Electronic Supplementary Information

Pendant chain engineering to fine-tune nanomorphology and solid state luminescence in naphthalimide AIEEgens: application to phenolic nitro-explosive detection in water

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1. Materials, Apparatus and methods

All starting materials, reagents and analytes (4-bromo-1,8-naphthalene anhydride, 8-hydroxyquinolene, α-naphthol, alkylamines, nitroaromatics, deuterated solvents) were purchased from Sigma Aldrich (INDIA). HPLC grade solvents and potassium carbonate were purchased from Zenith India and Northeast Chemicals. The chemicals purchased were of reagent grade and used without additional purification.

(Caution! Nitroaromatic analytes, especially TNP, are categorized as secondary chemical explosives and should be handled carefully with safety measures)

NMR ($^1$H, $^{13}$C) spectra were recorded with a Bruker Avance 600 MHz NMR spectrometer by taking residual solvent signal as internal reference. Electro spray ionization mass (ESI-MS) spectra were recorded on a Waters (Micro mass MS-Technologies) Q-Tof MS Analyzer spectrometer. Perkin-Elmer Model Lambda-35 spectrophotometer and Horiba Fluoromax-4 spectrofluorometer have been used to record UV/vis and PL spectra respectively in a 3 ml quartz cuvettes of path length 1 cm at 298 K. Fluorescence quantum yields in solutions were calculated by standard methods using Quinine sulphate (Φ_F = 0.577 in 0.1 M H_2SO_4, λ_ex= 350 nm). Solid state absorbance and emission were recorded with Fluoromax-4 fluorescence spectrophotometer equipped with a Quanta-ϕ integrating sphere to get solid state fluorescence quantum yield. Hydrodynamic diameters of the nanoaggregates were obtained in a Malvern Zetasizer instrument. Life-time measurements were performed using a MicroTime-200 instrument. FE-SEM images were obtained on Sigma Carl ZEISS field emission scanning electron microscope by drop casting the aqueous solution on aluminium foil and were left for drying at room temperature. The ground state optimized geometries were obtained using B3LYP hybrid functional incorporated in the Gaussian 09 package.1,2 The 6-31G(d) basis set for all the atoms has been used in all calculations, which offers reasonably high quality outcomes at a reasonable time.

2. Synthesis
**Alkylation:** To a suspension of 4-bromonaphthalene anhydride (554.2 mg, 2 mmol) in ethanol, butylamine (146.28 mg, 2 mmol) was added drop wise at room temperature. The temperature was increased and stirred for 8 hours at 85 °C. The mixture was cooled and the solvent was evaporated under reduced pressure. The solid residue was dissolved in chloroform and washed with water for two times. The organic layer was concentrated after drying over anhydrous Na₂SO₄. Finally column purification was performed to obtain the pure product (BN).

Similar procedures were followed by taking equal equivalents of respective alkyl or cycloalkylamines to get the other Alkylated 4-bromonaphthalimides derivatives (HN, ON, CHN and MCHN) as mentioned in Scheme 1.

**BN:** Light grey solid (595 mg, 89% yield); M.p. 100-102 °C; HRMS (m/z): calcd for C₁₆H₁₄BrNO₂ 331.0208; found 332.0280 [M+H]+; ¹H NMR (600 MHz, CDCl₃, δ ppm) 8.44 (d, 1H), 8.34 (d, 1H), 8.20 (d, 1H), 7.82 (d, 1H), 7.63 (t, 1H), 3.97 (t, 2H) 1.52 (m, 2H), 1.26 (m, 2H), 0.78 (t, 3H); ¹³C NMR (150.00 MHz, CDCl₃, δ ppm) 163.79, 133.35, 132.16, 131.36, 131.25, 130.77, 130.34, 129.14, 128.24, 123.32, 122.46, 40.57, 30.35, 20.56, 14.02.

**HN:** Light green solid (615 mg, 85% yield); M.p. 92-93 °C; HRMS (m/z): calcd for C₁₈H₁₈BrNO₂ 359.0521; found 360.0600 [M+H]+; ¹H NMR (600 MHz, CDCl₃, δ ppm) 8.57 (d, 1H), 8.46 (d, 1H), 8.32 (d, 1H), 7.94 (d, 1H), 7.77 (t, 1H), 4.12 (t, 3H) 1.70 (m, 2H), 1.31 (m, 6H), 0.87 (t, 3H); ¹³C NMR (150.00 MHz, CDCl₃, δ ppm) 163.63, 163.60, 133.22, 132.06, 131.26, 131.16, 130.61, 130.24, 128.98, 128.15, 123.21, 122.34, 40.78, 31.71, 28.18, 26.96, 22.74, 14.25.

