RSC Advances

Electronic Supplementary Material

Removal of Endocrine Disruptor Di-(2-Ethylhexyl) Phthalate by Modified Polythiophene Coated Magnetic Nanoparticles: Characterization, Adsorption Isotherm, Kinetic Study, Thermodynamics

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Preparation of 3-(6-bromohexylthiophene) **(S1)**

Compound **(1)** was prepared from 3-bromothiophene according to the procedure reported in [27, 28]. 3-bromothiophene (2 mL, 21.3 mmol) was added to the dry, degassed hexane (50 mL). The reaction was started by cooling the flask to -78^{o}C . *n*-butylithium in hexane (2.0 M, 10.16 mL) was injected into the reaction flask using air tight gas syringes and stirred for 10 minutes. THF (5 mL) was injected drop-wise for 15 minutes, and continuously stirred for 1 hour, resulting in a white precipitate and clear supernatant liquid. The supernatant liquid was removed and exchanged with hexane/THF (10:1 v/v, 55 mL). 1,6-dibromohexanes (32.7 mL, 213 mmol) was added and stirred for 2 hours. The reaction was stopped with the addition of saturated $NaHCO_3$ (50 mL) and diethyl ether (100 mL) were added to separate the organic and inorganic layers. The organic layer was washed with water (100 mL), brine solution (100 mL), dried with magnesium sulfate anhydrous, treated with decolorizing charcoal, filtered, and concentrated in vacuum to produce orange oil. The excess 1,6-dibromohexane was removed by vacuum distillation (0.04 torr, 55 ^{o}C), and purified silica gel column chromatography system (ethyl acetate/hexane, 1/99 to 5/95 v/v) was used to obtain an oily product. Yield: 52%. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 1.38-1.46 (4H, m), 1.62 (2H, m), 2.59 (2H, t), 3.35 (2H, t), 6.86 (2H, m), 7.15–7.17 (1H, m). FT-IR (cm^{-1}): 3005.47, 2959.71, 2933.71, 2857.26, 1551.4, 1459.60, 1437.01, 1420, 1246.85, 1216, 1031.13, 859.61, 773.32, 643.35 and 559.77.

Preparation of 4-((phenylimino)methyl)phenol **(S2)**

4-hydroxybenzaldehyde (122 mg, 10 mmol) was added to (112 mg, 10 mmol) 2-aminobenzenethiol in 50-mL of ethanol. The mixture was refluxed for 3 hours. Yellow crystal was obtained after recrystallization with ethanol, resulting in a yield of 95%. m.p: 203.8–205.5 ^{o}C.^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 6.7 (2H-Ar), 7.5 (2H-Ar), 7.2 (2H-Ar), 7.8 (H-Ar-S), 8.9 (H-C=N), 9.7 (OH). FT-IR (cm^{-1}): 1609, 1588 & 1504, 749, 3411.

