

Supporting information

Probing the influence of substrate binding on photocatalytic dehalogenation with a heteroleptic supramolecular square containing PDI photosensitizers as linker

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Characterization

$^1\text{H-NMR}$

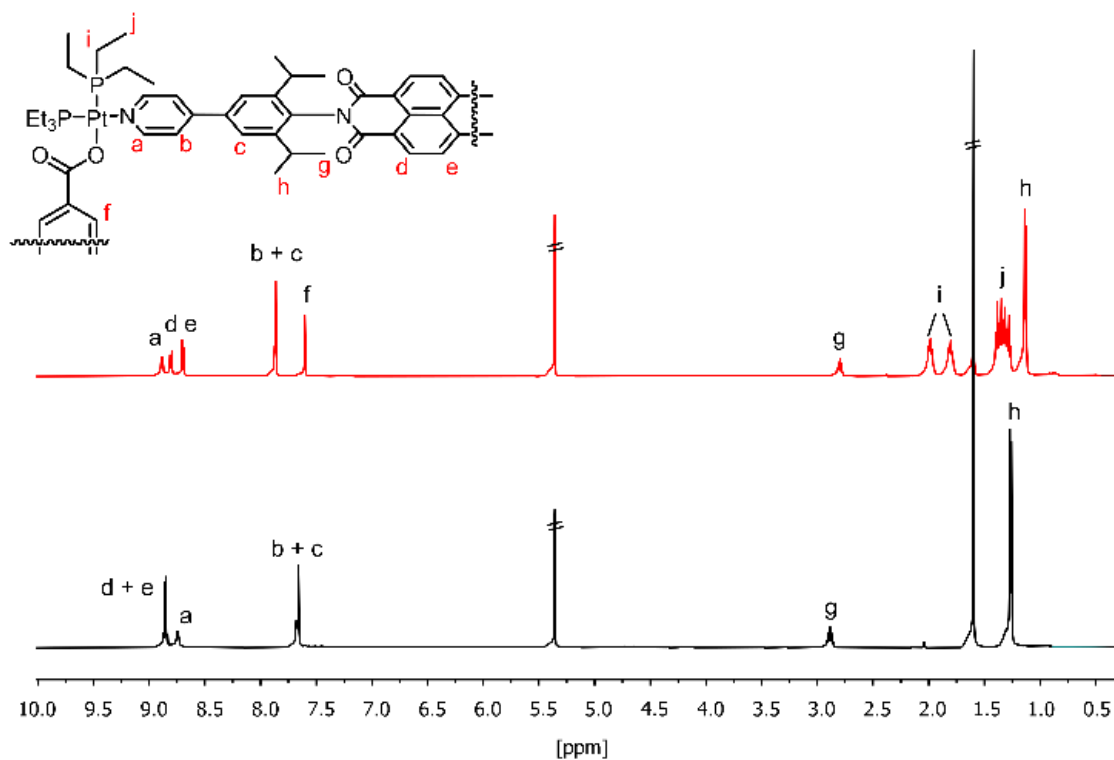


Figure S1. $^1\text{H-NMR}$ spectrum of free **PDI-Py₂** (bottom) and heteroleptic square **2** (top) in CD_3CN .

$^{31}\text{P-NMR}$

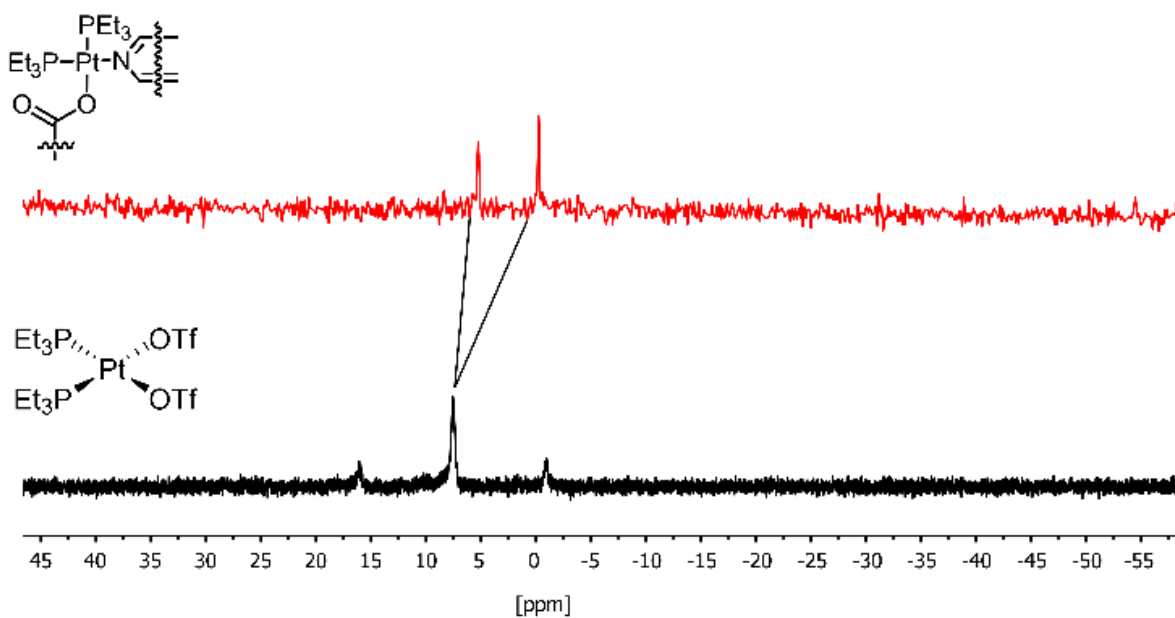


Figure S2. $^{31}\text{P-NMR}$ showing splitting of phosphine chemical shift due to heteroleptic coordination mode in CD_3CN . Shown in black (bottom) is the Pt(II) precursor $\text{cis-}[\text{Pt}(\text{PEt}_3)_2(\text{OTf})_2]$.

