Supporting Information

Novel pyrazolyazoindole derivatives as photoswitches: design, synthesis, and photoswitching behavior research combine with theoretical methods

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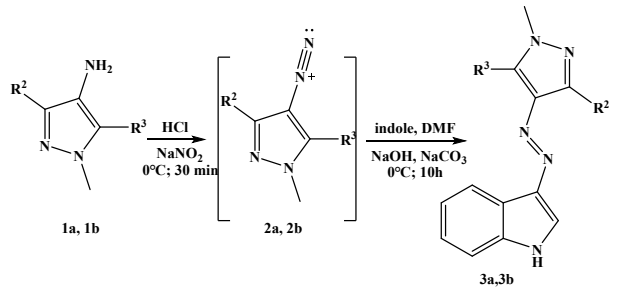
1 Synthesis

1.1 Specific synthesis steps

Synthesis of intermediates **3a** and **3b** (**A1** and **B1**)

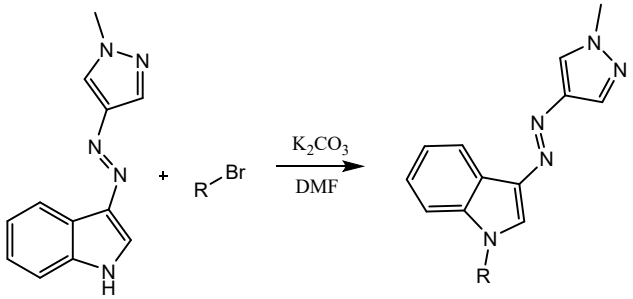


1 (**1a** and **1b**, 10 mmol, 1 eq.) was dissolved in 30 mL of water,followed by the addtion of 5 mL of HCl (12.2 mol/L, 57 mmol). After the solution was cooled under 0°C, a pre-cooling solution of $NaNO_2$ (0.9 g, 13 mmol, 1.3 eq.) in 30 mL water was slowly added. After the mixture was stirred for 30 min in a 0°C ice-salt bath, a pre-cooling solution of indole (1.4 g, 12 mmol, 1.2 eq.) and NaOH (1 g, 27 mmol) in 20 mL of water was slowly added. Then, a pre-cooling solution of Na_2CO_3 (3.8 g, 33 mmol) in 30 mL of water was slowly drip added. The brownish yellow solid precipitated continuously. After stirred for 3 hours, filtered and wash with water and dry to obtained yellow solid.[S1] The crude product was subjected to flash silica gel column chromatography (ethyl acetate-Petroleum ether: 2:1) to afford the pure compounds **3** (**3a** and **3b**).

3a (**A1**): Yellow solid, yield 95 %; ^{1}H NMR (500 MHz, DMSO) δ 11.85 (s, 1H), 8.27 (d, *J* = 7.9 Hz), 8.25 (s, 1H), 8.15 (s, 1H), 7.85 (s, 1H), 7.46 (d, *J* = 8.1 Hz, 1H), 7.24 (t, *J* = 7.5 Hz, 1H), 7.18 (t, *J* = 7.5 Hz, 1H), 3.91 (s, 3H,); ^{13}C NMR (126 MHz, DMSO) δ 142.31, 136.92, 135.64, 131.69, 131.17, 126.26, 123.88, 122.46, 122.32, 118.81, 112.55, 39.50; HRMS (ESI) *m/z* calcd for $C_{12}H_{11}N_5$ $[M + H]^+$ 226.1087, found 226.1086.

3b (**B1**): Light yellow solid, yield 92 %; ^{1}H NMR (500 MHz, DMSO) *δ* 11.72 (s, 1H), 8.29 (d, *J* = 7.9 Hz, 1H), 8.07 (s, 1H), 7.44 (d, *J* = 7.9 Hz, 1H), 7.22 (t, *J* = 7.3 Hz, 1H), 7.17 (t, *J* = 7.3 Hz, 1H), 3.73 (s, 3H), 2.55 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 139.79, 136.85, 136.35, 136.12, 135.02, 129.81, 127.79, 123.57, 122.40, 122.07, 118.78, 112.44, 99.99, 36.25, 14.10, 10.03; HRMS (ESI) *m/z* calcd for $C_{12}H_{11}N_5$ $[M + H]^+$ 372.1712, found 372.1700; HRMS (ESI) *m/z* calcd for $C_{12}H_{11}N_5$ $[M + H]^+$ 254.1400, found 254.1397.

Synthesis of title compounds **A2-A5**, **B2**, and **B3.**



intermediate **3** (3 mmol) was dissolved in DMF (30ml) and added to a single-necked flask, and then the corresponding bromide, KOH. Reacted at 80° for 3-5 hours, After the reaction, added 40ml of water, extracted ethyl acetate (40ml×3), dried and evaporated solvent, purification by column chromatography (ethyl acetate-Petroleum ether: 1:1) gave the products **A2-A5, B2, and B3**.[S2]

A2: yellow solid, yield 89 %; ^{1}H NMR (500 MHz, DMSO-*d6*) δ 8.26 (d, *J* = 7.8 Hz, 1H), 8.24 (s, 1H), 8.15 (s, 1H), 7.84 (s, 1H), 7.52 (d, *J* = 8.1 Hz, 1H), 7.30 (t, *J* = 7.6 Hz, 1H), 7.22 (t, *J* = 7.5 Hz, 1H), 3.89 (s, 3H), 3.87 (s, 3H). 13C NMR (126 MHz, DMSO) δ 142.31, 137.43, 134.56, 134.49, 131.81, 126.17, 123.91, 122.60, 122.53, 119.30, 110.83, 39.51, 33.45; HRMS (ESI) *m*/*z* calcd for $C_{12}H_{11}N_5$ $[M + H]^+$ 240.1244, found 240.1241.

A3: yellow solid, yield 92 %; ^{1}H NMR (500 MHz, DMSO-*d6*) δ 8.29 (d, *J* = 7.9 Hz, 1H), 8.24 (s, 1H), 8.23 (s, 1H), 7.59 (d, *J* = 8.3 Hz, 1H), 7.30 (t, *J* = 7.6 Hz, 1H), 7.22 (t, *J* = 7.4 Hz, 1H), 4.30 (q, *J* = 7.2 Hz, 2H), 3.90 (s, 3H), 1.49 – 1.39 (m, 3H); ^{13}C NMR (126 MHz, DMSO) δ 142.32, 136.44, 134.66, 133.08, 131.70, 126.24, 123.88, 122.67, 122.53, 119.43, 110.83, 41.30, 39.51, 15.61; HRMS (ESI) *m*/*z* calcd for $C_{12}H_{11}N_5$ $[M + H]^+$ 254.1400, found 254.1397.

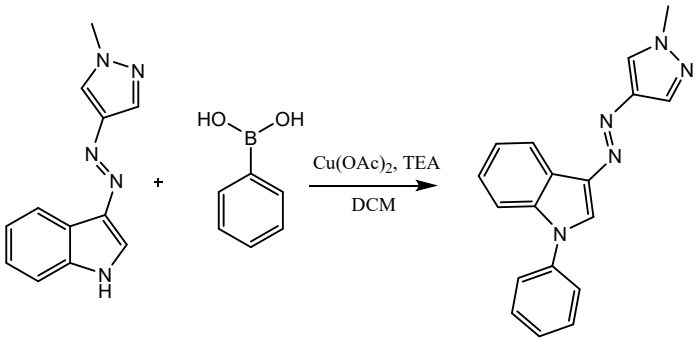
A4: yellow solid, yield 87 %; ^{1}H NMR (500 MHz, DMSO) δ 8.28 (t, *J* = 7.5 Hz, 1H), 8.25 (s, 1H), 8.22 (s, 1H), 7.85 (s, 1H), 7.60 (d, *J* = 8.2 Hz, 1H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.22 (t, *J* = 7.5 Hz, 1H), 4.24 (t, *J* = 6.9 Hz, 1H), 3.90 (s, 1H), 1.85 (dt, *J* = 14.6, 7.2 Hz, 1H), 0.89 (t, *J* = 7.3 Hz, 1H); ^{13}C NMR (126 MHz, DMSO) δ 142.34, 136.79, 133.79, 133.77, 131.69, 126.27, 123.87, 122.64, 122.52, 119.37, 110.97, 47.91, 39.51, 23.29, 11.52; HRMS (ESI) *m*/*z* calcd for $C_{12}H_{11}N_5$ $[M + H]^+$ 268.1557, found 268.1551.

A5: yellow solid, yield 85 %; ^{1}H NMR (500 MHz, DMSO) δ 8.30 (d, J = 7.8 Hz, 1H), 8.26 (s, 1H), 8.18 (s, 1H), 7.87 (s, 1H), 7.53 (d, J = 8.1 Hz, 1H), 7.29 (t, J = 7.4 Hz, 1H), 7.22 (t, J = 7.5 Hz, 1H), 6.07 (ddd, J = 13.4, 10.2, 4.0 Hz, 1H), 5.21 (d, J = 10.2 Hz, 1H), 5.13 (d, J = 17.1 Hz, 1H), 4.93 (s, 2H), 3.90 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 142.35, 136.76, 134.79, 134.09, 133.60, 131.81, 126.33, 122.69, 122.66, 119.53, 117.90, 111.18, 48.89, 39.52; HRMS (ESI) *m*/*z* calcd for $C_{12}H_{11}N_5$ $[M + H]^+$ 266.1445, found 266.1440.

B2: yellow solid, yield 84 %; ^{1}H NMR (500 MHz, DMSO) δ 8.29 (d, *J* = 7.9 Hz, 1H), 8.08 (s, 1H), 7.52 (d, *J* = 8.3 Hz, 1H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.22 (t, *J* = 7.5 Hz, 1H), 3.88 (s, 3H), 3.72 (s, 3H), 2.53 (d, *J* = 17.3 Hz, 3H), 2.38 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 136.80, 136.26, 129.97, 128.47, 125.35, 125.00, 121.41, 120.74, 119.31, 110.06, 100.66, 36.09, 32.88, 11.24, 8.86; HRMS (ESI) *m*/*z* calcd for $C_{12}H_{11}N_5$ $[M + H]^+$ 268.1557, found 268.1551.

B3: yellow solid, yield 80 %; ^{1}H NMR (500 MHz, DMSO) δ 8.30 (d, J = 7.8 Hz, 1H), 8.12 (s, 1H), 7.57 (d, J = 8.1 Hz, 1H), 7.27 (t, J = 7.6 Hz, 1H), 7.21 (t, J = 7.5 Hz, 1H), 4.22 (t, J = 6.9 Hz, 2H), 3.72 (s, 3H), 2.55 (s, 3H), 2.39 (s, 3H), 1.85 (h, J = 7.1 Hz, 2H), 0.88 (t, J = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, DMSO) δ 139.79, 136.72, 136.41, 135.07, 135.04, 132.40, 123.57, 122.56, 122.25, 119.36, 110.82, 47.81, 36.25, 23.35, 14.10, 11.55, 10.03; HRMS (ESI) *m*/*z* calcd for $C_{12}H_{11}N_5$ $[M + H]^+$ 260.1870, found 260.1871.

Synthesis of title compounds **A6** and **B4.**

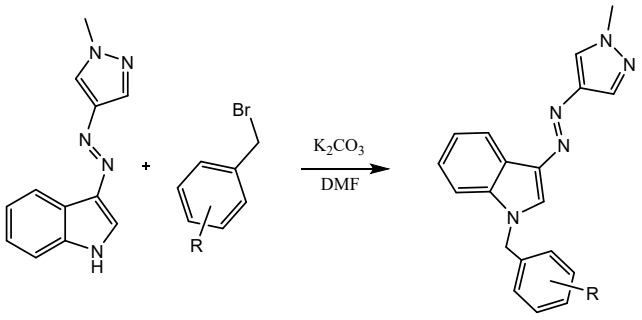


intermediate **3** (3 mmol) was dissolved in DCM (30ml) and added to a flask, and then the phenylboronic acid and TEA (1.3 ml, 9 mmol) and $Cu(OAc)_2$ (1.2 g, 6 mmol) in dichloromethane was slowly added dropwise to the mixed solution. Reacted at r.t. for 24 hours, After the reaction, filter and wash the solution, purification by column chromatography (ethyl acetate-Petroleum ether: 1:1) gave the products **A6** and **B4**.[S3]

A6: yellow solid, yield 63 %; ^{1}H NMR (500 MHz, DMSO) *δ* 8.47 (s, 1H), 8.41 (d, *J* = 7.4 Hz, 1H), 8.34 (s, 1H), 7.91 (s, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.58 (d, *J* = 7.9 Hz, 1H), 7.51 (t, *J* = 7.3 Hz, 1H), 7.38 – 7.30 (m, 1H), 3.93 (s, 1H). ^{13}C NMR (126 MHz, DMSO) *δ* 141.92, 138.09, 136.06, 135.85, 132.61, 131.53, 130.10, 127.68, 126.56, 124.65, 123.16, 122.71, 119.90, 111.03, 56.17; HRMS (ESI) *m/z* calcd for $C_{12}H_{11}N_5$ $[M + H]^+$ 302.1400, found 302.1402.

B4: yellow solid, yield 46 %; ^{1}H NMR (500 MHz, DMSO) δ 8.42 (d, *J* = 6.7 Hz, 1H), 8.37 (s, 1H), 7.72 (d, *J* = 7.6 Hz, 2H), 7.64 (t, *J* = 7.3 Hz, 3H), 7.58 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 6.7 Hz, 2H), 7.32 (s, 2H), 3.75 (s, 3H), 2.59 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 135.22, 134.52, 130.44, 130.38, 127.79, 124.86, 124.70, 123.29, 122.92, 120.37, 118.85, 111.28, 36.31, 14.15, 10.10; HRMS (ESI) *m/z* calcd for $C_{12}H_{11}N_5$ $[M + H]^+$ 330.1713, found 330.1715.

Synthesis of title compounds **A7**, **A8**, and **B5**.



intermediate 3 (3 mmol) was dissolved in CH_3CN (20 ml), and then the benzyl bromideand or 3-Bromobenzyl bromide (3.6 mmol) and K_2CO_3 (1.3 g, 9 mmol) was added to the solvent at 80℃ for 4h, adding the reaction solution to 50ml of cold water, a large amount of yellow solid was

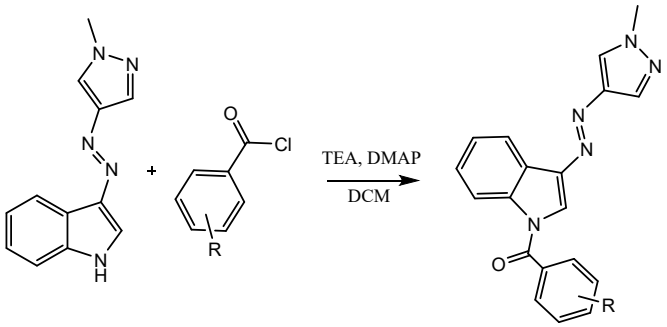
precipitated and purification by column chromatography (ethyl acetate-Petroleum ether: 1:1) gave the products **A7**, **A8**, and **B5**.

A7: yellow solid, yield 85 %; ^{1}H NMR (500 MHz, DMSO) *δ* 8.37 (s, 1H), 8.27 (s, 1H), 8.27 (s, 1H), 7.87 (s, 1H), 7.56 (d, *J* = 8.1 Hz, 1H), 7.34 (d, *J* = 4.3 Hz, 1H), 7.30 – 7.19 (m, 1H), 5.53 (s, 1H), 3.91 (s, 1H); ^{13}C NMR (126 MHz, DMSO) δ 142.34, 137.69, 136.72, 134.87, 133.91, 131.77, 129.14, 128.12, 127.73, 126.43, 122.72, 122.70, 119.69, 111.35, 50.00, 39.53; HRMS (ESI) *m/z* calcd for $C_{12}H_{11}N_5$ $[M + H]^+$ 316.1557, found 316.1550.

A8: yellow solid, yield 79 %; ^{1}H NMR (500 MHz, DMSO) δ 8.41 (s, 1H), 8.29 (d, *J* = 5.9 Hz, 1H), 8.28 (s, 1H), 7.87 (s, 1H), 7.58 (d, *J* = 10.8 Hz, 2H), 7.49 (d, *J* = 6.9 Hz, 1H), 7.32 (d, *J* = 6.1 Hz, 1H), 7.31 – 7.19 (m, 3H), 5.54 (s, 2H), 3.91 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 142.28, 140.50, 136.63, 134.95, 133.82, 131.76, 131.36, 131.04, 130.49, 126.82, 126.51, 124.19, 122.83, 122.73, 122.36, 119.68, 111.27, 49.23, 39.54; HRMS (ESI) *m/z* calcd for $C_{12}H_{11}N_5$ $[M + H]^+$ 394.0662, found 394.0658.

B5: yellow solid, yield 80 %; ^{1}H NMR (500 MHz, DMSO) δ 8.31 (d, *J* = 7.4 Hz, 1H), 8.27 (s, 1H), 7.54 (d, *J* = 7.9 Hz, 1H), 7.34 (d, *J* = 5.5 Hz, 4H), 7.28 (d, *J* = 4.0 Hz, 1H), 7.26 – 7.18 (m, 2H), 5.51 (s, 2H), 3.73 (s, 3H), 2.55 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 139.86, 137.92, 136.66, 135.40, 135.10, 132.56, 129.13, 128.08, 127.75, 123.79, 122.62, 122.46, 111.21, 49.89, 36.27, 14.13, 10.04; HRMS (ESI) *m/z* calcd for $C_{12}H_{11}N_5$ $[M + H]^+$ 344.1870, found 344.1865.

Synthesis of title compounds **A9**-**A11**, **B6** and **B7**.



intermediate 3 (3 mmol) was dissolved in DCM (20 ml), and then the acid chloride or (3.6 mmol), DMAP (1.0，8 g, 9 mmol) and TEA (1.3 ml, 9 mmol) was added to the solvent at 0℃ to r.t. for 10h, concentrated solvent purification by column chromatography (ethyl acetate-Petroleum ether: 1:1) gave the products **A9**-**A11**, **B6** and **B7**.[S4]

A9: yellow solid, yield 80 %; ^{1}H NMR (500 MHz, DMSO) δ 8.44 (s, 1H), 8.38 (t, *J* = 7.4 Hz, 2H), 8.03 (s, 1H), 7.94 (s, 1H), 7.90 (d, *J* = 7.6 Hz, 2H), 7.76 (t, *J* = 7.4 Hz, 1H), 7.66 (t, *J* = 7.6 Hz, 2H), 7.53 (t, *J* = 7.7 Hz, 1H), 7.47 (t, *J* = 7.4 Hz, 1H), 3.92 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 168.79, 142.09, 137.61, 136.43, 133.82, 132.99, 132.10, 130.70, 130.69, 129.78, 129.31, 128.14, 126.81, 125.80, 122.99, 122.79, 116.34, 39.64; HRMS (ESI) *m/z* calcd for $C_{12}H_{11}N_5$ $[M + H]^+$ 330.1350, found 330.1346.

A10: yellow solid, yield 75 %; ^{1}H NMR (500 MHz, DMSO) δ 8.45 (s, 1H), 8.38 (d, *J* = 8.1 Hz, 2H), 8.09 (s, 1H), 8.05 (s, 1H), 7.95 (s, 1H), 7.93 (s, 1H), 7.89 (d, *J* = 7.6 Hz, 1H), 7.61 (t, *J* = 7.9 Hz, 1H), 7.53 (t, *J* = 7.7 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 1H), 3.93 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 167.34, 142.07, 137.83, 136.41, 136.12, 135.56, 132.12, 132.11, 131.43, 130.72, 128.22, 126.93, 125.96, 123.06, 122.88, 122.39, 116.42, 39.65; HRMS (ESI) *m/z* calcd for $C_{12}H_{11}N_5$ $[M + H]^+$ 408.0455, found 408.0451.

A11: yellow solid, yield 85 %; ^{1}H NMR (500 MHz, DMSO) δ 8.57 (s, 1H), 8.45 (s, 1H), 8.28 (d, *J* = 7.9 Hz, 1H), 8.06 – 8.00 (m, 3H), 7.95 (s, 1H), 7.49 – 7.36 (m, 4H), 3.93 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 145.54, 142.37, 138.85, 135.20, 134.79, 133.18, 130.11, 128.45, 127.09, 126.09, 124.87, 123.37, 122.84, 113.41, 39.63, 21.63; HRMS (ESI) *m/z* calcd for $C_{12}H_{11}N_5$ $[M + H]^+$ 380.1176, found 380.1173.

B6: yellow solid, yield 84 %; ^{1}H NMR (500 MHz, DMSO) δ 8.40 (d, *J* = 7.8 Hz, 1H), 8.37 (d, *J* = 8.0 Hz, 1H), 7.96 (s, 1H), 7.88 (d, *J* = 7.7 Hz, 2H), 7.75 (t, *J* = 6.9 Hz, 1H), 7.66 (t, *J* = 7.0 Hz, 2H), 7.52 – 7.44 (m, 2H), 3.74 (s, 3H), 2.57 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.75, 142.08, 139.04, 136.67, 135.76, 134.77, 134.14, 132.32, 129.36, 128.85, 128.36, 126.27, 125.29, 123.26, 122.93, 116.33, 36.05, 13.93, 10.22; HRMS (ESI) *m/z* calcd for $C_{12}H_{11}N_5$ $[M + H]^+$ 358.1663, found 358.1660.

B7: yellow solid, yield 78 %; ^{1}H NMR (500 MHz, DMSO) δ 8.44 (s, 1H), 8.28 (d, *J* = 7.4 Hz, 1H), 8.03 – 7.98 (m, 1H), 7.49 – 7.36 (m, 2H), 3.75 (s, 1H), 2.57 (s, 1H), 2.40 (s, 1H), 2.33 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 145.36, 142.33, 139.38, 135.65, 135.23, 134.94, 130.05, 127.06, 126.58, 125.81, 124.66, 123.23, 123.16, 113.45, 36.04, 21.63, 13.86, 10.21; HRMS (ESI) *m/z* calcd for $C_{12}H_{11}N_5$ $[M + H]^+$ 408.1489, found 408.1484.

1.2 spectrograms of target compounds

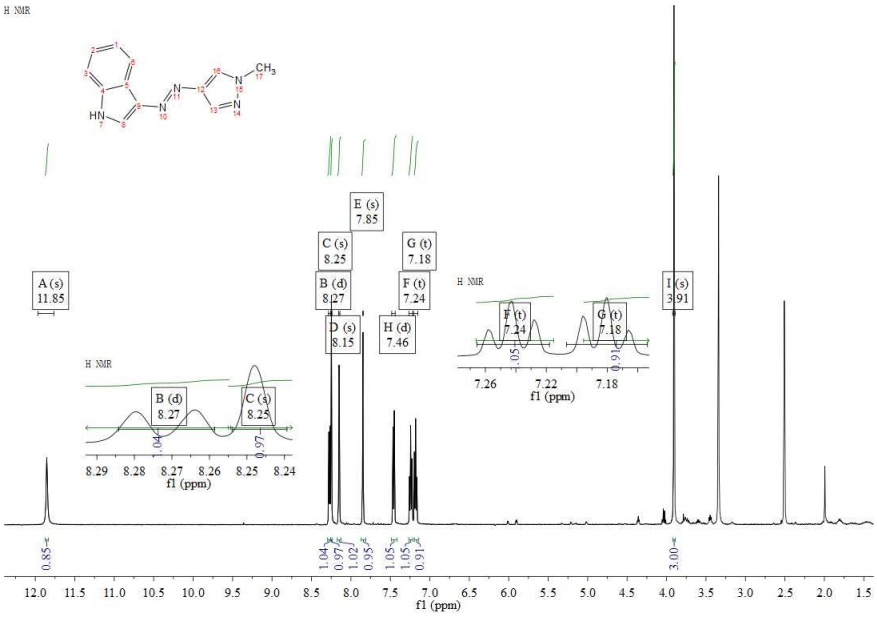


Figure S1. ^{1}H NMR sprectrum of **A1** in DMSO-d_6.

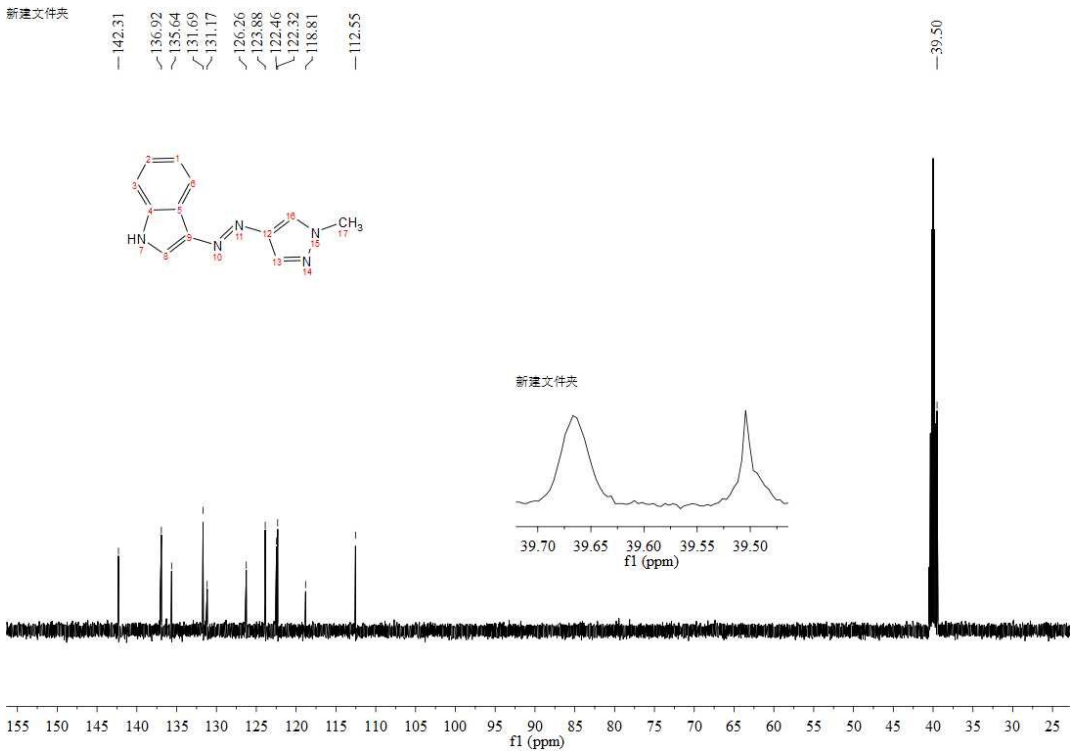


Figure S2. ^{13}C NMR sprectrum of **A1** in DMSO-d_6.

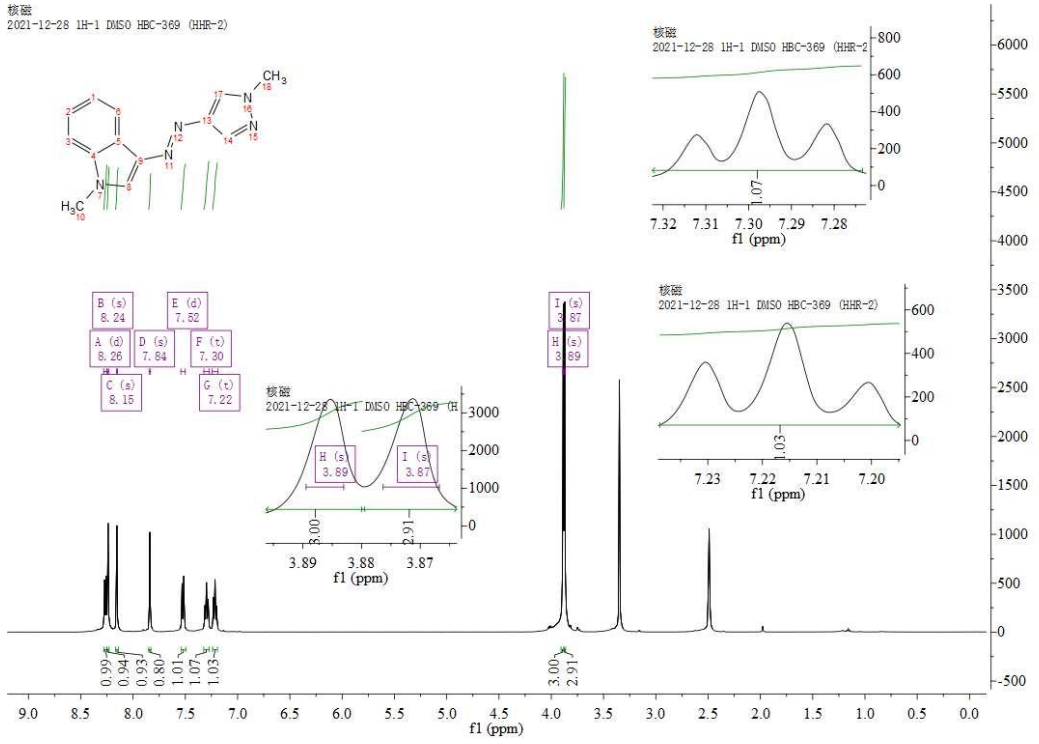


Figure S3. ^{1}H NMR sprectrum of **A2** in DMSO-d_6.

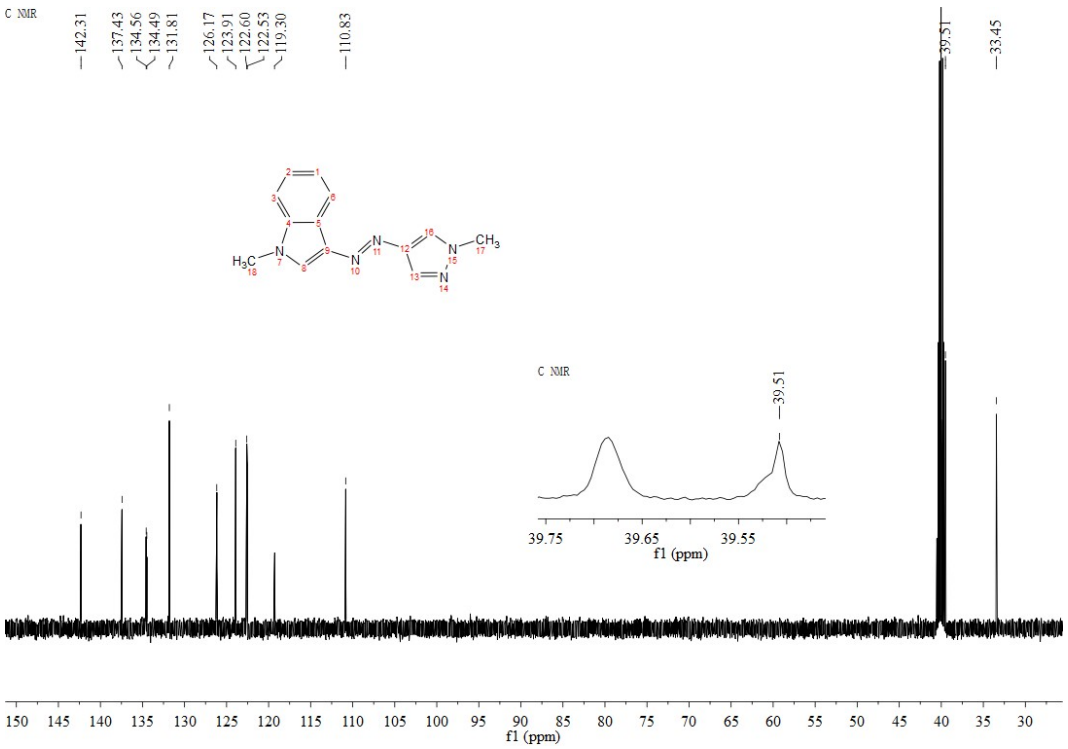


Figure S4. ^{13}C NMR sprectrum of **A2** in DMSO-d_6.

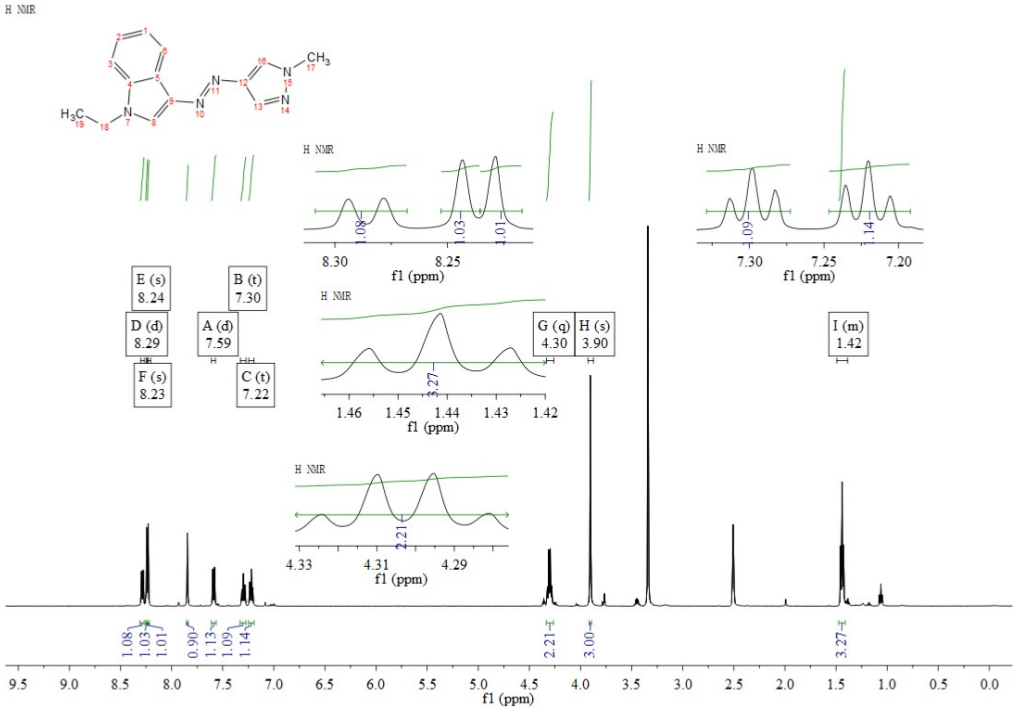


Figure S5. ^{1}H NMR sprectrum of **A3** in DMSO-d_6.

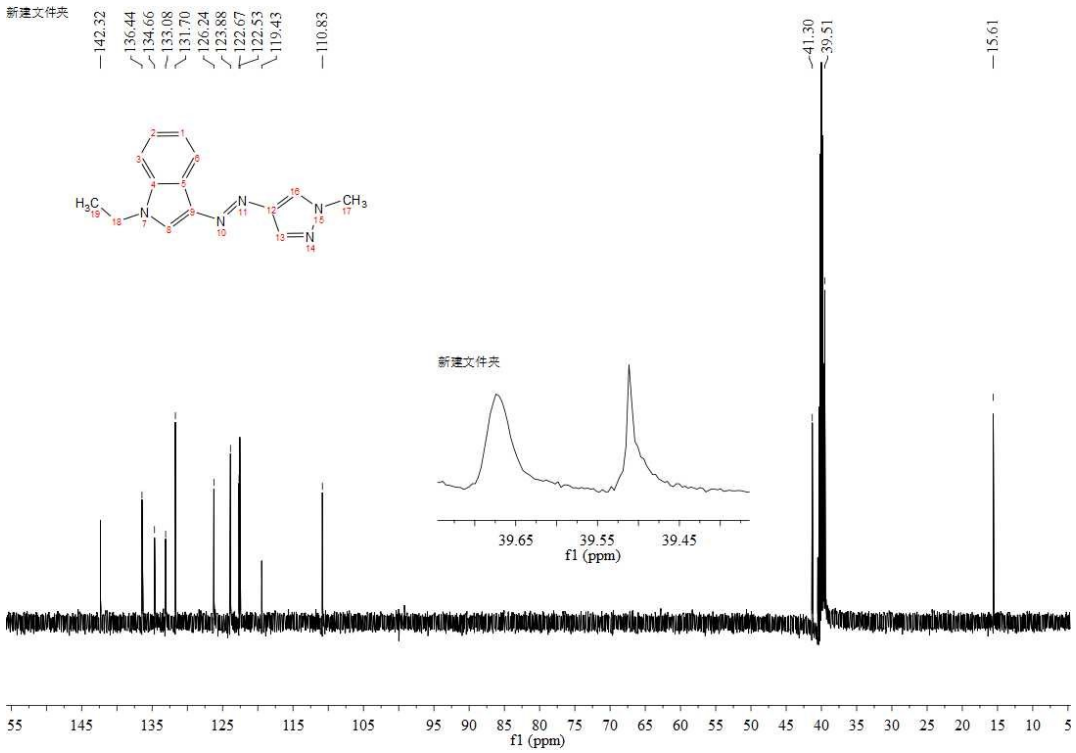


Figure S6. ^{13}H NMR sprectrum of **A3** in DMSO-d_6.

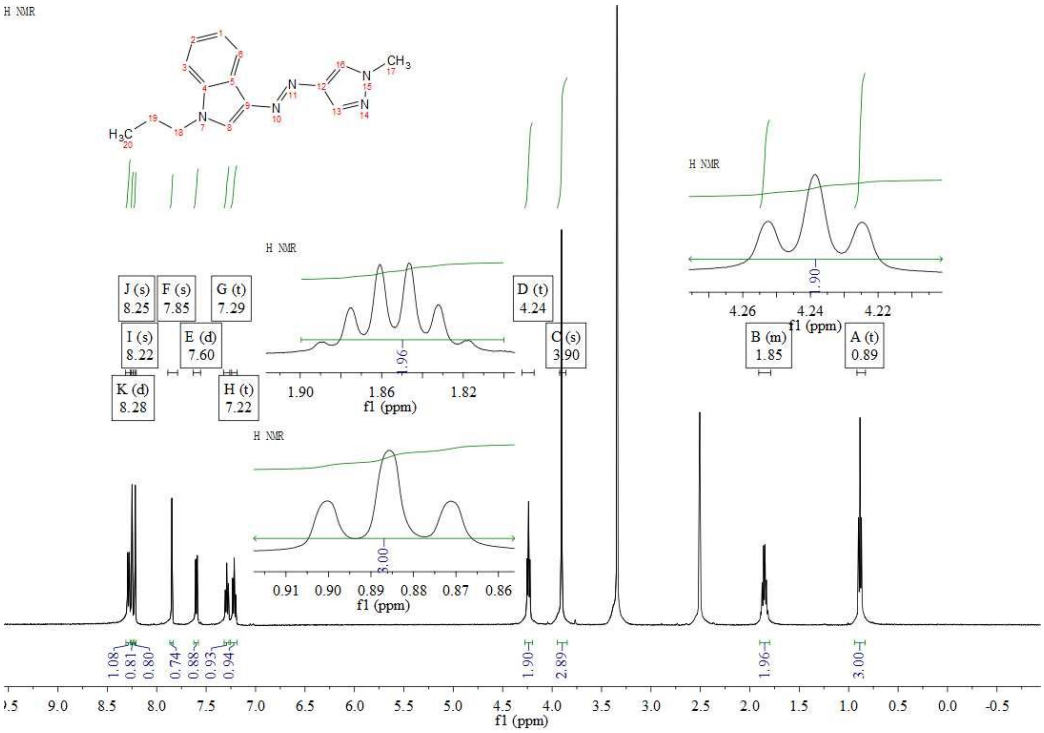


Figure S7. ^{1}H NMR sprectrum of **A4** in DMSO-d_6.

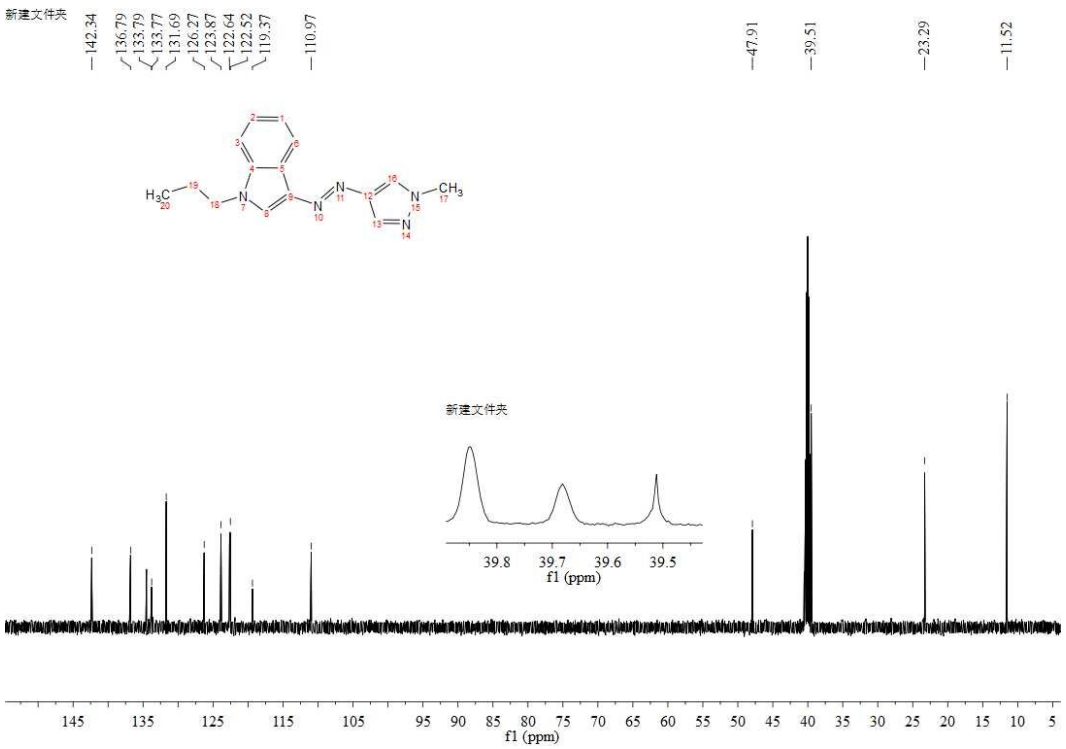


Figure S8. ^{13}C NMR sprectrum of **A4** in DMSO-d_6.

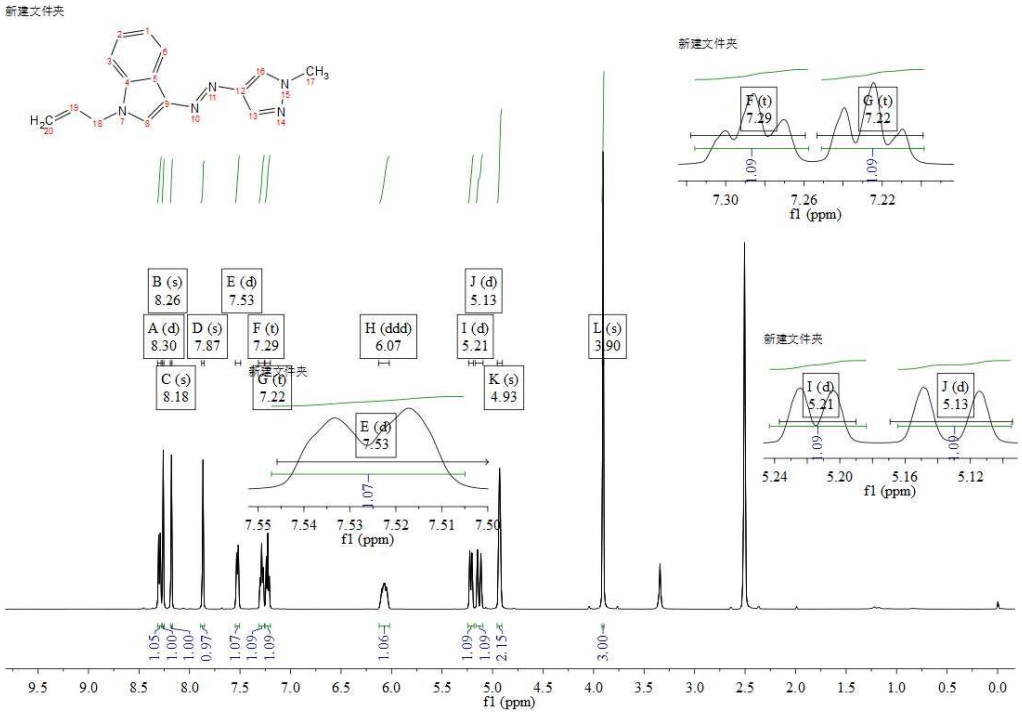


Figure S9. ^{1}H NMR sprectrum of **A5** in DMSO-d_6.

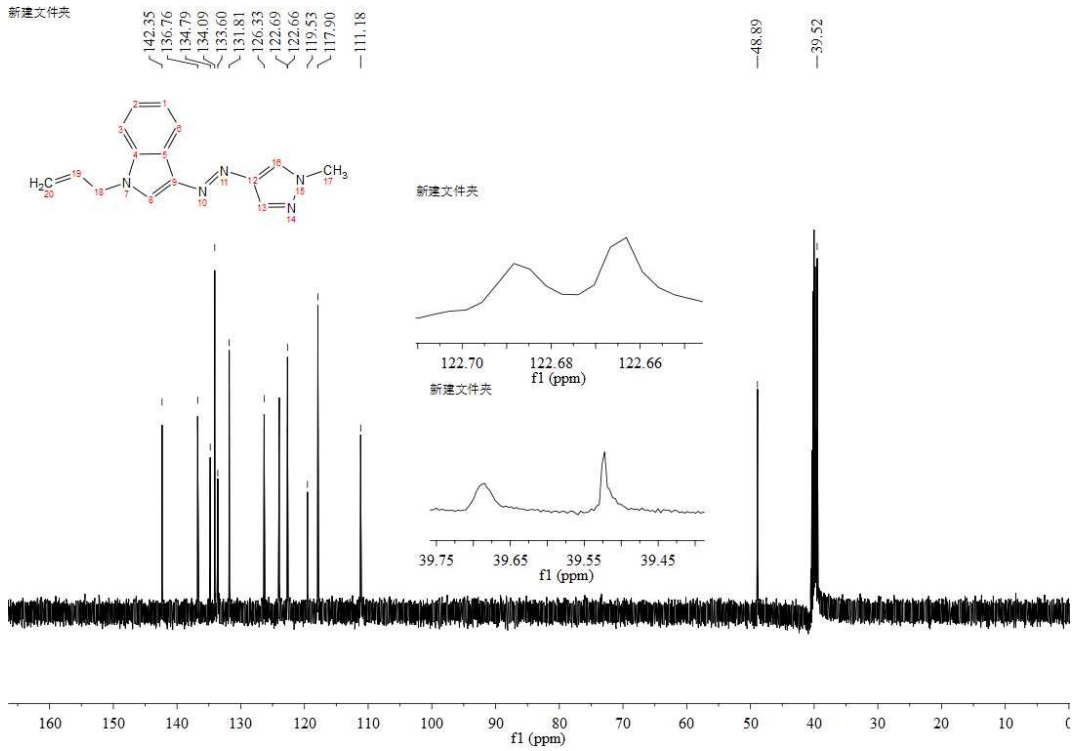


Figure S10. ^{13}C NMR sprectrum of **A5** in DMSO-d_6.