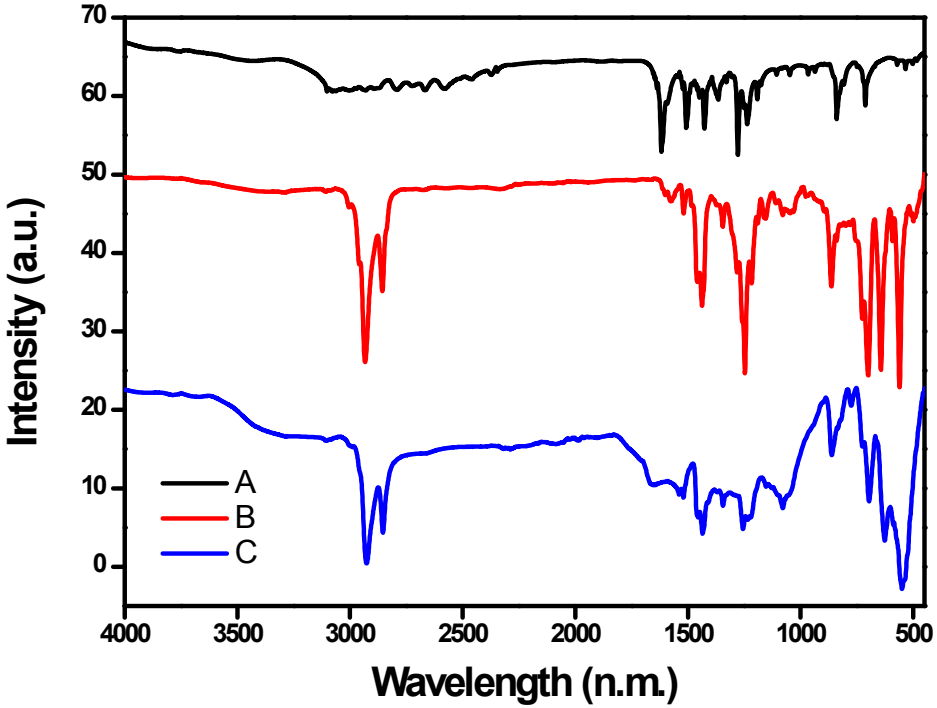

Figure S1: FT-IR for compounds (**A**) 4-((phenylimino)methyl)phenol, (**B**) 3-bromohexylthiophene and (**C**) N-(4-(6-(thiophen-3-yl)hexyloxy)benzylidene)benzenamine.

