Electronic Supplementary Information for:

# New excited state intramolecular proton transfer (ESIPT) dyes based on naphthalimide and observation of triplet excited states

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## General.

All the chemicals used in synthesis are analytical pure and were used as received. Solvents were dried and distilled. NMR spectra were recorded on a 400 MHz Varian Unity Inova NMR spectrophotometer. $^{13}C$ NMR spectra were recorded on the same instrument (100 MHz) with total proton decoupling. Mass spectra were recorded with Q-TOF Micro MS spectrometer. UV-Vis absorption spectra were measured with a HP8453 UV-visible spectrophotometer. Fluorescence spectra were recorded on Shimadzu 5301 PC spectrofluorometer.

The nanosecond time-resolved transient absorption (TA) spectra were measured on LP 920 laser flash photolysis spectrometer (Edinburgh Instruments, UK) and the signals were recorded on a Tektronix TDS 3012B oscilloscope. The lifetime values were obtained by monitoring the decay trace of the transients at a specific wavelength with the LP900 software. All samples in flash photolysis experiments were deaerated with argon for ca. 15 min before measurement and the argon gas flow was kept during the measurement.

The density functional theory (DFT) calculations were used for optimization of the geometries for both singlet states and triplet states. All the calculations were performed with Gaussian 09W.[1]

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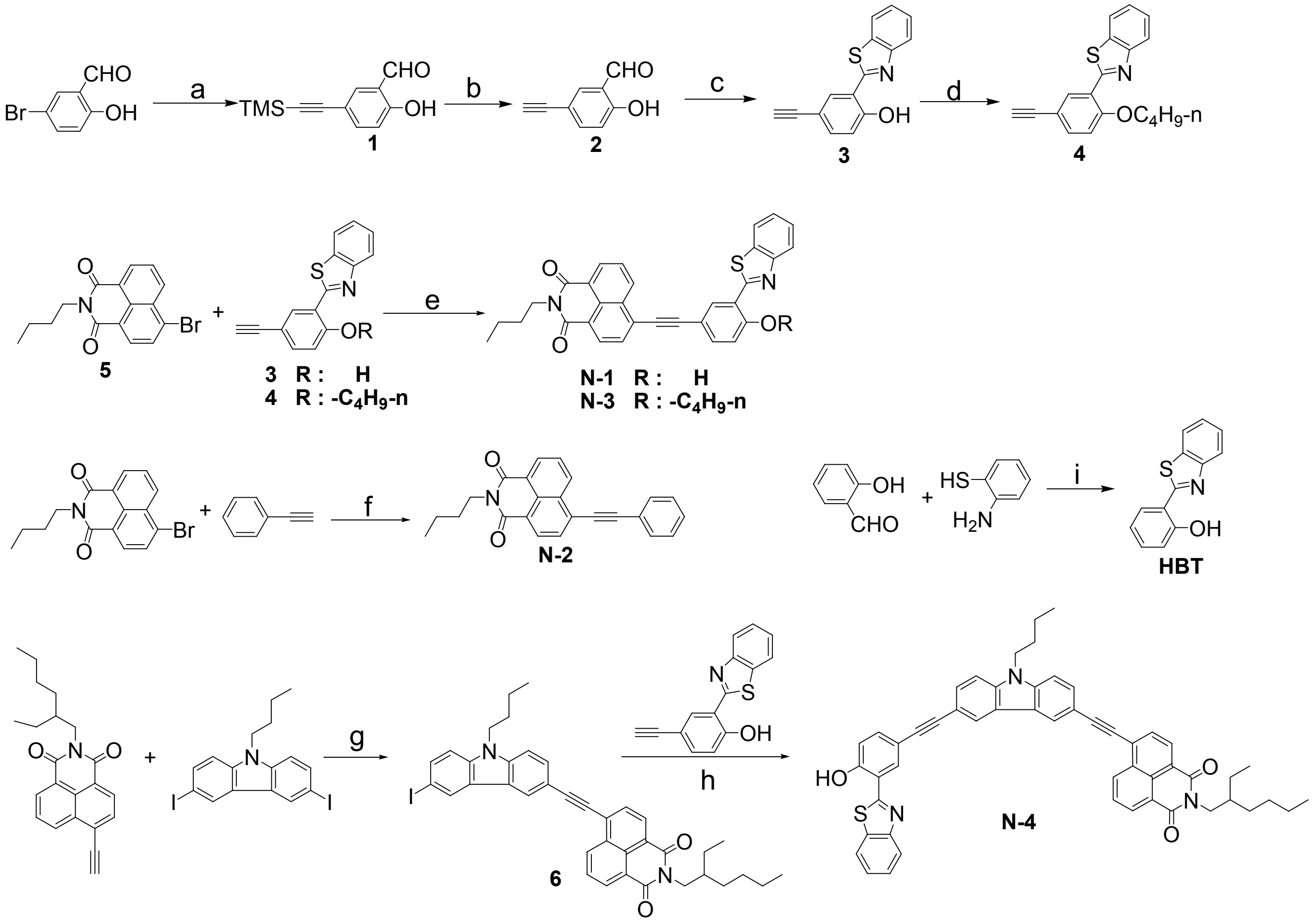
[1] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, et al., GAUSSIAN 09 (Revision A.1), Gaussian, Inc., Wallingford, CT, 2009.

## Experimental Section

### *Synthesis:*



***Scheme S1***. Synthesis of **N-1, N-2, N-3, N-4** and **HBT**. a) trimethylsilylacetylene, CuI, $Pd(PPh_3)_2Cl_2$, $PPh_3$, $NEt_3$, reflux, 6 h; b) TBAF, THF; c) 2-aminothiophenol, MeOH ; d) $n$-$C_4H_9Br$, $K_2CO_3$, DMF; e) $Pd(PPh_3)_2Cl_2$, $PPh_3$, CuI, $NEt_3$, reflux, 6 h; f) $Pd(PPh_3)_2Cl_2$, $PPh_3$, CuI, $NEt_3$, reflux, 6 h; g) $Pd(PPh_3)_2Cl_2$, $PPh_3$, CuI, $NEt_3$, reflux, 8 h; h) $Pd(PPh_3)_4$, $PPh_3$, CuI, $NEt_3$, reflux, 8 h; i) 2-aminothiophenol, MeOH.

## *Synthesis Procedures*

### Synthesis of compound 2-(5’-ethnyl-2’-hydroxyphenyl)benzothiazole (3)

**2** (100 mg, 0.69 mmol) and 2-aminothiophenol (170 mg, 1.30 mmol) were mixed in methanol (10 mL) and stirred for 6 h at 30 °C. Methanol was evaporated under reduced pressure and the residue was purified by column chromatography (silica gel, petroleum /$CH_2Cl_2$, 3:1, v / v) to give the product as white solid. Yield: 62.2 mg, 36.0 %. Mp: 143.7−144.6 °C. $^1$H NMR (400 MHz, $CDCl_3/CD_3OD$): $\delta$ 8.02 (d, 1H, $J$ = 8.4 Hz), 7.95 (d, 1H, $J$ = 8.0 Hz), 7.87 (s, 1H), 7.55−7.43 (m, 3H), 7.08 (d, 1H, $J$ = 8.4 Hz), 3.07 (s, 1H). TOF HRMS EI$^+$ ($[C_{15}H_9NOS]^+$): calcd $m/z$ = 251.0405, found $m/z$ = 251.0408.

**Synthesis of compound 3. 4. 2-(5'-ethnyl-2'-butoxyphenyl)benzothiazole (4)**

The mixture of compound **3** (50 mg, 0.20 mmol), $K_2CO_3$ (50 mg, 0.36 mmol) and *N*,*N*-dimethyl formamide (0.25 mL) were stirred at room temperature, then *n*-butyl bromide (122 mg, 0.90 mmol) was added. The mixture were stirred at 50 °C for 4 h, then the resulting solution was added dropwise into ice water. The mixture was extracted with $CH_2Cl_2$. The organic layer was washed with water and then dried over anhydrous $Na_2SO_4$. The solvent was removed under reduced pressure then the crude product was purified by column chromatography (silica gel, petroleum : $CH_2Cl_2$, 1 : 1, v/v) to give the product as white solid. Yield: 50 mg, 81.4%. M. p. 134.2−135.4 °C. $^1$H NMR (400 MHz, $CDCl_3/CD_3OD$): $\delta$ 8.73 (s, 1H), 8.11 (d, 1H, $J$ = 8.0 Hz), 7.95 (d, 1H, $J$ = 8.0 Hz), 7.56 (d, 1H, $J$ = 8.8 Hz), 7.52 (t, 1H, $J_1$ = 7.2 Hz, $J_2$ = 8.0 Hz), 7.40 (t, 1H, $J_1$ = 8.0 Hz, $J_2$ = 7.2 Hz), 7.00 (d, 1H, $J$ = 8.8 Hz), 4.24−4.21 (m, 2H), 3.04 (s, 1H), 2.04−1.99 (m, 2H), 1.66−1.61 (m, 2H), 1.06 (t, 3H, $J$ = 7.2 Hz). TOF HRMS EI$^+$ ($[C_{19}H_{17}NOS]^+$): calculated $m/z$ = 307.1031, found $m/z$ = 307.1031.

