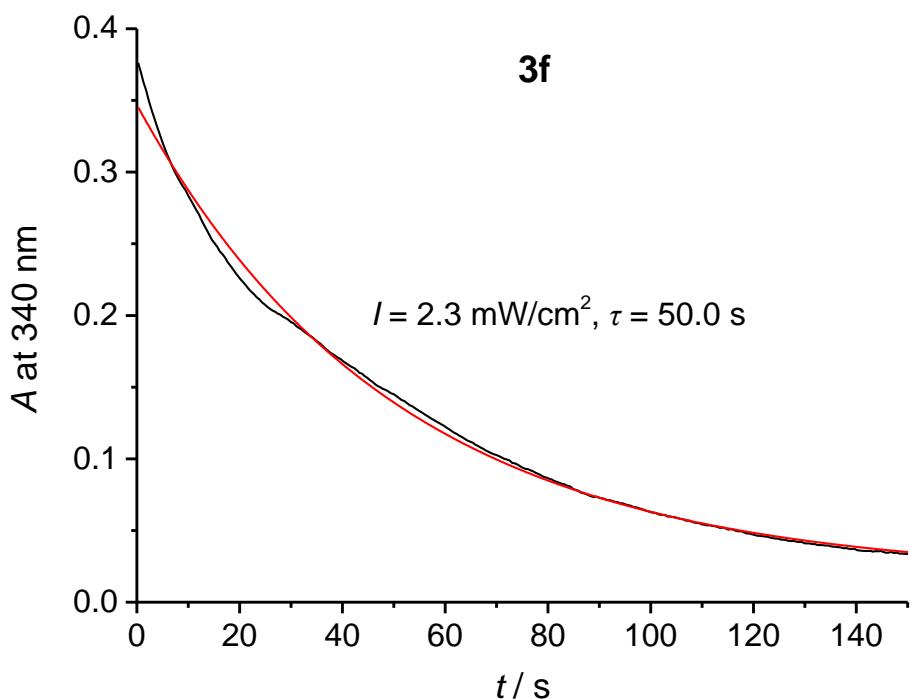


Figure S31. Isomerization kinetics of **3e** in aqueous solution with 50% DMSO. Sample exposed to 365 nm irradiation (top), and subsequently to 460 nm irradiation (bottom) while the absorption changes were monitored at 340 nm. Black lines are the experimental data, red lines are the fitting to mono-exponential kinetics.



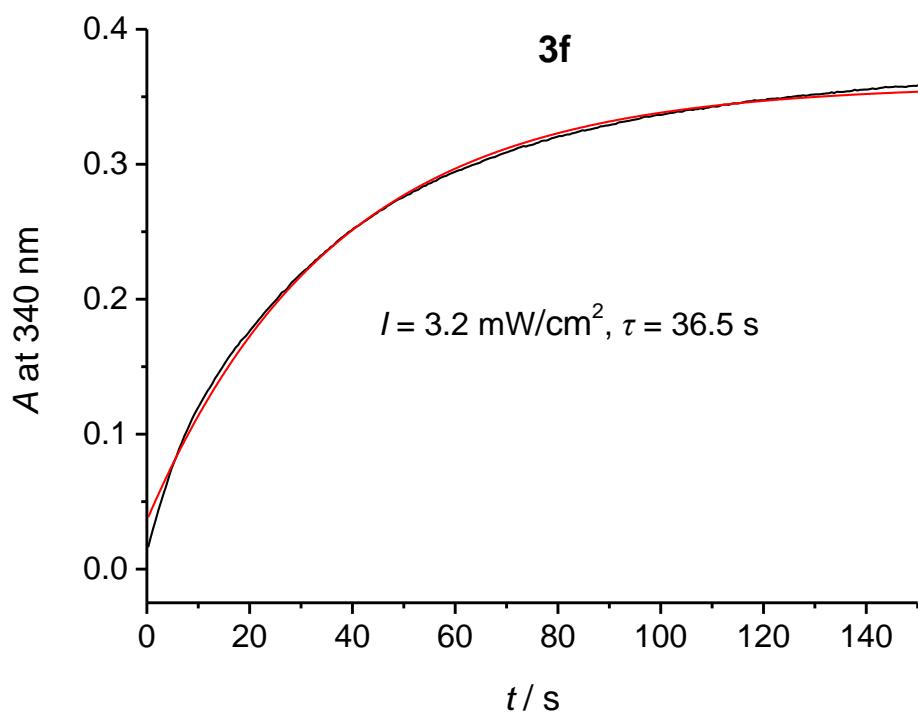
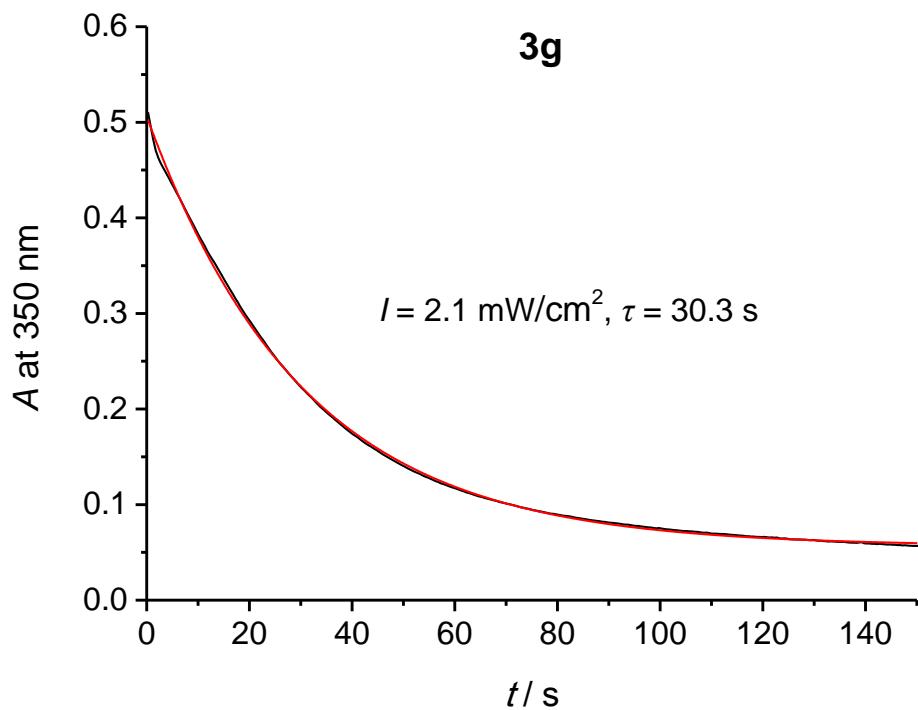


Figure S32. Isomerization kinetics of **3f** in aqueous solution with 50% DMSO. Sample exposed to 365 nm irradiation (top), and subsequently to 460 nm irradiation (bottom) while the absorption changes were monitored at 340 nm. Black lines are the experimental data, red lines are the fitting to mono-exponential kinetics.



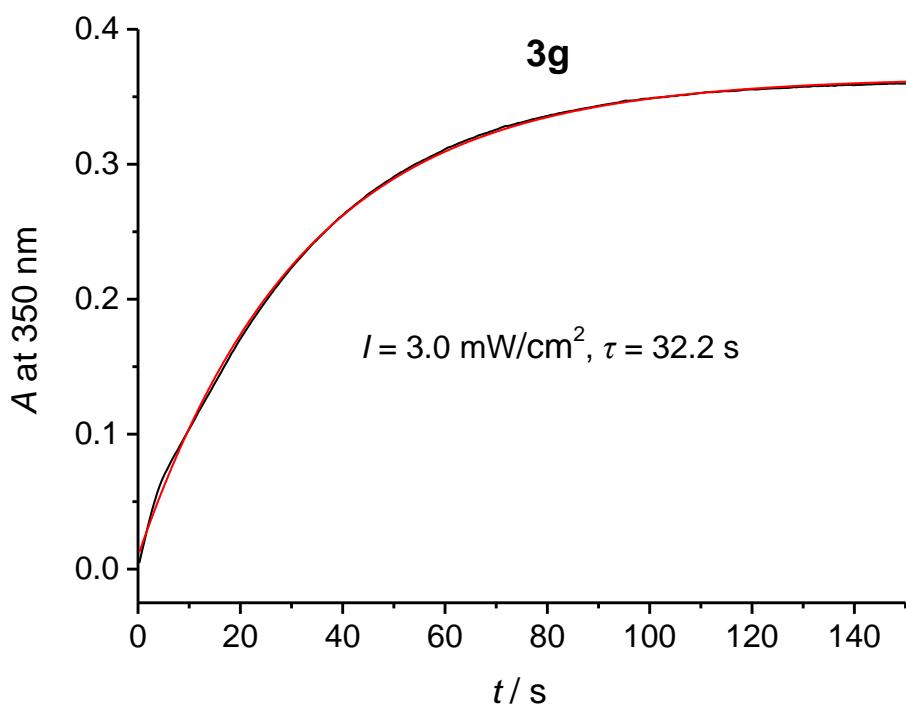
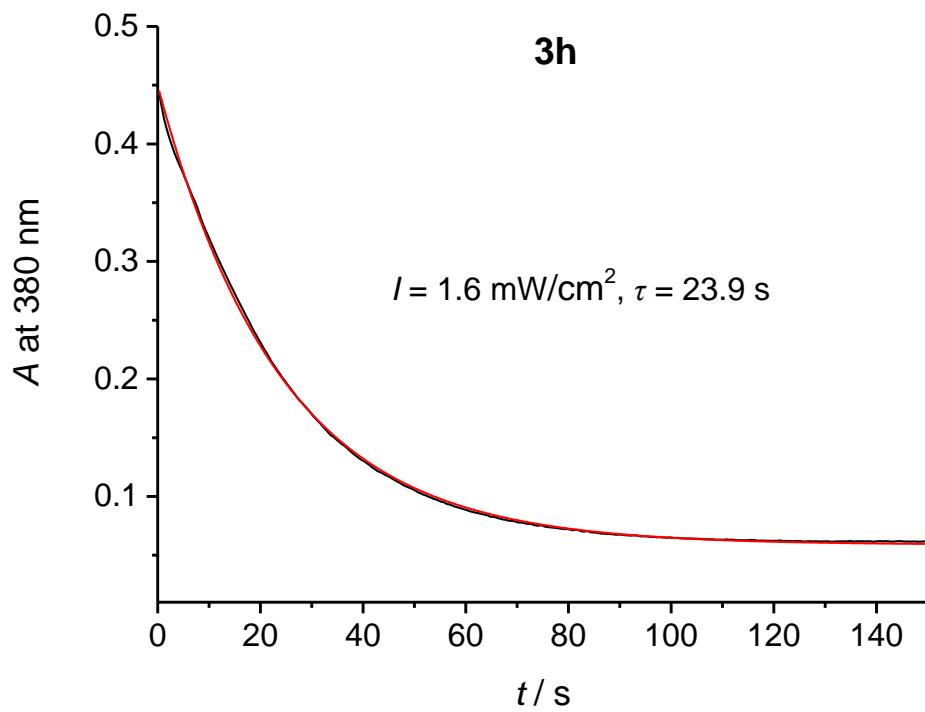


Figure S33. Isomerization kinetics of **3g** in 100% DMSO. Sample exposed to 365 nm irradiation (top), and subsequently to 460 nm irradiation (bottom) while the absorption changes were monitored at 350 nm. Black lines are the experimental data, red lines are the fitting to mono-exponential kinetics.



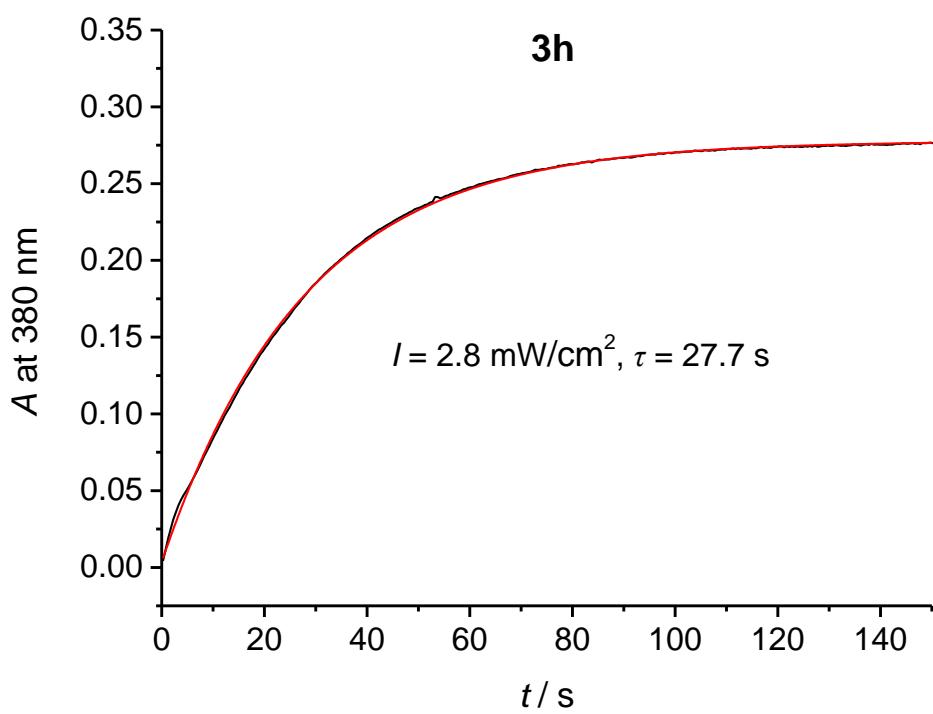
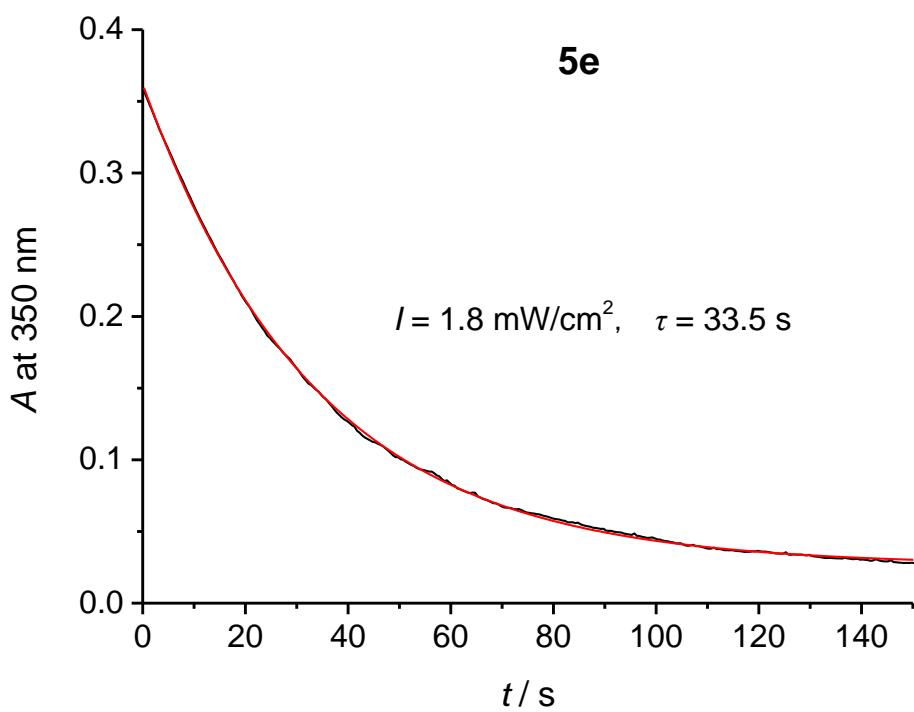


Figure S34. Isomerization kinetics of **3h** in aqueous solution with 20% DMSO. Sample exposed to 365 nm irradiation (top), and subsequently to 460 nm irradiation (bottom) while the absorption changes were monitored at 380 nm. Black lines are the experimental data, red lines are the fitting to mono-exponential kinetics.



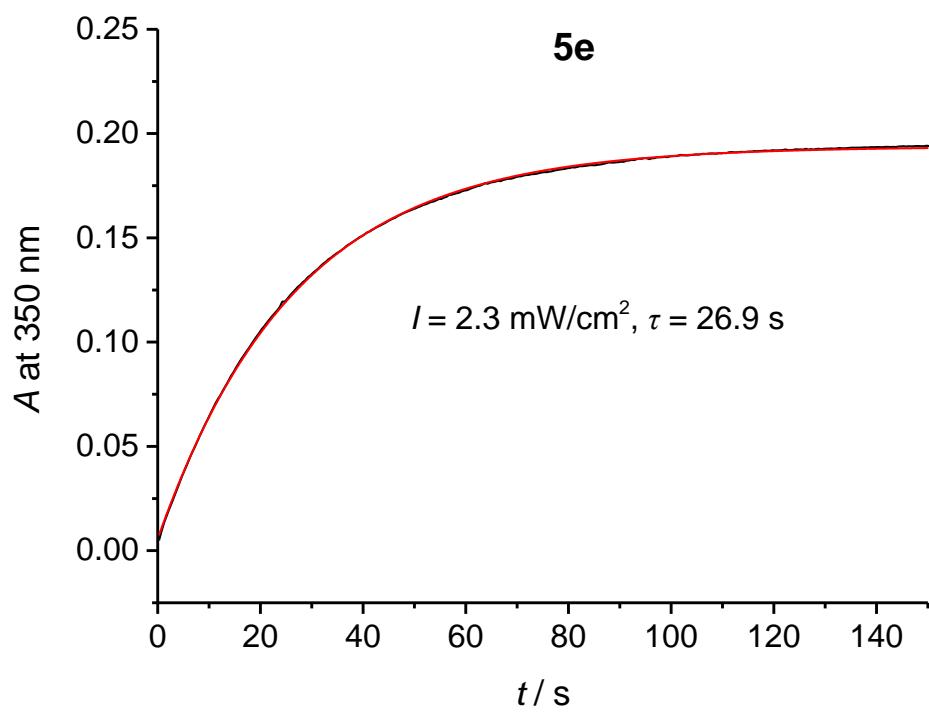
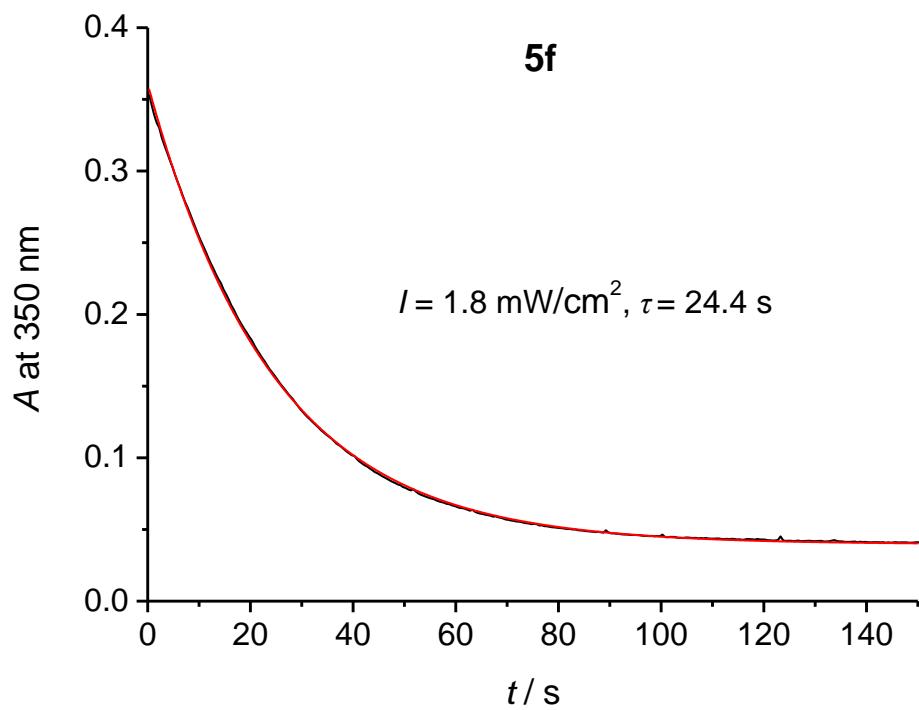


Figure S35. Isomerization kinetics of **5e** in aqueous solution with 5% DMSO. Sample exposed to 365 nm irradiation (top), and subsequently to 460 nm irradiation (bottom) while the absorption changes were monitored at 350 nm. Black lines are the experimental data, red lines are the fitting to mono-exponential kinetics.



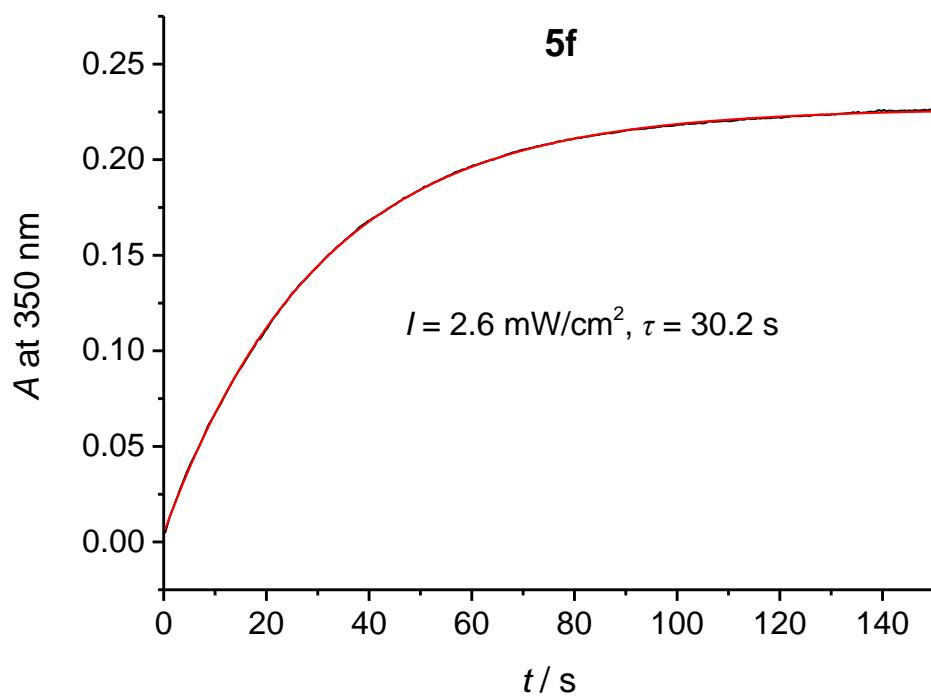
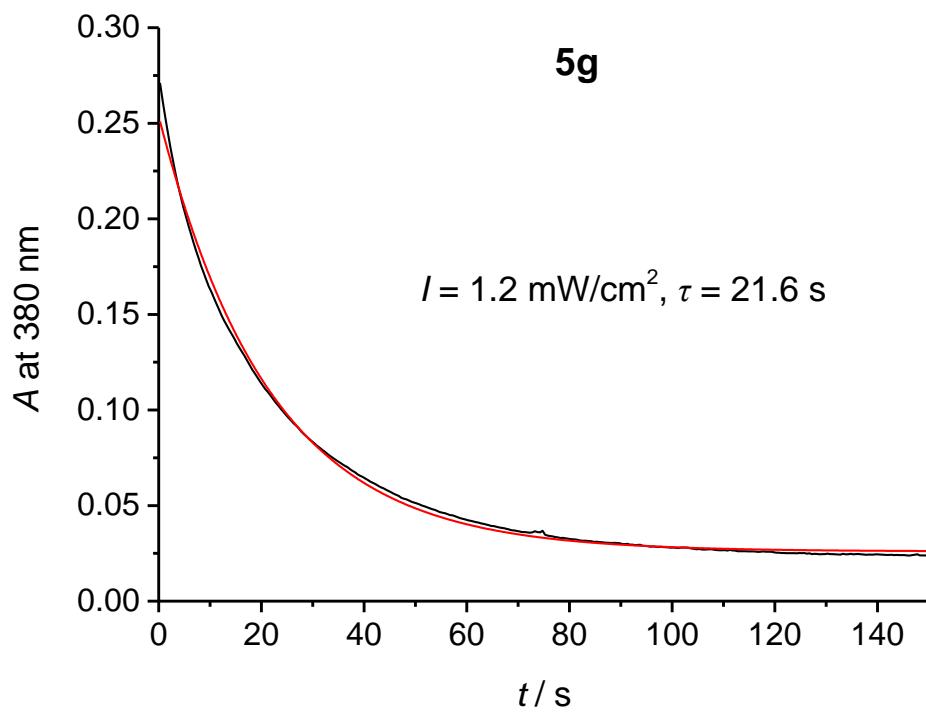


Figure S36. Isomerization kinetics of **5f** in aqueous solution with 7.5% DMSO. Sample exposed to 365 nm irradiation (top), and subsequently to 460 nm irradiation (bottom) while the absorption changes were monitored at 350 nm. Black lines are the experimental data, red lines are the fitting to mono-exponential kinetics.



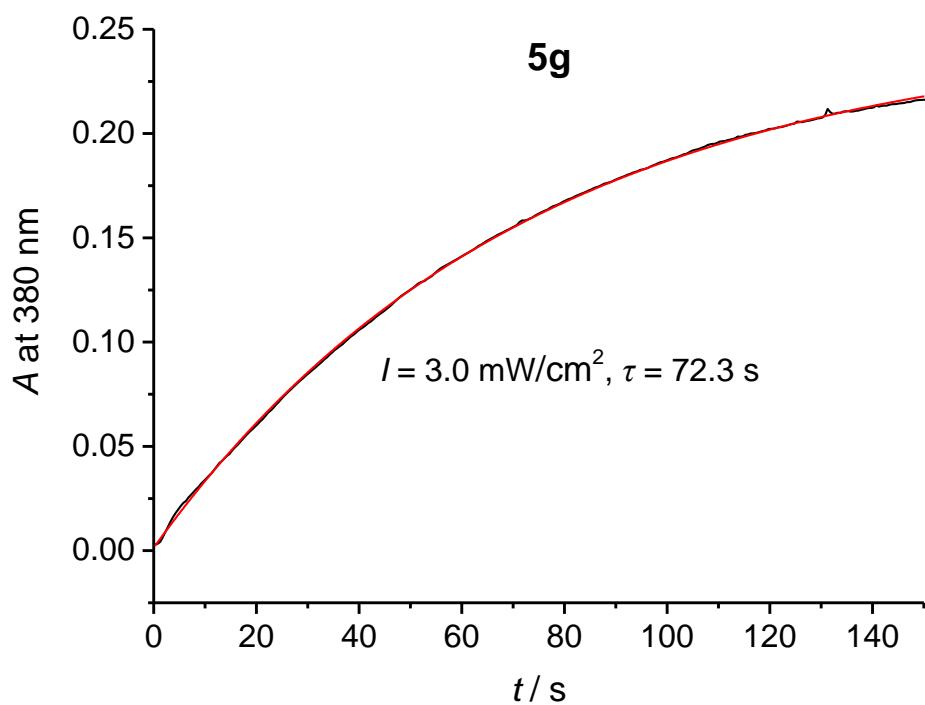
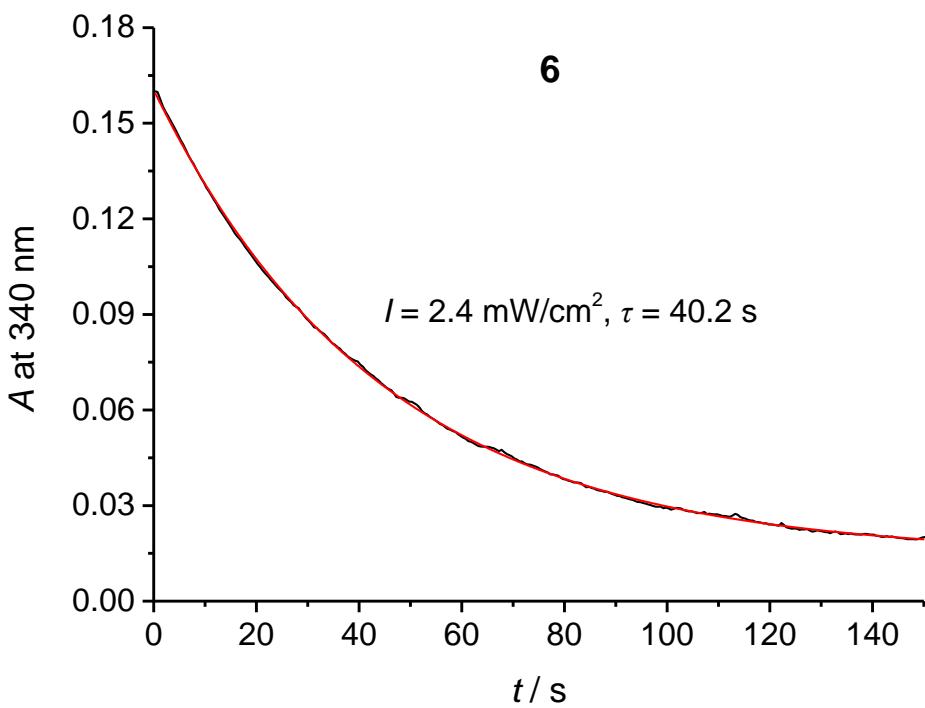


Figure S37. Isomerization kinetics of **5g** in aqueous solution with 33.3% DMSO. Sample exposed to 405 nm irradiation (top), and subsequently to 523 nm irradiation (bottom) while the absorption changes were monitored at 380 nm. Black lines are the experimental data, red lines are the fitting to mono-exponential kinetics.



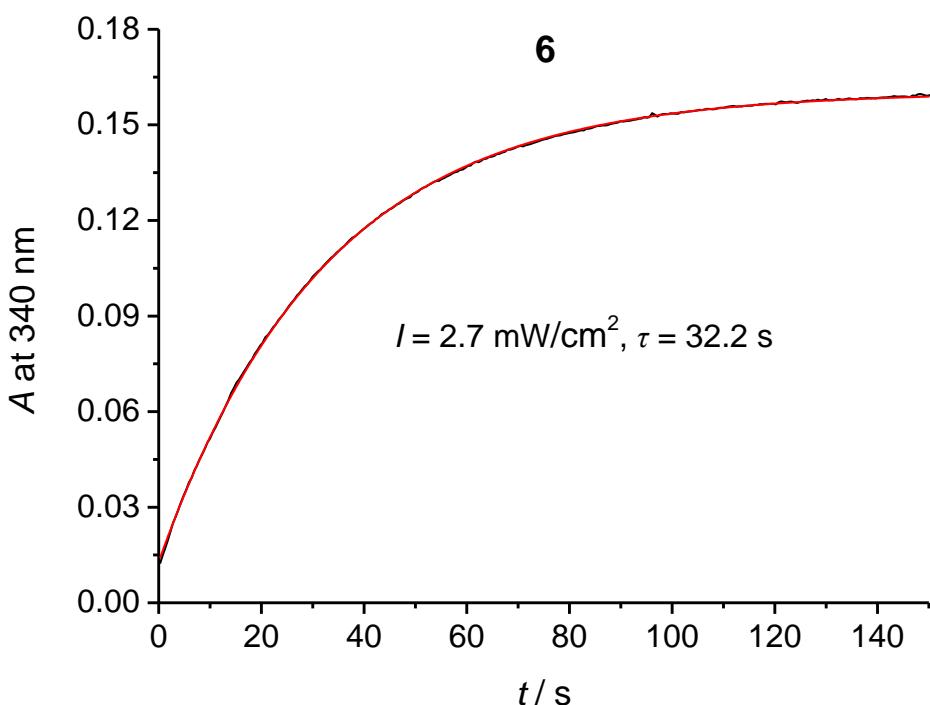
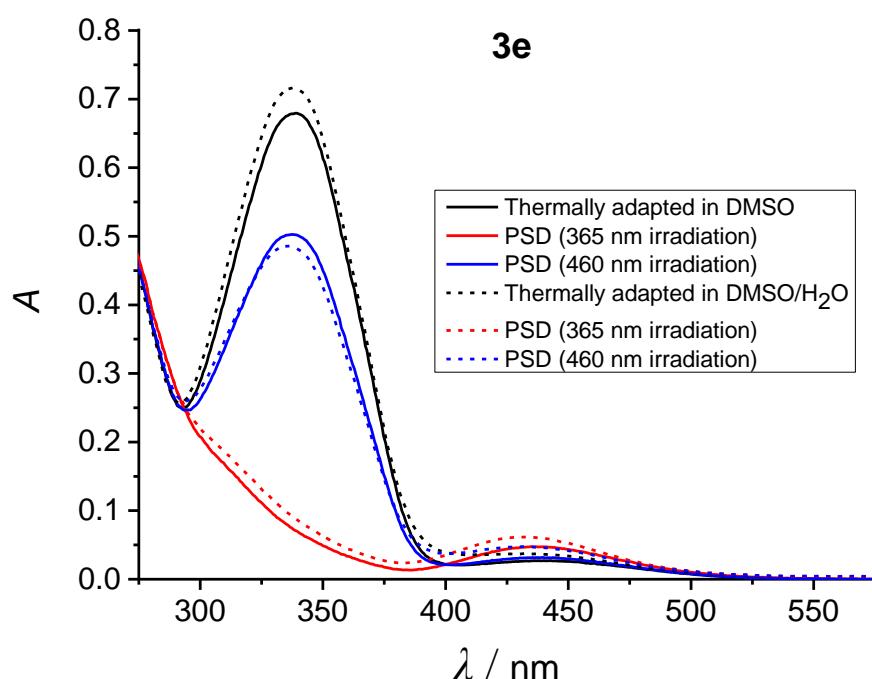


Figure S38. Isomerization kinetics of **6** in aqueous solution with 1% DMSO. Sample exposed to 365 nm irradiation (top), and subsequently to 460 nm irradiation (bottom) while the absorption changes were monitored at 340 nm. Black lines are the experimental data, red lines are the fitting to mono-exponential kinetics.

3.4. Determination of PSD



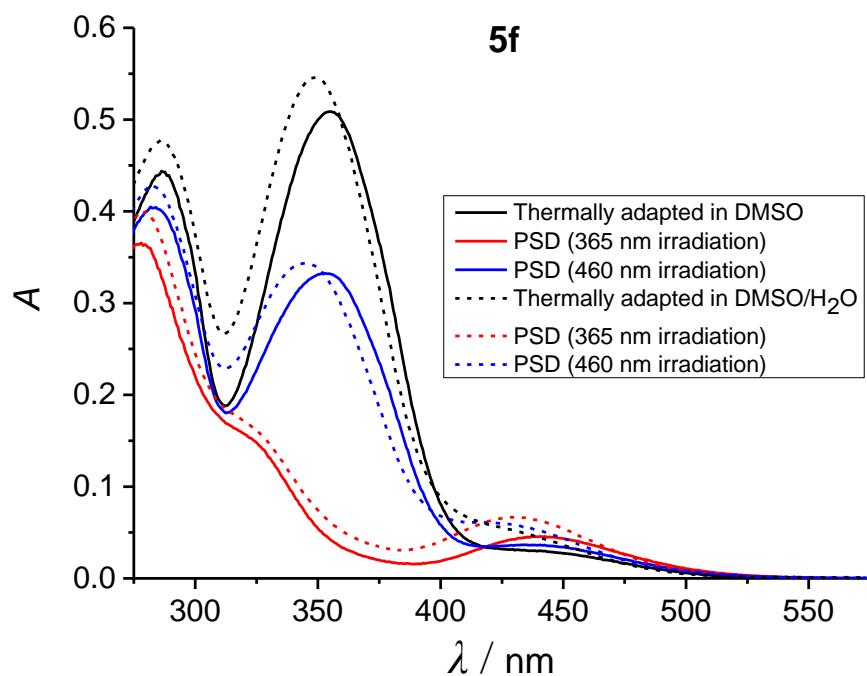
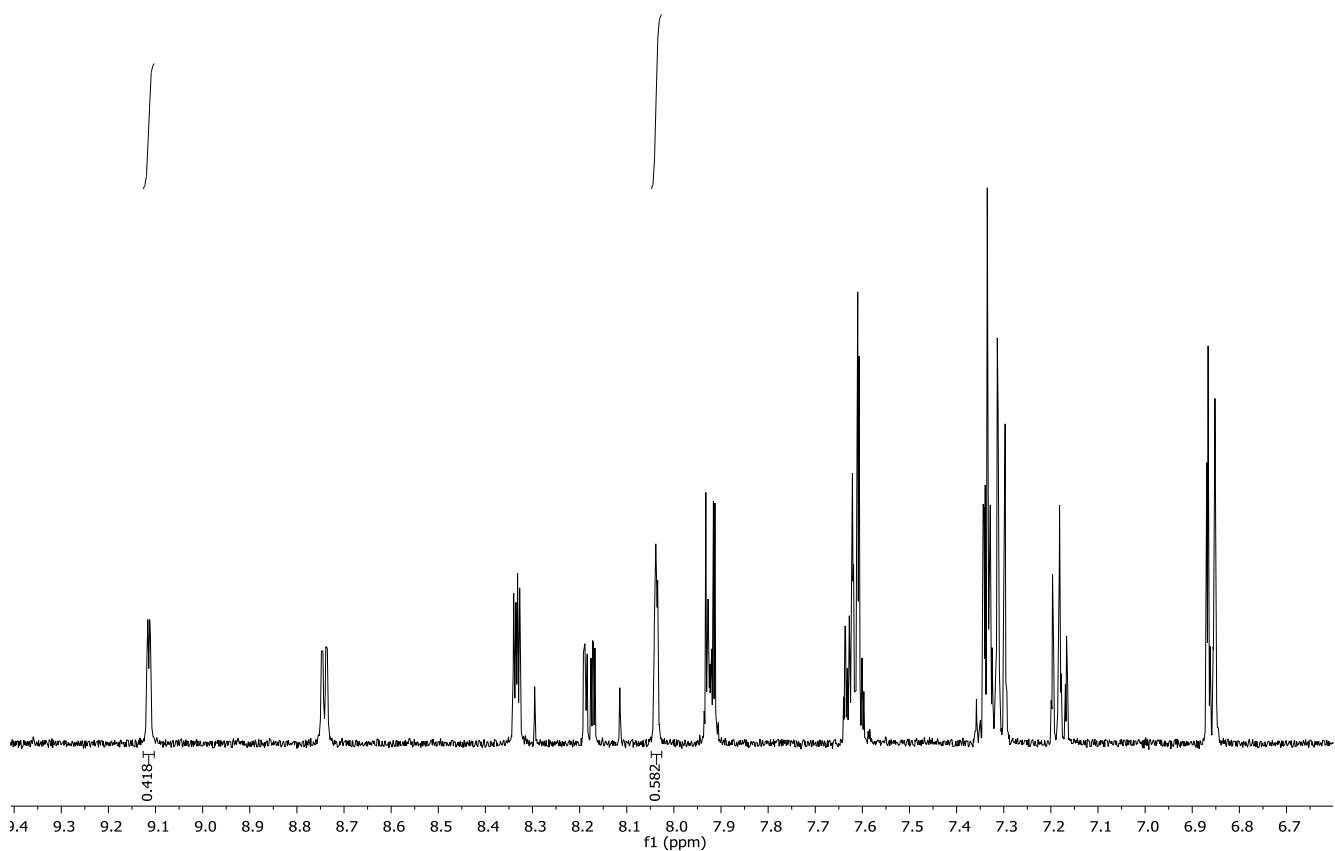
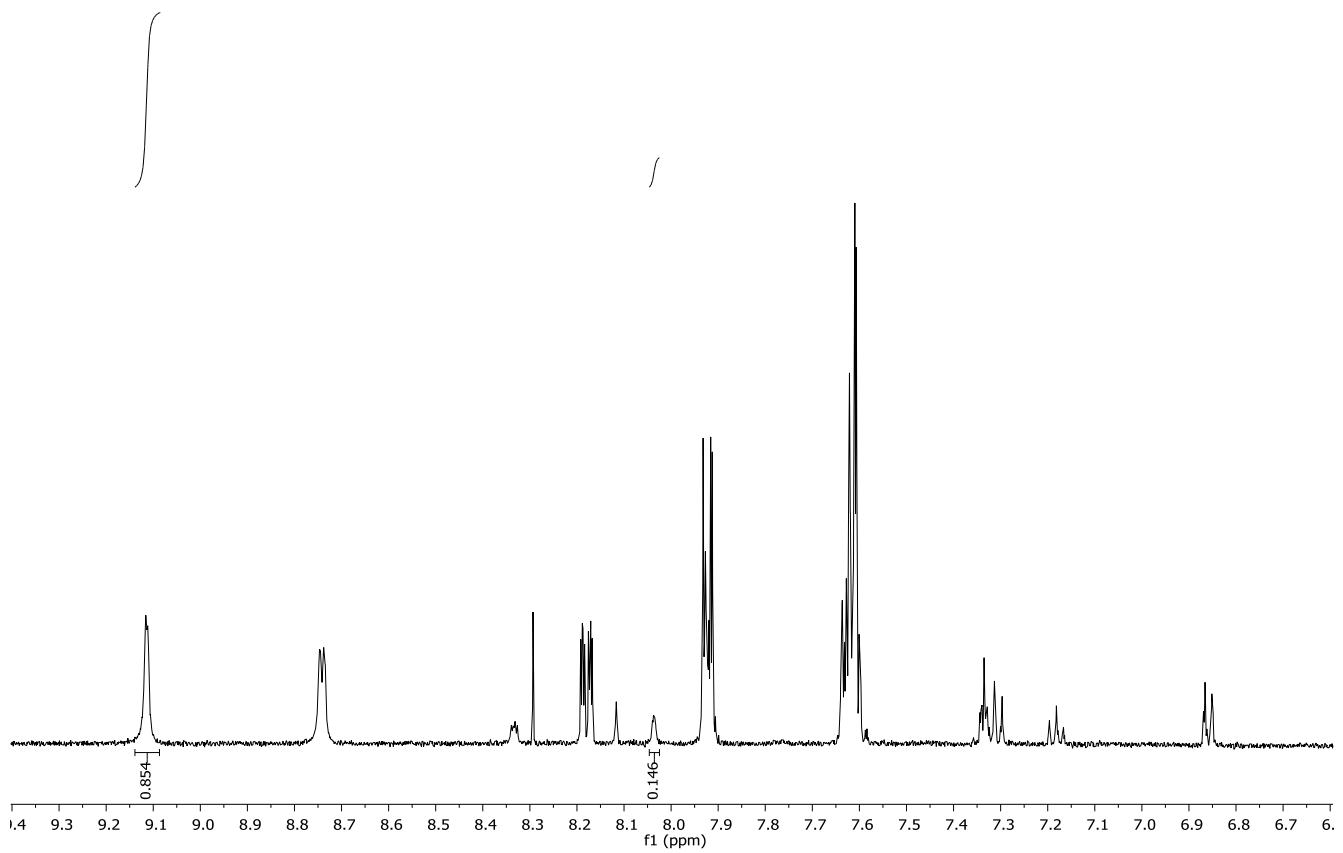


Figure S39. Photostationary distributions (PSD) were determined by ¹H-NMR spectroscopy (500 MHz) in DMSO-d₆ solution. In order to compare the PSD in DMSO-d₆ and in aqueous solution, the absorption spectra at the respective PSD were recorded in both solvent systems and compared (at the same concentration). Above are the results for two typical samples. Solid lines: UV-Vis absorption spectra in DMSO solution. Dashed lines: UV-Vis absorption spectra in aqueous solution. Black lines: After thermal adaption (at 50 °C for 72 h). Red lines: After exposure to 365 nm UV to yield the PSD. Blue lines: After exposure to 460 nm light to yield the PSD.