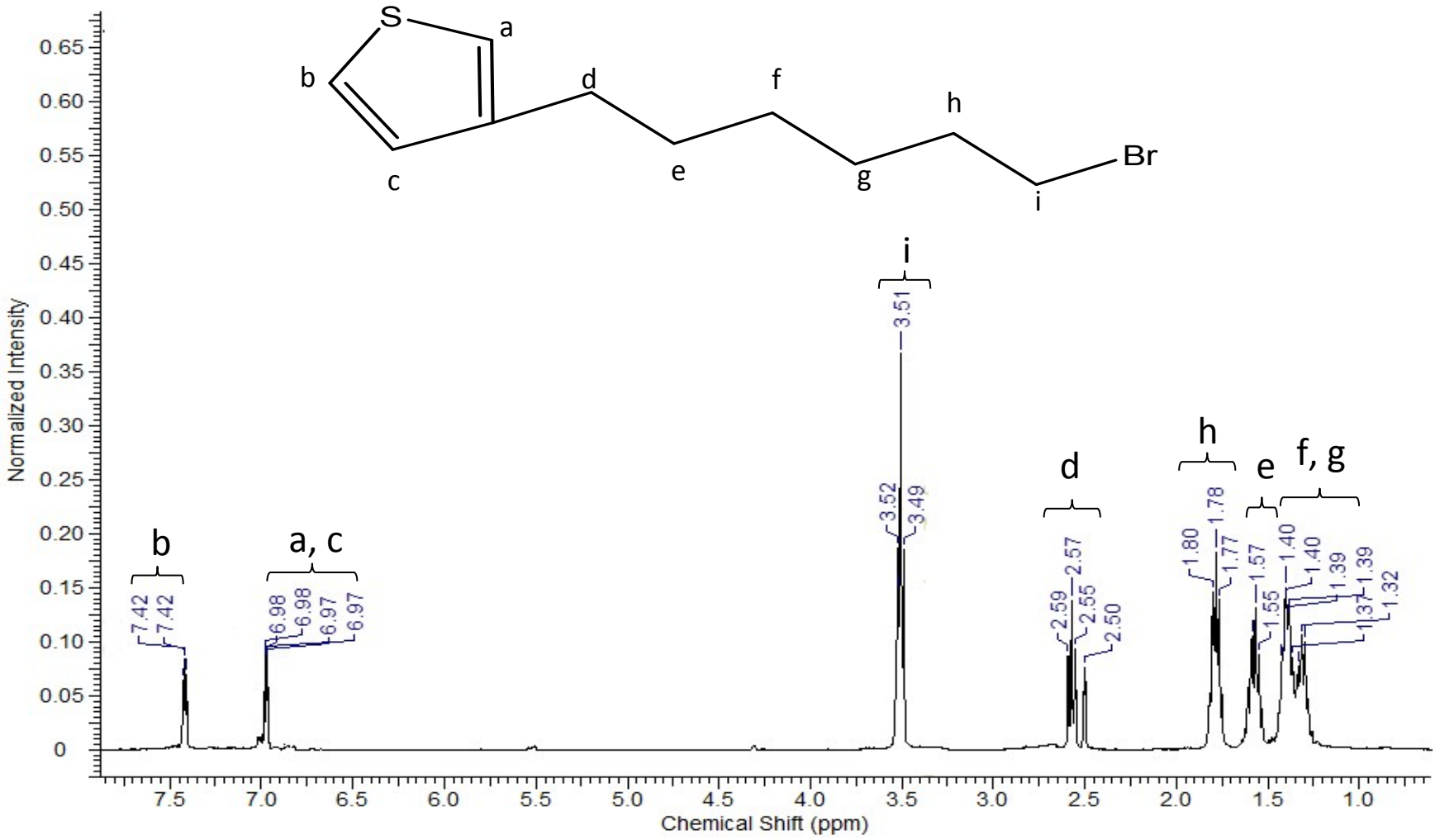

Figure S2: ^{1}H NMR for 3-bromohexylthiophene (1)