**Synthesis of compound 9-Butyl-3-iodo-9H-carbazole-naphthalimide (6)**

4-ethynylnaphthalimide (166.0 mg, 0.50 mmol), 9-butyl-3, 6-diiodo-9H-carbazole (715.0 mg, 1.5 mmol), CuI (10.0 mg, 0.05 mmol), $Pd(PPh_3)_2Cl_2$ (3.5 mg, 0.05 mmol), triphenylphosphine (5.0 mg, 0.02 mmol), and dry triethylamine (60 mL) were mixed, then the mixture was refluxed under $N_2$ for 8 h. Then the reaction mixture was filtered and the organic phase was evaporated under reduced pressure. The residue was purified through column chromatography (silica gel, hexane: $CH_2Cl_2$ = 1:2, v/v). A yellow solid was obtained. Yield: 110.0 mg, 31.6 %. M.p.: 141.0 − 142.6 °C. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 8.83 (d, 1H, $J$ = 8.0 Hz), 8.66 (d, 1H, $J$ = 4.0 Hz), 8.57 (d, 1H, $J$ = 8.0 Hz), 8.44 (s, 1H), 8.37 (s, 1H), 7.98−7.95 (m, 1H), 7.79−7.76 (m, 1H), 7.45 (d, 1H, $J$ = 8.0 Hz), 7.24 (d, 2H, $J$ = 8.0 Hz), 4.32−4.29 (m, 2H), 4.16−4.12 (m, 2H), 1.97−1.95 (m, 1H), 1.89−1.85 (m, 2H), 1.42−1.26 (m, 10H), 0.98−0.87 (m, 9H). ESI−MS $C_{38}H_{37}N_2O_2I$ Calculated $m/z$ = 680.1900, found $m/z$ = 680.1901.

**Synthesis of compound N-1**

Under argon atmosphere, $Pd(PPh_3)_2Cl_2$ (2.4 mg, 0.003 mmol, 3.0 mol%), $PPh_3$ (1.3 mg, 0.005 mmol, 5.0 mol%), CuI (1.0 mg, 0.005 mmol, 5.0 mol% ), TEA (2 mL, 1.40 mmol) and **5** (50 mg, 0.15 mmol) were added to a solution of **3** (25.0 mg, 0.10 mmol) in anhydrous THF (5 mL). The mixture was stirred at 70 °C for 6 h. The resulting solution was cooled to rt., the solvent was removed under reduced pressure and the compound was purified by column chromatography (silica gel, $CH_2Cl_2$ as the eluent) to give the product as yellow solid. Yield: 34 mg, 67.7%. M.p.: 236.3−237.3 °C. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 8.71 (d, 1H, $J$ = 12 Hz), 8.61 (d, 1H, $J$ = 8 Hz), 8.53 (d, 1H, $J$ = 12 Hz), 7.98−7.89 (m, 4H), 7.81 (t, 1H, $J$ = 8 Hz), 7.64 (d, 1H, $J$ = 8 Hz), 7.50 (t, 1H, $J$ = 8 Hz), 7.43−7.39 (m, 1H), 7.14 (d, 1H, $J$ = 4 Hz), 4.14 (t, 2H, $J$ = 8 Hz), 1.70−1.66 (m, 2H), 1.45−1.39 (m, 2H), 0.94 (t, 3H, $J$ = 8 Hz). $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 168.1, 164.0, 163.8, 159.0, 151.6, 136.2, 132.6, 132.3, 132.0, 131.6, 130.6, 130.4, 128.7, 128.6, 127.6, 127.5, 127.1, 126.1, 123.1, 122.4, 121.7, 118.7, 117.2, 113.5, 98.5, 94.6, 85.8, 40.4, 30.4, 20.6, 14.0. TOF HRMS EI$^+$ calcd ($[C_{31}H_{22}N_2O_3S]$): calculated $m/z$ = 502.1351, found $m/z$ = 502.1353.

### Synthesis of compound N-2

**N-2** was obtained following the procedure similar to that of **N-1**, except benzene acetylene (50.0 mg, 0.49 mmol) was used instead of **3**. Yellow solid, yield: 67.3 mg, 38.9%. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.66 (d, 1H, *J* = 8 Hz), 8.57 (d, 1H, *J* = 8 Hz), 8.48 (d, 1H, *J* = 4 Hz), 7.88 (d, 1H, *J* = 8 Hz), 7.76 (t, 1H, *J* = 8 Hz), 7.62–7.59 (m, 2H), 7.37 (t, 3H, *J* = 4 Hz), 4.14 (t, 2H, *J* = 8 Hz), 1.69–1.62 (m, 2H), 1.43–1.33 (m, 2H), 0.91 (t, 3H, *J* = 8 Hz). $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$164.1, 163.9, 132.5, 132.1, 131.7, 130.9, 130.5, 129.6, 128.8, 128.2, 127.7, 127.6, 123.1, 122.4, 122.3, 99.2, 94.6, 86.4, 40.5, 30.4, 20.6, 14.0.

### Synthesis of compound N-3

**N-3** was obtained following the procedure similar to that of **N-1**, except **4** (50.0 mg, 0.16 mmol) was used instead of **3**. Yellow solid, yield: 28 mg, 30.8%. Mp: 217.8–218.9°C. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$8.92 (s, 1H), 8.82 (d, 1H, *J* = 8 Hz), 8.66 (d, 1H, *J* = 4 Hz), 8.58 (d, 1H, *J* = 8 Hz), 8.16 (s, 1H), 8.00–7.95 (m, 2H), 7.87 (d, 1H, *J* = 8 Hz), 7.76 (d, 1H, *J* = 8 Hz), 7.55 (d, 1H, *J* = 8 Hz), 7.42 (t, 1H, *J* = 8 Hz), 7.13 (d, 1H, *J* = 8 Hz), 4.30 (t, 2H, *J* = 4 Hz), 4.20 (t, 2H, *J* = 8 Hz), 2.10–2.04 (m, 2H), 1.77–1.65 (m ,4H), 1.50–1.44 (m, 2H), 1.08 (t, 3H, *J* = 4 Hz), 0.99 (t, 3H, *J* = 8 Hz). $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$164.2, 163.9, 157.4, 135.2, 133.3, 132.7, 131.7, 130.7, 130.5, 128.2, 127.9, 127.5, 126.3, 125.1, 123.1, 123.0, 122.0, 121.5, 115.1, 112.7, 98.9, 86.0, 69.6, 40.5, 31.3, 30.4, 29.9, 20.6, 19.7, 14.0. TOF HRMS EI$^+$: ([$C_{35}H_{30}N_2O_3S$]) calculated *m*/*z* = 558.1977, found *m*/*z* = 558.1984.

### Synthesis of compound N-4

Under argon atmosphere, Pd (PPh$_3$)$_4$ (12.0 mg, 0.01mmol), CuI (1.0 mg, 0.005 mmol) and **6** (68.0 mg, 0.1 mmol ) were added to a solution of **3** (25.0 mg, 0.1 mmol) in anhydrous TEA (15 mL). The mixture was stirred at 90 °C for 8 h. The resulting solution was cooled to rt., removed the solvent under reduced pressure and the compound was purified by column chromatography (silica gel, CH$_2$Cl$_2$ and petroleum as the eluent) to give the product as yellow solid. Yield: 27 mg, 33.8%. M.p.: > 250 °C. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 12.75 (s, 1H), 8.85 (d, 1H, *J* = 8 Hz), 8.67 (m, 1H), 8.65 (d, 1H, *J* = 4 Hz), 8.58 (d, 1H, *J* = 8 Hz), 8.43 (d, 1H, *J* = 4 Hz), 8.36 (d, 1H, *J* = 4 Hz), 8.03 (d, 1H, *J* = 8 Hz), 7.99 (d, 1H, *J* = 8 Hz), 7.94 (d, 1H, *J* = 4 Hz), 7.87 (t, 1H, *J* = 8 Hz), 7.80 (d, 1H, *J* = 8 Hz), 7.73–7.69 (m, 2H), 7.60 (d, 1H, *J* = 8 Hz), 7.53 (t, 1H, *J* = 4 Hz), 7.47 (d, 1H, *J* = 8 Hz), 7.43 (d, 1H, *J* = 8 Hz), 7.13 (d, 1H, *J* = 8 Hz), 4.32–4.29 (m, 2H), 4.19–4.08 (m, 2H), 1.94–1.87 (m, 1H), 1.75–1.68 (m, 2H), 1.47–1.38 (m, 10H), 1.01–0.95 (m, 9H). $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 168.68, 164.57, 164.30, 157.92, 151.77, 141.11, 140.50,135.84, 132.76, 132.54, 131.61, 131.48, 131.04, 130.61, 129.97, 128.34, 128.26, 126.95, 125.90, 124.84, 124.20, 123.07, 122.79, 122.51, 122.38, 121.72, 121.59, 118.37, 116.98, 115.68, 114.39, 112.86, 109.35, 109.29, 101.20, 94.57, 89.58, 87.26, 85.49, 65.71, 44.35, 43.32, 38.11, 31.23, 30.92, 30.72, 28.87, 24.23, 23.25, 20.68, 19.34, 14.27. MALDI-HRMS: [$C_{53}H_{46}N_3O_3S+H^+$] Calcd *m*/*z* = 804.3260, found *m*/*z* = 804.3288.

### Synthesis of compound HBT

Salicylaldehyde (250 mg, 2.0 mmol) and 2-aminothiophenol (500 mg, 4.0 mmol) were combined in methanol (20 mL) and stirred for 12 h at 30 °C. Then methanol was evaporated under reduced pressure and the compound was purified by column chromatography (silica gel, petroleum / $CH_2Cl_2$, 3 : 1, v / v) to give the product as white solid. Yield: 107 mg, 23.6%. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 12.52 (s, 1H), 8.00 (d, 1H, *J* = 8 Hz), 7.91 (d, 1H, *J* =8 Hz), 7.71 (d, 1H, *J* = 8 Hz), 7.51 (d, 1H, *J* = 8 Hz), 7.43−7.36 (m, 2H), 7.12 (d, 1H, *J* = 8 Hz), 6.96 (t, 1H, *J* = 8 Hz). $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ 169.5, 158.1, 152.0, 132.9, 128.6, 126.8, 125.7, 122.3, 121.7, 119.7, 118.0, 116.9.