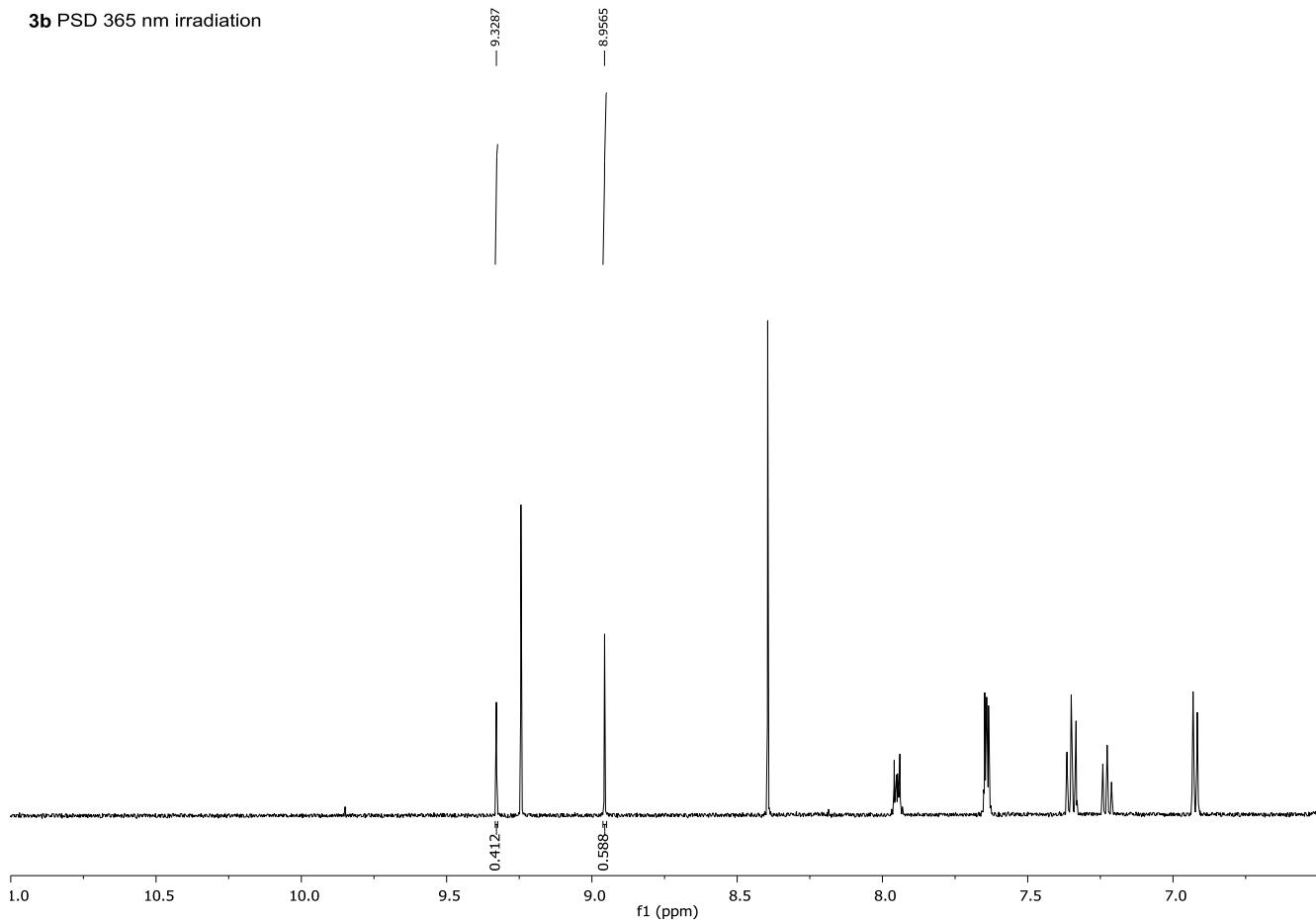
3a PSD 365 nm irradiation



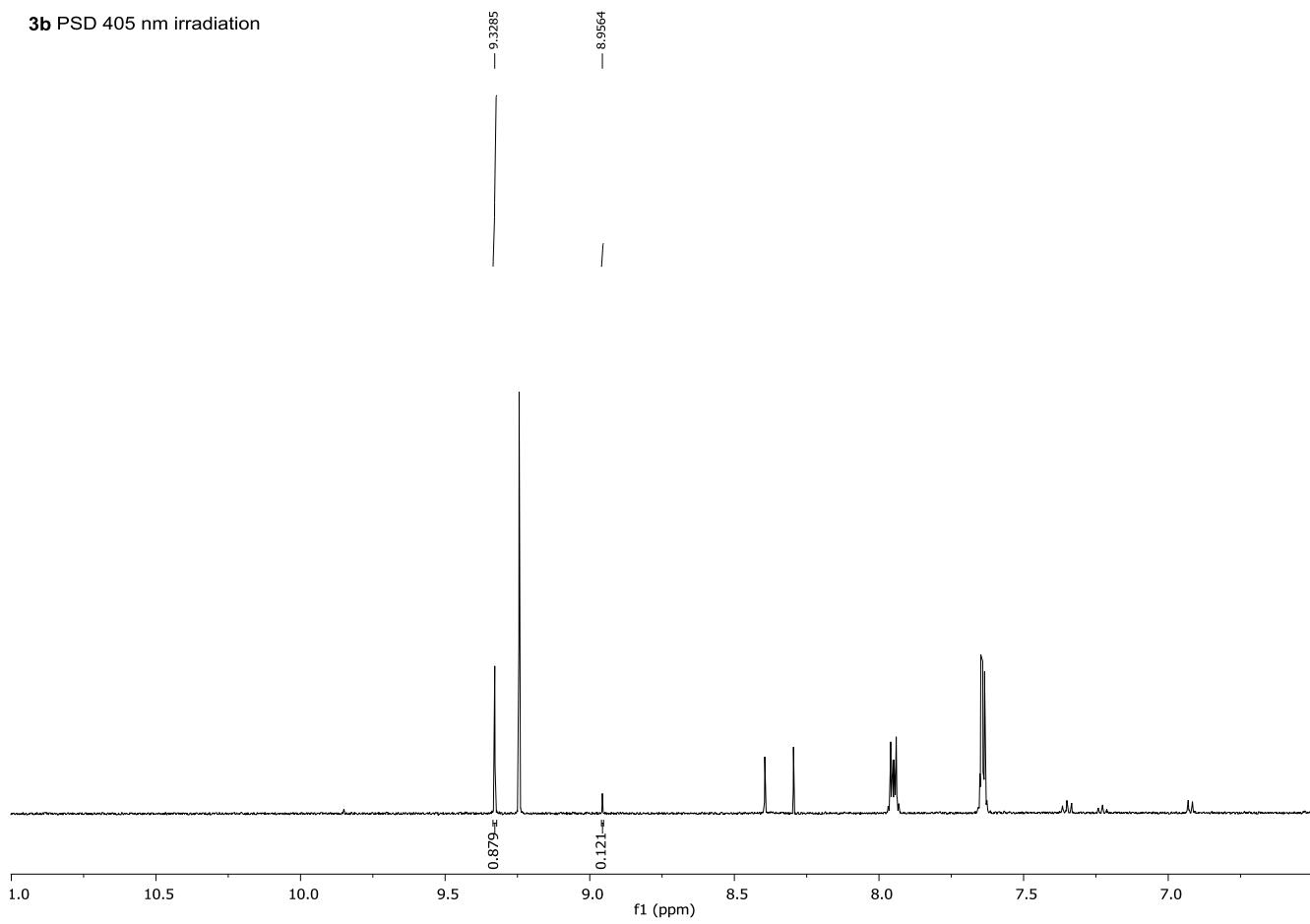
3a PSD 405 nm irradiation



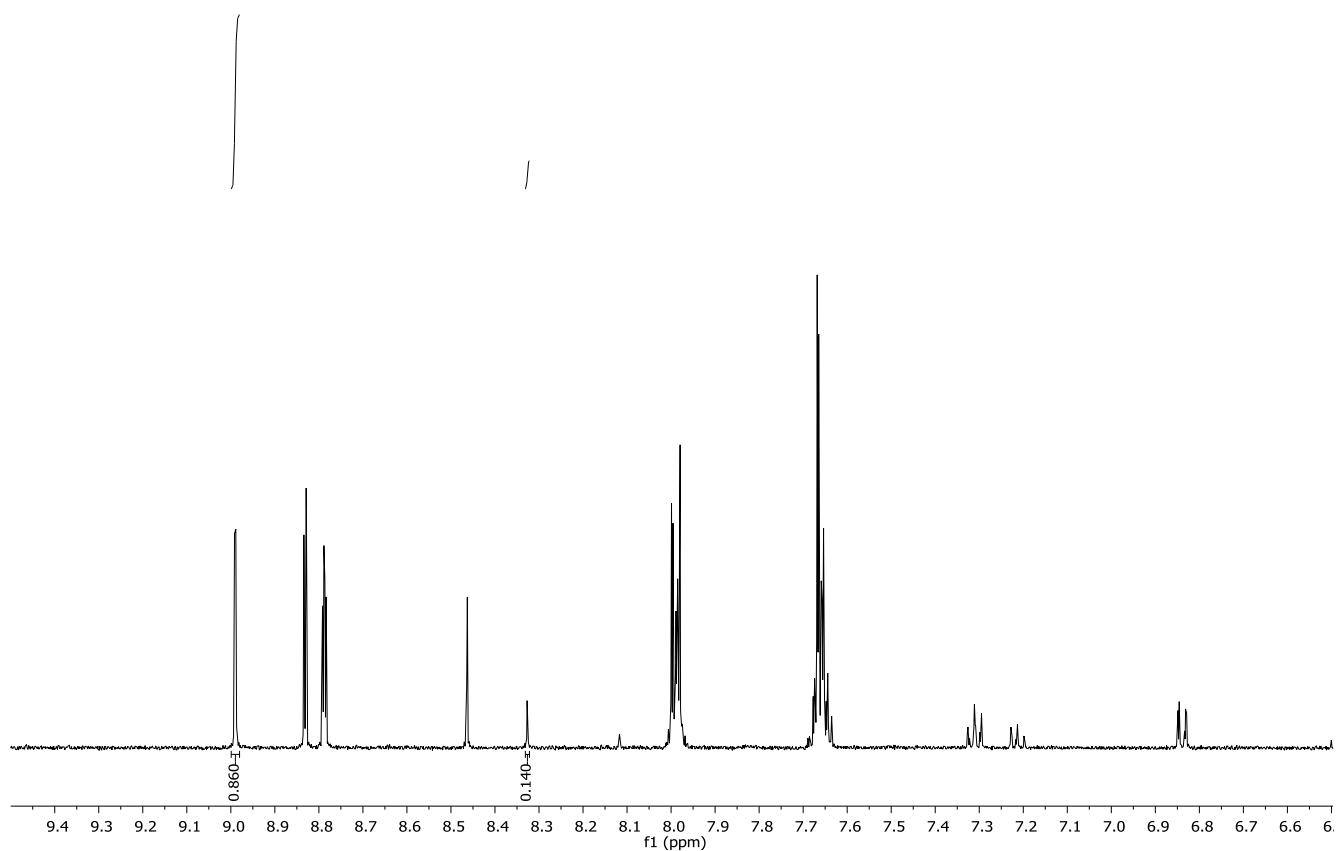
3b PSD 365 nm irradiation



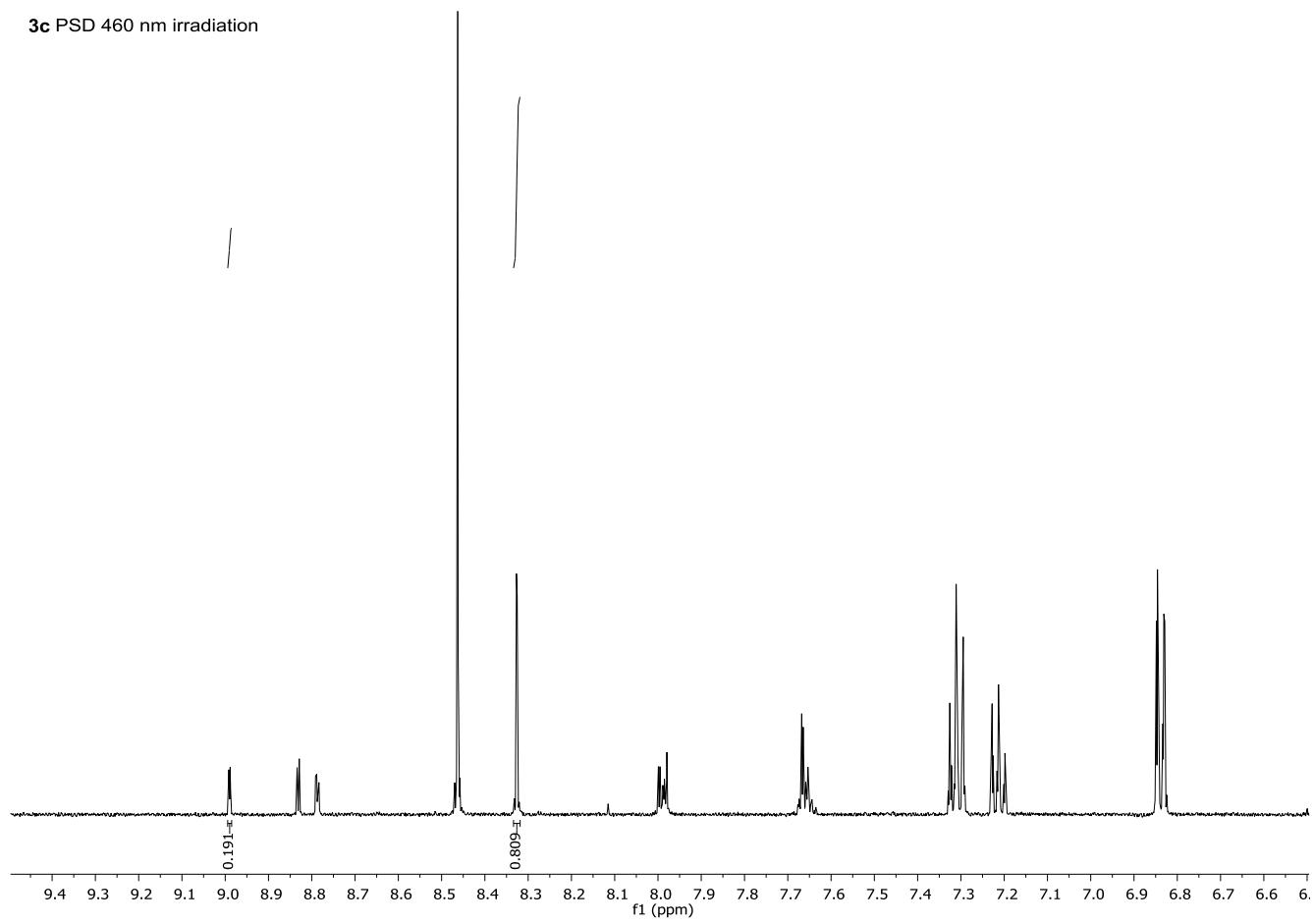
3b PSD 405 nm irradiation



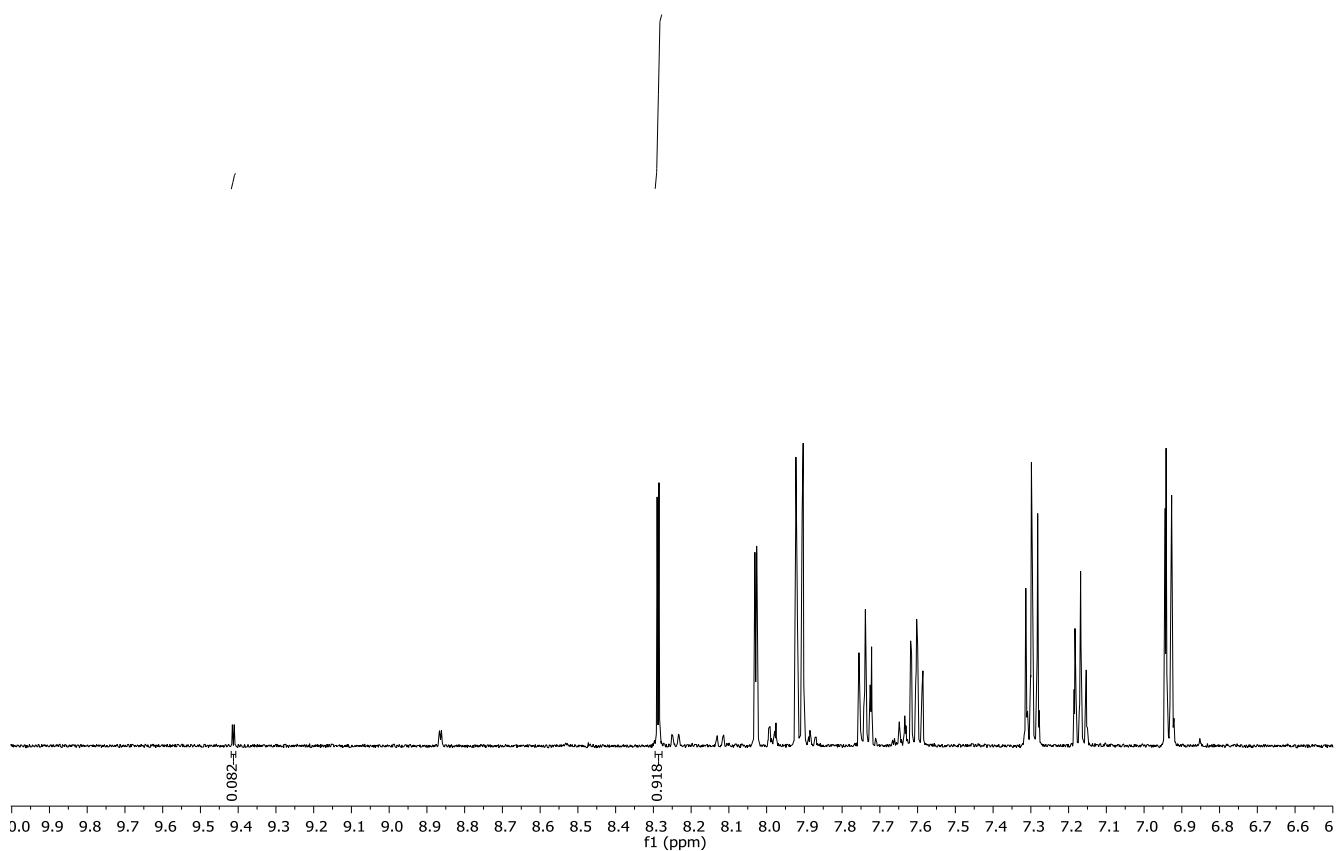
3c PSD 365 nm irradiation



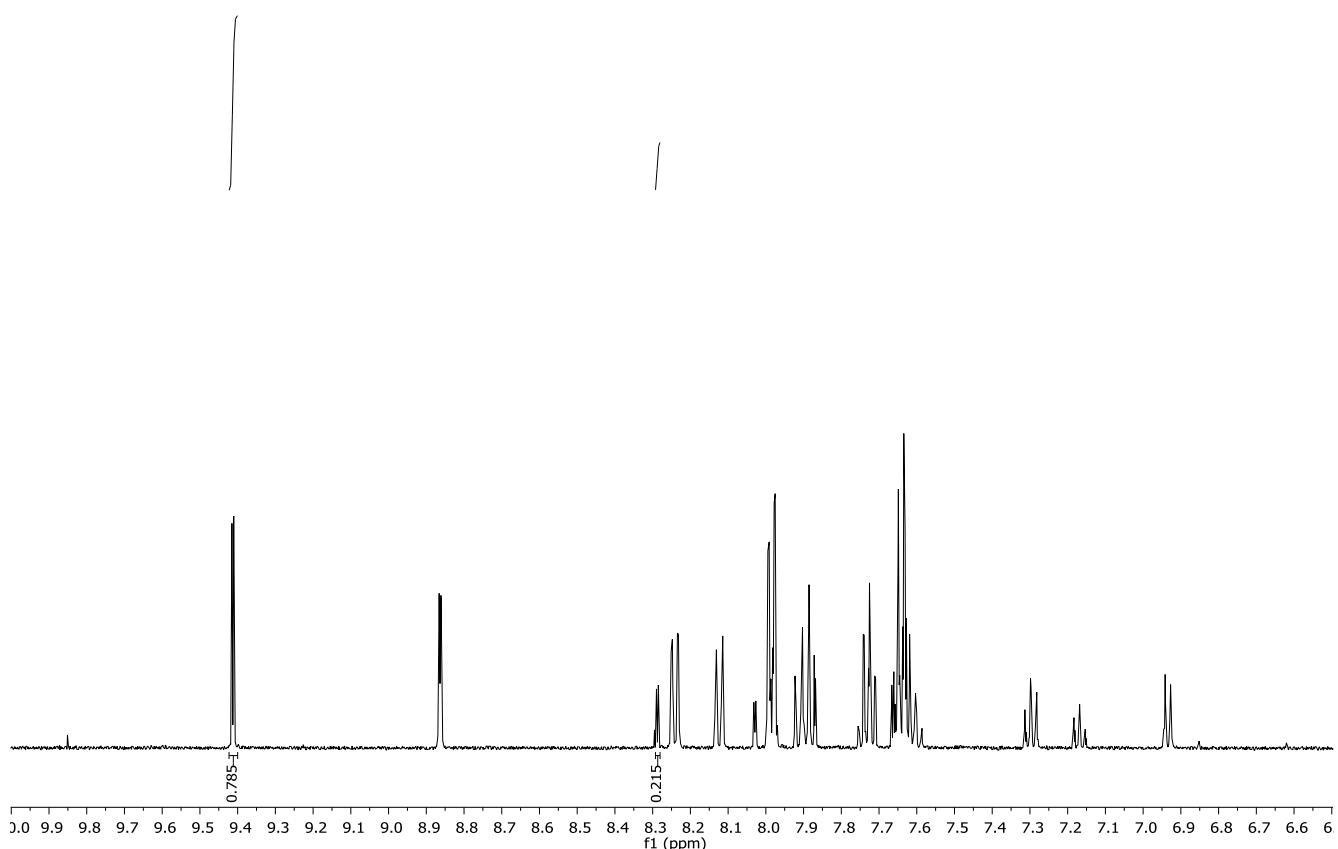
3c PSD 460 nm irradiation



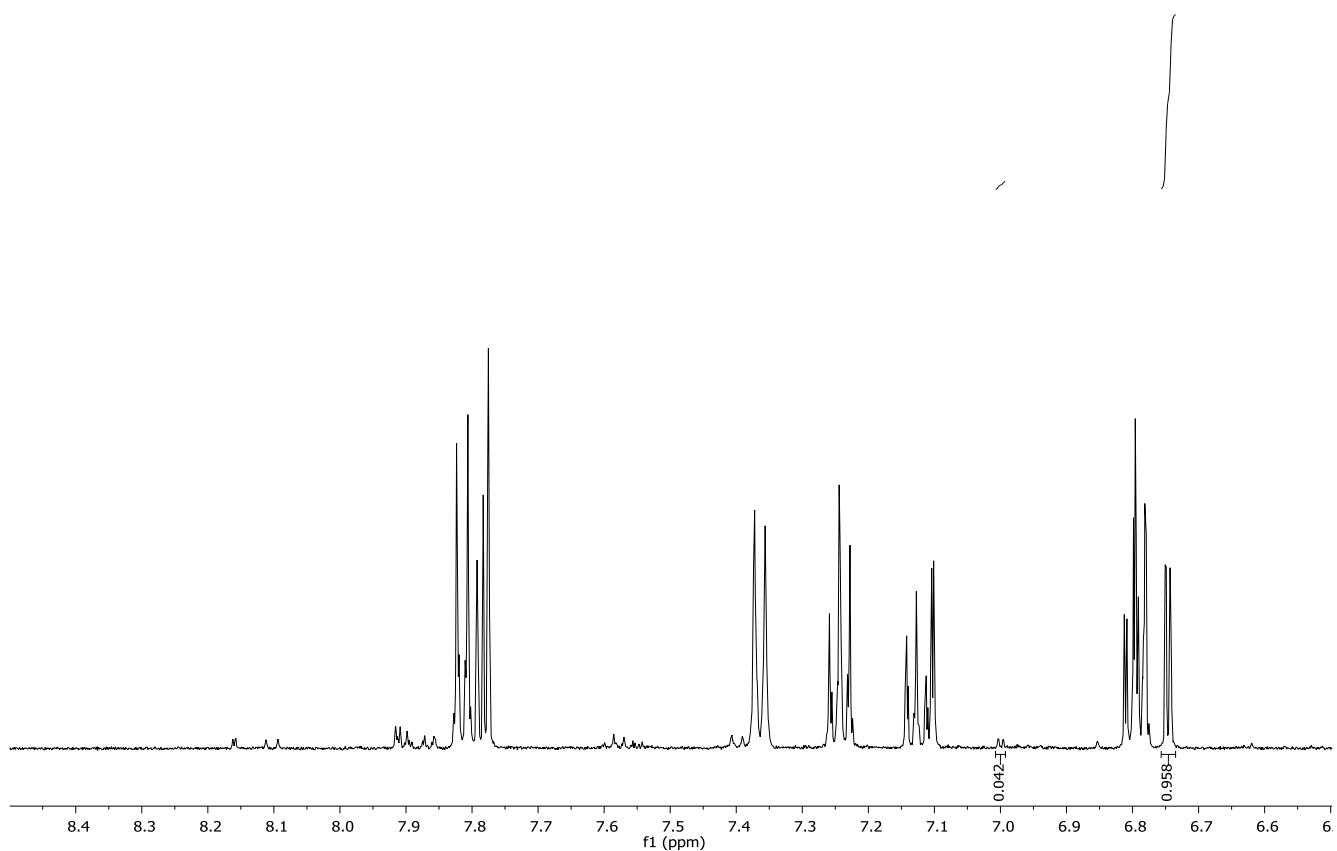
3d PSD 365 nm irradiation



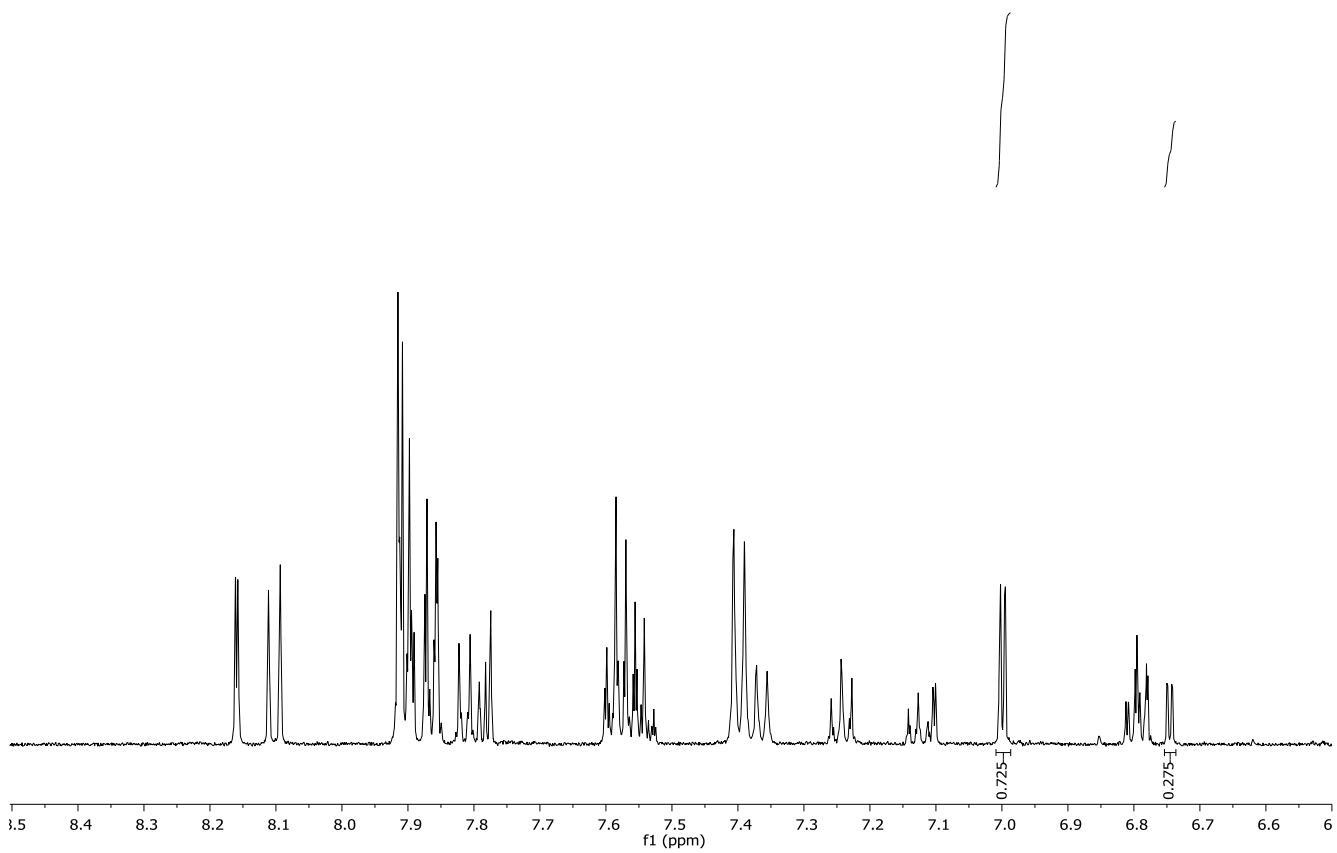
3d PSD 460 nm irradiation



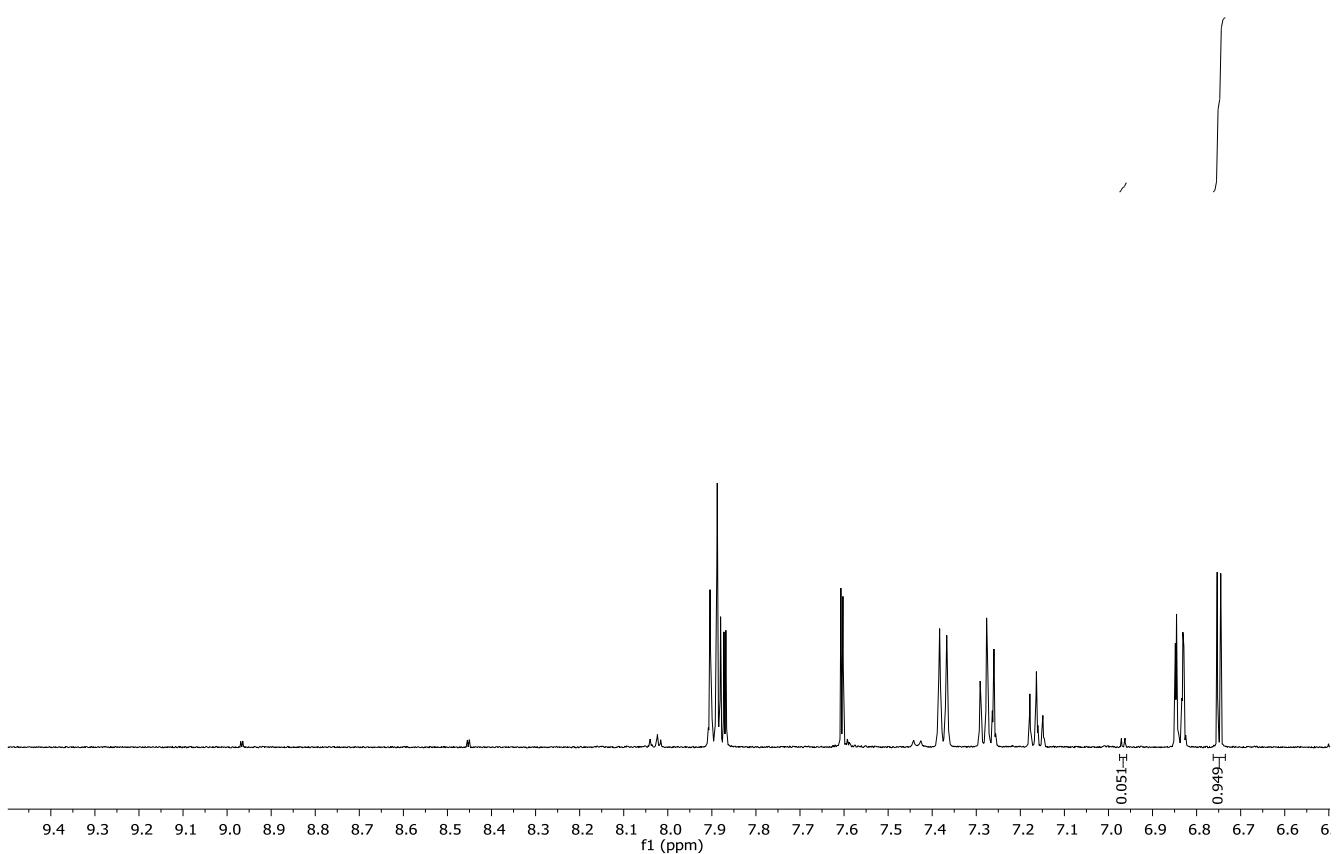
3e PSD 365 nm irradiation



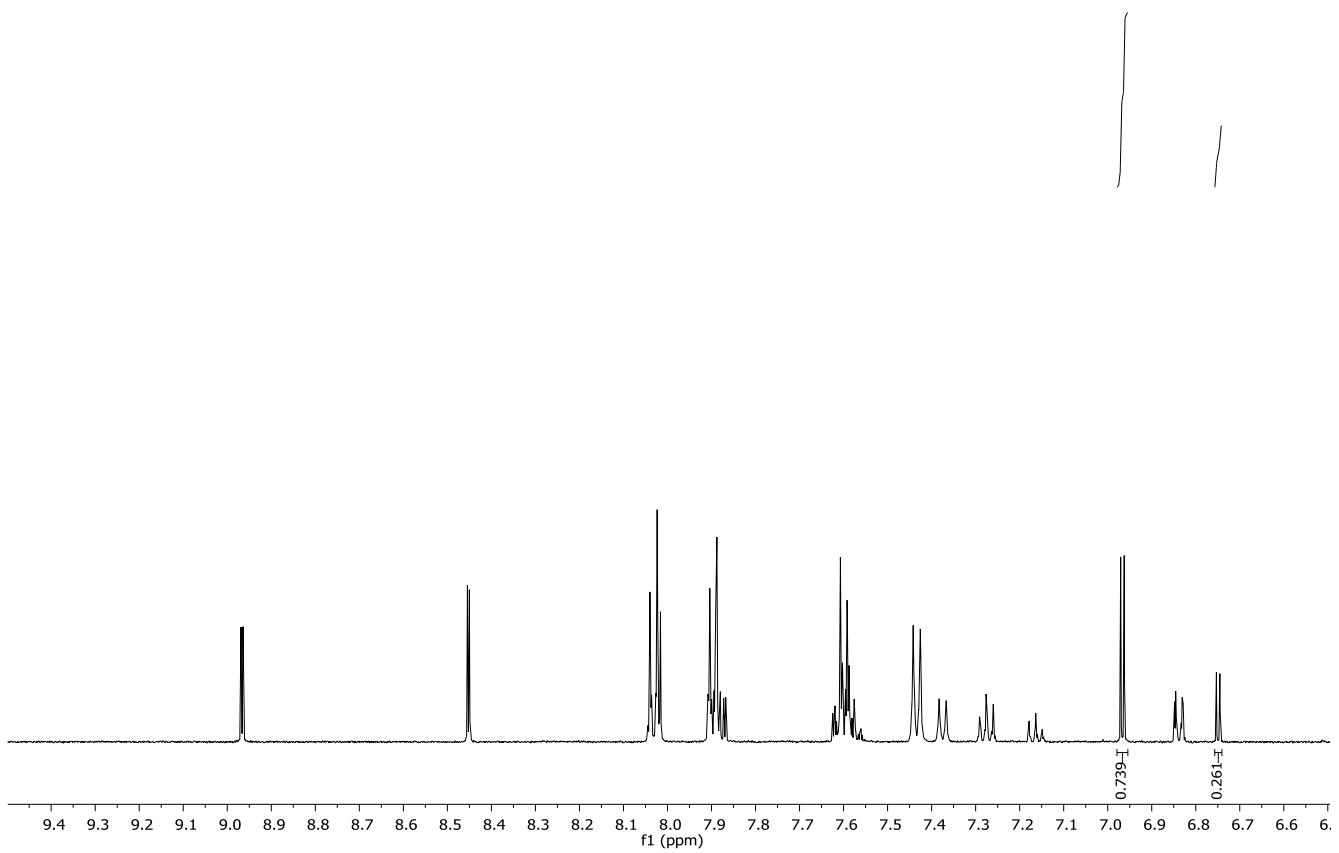
3e PSD 460 nm irradiation



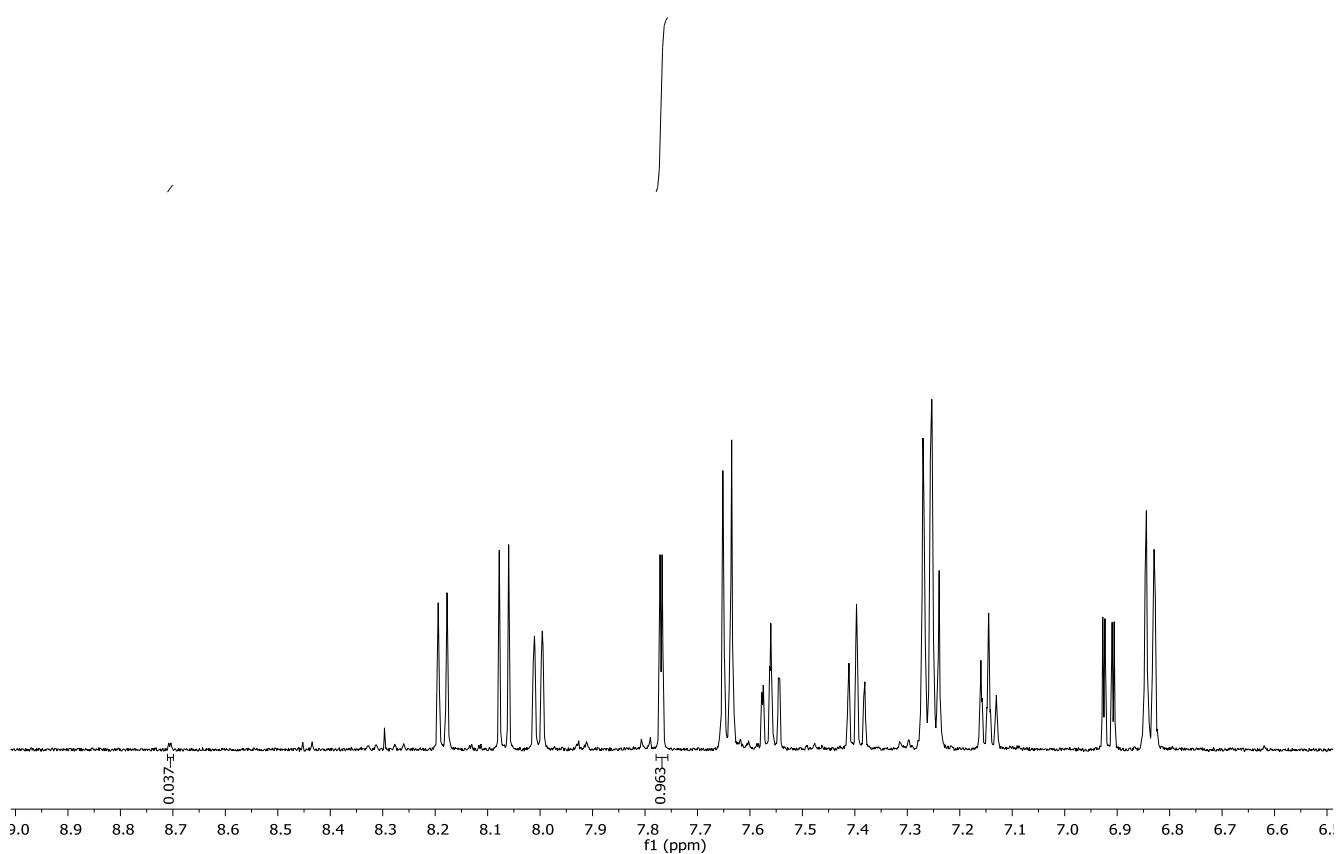
3f PSD 365 nm irradiation



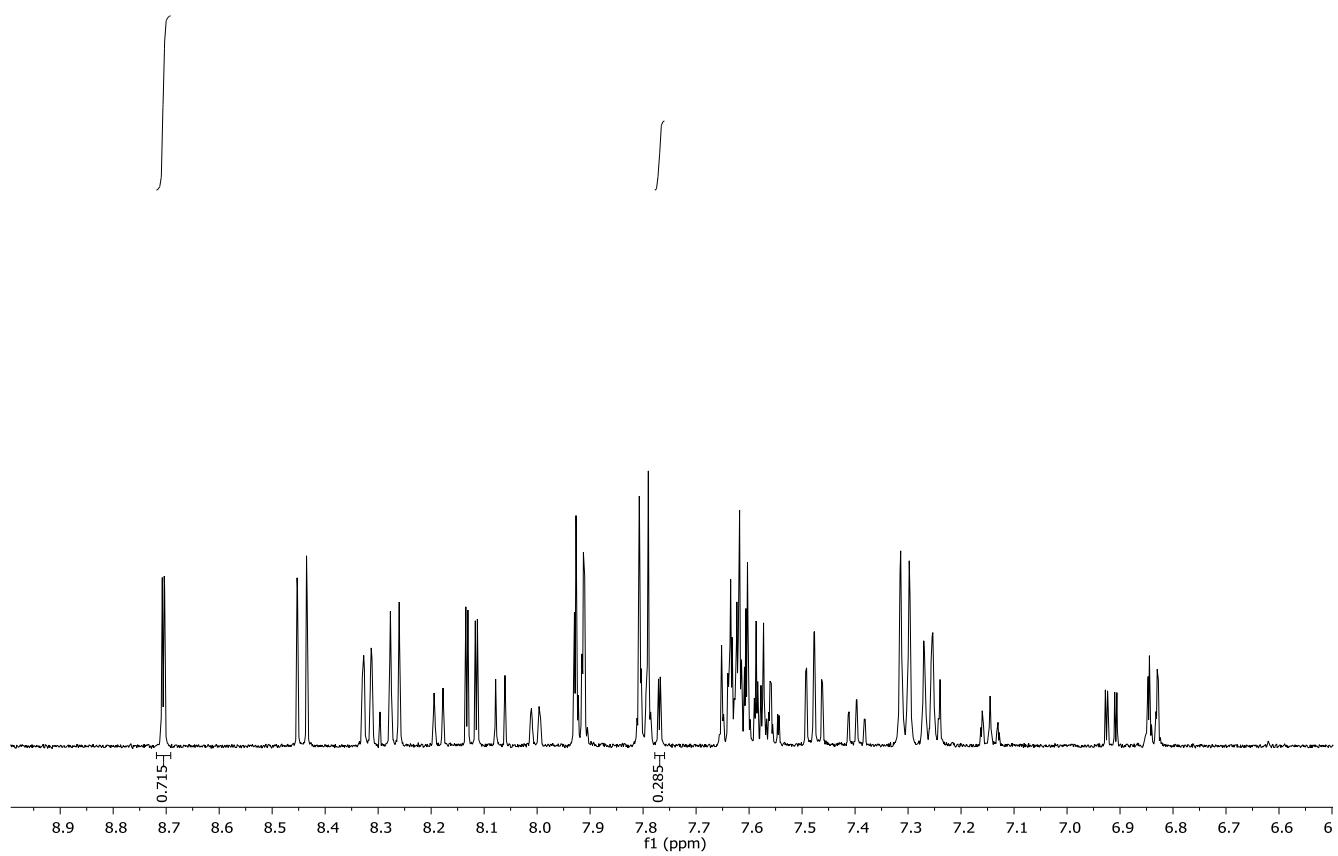
3f PSD 460 nm irradiation



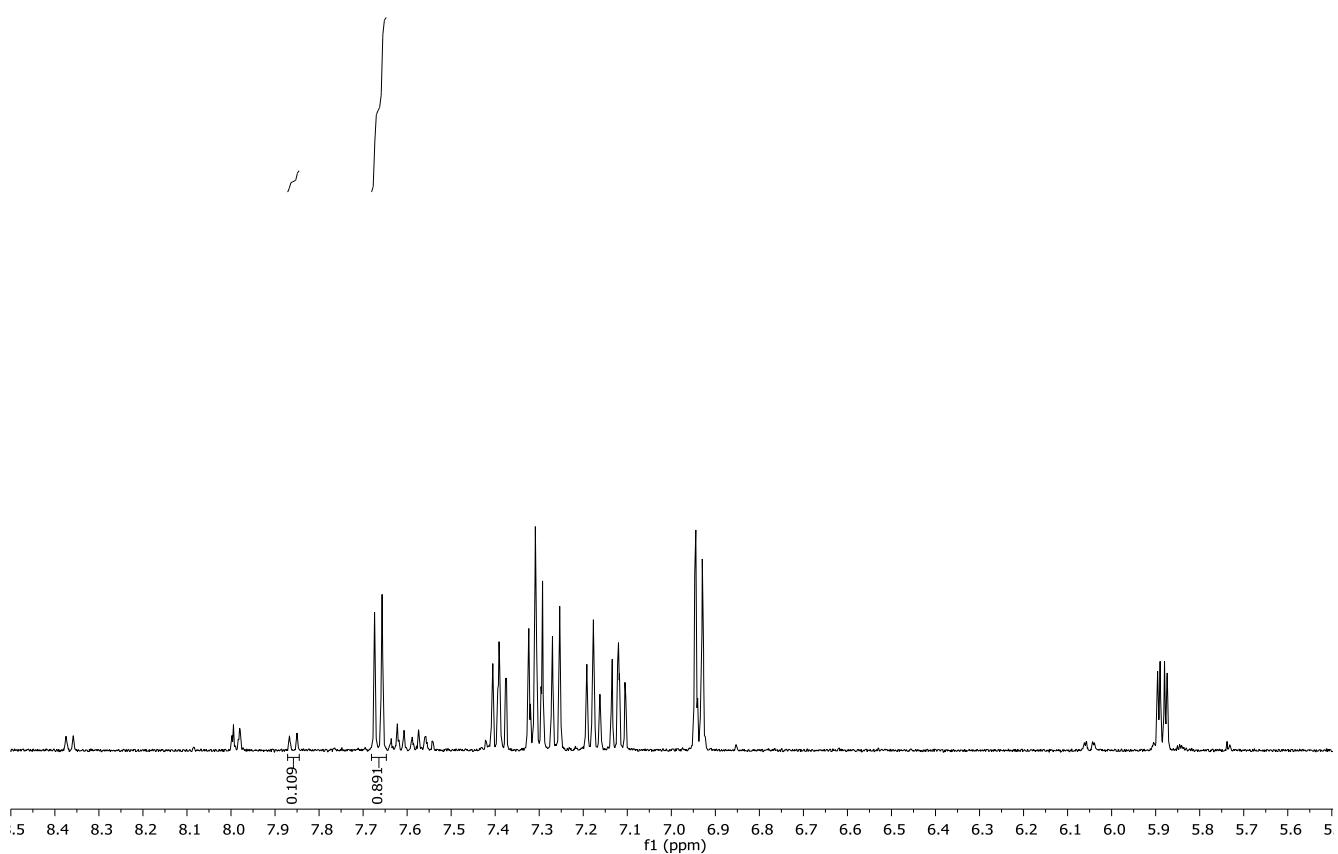
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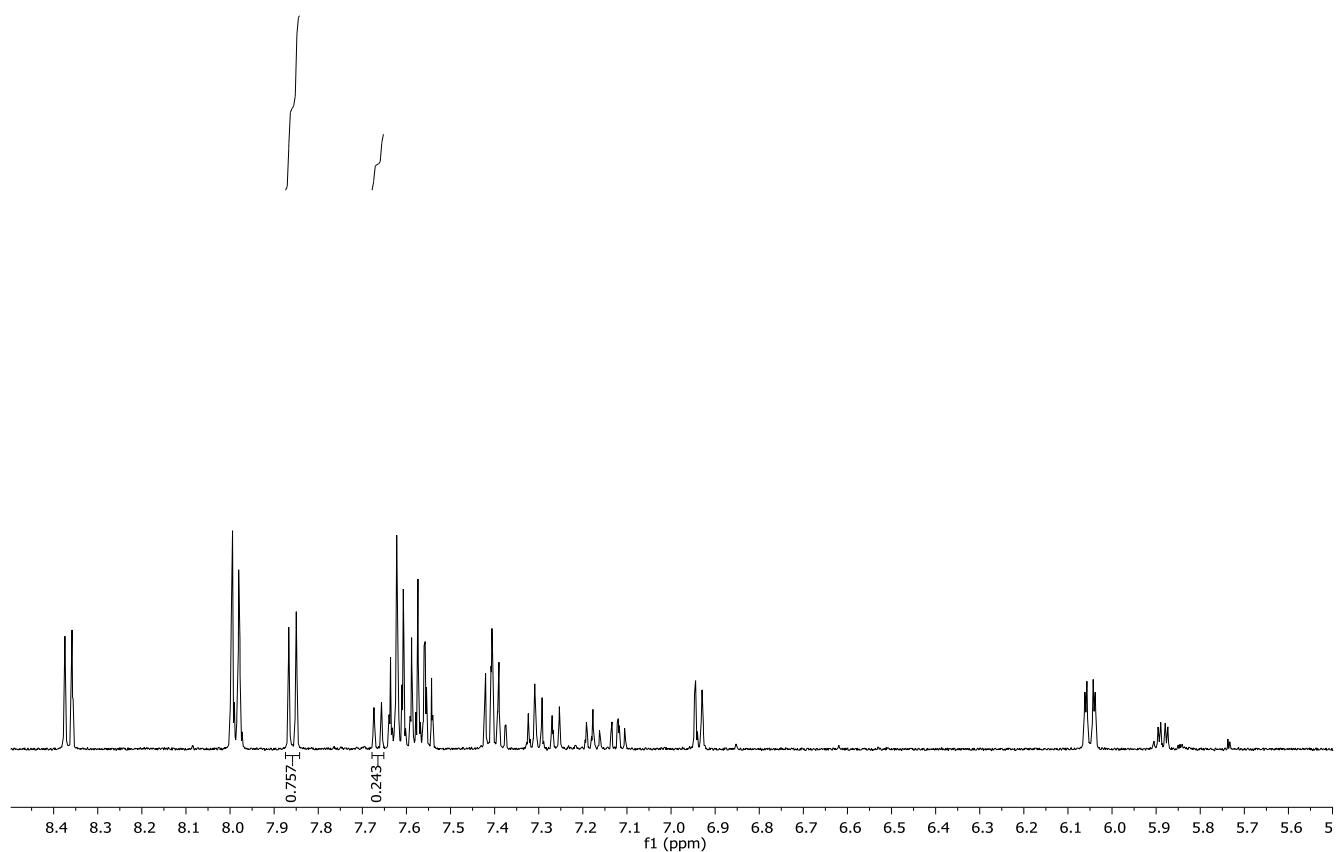
3g PSD 460 nm irradiation



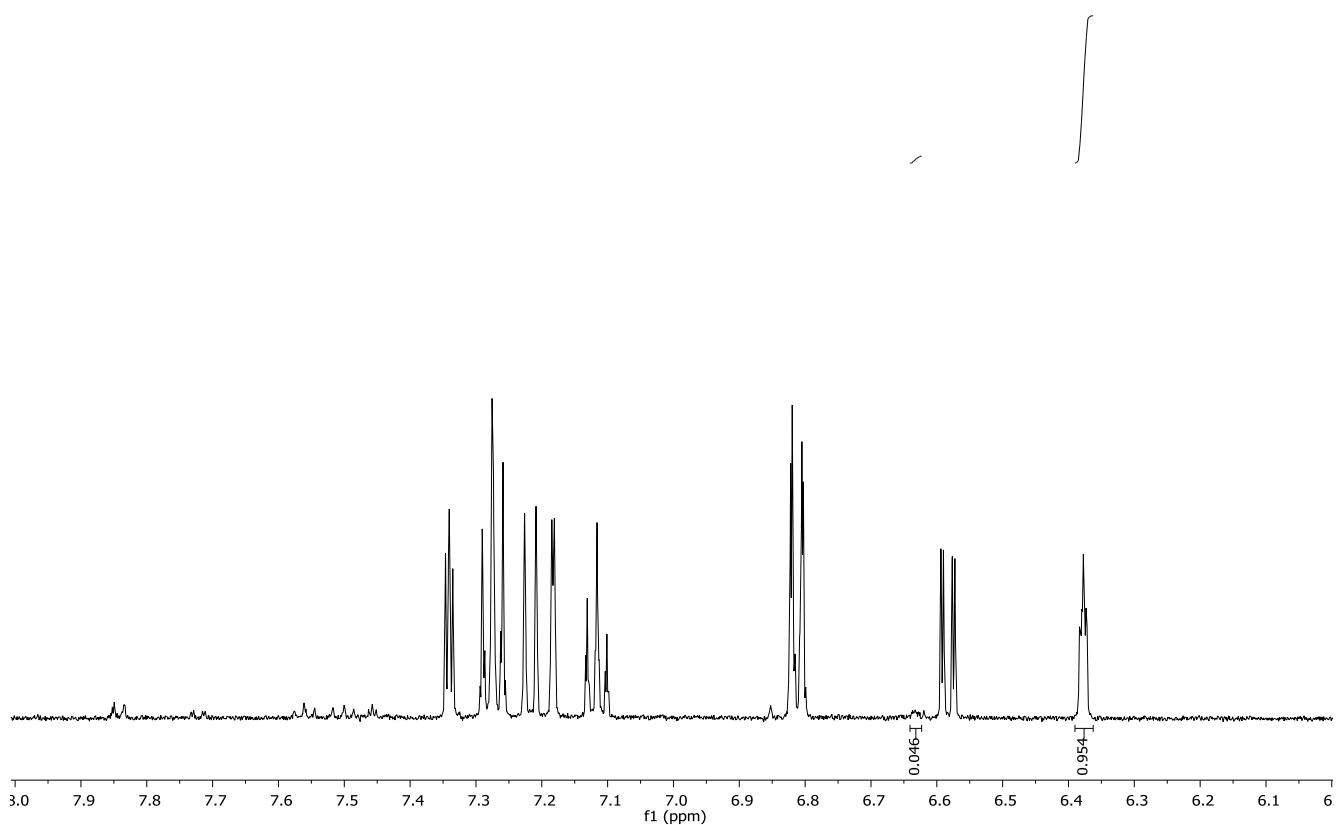
3h PSD 365 nm irradiation



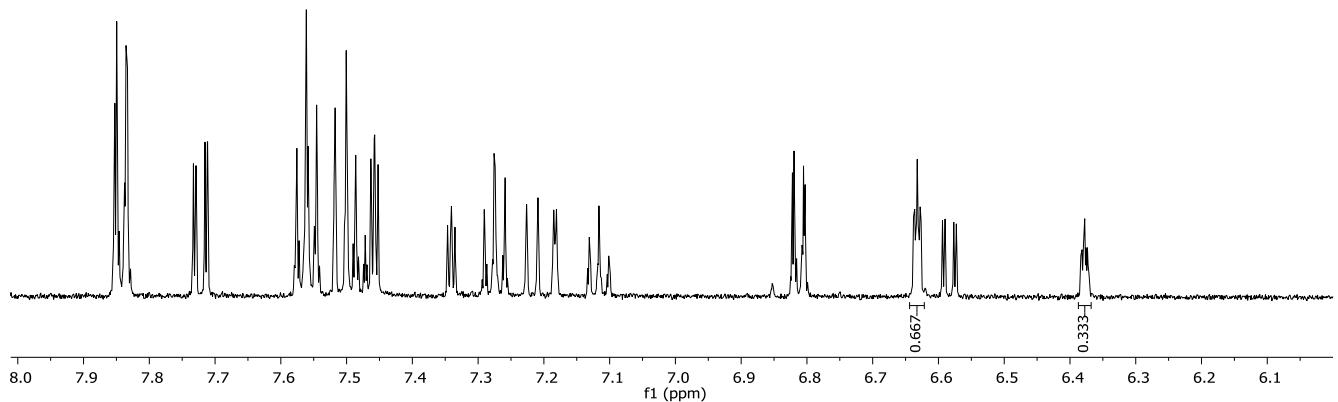
3h PSD 460 nm irradiation



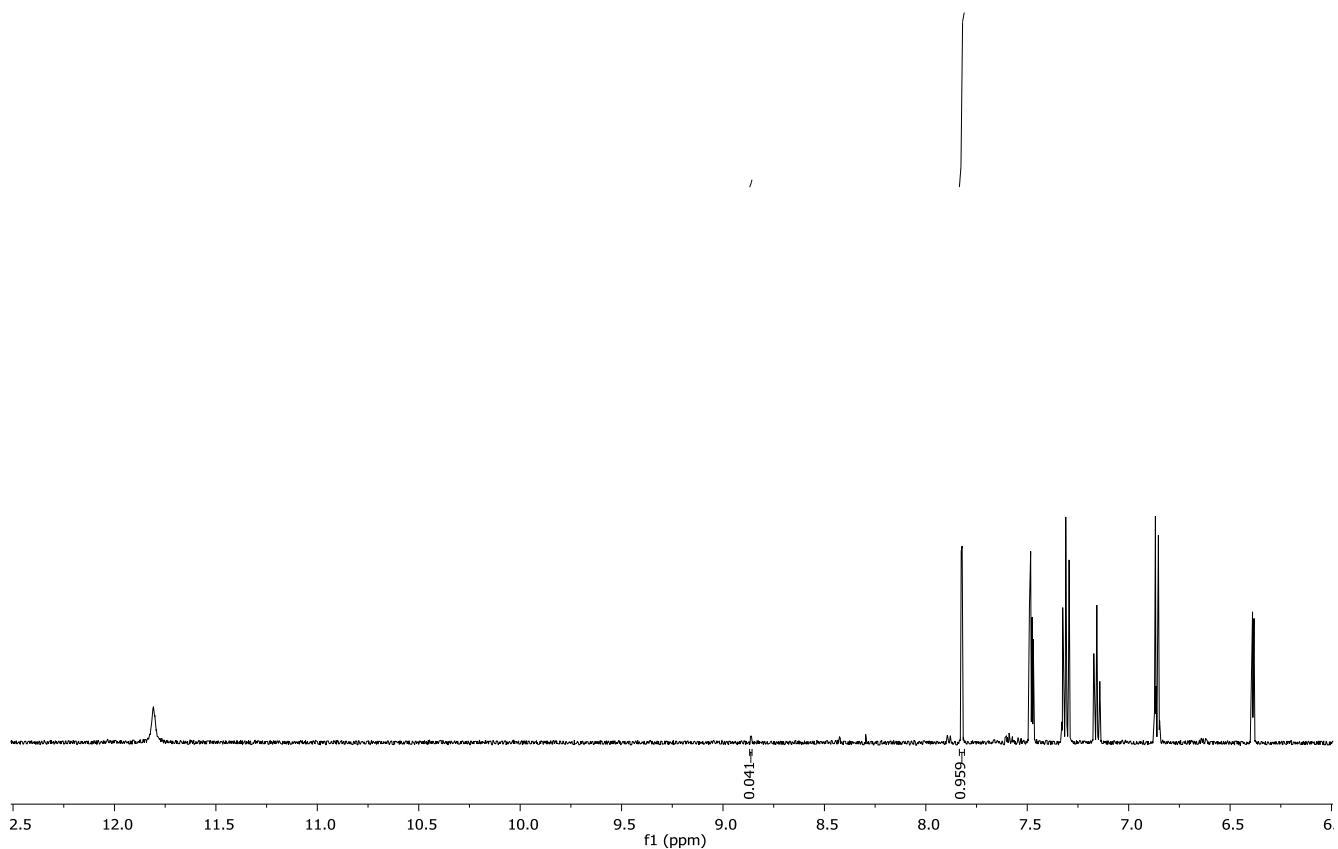
5e PSD 365 nm irradiation



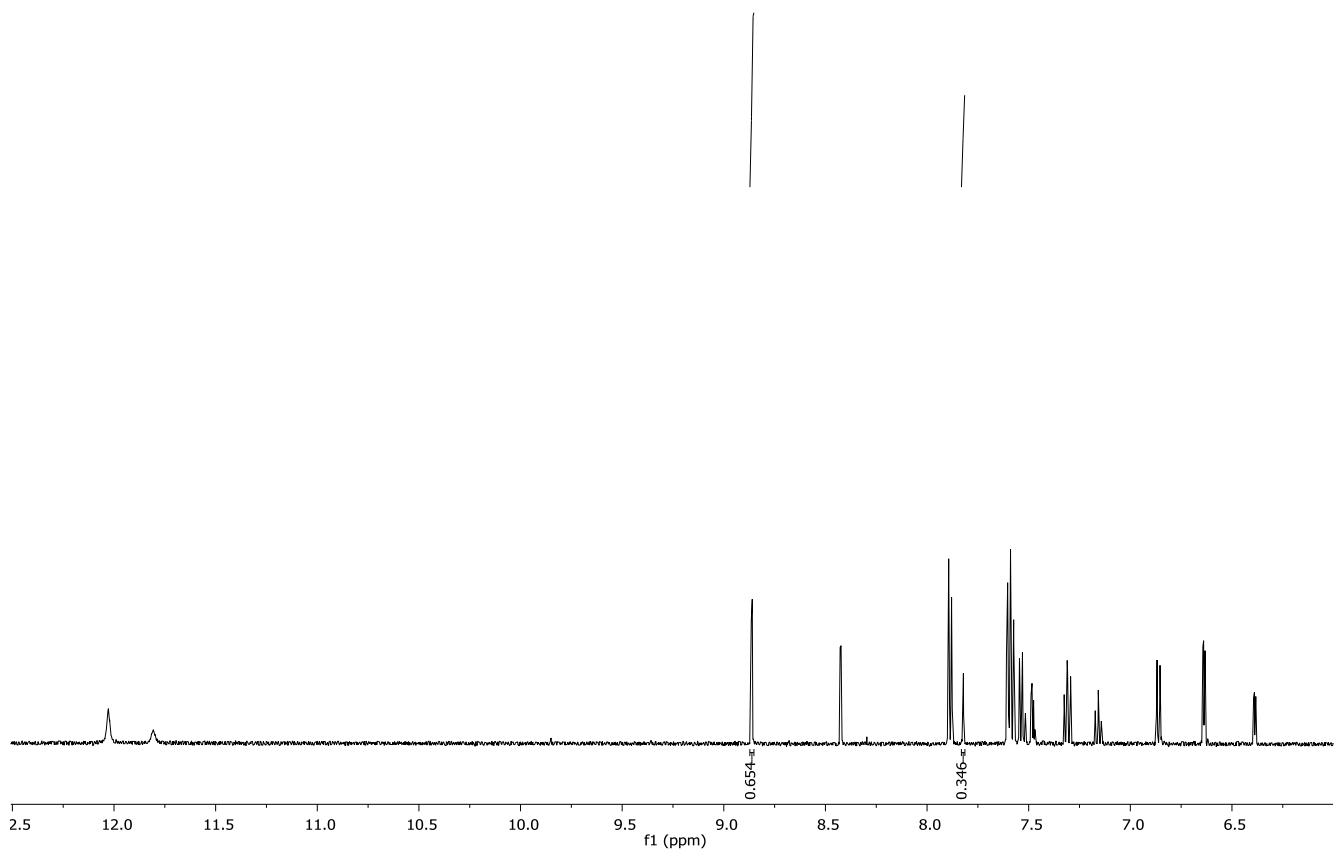
5e PSD 460 nm irradiation



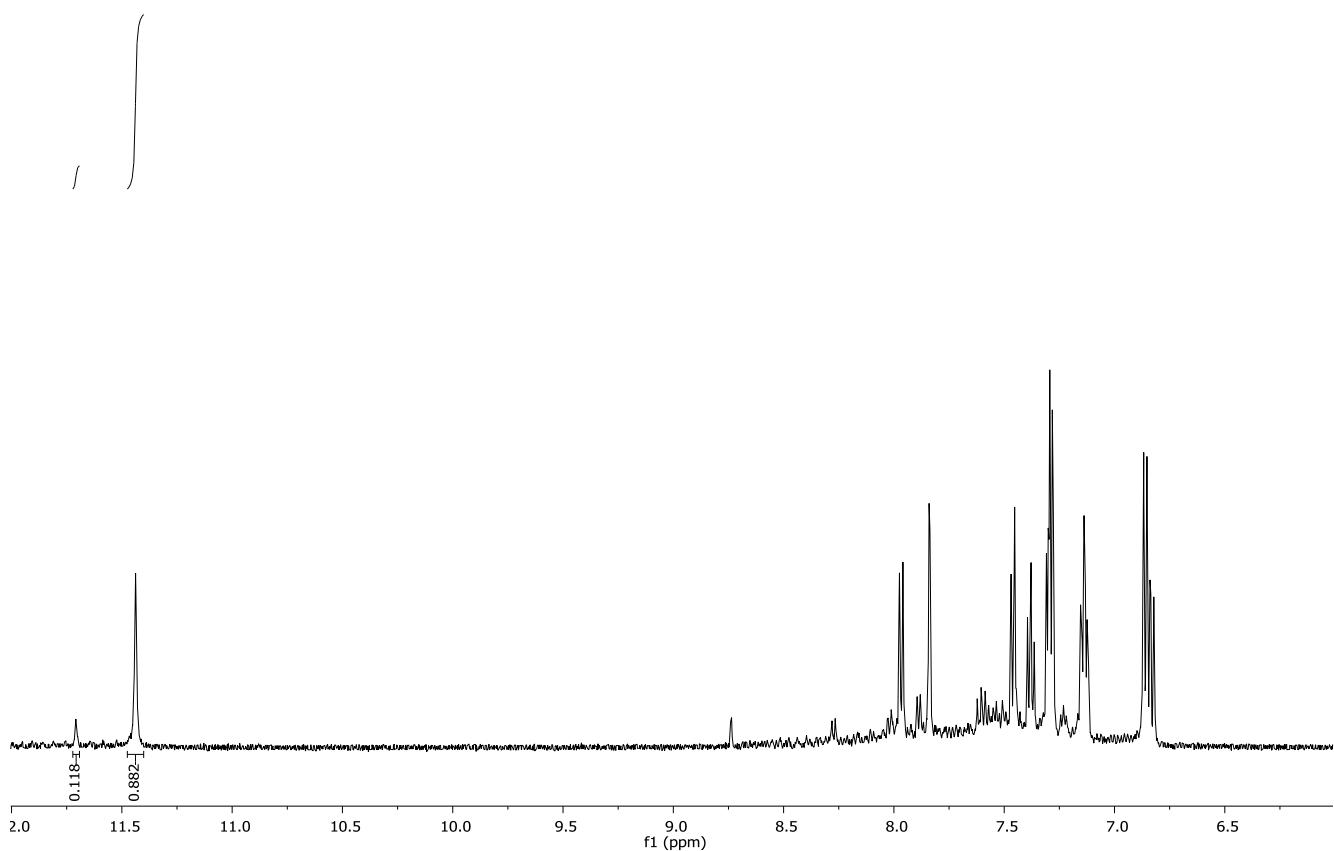
5f PSD 365 nm irradiation



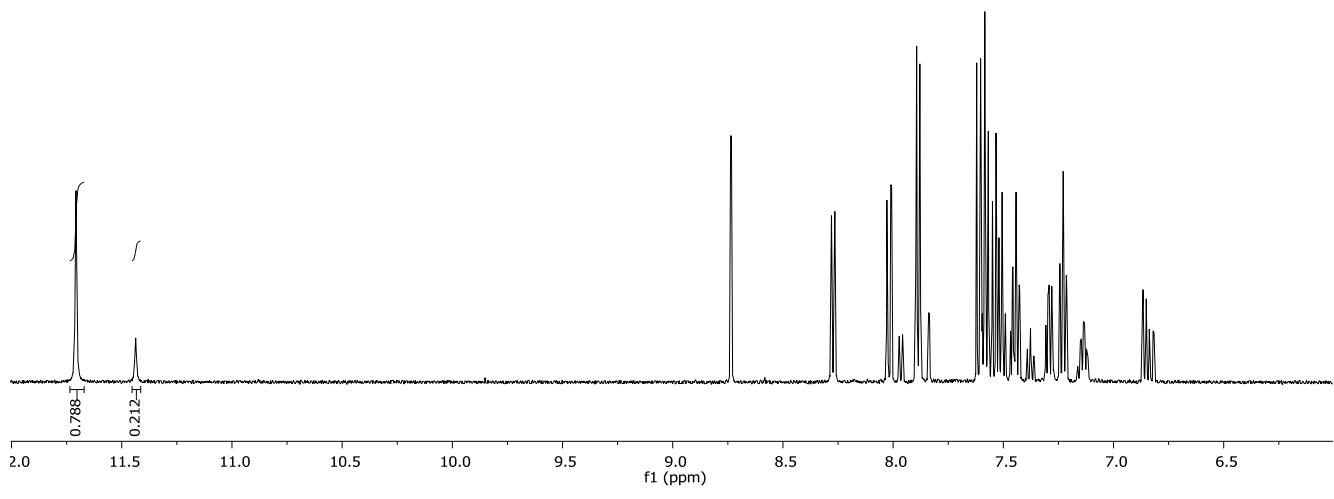
5f PSD 460 nm irradiation



5g PSD 405 nm irradiation



5g PSD 523 nm irradiation



4. Computational details

Quantum chemical calculations were performed with the Gaussian 16 suite^[13] of programs. All compounds were fully optimized by using B3LYP/6-31G(d)^[14] functions. The optimized structures were used for analysis of geometric properties and for subsequent TDDFT calculations. TDDFT calculations were carried out to investigate the electronic properties of the compounds and plot the frontier molecular orbitals (FMO).

Transition states were optimized by using the Berny algorithm at B3LYP/6-31G(d)^[14] level.

Intrinsic reaction path (IRC) calculations^[15] were further carried out to confirm the transition state leading to the corresponding Z/E minima. The IRC calculations were performed at the same level of theory as transition state optimization. The aim of this part is to investigate the potential transition states assuming that the compounds isomerize via inversion, since this isomerization mechanism has been suggested to dominate for azoheteroarene compounds^[17,18]. However, it should be mentioned that the rotation mechanisms has also been proposed for azo compounds, while some studies have pointed out that azoindazole compounds^[19], and azopyrrole compounds may isomerize via the rotation mechanism as well^[17]. Furthermore, tautomerism has been suggested to be a viable mechanism.^[20,21]

All the above theoretical calculations were carried out in gas phase. Please note that the current basis set was chosen to allow for a relative, qualitative, comparison between the studied compounds, and not for more a more quantitative analysis.

4.1. Optimized ground state geometry

All the ground state structures were fully optimized. The N₁=N₂ bond distances, N₁-N₂-C₃ angles, C₄-N₁-N₂-C₃ dihedrals are summarized in Table S1. Except for the symmetric compound **3b** two conformers are considered for each isomer (referred to as I and II), interconverted by rotation of the respective heterocycle (Figure S40a).

The relative ground state energy differences ($\Delta G(Z-E)$) between the *E*- and *Z*-isomers were calculated. As expected, all *E*-isomers are more stable than the corresponding *Z*-isomers, with a typical energy difference around 15 kcal/mol. The energy differences between the two conformations of each isomer (I and II) are listed in Table S2.

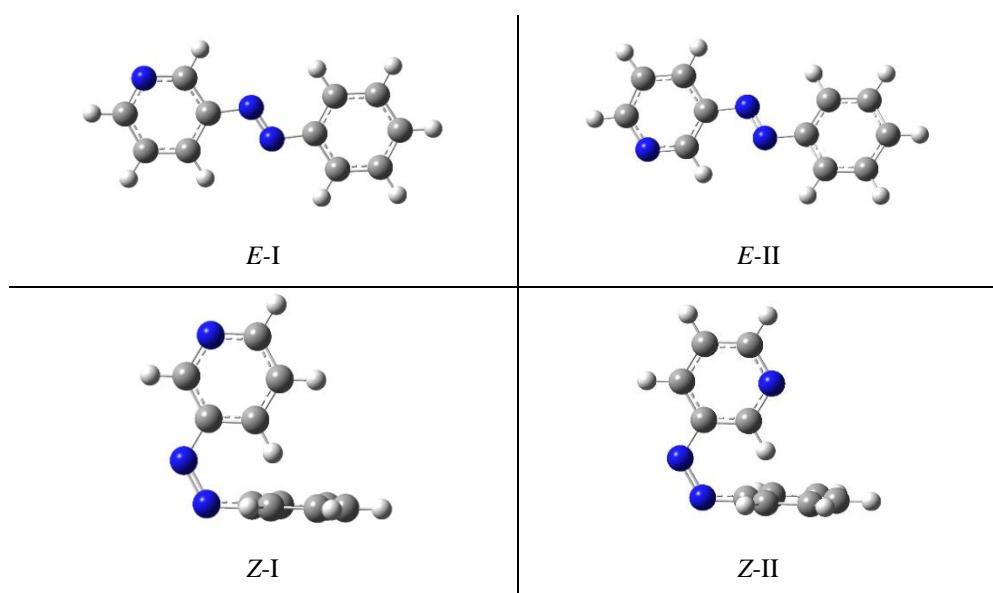


Figure S40a. Representation of **3a** to exemplify the two conformations (I and II) of each isomer.

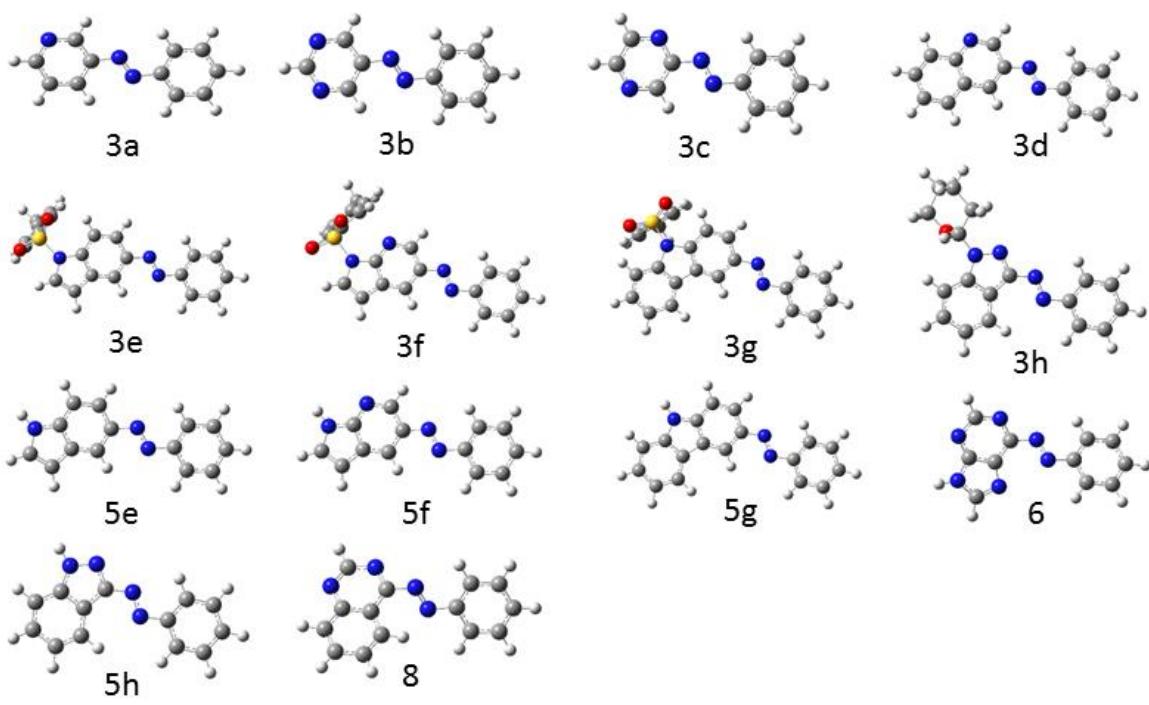
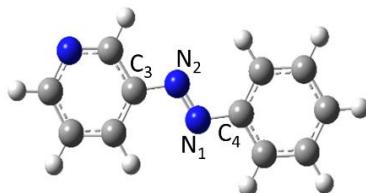


Figure S40b. Representation of all compounds in the *E*-I conformation.

Table S1. Selected structural parameters and the relative energy differences between the *E*- and *Z*-isomer ($\Delta G(Z-E)$). The two conformations for the respective isomer are referred to as I and II as indicated in Figure S40.



Compound	<i>E</i>			<i>Z</i>			$\Delta G(Z-E)$ (kcal/mol)
	R(N ₁ N ₂)(Å)	A(N ₁ N ₂ C ₃)(°)	D(C ₄ N ₁ N ₂ C ₃)(°)	R(N ₁ N ₂)(Å)	A(N ₁ N ₂ C ₃)(°)	D(C ₄ N ₁ N ₂ C ₃)(°)	
3a-I	1.261	114.4	179.9	1.249	124	9.7	-15.56
3a-II	1.261	114.5	179.9	1.25	123.9	10.02	-14.56
3b-I	1.262	114.1	179.9	1.25	123.9	9.8	-14.87
3c-I	1.261	113.5	179	1.248	123.4	10.32	-13.74
3c-II	1.26	114.7	179.3	1.25	123.6	11.78	-12.36
3d-I	1.261	115.4	179.7	1.249	124.3	9.95	-15.19
3d-II	1.262	114.5	179.9	1.251	123.9	10.44	-15.19
3e-I	1.261	115	179.9	1.249	124.3	9.92	-15.56
3e-II	1.262	115	179.9	1.25	124.2	10.1	-15.81
3f-I	1.261	114.7	179.9	1.25	124.2	9.86	-22.15
3f-II	1.261	114.9	179.9	1.25	123.9	9.8	-15.12
3g-I	1.261	114.9	179.9	1.25	124.2	10.13	-15.5
3g-II	1.262	114.9	179.9	1.25	124.2	10.147	-15.81

3h-I	1.266	113.9	179.9	1.25	123.2	11.31	-17.19
3h-II	1.264	115.7	179.8	1.253	124.7	9.62	-12.61
5e-I	1.262	115.3	179.9	1.252	123.2	11.31	-15.44
5e-II	1.262	115.2	179.9	1.251	124.5	10.27	-15.94
5f-I	1.262	114.9	179.9	1.251	124.5	9.89	-15.81
5f-II	1.262	115.2	179.9	1.251	124.1	10	-15.44
5g-I	1.262	115.2	179.9	1.251	124.7	10.25	-15.81
5g-II	1.263	115.2	179.9	1.252	124.6	10.33	-16.06
6-I	1.26	113.5	179.9	1.245	124.3	9.96	-10.48
6-II	1.261	114.3	179.9	1.245	124.1	11.92	-10.67
5h-I	1.266	113.9	179.9	1.252	123.5	11.56	-17.51
5h-II	1.263	115.6	179.9	1.252	124.5	10.35	-12.8
8-I	1.257	115	179.3	1.246	124.4	12.19	-9.287
8-II	1.259	114	176.5	1.245	125.7	6.002	-11.61

Table S2. The relative energies between the two conformations (I and II) of each isomer.

Compound	E			Z		
	E_I (a.u)	E_{II} (a.u)	ΔE_E (kcal/mol)	Z_I (a.u)	Z_{II} (a.u)	ΔE_Z (kcal/mol)
3a	-588.7974	-588.7961	-0.81575	-588.7726	-588.7729	0.18825
3b	-604.8342			-604.8105		
3c	-604.8284	-604.827	-0.8785	-604.8065	-604.8073	0.502
3d	-742.443	-742.4433	0.18825	-742.4188	-742.4191	0.18825
3e	-1523.2624	-1523.263	0.31375	-1523.238	-1523.2377	0.06275
3f	-1539.3031	-1539.302	-0.6275	-1539.268	-1539.278	6.33775
3g	-1676.9147	-1676.915	0.06275	-1676.89	-1676.8896	-0.251
3h	-990.9353	-990.9302	-3.20025	-990.9079	-990.9101	1.3805
5e	-704.3311	-704.332	0.56475	-704.3065	-704.3066	0.06275
5f	-720.3743	-720.3735	-0.502	-720.3491	-720.3489	-0.1255
5g	-857.9855	-857.9859	0.251	-857.9603	-857.9603	0
6	-720.3581	-720.3529	-3.263	-720.3302	-720.3325	1.44325
5h	-752.4536	-752.4534	-0.1255	-752.4369	-752.4364	-0.31375
8	-758.4772	-758.4794	1.3805	-758.4624	-758.4609	-0.94125

$$\Delta E_E = (E_I - E_{II}) \times 627.5; \Delta E_Z = (Z_I - Z_{II}) \times 627.5$$

4.2. Absorption Spectra

The TDDFT calculations of the predicted absorption maxima (λ_{\max}) of all isomers are summarized in Table S3. The first transition ($n-\pi^*$) has a very weak oscillator strength for all *E*-isomers; compounds with pronounced symmetry breaking out-of-plane rotated heterocycles (see Table S6) displaying the strongest transitions. Compared to the experimental data, it is seen that the calculations correctly predict the spectral shifts induced by an increase in the ring-size, and by the introduction of electron withdrawing/donating groups.

Table S3. Spectral properties of the *E*- and *Z*-isomers, including the wavelengths of absorption maxima (λ_{\max}) and oscillator strengths (f).

Compound	<i>E</i>				<i>Z</i>			
	$\pi-\pi^*$		$n-\pi^*$		$\pi-\pi^*$		$n-\pi^*$	
	λ_{\max} (nm)	f						
3a-I	333	0.7618	494	0.0000	312	0.0021	482	0.0352
3a-II	323	0.4950	511	0.0021	309	0.1065	480	0.0280
3b	319	0.6014	508	0.0016	335	0.0343	481	0.0292
3c-I	322	0.0210	530	0.0017	334	0.0083	487	0.0205
3c-II	330	0.6405	524	0.0013	344	0.0012	508	0.0382
3d-I	368	0.3879	509	0.0002	327	0.0431	488	0.0532
3d-II	349	0.5364	516	0.0000	343	0.0074	495	0.0496
3e-I	369	0.1297	481	0.0000	347	0.0182	484	0.0481
3e-II	360	0.0511	475	0.0000	346	0.0085	485	0.0484
3f-I	355	0.0119	477	0.0000	334	0.0018	485	0.0536
3f-II	351	0.0393	487	0.0000	336	0.0166	484	0.0491
3g-I	371	0.6747	481	0.0000	345	0.0327	487	0.0691
3g-II	366	0.7621	478	0.0000	345	0.0104	488	0.0584
3h-I	360	0.6933	470	0.0000	342	0.0390	493	0.0470
3h-II	370	0.6455	499	0.0000	337	0.1353	497	0.0423
5e-I	380	0.0887	477	0.0000	356	0.0084	483	0.0489
5e-II	366	0.0326	469	0.0000	352	0.0042	483	0.0547
5f-I	360	0.0245	475	0.0000	341	0.0019	486	0.0451
5f-II	354	0.0366	484	0.0000	340	0.0122	482	0.0461
5g-I	384	0.5440	475	0.0000	352	0.0525	488	0.0610
5g-II	373	0.7984	470	0.0000	347	0.0222	487	0.0756
6-I	346	0.0331	527	0.0076	313	0.0019	466	0.0235
6-II	375	0.0006	563	0.0000	321	0.0007	484	0.0367
5h-I	353	0.6360	468	0.0000	313	0.0616	491	0.0399
5h-II	361	0.6145	497	0.0000	330	0.1313	492	0.0460
8-I	362	0.1256	513	0.0140	354	0.0211	515	0.0399
8-II	375	0.011	524	0.0151	345	0.0455	464	0.0111

The calculations show that the two conformations (I and II) of each isomer have similar FMO topologies, indicating that the orientation of the heteroarene does not have a dramatic impact on the FMO (see Figure S41). The HOMO-1, HOMO and LUMO of **3a** *E*-isomer are clearly π , n, and π^* orbitals, respectively, while the HOMO-1 and HOMO of the *Z*-isomer shows n/ π character, and LUMO shows clearly π^* character. For the *E*-isomer of **3a-3c**, **6** and **8**, the contribution to the highest occupied molecular orbital HOMO and the lowest unoccupied molecular orbital LUMO originates from $N_1=N_2$ bond lone-pair n orbital and π^* antibonding orbital, respectively. For the rest of the compounds, the contribution to the HOMO and the LUMO originates from π conjugated orbital and π^* antibonding orbital, respectively (Figure S42). However, for *Z*-isomers, all the compounds have the contribution to the HOMO and the LUMO originating from n/ π mixed orbital and π^* antibonding orbital, respectively.

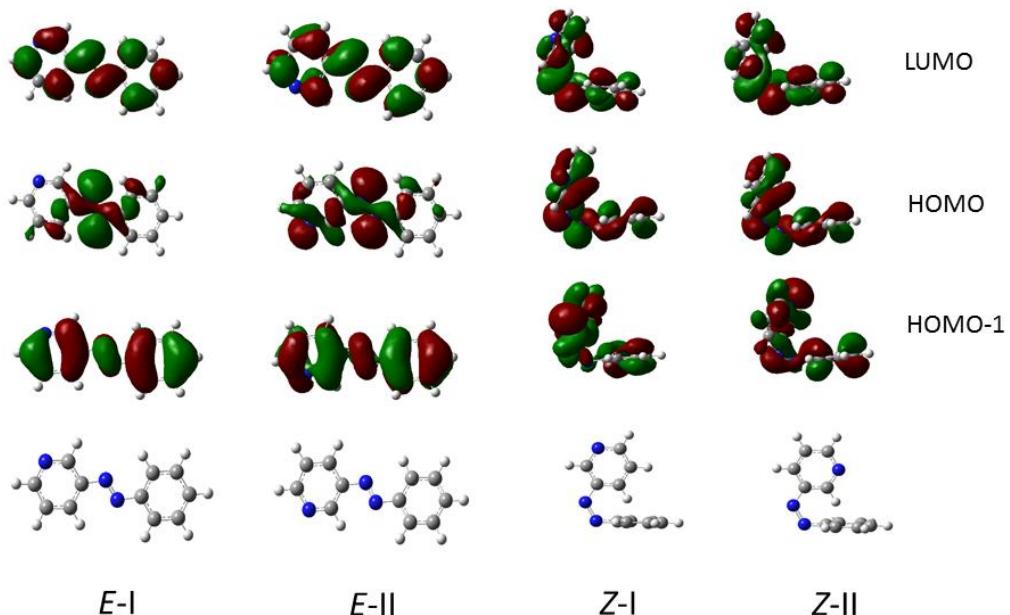


Figure S41. FMO of compound **3a** in conformation I and II of the *E*- and *Z*-isomer.

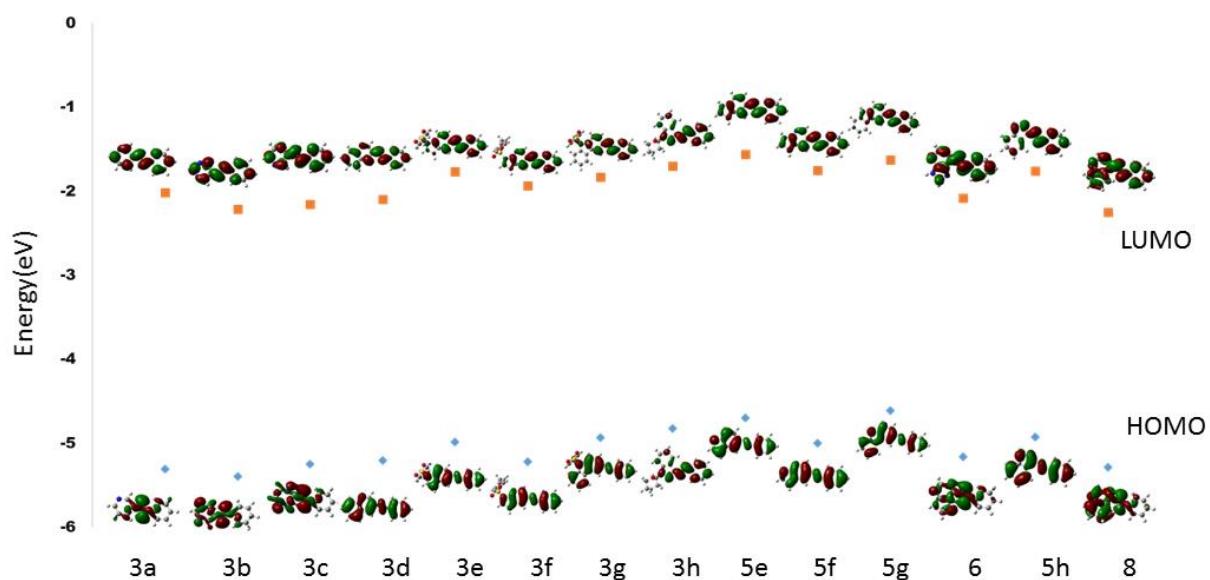


Figure S42. FMO surfaces and molecular orbital energy level diagram for all compounds in the *E*-I conformation. The HOMO to LUMO for **3a**, **3b**, **3c**, **6** and **8** originates from n- π^* , the other originates from π to π^* .

Table S4. Energy levels of HOMO and LUMO, and the HOMO-LUMO energy gap.

Compound	E			Z		
	HOMO(eV)	LUMO(eV)	HOMO-LUMO(eV)	HOMO(eV)	LUMO(eV)	HOMO-LUMO(eV)
3a-I	-5.31	-2.02	-3.29	-5.02	-1.83	-3.19
3a-II	-5.16	-1.98	-3.18	-4.99	-1.78	-3.21
3b	-5.4	-2.21	-3.19	-5.23	-2.02	-3.21
3c-I	-5.25	-2.15	-3.1	-5.13	-1.94	-3.19
3c-II	-5.36	-2.21	-3.15	-5.08	-2.03	-3.05
3d-I	-5.2	-2.1	-3.1	-4.94	-1.85	-3.09
3d-II	-5.1	-1.99	-3.11	-4.9	-1.85	-3.05
3e-I	-4.99	-1.76	-3.23	-4.73	-1.58	-3.15
3e-II	-5.01	-1.73	-3.28	-4.73	-1.6	-3.13
3f-I	-5.22	-1.93	-3.29	-4.82	-1.67	-3.15
3f-II	-5.2	-1.89	-3.31	-4.87	-1.71	-3.16
3g-I	-4.93	-1.83	-3.1	-4.73	-1.64	-3.09
3g-II	-4.93	-1.81	-3.12	-4.75	-1.67	-3.08
3h-I	-4.82	-1.7	-3.12	-4.66	-1.62	-3.04
3h-II	-4.81	-1.76	-3.05	-4.65	-1.63	-3.02
5e-I	-4.7	-1.56	-3.14	-4.72	-1.58	-3.14
5e-II	-4.74	-1.52	-3.22	-4.69	-1.55	-3.14
5f-I	-5	-1.75	-3.25	-4.5	-1.37	-3.13
5f-II	-5	-1.7	-3.3	-4.5	-1.38	-3.12
5g-I	-4.61	-1.63	-2.98	-4.49	-1.45	-3.04
5g-II	-4.63	-1.6	-3.03	-4.49	-1.45	-3.04
6-I	-5.17	-2.08	-3.09	-5.09	-1.78	-3.31
6-II	-5.2	-2.19	-3.01	-5.05	-1.88	-3.17
5h-I	-4.92	-1.76	-3.16	-4.74	-1.68	-3.06
5h-II	-4.9	-1.8	-3.1	-4.73	-1.67	-3.06
8-I	-5.28	-2.25	-3.03	-5.12	-2.13	-2.99
8-II	-5.35	-2.31	-3.04	-5.22	-1.88	-3.34

4.3. Thermal stability of the Z-isomers

Azobenzene derivatives undergo a thermal *Z* to *E* isomerization in the ground state.^[16] Two reaction pathways are usually considered: rotation about the azo bridge and inversion at one of the N=N nitrogen atoms. The inversion mechanism has been suggested to dominate for azoheteroarene compounds^[17,18], and our calculations are based on this mechanism. However, it should be mentioned that the rotation mechanisms has also been proposed for azo compounds, while some studies have pointed out that azoindazole compounds^[19], and azopyrrole compounds may isomerize via the rotation mechanism as well^[17]. Furthermore, tautomerism has been suggested to be a viable mechanism.^[20,21]

Both sides of the azo nitrogen could undergo inversion and two types of transition states are proposed: type I transition state is *Z*-isomer-like with the heteroarenes more perpendicularly oriented to the benzene ring, while type II transition state is *E*-isomer-like with the two ring systems coplanar^[18] (Figure S43). Thus, four possible transition states need to be considered (for non-symmetric compounds, i.e., for all compounds studied here except **3b**).

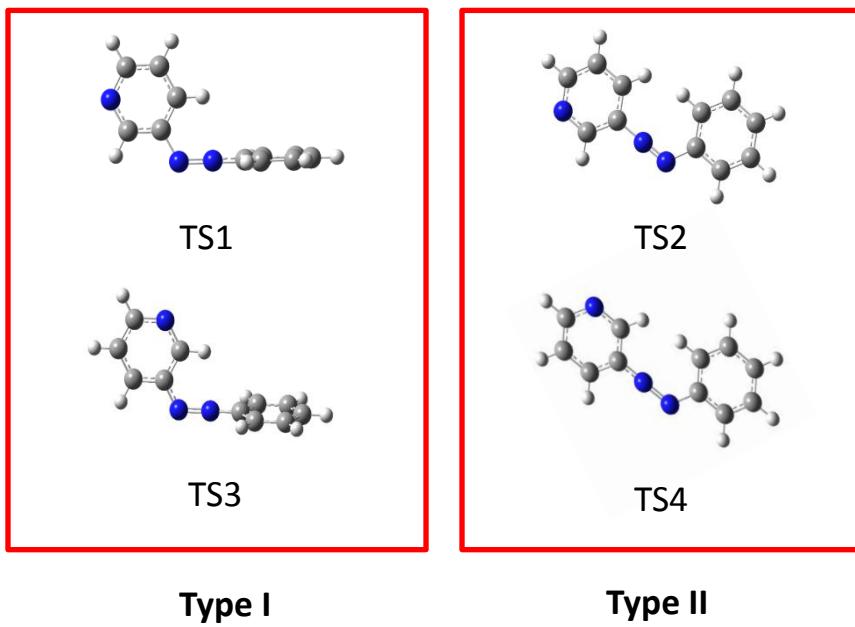


Figure S43. The four different transition states of **3a**. TS1 and TS3 are categorized as Type I transition states while TS2 and TS4 are categorized as Type II transition states.

All the transition states were optimized and the resulting structures are characterized by one imaginary frequency ranging from 400 to 500 cm⁻¹. IRC calculations were further carried out to confirm that the transition states proceed along to the *Z* and *E* minima.

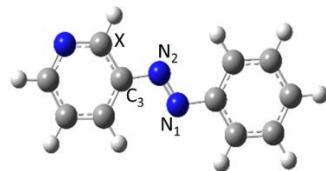
The computed activation energies corresponding to different transition states are summarized in Table S5. Comparing the lower energy barrier for each compound, it is seen that **3c**, **3g**, **3h**, **5e**, and **5g** have the lowest activation energies; around 24 to 25 kcal/mol. With the exception of **6**, compounds **3c**, **3g**, **3h**, and **5e** have the fastest experimentally observed thermal *Z* → *E* isomerization, while **5g** decomposes. Compound **6**, which has the shortest lifetime of the *Z*-isomer, has a very high energy barrier associated with the inversion mechanism (close to 31 kcal/mol). This makes it very likely that **6** instead undergo thermal isomerization by a rotation mechanism. This notion is supported by the dihedral angle X-C₃-N₁=N₂ twisting: the *Z*-isomer of **6**, together with **8**, is much more twisted than the rest of the compounds (Table S6). Thus, these two compounds may prefer to go undergo a rotation mechanism, rather than of the inversion mechanism considered here.

Table S5. Activation energies for the thermal $Z \rightarrow E$ isomerization through inversion.

Compounds	$\Delta G_{\ddagger, TS1}^{\ddagger}$ (kcal/mol)	$\Delta G_{\ddagger, TS2}^{\ddagger}$ (kcal/mol)	$\Delta G_{\ddagger, TS3}^{\ddagger}$ (kcal/mol)	$\Delta G_{\ddagger, TS4}^{\ddagger}$ (kcal/mol)
3a	26.1	34.45	26.92	30.06
3b	27.92	29.81		
3c	24.79	35.45	27.17	28.43
3d	26.23	31.88	26.42	28.93
3e	29.87	36.14	29.93	42.48
3f	36.27	29.99	48.94	36.39
3g	25.1	37.65	24.85	37.4
3h	25.03	41.98	26.42	30.81
5e	24.16	33.57	24.22	33.63
5f	25.16	33.32	25.04	32.57
5g	24.66	33.45	24.03	33.45
6	31.31	37.59	30.37	34.76
5h	27.85	32.13	27.3	36.08
8	35.39	31.63	39.47	37.59

$$\Delta G_{\ddagger, TS1}^{\ddagger} = E_{TS1} - E_{ZI}; \Delta G_{\ddagger, TS2}^{\ddagger} = E_{TS2} - E_{ZI}; \Delta G_{\ddagger, TS3}^{\ddagger} = E_{TS3} - E_{ZII}; \Delta G_{\ddagger, TS4}^{\ddagger} = E_{TS4} - E_{ZII}$$

Table S6. The dihedral angle $XC_3N_1=N_2$. Please note that the dihedral angle is defined such that atom “X” is always positioned above N_2 , i.e., atom X is changed in going from conformer I to conformer II so that the dihedral angle is always $> 90^\circ$.

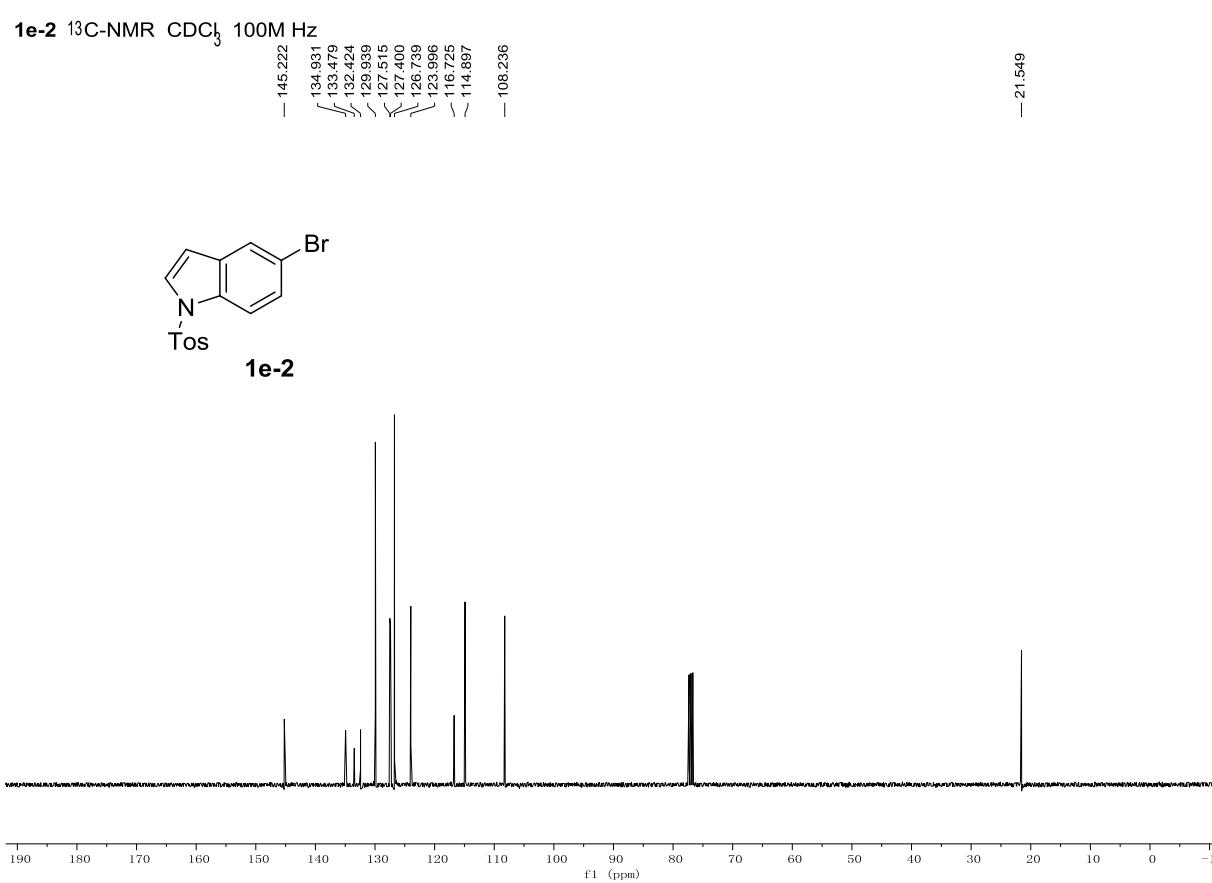
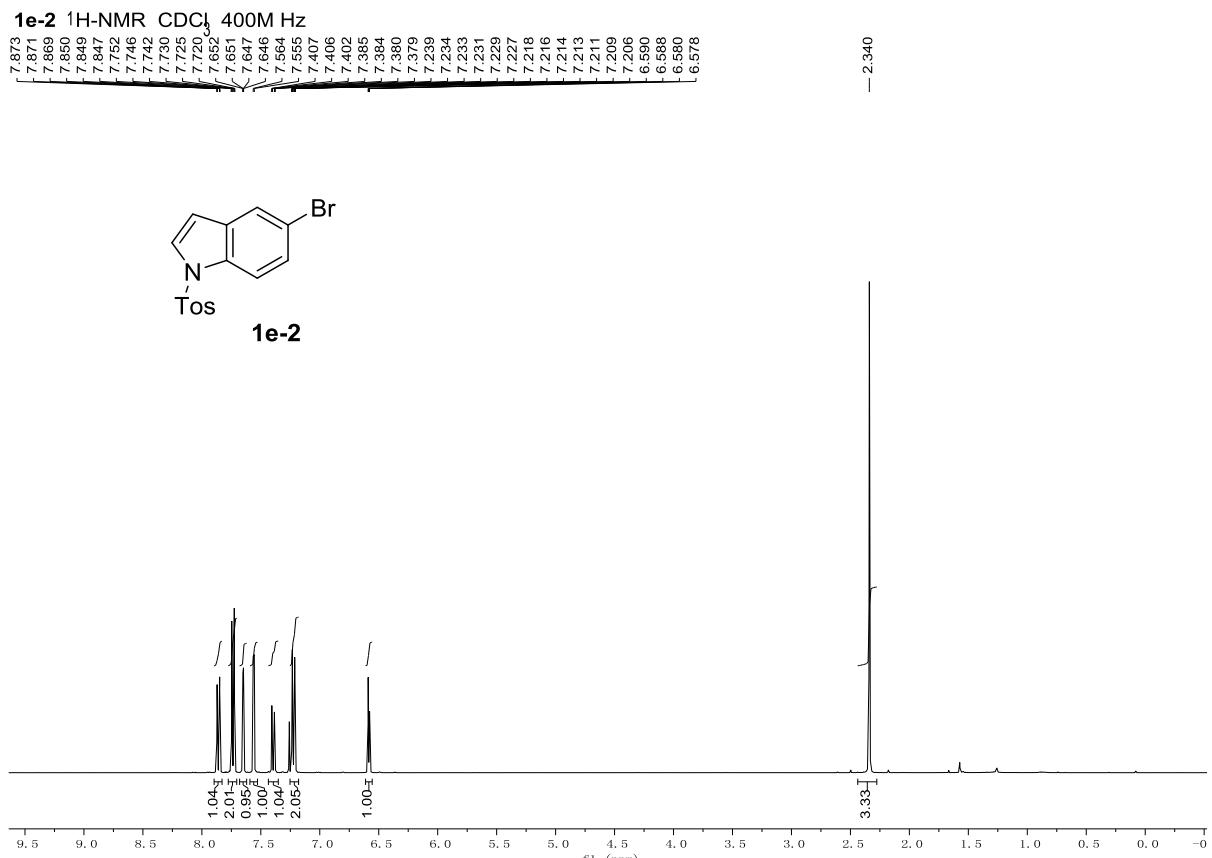


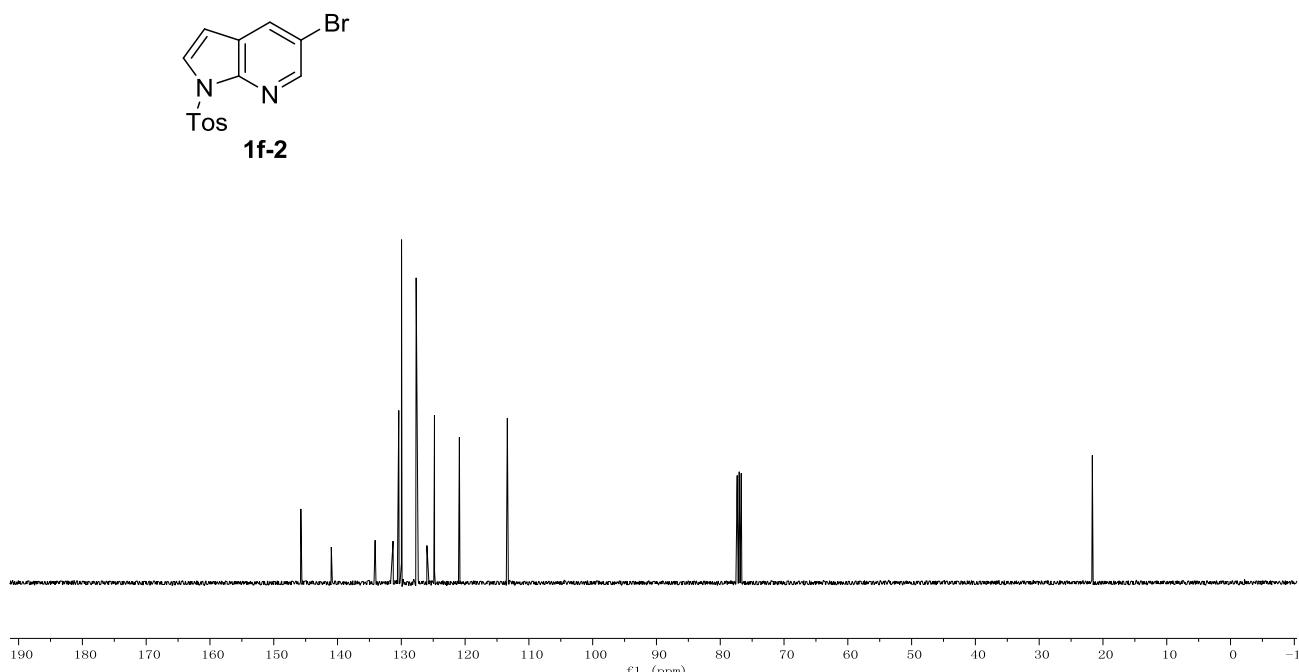
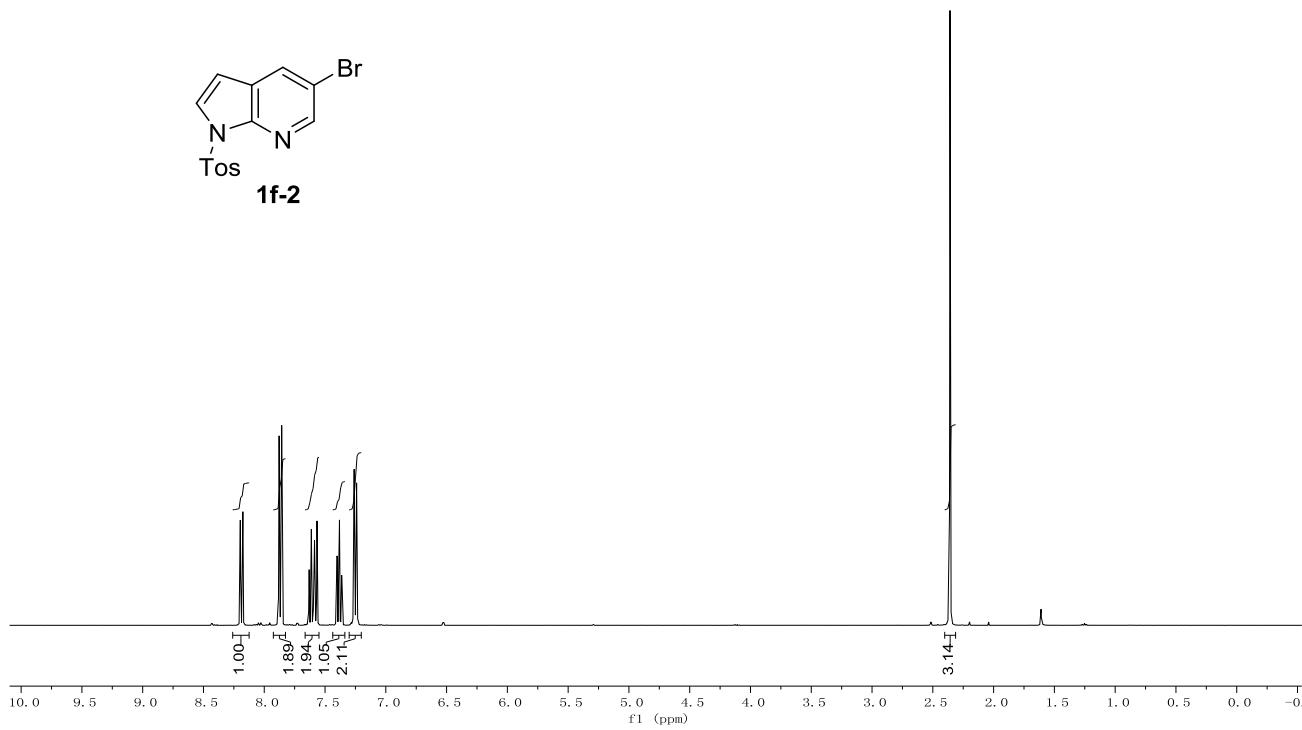
Compound	$E(XC_3N_1=N_2)(^\circ)$	$Z(XC_3N_1=N_2)(^\circ)$
3a-I	179.5	137.9
3a-II	165.3	135.5
3b	166.4	136.3
3c-I	179.6	124.2
3c-II	172	141.3
3d-I	179.9	140.3
3d-II	180	141.1
3e-I	180	143.2
3e-II	179.2	143.8
3f-I	179.8	144.5
3f-II	179.5	141.6
3g-I	179.8	142.1
3g-II	179.1	143.8
3h-I	179.9	139.4
3h-II	179.2	160.9
5e-I	180	145.2
5e-II	180	146.6
5f-I	180	147.5
5f-II	180	143.6
5g-I	180	147.9
5g-II	180	147.7
6-I	149.2	119.8
6-II	179.9	129.2
5h-I	180	141.6
5h-II	179.9	156.8
8-I	139.6	134.1
8-II	151.3	104.4

