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Supplementary Material

Synthesis and Multiple Functionalities of a Tetraphenylethene-Substituted Tetrapyridinium Salt: Mechanochromic, Cancer Cell Imaging and DNA Marker

Anushri Rananaware, Amanda N. Abraham, Duong Duc La, Vishal Mistry, Ravi Shukla,* and Sheshanath V. Bhosale*

School of Science, RMIT University, GPO BOX 2476, Melbourne, VIC-3001, Australia.

*Email: sheshanath.bhosale@rmit.edu.au; ravi.shukla@rmit.edu.au

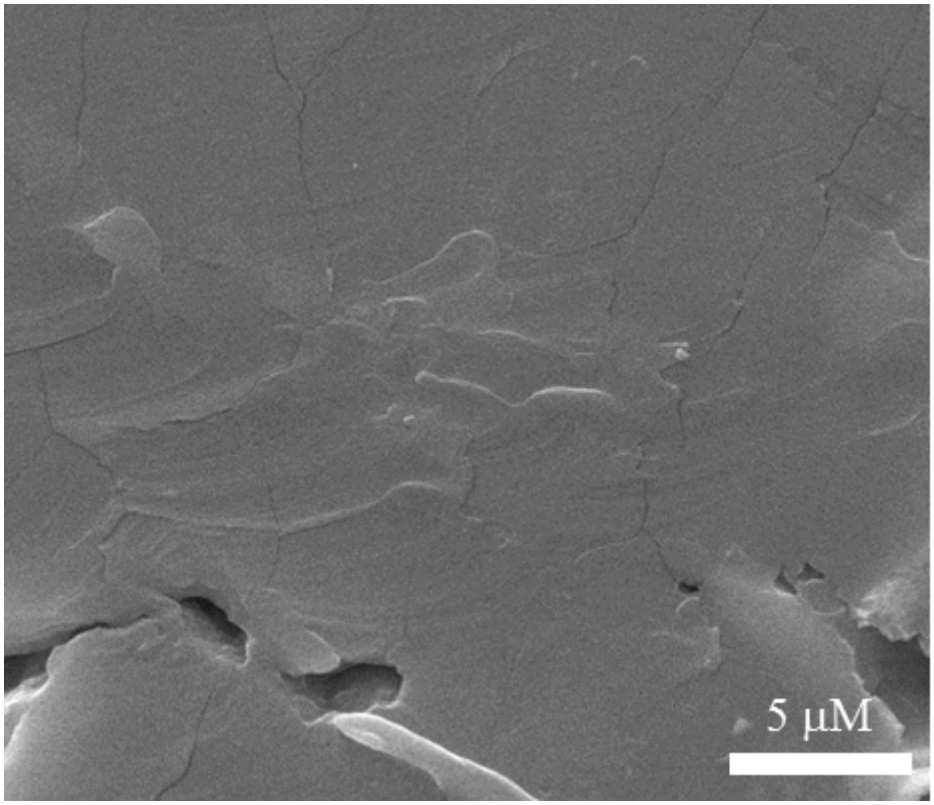
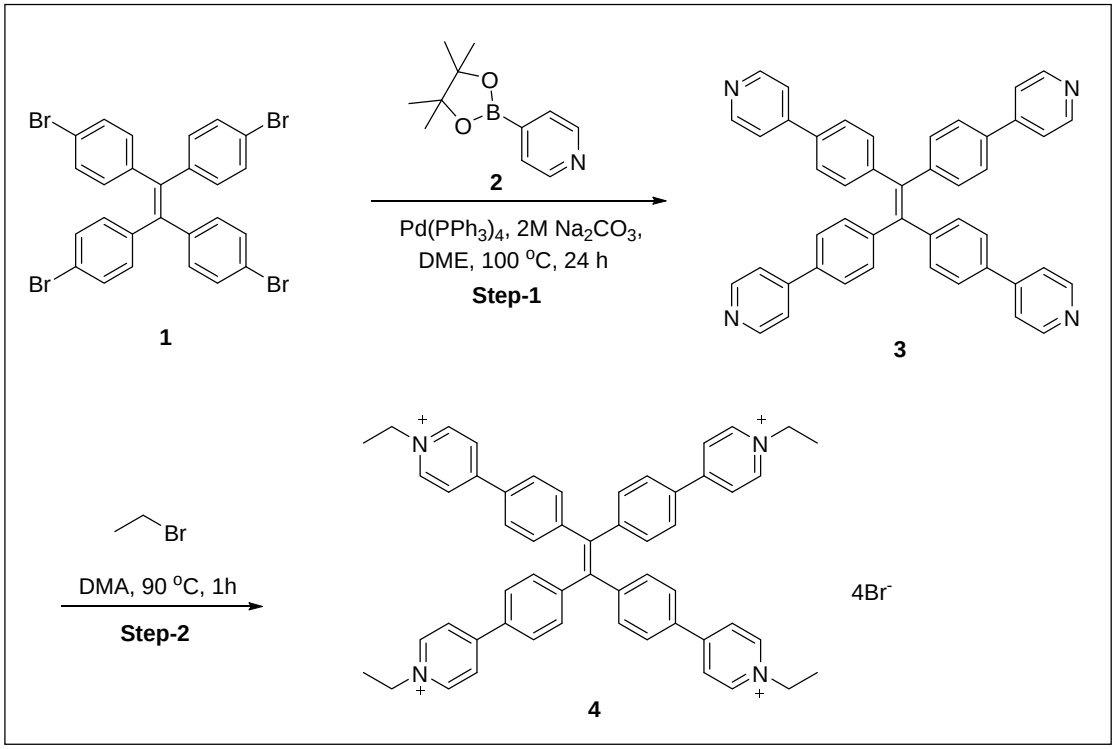