¹H-NMR DOSY

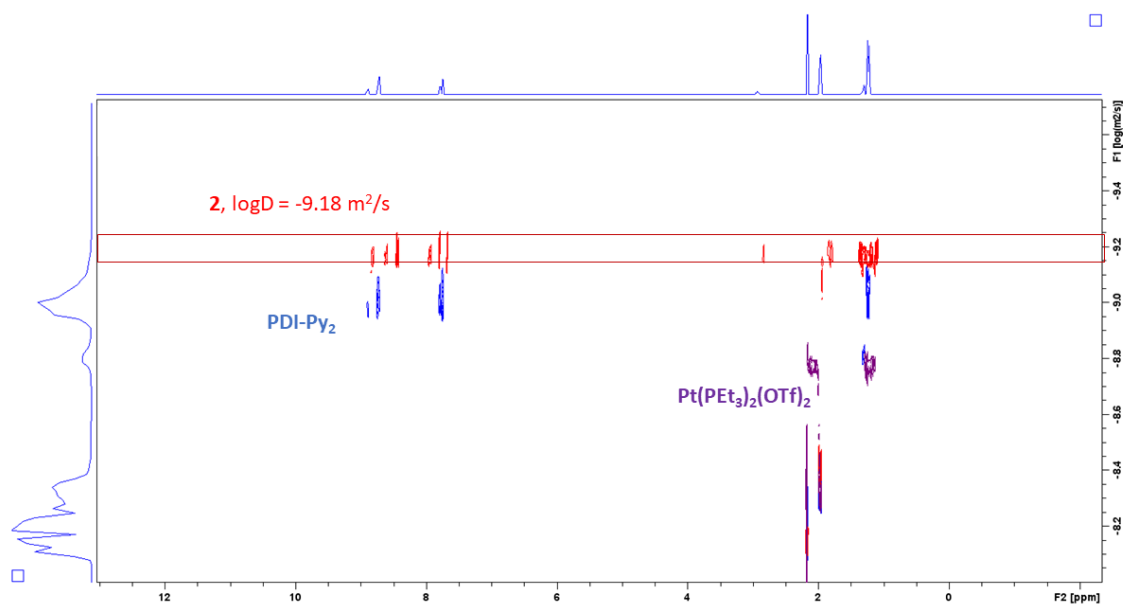


Figure S3. ¹H-DOSY comparing **PDI-Py₂**, *cis*-[Pt(PEt₃)₂(OTf)₂] and heteroleptic square **2** in CD₃CN.