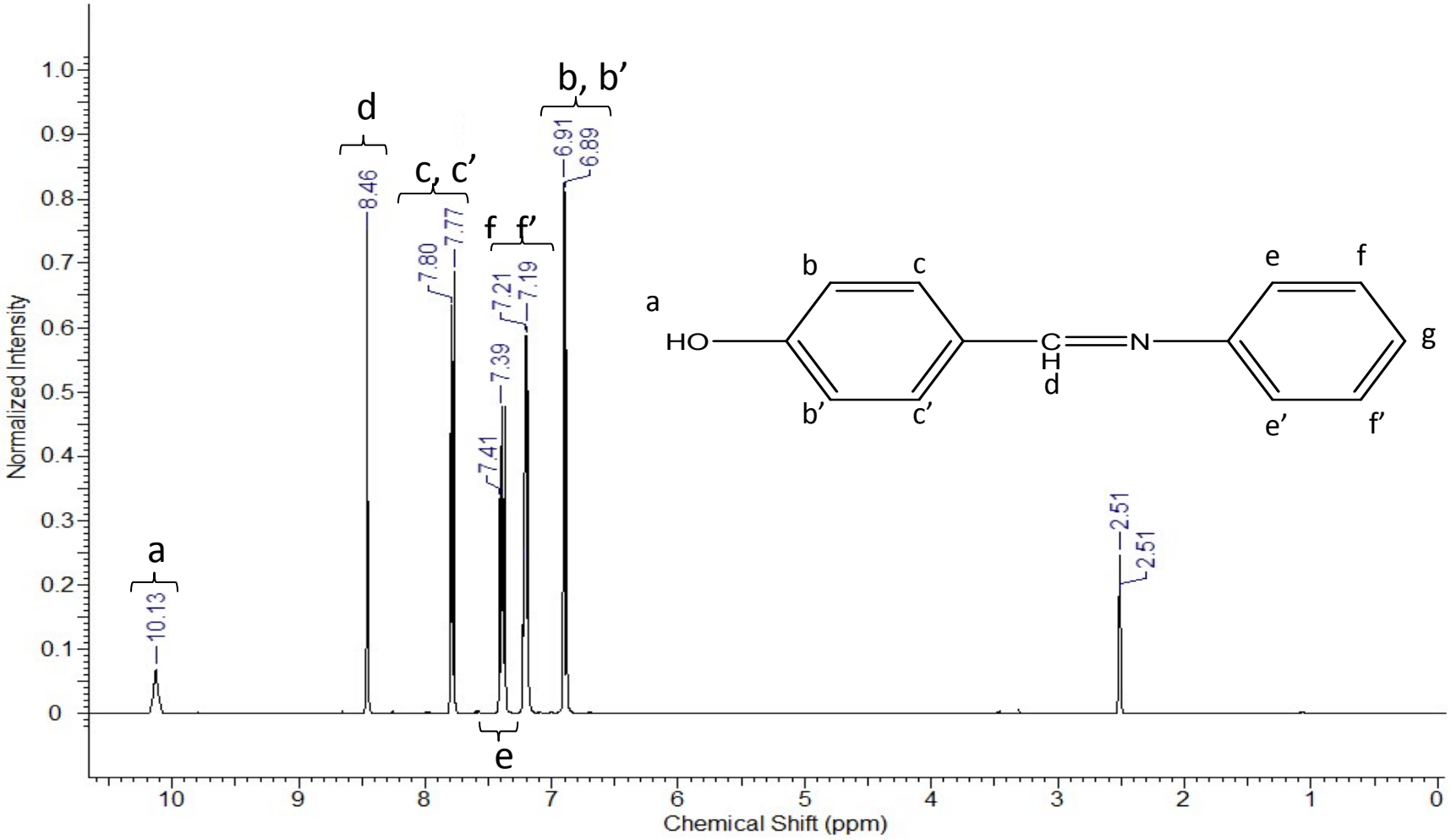

Figure S3: ^{1}H NMR for 4-((phenylimino)methyl)phenol (2)