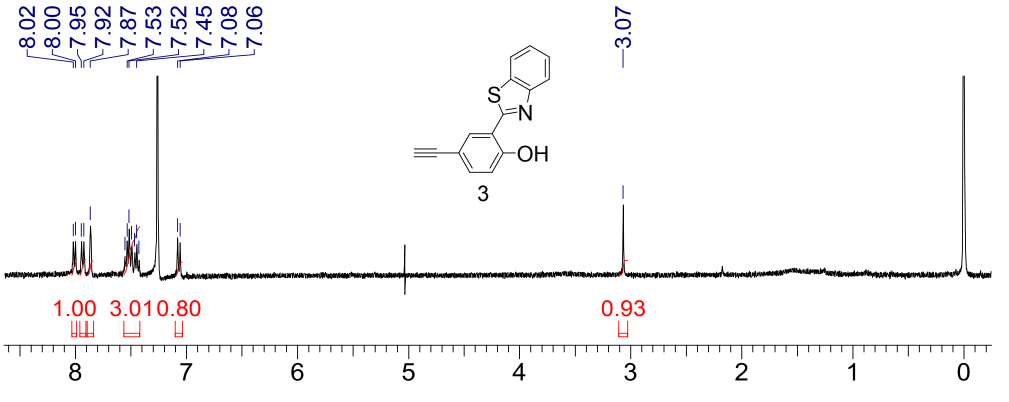


**Fig. S1** $^1$H NMR of compound **3** ($CDCl_3$, 400 MHz).

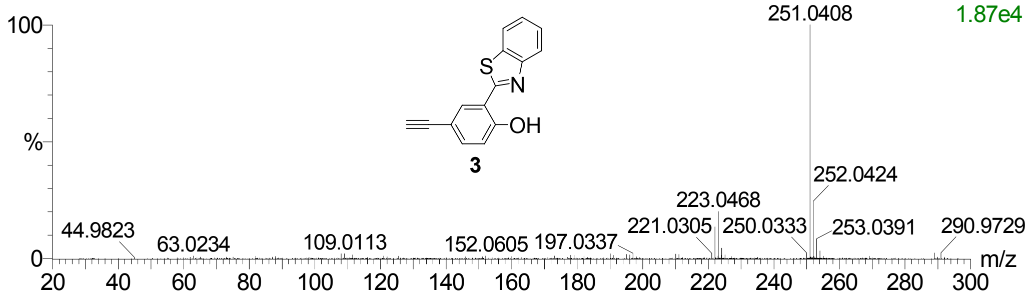
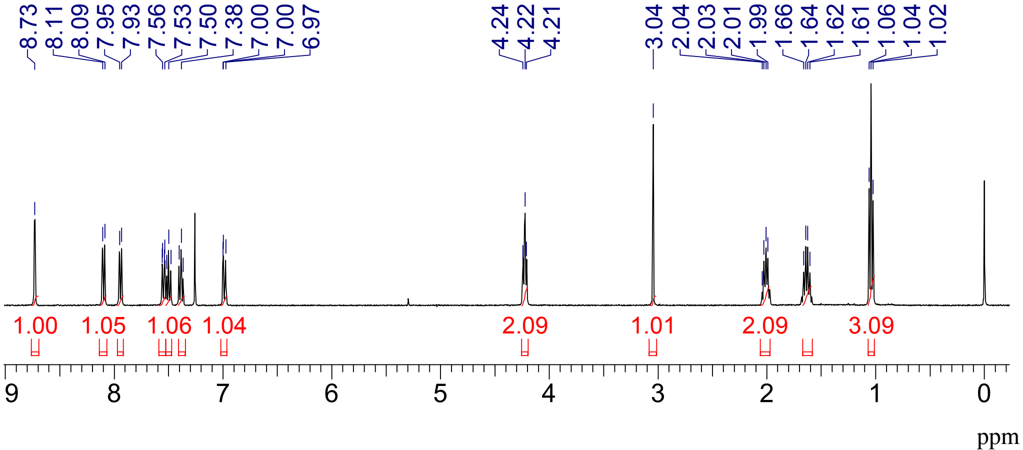
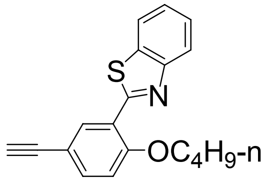


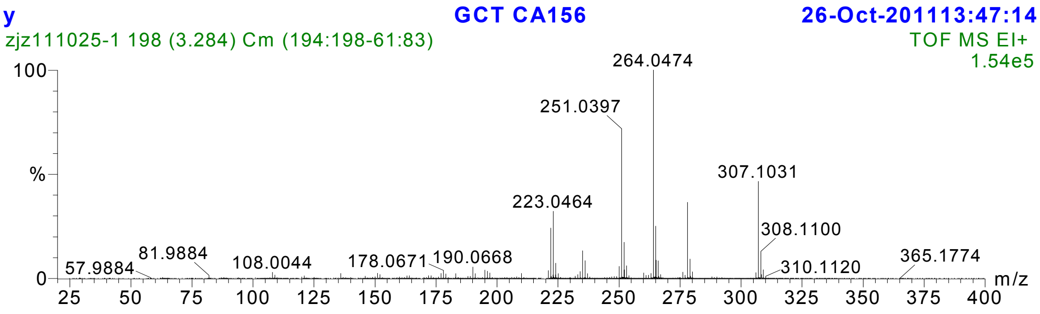
**Fig. S2** TOF HRMS EI$^+$ of compound **3**.