**ON:** Light brown solid (620 mg, 80% yield); M.p. 85-86 °C; HRMS (m/z): calcd for C₂₀H₂₂BrNO₂ 387.083; found 388.0950 [M+H]+; ¹H NMR (600 MHz, CDCl₃, δ ppm) 8.64 (d, 1H), 8.52 (d, 1H), 8.39 (d, 1H), 8.02 (d, 1H), 7.83 (t, 1H), 4.15 (t, 2H) 1.71 (m, 2H), 1.34 (m, 10H), 0.87 (t, 3H); ¹³C NMR (150.00 MHz, CDCl₃, δ ppm) 163.73, 133.32, 132.15, 131.34, 131.24, 130.74, 130.32, 129.11, 128.22, 123.31, 122.45, 40.82, 32.00, 29.51, 29.40, 28.27, 27.32, 22.83, 14.28.

**CHN:** White solid (586 mg, 82% yield); M.p. 82-83 °C; HRMS (m/z): calcd for C₁₈H₁₆BrNO₂ 357.063; found 358.0455 [M+H]+; ¹H NMR (600 MHz, CDCl₃, δ ppm) 8.62 (d, 1H), 8.52 (d, 1H), 8.37 (d, 1H), 8.01 (d, 1H), 7.83 (t, 1H), 4.15 (m, 1H) 2.54 (m, 2H) 1.90 (m, 2H), 1.74 (m, 2H), 1.45 (m, 2H), 0.87 (m, 2H); ¹³C NMR (150.00 MHz, CDCl₃, δ ppm) 164.02, 163.98, 132.82,
MCHN: White solid (645 mg, 86% yield); M.p. 72-74 °C; HRMS (m/z): calcd for C\textsubscript{18}H\textsubscript{16}BrNO\textsubscript{2} 371.053; found 372.0633 [M+H]\textsuperscript{+}; \textsuperscript{1}H NMR (600 MHz, CDCl\textsubscript{3}, δ ppm) 8.63 (d, 1H), 8.53 (d, 1H), 8.38 (d, 1H), 8.01 (d, 1H), 7.82 (t, 1H), 4.04 (d, 2H) 1.88  (m, 1H) 1.67 (m, 5H), 1.17 (m, 5H); \textsuperscript{13}C NMR (150.00 MHz, CDCl\textsubscript{3}, δ ppm) 164.12, 133.35, 132.28, 131.48, 131.26, 130.79, 130.34, 129.21, 128.26, 123.29, 122.43, 46.34, 36.88, 32.11, 31.14, 29.89, 26.53, 26.06.

**Post functionalization:** To different round bottom flasks, each containing the solution of BN, HN, ON, CHN and MCHN (0.5 mmol) in dry DMF (5 mL), 1 mmol of 8-hydroxyquinoline (for HNN, α-naphthol was taken) and 200 mg of K\textsubscript{2}CO\textsubscript{3} were added to them separately and were refluxed for 15 hours. The solvents were vaporized under vacuum and the residues were extracted with chloroform (30×3 mL). The organic layers were washed with H\textsubscript{2}O for several times followed by washing with brine and dried over anhydrous Na\textsubscript{2}SO\textsubscript{4}. The crude products were concentrated and purified through column chromatography over silica gel to get the final products (BNQ, HNQ, ONQ, CHNQ, MCHNQ and HNN) respectively.

BNQ: Light yellow solid (164 mg, 82 % yield); M.p. 177-179 °C; HRMS (m/z): calcd for C\textsubscript{25}H\textsubscript{20}N\textsubscript{2}O\textsubscript{3} 396.147; found 397.1581 [M+H]\textsuperscript{+}; \textsuperscript{1}H NMR (600 MHz, CDCl\textsubscript{3}, δ ppm) 8.87 (m, 2H), 8.67 (d, 1H), 8.39 (d, 1H), 8.27 (d, 1H), 7.79 (m, 2H), 07.58 (d, 1H), 7.49 (d, 1H), 7.46 (d, 1H), 6.75 (d, 1H), 4.18 (t, 2H), 1.72 (m, 2H), 1.45 (m, 2H), 0.98 (t, 3H), \textsuperscript{13}C NMR (150.00 MHz, CDCl\textsubscript{3}, δ ppm) 164.71, 164.06, 160.58, 151.30, 150.99, 141.41, 136.48, 132.90, 132.05, 129.24, 129.18, 129.05, 126.95, 126.71, 126.65, 125.64, 124.06, 122.36, 120.28, 116.84, 111.57 40.53, 30.45, 20.60, 14.05.