ESI-MS

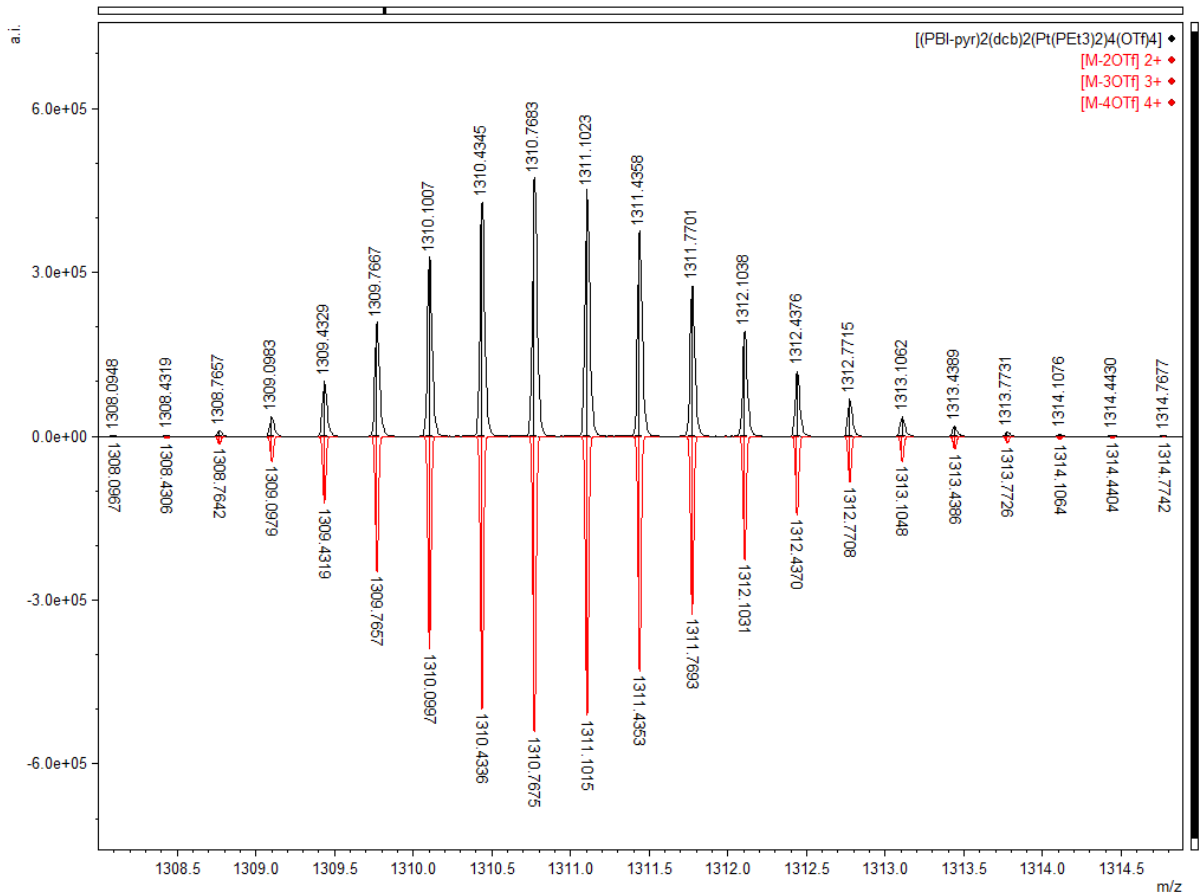
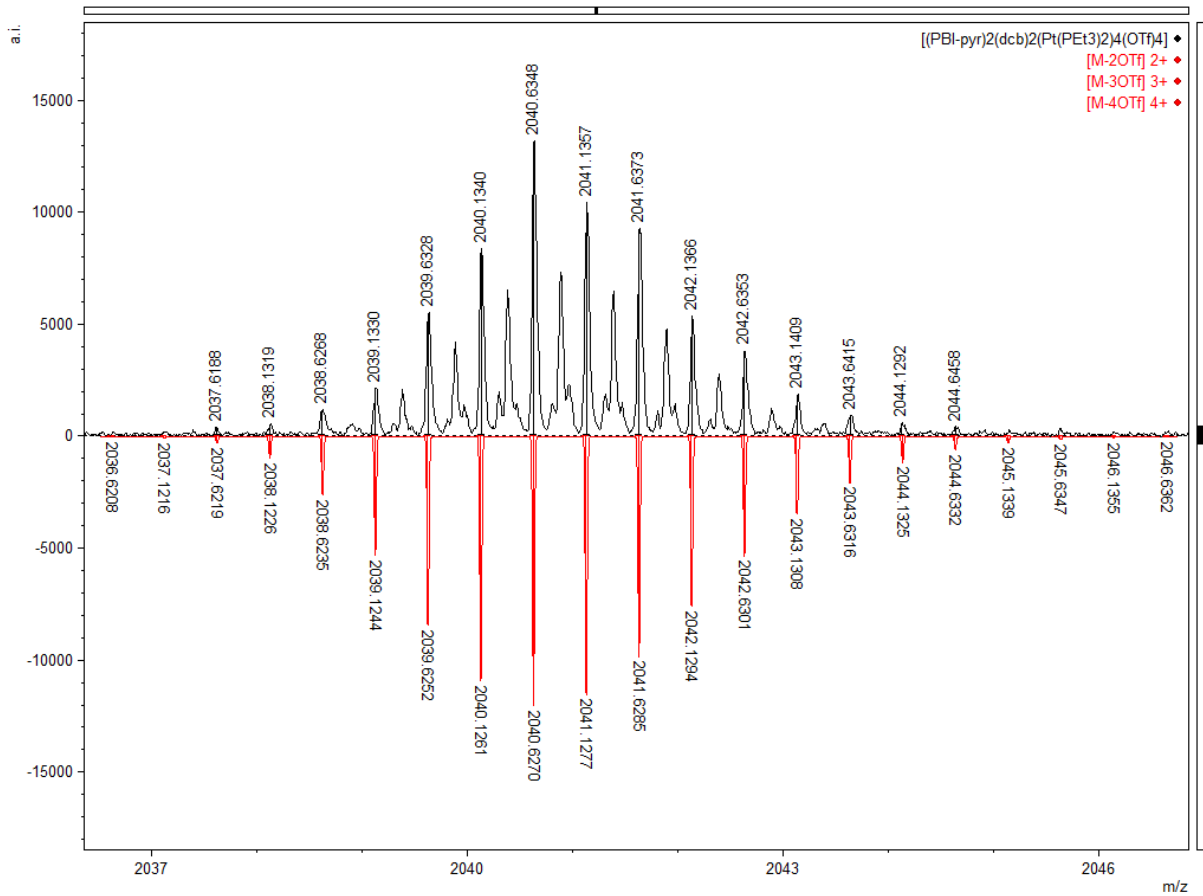


Figure S4. Sections from ESI-MS spectra of 2.