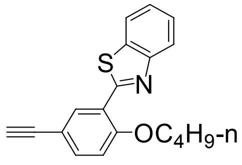




**4**

**Fig. S3** $^1$H NMR of compound **4** ($CDCl_3$, 400 MHz).





**4**

**Fig. S4** TOF HRMS EI$^+$ of compound **4.**

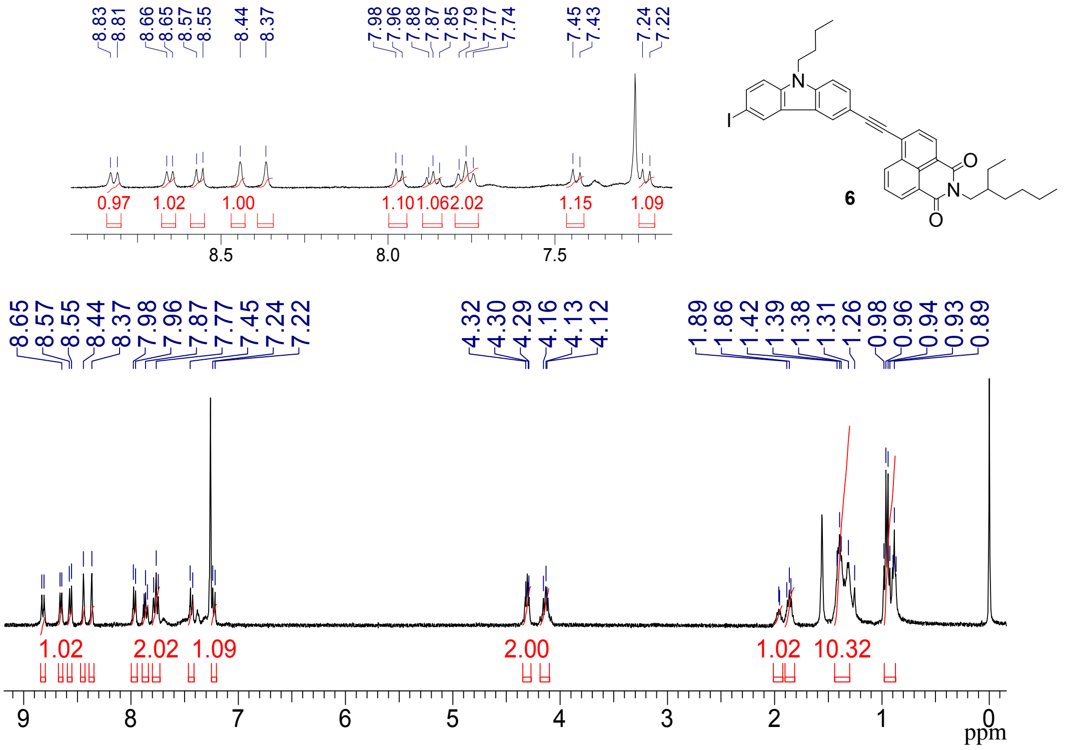


**Fig. S5** $^1$H NMR of compound **6** ($CDCl_3$, 400 MHz).

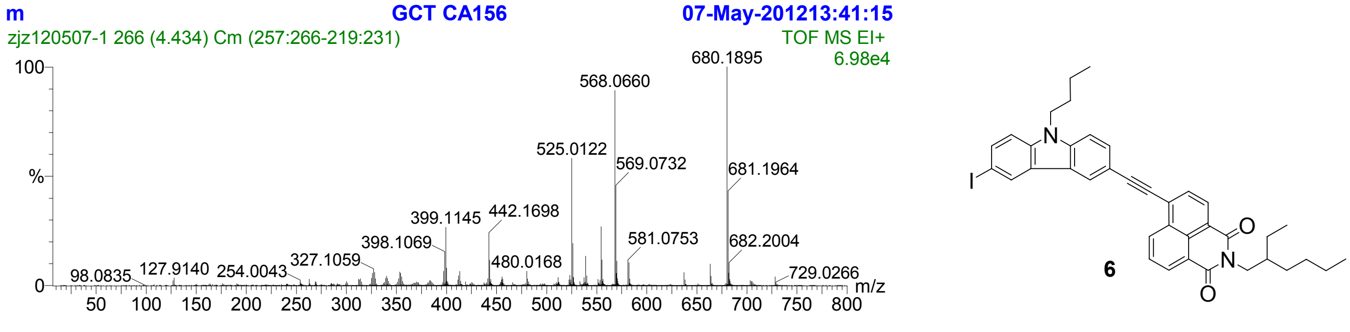


**Fig. S6** TOF HRMS $EI^+$ of compound **6**.

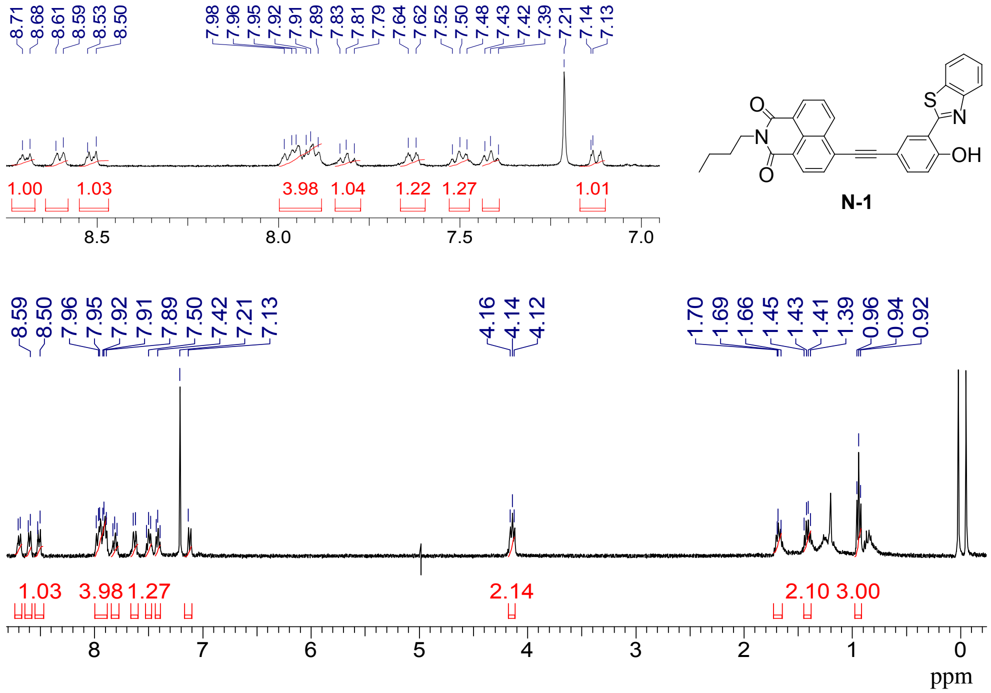


**Fig. S7** $^{1}$H NMR of compound **N–1** ($CDCl_3$, 400 MHz).

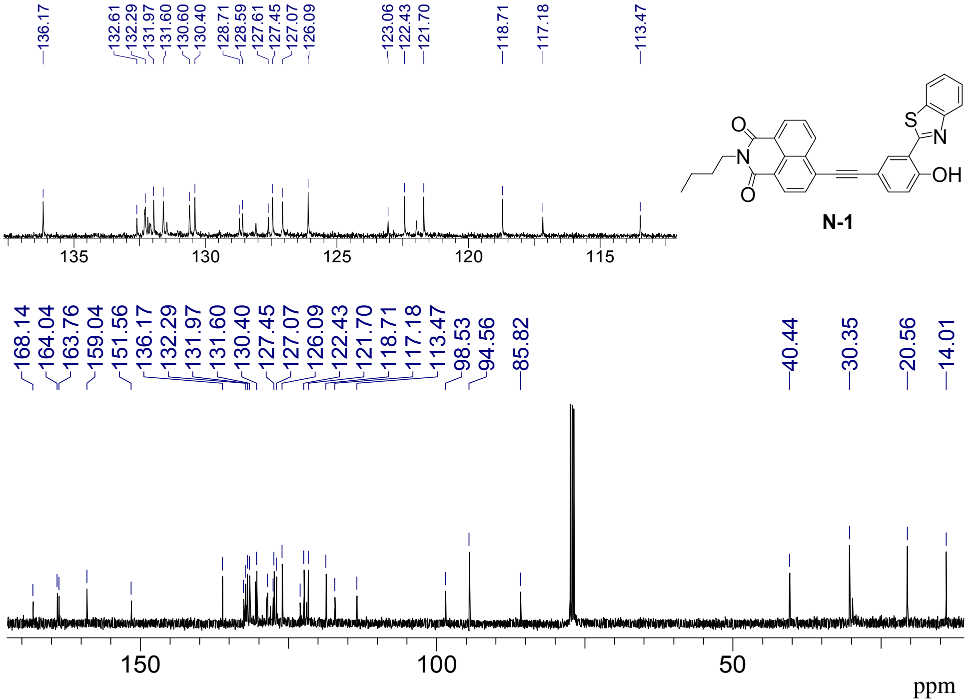


**Fig. S8** $^{13}$C NMR of compound **N–1** ($CDCl_3$, 100 MHz).

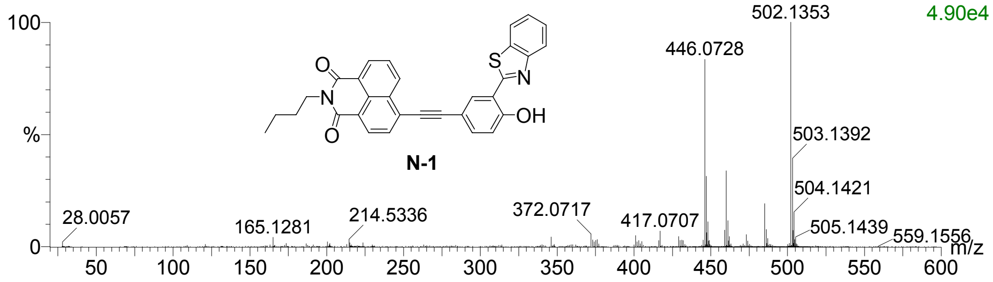