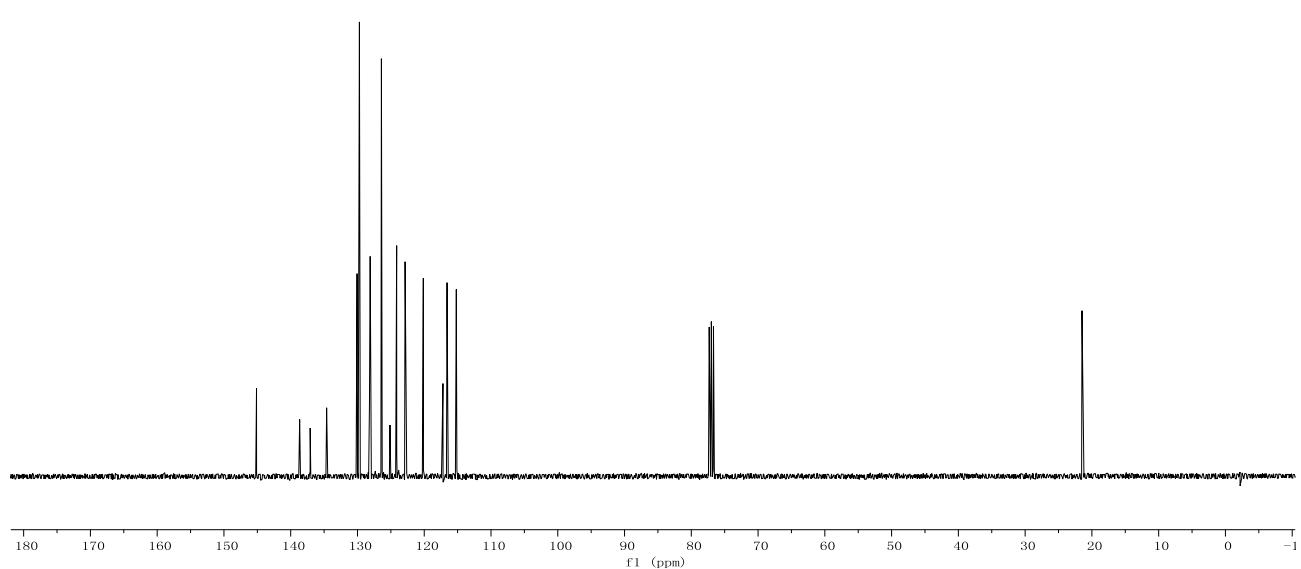
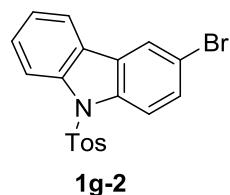
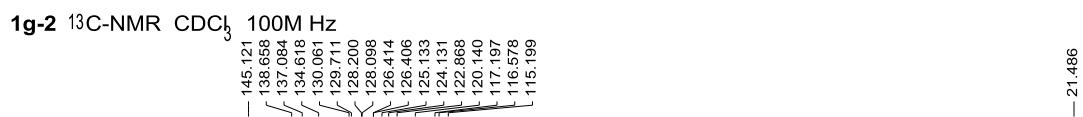
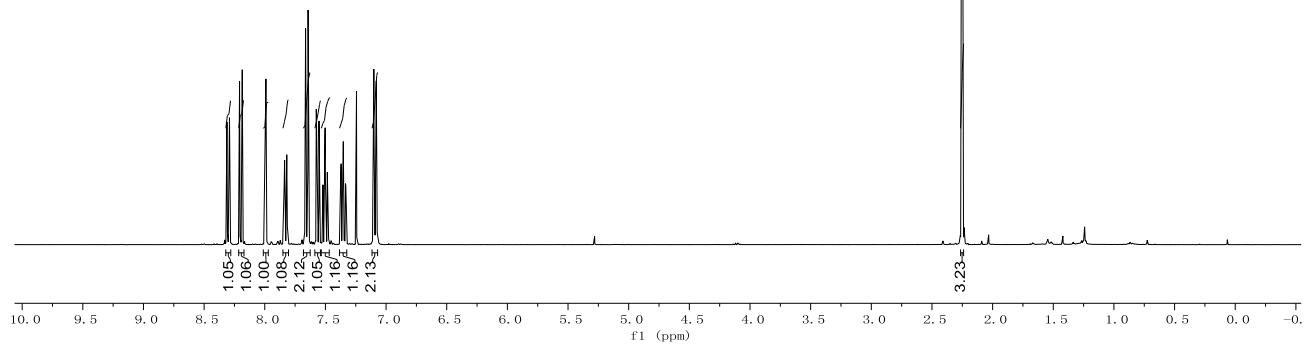
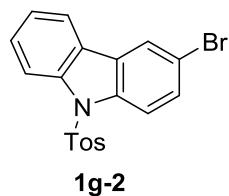
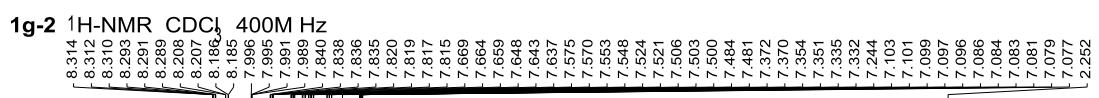
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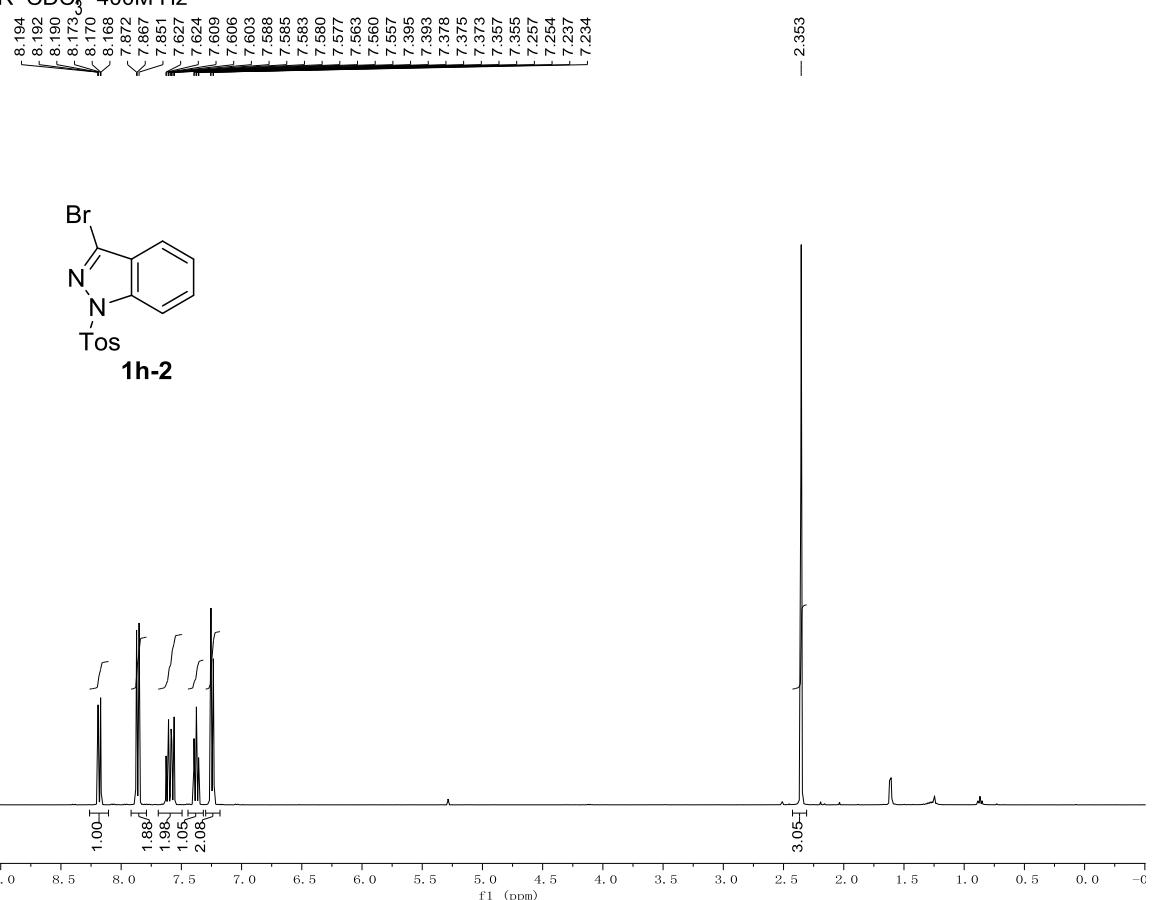
6. ^1H , ^{13}C NMR spectra







1h-2 $^1\text{H-NMR}$ CDCl_3 , 400M Hz

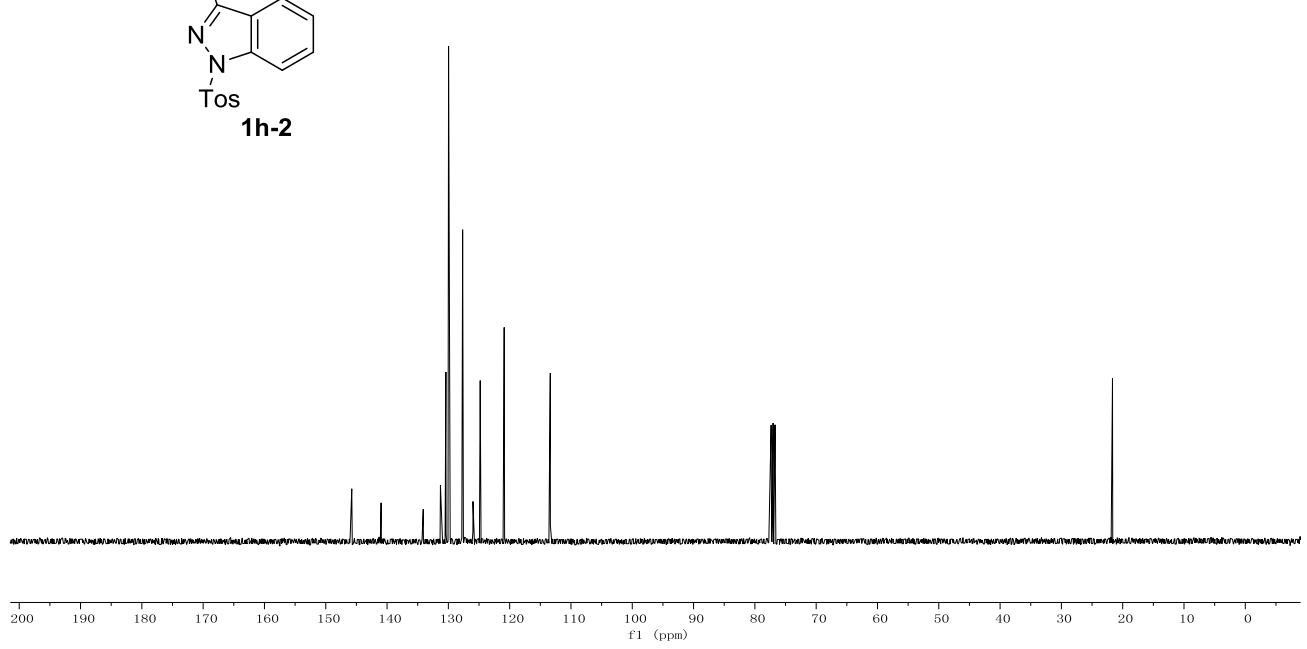


1h-2 ^{13}C -NMR CDCl_3 100M Hz

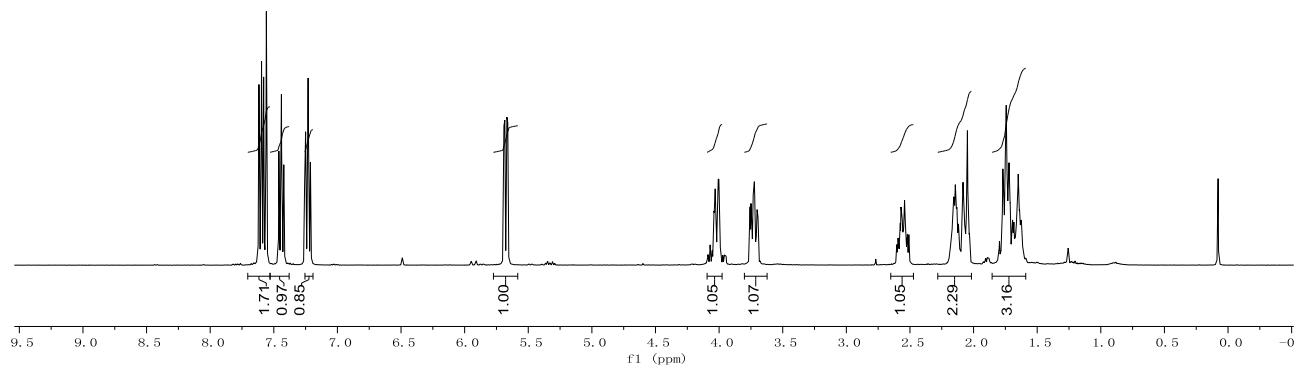
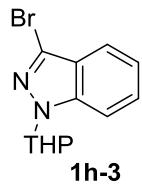


BrC1=NN(Tos)c2ccccc12

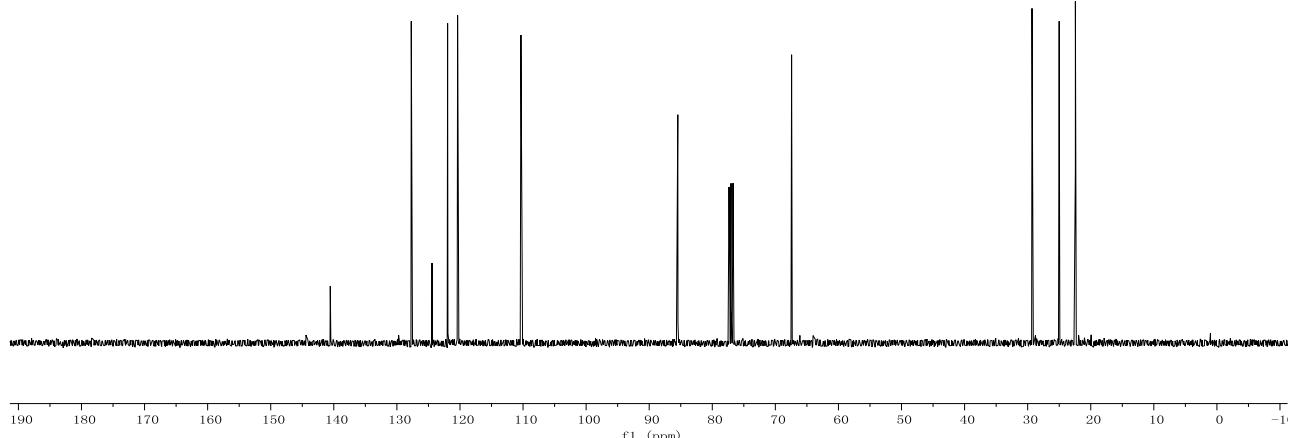
1h-2



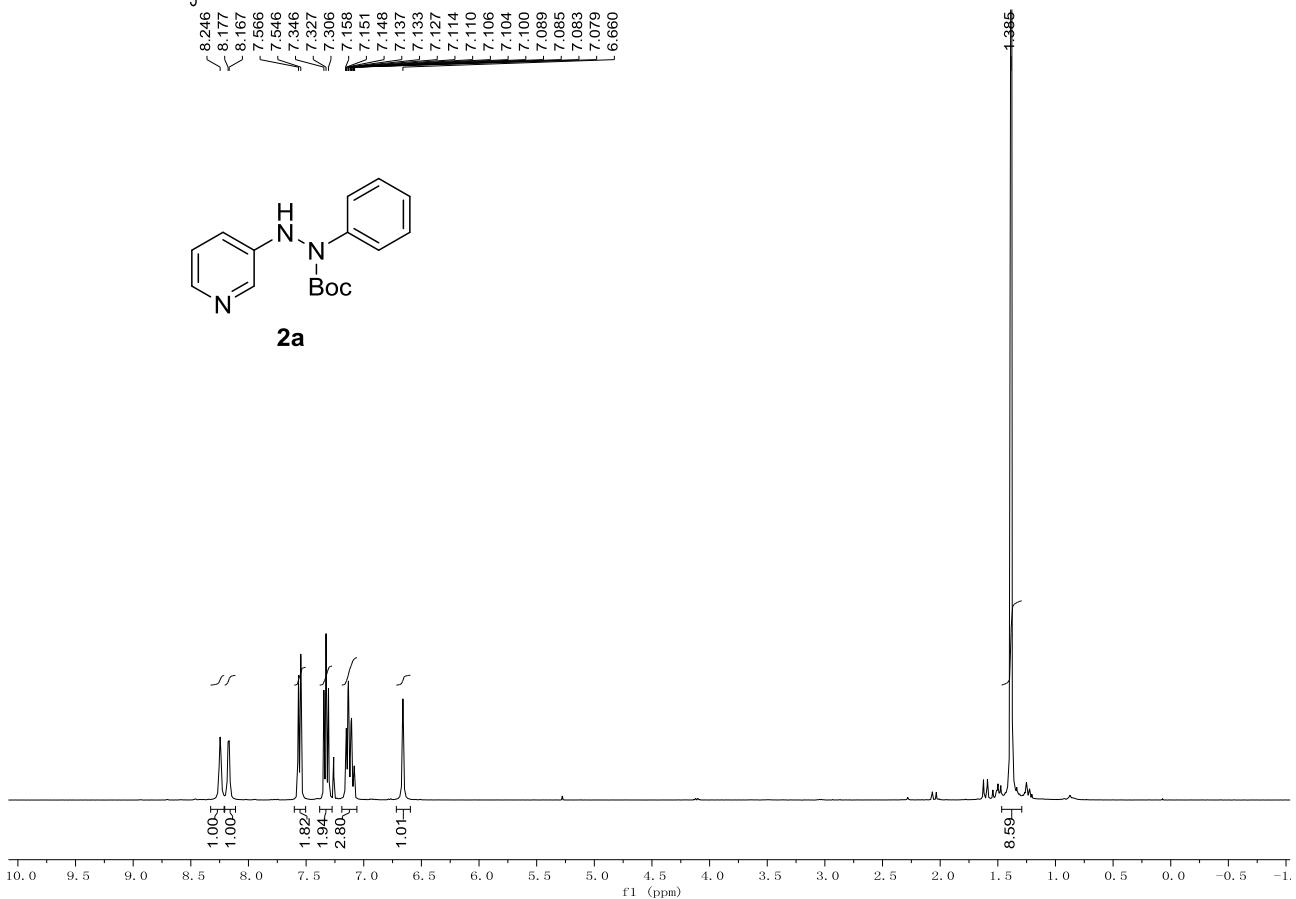
1h-3 $^1\text{H-NMR}$ CDCl_3 400M Hz



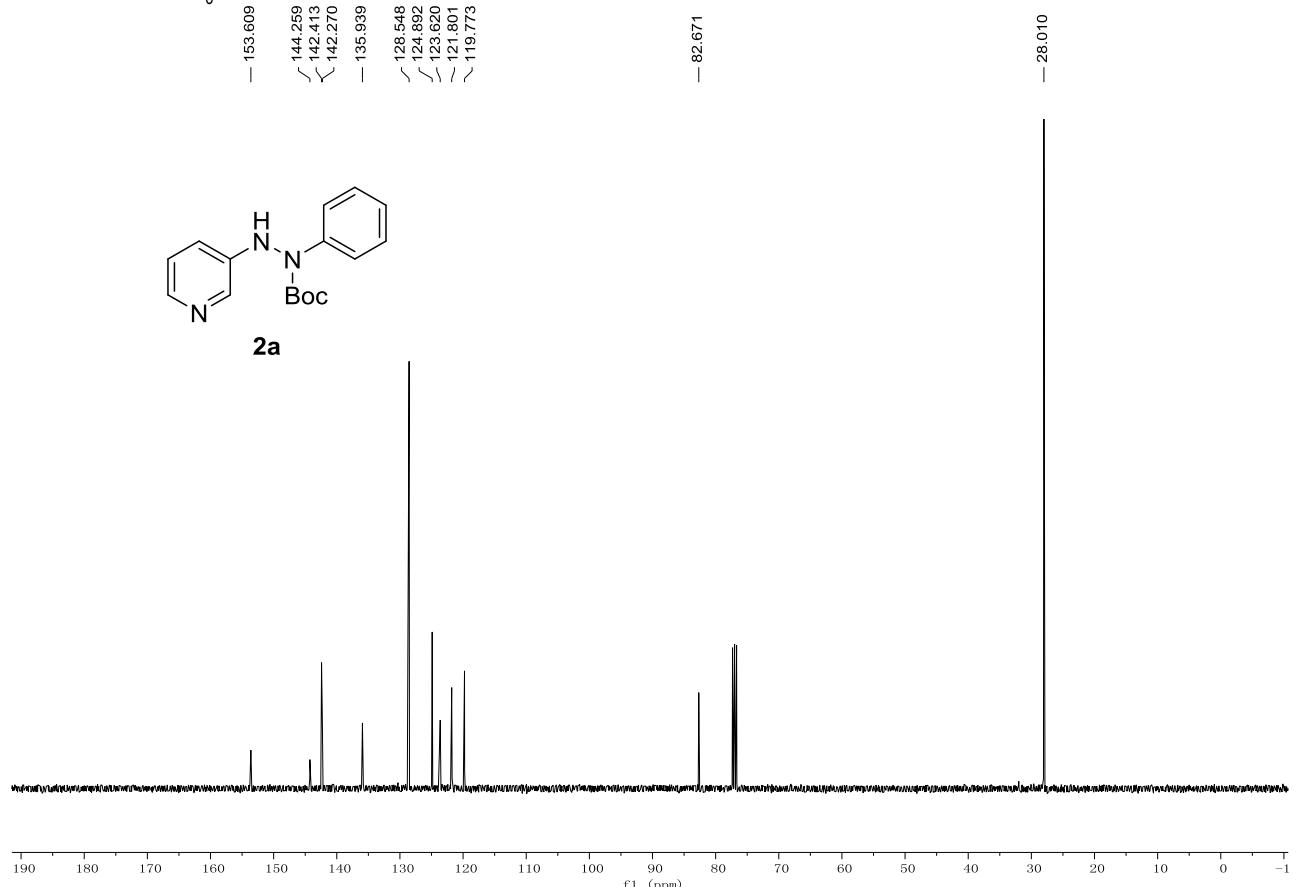
1h-3 $^{13}\text{C-NMR}$ CDCl_3 100M Hz



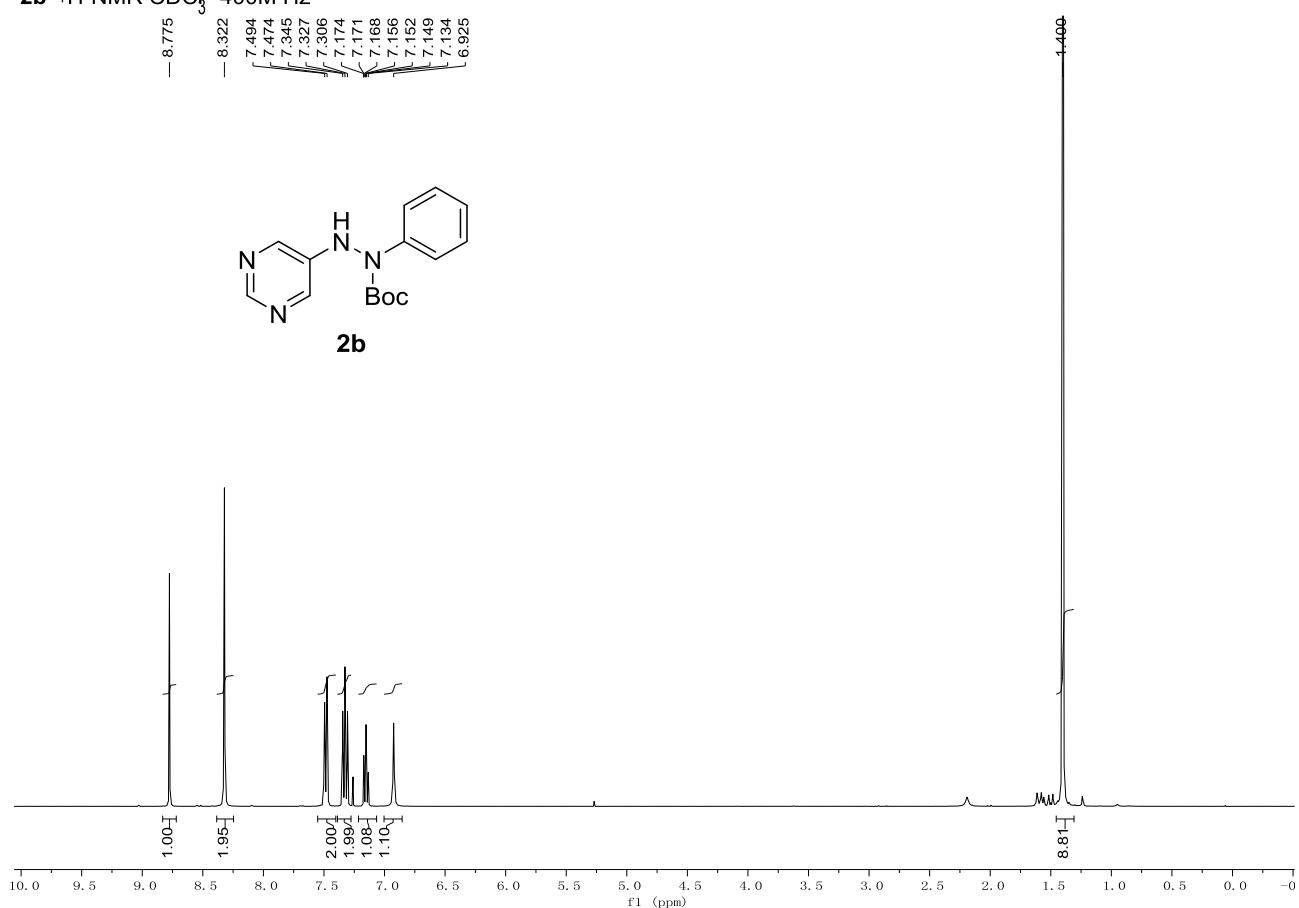
2a $^1\text{H-NMR}$ CDCl_3 400M Hz



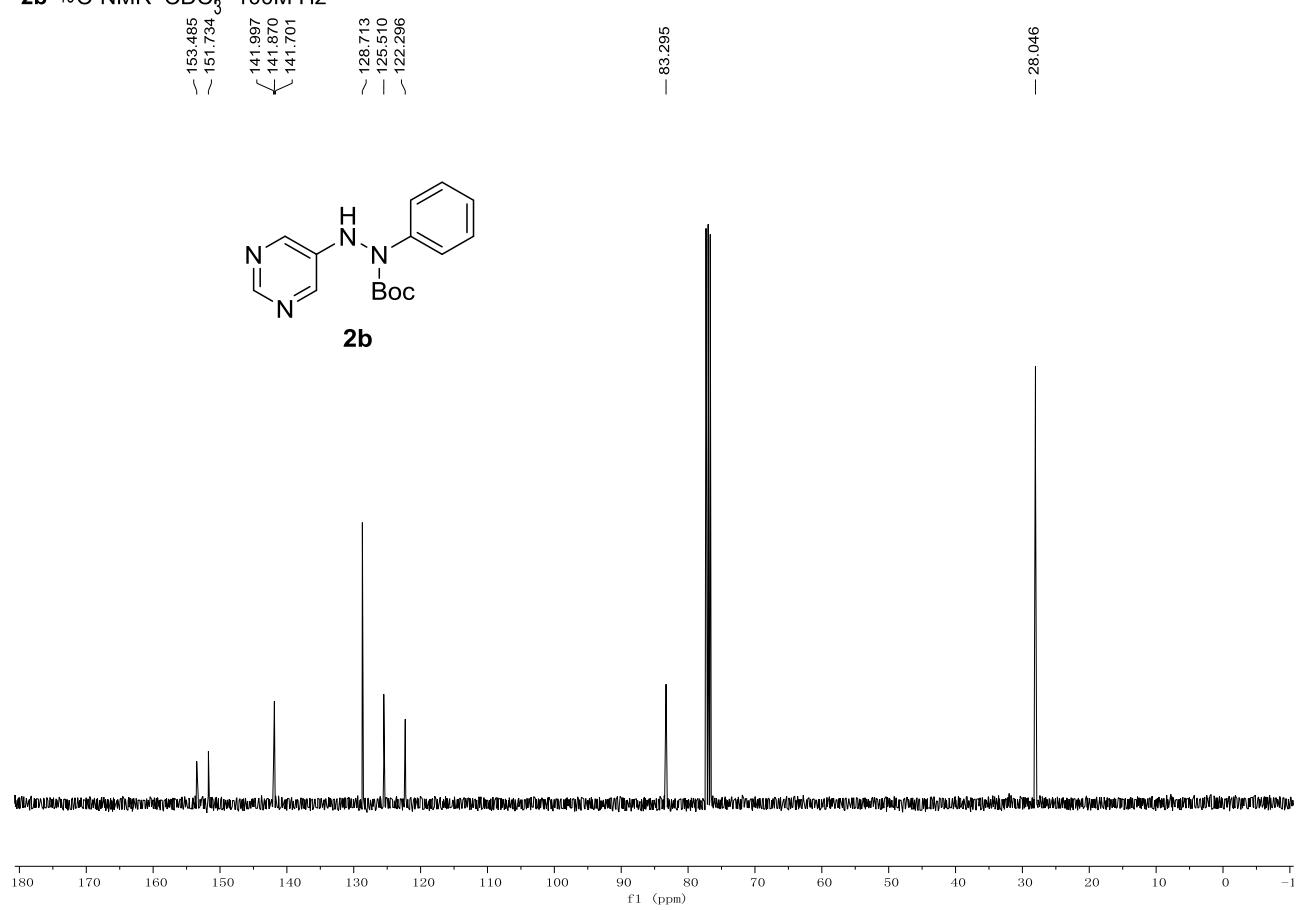
2a $^{13}\text{C-NMR}$ CDCl_3 100M Hz



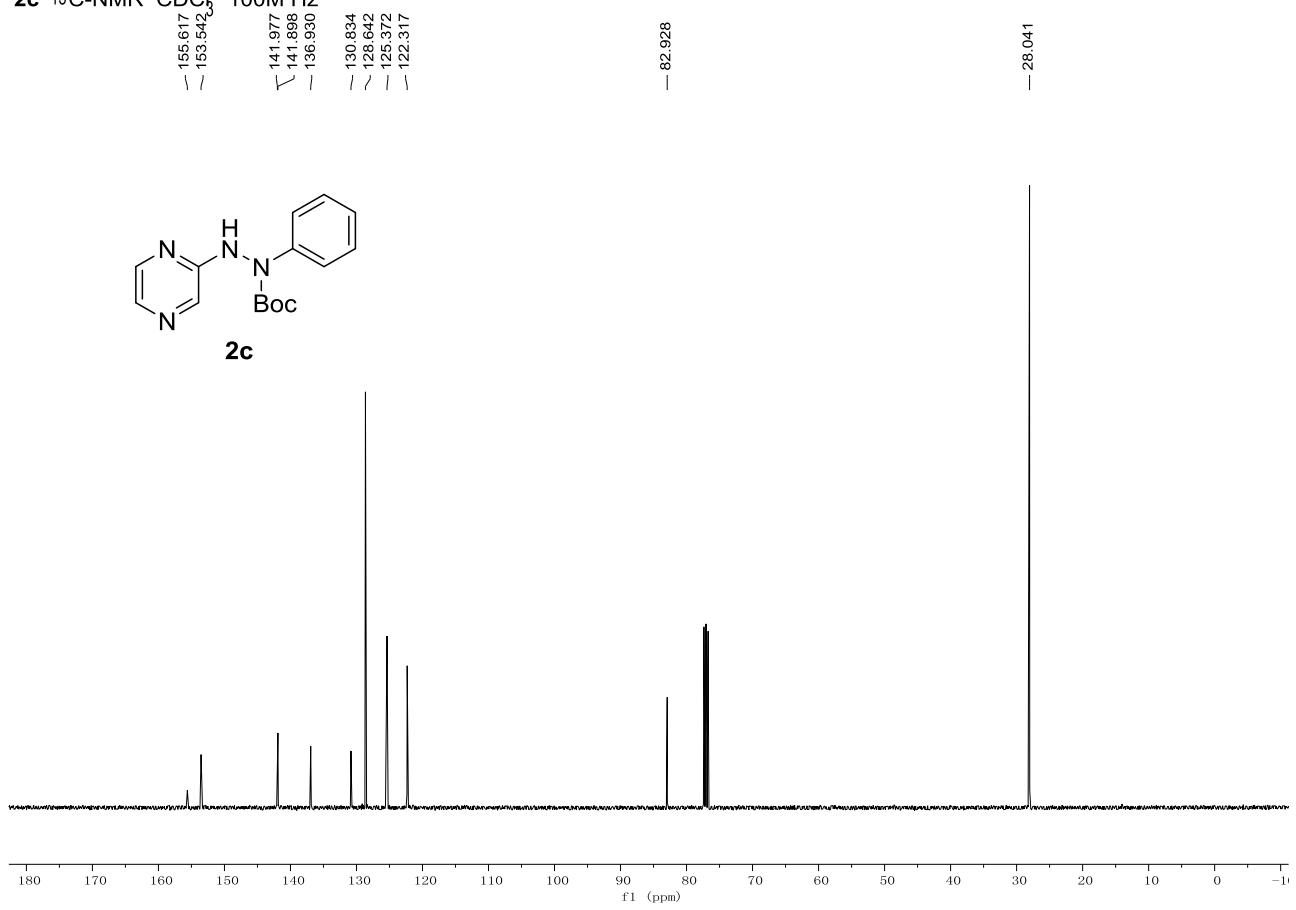
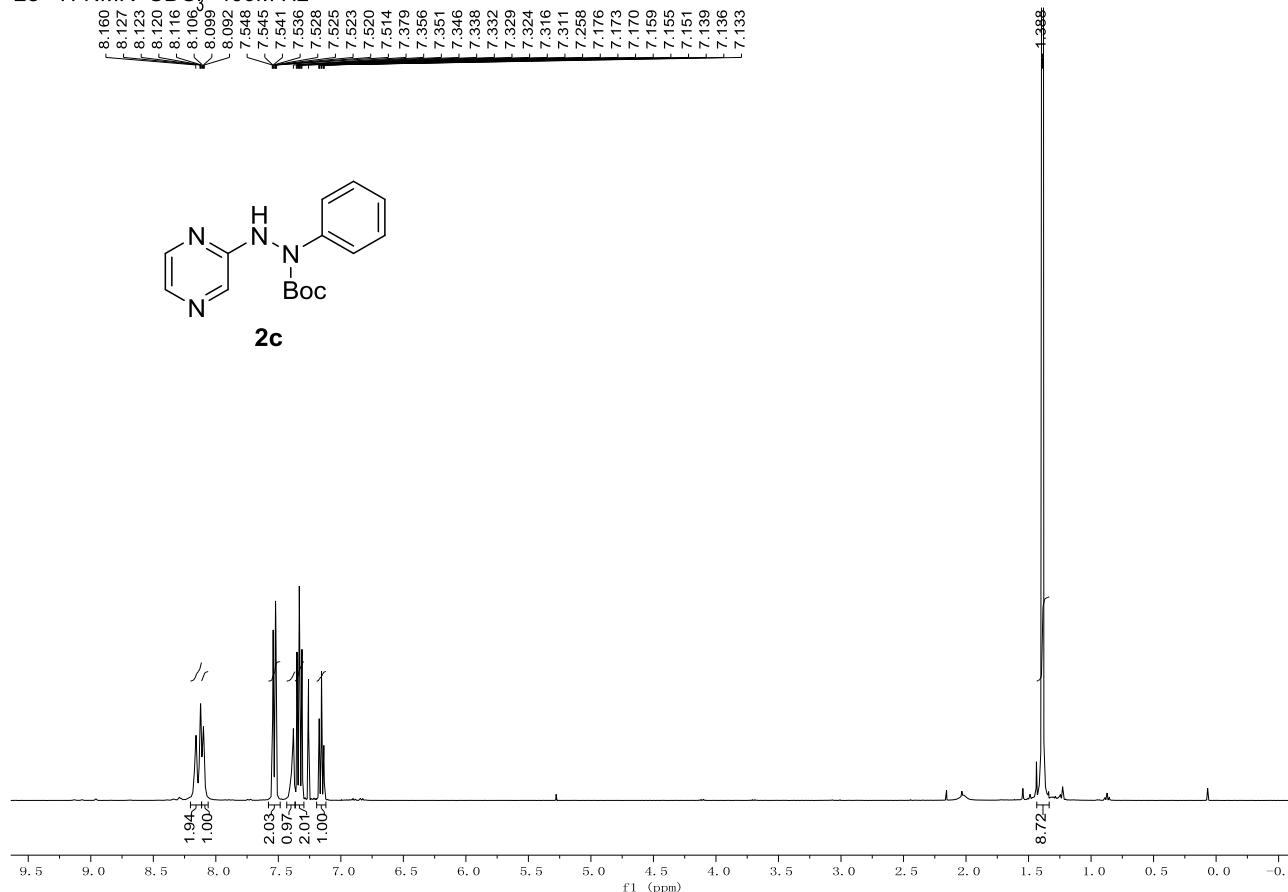
2b $^1\text{H-NMR}$ CDCl_3 400M Hz



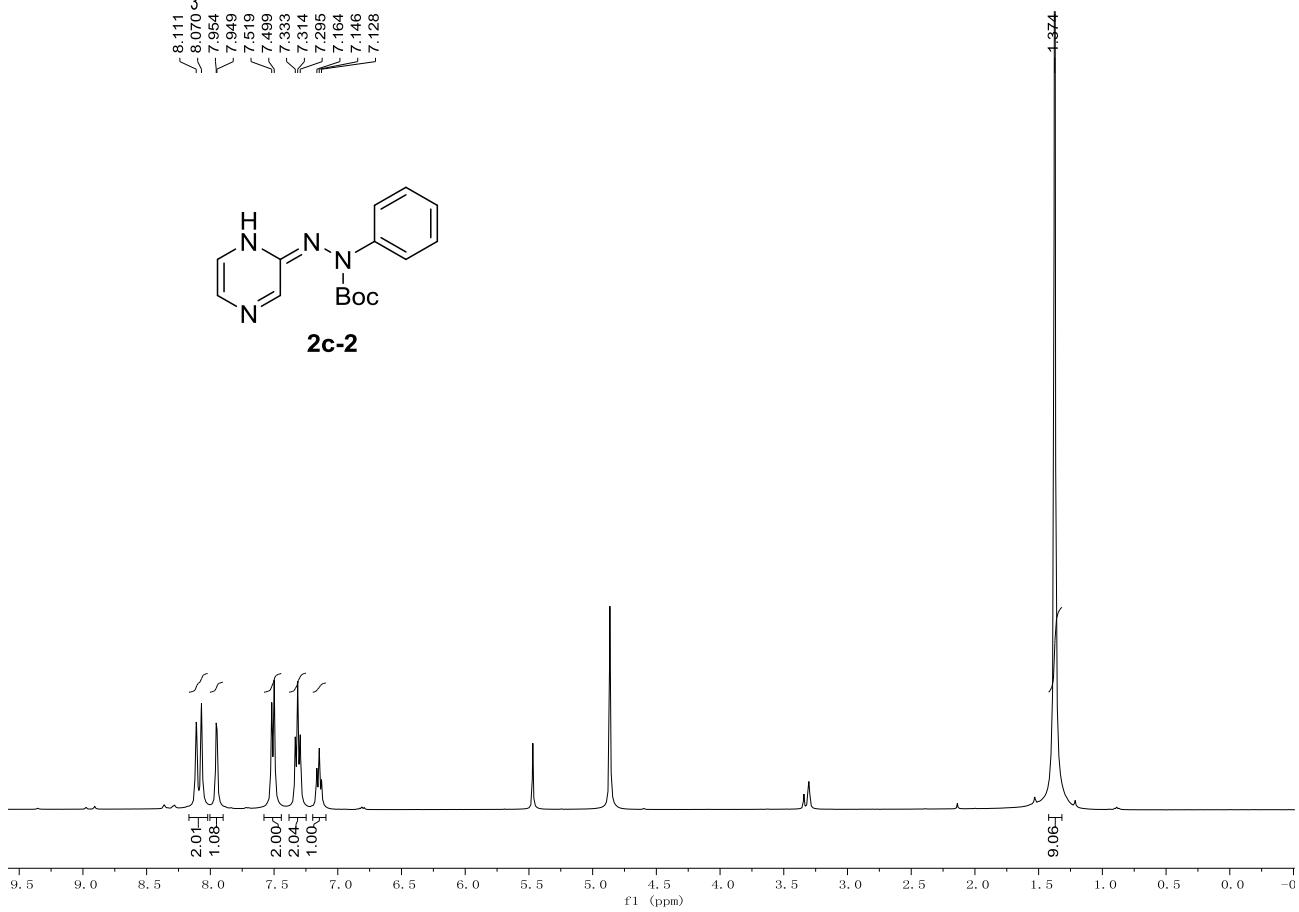
2b $^{13}\text{C-NMR}$ CDCl_3 100M Hz



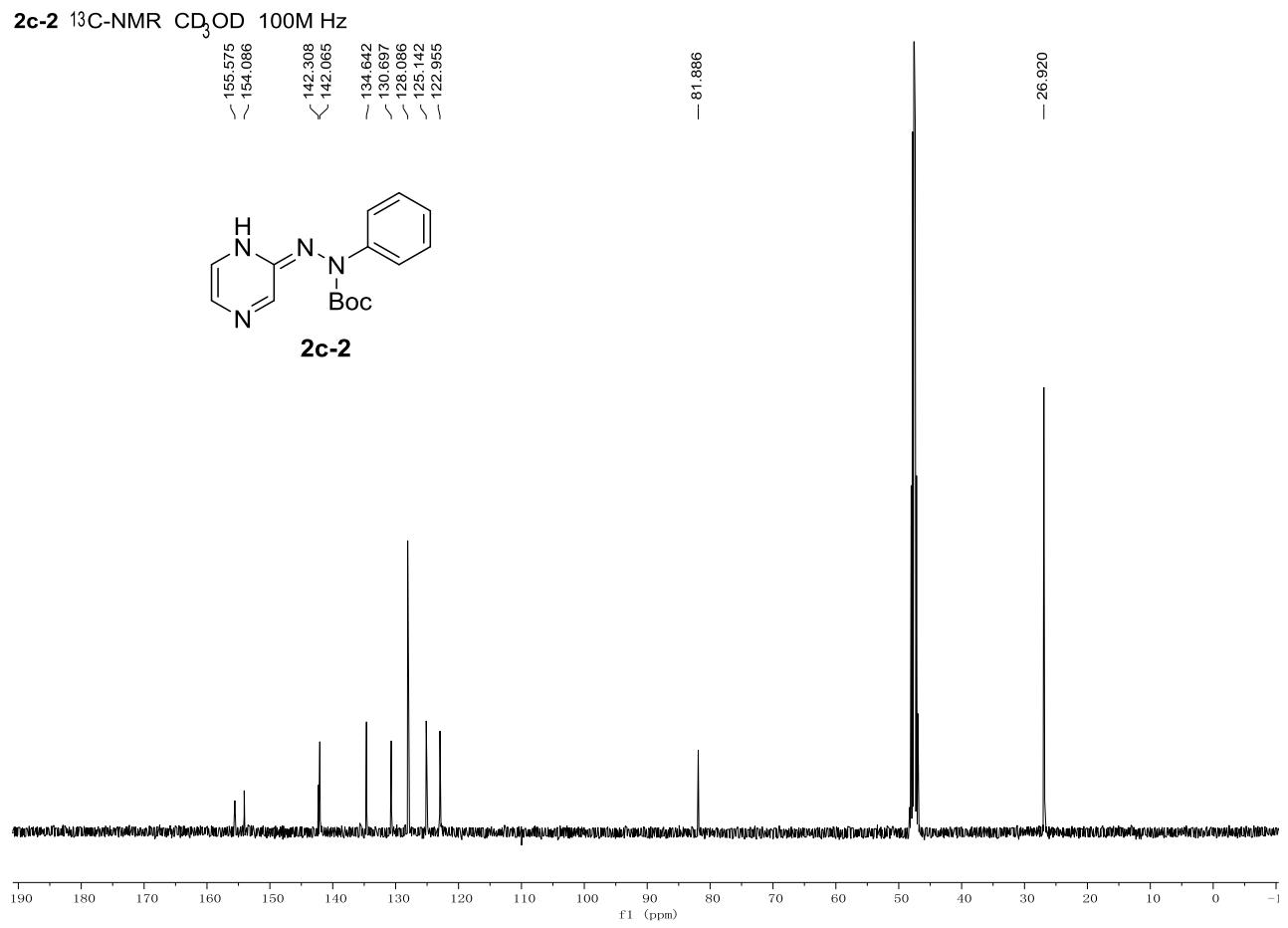
2c $^1\text{H-NMR}$ CDCl_3 400M Hz



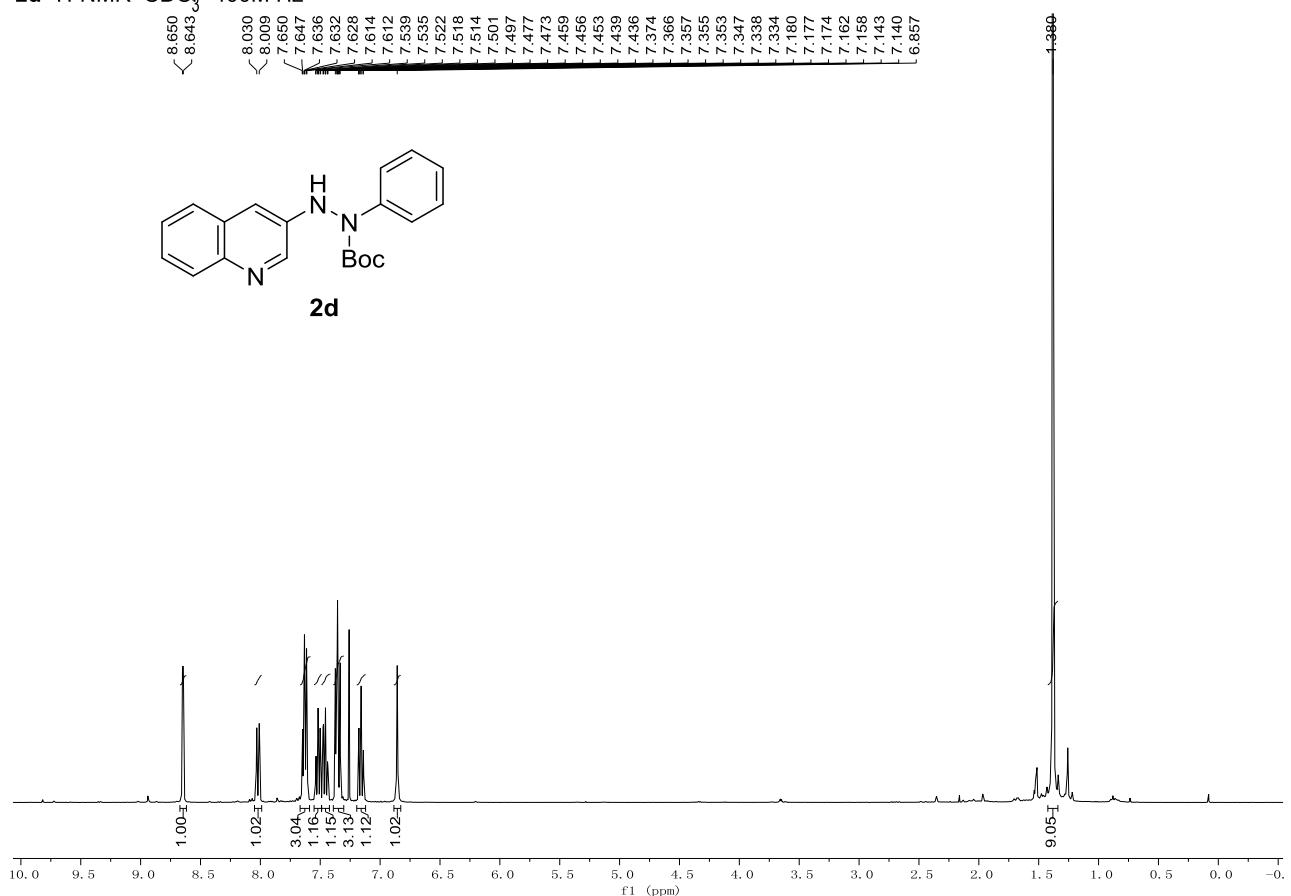
2c-2 $^1\text{H-NMR}$ CD_3OD 400M Hz



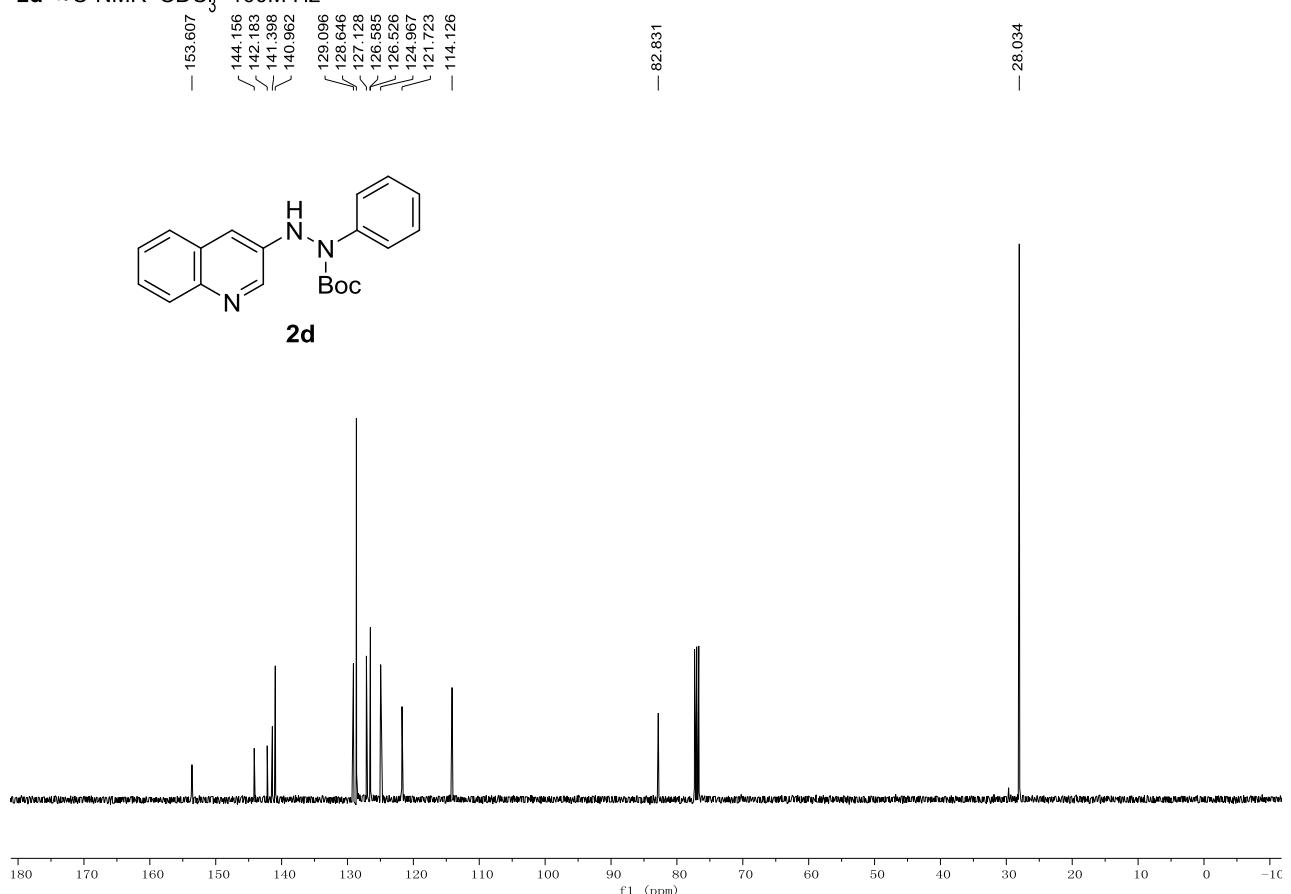
2c-2 $^{13}\text{C-NMR}$ CD_3OD 100M Hz

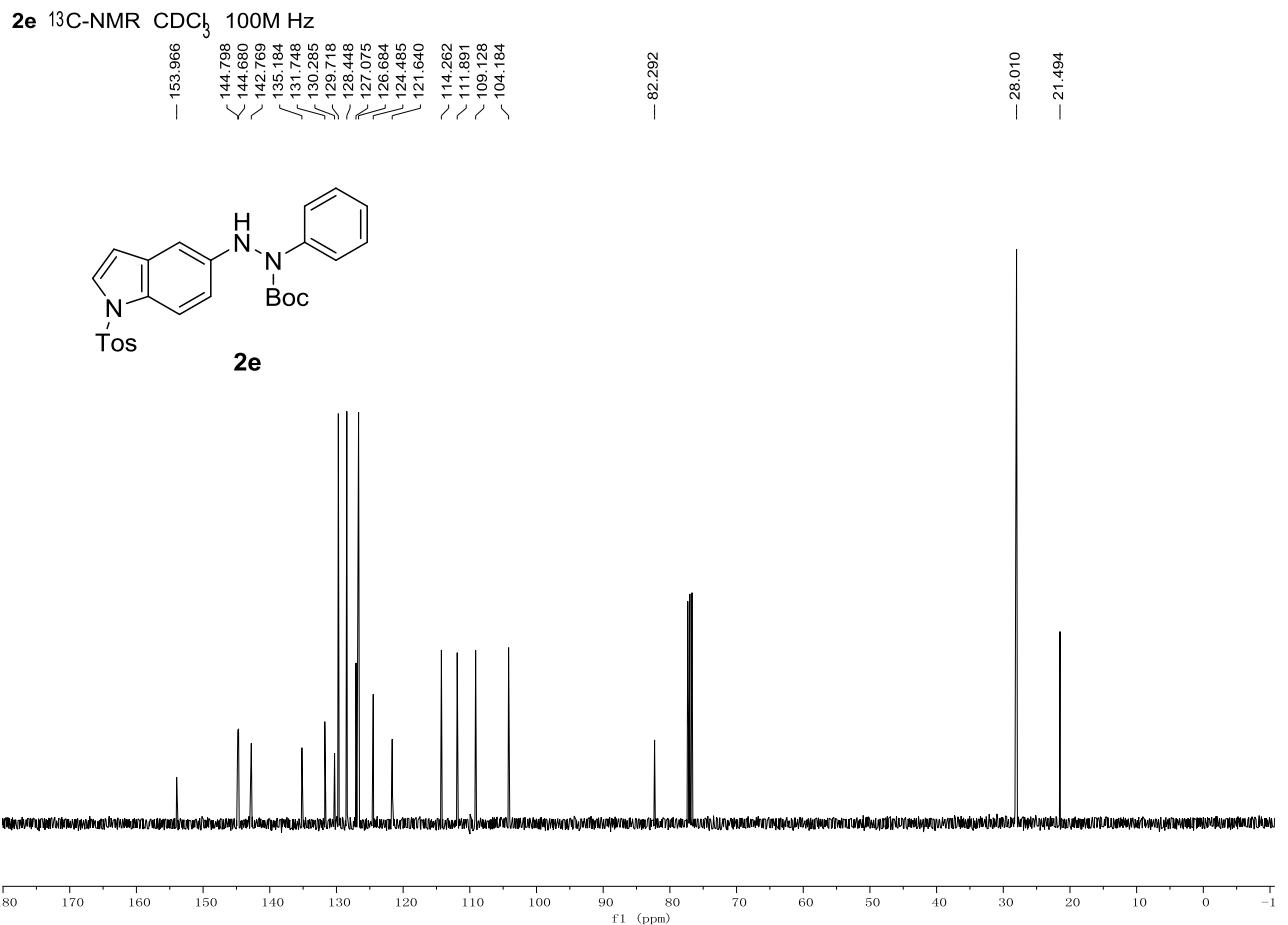
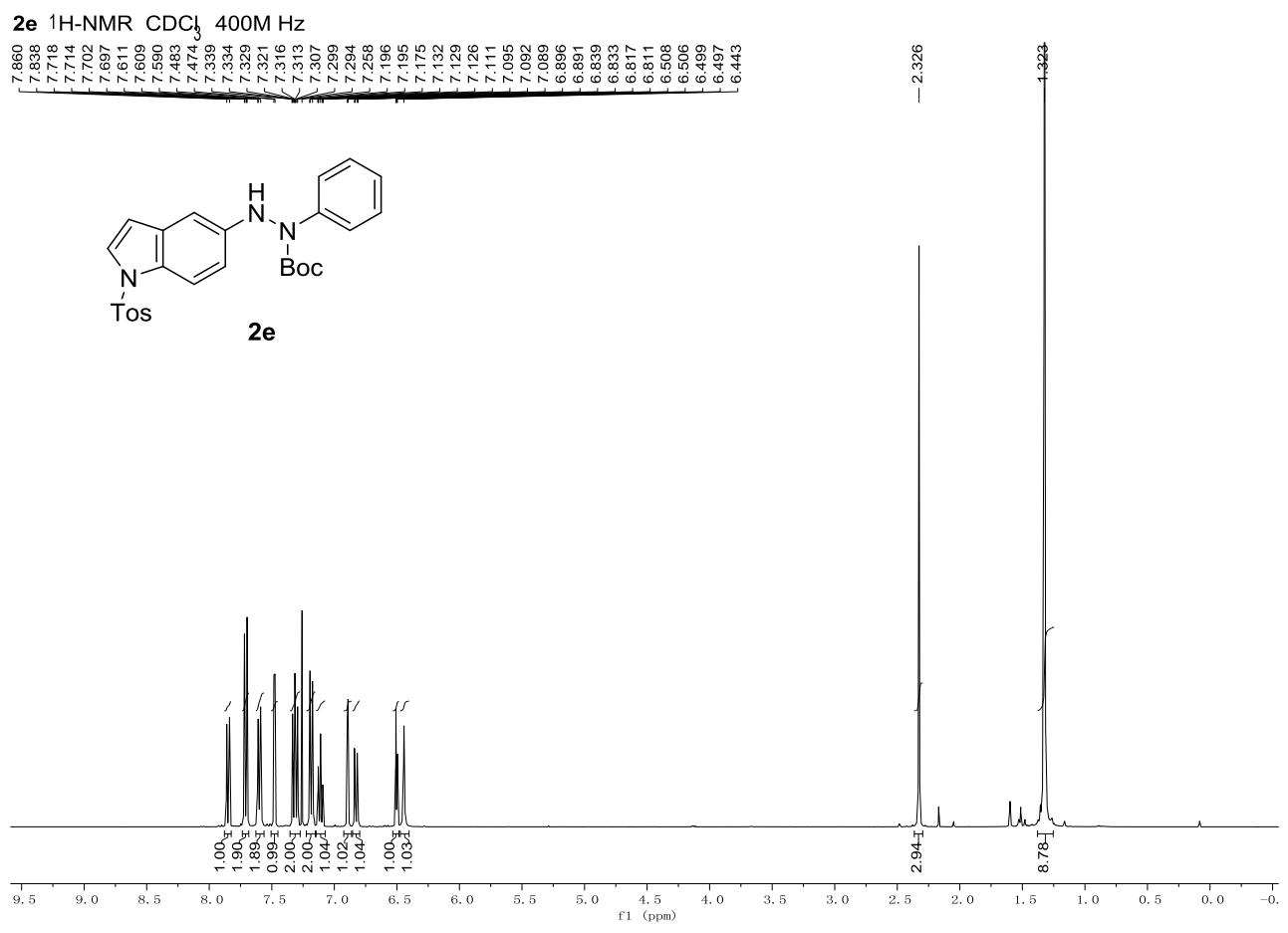


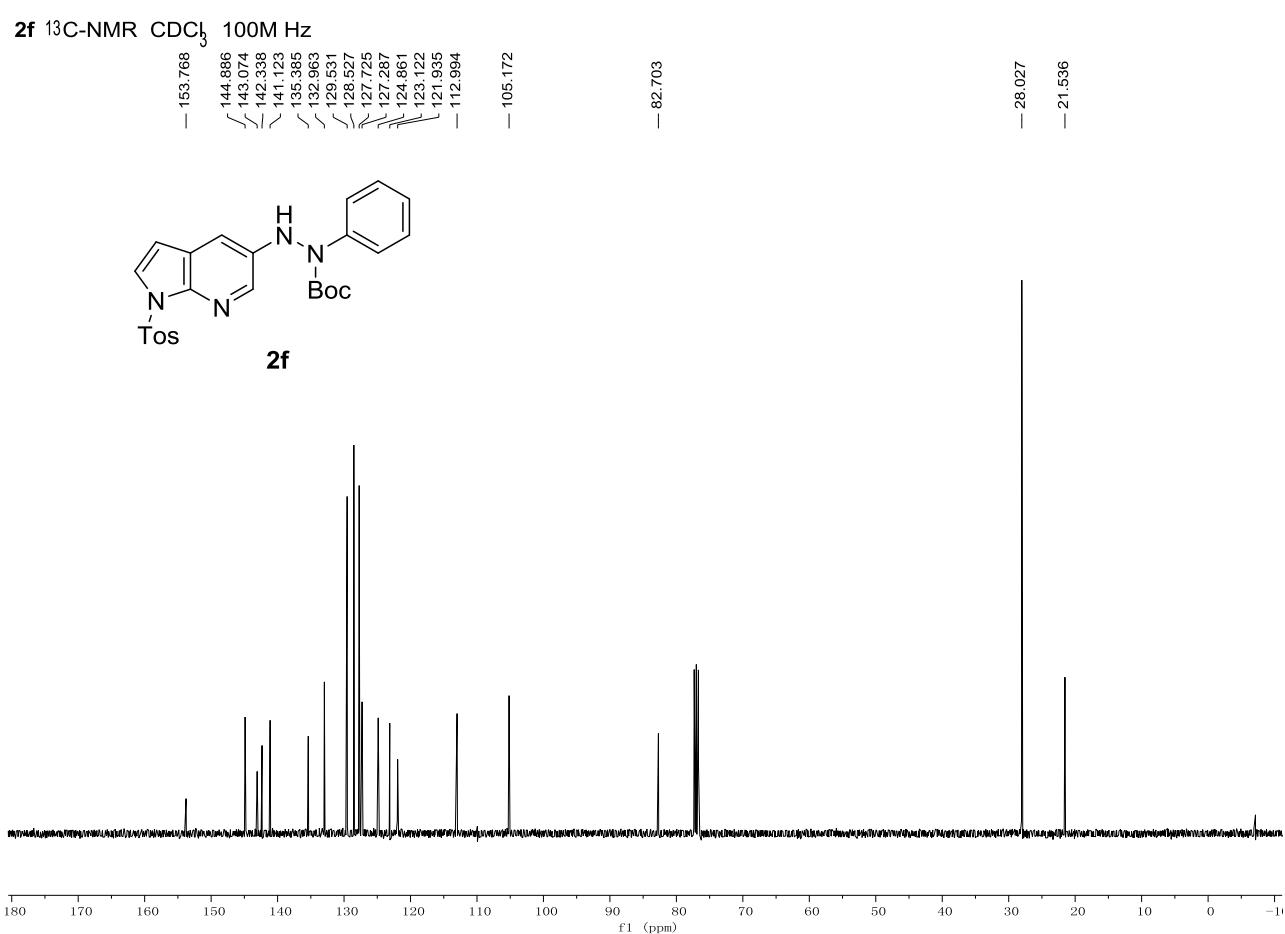
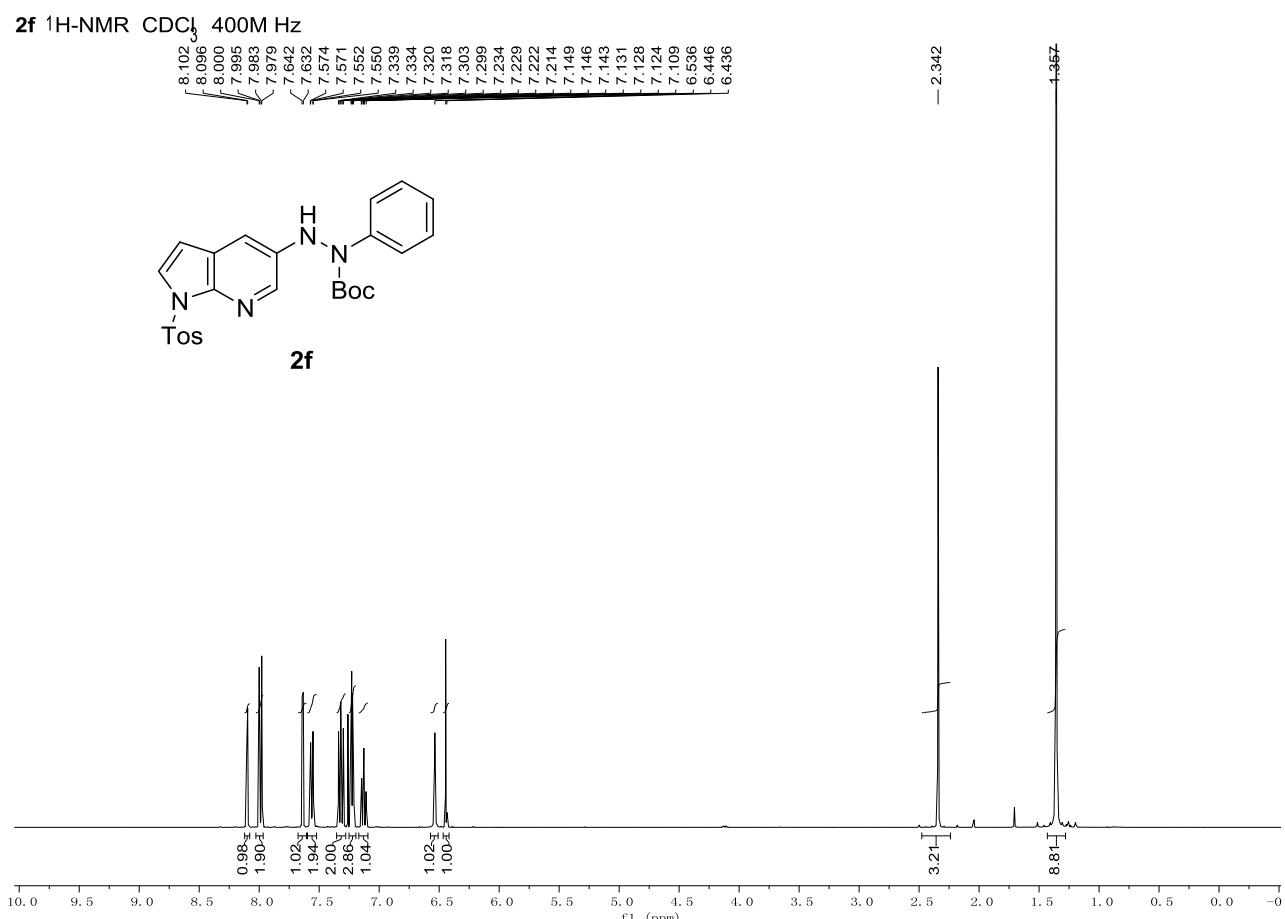
2d $^1\text{H-NMR}$ CDCl_3 400M Hz

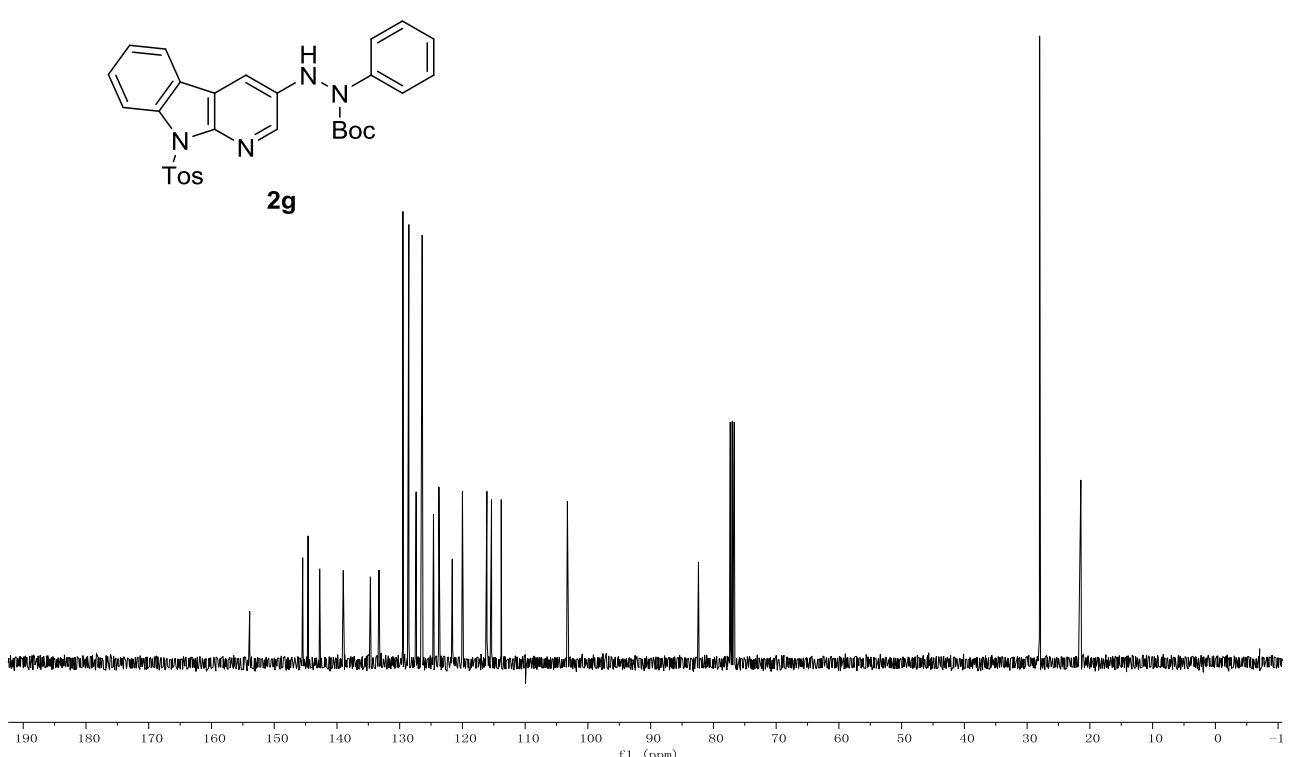
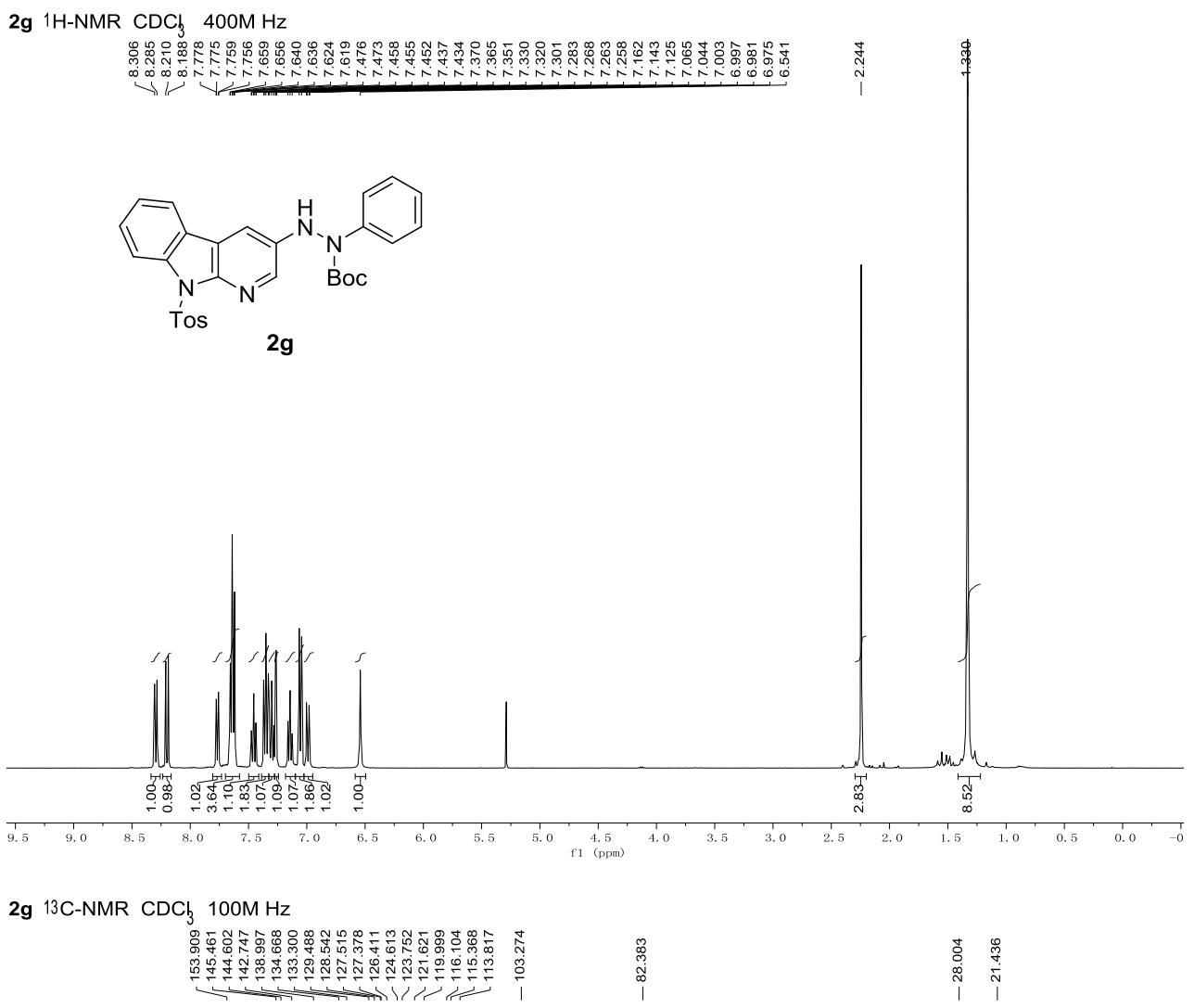