¹H-NMR titrations

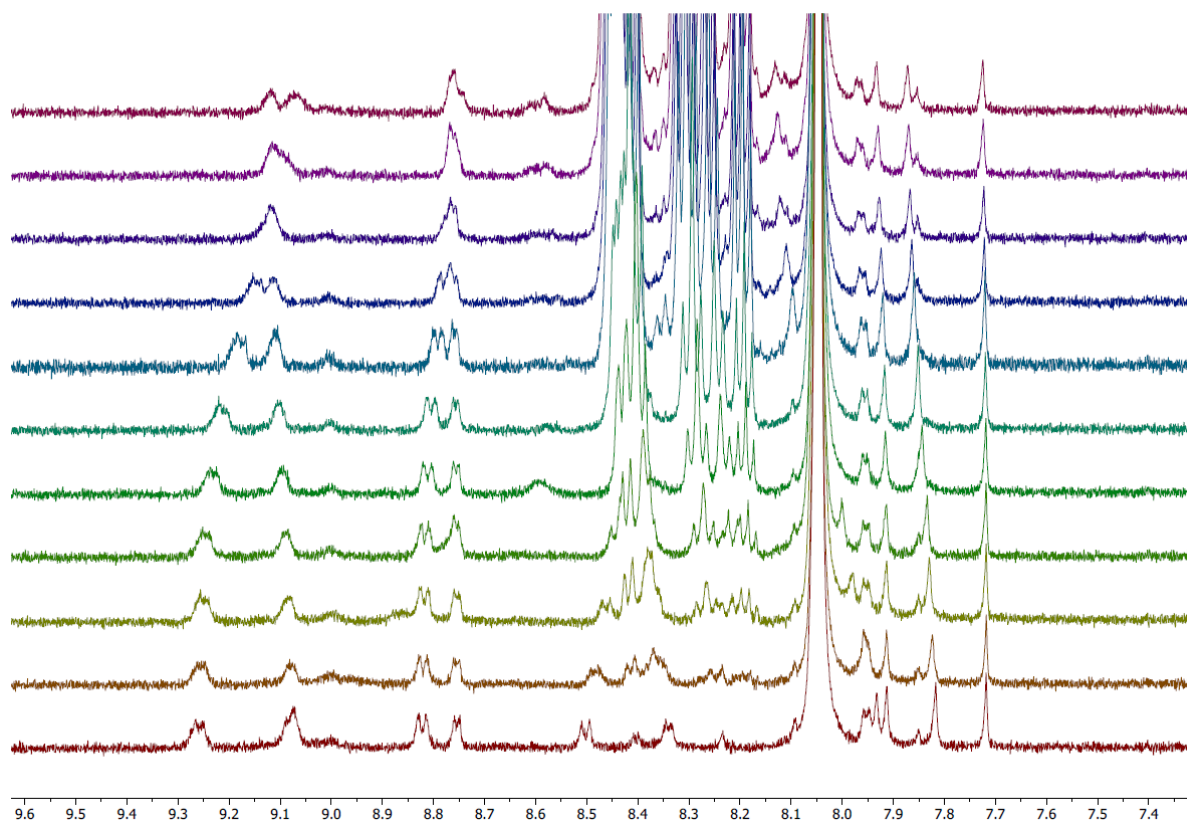


Figure S5. ¹H-NMR titration of 1-bromopyrene **5** to square **2** in CD₃CN..