Fig. S1 SEM image of TPy-TPE after heating: the amorphous sate is maintained even when the grounded material was heated at high temperature.

Experimental Procedure for synthesis of TPy-TPE



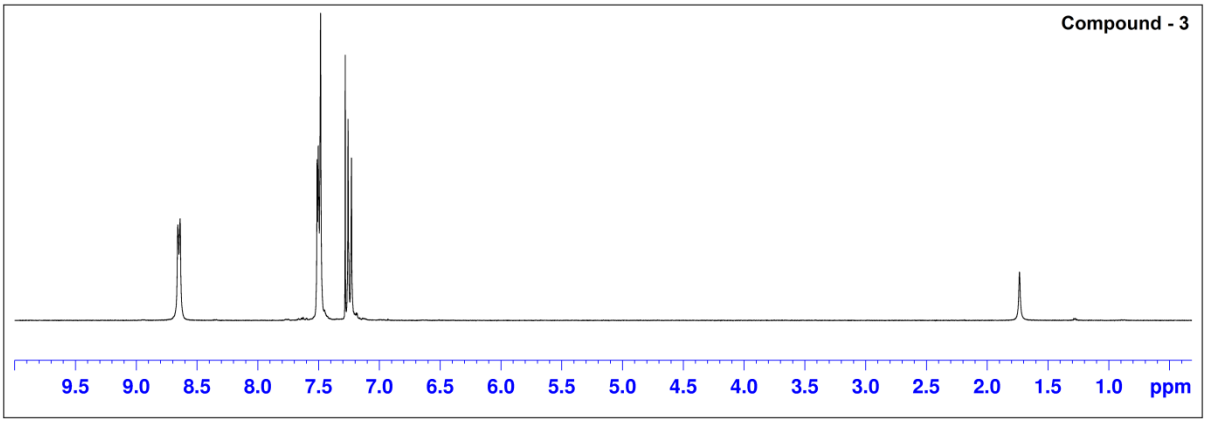
Step-1: Synthesis of 1,1,2,2-tetrakis(4-(pyridin-4-yl)phenyl)ethene, **3.**