HNQ: Yellow solid (155 mg, 73 % yield); M.p. 168-170 °C; HRMS (m/z): calcd for C\textsubscript{27}H\textsubscript{24}N\textsubscript{2}O\textsubscript{3} 424.1787; found 425.1894 [M+H]\textsuperscript{+}; \textsuperscript{1}H NMR (600 MHz, CDCl\textsubscript{3}, δ ppm) 8.85 (d, 2H), 8.64 (d, 1H), 8.37 (d, 1H), 8.24 (d, 1H), 7.76-7.79 (m, 2H), 07.57 (t, 1H), 7.46 (d, 2H), 6.72(d, 1H), 4.14 (t, 2H), 1.70 (m, 2H), 1.32 (m, 6H), 86 (t, 3H), \textsuperscript{13}C NMR (150.00 MHz, CDCl\textsubscript{3}, δ ppm) 164.58, 163.93, 160.51, 151.11, 150.91, 141.31, 136.42, 132.84, 131.95, 130.24, 129.81, 129.16, 126.89, 126.62, 125.63, 123.91, 122.72, 122.29, 120.32, 116.84, 111.39, 40.53, 31.72, 28.25, 26.97, 22.73, 14.25.
**ONQ:** White solid (182 mg, 80 % yield); M.p. 150-153 °C; HRMS (m/z): calcd for C_{29}H_{28}N_{2}O_{3} 452.210; found 453.2165 [M+H]+; \(^1^H\) NMR (600 MHz, CDCl\(_3\), \(\delta\) ppm) 8.86 (d, 2H), 8.66 (d, 1H), 8.39 (d, 1H), 8.26 (d, 1H), 7.79 (d, 2H), 07.59 (t, 1H), 7.48 (m, 2H), 6.74(d, 1H), 4.16 (t, 2H), 1.72 (m, 2H), 1.25-1.43 (m, 10H), 0.87 (t, 3H); \(^{13}\)C NMR (150.00 MHz, CDCl\(_3\), \(\delta\) ppm) 164.69, 164.04, 160.56, 151.30, 150.98, 141.41, 136.51, 132.89, 132.04, 130.35, 129.94, 129.22, 126.96, 126.69, 125.65, 123.89, 122.76, 122.37, 120.30, 116.94, 111.35, 40.62, 32.02, 29.55, 29.43, 28.37, 27.37, 22.83, 14.28.

**CHNQ:** Light pink solid (170 mg, 80.5 % yield); M.p. 167-169 °C; HRMS (m/z): calcd for C_{27}H_{22}N_{2}O_{3} 422.163; found 423.1719 [M+H]+; \(^1^H\) NMR (600 MHz, CDCl\(_3\), \(\delta\) ppm) 8.87 (d, 1H), 8.84 (d, 1H), 8.64 (d, 1H), 8.37 (d, 1H), 8.26 (d, 1H), 7.78 (m, 2H), 7.58 (t, 1H), 7.44 (d, 1H), 7.43 (d, 1H), 6.75(d, 1H), 5.02 (m, 1H), 2.55 (m, 2H), 1.87 (m, 2H), 1.72 (m, 3H), 0.88 (m, 3H); \(^{13}\)C NMR (150.00 MHz, CDCl\(_3\), \(\delta\) ppm) 165.11, 164.49, 160.24, 151.45, 150.95, 141.38, 136.47, 132.76, 131.92, 130.33, 129.91, 128.91, 126.93, 126.71, 125.50, 123.94, 122.73, 122.53, 120.08, 116.92, 111.79, 53.84, 29.89, 29.34, 26.78, 25.69, 22.88.