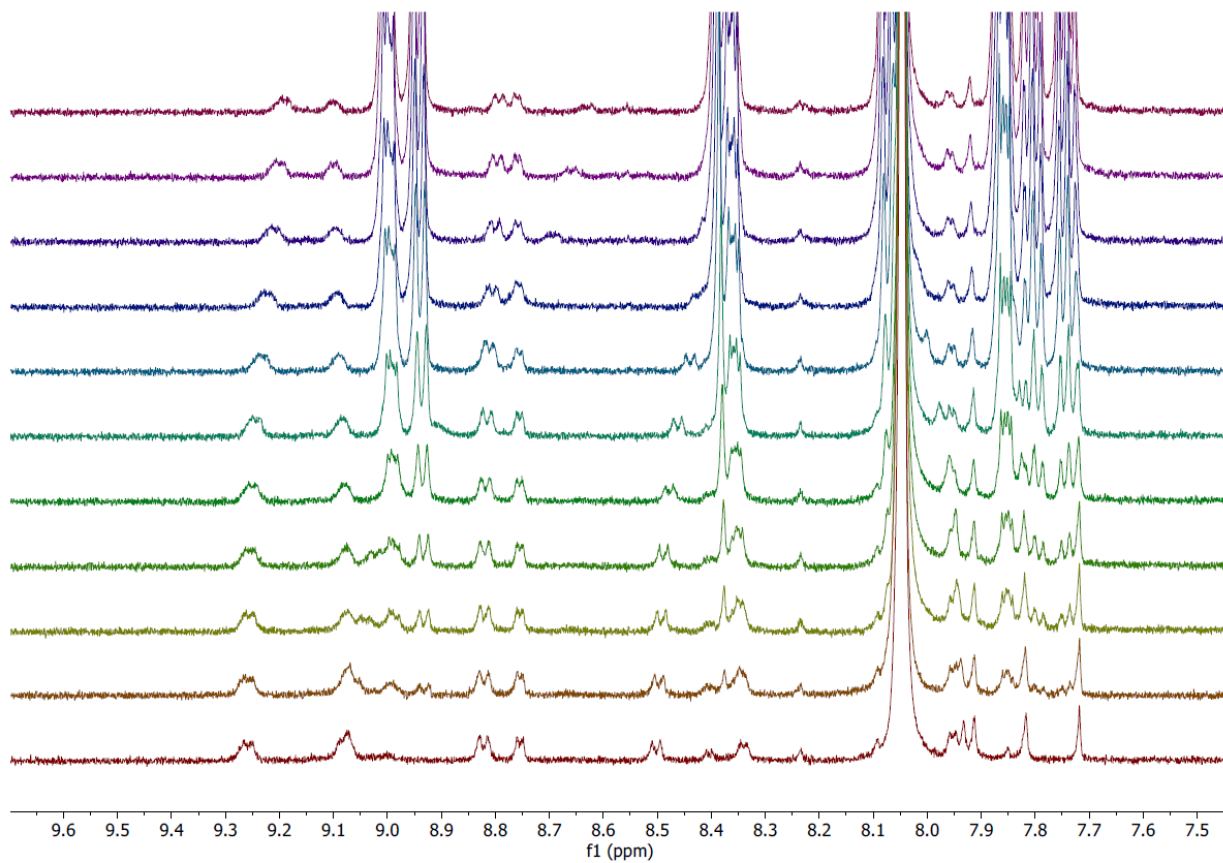


Figure S6. ¹H-NMR titration 9-bromophenanthrene **4** to square **2**.

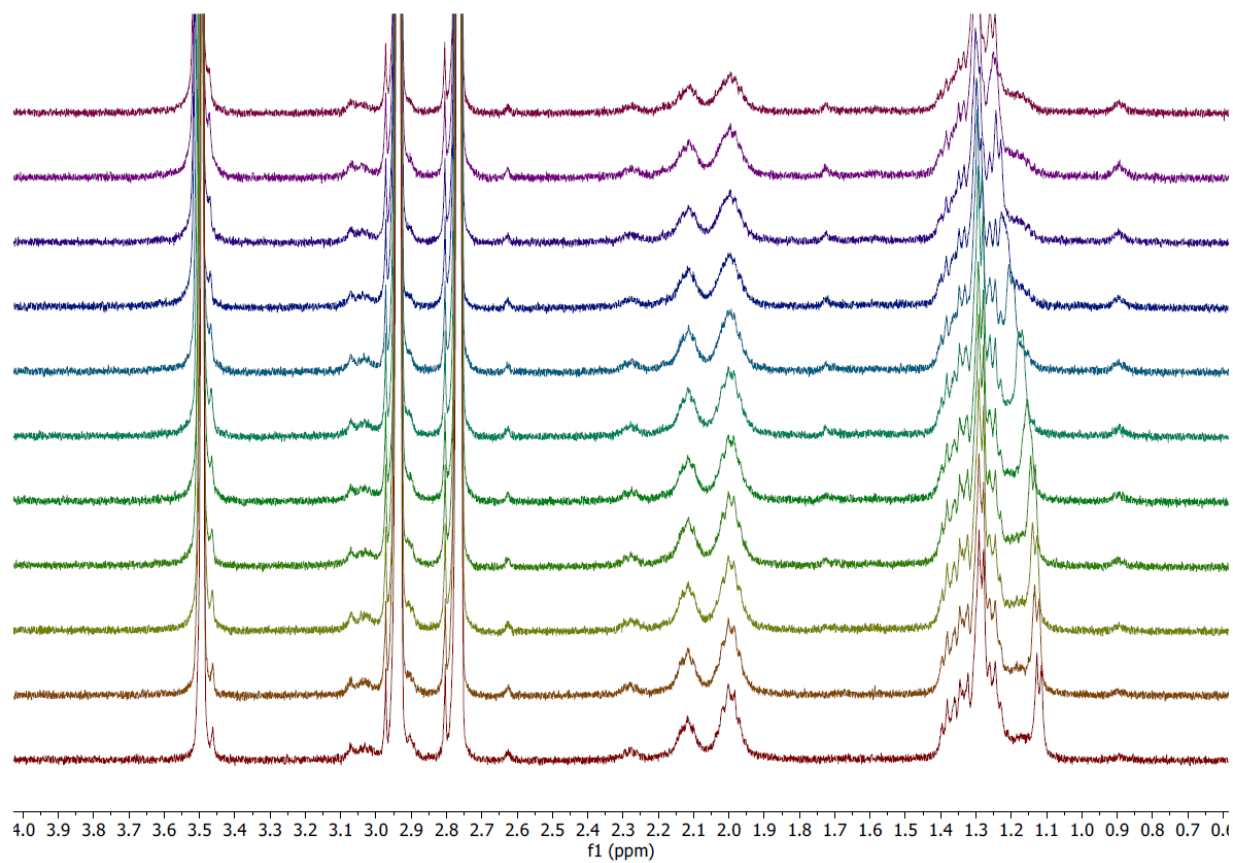


Figure S7. ¹H-NMR titration 9-bromophenanthrene **4** to square **2**.