2d $^{13}\text{C-NMR}$ CDCl_3 100M Hz

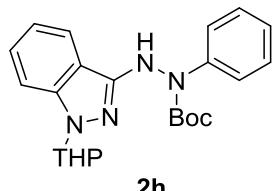




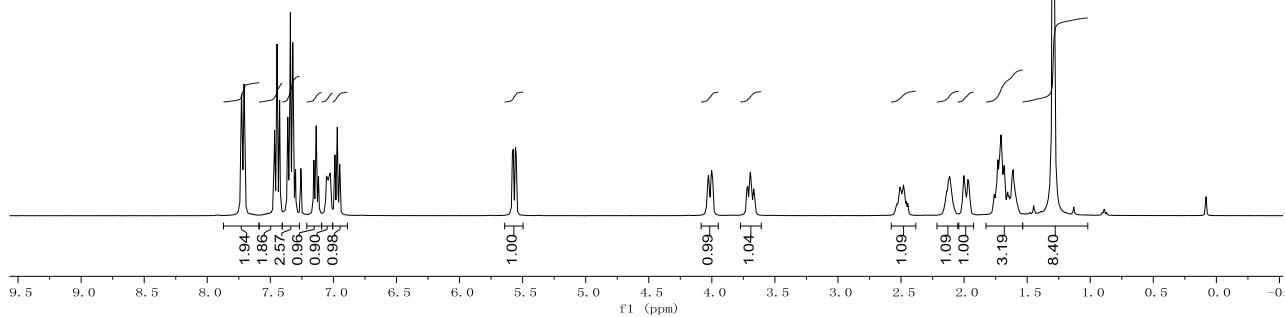




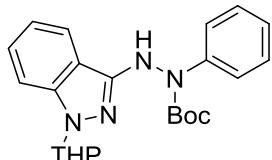
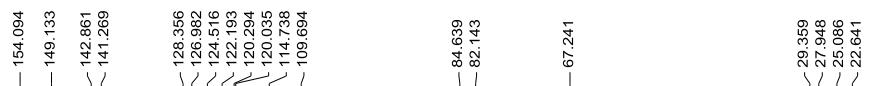
2h $^1\text{H-NMR}$ CDCl_3 , 400M Hz



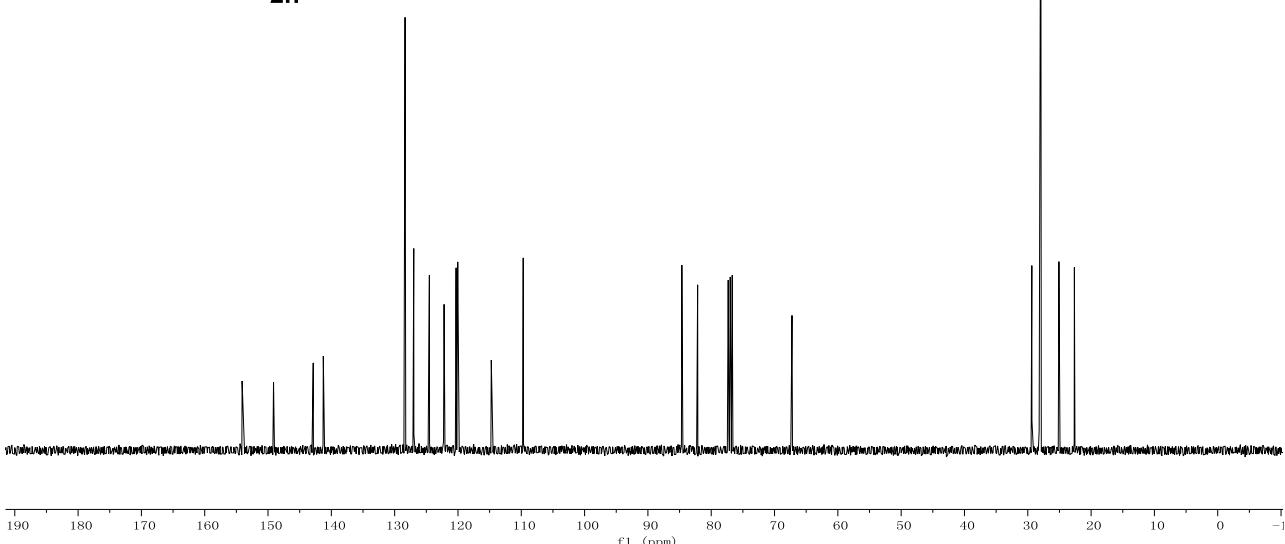
2h



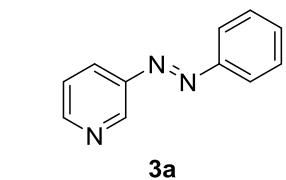
2h ^{13}C -NMR CDCl_3 100M Hz



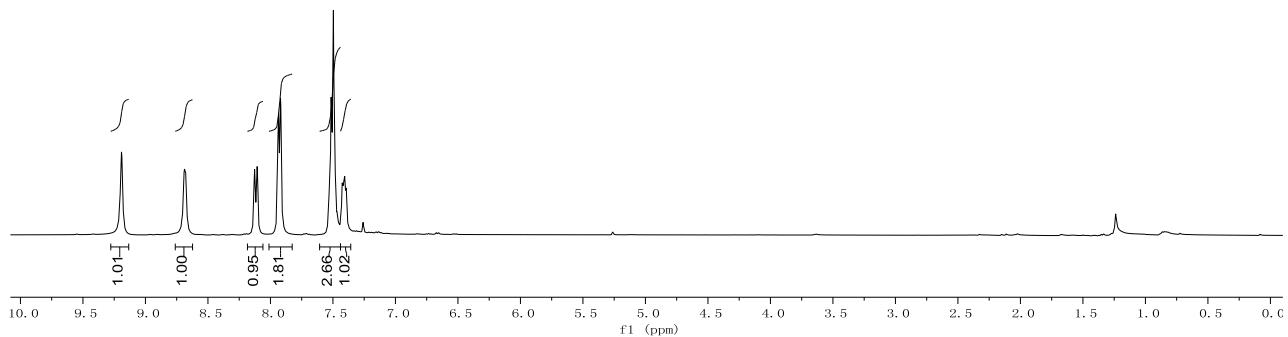
2h



3a $^1\text{H-NMR}$ CDCl_3 400M Hz

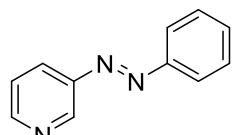


3a

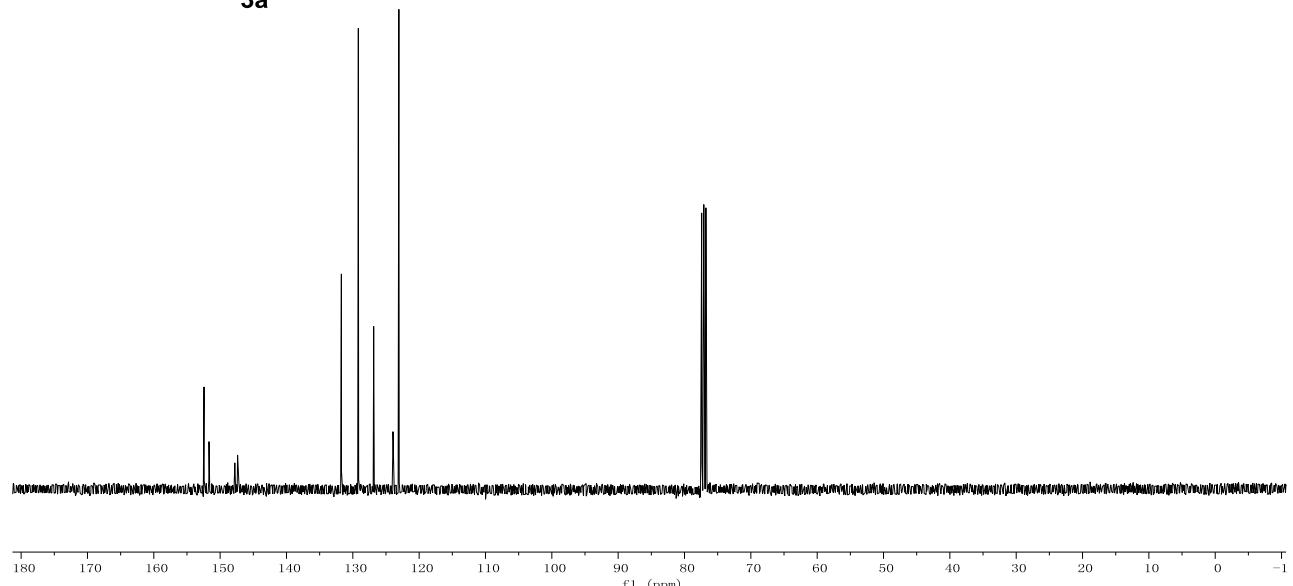


3a $^{13}\text{C-NMR}$ CDCl_3 100M Hz

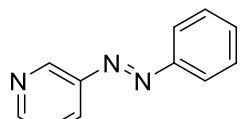
152.427
151.675
147.787
147.372
131.729
129.169
126.854
123.941
123.058



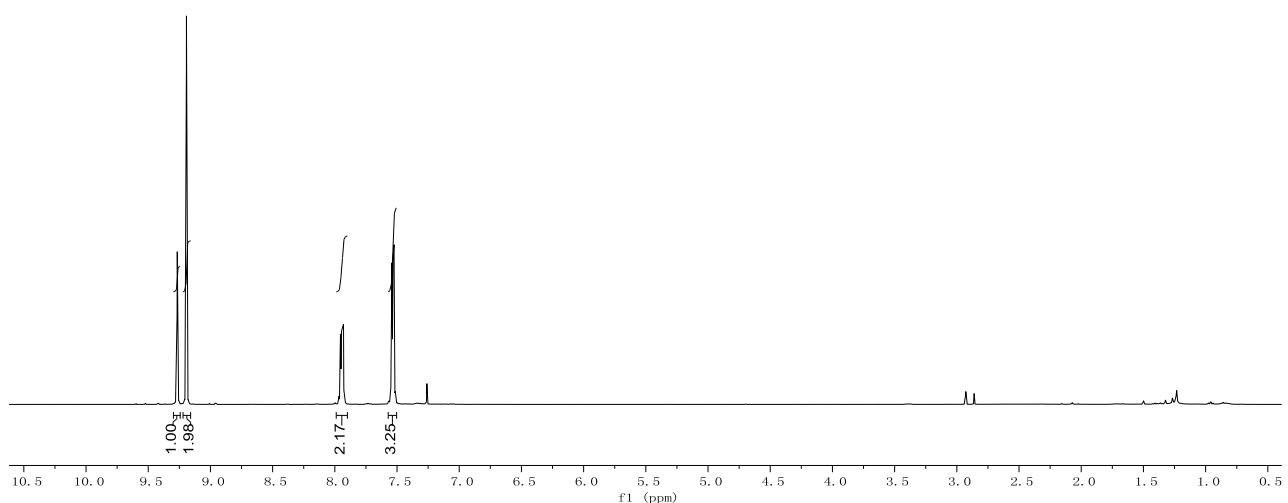
3a



3b $^1\text{H-NMR}$ CDCl_3 400M Hz

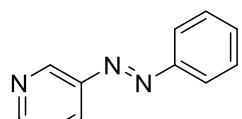


3b

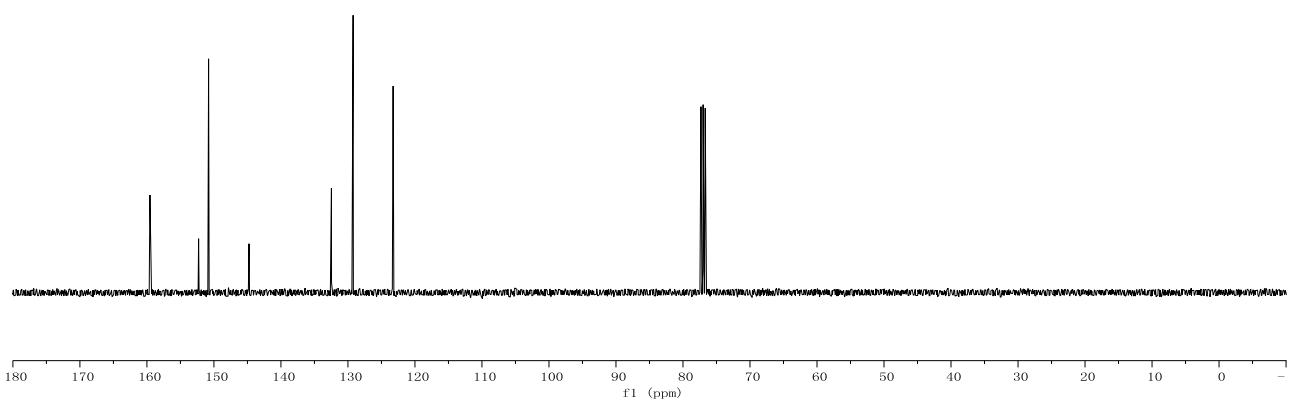


3b $^{13}\text{C-NMR}$ CDCl_3 100M Hz

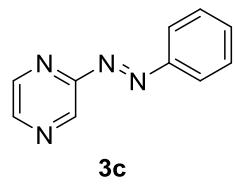
— 159.550
— 152.283
— 150.794
— 144.762
— 144.463
— 144.228
— 132.463
— 129.228
— 123.262



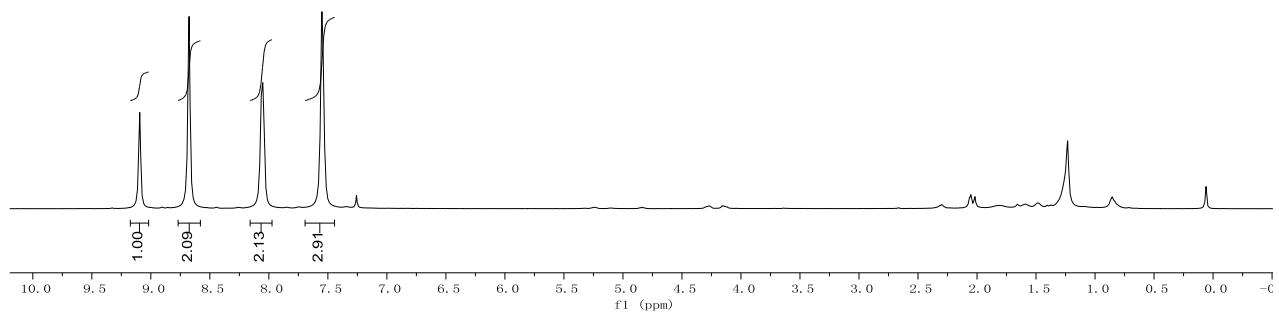
3b



3c $^1\text{H-NMR}$ CDCl_3 400M Hz

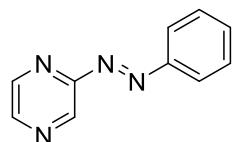


3c

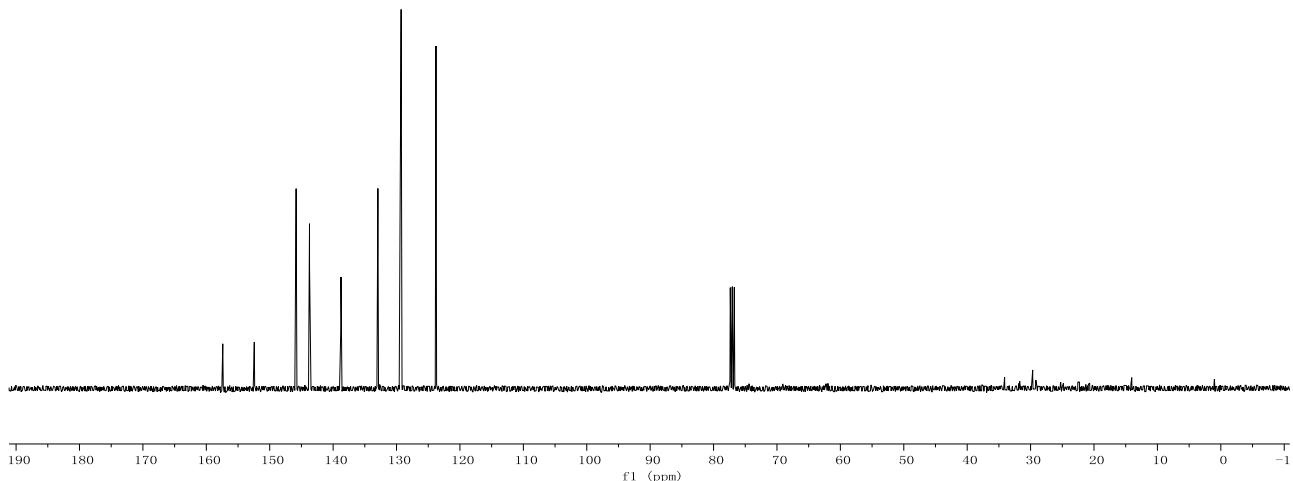


3c $^{13}\text{C-NMR}$ CDCl_3 100M Hz

Peak assignments (ppm):
157.404, 152.431, 145.837, 143.724, 138.763
132.941, 129.276, 123.781



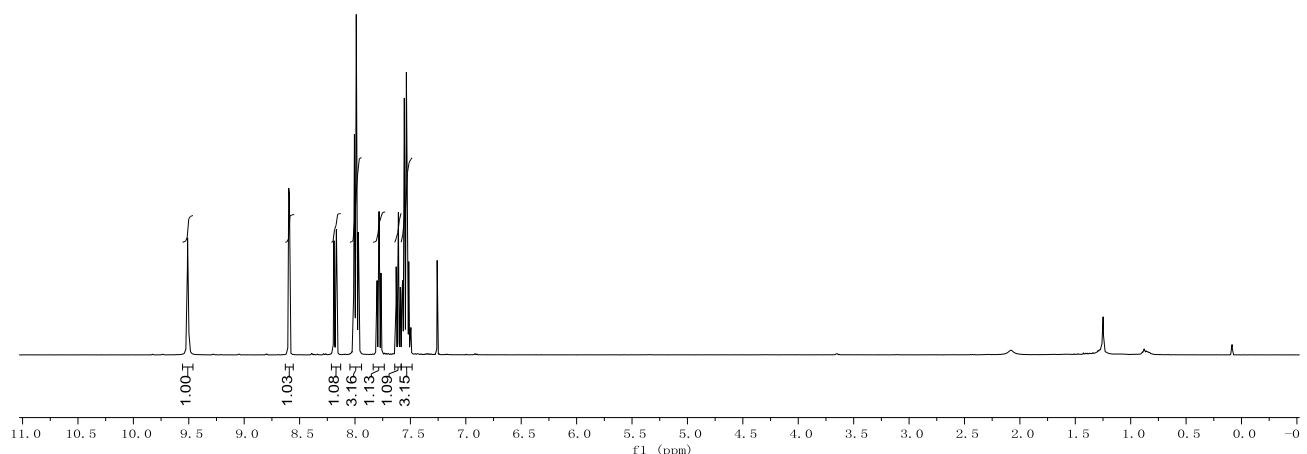
3c



3d $^1\text{H-NMR}$ CDCl_3 400M Hz



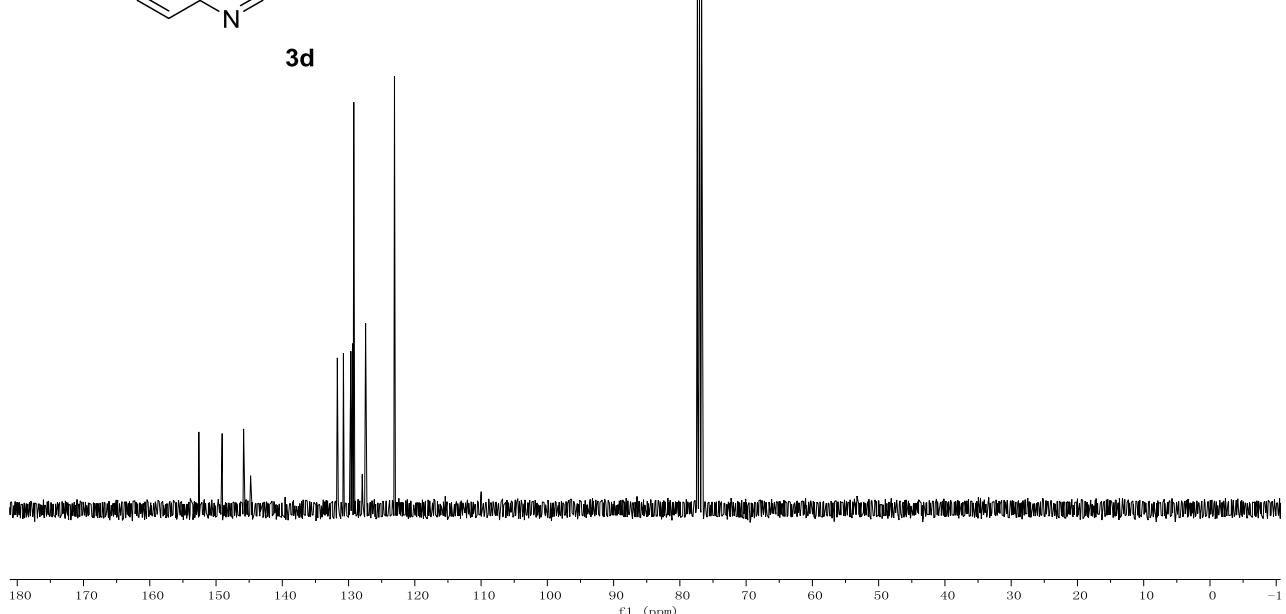
3d



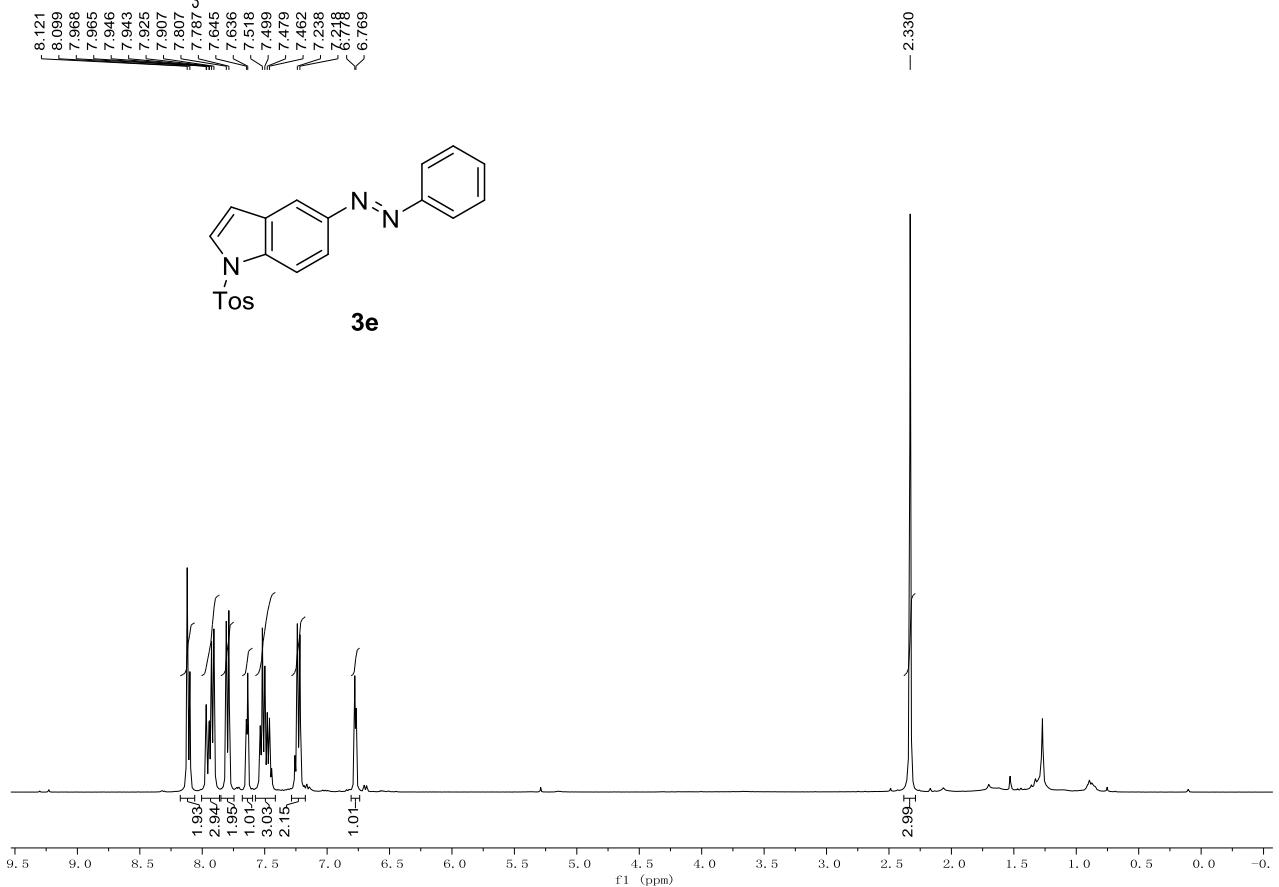
3d $^{13}\text{C-NMR}$ CDCl_3 100M Hz



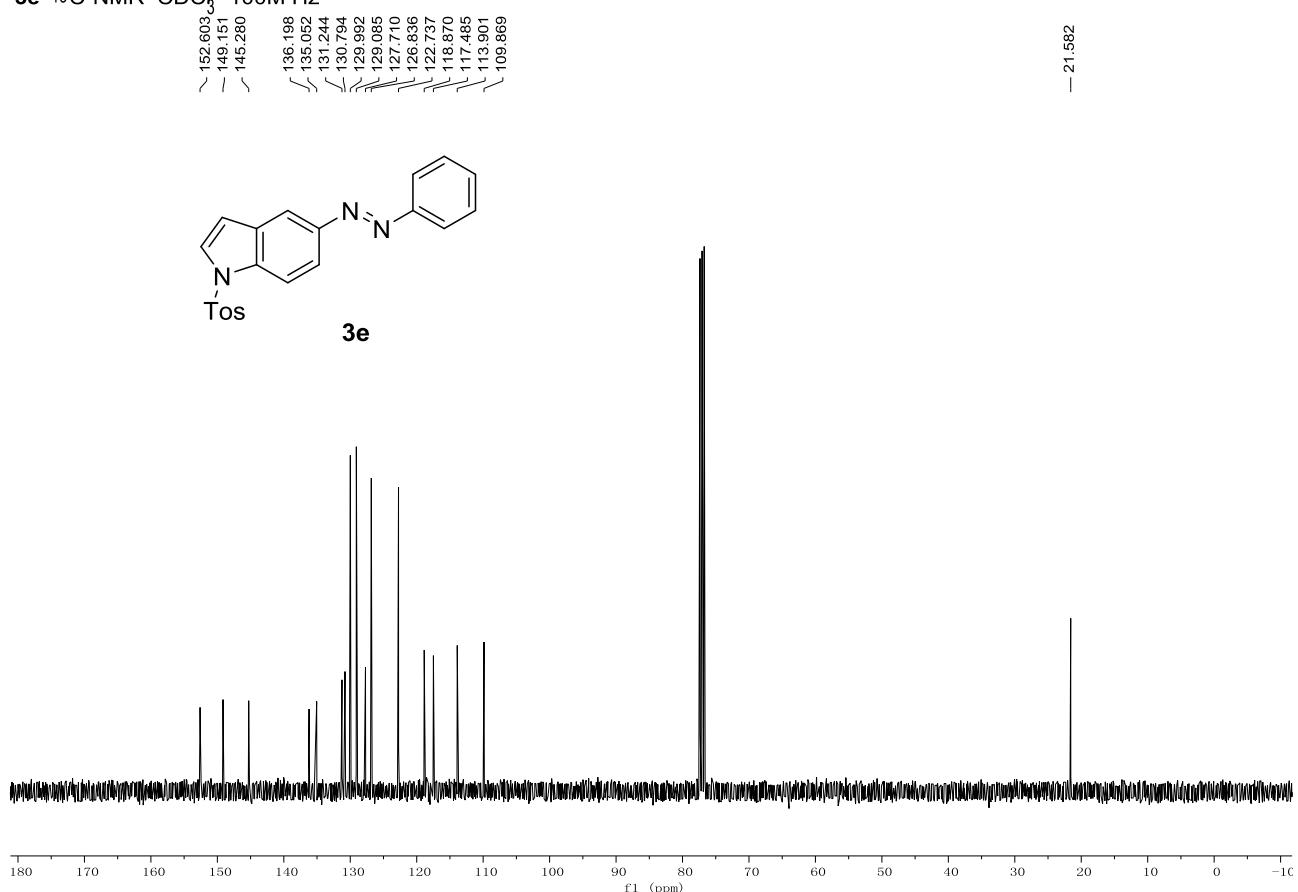
3d



3e $^1\text{H-NMR}$ CDCl_3 400M Hz



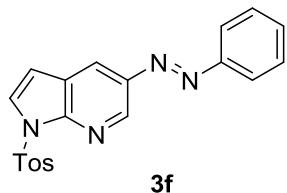
3e $^{13}\text{C-NMR}$ CDCl_3 100M Hz



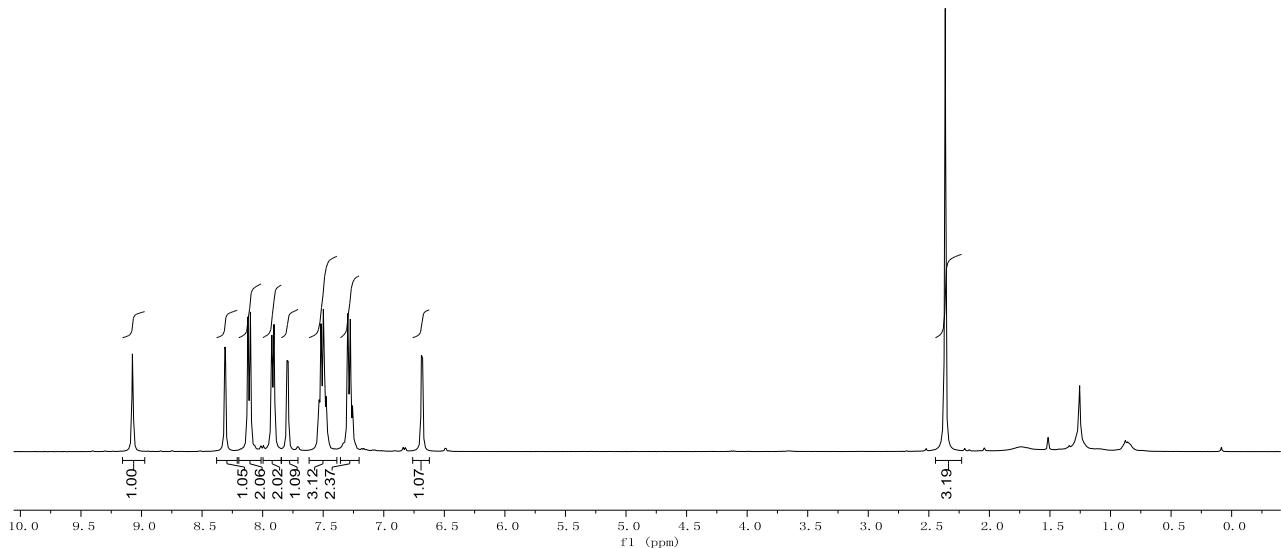
3f $^1\text{H-NMR}$ CDCl_3 400M Hz

9.075
9.071
8.312
8.122
8.101
7.924
7.906
7.799
7.789
7.534
7.518
7.499
7.476
7.297
7.276
6.689
6.679

— 2.364



3f

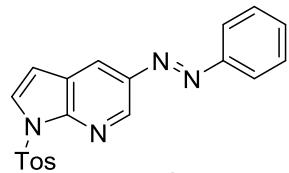


3f $^{13}\text{C-NMR}$ CDCl_3 100M Hz

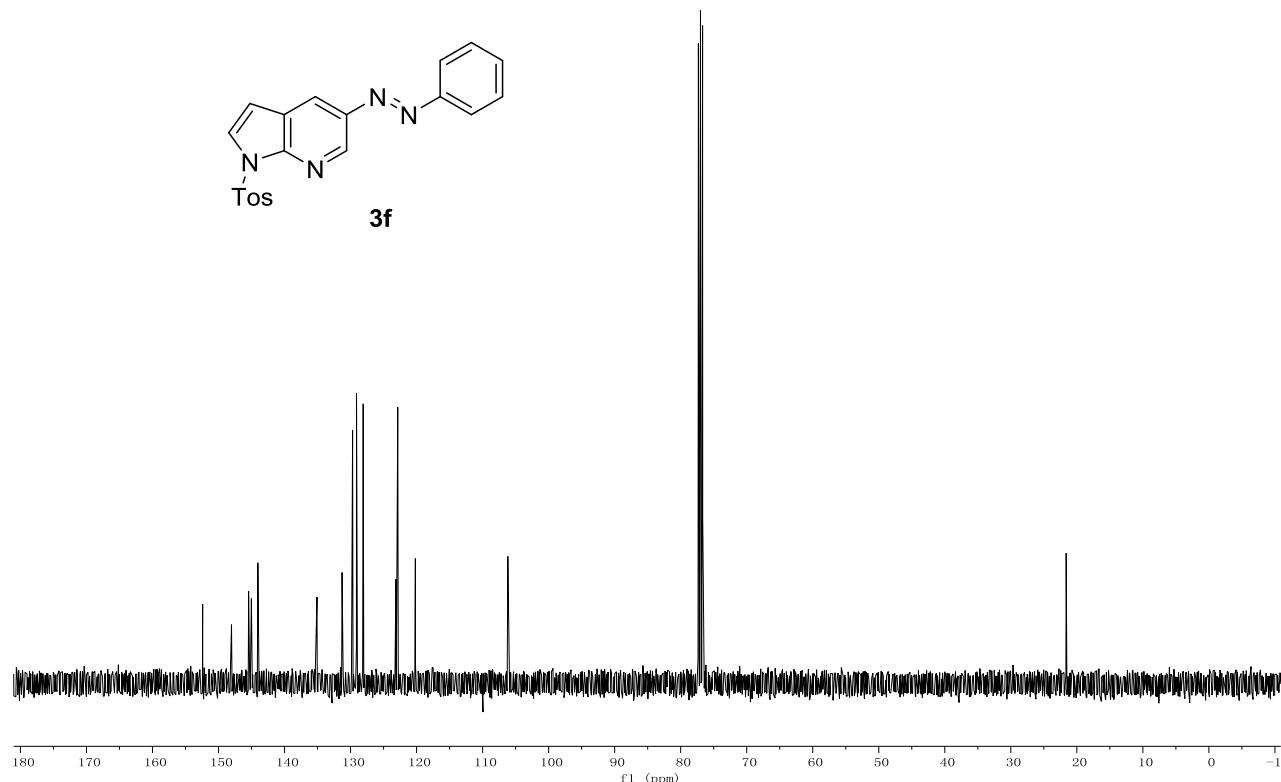
152.400
148.033
145.441
145.020
144.039
135.083
131.284
129.687
129.097
128.116
128.088
123.131
122.850
120.187

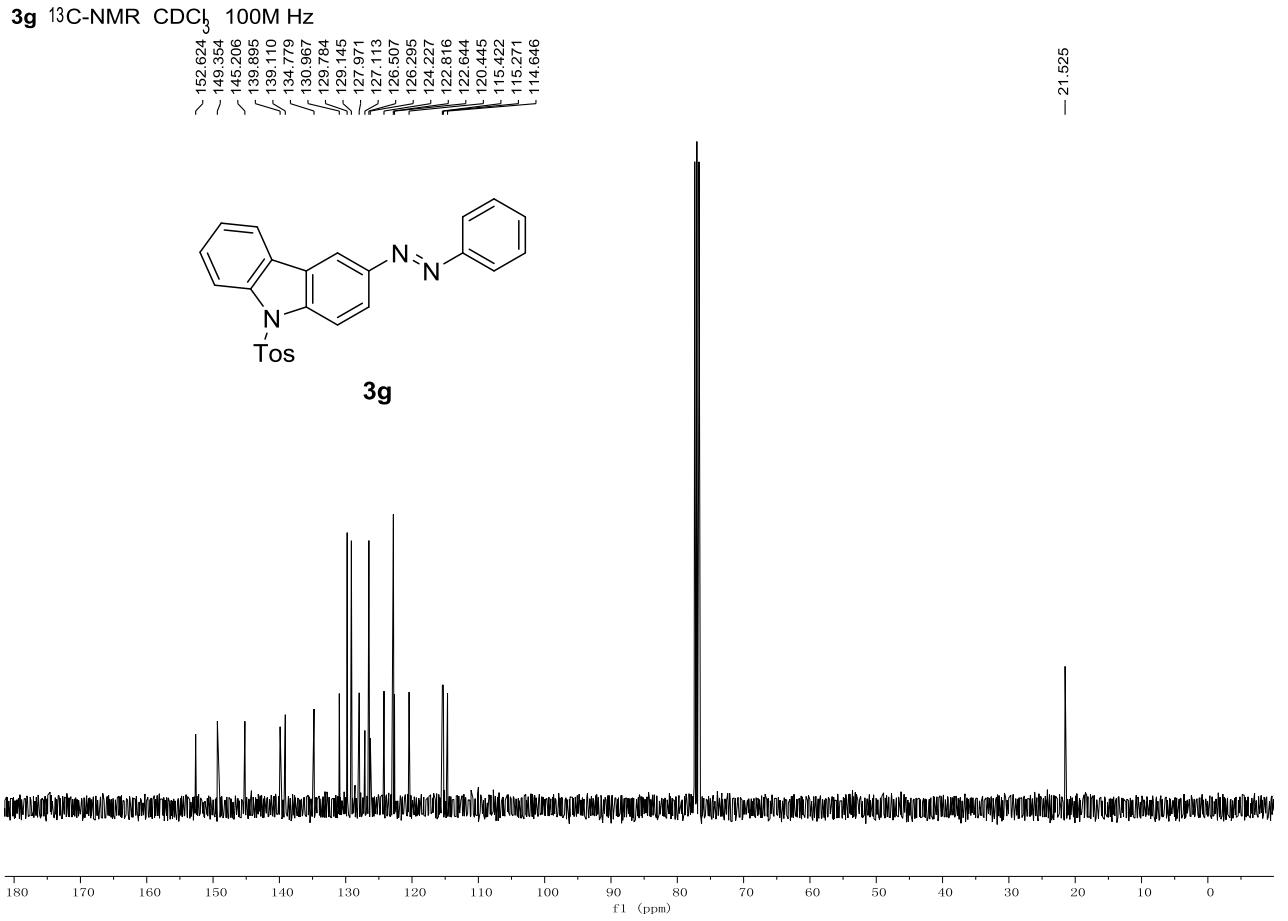
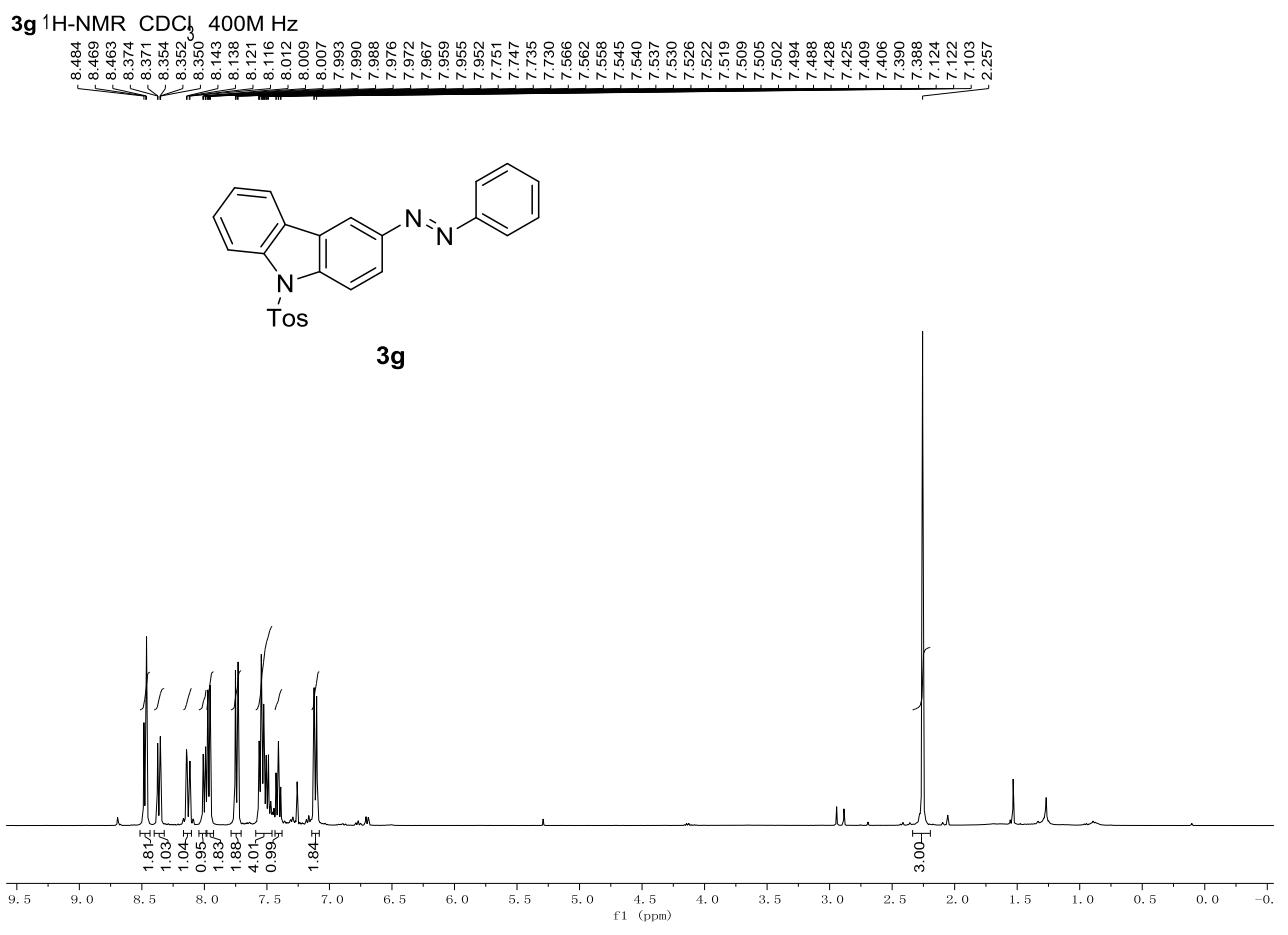
— 106.181

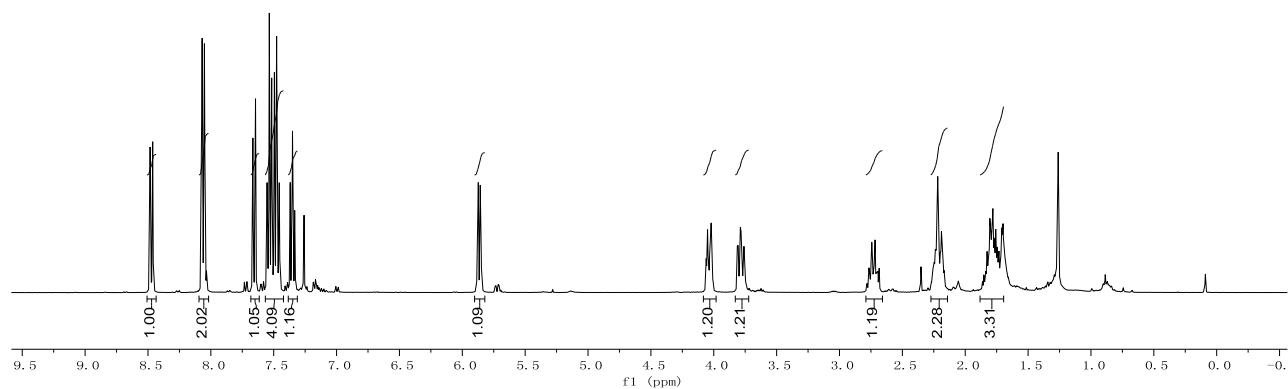
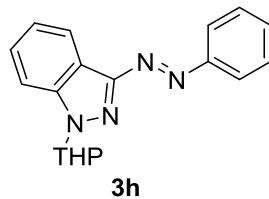
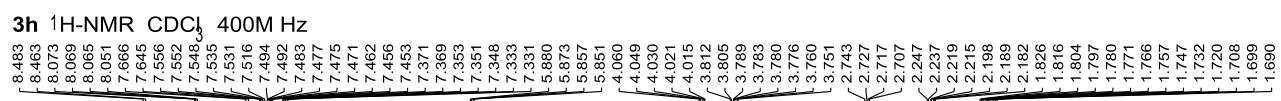
— 21.617



3f



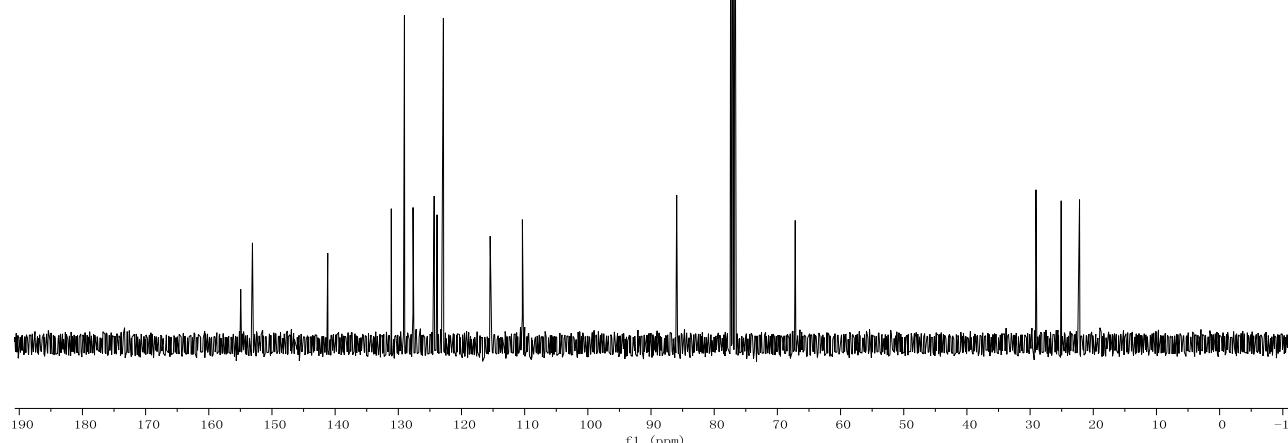
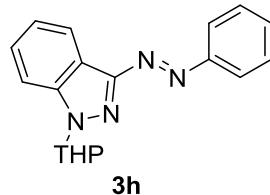




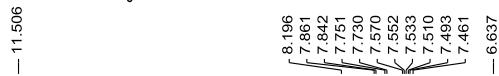
3h $^{13}\text{C-NMR}$ CDCl_3 100M Hz

-154.948
-153.090
-141.171
131.114
129.034
127.672
124.324
123.869
122.864
-115.461
-110.361

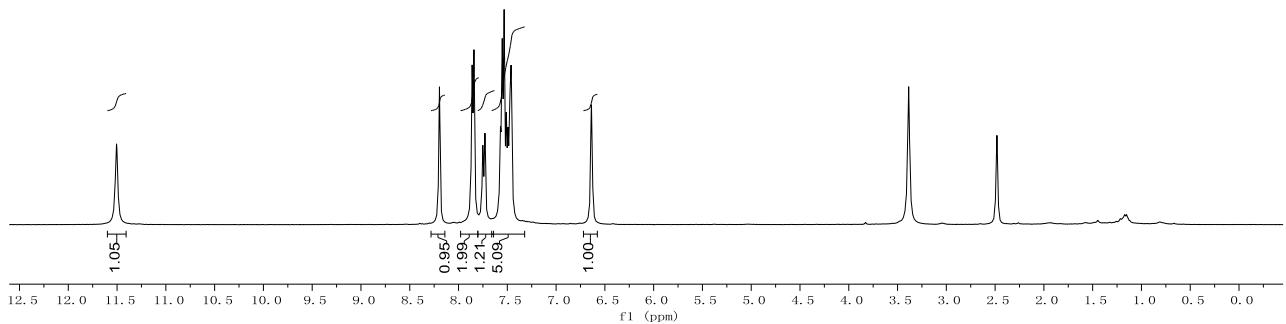
-85.941
-67.175
-29.073
-25.078
-22.173



5e $^1\text{H-NMR}$ DMSO- d_6 400M Hz



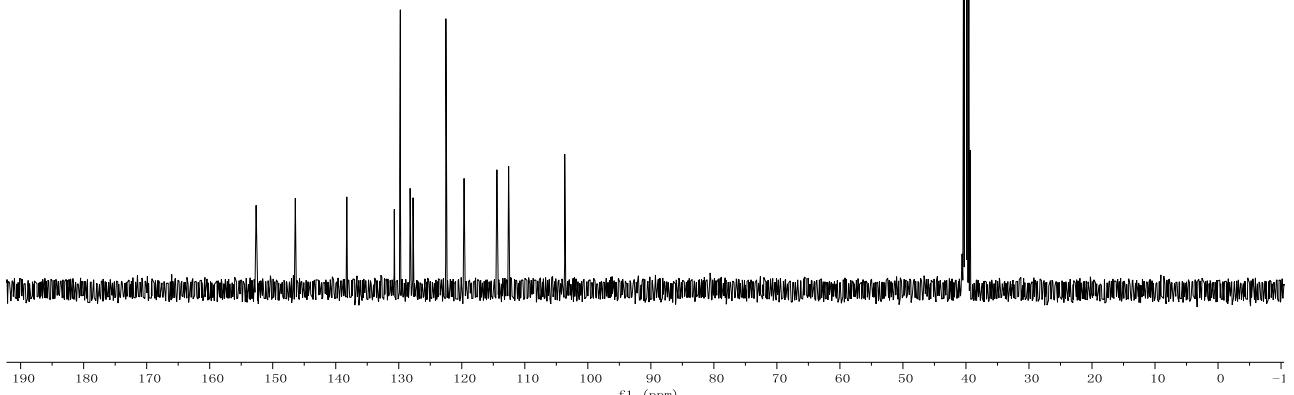
5e



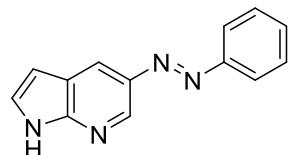
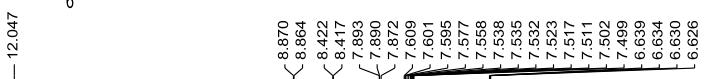
5e $^{13}\text{C-NMR}$ DMSO- d_6 100M Hz



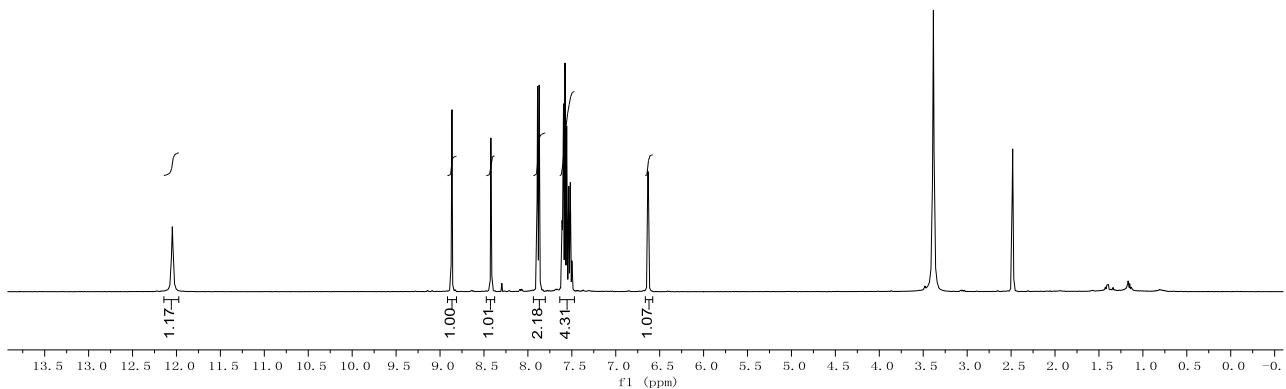
5e



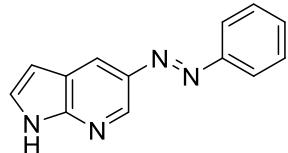
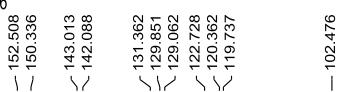
5f $^1\text{H-NMR}$ DMSO- d_6 400M Hz



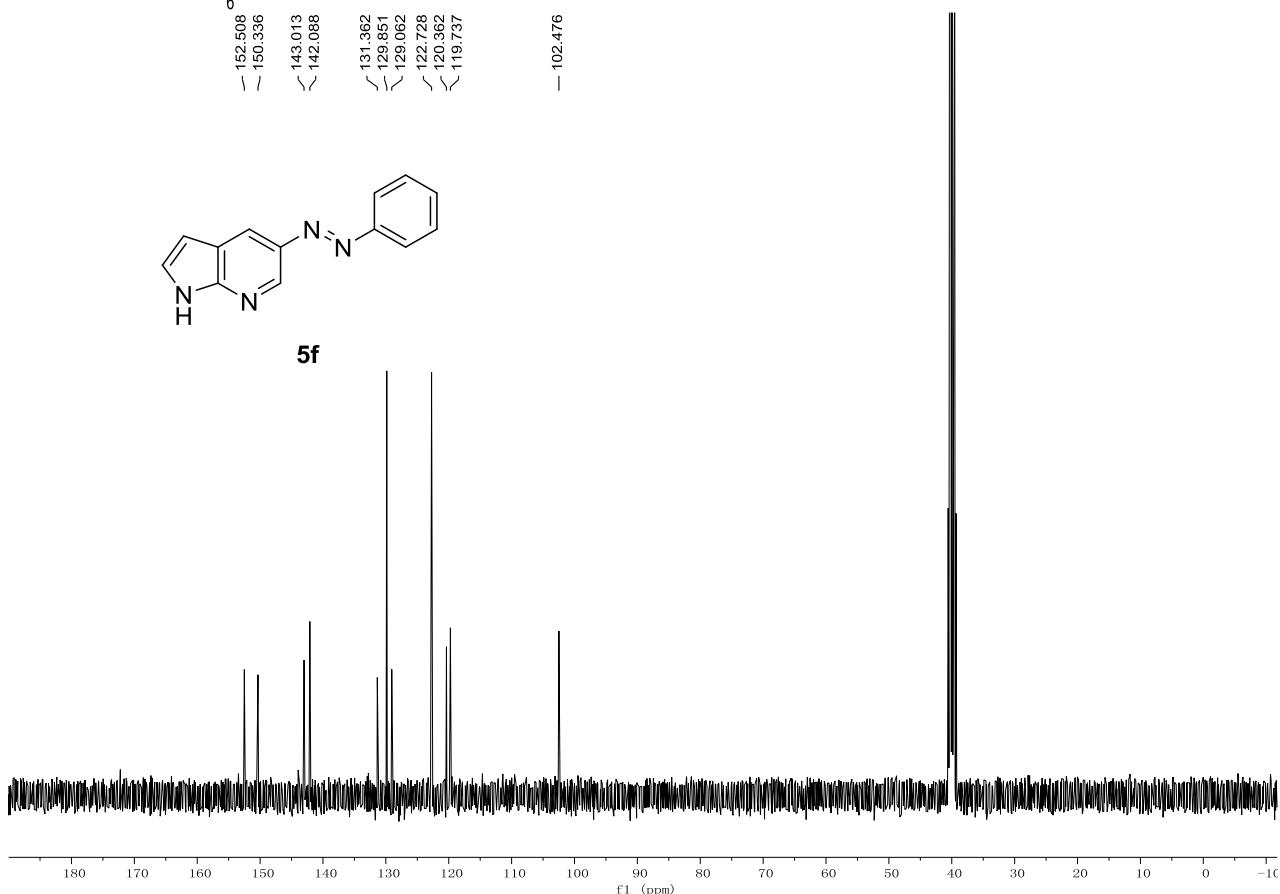
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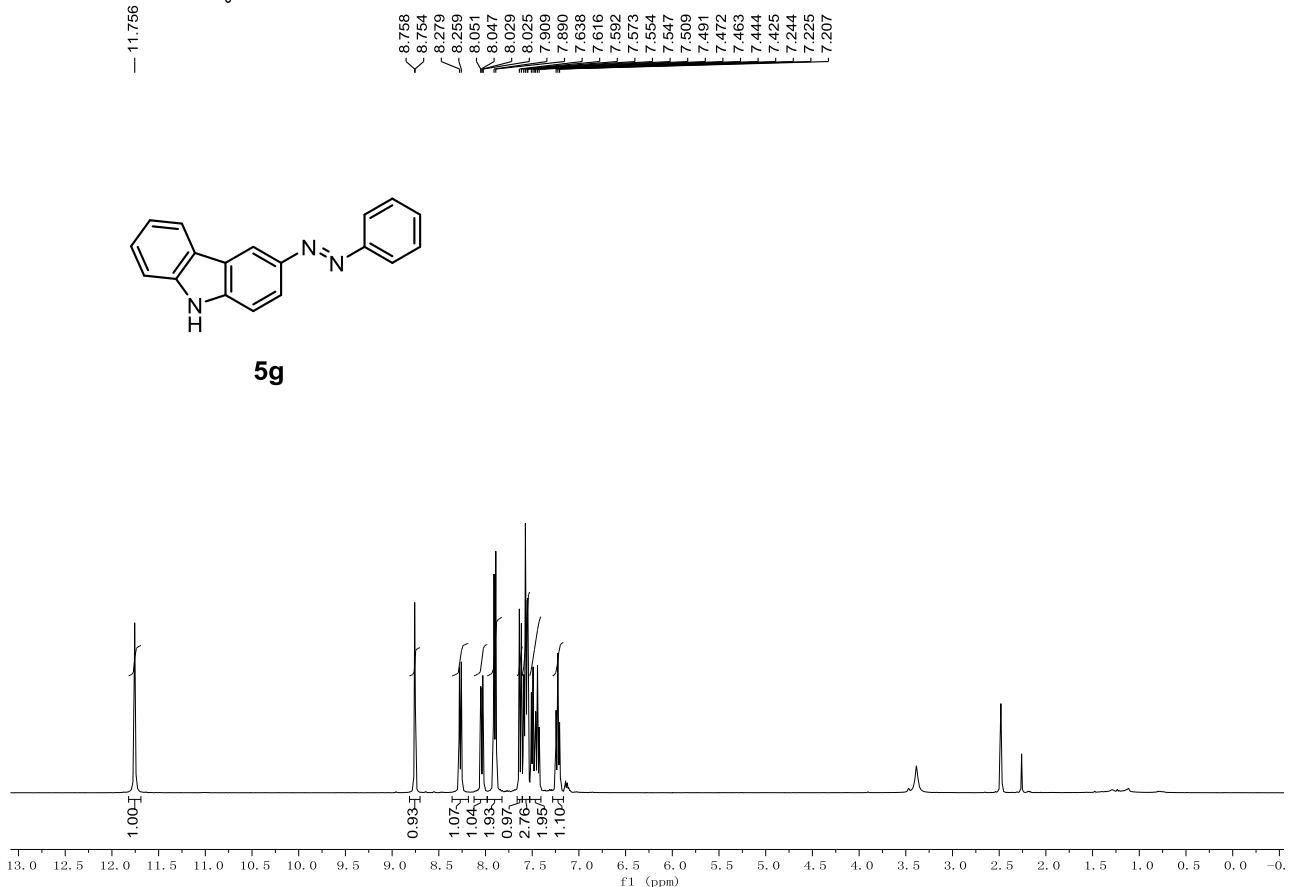
5f $^{13}\text{C-NMR}$ DMSO- d_6 100M Hz



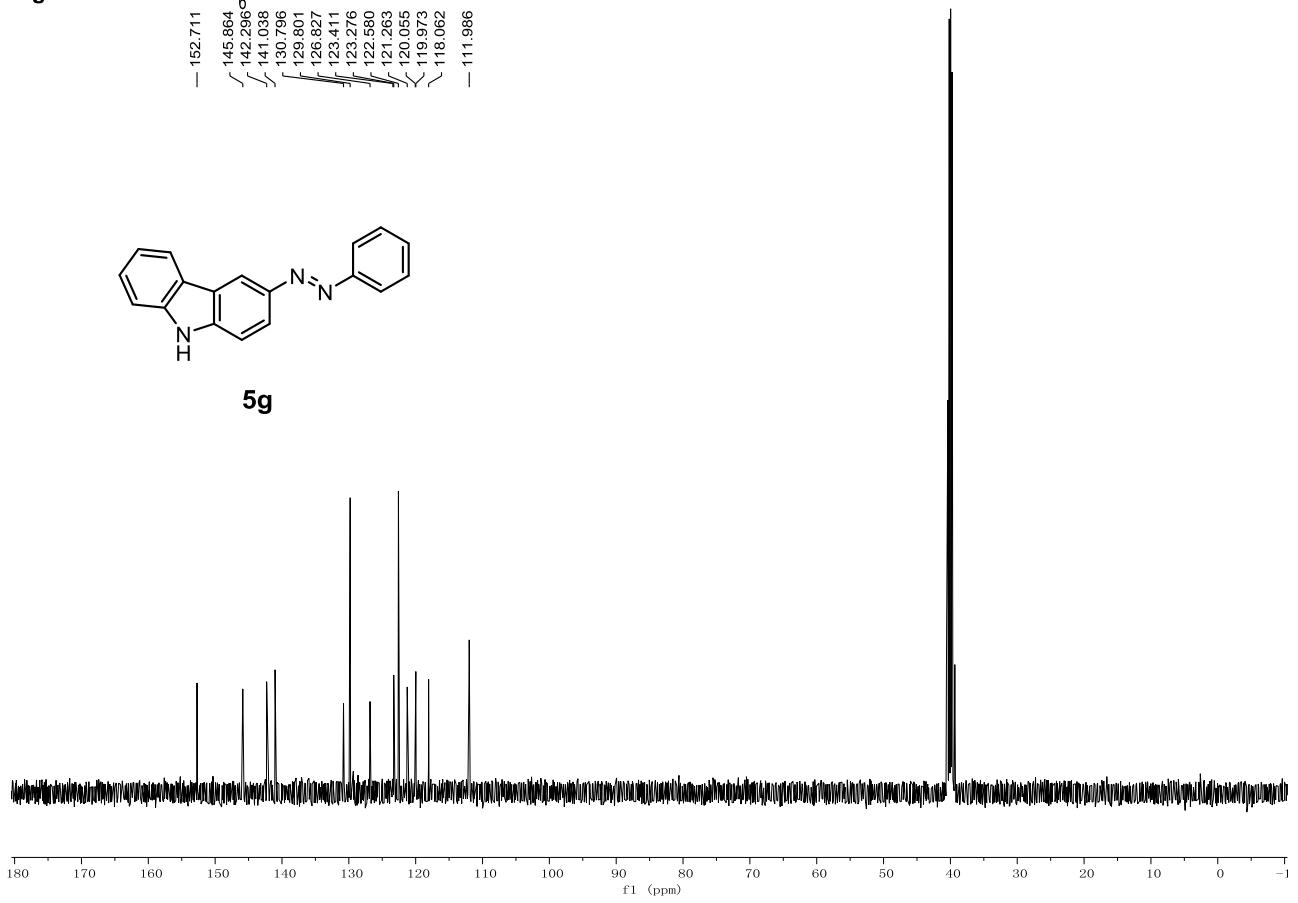
5f



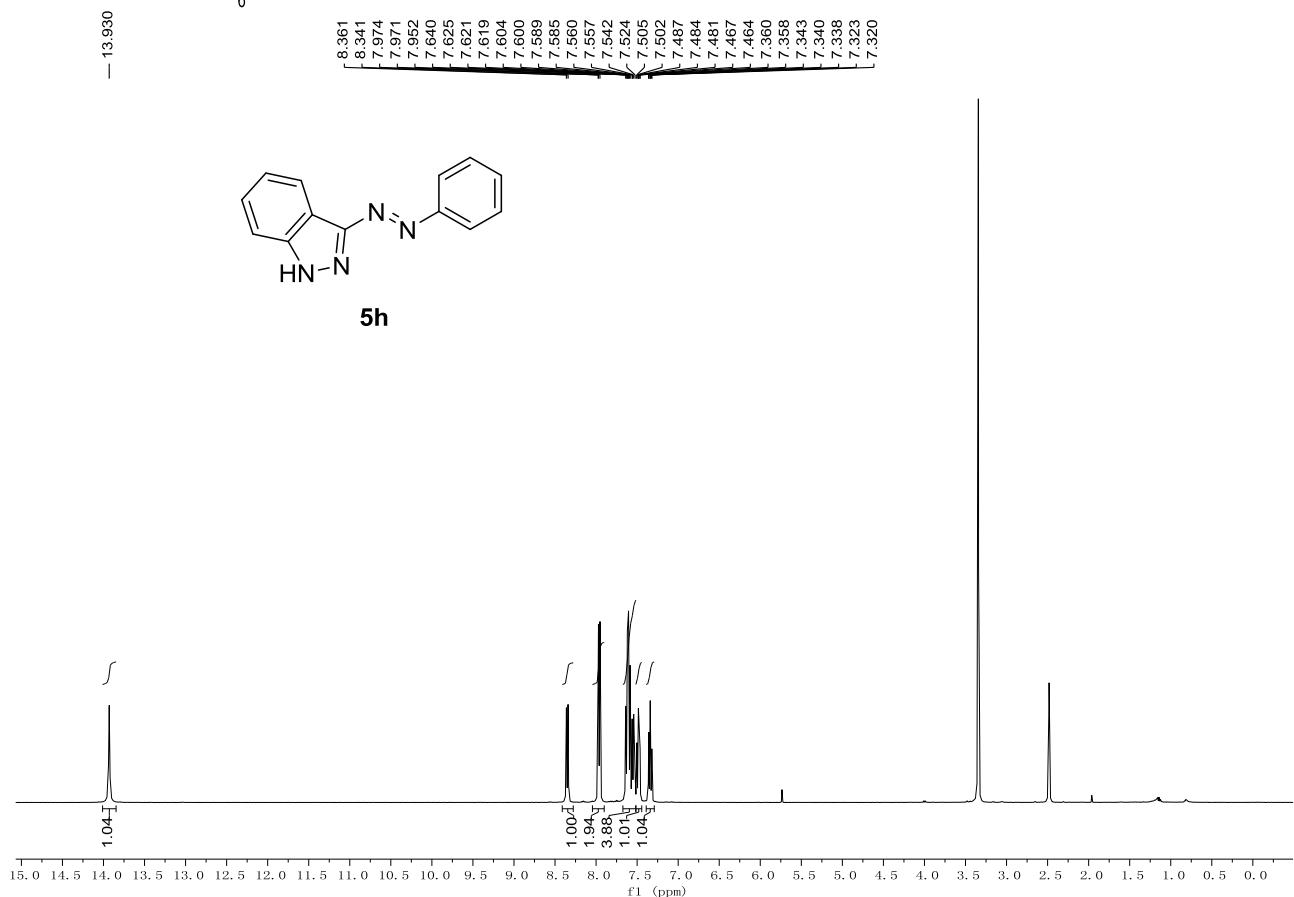
5g $^1\text{H-NMR}$ DMSO- d_6 400M Hz



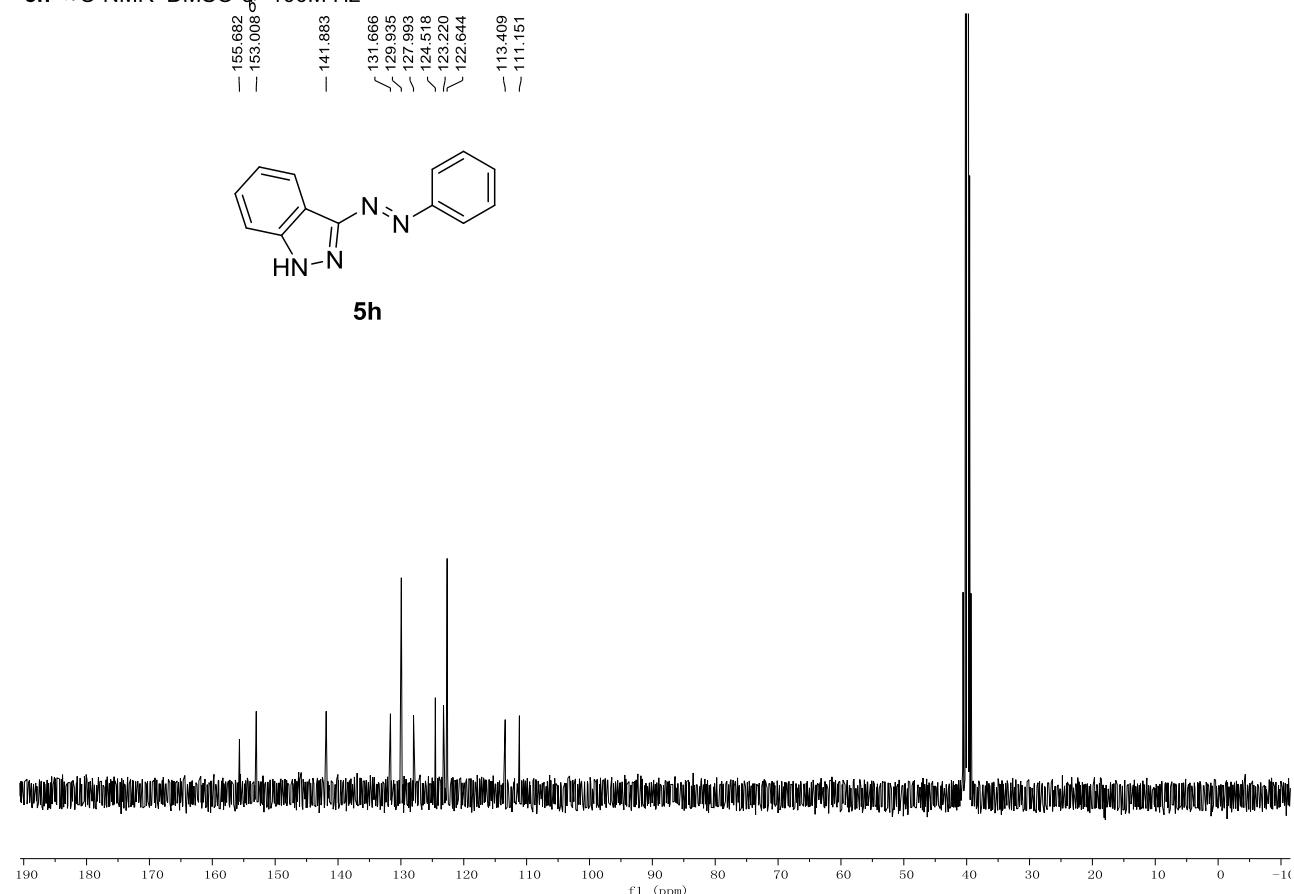
5g $^{13}\text{C-NMR}$ DMSO- d_6 100M Hz



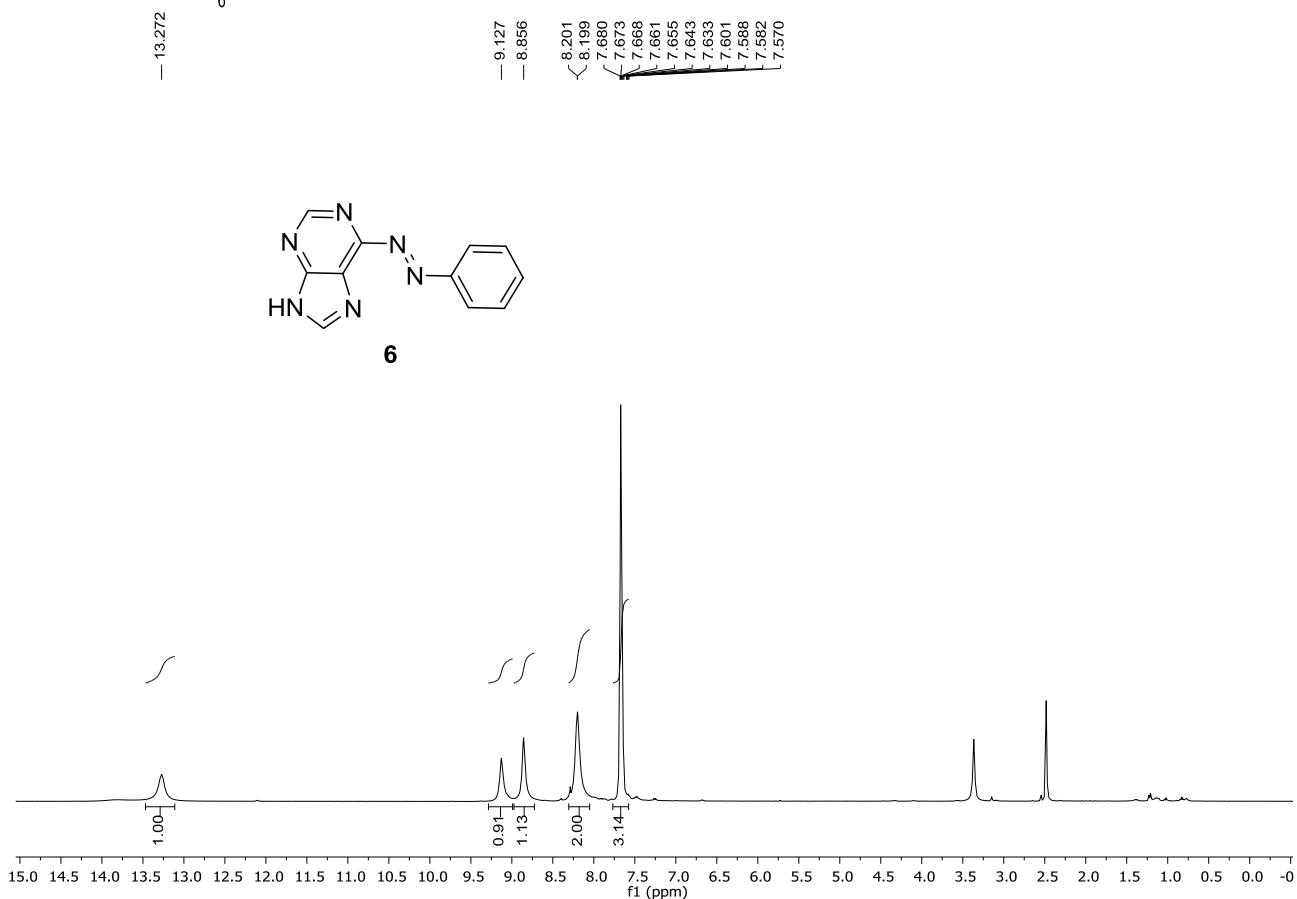
5h $^1\text{H-NMR}$ DMSO-d₆ 400M Hz



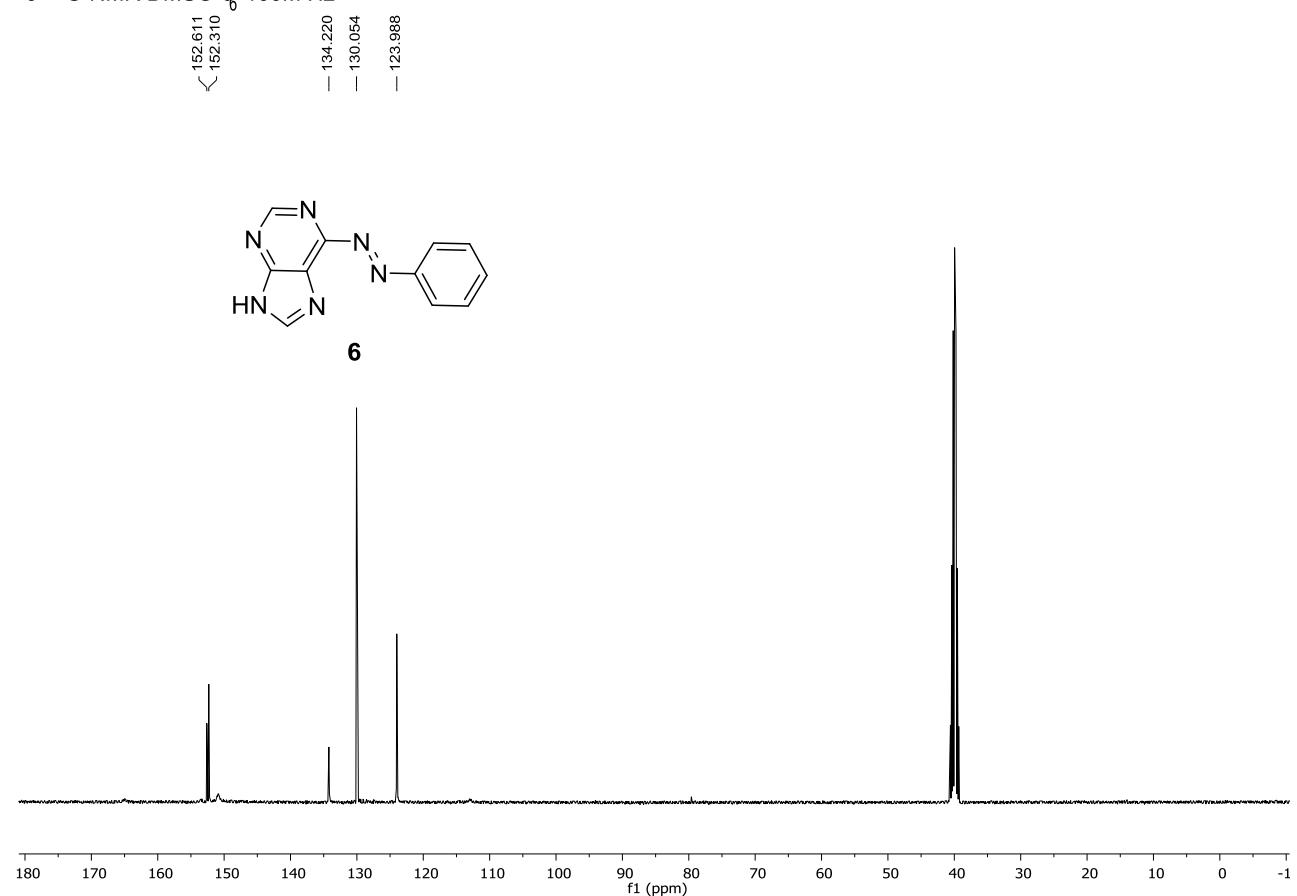
5h $^{13}\text{C-NMR}$ DMSO-d₆ 100M Hz

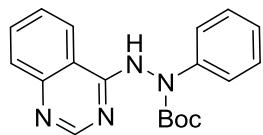
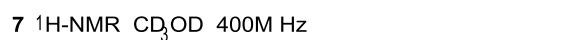


