Supplementary Information

Cyclic Tetra [(Indolyl)-tetramethyl]-diethane-1,2-diamine (CTet) Impregnated Hydrous Zirconium Oxide as a Novel Hybrid Material for Enhanced Removal of Fluoride from Water.

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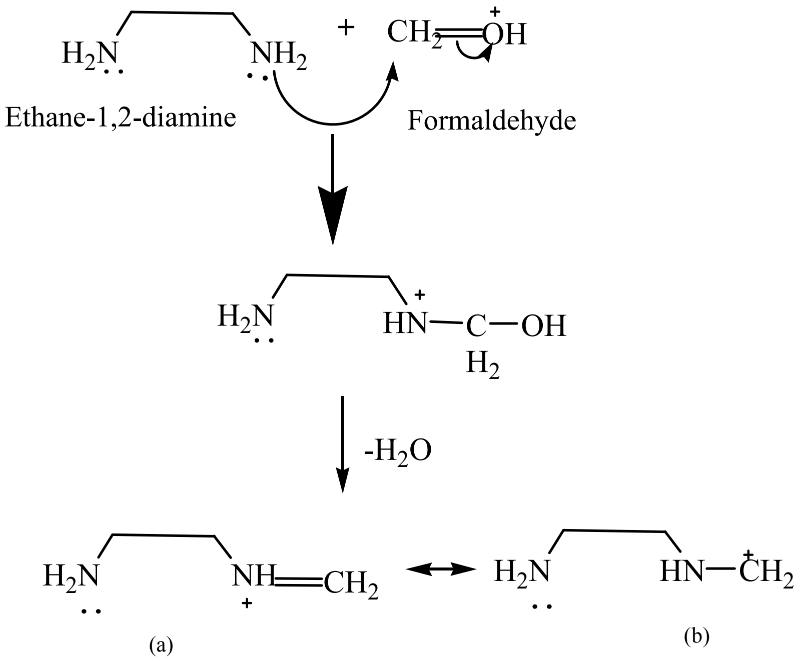
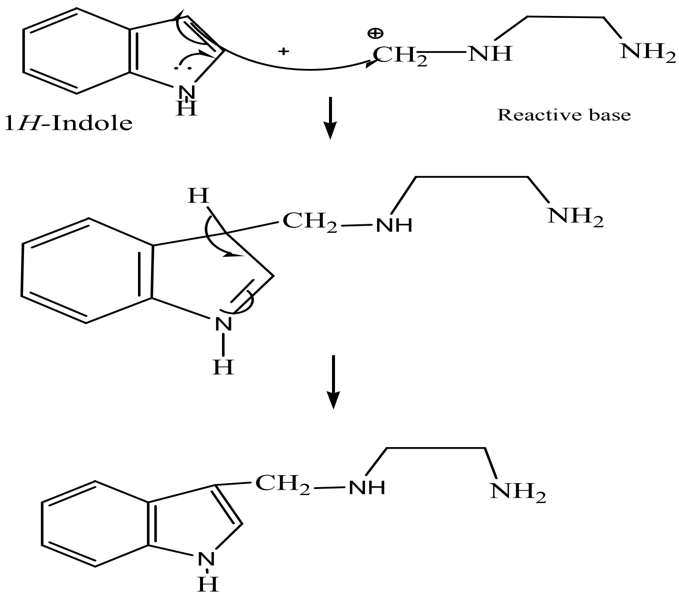
This file includes the Supplementary information of CTet-HZO Reaction mechanism. Figure S1 to Figure S8, Table S1 , S2 and Scheme S1.