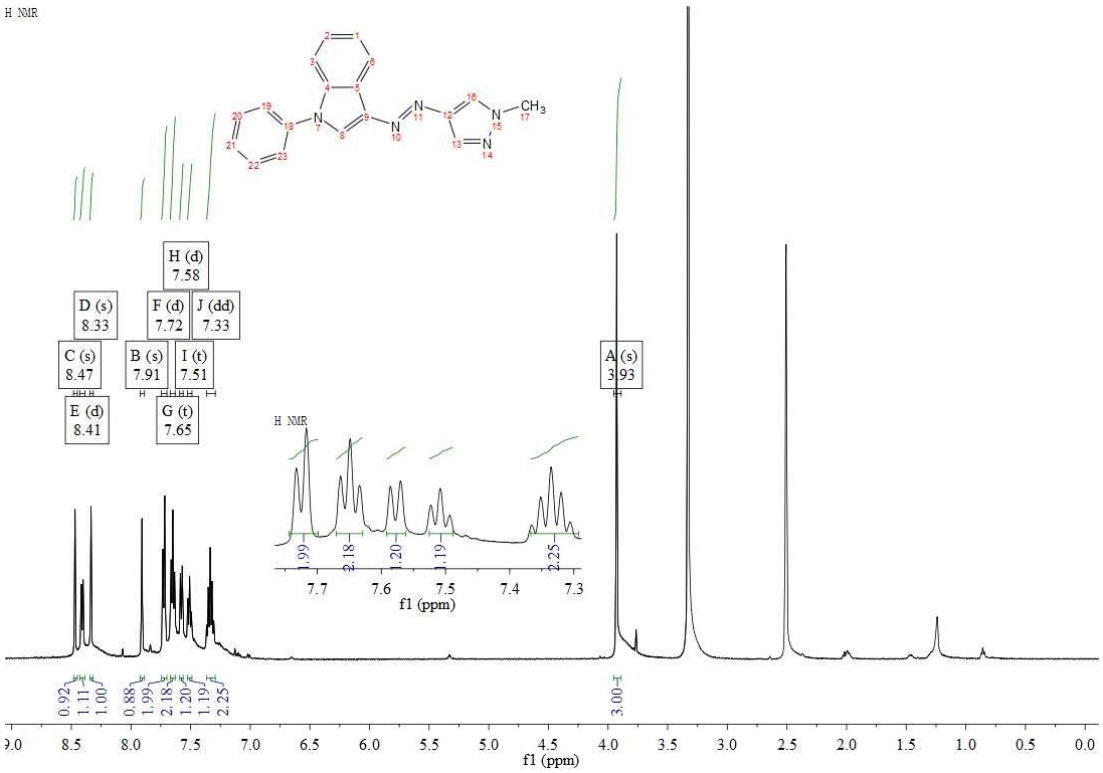


Figure S11. ^{1}H NMR sprectrum of compound **A6** DMSO-d_6.

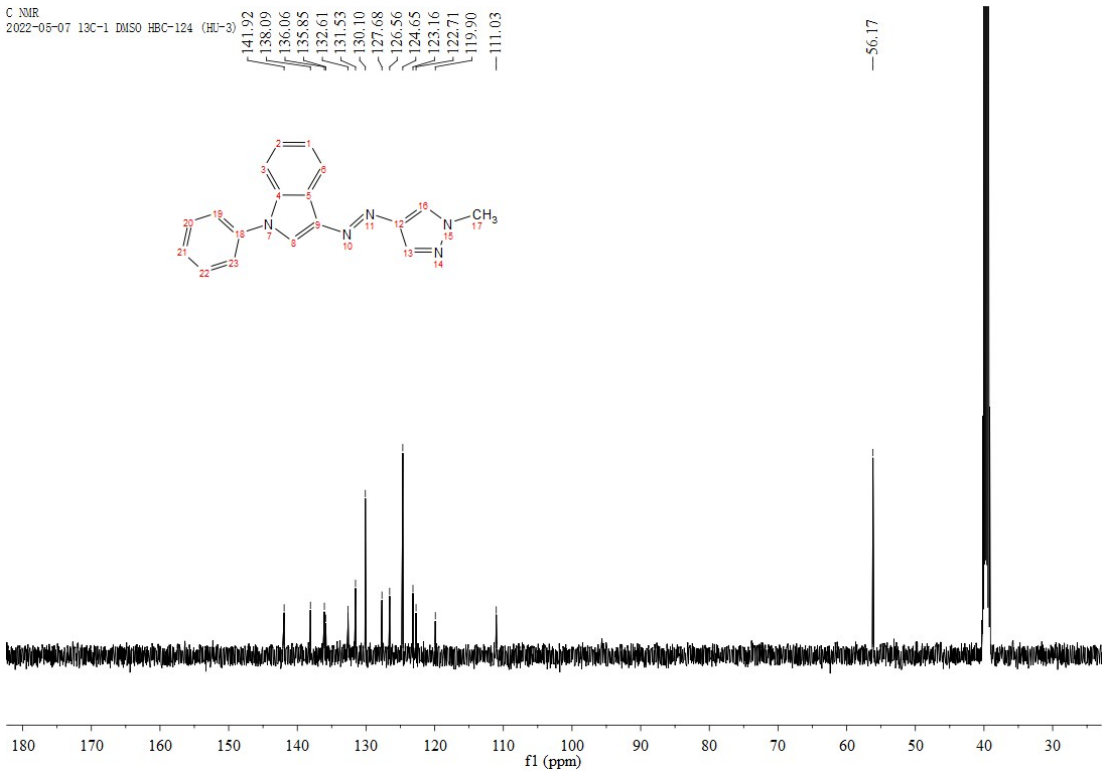


Figure S12. ^{13}C NMR sprectrum of compound **A6** DMSO-d_6.

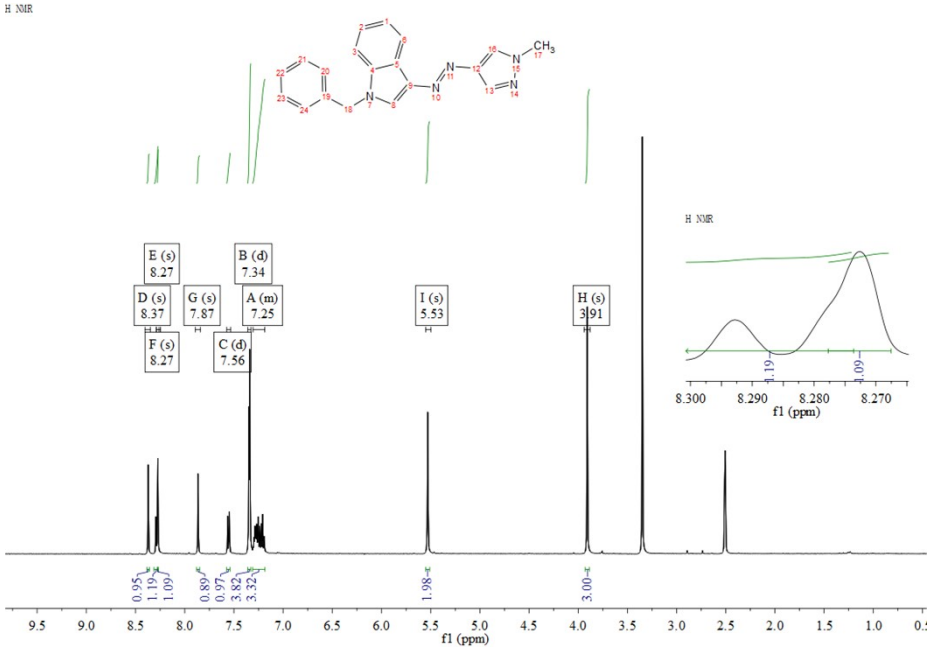


Figure S13. ^{1}H NMR sprectrum of **A7** in DMSO-d_6.

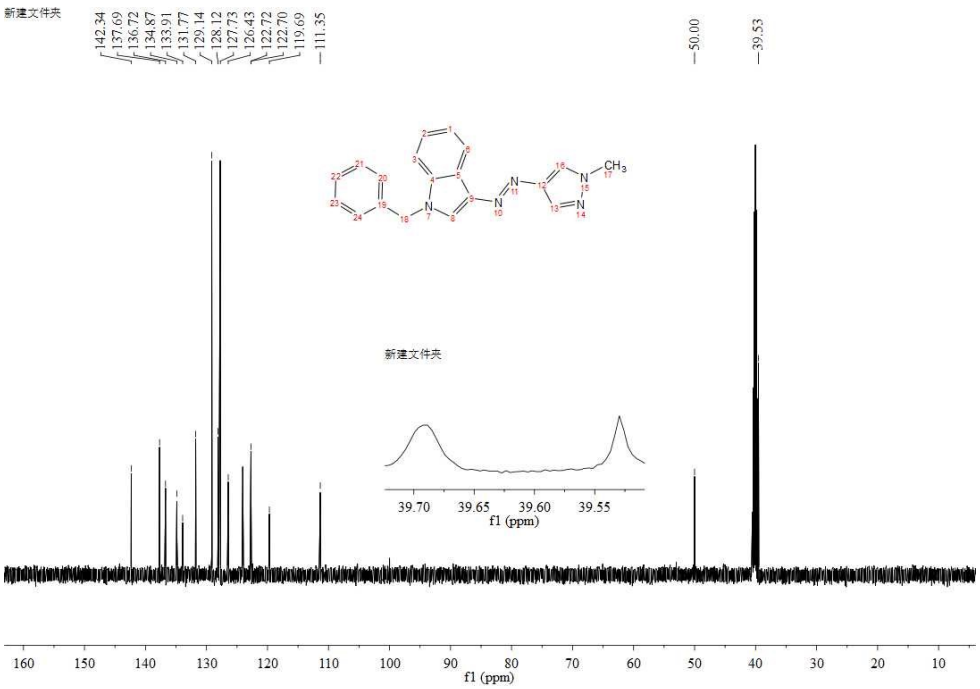


Figure S14. ^{13}C NMR sprectrum of **A7** in DMSO-d_6.

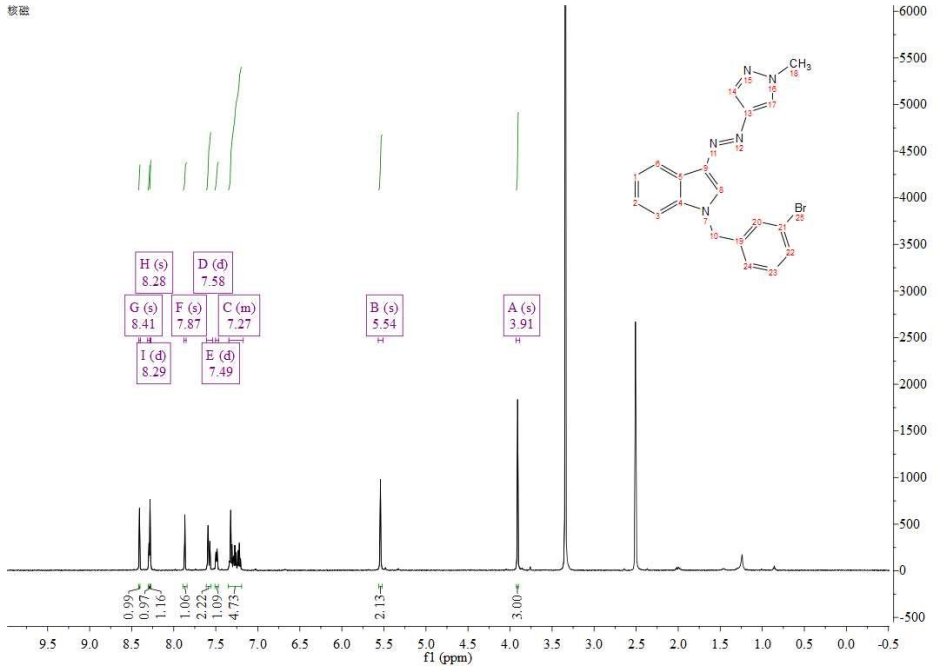


Figure S15. ^{1}H NMR sprectrum of **A8** in DMSO-d_6.

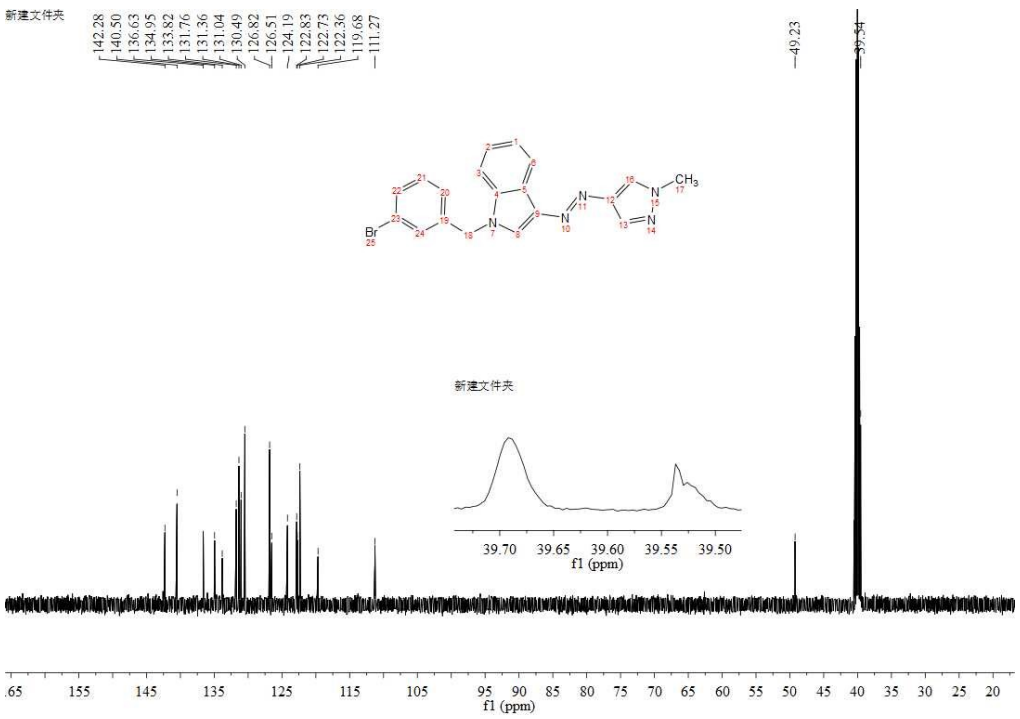


Figure S16. ^{13}C NMR sprectrum of **A8** in DMSO-d_6.

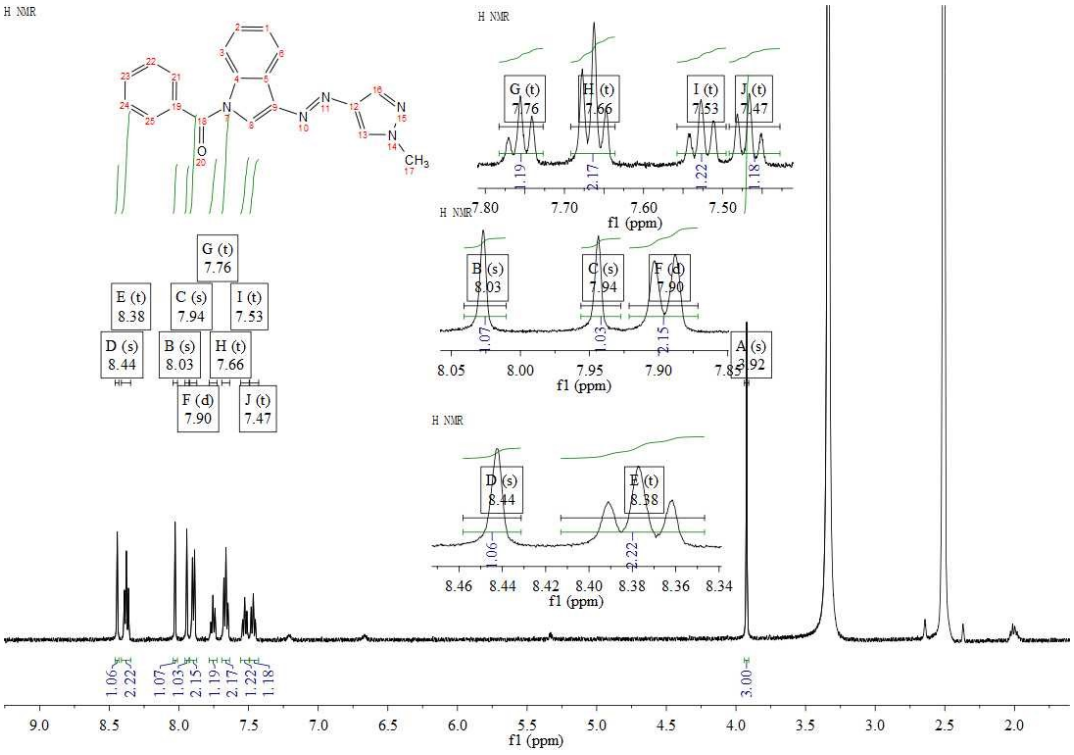


Figure S17. ^{1}H NMR sprectrum of **A9** in DMSO-d_6.

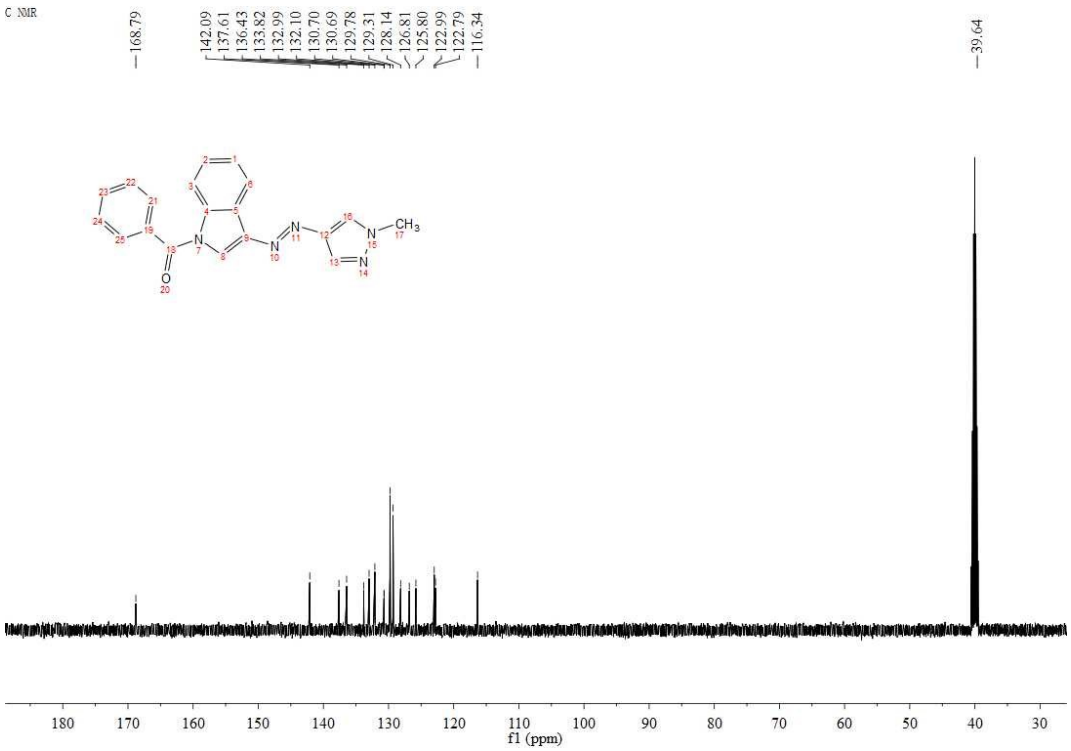


Figure S18. ^{13}C NMR sprectrum of **A9** in DMSO-d_6.

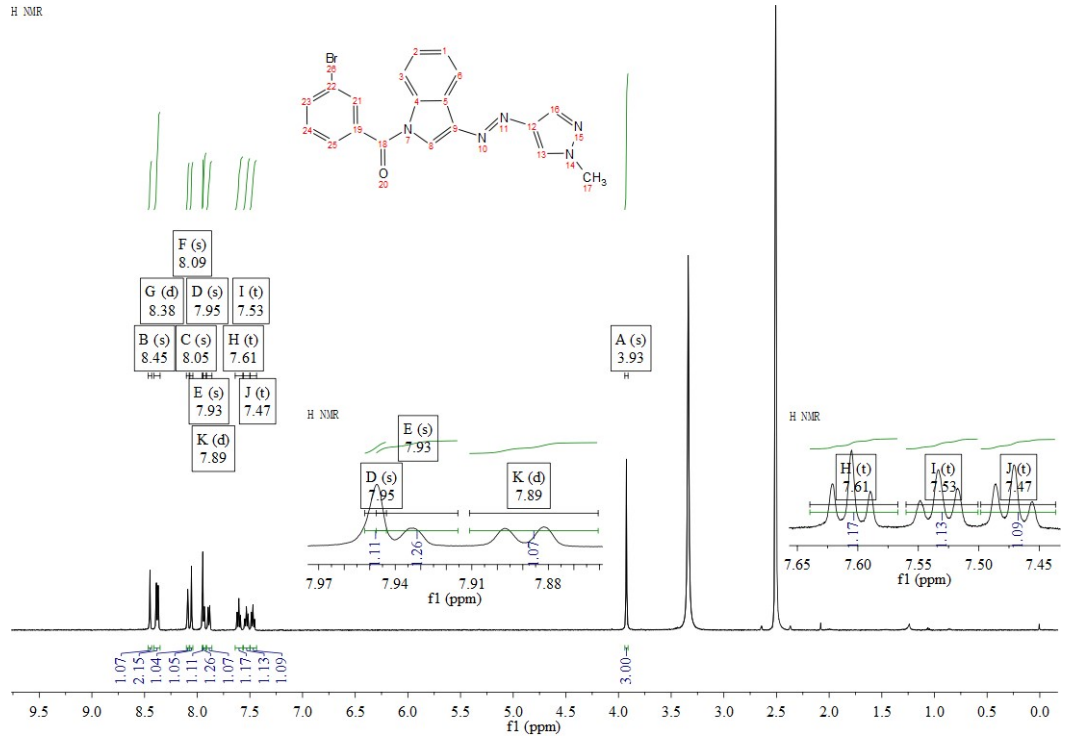


Figure S19. ^{1}H NMR sprectrum of **A10** in DMSO-d_6.

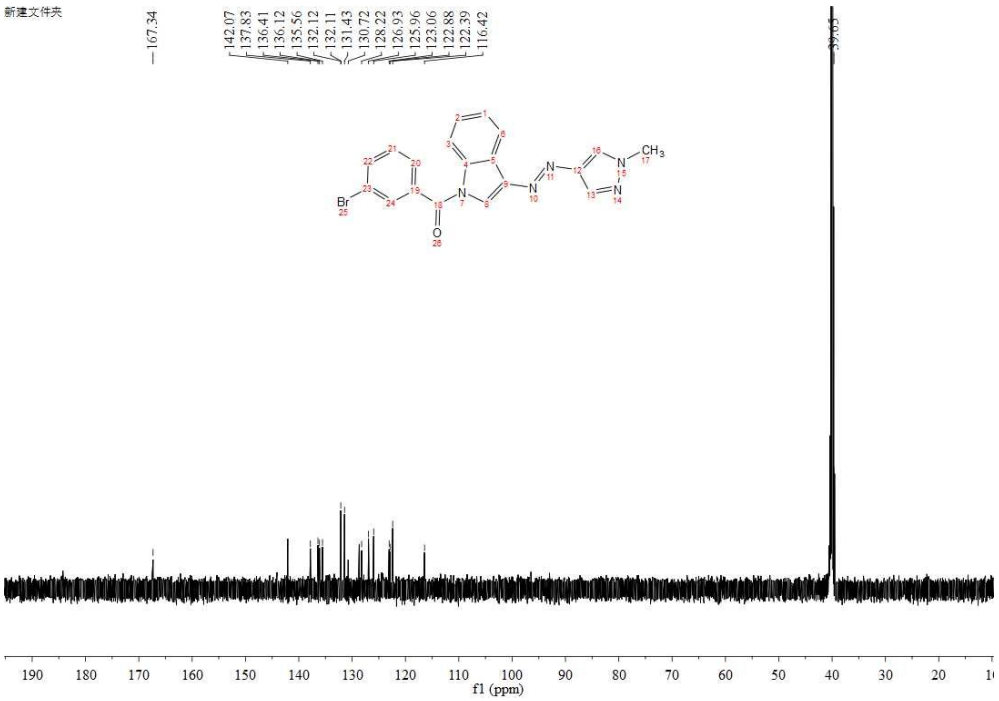


Figure S20. ^{13}C NMR sprectrum of **A10** in DMSO-d_6.

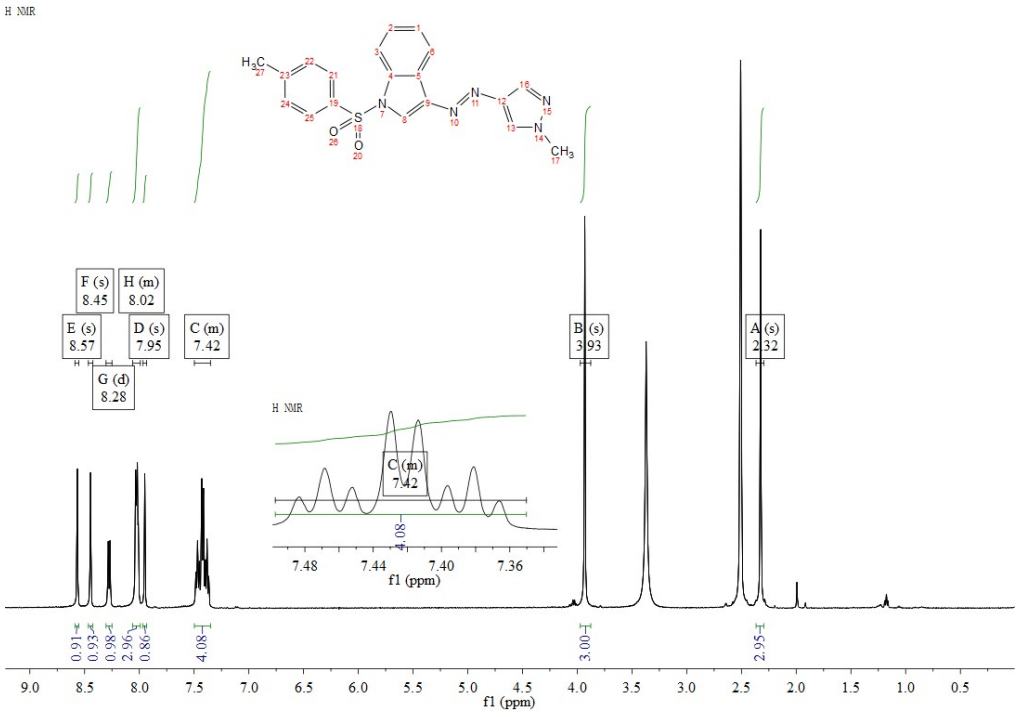


Figure S21. ^{1}H NMR sprectrum of **A11** in DMSO-d_6.

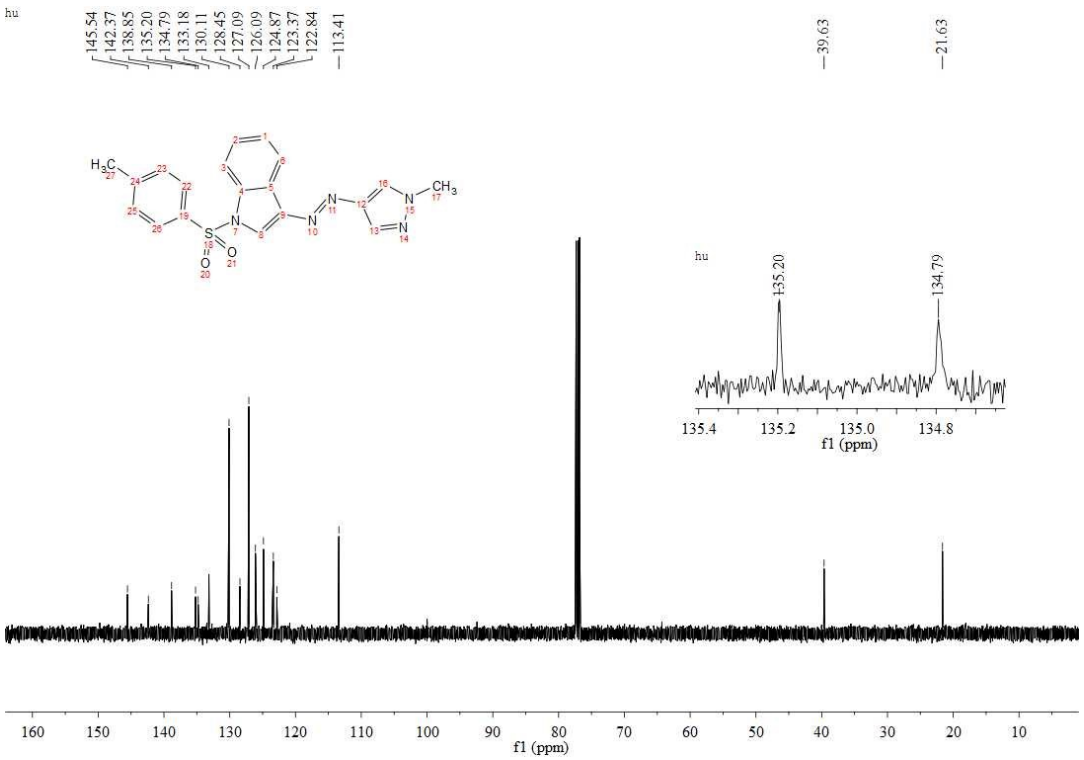


Figure S22. ^{13}C NMR sprectrum of **A11** in $CDCl_3$.

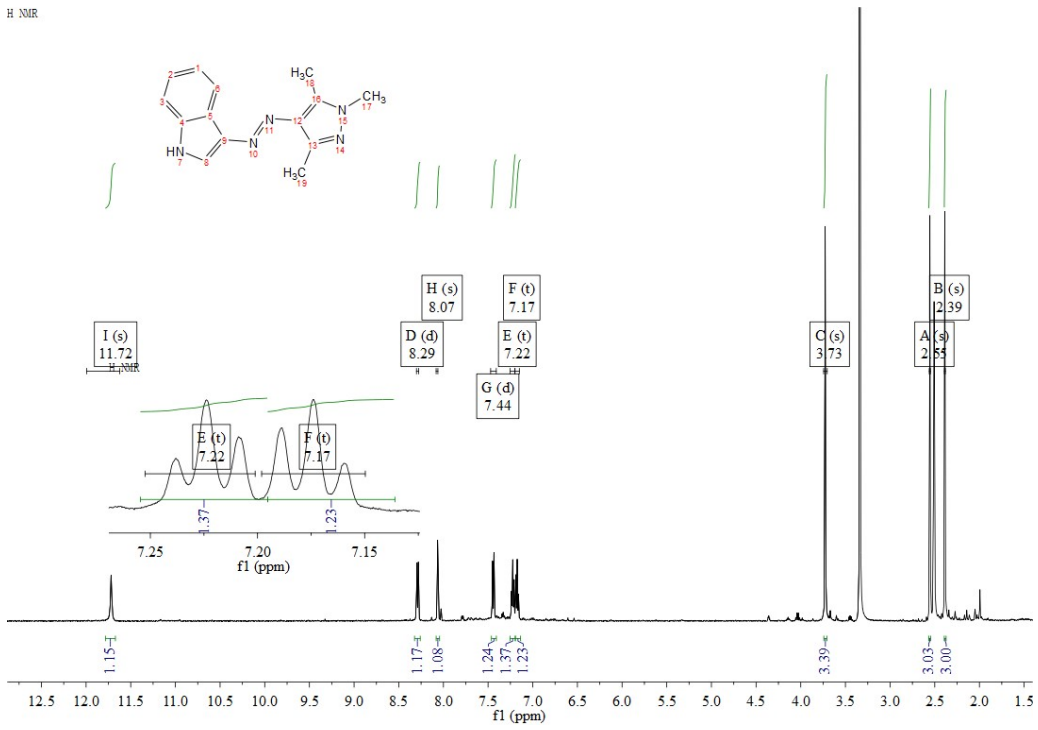


Figure S23. ^{1}H NMR sprectrum of **B1** in DMSO-d_6.

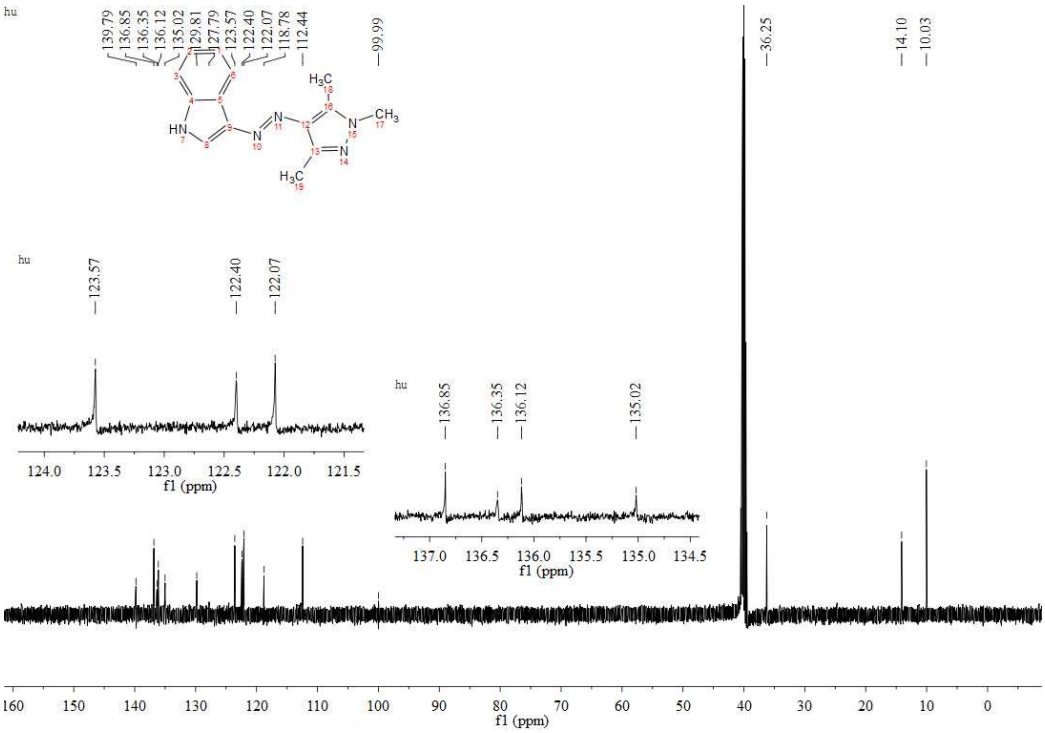


Figure S24. ^{13}C NMR sprectrum of **B1** in DMSO-d_6.

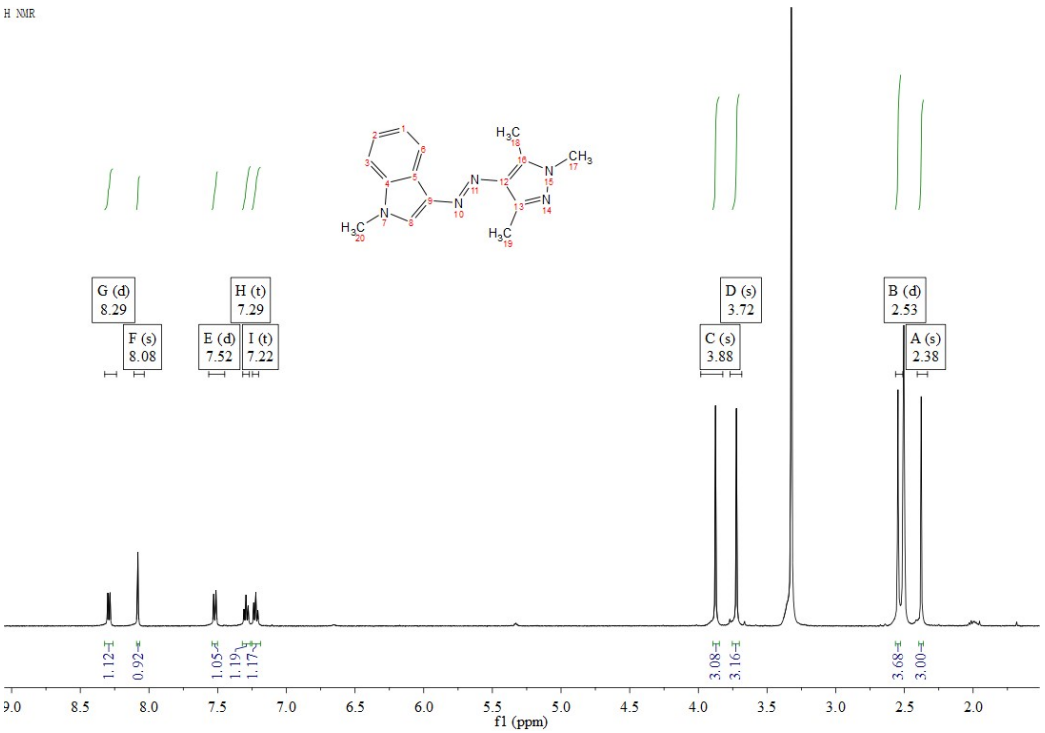


Figure S25. ^{1}H NMR sprectrum of **B2** in DMSO-d_6.

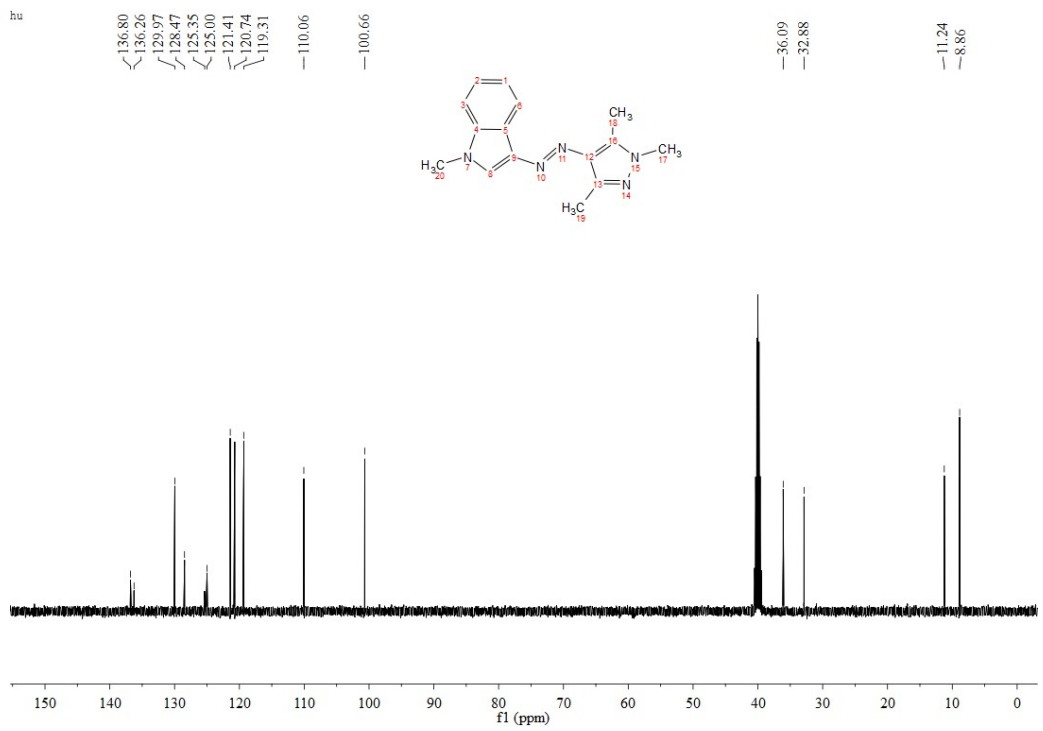


Figure S26. ^{13}C NMR sprectrum of **B2** in DMSO-d_6.

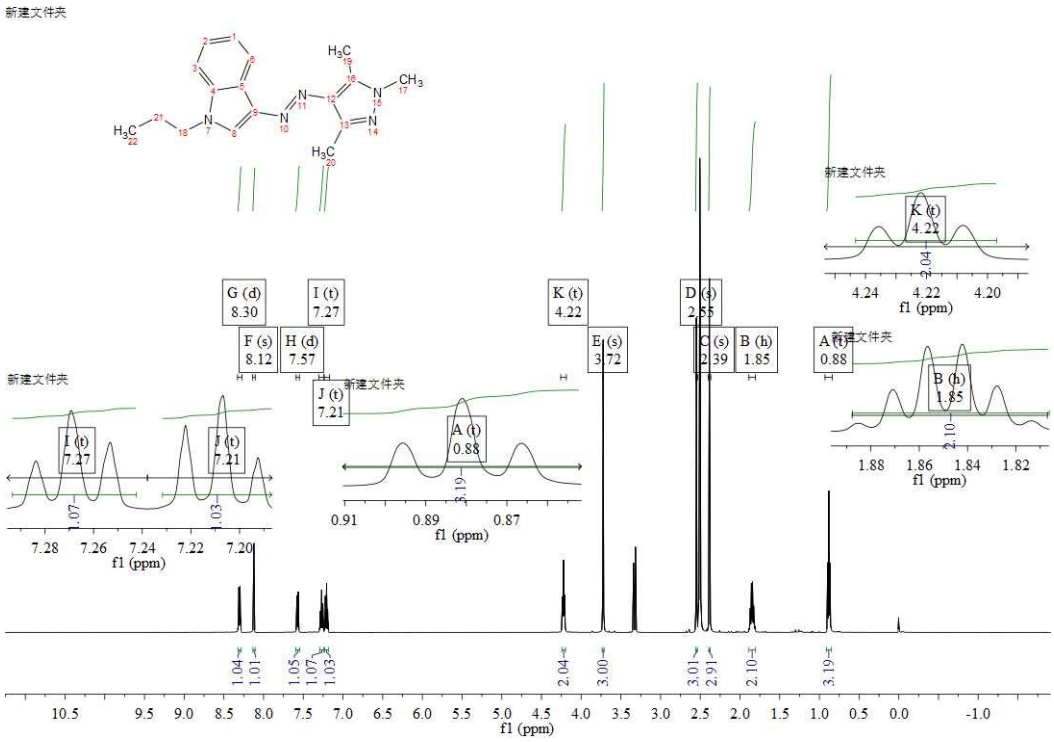


Figure S27. ^{1}H NMR sprectrum of **B3** in DMSO-d_6.

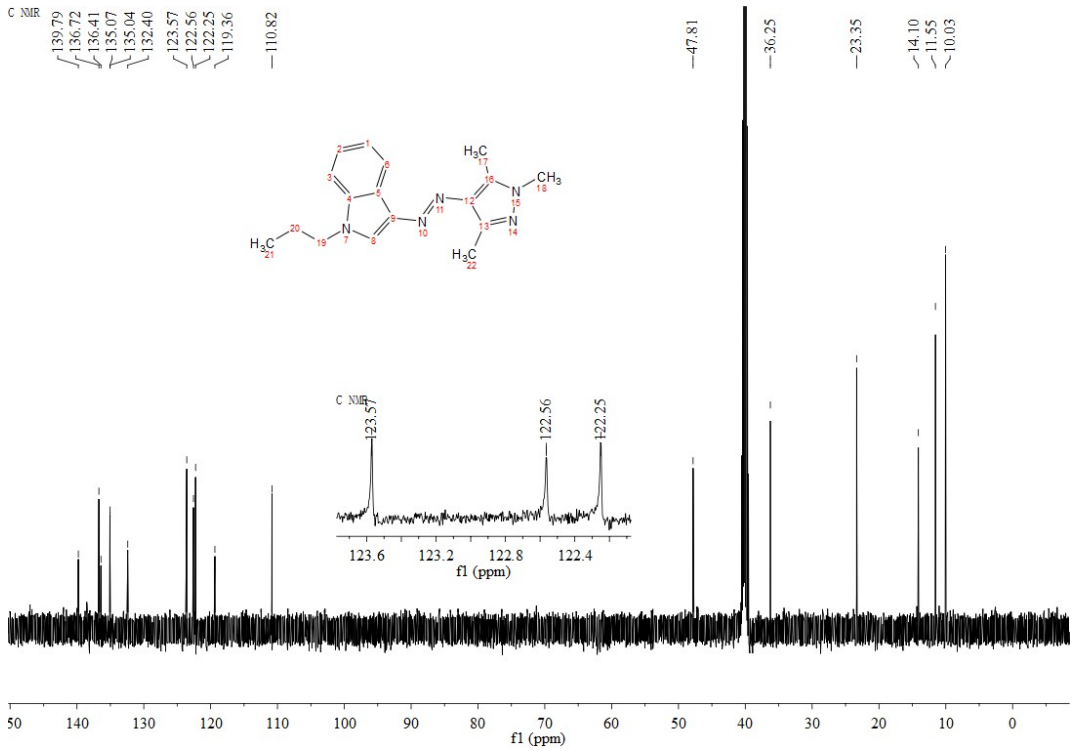


Figure S28. ^{13}C NMR sprectrum of **B3** in DMSO-d_6.

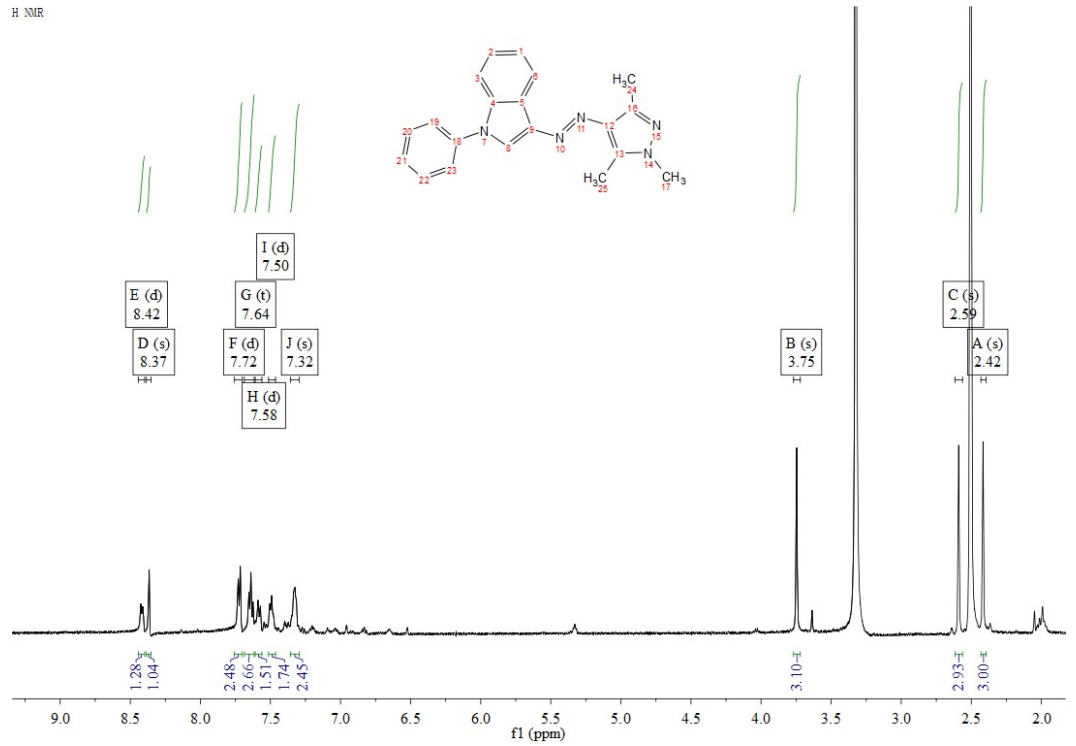


Figure S29. ^{1}H NMR sprectrum of **B4** in DMSO-d_6.

