

### Supplementary Material

#### **Highly sheared anti-parallel dipolar carbonyl···carbonyl interaction in the crystal packing of strapped crown-3-pyromellitimide**

Ethan Nam Wei Howe,<sup>A</sup> Mohan Bhadbhade<sup>B</sup> and Pall Thordarson<sup>A,C</sup>

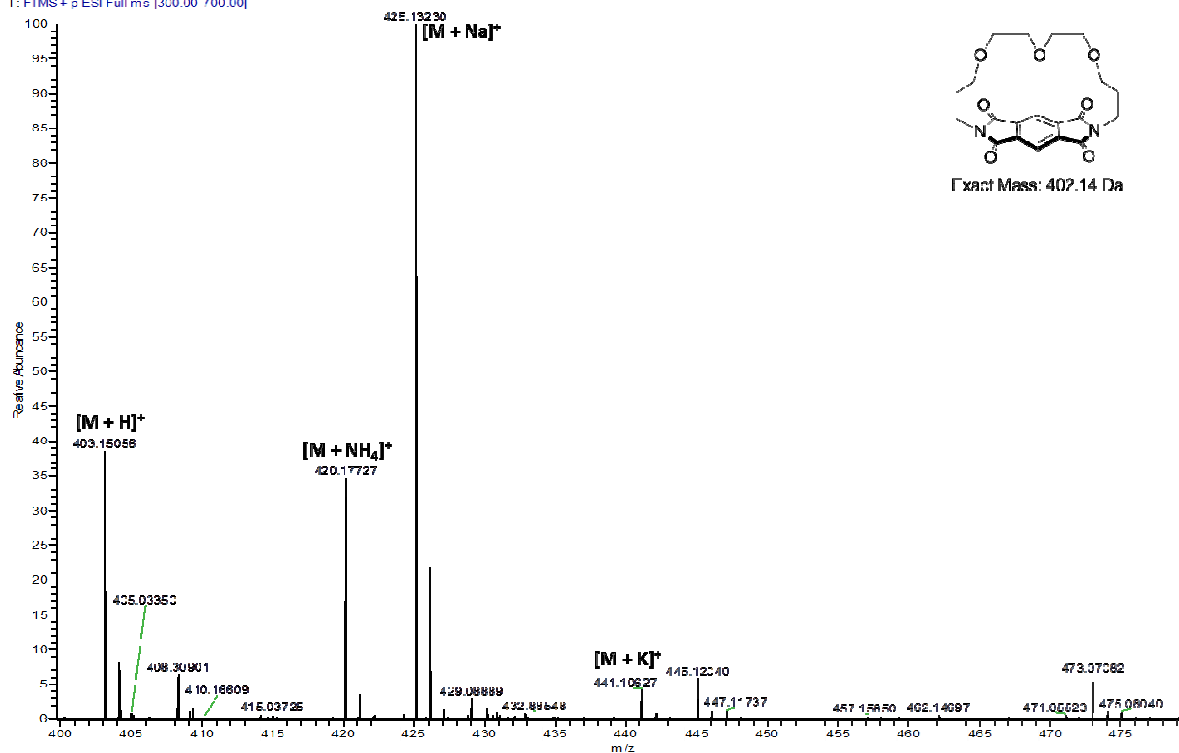
<sup>A</sup>School of Chemistry, The University of New South Wales, Sydney, NSW 2052, Australia

<sup>B</sup>Analytical Centre, The University of New South Wales, Sydney, NSW 2052, Australia

<sup>C</sup>Corresponding author. Email: [p.thordarson@unsw.edu.au](mailto:p.thordarson@unsw.edu.au)