**Fig. S9** TOF HRMS EI$^+$ of compound **N–1**.

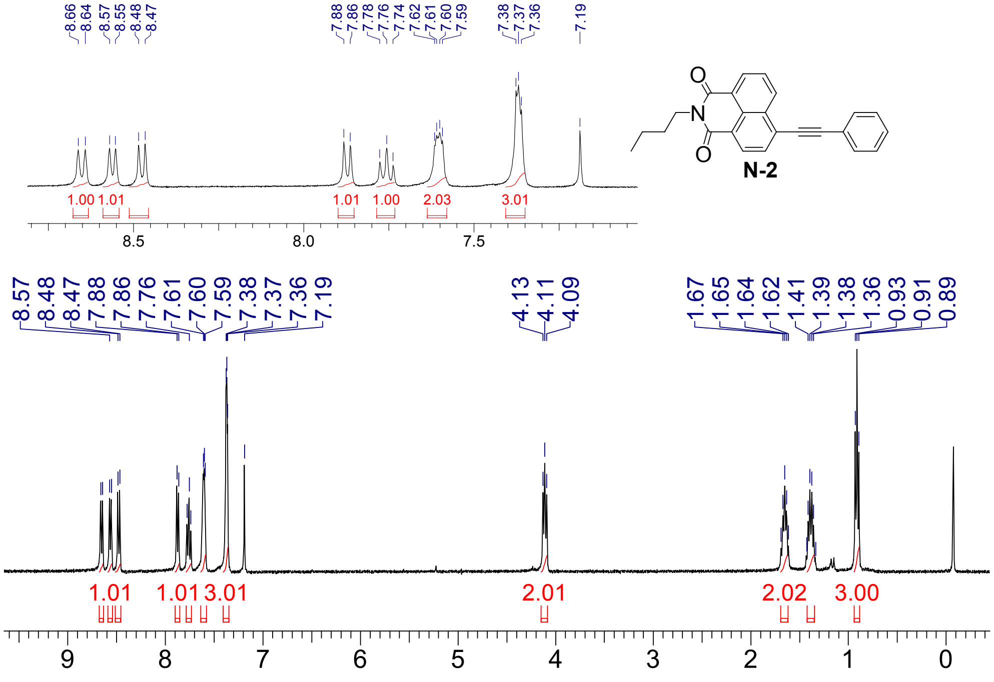


**Fig. S10** $^1$H NMR of compound **N–2** ($CDCl_3$, 400 MHz).

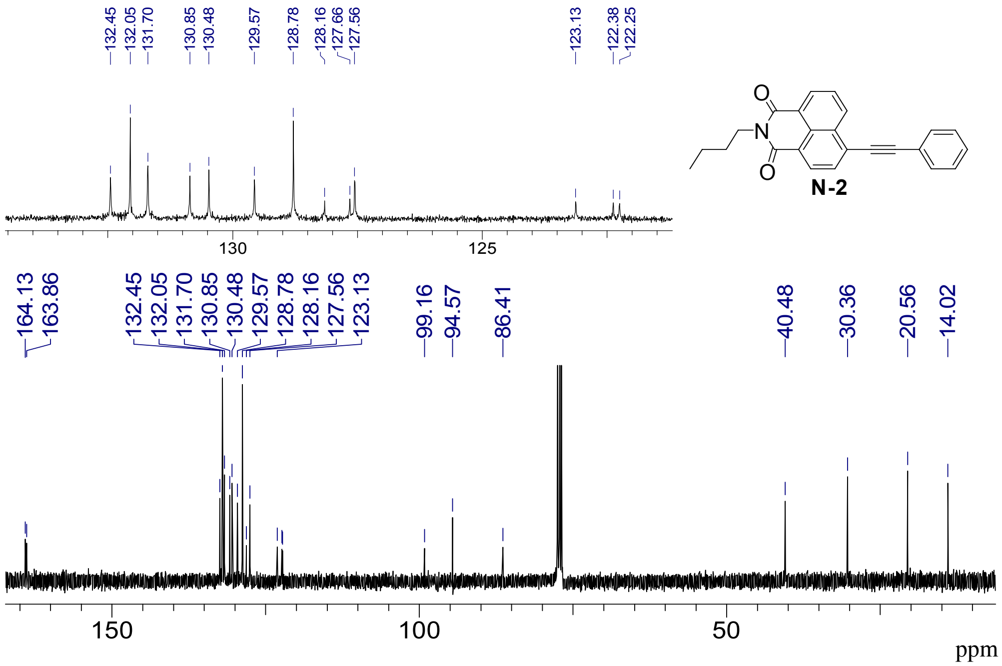


**Fig. S11** $^{13}$C NMR of compound **N–2** ($CDCl_3$, 100 MHz).

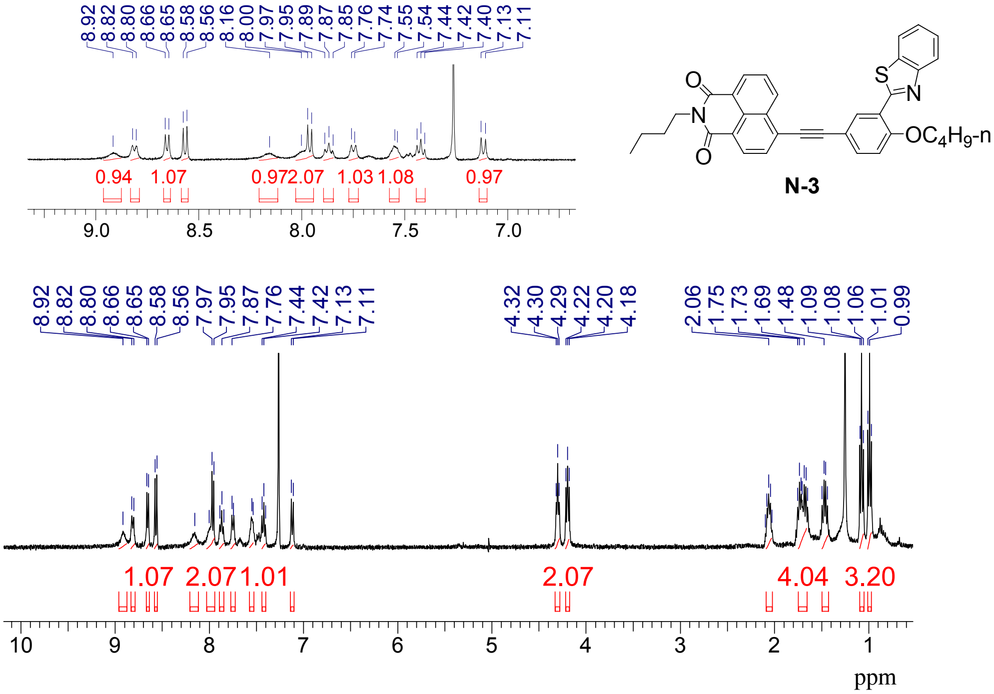


**Fig. S12** $^{1}$H NMR of compound **N–3** ($CDCl_3$, 400 MHz).

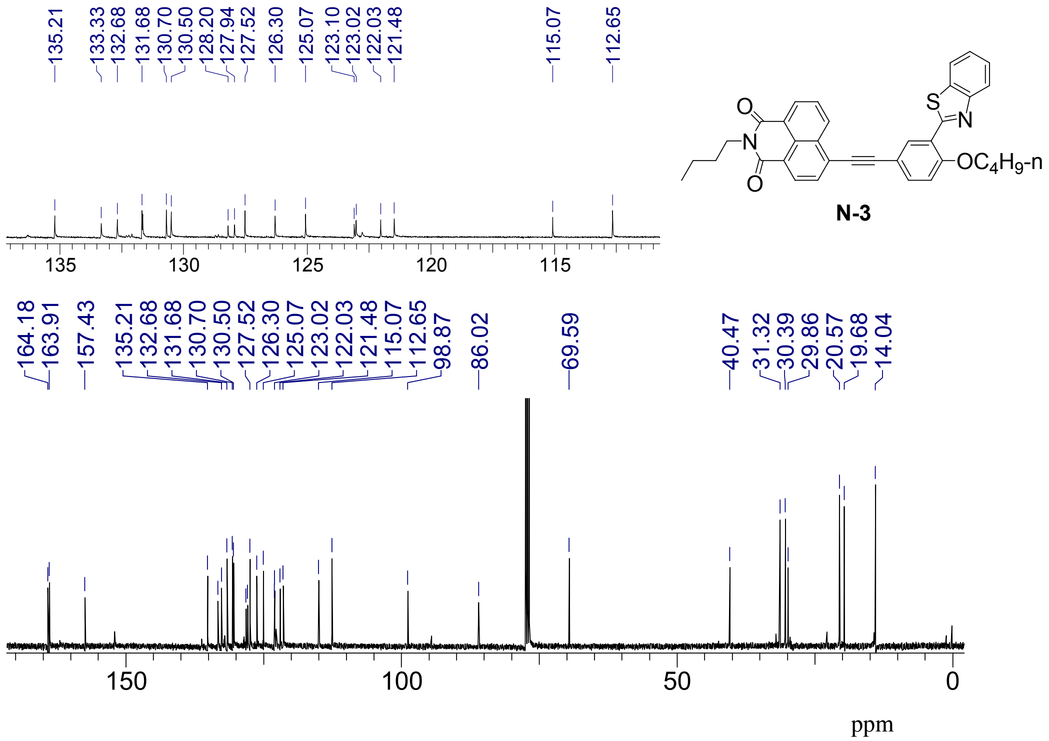


**Fig. S13** $^{13}$C NMR of compound **N–3** (CDCl$_3$, 100 MHz).

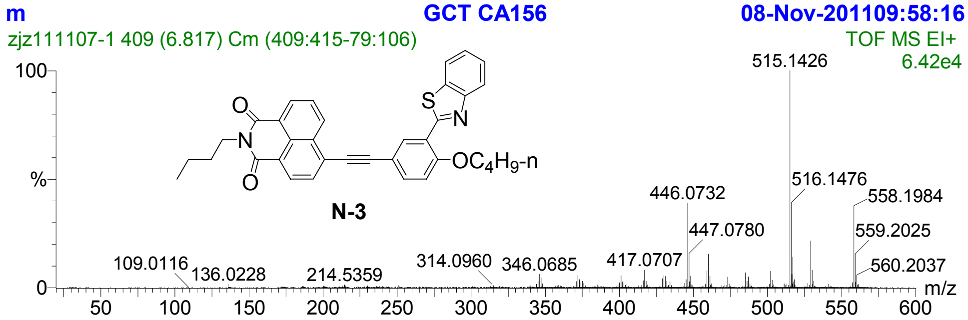


**Fig. S14** TOF HRMS EI$^+$ compound **N–3**.

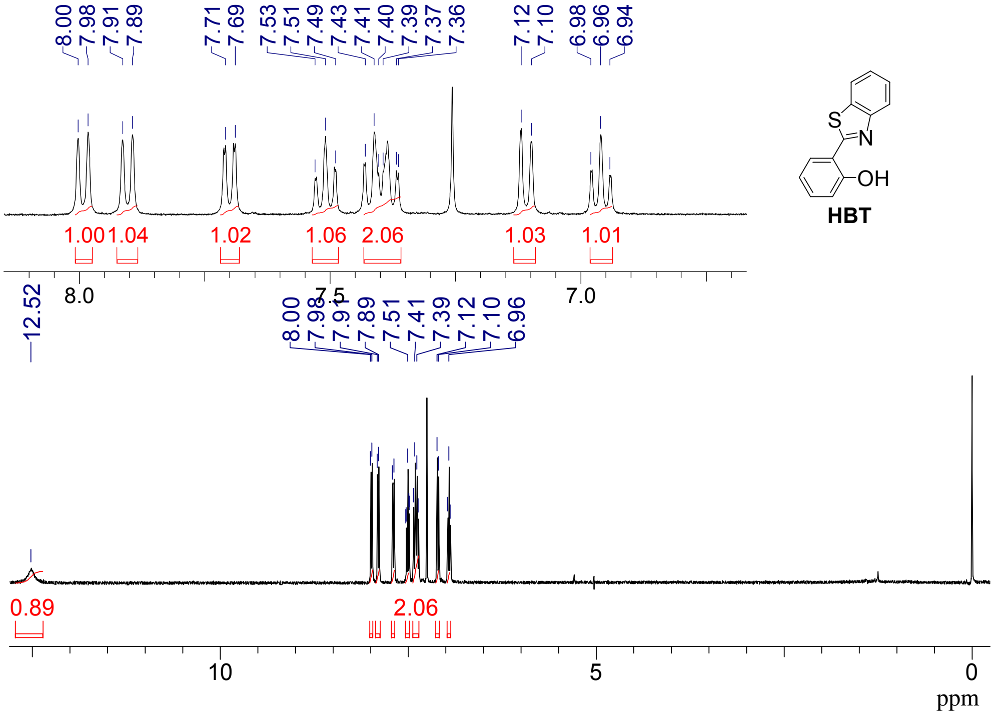


**Fig. S15** $^{1}$H NMR of compound **HBT** ($CDCl_3$, 400 MHz).

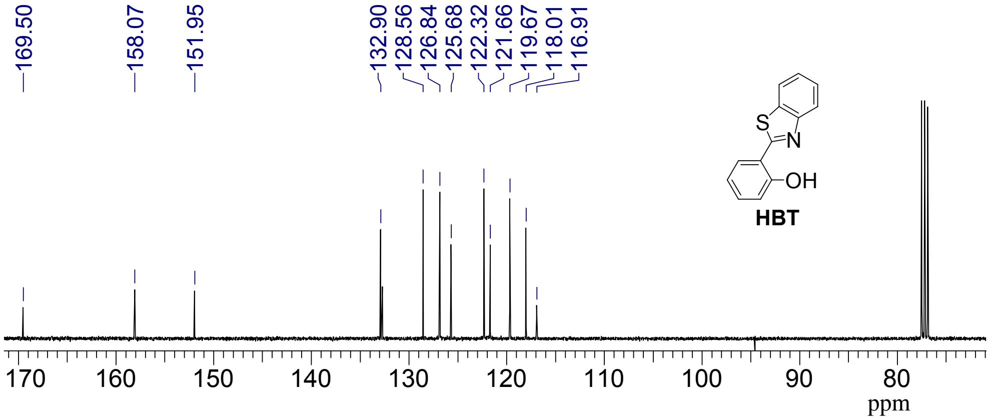