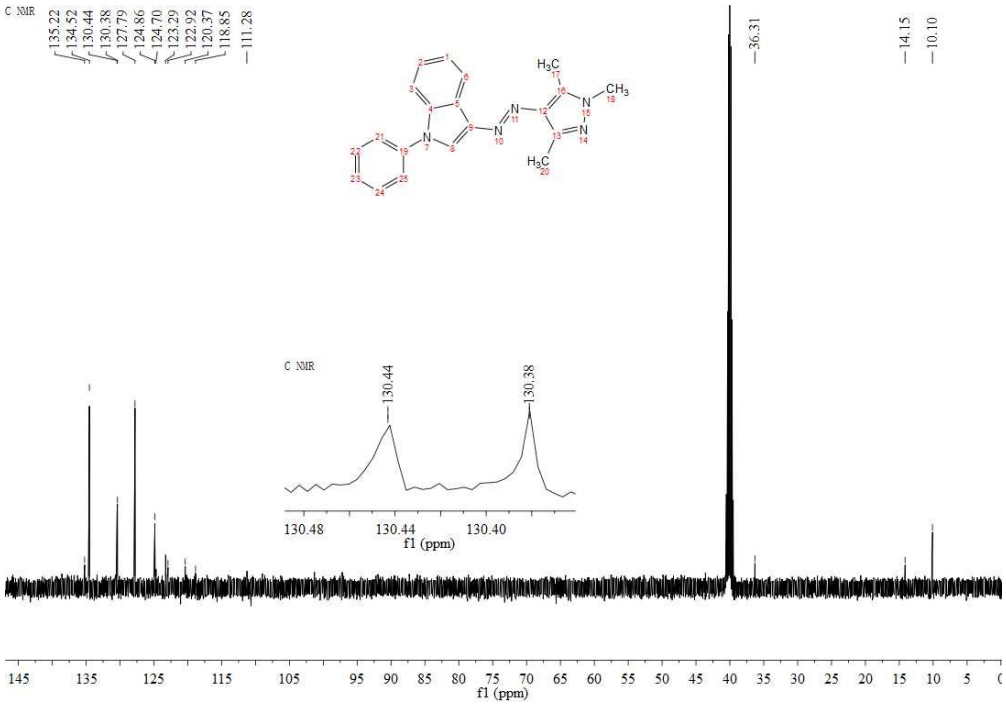


Figure S30. ^{13}C NMR sprectrum of **B4** in DMSO-d_6.

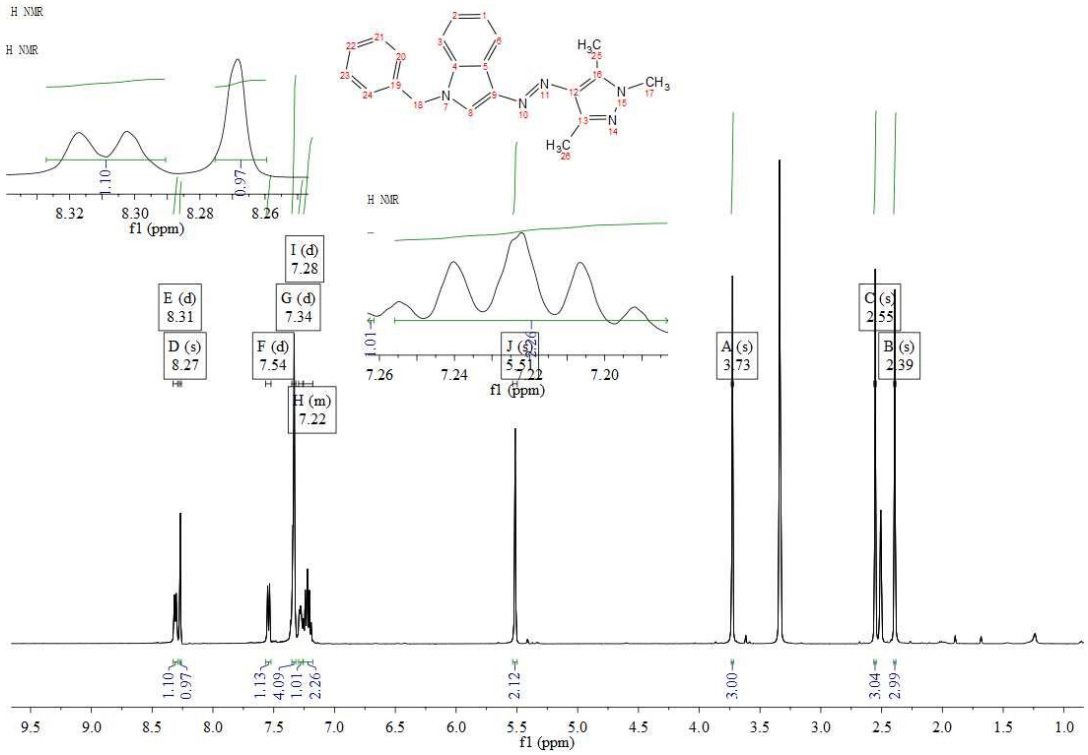


Figure S31. ^{1}H NMR sprectrum of **B5** in DMSO-d_6.

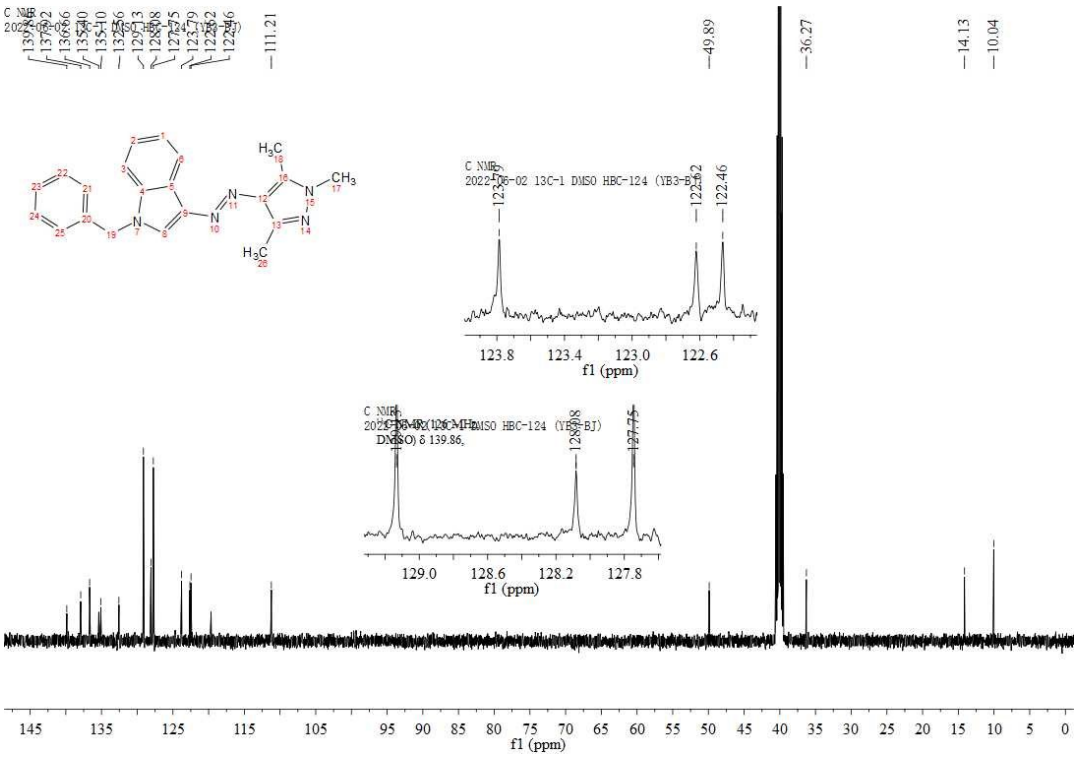


Figure S32. ^{13}C NMR sprectrum of **B5** in DMSO-d_6.

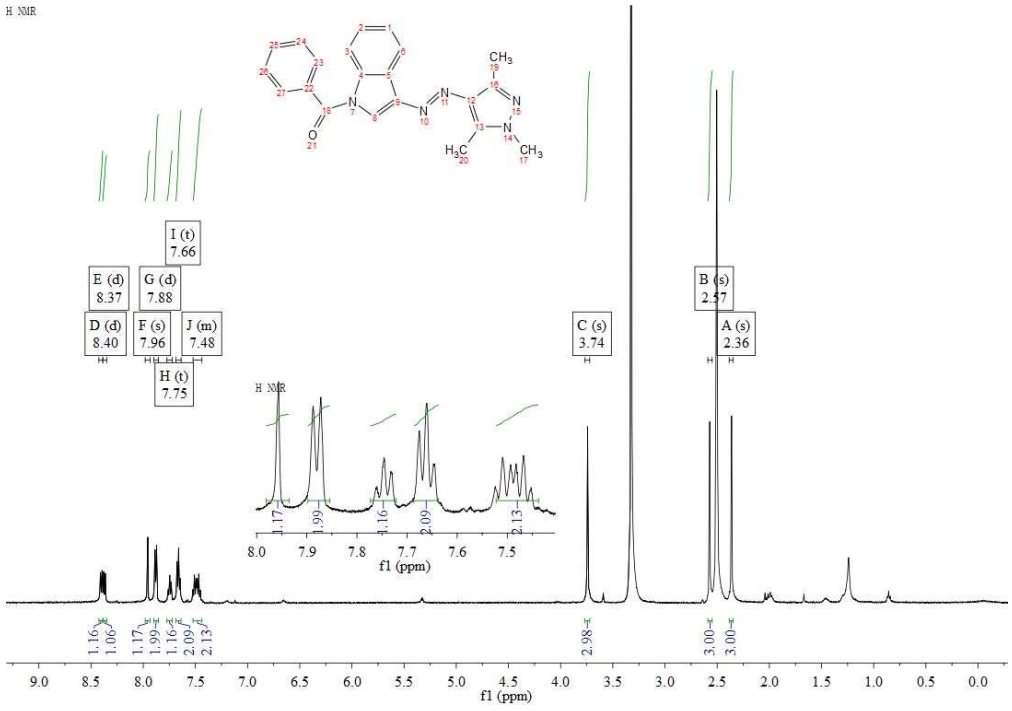


Figure S33. ^{1}H NMR sprectrum of **B6** in DMSO-d_6.

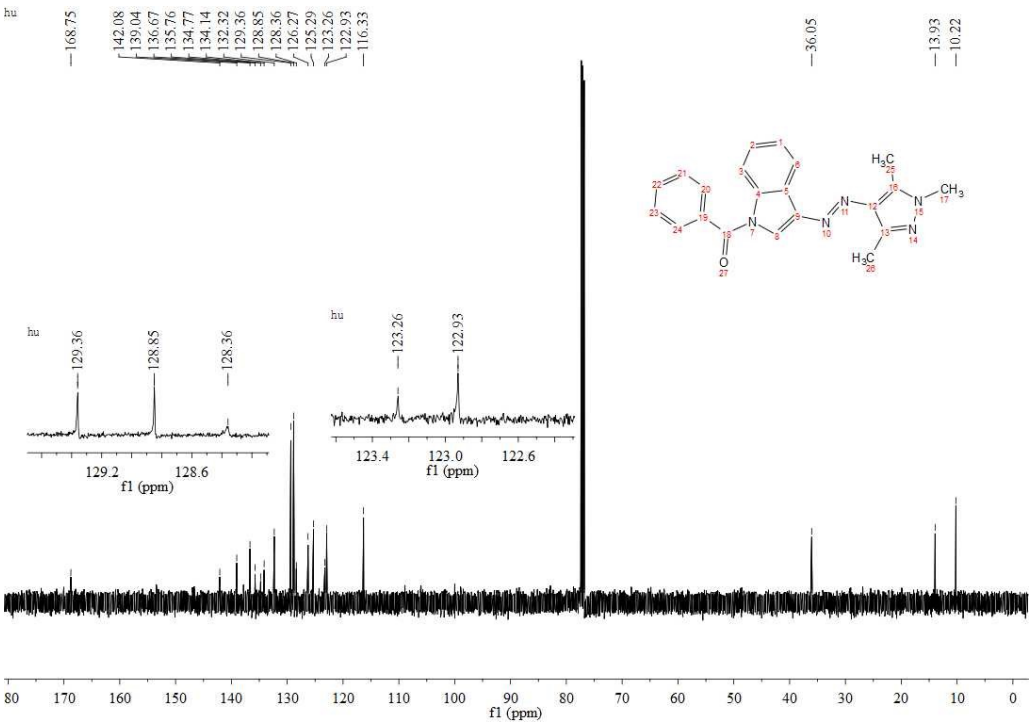


Figure S34. ^{13}C NMR sprectrum of **B6** in $CDCl_3$.

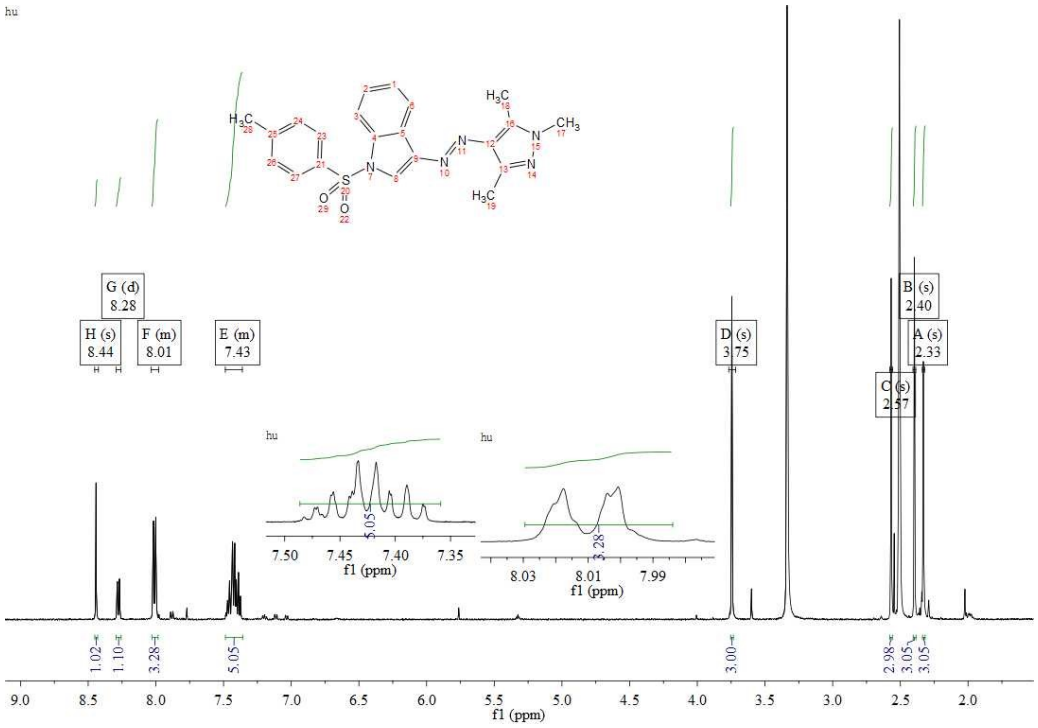


Figure S35. ^{1}H NMR sprectrum of **B7** in DMSO-d_6.

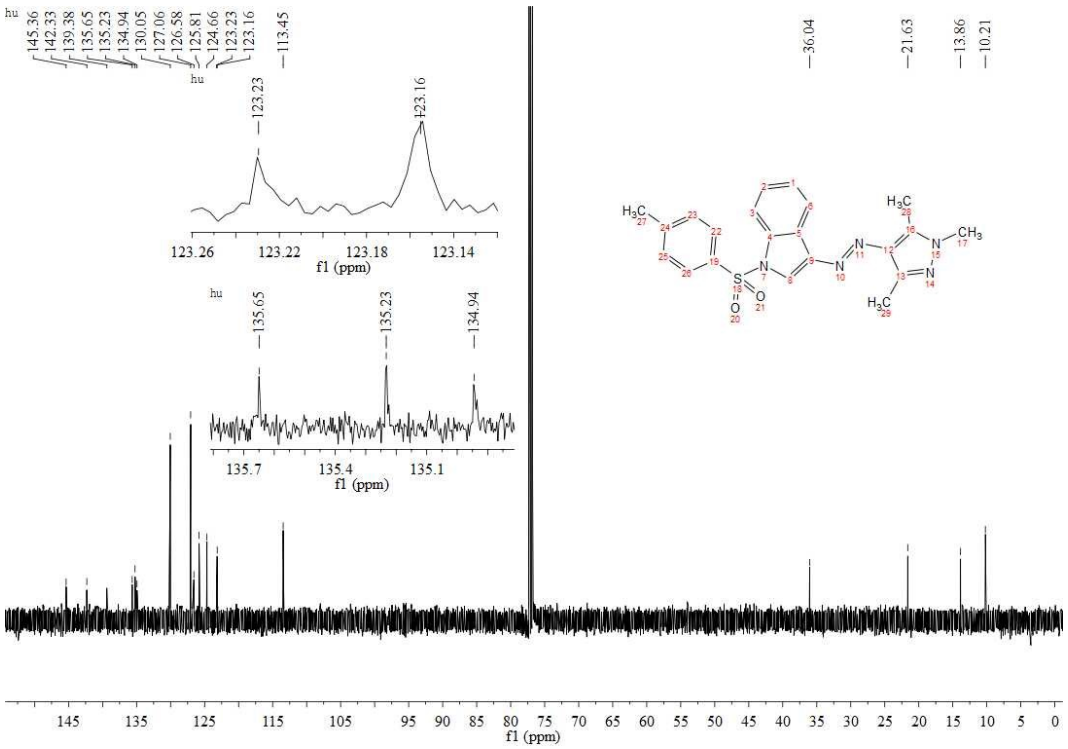


Figure S36. ^{13}C NMR sprectrum of **B7** in $CDCl_3$.

1.3. Crystal structure information

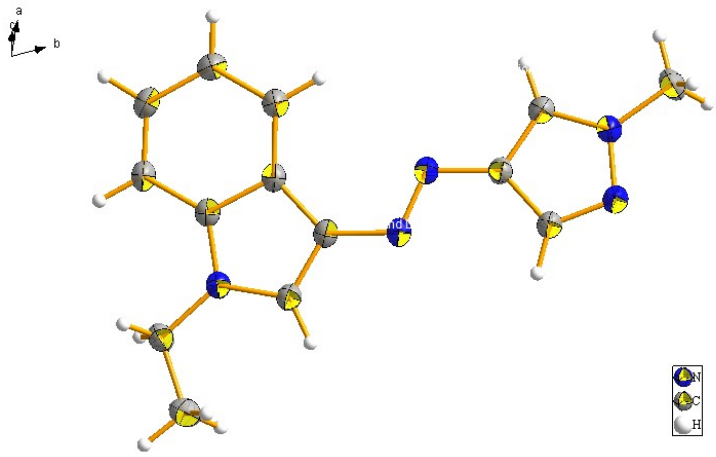


Figure S37. Molecular ellipsoid diagram of target compound (*E*)-**A3** (CCDC number: 2184785).

Table S1. Crystal structure information of compound **A3**

Formula	$C_{14}H_{15}N_5$
Formula weight	253.31
Temperature/K	193.00
Crystal system	triclinic

Space group	P-1
a(Å)	8.7299(5)
b(Å)	9.2355(5)
c(Å)	9.5254(5)
α(°)	65.084(2)
β(°)	68.436(2)
γ(°)	73.691(2)
Volume(Å^3)	640.49(6)
Z	2
ρ_{calc}(g/cm^3)	1.313
μ(mm^{-1})	0.084
F(000)	268.0
Crystal size(mm^3)	0.16 × 0.15 × 0.13
Radiation	MoKα (λ = 0.71073)
2ϑ range for data collection(°)	4.918 to 54.976
Index ranges	-11 ≤ h ≤ 11, -11 ≤ k ≤ 11, -12 ≤ l ≤ 12
Reflections collected	20760
Independent reflections	2926 [R_{int} = 0.0380, R_{sigma} = 0.0229]
Data/restraints/parameters	2926/0/174
Goodness-of-fit on F^2	1.100
Final *R* indexes [I>=2σ (I)]	R_1 = 0.0401, wR_2 = 0.1099
Final *R* indexes [all data]	R_1 = 0.0436, wR_2 = 0.1127
Largest diff. peak/hole (e Å^{-3})	0.26/-0.22

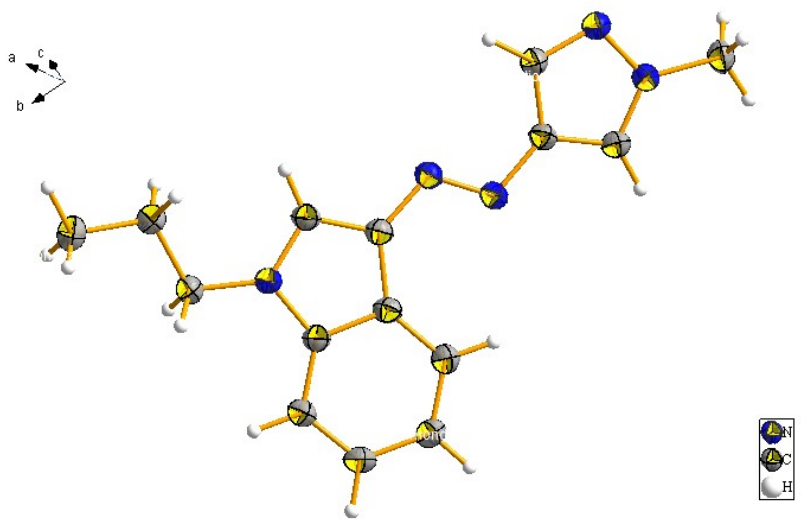


Figure S38. Molecular ellipsoid diagram of target compound (*E*)-**A4** (CCDC number: 2184786).

Table S2. Crystal structure information of compound **A4**

Formula	$C_{15}H_{17}N_5$
Formula weight	267.33
Temperature/K	193.00
Crystal system	triclinic
Space group	P-1
a(Å)	9.2845(5)
b(Å)	9.2942(5)
c(Å)	9.4489(4)
α(°)	67.465(2)
β(°)	69.500(2)
γ(°)	70.108(2)
Volume(Å^3)	685.12(6)
Z	2
ρ_{calc}(g/cm^3)	1.296
μ(mm^{-1})	0.082
F(000)	284.0
Crystal size(mm^3)	0.2 × 0.18 × 0.15
Radiation	MoKα (λ = 0.71073)
2ϑ range for data collection(°)	4.822 to 54.972
Index ranges	-12 ≤ h ≤ 12, -12 ≤ k ≤ 12, -12 ≤ l ≤ 12
Reflections collected	22511

Independent reflections	3127 [R_{int} = 0.0419, R_{sigma} = 0.0279]
Data/restraints/parameters	3127/0/183
Goodness-of-fit on F^2	1.059
Final R indexes [I>=2σ (I)]	R_1 = 0.0404, wR_2 = 0.1083
Final R indexes [all data]	R_1 = 0.0438, wR_2 = 0.1112
Largest diff. peak/hole (e Å^{-3})	0.26/-0.22

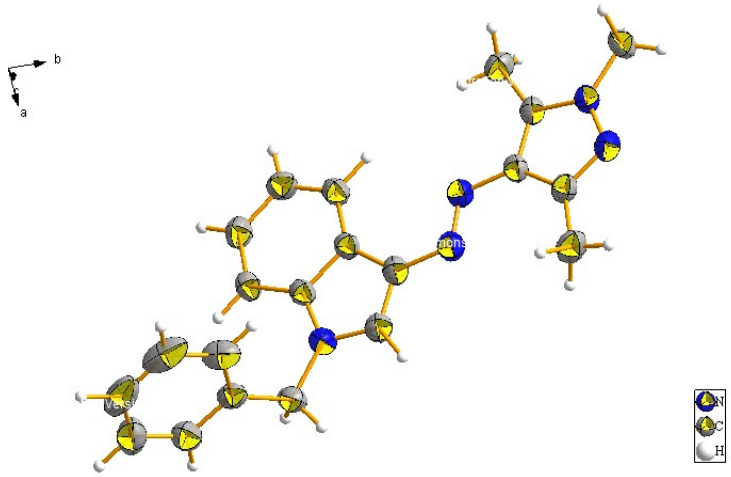


Figure S39. Molecular ellipsoid diagram of target compound (*E*)-**B5** (CCDC number: 2184787).

Table S3. Crystal structure information of compound **B5**

Formula	$C_{21}H_{21}N_5$
Formula weight	343.43
Temperature/K	193.00
Crystal system	triclinic
Space group	P-1
a(Å)	5.4109(4)
b(Å)	12.3109(6)
c(Å)	14.8982(9)
α(°)	67.826(2)
β(°)	83.410(2)
γ(°)	88.031(2)
Volume(Å^3)	912.90(10)
Z	2
ρ_{calc}(g/cm^3)	1.249

μ(mm^{-1})	0.077
F(000)	364.0
Crystal size(mm^3)	0.16 × 0.15 × 0.12
Radiation	MoKα (λ = 0.71073)
2ϑ range for data collection(°)	5.438 to 54.902
Index ranges	-7 ≤ h ≤ 7, -15 ≤ k ≤ 14, -19 ≤ l ≤ 19
Reflections collected	18968
Independent reflections	4149 [R_{int} = 0.0703, R_{sigma} = 0.0510]
Data/restraints/parameters	4149/0/319
Goodness-of-fit on F^2	1.033
Final *R* indexes [I>=2σ (I)]	R_1 = 0.0533, wR_2 = 0.1216
Final *R* indexes [all data]	R_1 = 0.0903, wR_2 = 0.1498
Largest diff. peak/hole (e Å^{-3})	0.29/-0.18

2 Photochemical research

General information

The light sources used for photoisomerization are: 365 nm LED lamp (3 W), 460 nm LED lamp (5 W), 254 nm lamp (3 W), 302 nm LED lamp (3 W), 515 nm laser (80 mW), 650 nm laser (200 mW).

Photochemical isomerizations (PSSs)

PSS compositions at different wavelengths were determined as follows: 365 and 460 nm PSSs were determined by ^{1}H NMR in DMSO. The sample (1-2 mg/mL in DMSO-*d6*) was sealed in a quartz cuvette and then irradiated with 365 nm or 460 nm LED light typically for 30-40 min to ensure the establishment of PSS. Then we used the UV-Vis spectra of a trans isomer and a 365 nm PSS state to deduce the spectrum of the cis isomer. A pair of trans and cis spectra were used for fitting the respective spectra at 254, 302, 515, and 650 nm PSS states. According to the fitting results, isomer fractions in the respective PSS states were obtained.

Spectral fitting follows the equation: $\alpha \times Abs_{trans}(\lambda) + (1-\alpha) \times Abs_{cis}(\lambda) = Abs_{pss}(\lambda)$.

With α the content of trans isomer in a PSS state, Abstrans (λ), Abscis (λ) and Abspss (λ) the srectra of pure trans, pure cis and pss state (at the same concentratin).

Optical cycle

To check the photostability, solutions of the synthesized switches in DMSO were exposed to 365 nm and 460 nm light alternately. After 8-10 times cycles of photolysis, noticeable photobleaching was not found for any of these switches.

Thermal isomerization kinetics[s1]

Thermal cis-trans isomerization kinetics was studied at elevated temperatures. The trans sample was thermally equilibrated for at least 10 min to reach the equilibrium temperature, and the absorbance at π−π* λmax was recorded. It was then irradiated for 10 s by 365 nm UV light to reach a cis-rich state and thermally equilibrated again for 2 min. The absorbance was read at a certain interval (typically, 60 s) with a sampling time of 1 s.

The absorbance data were fitted following first-order rate equation:

$$\ln [(A_\infty - A_0)/ (A_\infty - A_t)] = kt$$

A_∞, A_0 and A_t represent the absorbances of pure trans state, at initial state (PSS_{cis}) and at reaction time *t*.

The thermal half-life $t_{1/2}$ of a first-order kinetics reaction was calculated as:

$$t_{1/2} = \ln 2/k$$

The Arrhenius equation can be used to analyse the relationship between *k* and reaction temperature *T*:

$$\ln k = (-E_a/RT)\ln A$$

E_a is the apparent activation energy, *R* is the gas constant and *A* is the pre-exponential factor.

2.1 UV/Vis spectra for the manuscript text.

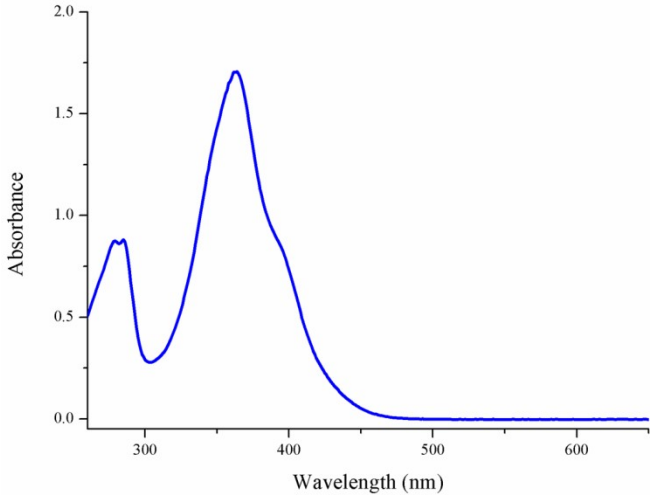


Fig. S40. UV/Vis sprectrum at ambient light of compound **A1** in DMSO at room temperature (0.1 mM).

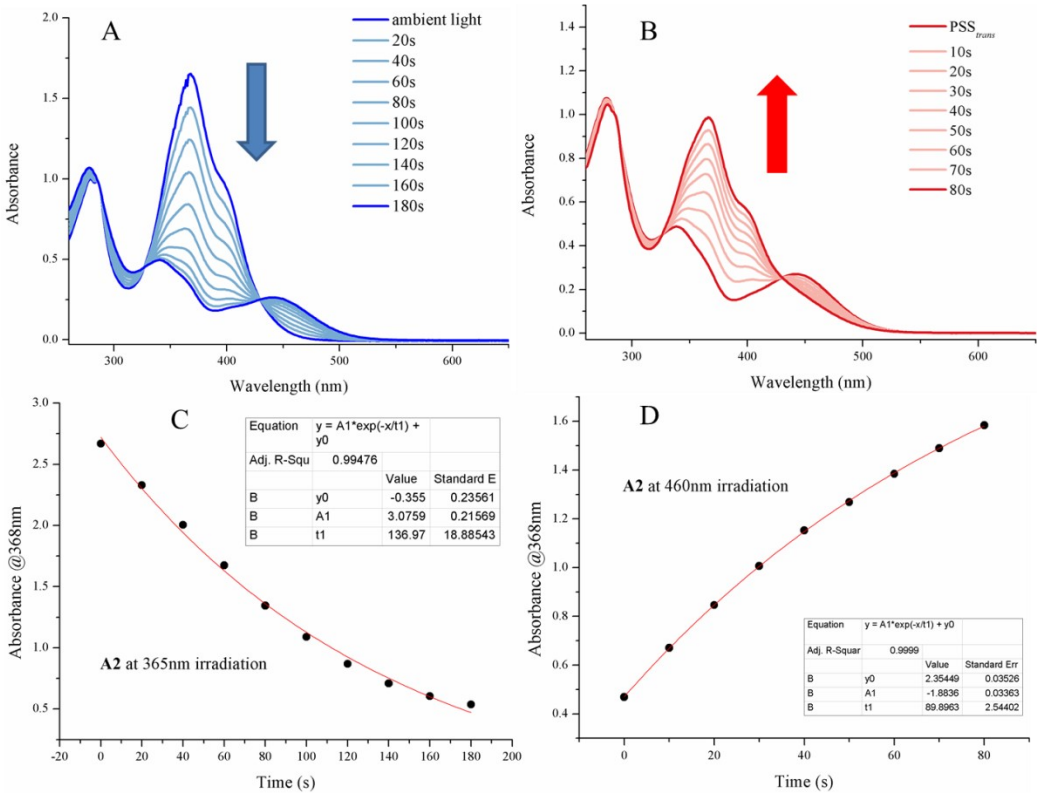


Fig. S41. UV/Vis spectral changes during (A) UV (365 nm) and (B) visible light (460 nm) irradiation of compound **A2** in DMSO at room temperature. Kinetics of the photoisomerization for compound **A2** at (C) 365 nm irradiation and at (D) 460 nm irradiation (0.108 mM).

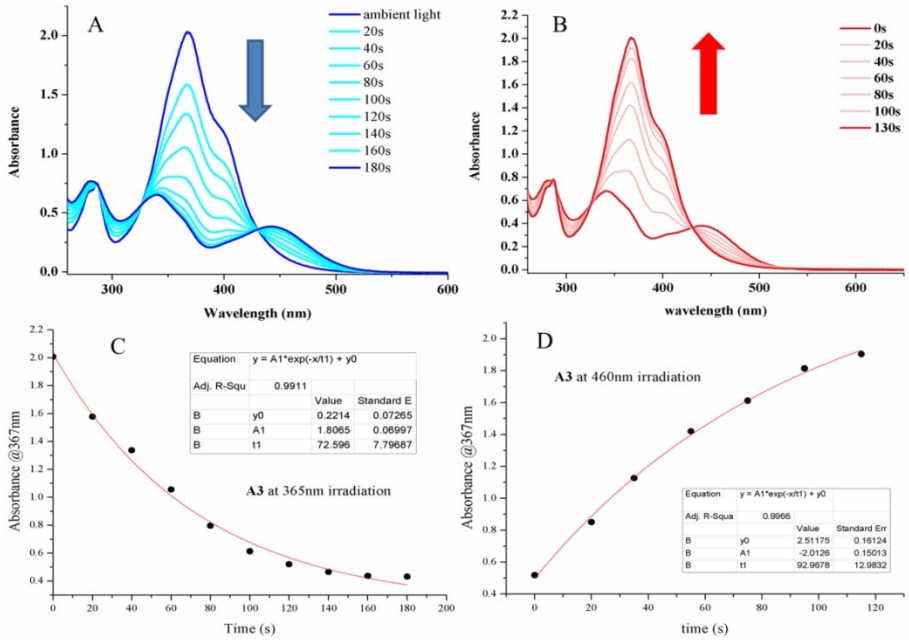


Fig. S42. UV/Vis spectral changes during (A) UV (365 nm) and (B) visible light (460 nm) irradiation of compound **A3** in DMSO at room temperature. Kinetics of the photoisomerization for compound **A3** at (C) 365 nm irradiation and at (D) 460 nm irradiation (0.098 mM).

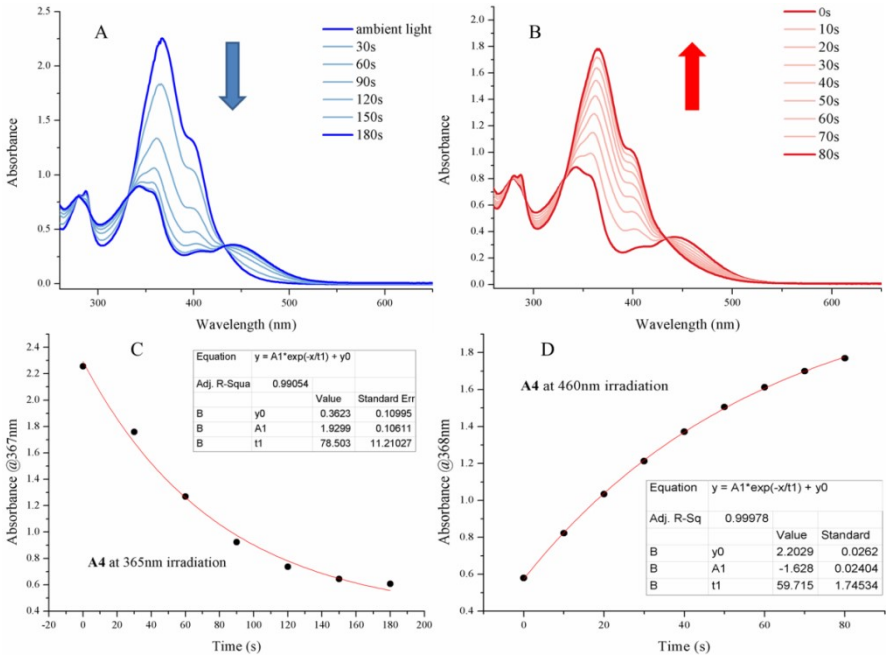


Fig. S43. UV/Vis spectral changes during (A) UV (365 nm) and (B) visible light (460 nm) irradiation of compound **A4** in DMSO at room temperature. Kinetics of the photoisomerization for compound **A4** at (C) 365 nm irradiation and at (D) 460 nm irradiation (0. 100 mM).

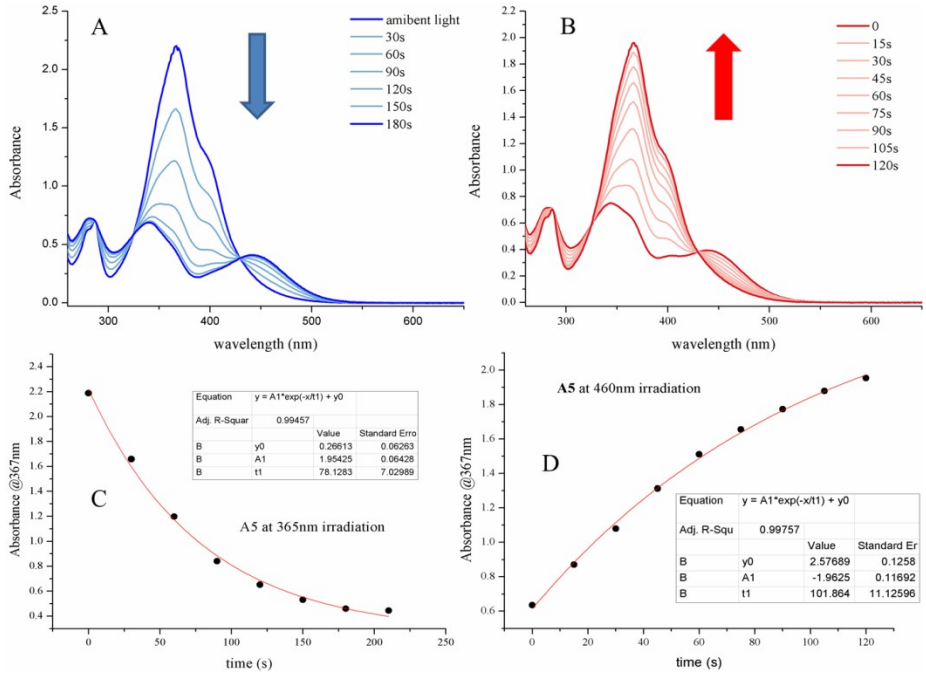


Fig. S44. UV/Vis spectral changes during (A) UV (365 nm) and (B) visible light (460 nm) irradiation of compound **A5** in DMSO at room temperature. Kinetics of the photoisomerization for compound **A5** at (C) 365 nm irradiation and at (D) 460 nm irradiation (0.100 mM).

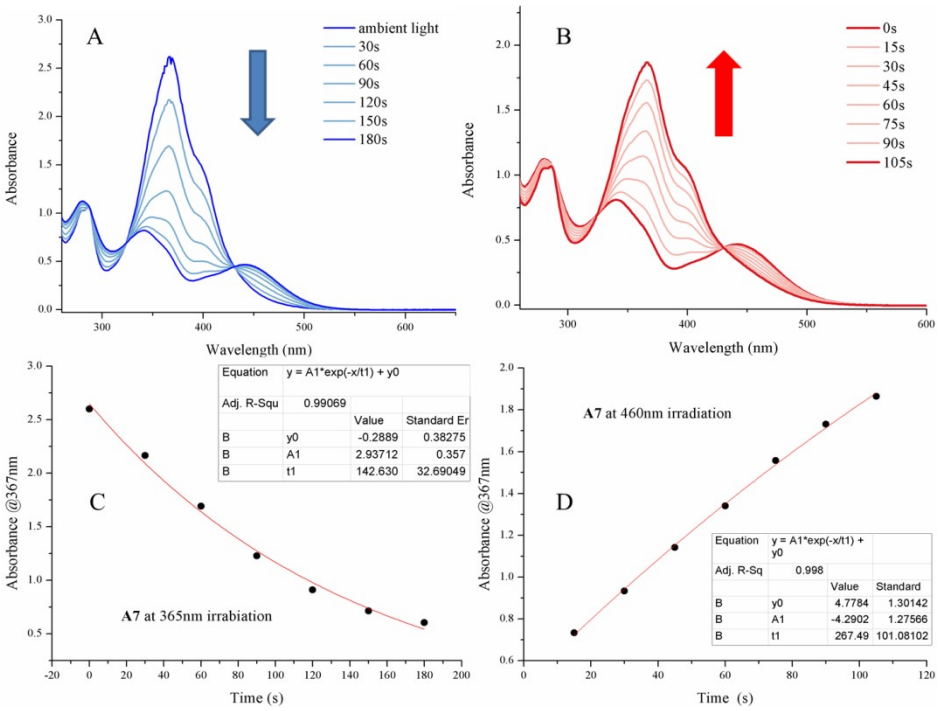


Fig. S45. UV/Vis spectral changes during (A) UV (365 nm) and (B) visible light (460 nm) irradiation of compound **A7** in DMSO at room temperature. Kinetics of the photoisomerization for compound **A7** at (C) 365 nm irradiation and at (D) 460 nm irradiation (0.100 mM).

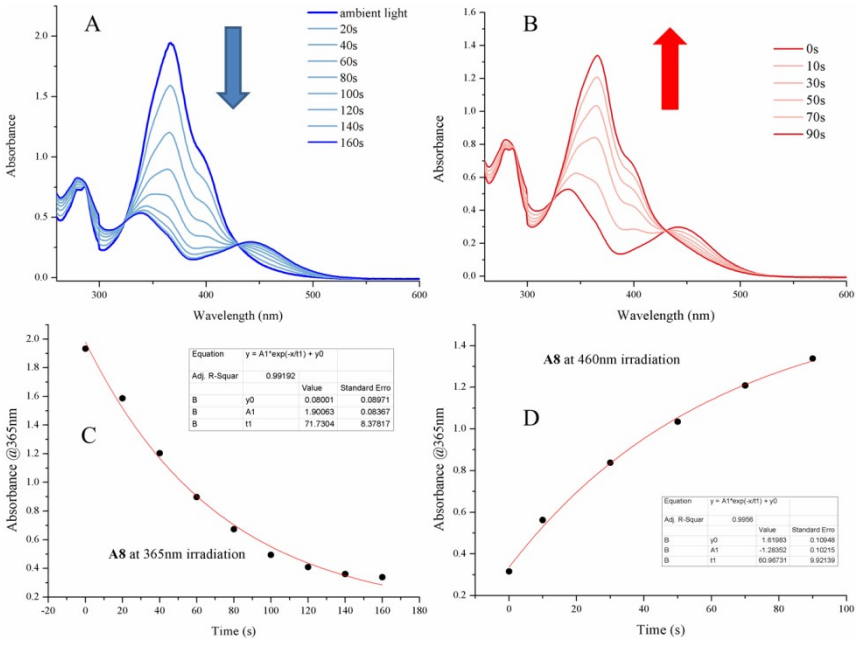


Fig. S46. UV/Vis spectral changes during (A) UV (365 nm) and (B) visible light (460 nm) irradiation of compound **A8** in DMSO at room temperature. Kinetics of the photoisomerization for compound **A8** at (C) 365 nm irradiation and at (D) 460 nm irradiation (0.095 mM).

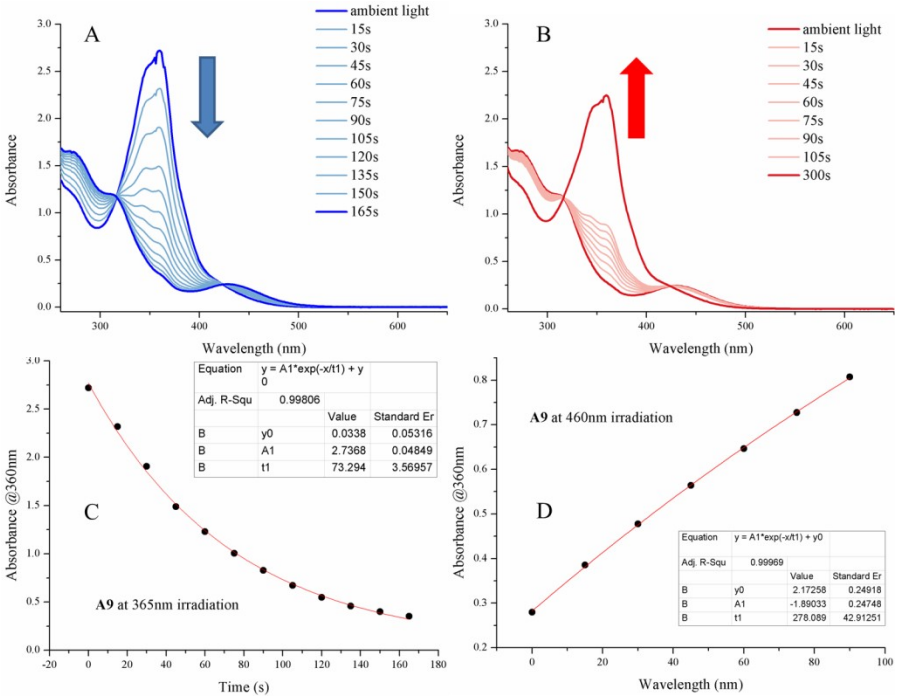


Fig. S47. UV/Vis spectral changes during (A) UV (365 nm) and (B) visible light (460 nm) irradiation of compound **A9** in DMSO at room temperature. Kinetics of the photoisomerization for compound **A9** at (C) 365 nm irradiation and at (D) 460 nm irradiation (0.097 mM).

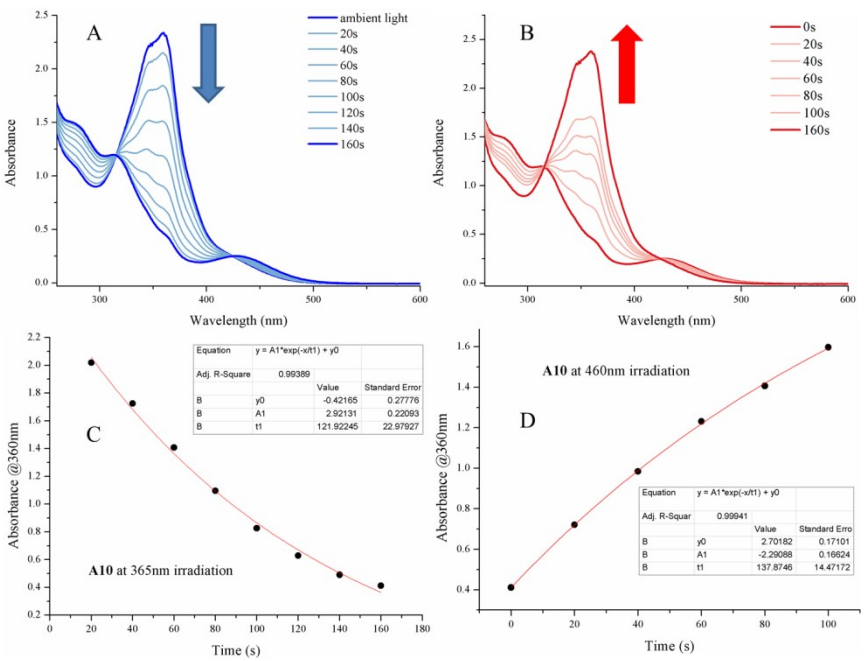


Fig. S48. UV/Vis spectral changes during (A) UV (365 nm) and (B) visible light (460 nm) irradiation of compound **A10** in DMSO at room temperature. Kinetics of the photoisomerization for compound **A10** at (C) 365 nm irradiation and at (D) 460 nm irradiation (0.1 mM).

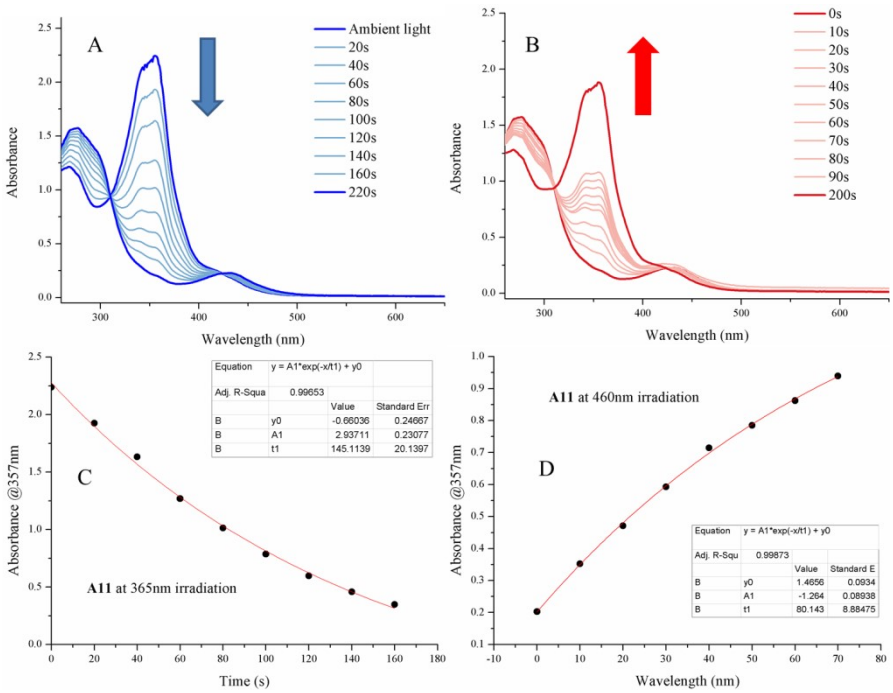


Fig. S49. UV/Vis spectral changes during (A) UV (365 nm) and (B) visible light (460 nm) irradiation of compound **A11** in DMSO at room temperature. Kinetics of the photoisomerization for compound **A11** at (C) 365 nm irradiation and at (D) 460 nm irradiation (0.1 mM).