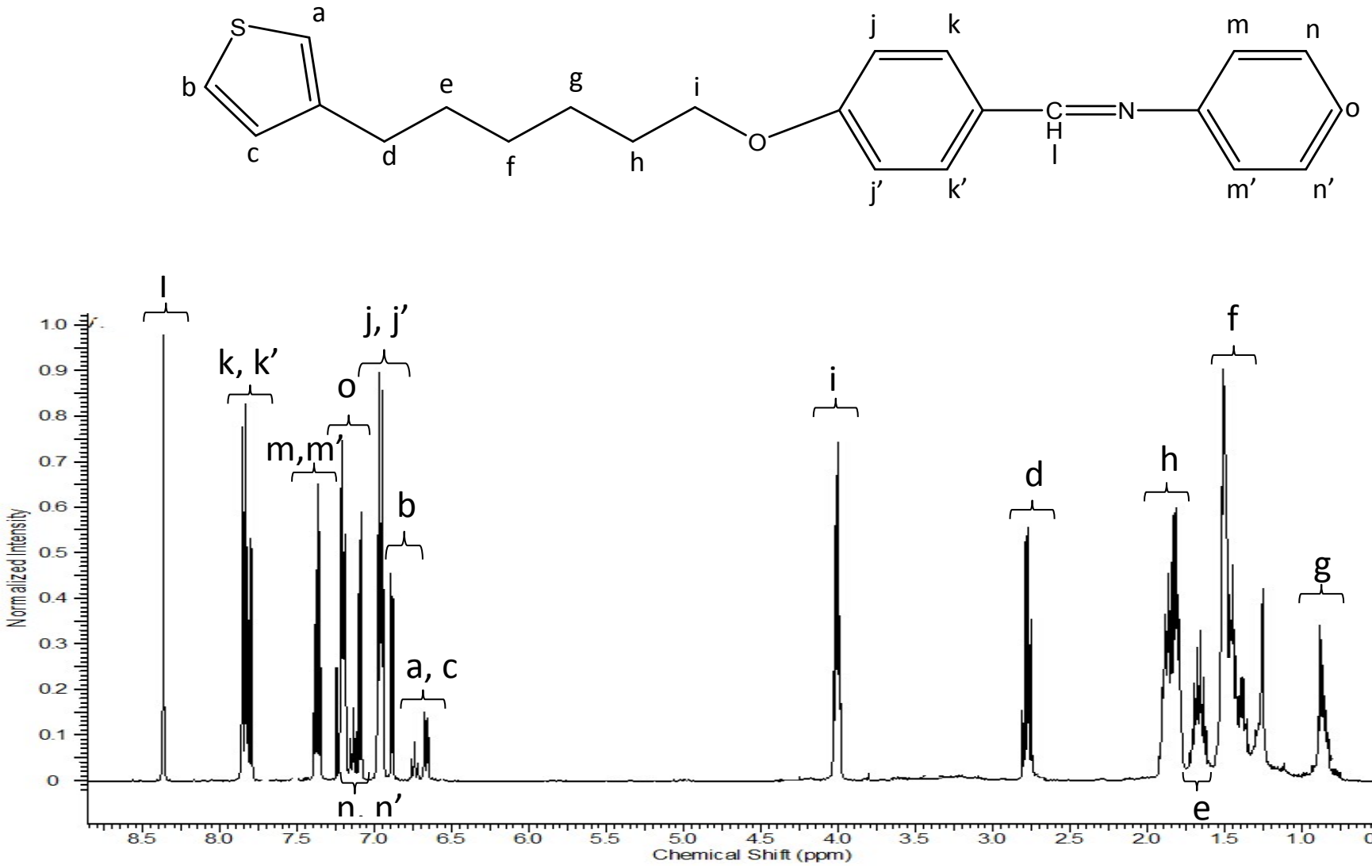

Figure S4: ^{1}H NMR for N-(4-(6-(thiophen-3-yl)hexyloxy)benzylidene)benzenamine(3)