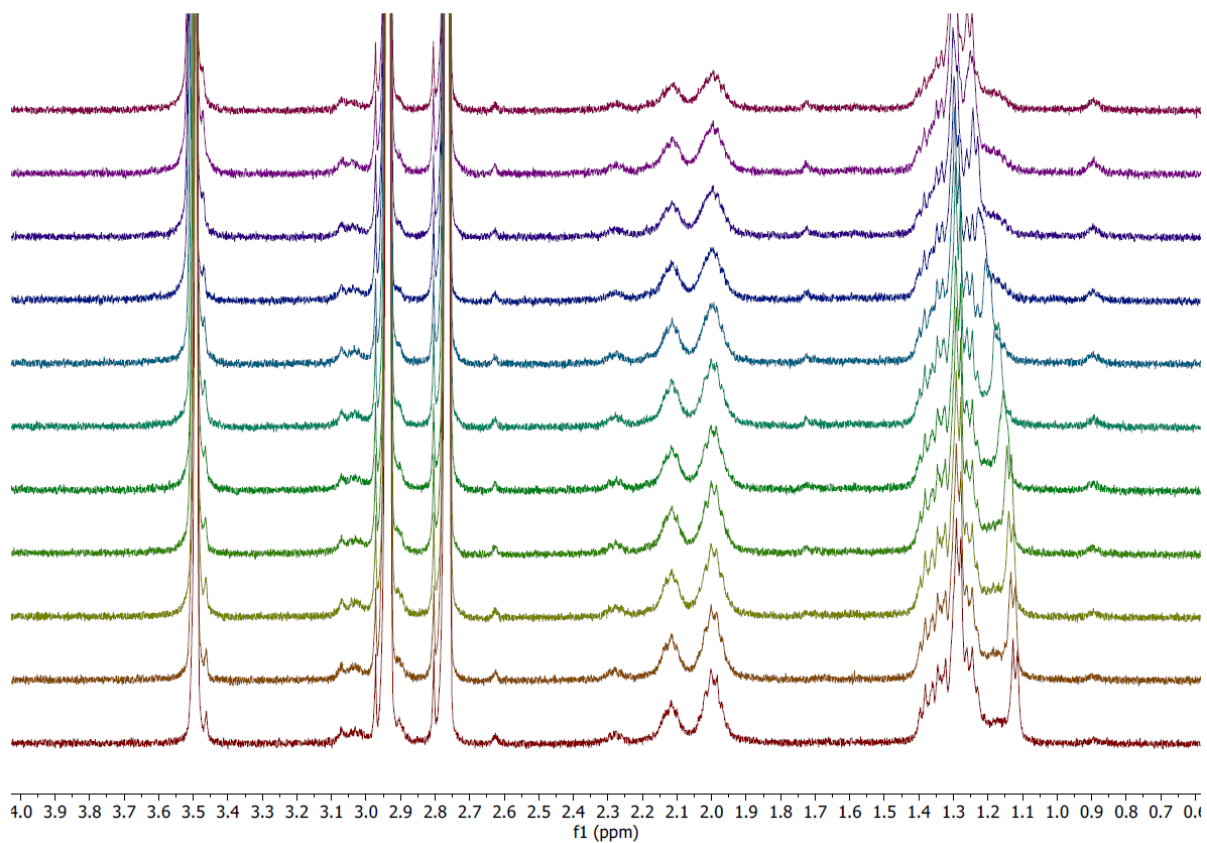


Figure S8. ¹H-NMR titration 4-bromo-benzaldehyde **3** to square **2**.

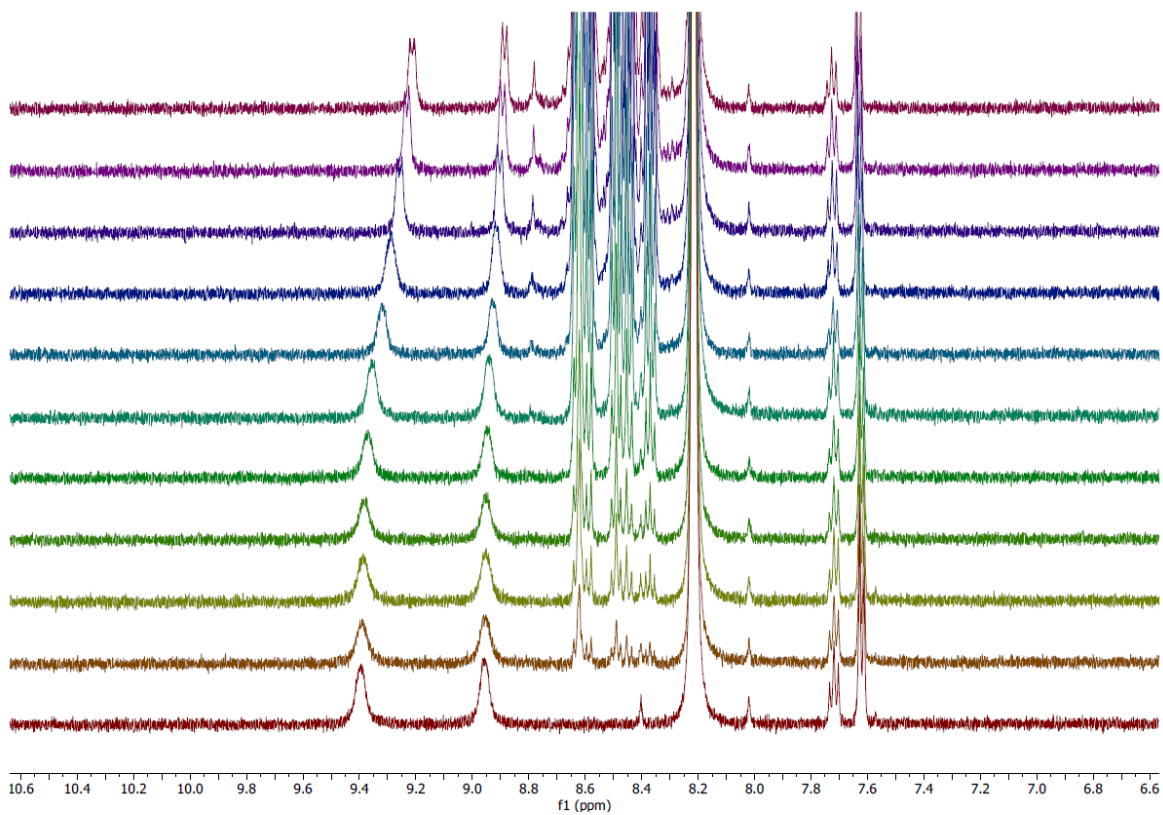


Figure S9. ¹H-NMR titration 1-bromopyrene **5** to free PDI **1**.