6 $^1\text{H-NMR}$ DMSO- d_6 400M Hz

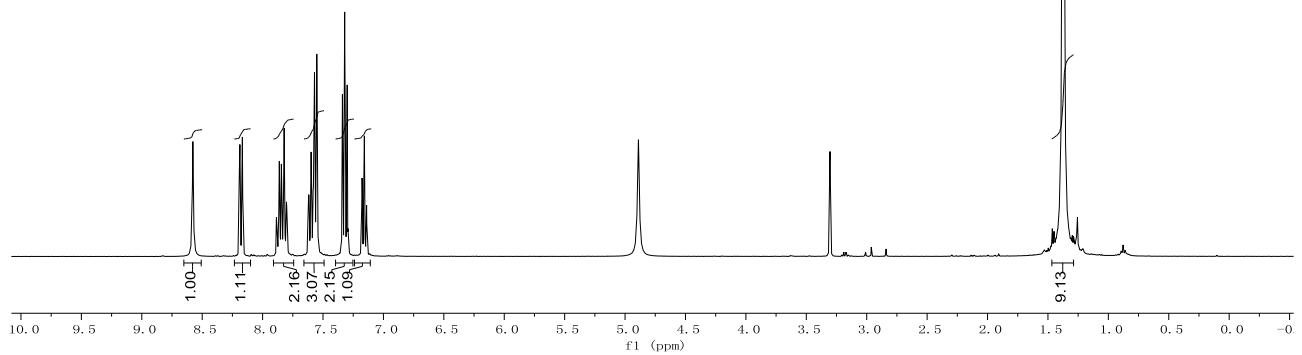


6 $^{13}\text{C-NMR}$ DMSO- d_6 100M Hz

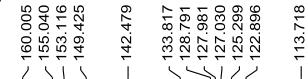




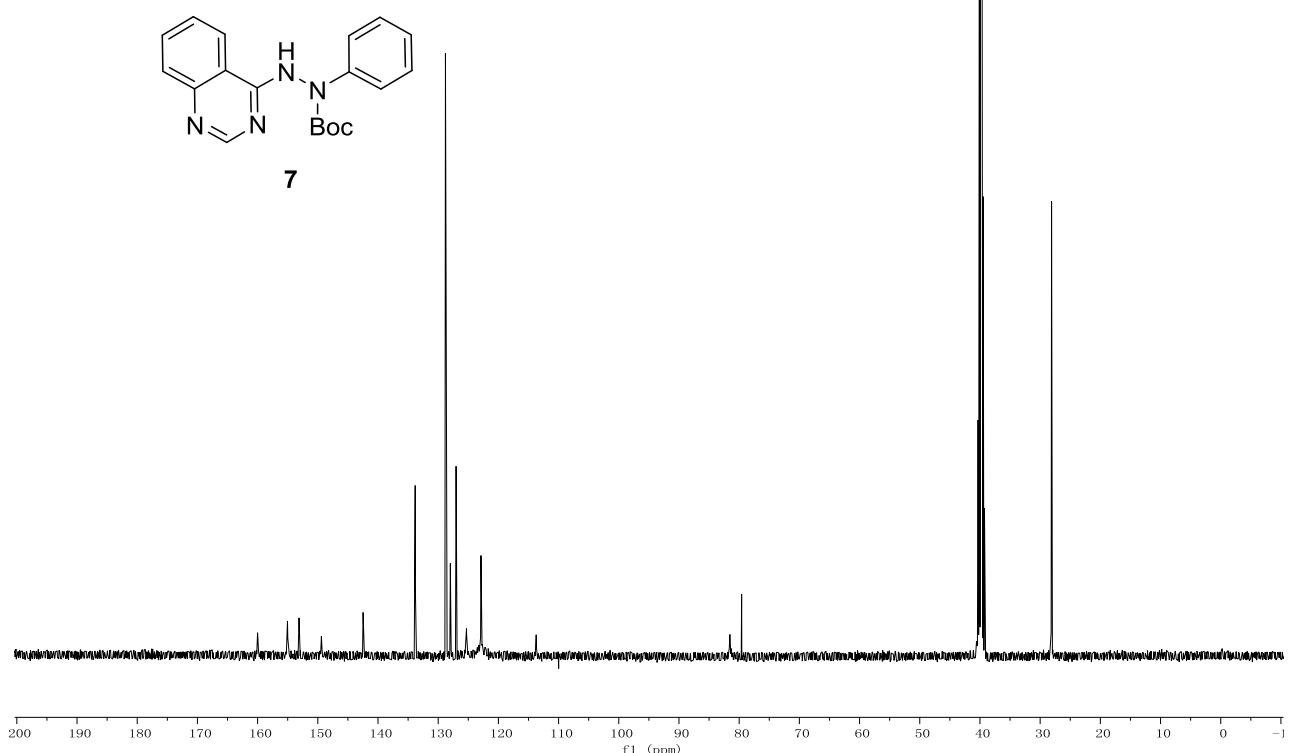
7



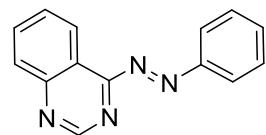
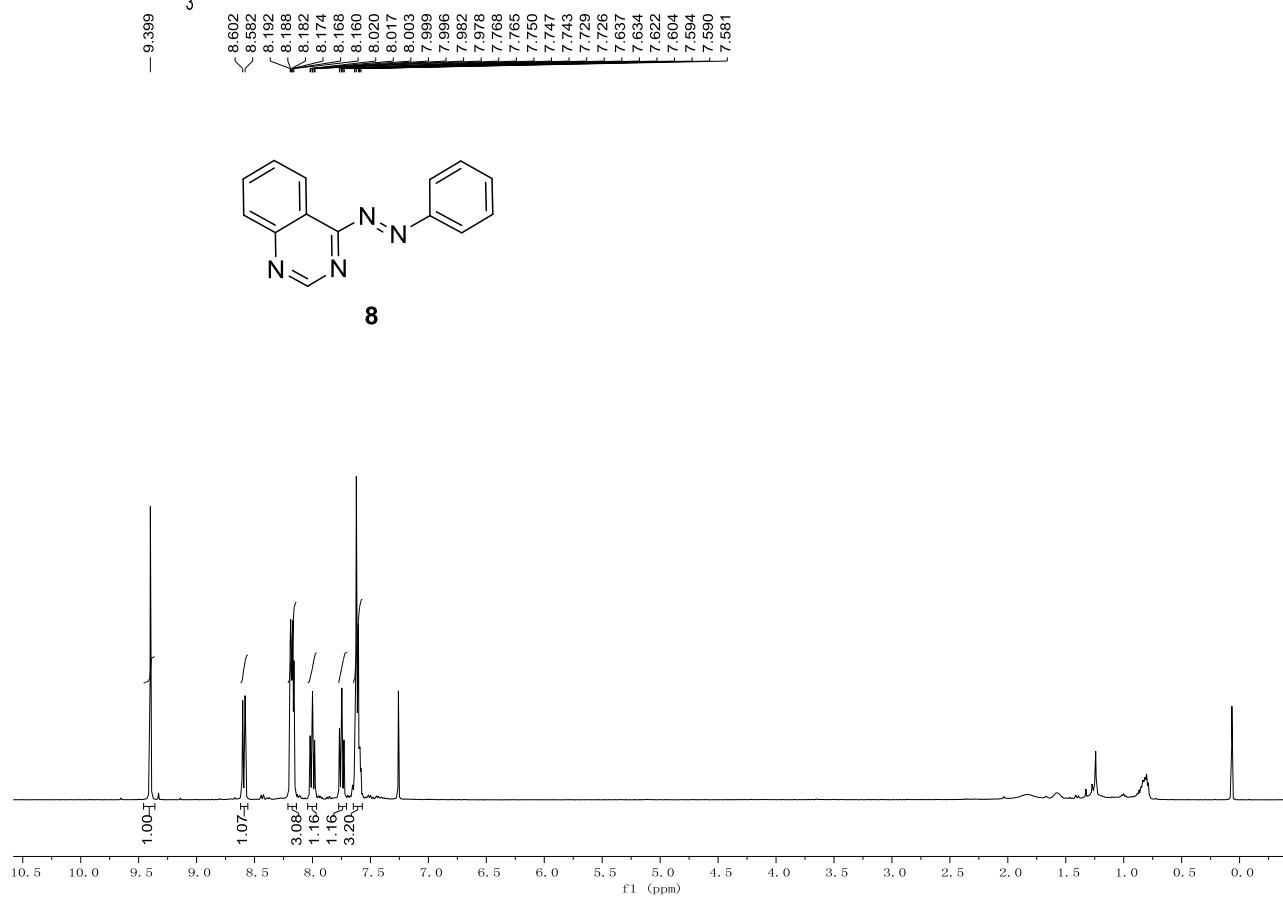
7 ^{13}C -NMR DMSO- d_6 100M Hz



7

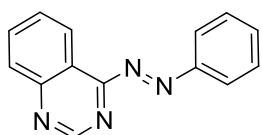
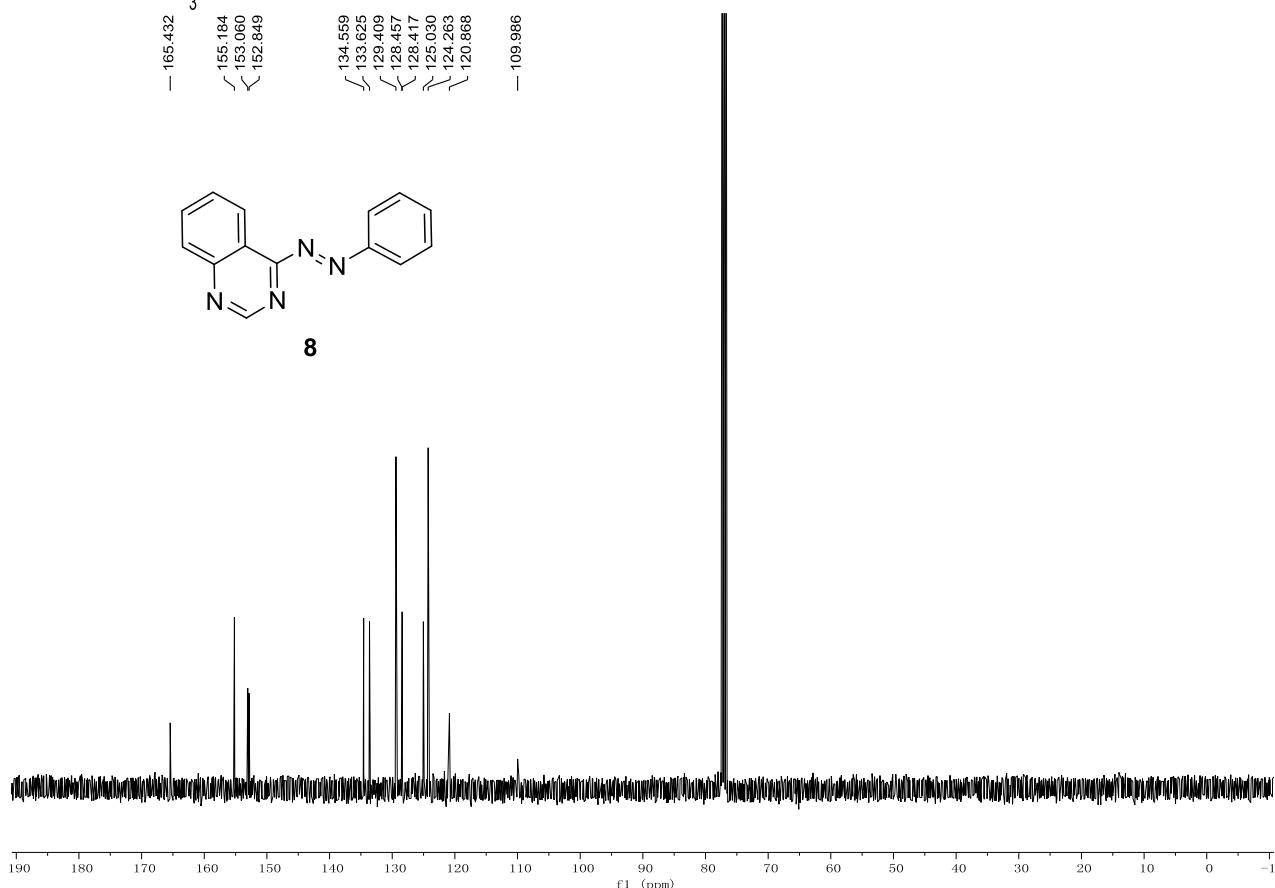


8 $^1\text{H-NMR}$ CDCl_3 400M Hz



8

8 $^{13}\text{C-NMR}$ CDCl_3 100M Hz



8

7. Cartesian coordinates

Table S1 Cartesian coordinates of compound **3a-E-I**

N	0.40433300	0.26801000	0.35826600
N	-0.43529600	-0.31453900	-0.36727200
C	-4.52254700	0.49977000	0.18308700
H	-5.58211900	0.69263500	0.30551100
C	-4.08521400	-0.41082500	-0.77779600
H	-4.80162500	-0.92841800	-1.40471700
C	-2.72272600	-0.65484900	-0.93174800
H	-2.36013700	-1.35814400	-1.67225100
C	-1.79332800	0.01136500	-0.12343000
C	-2.23429200	0.92911000	0.84456900
H	-1.51018600	1.44070600	1.46467500
C	-3.59413600	1.16702600	0.99127400
H	-3.93867900	1.87462900	1.73671000
C	4.43877200	-0.48594000	-0.13290100
H	5.51158200	-0.63507600	-0.20530300
C	1.75645100	-0.06616200	0.10136200
C	2.20854400	-0.96083300	-0.87782900
H	1.50058600	-1.46737600	-1.52058600
C	2.70319400	0.57003300	0.91231800
H	2.36244400	1.26546500	1.67355100
C	3.57418200	-1.16993900	-0.99187400
H	3.97460800	-1.85113600	-1.73271200
N	4.01973000	0.37136600	0.80621300

Table S2 Cartesian coordinates of compound **3a-E-II**

N	0.40664000	0.29556400	0.42492200
N	-0.40531200	-0.23502600	-0.36881800
C	-4.51699500	0.46852700	0.15126200
H	-5.58204200	0.63540000	0.26392600
C	-4.03770300	-0.28164700	-0.92170500
H	-4.72679900	-0.69946500	-1.64607400
C	-2.66856800	-0.49553600	-1.06093900
H	-2.27386400	-1.07674100	-1.88605100
C	-1.77468000	0.04444100	-0.12819200
C	-2.25788200	0.79836100	0.95409700
H	-1.56097200	1.20760900	1.67341500
C	-3.62418600	1.00545800	1.08661000
H	-4.00161500	1.58536700	1.92106000
C	4.41125900	-0.57721800	-0.18131100
H	5.45399800	-0.82114700	-0.35791900
C	4.06736000	0.49899700	0.63294900
H	4.83829900	1.09862400	1.10040700
C	1.76845800	-0.01993900	0.19251700
C	2.21587500	-1.09455200	-0.59360800
H	1.49546500	-1.75122000	-1.06732500
N	3.50692400	-1.37023500	-0.77866800
C	2.72033600	0.77797600	0.83082900
H	2.39477400	1.59979800	1.45783300

Table S3 Cartesian coordinates of compound **3a-Z-I**

C	0.56608800	1.19321600	-0.40134000
H	1.09458800	2.02659200	-0.84740300
C	-0.39327000	1.41776600	0.58496000
H	-0.61056600	2.42696300	0.91973900
N	-1.10432200	0.43500900	1.15446100
C	-0.87165600	-0.81433100	0.74718700
H	-1.47086400	-1.60248200	1.19310400
C	0.10688700	-1.14402200	-0.19711500
N	0.16224700	-2.51048000	-0.62802100
C	0.82921800	-0.11100000	-0.80068300
H	1.56230900	-0.32001100	-1.56930700
N	1.22035200	-3.14689000	-0.78913800
C	5.11955000	-2.02832700	0.36288800
H	6.13250600	-1.77625600	0.65400300
C	4.86229900	-2.52563100	-0.91594200
H	5.67387400	-2.65959900	-1.62154700
C	3.56594100	-2.87585300	-1.28142400
H	3.35635000	-3.29455100	-2.25885900
C	2.51231500	-2.66975300	-0.38469600
C	2.76664400	-2.18600000	0.90461300
H	1.95834400	-2.07387700	1.61601600
C	4.07270500	-1.87625900	1.27375700
H	4.27256100	-1.51512200	2.27594500

Table S4 Cartesian coordinates of compound **3a-Z-II**

N	0.49989800	1.14081900	-0.78437500
C	-0.38952300	1.47429500	0.16099000
H	-0.51774600	2.53522800	0.34958600
C	-1.13710000	0.53481300	0.86896900
H	-1.85986300	0.85697600	1.60815000
C	-0.94957300	-0.81384500	0.59374400
H	-1.52507300	-1.58044000	1.09921300
C	0.01980300	-1.17227600	-0.34384100
N	0.12418800	-2.54968300	-0.72604000
C	0.70166200	-0.15538600	-1.02605000
H	1.41249000	-0.40332200	-1.80722800
N	1.20506200	-3.15892100	-0.83299500
C	5.02806600	-1.87957100	0.40564900
H	6.02258000	-1.58522200	0.71975900
C	4.83016100	-2.43832400	-0.85831100
H	5.66954800	-2.57796200	-1.52942400
C	3.55787000	-2.84188000	-1.25196900
H	3.39445600	-3.30730800	-2.21697700
C	2.46776900	-2.62934600	-0.40150600
C	2.66290900	-2.08397700	0.87356500
H	1.82818200	-1.96726600	1.55266400
C	3.94601600	-1.72008600	1.27290500
H	4.10011800	-1.31111400	2.26471900

Table S5 Cartesian coordinates of compound **3b-E**

N	-5.35563900	8.61925400	-0.68390500
C	-5.47587700	7.29638300	-0.55081200
H	-4.75602900	6.78228500	0.07895200
C	-6.47984500	6.57299700	-1.19648600
N	-6.51651100	5.17643300	-0.98100000
C	-7.38626200	7.31015100	-1.96948400
H	-8.21391400	6.81921400	-2.46828000
N	-7.27585400	8.63167600	-2.10449900
C	-6.25973000	9.21952200	-1.46148600
H	-6.16708200	10.29437500	-1.57885100
N	-7.25217000	4.54545200	-1.77660700
C	-7.63456500	0.38573600	-1.34798500
H	-7.74923400	-0.68832800	-1.25834500
C	-6.85460100	1.08308000	-0.41716100
H	-6.36945700	0.54607600	0.38972700
C	-6.69994100	2.45834300	-0.51997500
H	-6.10068800	3.00586100	0.19528300
C	-7.33341800	3.14751100	-1.56787400
C	-8.11586400	2.44993800	-2.49671800
H	-8.59660500	3.00375000	-3.29445600
C	-8.26432800	1.06987000	-2.38680100
H	-8.86888700	0.53152100	-3.10693700

Table S6 Cartesian coordinates of compound **3b-Z**

N	-2.99660400	4.51768200	-2.55773800
C	-4.20292000	4.96739000	-2.20796600
H	-4.58116000	5.84696700	-2.71957100
C	-4.97429400	4.33019100	-1.23426300
N	-6.19443800	4.94307100	-0.80987500
C	-4.38235800	3.24803600	-0.57495200
H	-4.88847100	2.74641700	0.24300300
N	-3.16697400	2.80933900	-0.90366000
C	-2.54117100	3.45189100	-1.89387100
H	-1.56148900	3.08044200	-2.17568900
N	-7.25974700	4.32052600	-0.64083200
C	-8.11548500	0.34343400	-1.74186700
H	-8.36909300	-0.67326100	-2.01804700
C	-8.45895500	0.83145300	-0.47966600
H	-8.97793200	0.19515800	0.22744800
C	-8.15910900	2.14531600	-0.13411100
H	-8.44835900	2.54906000	0.82904500
C	-7.45617600	2.95544800	-1.03268300
C	-7.12407600	2.47655300	-2.30638600
H	-6.63286700	3.12064600	-3.02421800
C	-7.46502500	1.17312100	-2.65651300
H	-7.22289600	0.80622200	-3.64708800

Table S7 Cartesian coordinates of compound **3c-E-I**

N	0.43378400	0.29155000	0.45217800
N	-0.37422400	-0.20034900	-0.36979000
C	-4.48605200	0.46311500	0.15126800
H	-5.55247100	0.62071100	0.26403500
C	-3.99940700	-0.25407700	-0.94080300
H	-4.68373800	-0.65525800	-1.67872800
C	-2.62886200	-0.45508400	-1.08090200
H	-2.22617200	-1.00978300	-1.92011100
C	-1.74352600	0.06385600	-0.12778300
C	-2.23376600	0.78585100	0.97348500
H	-1.54140400	1.18051400	1.70521700
C	-3.60115300	0.98068600	1.10552600
H	-3.98640700	1.53589800	1.95287900
C	4.37272600	-0.58504500	-0.19119600
H	5.42559800	-0.79162000	-0.34812000
C	3.96403700	0.51000500	0.56867100
H	4.69179200	1.17302000	1.02408300
C	1.79170300	-0.03460200	0.19508600
C	2.20004200	-1.15350800	-0.54986300
H	1.46811200	-1.82998900	-0.97304200
N	3.48887600	-1.42514400	-0.74275200
N	2.67450800	0.78285200	0.77204500

Table S8 Cartesian coordinates of compound **3c-E-II**

C	3.69995500	-12.26103000	46.45260300
N	4.89219200	-11.49285400	46.48621900
C	2.50638100	-11.52143900	46.44658700
H	2.54427200	-10.43506600	46.46277400
N	1.30667200	-12.10612900	46.41749800
C	1.31026900	-13.44355700	46.40451000
H	0.34368800	-13.94260700	46.38483900
C	2.50062000	-14.18118400	46.42301800
H	2.47904100	-15.26981400	46.42287600
N	3.69928000	-13.60080200	46.44678900
N	5.95110400	-12.15806100	46.33112900
C	9.61174000	-10.09566300	46.43776700
H	10.57187400	-9.58715100	46.46099400
C	9.55694300	-11.47350100	46.22008000
H	10.47183800	-12.04048700	46.07348900
C	8.32315800	-12.12091100	46.19172800
H	8.24362800	-13.19079400	46.02584800
C	7.14096800	-11.39148100	46.38048000
C	7.19763200	-10.00326800	46.60028300
H	6.27229500	-9.45694600	46.74469600
C	8.43093200	-9.36456900	46.62740400
H	8.48051800	-8.29228300	46.79699000

Table S9 Cartesian coordinates of compound **3c-Z-I**

N	0.39862900	1.11796000	-0.77571500
C	-0.37400900	1.40639800	0.27879200
H	-0.55075500	2.45299200	0.49922600
C	-0.94462800	0.40326600	1.05851400
H	-1.58208900	0.64708900	1.90142600
C	0.05784300	-1.17218600	-0.22468600
N	0.13962100	-2.55641400	-0.59877900
C	0.62014900	-0.16866000	-1.02918200
H	1.23824800	-0.41752800	-1.88463000
N	1.21369200	-3.16798000	-0.74106400
C	5.05633000	-1.82863300	0.34735500
H	6.05675400	-1.51367100	0.61984200
C	4.83289700	-2.46388600	-0.87595100
H	5.65756000	-2.64104100	-1.55612800
C	3.55455200	-2.89491300	-1.21412800
H	3.36904800	-3.41826900	-2.14465400
C	2.48354200	-2.63154100	-0.35260200
C	2.70481000	-2.01101600	0.88422100
H	1.88897500	-1.86680300	1.58074400
C	3.99548200	-1.62056300	1.23006500
H	4.17243200	-1.15554200	2.19273800
N	-0.74818600	-0.89196000	0.79579400

Table S10 Cartesian coordinates of compound **3c-Z-II**

C	3.52646300	-12.38787600	46.20620400
N	4.72245100	-11.73376200	45.76698900
C	2.72524700	-11.71725800	47.14507200
H	3.06269300	-10.78341300	47.58862900
N	1.54388100	-12.20062900	47.52886500
C	1.14209500	-13.32962700	46.92855100
H	0.17340200	-13.72828600	47.22092300
C	1.91743400	-13.96248500	45.95448000
H	1.56302700	-14.85991200	45.45133400
N	3.11925200	-13.50354700	45.59371800
N	5.79794000	-12.33107100	45.55657100
C	6.86361500	-16.25166700	46.68323900
H	7.17997200	-17.25101900	46.96848000
C	7.14532700	-15.76572900	45.40338500
H	7.67882300	-16.38708200	44.68948200
C	6.76884800	-14.47365900	45.04729800
H	7.00972600	-14.06471500	44.07091300
C	6.04787600	-13.68335000	45.95179900
C	5.77868900	-14.16106600	47.24255800
H	5.27173300	-13.52612500	47.96247300
C	6.19591100	-15.44008100	47.60388100
H	5.99929500	-15.80383900	48.60875500

Table S11 Cartesian coordinates of compound **3d-E-I**

N	5.53693000	0.05779800	-0.21252300
N	6.06214200	-1.07671900	-0.11408900
C	10.24952300	-1.40580400	-0.28374700
H	11.32695000	-1.51681100	-0.32465300
C	9.67521500	-0.13234300	-0.37852300
H	10.31066100	0.73849700	-0.49231200
C	8.29676100	0.02353100	-0.32740200
H	7.84496500	1.00392900	-0.39941600
C	7.47723300	-1.10822900	-0.17932800
C	8.05308000	-2.38141600	-0.08369300
H	7.40238600	-3.24044900	0.03082000
C	9.43690100	-2.52909900	-0.13636500
H	9.87868300	-3.51578500	-0.06248300
C	1.40577100	0.51952600	-0.05841000
N	2.23719700	1.58693400	-0.25648200
C	3.53043400	1.36313100	-0.29261200
H	4.18573500	2.21607700	-0.44977800
C	4.12400000	0.08038200	-0.14133700
C	3.29997100	-1.01011200	0.06146100
H	3.72044200	-2.00088300	0.18382300
C	1.90493300	-0.81352700	0.10821900
C	0.98469500	-1.87832800	0.31243300
H	1.36782500	-2.88506400	0.43779900
C	-0.36602500	-1.63138900	0.34860900
H	-1.06407000	-2.44552800	0.50411800
C	-0.85707100	-0.31236000	0.18322600
H	-1.92589500	-0.13492400	0.21452100
C	0.00703400	0.73969800	-0.01549000

H

-0.35690800 1.75236700 -0.14298400

Table S12 Cartesian coordinates of compound **3d-E-II**

C	1.36109100	0.49083300	-0.17087300
N	1.92241800	-0.75093800	-0.32563300
C	3.22918900	-0.85546400	-0.31117000
H	3.65287300	-1.84563400	-0.43551300
C	4.10854600	0.25769300	-0.14269900
N	5.51869900	0.17198000	-0.12338000
C	3.55988800	1.51268800	0.01224900
H	4.20937500	2.37175700	0.14060900
C	2.15561200	1.66665900	0.00308700
N	5.98944200	-0.98405400	-0.25409800
C	10.16279500	-1.49474400	-0.23241500
H	11.23514000	-1.65262200	-0.22997100
C	9.64770500	-0.19975800	-0.09916200
H	10.32367500	0.64119500	0.00583000
C	8.27615500	0.01582700	-0.10081600
H	7.87022800	1.01353300	0.00109400
C	7.40381300	-1.07700600	-0.23757600
C	7.92047600	-2.37183400	-0.37154200
H	7.22982700	-3.20040000	-0.47627600
C	9.29757100	-2.57955100	-0.36845800
H	9.69336900	-3.58297700	-0.47196100
C	1.51388900	2.92289600	0.15754900
H	2.12199700	3.81114400	0.28894300
C	0.14085900	3.00721500	0.14016200
H	-0.34629500	3.96790600	0.25851000
C	-0.64390500	1.84264400	-0.03200700
H	-1.72456900	1.92537000	-0.04347800
C	-0.04834500	0.60965500	-0.18461400

H

-0.63911900 -0.28901300 -0.31729000

Table S13 Cartesian coordinates of compound **3d-Z-I**

C	1.11180100	0.78223600	0.47025600
N	1.49490800	-0.44330900	0.94322000
C	2.63812100	-0.93815200	0.53210700
H	2.91830700	-1.92379600	0.89454400
C	3.53187200	-0.25308700	-0.33683100
N	4.66763900	-0.99673000	-0.79026400
C	3.15679300	0.97111800	-0.84383600
H	3.78561500	1.50595700	-1.54551300
C	1.91614200	1.52344700	-0.45135800
N	5.81855300	-0.53089100	-0.88323500
C	7.24591600	3.14803000	0.60639100
H	7.64729100	4.08085100	0.98467700
C	7.50111800	2.75872500	-0.70949000
H	8.09981800	3.38839000	-1.35728300
C	7.00854000	1.54799700	-1.18848300
H	7.22603100	1.21849200	-2.19783200
C	6.20634100	0.75144900	-0.36536500
C	5.96079900	1.12863900	0.96044100
H	5.38153000	0.48745900	1.61298200
C	6.48997100	2.32299500	1.44127600
H	6.31144700	2.60914500	2.47135500
C	1.44976900	2.77831100	-0.92524600
H	2.06172000	3.33603600	-1.62570700
C	0.24259900	3.27700100	-0.49585400
H	-0.10808500	4.23639600	-0.85782900
C	-0.55076500	2.54374300	0.41950500
H	-1.50017400	2.95108100	0.74737200
C	-0.12783600	1.32221100	0.89174100

H -0.72657900 0.74865400 1.58946000

Table S14 Cartesian coordinates of compound **3d-Z-II**

C	3.64136500	-1.91529400	2.19578400
N	4.91102200	-1.29120900	2.41413100
C	2.68430500	-1.22373900	1.48961600
H	2.92650900	-0.27325300	1.02675200
C	1.39141500	-1.77734900	1.35123200
C	1.12118400	-3.01348600	2.01704800
N	2.06638500	-3.64700200	2.77747200
C	3.26691200	-3.12510000	2.85154500
H	3.99071600	-3.64004300	3.47556000
N	6.00094100	-1.89255400	2.34000000
C	6.72842400	-5.75757900	0.81865100
H	6.95102600	-6.74305600	0.42668800
C	7.28949500	-5.34225700	2.02787800
H	7.94767100	-6.00419000	2.57845100
C	7.02571000	-4.06733300	2.51856800
H	7.47987600	-3.71934900	3.43901100
C	6.14757300	-3.22444400	1.82822600
C	5.59561000	-3.62996900	0.60592900
H	4.95910000	-2.95918000	0.04326800
C	5.89720200	-4.89328800	0.10437800
H	5.48167100	-5.20230100	-0.84776400
C	-0.16656400	-3.59131000	1.90229400
H	-0.35688300	-4.52808100	2.41270900
C	-1.14345800	-2.96873300	1.15886200
H	-2.12640700	-3.41739300	1.07358000
C	-0.87917700	-1.74174800	0.50360200
H	-1.66224100	-1.26542700	-0.07463200
C	0.36108900	-1.15549500	0.59809700

H 0.56942900 -0.21584000 0.09836500

Table S15 Cartesian coordinates of compound **3e-E-I**

C	-1.50881400	-1.70331600	1.88603900
N	-0.12205900	-1.66663000	2.17380100
C	-1.99811500	-0.58108200	1.18206300
H	-1.29050200	0.20305700	0.93248900
C	-3.33585700	-0.46499700	0.82844500
H	-3.71117700	0.41385700	0.31917200
C	-4.18407900	-1.51624300	1.18843300
C	-3.71612100	-2.65542100	1.90329700
C	-2.36906300	-2.74345600	2.25662700
H	-1.97410500	-3.59067000	2.80622100
C	-4.85075100	-3.52154100	2.11994800
H	-4.84937500	-4.46117500	2.65543200
C	-5.93599600	-2.93025300	1.55683000
H	-6.97093200	-3.23353300	1.51572600
N	-5.56289600	-1.69408600	0.99929400
S	-6.57111000	-0.84638600	-0.10532300
O	-7.92881000	-1.24713300	0.25374500
O	-6.12439400	0.54297600	-0.07473900
C	-5.54365600	-2.65227000	-4.19128800
C	-5.22313200	-3.23737100	-5.54539100
H	-5.89427800	-2.83334500	-6.31476900
H	-5.34215900	-4.32574000	-5.54974900
H	-4.19828600	-3.00425500	-5.85059600
C	-6.53804500	-3.22251400	-3.38211500
H	-7.06952100	-4.10511000	-3.72891600
C	-6.86188000	-2.67579000	-2.14374700
H	-7.64379400	-3.11063600	-1.53057400
C	-6.17650400	-1.53997500	-1.70537500

C	-5.18602100	-0.94643300	-2.48996600
H	-4.67816400	-0.05332500	-2.14406700
C	-4.87722500	-1.51015300	-3.72597300
H	-4.10694300	-1.05187800	-4.34084500
N	0.31907500	-2.66716200	2.80229900
C	4.41911700	-2.75176100	3.75666000
H	5.47368400	-2.79751300	4.01515600
C	3.91603000	-1.64194100	3.06530600
H	4.58295600	-0.82910100	2.78956400
C	2.56903500	-1.57221200	2.72976200
H	2.16072300	-0.72159700	2.19564100
C	1.70798300	-2.62423100	3.08796500
C	2.21338000	-3.73295800	3.77996300
H	1.52524900	-4.53020000	4.04451700
C	3.56535500	-3.79691500	4.11331800
H	3.95157700	-4.65908600	4.65002300

Table S16 Cartesian coordinates of compound **3e-E-II**

C	0.77333200	1.22274500	0.55895000
N	2.05372300	1.74357400	0.23921300
C	-0.44204400	1.70908200	0.04644300
H	-0.42075000	2.54366500	-0.64535200
C	-1.63792600	1.11590400	0.43373200
H	-2.57847600	1.49109800	0.03857200
C	-1.63891000	0.03898300	1.32976600
H	-2.57876400	-0.41835500	1.62732800
C	-0.43295200	-0.44485700	1.83971800
H	-0.42947200	-1.27950600	2.53535400
C	0.76978100	0.14560700	1.45520800
H	1.72311300	-0.20862600	1.83570500
N	2.04284600	2.71174000	-0.56946700
C	5.72989800	4.38047000	-1.63295200
C	4.52072600	4.87852400	-2.18478600
C	3.30729000	4.29769400	-1.79967600
H	2.35537300	4.64649300	-2.18804700
C	3.31684700	3.23744500	-0.89170900
C	4.53656300	2.76178100	-0.34925900
H	4.49514000	1.94752900	0.36469800
C	5.74885000	3.32800000	-0.70588200
H	6.67803900	2.98822200	-0.26464600
C	4.86496500	5.95896100	-3.07547500
H	4.17674400	6.57347700	-3.63980900
C	6.21771900	6.09220200	-3.05829700
H	6.87155500	6.78788000	-3.56131400
N	6.76905800	5.15382700	-2.16967600
S	8.45020200	4.78953300	-2.14671000

O	9.09695200	6.00853500	-2.62463800
O	8.72149200	4.21585300	-0.83229100
C	8.94311200	1.52577600	-5.32709300
C	9.06995100	0.45376900	-6.38215700
H	9.72606000	0.77071000	-7.19920100
H	8.09095800	0.22089700	-6.82147300
H	9.46883400	-0.47570500	-5.96385000
C	9.01678800	2.88366200	-5.67232600
H	9.19781100	3.16395300	-6.70686700
C	8.87202100	3.88115900	-4.71225600
H	8.95066100	4.92882500	-4.98185100
C	8.65137200	3.51345600	-3.38270300
C	8.58648800	2.17080300	-3.00561300
H	8.44459100	1.90264500	-1.96483400
C	8.73360700	1.18865100	-3.98247000
H	8.69123300	0.14181900	-3.69310900

Table S17 Cartesian coordinates of compound **3e-Z-I**

C	-2.29649300	-1.09773100	2.69564000
N	-1.06126600	-1.03496500	3.42400700
C	-2.41170700	-0.17699100	1.63041900
H	-1.54897000	0.43698300	1.39160500
C	-3.58956500	-0.04244900	0.90835900
H	-3.67463200	0.67492100	0.10146000
C	-4.67898900	-0.82401700	1.30594900
C	-4.60347500	-1.71339600	2.41067700
C	-3.39727200	-1.85188300	3.10731800
H	-3.32492900	-2.52107200	3.95761900
C	-5.90489500	-2.31459100	2.56917500
H	-6.19891700	-3.02216800	3.33241900
C	-6.71250000	-1.81321800	1.59747800
H	-7.75479800	-1.98745200	1.37846600
N	-5.99674800	-0.88411200	0.82512100
S	-6.57164300	-0.30815000	-0.68835600
O	-8.02527500	-0.40985100	-0.59287100
O	-5.88215400	0.95615100	-0.92697900
C	-5.08699700	-3.39963600	-3.73031900
C	-4.61363500	-4.40722300	-4.74985300
H	-5.03835100	-4.19138900	-5.73908100
H	-4.91898300	-5.42358400	-4.48044300
H	-3.52405700	-4.39304100	-4.85214600
C	-6.30881900	-3.57615400	-3.06323700
H	-6.91008800	-4.45749300	-3.27164300
C	-6.77030700	-2.63935700	-2.14308500
H	-7.72456900	-2.77212500	-1.64480500
C	-5.99382000	-1.50750100	-1.88231200

C	-4.77630500	-1.30130100	-2.53329800
H	-4.19696800	-0.40660700	-2.33523300
C	-4.33291500	-2.25150700	-3.45072400
H	-3.38643400	-2.09490400	-3.96174600
N	-0.46620600	-2.03125900	3.88838300
C	-1.17201800	-6.12768900	3.12995100
H	-1.31122000	-7.18988200	2.94925000
C	-1.03266300	-5.65005300	4.43541400
H	-1.06330500	-6.33953300	5.27479400
C	-0.82647500	-4.29120200	4.66594300
H	-0.67636200	-3.90835200	5.67122300
C	-0.81575800	-3.39207000	3.59146000
C	-0.94109600	-3.87093700	2.27887300
H	-0.89368500	-3.17792100	1.44514600
C	-1.11009900	-5.23584600	2.05579000
H	-1.19663700	-5.60464800	1.03709200

Table S18 Cartesian coordinates of compound **3e-Z-II**

N	2.54426900	3.40509100	0.38607100
C	5.84956700	4.85673800	-1.76408900
C	4.53117700	5.02133800	-2.26480500
C	3.45307200	4.51863400	-1.52789300
H	2.42612800	4.66877700	-1.84708900
C	3.70593900	3.80248900	-0.35713400
C	5.02602400	3.66739700	0.13335400
H	5.19501700	3.16282500	1.07762000
C	6.10609300	4.20689500	-0.55220300
H	7.10932400	4.14678500	-0.14841800
C	4.62724100	5.76577400	-3.49600800
H	3.80516200	6.08626500	-4.12144600
C	5.94296600	6.02557200	-3.71906200
H	6.43643800	6.56889700	-4.51026900
N	6.71052000	5.50194500	-2.66610500
S	8.41681800	5.32347200	-2.77364000
O	8.83920700	6.37113400	-3.69903700
O	8.90024900	5.24232800	-1.39868800
C	9.02212600	1.25702000	-4.80132400
C	9.19046300	-0.08369600	-5.47426800
H	9.78226400	0.00008500	-6.39171700
H	8.21621700	-0.50607200	-5.75370900
H	9.68291500	-0.80490500	-4.81473300
C	8.88515800	2.42759900	-5.56304200
H	8.93006500	2.36901200	-6.64760000
C	8.70358800	3.66652000	-4.95542100
H	8.62029800	4.57072300	-5.54868300
C	8.65965300	3.73629600	-3.56061800

C	8.80503500	2.59153600	-2.77520500
H	8.79826200	2.66712700	-1.69374600
C	8.98541700	1.36129300	-3.40396400
H	9.10768200	0.46809700	-2.79682000
N	2.44144000	2.32354300	1.00521400
C	4.92972900	-1.08554100	0.81968300
H	5.53350500	-1.98825300	0.78841900
C	4.53276400	-0.54909100	2.04733700
H	4.82801700	-1.03226200	2.97480700
C	3.73360800	0.59156200	2.08763900
H	3.38247600	0.99851400	3.03142400
C	3.37411400	1.23808300	0.89739900
C	3.76057100	0.69400500	-0.33674700
H	3.44824900	1.17299100	-1.25896200
C	4.52793900	-0.46873500	-0.36807500
H	4.81463400	-0.89430900	-1.32624800

Table S19 Cartesian coordinates of compound **3f-E-I**

C	-1.57779300	-1.98709900	1.81508400
N	-0.17972500	-1.90846800	2.00694700
C	-2.08658600	-1.15030000	0.79824900
H	-1.38841000	-0.52358600	0.24896600
C	-4.18003000	-1.85937100	1.16619700
C	-3.80268500	-2.75704300	2.20874000
C	-2.45080300	-2.81327100	2.53704900
H	-2.05900500	-3.46066500	3.31419000
C	-5.00427000	-3.40625600	2.66389000
H	-5.08629900	-4.14479300	3.44937300
C	-6.03737000	-2.91522400	1.92393800
H	-7.09518700	-3.12591400	1.95361200
N	-5.55829000	-1.97315900	1.00360400
S	-6.58541200	-1.05679400	-0.05795800
O	-7.92256200	-1.56673700	0.24392900
O	-6.23614100	0.34694900	0.10524500
C	-5.42494800	-2.42752200	-4.26545100
C	-5.06985600	-2.85275600	-5.66977300
H	-5.58905300	-2.22962600	-6.40994800
H	-5.35664100	-3.89195500	-5.85934400
H	-3.99593000	-2.75412200	-5.85862100
C	-6.48722200	-3.03369700	-3.57934900
H	-7.04880400	-3.83169200	-4.05836300
C	-6.84059600	-2.62737200	-2.29504400
H	-7.67241700	-3.08599200	-1.77160400
C	-6.11281800	-1.60063300	-1.69007400
C	-5.05115600	-0.97317200	-2.34581000
H	-4.49667400	-0.18610900	-1.84900900

C	-4.71614600	-1.39783700	-3.62884500
H	-3.88870700	-0.91905400	-4.14635700
N	0.27179300	-2.66063800	2.91346400
C	4.41189900	-2.59326100	3.66558500
H	5.47735300	-2.59416300	3.87938800
C	3.90033400	-1.75499300	2.66624100
H	4.57145200	-1.10761800	2.10785300
C	2.53957000	-1.74479700	2.38410800
H	2.12484800	-1.10271700	1.61518200
C	1.67395200	-2.58284100	3.10875700
C	2.18761000	-3.41998300	4.10833000
H	1.49534300	-4.05559000	4.65219000
C	3.55348600	-3.42549100	4.38598200
H	3.94684700	-4.07630000	5.16190500
N	-3.37434900	-1.07453900	0.45865400

Table S20 Cartesian coordinates of compound **3f-E-II**

C	0.91675800	1.17282600	0.37207900
N	2.15105900	1.72371700	-0.05640000
C	-0.33581900	1.79177900	0.21542300
H	-0.38393500	2.76227300	-0.26557400
C	-1.47992300	1.15226300	0.67738300
H	-2.44947100	1.62867600	0.55768700
C	-1.39134700	-0.10159700	1.29632100
H	-2.29139300	-0.59392000	1.65471800
C	-0.14827700	-0.71705000	1.45257100
H	-0.07609100	-1.68899600	1.93260300
C	1.00318400	-0.08127900	0.99132700
H	1.98392100	-0.53456900	1.09922200
N	2.06266600	2.85500200	-0.60792700
C	5.59643800	4.50972800	-1.87016000
C	4.40352100	5.25306900	-2.08325700
C	3.21663700	4.66505400	-1.64294400
H	2.24751300	5.14283300	-1.75236700
C	3.29191600	3.40736000	-1.03733500
C	4.55165100	2.77151300	-0.89787200
H	4.59859100	1.79199900	-0.43376100
N	5.69991900	3.30597400	-1.30912000
C	4.77613900	6.47812200	-2.73758400
H	4.11784400	7.27962300	-3.04338500
C	6.12958500	6.45454500	-2.90277000
H	6.80506300	7.17683300	-3.33418000
N	6.64927900	5.26299500	-2.38331600
S	8.34914200	4.90066400	-2.32200800
O	8.96497100	6.06369300	-2.96012600

O	8.66031300	4.51185700	-0.95414500
C	8.87182500	1.28797900	-5.07936700
C	9.02950300	0.09738500	-5.99404000
H	9.69971800	0.31928000	-6.83042600
H	8.06165900	-0.19963400	-6.41924600
H	9.42756000	-0.77002700	-5.45738800
C	9.06191100	2.59188500	-5.55895800
H	9.35447100	2.74473000	-6.59462200
C	8.89199000	3.69692800	-4.72843600
H	9.05767100	4.70399800	-5.09528400
C	8.52606700	3.48803600	-3.39728100
C	8.33921400	2.20247900	-2.88389300
H	8.05373000	2.06917500	-1.84733000
C	8.51375400	1.11384000	-3.73409800
H	8.37367700	0.10896200	-3.34383500

Table S21 Cartesian coordinates of compound **3f-Z-I**

N	2.62534500	1.40325600	0.50475600
N	3.79812900	0.97157800	0.46708500
C	7.38251200	2.96425700	0.27175200
N	7.22467000	1.87204100	-0.46702500
C	6.02899100	1.29560700	-0.36468900
H	5.87279300	0.37844300	-0.92737900
C	4.96199000	1.80478200	0.41243700
C	5.16607600	2.93788500	1.20578200
H	4.38248100	3.32009600	1.85108000
C	6.42602700	3.53882500	1.15401300
C	7.05952800	4.65509800	1.79896000
H	6.61926400	5.32574200	2.52413600
C	8.33160800	4.73443700	1.31356300
H	9.11482900	5.44065400	1.54158700
N	8.54519500	3.73489000	0.35604700
S	10.08608300	3.28119200	-0.34168600
O	10.71544100	2.30995200	0.54932400
O	9.82999400	2.98983500	-1.74566900
C	12.43492600	7.20653700	-0.09067400
C	13.24005500	8.48226700	-0.03799100
H	13.59102700	8.69432200	0.97659300
H	12.65462300	9.34022500	-0.38465300
H	14.12527500	8.41107500	-0.68347000
C	12.61135600	6.20490300	0.87434700
H	13.32465900	6.35753500	1.68014300
C	11.89316600	5.01159000	0.81545100
H	12.03949300	4.22986900	1.55336200
C	10.97973200	4.82586700	-0.22332100

C	10.78737500	5.80110900	-1.20541000
H	10.08880200	5.62586700	-2.01688200
C	11.51361000	6.98567800	-1.12690500
H	11.36871000	7.75040400	-1.88576200
C	1.24747000	5.34001700	-0.16695700
H	0.85285400	6.33594900	-0.34747900
C	0.83940300	4.61643900	0.95649100
H	0.12595800	5.04765200	1.65353600
C	1.32375600	3.32797900	1.17402800
H	0.98689100	2.73637500	2.02031100
C	2.26623100	2.77741900	0.29544500
C	2.66615700	3.49549300	-0.84139100
H	3.36352300	3.05064600	-1.54395300
C	2.14824600	4.76882900	-1.06980700
H	2.45165000	5.31798700	-1.95712600

Table S22 Cartesian coordinates of compound **3f-Z-II**

N	2.36566300	1.96511700	-1.25249100
C	5.84501500	4.05233000	-1.94701300
C	4.62438500	4.78057000	-1.99361500
C	3.45605100	4.06111400	-1.73469600
H	2.46998600	4.51400200	-1.78378100
C	3.58178700	2.71166600	-1.39463000
C	4.85873700	2.10231300	-1.41577600
H	4.95347000	1.03816100	-1.22183500
N	5.98619800	2.75419900	-1.70157700
C	4.95112600	6.13662200	-2.34221300
H	4.26326000	6.96226300	-2.46210000
C	6.30533000	6.20246700	-2.49113500
H	6.95262000	7.03130800	-2.73260300
N	6.87093800	4.94417400	-2.25852100
S	8.58121200	4.63999200	-2.26495100
O	9.15604600	5.94596800	-2.58582100
O	8.89882600	3.93469700	-1.03147600
C	9.25034900	1.84434400	-5.82380800
C	9.45450600	0.92450700	-7.00326900
H	10.13366600	1.36254200	-7.74145800
H	8.50225300	0.72475000	-7.51224300
H	9.86468200	-0.04159200	-6.69166400
C	9.39234000	3.23249100	-5.96337000
H	9.68136300	3.64765400	-6.92547900
C	9.17878300	4.09038500	-4.88732600
H	9.30706000	5.16223900	-4.99172900
C	8.81785500	3.54523600	-3.65351200
C	8.67853200	2.16674000	-3.47666400

H	8.39691100	1.77029000	-2.50854100
C	8.89611700	1.32960500	-4.56777600
H	8.79339400	0.25497100	-4.44009500
N	2.18033300	1.09068800	-0.37742100
C	4.55403400	0.21173100	3.00366300
H	5.13454600	-0.03511800	3.88800100
C	4.27222400	1.54656400	2.70178800
H	4.62854400	2.33900000	3.35415900
C	3.53921300	1.87358400	1.56281800
H	3.31813200	2.91032300	1.33196800
C	3.06905600	0.85207500	0.72355100
C	3.30511100	-0.48887200	1.05517200
H	2.88804800	-1.26587900	0.42128100
C	4.07012200	-0.80449500	2.17580900
H	4.27177600	-1.84512600	2.41457800

Table S23 Cartesian coordinates of compound **3g-E-I**

C	3.45143400	-0.02715400	-2.67413400
N	4.61005800	0.74412900	-2.41726600
C	2.28234700	0.71455100	-2.93085000
H	2.35609700	1.79715300	-2.90411400
C	1.06328200	0.09861400	-3.19572600
H	0.16646000	0.67970300	-3.36277700
C	1.03694400	-1.29835900	-3.21490700
C	2.20362400	-2.06173300	-2.95053300
C	3.41087700	-1.42858300	-2.67648400
H	4.31725800	-1.98532700	-2.46576300
N	5.65360600	0.07443100	-2.18392500
C	9.21574300	2.17390300	-1.39304300
H	10.14806200	2.69228200	-1.18558200
C	9.17907200	0.77855100	-1.40613000
H	10.08143300	0.20630600	-1.20920800
C	7.98050500	0.11857000	-1.67203900
H	7.92110700	-0.96554200	-1.68826600
C	6.81259600	0.85002400	-1.92671100
C	6.85108600	2.25540700	-1.91288200
H	5.93793800	2.80539600	-2.11085700
C	8.04934300	2.90737000	-1.64680500
H	8.08077600	3.99380000	-1.63511800
C	1.82940700	-3.46269500	-3.01659900
C	0.45094200	-3.52164100	-3.31801700
N	-0.04625800	-2.18918400	-3.42566500
S	-1.44027200	-1.77474100	-4.35495600
O	-2.40055300	-2.85147500	-4.13280600
O	-1.74906200	-0.38934500	-4.01360100

C	0.01387500	-1.94671700	-8.69959200
C	0.52878400	-2.01275100	-10.11704700
H	-0.00018200	-2.77252200	-10.70117600
H	1.59559200	-2.27229400	-10.13312300
H	0.42027900	-1.05097000	-10.62848800
C	-0.52124200	-3.08349700	-8.07665200
H	-0.59217000	-4.01508500	-8.63224900
C	-0.97296900	-3.04083700	-6.76008500
H	-1.40105700	-3.91932900	-6.29082500
C	-0.88934700	-1.83763100	-6.05508200
C	-0.37139600	-0.68549200	-6.65186000
H	-0.33762300	0.24665500	-6.09944500
C	0.07438300	-0.75086500	-7.96949000
H	0.47013400	0.14504000	-8.44097500
C	-0.22130100	-4.74120800	-3.41766800
H	-1.28454600	-4.78126700	-3.61340900
C	0.52453900	-5.90607400	-3.23284100
H	0.02207500	-6.86660900	-3.30563500
C	1.89567800	-5.86373300	-2.94046300
H	2.44415900	-6.78975500	-2.79394400
C	2.55354700	-4.64269000	-2.82327400
H	3.61253300	-4.60298000	-2.58351300

Table S24 Cartesian coordinates of compound **3g-E-II**

C	0.79437300	1.20226000	0.59474100
N	2.06412500	1.76766300	0.31327300
C	-0.41128500	1.59297800	-0.01384000
H	-0.39036500	2.38365000	-0.75542300
C	-1.59749400	0.96351900	0.34452600
H	-2.53062100	1.26459100	-0.12464200
C	-1.59829100	-0.05519800	1.30631300
H	-2.53066600	-0.54145200	1.58057600
C	-0.40209000	-0.44398900	1.91168000
H	-0.39880400	-1.23316600	2.65845400
C	0.79100500	0.18324700	1.55675100
H	1.73664000	-0.09716600	2.01084500
N	2.05504700	2.68203500	-0.55612100
C	5.72272900	4.47374000	-1.52142100
C	4.52419500	4.86306800	-2.16281300
C	3.32078500	4.25067100	-1.81437200
H	2.37985600	4.52659100	-2.28044000
C	3.31978900	3.25015700	-0.83831900
C	4.52508400	2.87954300	-0.20045100
H	4.48531200	2.11261100	0.56448000
C	5.72937500	3.48686300	-0.52520500
H	6.64393700	3.21992800	-0.01237000
C	4.85414900	5.91487800	-3.10492600
C	6.24590100	6.14228500	-3.01566400
N	6.78339300	5.26662800	-2.02785100
S	8.43386200	4.76002700	-2.01154000
O	9.21378000	5.93409000	-2.39102000
O	8.63204500	4.08910300	-0.73033300

C	8.68701500	1.65270100	-5.37274900
C	8.73251000	0.63398500	-6.48576300
H	9.40215500	0.94986300	-7.29191200
H	7.73635500	0.49086800	-6.92493900
H	9.07067200	-0.34188800	-6.12261400
C	8.92778900	3.00980600	-5.63081600
H	9.17857900	3.32665200	-6.63989500
C	8.86055100	3.96138500	-4.61613400
H	9.06457300	5.00642200	-4.81985900
C	8.54878500	3.54605500	-3.31938600
C	8.31454700	2.19966000	-3.02873900
H	8.09932300	1.89048500	-2.01219900
C	8.38695700	1.26533500	-4.05855400
H	8.21394800	0.21555700	-3.83581700
C	6.87384900	7.12673300	-3.78154200
H	7.93344400	7.32210300	-3.68422500
C	6.08017500	7.86497900	-4.65984900
H	6.54733900	8.63649400	-5.26555400
C	4.69845700	7.64579500	-4.76494200
H	4.10898800	8.24489700	-5.45302500
C	4.07717400	6.67611500	-3.98370200
H	3.00524800	6.51184600	-4.05147400

Table S26 Cartesian coordinates of compound **3g-Z-I**

C	3.93055000	-0.64684100	-3.51427800
N	5.21427700	-0.01729600	-3.63161900
C	2.82380200	0.22366600	-3.49236800
H	3.01282900	1.29230300	-3.46024800
C	1.51740100	-0.25408100	-3.48690000
H	0.67653200	0.42288700	-3.41660700
C	1.33042200	-1.63596500	-3.58367600
C	2.43232400	-2.52102400	-3.65303900
C	3.73650500	-2.02913000	-3.60553900
H	4.58433000	-2.70381100	-3.65090300
C	1.90342500	-3.86909500	-3.73874000
C	0.49389100	-3.77423100	-3.71495000
N	0.13380700	-2.40020800	-3.60263000
S	-1.37274200	-1.77319800	-4.16462400
O	-2.37584700	-2.77239400	-3.80902700
O	-1.44312000	-0.40364000	-3.66345900
C	-0.92603000	-1.66831300	-8.72619200
C	-0.74229700	-1.64710600	-10.22431600
H	-1.45307700	-2.31183500	-10.72534400
H	0.26718800	-1.98093600	-10.49847300
H	-0.87233000	-0.63865500	-10.63004500
C	-1.43866400	-2.80315200	-8.08135000
H	-1.73410300	-3.66670900	-8.67170500
C	-1.58565300	-2.84317900	-6.69707100
H	-1.99858100	-3.71760700	-6.20711800
C	-1.21480900	-1.72579000	-5.94508800
C	-0.71137800	-0.57645700	-6.55967000
H	-0.45294300	0.29177200	-5.96427000

C	-0.57274000	-0.55833200	-7.94503600
H	-0.18949100	0.33669000	-8.42835000
C	-0.31288100	-4.91364900	-3.74664500
H	-1.39078200	-4.83867300	-3.69210800
C	0.32287900	-6.15277000	-3.82861900
H	-0.28518700	-7.05273800	-3.85484700
C	1.72118000	-6.26235800	-3.86022000
H	2.18345500	-7.24371800	-3.91531200
C	2.51850700	-5.12306300	-3.80697900
H	3.60204100	-5.20364400	-3.81576500
N	6.24519300	-0.40387900	-3.03924200
C	6.58828400	-3.21180800	0.09878600
H	6.71524000	-3.91727100	0.91510000
C	7.43454600	-3.26354300	-1.01167900
H	8.22328600	-4.00932000	-1.06231400
C	7.28879500	-2.34155800	-2.04637400
H	7.96266600	-2.34112600	-2.89820600
C	6.25503600	-1.39659400	-2.00208800
C	5.41397700	-1.33273000	-0.88095400
H	4.63958300	-0.57454600	-0.82810900
C	5.59093100	-2.23512700	0.16576800
H	4.94387500	-2.17701900	1.03684200

Table S27 Cartesian coordinates of compound **3g-Z-II**

N	2.42898600	2.43761400	1.02770900
N	2.56471200	3.53378300	0.44150300
C	5.99245500	5.06046000	-1.46948700
C	4.70672500	5.21981900	-2.03706600
C	3.58955600	4.69499600	-1.38840500
H	2.58486800	4.84578300	-1.77164100
C	3.76780000	3.95162700	-0.21832400
C	5.05318100	3.82001700	0.34755200
H	5.17155700	3.29609800	1.28918100
C	6.17043800	4.38687900	-0.25708400
H	7.14534500	4.31892000	0.20698400
C	4.85816400	6.00426700	-3.24742500
C	6.23168900	6.30442600	-3.38900300
N	6.93454400	5.74065500	-2.28512900
S	8.60473400	5.31444200	-2.34854600
O	9.25939600	6.38146100	-3.09932100
O	8.98549300	4.99640500	-0.97549300
C	8.70958800	1.46763800	-4.84155900
C	8.70968700	0.20376100	-5.66713100
H	9.34972300	0.30174100	-6.54996700
H	7.69782000	-0.03071200	-6.02335000
H	9.05864600	-0.65544900	-5.08575600
C	8.83487900	2.72323600	-5.45405000
H	8.96151200	2.78297200	-6.53203100
C	8.81031300	3.89743200	-4.70616300
H	8.92603100	4.86347300	-5.18424800
C	8.65939500	3.81346000	-3.31966900
C	8.54221300	2.57741700	-2.67964900

H	8.45186900	2.52826900	-1.60041500
C	8.56959200	1.41557100	-3.44735400
H	8.48924700	0.45091100	-2.95281900
C	6.70156000	7.08078200	-4.45035100
H	7.74880800	7.33861900	-4.53560400
C	5.76727900	7.53192200	-5.38303900
H	6.11027800	8.13826100	-6.21673200
C	4.40136700	7.23631900	-5.25957800
H	3.70009300	7.61140700	-5.99935100
C	3.93861700	6.47797600	-4.18848200
H	2.88009500	6.25748800	-4.08117800
C	4.94645500	-0.95280300	0.91219500
H	5.55767900	-1.85083800	0.89630000
C	4.47439700	-0.44691300	2.12616200
H	4.71859100	-0.94925600	3.05822200
C	3.66591700	0.68769100	2.14515000
H	3.25739500	1.07098700	3.07561700
C	3.37243900	1.35899700	0.95057600
C	3.83407900	0.84557800	-0.27077000
H	3.57193100	1.34280600	-1.19897900
C	4.61026400	-0.31166500	-0.28301700
H	4.95479700	-0.71412900	-1.23208400

Table S28 Cartesian coordinates of compound **3h-E-I**

C	0.75302700	-1.63992700	-5.71653200
H	1.59721100	-1.09067700	-5.31933100
C	-0.55558300	-1.27982000	-5.42661500
H	-0.74663900	-0.42431700	-4.78486600
C	-1.65012000	-2.00845900	-5.94310000
H	-2.66020200	-1.70252500	-5.68442400
C	-1.46582300	-3.11152500	-6.76452500
H	-2.30558100	-3.68675300	-7.13964200
C	-0.14210900	-3.46190300	-7.06273700
C	0.96558100	-2.75222100	-6.54857000
C	2.10431500	-3.45397600	-7.09109000
N	3.47400700	-3.25824600	-6.96742600
N	1.72036800	-4.47611900	-7.85330000
N	0.37364600	-4.47459900	-7.85067200
N	3.78784400	-2.27356100	-6.23546700
C	7.88885200	-1.48043800	-5.70453500
H	8.94109800	-1.25548300	-5.55213400
C	6.90967400	-0.68729700	-5.10394200
H	7.19560900	0.15697400	-4.48261000
C	5.56143600	-0.98009700	-5.30205900
H	4.77962700	-0.37976900	-4.84642300
C	5.18445500	-2.06727400	-6.10214900
C	6.17198800	-2.86548000	-6.70636200
H	5.86261500	-3.70300000	-7.32161200
C	7.51455100	-2.56797900	-6.50436000
H	8.27883400	-3.18442300	-6.97061100
C	-1.08683900	-8.20977900	-9.15987900
H	-1.79589400	-8.91893500	-9.60541400

H	-0.31649700	-8.79569100	-8.64252200
C	-1.80755300	-7.33286000	-8.13587000
H	-2.18391600	-7.91540400	-7.29051800
H	-2.66639000	-6.82425900	-8.60914100
O	-0.92612800	-6.36242200	-7.56870000
C	-0.38981300	-5.48434100	-8.55266600
H	-1.22731900	-4.96426600	-9.05004500
C	0.43487400	-6.23935400	-9.59404100
H	1.30055300	-6.68193300	-9.09309700
H	0.81558600	-5.53779200	-10.34398200
C	-0.43666300	-7.33021600	-10.23850300
H	0.16931700	-7.93636100	-10.92131700
H	-1.22280300	-6.86159200	-10.84881300

Table S29 Cartesian coordinates of compound **3h-E-II**

C	0.40386500	-1.16301200	-6.50613900
C	-0.72248200	-1.74167700	-5.88354700
C	-1.81868700	-0.90852100	-6.29078100
N	-3.13222200	-1.14514100	-5.88284100
N	-1.40583500	0.07815900	-7.08318200
N	-0.07162600	-0.08420600	-7.22451400
N	-3.99804400	-0.33996700	-6.33065000
C	-8.00246000	-0.92630200	-5.17473700
H	-9.04391400	-1.05488300	-4.89193900
C	-7.63246400	0.11519300	-6.02743100
H	-8.38359800	0.80024400	-6.41097000
C	-6.29538600	0.27589400	-6.38671400
H	-5.97542000	1.07584200	-7.04740500
C	-5.32081700	-0.60404700	-5.89572200
C	-5.69567100	-1.65245000	-5.03650200
H	-4.92949100	-2.32368100	-4.66502600
C	-7.03047000	-1.80712200	-4.68205100
H	-7.32191800	-2.61678300	-4.01786800
C	-0.57463100	-2.88614400	-5.08389300
H	-1.43770700	-3.33572400	-4.60344300
C	0.69829700	-3.41315500	-4.93029400
H	0.84556500	-4.29741500	-4.31669800
C	1.81914000	-2.81543600	-5.55405700
H	2.80275500	-3.25113700	-5.40123200
C	1.69679200	-1.68352200	-6.34628300
H	2.56196800	-1.21376400	-6.80190000
C	1.65826600	3.49175700	-8.64516000
H	2.39357700	4.12830800	-9.15342300

H	1.01204900	4.14741600	-8.04778200
C	2.37568300	2.52160500	-7.70662100
H	2.89651500	3.04296900	-6.89878400
H	3.12163000	1.93153200	-8.26851700
O	1.45330200	1.64246400	-7.06124200
C	0.72711400	0.84784600	-7.99293100
H	1.44742700	0.24667800	-8.57526800
C	-0.10721800	1.70809700	-8.94074400
H	-0.86584600	2.23186400	-8.35241100
H	-0.63484900	1.06622400	-9.65428100
C	0.81167800	2.70938100	-9.66042700
H	0.21188900	3.39108100	-10.27395600
H	1.47724800	2.16983700	-10.35043100

Table S30 Cartesian coordinates of compound **3h-Z-I**

C	-0.12342800	-0.89672400	-7.04920400
H	0.60741300	-0.12331700	-6.83977200
C	-1.47808100	-0.65335500	-6.88709200
H	-1.81131500	0.32390300	-6.55006500
C	-2.43837100	-1.65838900	-7.14404200
H	-3.49136800	-1.43508900	-6.99597700
C	-2.06876600	-2.92176300	-7.57832600
H	-2.80886600	-3.69252800	-7.76722000
C	-0.69690000	-3.15971700	-7.75437400
C	0.27896900	-2.17321400	-7.47976300
C	1.52431500	-2.82780400	-7.79669000
N	2.84306600	-2.30311300	-7.90130300
N	1.32294900	-4.05450100	-8.25119100
N	-0.01870400	-4.26627700	-8.21512800
N	3.38554800	-1.62432100	-6.99900900
C	-0.63374400	-8.43853100	-8.32214100
H	-1.18530400	-9.37738200	-8.45839900
H	0.30970300	-8.68134100	-7.81675800
C	-1.43828800	-7.49067500	-7.43247100
H	-1.56716700	-7.88889700	-6.42210000
H	-2.44206400	-7.32650400	-7.86390900
O	-0.77410200	-6.23739900	-7.26833200
C	-0.57888300	-5.56368100	-8.50894800
H	-1.56502300	-5.38358100	-8.97015100
C	0.28897400	-6.38338600	-9.46439700
H	1.28710900	-6.47602500	-9.02725000
H	0.39626400	-5.84676100	-10.41357300
C	-0.34416700	-7.76871000	-9.67360200

H	0.31763300	-8.39355700	-10.28396200
H	-1.28360700	-7.66403700	-10.23645700
C	2.13254700	-1.09714700	-3.00440000
H	1.84776100	-0.94839300	-1.96653200
C	2.01342500	-2.36104200	-3.58818700
H	1.64175600	-3.19769600	-3.00289500
C	2.36606500	-2.56084100	-4.92138400
H	2.28120300	-3.54492900	-5.36959000
C	2.85886700	-1.48462100	-5.67608400
C	3.03004300	-0.22973100	-5.07380200
H	3.46654300	0.57365000	-5.66011900
C	2.63981000	-0.03078900	-3.75182100
H	2.75208600	0.94981200	-3.29738200

Table S31 Cartesian coordinates of compound **3h-Z-II**

C	0.56065300	-1.05902700	-6.41972100
C	-0.63322000	-1.69376200	-6.01448500
C	-1.64963700	-1.07660200	-6.81855000
N	-2.98472200	-1.53504400	-6.81971400
N	-1.12796100	-0.18159100	-7.65058100
N	0.20463600	-0.17710000	-7.41998800
N	-3.96996200	-0.86481400	-7.20954300
C	-0.60315400	-2.68685400	-5.02219300
H	-1.51740100	-3.18415300	-4.71453600
C	0.62357300	-3.00855400	-4.46264500
H	0.68140600	-3.77501000	-3.69510100
C	1.80956000	-2.35142200	-4.86818700
H	2.74991200	-2.62164200	-4.39553800
C	1.80311400	-1.36742100	-5.84569800
H	2.70866600	-0.84599500	-6.13559800
C	2.06279700	3.24826600	-9.03171300
H	2.86011900	3.84486900	-9.49262700
H	1.30275500	3.94653400	-8.65873300
C	2.62608700	2.45822600	-7.85060600
H	2.97809000	3.11373300	-7.04937000
H	3.47618700	1.83523900	-8.18072200
O	1.62548800	1.63034600	-7.25425800
C	1.10327300	0.67577400	-8.17250700
H	1.93627900	0.04243700	-8.52637500
C	0.42697900	1.34998000	-9.36495100
H	-0.43864800	1.91084800	-9.00031700
H	0.05318400	0.58955600	-10.05833300
C	1.43315600	2.28818000	-10.05224800

H	0.93467100	2.84519800	-10.85346100
H	2.22572500	1.69338800	-10.52977000
C	-4.15285500	3.25372600	-8.11374300
H	-4.24534100	4.31224400	-8.34082800
C	-4.54853400	2.29692400	-9.05103800
H	-4.94862500	2.60806500	-10.01251400
C	-4.45644500	0.93885400	-8.75060600
H	-4.78992500	0.18420700	-9.45669000
C	-3.91517000	0.53114900	-7.52629800
C	-3.53231600	1.48815200	-6.57589500
H	-3.14825900	1.16677300	-5.61247700
C	-3.65852700	2.84285400	-6.87219000
H	-3.36810500	3.58197100	-6.13005200

Table S32 Cartesian coordinates of compound **5e-E-I**

C	4.41136000	5.29984000	0.98464200
N	5.60090400	6.06505100	0.97614300
C	3.22348600	6.05405400	0.82139500
H	3.32381600	7.12857900	0.70648200
C	1.97734500	5.44903000	0.80801900
H	1.06985100	6.03331000	0.68240900
C	1.93654600	4.05789200	0.96258200
C	3.11900500	3.27340200	1.12883300
C	4.36313700	3.90946800	1.13861400
H	5.28934600	3.35886200	1.26165400
N	6.66738900	5.40602700	1.12124100
C	10.30876400	7.52419800	1.12025600
H	11.26144200	8.04720700	1.12353300
C	10.27055100	6.13763700	1.27673700
H	11.19252600	5.57639700	1.40236100
C	9.04594700	5.47163900	1.27171900
H	8.98555500	4.39400900	1.39125100
C	7.85193300	6.18719300	1.11041700
C	7.89243000	7.58362200	0.95290600
H	6.95936300	8.12184000	0.82915100
C	9.11669900	8.24201800	0.95871000
H	9.14835300	9.32182000	0.83688900
C	2.69416400	1.90361300	1.25573800
H	3.32840200	1.03930400	1.39503100
C	1.32987300	1.89568100	1.16706300
H	0.63228500	1.07105600	1.21445600
N	0.86812700	3.19140800	0.99034400
H	-0.10019800	3.45574400	0.89702500

Table S33 Cartesian coordinates of compound **5e-E-II**

C	5.10198700	-0.16315700	1.12039700
N	6.30283200	0.58932600	1.19558200
C	3.92253900	0.56229500	1.33550700
H	4.00476700	1.62558500	1.54025700
C	2.68429000	-0.07599800	1.28513100
H	1.77377000	0.49290100	1.45290900
C	2.61765400	-1.44472400	1.01923000
H	1.65423900	-1.94610300	0.97914600
C	3.79506400	-2.17241800	0.80390000
H	3.74145600	-3.23831500	0.59699400
C	5.03286600	-1.54154100	0.85279600
H	5.95487500	-2.08800700	0.68879900
N	7.35564500	-0.07905200	0.99851100
C	11.00499700	1.94934800	1.17578600
C	10.96628300	0.55261800	0.90110600
C	9.72063400	-0.08684200	0.85111700
H	9.62700000	-1.14904100	0.64622800
C	8.55928700	0.65661400	1.07016600
C	8.62548900	2.05000200	1.34243500
H	7.69587100	2.58254900	1.50536000
C	9.84132700	2.70413500	1.39724100
H	9.89358800	3.76991300	1.60544900
C	12.32761900	0.12197000	0.73170500
H	12.66878200	-0.88010400	0.51186200
C	13.12134600	1.22397500	0.90129600
H	14.19673700	1.32387700	0.85472800
N	12.32746800	2.32772500	1.16930600
H	12.66789000	3.26237100	1.33375500

Table S34 Cartesian coordinates of compound **5e-Z-I**

C	4.13533000	5.02162800	0.64280400
N	5.35051400	5.65820500	0.22550000
C	3.19541100	5.88808500	1.25354600
H	3.49429600	6.91597400	1.43345100
C	1.93518200	5.44352900	1.61850100
H	1.22714300	6.10858500	2.10561100
C	1.60089700	4.12010300	1.30593700
C	2.50836800	3.24563200	0.64040900
C	3.79217600	3.70753700	0.31842800
H	4.49943600	3.06102200	-0.18917300
N	6.47923800	5.11994000	0.25651300
C	1.82283900	1.99512700	0.45601100
H	2.21539300	1.10338900	-0.01243300
C	0.57337600	2.13845000	0.99587800
H	-0.24216600	1.43191100	1.06311800
N	0.43454700	3.41650600	1.51059000
H	-0.39742400	3.78014500	1.94847100
C	7.66315100	1.53632100	2.15848600
H	8.01109100	0.63053000	2.64719900
C	6.90052200	2.46790600	2.86831200
H	6.65750700	2.28922600	3.91251700
C	6.44244000	3.62762800	2.24675500
H	5.84819200	4.35009600	2.79691000
C	6.76245600	3.86897900	0.90225400
C	7.56839700	2.95979200	0.20448600
H	7.84856300	3.18674200	-0.82013700
C	7.99269700	1.78554600	0.82402400
H	8.59872800	1.07376600	0.26973300

Table S35 Cartesian coordinates of compound **5e-Z-II**

N	6.56768200	0.61947100	2.03804000
N	7.66692500	0.04985000	1.85391700
C	11.45017300	1.79153200	1.31426600
C	11.07682600	0.62640200	0.58485300
C	9.80194600	0.08269900	0.79165200
H	9.48383500	-0.83044500	0.29726300
C	8.91105200	0.73178200	1.64759200
C	9.31202900	1.88252000	2.37484000
H	8.62297300	2.33925500	3.07521400
C	10.58379300	2.41112200	2.22416900
H	10.89418400	3.27962600	2.79916100
C	12.20856100	0.25771500	-0.22130200
H	12.27629700	-0.58065200	-0.90051100
C	13.19556500	1.17213400	0.03083900
H	14.19541400	1.24793600	-0.37330800
N	12.74417000	2.09815100	0.95624300
H	13.28126700	2.87289400	1.31336500
C	5.55378700	4.68540100	1.49401300
H	5.24841500	5.71801300	1.34959000
C	6.27032000	4.01940900	0.49601800
H	6.51981100	4.53273700	-0.42900800
C	6.67366000	2.69797100	0.67686300
H	7.23131800	2.18086700	-0.09726100
C	6.34358100	2.02588600	1.86371400
C	5.58215700	2.67743700	2.84342300
H	5.29230400	2.12662400	3.73361500
C	5.21411100	4.01018600	2.66916400
H	4.64324100	4.51617500	3.44327700