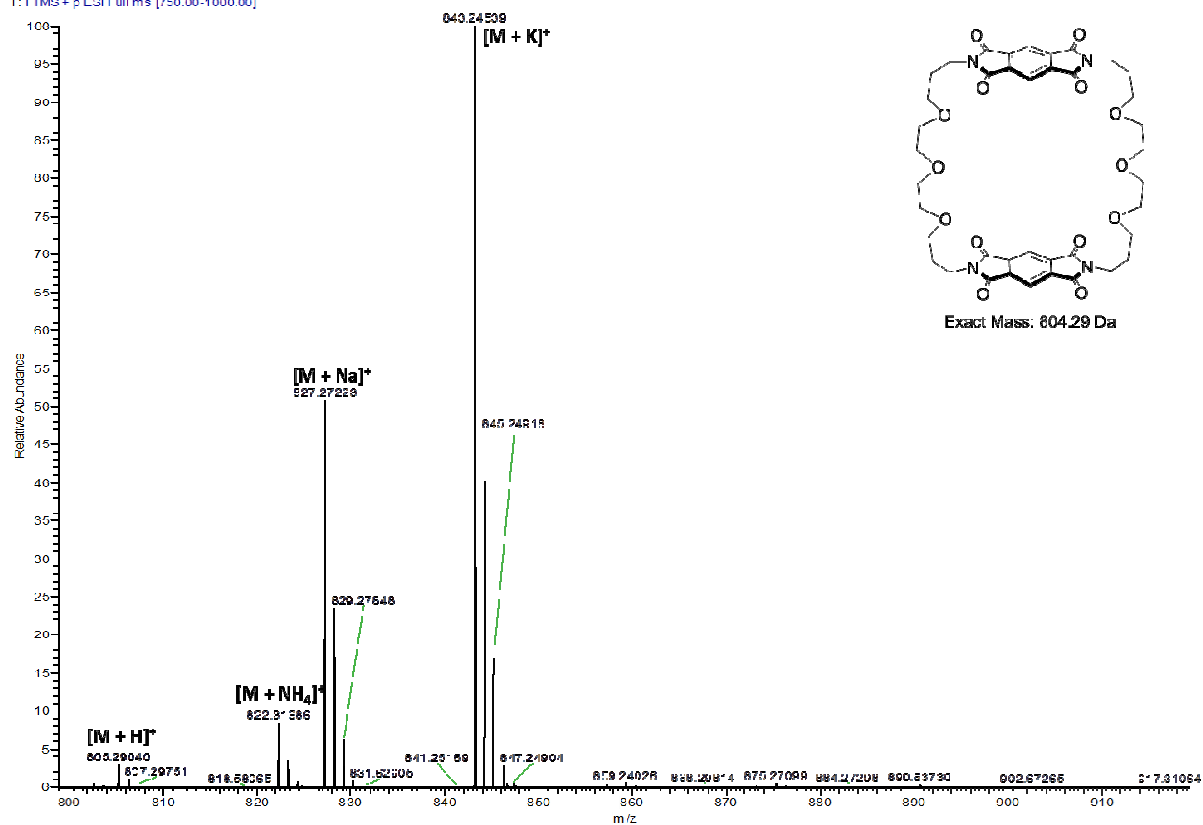
The cation recognition selectivity of crown-3-pyromellitimide **4** and crown-6-bispyromellitimide **5** was investigated using HR-MS (ESI) recorded on a Thermo Scientific Linear Quadrupole Ion Trap with Orbitrap Mass Analyser (LTQ ORBITRAP XL) mass spectrometer. Samples were prepared with 10 mole excess of NaClO<sub>4</sub>, KPF<sub>6</sub> and NH<sub>4</sub>PF<sub>6</sub> dissolved in a solution of formic acid (0.1% v/v) in acetonitrile (HPLC grade).

11-1-25\_110210 #1-32 RT: 0.01-0.50 AM: 32 NL: 4.15C6  
1: FIMS+ p ESI Full ms (300.00 / 00.00)



**Figure S1.** Mass spectrum of strapped crown-3-pyromellitimide **4** showing cation recognition selectivity.

11-1-09\_10021910-236 #1-15 RT: 0.02-0.40 AV: 15 NL: 2.51CG  
T: FTMS + p ESI Full ms [750.00-1000.00]



**Figure S2.** Mass spectrum of macrocyclic crown-6-bispyromellitimide **5** showing cation recognition selectivity.