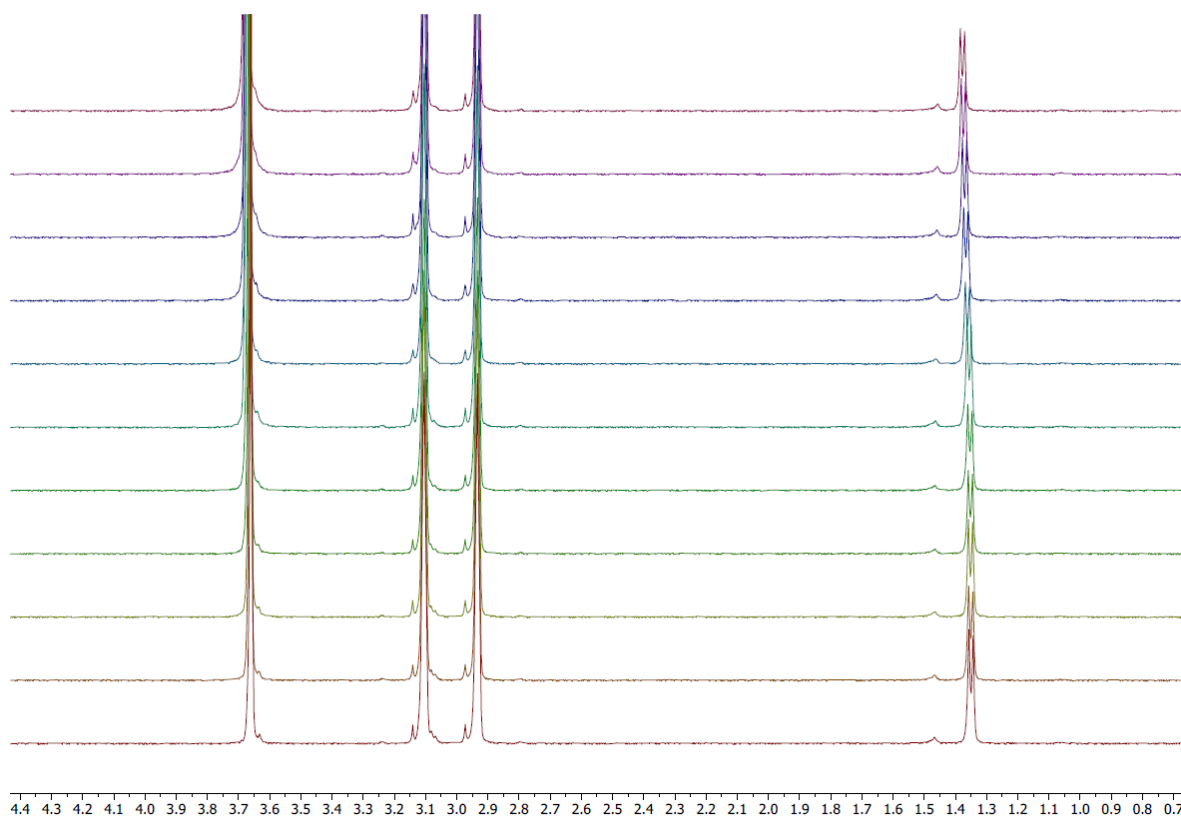


Figure S10. ¹H-NMR titration 1-bromopyrene **5** to free PDI **1**

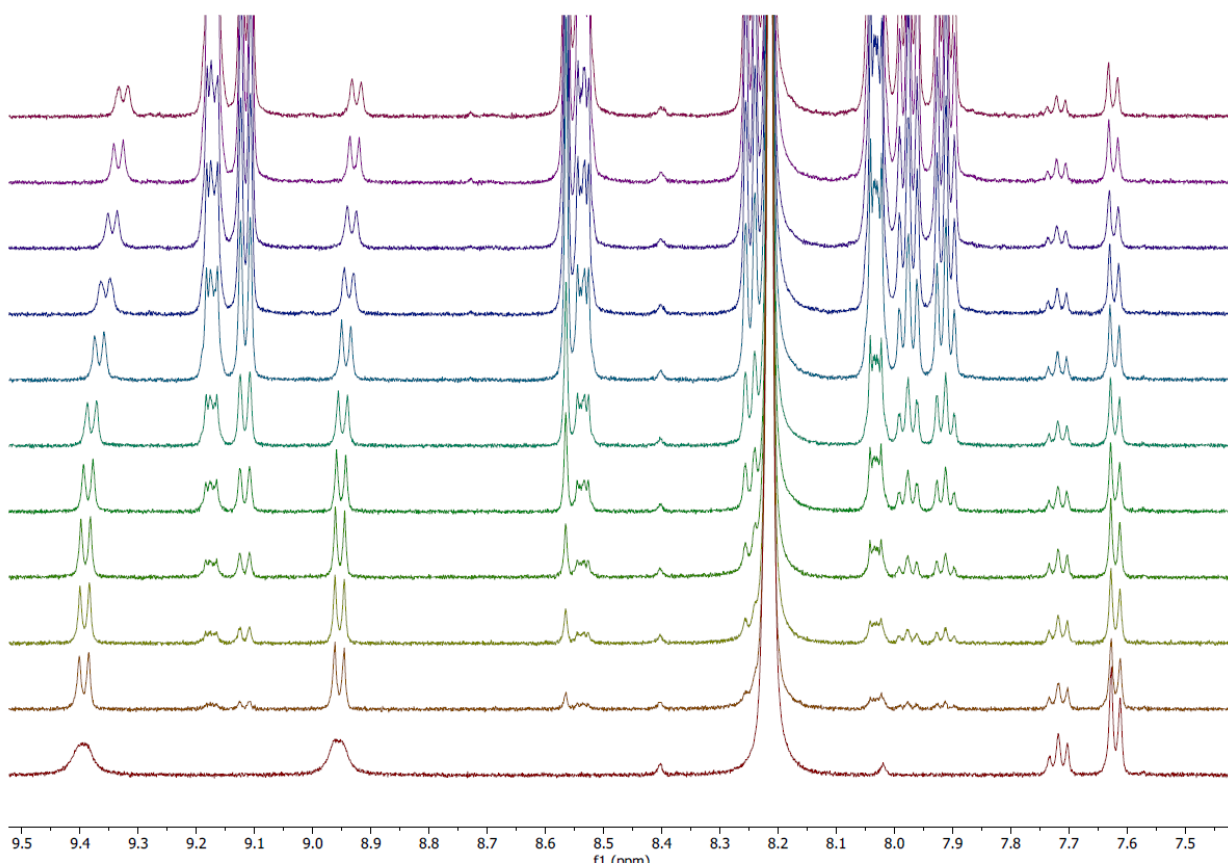