Table S36 Cartesian coordinates of compound **5f-E-I**

C	10.69126700	-4.26246500	2.04831900
N	11.86147700	-3.47335100	2.02759700
C	9.48805200	-3.54552400	1.84496800
H	9.55195400	-2.47068200	1.69217500
N	8.27491700	-4.09529700	1.82693200
C	8.26961800	-5.41450500	2.02036100
C	9.40106900	-6.26232400	2.23713500
C	10.65224400	-5.64973200	2.24904600
H	11.57707000	-6.19503100	2.40451800
N	12.93654700	-4.10940900	2.20817800
C	16.54421400	-1.93858500	2.18271400
H	17.48884800	-1.40130000	2.18059700
C	16.52531500	-3.31994400	2.38261900
H	17.45398200	-3.86254900	2.53667800
C	15.31096300	-4.00429100	2.38447800
H	15.26511000	-5.07836200	2.53745800
C	14.10907200	-3.31150700	2.18641200
C	14.12972400	-1.92022000	1.98526800
H	13.19068700	-1.39986200	1.83364600
C	15.34394100	-1.24376700	1.98460700
H	15.36137600	-0.16809700	1.82922600
C	8.89323200	-7.59822500	2.39202600
H	9.46581000	-8.49758400	2.57078600
C	7.53150300	-7.52196500	2.26989400
H	6.78600900	-8.30289100	2.32388600
N	7.15132000	-6.20818800	2.04585400
H	6.21067900	-5.86594300	1.91892300

Table S37 Cartesian coordinates of compound **5f-E-II**

C	14.93083700	-7.96798400	-0.13396000
N	16.14568500	-7.23837200	-0.07007100
C	13.76781800	-7.21714300	0.08340000
H	13.87231000	-6.15455400	0.28099700
C	12.51719000	-7.83149800	0.04397100
H	11.61887600	-7.24419900	0.21325900
C	12.42300300	-9.20026000	-0.21303700
H	11.44983200	-9.68293700	-0.24457200
C	13.58437900	-9.95295300	-0.43062200
H	13.50820300	-11.01869500	-0.63053400
C	14.83443200	-9.34645000	-0.39269200
H	15.74436400	-9.91223600	-0.55854700
N	17.18523000	-7.92646000	-0.26820700
C	20.74076300	-5.90012200	-0.10068400
C	20.78897700	-7.29811400	-0.37468800
C	19.56028800	-7.96016000	-0.42515700
H	19.46996300	-9.02386700	-0.62554600
C	18.40086100	-7.20997200	-0.20640800
C	18.50127000	-5.81667700	0.05733500
H	17.59208600	-5.24846800	0.22510800
N	19.65282400	-5.15382700	0.11291400
C	22.17378500	-7.64413000	-0.52939200
H	22.58392500	-8.62098600	-0.74470700
C	22.89284200	-6.49064900	-0.35138100
H	23.96062400	-6.32677000	-0.38723100
N	22.03214100	-5.43749500	-0.09279900
H	22.28869200	-4.47652300	0.07725100

Table S38 Cartesian coordinates of compound **5f-Z-I**

C	10.37385100	-4.44742800	2.29599500
N	11.51815900	-3.67271800	2.66969800
C	9.52392800	-3.81821500	1.35313600
H	9.83876200	-2.86778800	0.92863100
N	8.36152300	-4.31569400	0.93566400
C	8.00946000	-5.45944500	1.52339400
C	8.73546600	-6.17132600	2.52444100
C	9.96742200	-5.63761800	2.91050600
H	10.57940400	-6.11460000	3.66812400
N	12.63189800	-4.15394200	2.97475700
C	7.94461400	-7.31768800	2.87437700
H	8.18738500	-8.08282500	3.59847200
C	6.81309800	-7.26935700	2.10242900
H	5.97304800	-7.94844000	2.06182500
N	6.84800900	-6.15198500	1.28626200
H	6.13749100	-5.86037300	0.63196200
C	14.02057300	-8.11503500	2.49064000
H	14.41928400	-9.11820400	2.36869900
C	14.13328800	-7.45914300	3.71908600
H	14.62034900	-7.95062300	4.55704200
C	13.64565800	-6.16210500	3.86909800
H	13.75956400	-5.62419800	4.80579800
C	12.99066400	-5.53297900	2.80208700
C	12.88959700	-6.18343100	1.56320600
H	12.41747400	-5.67880000	0.72627100
C	13.41142800	-7.46669600	1.41290400
H	13.33970200	-7.96354200	0.44899900

Table S39 Cartesian coordinates of compound **5f-Z-II**

N	16.42588300	-7.22163700	0.76872200
N	17.50911900	-7.82096200	0.58583400
C	21.22632100	-6.11566500	0.14968800
C	20.91180400	-7.22678000	-0.68701600
C	19.63774500	-7.77879300	-0.53214400
H	19.30696800	-8.65296800	-1.08588100
C	18.76394100	-7.16399900	0.36865700
C	19.21651000	-6.07228300	1.15324700
H	18.56083400	-5.63745100	1.90163500
N	20.43845700	-5.55018500	1.06419800
C	22.07770800	-7.49244600	-1.48084600
H	22.19995800	-8.26662100	-2.22548000
C	23.02373400	-6.56902200	-1.11672500
H	24.03222600	-6.43112800	-1.48063600
N	22.51572100	-5.73715600	-0.13485500
H	22.99847500	-4.97803300	0.32177400
C	15.55388800	-3.12541400	0.21430200
H	15.28808100	-2.08199600	0.07003400
C	15.17330900	-3.79175600	1.38184900
H	14.61016700	-3.26831400	2.14974100
C	15.49173100	-5.13696300	1.55618700
H	15.17131400	-5.68026100	2.44034600
C	16.24478400	-5.81012000	0.58506500
C	16.61472100	-5.14744600	-0.59520500
H	17.16137400	-5.68106200	-1.36582100
C	16.26043400	-3.81206100	-0.77653200
H	16.54039100	-3.30457700	-1.69583600

Table S40 Cartesian coordinates of compound **5g-E-I**

C	19.39391500	-9.01910300	-0.99025300
N	20.56839200	-8.22750400	-1.06309400
C	18.18632300	-8.31446000	-1.08704500
H	18.23011800	-7.23622900	-1.20833400
C	16.96944700	-8.99171900	-1.02766700
H	16.03699400	-8.43894000	-1.10334400
C	16.95238000	-10.37871700	-0.87108100
H	16.00572600	-10.91047100	-0.82435600
C	18.15788100	-11.08568000	-0.77410800
H	18.14264400	-12.16580700	-0.65222800
C	19.37462800	-10.41611400	-0.83259900
H	20.31761900	-10.94618800	-0.75932100
N	21.64816000	-8.87631100	-0.97416200
C	25.28355600	-6.81585600	-1.15476900
C	25.26768100	-8.20502800	-0.99840900
H	26.18804400	-8.77692100	-0.92086600
C	24.02911300	-8.82998000	-0.94555800
H	23.95429000	-9.90613800	-0.82530300
C	22.82486700	-8.09884800	-1.04511300
C	22.85058600	-6.70398300	-1.20200400
H	21.91146200	-6.16652100	-1.27595000
C	24.08011400	-6.05634100	-1.25750700
C	24.47826000	-4.66744200	-1.40837900
C	25.89681200	-4.64507500	-1.39068300
N	26.35498500	-5.94901600	-1.23722200
H	27.32500500	-6.22065100	-1.19265400
C	26.61918100	-3.45760100	-1.51419700
H	27.70576000	-3.45199800	-1.49933100

C	25.89542200	-2.27505700	-1.65778000
H	26.43094800	-1.33477700	-1.75609800
C	24.49013300	-2.27599500	-1.67772500
H	23.95626200	-1.33694500	-1.79116700
C	23.77669700	-3.46587900	-1.55380700
H	22.69009500	-3.46180700	-1.56978400

Table S41 Cartesian coordinates of compound **5g-E-II**

C	18.03689800	-2.70721900	0.12456200
N	19.23968300	-1.95881200	0.19539600
C	16.86021900	-1.97723800	0.34054400
H	16.94632100	-0.91376000	0.54259400
C	15.61987300	-2.61158200	0.29431500
H	14.71158800	-2.03935500	0.46265500
C	15.54828500	-3.98074100	0.03183800
H	14.58319300	-4.47906500	-0.00496900
C	16.72280600	-4.71293700	-0.18427600
H	16.66515900	-5.77911200	-0.38844900
C	17.96274700	-4.08614700	-0.13959000
H	18.88242800	-4.63627200	-0.30429100
N	20.29078600	-2.63033500	-0.00316700
C	23.95157900	-0.61136100	0.16228300
C	23.90012800	-2.00582500	-0.10967900
C	22.65979200	-2.64213700	-0.15625100
H	22.56401900	-3.70442400	-0.35978000
C	21.49519100	-1.89785400	0.06474200
C	21.57032500	-0.50827800	0.33421200
H	20.64405300	0.02987500	0.49935600
C	22.79065500	0.14340800	0.38517300
H	22.84548500	1.20903900	0.59202700
C	25.27105300	-2.44766500	-0.28424100
C	26.09241200	-1.30274300	-0.11059500
N	25.27318200	-0.21246000	0.15671700
H	25.59590500	0.72841400	0.32240000
C	27.48306900	-1.36723500	-0.21199400
H	28.10160200	-0.48398200	-0.07709400

C	28.05169300	-2.60773100	-0.49315600
H	29.13183800	-2.68888600	-0.57805600
C	27.25596300	-3.75353800	-0.66863400
H	27.73097800	-4.70562500	-0.88690400
C	25.86925200	-3.68131100	-0.56595000
H	25.25944100	-4.57040500	-0.70263700

Table S42 Cartesian coordinates of compound **5g-Z-I**

N	20.78516900	-8.20427100	-1.98957200
N	21.95892500	-8.62462500	-1.87927600
C	25.46917700	-6.60645900	-0.76317200
C	25.25280900	-7.92772100	-0.36013100
H	25.99658100	-8.47492000	0.21229400
C	24.06483800	-8.53221400	-0.74725300
H	23.86617500	-9.56966700	-0.49681100
C	23.07505500	-7.82707600	-1.46802300
C	23.30596300	-6.50866400	-1.88224000
H	22.56812000	-5.98046400	-2.47541000
C	24.51105200	-5.89548600	-1.53872600
C	25.07665900	-4.58439900	-1.79896900
C	26.34774200	-4.55649800	-1.16765600
N	26.55842000	-5.78290800	-0.54999800
H	27.39138100	-6.04221500	-0.04455600
C	27.17254600	-3.43132700	-1.21666800
H	28.14386500	-3.42053300	-0.72953300
C	26.70518800	-2.31944200	-1.91424000
H	27.32598000	-1.42945700	-1.96990400
C	25.44876000	-2.32679000	-2.54516800
H	25.11413600	-1.44293500	-3.08042000
C	24.63101200	-3.45239400	-2.49094300
H	23.66003300	-3.45207600	-2.97906500
C	19.13128400	-4.56166900	-0.62797600
H	18.66539100	-3.64431700	-0.27919500
C	19.90781900	-5.32968400	0.24407200
H	20.04343500	-5.01202800	1.27458400
C	20.51657600	-6.50250400	-0.19753200

H	21.12071300	-7.09867200	0.47888100
C	20.33633400	-6.92315400	-1.52396800
C	19.51752400	-6.18013700	-2.38474800
H	19.34774800	-6.54638100	-3.39315300
C	18.94077100	-4.99019900	-1.94391500
H	18.32502200	-4.40711400	-2.62361200

Table S43 Cartesian coordinates of compound **5g-Z-II**

N	19.51789200	-1.88980200	1.22330900
N	20.64094500	-2.44295800	1.21054900
C	24.43530700	-0.68615600	0.77010800
C	24.14345700	-1.95347400	0.19500000
C	22.86930900	-2.49700800	0.35767700
H	22.61422400	-3.48157100	-0.02309600
C	21.88384000	-1.75699900	1.02103900
C	22.19980300	-0.50491700	1.59970700
H	21.44275400	0.03322700	2.15763900
C	23.47538900	0.03229800	1.49067400
H	23.71517900	0.98441600	1.95608800
C	25.36221800	-2.41185300	-0.44477800
C	26.33807300	-1.40311800	-0.23029300
N	25.75551900	-0.37697000	0.50278900
H	26.22719600	0.46257700	0.80146400
C	27.64093400	-1.51986000	-0.71804600
H	28.38039400	-0.74204200	-0.54753400
C	27.96096000	-2.67253300	-1.43212600
H	28.96759000	-2.79109800	-1.82348700
C	27.00878700	-3.68276400	-1.65552000
H	27.29121200	-4.56888800	-2.21645800
C	25.71113700	-3.55934400	-1.16649100
H	24.97905500	-4.34304500	-1.34231600
C	18.47660300	2.03477600	0.05391600
H	18.16539900	3.02935300	-0.25315500
C	18.05775100	1.51533300	1.28148000
H	17.41919000	2.10508000	1.93381800
C	18.43443800	0.22925300	1.66411200

H	18.08570700	-0.20371000	2.59724900
C	19.28139800	-0.52705900	0.84266000
C	19.69121700	-0.01286600	-0.39710200
H	20.31580500	-0.61444300	-1.04964800
C	19.28044700	1.26026200	-0.78692100
H	19.59216900	1.65040700	-1.75230700

Table S44 Cartesian coordinates of compound **5g-z-II**

C	23.28812600	-1.65299800	-0.03815400
N	24.46936600	-0.86826200	-0.03787100
C	22.08504900	-0.93420700	-0.03745600
H	22.13238900	0.15067000	-0.03677000
C	20.86454100	-1.60729900	-0.03764700
H	19.93496300	-1.04479800	-0.03710500
C	20.84064900	-3.00300000	-0.03853500
H	19.89102100	-3.53139500	-0.03868600
C	22.04205300	-3.72361100	-0.03923100
H	22.02059800	-4.81032300	-0.03991900
C	23.26267200	-3.05894100	-0.03904600
H	24.20293500	-3.59891600	-0.03957300
N	25.54206000	-1.54068100	-0.03854700
N	28.81110600	-0.47974700	-0.03886000
H	29.77617500	-0.77389000	-0.03928200
N	27.85326600	-1.42194800	-0.03913700
C	26.69359100	-0.76304200	-0.03843300
C	26.90476300	0.66567300	-0.03768900
C	28.31305400	0.80191100	-0.03799800
C	28.95353200	2.04861100	-0.03747000
H	30.03627400	2.13477400	-0.03771700
C	28.13607900	3.16942200	-0.03661300
H	28.58926700	4.15692700	-0.03617900
C	26.72738300	3.05671000	-0.03628700
H	26.12639800	3.96157900	-0.03560800
C	26.10052500	1.81858100	-0.03681600
H	25.02186300	1.72600000	-0.03657000

Table S45 Cartesian coordinates of compound **5h-E-I**

C	23.28812600	-1.65299800	-0.03815400
N	24.46936600	-0.86826200	-0.03787100
C	22.08504900	-0.93420700	-0.03745600
H	22.13238900	0.15067000	-0.03677000
C	20.86454100	-1.60729900	-0.03764700
H	19.93496300	-1.04479800	-0.03710500
C	20.84064900	-3.00300000	-0.03853500
H	19.89102100	-3.53139500	-0.03868600
C	22.04205300	-3.72361100	-0.03923100
H	22.02059800	-4.81032300	-0.03991900
C	23.26267200	-3.05894100	-0.03904600
H	24.20293500	-3.59891600	-0.03957300
N	25.54206000	-1.54068100	-0.03854700
N	28.81110600	-0.47974700	-0.03886000
H	29.77617500	-0.77389000	-0.03928200
N	27.85326600	-1.42194800	-0.03913700
C	26.69359100	-0.76304200	-0.03843300
C	26.90476300	0.66567300	-0.03768900
C	28.31305400	0.80191100	-0.03799800
C	28.95353200	2.04861100	-0.03747000
H	30.03627400	2.13477400	-0.03771700
C	28.13607900	3.16942200	-0.03661300
H	28.58926700	4.15692700	-0.03617900
C	26.72738300	3.05671000	-0.03628700
H	26.12639800	3.96157900	-0.03560800
C	26.10052500	1.81858100	-0.03681600
H	25.02186300	1.72600000	-0.03657000

Table S46 Cartesian coordinates of compound **5h-E-II**

C	22.51392100	5.07879200	-1.31425200
N	23.71535100	5.82664900	-1.24040100
C	21.33690000	5.83488300	-1.22470400
H	21.42784900	6.91049100	-1.10829800
C	20.09332900	5.20832500	-1.28508500
H	19.18406400	5.79897000	-1.21516900
C	20.02026600	3.82242400	-1.43538100
H	19.05254900	3.33009700	-1.48290700
C	21.19521900	3.06419700	-1.52521500
H	21.13441900	1.98522100	-1.64225100
C	22.43822200	3.68264800	-1.46568800
H	23.35817600	3.11282700	-1.53343500
N	24.76800600	5.13193700	-1.32229100
C	28.18157400	6.25718400	-1.22178900
C	27.24922500	5.20038900	-1.33185100
C	25.96717100	5.84341500	-1.25215500
N	26.09587500	7.16292800	-1.10749400
N	27.42378800	7.39463500	-1.09118500
H	27.74221800	8.34679700	-0.98768100
C	27.70393500	3.87997300	-1.48074000
H	26.99535500	3.06238500	-1.56602100
C	29.07208200	3.66009900	-1.51458700
H	29.45294300	2.64926800	-1.62876800
C	29.99113900	4.73102400	-1.40288200
H	31.05615000	4.51819700	-1.43382600
C	29.56792500	6.04322600	-1.25513500
H	30.27634900	6.86201800	-1.16980800

Table S47 Cartesian coordinates of compound **5h-Z-I**

N	24.69622200	-0.58472000	-1.00702200
N	25.81327300	-1.11453500	-0.80645700
N	28.66480200	-0.39779200	1.03867900
H	29.36203300	-0.77904400	1.65965000
N	27.63345300	-1.18870100	0.66504000
C	26.89048100	-0.45375700	-0.15394600
C	27.48544400	0.84181200	-0.38151200
C	28.65274400	0.82457200	0.42159100
C	29.54868800	1.90341200	0.47416900
H	30.43977900	1.87252600	1.09441500
C	29.25066500	3.00468000	-0.31219500
H	29.91975000	3.86063300	-0.30386800
C	28.09786100	3.03807500	-1.13057700
H	27.90304200	3.92024900	-1.73334500
C	27.21415300	1.97145900	-1.17494900
H	26.33089400	2.01219100	-1.80250000
C	23.13194900	2.95649900	0.67093300
H	22.69058700	3.85509500	1.09286800
C	23.86275600	2.08728600	1.48500200
H	23.98402600	2.30601700	2.54250400
C	24.44096100	0.93700800	0.95175600
H	24.99839800	0.25676200	1.58688400
C	24.27302700	0.64445800	-0.41068800
C	23.49304100	1.48816500	-1.21481500
H	23.32808700	1.21237800	-2.25233300
C	22.95057300	2.65483100	-0.68159100
H	22.36701300	3.31734000	-1.31499400

Table S48 Cartesian coordinates of compound **5h-Z-II**

N	24.01938300	5.91122400	-0.31386200
N	25.10859300	5.29886700	-0.40432100
C	28.55990600	6.12448200	-1.04522900
C	27.47922300	5.22271000	-1.18127600
C	26.36133100	5.91946200	-0.60957400
N	26.72021800	7.11189000	-0.14307500
N	28.03864800	7.22706700	-0.41490400
H	28.52540100	8.04786300	-0.08656000
C	27.68226600	3.96949700	-1.78230200
H	26.85984200	3.26830000	-1.88135700
C	28.95705200	3.66027200	-2.22999100
H	29.14624500	2.69685100	-2.69434200
C	30.02608600	4.57764600	-2.09214300
H	31.01051400	4.29941400	-2.45809700
C	29.85161800	5.81974800	-1.50065500
H	30.67562600	6.51939700	-1.39623600
C	23.18843900	9.94370600	-1.23615700
H	22.92963000	10.97070200	-1.47847700
C	22.85636000	9.41158100	0.01172100
H	22.33999200	10.02424500	0.74592800
C	23.16249600	8.08606100	0.31401700
H	22.88165900	7.64823500	1.26717500
C	23.85517900	7.30185100	-0.61523900
C	24.17733100	7.82722700	-1.87454400
H	24.67745200	7.20147600	-2.60767200
C	23.83601600	9.14213900	-2.18047000
H	24.07739400	9.54348900	-3.16135500

Table S49 Cartesian coordinates of compound **6-E-I**

C	-0.47030500	2.28826000	-8.14529200
N	0.70500200	3.06846500	-8.24786900
N	-1.59051100	2.99064200	-7.93119800
C	-2.75671700	2.33696100	-7.85064800
H	-3.63279900	2.94927500	-7.65124900
N	-2.97732500	1.02265100	-7.99320400
C	-1.85328300	0.35751600	-8.24046200
C	-0.54671000	0.89461000	-8.33163400
N	1.73964700	2.47422200	-7.84236700
C	5.41691500	4.47993100	-8.17069200
H	6.38067300	4.97670700	-8.24470900
C	5.33949500	3.17996700	-7.66757700
H	6.24026400	2.66194400	-7.35091500
C	4.10083200	2.54847700	-7.57097200
H	4.00236400	1.53829800	-7.18600100
C	2.93971600	3.21547600	-7.98336100
C	3.01710600	4.52515600	-8.48889700
H	2.10416800	5.02377400	-8.79534200
C	4.25502300	5.14930400	-8.57885900
H	4.32254500	6.16225400	-8.96650900
N	0.37020500	-0.10260900	-8.62315500
C	-0.35091100	-1.19251100	-8.69295200
H	0.03951200	-2.17886300	-8.90954700
N	-1.69672900	-0.99053800	-8.46610400
H	-2.43647500	-1.67836800	-8.47708500

Table S50 Cartesian coordinates of compound **6-E-II**

C	0.01348700	0.94919100	-8.76160200
N	1.22339400	1.68635900	-8.79009800
C	-1.18942700	1.67108600	-8.81907900
C	-2.36737400	0.88525300	-8.78735900
N	-2.43521500	-0.43789700	-8.71026100
C	-1.21385600	-0.99772900	-8.66214100
H	-1.19383000	-2.08324500	-8.59805200
N	-0.02417800	-0.38903800	-8.68325500
N	2.26534600	0.97766700	-8.73310000
C	5.96986200	2.95652700	-8.80495800
H	6.94121200	3.44373600	-8.82180900
C	5.88916800	1.56516400	-8.72182100
H	6.79470400	0.96703700	-8.67388100
C	4.64135400	0.94529400	-8.70047000
H	4.54029600	-0.13369200	-8.63644900
C	3.47186700	1.71640600	-8.76233300
C	3.55409900	3.11882600	-8.84616900
H	2.63622500	3.69433700	-8.89288700
C	4.80161700	3.72909900	-8.86687500
H	4.87260300	4.81160800	-8.93142300
N	-3.39762200	1.79501800	-8.85374800
H	-4.38371400	1.57573600	-8.85302500
C	-2.80957100	3.04250600	-8.91996000
H	-3.41021600	3.94140700	-8.98036500
N	-1.50103200	3.01824200	-8.90227700

Table S51 Cartesian coordinates of compound **6-Z-I**

C	-0.69436300	1.83806100	-8.47228800
N	0.34041500	2.42016300	-9.26358300
N	-1.17284400	2.55945300	-7.45307400
C	-2.26988300	2.11316100	-6.81819300
H	-2.60910900	2.72030700	-5.98244200
N	-2.99711600	1.02247700	-7.08710400
C	-2.50284700	0.34301600	-8.12069200
C	-1.35748800	0.66897900	-8.87570300
N	1.47670700	1.92984500	-9.40399600
N	-1.13459600	-0.26613100	-9.87223200
C	-2.11035400	-1.12560500	-9.72306500
H	-2.26073600	-2.00463900	-10.33660900
N	-2.97023800	-0.82097300	-8.68628600
H	-3.78876500	-1.33542900	-8.39266800
C	3.07497500	-1.28752400	-7.19971000
H	3.51781000	-2.11133200	-6.64678600
C	3.24855500	-1.20106100	-8.58445400
H	3.82163200	-1.95931100	-9.11066800
C	2.70797500	-0.12992300	-9.28963600
H	2.85220200	-0.02598300	-10.36036700
C	1.93888200	0.82837800	-8.61669000
C	1.77434200	0.75563500	-7.22542200
H	1.23305400	1.53524000	-6.70038200
C	2.35271900	-0.30168900	-6.52380000
H	2.24126800	-0.35181500	-5.44414800

Table S52 Cartesian coordinates of compound **6-Z-II**

C	-0.41957100	0.68957600	-9.70181000
N	0.82947200	1.18929900	-10.17756100
C	-1.24595300	1.46480500	-8.87549600
C	-2.53830700	0.94154000	-8.66549400
N	-3.03891100	-0.17975500	-9.18267400
C	-2.14919600	-0.80842800	-9.95894700
H	-2.48531900	-1.73282000	-10.42243700
N	-0.88673300	-0.44313300	-10.23962300
N	1.90876200	0.57583800	-10.08293400
N	-3.14313400	1.84076600	-7.81736500
H	-4.08694300	1.77801600	-7.46232900
C	-2.20983200	2.82538100	-7.56071800
H	-2.43935400	3.66075700	-6.91155400
N	-1.06411800	2.64100700	-8.16750100
C	2.64798000	-2.83550400	-7.72059400
H	2.87327100	-3.71049500	-7.11734500
C	1.90195100	-1.78645700	-7.17809200
H	1.55526300	-1.83972500	-6.14967800
C	1.60066500	-0.66457500	-7.94798300
H	1.04347600	0.16314400	-7.52112000
C	2.06595200	-0.58947800	-9.26833000
C	2.86371700	-1.61307600	-9.79509400
H	3.25083800	-1.50894900	-10.80393200
C	3.12545800	-2.74710600	-9.03148900
H	3.71916800	-3.55432700	-9.45119800

Table S53 Cartesian coordinates of compound **8-E-I**

C	1.43007800	0.54804100	-0.03393700
N	2.61833600	1.30786900	0.14875400
N	0.36494900	1.30134600	-0.23606100
C	-0.81594100	0.65945200	-0.40465600
H	-1.67187900	1.30175100	-0.60278100
N	-1.04071200	-0.63513800	-0.35020700
C	0.04231700	-1.42434200	-0.09154300
C	1.35535900	-0.87910500	0.07903600
N	3.64106200	0.83976400	-0.41380100
C	7.26590200	2.91888700	0.05088100
H	8.21492100	3.43760700	0.15633500
C	7.19432700	1.74173700	-0.69591900
H	8.08442400	1.34173100	-1.17289900
C	5.97412500	1.08145200	-0.83045800
H	5.88339000	0.16671100	-1.40834500
C	4.82687300	1.59723700	-0.21410400
C	4.89702600	2.78463700	0.53447600
H	3.99363300	3.16961000	0.99451300
C	6.11664800	3.43759200	0.66294700
H	6.17891000	4.35654900	1.23936300
C	2.43318000	-1.75478900	0.37343700
H	3.42754800	-1.35081700	0.51079100
C	2.21379200	-3.11117300	0.47265600
H	3.04272700	-3.77516300	0.70097300
C	0.91828200	-3.65125000	0.28333700
H	0.76916900	-4.72461300	0.36429500
C	-0.14840500	-2.82657400	0.00957800
H	-1.15464200	-3.20880900	-0.12816200

Table S54 Cartesian coordinates of compound **8-E-II**

C	15.38306100	1.79441800	-2.69701200
N	16.59399800	2.53595400	-2.65715900
C	14.17449000	2.53923800	-2.85411200
C	12.97452500	1.76517700	-2.85136400
N	13.00045100	0.41085000	-2.68359700
C	14.18936600	-0.13316800	-2.52656300
H	14.21995100	-1.21116200	-2.37893500
N	15.39595800	0.48581000	-2.52415300
N	17.59655500	1.90242400	-3.07979800
C	21.35947100	3.76040400	-2.88235200
H	22.34468500	4.21720300	-2.84246000
C	21.18981200	2.52175000	-3.50350600
H	22.03974000	2.01226500	-3.94826500
C	19.92521600	1.93797900	-3.54761000
H	19.75723300	0.97384600	-4.01727300
C	18.82715800	2.59602700	-2.97650000
C	18.99965600	3.84237400	-2.34817600
H	18.13975700	4.33139300	-1.90409300
C	20.26378300	4.41652800	-2.30449700
H	20.40463500	5.37780200	-1.81772800
C	11.72916000	2.42239800	-3.02318800
H	10.82975900	1.81514900	-3.01916500
C	11.68961800	3.78893600	-3.18735900
H	10.73489100	4.29133600	-3.31788000
C	12.88251200	4.55531400	-3.18322800
H	12.82571100	5.63306500	-3.30763200
C	14.10677300	3.94542900	-3.02000000
H	15.02557500	4.52096200	-3.01049400

Table S55 Cartesian coordinates of compound **8-Z-I**

C	9.00440200	4.19167500	-1.01518900
N	10.24497600	4.76044200	-0.59123400
C	8.10955900	5.01250000	-1.76633300
C	6.83135800	4.43571500	-2.02493200
N	6.49007000	3.20438000	-1.53693400
C	7.40534600	2.58823300	-0.82245200
H	7.13968400	1.61634600	-0.41102700
N	8.66530800	3.01100400	-0.53646100
N	11.35172900	4.19606400	-0.69547600
C	12.27680600	0.76729900	-2.96411500
H	12.55313000	-0.10881400	-3.54398300
C	11.40785200	1.71794500	-3.50654000
H	11.01469900	1.58624700	-4.51077600
C	11.04044600	2.83891400	-2.76628200
H	10.37856100	3.58448400	-3.19509800
C	11.56187700	3.01713700	-1.47655100
C	12.47949900	2.09551700	-0.95536800
H	12.90645800	2.28146600	0.02522200
C	12.80883500	0.95720600	-1.68582400
H	13.49706400	0.22822400	-1.26748800
C	5.89473500	5.16508200	-2.79963200
H	4.92742500	4.71078800	-2.98856200
C	6.22375700	6.41330900	-3.28243600
H	5.50263300	6.97148700	-3.87342600
C	7.49014200	6.98782800	-3.01061500
H	7.72149400	7.97886800	-3.39034900
C	8.42292300	6.30127600	-2.26318700
H	9.39093500	6.73657700	-2.03575100

Table S56 Cartesian coordinates of compound **8-Z-II**

C	13.89990500	2.61303500	-1.45444900
N	14.74291000	3.29432200	-0.52135100
N	13.58554000	3.24896000	-2.56494900
C	12.63669600	2.66293200	-3.34430500
H	12.40018200	3.19799000	-4.26208900
N	11.98859000	1.54302400	-3.12198500
C	12.29686500	0.88857800	-1.96096900
C	13.26910700	1.39548900	-1.04861100
N	15.95282500	3.06501900	-0.33203700
C	18.39478100	0.39192200	-2.49396600
H	19.04860200	-0.29246100	-3.02725800
C	18.47676200	0.49584800	-1.10231700
H	19.19243000	-0.10704200	-0.55061800
C	17.65889200	1.39424300	-0.42368000
H	17.72966100	1.52129100	0.65234000
C	16.70933200	2.14746300	-1.12942800
C	16.63767200	2.06170900	-2.52894900
H	15.95465900	2.69779600	-3.07866700
C	17.49062800	1.18706900	-3.20148100
H	17.44849500	1.12978700	-4.28554900
C	13.54562000	0.69707500	0.15267800
H	14.27281200	1.09730500	0.85185600
C	12.88219900	-0.47901300	0.42751000
H	13.08972800	-1.01615200	1.34846000
C	11.92474900	-0.99230100	-0.48123200
H	11.41219600	-1.92118500	-0.24619600
C	11.63370800	-0.32522300	-1.65118000
H	10.89905300	-0.69598000	-2.35867500

Table S57 Cartesian coordinates of compound **3a-TS1**

C	1.54880000	0.93360000	-0.52630000
N	2.78500000	1.64830000	-0.52630000
C	0.34080000	1.63160000	-0.52630000
H	0.34080000	2.71860000	-0.52630000
N	-0.86720000	0.93460000	-0.52630000
C	-0.86720000	-0.46140000	-0.52630000
H	-1.80820000	-1.00440000	-0.52630000
C	0.34080000	-1.15840000	-0.52630000
H	0.34080000	-2.24540000	-0.52630000
C	1.54880000	-0.46140000	-0.52630000
H	2.48980000	-1.00440000	-0.52630000
N	4.02210000	0.93500000	-0.52630000
C	7.61720000	-1.13790000	-0.52550000
H	8.55880000	-1.68080000	-0.52470000
C	7.01300000	-0.78950000	0.68280000
H	7.48360000	-1.06090000	1.62430000
C	5.80480000	-0.09290000	0.68280000
H	5.33380000	0.17870000	1.62350000
C	5.20030000	0.25560000	-0.52630000
C	5.80490000	-0.09300000	-1.73370000
H	5.33430000	0.17840000	-2.67520000
C	7.01310000	-0.78960000	-1.73380000
H	7.48410000	-1.06120000	-2.67440000

Table S58 Cartesian coordinates of compound **3a-TS2**

N	0.40690700	-0.10289800	0.97108500
N	-0.78327100	-0.40249600	0.76164600
C	-3.70926400	2.11769500	2.50070100
H	-4.46966400	2.75754100	2.92958000
C	-3.87701000	1.60053400	1.21612600
H	-4.76470100	1.85355400	0.63214100
C	-2.91664000	0.74573200	0.67536700
H	-3.04048700	0.31329100	-0.31537000
C	-1.75763900	0.46622800	1.40157500
C	-1.58545100	0.97778300	2.68522500
H	-0.70861300	0.70076900	3.26332100
C	-2.57194400	1.78907000	3.24259900
H	-2.46333500	2.14843400	4.26674200
C	4.25415000	1.30833300	1.09774200
H	5.24822200	1.73908100	1.14041500
C	1.69563200	0.30376700	1.02089000
C	2.74190400	-0.41892200	0.38060400
H	2.51806400	-1.36719700	-0.11858300
C	2.05007200	1.50909700	1.67846200
H	1.27088200	2.09192400	2.16572600
C	4.02691200	0.11022800	0.40411500
H	4.83674900	-0.39771100	-0.08590800
N	3.28757800	2.00020500	1.74049900

Table S59 Cartesian coordinates of compound **3a-TS3**

N	-3.94651000	5.41291100	-1.17468600
C	-7.57070600	3.36829300	-1.18432800
H	-8.50547800	2.81704000	-1.18687300
C	-7.57764600	4.76127700	-1.18066600
H	-8.51506500	5.30273400	-1.18037700
C	-6.35833500	5.42895800	-1.17742300
H	-6.29538200	6.51105900	-1.17444400
C	-5.19182900	4.66948000	-1.17812800
C	-5.28239700	3.27365900	-1.18195500
H	-4.38306500	2.66628100	-1.18254500
N	-6.44917900	2.62882500	-1.18497300
N	-2.90613800	4.77790600	-1.17565600
C	0.67094100	2.66300200	-1.17914300
H	1.60675100	2.11836200	-1.18003300
C	0.05195400	3.01834500	0.02224000
H	0.50971400	2.74830600	0.96820000
C	-1.14807900	3.71636000	0.04752700
H	-1.61766700	3.98619800	0.98472800
C	-1.76899100	4.08417500	-1.17681900
C	-1.14635300	3.72331700	-2.40235500
H	-1.61464900	3.99846600	-3.33865300
C	0.05363600	3.02514400	-2.37935100
H	0.51267400	2.76040400	-3.32618800

Table S60 Cartesian coordinates of compound **3a-TS4**

C	-1.34713800	3.41024900	-0.54793800
H	-2.06903400	3.42797300	0.26361400
C	-1.73137200	3.78294200	-1.86735600
N	-2.93011900	4.29072400	-2.19702600
C	-0.72874800	3.68841500	-2.86077800
H	-0.98300000	3.97889100	-3.88565500
N	0.51209900	3.29251300	-2.63690000
C	0.86904600	3.00352900	-1.37515500
H	1.91104200	2.74281100	-1.21382300
C	-0.02527700	3.05206500	-0.31366600
H	0.28751700	2.76066100	0.68359500
N	-4.04460800	4.78226200	-2.41778500
C	-7.52067500	4.00216900	-0.17266300
H	-8.41622600	3.90845900	0.44551500
C	-7.58105000	4.67893800	-1.38971100
H	-8.52601900	5.07197700	-1.75812800
C	-6.42106500	4.86127000	-2.14033000
H	-6.43593700	5.42298100	-3.06372300
C	-5.19929300	4.36091700	-1.68051300
C	-5.14814800	3.63065800	-0.44185500
H	-4.20245800	3.24688000	-0.09496000
C	-6.30477200	3.47938700	0.29419000
H	-6.26236400	2.95493000	1.24025100

Table S61 Cartesian coordinates of compound **3b-TS1**

N	-8.44956000	8.46814900	-3.87343800
C	-7.71417700	7.75717900	-3.01465100
H	-6.95179100	8.27733000	-2.44239000
C	-7.90541000	6.38991300	-2.84652100
N	-7.04532600	5.72661300	-1.88659300
C	-8.90177200	5.78046400	-3.60980700
H	-9.10307900	4.71735900	-3.52455800
N	-9.64154400	6.48122500	-4.46913900
C	-9.37549900	7.79111300	-4.55663800
H	-9.97740900	8.36072200	-5.25712300
N	-7.19249100	4.52594500	-1.74173300
C	-7.65752400	0.43129800	-1.21220500
H	-7.77438700	-0.63567700	-1.07005200
C	-6.76708500	0.93132700	-2.16558500
H	-6.18314700	0.24796900	-2.77311500
C	-6.60076700	2.29553200	-2.36511900
H	-5.90760800	2.67178100	-3.10632700
C	-7.35330300	3.21074800	-1.58280700
C	-8.26156200	2.71086700	-0.61266600
H	-8.83787100	3.40468300	-0.01445100
C	-8.39433400	1.33852300	-0.44681600
H	-9.09275600	0.97613800	0.30013500

Table S62 Cartesian coordinates of compound **3b-TS2**

N	-4.05175900	7.67062400	0.40851800
C	-4.63413800	6.95714000	-0.55905800
H	-4.88451400	7.47968100	-1.46986700
C	-4.92645700	5.58400000	-0.40020100
N	-5.56011700	4.80818000	-1.29372600
C	-4.53623300	5.02295100	0.84878500
H	-4.76262100	3.96789500	1.04415200
N	-3.93247800	5.73235000	1.79454900
C	-3.72859600	7.02155300	1.53458600
H	-3.24506500	7.59815700	2.31669700
N	-6.10813800	4.08639000	-2.14070100
C	-6.61643800	5.45337300	-6.10414800
H	-6.79031300	5.77885200	-7.11939200
C	-6.61315100	6.37192600	-5.05990100
H	-6.79162200	7.42277500	-5.26170100
C	-6.38077800	5.93598200	-3.75656200
H	-6.44134400	6.65381600	-2.92128600
C	-6.18256700	4.58461200	-3.49456200
C	-6.22379700	3.66297900	-4.52736400
H	-6.09430700	2.58283400	-4.29640300
C	-6.40146700	4.06842800	-5.83620000
H	-6.41966200	3.37372800	-6.64480000

Table S63 Cartesian coordinates of compound **3c-TS1**

C	1.64831700	0.82122300	-0.52607600
N	2.88638600	1.59660000	-0.52583000
C	0.46488500	1.55515500	-0.52585000
H	0.48743900	2.63932500	-0.52555000
N	-0.72371600	0.94410500	-0.52599100
C	-0.70463900	-0.38965600	-0.52640300
H	-1.65921200	-0.90427900	-0.52651500
C	0.49383500	-1.11550900	-0.52670000
H	0.48502100	-2.20014000	-0.52707400
N	3.92101800	0.95846100	-0.52574900
C	7.51926300	-1.11440800	-0.52533500
H	8.46013200	-1.65019300	-0.52522500
C	6.89769800	-0.76160800	0.67529700
H	7.35829600	-1.02462100	1.62181300
C	5.69096800	-0.07525700	0.69955500
H	5.21827600	0.19171200	1.63587600
C	5.06613200	0.28118700	-0.52561800
C	5.69117700	-0.07537800	-1.75064800
H	5.21864700	0.19150600	-2.68707800
C	6.89790900	-0.76171600	-1.72611300
H	7.35866500	-1.02482600	-2.67252500
N	1.67641300	-0.50633200	-0.52652500

Table S64 Cartesian coordinates of compound **3c-TS2**

N	0.40690700	-0.10289800	0.97108500
N	-0.78327100	-0.40249600	0.76164600
C	-3.70926400	2.11769500	2.50070100
H	-4.46966400	2.75754100	2.92958000
C	-3.87701000	1.60053400	1.21612600
H	-4.76470100	1.85355400	0.63214100
C	-2.91664000	0.74573200	0.67536700
H	-3.04048700	0.31329100	-0.31537000
C	-1.75763900	0.46622800	1.40157500
C	-1.58545100	0.97778300	2.68522500
H	-0.70861300	0.70076900	3.26332100
C	-2.57194400	1.78907000	3.24259900
H	-2.46333500	2.14843400	4.26674200
C	4.25415000	1.30833300	1.09774200
H	5.24822200	1.73908100	1.14041500
C	1.69563200	0.30376700	1.02089000
C	2.05007200	1.50909700	1.67846200
H	1.27088200	2.09192400	2.16572600
C	4.02691200	0.11022800	0.40411500
H	4.83674900	-0.39771100	-0.08590800
N	3.28757800	2.00020500	1.74049900
N	2.74190400	-0.41892200	0.38060400

Table S65 Cartesian coordinates of compound **3c-TS3**

C	-1.70598000	0.71515000	-0.00021400
N	-0.47724300	1.49502900	0.00002700
C	-2.88959300	1.45176200	0.00001000
H	-2.86438400	2.53584600	0.00030900
N	-4.07890200	0.84310300	-0.00013100
C	-4.06057300	-0.49095800	-0.00054300
H	-5.01550700	-1.00488900	-0.00065600
C	-2.86307600	-1.21847800	-0.00084000
H	-2.87395400	-2.30301700	-0.00121500
N	0.58487200	0.90003500	0.00011800
C	4.16247000	-1.21414000	0.00052500
H	5.10550000	-1.74615000	0.00063400
C	3.53971700	-0.86312000	1.20104400
H	4.00168400	-1.12339200	2.14765800
C	2.32984500	-0.18188300	1.22505900
H	1.85998900	0.08906700	2.16170700
C	1.70027300	0.16740900	0.00024100
C	2.33005400	-0.18200300	-1.22443200
H	1.86036100	0.08886200	-2.16119000
C	3.53992800	-0.86322800	-1.20014000
H	4.00205300	-1.12359700	-2.14665000
N	-1.67891700	-0.61181300	-0.00066400

Table S66 Cartesian coordinates of compound **3c-TS4**

C	-1.73137200	3.78294200	-1.86735600
N	-2.93011900	4.29072400	-2.19702600
C	-0.72874800	3.68841500	-2.86077800
H	-0.98300000	3.97889100	-3.88565500
N	0.51209900	3.29251300	-2.63690000
C	0.86904600	3.00352900	-1.37515500
H	1.91104200	2.74281100	-1.21382300
C	-0.02527700	3.05206500	-0.31366600
H	0.28751700	2.76066100	0.68359500
N	-4.04460800	4.78226200	-2.41778500
C	-7.52067500	4.00216900	-0.17266300
H	-8.41622600	3.90845900	0.44551500
C	-7.58105000	4.67893800	-1.38971100
H	-8.52601900	5.07197700	-1.75812800
C	-6.42106500	4.86127000	-2.14033000
H	-6.43593700	5.42298100	-3.06372300
C	-5.19929300	4.36091700	-1.68051300
C	-5.14814800	3.63065800	-0.44185500
H	-4.20245800	3.24688000	-0.09496000
C	-6.30477200	3.47938700	0.29419000
H	-6.26236400	2.95493000	1.24025100
N	-1.34713800	3.41024900	-0.54793800

Table S67 Cartesian coordinates of compound **3d-TS1**

C	1.32411000	0.71516100	0.00134900
N	1.38287800	-0.65109400	0.00072300
C	2.56774800	-1.21776600	-0.00030500
H	2.61151700	-2.30385100	-0.00079400
C	3.78357100	-0.49162700	-0.00083400
N	4.98185300	-1.30119800	-0.00206400
C	3.75363200	0.88488500	-0.00027700
H	4.67202500	1.46196200	-0.00073200
C	2.50208000	1.53348000	0.00088200
N	6.05608400	-0.72368100	-0.00264600
C	9.74110000	1.19863800	-0.00216100
H	10.70379500	1.69419900	-0.00200700
C	9.10493800	0.87265400	-1.20303000
H	9.57666700	1.11601100	-2.14940300
C	7.87044100	0.23768400	-1.22732600
H	7.38777000	-0.00922100	-2.16423300
C	7.22907600	-0.09362000	-0.00257100
C	7.87114100	0.23560500	1.22240600
H	7.38898500	-0.01290700	2.15915200
C	9.10561500	0.87061900	1.19850900
H	9.57787700	1.11234900	2.14503600
C	2.36779300	2.94856800	0.00159100
H	3.26272700	3.56062500	0.00122300
C	1.12151800	3.52539000	0.00272800
H	1.02125200	4.60424500	0.00327900
C	-0.04164300	2.71583600	0.00319800
H	-1.01725500	3.18800100	0.00411700
C	0.05454800	1.34358700	0.00251800

H -0.82854200 0.71596500 0.00287300

Table S68 Cartesian coordinates of compound **3d-TS2**

C	1.90762000	1.35375300	-0.60827700
N	2.78909200	0.62838000	-1.36458300
C	3.87302500	0.17909000	-0.79439200
H	4.54368400	-0.39607700	-1.43962100
C	4.22749500	0.36984300	0.58518700
N	5.37877400	-0.10979500	1.08019900
C	3.29908200	1.06955100	1.38763400
H	3.49879000	1.21817400	2.44625200
C	2.12490900	1.58409400	0.80030400
N	6.40178800	-0.67434600	1.50872000
C	9.50465200	-1.62989500	-1.20600000
H	10.26934600	-1.97343100	-1.90574000
C	8.29914100	-1.12912500	-1.69767400
H	8.12048800	-1.05777300	-2.78178900
C	7.30533800	-0.72925400	-0.82127300
H	6.36842000	-0.35609200	-1.20354300
C	7.47858600	-0.88080200	0.55438200
C	8.69286600	-1.35987800	1.05468200
H	8.83186400	-1.46665900	2.13296500
C	9.70365500	-1.73204500	0.17221900
H	10.64606500	-2.10218700	0.55503300
C	1.11606200	2.26211700	1.53300600
H	1.24081100	2.38580200	2.60703400
C	-0.01511500	2.73280600	0.90773000
H	-0.77470600	3.24036900	1.48026700
C	-0.18272100	2.57000600	-0.48772900
H	-1.05791000	2.97781200	-0.96697100
C	0.76114300	1.88561300	-1.22764500

H 0.65075900 1.74264800 -2.30037900

Table S69 Cartesian coordinates of compound **3d-TS3**

C	3.89340400	-1.78574700	1.48787400
N	5.13075300	-1.04359500	1.48785200
C	2.73788600	-1.04170300	1.48784000
H	2.79058200	0.04181100	1.48778300
C	1.49267500	-1.70876700	1.48788400
C	1.50828700	-3.13970100	1.48794400
N	2.67568700	-3.85938400	1.48796100
C	3.81202500	-3.20530400	1.48792700
H	4.72501400	-3.79330100	1.48794400
N	6.17510800	-1.67569700	1.48806800
C	9.75703200	-3.78415200	1.48857200
H	10.69401600	-4.32680600	1.48870100
C	9.13795800	-3.42616200	2.68925400
H	9.59691900	-3.69240000	3.63576900
C	7.93648300	-2.73064700	2.71305800
H	7.46717400	-2.45881800	3.64990000
C	7.31287900	-2.36718700	1.48823500
C	7.93613300	-2.73183500	0.26358500
H	7.46655100	-2.46094400	-0.67339200
C	9.13765900	-3.42725600	0.28772100
H	9.59638700	-3.69435400	-0.65866600
C	0.27844300	-3.83852300	1.48798400
H	0.30208100	-4.92169200	1.48804000
C	-0.91295300	-3.14725200	1.48796500
H	-1.85106900	-3.69008200	1.48800400
C	-0.92947200	-1.73243100	1.48790500
H	-1.87804100	-1.20879500	1.48789100
C	0.24979200	-1.02473000	1.48786800

H 0.24650500 0.05955500 1.48782800

Table S70 Cartesian coordinates of compound **3d-TS4**

C	4.12828500	-2.32898200	0.04950400
N	5.44964600	-2.23686500	-0.05983500
C	3.55858200	-1.95099900	1.26836400
H	4.17658900	-1.54553000	2.05572700
C	2.18305500	-2.11436800	1.48551400
C	1.38850400	-2.66760300	0.42821900
N	1.93471000	-2.95725500	-0.80470000
C	3.22104800	-2.78830400	-0.98591700
H	3.60867900	-3.01477100	-1.98089800
N	6.63351600	-1.94544200	-0.28298400
C	9.34657600	-2.47440200	2.92739100
H	10.03757000	-2.49526000	3.76433600
C	7.99009700	-2.73459500	3.13516000
H	7.63306600	-2.96688200	4.13732200
C	7.09114900	-2.65953100	2.07816700
H	6.03860900	-2.83955400	2.24777000
C	7.53862600	-2.27793600	0.80343100
C	8.89608600	-2.04230100	0.58042800
H	9.22731700	-1.75492800	-0.41097700
C	9.79926600	-2.14835200	1.64276200
H	10.85138500	-1.95782000	1.47857900
C	0.02120800	-2.94400500	0.67468800
H	-0.58319400	-3.35637000	-0.13671100
C	-0.50118300	-2.77149500	1.93701700
H	-1.53704300	-3.02572000	2.12833100
C	0.29632300	-2.25037300	2.99191500
H	-0.11789200	-2.15660900	3.99526100
C	1.60745300	-1.90957800	2.77229800

H

2.22836700 -1.51006800 3.56773900

Table S71 Cartesian coordinates of compound **3e-TS4**

C	3.54450000	-0.04860000	-2.77030000
N	4.72150000	0.69730000	-2.47970000
C	2.42990000	0.67010000	-3.27160000
H	2.51290000	1.71840000	-3.40090000
C	1.24740000	0.02480000	-3.58540000
H	0.41390000	0.57110000	-3.94830000
C	1.18820000	-1.36580000	-3.39450000
C	2.26520000	-2.09360000	-2.89690000
C	3.45920000	-1.42880000	-2.58110000
H	4.28100000	-1.97890000	-2.20440000
N	5.76300000	1.35730000	-2.22250000
C	5.90260000	5.53470000	-2.80690000
H	5.95390000	6.58430000	-2.94910000
C	7.01170000	4.84230000	-2.32840000
H	7.90720000	5.36500000	-2.10640000
C	6.94470000	3.46500000	-2.14180000
H	7.78770000	2.93700000	-1.77800000
C	5.76940000	2.76810000	-2.43210000
C	4.65650000	3.47240000	-2.91320000
H	3.75770000	2.95990000	-3.13790000
C	4.72590000	4.84980000	-3.09880000
H	3.88210000	5.37850000	-3.46300000
C	1.86910000	-3.44630000	-2.82480000
H	2.46870000	-4.25150000	-2.48260000
C	0.59160000	-3.53820000	-3.27090000
H	-0.03890000	-4.38640000	-3.36750000
N	0.14060000	-2.26670000	-3.63000000
S	-1.37390000	-1.92400000	-4.38380000

O	-2.27910000	-2.99930000	-4.14720000
O	-1.83050000	-0.62960000	-3.99940000
C	-0.35770000	-1.85140000	-8.88190000
C	-0.00490000	-1.82930000	-10.35350000
H	-0.49230000	-2.66850000	-10.85010000
H	1.07820000	-1.91010000	-10.44340000
H	-0.35520000	-0.89080000	-10.78390000
C	-0.71850000	-3.04370000	-8.26100000
H	-0.75890000	-3.94300000	-8.82190000
C	-1.03020000	-3.06370000	-6.90490000
H	-1.31410000	-3.97700000	-6.44450000
C	-0.97560000	-1.89260000	-6.14480000
C	-0.62510000	-0.69730000	-6.77790000
H	-0.59900000	0.20540000	-6.22130000
C	-0.31260000	-0.67880000	-8.13380000
H	-0.04070000	0.23540000	-8.59750000

Table S72 Cartesian coordinates of compound **3f-TS1**

C	3.54450000	-0.04860000	-2.77030000
N	4.72150000	0.69730000	-2.47970000
C	2.42990000	0.67010000	-3.27160000
H	2.51290000	1.71840000	-3.40090000
C	1.24740000	0.02480000	-3.58540000
H	0.41390000	0.57110000	-3.94830000
C	1.18820000	-1.36580000	-3.39450000
C	2.26520000	-2.09360000	-2.89690000
C	3.45920000	-1.42880000	-2.58110000
H	4.28100000	-1.97890000	-2.20440000
N	5.76300000	1.35730000	-2.22250000
C	5.90260000	5.53470000	-2.80690000
H	5.95390000	6.58430000	-2.94910000
C	7.01170000	4.84230000	-2.32840000
H	7.90720000	5.36500000	-2.10640000
C	6.94470000	3.46500000	-2.14180000
H	7.78770000	2.93700000	-1.77800000
C	5.76940000	2.76810000	-2.43210000
C	4.65650000	3.47240000	-2.91320000
H	3.75770000	2.95990000	-3.13790000
C	4.72590000	4.84980000	-3.09880000
H	3.88210000	5.37850000	-3.46300000
C	1.86910000	-3.44630000	-2.82480000
H	2.46870000	-4.25150000	-2.48260000
C	0.59160000	-3.53820000	-3.27090000
H	-0.03890000	-4.38640000	-3.36750000
N	0.14060000	-2.26670000	-3.63000000
S	-1.37390000	-1.92400000	-4.38380000

O	-2.27910000	-2.99930000	-4.14720000
O	-1.83050000	-0.62960000	-3.99940000
C	-0.35770000	-1.85140000	-8.88190000
C	-0.00490000	-1.82930000	-10.35350000
H	-0.49230000	-2.66850000	-10.85010000
H	1.07820000	-1.91010000	-10.44340000
H	-0.35520000	-0.89080000	-10.78390000
C	-0.71850000	-3.04370000	-8.26100000
H	-0.75890000	-3.94300000	-8.82190000
C	-1.03020000	-3.06370000	-6.90490000
H	-1.31410000	-3.97700000	-6.44450000
C	-0.97560000	-1.89260000	-6.14480000
C	-0.62510000	-0.69730000	-6.77790000
H	-0.59900000	0.20540000	-6.22130000
C	-0.31260000	-0.67880000	-8.13380000
H	-0.04070000	0.23540000	-8.59750000

Table S73 Cartesian coordinates of compound **3f-TS2**

C	7.29300000	9.97490000	-1.55850000
N	8.53430000	10.66990000	-1.60770000
C	6.32760000	10.43040000	-0.67330000
H	6.50520000	11.27020000	-0.05320000
C	5.11310000	9.74040000	-0.62810000
C	4.93750000	8.64210000	-1.46660000
N	5.86610000	8.18110000	-2.33700000
C	7.01590000	8.83910000	-2.37720000
H	7.75460000	8.49270000	-3.05360000
N	9.63210000	11.28450000	-1.65130000
C	10.37980000	14.59640000	0.85660000
H	10.58330000	15.42950000	1.48050000
C	11.33330000	14.16510000	-0.06160000
H	12.26260000	14.67010000	-0.13670000
C	11.06680000	13.07190000	-0.88010000
H	11.79220000	12.74390000	-1.57860000
C	9.84560000	12.40030000	-0.78780000
C	8.89000000	12.84090000	0.13880000
H	7.95860000	12.34420000	0.22300000
C	9.15900000	13.93440000	0.95610000
H	8.43370000	14.26410000	1.65570000
N	3.67370000	8.12800000	-1.23350000
C	3.06400000	8.91380000	-0.24790000
H	2.07970000	8.69920000	0.08780000
C	3.92690000	9.89330000	0.12490000
H	3.74220000	10.64190000	0.85370000
S	3.00250000	6.75260000	-2.01570000
O	1.76950000	6.41310000	-1.38440000

O	2.93350000	6.97440000	-3.42130000
C	5.99590000	3.33940000	-1.18170000
C	6.98800000	2.23120000	-0.90320000
H	7.22230000	1.72680000	-1.84080000
H	6.54450000	1.52330000	-0.20260000
H	7.88470000	2.68040000	-0.47580000
C	6.06480000	4.05630000	-2.37250000
H	6.80760000	3.82150000	-3.09180000
C	5.16250000	5.08460000	-2.62700000
H	5.22170000	5.62470000	-3.53930000
C	4.18290000	5.42130000	-1.68990000
C	4.11280000	4.68960000	-0.50140000
H	3.36180000	4.91760000	0.21270000
C	5.01590000	3.66160000	-0.24700000
H	4.95300000	3.12150000	0.66330000

Table S74 Cartesian coordinates of compound **3f-TS3**

C	-1.60240000	-1.94650000	1.82560000
N	-0.20350000	-1.88190000	2.02220000
C	-2.10830000	-1.04150000	0.87120000
H	-1.41560000	-0.37840000	0.36380000
C	-4.20280000	-1.77210000	1.19050000
N	-3.82260000	-2.74060000	2.16220000
C	-2.47410000	-2.82030000	2.48780000
H	-2.11320000	-3.52650000	3.22090000
N	0.25680000	-2.66650000	2.88510000
C	-3.39780000	-0.94200000	0.54360000
C	-4.07090000	-0.12860000	-0.34930000
H	-3.64800000	0.62410000	-0.99810000
C	-5.43790000	-0.49530000	-0.22990000
H	-6.26140000	-0.06390000	-0.77960000
N	-5.53160000	-1.52920000	0.73960000
S	-6.51280000	-1.03390000	2.03650000
O	-6.21920000	0.36310000	2.29860000
O	-7.87370000	-1.43830000	1.73480000
C	-5.15930000	-3.39390000	5.60820000
C	-4.72840000	-4.14380000	6.74450000
H	-4.10720000	-3.51390000	7.38120000
H	-4.15100000	-5.00660000	6.41270000
H	-5.59820000	-4.48320000	7.30690000
C	-4.76770000	-2.06270000	5.46290000
H	-4.13510000	-1.59690000	6.21410000
C	-5.18800000	-1.32940000	4.35350000
H	-4.88330000	-0.29280000	4.23980000
C	-6.00050000	-1.92770000	3.38880000

C	-6.39150000	-3.25840000	3.53480000
H	-7.02420000	-3.72430000	2.78350000
C	-5.97130000	-3.99170000	4.64410000
H	-6.27590000	-5.02840000	4.75780000
C	1.78030000	-5.26280000	5.74160000
H	2.17920000	-5.94220000	6.49020000
C	1.33010000	-3.99720000	6.11900000
H	1.37820000	-3.69130000	7.16090000
C	0.81790000	-3.12450000	5.15920000
H	0.46720000	-2.13900000	5.45250000
C	0.75610000	-3.51750000	3.82110000
C	1.20640000	-4.78260000	3.44460000
H	1.15830000	-5.08860000	2.40270000
C	1.71850000	-5.65540000	4.40450000
H	2.06920000	-6.64090000	4.11120000

Table S75 Cartesian coordinates of compound **3f-TS4**

C	6.49480000	7.99070000	-1.53280000
N	7.67130000	8.71150000	-1.17620000
C	5.24040000	8.59820000	-1.25370000
H	5.22780000	9.55270000	-0.79270000
N	4.07730000	8.03320000	-1.54200000
C	4.13050000	6.81450000	-2.12890000
C	5.30590000	6.13560000	-2.44190000
C	6.53010000	6.73700000	-2.13640000
H	7.44290000	6.24970000	-2.36070000
N	8.71090000	9.34850000	-0.86110000
C	8.48970000	13.11860000	1.02450000
H	8.45130000	14.06760000	1.49680000
C	9.71970000	12.54750000	0.70940000
H	10.61760000	13.06150000	0.94210000
C	9.77030000	11.30300000	0.08910000
H	10.70570000	10.86820000	-0.15130000
C	8.59290000	10.61890000	-0.22220000
C	7.35790000	11.19990000	0.09930000
H	6.45500000	10.69570000	-0.12810000
C	7.30990000	12.44470000	0.71970000
H	6.37390000	12.88100000	0.96050000
C	4.94070000	4.90990000	-3.04310000
H	5.60820000	4.16340000	-3.39370000
C	3.58510000	4.85430000	-3.09300000
H	2.94070000	4.09890000	-3.46940000
N	3.06590000	6.02690000	-2.53150000
S	1.40710000	6.44720000	-2.37580000
O	0.61510000	5.48030000	-3.06250000

O	1.07990000	6.64820000	-1.00390000
C	0.97790000	10.45770000	-4.62030000
C	0.84720000	11.77250000	-5.35830000
H	0.37760000	12.50170000	-4.69770000
H	0.22830000	11.62260000	-6.24330000
H	1.84710000	12.10160000	-5.64210000
C	1.17970000	10.44390000	-3.24330000
H	1.23540000	11.35590000	-2.70520000
C	1.30910000	9.23630000	-2.56400000
H	1.45870000	9.23550000	-1.51280000
C	1.25120000	8.02180000	-3.25200000
C	1.03990000	8.04360000	-4.63320000
H	0.97330000	7.13000000	-5.16910000
C	0.91040000	9.25170000	-5.31210000
H	0.75640000	9.25000000	-6.36130000

Table S76 Cartesian coordinates of compound **3g-TS1**

C	17.30880000	4.28550000	0.56920000
C	16.07090000	4.94300000	0.64940000
H	15.99620000	5.95800000	0.94690000
C	14.93020000	4.22950000	0.31700000
H	13.98060000	4.69710000	0.36700000
C	15.00630000	2.87970000	-0.09260000
N	13.78310000	2.22140000	-0.40040000
C	16.25020000	2.24690000	-0.17550000
H	16.32610000	1.23720000	-0.48300000
C	17.40540000	2.96040000	0.15930000
N	13.79510000	1.01510000	-0.76400000
C	18.77790000	2.59180000	0.19250000
C	19.50800000	3.69140000	0.62650000
N	18.60900000	4.76330000	0.86730000
S	18.95900000	6.18860000	1.77040000
O	20.32910000	6.54950000	1.61590000
O	18.01640000	7.21160000	1.45840000
C	18.28320000	4.85350000	6.13220000
C	18.07350000	4.40550000	7.56270000
H	18.35820000	3.35570000	7.63760000
H	17.02500000	4.52900000	7.83460000
H	18.70480000	5.01940000	8.20580000
C	19.52110000	4.66890000	5.52440000
H	20.31370000	4.21650000	6.06490000
C	19.72730000	5.07660000	4.20990000
H	20.67760000	4.93540000	3.75890000
C	18.69500000	5.67050000	3.47950000
C	17.45930000	5.86720000	4.10140000

H	16.66960000	6.33350000	3.56760000
C	17.25440000	5.45890000	5.41600000
H	16.30880000	5.61340000	5.87080000
C	20.90270000	3.63780000	0.77310000
H	21.46370000	4.47810000	1.09350000
C	21.54660000	2.44600000	0.47450000
H	22.60010000	2.37570000	0.57390000
C	20.81670000	1.32560000	0.03540000
H	21.32790000	0.42410000	-0.18840000
C	19.43750000	1.39370000	-0.10740000
H	18.88700000	0.55100000	-0.43780000
C	13.83470000	-2.95780000	-1.96220000
H	13.84510000	-3.99820000	-2.27670000
C	13.91320000	-1.94140000	-2.91480000
H	13.98470000	-2.18990000	-3.97060000
C	13.89990000	-0.60610000	-2.51240000
H	13.96100000	0.18570000	-3.25370000
C	13.80810000	-0.28700000	-1.15650000
C	13.72960000	-1.30350000	-0.20490000
H	13.65810000	-1.05500000	0.85090000
C	13.74290000	-2.63880000	-0.60730000
H	13.68180000	-3.43070000	0.13400000

Table S77 Cartesian coordinates of compound **3g-TS2**

C	-0.29740000	2.76880000	-0.74340000
N	0.89640000	2.22310000	-0.18630000
C	-0.29900000	3.87140000	-1.60950000
H	0.61160000	4.33960000	-1.87890000
C	-1.49790000	4.35880000	-2.12060000
H	-1.49460000	5.19310000	-2.77510000
C	-2.70220000	3.75230000	-1.77360000
H	-3.61490000	4.12520000	-2.16420000
C	-2.70860000	2.65670000	-0.91440000
H	-3.62630000	2.19530000	-0.65090000
C	-1.51110000	2.16770000	-0.40170000
H	-1.51460000	1.33440000	0.25200000
N	2.00940000	2.72580000	-0.49490000
C	5.67580000	4.45680000	-1.59350000
C	4.48510000	4.92220000	-2.13970000
C	3.27110000	4.34050000	-1.76220000
H	2.36100000	4.68970000	-2.17460000
C	3.26650000	3.29360000	-0.84350000
C	4.49040000	2.83220000	-0.29430000
H	4.48470000	2.04000000	0.40880000
C	5.69710000	3.40690000	-0.66140000
H	6.60260000	3.05740000	-0.23520000
C	4.80020000	5.96660000	-3.05100000
C	6.17970000	6.13180000	-3.05470000
N	6.74770000	5.20150000	-2.14540000
S	8.41420000	4.77240000	-2.05430000
O	9.23210000	5.89390000	-2.37770000
O	8.69400000	4.14950000	-0.80300000

C	8.87730000	1.62360000	-5.39040000
C	9.01030000	0.59080000	-6.48870000
H	9.67500000	0.97770000	-7.26160000
H	8.01730000	0.40320000	-6.89820000
H	9.42790000	-0.32280000	-6.06480000
C	9.02770000	2.97760000	-5.67580000
H	9.24660000	3.29020000	-6.66540000
C	8.89390000	3.92740000	-4.66770000
H	9.01910000	4.95620000	-4.89570000
C	8.59650000	3.53870000	-3.35910000
C	8.45580000	2.17720000	-3.07820000
H	8.24540000	1.86300000	-2.08660000
C	8.59010000	1.22830000	-4.08720000
H	8.47350000	0.19920000	-3.85880000
C	6.80470000	7.08810000	-3.86980000
H	7.85580000	7.22350000	-3.86710000
C	6.00550000	7.87510000	-4.68600000
H	6.44880000	8.60750000	-5.31170000
C	4.60720000	7.71570000	-4.69090000
H	4.01380000	8.32770000	-5.32140000
C	4.00220000	6.76710000	-3.87740000
H	2.94980000	6.64660000	-3.88050000

Table S78 Cartesian coordinates of compound **3g-TS3**

N	1.96770000	1.74940000	0.29980000
N	2.00940000	2.72580000	-0.49490000
C	5.67580000	4.45680000	-1.59350000
C	4.48510000	4.92220000	-2.13970000
C	3.27110000	4.34050000	-1.76220000
H	2.36100000	4.68970000	-2.17460000
C	3.26650000	3.29360000	-0.84350000
C	4.49040000	2.83220000	-0.29430000
H	4.48470000	2.04000000	0.40880000
C	5.69710000	3.40690000	-0.66140000
H	6.60260000	3.05740000	-0.23520000
C	4.80020000	5.96660000	-3.05100000
C	6.17970000	6.13180000	-3.05470000
N	6.74770000	5.20150000	-2.14540000
S	8.41420000	4.77240000	-2.05430000
O	9.23210000	5.89390000	-2.37770000
O	8.69400000	4.14950000	-0.80300000
C	8.87730000	1.62360000	-5.39040000
C	9.01030000	0.59080000	-6.48870000
H	9.67500000	0.97770000	-7.26160000
H	8.01730000	0.40320000	-6.89820000
H	9.42790000	-0.32280000	-6.06480000
C	9.02770000	2.97760000	-5.67580000
H	9.24660000	3.29020000	-6.66540000
C	8.89390000	3.92740000	-4.66770000
H	9.01910000	4.95620000	-4.89570000
C	8.59650000	3.53870000	-3.35910000
C	8.45580000	2.17720000	-3.07820000

H	8.24540000	1.86300000	-2.08660000
C	8.59010000	1.22830000	-4.08720000
H	8.47350000	0.19920000	-3.85880000
C	6.80470000	7.08810000	-3.86980000
H	7.85580000	7.22350000	-3.86710000
C	6.00550000	7.87510000	-4.68600000
H	6.44880000	8.60750000	-5.31170000
C	4.60720000	7.71570000	-4.69090000
H	4.01380000	8.32770000	-5.32140000
C	4.00220000	6.76710000	-3.87740000
H	2.94980000	6.64660000	-3.88050000
C	1.83020000	-1.46690000	2.91850000
H	1.79410000	-2.30890000	3.60490000
C	1.70000000	-0.16570000	3.40490000
H	1.56260000	0.00570000	4.46940000
C	1.74620000	0.91540000	2.52500000
H	1.64490000	1.92880000	2.90320000
C	1.92270000	0.69520000	1.15780000
C	2.05270000	-0.60580000	0.67250000
H	2.19010000	-0.77720000	-0.39210000
C	2.00660000	-1.68690000	1.55230000
H	2.10790000	-2.70040000	1.17420000

Table S79 Cartesian coordinates of compound **3g-TS4**

C	3.49580000	-0.00130000	-2.69280000
N	4.67970000	0.73470000	-2.40710000
C	2.34410000	0.73270000	-3.05420000
H	2.40150000	1.79010000	-3.09270000
C	1.15090000	0.09310000	-3.35190000
H	0.29370000	0.66040000	-3.61180000
C	1.11760000	-1.30910000	-3.28690000
C	2.23980000	-2.04820000	-2.93000000
C	3.43950000	-1.39680000	-2.62940000
H	4.29140000	-1.96370000	-2.36030000
N	5.72770000	1.38620000	-2.15420000
C	5.81270000	5.59650000	-2.42130000
H	5.85060000	6.65440000	-2.48380000
C	6.94030000	4.88210000	-2.02590000
H	7.83650000	5.39620000	-1.78730000
C	6.89090000	3.49410000	-1.94430000
H	7.74810000	2.94930000	-1.64380000
C	5.71470000	2.80820000	-2.25650000
C	4.58320000	3.53440000	-2.65410000
H	3.68360000	3.03030000	-2.89480000
C	4.63530000	4.92260000	-2.73520000
H	3.77730000	5.46800000	-3.03650000
C	1.88820000	-3.42450000	-2.96690000
C	0.55510000	-3.51750000	-3.34630000
N	0.05150000	-2.20580000	-3.54930000
S	-1.41240000	-1.80780000	-4.36640000
O	-2.39910000	-2.80840000	-4.12840000
O	-1.80390000	-0.47350000	-4.05270000

C	-0.22140000	-1.96380000	-8.81800000
C	0.18650000	-2.01670000	-10.27440000
H	-0.37680000	-2.80590000	-10.77290000
H	1.25590000	-2.22470000	-10.31880000
H	-0.03540000	-1.05480000	-10.73750000
C	-0.69150000	-3.10610000	-8.17640000
H	-0.77500000	-4.01850000	-8.71080000
C	-1.05580000	-3.05870000	-6.83420000
H	-1.42120000	-3.93390000	-6.35800000
C	-0.94570000	-1.86950000	-6.10900000
C	-0.48110000	-0.72500000	-6.76200000
H	-0.40640000	0.19060000	-6.23080000
C	-0.11680000	-0.77380000	-8.10410000
H	0.24070000	0.10230000	-8.58310000
C	-0.08650000	-4.75810000	-3.48210000
H	-1.10660000	-4.83180000	-3.76020000
C	0.65000000	-5.90640000	-3.23000000
H	0.19220000	-6.85840000	-3.32270000
C	2.00190000	-5.82350000	-2.84700000
H	2.54720000	-6.71310000	-2.65840000
C	2.62280000	-4.58910000	-2.71340000
H	3.64010000	-4.52500000	-2.42480000

Table S80 Cartesian coordinates of compound **4h-TS1**

N	-2.63640000	-0.88167700	0.35194700
N	-1.56921400	-1.39967900	0.70692300
N	1.77968900	-0.34770700	0.51363900
N	0.80506600	-1.23826700	0.84734900
C	-0.35688100	-0.67493900	0.48870400
C	-0.15101300	0.62013000	-0.08187200
C	1.24498000	0.80152700	-0.04443100
C	1.85189100	1.97378500	-0.51975100
H	2.92952400	2.08325200	-0.51147100
C	1.02337300	2.96227500	-1.03199800
H	1.46392300	3.87971200	-1.41263200
C	-0.37761200	2.79132600	-1.07386500
H	-1.00257200	3.57977800	-1.48320500
C	-0.97148000	1.63055700	-0.60523200
H	-2.04686100	1.51244800	-0.64834500
C	5.76533400	-1.81460300	0.16429300
H	6.85061500	-1.89426800	0.30463400
H	5.48089500	-2.53058800	-0.61737800
C	5.38382600	-0.41575900	-0.30441800
H	5.77389800	-0.18731000	-1.30026000
H	5.75311700	0.35220500	0.39592900
O	3.94951400	-0.32464600	-0.43497300
C	3.21879600	-0.57185400	0.77839700
H	3.52918300	0.17597300	1.52794000
C	3.49728900	-1.98182300	1.27727900
H	3.12552800	-2.68419100	0.52339400
H	2.95276300	-2.18004700	2.20515100
C	5.01424900	-2.14646900	1.46260400

H	5.23835900	-3.16973600	1.78322600
H	5.36151700	-1.48280400	2.26838800
C	-6.22597700	0.88315400	-0.86745600
H	-7.16195100	1.33440600	-1.18085400
C	-5.42771200	0.18807400	-1.77922600
H	-5.74112400	0.09486700	-2.81654000
C	-4.22196000	-0.39300700	-1.39829600
H	-3.61299000	-0.93306200	-2.11562900
C	-3.77815700	-0.29499800	-0.04828200
C	-4.59872500	0.40937300	0.87943500
H	-4.27769100	0.48587000	1.91292600
C	-5.79328000	0.98286000	0.45806800
H	-6.39711200	1.51580800	1.18899900

Table S81 Cartesian coordinates of compound **4h-TS2**

N	21.79590000	13.21510000	-0.19120000
N	22.84550000	13.81830000	0.16900000
C	22.70470000	17.64570000	1.98120000
H	22.68820000	18.62260000	2.44450000
C	23.93570000	16.99980000	1.74750000
H	24.86560000	17.47440000	2.02840000
C	23.94000000	15.72870000	1.14370000
H	24.87060000	15.21440000	0.95370000
C	22.75130000	15.10300000	0.77500000
C	21.53330000	15.74950000	1.00940000
H	20.61280000	15.26430000	0.72280000
C	21.49580000	17.02130000	1.61200000
H	20.54990000	17.51370000	1.78940000
C	18.45970000	12.13030000	-0.94410000
C	19.32320000	13.06650000	-0.43380000
C	20.62090000	12.53980000	-0.59440000
N	20.58440000	11.35340000	-1.15460000
N	19.25860000	11.09300000	-1.38780000
C	18.80440000	14.25790000	0.10640000
H	19.48970000	14.99140000	0.50520000
C	17.40590000	14.47450000	0.11660000
H	17.00330000	15.38960000	0.52730000
C	16.53180000	13.49190000	-0.41930000
H	15.46360000	13.65690000	-0.42250000
C	17.06750000	12.30160000	-0.95720000
H	16.43350000	11.54160000	-1.39140000
C	18.26730000	8.11890000	-4.27740000
H	17.82630000	7.22070000	-4.71110000

H	18.76590000	8.67770000	-5.07180000
C	19.29860000	7.72260000	-3.20950000
H	20.09480000	7.13910000	-3.67570000
H	18.82110000	7.10750000	-2.44400000
C	19.90460000	8.98370000	-2.56680000
H	20.42270000	9.57760000	-3.32200000
H	20.60870000	8.70310000	-1.78260000
C	18.74540000	9.81450000	-1.96380000
H	18.23510000	9.25490000	-1.19220000
O	17.82670000	10.12010000	-3.07530000
C	17.15560000	8.99160000	-3.68360000
H	16.48820000	9.33740000	-4.47500000
H	16.58620000	8.43470000	-2.93720000