**Fig. S16** $^{13}$C NMR of compound **HBT** ($CDCl_3$, 100 MHz).

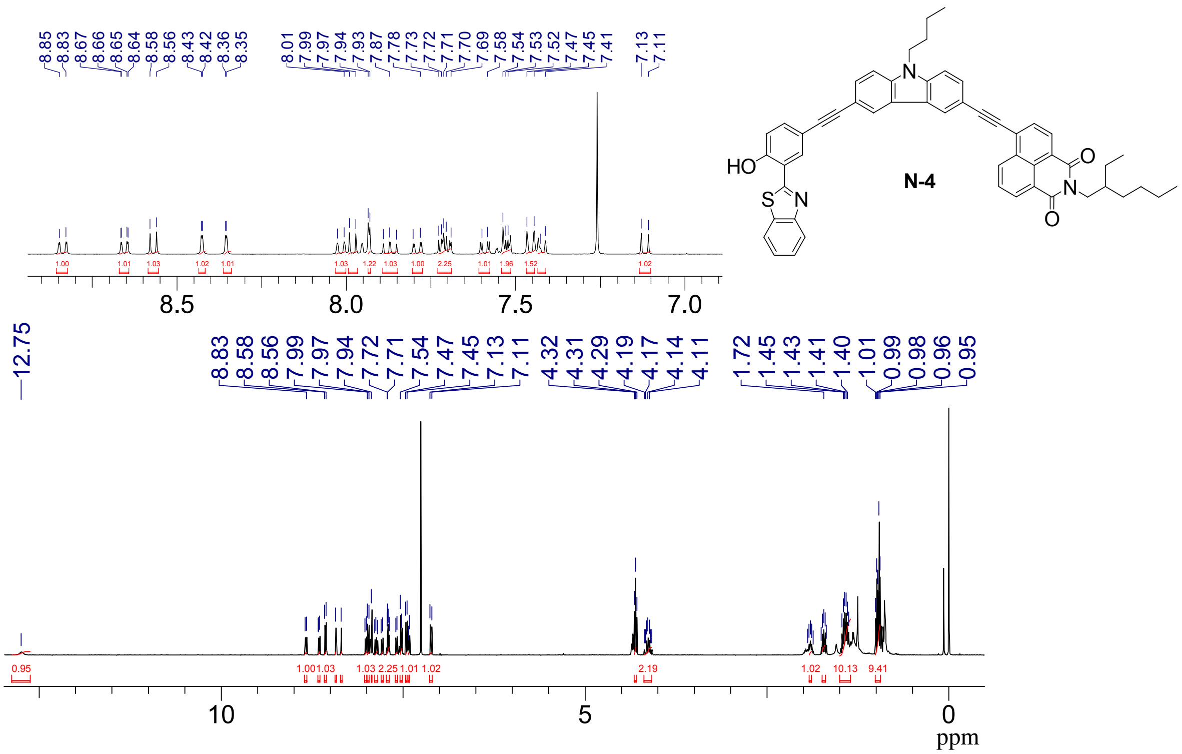


**Fig. S17** $^1$H NMR of compound **N-4** ($CDCl_3$, 400 MHz).

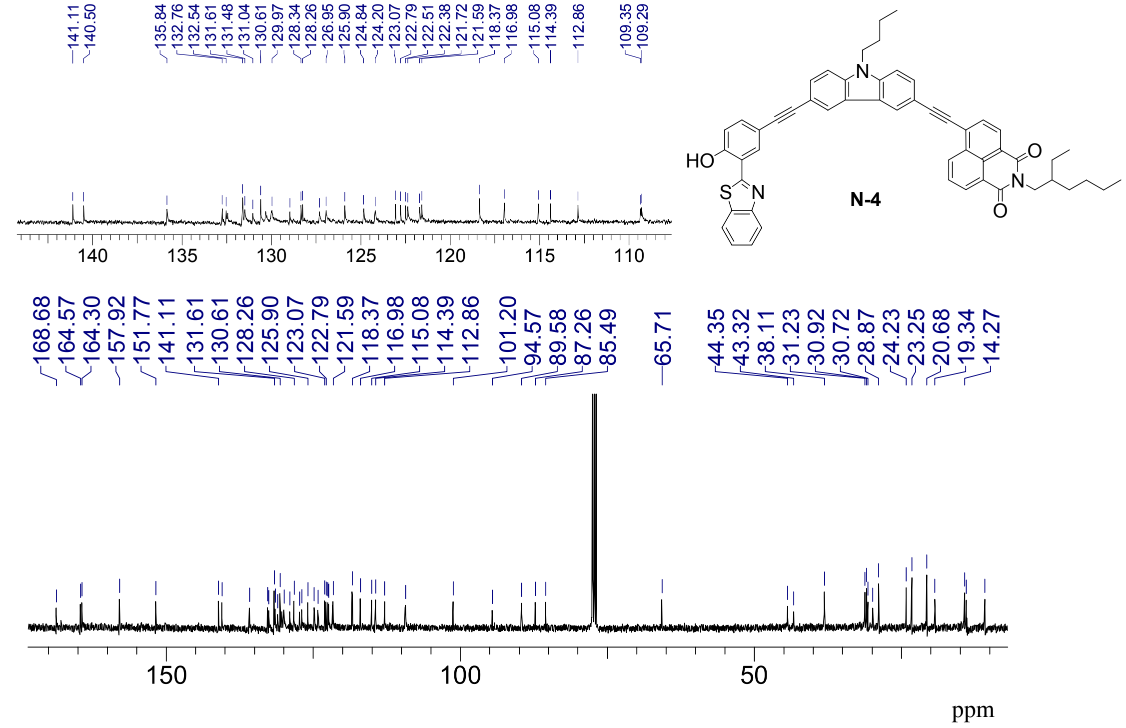


**Fig. S18** $^{13}$C NMR of compound **N-4** ($CDCl_3$, 100 MHz).

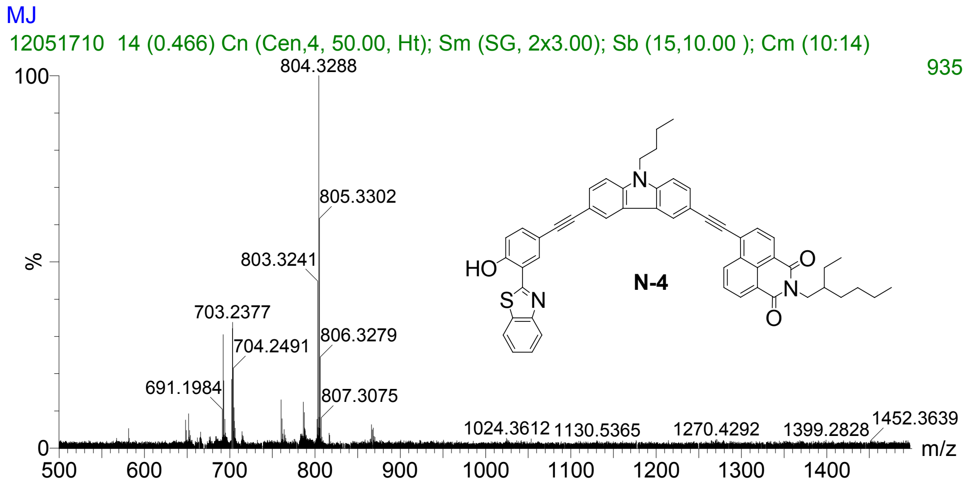


**Fig. S19** MALDI–HRMS of compound **N-4**.

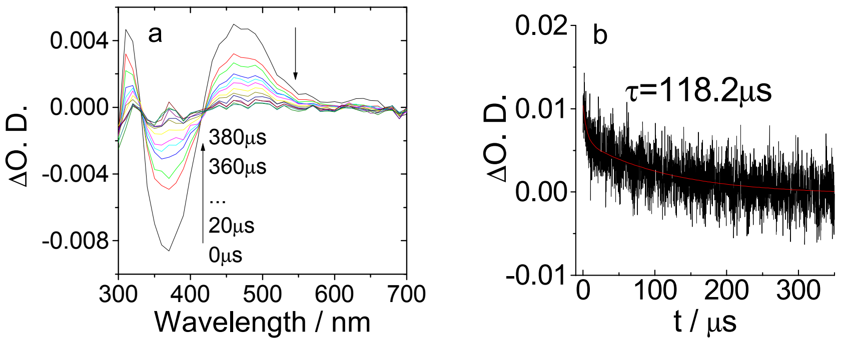


**Fig. S20** (a) Nanosecond time-resolved transient absorption difference spectra of **N-1** in *deaerated* methanol ($\lambda_{ex}$ = 355 nm) and (b) decay traces of the transient absorption at 380 nm; $c = 2.0 \times 10^{-5}$ M; 20 °C.