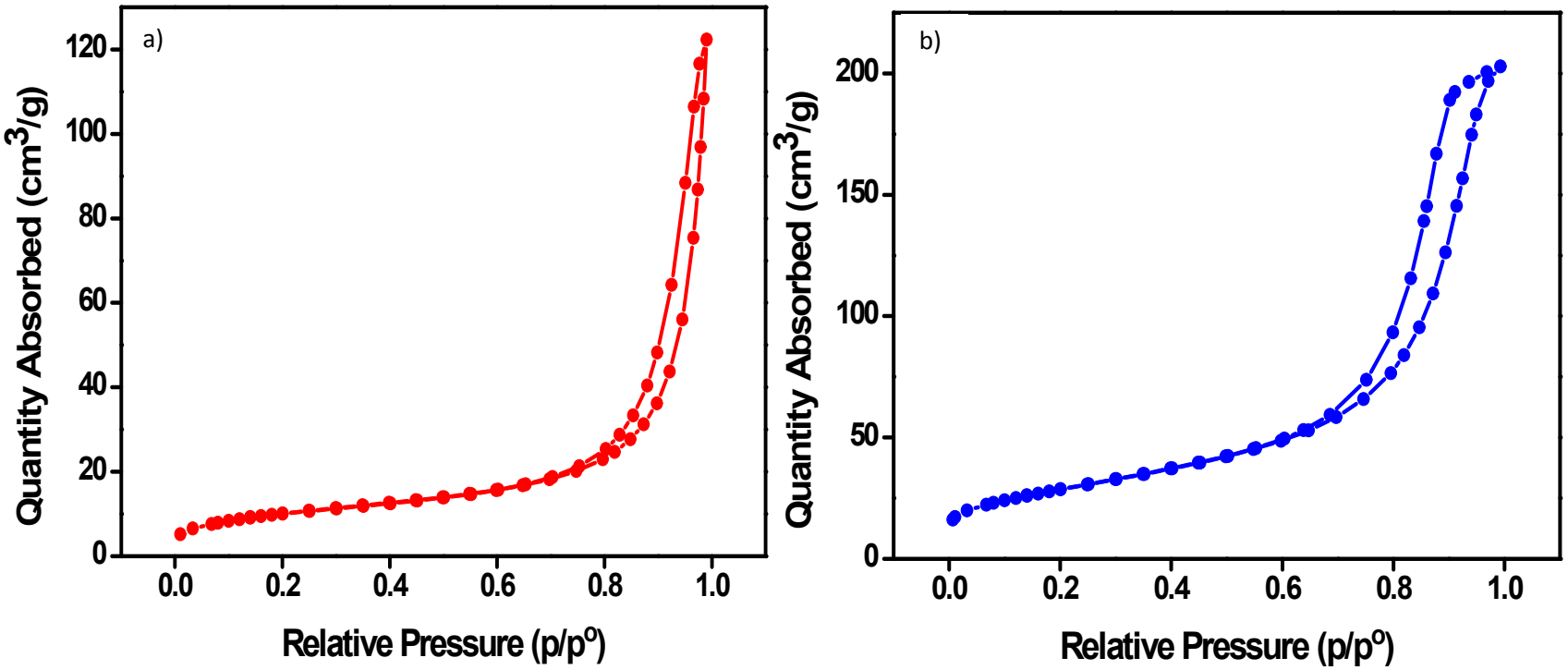

Figure S5: BET profile (a) Fe_3O_4 and (b) Fe_3O_4@P3TArH

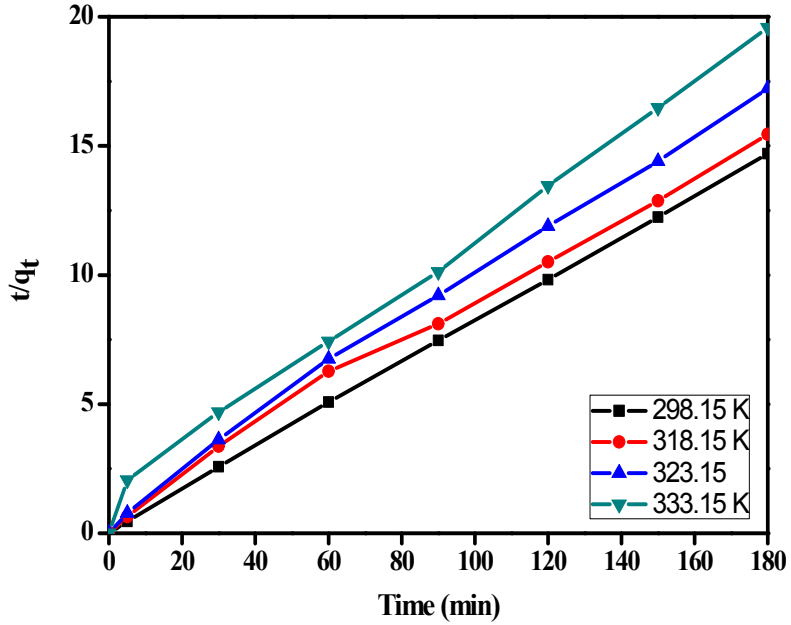

Figure S6: Pseudo second-order kinetics model