Table S82 Cartesian coordinates of compound **4h-TS3**

N	21.79590000	13.21510000	-0.19120000
N	22.91240000	12.65660000	-0.38270000
C	18.45970000	12.13030000	-0.94410000
C	19.32320000	13.06650000	-0.43380000
C	20.62090000	12.53980000	-0.59440000
N	20.58440000	11.35340000	-1.15460000
N	19.25860000	11.09300000	-1.38780000
C	18.80440000	14.25790000	0.10640000
H	19.48970000	14.99140000	0.50520000
C	17.40590000	14.47450000	0.11660000
H	17.00330000	15.38960000	0.52730000
C	16.53180000	13.49190000	-0.41930000
H	15.46360000	13.65690000	-0.42250000
C	17.06750000	12.30160000	-0.95720000
H	16.43350000	11.54160000	-1.39140000
C	18.26730000	8.11890000	-4.27740000
H	17.82630000	7.22070000	-4.71110000
H	18.76590000	8.67770000	-5.07180000
C	19.29860000	7.72260000	-3.20950000
H	20.09480000	7.13910000	-3.67570000
H	18.82110000	7.10750000	-2.44400000
C	19.90460000	8.98370000	-2.56680000
H	20.42270000	9.57760000	-3.32200000
H	20.60870000	8.70310000	-1.78260000
C	18.74540000	9.81450000	-1.96380000
H	18.23510000	9.25490000	-1.19220000
O	17.82670000	10.12010000	-3.07530000
C	17.15560000	8.99160000	-3.68360000

H	16.48820000	9.33740000	-4.47500000
H	16.58620000	8.43470000	-2.93720000
C	26.58070000	10.82120000	-1.01130000
H	27.54150000	10.34020000	-1.17540000
C	25.89640000	10.61930000	0.18760000
H	26.32390000	9.98140000	0.95700000
C	24.66360000	11.23600000	0.39920000
H	24.13020000	11.07910000	1.33260000
C	24.11460000	12.05520000	-0.58890000
C	24.79930000	12.25660000	-1.78710000
H	24.37180000	12.89450000	-2.55650000
C	26.03220000	11.63990000	-1.99870000
H	26.56550000	11.79670000	-2.93210000

Table S83 Cartesian coordinates of compound **4h-TS4**

C	0.83830000	-1.82080000	-5.66810000
H	1.66000000	-1.27900000	-5.27860000
C	-0.45480000	-1.49020000	-5.29700000
H	-0.62290000	-0.69200000	-4.62030000
C	-1.56000000	-2.20840000	-5.80910000
H	-2.54110000	-1.94220000	-5.50870000
C	-1.36440000	-3.25410000	-6.69160000
H	-2.18260000	-3.80810000	-7.07510000
C	-0.04340000	-3.56620000	-7.05390000
C	1.05210000	-2.88660000	-6.57050000
C	2.18230000	-3.49590000	-7.17040000
N	3.54830000	-3.18040000	-7.01160000
N	1.82660000	-4.46820000	-7.97040000
N	0.45970000	-4.53260000	-7.90090000
N	4.76910000	-2.89840000	-6.86970000
C	7.73730000	-5.08350000	-8.92510000
H	8.49480000	-5.62330000	-9.43390000
C	8.08060000	-4.03780000	-8.07240000
H	9.10000000	-3.78170000	-7.93240000
C	7.08650000	-3.32950000	-7.40450000
H	7.34780000	-2.53420000	-6.75560000
C	5.74050000	-3.65920000	-7.58190000
C	5.40330000	-4.71390000	-8.44300000
H	4.38820000	-4.97880000	-8.59050000
C	6.39910000	-5.42070000	-9.10970000
H	6.13840000	-6.21750000	-9.75910000
C	-1.43700000	-8.14080000	-9.15030000
H	-2.10870000	-8.80940000	-9.69000000

H	-0.89580000	-8.72360000	-8.40230000
C	-2.26260000	-7.06550000	-8.43420000
H	-2.89950000	-7.52510000	-7.67620000
H	-2.87690000	-6.51300000	-9.14740000
O	-1.29970000	-6.18770000	-7.80370000
C	-0.38080000	-5.46950000	-8.70480000
H	-0.93600000	-4.90730000	-9.44280000
C	0.50010000	-6.54600000	-9.38490000
H	1.06880000	-7.08430000	-8.62440000
H	1.18940000	-6.07430000	-10.08630000
C	-0.43340000	-7.51550000	-10.13210000
H	0.16320000	-8.30590000	-10.59150000
H	-0.96910000	-6.98340000	-10.92090000

Table S84 Cartesian coordinates of compound **5e-TS1**

C	4.37947600	5.27177100	0.99373200
N	5.59646800	6.05123800	0.99110200
C	3.20445100	6.03800300	0.83342000
H	3.31270400	7.11263500	0.72512600
C	1.95693500	5.43497300	0.81547000
H	1.05022000	6.02074000	0.69254700
C	1.91398400	4.04273900	0.96208800
C	3.09327300	3.25058000	1.12523500
C	4.33880200	3.88514300	1.13984200
H	5.26166200	3.32526400	1.26146700
N	6.65700400	5.44769500	1.12713900
C	2.66365700	1.88267600	1.24365400
H	3.29409400	1.01509500	1.37863300
C	1.29947100	1.88205100	1.15343000
H	0.59833200	1.06025600	1.19551200
N	0.84347800	3.18052600	0.98377700
H	-0.12394100	3.44909700	0.89121600
C	10.28822500	3.46454200	1.58725800
H	11.23677900	2.95099900	1.70701100
C	9.58177600	3.93216400	2.69911600
H	9.98267300	3.78297100	3.69923100
C	8.36633700	4.59225900	2.56918900
H	7.82900700	4.95419100	3.43945900
C	7.81538200	4.80540000	1.27483700
C	8.53249200	4.33284000	0.14049500
H	8.12258100	4.49599200	-0.85068500
C	9.74461200	3.67748900	0.31718300
H	10.27426700	3.32697000	-0.56588400

Table S85 Cartesian coordinates of compound **5e-TS2**

C	6.28260000	-2.08390000	0.65300000
N	6.27370000	-0.68620000	0.93910000
C	5.05230000	-2.74050000	0.57340000
H	4.15840000	-2.19330000	0.72600000
C	4.99640000	-4.10260000	0.29480000
H	4.05850000	-4.59380000	0.23480000
C	6.17200000	-4.82110000	0.09470000
H	6.12910000	-5.85930000	-0.11760000
C	7.40400000	-4.17700000	0.17320000
H	8.29870000	-4.72520000	0.02120000
C	7.46230000	-2.81460000	0.45110000
H	8.40370000	-2.33330000	0.50890000
N	7.36470000	-0.05970000	0.99680000
C	11.03950000	1.94370000	1.17630000
C	11.00690000	0.58170000	0.89620000
C	9.76700000	-0.07240000	0.83860000
H	9.72330000	-1.10800000	0.62710000
C	8.59850000	0.64880000	1.06200000
C	8.66330000	2.04470000	1.34530000
H	7.77000000	2.58760000	1.51310000
C	9.88090000	2.69910000	1.40430000
H	9.93830000	3.73610000	1.61470000
C	12.34490000	0.15820000	0.72540000
H	12.66070000	-0.82800000	0.50100000
C	13.15540000	1.23490000	0.89840000
H	14.21190000	1.30570000	0.84750000
N	12.36490000	2.33020000	1.17460000
H	12.70340000	3.28980000	1.35280000

Table S86 Cartesian coordinates of compound **5e-TS3**

N	6.28150000	0.55230000	1.19270000
N	7.36470000	-0.05970000	0.99680000
C	11.03950000	1.94370000	1.17630000
C	11.00690000	0.58170000	0.89620000
C	9.76700000	-0.07240000	0.83860000
H	9.72330000	-1.10800000	0.62710000
C	8.59850000	0.64880000	1.06200000
C	8.66330000	2.04470000	1.34530000
H	7.77000000	2.58760000	1.51310000
C	9.88090000	2.69910000	1.40430000
H	9.93830000	3.73610000	1.61470000
C	12.34490000	0.15820000	0.72540000
H	12.66070000	-0.82800000	0.50100000
C	13.15540000	1.23490000	0.89840000
H	14.21190000	1.30570000	0.84750000
N	12.36490000	2.33020000	1.17460000
H	12.70340000	3.28980000	1.35280000
C	2.71240000	2.56880000	1.83760000
H	1.77750000	3.09710000	2.00590000
C	3.23860000	2.47760000	0.54870000
H	2.71400000	2.93460000	-0.28650000
C	4.43810000	1.80000000	0.33170000
H	4.84840000	1.72860000	-0.67170000
C	5.11180000	1.21310000	1.40430000
C	4.58510000	1.30470000	2.69240000
H	5.10960000	0.84770000	3.52760000
C	3.38560000	1.98230000	2.90950000
H	2.97530000	2.05370000	3.91290000

Table S87 Cartesian coordinates of compound **5e-TS4**

C	4.36290000	5.32230000	0.97810000
N	5.58270000	6.05760000	0.97450000
C	3.16110000	6.06190000	0.82330000
H	3.21740000	7.11350000	0.71260000
C	1.93140000	5.42840000	0.81630000
H	1.03070000	5.97490000	0.70140000
C	1.91670000	4.03490000	0.96700000
C	3.07630000	3.28150000	1.11940000
C	4.31870000	3.93420000	1.12540000
H	5.20520000	3.36890000	1.24110000
N	6.66160000	6.70800000	0.97130000
C	6.68760000	10.90030000	0.48570000
H	6.71120000	11.95360000	0.36460000
C	7.87460000	10.19280000	0.65670000
H	8.80150000	10.70790000	0.66610000
C	7.84380000	8.81090000	0.81550000
H	8.74590000	8.27130000	0.94570000
C	6.62770000	8.12400000	0.80450000
C	5.43660000	8.84340000	0.63200000
H	4.50590000	8.33860000	0.62120000
C	5.46970000	10.22560000	0.47340000
H	4.56670000	10.76560000	0.34300000
C	2.68220000	1.92910000	1.24180000
H	3.33180000	1.10200000	1.37070000
C	1.32680000	1.87420000	1.16570000
H	0.67630000	1.03850000	1.21690000
N	0.85140000	3.15730000	0.99780000
H	-0.14210000	3.42670000	0.90900000

Table S88 Cartesian coordinates of compound **5f-TS1**

C	-0.92035600	1.06961700	-0.23743700
N	0.29004200	1.83114400	-0.25018900
C	-2.13797100	1.77554000	-0.44786700
H	-2.09922500	2.84735300	-0.60795000
N	-3.33220100	1.19475500	-0.46000800
C	-3.33072300	-0.13303300	-0.25730500
C	-2.19431300	-0.92746900	-0.04037000
C	-0.95084800	-0.30381600	-0.03068700
H	-0.04191700	-0.86934700	0.13234700
N	1.39214200	1.27211400	-0.07534400
C	-2.64618600	-2.26251400	0.12548400
H	-2.02547500	-3.12364400	0.30936000
C	-4.00317500	-2.26108200	0.01091600
H	-4.70531400	-3.07643400	0.07611100
N	-4.42317600	-0.96195800	-0.22264800
H	-5.37395300	-0.64358500	-0.35114600
C	5.00394400	-0.70565700	0.51955100
H	5.95174400	-1.21177800	0.67412900
C	4.29633700	-0.19447700	1.60885000
H	4.69342600	-0.30216900	2.61530100
C	3.08095100	0.45488200	1.41791300
H	2.53056000	0.85688700	2.26163200
C	2.55519800	0.59684300	0.12188300
C	3.27284000	0.08624600	-0.97278300
H	2.87066000	0.20362000	-1.97329000
C	4.48725000	-0.56100300	-0.76887400
H	5.03373700	-0.95556500	-1.62194900

Table S89 Cartesian coordinates of compound **5f-TS2**

C	16.09880000	-9.93520000	-0.58240000
N	16.10670000	-8.53350000	-0.31560000
C	14.86220000	-10.58320000	-0.63440000
H	13.97420000	-10.02730000	-0.47790000
C	14.79230000	-11.94930000	-0.88960000
H	13.85020000	-12.43490000	-0.92800000
C	15.95970000	-12.67970000	-1.09510000
H	15.90640000	-13.72090000	-1.28940000
C	17.19740000	-12.04350000	-1.04570000
H	18.08580000	-12.60090000	-1.20240000
C	17.27000000	-10.67750000	-0.79080000
H	18.21620000	-10.20330000	-0.75500000
N	17.20420000	-7.91810000	-0.26550000
C	20.78690000	-5.88930000	-0.09810000
C	20.82020000	-7.25360000	-0.37060000
C	19.60790000	-7.94670000	-0.42820000
H	19.57910000	-8.98500000	-0.63160000
C	18.44540000	-7.22210000	-0.20880000
C	18.52730000	-5.82110000	0.06340000
H	17.63720000	-5.27170000	0.23080000
N	19.67280000	-5.15740000	0.11980000
C	22.18050000	-7.61090000	-0.53050000
H	22.54910000	-8.58080000	-0.74710000
C	22.93320000	-6.49120000	-0.35750000
H	23.98500000	-6.36250000	-0.40070000
N	22.07870000	-5.43570000	-0.09250000
H	22.33830000	-4.45300000	0.08530000

Table S90 Cartesian coordinates of compound **5f-TS3**

N	16.13510000	-7.27970000	-0.07790000
N	17.20420000	-7.91810000	-0.26550000
C	20.78690000	-5.88930000	-0.09810000
C	20.82020000	-7.25360000	-0.37060000
C	19.60790000	-7.94670000	-0.42820000
H	19.57910000	-8.98500000	-0.63160000
C	18.44540000	-7.22210000	-0.20880000
C	18.52730000	-5.82110000	0.06340000
H	17.63720000	-5.27170000	0.23080000
N	19.67280000	-5.15740000	0.11980000
C	22.18050000	-7.61090000	-0.53050000
H	22.54910000	-8.58080000	-0.74710000
C	22.93320000	-6.49120000	-0.35750000
H	23.98500000	-6.36250000	-0.40070000
N	22.07870000	-5.43570000	-0.09250000
H	22.33830000	-4.45300000	0.08530000
C	12.61200000	-5.17600000	0.54110000
H	11.68920000	-4.62510000	0.70390000
C	13.27240000	-5.76300000	1.62080000
H	12.86440000	-5.66950000	2.62400000
C	14.45640000	-6.47010000	1.41310000
H	14.97120000	-6.92740000	2.25340000
C	14.98050000	-6.59020000	0.12470000
C	14.31970000	-6.00310000	-0.95400000
H	14.72770000	-6.09660000	-1.95720000
C	13.13560000	-5.29600000	-0.74630000
H	12.62090000	-4.83860000	-1.58670000

Table S91 Cartesian coordinates of compound **5f-TS4**

C	10.62780000	-4.22820000	2.03350000
N	11.83620000	-3.47270000	2.02150000
C	9.40840000	-3.52440000	1.82320000
H	9.44660000	-2.47710000	1.66680000
N	8.21930000	-4.10790000	1.81190000
C	8.22140000	-5.44320000	2.01580000
C	9.35020000	-6.22860000	2.23070000
C	10.60050000	-5.60450000	2.24090000
H	11.48320000	-6.16580000	2.40100000
N	12.90400000	-2.80510000	2.01090000
C	12.87200000	1.36900000	1.38680000
H	12.88090000	2.41790000	1.23080000
C	14.06900000	0.68310000	1.57420000
H	14.98900000	1.21030000	1.56100000
C	14.05760000	-0.69310000	1.77870000
H	14.96780000	-1.21580000	1.92130000
C	12.85060000	-1.39580000	1.79740000
C	11.64910000	-0.69830000	1.60830000
H	10.72470000	-1.21430000	1.61990000
C	11.66310000	0.67820000	1.40400000
H	10.75230000	1.20190000	1.26120000
C	8.90250000	-7.56090000	2.39650000
H	9.51560000	-8.40640000	2.57740000
C	7.54710000	-7.56690000	2.28320000
H	6.86050000	-8.37250000	2.34820000
N	7.12970000	-6.26870000	2.05000000
H	6.16050000	-5.93990000	1.91840000

Table S92 Cartesian coordinates of compound **5g-TS1**

N	-1.96240500	-2.07297800	0.20542200
N	-0.87620600	-2.65214900	0.28103600
C	2.80361300	-0.59886300	0.11216100
C	2.78916700	-1.98696200	0.27604300
H	3.71231400	-2.55290500	0.36168800
C	1.55269600	-2.62362200	0.32614600
H	1.48932200	-3.70028300	0.45199300
C	0.34891500	-1.88930700	0.21577700
C	0.37334700	-0.50568800	0.05225000
H	-0.56175400	0.04073600	-0.03121400
C	1.59656700	0.14362600	-0.00044200
C	1.97013800	1.52714200	-0.15753600
C	3.38262800	1.57772000	-0.13407100
N	3.86263300	0.28142400	0.02952700
H	4.83665500	0.02537100	0.08008900
C	4.07386000	2.78119800	-0.26236600
H	5.15962800	2.81370200	-0.24322900
C	3.32241700	3.94458600	-0.41669900
H	3.83521100	4.89680700	-0.51916100
C	1.91811900	3.90736000	-0.44229100
H	1.35948100	4.83048000	-0.56421800
C	1.23677500	2.70228400	-0.31322000
H	0.15083600	2.67443300	-0.33299100
C	-5.60835500	-0.05345200	-0.05114200
H	-6.56078200	0.46273400	-0.11710400
C	-4.98598100	-0.24628200	1.18513000
H	-5.45572400	0.12208700	2.09436700
C	-3.76575300	-0.90390900	1.28925100

H	-3.29216500	-1.05269000	2.25404400
C	-3.12014600	-1.39528900	0.12020500
C	-3.76121300	-1.20500300	-1.13590500
H	-3.28421900	-1.58543900	-2.03309600
C	-4.98094400	-0.54169500	-1.20049900
H	-5.44697400	-0.40688700	-2.17401400

Table S93 Cartesian coordinates of compound **5g-TS2**

C	19.22180000	-4.64080000	-0.32400000
N	19.21370000	-3.24110000	-0.05220000
C	17.99150000	-5.29880000	-0.38630000
H	17.09840000	-4.75080000	-0.23280000
C	17.93530000	-6.66410000	-0.64810000
H	16.99780000	-7.15700000	-0.69430000
C	19.11020000	-7.38340000	-0.84960000
H	19.06700000	-8.42400000	-1.04900000
C	20.34210000	-6.73740000	-0.78930000
H	21.23590000	-7.28670000	-0.94280000
C	20.40080000	-5.37190000	-0.52800000
H	21.34190000	-4.88860000	-0.48400000
N	20.30470000	-2.61390000	0.00220000
C	23.98100000	-0.60870000	0.16520000
C	23.94310000	-1.97250000	-0.10550000
C	22.70920000	-2.62830000	-0.15600000
H	22.66590000	-3.66550000	-0.35970000
C	21.53750000	-1.90520000	0.06370000
C	21.60380000	-0.51200000	0.33780000
H	20.71170000	0.03350000	0.50420000
C	22.82370000	0.14450000	0.39070000
H	22.88010000	1.18280000	0.59520000
C	25.28870000	-2.41000000	-0.28050000
C	26.11150000	-1.30280000	-0.11170000
N	25.30880000	-0.19740000	0.16190000
H	25.64360000	0.76240000	0.33420000
C	27.50380000	-1.37970000	-0.21690000
H	28.10950000	-0.52050000	-0.08400000

C	28.06420000	-2.61700000	-0.50030000
H	29.11610000	-2.71360000	-0.58720000
C	27.24670000	-3.75250000	-0.67500000
H	27.69400000	-4.68870000	-0.89090000
C	25.86450000	-3.65450000	-0.56680000
H	25.24980000	-4.50640000	-0.69800000

Table S94 Cartesian coordinates of compound **5g-TS3**

N	19.22230000	-1.99730000	0.18860000
N	20.30470000	-2.61390000	0.00220000
C	23.98100000	-0.60870000	0.16520000
C	23.94310000	-1.97250000	-0.10550000
C	22.70920000	-2.62830000	-0.15600000
H	22.66590000	-3.66550000	-0.35970000
C	21.53750000	-1.90520000	0.06370000
C	21.60380000	-0.51200000	0.33780000
H	20.71170000	0.03350000	0.50420000
C	22.82370000	0.14450000	0.39070000
H	22.88010000	1.18280000	0.59520000
C	25.28870000	-2.41000000	-0.28050000
C	26.11150000	-1.30280000	-0.11170000
N	25.30880000	-0.19740000	0.16190000
H	25.64360000	0.76240000	0.33420000
C	27.50380000	-1.37970000	-0.21690000
H	28.10950000	-0.52050000	-0.08400000
C	28.06420000	-2.61700000	-0.50030000
H	29.11610000	-2.71360000	-0.58720000
C	27.24670000	-3.75250000	-0.67500000
H	27.69400000	-4.68870000	-0.89090000
C	25.86450000	-3.65450000	-0.56680000
H	25.24980000	-4.50640000	-0.69800000
C	15.65620000	0.03400000	0.80330000
H	14.72220000	0.56590000	0.96500000
C	16.32350000	-0.54560000	1.88280000
H	15.90960000	-0.46520000	2.88460000
C	17.52200000	-1.22830000	1.67650000

H	18.04200000	-1.67990000	2.51670000
C	18.05360000	-1.33150000	0.38980000
C	17.38590000	-0.75190000	-0.68880000
H	17.79980000	-0.83220000	-1.69070000
C	16.18740000	-0.06910000	-0.48250000
H	15.66740000	0.38240000	-1.32270000

Table S95 Cartesian coordinates of compound **5g-TS4**

C	20.65150000	-10.93570000	-0.77080000
N	20.59850000	-9.51830000	-0.91880000
C	19.44160000	-11.62880000	-0.68700000
H	18.52940000	-11.09270000	-0.73450000
C	19.43040000	-13.01250000	-0.54200000
H	18.50830000	-13.53230000	-0.47900000
C	20.63060000	-13.71560000	-0.48010000
H	20.62190000	-14.77030000	-0.36980000
C	21.84230000	-13.03470000	-0.56280000
H	22.75540000	-13.57120000	-0.51570000
C	21.85600000	-11.65080000	-0.70760000
H	22.78230000	-11.14150000	-0.77020000
N	21.67160000	-8.86030000	-0.97430000
C	25.31800000	-6.80490000	-1.14330000
C	25.32060000	-8.19440000	-0.97890000
H	26.23000000	-8.73240000	-0.89710000
C	24.09520000	-8.84050000	-0.92710000
H	24.05560000	-9.89160000	-0.80350000
C	22.88380000	-8.11700000	-1.03700000
C	22.91060000	-6.72730000	-1.20080000
H	22.01520000	-6.17060000	-1.28480000
C	24.14300000	-6.06850000	-1.25430000
C	24.51070000	-4.69970000	-1.40980000
C	25.89880000	-4.63650000	-1.38840000
N	26.39420000	-5.92850000	-1.22500000
H	27.39030000	-6.18930000	-1.17330000
C	26.59720000	-3.43170000	-1.51670000
H	27.65630000	-3.40970000	-1.49670000

C	25.85770000	-2.26780000	-1.67090000
H	26.35290000	-1.33620000	-1.77130000
C	24.44850000	-2.31080000	-1.69590000
H	23.90160000	-1.41080000	-1.81480000
C	23.77340000	-3.51890000	-1.56640000
H	22.71520000	-3.55260000	-1.58500000

Table S96 Cartesian coordinates of compound **5h-TS1**

N	-0.91271800	-1.44786600	-0.00055800
N	0.16662200	-2.05344400	-0.00094200
N	3.47950100	-0.97963500	-0.00197400
H	4.45223200	-1.25009100	-0.00273000
N	2.53980500	-1.94420100	-0.00198400
C	1.37060700	-1.29655700	-0.00093100
C	1.55990500	0.11901600	-0.00009600
C	2.95600000	0.29089200	-0.00094200
C	3.55859500	1.55435800	-0.00068900
H	4.63861000	1.66644400	-0.00142000
C	2.71663400	2.65549900	0.00047000
H	3.14488800	3.65371300	0.00068100
C	1.31395900	2.49918100	0.00149800
H	0.67960200	3.38043700	0.00246100
C	0.72835700	1.24471900	0.00117200
H	-0.34954600	1.14621200	0.00198200
C	-4.53539900	0.63030600	0.00152000
H	-5.48099000	1.16285600	0.00199900
C	-3.91369100	0.28305100	1.20348900
H	-4.37628200	0.54546600	2.15208100
C	-2.70153900	-0.39795000	1.22219300
H	-2.22771000	-0.66943600	2.15950900
C	-2.06764000	-0.75647400	0.00020900
C	-2.70588200	-0.40340400	-1.22101200
H	-2.23537200	-0.67906500	-2.15877700
C	-3.91783300	0.27779300	-1.20106700
H	-4.38373700	0.53601200	-2.14918500

Table S97 Cartesian coordinates of compound **5h-TS2**

C	23.72780000	3.08230000	-1.53520000
N	23.70560000	4.49710000	-1.38020000
C	22.50190000	2.41860000	-1.62360000
H	21.60360000	2.97790000	-1.57350000
C	22.45670000	1.03650000	-1.77640000
H	21.52170000	0.54070000	-1.84270000
C	23.63920000	0.30460000	-1.84190000
H	23.60460000	-0.74880000	-1.95830000
C	24.86700000	0.95550000	-1.75460000
H	25.76670000	0.39670000	-1.80430000
C	24.91450000	2.33790000	-1.60190000
H	25.85310000	2.82340000	-1.53620000
N	24.79400000	5.13440000	-1.31530000
C	28.20370000	6.24790000	-1.21590000
C	27.28170000	5.23460000	-1.32710000
C	26.01230000	5.84780000	-1.24260000
N	26.12480000	7.15050000	-1.08970000
N	27.46100000	7.39160000	-1.07370000
H	27.85760000	8.34260000	-0.96530000
C	27.74140000	3.91190000	-1.48900000
H	27.04700000	3.11630000	-1.57680000
C	29.10590000	3.67180000	-1.53150000
H	29.46520000	2.68180000	-1.65300000
C	30.03280000	4.73600000	-1.41400000
H	31.07200000	4.52800000	-1.44930000
C	29.59010000	6.03710000	-1.25450000
H	30.27220000	6.84370000	-1.16530000

Table S98 Cartesian coordinates of compound **5h-TS3**

N	23.70880000	5.77600000	-1.23970000
N	24.79400000	5.13440000	-1.31530000
C	28.20370000	6.24790000	-1.21590000
C	27.28170000	5.23460000	-1.32710000
C	26.01230000	5.84780000	-1.24260000
N	26.12480000	7.15050000	-1.08970000
N	27.46100000	7.39160000	-1.07370000
H	27.85760000	8.34260000	-0.96530000
C	27.74140000	3.91190000	-1.48900000
H	27.04700000	3.11630000	-1.57680000
C	29.10590000	3.67180000	-1.53150000
H	29.46520000	2.68180000	-1.65300000
C	30.03280000	4.73600000	-1.41400000
H	31.07200000	4.52800000	-1.44930000
C	29.59010000	6.03710000	-1.25450000
H	30.27220000	6.84370000	-1.16530000
C	20.14290000	7.88390000	-0.99050000
H	19.20900000	8.43600000	-0.92450000
C	20.74400000	7.39110000	0.16810000
H	20.27850000	7.55910000	1.13590000
C	21.94240000	6.68260000	0.08470000
H	22.41090000	6.29860000	0.98650000
C	22.54020000	6.46680000	-1.15830000
C	21.93870000	6.95980000	-2.31600000
H	22.40420000	6.79180000	-3.28380000
C	20.74030000	7.66830000	-2.23250000
H	20.27180000	8.05230000	-3.13440000

Table S99 Cartesian coordinates of compound **5h-TS4**

C	24.54830000	-3.59820000	-0.03900000
N	24.49600000	-2.17480000	-0.03820000
C	23.33720000	-4.29470000	-0.03920000
H	22.42560000	-3.75560000	-0.03890000
C	23.32310000	-5.68580000	-0.03990000
H	22.39980000	-6.20730000	-0.04020000
C	24.52150000	-6.39420000	-0.04050000
H	24.51080000	-7.45460000	-0.04110000
C	25.73450000	-5.71070000	-0.04020000
H	26.64690000	-6.25110000	-0.04070000
C	25.75130000	-4.31940000	-0.03950000
H	26.67980000	-3.80930000	-0.03930000
N	25.57490000	-1.52210000	-0.03820000
N	28.87540000	-0.44910000	-0.03920000
H	29.89150000	-0.65200000	-0.03990000
N	27.93170000	-1.42340000	-0.03920000
C	26.78190000	-0.79190000	-0.03820000
C	26.97060000	0.61550000	-0.03730000
C	28.33300000	0.80820000	-0.03820000
C	28.94150000	2.07220000	-0.03790000
H	29.99650000	2.17530000	-0.03870000
C	28.11270000	3.17870000	-0.03680000
H	28.52660000	4.15490000	-0.03650000
C	26.70680000	3.01830000	-0.03570000
H	26.08680000	3.87830000	-0.03490000
C	26.13580000	1.75540000	-0.03610000
H	25.08260000	1.64540000	-0.03530000

Table S100 Cartesian coordinates of compound **6-TS1**

N	-0.91020300	-1.31852500	0.10034400
N	0.17624000	-1.88977700	0.20125200
N	3.89175200	0.13532100	0.15427900
C	3.70070800	-1.17979300	0.29220900
H	4.59107600	-1.79324300	0.40436200
N	2.51885600	-1.81790300	0.30618700
C	1.39867400	-1.09585000	0.17223000
C	1.45606800	0.29568300	0.01740700
C	2.76288800	0.81631700	0.02265700
N	0.53230700	1.31579400	-0.14268800
N	2.60548700	2.17037400	-0.13697200
H	3.35531400	2.84617300	-0.17610600
C	1.25481900	2.40429300	-0.22962400
H	0.86199400	3.40462300	-0.36144600
C	-4.57875300	0.63879900	-0.24045600
H	-5.53726400	1.14022100	-0.32863000
C	-3.98625000	0.45413200	1.01068400
H	-4.48357100	0.81360000	1.90847500
C	-2.75847600	-0.18485800	1.14139500
H	-2.30268400	-0.32573900	2.11530600
C	-2.08251000	-0.65906300	-0.01168500
C	-2.69014300	-0.47996400	-1.28081300
H	-2.18167200	-0.84723100	-2.16549400
C	-3.91802000	0.16472100	-1.37599400
H	-4.36172900	0.29566400	-2.36015000

Table S101 Cartesian coordinates of compound **6-TS2**

C	-0.03600000	0.94210000	-8.76170000
N	1.20660000	1.63730000	-8.78670000
C	-1.24370000	1.66480000	-8.81800000
C	-2.39960000	0.92190000	-8.79050000
N	-2.44810000	-0.41900000	-8.71460000
C	-1.27690000	-1.03220000	-8.66450000
H	-1.26500000	-2.09270000	-8.60370000
N	-0.08010000	-0.39240000	-8.68580000
N	2.30790000	2.25350000	-8.80890000
C	2.44160000	6.46230000	-9.05620000
H	2.49190000	7.51950000	-9.11770000
C	3.61330000	5.71240000	-8.99130000
H	4.55540000	6.19900000	-9.00360000
C	3.54670000	4.32500000	-8.91040000
H	4.43630000	3.75160000	-8.86100000
C	2.30990000	3.67580000	-8.89320000
C	1.13420000	4.43750000	-8.95910000
H	0.18790000	3.96110000	-8.94740000
C	1.20330000	5.82500000	-9.04030000
H	0.31190000	6.39730000	-9.09000000
N	-3.41060000	1.80600000	-8.85350000
H	-4.41290000	1.56410000	-8.85250000
C	-2.86510000	3.05530000	-8.91710000
H	-3.48480000	3.91580000	-8.97350000
N	-1.56900000	3.01850000	-8.89890000

Table S102 Cartesian coordinates of compound **6-TS3**

N	13.94030000	8.11580000	-8.43170000
N	15.02050000	7.46900000	-8.52140000
N	18.67880000	9.51900000	-8.45870000
C	18.62620000	8.18270000	-8.59120000
C	17.46880000	7.44210000	-8.61970000
C	16.26430000	8.16210000	-8.50030000
N	16.31250000	9.49220000	-8.36840000
C	17.51040000	10.12990000	-8.35110000
H	17.50180000	11.18670000	-8.24420000
N	17.78980000	6.09310000	-8.76800000
C	19.08490000	6.05670000	-8.82360000
H	19.70180000	5.19940000	-8.93460000
N	19.63370000	7.30190000	-8.72020000
H	20.63610000	7.54300000	-8.73610000
C	10.38890000	10.24220000	-8.13720000
H	9.45870000	10.79920000	-8.06070000
C	10.94970000	9.99150000	-9.38990000
H	10.45660000	10.35300000	-10.28860000
C	12.14320000	9.27690000	-9.48910000
H	12.58030000	9.08140000	-10.46430000
C	12.77650000	8.81260000	-8.33490000
C	12.21530000	9.06360000	-7.08310000
H	12.70830000	8.70210000	-6.18430000
C	11.02170000	9.77830000	-6.98380000
H	10.58460000	9.97380000	-6.00860000

Table S103 Cartesian coordinates of compound **6-TS4**

C	20.57270000	13.74190000	-0.15550000
N	21.77690000	14.50190000	-0.18180000
C	19.37050000	14.43760000	-0.25860000
H	19.40650000	15.51340000	-0.35240000
C	18.13680000	13.76030000	-0.24180000
H	17.21010000	14.31110000	-0.32280000
C	18.12520000	12.35560000	-0.11860000
H	17.18420000	11.82370000	-0.10490000
C	19.33750000	11.64300000	-0.01360000
H	19.33280000	10.56600000	0.08110000
C	20.55520000	12.34890000	-0.03310000
H	21.48880000	11.81250000	0.04630000
N	22.88770000	13.91680000	-0.07890000
N	26.43820000	11.73100000	0.28680000
C	25.22410000	11.21000000	0.30480000
H	25.12830000	10.15840000	0.42070000
N	24.08370000	11.93430000	0.18440000
C	24.14110000	13.25660000	0.03720000
C	25.40610000	13.89420000	0.00720000
C	26.49640000	13.06480000	0.13770000
N	25.85960000	15.21050000	-0.12740000
N	27.58180000	13.85620000	0.08420000
H	28.53500000	13.53970000	0.15230000
C	27.15200000	15.13910000	-0.07600000
H	27.84530000	15.94060000	-0.14400000

Table S104 Cartesian coordinates of compound **8-TS1**

N	0.69624207	1.64819373	-1.11573094
N	0.24264700	0.60642400	-1.61732300
N	4.57808389	2.41501584	0.17914180
C	2.02410982	1.80029360	-0.60721060
N	3.01961329	1.60660187	-1.44557143
C	2.20024174	2.35389831	0.69328396
C	4.25947677	1.93644639	-0.99949626
H	5.06675233	1.77500164	-1.70754665
C	3.54908217	2.63276349	1.05446685
C	3.82007327	3.15282238	2.34240180
H	4.84893236	3.36053132	2.61019366
C	2.78611796	3.38505992	3.22076313
H	2.99622778	3.78506926	4.20590536
C	1.44603349	3.11463375	2.85485913
H	0.64913929	3.31368977	3.56121510
C	1.15235837	2.60579725	1.61050634
H	0.12841125	2.39988219	1.32374313
C	-1.51898299	-2.78252909	-3.38604163
H	-1.99962728	-3.63644517	-3.84878430
C	-0.88124480	-2.92603123	-2.15207723
H	-0.87698575	-3.88689086	-1.65111999
C	-0.25200979	-1.83842508	-1.55507958
H	0.22203086	-1.95294049	-0.58878535
C	-0.27939609	-0.59255000	-2.19460589
C	-0.97020508	-0.43213620	-3.40138553
H	-1.02030207	0.55079791	-3.85456465
C	-1.55945589	-1.53474330	-4.01079733
H	-2.06797194	-1.41710372	-4.96031939

Table S105 Cartesian coordinates of compound **8-TS2**

N	-0.23906209	-0.44408469	-0.51053579
N	-1.10306509	-1.01845769	-1.21565379
C	-5.20885809	-0.22208069	-0.69808479
H	-6.26892009	-0.03105369	-0.57617979
C	-4.77164209	-1.13447769	-1.66077879
H	-5.49089909	-1.65124669	-2.28523979
C	-3.40924309	-1.37902969	-1.81697679
H	-3.04555009	-2.08314669	-2.55713079
C	-2.48577909	-0.70447469	-1.00447379
C	-2.92447909	0.20802031	-0.03714479
H	-2.18850609	0.71118031	0.58056921
C	-4.28302909	0.44642431	0.11160621
H	-4.62975009	1.15217631	0.85786921
N	2.26589091	1.63478631	2.04066621
C	0.59678991	0.22883531	0.31606121
C	2.03114891	0.03696631	0.20930121
N	0.09901991	1.06523531	1.23033621
C	2.83150291	0.79157731	1.12781621
C	0.95126191	1.72234231	2.04243021
H	0.49735891	2.39256931	2.76703321
C	4.24596791	0.65213231	1.07945421
H	4.84159291	1.22789731	1.77757721
C	4.83598591	-0.19256869	0.16702221
H	5.91527591	-0.28900869	0.14069821
C	4.04462691	-0.93978769	-0.74027279
H	4.52397891	-1.60182869	-1.45189279
C	2.67075491	-0.82656369	-0.71791779
H	2.05287491	-1.39159769	-1.40509679

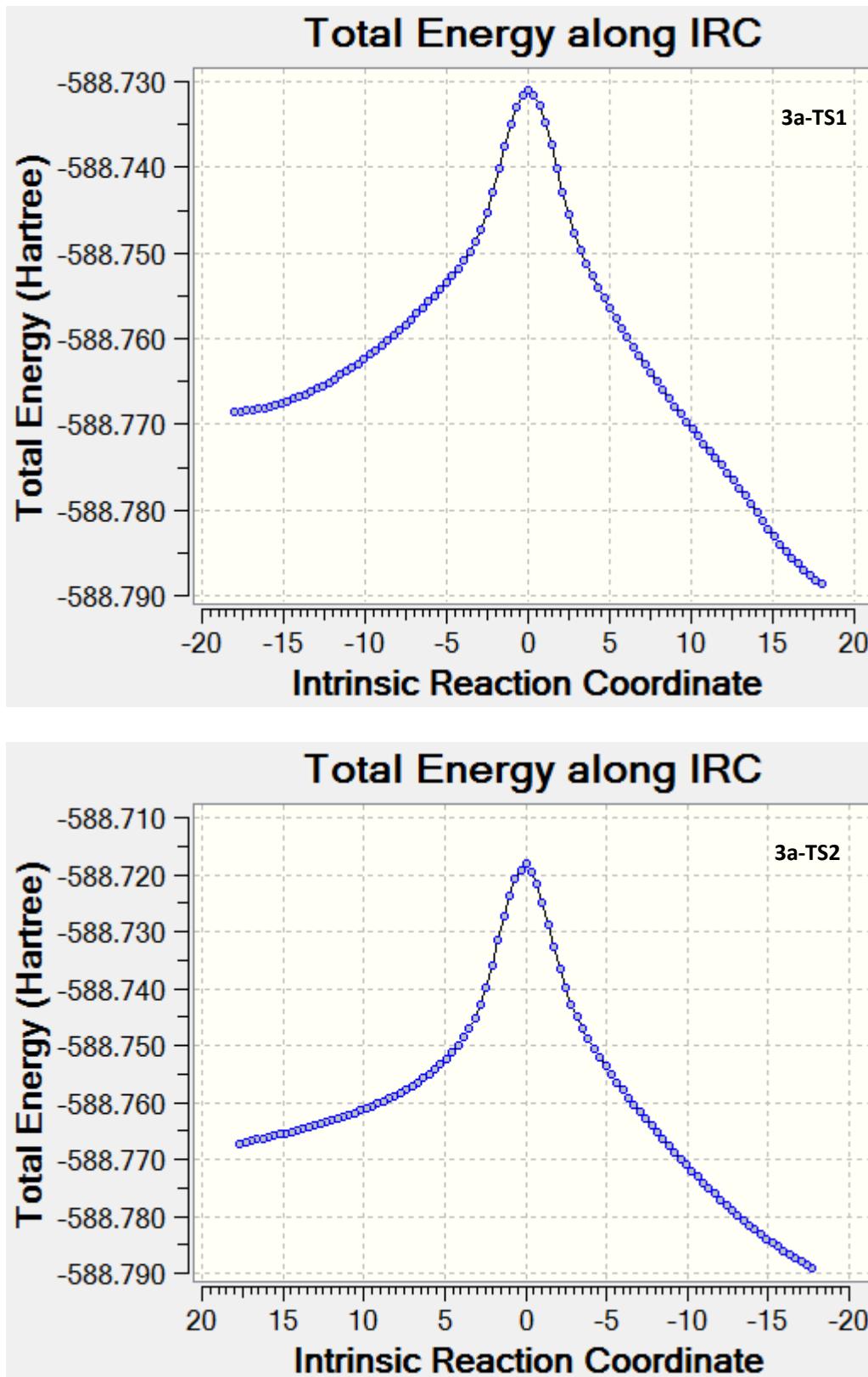
Table S106 Cartesian coordinates of compound **8-TS3**

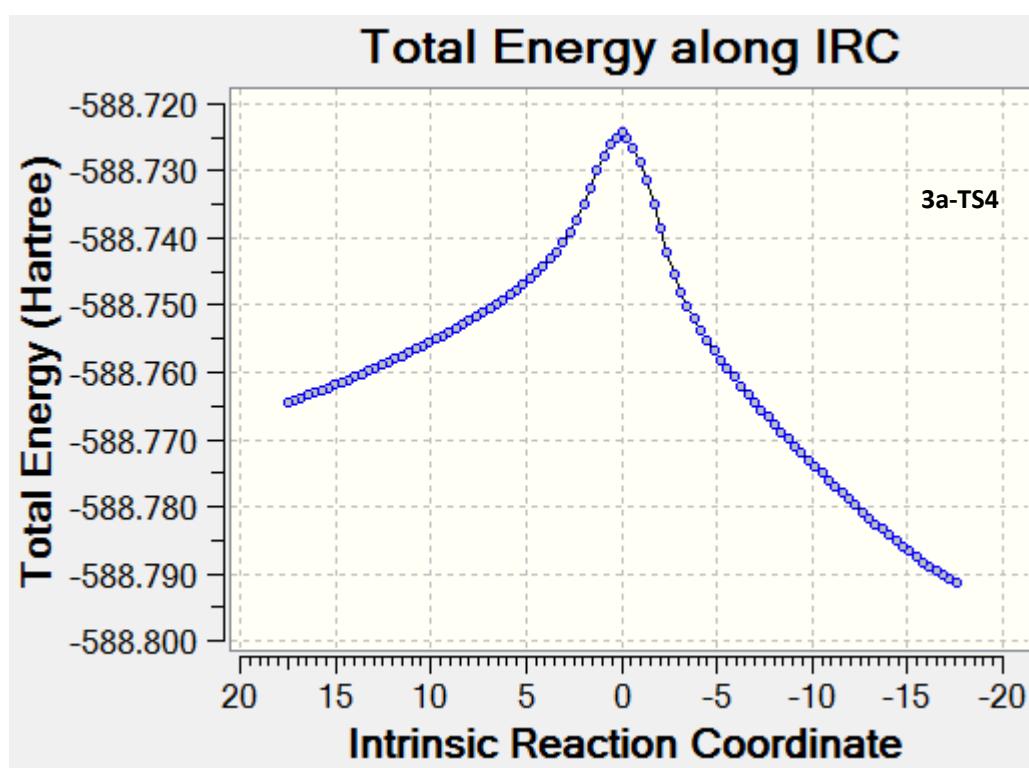
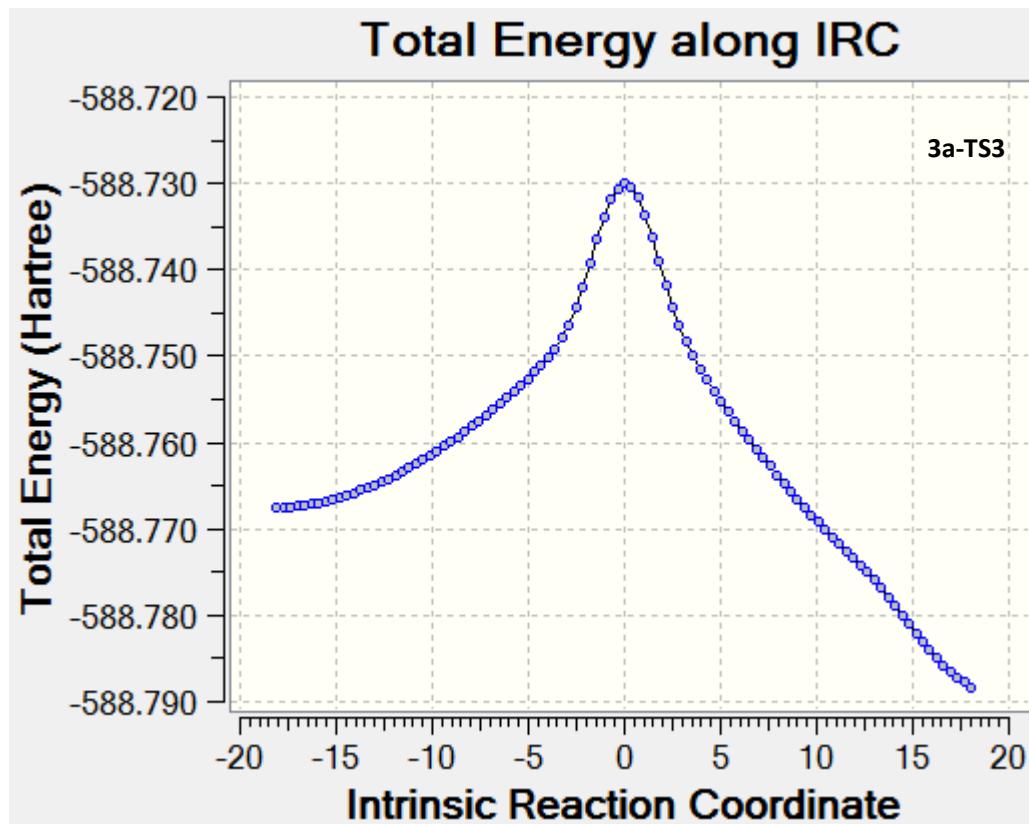
N	-1.94401100	0.49721700	0.38964000
N	0.88859900	2.47013400	2.89333300
C	-0.86939100	1.14944400	1.22972800
C	0.51275900	0.89938600	1.06956100
N	-1.33527900	1.98386300	2.13815300
C	1.38260100	1.60804500	1.95585000
C	-0.41858200	2.61021500	2.93463100
H	-0.82607000	3.29194500	3.67433600
C	2.77898100	1.39517900	1.83926500
H	3.43980000	1.93115500	2.50951400
C	3.27835300	0.52673900	0.89476800
H	4.34856900	0.37520800	0.81853400
C	2.41527000	-0.16818500	0.02490000
H	2.81729400	-0.84930500	-0.71515100
C	1.06444200	0.01631000	0.11280200
H	0.45369500	-0.53036500	-0.56769200
N	-1.66394300	-0.30466800	-0.49755700
C	-0.66338100	-3.06021500	-3.54226600
H	-0.42029700	-3.76772700	-4.32518300
C	-0.89422500	-3.48350900	-2.23233400
H	-0.82832100	-4.53695300	-1.98157600
C	-1.21094600	-2.58728900	-1.21000900
H	-1.38181000	-2.95095000	-0.20483300
C	-1.32657800	-1.19340300	-1.47836500
C	-1.06427600	-0.76505200	-2.81104800
H	-1.12147200	0.28885000	-3.05182100
C	-0.75010400	-1.69228600	-3.80621200
H	-0.56935400	-1.31920900	-4.80875200

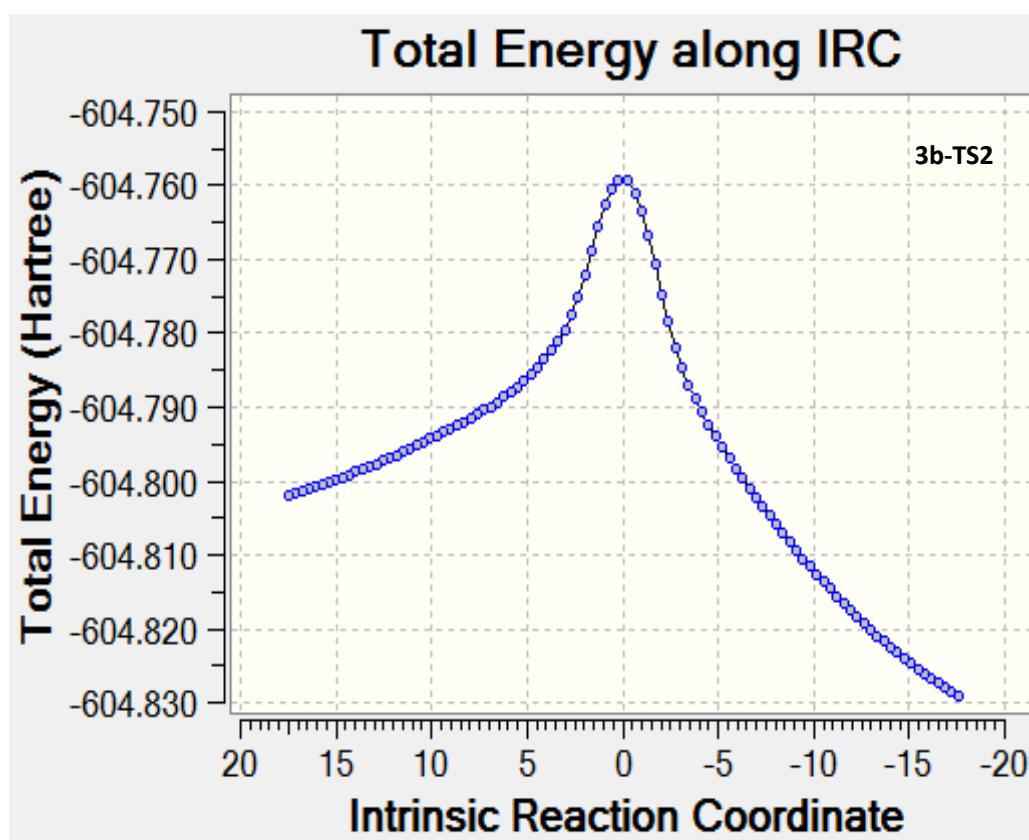
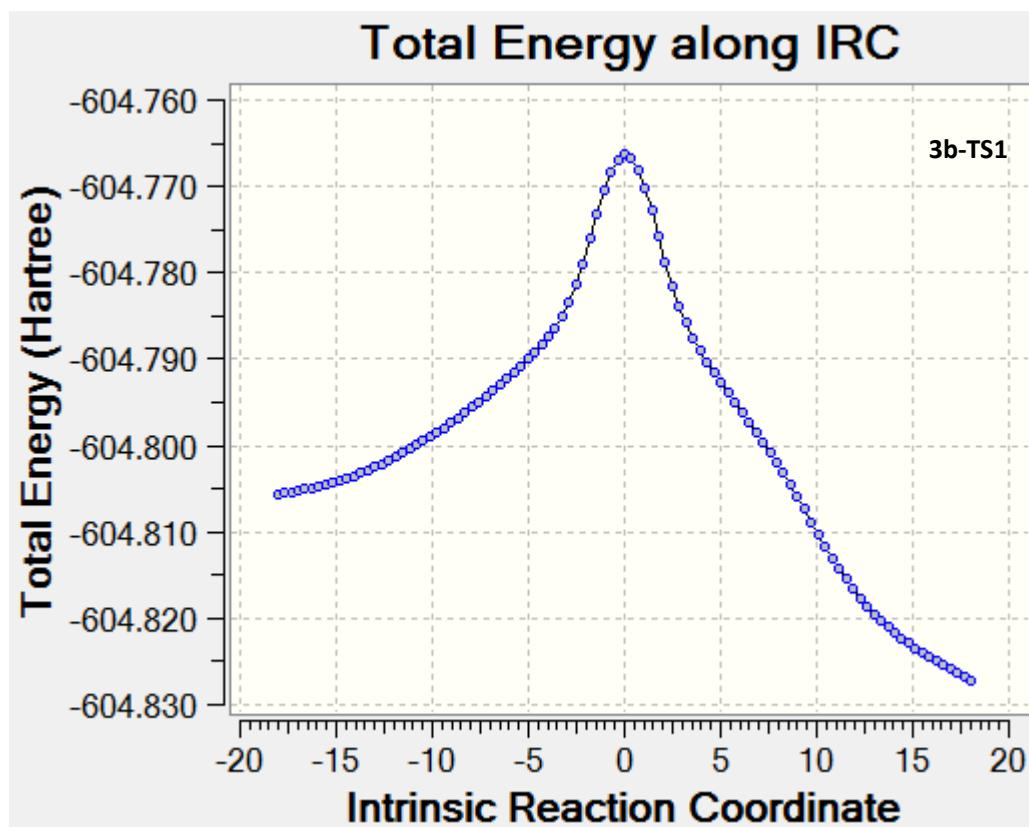
Table S107 Cartesian coordinates of compound **8-TS4**

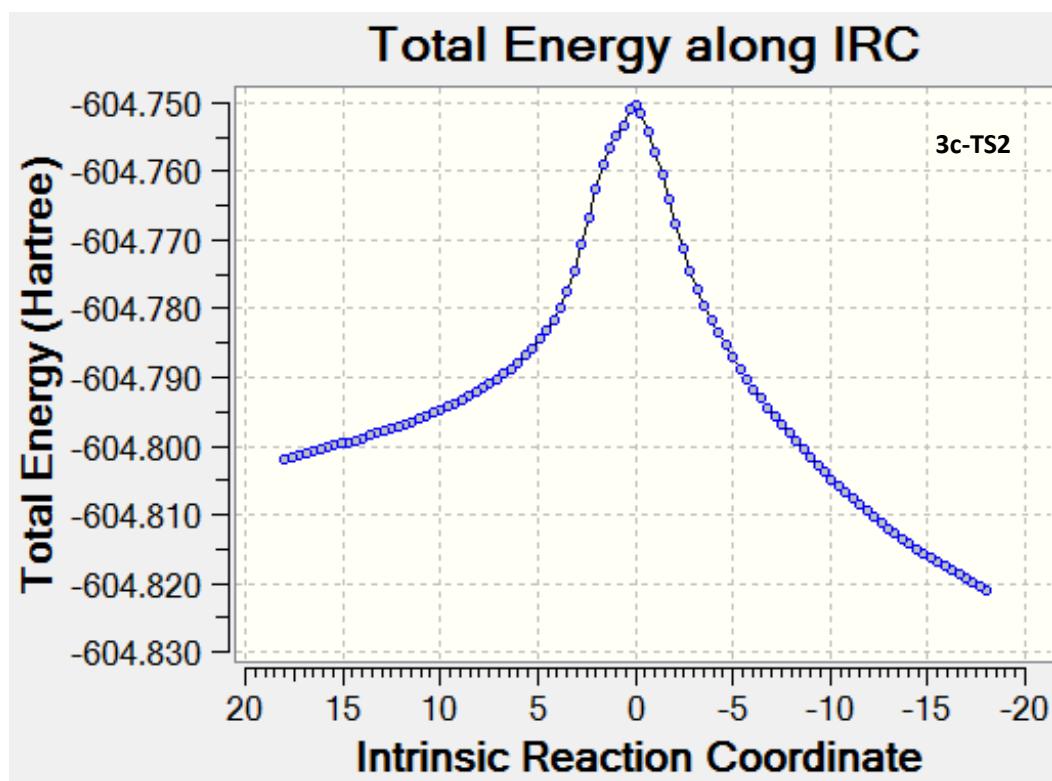
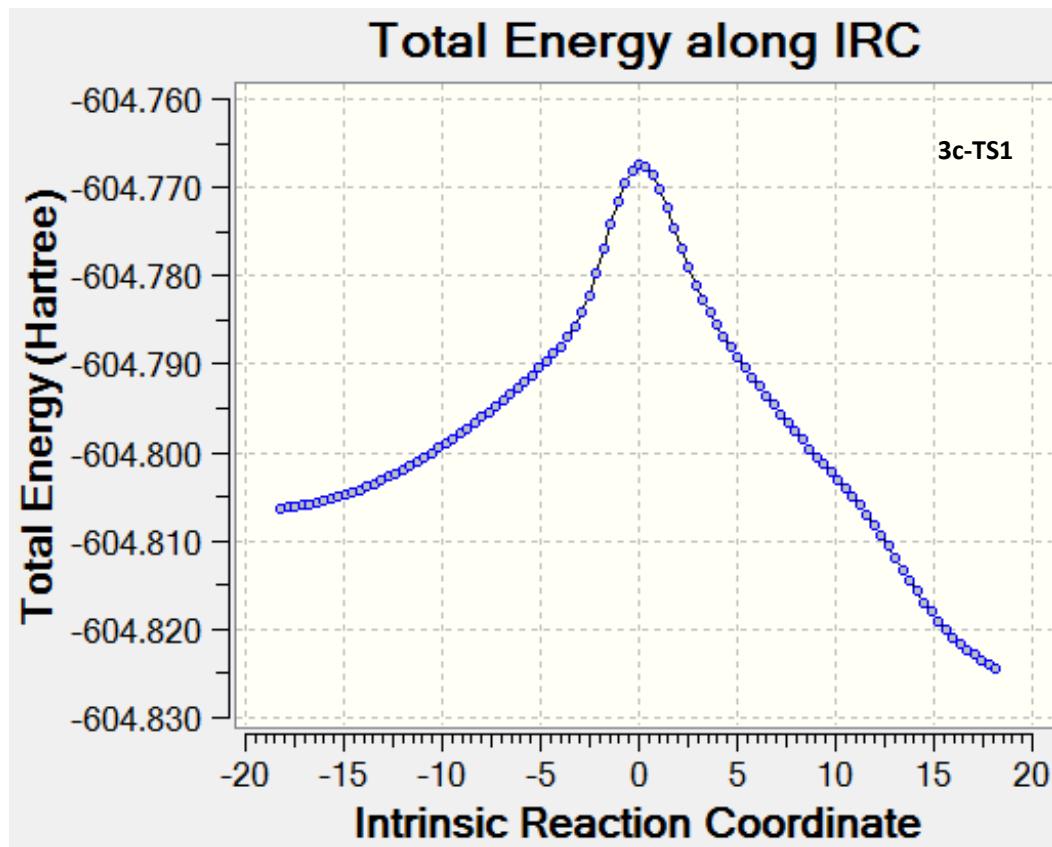
C	-0.76416900	-0.34711800	-0.00008100
N	0.46195500	0.37236900	0.00103500
C	-2.01017100	0.39593500	-0.00059800
C	-3.23341700	-0.35375800	-0.00020900
N	-3.22402200	-1.72920900	-0.00006100
C	-2.03710400	-2.32233400	0.00028600
H	-2.01975700	-3.41188000	0.00053300
N	-0.81463800	-1.70008200	0.00103100
C	-4.45997700	0.38546200	0.00002200
H	-5.38861800	-0.17671800	-0.00003800
C	-4.46613000	1.76784100	-0.00004700
H	-5.41131700	2.30437500	-0.00002500
C	-3.24869300	2.49023500	0.00002500
H	-3.26067700	3.57653800	0.00036700
C	-2.05014000	1.81147700	-0.00004900
H	-1.10163300	2.33850200	0.00041800
N	1.54026000	1.07918500	-0.00315000
C	5.24971100	-0.96870600	-0.00065000
H	6.19386300	-1.50684900	-0.00074400
C	5.23516100	0.41971900	-0.16851000
H	6.16853600	0.95993800	-0.30128500
C	4.02142100	1.11525400	-0.16611800
H	3.99299700	2.19349300	-0.29741100
C	2.81433700	0.39546400	-0.00137400
C	2.84515900	-0.98608800	0.16977800
H	1.89536800	-1.50091900	0.28872700
C	4.04959700	-1.66616600	0.16948900
H	4.06054700	-2.74455600	0.30198900

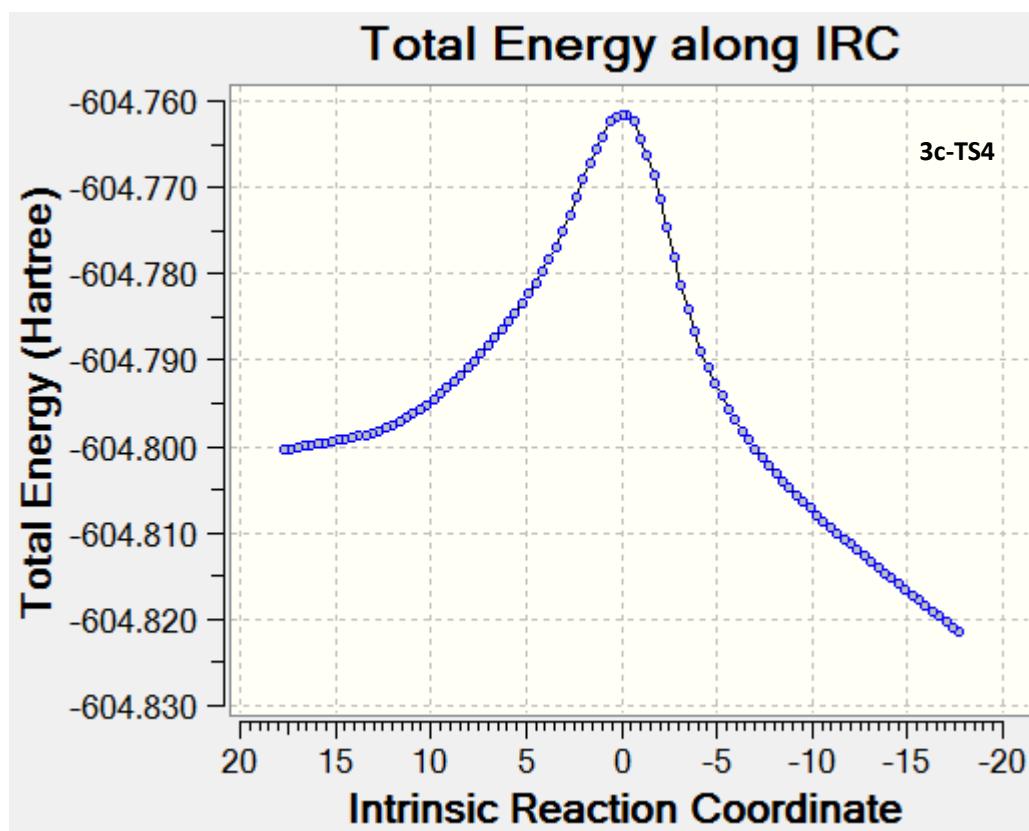
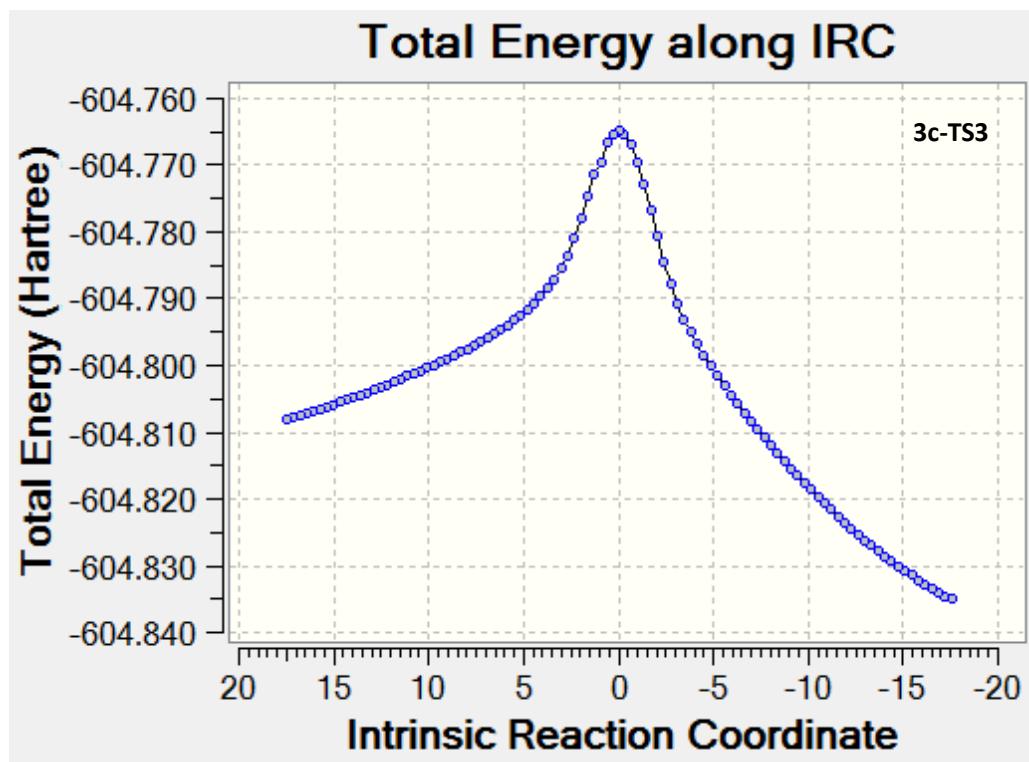
8. IRC figures

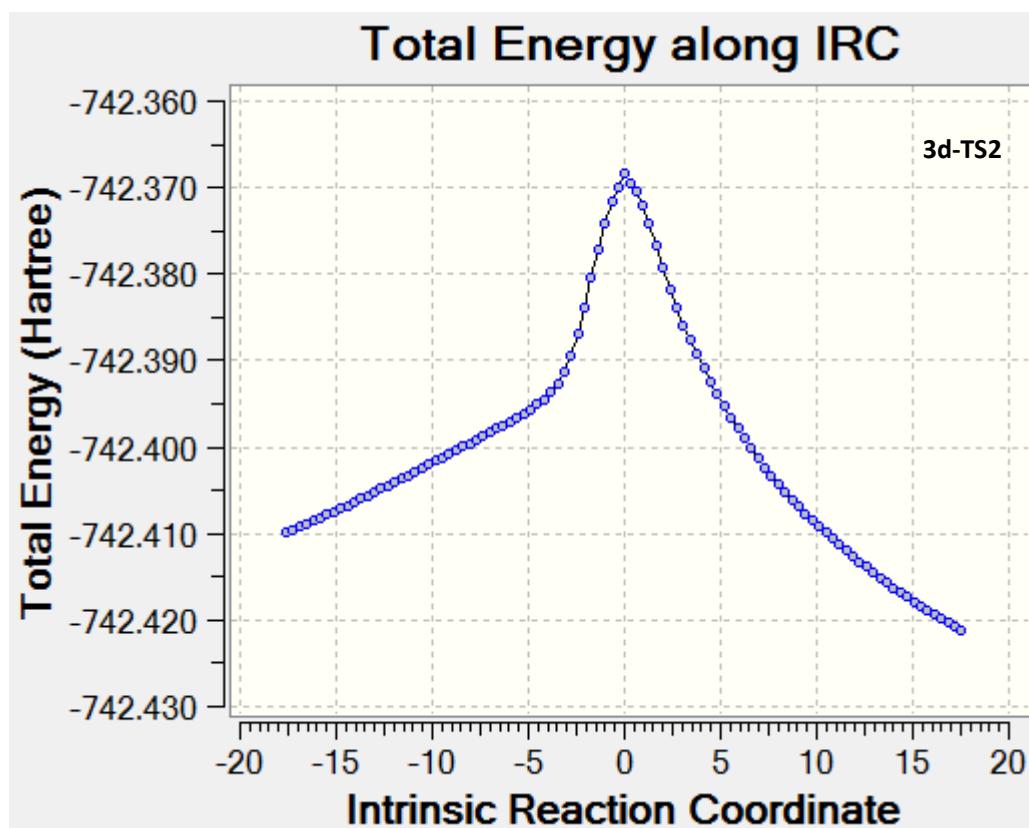
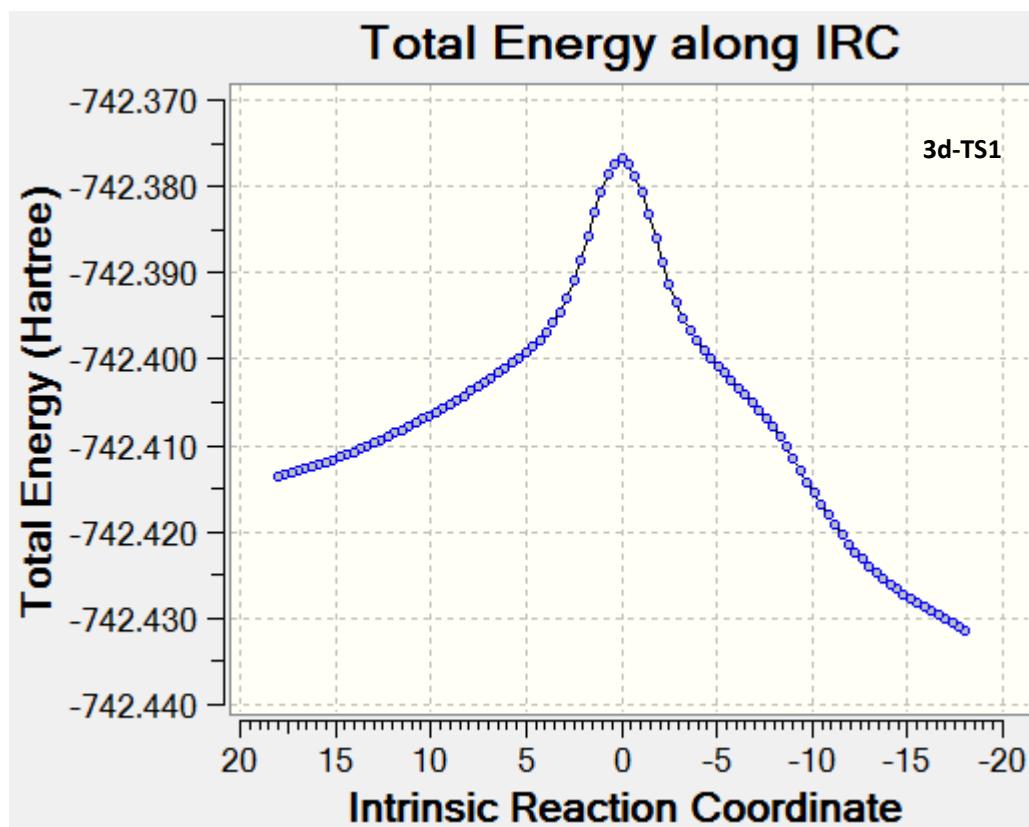


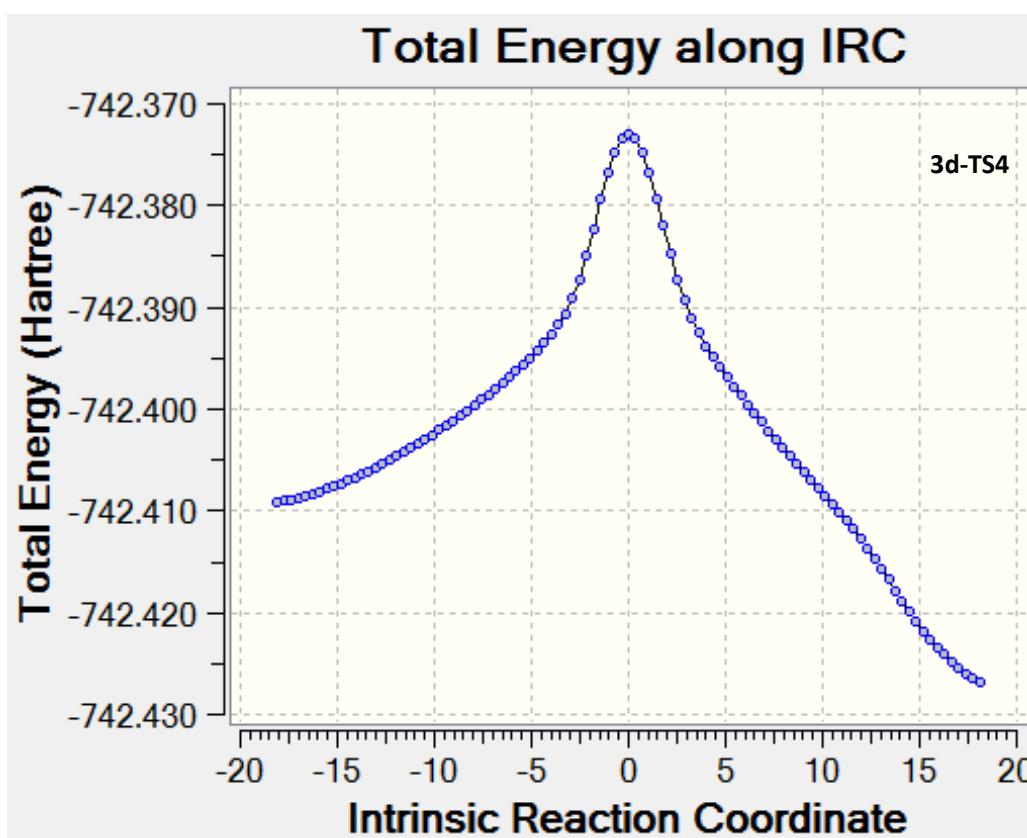
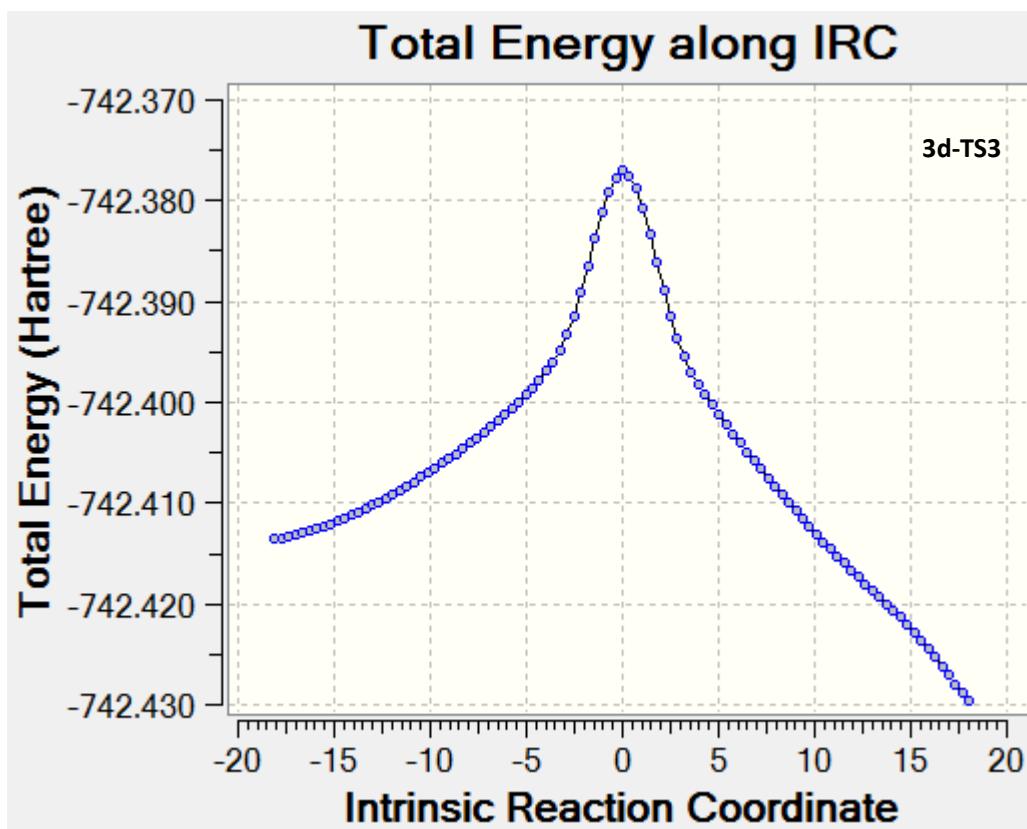