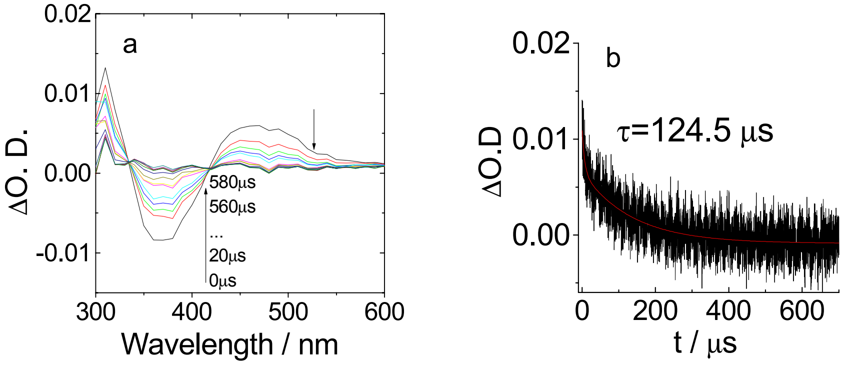


**Fig. S21** (a) Nanosecond time-resolved transient absorption difference spectra of **N-1** in *aerated* methanol ($\lambda_{ex}$ = 355 nm) and (b) decay traces of the transient absorption at 380 nm; $c = 2.0 \times 10^{-5}$ M; 20 °C.

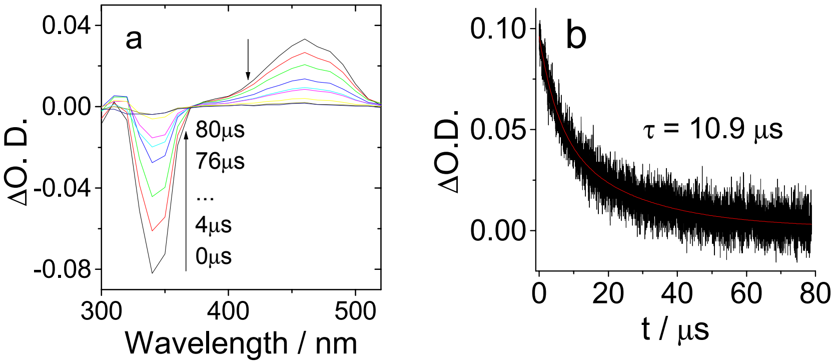


**Fig. S22** (a) Nanosecond time-resolved transient absorption difference spectra of **HBT** in aerated benzene ($\lambda_{ex}$ = 355 nm) and (b) decay traces of the transient absorption at 340 nm; $c = 2.0 \times 10^{-5}$ M; 20 °C.

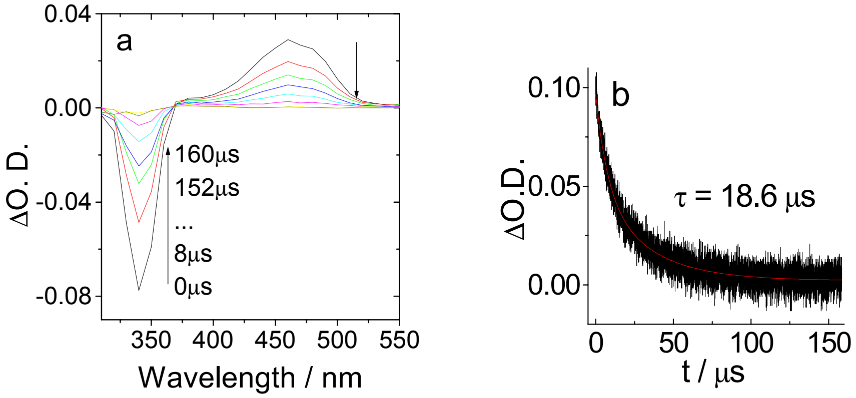


**Fig. S23** (a) Nanosecond time-resolved transient absorption difference spectra of **HBT** in deaerated benzene ($\lambda_{ex}$ = 355 nm) and (b) decay traces of the transient absorption at 340 nm; $c = 2.0 \times 10^{-5}$ M; 20 °C.

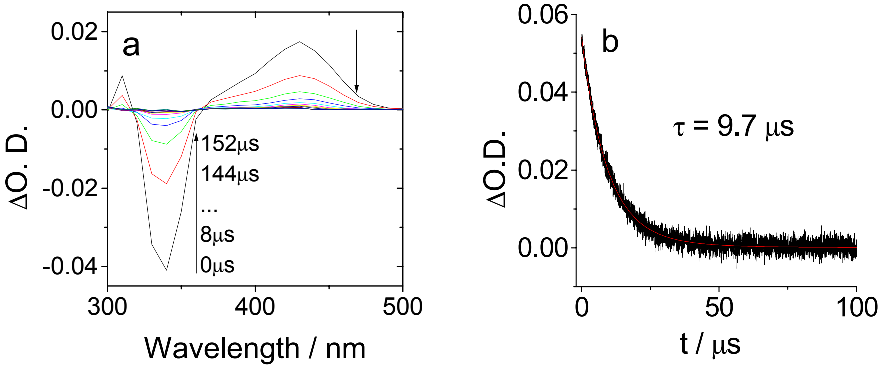


**Fig. S24** (a) Nanosecond time-resolved transient absorption difference spectra of **HBT** in aerated methanol ($\lambda_{ex}$ = 355 nm) and (b) decay traces of the transient absorption at 340 nm; $c = 2.0 \times 10^{-5}$ M; 20 °C.

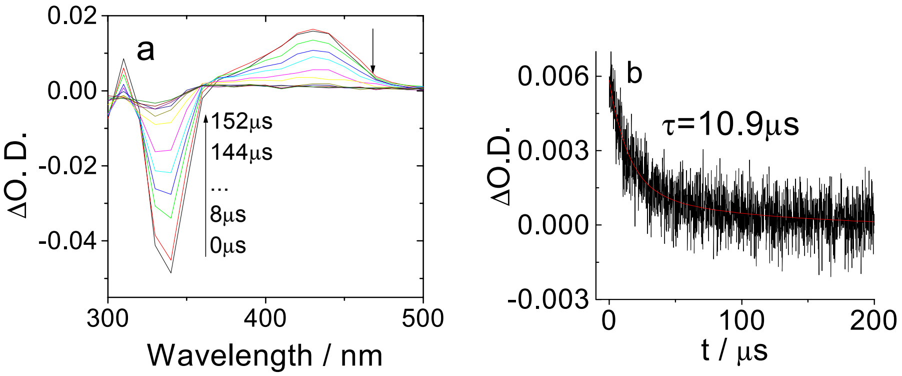


**Fig. S25** (a) Nanosecond time-resolved transient absorption difference spectra of **HBT** in deaerated methanol ($\lambda_{ex}$ = 355 nm) and (b) decay traces of the transient absorption at 340 nm; *c* = 2 ×$10^{-5}$ M; 20 °C.

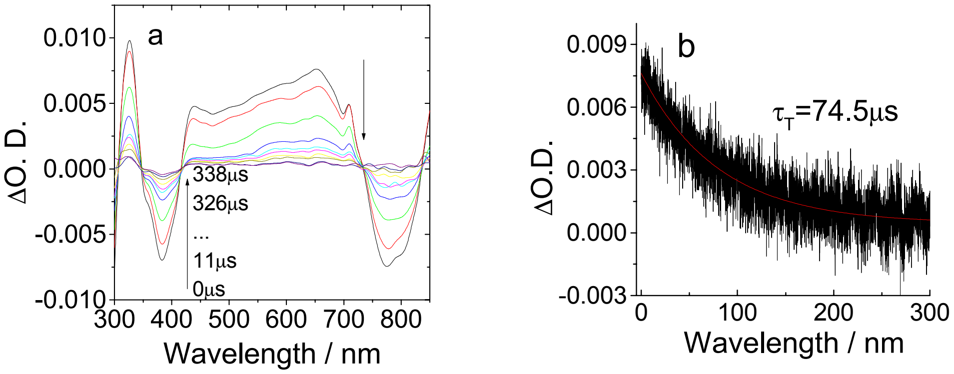


**Fig. S26** (a) Nanosecond time-resolved transient absorption difference spectra of **N-3** in deaerated benzene ($\lambda_{ex}$ = 355 nm) and (b) decay traces of the transient absorption at 380 nm; *c* = 2.0 × $10^{-5}$ M; 20 °C.

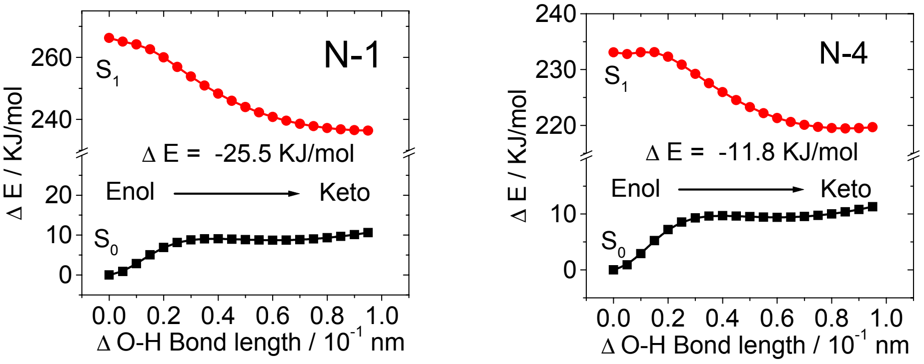


**Fig. S27** Potential energy curves from enol form to keto form of the compounds **N-1** and **N-4** at the Excited State and Ground State. The calculations are based on the optimized ground state geometry ($S_0$ state) at the B3LYP/6-31G(d)/ level using Gaussian 09W.

**Table S1.** Free energy changes for the transformation from enol form to keto form of the compounds at the Excited State and Ground States.

| Compounds | $\Delta E$ / kJ mol-1 [a] | $\Delta E$ / kJ mol-1 [b] |
|---|---|---|
| **N-1** | 9.1 | −25.5 |
| **N-4** | 9.7 | −11.8 |

[a] At $S_0$ (ground state) state. [b] At $S_1$ state.