**MCHNQ:** Yellow solid (162 mg, 74 % yield); M.p. 189-191 °C; HRMS (m/z): calcd for C_{28}H_{24}N_{2}O_{3} 436.178; found 437.1878 [M+H]+; \(^1^H\) NMR (600 MHz, CDCl\(_3\), \(\delta\) ppm) 8.87 (m, 2H), 8.66 (d, 1H), 8.39 (d, 1H), 8.27 (d, 1H), 7.80 (m, 2H), 7.59 (d, 1H), 7.46 (d, 1H), 7.45 (d, 1H), 6.75(d, 1H), 4.05 (d, 2H), 1.72 (m, 1H), 1.63 (m, 2H), 1.22 (m, 4H), 0.88 (m, 3H); \(^{13}\)C NMR (150.00 MHz, CDCl\(_3\), \(\delta\) ppm) 165.03, 164.39, 160.54, 151.30, 150.98, 141.39, 136.51, 133.00, 132.15, 130.34, 129.97, 129.22, 126.96, 126.70, 125.64, 123.99, 122.70, 122.37, 120.28, 116.95, 111.58, 46.23, 36.96, 32.12, 31.19, 29.89, 26.59, 26.11.

**HNN:** Light grey solid (189 mg, 89 % yield); M.p. 112-114 °C; HRMS (m/z): calcd for C_{28}H_{25}NO_{3} 423.183; found 424.1926 [M+H]+; \(^1^H\) NMR (600 MHz, CDCl\(_3\), \(\delta\) ppm) 8.88 (dd, 1H), 8.70 (dd, 1H), 8.38 (d, 1H), 7.93 (m, 2H), 7.83 (m, 2H), 7.54 (m, 2H), 7.28 (t, 1H), 6.77(d, 1H), 4.16 (t, 2H), 1.72 (m, 2H), 1.62 (m, 2H), 1.32 (m, 5H), 0.88 (t, 3H); \(^{13}\)C NMR (150.00 MHz, CDCl\(_3\), \(\delta\) ppm) 164.41, 163.73, 160.19, 150.36, 135.21, 132.91, 131.91, 129.71, 128.47, 128.24, 126.99, 126.75, 126.73, 126.63, 125.91, 125.90, 123.54, 122.74, 121.44, 116.90, 116.61, 110.31, 40.42, 31.58, 28.09, 26.82, 22.59, 14.10.
3. Preparation of stock solutions for aggregation and sensing studies

Stock solutions of all the naphthalimides were prepared in DMF at a concentration of $1 \times 10^{-2}$ M. Stock solutions of nitroaromatic compounds like trinitrophenol (TNP), 2,4-dinitrophenol (2,4-DNP), 2,6-dinitrophenol (2,6-DNP), 4-nitrophenol (p-NP), 2-nitrophenol (o-NP) and phenol were prepared in Milli-Q water at a concentrations of $1 \times 10^{-2}$ M. Nitroaromatics, namely, trinitrotoluene (TNT), 2,4-dinitrotoluene (2,4-DNT), 2,4-dinitrobenzene (1,3-DNB), 2-nitrotoluene (o-NT), 3-nitrotoluene (m-NT), 4-nitrotoluene (p-NT), nitrobenzene (NB), nitromethane (NM), 2,3-dimethyl-2,3-dinitrobutane (DMNB), 2,6-dinitrotoluene (2,6-DNT), 1,4-dinitrobenzene (1,4-DNB) were prepared at concentrations of $1 \times 10^{-2}$ M in 1:1 methanol:water solvent system. The stock solution of each naphthalimide was diluted to 20 µM in water and HEPES buffer (pH 7) for each titration in a 3 mL quartz cuvette (1 cm × 1 cm). The stock solutions of nitroaromatics were introduced in portions and the fluorescence intensity changes were recorded at room temperature ($\lambda_{ex} = 360$ nm).

4. Quantum Yield Calculations

PL quantum yields ($\Phi_s$) of naphthalimides were calculated by taking quinine sulfate ($\Phi_s = 0.57$ in 0.1 M H$_2$SO$_4$) as standard and using the equation shown below:

$$\Phi_s = \Phi_r \left(\frac{A_r F_s}{A_s F_r}\right) \left(\frac{\eta_s^2}{\eta_r^2}\right)$$

Where, s and r represent sample and reference, $\Phi$ signifies the quantum yield, A denotes absorbance, F signifies relative integrated fluorescence intensity, and $\eta$ represents the refractive index of the medium.