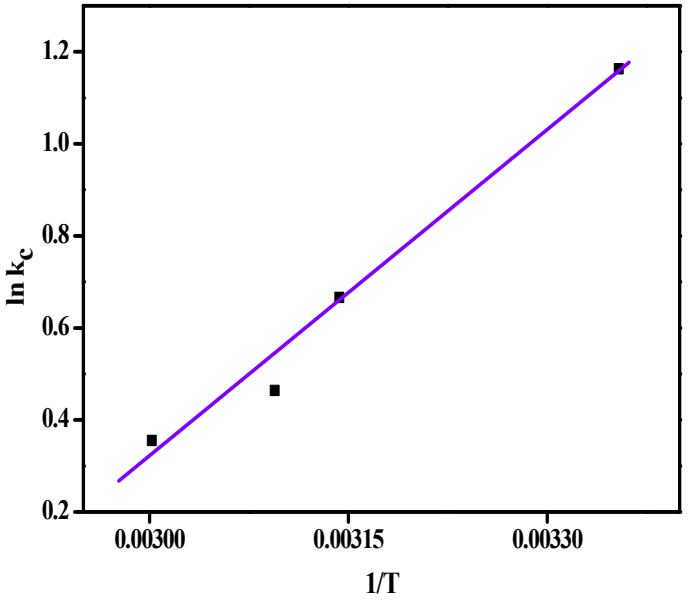

Figure S7: Van't Hoff function

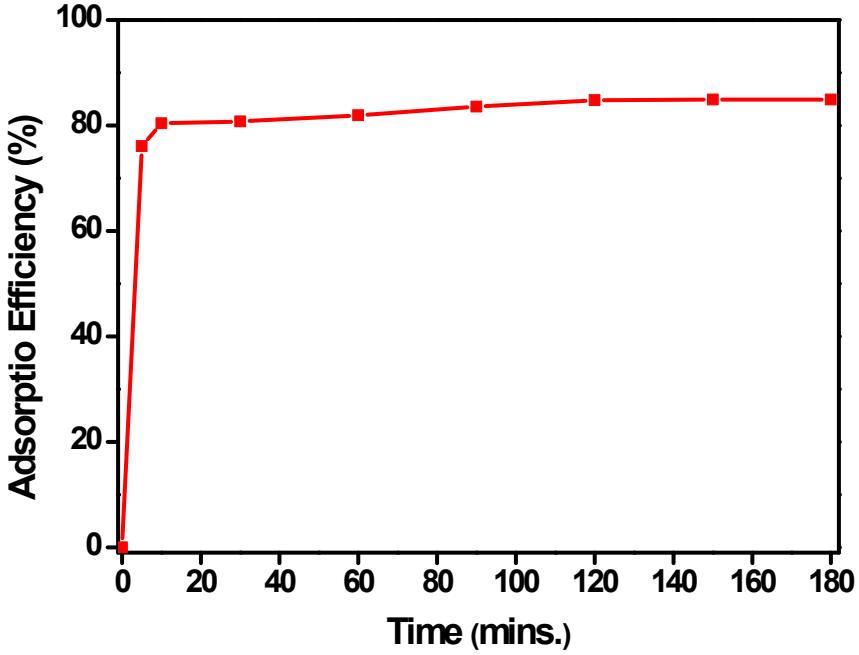

Figure S8: Adsorption Efficiency over time

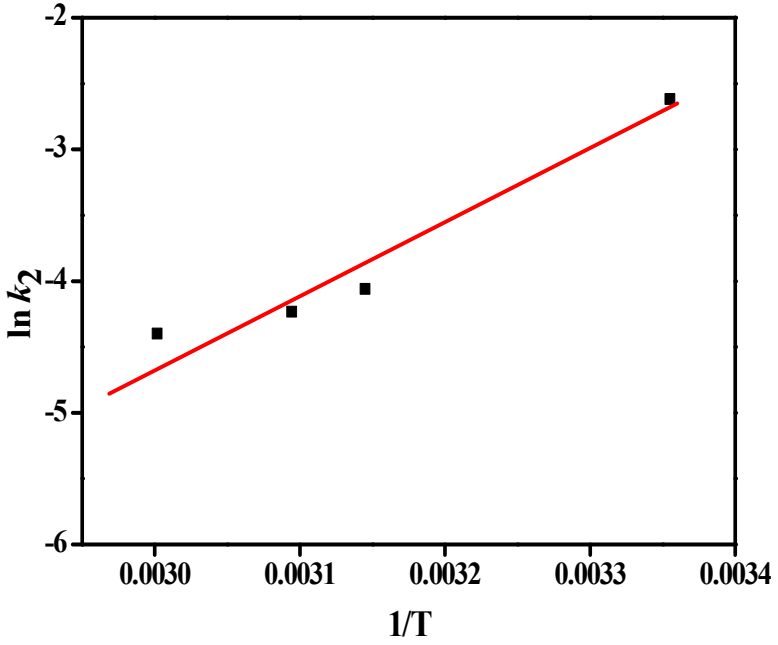