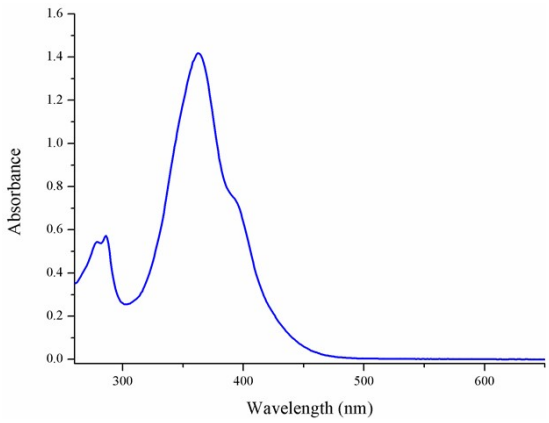


Fig. S50. UV/Vis spectra at ambient light of compound **B1** in DMSO at room temperature (0.1 mM).

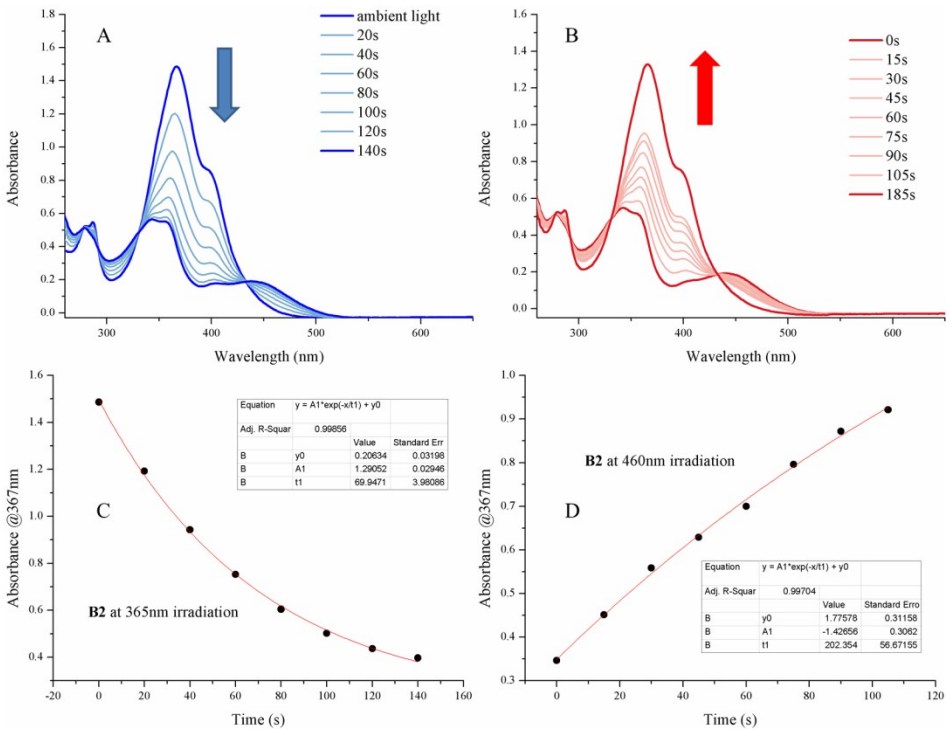


Fig. S51. UV/Vis spectral changes during (A) UV (365 nm) and (B) visible light (460 nm) irradiation of compound **B2** in DMSO at room temperature. Kinetics of the photoisomerization for compound **B2** at (C) 365 nm irradiation and at (D) 460 nm irradiation (0.1 mM).

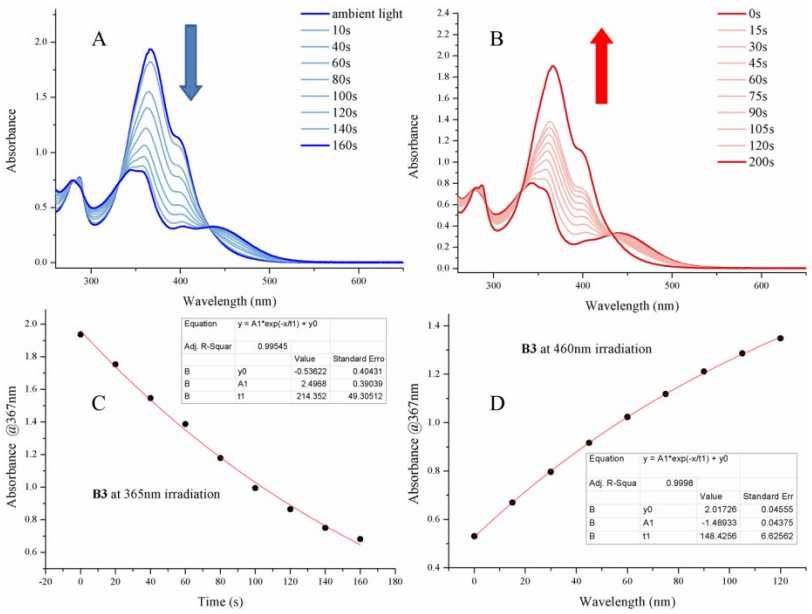


Fig. S52. UV/Vis spectral changes during (A) UV (365 nm) and (B) visible light (460 nm) irradiation of compound **B3** in DMSO at room temperature. Kinetics of the photoisomerization for compound **B3** at (C) 365 nm irradiation and at (D) 460 nm irradiation (0.1 mM).

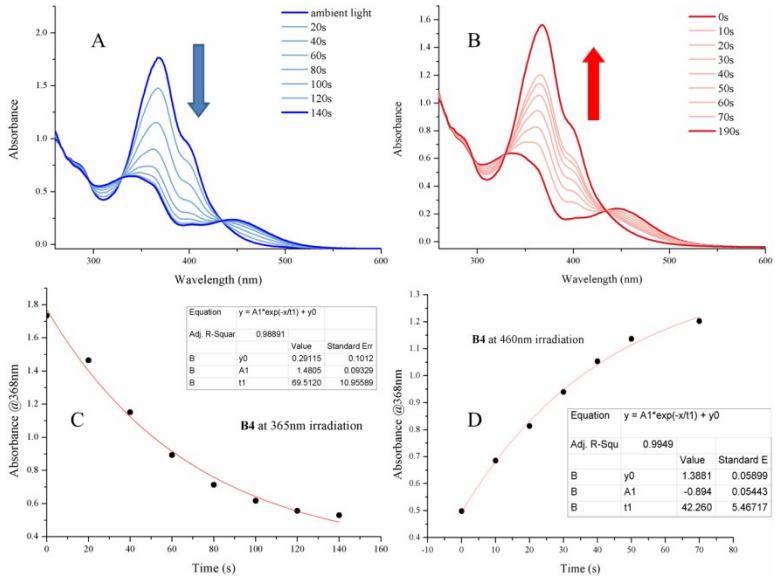


Fig. S53. UV/Vis spectral changes during (A) UV (365 nm) and (B) visible light (460 nm) irradiation of compound **B4** in DMSO at room temperature. Kinetics of the photoisomerization for compound **B4** at (C) 365 nm irradiation and at (D) 460 nm irradiation (0.1 mM).

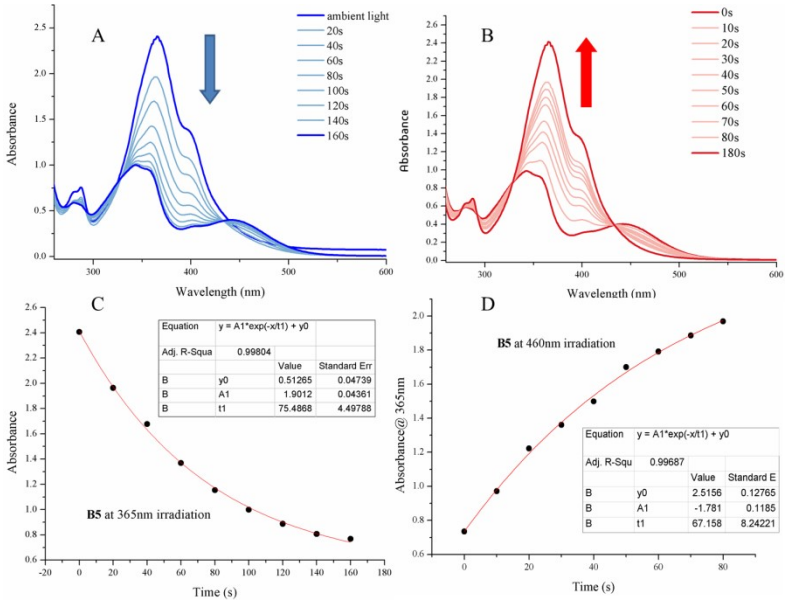


Fig. S54. UV/Vis spectral changes during (A) UV (365 nm) and (B) visible light (460 nm) irradiation of compound **B5** in DMSO at room temperature. Kinetics of the photoisomerization for compound **B5** at (C) 365 nm irradiation and at (D) 460 nm irradiation (0.1 mM).

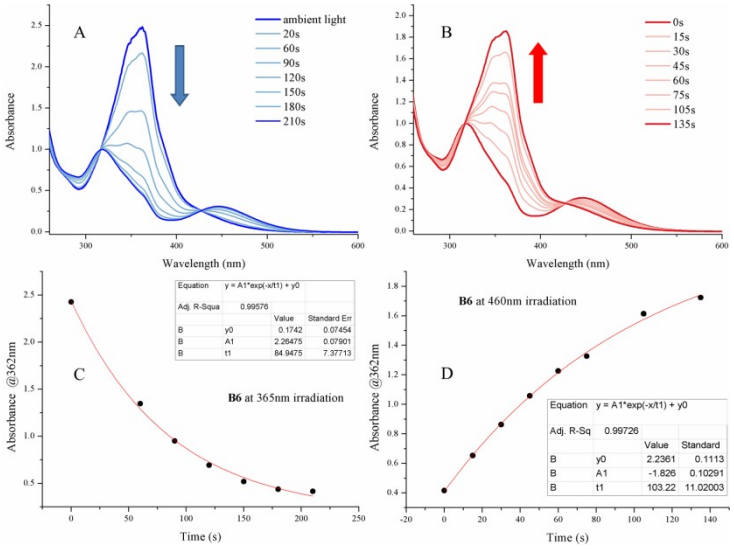


Fig. S55. UV/Vis spectral changes during (A) UV (365 nm) and (B) visible light (460 nm) irradiation of compound **B6** in DMSO at room temperature. Kinetics of the photoisomerization for compound **B6** at (C) 365 nm irradiation and at (D) 460 nm irradiation (0.1 mM).

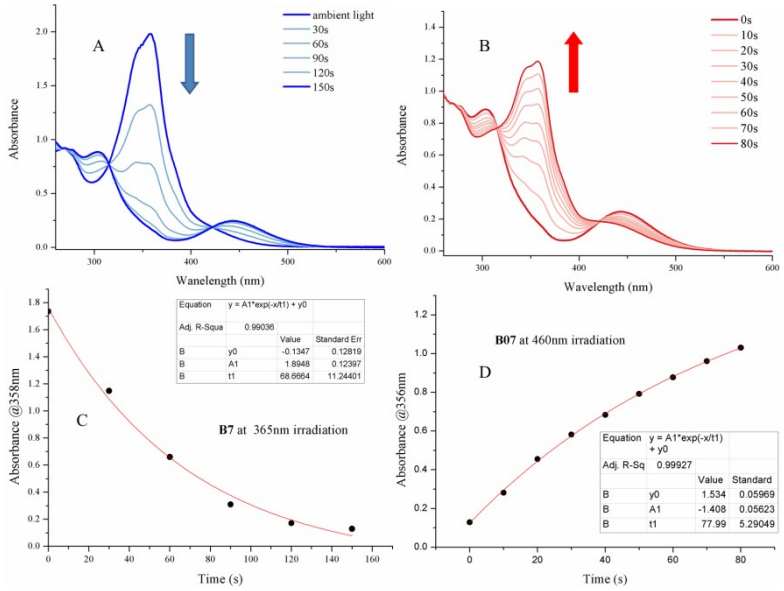


Fig. S56. UV/Vis spectral changes during (A) UV (365 nm) and (B) visible light (460 nm) irradiation of compound **B7** in DMSO at room temperature. Kinetics of the photoisomerization for compound **B7** at (C) 365 nm irradiation and at (D) 460 nm irradiation (0.1 mM).

2.2

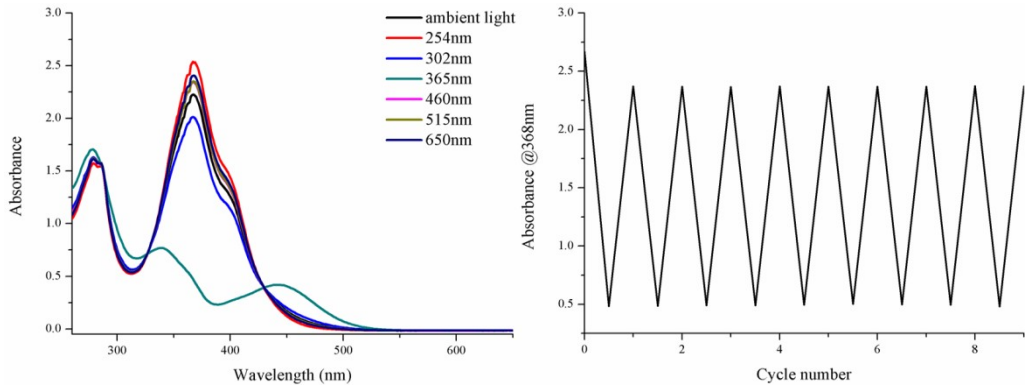


Fig. S57. UV/Vis absorption spectra of **A3** in PSSs generated by irradiations with various wavelengths of light in DMSO (left). Multiple rounds of photoswitching of **A3** by alternating 365 nm and 460 nm light irradiations in DMSO (right).

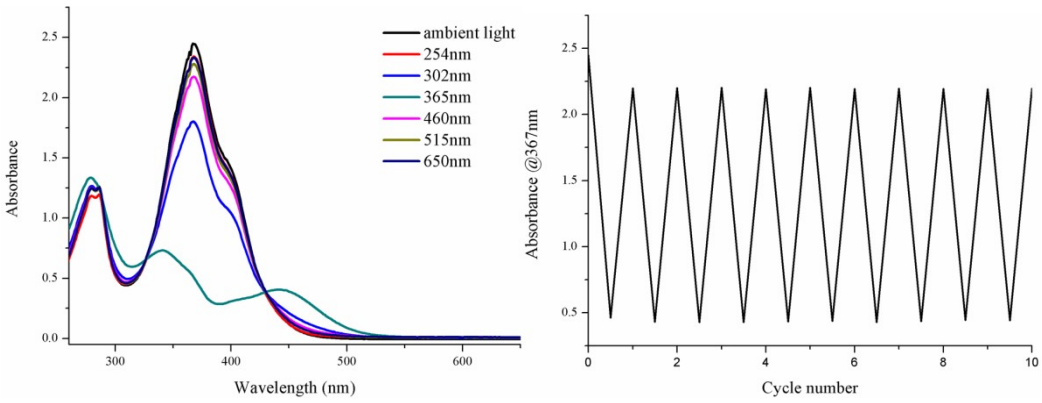


Fig. S58. UV/Vis absorption spectra of **A2** in PSSs generated by irradiations with various wavelengths of light in DMSO (left). Multiple rounds of photoswitching of **A2** by alternating 365 nm and 460 nm light irradiations in DMSO (right).

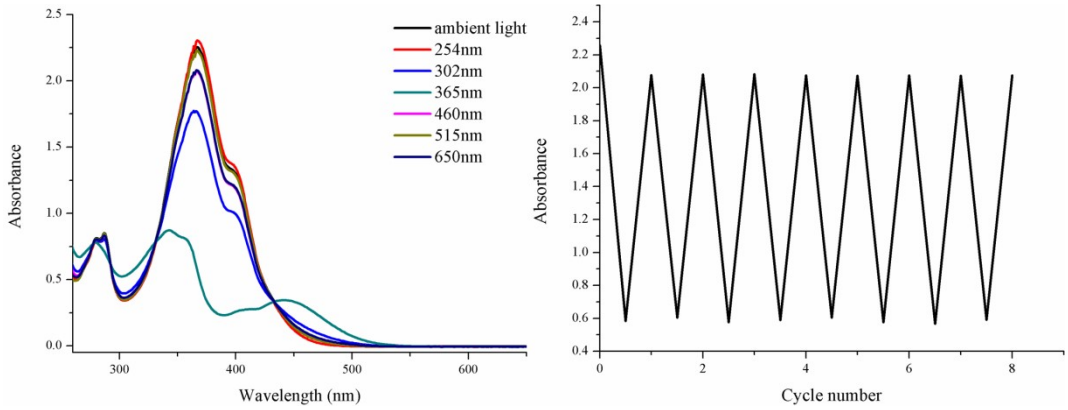


Fig. S59. UV/Vis absorption spectra of **A4** in PSSs generated by irradiations with various wavelengths of light in DMSO (left). Multiple rounds of photoswitching of **A4** by alternating 365 nm and 460 nm light irradiations in DMSO (right).

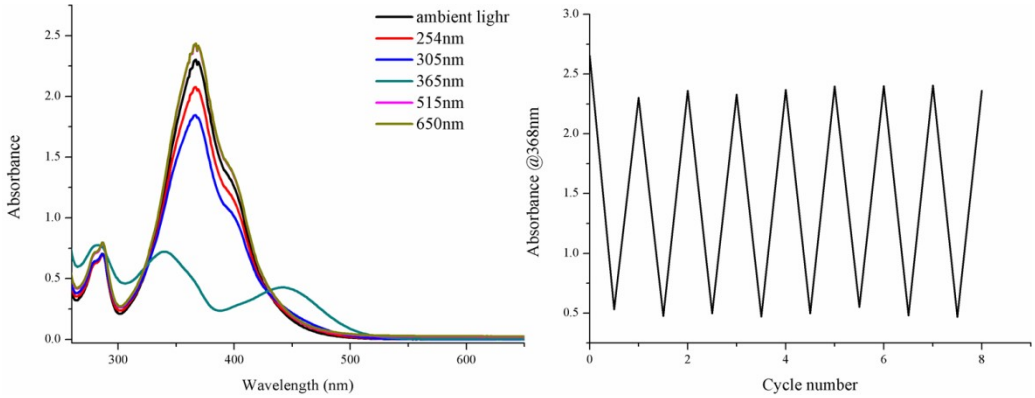


Fig. S60. UV/Vis absorption spectra of **A5** in PSSs generated by irradiations with various wavelengths of light in DMSO (left). Multiple rounds of photoswitching of **A5** by alternating 365 nm and 460 nm light irradiations in DMSO (right).

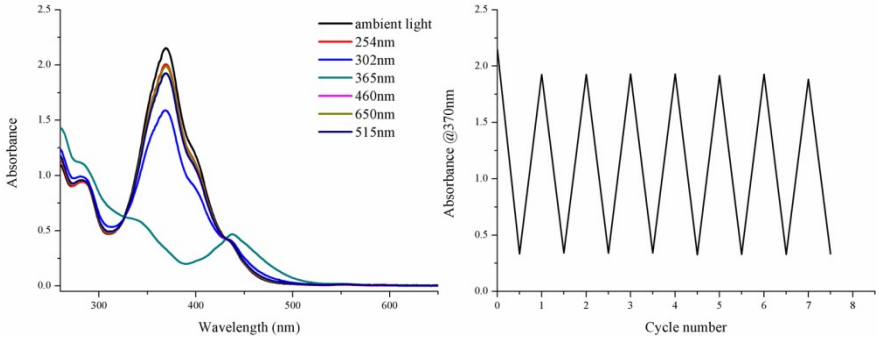


Fig. S61. UV/Vis absorption spectra of **A6** in PSSs generated by irradiations with various wavelengths of light in DMSO (left). Multiple rounds of photoswitching of **A6** by alternating 365 nm and 460 nm light irradiations in DMSO (right).

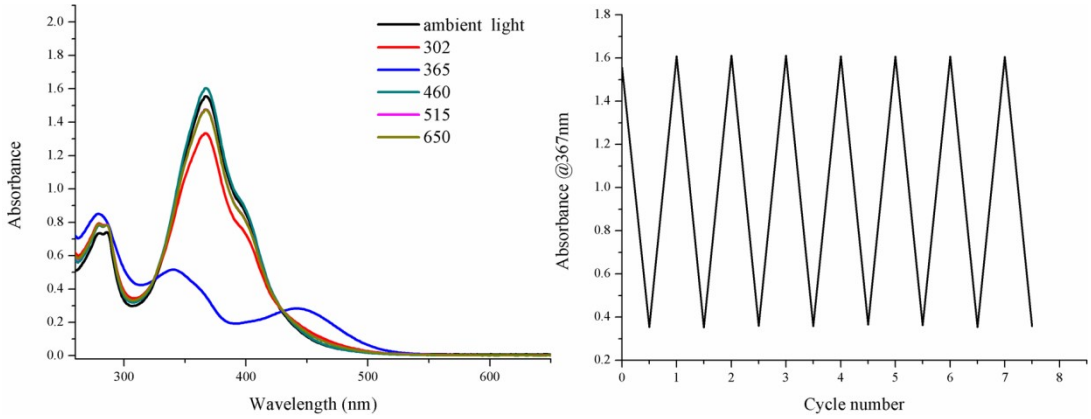


Fig. S62. UV/Vis absorption spectra of **A7** in PSSs generated by irradiations with various wavelengths of light in DMSO (left). Multiple rounds of photoswitching of **A7** by alternating 365 nm and 460 nm light irradiations in DMSO (right).

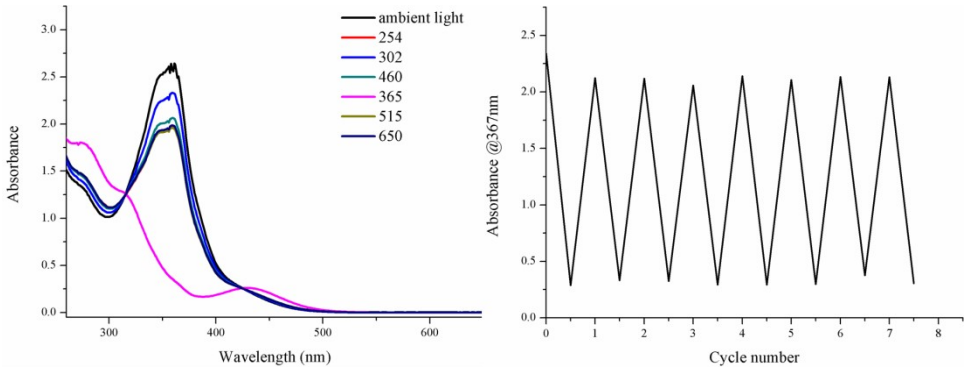


Fig. S63. UV/Vis absorption spectra of **A8** in PSSs generated by irradiations with various wavelengths of light in DMSO (left). Multiple rounds of photoswitching of **A8** by alternating 365 nm and 460 nm light irradiations in DMSO (right).

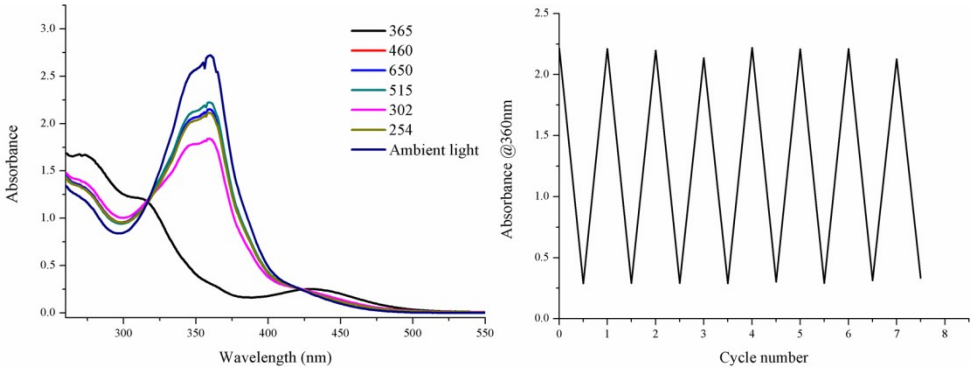


Fig. S64. UV/Vis absorption spectra of **A9** in PSSs generated by irradiations with various wavelengths of light in DMSO (left). Multiple rounds of photoswitching of **A9** by alternating 365 nm and 460 nm light irradiations in DMSO (right).

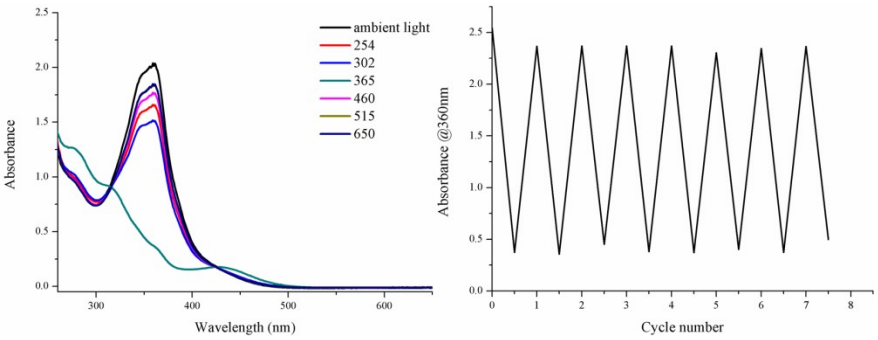


Fig. S65. UV/Vis absorption spectra of **A10** in PSSs generated by irradiations with various wavelengths of light in DMSO (left). Multiple rounds of photoswitching of **A10** by alternating 365 nm and 460 nm light irradiations in DMSO (right).

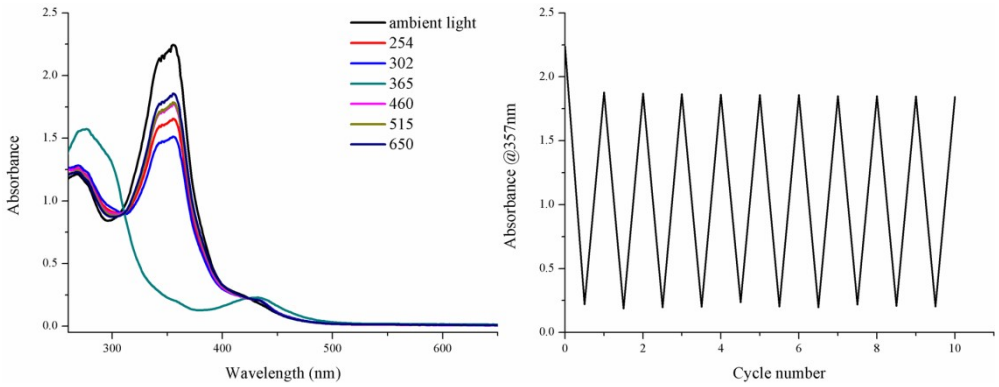


Fig. S66. UV/Vis absorption spectra of **A11** in PSSs generated by irradiations with various wavelengths of light in DMSO (left). Multiple rounds of photoswitching of **A11** by alternating 365 nm and 460 nm light irradiations in DMSO (right).

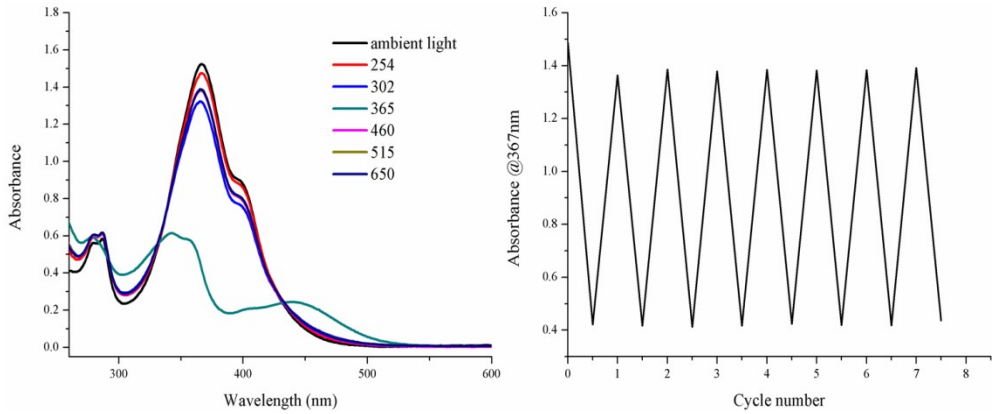


Fig. S67. UV/Vis absorption spectra of **B2** in PSSs generated by irradiations with various wavelengths of light in DMSO (left). Multiple rounds of photoswitching of **B2** by alternating 365 nm and 460 nm light irradiations in DMSO (right).

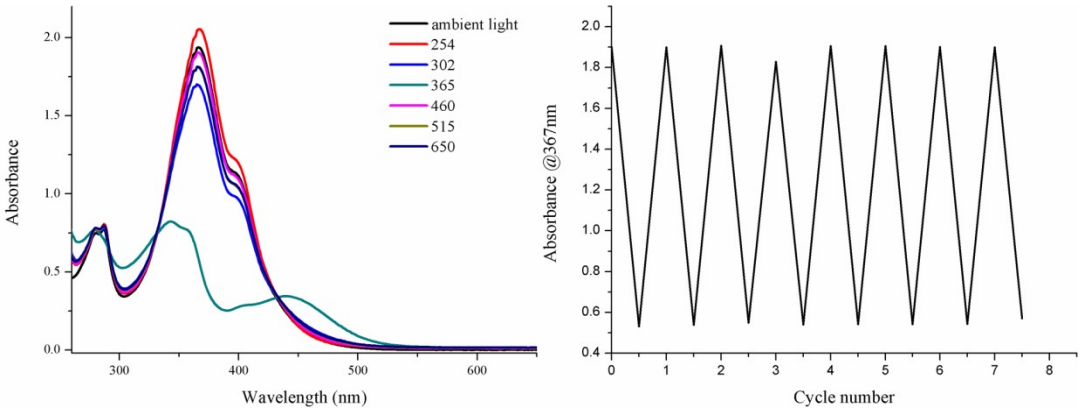


Fig. S68. UV/Vis absorption spectra of **B3** in PSSs generated by irradiations with various wavelengths of light in DMSO (left). Multiple rounds of photoswitching of **B3** by alternating 365 nm and 460 nm light irradiations in DMSO (right).

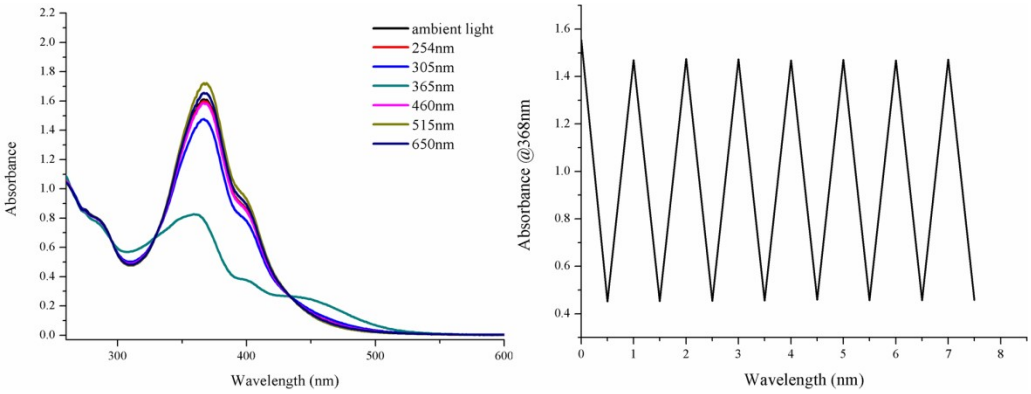


Fig. S69. UV/Vis absorption sprectrum of **B4** in PSSs generated by irradiations with various wavelengths of light in DMSO (left). Multiple rounds of photoswitching of **B4** by alternating 365 nm and 460 nm light irradiations in DMSO (right).

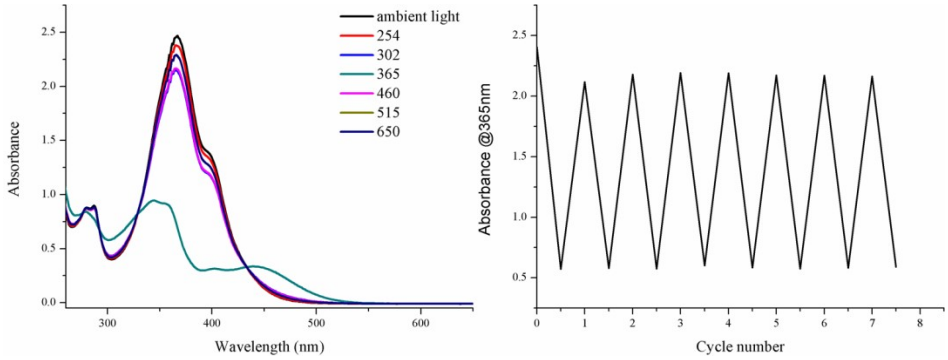


Fig. S70. UV/Vis absorption spectra of **B5** in PSSs generated by irradiations with various wavelengths of light in DMSO (left). Multiple rounds of photoswitching of **B5** by alternating 365 nm and 460 nm light irradiations in DMSO (right).

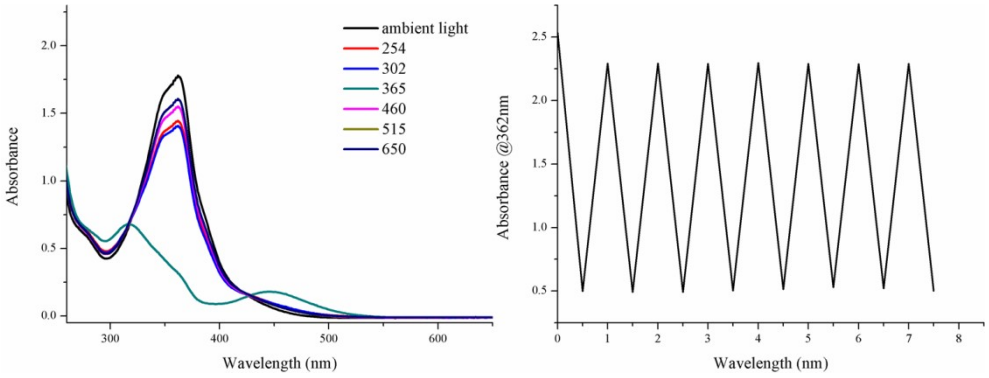


Fig. S71. UV/Vis absorption spectra of **B6** in PSSs generated by irradiations with various wavelengths of light in DMSO (left). Multiple rounds of photoswitching of **B6** by alternating 365 nm and 460 nm light irradiations in DMSO (right).

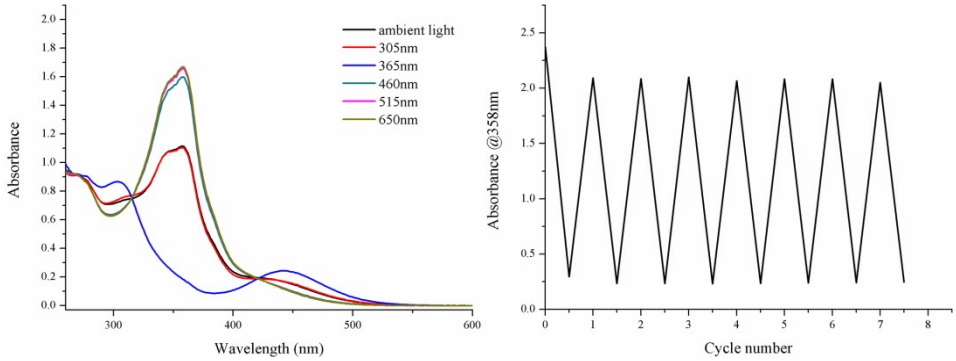


Fig. S72. UV/Vis absorption spectra of **B7** in PSSs generated by irradiations with various wavelengths of light in DMSO (left). Multiple rounds of photoswitching of **B7** by alternating 365 nm and 460 nm light irradiations in DMSO (right).

2.2 Determination of PSS compositions using ^{1}H NMR in DMSO-d_6.

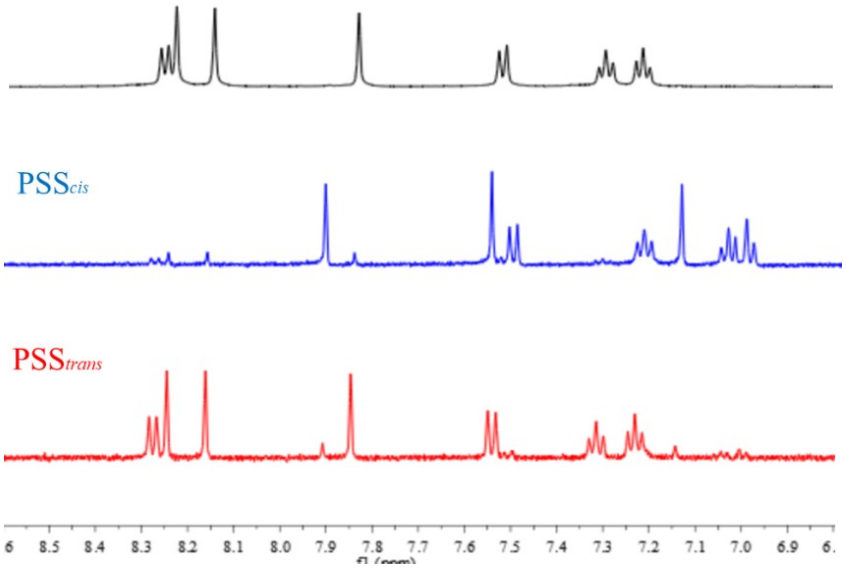


Figure S73. Expanded ^{1}H NMR spectra showing proton signals of **A2** in DMSO.

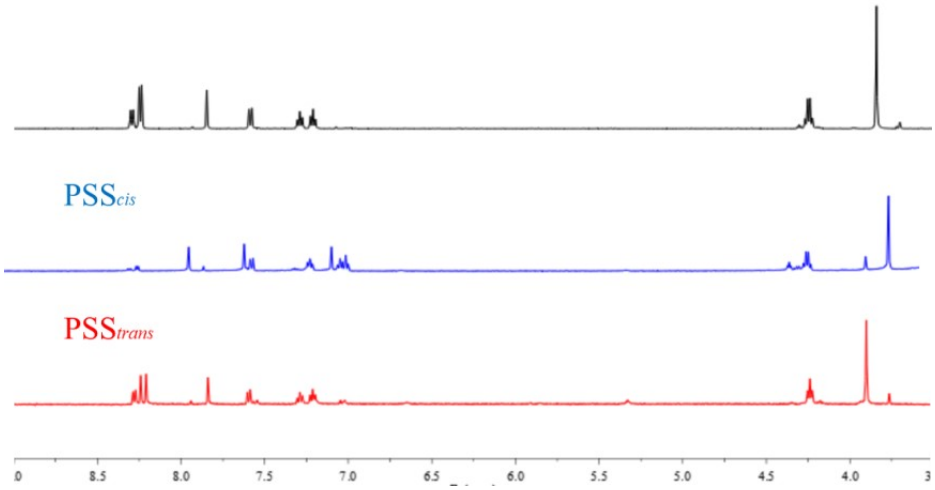


Figure S74. Expanded ^{1}H NMR spectra showing proton signals of **A3** in DMSO.

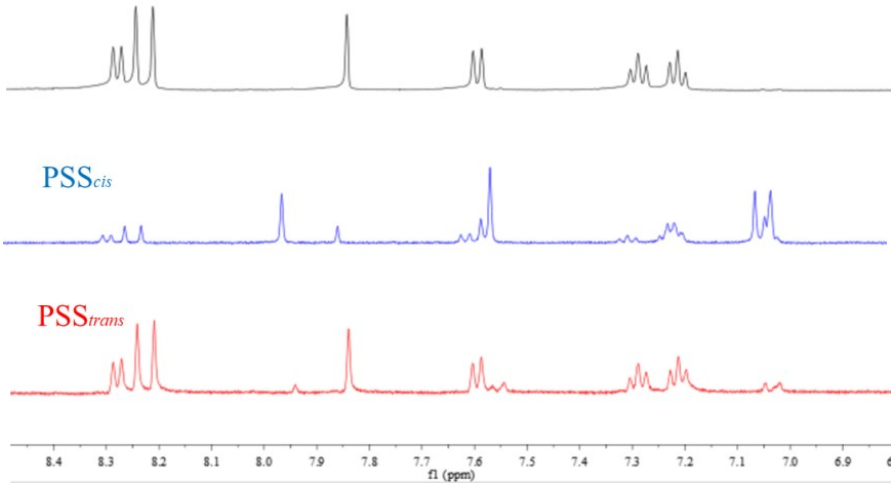


Figure S75. Expanded ^{1}H NMR spectra showing proton signals of **A4** in DMSO.

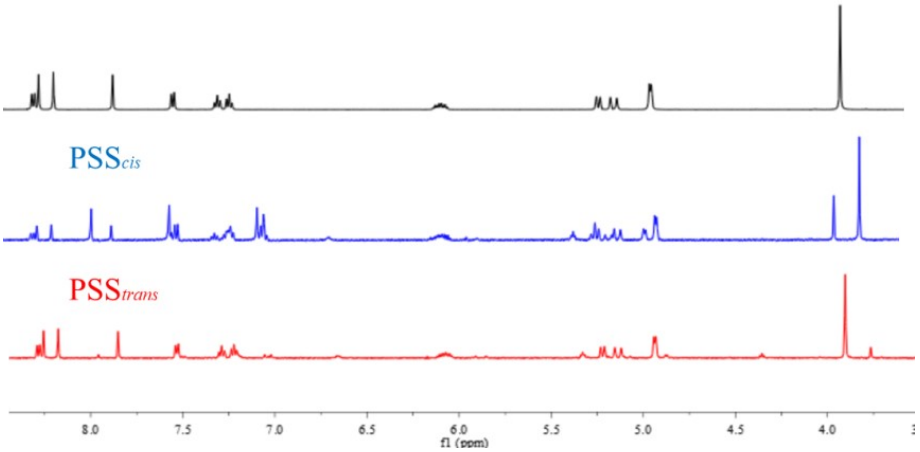


Figure S76. Expanded ^{1}H NMR spectra showing proton signals of **A5** in DMSO.

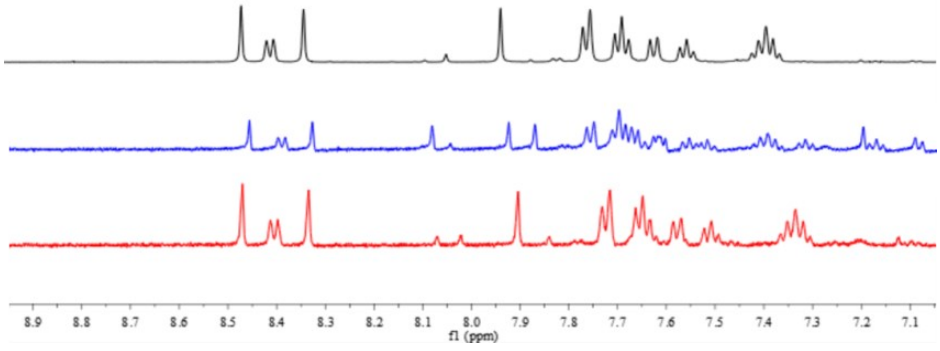


Figure S77. Expanded ^{1}H NMR spectra showing proton signals of **A6** in DMSO.

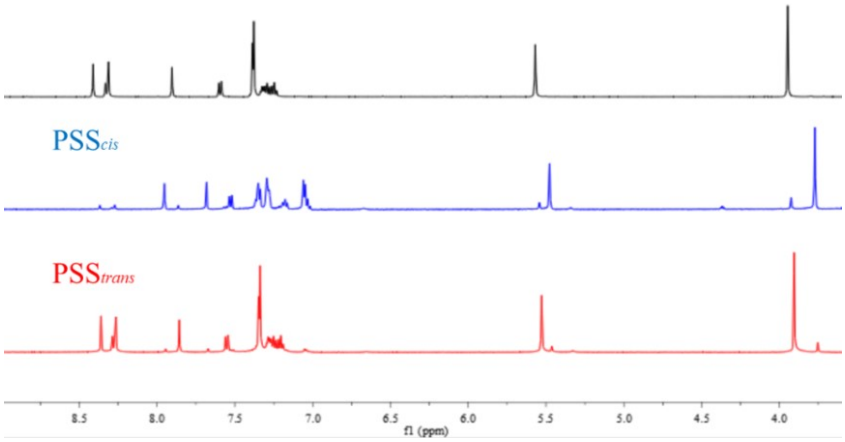


Figure S78. Expanded ^{1}H NMR spectra showing proton signals of **A7** in DMSO.

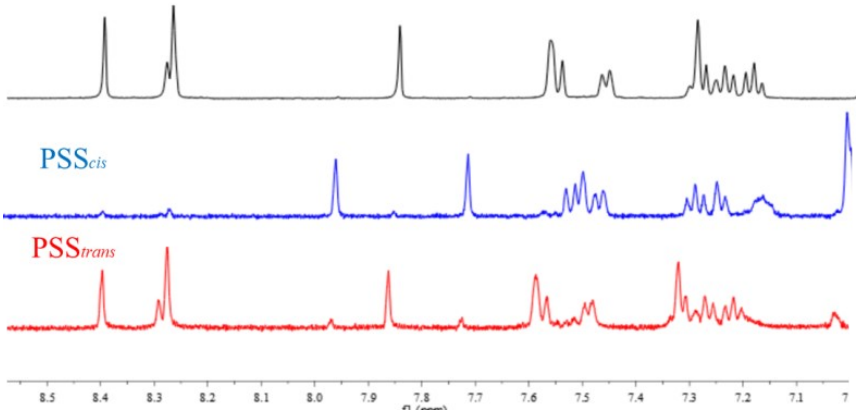


Figure S79. Expanded 1H NMR spectra showing proton signals of **A8** in DMSO.

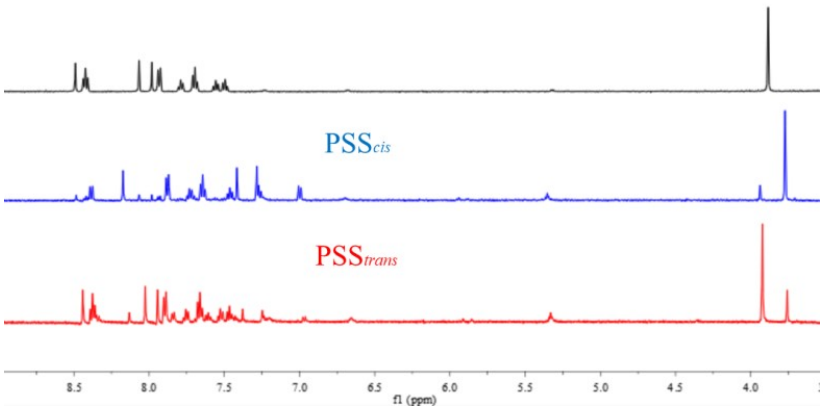


Figure S80. Expanded ^{1}H NMR spectra showing proton signals of **A9** in DMSO.