5. Cyclic Voltammetry Studies

Electrochemical measurements were performed in a three-electrode cell with platinum wire as counter electrode, glassy carbon as working electrode and saturated Ag/AgNO$_3$ electrode as reference electrode. The Fc$^+$/Fc couple was employed as internal reference and Tetrabutylammoniumhexafluorophosphate (0.1 M) in acetonitrile was taken as supporting electrolyte. All the measurements were carried out at room temperature under inert atmosphere. Single reduction peak was observed for HNQ. The LUMO level (-3.0234 eV) was calculated from
the onset method \[ E_{\text{LUMO}} = -(E_{\text{onset, red vs Fc+/Fc}} + 4.8) \text{ (eV)} \]. Band gap (3.1234 eV) of HNQ was determined from the onset of UV–visible spectrum to calculate its HOMO level (-6.1468 eV).

6. Computational study

**Figure S1.** Optimized structures in electronic ground state with electron density of HOMO and LUMO (Gaussian 09, DFT B3LYP 6-31G basis set). Energy of HOMO, LUMO and band gaps are in eV, dipole moments are in debye and dihedral angels are in “o” with respect to naphthalimide and quinoline/naphthalene plane. (Left to Right: BNQ, HNQ, ONQ, CHNQ, MCHNQ and HNN).

7. Aggregation study

**Table S1.** Photophysical properties of Naphthalimide AIEgens with various \( f_w \) in DMF at 20 \( \mu \text{M} \) concentration.

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<th>Compound</th>
<th>( f_w ) in</th>
<th>( \lambda_{\text{abs. max}} )</th>
<th>( \epsilon )</th>
<th>( \lambda_{\text{em. max}} )</th>
<th>Stokes shift</th>
<th>( \Phi_{\text{FL}} )</th>
<th>( \Phi_{\text{FL}} ) (%)</th>
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<td>26.1±1.1</td>
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<tr>
<td>MCHNQ</td>
<td>0%</td>
<td>363</td>
<td>2721.125</td>
<td>438</td>
<td>75</td>
<td>4.05</td>
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<td>20%</td>
<td>365</td>
<td>2652.25</td>
<td>444</td>
<td>79</td>
<td>3.50</td>
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<tr>
<td></td>
<td>40%</td>
<td>366</td>
<td>2310.225</td>
<td>444</td>
<td>78</td>
<td>2.13</td>
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<tr>
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<td>60%</td>
<td>368</td>
<td>2474.075</td>
<td>442</td>
<td>74</td>
<td>1.32</td>
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<td></td>
<td>80%</td>
<td>365</td>
<td>1940.35</td>
<td>444</td>
<td>79</td>
<td>1.27</td>
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<td></td>
<td></td>
<td>27.0±0.9</td>
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<td>Water Fraction</td>
<td>HNN</td>
<td>Absorption (%)</td>
<td>Absorbance</td>
<td>Excitation Max.</td>
<td>Fluorescence (µM)</td>
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<tr>
<td>0%</td>
<td>362</td>
<td>99.8%</td>
<td>3400.925</td>
<td>412</td>
<td>50</td>
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<tr>
<td>20%</td>
<td>364</td>
<td>11.7±0.8</td>
<td>3457.475</td>
<td>411</td>
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<tr>
<td>40%</td>
<td>366</td>
<td>20%</td>
<td>3404.375</td>
<td>429</td>
<td>1.16</td>
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<tr>
<td>60%</td>
<td>368</td>
<td>40%</td>
<td>3069.7</td>
<td>429</td>
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<tr>
<td>80%</td>
<td>370</td>
<td>60%</td>
<td>3601.175</td>
<td>482</td>
<td>15.42</td>
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<tr>
<td>99.8%</td>
<td>383</td>
<td>80%</td>
<td>3915.85</td>
<td>481</td>
<td>12.16</td>
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Measured at each absorption maximum. Excited at 360 nm for all compounds. Quantum yields were calculated by using quinine sulfate (0.1 M H₂SO₄, λ<sub>ex</sub>=350 nm, Φ<sub>FL</sub> = 57.7%) solution as reference together with the following formula: Φ<sub>FL</sub>=Φ<sub>FL</sub>(I/I<sub>R</sub>)(A<sub>R</sub>/A)(η<sup>2</sup>/η<sub>R</sub>²), where Φ = quantum yield, I = Intensity of emission, A = absorbance at λ<sub>ex</sub>, η = refractive index of solvent, R = reference. (20 µM)

**Absorption and emission spectra at different water fraction in DMF** (at 25 °C, 20 µM, λ<sub>ex</sub> = 360 nm)

![Figure S2. Absorption (left) and emission spectra (right) of BNQ.](image)
Figure S3. Absorption (left) and emission spectra (right) of HNQ.