To a stirred solution of 1 (1.0 g, 1.553 mmol) in DME (75 mL) was added 2 (1.44 g, 7.024 mmol) and 2M Na_2CO_3 solution (25 mL) and resultant was degassed for 15 min using argon atmosphere. Then to it was added Pd-tetrakis (0.36 g, 0.310 mmol) and reaction mixture was allowed to reflux for 24 h. Reaction completion was checked by TLC analysis. After completion, reaction was quenched with water and extracted with DCM (3X40 mL). Organic layer was washed with water, dried over sodium sulphate and evaporated. Crude residue obtained was purified by flash column chromatography to give **3** as a pale yellow solid (0.7 g, 70.4 %); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.65 (d, *J* = 5.7 Hz, 8H), 7.50 (dd, *J* = 5.0, 3.5 Hz, 16H), 7.22 (t, 8H); ^{13}C NMR (300 MHz, $CDCl_3$): δ 150.32, 147.44, 144.03, 140.79, 136.49, 132.13, 126.54, 121.27; HRMS (MALDI-TOF, m/z): [M^+] calcd for $C_{46}H_{32}N_4$: 640.26, found: 640.89 [M^+].

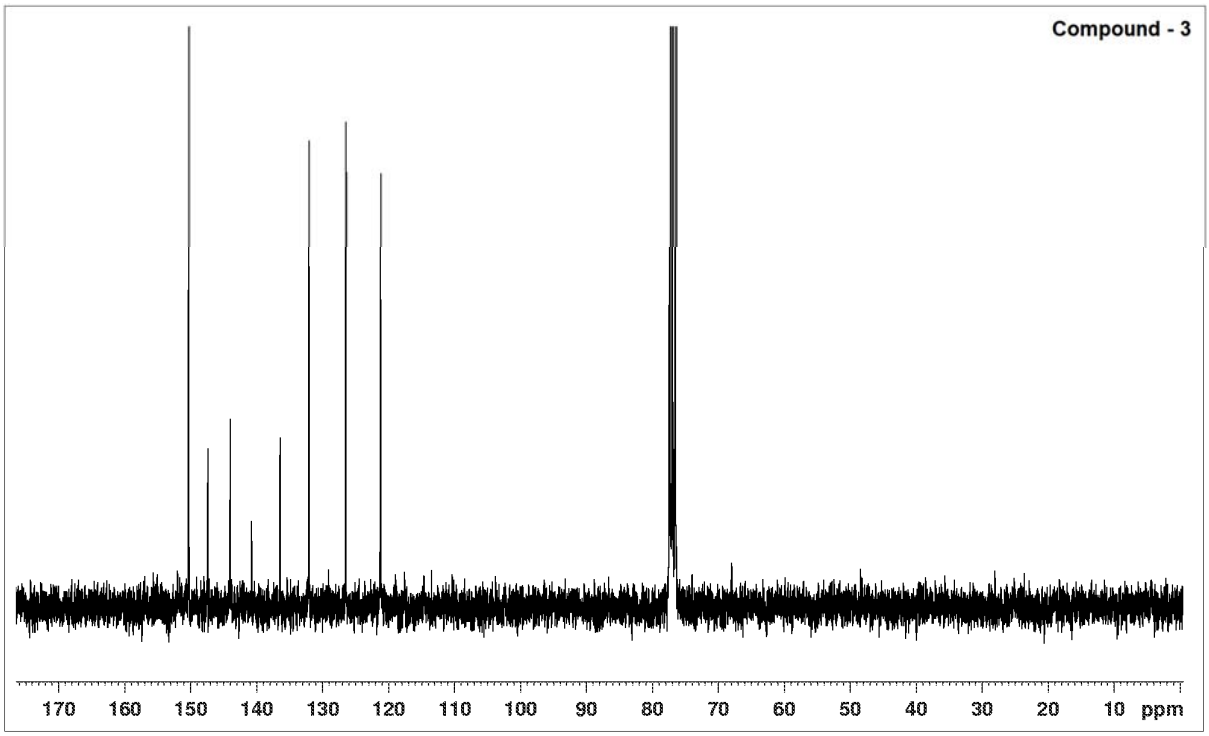
Step-2: Synthesis of 4,4',4",4'"-(ethene-1,1,2,2-tetrayltetrakis(benzene-4,1-diyl))tetrakis(1-ethylpyridin-1-ium), **4.**