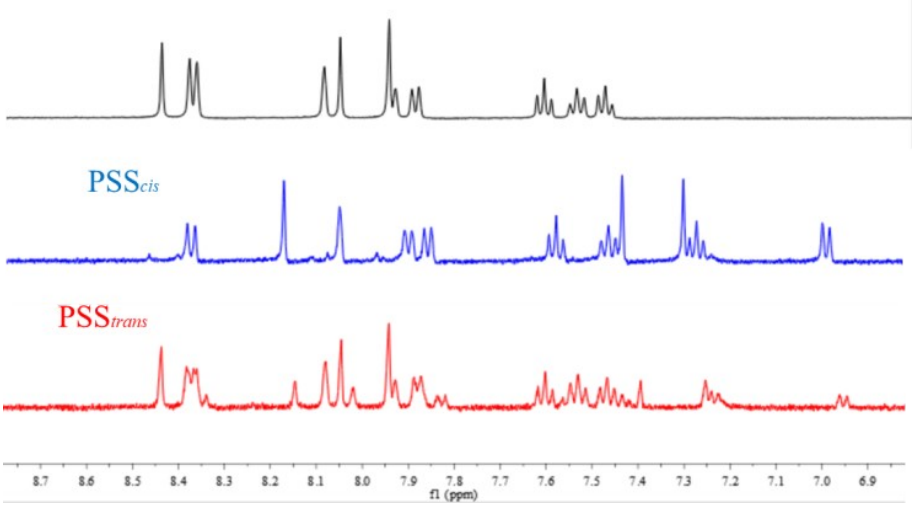


Figure S81. Expanded ^{1}H NMR spectra showing proton signals of **A10** in DMSO.

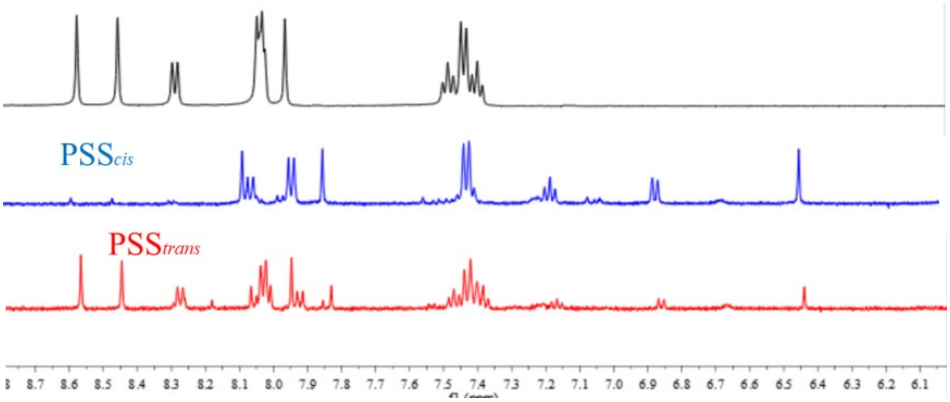


Figure S82. Expanded ^{1}H NMR spectra showing proton signals of **A11** in DMSO.

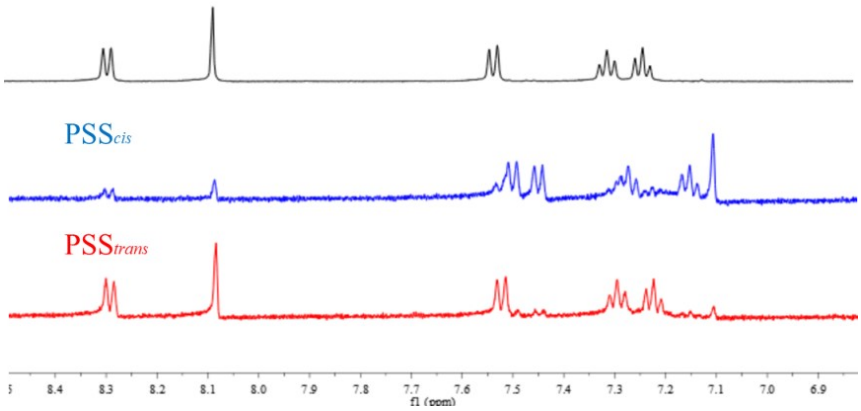


Figure S83. Expanded ^{1}H NMR spectra showing proton signals of **B2** in DMSO.

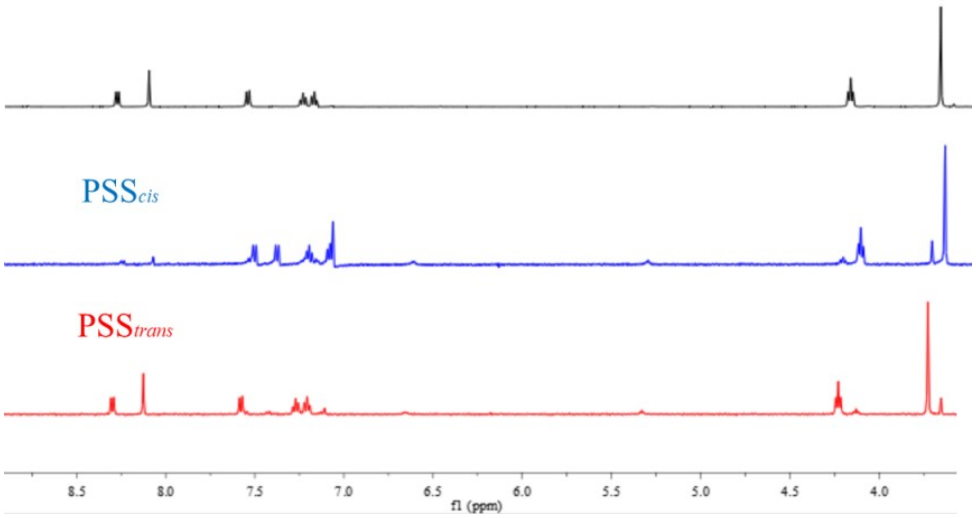


Figure S84. Expanded ^{1}H NMR spectra showing proton signals of **B3** in DMSO-*d6*.

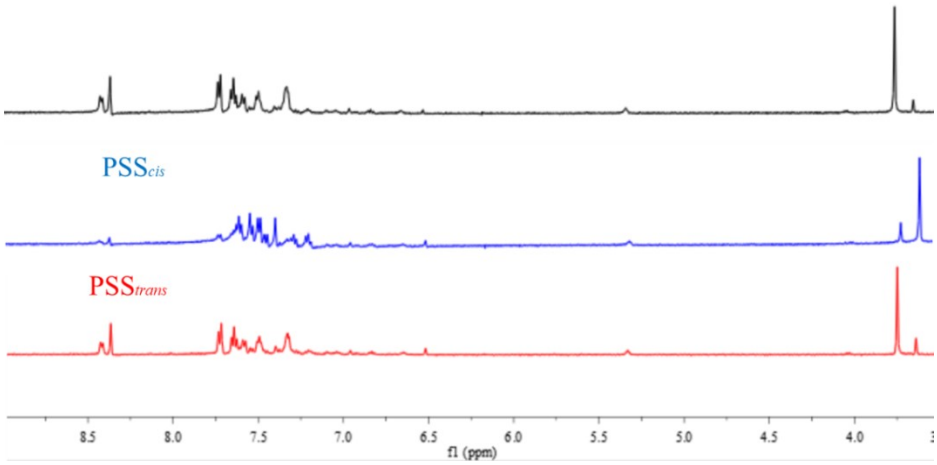


Figure S85. Expanded ^{1}H NMR spectra showing proton signals of **B4** in DMSO-*d6*.

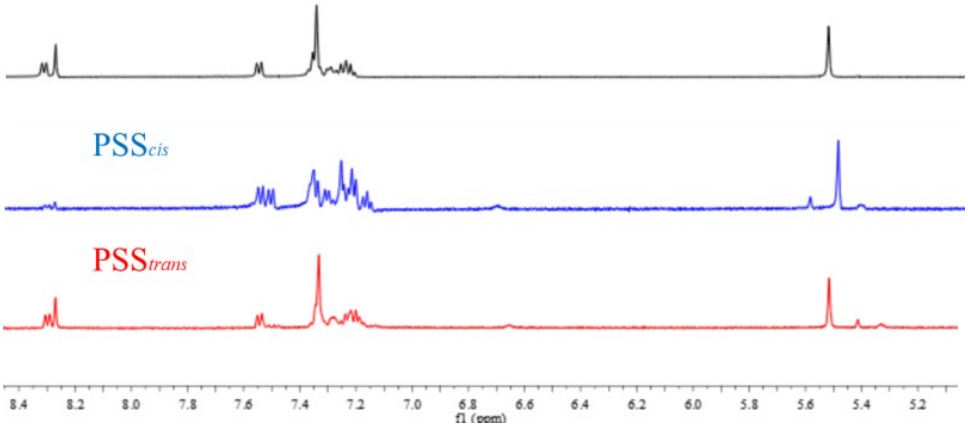


Figure S86. Expanded ^{1}H NMR spectra showing proton signals of **B5** in DMSO-*d6*.

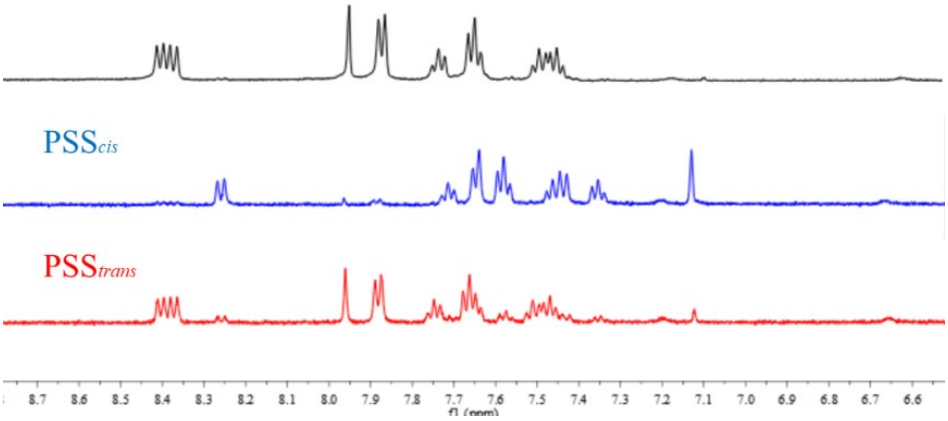


Figure S87. Expanded ^{1}H NMR spectra showing proton signals of **B6** in DMSO-*d6*.

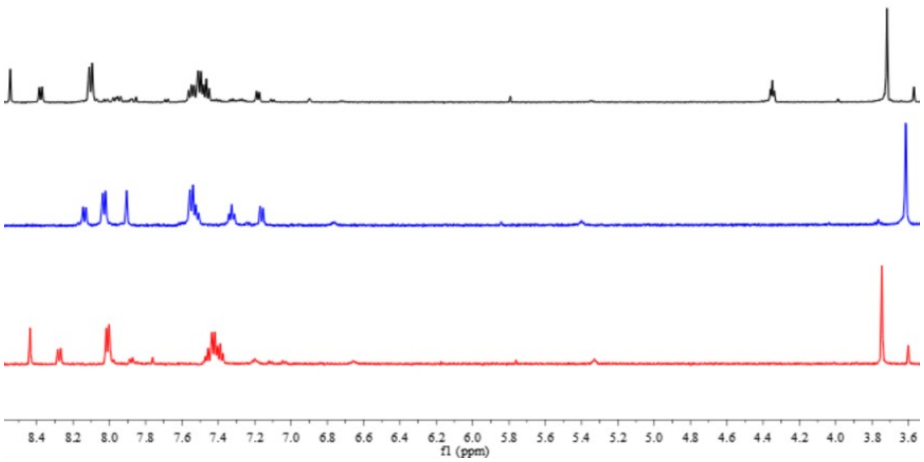


Figure S88. Expanded ^{1}H NMR spectra showing proton signals of **B7** in DMSO-*d6*.

2.3 The thermal half-lives of title compounds

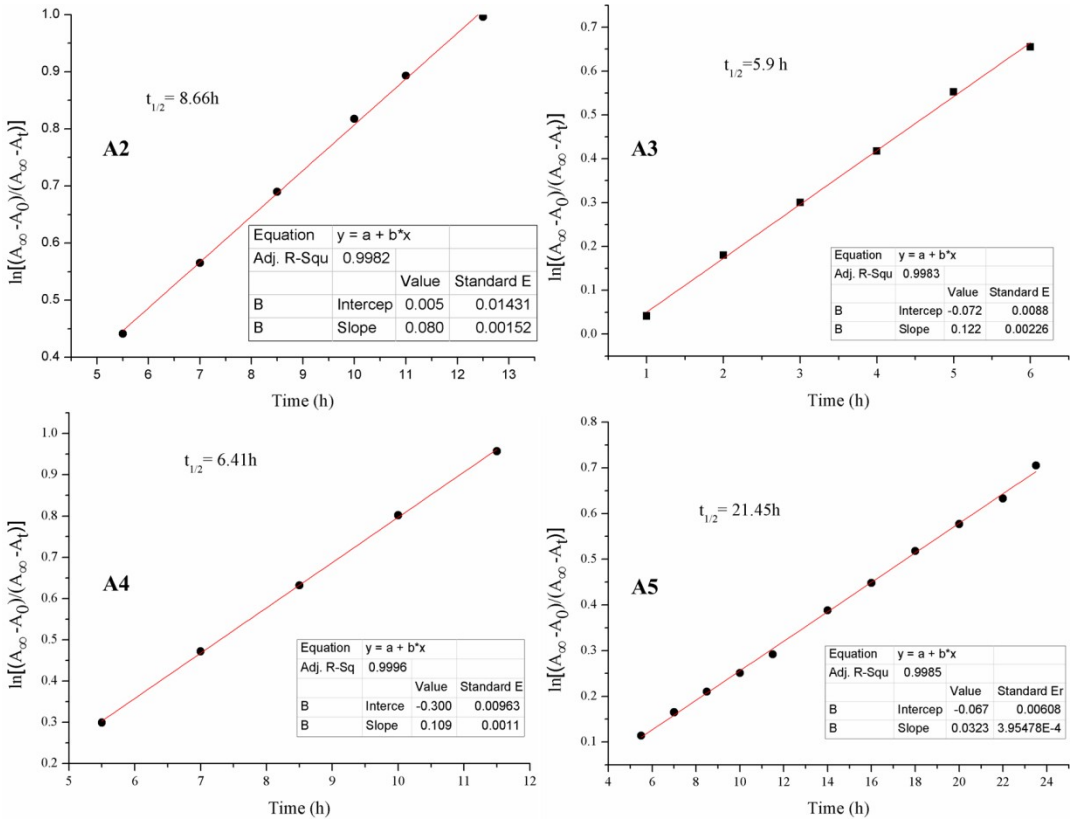


Figure S89. First-order kinetics analysis of compounds **A2**, **A3**, **A4**, and **A5**.

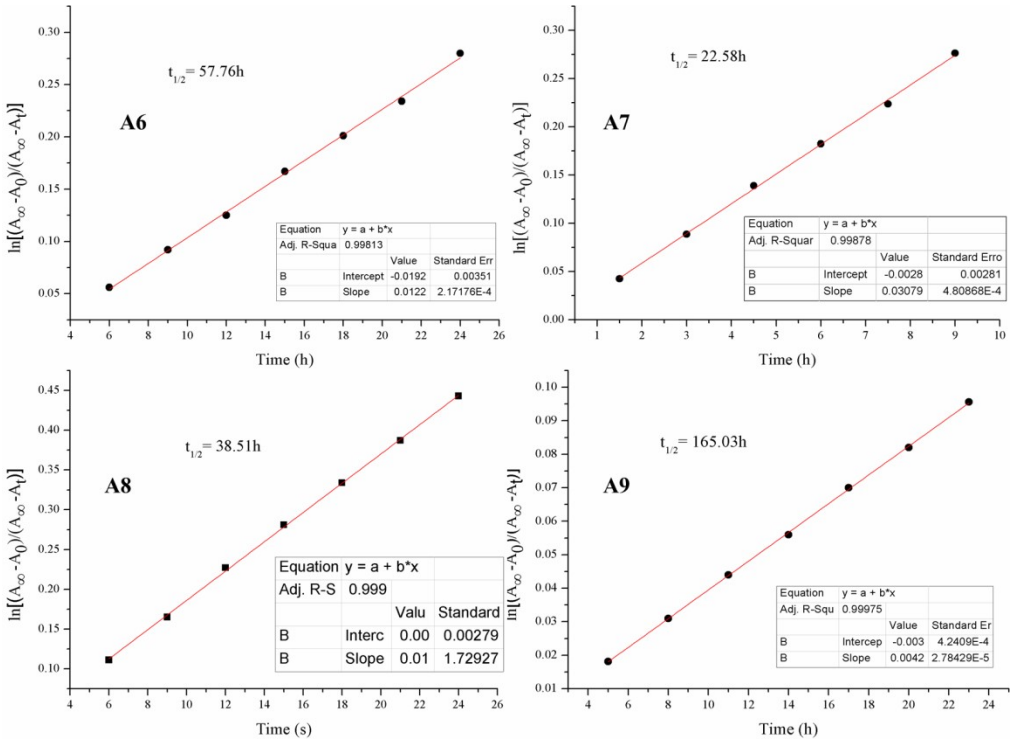


Figure S90. First-order kinetics analysis of compounds **A6**, **A7**, **A8**, and **A9**.

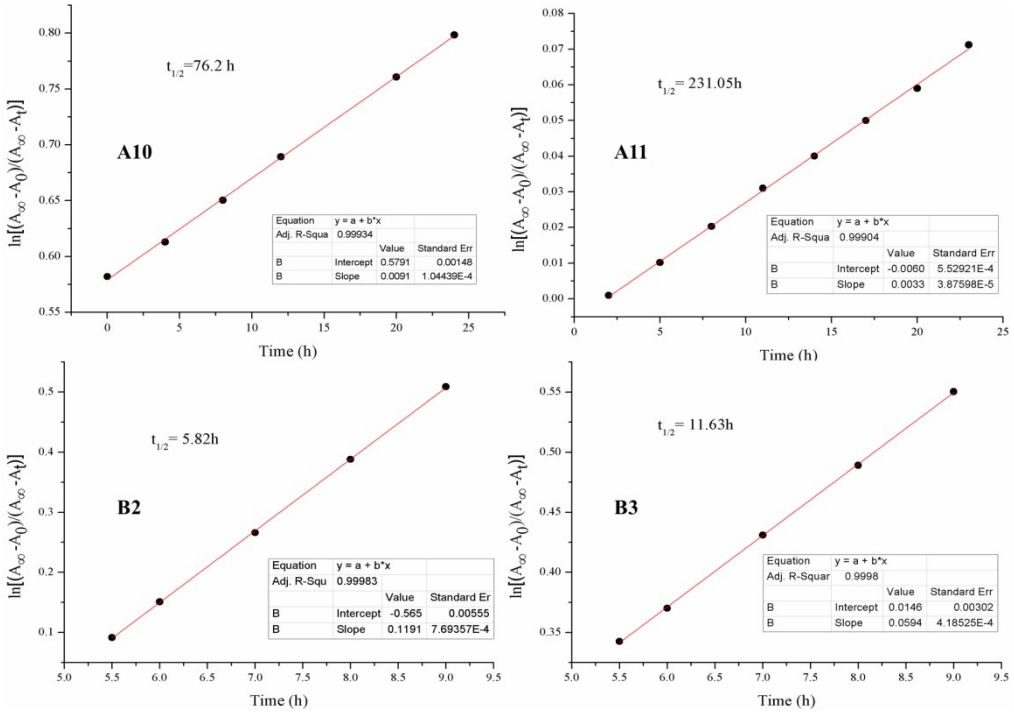


Figure S91. First-order kinetics analysis of compounds **A10**, **A11**, **B2**, and **B3**.

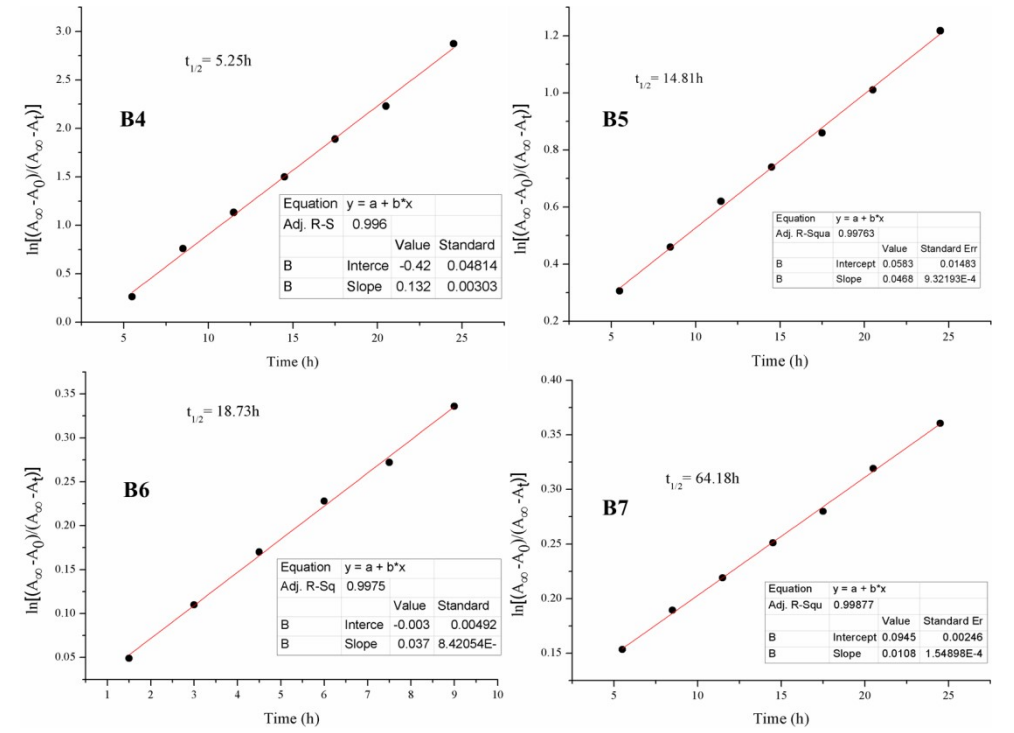


Figure S92. First-order kinetics analysis of compounds **B4**, **B5**, **B6**, and **B7**.

2.4 First-order kinetics analysis thermal isomerization of A9, A11, and B7

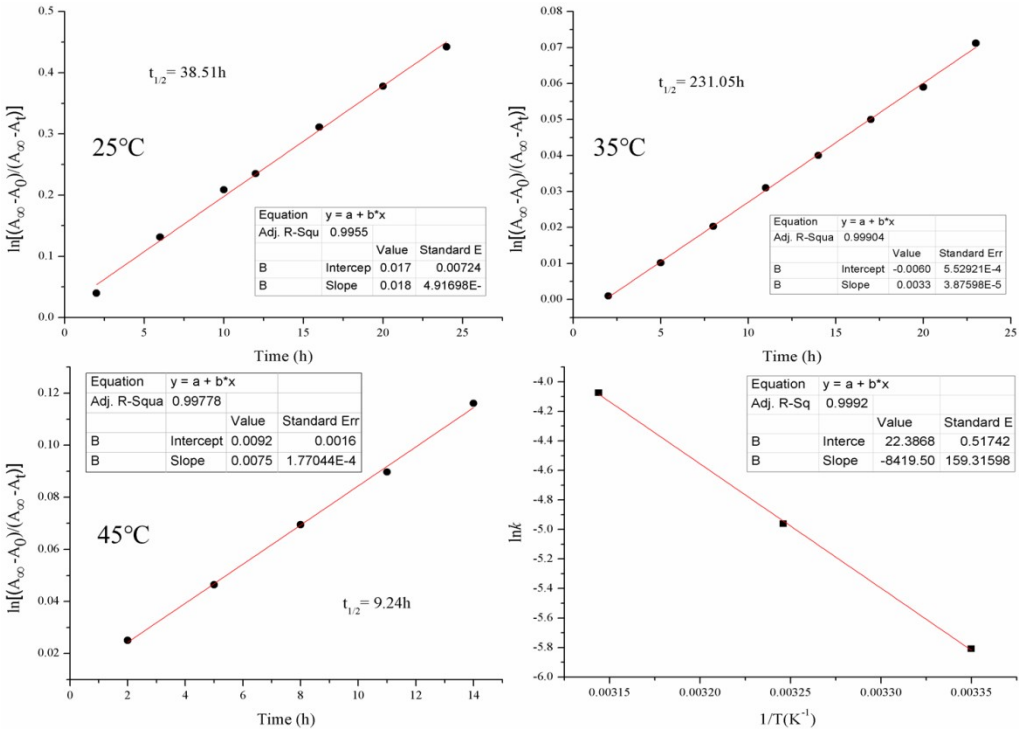


Figure S93. First-order kinetics analysis and Arrhenius plot for thermal isomerization of compound **A9** in DMSO.

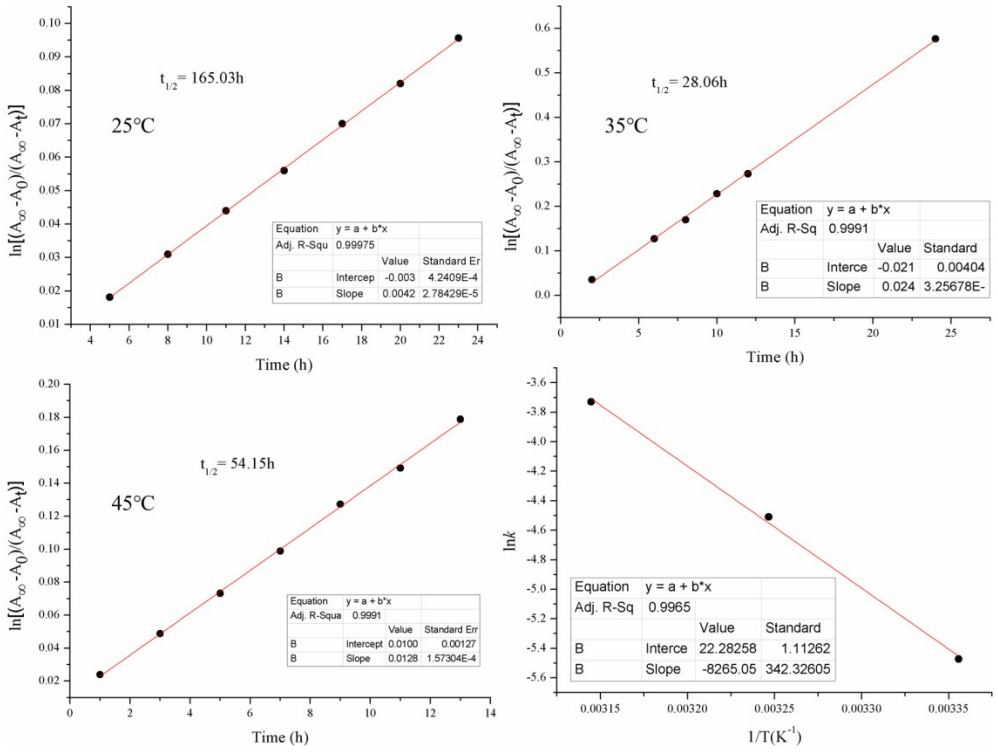


Figure S94. First-order kinetics analysis and Arrhenius plot for thermal isomerization of compound **A11** in DMSO.

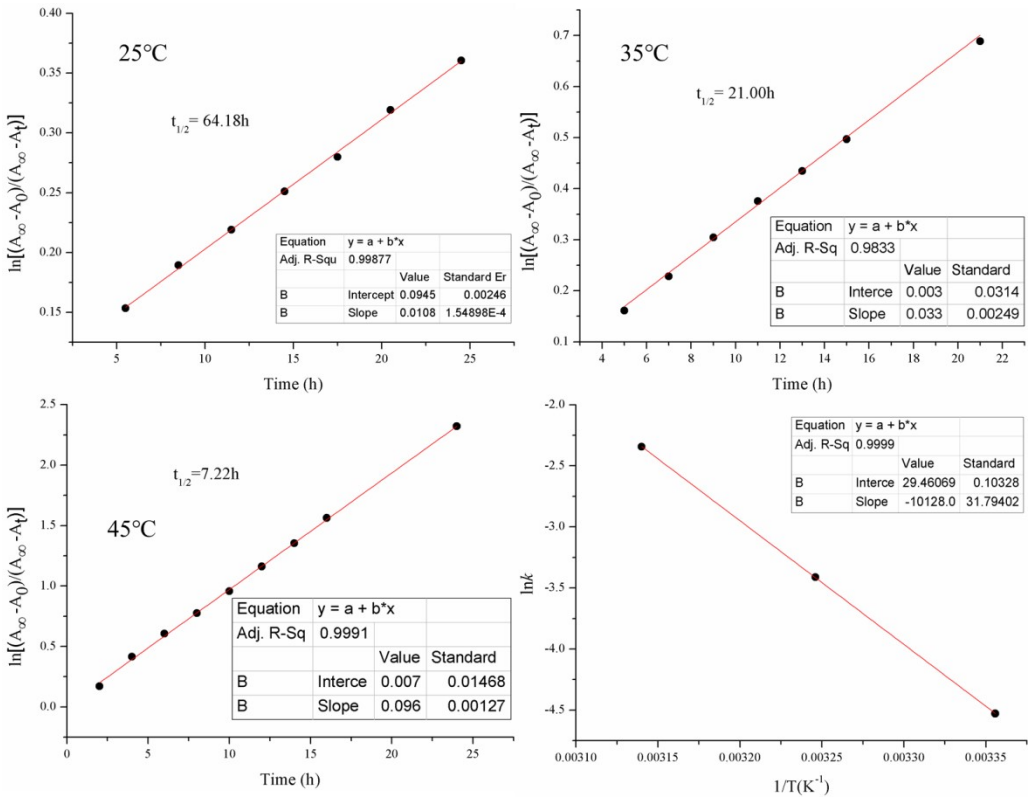


Figure S95. First-order kinetics analysis and Arrhenius plot for thermal isomerization of compound **B7** in DMSO.

3 Biological application

3.1 Photoisomerization and half-lives in 10% phosphate buffer (pH 7.5)-DMSO mixture

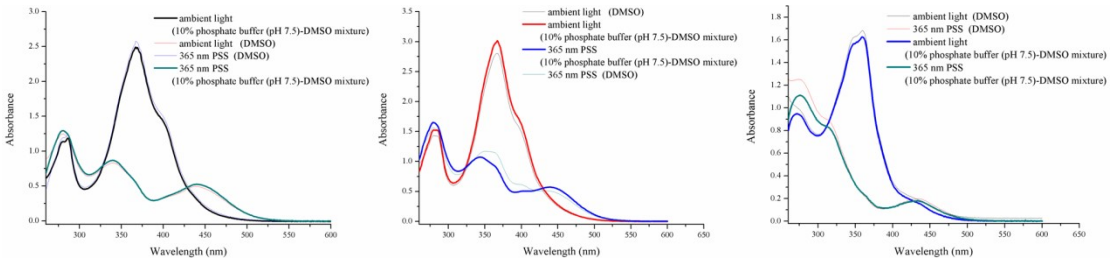


Figure S96. UV-vis absorption spectra of **A3**, **A8**, and **A10** in PSSs generated by irradiations with 365 and 460 nm of light in 10% phosphate buffer (pH 7.5)-DMSO mixture and DMSO.

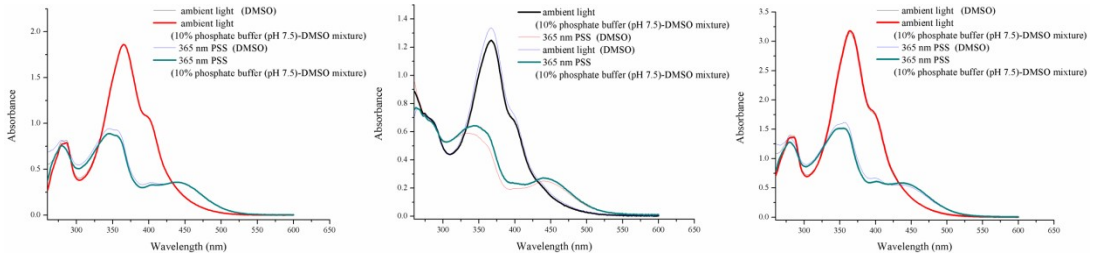


Figure S97. UV-vis absorption spectra of **B2**, **B4**, and **B7** in PSSs generated by irradiations with 365 and 460 nm of light in 10% phosphate buffer (pH 7.5)-DMSO mixture and DMSO.

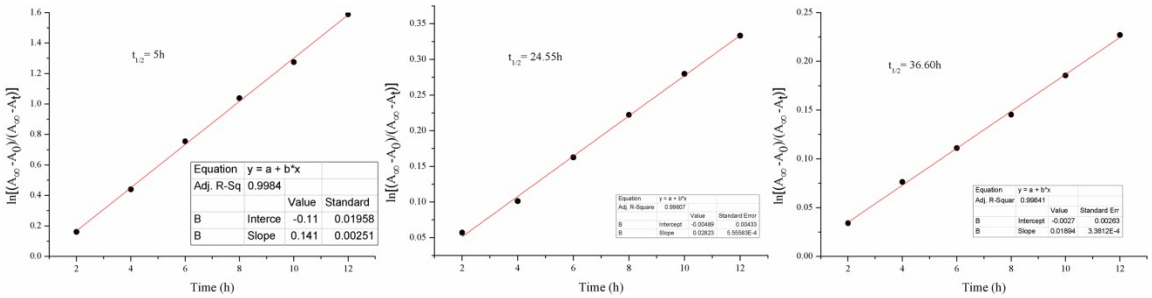


Figure S98. First-order kinetics analysis of compounds **A3**, **A8**, and **A10** in 10% phosphate buffer (pH 7.5)-DMSO mixture.

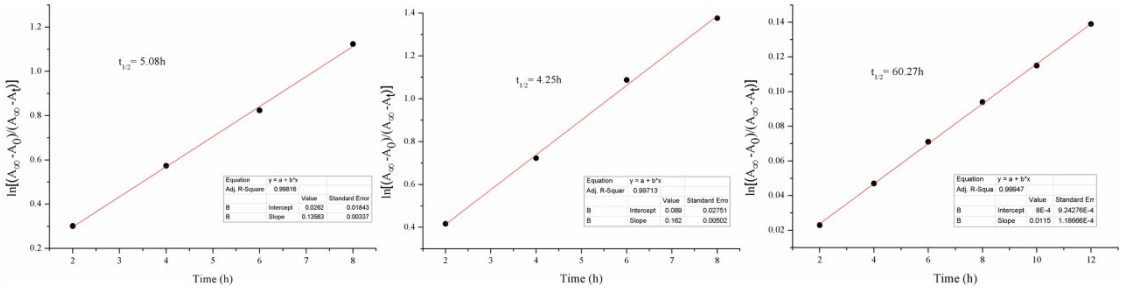
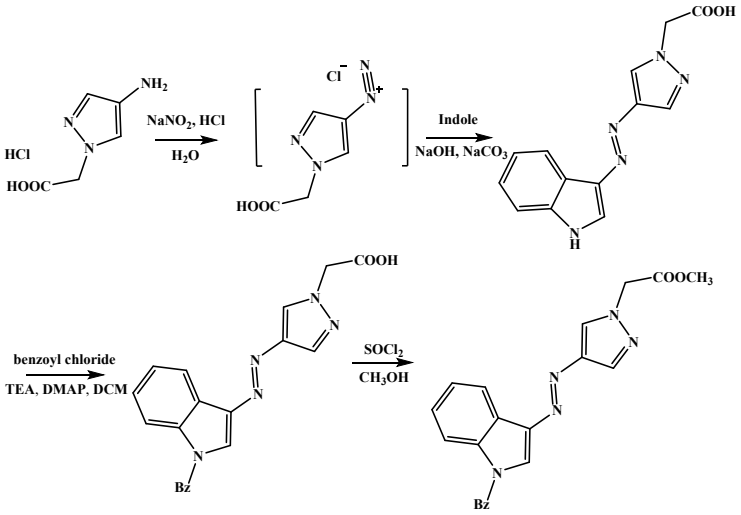


Figure S99. First-order kinetics analysis of compounds **B2**, **B4**, and **B7** in 10% phosphate buffer (pH 7.5)-DMSO mixture.

3.2 the information of bi-functional model molecule C1.



The synthesize route to 2-(4-((1H-indol-3-yl)diazenyl)-1H-pyrazol-1-yl)acetic acid is similar to **3**. To a solution of 2-(4-((1H-indol-3-yl)diazenyl)-1H-pyrazol-1-yl)acetic (0.81 g, 3 mmol) in DCM (20 mL), DMAP (1.1 g, 9 mmol), TEA (1.4 mL, 10 mmol) were added. After 3 min benzoyl chloride (0.5 g, 3.6 mmol) was added and the reaction mixture was stirred overnight from 0℃ to room temperature. The solvent was removed under reduced pressure, gave the intermediate Indoleamide (0.97 g， yield with 87％).

2-(4-((1-benzoyl-1H-indol-3-yl)diazenyl)-1H-pyrazol-1-yl)acetic acid (0.75 g, 2 mmol) was dissolved in 30 methanol, $SOCl_2$ (0.9 mL, 12 mmol) was added and the reaction mixture was stirred for 4 h at 80 ℃. purification by column chromatography (ethyl acetate-Petroleum ether: 1:3) gave the product **C1** (0.69 g, yield with 90％).

C1: ^{1}H NMR (500 MHz, DMSO) δ 8.49 (s, 1H), 8.42 – 8.33 (m, 2H), 8.06 (s, 1H), 8.00 (s, 1H), 7.89 (d, *J* = 6.9 Hz, 2H), 7.74 (d, *J* = 7.1 Hz, 1H), 7.66 (d, *J* = 6.8 Hz, 2H), 7.50 (dd, *J* = 22.0, 7.2 Hz, 2H), 5.19 (s, 2H), 3.72 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 168.84, 168.78, 137.62, 136.44, 133.75, 133.05, 132.58, 131.19, 131.19, 129.79, 129.34, 129.17, 126.90, 125.91, 123.00, 122.65, 116.34, 53.48, 52.87; Elemental analysis (%) calcd. for $C_{21}H_{17}N_5O_3$ (387.13): C 65.11, H 4.42, N 18.08, O 12.39; Found: C 65.17, H 4.40, N 18.07, O 12.36.

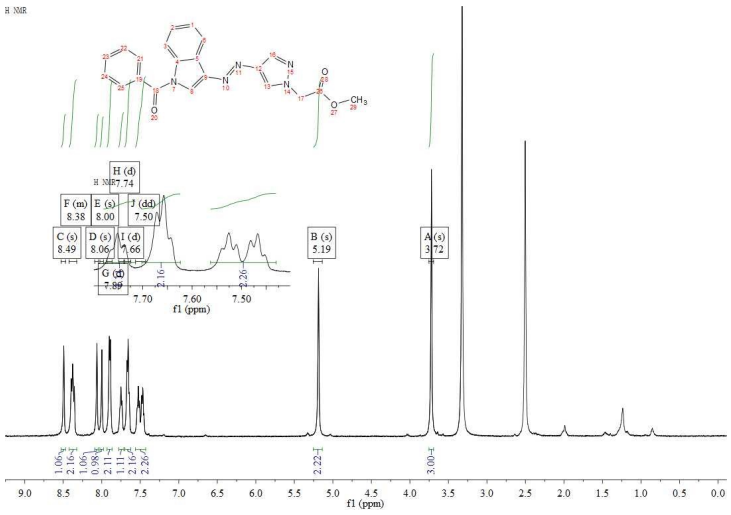


Figure S100. Expanded ^{1}H NMR spectra showing proton signals of **C1** in DMSO.

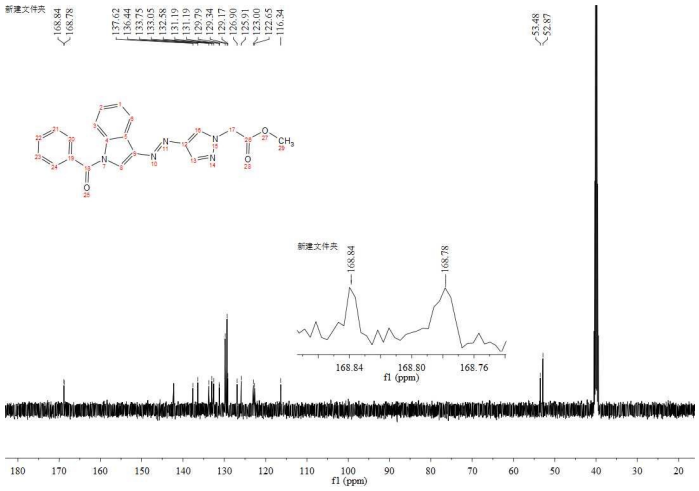


Figure S101. Expanded ^{13}C NMR spectra showing proton signals of **C1** in DMSO.

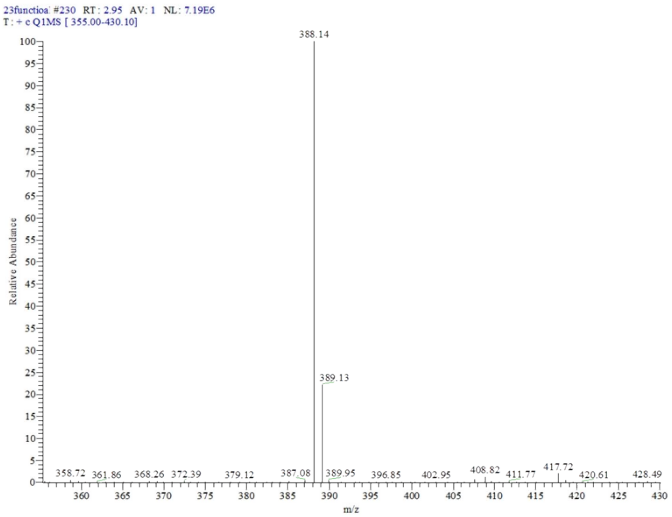


Figure S102. The mass spectrum of

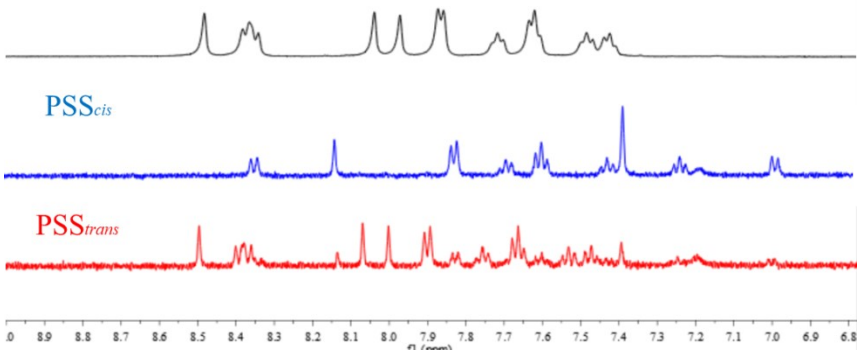


Figure S103. Expanded ^{1}H NMR spectra showing proton signals of **C1** in DMSO-*d6*.

4 DFT calculations[S5]

4.1 Computed and experimental UV/Vis Spectra

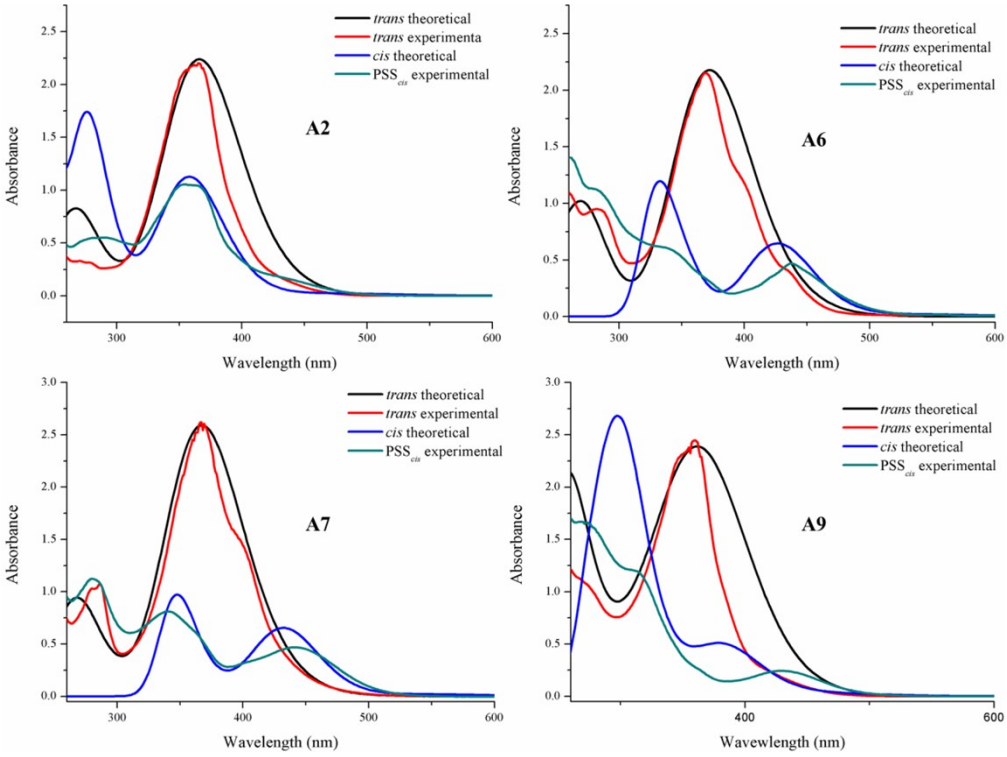


Figure S104. Comparison between the calculated and experimental absorption spectra of **A2, A6**, **A7**, **A9**.

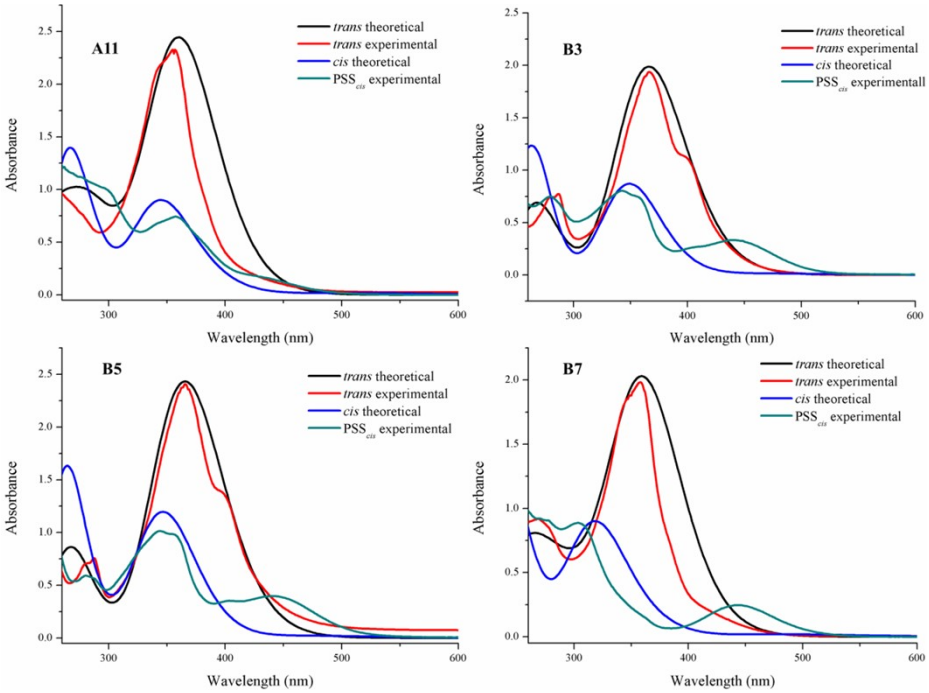


Figure S105. Comparison between the calculated and experimental absorption spectra of **A11, B3**, **B5**, **B7**.