Figure S9: Arrhenius function

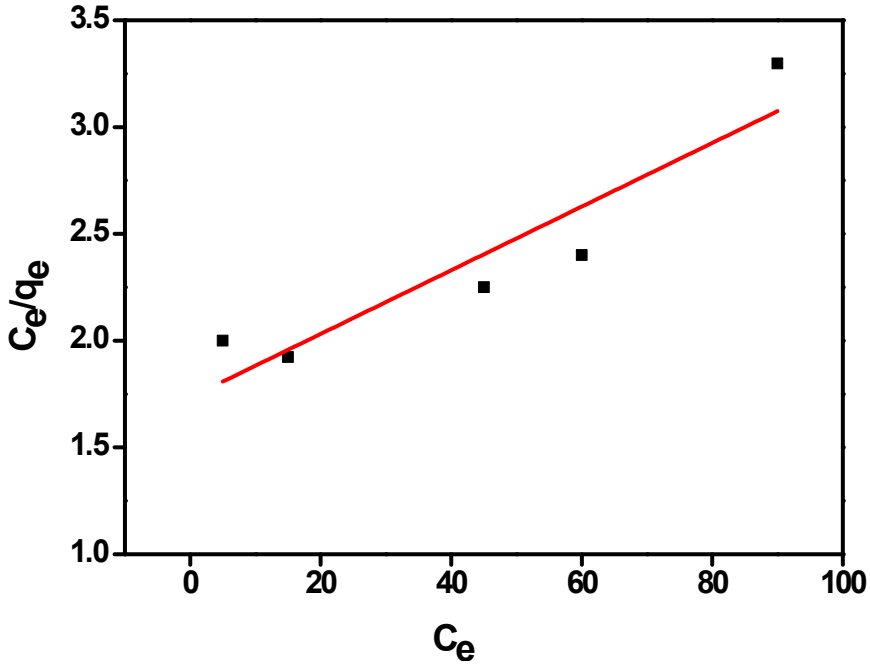

Figure S10: Langmuir isotherm model

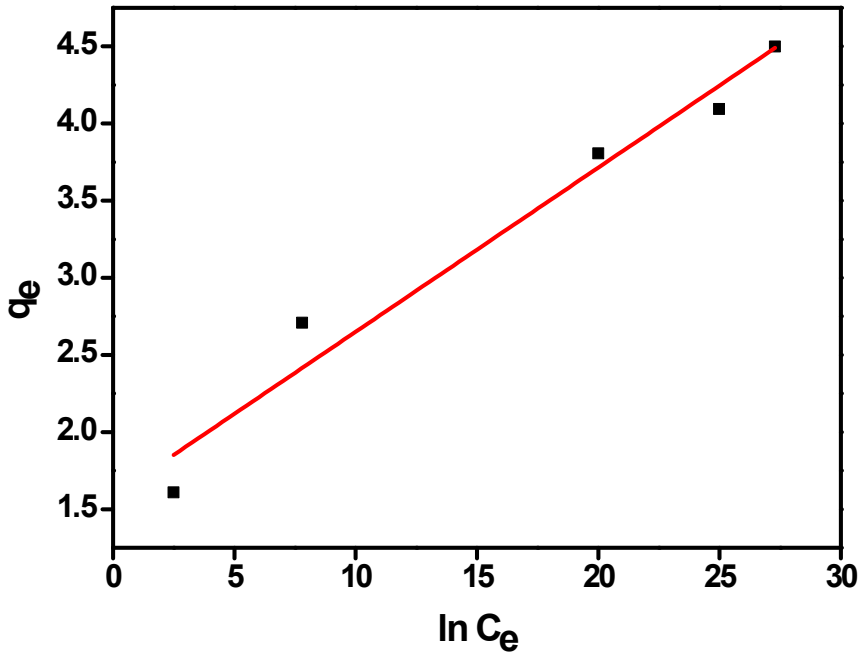

Figure S11: Temkin isotherm model