Figure S11. ¹H-NMR titration 9-bromophenanthrene **4** to free PDI **1**

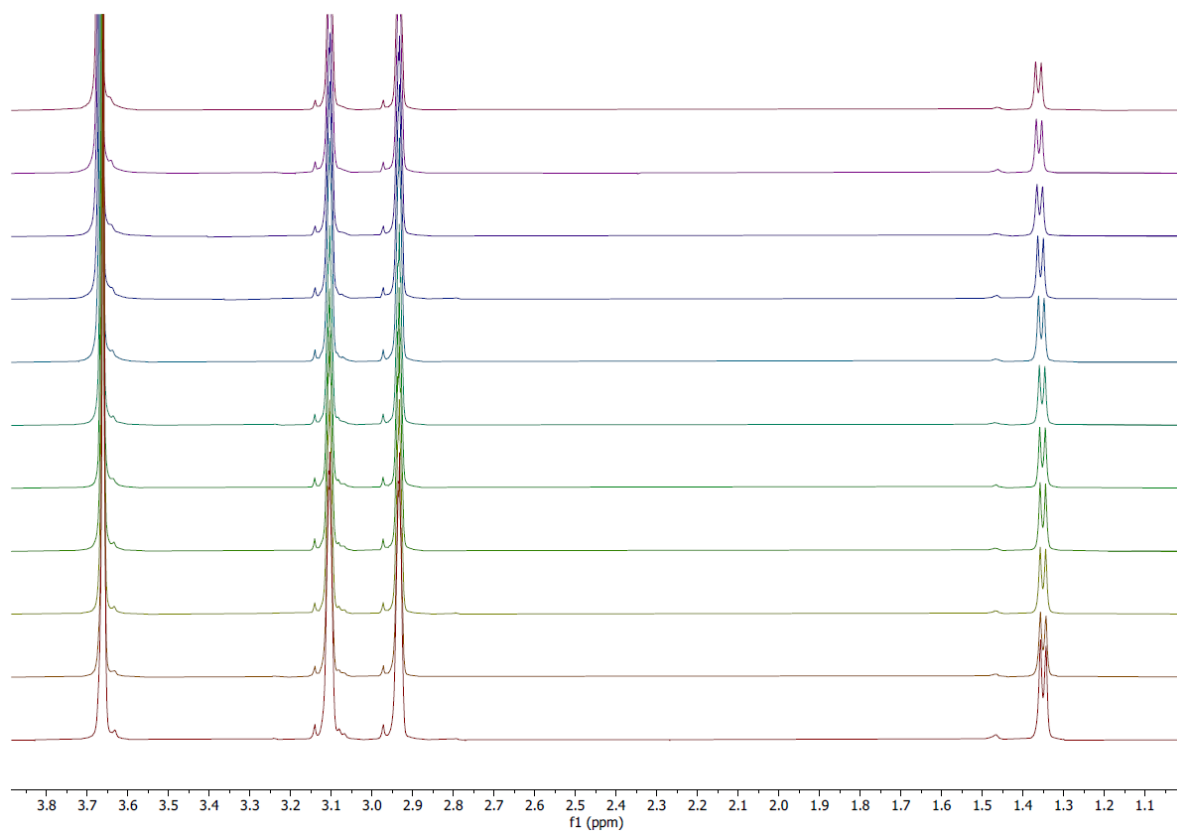


Figure S12. ¹H-NMR titration 9-bromophenanthrene **4** to free PDI **1**