4.2 the energy of calculations

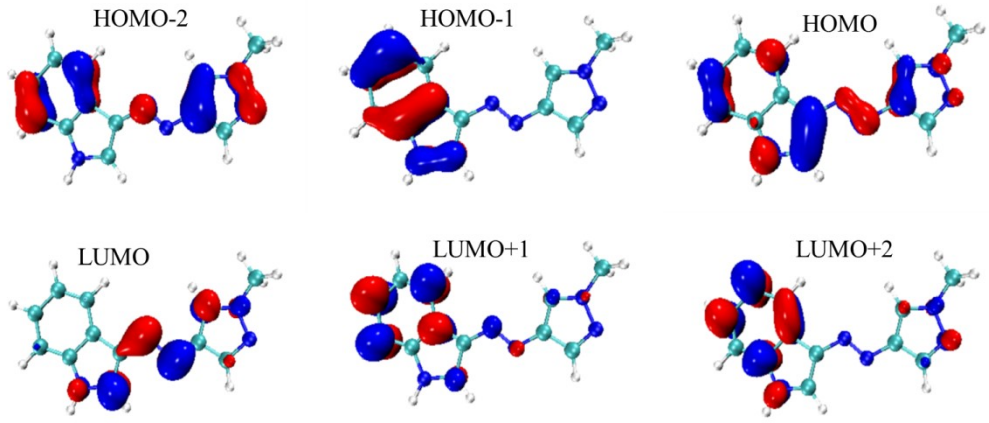
Table S4. The energy (Hartree) TS-1, TS-2, and *cis*-isomer by Gauss calculations (**A9**, **A11**, and **B7**).

Compd.	TS-1	TS-2	*Cis*-isomer
A9	-1540.1519	-1540.1105	-1540.1981
A11	-1069.1888	-1069.1456	-1069.2353
B7	-1578.9520	-1578.3637	-1617.8487

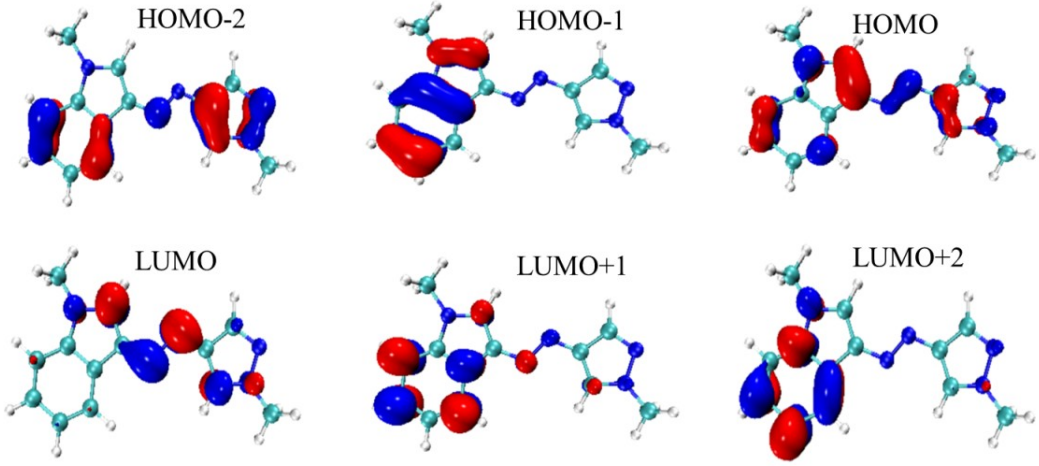
4.3 The diagrams and energy for Frontier MOs of compounds

Table S5. The energy (eV) of Frontier MOs (**A1**—**A5**).

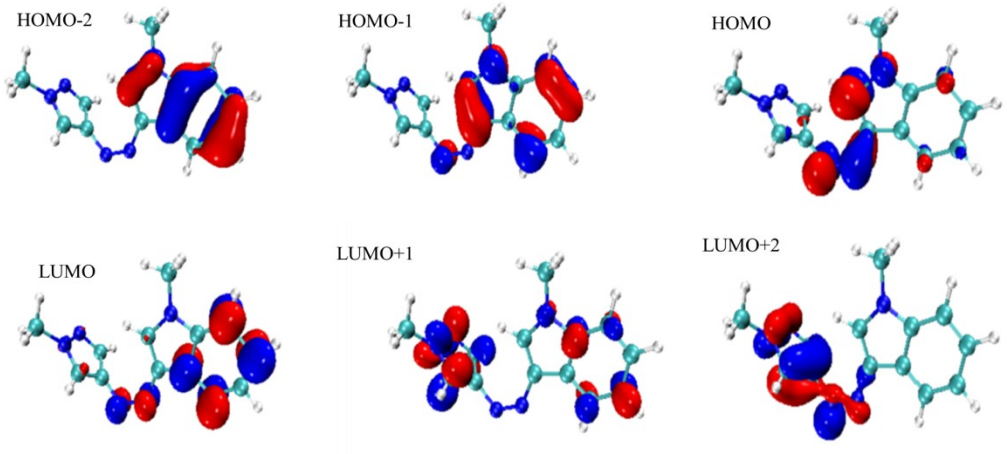
Compd.	**A1**	**A2**		**A3**		**A4**		**A5**	
		trans	*cis*	*trans*	*cis*	*trans*	*cis*	*trans*	*cis*
HOMO-2	-9.400	-9.385	-9.067	-9.384	-9.065	-9.384	-9.066	-9.393	-9.081
HOMO-1	-8.713	-8.649	-8.743	-8.628	-8.720	-8.625	-8.717	-8.626	-8.710
HOMO	-7.632	-7.527	-8.045	-7.525	-8.042	-7.525	8.037	-7.567	-8.057
LUMO	2.121	2.136	2.340	2.125	2.320	2.123	2.325	2.103	2.292
LUMO+1	3.548	3.551	3.617	3.538	3.605	3.537	3.602	3.541	3.603
LUMO+2	4.571	4.520	4.393	4.538	4.391	4.535	4.399	4.410	4.350



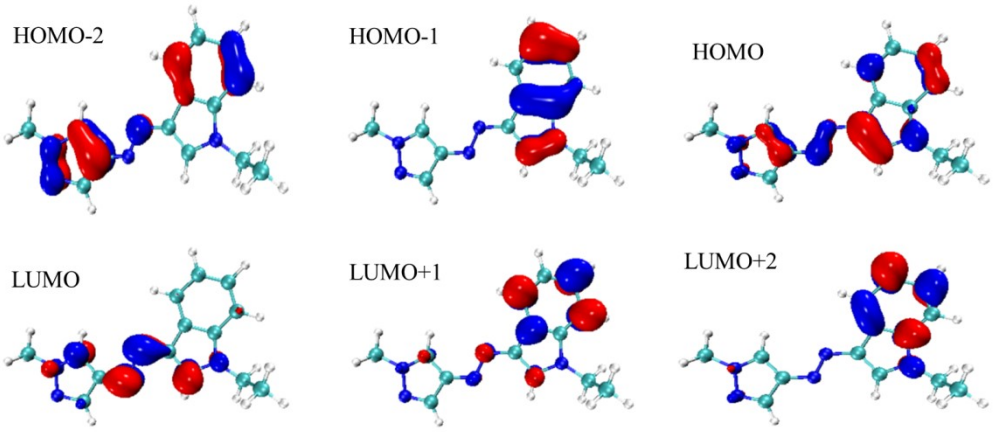
Frontier MOs of **A1**



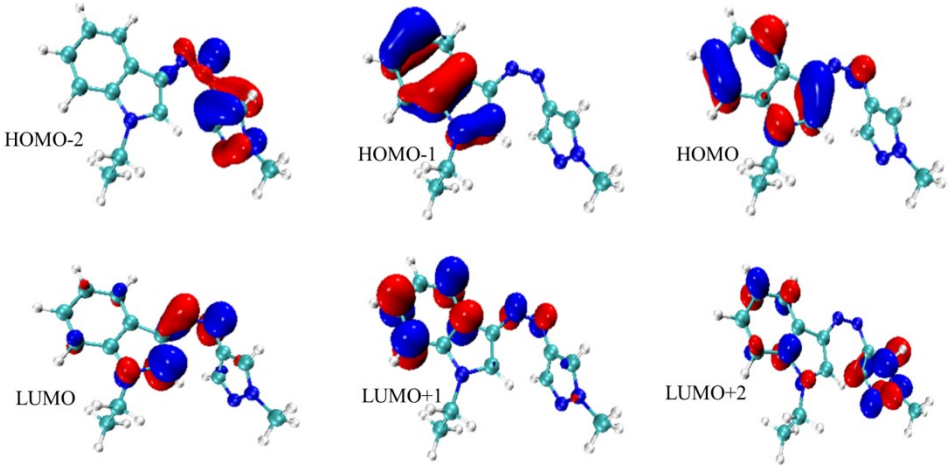
Frontier MOs of **A2** *trans*



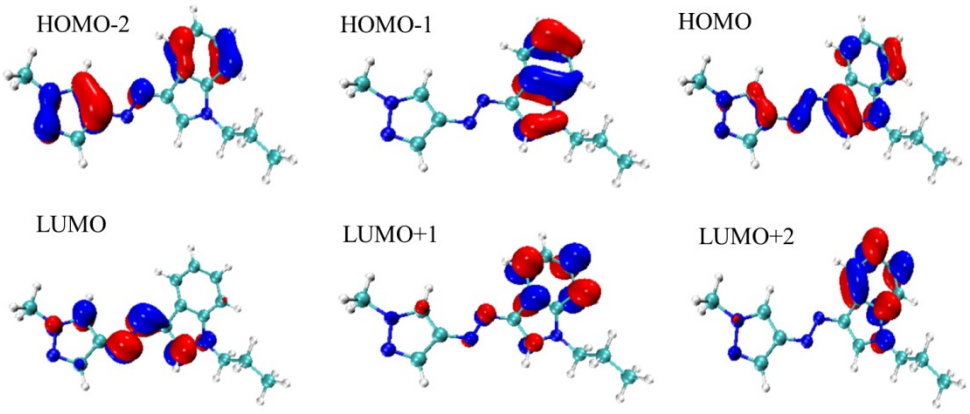
Frontier MOs of **A2** *cis*



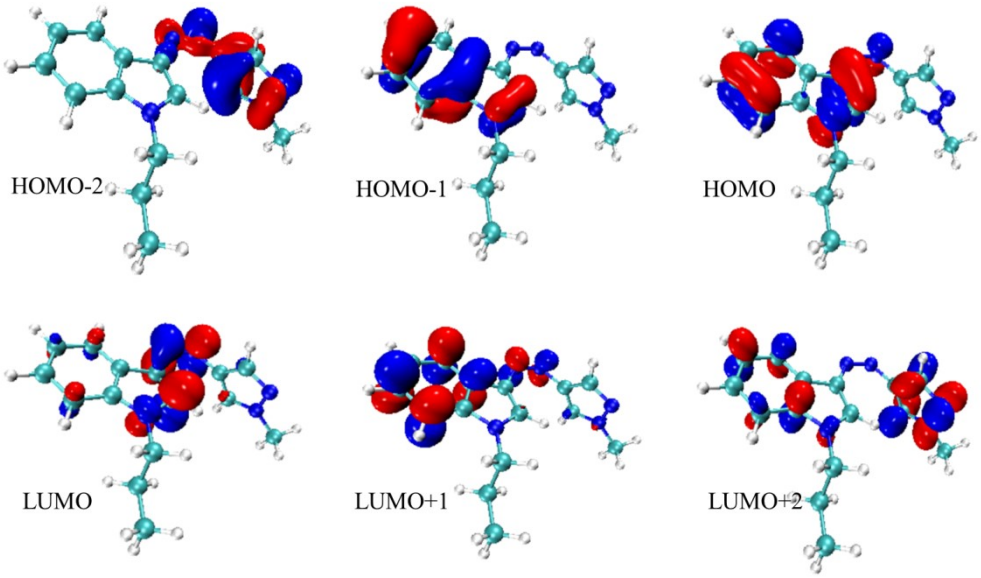
Frontier MOs of **A3** *trans*



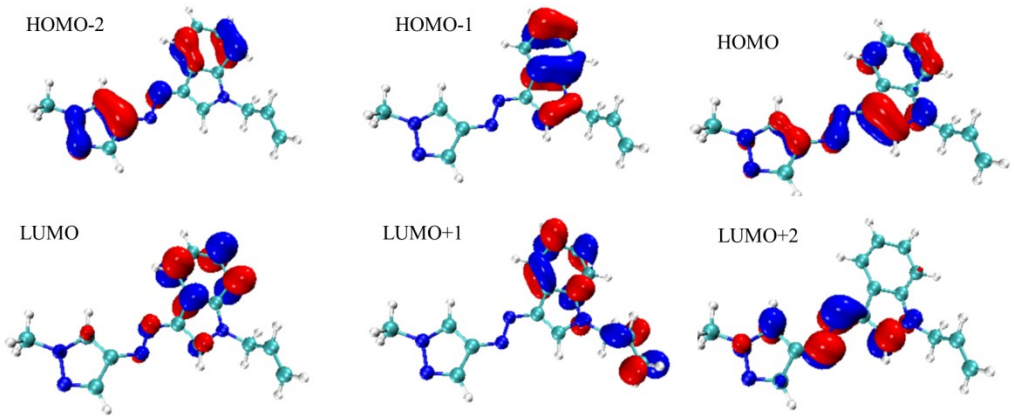
Frontier MOs of **A3** *cis*



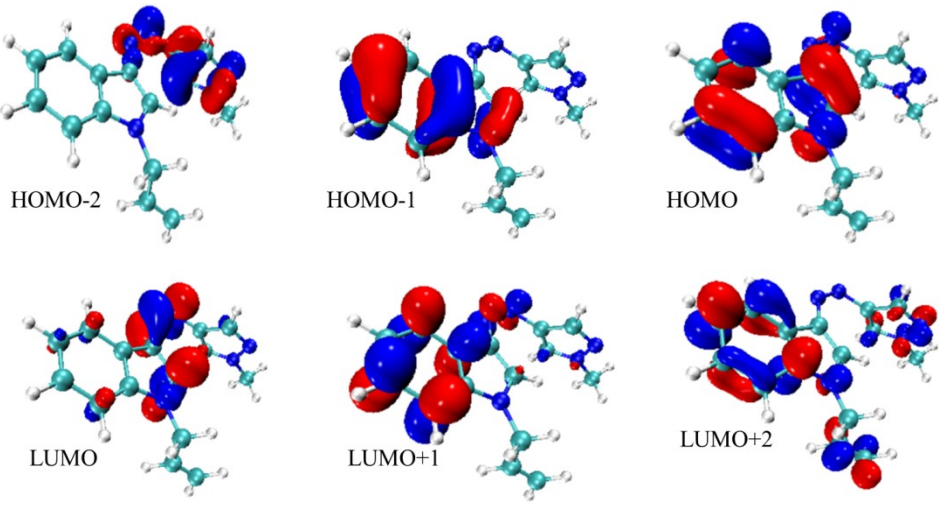
Frontier MOs of **A4** *trans*



Frontier MOs of **A4** *cis*



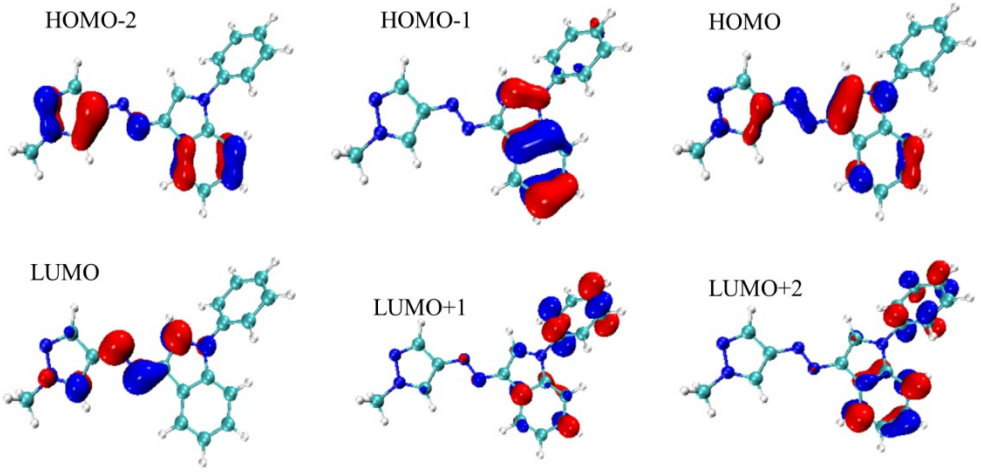
Frontier MOs of **A5** *trans*



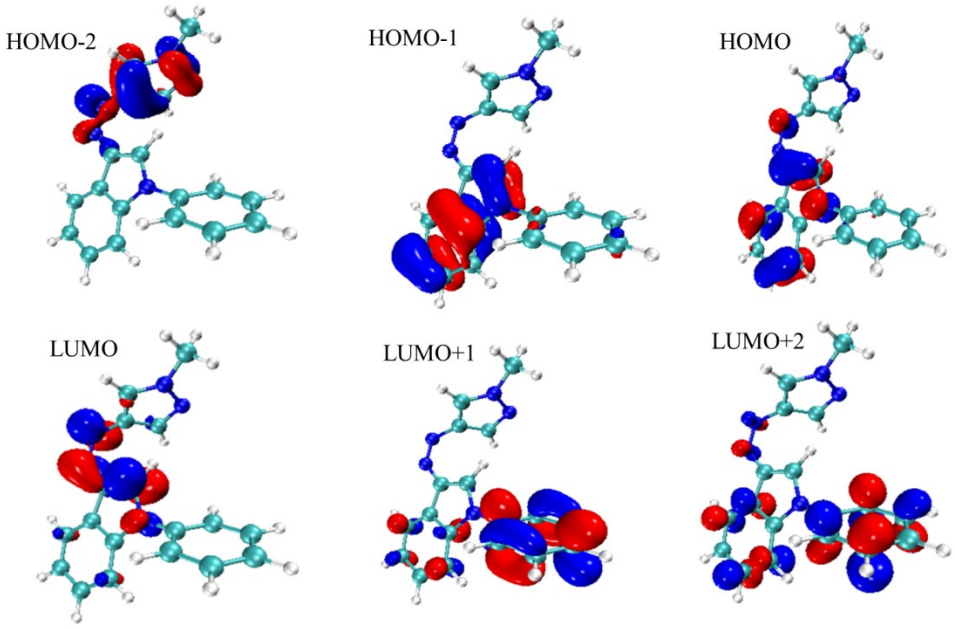
Frontier MOs of **A5** *cis*

Table S6. The energy (eV) of Frontier MOs (**A6**—**A10**).

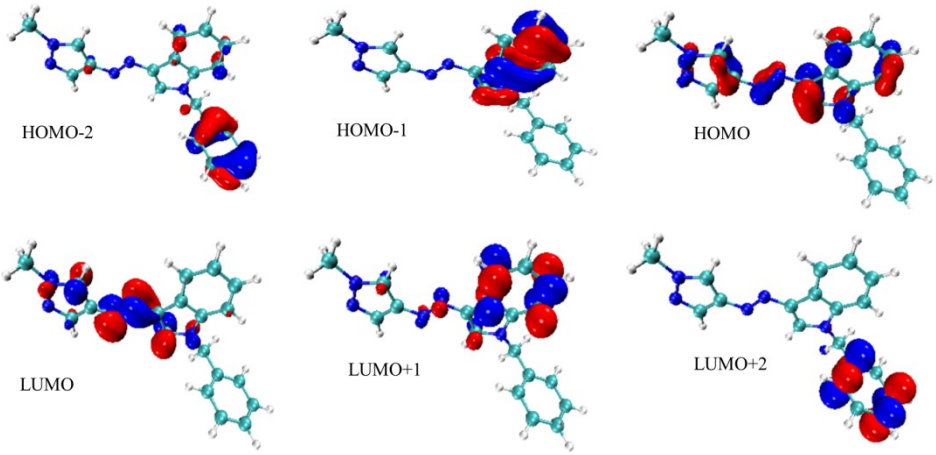
Compd.	**A6**		**A7**		**A8**		**A9**		**A10**	
	trans	*cis*	*trans*	*cis*	*trans*	*cis*	*trans*	*cis*	*trans*	*cis*
HOMO-2	-9.410	-9.113	-9.328	-9.092	-9.320	-9.110	-9.478	-9.434	-9.461	-9.444
HOMO-1	-8.680	-8.766	-8.694	-8.781	-8.721	-8.808	-9.024	-9.045	-9.059	-9.080
HOMO	-7.634	-8.119	-7.584	-8.082	-7.614	-8.107	-7.992	-8.422	-8.021	-8.569
LUMO	2.011	2.185	2.089	2.280	2.070	2.251	1.663	2.160	1.614	1.960
LUMO+1	3.459	3.434	3.520	3.562	3.358	3.328	2.392	2.501	2.259	2.480
LUMO+2	3.484	3.493	3.697	3.669	3.454	3.439	3.262	3.000	3.107	2.913



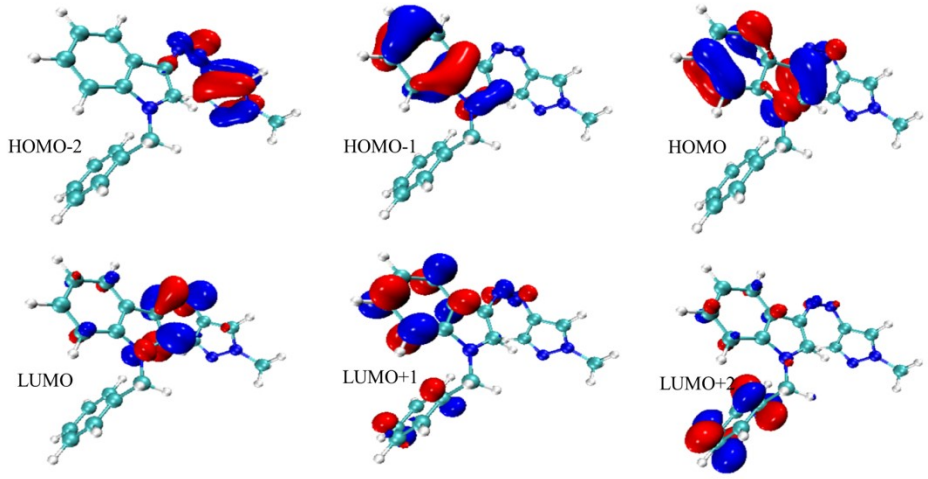
Frontier MOs of **A6** *trans*



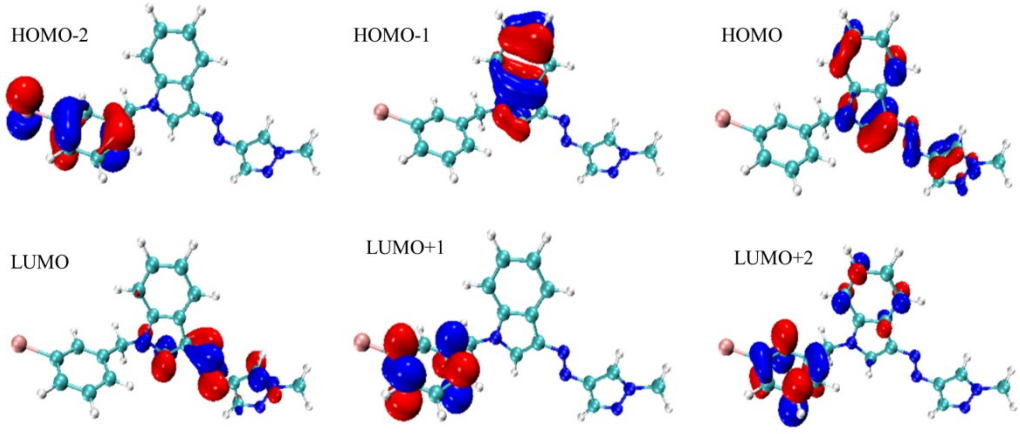
Frontier MOs of **A6** *cis*



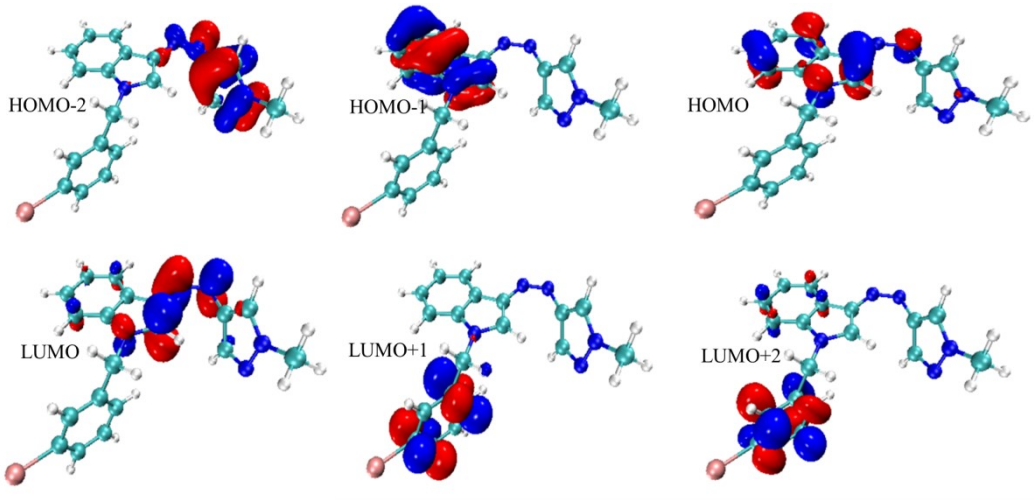
Frontier MOs of **A7** *trans*



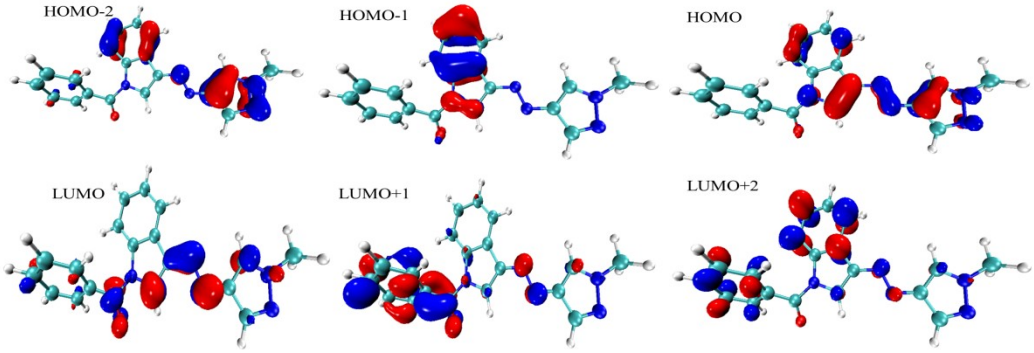
Frontier MOs of **A7** *cis*



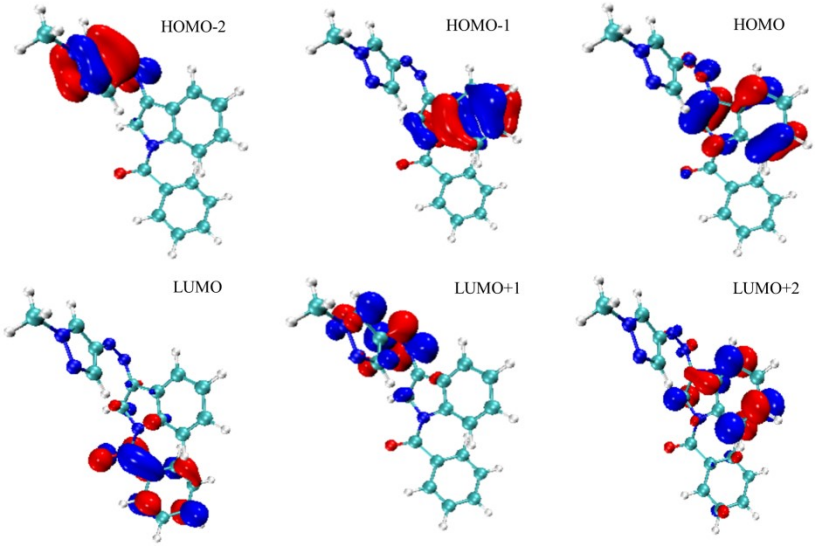
Frontier MOs of **A8** *trans*



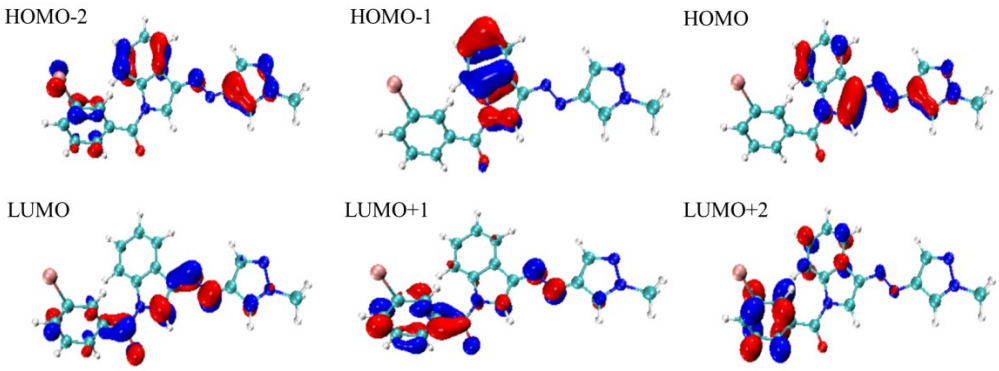
Frontier MOs of **A8** *cis*



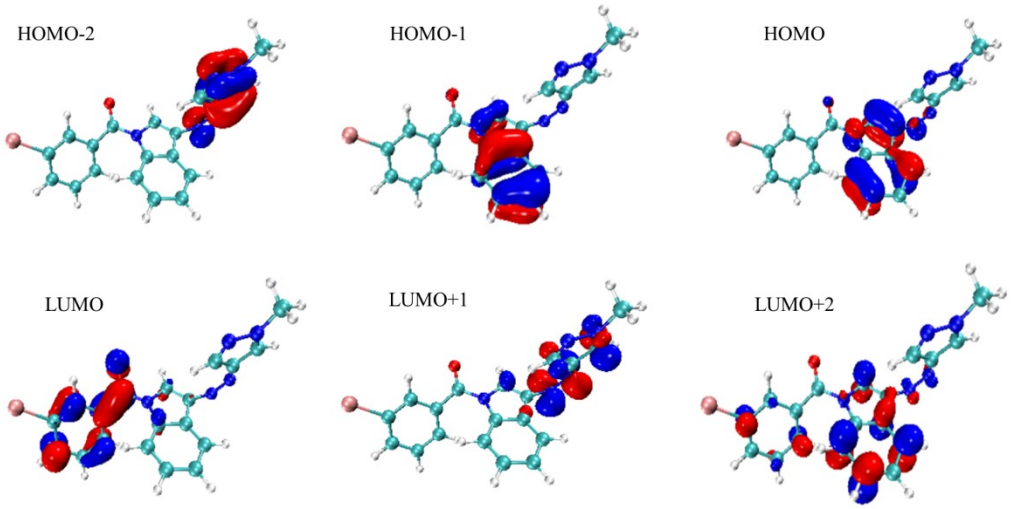
Frontier MOs of **A9** *trans*



Frontier MOs of **A9** *cis*



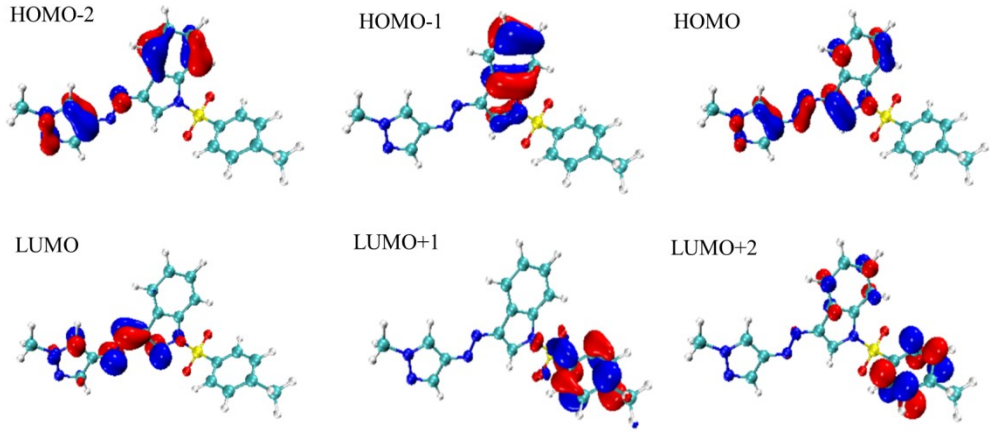
Frontier MOs of **A10** *trans*



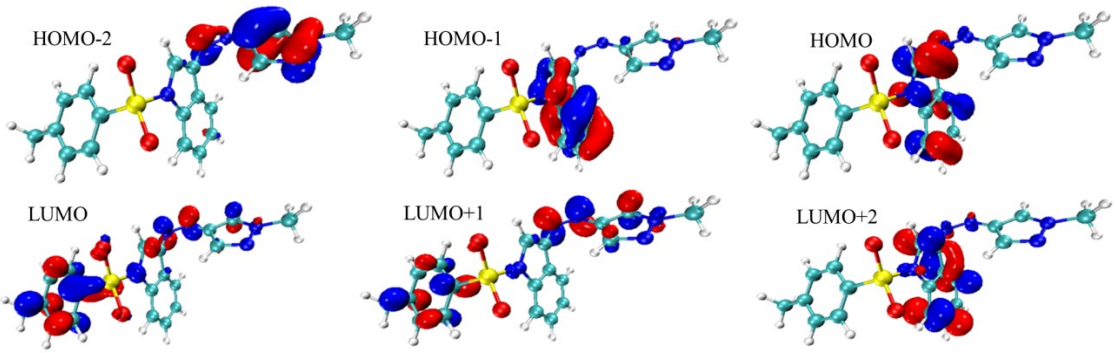
Frontier MOs of **A10** *cis*

Table S7. The energy (eV) of Frontier MOs (**A11**—**B4**).

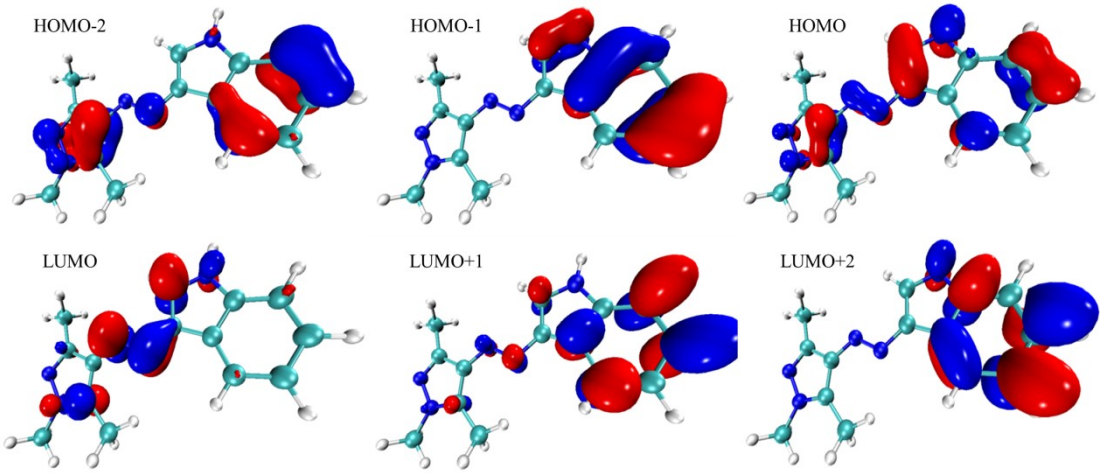
Compd.	**B1**	**A11**		**B2**		**B3**		**B4**	
		trans	*cis*	*trans*	*cis*	*trans*	*cis*	*trans*	*cis*
HOMO-2	-9.247	-9.580	-9.4754	-9.232	-8.826	-9.240	-8.826	-9.223	-8.864
HOMO-1	-8.677	-9.200	-9.2220	-8.615	-8.734	-8.593	-8.689	-8.641	-8.770
HOMO	-7.515	-8.119	-8.5843	-7.418	-8.046	-7.424	-8.043	-7.504	-8.137
LUMO	2.199	1.754	2.2792	2.211	2.326	2.187	2.296	2.156	2.176
LUMO+1	3.571	2.398	2.5174	3.571	3.624	3.556	3.624	3.484	3.434
LUMO+2	4.597	3.176	2.9029	4.541	4.474	4.557	4.500	3.518	3.500



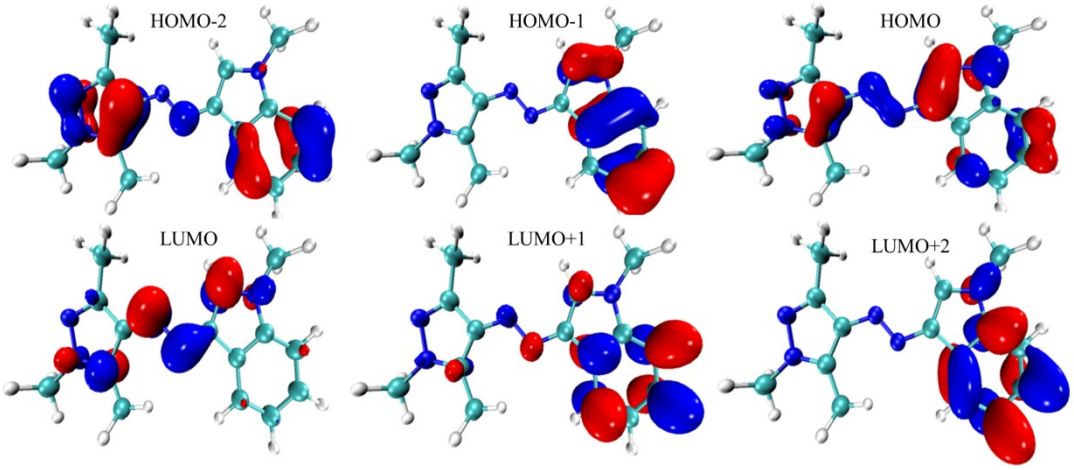
Frontier MOs of **A11** *trans*



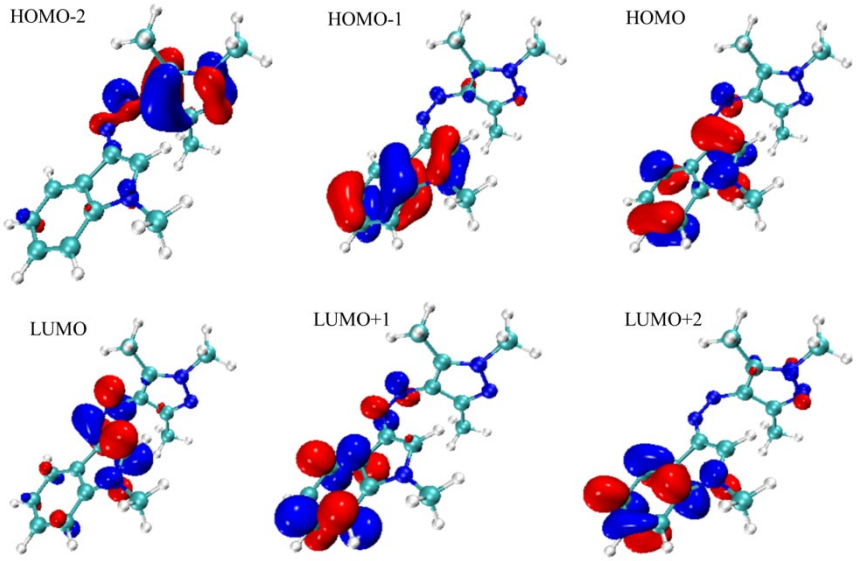
Frontier MOs of **A11** *cis*



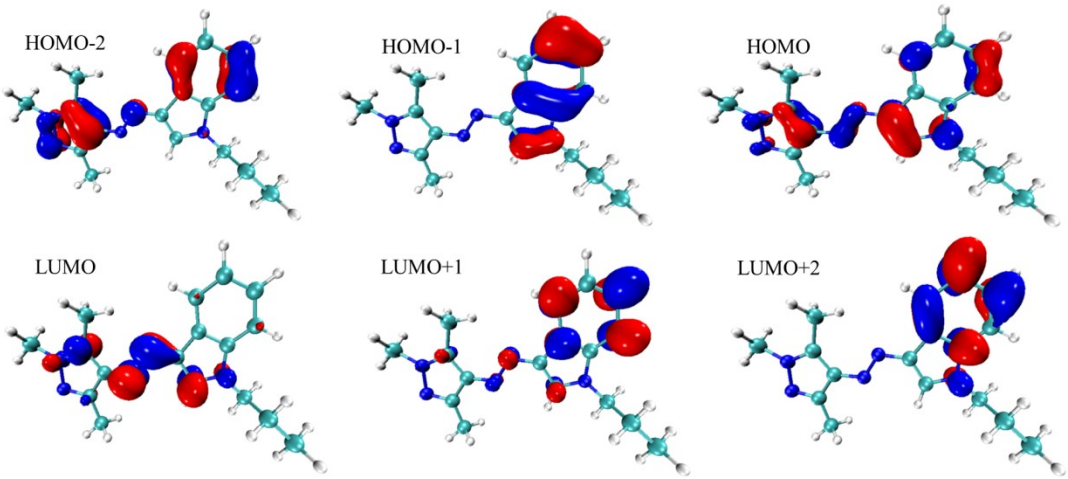
Frontier MOs of **B1** *trans*



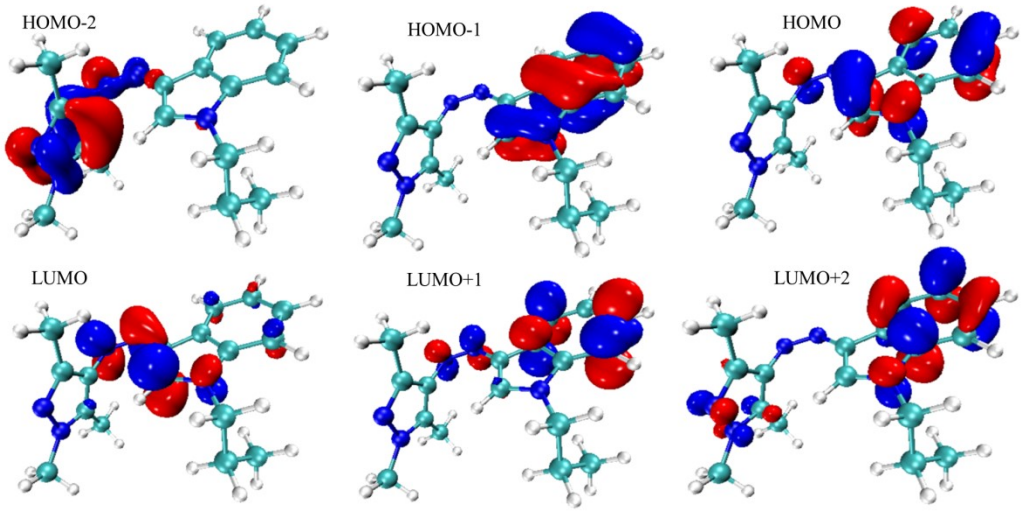
Frontier MOs of **B2** *trans*



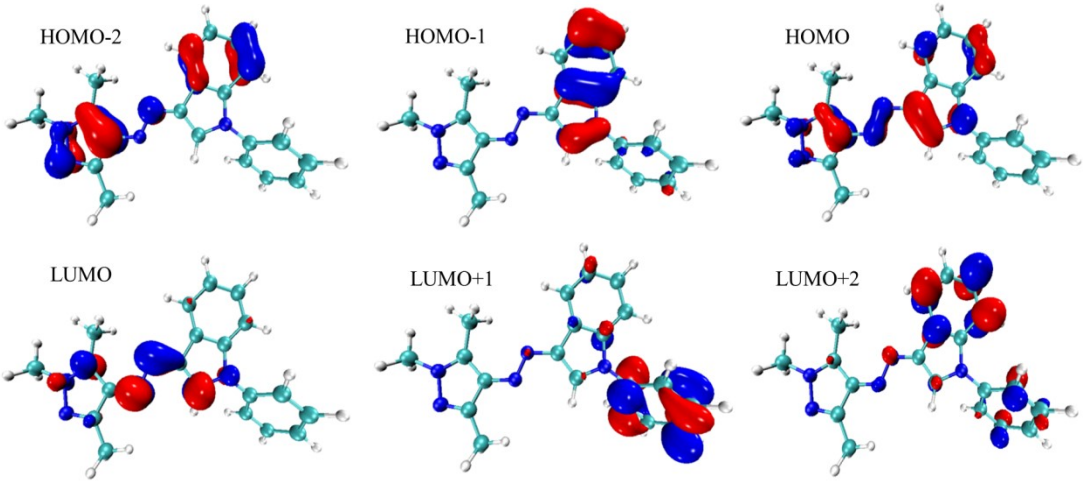
Frontier MOs of **B2** *cis*



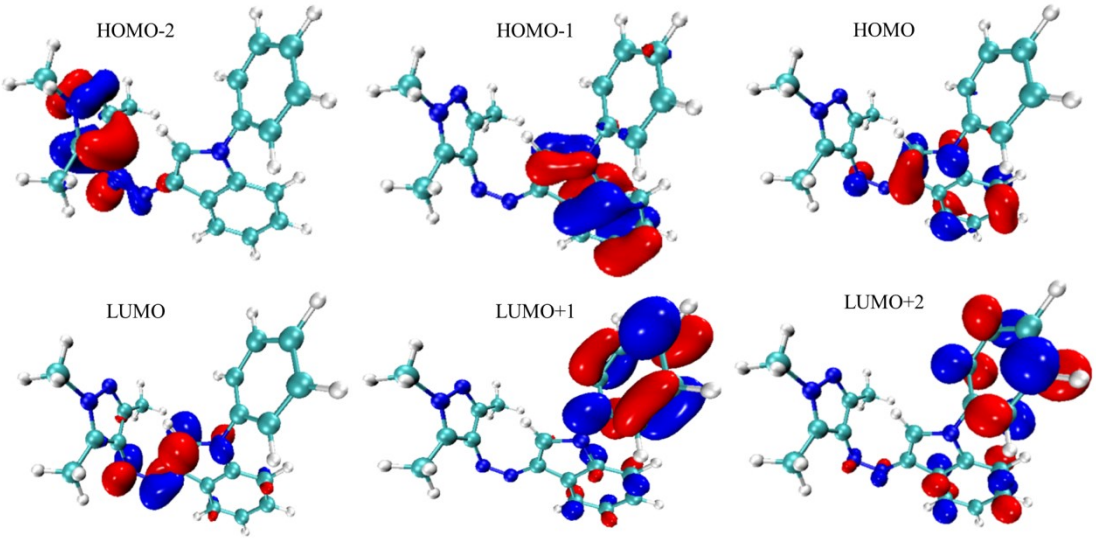
Frontier MOs of **B3** *trans*



Frontier MOs of **B3** *cis*



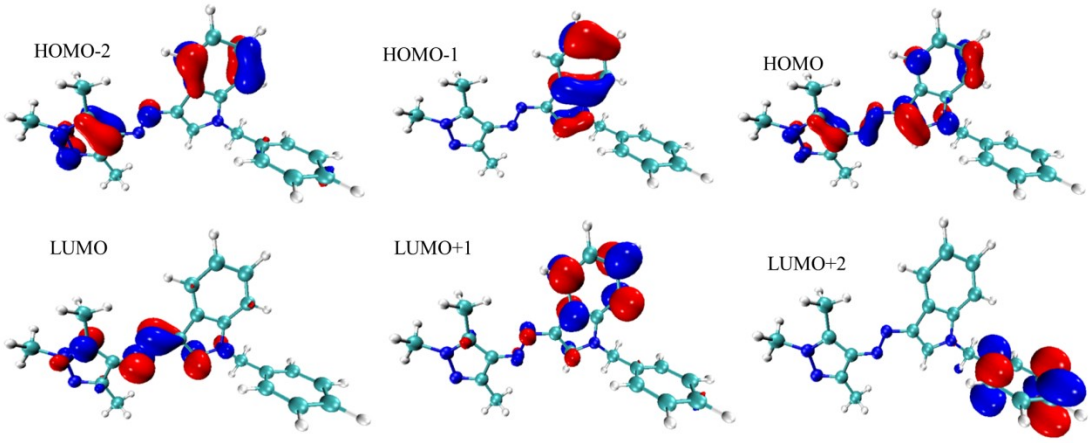
Frontier MOs of **B4** *trans*



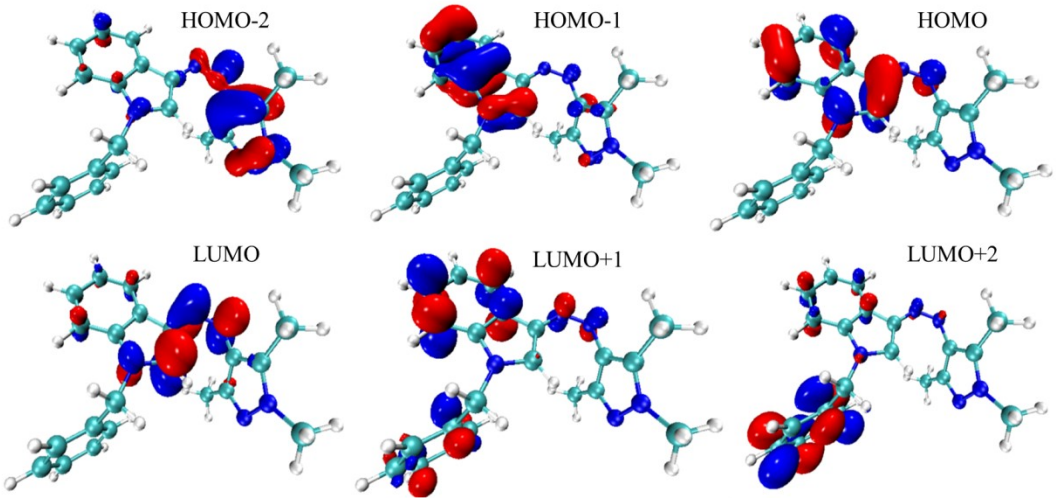
Frontier MOs of **B4** *cis*

Table S8. The energy (eV) of Frontier MOs (**B5**—**B7**).