Figure S4. Absorption (left) and emission spectra (right) of ONQ.

Figure S5. Absorption (left) and emission spectra (right) of CHNQ.
Figure S6. Absorption (left) and emission spectra (right) of MCHNQ.

Figure S7. Absorption (left) and emission spectra (right) of HNN.

Figure S8. Emission spectra in 99.8% water-0.2% DMF. (20 µM, λ<sub>ex</sub> 360 nm)
8. DLS Studies of Aggregates (99.8% Water-0.2% DMF mixture solution at 25 °C, 20 μM)

![Figure S9. Size distribution by DLS of BNQ aggregate [Left] and HNQ aggregate [Right].](image)

![Figure S10. Size distribution by DLS of ONQ aggregate [Left] and CHNQ aggregate [Right].](image)

![Figure S11. Size distribution by DLS of MCHNQ aggregate [Left] and HNN aggregate [Right].](image)

9. Sensing studies
Figure S12. [Left] Effect of increasing concentration of 2,4-DNP on the fluorescence spectra of HNQ (20 µM at pH 7) at room temperature. [Right] Stern–Volmer plots for the fluorescence quenching of HNQ by 2,4-DNP.

Figure S13. [Left] Effect of increasing concentration of p-NP on the fluorescence spectra of HNQ (20 µM at pH 7) at room temperature. [Right] Stern–Volmer plots for the fluorescence quenching of HNQ by p-NP.
**Figure S14.** Extent of fluorescence quenching of the naphthalimides nanoaggregates observed upon the addition of 70 µM TNP in aqueous media.

10. Detection limit calculations

**Figure S15.** Change in fluorescence emission intensity of HNQ at different concentrations of TNP.

\[
\text{LOD} = 3 \times \text{S.D.} / k
\]

LOD for TNP = \[3 \times 1015.514 / 4.12 \times 10^{10}\]

\[= 73.79 \times 10^{-9} \text{ M} \quad (16.8 \text{ ppb})\]
Using the above formula \((\text{LOD} = 3 \times \text{S.D.} / k)\), LOD for TNP was also calculated in other N-atom containing congeners.

**Figure S16.** Change in fluorescence emission intensity of BNQ at lower concentrations of TNP. LOD = 123.32 nM  (28.2 ppb)

**Figure S17.** Change in fluorescence emission intensity of CHNQ at lower concentrations of TNP. LOD = 86.03 nM  (19.7 ppb)
Figure S18. Change in fluorescence emission intensity of MCHNQ at lower concentrations of TNP. LOD = 78.08 nM (17.9 ppb)

Figure S19. Change in fluorescence emission intensity of ONQ at lower concentrations of TNP. LOD = 113.74 nM (26.0 ppb)
11. $^1$H-NMR, $^{13}$C-NMR, Mass and IR Spectra

$^1$H spectra of BN

$^{13}$C spectra of BN
Mass spectra of BN

$^1$H spectra of HN
$^{13}$C spectra of HN
Mass spectra of HN

$^{13}$C spectra of ON
Mass spectra of ON

\[ \text{\textsuperscript{1}H spectra of CHN} \]

[S21]
$^{13}$C spectra of CHN

Mass spectra of CHN
$^1$H spectra of MCHN

$^{13}$C spectra of MCHN
Mass spectra of MCHN

$^1$H spectra of BNQ
$^{13}$C spectra of BNQ

Mass spectra oh BNQ
IR Spectra of BNQ

\[1^H\] spectra of HNQ
$^{13}$C spectra of HNQ

Mass spectra of HNQ
IR Spectra of HNQ

$^1$H spectra of ONQ
\(^{13}\)C spectra of ONQ

Mass spectra of ONQ
IR Spectra of ONQ

$^1$H spectra of CHNQ
$^{13}$C spectra of CHNQ

Mass spectra of CHNQ
IR Spectra of CHNQ

$^1$H spectra of MCHNQ
$^{13}$C spectra of MCHNQ

Mass spectra of MCHNQ
IR Spectra of MCHNQ

$^1$H spectra of HNN
$^{13}$C spectra of HNN

Mass spectra of HNN
12. References


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Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.;
Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision A.02,