Supporting Information

Triphenylene Derivatives: Chemosensors for Sensitive Detection of Nitroaromatic Explosives.

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S1
Spectral overlaps for compound 3 and 5.

**Figure S1**: Spectral overlap of the absorption spectrum of picric acid (red line) with the emission spectrum of compound 3 (blue line).

**Figure S2**: Spectral overlap of the absorption spectrum of picric acid (red line) with the emission spectrum of compound 5 (blue line)
Fluorescence spectra of compound 5 in different solvents

Intensity (a.u.)

Wavelength (nm)

THF
DCM
Cyclohexane
Fluorescence response of derivative 3 with other nitroaromatic derivatives

4-Nitrotoluene (90 equiv.)

Dinitrotoluene (260 equiv.)

Dinitrobenzene (200 equiv.)

Trinitrotoluene (300 equiv.)
Fluorescence response of derivative 3 with other nitroaromatic derivatives

- Benzoquinone (1500 equiv.)
- Dimethyldinitrobutane (1500 equiv.)
- Benzoic acid (1500 equiv.)
Fluorescence response of derivative 5 with other nitroaromatic derivatives

4-Nitrotoluene (75 equiv.)

Dinitrotoluene (110 equiv.)

Trinitrotoluene (140 equiv.)

Dinitrobenzene (80 equiv.)
Fluorescence response of derivative 5 with other nitroaromatic derivatives

Benzoquinone (2500 equiv.)

dimethyldinitrobutane (2500 equiv.)

Benzoic acid (2500 equiv.)
Calculated Stern-Volmer constant for compounds 3 and 5 with various nitroaromatic derivatives

<table>
<thead>
<tr>
<th>Calculated Ksv for Compound</th>
<th>PA</th>
<th>4-NT</th>
<th>DNT</th>
<th>TNT</th>
<th>DNB</th>
<th>NB</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>$2.91 \times 10^5$ M$^{-1}$</td>
<td>$1.85 \times 10^4$ M$^{-1}$</td>
<td>$3.41 \times 10^3$ M$^{-1}$</td>
<td>$2.4 \times 10^3$ M$^{-1}$</td>
<td>$4.02 \times 10^3$ M$^{-1}$</td>
<td>$1.81 \times 10^3$ M$^{-1}$</td>
</tr>
<tr>
<td>5</td>
<td>$2.93 \times 10^5$ M$^{-1}$</td>
<td>$1.95 \times 10^4$ M$^{-1}$</td>
<td>$2.20 \times 10^3$ M$^{-1}$</td>
<td>$8.29 \times 10^3$ M$^{-1}$</td>
<td>$1.92 \times 10^4$ M$^{-1}$</td>
<td>$1.32 \times 10^4$ M$^{-1}$</td>
</tr>
</tbody>
</table>

**Table 2:** Calculated Stern-Volmer constants for compounds 3 and 5 with various nitroaromatics
$^1$H NMR of compound 3
\textsuperscript{13}C NMR of compound 3
MALDI-TOF Mass Spectrum of compound 3.
$^1$H NMR spectrum of Compound 5
$^{13}$C NMR spectrum of compound 5
Mass Spectrum of compound 5
Table: 1 Comparison of derivative 5 with previous reports

<table>
<thead>
<tr>
<th>S.No.</th>
<th>Reference</th>
<th>Detection limit</th>
<th>Calculated Stern-Volmer constant with PA</th>
<th>Contact mode detection of explosives with test strips.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Derivative 5</td>
<td>50 nM</td>
<td>$2.93 \times 10^5$ M$^{-1}$ for 5</td>
<td>YES</td>
</tr>
<tr>
<td>2</td>
<td><em>Dalton Trans.</em>, 2011, 40, 12333</td>
<td>*</td>
<td>$2.0 \times 10^4$ M$^{-1}$ and $5.0 \times 10^4$ M$^{-1}$</td>
<td>No</td>
</tr>
</tbody>
</table>
| 3     | *Dalton Trans.*, 2011, 40, 2257 | *              | $3.1 \times 10^4$ M$^{-1}$  
$1.9 \times 10^4$ M$^{-1}$ | No                                                   |
| 4     | *Chem. Commun.*, 2012, 48, 5007 | 0.87 µM         | $9.9 \times 10^4$ M$^{-1}$               | No                                                   |
| 5     | *Polym. Chem.*, 2010, 1, 426    | 4.3 µM          | $1.5 \times 10^5$ M$^{-1}$               | No                                                   |
| 6     | *Sensors and Actuators B*, 2012, 161 251. | *              | $6.21 \times 10^3$ M$^{-1}$               | No                                                   |

* No data available