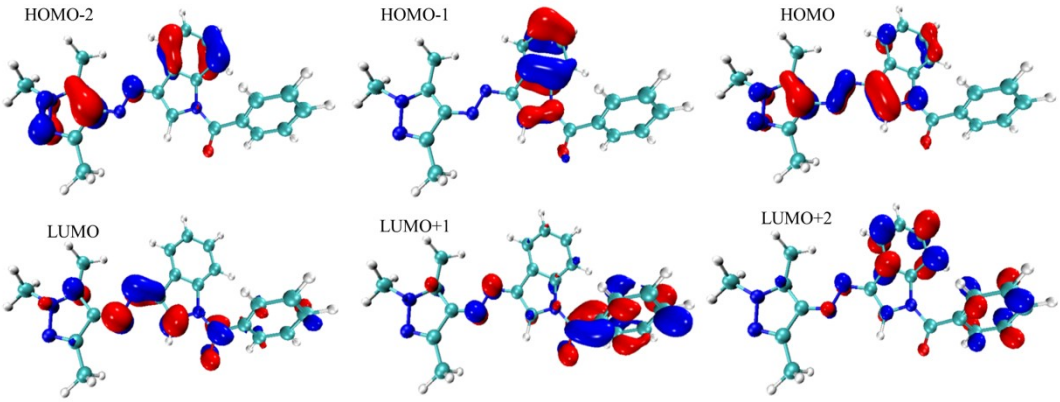
Compd.	**B5**		**B6**		**B7**	
	trans	*cis*	*trans*	*cis*	*trans*	*cis*
HOMO-2	-9.250	-8.852	-9.354	-9.106	-9.452	-9.293
HOMO-1	-8.664	-8.771	-8.999	-8.972	-9.162	-9.002
HOMO	-7.482	-8.091	-7.873	-8.537	-7.999	-8.662
LUMO	2.152	2.270	1.717	1.705	1.787	1.882
LUMO+1	3.537	3.568	2.418	2.462	2.344	2.354
LUMO+2	3.712	3.672	3.276	3.490	3.176	3.180



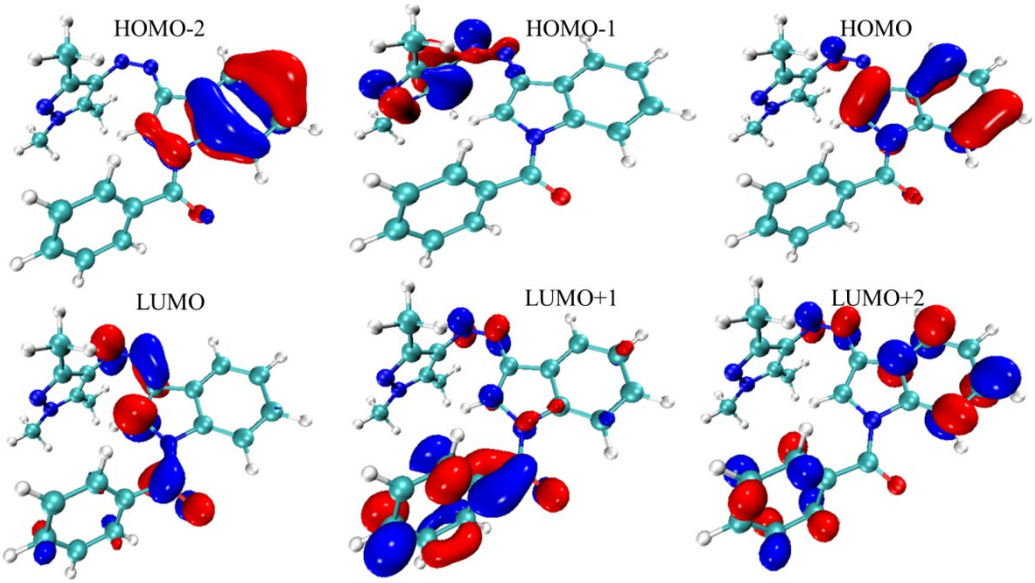
Frontier MOs of **B5** *trans*



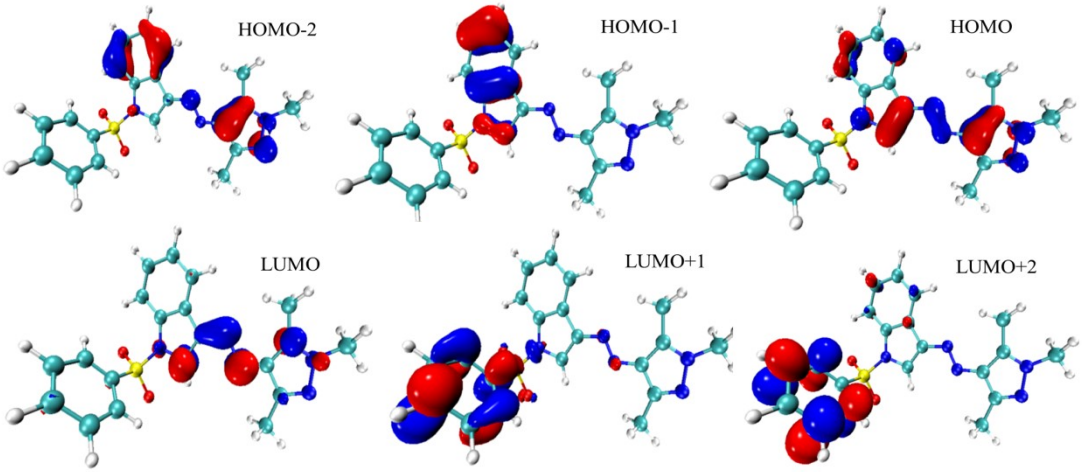
Frontier MOs of **B5** *cis*



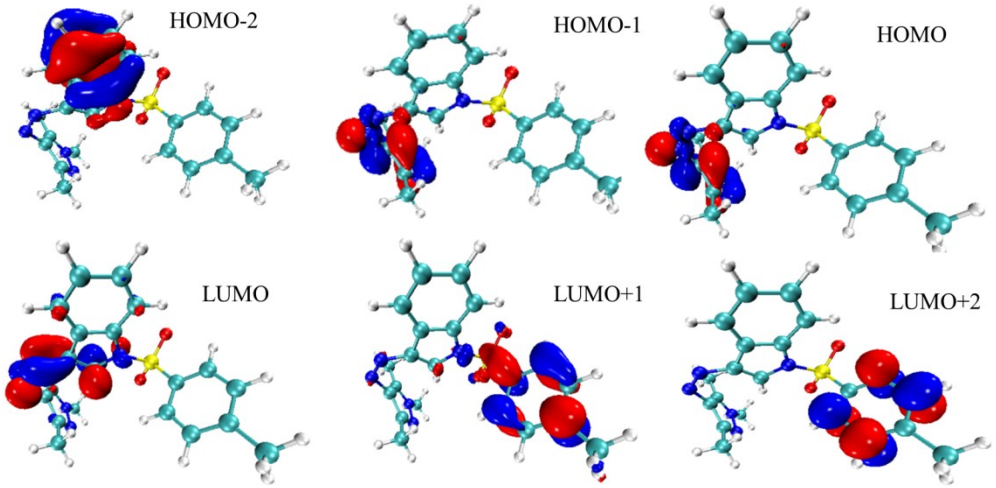
Frontier MOs of **B6** *trans*



Frontier MOs of **B6** *cis*



Frontier MOs of **B7** *trans*



Frontier MOs of **B7** *cis*

calculations of transition state

Table S9. The energy (Hartree) TS-1, TS-2, and *cis*-isomer by Gauss calculations (**A9**, **A11**, and **B7**).

Compd.	TS-1	TS-2	*Cis*-isomer
A9	-1540.1519	-1540.1105	-1540.1981
A11	-1069.1888	-1069.1456	-1069.2353
B7	-1578.9520	-1578.3637	-1617.8487

4.4 XYZ coordinates optimized molecular geometry of title compounds

Table S10. XYZ coordinates optimized molecular geometry of **A1**.

C	2.44815	0.03523	-0.94145
C	3.36786	1.03629	-1.08284
C	2.94823	2.17394	-0.16807
C	1.78617	1.79081	0.42332
N	1.51649	0.34583	0.16657
H	0.5609	0.15639	-0.05919
H	1.14985	2.43754	0.99053
C	3.51968	-1.20032	-2.69996
C	4.52248	-0.19749	-2.7772
C	4.44622	0.94556	-1.95554
C	2.46412	-1.08406	-1.76949
H	3.56611	-2.05019	-3.34839
H	5.33599	-0.30807	-3.46341
H	5.18607	1.71686	-2.00664
H	1.70517	-1.83495	-1.69827
N	3.64902	3.45238	0.02009

N	4.23634	4.52383	0.17779
C	5.48425	4.79222	-0.5513
C	6.10705	3.98139	-1.40479
C	6.33882	6.04218	-0.47305
H	5.8575	2.95651	-1.58437
H	6.12791	6.90463	0.12411
N	7.37832	5.88834	-1.24283
N	7.20686	4.72707	-2.05671
C	8.43276	3.92203	-2.15663
H	8.2426	3.0554	-2.75469
H	9.20665	4.50549	-2.61004
H	8.74137	3.61923	-1.17787

Zero-point correction=	0.236939 (Hartree/Particle)
Thermal correction to Energy=	0.249475
Thermal correction to Enthalpy=	0.250419
Thermal correction to Gibbs Free Energy=	0.195632
Sum of electronic and zero-point Energies=	-728.648173
Sum of electronic and thermal Energies=	-728.635638
Sum of electronic and thermal Enthalpies=	-728.634694
Sum of electronic and thermal Free Energies=	-728.689481

Table S11. XYZ coordinates optimized molecular geometry of **A2**-*trans*.

C	-3.12979	0.29402	0.00005
C	-2.01985	-0.56163	-0.00007
C	-0.8516	0.28285	-0.00014
C	-1.29538	1.57226	-0.00008
N	-2.663	1.59433	0.00004
H	-0.72888	2.47336	-0.00011
C	-4.5931	-1.56888	0.00012
C	-3.48881	-2.43474	0.00001
C	-2.20417	-1.9419	-0.00009
C	-4.42917	-0.20236	0.00015
H	-5.58281	-1.98059	0.0002
H	-3.65464	-3.49372	-0.00001
H	-1.35802	-2.59939	-0.00018
H	-5.27548	0.45392	0.00024
N	0.45026	-0.21538	-0.00026
N	1.37388	0.62608	-0.0003
C	2.66807	0.10692	-0.00012
C	3.81209	0.86574	-0.00015
C	3.12111	-1.23635	0.00006

H	3.92815	1.92365	-0.00029
H	2.52509	-2.11707	0.00011
N	4.85487	0.02268	0.00006
C	-3.50188	2.79366	0.00013
H	-4.12725	2.81361	0.88247
H	-2.86449	3.66437	0.00007
H	-4.12744	2.81362	-0.88207
N	4.43197	-1.29566	0.00024
C	5.90062	-1.35876	0.00047
H	6.27848	-0.86998	0.87409
H	6.21365	-2.38195	0.00069
H	6.27873	-0.87029	-0.87322

Zero-point correction=	0.266727 (Hartree/Particle)
Thermal correction to Energy=	0.280943
Thermal correction to Enthalpy=	0.281887
Thermal correction to Gibbs Free Energy=	0.223483
Sum of electronic and zero-point Energies=	-767.432402
Sum of electronic and thermal Energies=	-767.418186
Sum of electronic and thermal Enthalpies=	-767.417242
Sum of electronic and thermal Free Energies=	-767.475646

Table S12. XYZ coordinates optimized molecular geometry of **A2**-*cis*.

C	2.35418000	0.74548300	0.00739300
C	2.01413300	-0.60836800	0.05598700
C	0.56993400	-0.68137900	0.01938400
C	0.12083300	0.61617600	-0.04721400
N	1.17706000	1.47195600	-0.05364300
H	-0.86885200	0.99572900	-0.09281300
C	4.65507300	0.19859500	0.09370400
C	4.32524400	-1.16404300	0.14436600
C	3.01223200	-1.57577800	0.12646000
C	3.67883200	1.16678700	0.02495400
H	5.68635700	0.49023700	0.10886200
H	5.11169600	-1.89039300	0.19789500
H	2.75311000	-2.61424400	0.16522800
H	3.93431500	2.20604000	-0.01313300
N	-0.04470200	-1.93259700	0.08207700
N	-1.26365900	-2.19072800	0.05027400
C	-2.23423500	-1.15161300	-0.11466300
C	-3.04027200	-0.60871000	0.84631300
C	-2.63730700	-0.53826100	-1.32374000
H	-3.08194600	-0.79075600	1.89391800

H	-2.24750700	-0.70978100	-2.29964400
N	-3.60754000	0.32762200	-1.11528400
N	-3.85001900	0.28310600	0.23448200
C	-4.89622300	1.12228800	0.81333200
H	-4.91533400	0.96575900	1.88038600
H	-4.68420100	2.15955600	0.60269900
H	-5.85278100	0.85392800	0.39038900
C	1.09245600	2.93355600	-0.11664800
H	1.59235400	3.29710200	-1.00382100
H	0.05351200	3.22265400	-0.15235200
H	1.55202300	3.37025600	0.75927000

Zero-point correction=	0.266267 (Hartree/Particle)
Thermal correction to Energy=	0.280552
Thermal correction to Enthalpy=	0.281496
Thermal correction to Gibbs Free Energy=	0.222143
Sum of electronic and zero-point Energies=	-767.407399
Sum of electronic and thermal Energies=	-767.393114
Sum of electronic and thermal Enthalpies=	-767.392170
Sum of electronic and thermal Free Energies=	-767.451523

Table S13. XYZ coordinates optimized molecular geometry of **A3**-*trans.*

C	2.89046	0.12334	-0.17818
C	1.72244	0.88697	-0.04594
C	0.61793	-0.03589	-0.11833
C	1.15126	-1.27895	-0.28704
N	2.51687	-1.20037	-0.3279
H	0.64898	-2.21255	-0.38439
C	4.21081	2.08393	0.00334
C	3.04692	2.85659	0.13616
C	1.80388	2.26831	0.11226
C	4.14851	0.71831	-0.154
H	5.16717	2.56767	0.02549
H	3.13424	3.918	0.25751
H	0.91132	2.85286	0.2121
H	5.04241	0.13709	-0.25292
N	-0.71505	0.36141	-0.0276
N	-1.57671	-0.53928	-0.11409
C	-2.9032	-0.1198	-0.02121
C	-3.99181	-0.95279	-0.09829
C	-3.44704	1.17639	0.16156
H	-4.03521	-2.00758	-0.23348

H	-2.913	2.09025	0.26445
N	-5.08944	-0.19333	0.03024
C	3.42823	-2.34567	-0.44906
H	2.89486	-3.13619	-0.95676
H	4.26085	-2.05153	-1.07218
C	3.92138	-2.82862	0.92382
H	4.59118	-3.67112	0.79816
H	4.45278	-2.03817	1.43879
H	3.08252	-3.13862	1.53449
N	-4.75837	1.14094	0.19402
C	-6.22729	1.09782	0.23028
H	-6.54594	0.47489	1.0398
H	-6.60982	2.08733	0.36971
H	-6.59531	0.69986	-0.69226

Zero-point correction=	0.297140 (Hartree/Particle)
Thermal correction to Energy=	0.312575
Thermal correction to Enthalpy=	0.313519
Thermal correction to Gibbs Free Energy=	0.251917
Sum of electronic and zero-point Energies=	-806.223575
Sum of electronic and thermal Energies=	-806.208140
Sum of electronic and thermal Enthalpies=	-806.207196
Sum of electronic and thermal Free Energies=	-806.268798

Table S14. XYZ coordinates optimized molecular geometry of **A3**-*cis*.

C	-2.29852900	0.41301500	-0.22795200
C	-1.90064500	-0.91366000	-0.04464700
C	-0.45609700	-0.91581700	0.02477500
C	-0.06232900	0.39257000	-0.12054900
N	-1.15244800	1.19150700	-0.27452200
H	0.90999100	0.81764600	-0.12720200
C	-4.57150100	-0.25136100	-0.26257600
C	-4.18193800	-1.58656600	-0.07933600
C	-2.85316400	-1.92590800	0.02960300
C	-3.64103000	0.75993700	-0.33882800
H	-5.61371100	-0.01478600	-0.34441800
H	-4.93427400	-2.34808000	-0.02462800
H	-2.54674700	-2.94278200	0.16812100
H	-3.94651500	1.77665900	-0.47788700
N	0.20990500	-2.13231600	0.18130200
N	1.43755300	-2.32845800	0.26873600
C	2.36230600	-1.23567000	0.26082200
C	3.15263500	-0.82474900	-0.77569200

C	2.72866100	-0.41396500	1.35213700
H	3.21090300	-1.17526900	-1.77872100
H	2.33822300	-0.43841500	2.34243900
N	3.66300500	0.44680700	1.00444200
N	3.91853000	0.19011000	-0.31893600
C	4.93332600	0.96531900	-1.02812400
H	4.96169200	0.63973700	-2.05612100
H	4.68009300	2.01380700	-0.98657600
H	5.89836700	0.80623700	-0.57058000
C	-1.11255300	2.65581000	-0.40811600
H	-0.15103300	2.92030900	-0.82318600
H	-1.87444900	2.94985500	-1.11554900
C	-1.32379500	3.35416700	0.94375600
H	-1.29347500	4.42883800	0.80912000
H	-2.28303900	3.08579200	1.36797700
H	-0.54391200	3.06816600	1.63841700

Zero-point correction=	0.296848 (Hartree/Particle)
Thermal correction to Energy=	0.312301
Thermal correction to Enthalpy=	0.313245
Thermal correction to Gibbs Free Energy=	0.251034
Sum of electronic and zero-point Energies=	-806.198379
Sum of electronic and thermal Energies=	-806.182926
Sum of electronic and thermal Enthalpies=	-806.181982
Sum of electronic and thermal Free Energies=	-806.244192

Table S15. XYZ coordinates optimized molecular geometry of **A4**-*trans*.

C	2.46616	0.75394	-0.2294
C	1.16712	1.25134	-0.06891
C	0.2766	0.1242	-0.17766
C	1.04929	-0.9721	-0.39374
N	2.37449	-0.61241	-0.43093
H	0.74237	-1.9823	-0.52849
C	3.34933	2.93696	0.03049
C	2.05261	3.44339	0.19174
C	0.96061	2.60989	0.14321
C	3.57155	1.59607	-0.17979
H	4.18396	3.60841	0.07279
H	1.91763	4.49408	0.35467
H	-0.03473	2.98642	0.26449
H	4.56686	1.21888	-0.29946
N	-1.11012	0.22836	-0.07306
N	-1.75497	-0.83485	-0.18883

C	-3.14083	-0.71957	-0.08266
C	-3.92619	0.3854	0.1303
C	-4.05075	-1.798	-0.18265
H	-3.64299	1.40155	0.26134
H	-3.81454	-2.82216	-0.34853
N	-5.29181	-1.39719	-0.04381
N	-5.2026	-0.03098	0.15126
C	-6.4241	0.73506	0.34266
H	-6.1684	1.77547	0.47866
H	-7.05835	0.62652	-0.5247
H	-6.94579	0.37137	1.21556
C	3.49602	-1.53438	-0.59519
H	3.14047	-2.39781	-1.14266
H	4.2531	-1.05052	-1.1991
C	4.09214	-1.97621	0.75312
H	4.41348	-1.09984	1.30322
H	3.31629	-2.45919	1.33571
C	5.27754	-2.93729	0.54637
H	6.06797	-2.45922	-0.02291
H	5.69052	-3.24686	1.49891
H	4.96464	-3.82756	0.01074

Zero-point correction=	0.327614 (Hartree/Particle)
Thermal correction to Energy=	0.344386
Thermal correction to Enthalpy=	0.345330
Thermal correction to Gibbs Free Energy=	0.280261
Sum of electronic and zero-point Energies=	-845.012827
Sum of electronic and thermal Energies=	-844.996055
Sum of electronic and thermal Enthalpies=	-844.995110
Sum of electronic and thermal Free Energies=	-845.060180

Table S16. XYZ coordinates optimized molecular geometry of **A4**-*cis*.

C	2.24247900	-0.05463400	0.20748500
C	1.74445400	-1.32790800	-0.07947900
C	0.30164400	-1.22919000	-0.07096400
C	0.00759300	0.08157700	0.21723100
N	1.15714800	0.78953600	0.38611600
H	-0.93129600	0.56506600	0.32155800
C	4.46239700	-0.86577400	0.05705600
C	3.97208400	-2.14784800	-0.23292600
C	2.61916900	-2.38741800	-0.30284600
C	3.60965000	0.19155000	0.27899700
H	5.52129500	-0.70696600	0.10552600

H	4.66584300	-2.94734700	-0.40140700
H	2.23610100	-3.36308700	-0.52303300
H	3.99147700	1.16778500	0.49714500
N	-0.45363900	-2.36803700	-0.35481300
N	-1.69469000	-2.47941100	-0.37744500
C	-2.54226200	-1.37621100	-0.04046700
C	-3.25820500	-0.58851700	-0.89763700
C	-2.90124100	-0.93349600	1.25408000
H	-3.29558400	-0.58476700	-1.96111200
H	-2.55708800	-1.31205200	2.18791000
N	-3.76122300	0.06212200	1.19279500
N	-3.97518200	0.27501200	-0.14571400
C	-4.90308600	1.31735200	-0.57735000
H	-4.91935900	1.34181500	-1.65560200
H	-5.89278600	1.09941200	-0.20472300
H	-4.57444800	2.27297100	-0.19774000
C	1.22653400	2.23120300	0.66553600
H	0.30785800	2.51601300	1.15904200
H	2.04348100	2.40329700	1.35278500
C	1.41799000	3.05860200	-0.61637400
H	2.32272800	2.73734800	-1.11863200
H	0.58436300	2.86939800	-1.28257900
C	1.50344100	4.56101900	-0.28894700
H	2.34376300	4.76424900	0.36619500
H	1.63327000	5.14095300	-1.19489400
H	0.59763700	4.89950400	0.20261100

Zero-point correction=	0.327276 (Hartree/Particle)
Thermal correction to Energy=	0.344063
Thermal correction to Enthalpy=	0.345007
Thermal correction to Gibbs Free Energy=	0.279312
Sum of electronic and zero-point Energies=	-844.987653
Sum of electronic and thermal Energies=	-844.970866
Sum of electronic and thermal Enthalpies=	-844.969922
Sum of electronic and thermal Free Energies=	-845.035617

Table S17. XYZ coordinates optimized molecular geometry of **A5**-*trans*.

C	-2.74107	-0.55028	-0.21817
C	-1.52371	-1.21982	-0.03005
C	-0.48438	-0.22912	-0.15702
C	-1.09854	0.96002	-0.40798
N	-2.45605	0.78357	-0.45432
H	-0.66173	1.91889	-0.55916

C	-3.92098	-2.58292	0.09554
C	-2.70716	-3.26131	0.28258
C	-1.50874	-2.58934	0.22157
C	-3.95401	-1.23008	-0.15417
H	-4.84145	-3.12961	0.14971
H	-2.72064	-4.31553	0.47574
H	-0.57779	-3.10056	0.36394
H	-4.88734	-0.72367	-0.29127
N	0.87223	-0.52773	-0.03261
N	1.66996	0.4241	-0.16828
C	3.02124	0.10638	-0.04066
C	4.04868	1.00995	-0.15548
C	3.65364	-1.13493	0.22104
H	4.01811	2.05589	-0.35032
H	3.18507	-2.0776	0.37164
N	5.1956	0.34018	0.02681
C	-3.4283	1.86541	-0.66285
H	-3.05786	2.5159	-1.44284
H	-4.34738	1.4159	-1.01156
C	-3.66626	2.64019	0.61104
H	-3.97154	2.05396	1.45863
C	-3.52569	3.9449	0.70737
H	-3.71529	4.46546	1.62638
H	-3.21777	4.54677	-0.12803
N	4.95846	-1.00343	0.26305
C	6.42001	-0.85306	0.30941
H	6.68332	-0.16487	1.08528
H	6.87022	-1.80329	0.50759
H	6.77034	-0.48155	-0.63088

Zero-point correction=	0.302851 (Hartree/Particle)
Thermal correction to Energy=	0.319061
Thermal correction to Enthalpy=	0.320005
Thermal correction to Gibbs Free Energy=	0.255707
Sum of electronic and zero-point Energies=	-843.846442
Sum of electronic and thermal Energies=	-843.830232
Sum of electronic and thermal Enthalpies=	-843.829288
Sum of electronic and thermal Free Energies=	-843.893585

Table S18. XYZ coordinates optimized molecular geometry of **A5**-*cis*.

C	2.36149100	0.31102200	0.21817900
C	2.00785300	-1.00395400	-0.09616800
C	0.56292100	-1.06407100	-0.10341900

C	0.12287200	0.19981900	0.19917200
N	1.18711200	1.02639000	0.39653700
H	-2.15371000	-1.48488400	2.17216900
C	4.65756700	-0.25305600	0.07108900
C	4.31201100	-1.57521100	-0.24530900
C	2.99358100	-1.95800400	-0.33101300
C	3.69396400	0.70147200	0.30465100
H	5.69246000	0.01949700	0.13085100
H	5.08953100	-2.29140000	-0.42236900
H	2.71939800	-2.96467300	-0.57285000
H	3.96953200	1.70840400	0.54159300
N	-0.05977300	-2.27233200	-0.42723500
N	-1.27984700	-2.52326100	-0.44892000
C	-2.24774400	-1.54615400	-0.05469900
C	-3.11169500	-0.86616400	-0.86671800
C	-2.59554100	-1.15766900	1.26050500
H	-3.20585100	-0.86798600	-1.92669800
H	-0.86437100	0.57829500	0.29085400
N	-3.58794600	-0.29271300	1.25246300
N	-3.90030300	-0.11099600	-0.07171100
C	-4.98380800	0.79460200	-0.44528700
H	-5.06921900	0.80776200	-1.52043000
H	-5.91048500	0.44898200	-0.01220600
H	-4.76394100	1.78884100	-0.08673100
C	1.07156500	2.46205100	0.70091300
H	0.31028900	2.59464600	1.45674400
H	2.01580200	2.78196200	1.11731100
C	0.74010900	3.25521600	-0.53959900
H	1.41926300	3.13161100	-1.36331700
C	-0.29797000	4.05834600	-0.63317200
H	-0.49744100	4.61827500	-1.52652500
H	-0.98901500	4.19158300	0.17892800

Zero-point correction=	0.302377 (Hartree/Particle)
Thermal correction to Energy=	0.318665
Thermal correction to Enthalpy=	0.319609
Thermal correction to Gibbs Free Energy=	0.253902
Sum of electronic and zero-point Energies=	-843.821231
Sum of electronic and thermal Energies=	-843.804944
Sum of electronic and thermal Enthalpies=	-843.804000
Sum of electronic and thermal Free Energies=	-843.869706

Table S19. XYZ coordinates optimized molecular geometry of **A6**-*trans*.

C	-1.94503	1.24337	-0.04594
C	-0.62404	1.70357	-0.05278
C	0.22468	0.53755	-0.01451
C	-0.58874	-0.54944	0.01228
N	-1.90701	-0.14628	-0.00322
H	-0.33231	-1.58121	0.05437
C	-2.74122	3.47143	-0.14948
C	-1.42039	3.94397	-0.14668
C	-0.35955	3.0696	-0.10088
C	-3.01946	2.12438	-0.10123
H	-3.54993	4.1736	-0.1917
H	-1.24191	5.0001	-0.18406
H	0.65218	3.42216	-0.10464
H	-4.02836	1.76775	-0.10698
N	1.61858	0.61475	-0.00457
N	2.23677	-0.46994	0.02697
C	3.62666	-0.37824	0.03661
C	4.47415	0.75793	0.01693
C	4.47813	-1.45532	0.069
H	4.18153	1.77998	-0.00945
H	4.25918	-2.49664	0.09164
C	-5.19262	-2.75417	0.05829
C	-4.24107	-2.85733	-0.94253
C	-3.16316	-1.98947	-0.97073
C	-3.02825	-1.0261	0.01587
C	-3.97282	-0.92622	1.02549
C	-5.05781	-1.78513	1.03891
H	-6.0302	-3.42204	0.07459
H	-4.3406	-3.60291	-1.70545
H	-2.43596	-2.05125	-1.75452
H	-3.85324	-0.19027	1.79386
H	-5.7874	-1.70364	1.81923
N	5.72999	-0.978	0.06795
N	5.738	0.40709	0.03552
C	7.15368	0.01172	0.05639
H	7.36855	-0.59031	-0.80169
H	7.76875	0.88713	0.04098
H	7.3542	-0.54947	0.94508

Zero-point correction=	0.323966 (Hartree/Particle)
Thermal correction to Energy=	0.340870
Thermal correction to Enthalpy=	0.341814
Thermal correction to Gibbs Free Energy=	0.275808
Sum of electronic and zero-point Energies=	-956.825619

Sum of electronic and thermal Energies=	-956.808715
Sum of electronic and thermal Enthalpies=	-956.807770
Sum of electronic and thermal Free Energies=	-956.873777

Table S20. XYZ coordinates optimized molecular geometry of **A6**-*cis*.

C	-2.02168200	-0.85084900	0.00133500
C	-1.28065800	-2.03208000	-0.02783200
C	0.11784400	-1.65960500	-0.05312200
C	0.15745600	-0.29232700	-0.04114000
N	-1.11788600	0.20829600	-0.01246600
H	0.98248900	0.37410900	-0.06273000
C	-4.03786000	-2.08694700	0.06412600
C	-3.30352800	-3.28135100	0.02409800
C	-1.92855600	-3.26375900	-0.01983900
C	-3.41041700	-0.86182800	0.05449900
H	-5.10802600	-2.12925400	0.10393600
H	-3.82592200	-4.21714700	0.03100100
H	-1.35896800	-4.17021400	-0.04516200
H	-3.97160000	0.04867300	0.08721000
N	1.08197900	-2.67169900	-0.12617000
N	2.32034900	-2.54707400	-0.10825400
C	2.93759400	-1.26748100	0.06193200
C	3.59977300	-0.53775200	-0.88517300
C	3.09155400	-0.53835700	1.26456400
H	3.74082100	-0.72384600	-1.92330700
H	2.72270500	-0.79355100	2.23021400
N	3.78320600	0.56373600	1.06396200
N	4.09022300	0.56188200	-0.27379000
C	4.87756400	1.65414200	-0.84074300
H	4.97684800	1.49477500	-1.90292600
H	4.37408500	2.59164700	-0.66012500
H	5.85565600	1.67280600	-0.38366300
C	-1.44430500	1.59825800	0.00867200
C	-0.98034600	2.39664000	1.04070900
C	-2.21286900	2.14412200	-1.00700600
C	-1.28123200	3.74779000	1.05201400
H	-0.39804000	1.96212900	1.82752300
C	-2.52451700	3.49212200	-0.98161000
H	-2.55462800	1.52170900	-1.80834200
C	-2.05686400	4.29663900	0.04471000
H	-0.91881600	4.36431200	1.84963700
H	-3.12076700	3.91241900	-1.76614800
H	-2.29463500	5.34118200	0.05873400

Zero-point correction=	0.323586 (Hartree/Particle)
Thermal correction to Energy=	0.340517
Thermal correction to Enthalpy=	0.341461
Thermal correction to Gibbs Free Energy=	0.274787
Sum of electronic and zero-point Energies=	-956.799929
Sum of electronic and thermal Energies=	-956.782997
Sum of electronic and thermal Enthalpies=	-956.782053
Sum of electronic and thermal Free Energies=	-956.848727

Table S21. XYZ coordinates optimized molecular geometry of A7-trans.

C	1.57979	1.27386	-0.45898
C	0.30141	1.66532	-0.04154
C	-0.58079	0.55933	-0.32157
C	0.17818	-0.42168	-0.88284
N	1.48364	-0.00878	-0.97131
H	-0.1208	-1.38313	-1.22826
C	2.46057	3.36736	0.21501
C	1.18384	3.76912	0.63599
C	0.10291	2.9272	0.51267
C	2.67425	2.12296	-0.3327
H	3.28591	4.04248	0.32479
H	1.05547	4.74551	1.05918
H	-0.87454	3.2282	0.83235
H	3.65209	1.81776	-0.64272
N	-1.94632	0.58351	-0.03911
N	-2.59706	-0.44185	-0.33205
C	-3.95996	-0.39927	-0.04287
C	-4.74542	0.62715	0.53921
C	-4.84148	-1.42238	-0.29079
H	-4.41536	1.58262	0.86938
H	-4.67012	-2.3802	-0.72201
C	2.58568	-0.78424	-1.54083
H	2.15217	-1.65279	-2.01817
H	3.07244	-0.19431	-2.30596
C	3.60346	-1.2253	-0.49865
C	4.95494	-1.21164	-0.80664
C	3.19648	-1.68116	0.7473
C	5.89087	-1.65299	0.11603
H	5.28044	-0.85568	-1.76531
C	4.1294	-2.1195	1.67007
H	2.15437	-1.68915	0.99705
C	5.48	-2.10745	1.35657

H	6.93327	-1.63612	-0.13338
H	3.80493	-2.46875	2.63028
H	6.20184	-2.44585	2.07301
N	-6.05237	-1.01799	0.11819
N	-6.00223	0.26397	0.63943
C	-7.40967	-0.14554	0.75045
H	-7.47955	-1.01928	1.36412
H	-7.97786	0.64656	1.19163
H	-7.79605	-0.36197	-0.2236

Zero-point correction=	0.354976 (Hartree/Particle)
Thermal correction to Energy=	0.373118
Thermal correction to Enthalpy=	0.374062
Thermal correction to Gibbs Free Energy=	0.304207
Sum of electronic and zero-point Energies=	-995.613725
Sum of electronic and thermal Energies=	-995.595583
Sum of electronic and thermal Enthalpies=	-995.594639
Sum of electronic and thermal Free Energies=	-995.664494

Table S22. XYZ coordinates optimized molecular geometry of **A7**-*cis*.

C	1.29373300	1.44632500	-0.51044800
C	0.34230200	2.30166500	0.04842100
C	-0.90070000	1.56428100	0.12014800
C	-0.64198600	0.32055600	-0.39797300
N	0.66559400	0.23899100	-0.77715700
H	-1.28397000	-0.51395200	-0.53061600
C	2.93939000	3.14087100	-0.36214700
C	1.99086400	4.00906100	0.19845800
C	0.69411000	3.59936100	0.40772800
C	2.60579100	1.85458500	-0.72127300
H	3.94319400	3.48556000	-0.51169000
H	2.28648300	5.00392100	0.46628700
H	-0.03636400	4.25549500	0.83532900
H	3.33393500	1.19177000	-1.14022200
N	-2.03778600	2.20588300	0.61735200
N	-3.17528300	1.72654700	0.78484300
C	-3.44582200	0.34700100	0.51713400
C	-4.14915700	-0.16804900	-0.53545900
C	-3.14046300	-0.76541800	1.33624800
H	-4.57788300	0.31650300	-1.38025300
H	-2.60820400	-0.76578300	2.25842800
N	-3.60889800	-1.88007600	0.81475700
N	-4.22915600	-1.50354000	-0.35012300

C	-4.88210700	-2.50868200	-1.18514900
H	-5.28263800	-2.02344300	-2.06134800
H	-4.16086800	-3.25508500	-1.48161200
H	-5.68262900	-2.97648900	-0.63178700
C	1.29930000	-0.93074900	-1.39110400
H	1.77199800	-0.62604500	-2.31486700
C	2.31752400	-1.59742200	-0.47821600
C	3.51428700	-2.06052300	-1.00190700
C	2.04855200	-1.78597800	0.87017000
C	4.43217400	-2.70938100	-0.19023700
H	3.73389200	-1.91513700	-2.04221100
C	2.96452300	-2.43064500	1.68184200
H	1.12835000	-1.42655600	1.28572400
C	4.15937900	-2.89517000	1.15324200
H	5.35501400	-3.06174200	-0.60640000
H	2.74809600	-2.57036400	2.72240100
H	4.86888400	-3.39329700	1.78352300
H	0.51124900	-1.63012800	-1.63526200

Zero-point correction=	0.354585 (Hartree/Particle)
Thermal correction to Energy=	0.372759
Thermal correction to Enthalpy=	0.373703
Thermal correction to Gibbs Free Energy=	0.303299
Sum of electronic and zero-point Energies=	-995.588441
Sum of electronic and thermal Energies=	-995.570268
Sum of electronic and thermal Enthalpies=	-995.569323
Sum of electronic and thermal Free Energies=	-995.639727

Table S23. XYZ coordinates optimized molecular geometry of **A8**-*trans.*

C	1.56969	3.1158	0.48896
C	1.22012	1.87622	-0.03998
C	-0.10125	1.62599	-0.42985
C	-1.09075	2.59468	-0.30119
C	-0.72827	3.81533	0.22144
C	0.59283	4.07637	0.61494
H	2.58037	3.30906	0.78781
H	-2.10212	2.39793	-0.59145
H	-1.46994	4.58119	0.33241
H	0.83805	5.03832	1.01913
C	1.09305	-0.22508	-0.84538
C	1.96673	0.67277	-0.31433
H	1.27501	-1.21971	-1.17814
N	-0.1598	0.33233	-0.92069

N	3.33162	0.54744	-0.05453
N	3.85567	-0.55107	-0.33554
C	5.21975	-0.65868	-0.07109
C	5.97322	-1.78228	-0.30617
C	6.12903	0.28505	0.46915
H	5.68487	-2.72474	-0.708
H	5.91666	1.28018	0.77826
C	-1.35099	-0.32127	-1.45562
H	-1.80469	0.32248	-2.19699
H	-1.02806	-1.22513	-1.95437
C	-2.36925	-0.67111	-0.37878
C	-3.72131	-0.58675	-0.66931
C	-1.97095	-1.11106	0.87415
C	-4.65426	-0.94442	0.27875
H	-4.0473	-0.24304	-1.62958
C	-2.91616	-1.4647	1.8191
H	-0.92873	-1.17286	1.11148
C	-4.2669	-1.38307	1.52311
H	-2.60686	-1.80387	2.78707
H	-5.00136	-1.65428	2.25159
Br	-6.53232	-0.8195	-0.14677
N	7.23012	-1.50965	0.07131
N	7.3377	-0.21747	0.55782
C	8.69099	-0.78303	0.65604
H	9.03035	-1.06722	-0.31811
H	9.35486	-0.05046	1.06535
H	8.67282	-1.64305	1.29238

Zero-point correction=	0.344774 (Hartree/Particle)
Thermal correction to Energy=	0.364254
Thermal correction to Enthalpy=	0.365198
Thermal correction to Gibbs Free Energy=	0.291161
Sum of electronic and zero-point Energies=	-3555.103352
Sum of electronic and thermal Energies=	-3555.083873
Sum of electronic and thermal Enthalpies=	-3555.082928
Sum of electronic and thermal Free Energies=	-3555.156965

Table S24. XYZ coordinates optimized molecular geometry of **A8-*cis*.**

C	-0.42814500	2.00262500	-0.46096400
C	-1.65927700	2.48622400	-0.01469600
C	-2.56994300	1.36193100	0.01890400
C	-1.85583200	0.27285400	-0.40913900
N	-0.57411000	0.64368000	-0.69839600

H	-2.15586800	-0.73704000	-0.53671000
C	0.50856700	4.16998500	-0.30185600
C	-0.72449200	4.66684800	0.14553500
C	-1.81071000	3.83504600	0.29238700
C	0.67292800	2.83810900	-0.60869600
H	1.33868500	4.84004000	-0.40481800
H	-0.81555500	5.70976100	0.37535400
H	-2.75577300	4.20607200	0.63321000
H	1.61753300	2.46106200	-0.94180400
N	-3.89781400	1.58012800	0.39762500
N	-4.80278600	0.73505600	0.53159800
C	-4.54586100	-0.66220400	0.36189300
C	-4.95387000	-1.45806200	-0.67162200
C	-3.91560500	-1.53898100	1.27631100
H	-5.47463600	-1.21149500	-1.56632500
H	-3.47635100	-1.29246900	2.21438500
N	-3.92396600	-2.77656800	0.82753100
N	-4.56402700	-2.71914800	-0.38520100
C	-4.76376500	-3.94129100	-1.16006100
H	-5.24078900	-3.68605300	-2.09314400
H	-3.80800400	-4.40312100	-1.35573400
H	-5.39102400	-4.62447500	-0.60708200
C	0.46986200	-0.24549600	-1.20761000
H	0.88833400	0.18441900	-2.10721300
C	1.57170600	-0.50246800	-0.18977600
C	2.88730800	-0.58039200	-0.61593400
C	1.27946200	-0.70071400	1.15113900
C	3.88955600	-0.85882300	0.28738400
H	3.13183200	-0.42433100	-1.64655900
C	2.29323100	-0.97653800	2.04922500
H	0.26653900	-0.63648500	1.49257500
C	3.60746500	-1.05767300	1.61817200
H	2.06639900	-1.12905200	3.08499000
H	4.39493500	-1.26983300	2.30994400
H	-0.00352600	-1.18061000	-1.47403900
Br	5.71544800	-0.96326600	-0.32722100

Zero-point correction=	0.344255 (Hartree/Particle)
Thermal correction to Energy=	0.363829
Thermal correction to Enthalpy=	0.364773
Thermal correction to Gibbs Free Energy=	0.289445
Sum of electronic and zero-point Energies=	-3555.078038
Sum of electronic and thermal Energies=	-3555.058464
Sum of electronic and thermal Enthalpies=	-3555.057520

Sum of electronic and thermal Free Energies= -3555.132848

Table S25. XYZ coordinates optimized molecular geometry of **A9**-*trans***.**

C	-0.79656	1.6877	0.19639
C	0.50948	1.76905	-0.28727
C	1.23011	0.61513	0.21338
C	0.37841	-0.1168	0.95725
N	-0.87223	0.50698	0.94499
H	0.52712	-1.01766	1.49949
C	-1.3493	3.72156	-0.8668
C	-0.04723	3.80987	-1.37177
C	0.88985	2.84258	-1.08263
C	-1.74172	2.66485	-0.07303
H	-2.05539	4.49483	-1.09337
H	0.22173	4.64715	-1.98364
H	1.8917	2.90792	-1.45513
H	-2.72489	2.61528	0.34187
N	2.5832	0.39742	-0.07507
N	3.09012	-0.62919	0.42146
C	4.43358	-0.85567	0.14516
C	5.33033	-0.11956	-0.59885
C	5.17367	-1.96409	0.61599
H	5.19074	0.79078	-1.13022
H	4.81913	-2.75924	1.22918
N	6.41788	-1.92002	0.2015
N	6.5007	-0.76119	-0.55665
C	7.77374	-0.40234	-1.17813
H	7.65023	0.5256	-1.71374
H	8.52501	-0.28427	-0.41222
H	8.07122	-1.18216	-1.86261
C	-2.04944	-0.04203	1.63324
C	-3.18107	-0.26834	0.61354
C	-4.31343	0.54635	0.63596
C	-3.07395	-1.28768	-0.33252
C	-5.3387	0.34125	-0.28707
H	-4.39792	1.3494	1.38243
C	-4.099	-1.49235	-1.25653
H	-2.18146	-1.92976	-0.35045
C	-5.23133	-0.6782	-1.23387
H	-6.23155	0.98295	-0.26905
H	-4.01408	-2.29587	-2.0026
H	-6.03982	-0.83969	-1.96158
O	-2.48808	0.87876	2.63556

Zero-point correction=	0.335007 (Hartree/Particle)
Thermal correction to Energy=	0.353610
Thermal correction to Enthalpy=	0.354554
Thermal correction to Gibbs Free Energy=	0.284415
Sum of electronic and zero-point Energies=	-1068.924581
Sum of electronic and thermal Energies=	-1068.905978
Sum of electronic and thermal Enthalpies=	-1068.905034
Sum of electronic and thermal Free Energies=	-1068.975173

Table S26. XYZ coordinates optimized molecular geometry of **A9-*cis*.**

C	-0.75866900	0.80490100	0.06358700
C	0.45111700	1.26220300	0.59611500
C	0.93633300	0.23659500	1.50379500
C	0.05108400	-0.76491500	1.49903100
N	-1.02170900	-0.44854900	0.64177000
H	0.04961100	-1.68627700	2.02925400
C	-0.88369100	2.75245800	-1.28759900
C	0.30624400	3.22911800	-0.73118800
C	0.98298200	2.48506600	0.20866600
C	-1.42657700	1.54413200	-0.90532200
H	-1.38804700	3.33612600	-2.03137500
H	0.69632400	4.17496100	-1.04872400
H	1.90512800	2.83199800	0.62998000
H	-2.33288000	1.19437600	-1.34540300
N	2.09356700	0.35956800	2.33712900
N	3.23995000	0.16163200	1.89580900
C	3.59062000	-0.24577700	0.60806300
C	4.92376200	-0.40799300	0.28808700
C	2.89337400	-0.59383000	-0.58664700
H	5.78095200	-0.25451100	0.90012900
H	1.84861500	-0.60224400	-0.76587700
N	3.72876000	-0.93271200	-1.53606900
N	4.99531000	-0.81115000	-0.97557200
C	6.16928600	-1.12116200	-1.78951800
H	7.05515600	-0.98048100	-1.19065400
H	6.11161400	-2.14618400	-2.12206300
H	6.19637900	-0.46160500	-2.64332000
C	-2.03538000	-1.37592100	0.39718200
C	-3.37510500	-0.87377600	0.01070400
C	-4.14008400	-1.66186100	-0.83655000
C	-3.91740200	0.27259700	0.57418400
C	-5.42783900	-1.28004300	-1.16138000