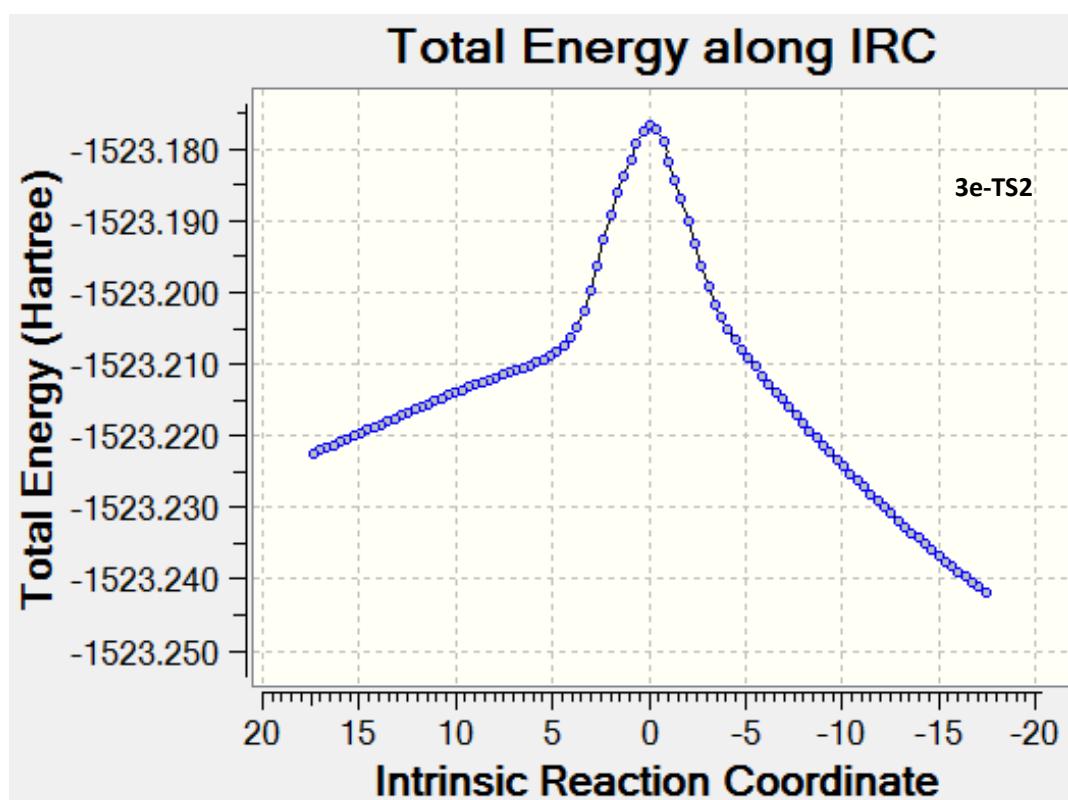
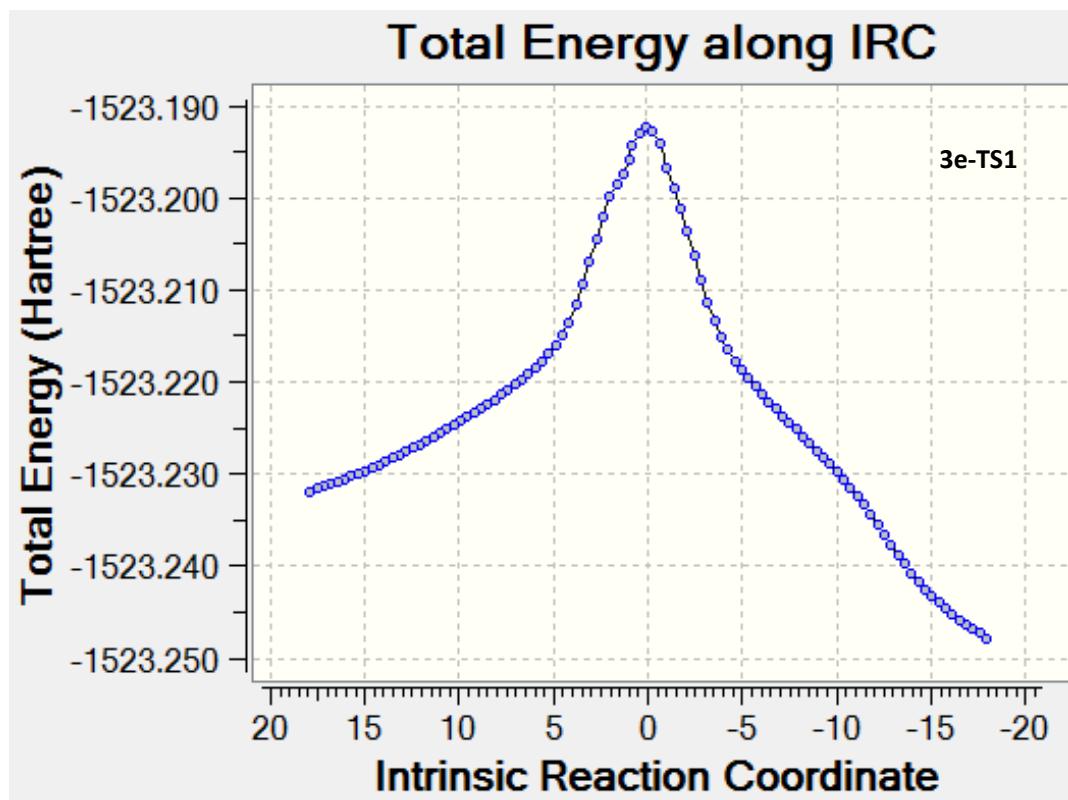


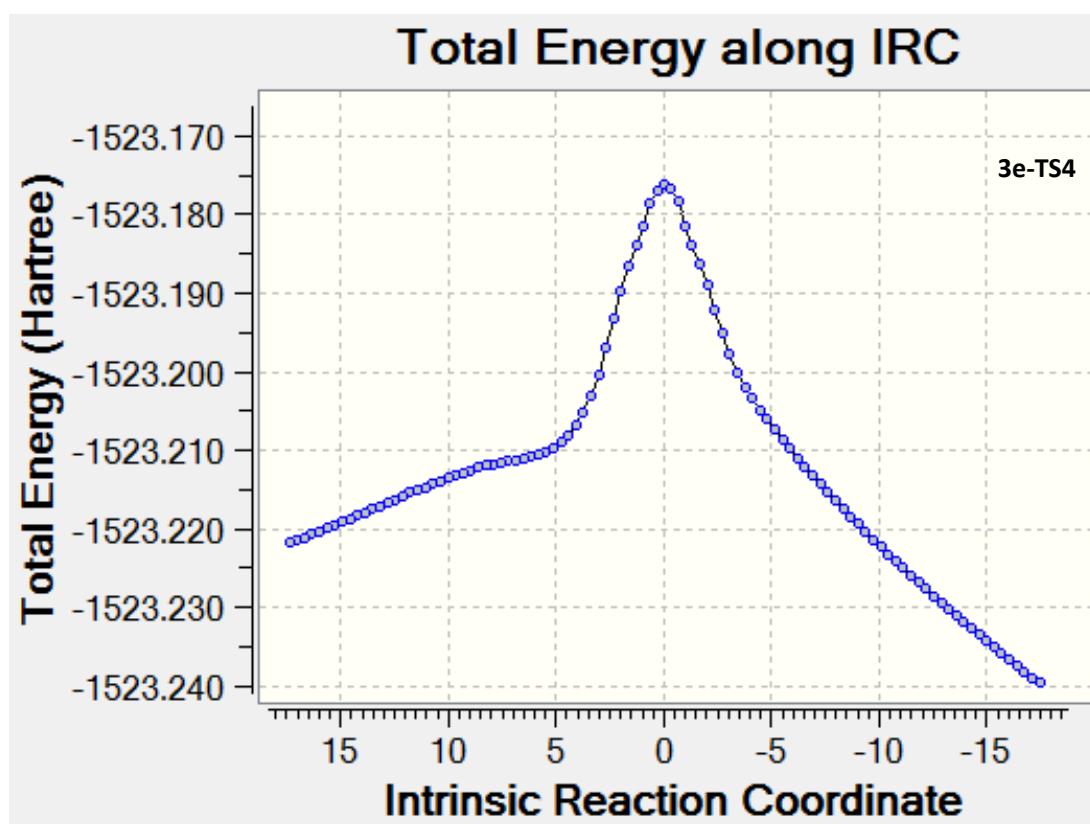
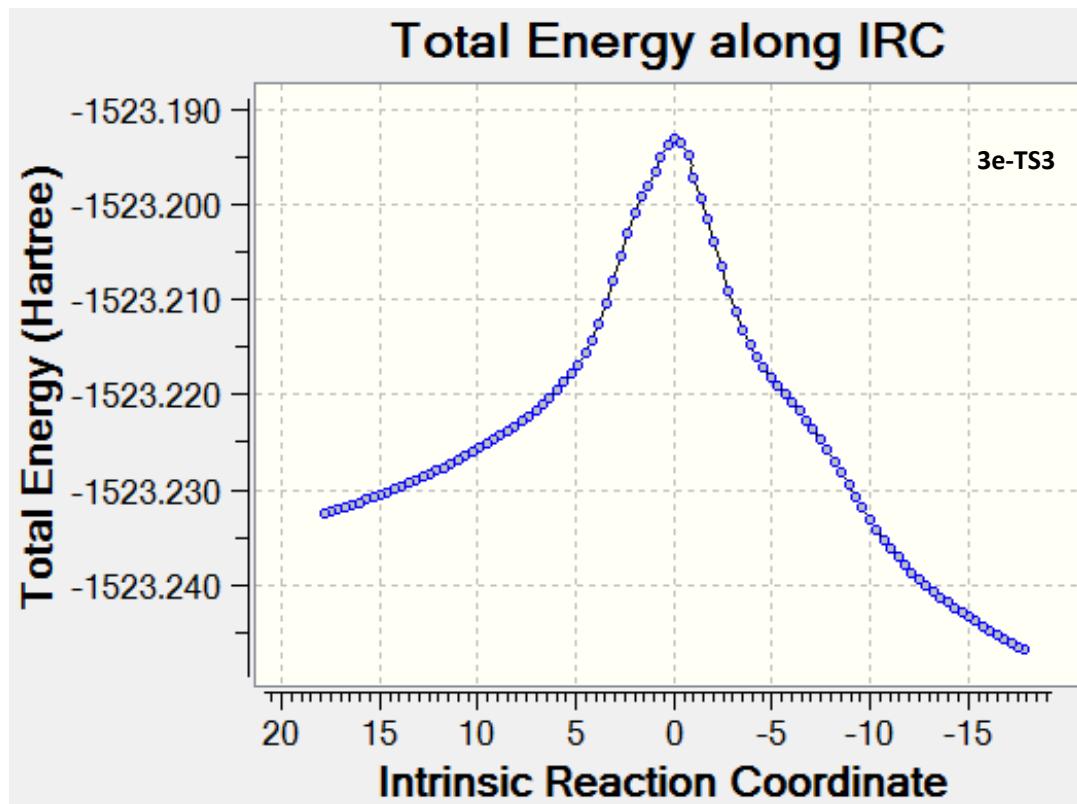


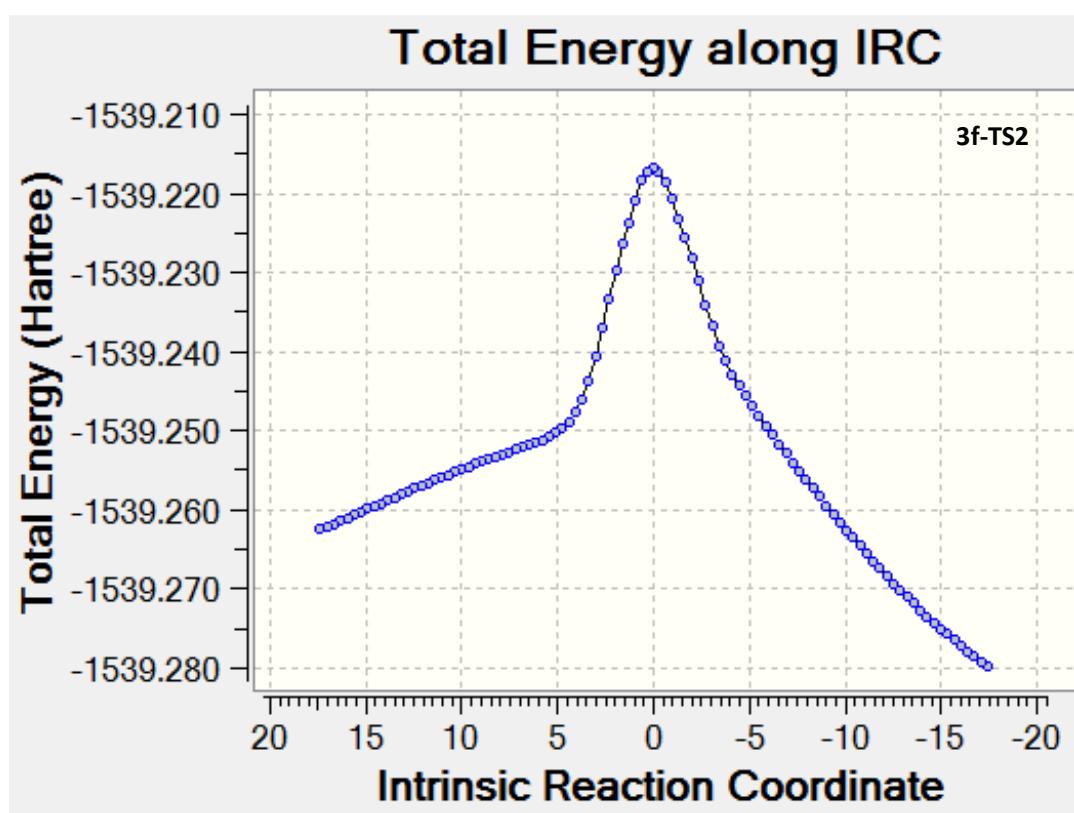
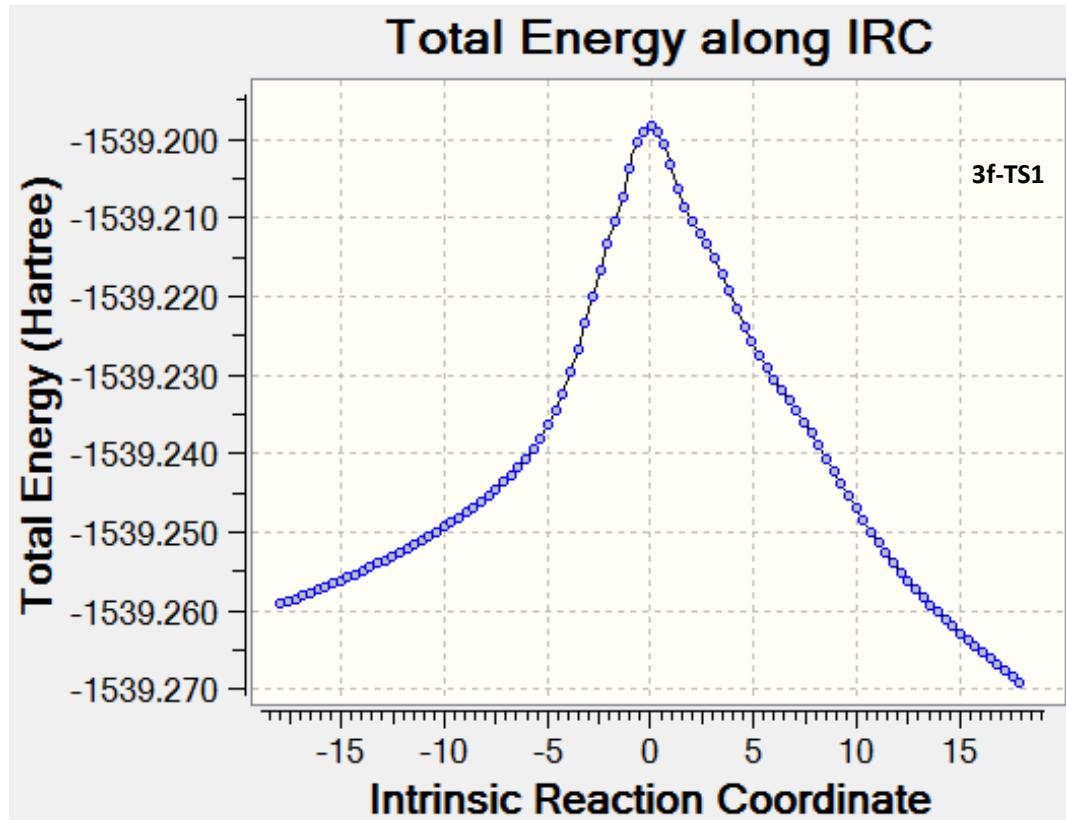


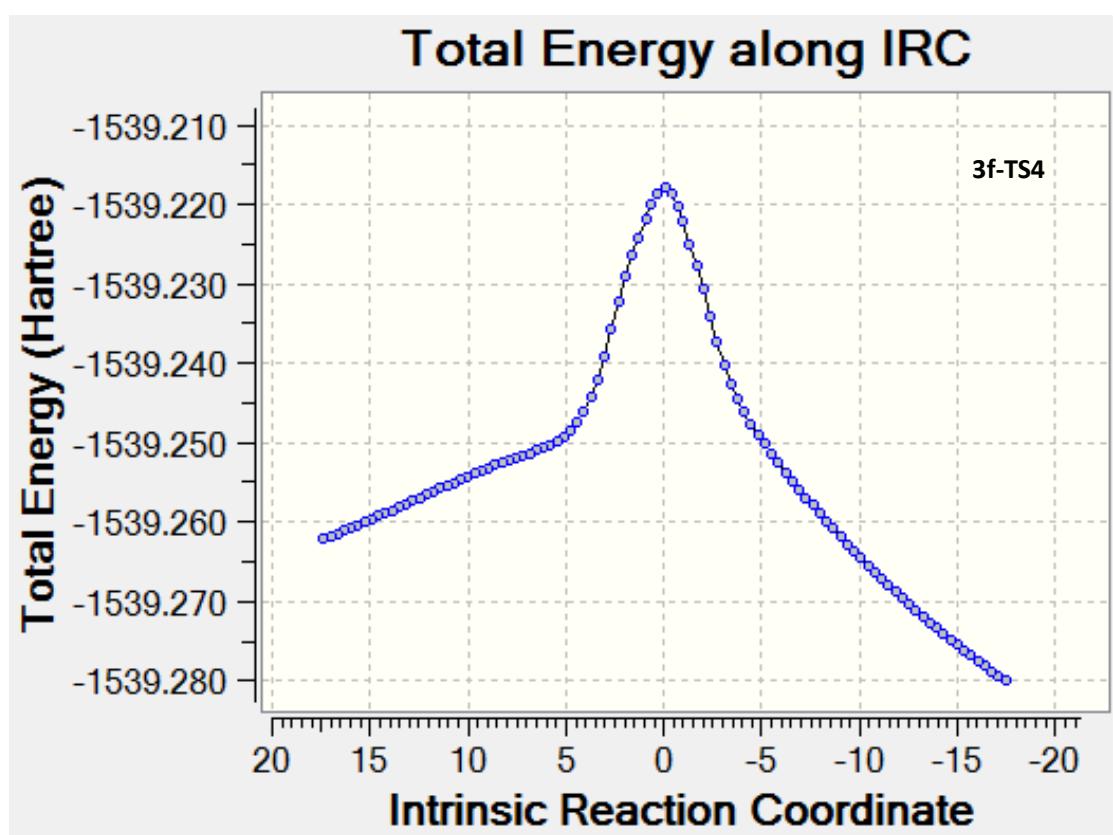
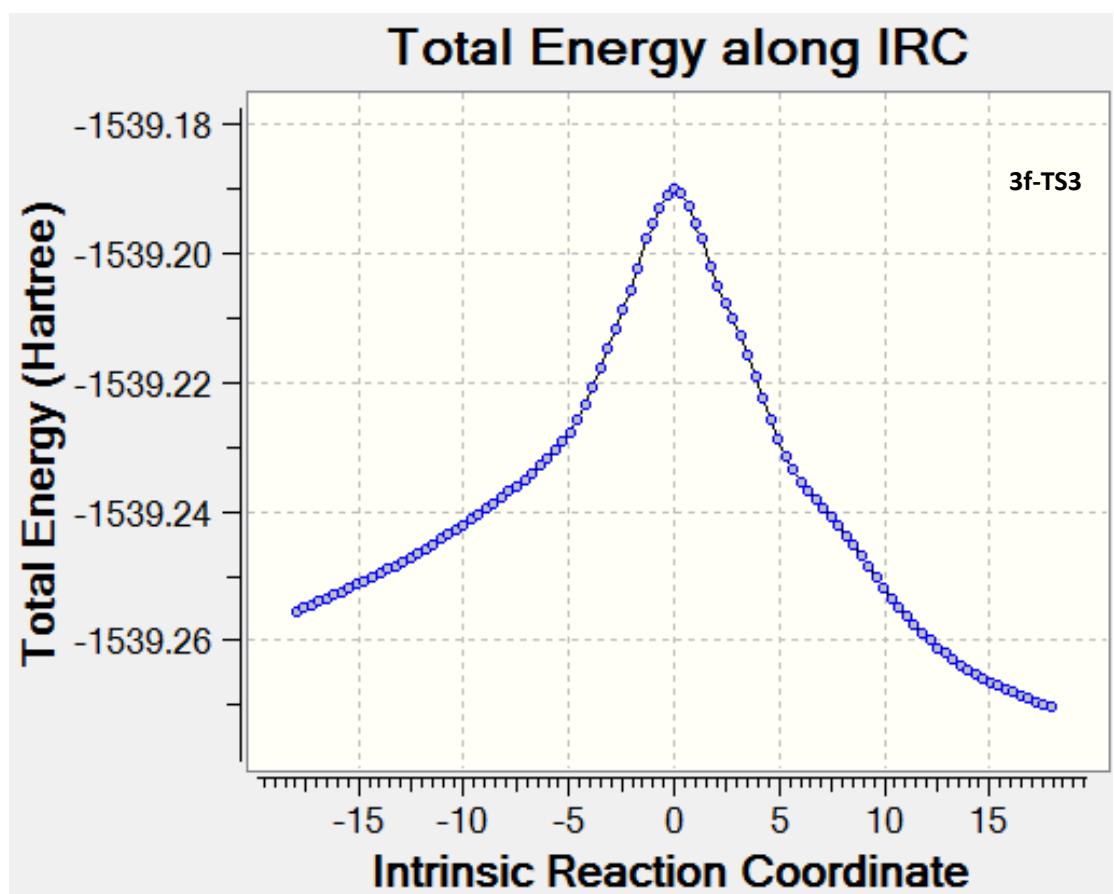


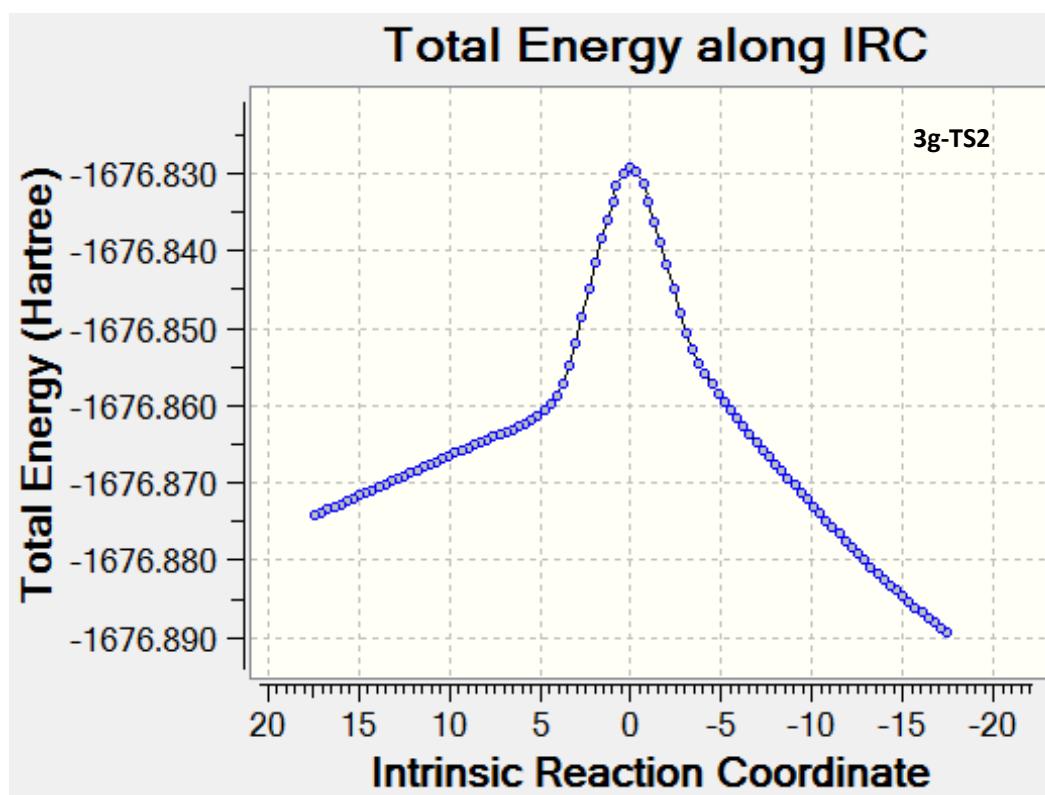
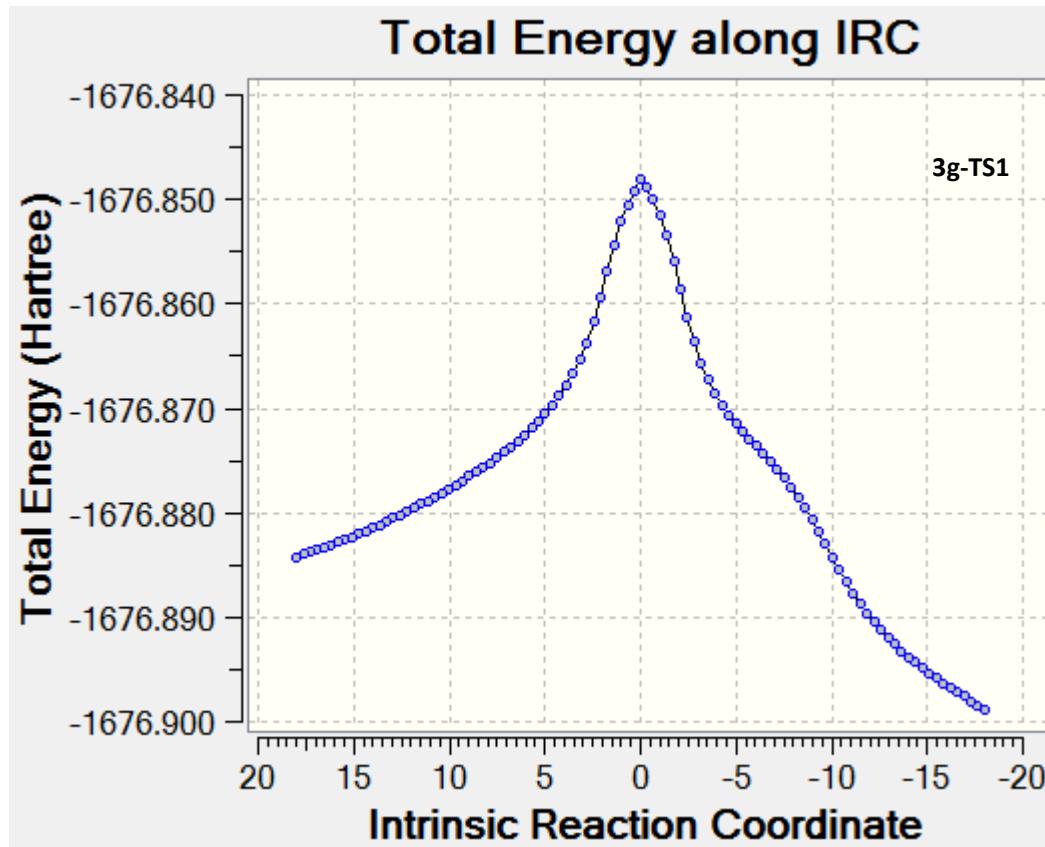


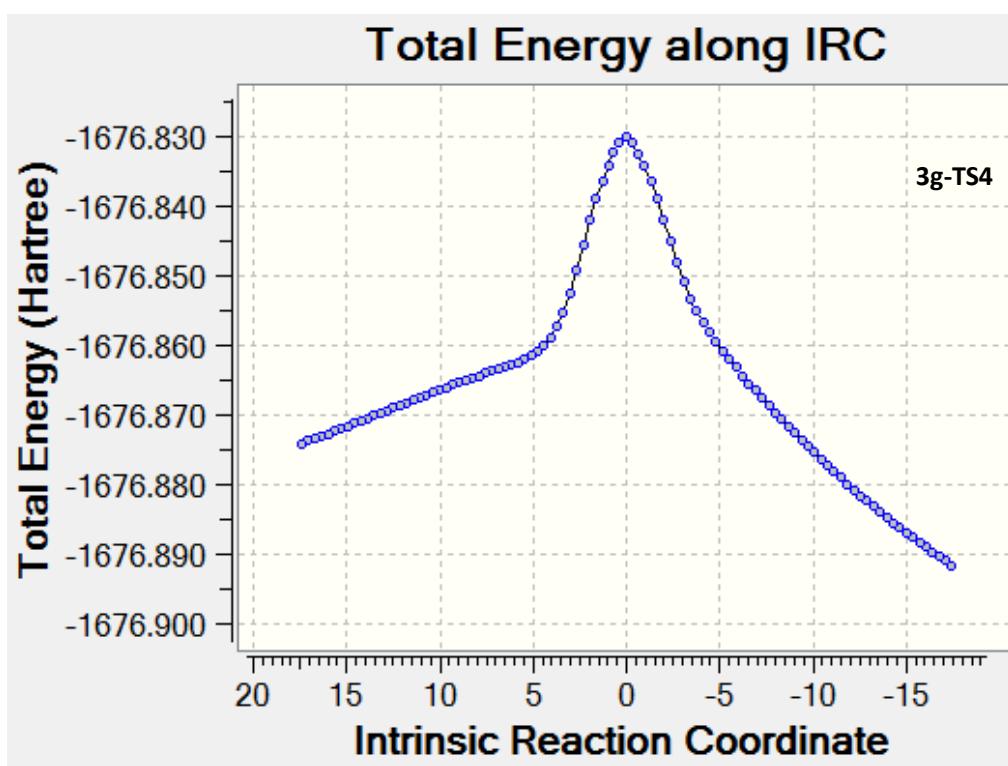
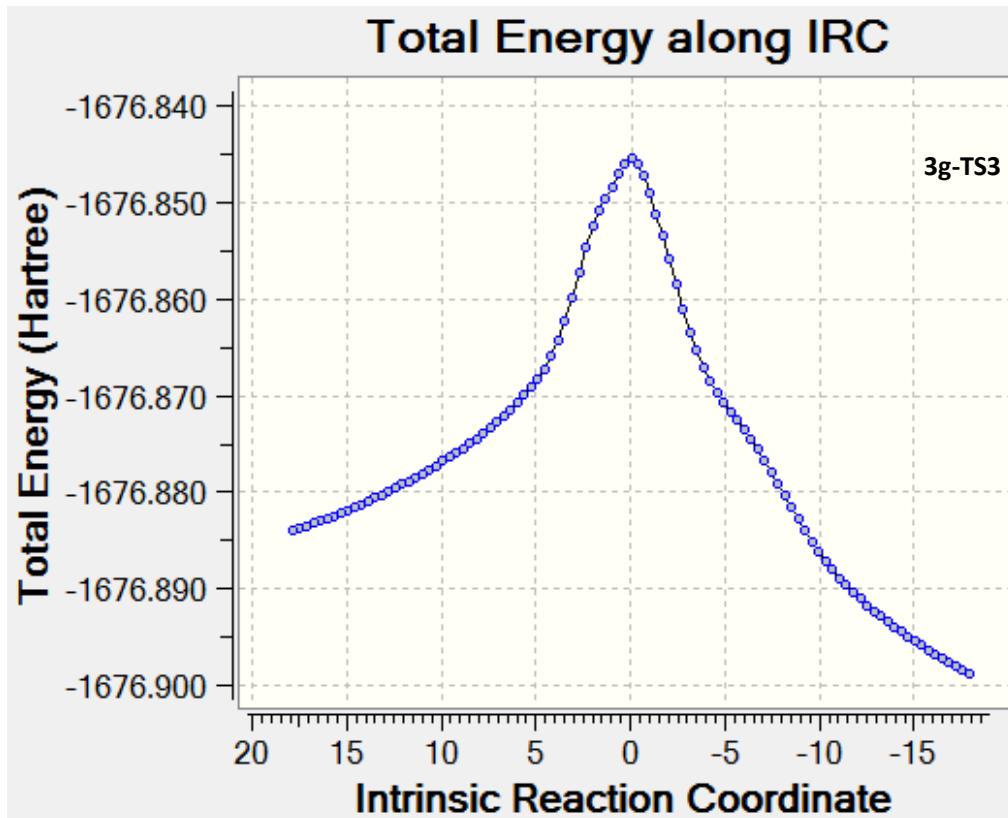


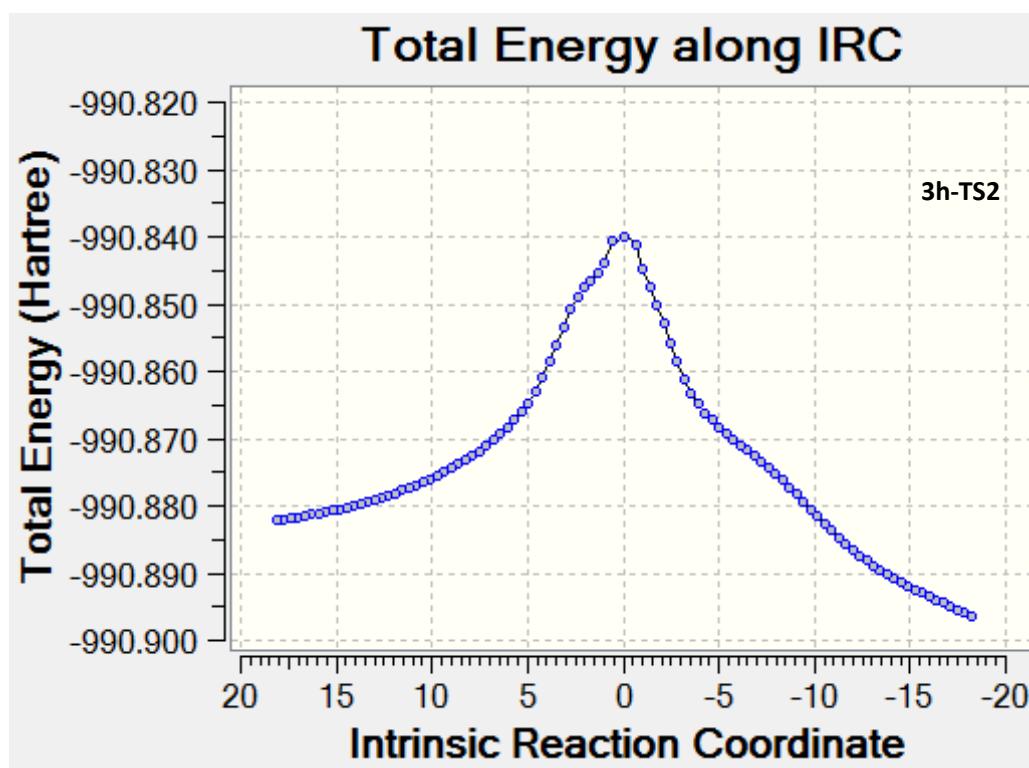
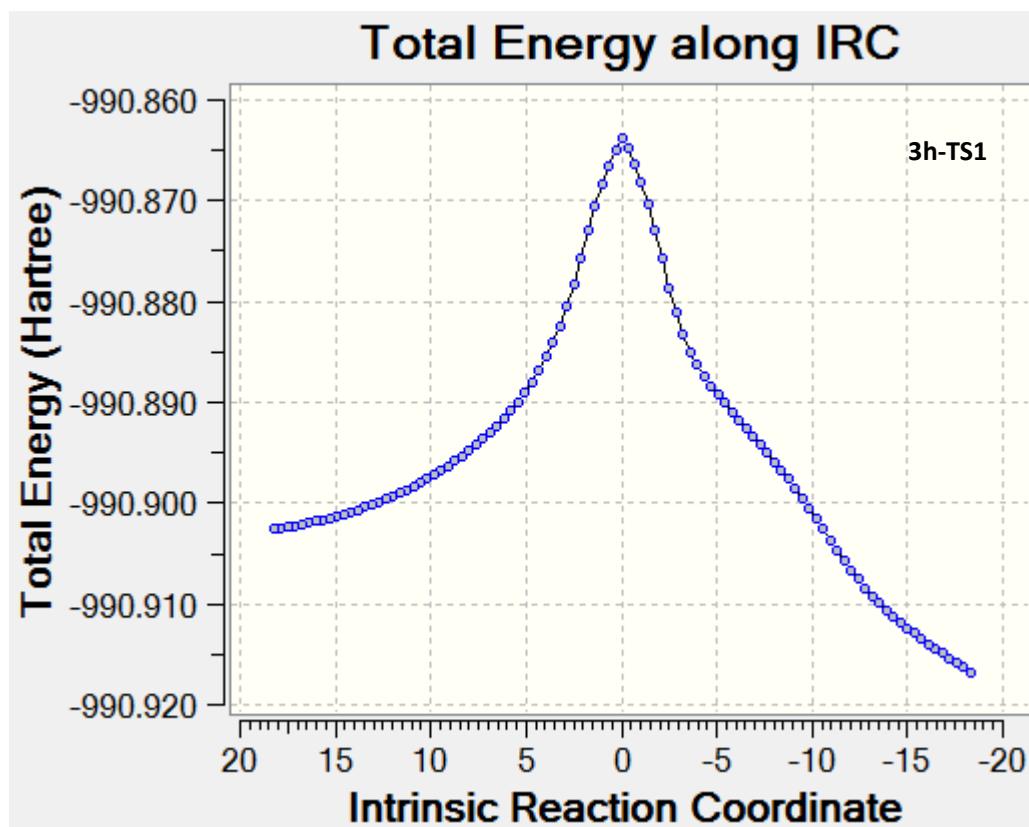


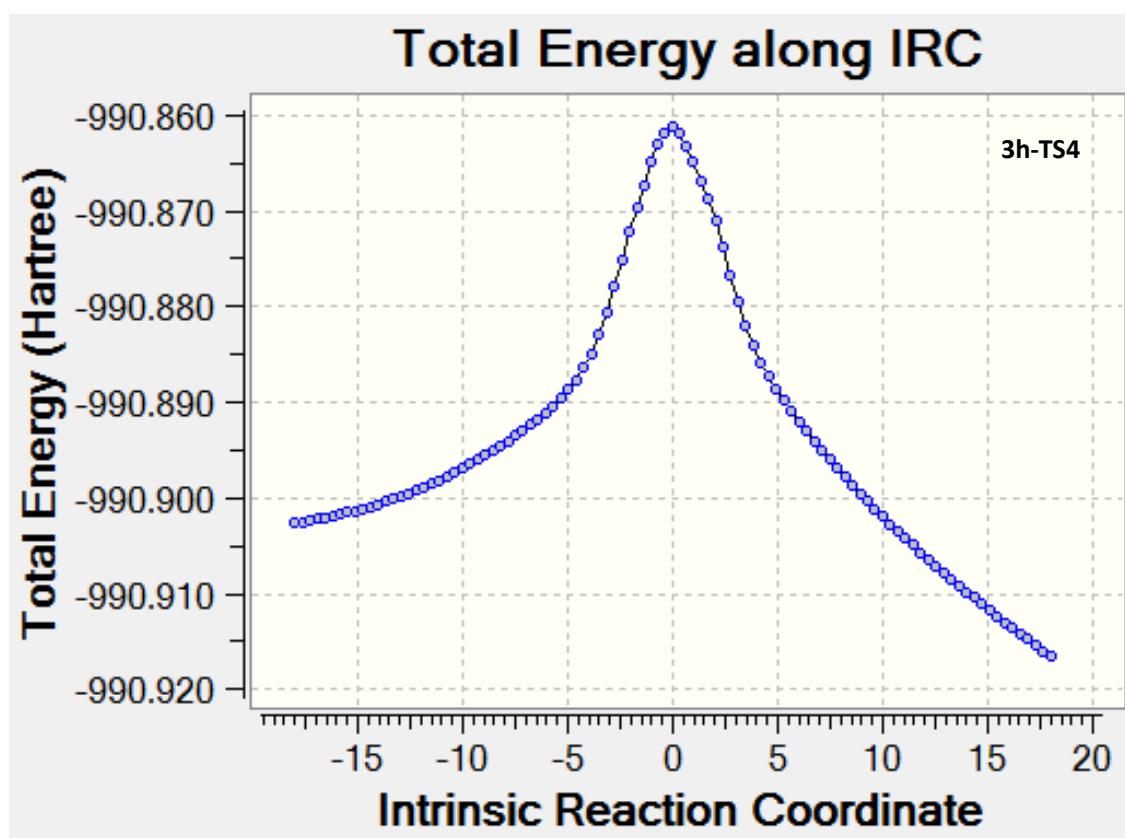
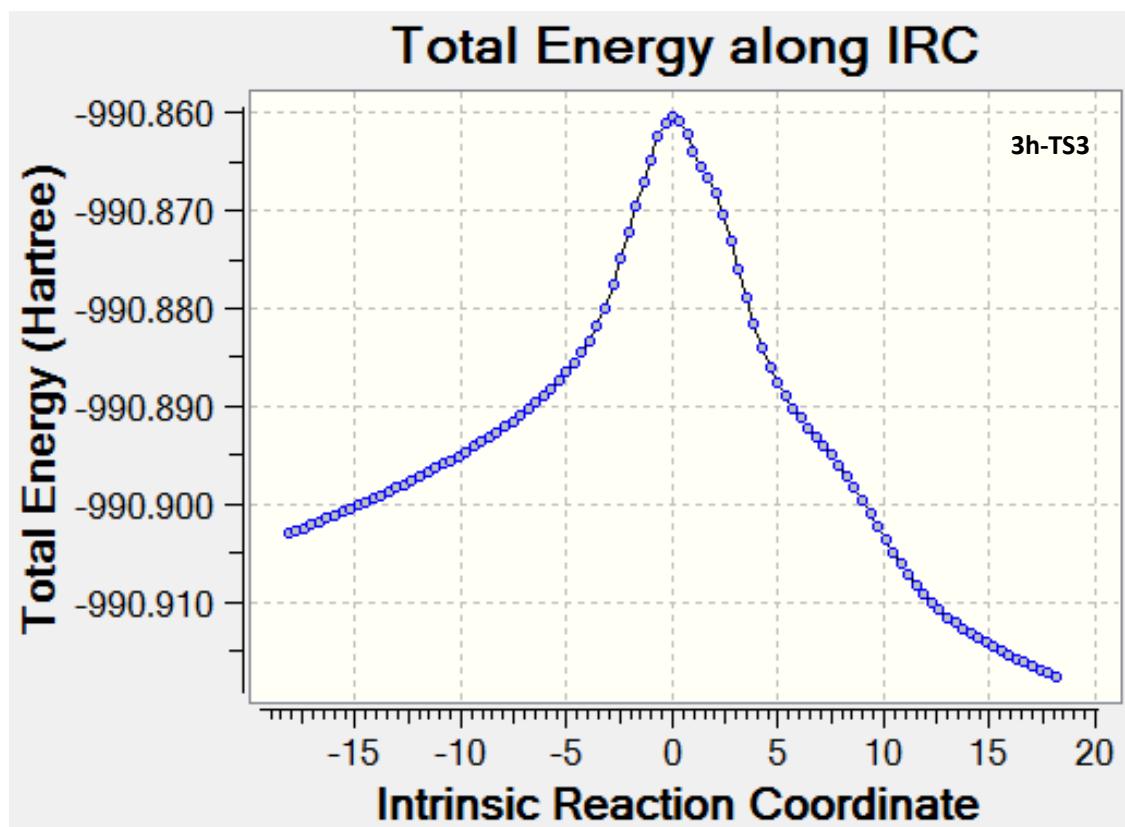


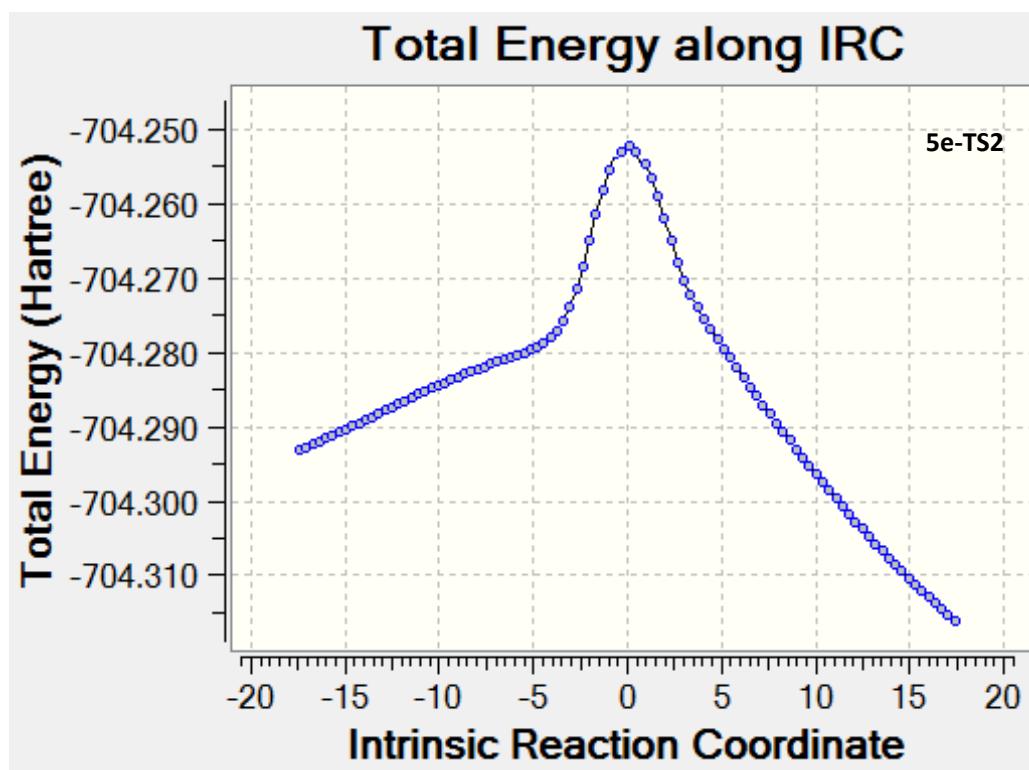
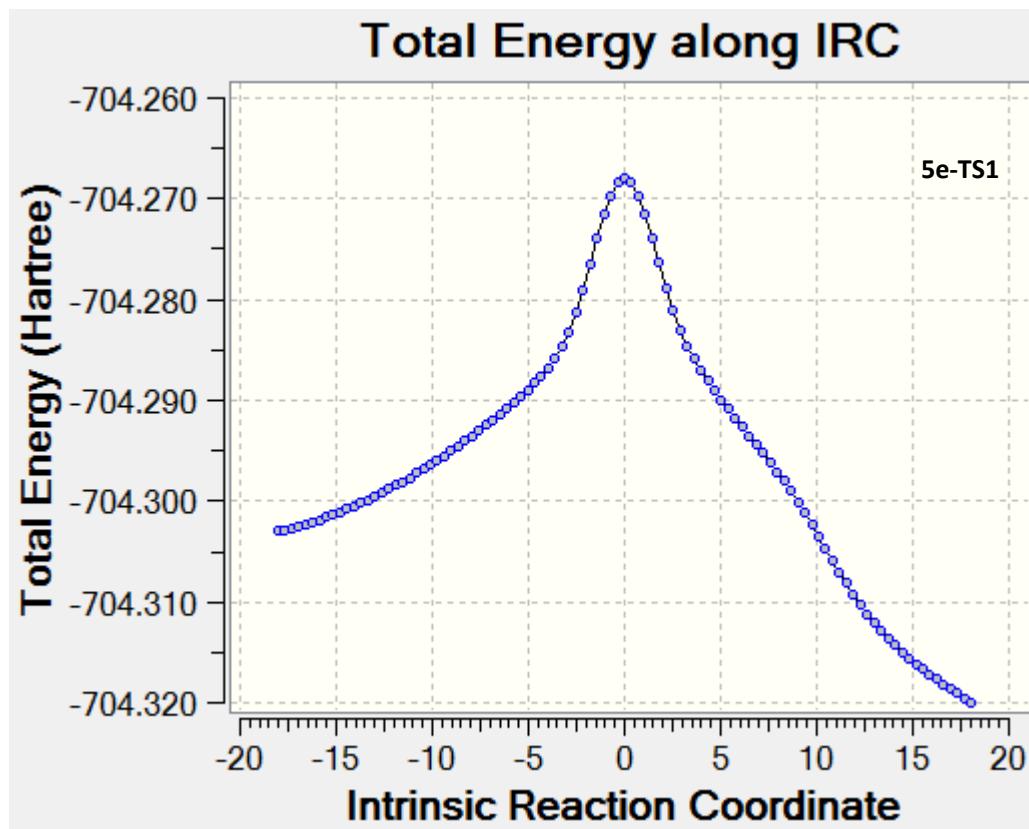


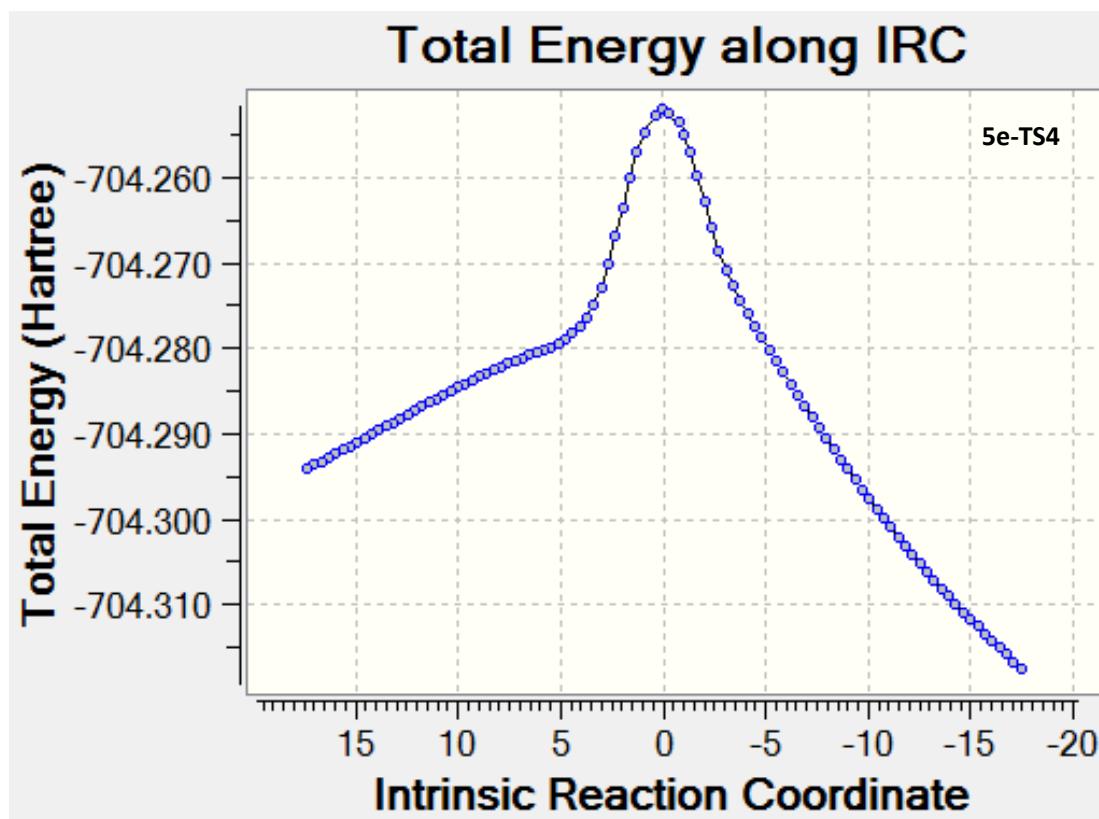
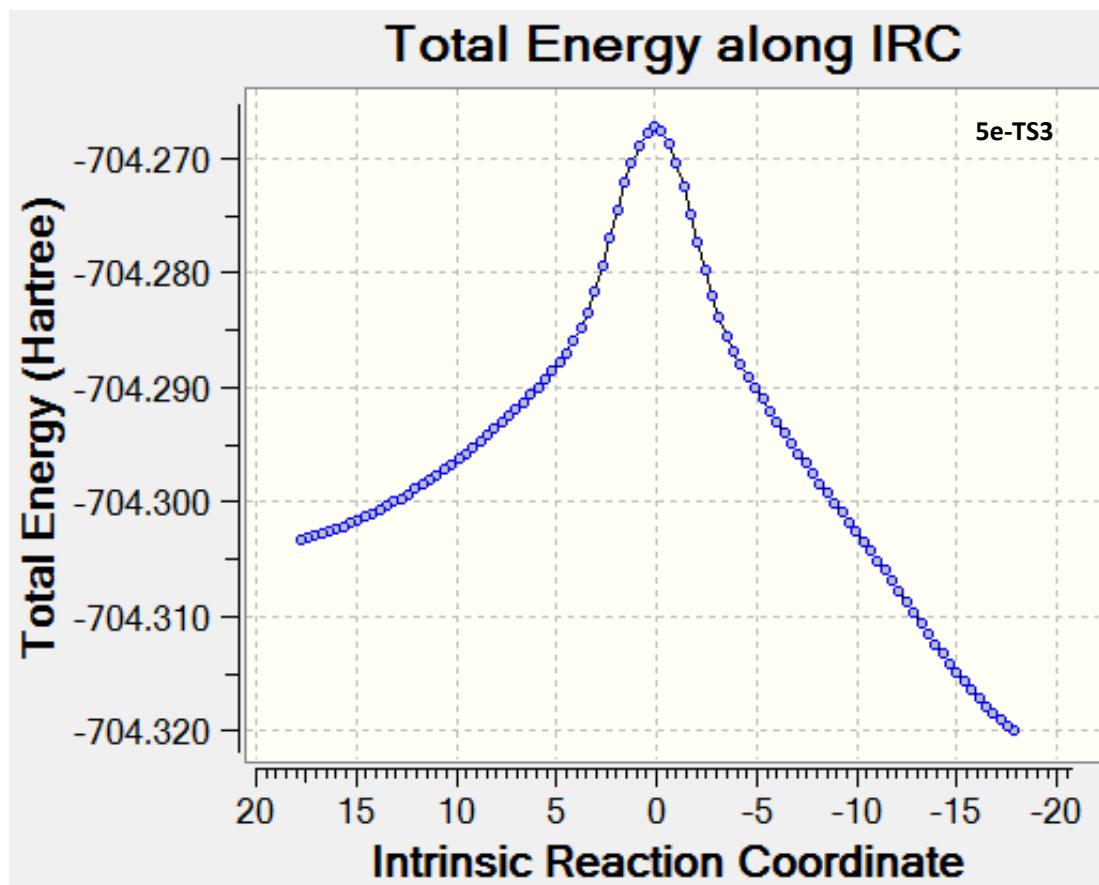


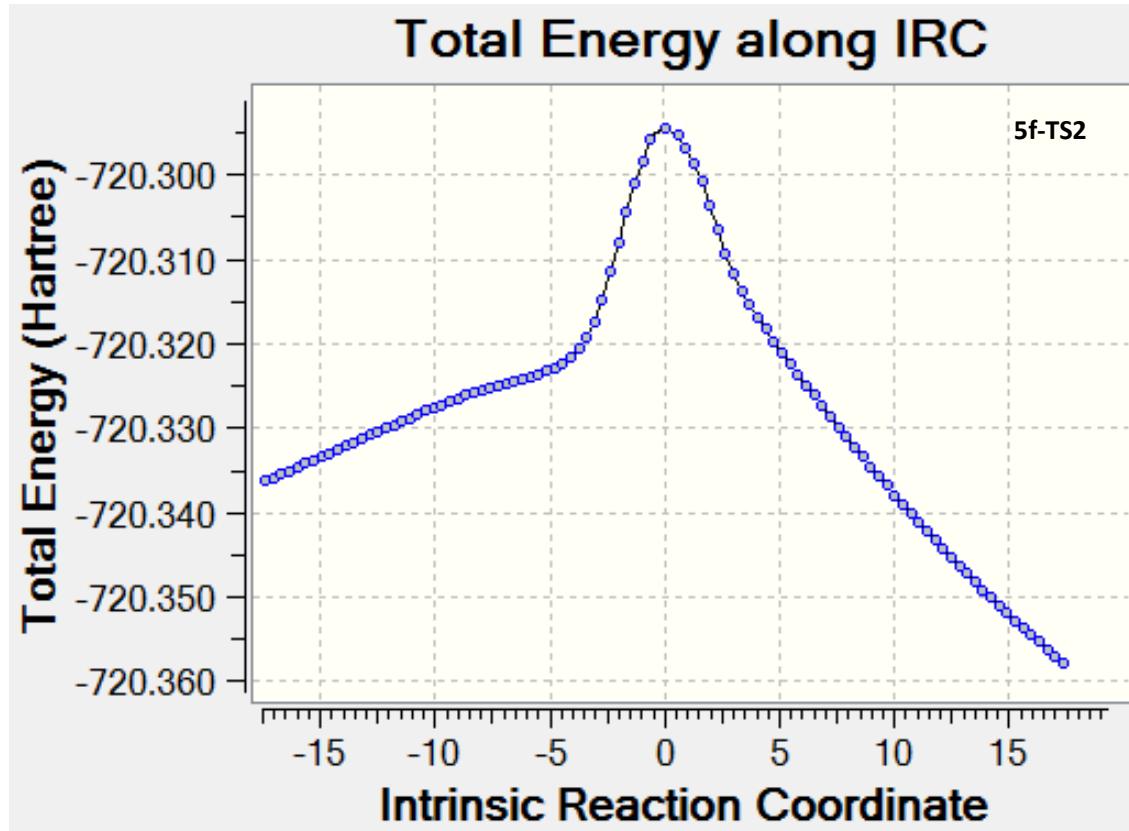
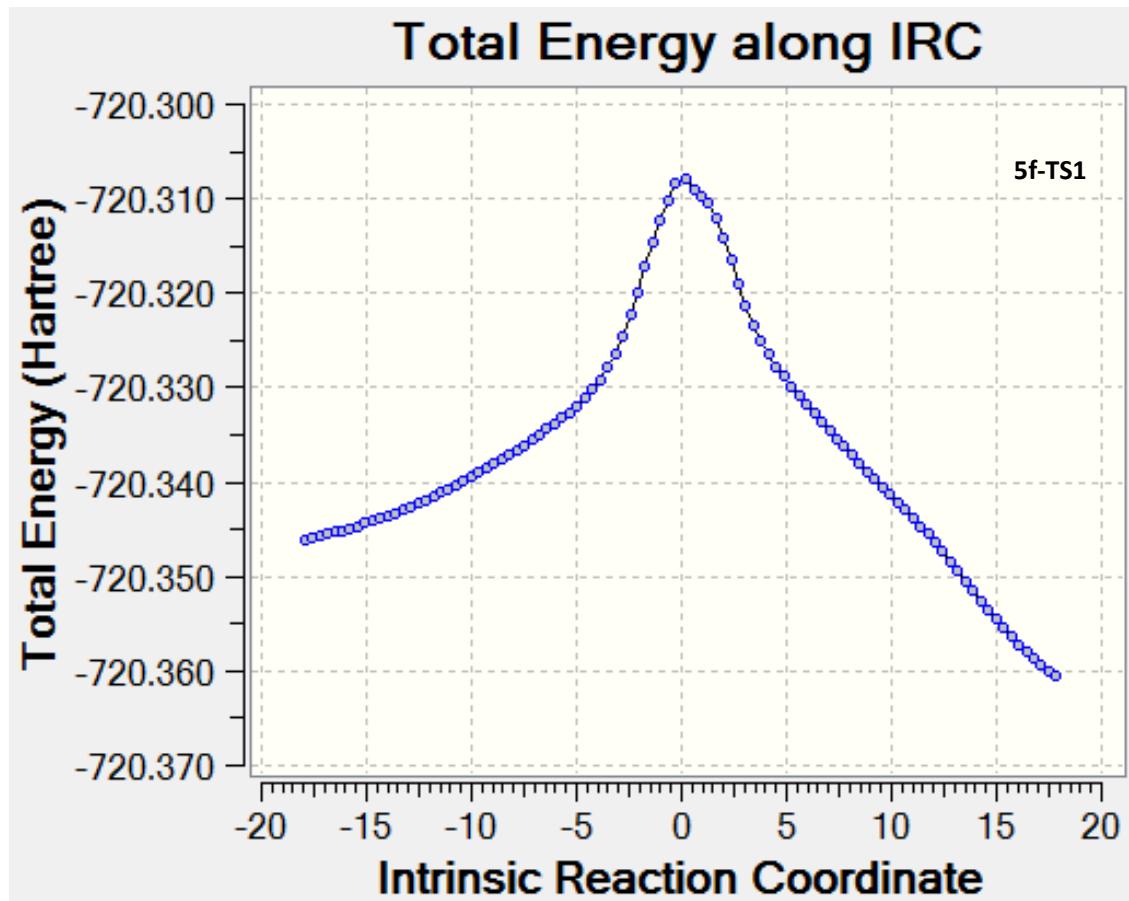


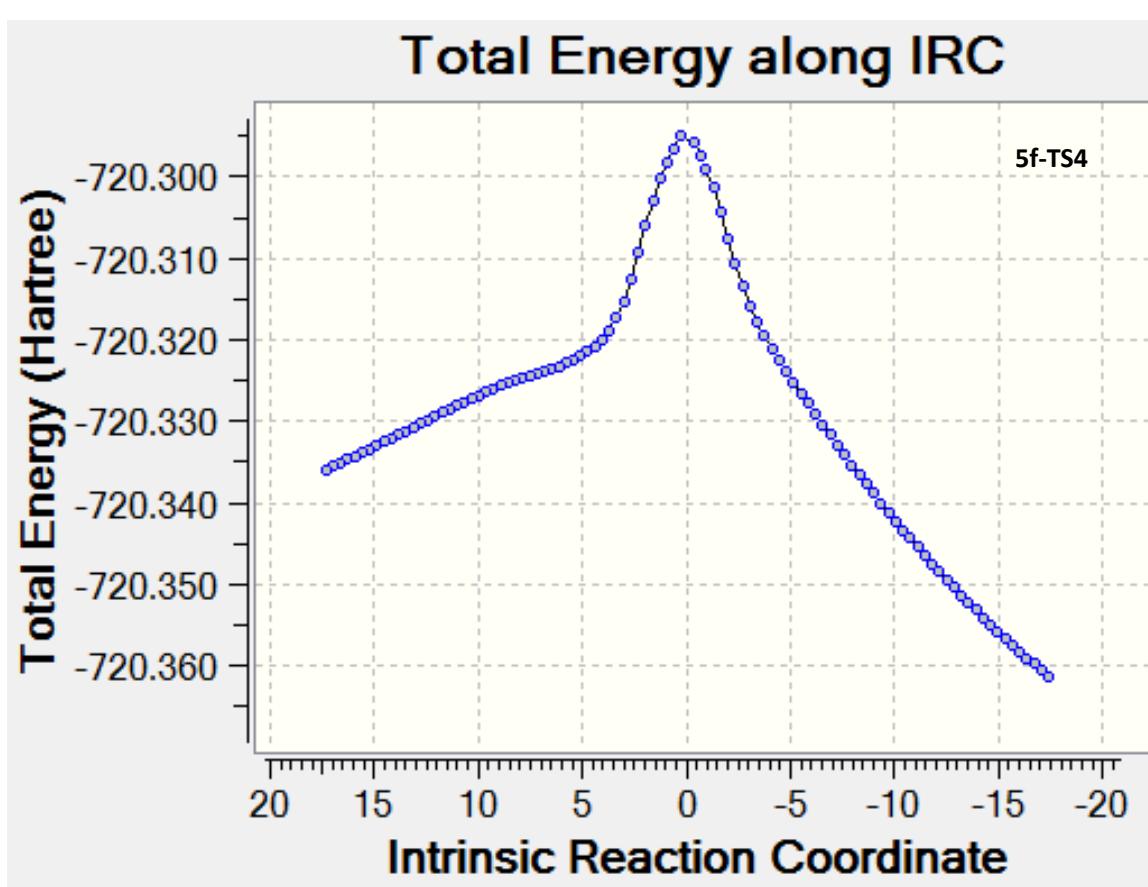
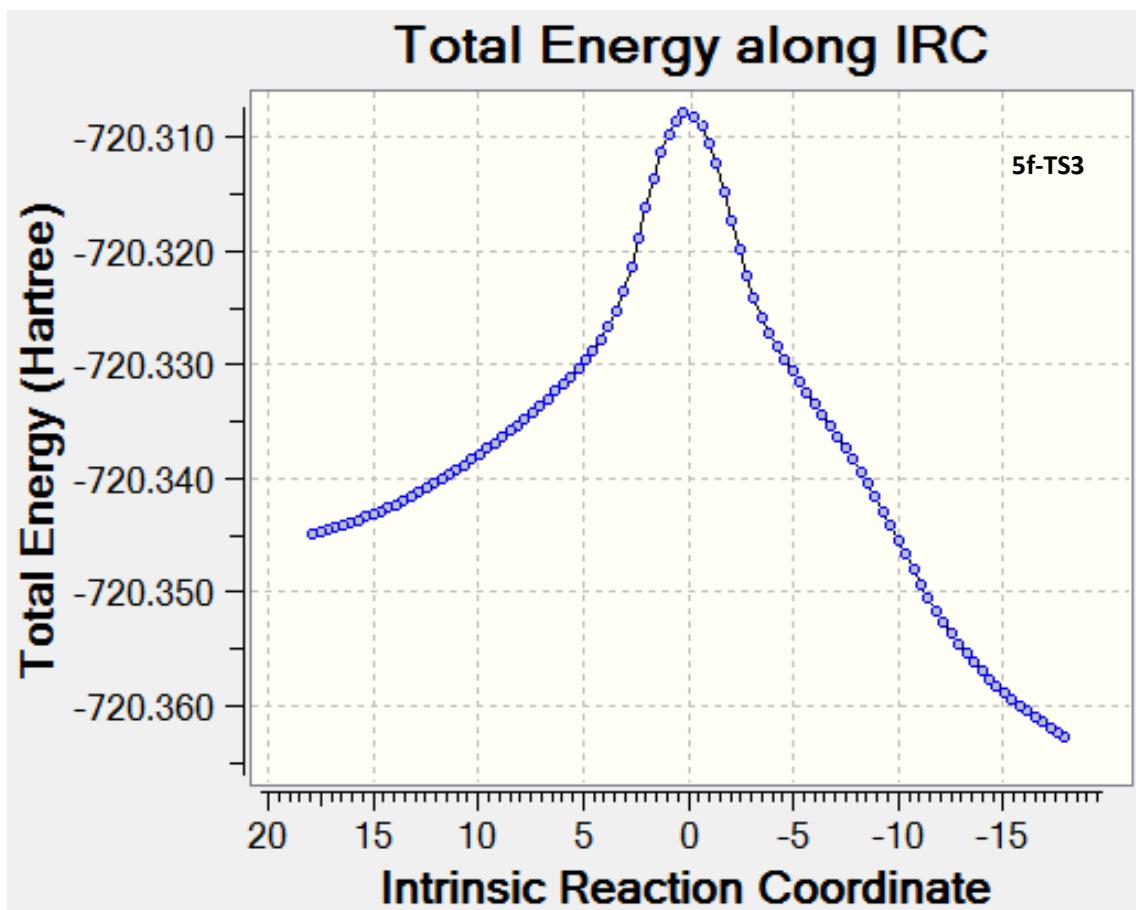




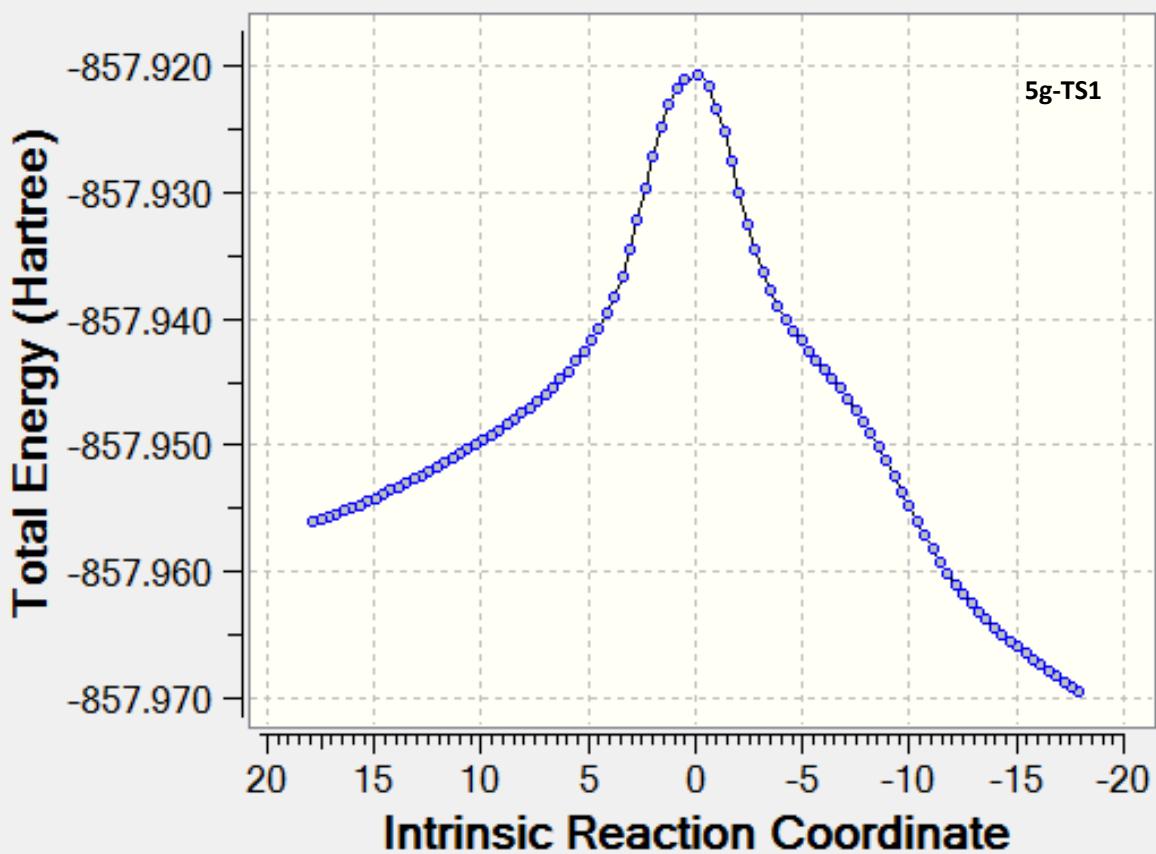




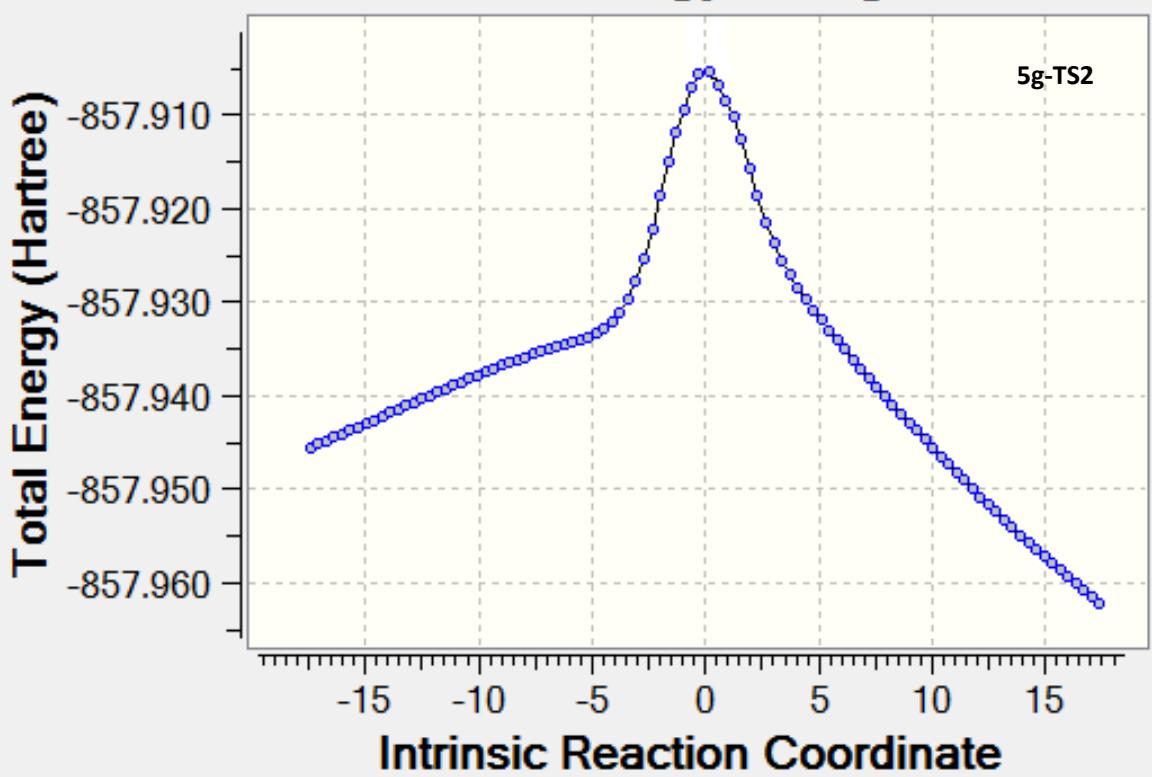




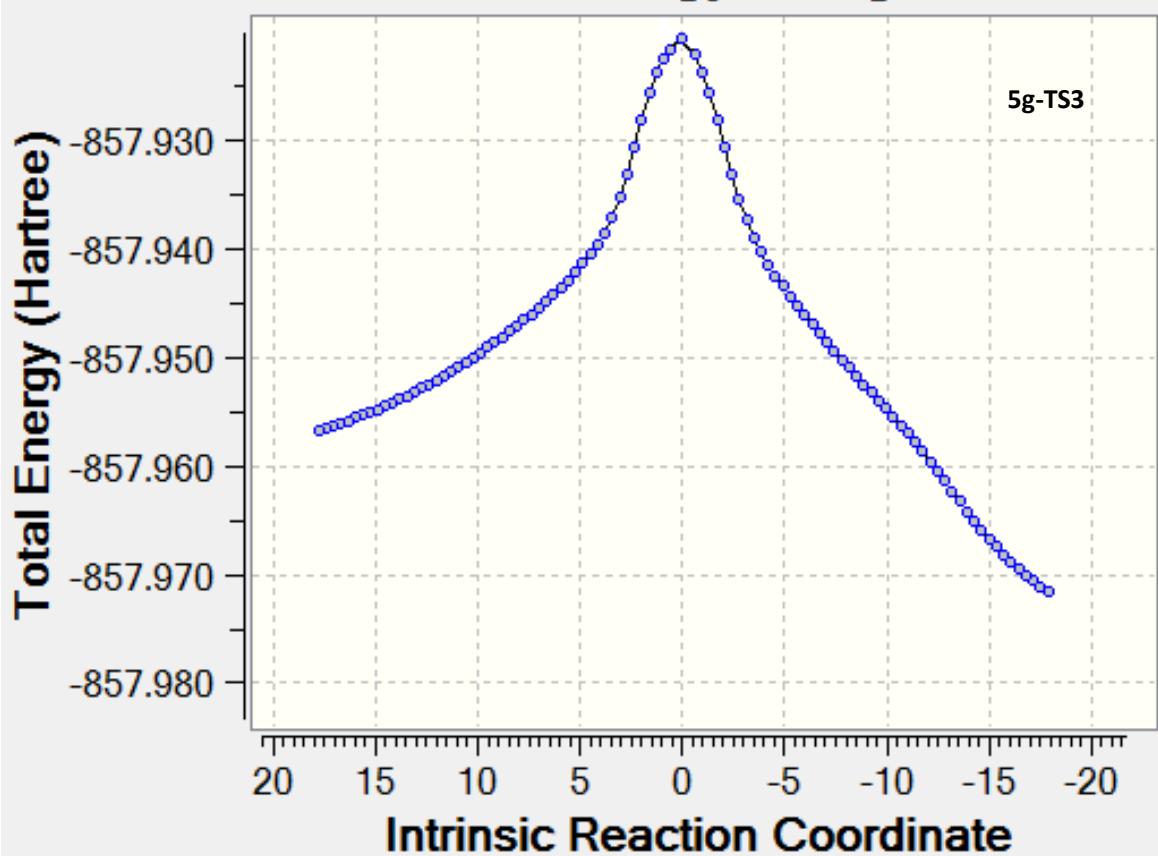
Total Energy along IRC



Total Energy along IRC



Total Energy along IRC



Total Energy along IRC