**Table S2.** Photophysical Properties of Compounds **N-1, N-2, N-3, N-4** and **HBT** in Different Solvents [a]

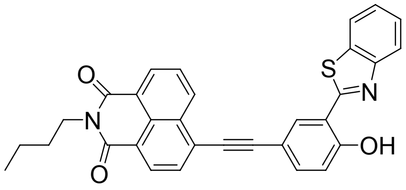
| Comp. | Solvents | $\lambda_{abs}{}^{b}$ (nm) | $\lambda_{em}{}^{c}$ (nm) | $\varepsilon^{d}$ ($M^{-1}cm^{-1}$) |
|---|---|---|---|---|
| **N-1** | $CH_2Cl_2$ | 390 | 545 | 34700 |
| | EtOAc | 380 | 592 | 36900 |
| | $CH_3CN$ | 396 | – [h] | 34400 |
| **N-2** | $CH_2Cl_2$ | 375 | 434 | 26700 |
| | EtOAc | 370 | 424 | 26300 |
| | $CH_3CN$ | 371 | 443 | 25700 |
| | MeOH | 374 | 459 | 23600 |
| **N-3** | $CH_2Cl_2$ | 392 | 483 | 17100 |
| | EtOAc | 384 | 469 | 16800 |
| | $CH_3CN$ | 392 | 550 | 18000 |
| **N-4** | $CH_2Cl_2$ | 440 | 568 | 20500 |
| | EtOAc | 428 | 548 | 20000 |
| | $CH_3CN$ | 424 | – [e] | 21100 |
| **HBT** | $CH_2Cl_2$ | 337 | 517 | 20200 |
| | EtOAc | 335 | 363 | 20500 |
| | $CH_3CN$ | 332 | 458 | 20000 |

[a] The excited wavelength for compound **N-1, N-2, N-3, N-4** and **HBT** were 370 nm, 350 nm, 370 nm, 410 nm and 315 nm. 1.0×$10^{-5}$ M, 20 °C. [b] Absorption wavelength. [c] Fluorescence emission wavelength. [d] Molar extinction coefficient. [e] Weak signal.

## Triplet state of compound N-1 **(DFT//B3LYP/6-31G(d))**

**Symbolic Z-matrix:**

**Charge = 0 Multiplicity = 3**

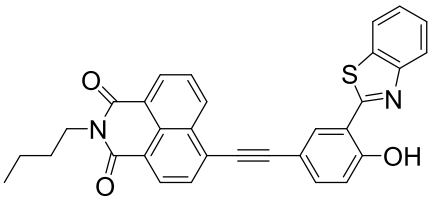


0 3

| | | | |
|---|---|---|---|
| C | -4.78143400 | 2.85559700 | -0.00000500 |
| C | -3.58856300 | 2.10434200 | -0.00008800 |
| C | -3.61487300 | 0.70942200 | -0.00010200 |
| C | -4.88635200 | 0.05010800 | -0.00003600 |
| C | -6.07115900 | 0.81481800 | 0.00004500 |
| C | -6.01185700 | 2.22414000 | 0.00006200 |
| H | -4.72589900 | 3.94025000 | 0.00000500 |
| H | -2.63102000 | 2.61600400 | -0.00014300 |
| C | -2.40650700 | -0.11532900 | -0.00017800 |
| C | -4.96256100 | -1.37455200 | -0.00005000 |
| H | -6.94098000 | 2.78215000 | 0.00012400 |
| C | -3.76431500 | -2.16616600 | -0.00015000 |
| C | -2.54454300 | -1.56651000 | -0.00021700 |
| H | -3.86832800 | -3.24483200 | -0.00017000 |
| H | -1.63542100 | -2.15928600 | -0.00029200 |
| C | -7.39392900 | 0.15976500 | 0.00011000 |

| | | | |
|---|---|---|---|
| C | -6.25490000 | -2.04735700 | 0.00003200 |
| N | -7.40148700 | -1.23910200 | 0.00013100 |
| C | -8.68989700 | -1.93838900 | 0.00024400 |
| H | -9.47502300 | -1.18622300 | 0.00036900 |
| H | -8.76821600 | -2.57266600 | -0.88611400 |
| H | -8.76800700 | -2.57275200 | 0.88655700 |
| O | -6.36890900 | -3.27914700 | 0.00004500 |
| O | -8.44338300 | 0.80462900 | 0.00022800 |
| C | -1.14715900 | 0.43565400 | -0.00019300 |
| C | -0.00385000 | 0.90994700 | -0.00019300 |
| C | 1.29180300 | 1.43779900 | -0.00018700 |
| C | 2.41937200 | 0.58693000 | -0.00010200 |
| C | 1.51388900 | 2.84611900 | -0.00025300 |
| C | 3.72320100 | 1.08699400 | -0.00008100 |
| H | 2.25205900 | -0.48555800 | -0.00004800 |
| C | 2.79190600 | 3.35769800 | -0.00022700 |
| H | 0.65879800 | 3.51406300 | -0.00031700 |
| C | 3.91524600 | 2.50428400 | -0.00013800 |
| H | 2.96999400 | 4.42796500 | -0.00027200 |
| O | 5.12253200 | 3.07515600 | -0.00011700 |
| H | 5.81004900 | 2.34962200 | -0.00004800 |
| C | 4.88540400 | 0.20227100 | -0.00000200 |
| C | 7.05237200 | -0.36562300 | 0.00014900 |
| C | 6.50358400 | -1.66920500 | 0.00009800 |
| C | 8.44434200 | -0.19292600 | 0.00024700 |
| C | 7.31948000 | -2.80230200 | 0.00014300 |
| C | 9.25588700 | -1.32068900 | 0.00029100 |
| H | 8.86185200 | 0.80891400 | 0.00028500 |
| C | 8.69959300 | -2.61250900 | 0.00024000 |
| H | 6.89477400 | -3.80096800 | 0.00010600 |
| H | 10.33544000 | -1.20414400 | 0.00036700 |
| H | 9.35470600 | -3.47857300 | 0.00027700 |
| S | 4.75198600 | -1.56943200 | -0.00001500 |
| N | 6.11526300 | 0.65136700 | 0.00009100 |

### Z-keto form of N-1 **(DFT//B3LYP/6-31G(d))**



**Symbolic Z-matrix:**

**Charge = 0 Multiplicity = 1**

0 1

| | | | |
|---|---|---|---|
| C | -4.69493600 | 2.83425200 | -0.00034000 |
| C | -3.54950400 | 2.06132200 | -0.00021200 |
| C | -3.62547900 | 0.64716500 | -0.00010500 |
| C | -4.91422800 | 0.03306200 | -0.00014000 |

| | | | |
|---|---|---|---|
| C | -6.07761500 | 0.84581400 | -0.00028200 |
| C | -5.96460600 | 2.22610500 | -0.00037000 |
| H | -4.61842400 | 3.91725900 | -0.00041800 |
| H | -2.57072500 | 2.53061800 | -0.00018500 |
| C | -2.45608700 | -0.19572800 | 0.00004500 |
| C | -5.03225100 | -1.37957200 | -0.00002200 |
| H | -6.86979000 | 2.82384000 | -0.00047500 |
| C | -3.89094400 | -2.16767000 | 0.00013500 |
| C | -2.61758500 | -1.58482800 | 0.00016300 |
| H | -4.00247200 | -3.24683300 | 0.00023000 |
| H | -1.73574700 | -2.21677200 | 0.00028200 |
| C | -7.42720600 | 0.23067400 | -0.00034000 |
| C | -6.36312100 | -2.01978200 | -0.00004400 |
| N | -7.47955300 | -1.17153800 | -0.00013400 |
| C | -8.79210200 | -1.82672900 | -0.00000500 |
| H | -9.55140600 | -1.04871500 | -0.00007500 |
| H | -8.89160800 | -2.45750800 | -0.88653400 |
| H | -8.89154600 | -2.45729100 | 0.88668500 |
| O | -6.52126000 | -3.23682400 | 0.00021800 |
| O | -8.45382600 | 0.90177000 | -0.00024900 |
| C | -1.15491700 | 0.36437300 | 0.00008700 |
| C | -0.02326800 | 0.82051900 | 0.00012900 |
| C | 1.29179500 | 1.34877800 | 0.00018000 |
| C | 2.40107500 | 0.51113100 | 0.00023800 |
| C | 1.51324300 | 2.76768200 | 0.00004700 |
| C | 3.71600400 | 1.02310200 | 0.00024000 |
| H | 2.24277000 | -0.56435300 | 0.00023200 |
| C | 2.77255800 | 3.29854400 | 0.00010100 |
| H | 0.64728300 | 3.42393100 | -0.00006700 |
| C | 3.95512800 | 2.47115400 | 0.00036600 |
| H | 2.93047500 | 4.37263600 | 0.00001200 |
| O | 5.11770000 | 2.97935600 | 0.00022800 |
| C | 4.84497800 | 0.16274400 | 0.00018200 |
| C | 6.60282200 | -1.62101500 | 0.00005100 |
| C | 7.11151700 | -0.30909400 | -0.00005200 |
| C | 7.45721400 | -2.72235500 | 0.00000700 |
| C | 8.48913200 | -0.07347000 | -0.00019100 |
| C | 8.83184200 | -2.48463400 | -0.00012700 |
| H | 7.06624000 | -3.73458900 | 0.00008700 |
| C | 9.33937700 | -1.17592400 | -0.00022300 |
| H | 8.87465200 | 0.94083300 | -0.00028200 |
| H | 9.51664300 | -3.32691400 | -0.00015900 |
| H | 10.41338700 | -1.01811500 | -0.00033700 |
| N | 6.09882000 | 0.63643500 | -0.00003700 |
| S | 4.83542700 | -1.59687400 | 0.00023700 |
| H | 6.14062700 | 1.68953500 | -0.00026600 |