H	-3.72036100	-2.56104700	-1.23914800
C	-5.21315100	0.64274100	0.26406000
H	-3.33905800	0.86377800	1.25399800
C	-5.96407500	-0.12702600	-0.61025500
H	-6.01081900	-1.87916900	-1.83091200
H	-5.63502800	1.52354000	0.70383700
H	-6.96509900	0.16697200	-0.85492300
O	-1.81007600	-2.56085000	0.54795500

Zero-point correction=	0.334786 (Hartree/Particle)
Thermal correction to Energy=	0.353246
Thermal correction to Enthalpy=	0.354190
Thermal correction to Gibbs Free Energy=	0.284755
Sum of electronic and zero-point Energies=	-1068.900545
Sum of electronic and thermal Energies=	-1068.882085
Sum of electronic and thermal Enthalpies=	-1068.881141
Sum of electronic and thermal Free Energies=	-1068.950576

Table S27. XYZ coordinates optimized molecular geometry of **A10**-*trans***.**

C	-0.41632	0.71088	-1.10355
C	0.83112	1.3022	-0.8916
C	1.75301	0.24901	-0.51727
C	1.07199	-0.91003	-0.52557
N	-0.26823	-0.66823	-0.84491
H	1.40178	-1.89822	-0.31762
C	-1.29905	2.81673	-1.74337
C	-0.06098	3.41829	-1.50299
C	1.01239	2.66479	-1.08205
C	-1.49266	1.46405	-1.55302
H	-2.11836	3.41543	-2.08762
H	0.05239	4.4721	-1.65966
H	1.97272	3.10721	-0.91181
H	-2.44217	1.02042	-1.75235
N	3.09955	0.50298	-0.23064
N	3.79155	-0.4901	0.07429
C	5.12936	-0.242	0.35694
C	5.86015	0.97295	0.35893
C	6.04214	-1.20692	0.71015
H	5.49373	1.94575	0.13482
H	5.91193	-2.25676	0.82735
C	-1.17144	-1.72358	-0.98687
C	-2.60722	-1.46251	-0.72134
C	-3.54313	-2.19916	-1.429

C	-3.01331	-0.60838	0.29237
C	-4.88815	-2.0456	-1.15424
H	-3.21466	-2.87775	-2.18861
C	-4.3532	-0.47854	0.56924
H	-2.29475	-0.06014	0.86254
C	-5.29392	-1.18237	-0.15114
H	-5.61855	-2.5973	-1.70909
H	-6.33326	-1.06422	0.0716
O	-0.76434	-2.82957	-1.27721
Br	-4.92035	0.69919	1.98343
N	7.21618	-0.59588	0.903
N	7.11336	0.7706	0.68544
C	8.51882	0.54329	1.05138
H	9.04439	1.47529	1.0445
H	8.56754	0.11357	2.03009
H	8.96756	-0.12444	0.34593

Zero-point correction=	0.324707 (Hartree/Particle)
Thermal correction to Energy=	0.344663
Thermal correction to Enthalpy=	0.345607
Thermal correction to Gibbs Free Energy=	0.271520
Sum of electronic and zero-point Energies=	-3628.412239
Sum of electronic and thermal Energies=	-3628.392283
Sum of electronic and thermal Enthalpies=	-3628.391339
Sum of electronic and thermal Free Energies=	-3628.465427

Table S28. XYZ coordinates optimized molecular geometry of **A10-*cis*.**

C	-0.55601400	1.18564700	0.14661200
C	-1.88470300	1.57022600	-0.05886200
C	-2.33236100	0.93361800	-1.28632500
C	-1.31373600	0.21665200	-1.77013300
N	-0.18930900	0.36083200	-0.93124500
H	-1.24722200	-0.38466300	-2.64428000
C	-0.53834300	2.38696200	2.19322900
C	-1.85369500	2.80342900	1.97314300
C	-2.53619500	2.39308600	0.85010800
C	0.12250000	1.57663300	1.29428900
H	-0.02839600	2.70028200	3.08197700
H	-2.33425500	3.43698600	2.69087500
H	-3.55098600	2.69164400	0.67940500
H	1.12427800	1.26336000	1.48390800
N	-3.60105100	1.15632000	-1.91021100
N	-4.62827200	0.56534700	-1.53129800

C	-4.72640400	-0.40138700	-0.53023100
C	-5.95857900	-0.95139300	-0.23828300
C	-3.82383200	-1.06031600	0.35616400
H	-6.90512700	-0.73794800	-0.67567200
H	-2.77694600	-0.92687100	0.45611300
N	-4.45414700	-1.92482000	1.11075200
N	-5.78876700	-1.84604600	0.72857600
C	-6.77406400	-2.69655500	1.39410100
H	-7.74123500	-2.52254800	0.94965100
H	-6.49401600	-3.73086500	1.26692900
H	-6.80538800	-2.45358200	2.44522700
C	0.97861000	-0.35587900	-1.17849600
C	2.26808900	0.20947700	-0.70911600
C	3.26350500	-0.68734800	-0.35432100
C	2.53663400	1.56842100	-0.75117900
C	4.50381100	-0.21961000	0.00434800
H	3.05838600	-1.73650600	-0.35755700
C	3.79498000	2.02535100	-0.40628200
H	1.77940600	2.25953400	-1.05737200
C	4.77746100	1.13083200	-0.01844200
H	4.01419000	3.07250300	-0.44128100
H	5.74898800	1.48327300	0.25675800
O	0.92836000	-1.39448500	-1.80667500
Br	5.87646500	-1.46306400	0.53116500

Zero-point correction=	0.324296 (Hartree/Particle)
Thermal correction to Energy=	0.344221
Thermal correction to Enthalpy=	0.345165
Thermal correction to Gibbs Free Energy=	0.270677
Sum of electronic and zero-point Energies=	-3628.388564
Sum of electronic and thermal Energies=	-3628.368639
Sum of electronic and thermal Enthalpies=	-3628.367695
Sum of electronic and thermal Free Energies=	-3628.442183

Table S29. XYZ coordinates optimized molecular geometry of **A11-*trans*.**

C	-0.89359	1.71335	0.1962
C	0.38399	1.89119	-0.33523
C	1.19952	0.78027	0.11507
C	0.42881	-0.01986	0.87667
N	-0.86073	0.51766	0.92373
H	0.65819	-0.91812	1.39453
C	-1.62297	3.72348	-0.80367
C	-0.3507	3.90848	-1.35616

C	0.65975	3.00182	-1.12279
C	-1.91203	2.62875	-0.01706
H	-2.38765	4.45105	-0.98741
H	-0.1626	4.7726	-1.96087
H	1.63935	3.14173	-1.53206
H	-2.87276	2.50546	0.43373
N	2.55135	0.65815	-0.23061
N	3.14767	-0.33313	0.23736
C	4.48862	-0.46078	-0.10233
C	5.31599	0.35831	-0.91152
C	5.30464	-1.48219	0.32218
H	5.04009	1.25039	-1.42038
H	5.08429	-2.31422	0.94836
S	-2.14878	-0.22247	1.76219
C	-3.1788	-0.89551	0.45355
C	-4.44165	-0.37984	0.29967
C	-2.70176	-1.92032	-0.33614
C	-5.25286	-0.89403	-0.69636
H	-4.78325	0.3997	0.94718
C	-3.51727	-2.4248	-1.32444
H	-1.72004	-2.32188	-0.18756
C	-4.80096	-1.91541	-1.51823
H	-6.23893	-0.49723	-0.82664
H	-3.16017	-3.21938	-1.94814
C	-5.67714	-2.48347	-2.6147
H	-5.21849	-2.31933	-3.58354
H	-5.80472	-3.55159	-2.48025
H	-6.65323	-2.01785	-2.61449
O	-1.45677	-1.34879	2.62113
O	-2.96502	0.89578	2.51211
N	6.51627	-1.27044	-0.20232
N	6.53458	-0.11965	-0.97765
C	7.90127	-0.65588	-1.05188
H	8.50143	-0.0188	-1.66738
H	8.3209	-0.70026	-0.0686
H	7.87629	-1.63891	-1.47371

Zero-point correction=	0.362636 (Hartree/Particle)
Thermal correction to Energy=	0.384867
Thermal correction to Enthalpy=	0.385811
Thermal correction to Gibbs Free Energy=	0.305216
Sum of electronic and zero-point Energies=	-1539.859690
Sum of electronic and thermal Energies=	-1539.837459
Sum of electronic and thermal Enthalpies=	-1539.836515

Sum of electronic and thermal Free Energies= -1539.917110

Table S30. XYZ coordinates optimized molecular geometry of **A11-*cis*.**

C	-0.09057900	0.93122000	-0.39190800
C	0.90349600	1.19661400	0.55230700
C	1.17375700	-0.04790700	1.25417700
C	0.36288200	-0.99160700	0.75992000
N	-0.43218400	-0.41447300	-0.25070500
H	0.25819000	-2.02161200	0.99966100
C	-0.01785900	3.17257600	-1.13460900
C	0.96540200	3.45792400	-0.18069500
C	1.43613300	2.47584600	0.66163200
C	-0.55537200	1.90990600	-1.25798000
H	-0.35610400	3.94988500	-1.78972200
H	1.35977300	4.45160300	-0.11423700
H	2.19632000	2.68697600	1.38646400
H	-1.28043700	1.68338900	-2.00878800
N	2.07291500	-0.18627700	2.35999300
N	3.30063300	-0.29714200	2.18926500
C	3.98235600	-0.36201900	0.97486600
C	5.35976100	-0.46047000	0.97459000
C	3.62471900	-0.37359000	-0.40620800
H	6.02727300	-0.48770400	1.80323700
H	2.66020000	-0.31725500	-0.84249100
N	4.68694200	-0.46864100	-1.16512800
N	5.76519900	-0.52044800	-0.28839600
C	7.11971900	-0.62620800	-0.82815400
H	7.81931100	-0.66214000	-0.00819200
H	7.19912000	-1.52722600	-1.41667400
H	7.32540600	0.23346900	-1.44726200
C	-3.17718800	-0.72819000	-0.33648800
C	-4.01453100	0.06806400	-1.07753300
C	-3.49215800	-1.13808700	0.94171400
C	-5.20276900	0.49219400	-0.50961600
H	-3.74956400	0.34074800	-2.07714100
C	-4.67740100	-0.71031800	1.49753100
H	-2.83576300	-1.78168100	1.49122900
C	-5.54431900	0.11306600	0.78003400
H	-4.93578300	-1.01867400	2.49055900
O	-1.34357600	-2.78821700	-0.75537800
S	-1.64071900	-1.27628600	-1.08684200
O	-1.62256300	-0.81055600	-2.59091600
H	-5.86293300	1.11534400	-1.07766400

C	-6.84040300	0.57342700	1.41326000
H	-6.63575400	1.16277700	2.30020400
H	-7.41706200	1.17732700	0.72599000
H	-7.43997700	-0.28024400	1.70841600

Zero-point correction=	0.362294 (Hartree/Particle)
Thermal correction to Energy=	0.384428
Thermal correction to Enthalpy=	0.385372
Thermal correction to Gibbs Free Energy=	0.306091
Sum of electronic and zero-point Energies=	-1539.835822
Sum of electronic and thermal Energies=	-1539.813688
Sum of electronic and thermal Enthalpies=	-1539.812744
Sum of electronic and thermal Free Energies=	-1539.892025

Table S31. XYZ coordinates optimized molecular geometry of **B1.**

C	3.47282	0.39801	-0.00001
C	2.41385	-0.52101	0.00005
C	1.19844	0.25426	0.00001
C	1.5662	1.56584	-0.00011
N	2.93286	1.66826	-0.00011
H	0.94781	2.43201	-0.00019
C	5.04182	-1.37762	0.00012
C	3.98958	-2.30622	0.00019
C	2.67875	-1.88842	0.00015
C	4.7989	-0.02305	0.00003
H	6.05375	-1.73138	0.00015
H	4.21658	-3.35386	0.00026
H	1.87309	-2.59502	0.0002
H	5.6059	0.68117	-0.00002
N	-0.07581	-0.31956	0.00006
N	-1.03836	0.47594	0.00004
C	-2.33007	-0.03438	-0.00001
C	-2.8612	-1.35526	-0.00016
C	-3.42446	0.8114	0.00007
C	-2.14014	-2.67222	-0.00031
H	-1.07608	-2.51607	-0.00022
H	-2.41735	-3.24797	0.8757
H	-2.41724	-3.24771	-0.87653
C	-3.40174	2.30799	0.00028
H	-2.87575	2.66589	0.87638
H	-2.87439	2.66609	-0.8749
H	-4.39365	2.73265	-0.00044
N	-4.51246	0.03603	0.

N	-4.17252	-1.31553	-0.00016
C	-5.64217	-1.28334	-0.00017
H	-5.9877	-0.77115	-0.87377
H	-6.02084	-2.2841	-0.00029
H	-5.98771	-0.77135	0.87354
H	3.4572	2.51977	-0.00017

Zero-point correction=	0.296115 (Hartree/Particle)
Thermal correction to Energy=	0.311172
Thermal correction to Enthalpy=	0.312116
Thermal correction to Gibbs Free Energy=	0.252025
Sum of electronic and zero-point Energies=	-806.241959
Sum of electronic and thermal Energies=	-806.226902
Sum of electronic and thermal Enthalpies=	-806.225958
Sum of electronic and thermal Free Energies=	-806.286048

Table S32. XYZ coordinates optimized molecular geometry of **B2-***trans*.

C	3.47282	0.39801	-0.00001
C	2.41385	-0.52101	0.00005
C	1.19844	0.25426	0.00001
C	1.5662	1.56584	-0.00011
N	2.93286	1.66826	-0.00011
H	0.94781	2.43201	-0.00019
C	5.04182	-1.37762	0.00012
C	3.98958	-2.30622	0.00019
C	2.67875	-1.88842	0.00015
C	4.7989	-0.02305	0.00003
H	6.05375	-1.73138	0.00015
H	4.21658	-3.35386	0.00026
H	1.87309	-2.59502	0.0002
H	5.6059	0.68117	-0.00002
N	-0.07581	-0.31956	0.00006
N	-1.03836	0.47594	0.00004
C	-2.33007	-0.03438	-0.00001
C	-2.8612	-1.35526	-0.00016
C	-3.42446	0.8114	0.00007
C	-2.14014	-2.67222	-0.00031
H	-1.07608	-2.51607	-0.00022
H	-2.41735	-3.24797	0.8757
H	-2.41724	-3.24771	-0.87653
C	-3.40174	2.30799	0.00028
H	-2.87575	2.66589	0.87638
H	-2.87439	2.66609	-0.8749

H	-4.39365	2.73265	-0.00044
C	3.69998	2.91402	-0.0002
H	4.32374	2.97136	-0.88221
H	3.01332	3.74668	-0.00043
H	4.32349	2.97164	0.88197
N	-4.51246	0.03603	0.
N	-4.17252	-1.31553	-0.00016
C	-5.64217	-1.28334	-0.00017
H	-5.9877	-0.77115	-0.87377
H	-6.02084	-2.2841	-0.00029
H	-5.98771	-0.77135	0.87354

Zero-point correction=	0.325774 (Hartree/Particle)
Thermal correction to Energy=	0.342519
Thermal correction to Enthalpy=	0.343463
Thermal correction to Gibbs Free Energy=	0.279920
Sum of electronic and zero-point Energies=	-845.026234
Sum of electronic and thermal Energies=	-845.009489
Sum of electronic and thermal Enthalpies=	-845.008545
Sum of electronic and thermal Free Energies=	-845.072088

Table S33. XYZ coordinates optimized molecular geometry of **B2**-*cis*.

C	2.65100000	0.75813100	0.03755000
C	2.27013800	-0.58317300	0.12089000
C	0.82542300	-0.61599500	0.05417900
C	0.41632000	0.69168100	-0.06392500
N	1.49753800	1.51579100	-0.07377000
H	-0.56076700	1.09796700	-0.14420300
C	4.93237200	0.14811000	0.19231700
C	4.56149900	-1.20217700	0.27770700
C	3.23758600	-1.57622500	0.24331100
C	3.98684100	1.14143300	0.07194800
H	5.97125400	0.41022000	0.22152300
H	5.32488100	-1.94882700	0.37104900
H	2.94716700	-2.60504700	0.30819900
H	4.27376200	2.17113700	0.00732900
N	0.17282600	-1.84698200	0.13965100
N	-1.05502300	-2.06598000	0.09589700
C	-1.98276300	-0.99334000	-0.10102400
C	-2.36412600	-0.41408900	-1.33653300
N	-3.28547100	0.50312700	-1.14587000
N	-3.51421000	0.52237500	0.21789300
C	-4.51507200	1.42373100	0.78011500

H	-4.07871100	2.03466500	1.55774700
H	-4.86130500	2.05427200	-0.02195500
H	-5.34761600	0.86558100	1.18645900
C	-1.83347900	-0.75403300	-2.69460800
H	-0.77882400	-0.51317800	-2.76854800
H	-1.95213400	-1.81241400	-2.89632300
H	-2.36935800	-0.19367600	-3.44852900
C	1.45702200	2.97608900	-0.18803300
H	1.98276800	3.29458100	-1.07763000
H	0.42762500	3.29294500	-0.25274000
H	1.91347400	3.42950300	0.68096700
C	-2.74447200	-0.38488300	0.85735900
C	-2.77494500	-0.60985000	2.33430200
H	-2.45683000	0.27810200	2.86984500
H	-3.77526900	-0.86445900	2.66597500
H	-2.10979700	-1.42215000	2.59088600

Zero-point correction=	0.325419 (Hartree/Particle)
Thermal correction to Energy=	0.342969
Thermal correction to Enthalpy=	0.343913
Thermal correction to Gibbs Free Energy=	0.278294
Sum of electronic and zero-point Energies=	-845.002041
Sum of electronic and thermal Energies=	-844.984491
Sum of electronic and thermal Enthalpies=	-844.983547
Sum of electronic and thermal Free Energies=	-845.049167

Table S34. XYZ coordinates optimized molecular geometry of **B3**-*trans*.

C	2.94001	0.60957	-0.2505
C	1.72204	1.285	-0.08737
C	0.68472	0.28705	-0.16045
C	1.3019	-0.91042	-0.35949
N	2.66038	-0.73385	-0.41922
H	0.8672	-1.87605	-0.46771
C	4.119	2.65718	-0.05125
C	2.90489	3.34172	0.11262
C	1.70717	2.66579	0.0954
C	4.15235	1.29364	-0.23278
H	5.03848	3.20806	-0.0336
H	2.91777	4.4044	0.2525
H	0.77695	3.18323	0.21913
H	5.08419	0.78017	-0.35454
N	-0.67407	0.58947	-0.04289
N	-1.46481	-0.37462	-0.12437

C	-2.82134	-0.10564	-0.01215
C	-3.53657	1.11142	0.18493
C	-3.7786	-1.09507	-0.08447
C	-2.99724	2.49946	0.33144
H	-2.3267	2.56128	1.17884
H	-2.43458	2.78539	-0.54804
H	-3.81686	3.1911	0.47203
C	-3.59428	-2.56253	-0.28331
H	-2.54019	-2.77901	-0.36692
H	-4.00253	-3.11982	0.55277
H	-4.09417	-2.89556	-1.18639
C	3.64595	-1.80926	-0.57717
H	4.45766	-1.4409	-1.18989
H	3.16711	-2.61995	-1.10892
C	4.18115	-2.30913	0.77544
H	3.34899	-2.66989	1.36881
H	4.63349	-1.48125	1.30872
C	5.2144	-3.43323	0.57447
H	6.05823	-3.07958	-0.00835
H	5.58688	-3.78426	1.52952
H	4.76979	-4.27519	0.0546
N	-4.96624	-0.49811	0.06016
N	-4.82547	0.8788	0.22898
C	-6.27322	0.6292	0.28035
H	-6.78963	1.55451	0.42875
H	-6.59174	0.18665	-0.6403
H	-6.49209	-0.03523	1.08999

Zero-point correction=	0.386714 (Hartree/Particle)
Thermal correction to Energy=	0.406821
Thermal correction to Enthalpy=	0.407765
Thermal correction to Gibbs Free Energy=	0.335637
Sum of electronic and zero-point Energies=	-922.606971
Sum of electronic and thermal Energies=	-922.586864
Sum of electronic and thermal Enthalpies=	-922.585920
Sum of electronic and thermal Free Energies=	-922.658048

Table S35. XYZ coordinates optimized molecular geometry of **B3**-*cis*.

C	2.52770100	0.06538000	-0.31295100
C	2.02431800	-1.12560400	0.21773700
C	0.58249600	-1.02508400	0.19234100
C	0.29239500	0.20510400	-0.34539200
N	1.44417900	0.86493500	-0.64802500

H	-0.64660000	0.65889600	-0.54317400
C	4.74331800	-0.71933400	-0.01022700
C	4.24637700	-1.91655900	0.52658900
C	2.89246100	-2.12704500	0.64375800
C	3.89747400	0.28010000	-0.43326400
H	5.80300500	-0.58022800	-0.09163800
H	4.93541400	-2.67244700	0.84705800
H	2.50218100	-3.03749400	1.05113200
H	4.28899200	1.19003500	-0.83848600
N	-0.17681900	-2.08572000	0.69162400
N	-1.42009600	-2.17802600	0.74119800
C	-2.25350500	-1.14143900	0.21119300
C	-2.63479600	-0.96425800	-1.14187100
N	-3.45889300	0.05288900	-1.25449100
N	-3.62343400	0.54194800	0.02851000
C	-4.51526200	1.67126000	0.27233000
H	-4.00320500	2.44144000	0.83156100
H	-4.80827700	2.05867400	-0.68937500
H	-5.39408900	1.35515400	0.81795500
C	-2.19805600	-1.78229600	-2.31728700
H	-1.13122800	-1.68136200	-2.48310200
H	-2.41570200	-2.83145400	-2.15360500
H	-2.71825500	-1.45335400	-3.20652200
C	1.49089800	2.21295900	-1.23908100
H	2.48730800	2.36967000	-1.62349600
H	0.80331600	2.23719700	-2.07372800
C	-2.91294800	-0.17861200	0.92321800
C	-2.89869400	0.09716200	2.39180800
H	-2.48082300	1.07619900	2.59972100
H	-3.90208600	0.06386400	2.80116600
H	-2.29685300	-0.64662100	2.89445000
C	1.13346300	3.31141100	-0.22393300
H	1.12483100	4.25709000	-0.75507000
H	0.12997400	3.13999600	0.14913100
C	2.12495800	3.38245000	0.94984100
H	1.84892000	4.17912300	1.63120000
H	2.13331100	2.45188100	1.50354200
H	3.12971500	3.57800000	0.59070000

Table S36. XYZ coordinates optimized molecular geometry of **B4**-*trans*.

C	-2.34869	1.25501	0.03681
C	-1.04178	1.75502	0.04301
C	-0.15713	0.61563	0.01601

C	-0.93606	-0.49507	-0.00348
N	-2.26891	-0.1322	0.00567
H	-0.64875	-1.51891	-0.03638
C	-3.21105	3.45976	0.12088
C	-1.90494	3.97173	0.11688
C	-0.81857	3.12881	0.08056
C	-3.44885	2.10471	0.08297
H	-4.0406	4.13766	0.15581
H	-1.7582	5.03302	0.14598
H	0.18222	3.51148	0.08367
H	-4.44682	1.71859	0.08985
N	1.2363	0.73888	0.00874
N	1.88174	-0.33043	-0.02073
C	3.26482	-0.25177	-0.02728
C	4.15468	0.86125	-0.00023
C	4.0671	-1.37413	-0.06499
C	3.82509	2.31967	0.04503
H	3.2418	2.5517	0.9269
H	4.74052	2.89537	0.05954
H	3.23609	2.60492	-0.81717
C	3.64734	-2.80685	-0.10345
H	4.02766	-3.3458	0.75687
H	2.56918	-2.85543	-0.0967
H	4.01383	-3.29453	-0.99968
C	-3.36111	-1.04658	-0.00717
C	-4.31597	-0.97615	-1.00981
C	-3.45872	-2.01561	0.97861
C	-5.37358	-1.86864	-1.01642
H	-4.22526	-0.23637	-1.77844
C	-4.50883	-2.91701	0.95699
H	-2.72445	-2.05558	1.75722
C	-5.47083	-2.84268	-0.0364
H	-6.11097	-1.80917	-1.79144
H	-4.57904	-3.66636	1.71954
H	-6.28712	-3.53653	-0.04748
N	5.33246	-0.9441	-0.06132
N	5.39754	0.44798	-0.01998
C	6.7962	-0.0039	-0.04166
H	6.97518	-0.5674	-0.93347
H	7.44596	0.84596	-0.02032
H	6.98552	-0.61917	0.81303

Zero-point correction= 0.382550 (Hartree/Particle)

Thermal correction to Energy= 0.400532

Thermal correction to Enthalpy=	0.401476
Thermal correction to Gibbs Free Energy=	0.333799
Sum of electronic and zero-point Energies=	-1034.418429
Sum of electronic and thermal Energies=	-1034.400447
Sum of electronic and thermal Enthalpies=	-1034.399503
Sum of electronic and thermal Free Energies=	-1034.467181

Table S37. XYZ coordinates optimized molecular geometry of **B4**-*cis*.

C	2.22649600	-0.94933500	0.05484600
C	1.39639700	-2.07009200	0.06737800
C	0.03034100	-1.59200300	0.03315500
C	0.09659400	-0.22522500	0.00274400
N	1.40678700	0.17573300	0.01819300
H	-0.67485500	0.50281400	-0.01921900
C	4.14276000	-2.33631700	0.08793500
C	3.31795200	-3.47057200	0.11073500
C	1.94772000	-3.34757100	0.09863000
C	3.61130300	-1.06689700	0.05861100
H	5.20725100	-2.46058900	0.09233300
H	3.76683200	-4.44347800	0.13482300
H	1.30979500	-4.20761600	0.11018500
H	4.24151500	-0.20237400	0.03871500
N	-1.01009000	-2.52776900	0.06712700
N	-2.23546200	-2.30322400	0.02823700
C	-2.73398900	-0.96773100	-0.10613300
C	-2.87285800	-0.22702900	-1.30600700
N	-3.42536900	0.93922800	-1.05976700
N	-3.65327500	0.96293000	0.30397400
C	-4.30366700	2.11794500	0.91532100
H	-3.75527900	2.43648300	1.79008000
H	-4.30474700	2.90840800	0.18317900
H	-5.32174200	1.88222300	1.19492300
C	-2.47020600	-0.65391500	-2.68339900
H	-1.39428100	-0.76949800	-2.75334200
H	-2.92824400	-1.60278700	-2.93762900
H	-2.78494900	0.08883200	-3.40364700
C	-3.25513300	-0.18763400	0.88835800
C	-3.38430900	-0.46994500	2.35021900
H	-2.78627300	0.22144700	2.93386200
H	-4.41569700	-0.38031700	2.67185800
H	-3.04535000	-1.47520700	2.55663400
C	1.83890000	1.53636000	-0.01060500
C	1.47234700	2.35013300	-1.06951700

C	2.61131900	2.03971400	1.02390400
C	1.87495800	3.67439100	-1.08915800
H	0.88604800	1.94761000	-1.87025500
C	3.02493900	3.35986300	0.99056100
H	2.87716000	1.40698300	1.84569200
C	2.65501500	4.18006900	-0.06282900
H	1.58775700	4.30300300	-1.90771600
H	3.62406900	3.74712600	1.78977600
H	2.97157900	5.20339200	-0.08308400

Zero-point correction=	0.382512 (Hartree/Particle)
Thermal correction to Energy=	0.402849
Thermal correction to Enthalpy=	0.403793
Thermal correction to Gibbs Free Energy=	0.329931
Sum of electronic and zero-point Energies=	-1034.394764
Sum of electronic and thermal Energies=	-1034.374426
Sum of electronic and thermal Enthalpies=	-1034.373482
Sum of electronic and thermal Free Energies=	-1034.447344

Table S38. XYZ coordinates optimized molecular geometry of **B5**-*trans*.

C	1.99563	1.25766	-0.56578
C	0.73036	1.71772	-0.1779
C	-0.18437	0.61822	-0.36384
C	0.54324	-0.4256	-0.84495
N	1.86162	-0.05805	-0.97136
H	0.21638	-1.40338	-1.10965
C	2.9379	3.37341	-0.06501
C	1.67498	3.84381	0.32564
C	0.57042	3.02551	0.27314
C	3.1139	2.08354	-0.51138
H	3.78239	4.03154	-0.01219
H	1.5761	4.85432	0.66926
H	-0.39633	3.37951	0.57023
H	4.08137	1.72695	-0.79848
N	-1.54952	0.70662	-0.07805
N	-2.22446	-0.32507	-0.28072
C	-3.58299	-0.27012	-0.00664
C	-4.41223	0.7799	0.48499
C	-4.4182	-1.35116	-0.19303
C	-4.02848	2.17742	0.85738
H	-3.28605	2.17308	1.64508
H	-3.59746	2.69388	0.00934
H	-4.90515	2.71354	1.19484

C	-4.08389	-2.71729	-0.69176
H	-3.02736	-2.76782	-0.90647
H	-4.32823	-3.46956	0.05028
H	-4.63765	-2.94396	-1.59633
C	2.93855	-0.90908	-1.47587
H	3.44352	-0.39686	-2.28401
H	2.47858	-1.79887	-1.88455
C	3.94292	-1.29815	-0.40032
C	5.2945	-1.34656	-0.704
C	3.52191	-1.64488	0.87581
C	6.21659	-1.7418	0.25296
H	5.63112	-1.07477	-1.68613
C	4.44092	-2.03717	1.83257
H	2.47967	-1.60388	1.12182
C	5.79172	-2.08736	1.52347
H	7.25933	-1.77357	0.00639
H	4.10565	-2.30203	2.81579
H	6.50292	-2.38974	2.26618
N	-5.64553	-0.95984	0.16411
N	-5.65205	0.36863	0.58869
C	-7.04607	-0.08203	0.70921
H	-7.64964	0.72044	1.07885
H	-7.40674	-0.38657	-0.25103
H	-7.09651	-0.908	1.38755

Zero-point correction=	0.414116 (Hartree/Particle)
Thermal correction to Energy=	0.435561
Thermal correction to Enthalpy=	0.436505
Thermal correction to Gibbs Free Energy=	0.359989
Sum of electronic and zero-point Energies=	-1073.207896
Sum of electronic and thermal Energies=	-1073.186451
Sum of electronic and thermal Enthalpies=	-1073.185507
Sum of electronic and thermal Free Energies=	-1073.262023

Table S39. XYZ coordinates optimized molecular geometry of **B5**-*cis*.

C	-1.54956600	1.49376200	0.50349000
C	-0.59426400	2.30591300	-0.11052400
C	0.63036500	1.53846000	-0.18544700
C	0.35733300	0.32003500	0.38449400
N	-0.94194500	0.28220400	0.79771100
H	0.98419100	-0.52382700	0.53110700
C	-3.16064600	3.21916800	0.33359400
C	-2.20831200	4.04381700	-0.28343500

C	-0.92674900	3.59704000	-0.50967100
C	-2.84626700	1.93970200	0.73229500
H	-4.15230300	3.59224100	0.49550400
H	-2.48898300	5.03446200	-0.58129900
H	-0.19342000	4.21980500	-0.98016000
H	-3.57755000	1.30970800	1.19418700
N	1.76646700	2.13349500	-0.74016200
N	2.89264000	1.62280900	-0.90345900
C	3.13766600	0.25715300	-0.55043400
C	2.83591900	-0.89117000	-1.32412600
N	3.26451000	-1.97517000	-0.71791200
N	3.85376400	-1.53774800	0.45419200
C	4.46566100	-2.49710100	1.36836700
H	4.05460300	-2.38706800	2.36202400
H	4.24131500	-3.48151600	0.99239100
H	5.53780500	-2.35990100	1.40573200
C	2.13643600	-0.93131000	-2.64723000
H	1.10827100	-0.60038000	-2.55113300
H	2.63284300	-0.28400500	-3.36093200
H	2.13913400	-1.94175800	-3.03261000
C	3.79661700	-0.19253700	0.55988000
C	4.36319300	0.57757000	1.70829900
H	3.86209800	0.31944900	2.63492800
H	5.42095800	0.37144800	1.82719300
H	4.23620200	1.63636800	1.53265500
C	-1.58500800	-0.84980300	1.46994100
H	-0.80757500	-1.56205400	1.71114000
H	-2.01879400	-0.50326200	2.39805500
C	-2.65000600	-1.51842100	0.61356000
C	-3.83722100	-1.93723500	1.19338000
C	-2.43435500	-1.75367700	-0.73704100
C	-4.79824100	-2.58837600	0.43530000
H	-4.01575000	-1.75550000	2.23581200
C	-3.39343800	-2.40068100	-1.49535400
H	-1.52219500	-1.42863700	-1.19622500
C	-4.57851000	-2.82083000	-0.91064400
H	-5.71307600	-2.90619000	0.89467200
H	-3.21805100	-2.57660200	-2.53813700
H	-5.32140500	-3.32078100	-1.49965600

Zero-point correction= 0.413665 (Hartree/Particle)
Thermal correction to Energy= 0.435168
Thermal correction to Enthalpy= 0.436112
Thermal correction to Gibbs Free Energy= 0.359342

Sum of electronic and zero-point Energies=	-1073.183210
Sum of electronic and thermal Energies=	-1073.161706
Sum of electronic and thermal Enthalpies=	-1073.160762
Sum of electronic and thermal Free Energies=	-1073.237532

Table S40. XYZ coordinates optimized molecular geometry of **B6**-*trans*.

C	1.84205	1.03584	-0.31628
C	0.55854	1.57444	-0.19456
C	-0.37654	0.46804	-0.16481
C	0.33454	-0.66677	-0.28027
N	1.70048	-0.36646	-0.34076
H	0.00917	-1.6774	-0.30985
C	2.74376	3.22754	-0.41709
C	1.46507	3.77051	-0.26511
C	0.36522	2.9484	-0.15888
C	2.9492	1.86375	-0.44869
H	3.58635	3.88235	-0.51538
H	1.34333	4.83482	-0.24267
H	-0.62331	3.34865	-0.06067
H	3.93141	1.46679	-0.57317
N	-1.75923	0.66361	-0.04577
N	-2.45454	-0.37431	-0.0438
C	-3.82513	-0.2383	0.06936
C	-4.6611	0.91036	0.19395
C	-4.676	-1.32563	0.07877
C	-4.26613	2.35259	0.23958
H	-3.60576	2.54061	1.07643
H	-3.73534	2.63154	-0.66157
H	-5.1519	2.96525	0.33791
C	-4.34086	-2.77586	-0.02385
H	-3.27123	-2.88819	-0.11391
H	-4.67813	-3.31167	0.85661
H	-4.81591	-3.22006	-0.89163
N	-5.91473	-0.84571	0.20058
C	2.64676	-1.37659	-0.53454
C	4.02019	-1.16513	-0.02067
C	5.06594	-1.75955	-0.71176
C	4.26055	-0.5151	1.18165
C	6.35718	-1.66333	-0.22934
H	4.8623	-2.28508	-1.6223
C	5.5506	-0.43684	1.67339
H	3.45001	-0.08385	1.73216
C	6.59888	-1.00167	0.96424

H	7.16619	-2.10635	-0.7737
H	5.73616	0.05846	2.60473
H	7.59851	-0.93227	1.34404
O	2.3119	-2.41177	-1.07575
N	-5.91698	0.5496	0.27262
C	-7.3313	0.15871	0.36103
H	-7.47565	-0.46668	1.21715
H	-7.93844	1.03497	0.45299
H	-7.60928	-0.37667	-0.52271

Zero-point correction=	0.393907 (Hartree/Particle)
Thermal correction to Energy=	0.415974
Thermal correction to Enthalpy=	0.416918
Thermal correction to Gibbs Free Energy=	0.338899
Sum of electronic and zero-point Energies=	-1146.519419
Sum of electronic and thermal Energies=	-1146.497352
Sum of electronic and thermal Enthalpies=	-1146.496408
Sum of electronic and thermal Free Energies=	-1146.574427

Table S41. XYZ coordinates optimized molecular geometry of **B6**-*cis*.

C	2.78294800	-0.41730800	-0.10252700
C	2.72950000	0.96667600	0.02781800
C	1.32840200	1.35335900	0.02398400
C	0.60019300	0.21734900	-0.08744900
N	1.45488700	-0.88197400	-0.15192800
H	-0.44721600	0.07719200	-0.15074400
C	5.14565500	-0.34476500	-0.04063900
C	5.10146100	1.04648100	0.09225000
C	3.89548700	1.71245400	0.12528800
C	3.99278400	-1.09553500	-0.14286500
H	6.09533800	-0.84052200	-0.06949900
H	6.01774000	1.59721700	0.16570200
H	3.84603900	2.77719100	0.22372600
H	4.02324500	-2.15389800	-0.26362500
N	1.02265000	2.72633700	0.08808500
N	-0.10598800	3.24665800	0.10583700
C	-1.29423300	2.44717100	0.10464400
C	-1.92913000	1.87759900	1.23562700
N	-3.03756500	1.27169200	0.87568800
N	-3.13194200	1.44775000	-0.49210600
C	-4.27914800	0.91342000	-1.22067200
H	-3.94737600	0.32456800	-2.06381800
H	-4.82606100	0.28654900	-0.53618600

H	-4.91769500	1.71379300	-1.56897300
C	-1.46229400	1.93261600	2.65715800
H	-0.50229400	1.44150800	2.77009300
H	-1.35484300	2.96083200	2.98329600
H	-2.18042600	1.43825200	3.29686800
C	-2.09468400	2.16877800	-0.96827300
C	-1.92636800	2.53871100	-2.40642300
H	-1.79846200	1.65509300	-3.02210700
H	-2.79215500	3.08139100	-2.76835200
H	-1.05394300	3.16609300	-2.52191900
C	1.08118900	-2.21110400	-0.35327500
C	-0.31020900	-2.59978700	-0.00980400
C	-0.92174000	-3.54945300	-0.81650500
C	-0.95196800	-2.14105500	1.13207500
C	-2.19162900	-4.00018100	-0.51334600
H	-0.40312900	-3.92031300	-1.67679000
C	-2.21716400	-2.60668200	1.44309100
H	-0.46512900	-1.44700000	1.78631100
C	-2.84043900	-3.52673200	0.61654600
H	-2.66924700	-4.71876900	-1.14781400
H	-2.70978000	-2.25532200	2.32664900
H	-3.82351600	-3.87939400	0.85592600
O	1.88286600	-3.00872000	-0.79724800

Zero-point correction=	0.393964 (Hartree/Particle)
Thermal correction to Energy=	0.415871
Thermal correction to Enthalpy=	0.416815
Thermal correction to Gibbs Free Energy=	0.339284
Sum of electronic and zero-point Energies=	-1146.496486
Sum of electronic and thermal Energies=	-1146.474579
Sum of electronic and thermal Enthalpies=	-1146.473635
Sum of electronic and thermal Free Energies=	-1146.551166

Table S42. XYZ coordinates optimized molecular geometry of **B7**-*trans*.

C	1.63934	1.56174	0.43667
C	0.35481	1.93714	0.04128
C	-0.51543	0.79496	0.24269
C	0.23023	-0.21386	0.73073
N	1.55647	0.22349	0.83987
H	-0.0384	-1.20007	1.0186
C	2.45563	3.71923	-0.06828
C	1.17635	4.10582	-0.48268
C	0.11947	3.22427	-0.42506

C	2.70536	2.44724	0.4013
H	3.25826	4.42795	-0.10716
H	1.02018	5.1037	-0.83995
H	-0.86556	3.5146	-0.72856
H	3.67297	2.16331	0.75283
N	-1.88705	0.84533	-0.04459
N	-2.52836	-0.19825	0.20116
C	-3.88303	-0.20775	-0.06401
C	-4.7546	0.78635	-0.59815
C	-4.67549	-1.31335	0.18033
S	2.8262	-0.79029	1.35725
O	2.1038	-2.02586	2.01642
C	-4.26608	-2.6346	0.74288
H	-3.20616	-2.61654	0.94524
H	-4.79522	-2.84238	1.66588
H	-4.47549	-3.43499	0.04242
C	-4.42464	2.17704	-1.03884
H	-3.68641	2.16083	-1.83033
H	-5.32193	2.66384	-1.39573
H	-4.00862	2.74818	-0.21884
C	3.65967	-1.27168	-0.16296
C	3.0753	-2.21998	-0.97251
C	4.87168	-0.69038	-0.45
C	3.72538	-2.57903	-2.13713
H	2.14569	-2.67675	-0.70139
C	5.51675	-1.05512	-1.61831
H	5.30288	0.01537	0.22778
C	4.94098	-1.99268	-2.45886
H	3.29058	-3.31267	-2.78373
H	6.46061	-0.61406	-1.86321
H	5.44211	-2.27441	-3.36246
O	3.81478	0.0747	2.22545
N	-5.91531	-0.98486	-0.18554
N	-5.97615	0.32284	-0.67239
C	-7.35307	-0.18429	-0.76093
H	-7.98844	0.57713	-1.16272
H	-7.37674	-1.04234	-1.39974
H	-7.69625	-0.45678	0.21522

Zero-point correction= 0.392696 (Hartree/Particle)
Thermal correction to Energy= 0.416392
Thermal correction to Enthalpy= 0.417336
Thermal correction to Gibbs Free Energy= 0.335770
Sum of electronic and zero-point Energies= -1578.661096

Sum of electronic and thermal Energies=	-1578.637399
Sum of electronic and thermal Enthalpies=	-1578.636455
Sum of electronic and thermal Free Energies=	-1578.718022

Table S43. XYZ coordinates optimized molecular geometry of **B7-*cis***.

C	0.86837800	1.96910900	-0.34047400
C	-0.13969800	2.53069000	0.43756600
C	-1.23347900	1.57484400	0.50241400
C	-0.86505200	0.48665600	-0.21711600
N	0.41468100	0.69856600	-0.71692600
H	-1.35896400	-0.42489400	-0.43515700
C	2.19107000	3.90579100	-0.08985200
C	1.19308400	4.47910300	0.70628900
C	0.02244800	3.80286300	0.97063900
C	2.04252500	2.64569700	-0.62894900
H	3.08587300	4.45890700	-0.29252900
H	1.34281600	5.46154500	1.10642300
H	-0.75208800	4.23696200	1.56830900
H	2.78959700	2.22065800	-1.26381500
N	-2.39284700	1.94473000	1.21038400
N	-3.42005100	1.26442700	1.37356500
C	-3.51481100	-0.07033400	0.86469300
C	-3.00123200	-1.24910600	1.46043200
N	-3.33761700	-2.29991200	0.74765700
N	-4.07727900	-1.81063600	-0.31322500
C	-4.63187700	-2.72844300	-1.30461200
H	-4.32487800	-2.43840000	-2.29939200
H	-4.24680800	-3.70904300	-1.07962800
H	-5.71180500	-2.74186400	-1.25008000
C	-2.19461800	-1.35323300	2.71755700
H	-1.22921900	-0.87345700	2.60070200
H	-2.71056900	-0.87611500	3.54268600
H	-2.03447000	-2.39423700	2.96245000
C	-4.20504900	-0.46927100	-0.24651700
C	-4.96340900	0.34672200	-1.24249100
H	-4.51106300	0.27709000	-2.22567400
H	-5.98991800	0.00641700	-1.31694400
H	-4.96559700	1.38373500	-0.93839100
C	2.55162900	-1.02357500	-0.57343500
C	3.84905600	-0.83644700	-0.98159400
C	2.23680700	-1.65474800	0.61152500
C	4.87319500	-1.28250400	-0.16528700
H	4.05169300	-0.35673400	-1.91570000

C	3.26382700	-2.09475000	1.41623000
H	1.21790800	-1.80212800	0.90671500
C	4.59383600	-1.91221900	1.03816100
H	5.88896000	-1.13914800	-0.47245400
H	3.03566800	-2.58405600	2.34163200
O	1.89989400	0.27114300	-2.89538800
C	5.70566800	-2.40354100	1.94071700
H	5.61002900	-3.47023300	2.10918300
H	6.67610700	-2.21013300	1.50445400
H	5.65567300	-1.90571900	2.90270800
S	1.24253900	-0.45841700	-1.66541600
O	0.15491100	-1.56421100	-1.95141300

Zero-point correction=	0.421192 (Hartree/Particle)
Thermal correction to Energy=	0.446840
Thermal correction to Enthalpy=	0.447785
Thermal correction to Gibbs Free Energy=	0.360746
Sum of electronic and zero-point Energies=	-1617.427565
Sum of electronic and thermal Energies=	-1617.401917
Sum of electronic and thermal Enthalpies=	-1617.400973
Sum of electronic and thermal Free Energies=	-1617.488012

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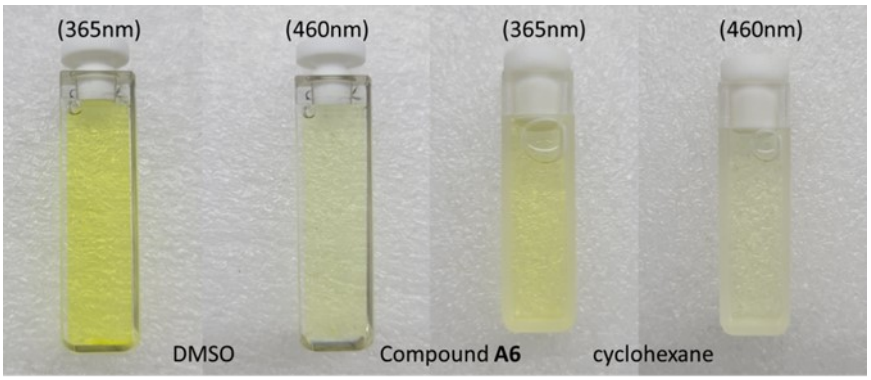
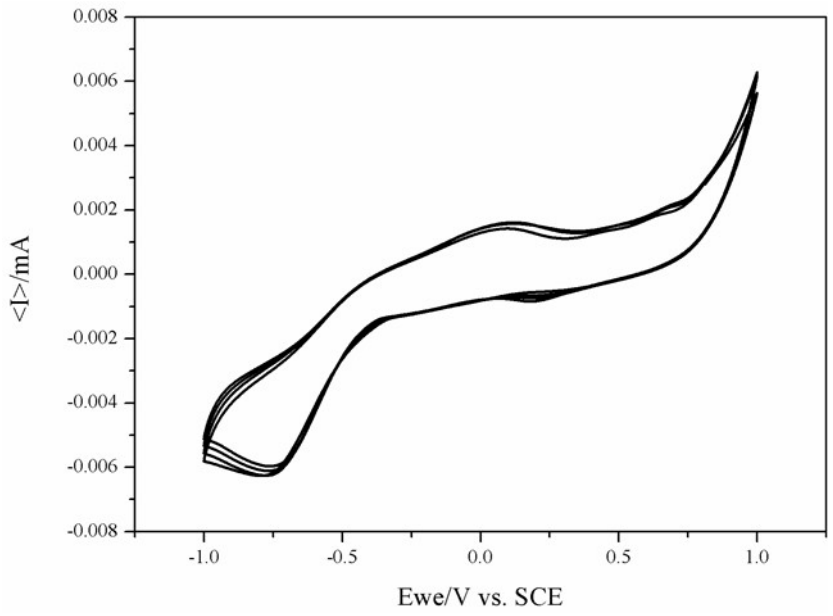


Photochromism of compounds in different polar solvents



Cyclic voltammetry of 0.01 mM compound **C1** and 0.05M tetrabutylammonium perchlorate in DMSO (25 mL), The working electrode is platinum electrode and the reference electrode is calomel electrode (cycle number: 4)