A stirred mixture of 3 (0.050 g, 0.0781 mmol), 1-bromoethane (0.051 g, 0.4685 mmol) in DMA (2 mL) was allowed to heat at 90 ^{o}C for 1h. Solid precipitates out in reaction mixture. Reaction mixture was allowed to cool at room temperature and then precipitates was filtered, washed with DCM to remove solvent and excess SM. Dried completely under vacuum to give **4** as a yellow solid (0.056 g, 94.9 %); ^{1}H NMR (300 MHz, MeOD): δ 8.96 (d, *J* = 7.0 Hz, 8H), 8.38 (d, *J* = 6.9 Hz, 8H), 7.92 (d, *J* = 8.4 Hz, 8H), 7.45 (d, *J* = 8.4 Hz, 8H), 4.66 (q, 8H), 1.68 (t, 12H); ^{13}C NMR (300 MHz, MeOD): δ 156.80, 147.75, 145.61, 143.20, 134.29, 133.85, 129.22, 126.02, 57.60, 16.69; HRMS (MALDI-TOF, m/z): [M^{+}] calcd for $C_{54}H_{5}N_{4}$: 756.42, found: 756.45.

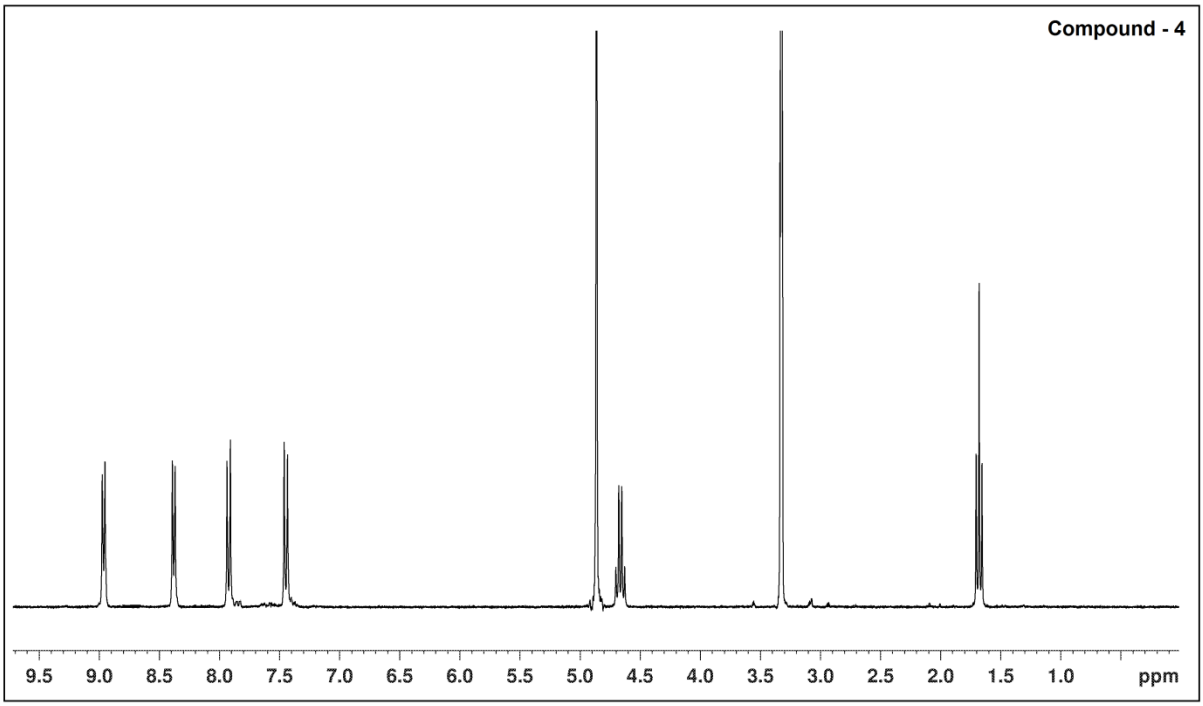
^{1}HNMR of **3**



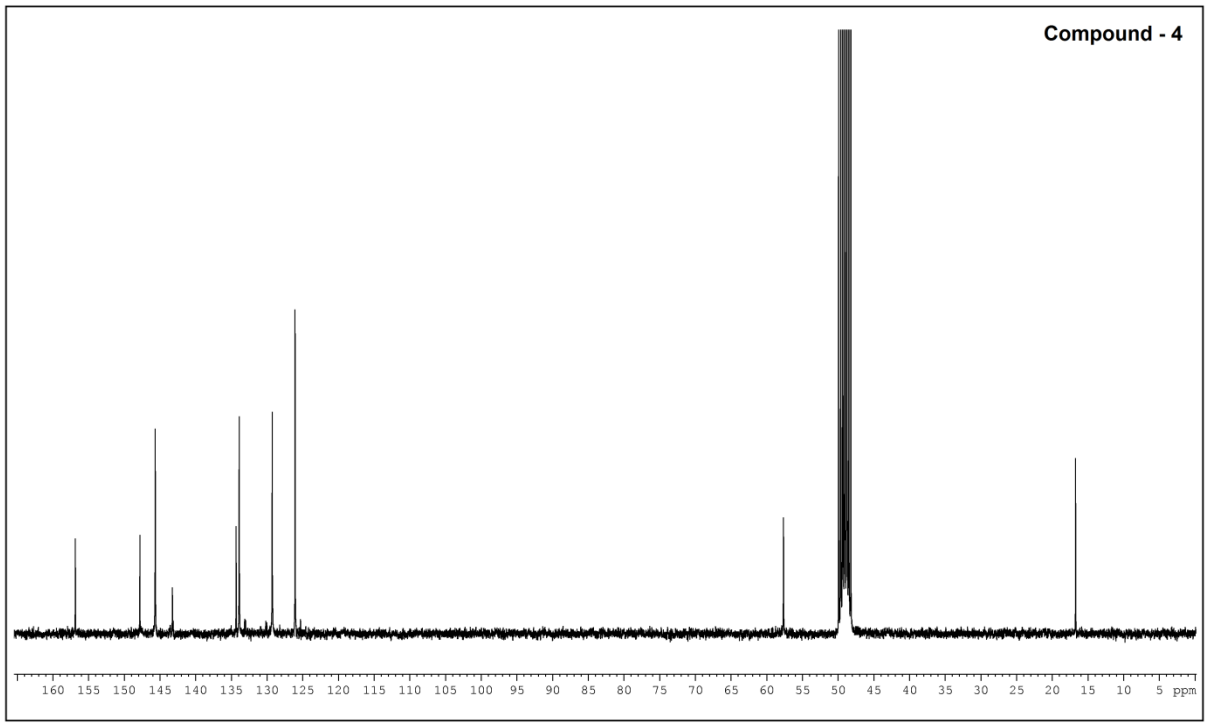
^{13}CNMR of **3**



^{1}HNMR of **4**



^{13}CNMR of **4**



S1 T. S. Reddy, H. Kulhari, V. G. Reddy, A.V. Subba Rao, V. Bansal, A. Kamal, and R. Shukla, *Org. Biomol. Chem.*, 2015, **13**, 10136.