Step I:



Resonance Structure

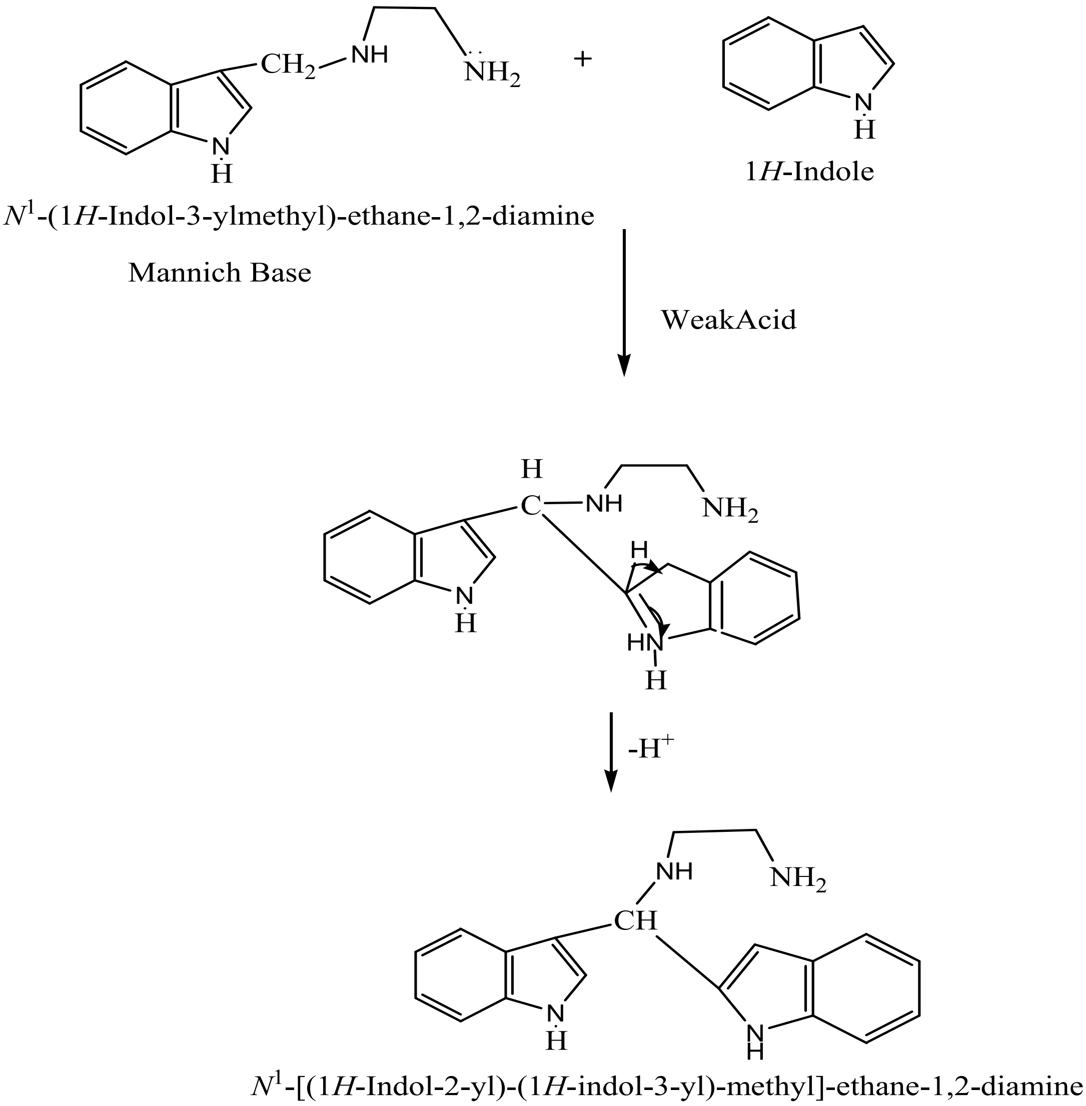
Step II :



N^1-(1*H*-Indol-3-ylmethyl)-ethane-1,2-diamine

Intermidiate of Mannich Base

Step III:



N^1-(1*H*-Indol-3-ylmethyl)-ethane-1,2-diamine

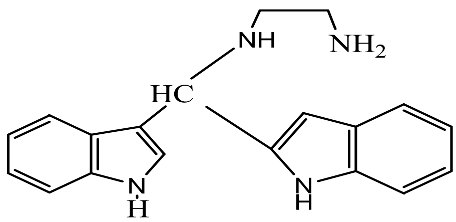
Mannich Base

1*H*-Indole

N^1-[(1*H*-Indol-2-yl)-(1*H*-indol-3-yl)-methyl]-ethane-1,2-diamine

2,3-Dimer of mannich Base

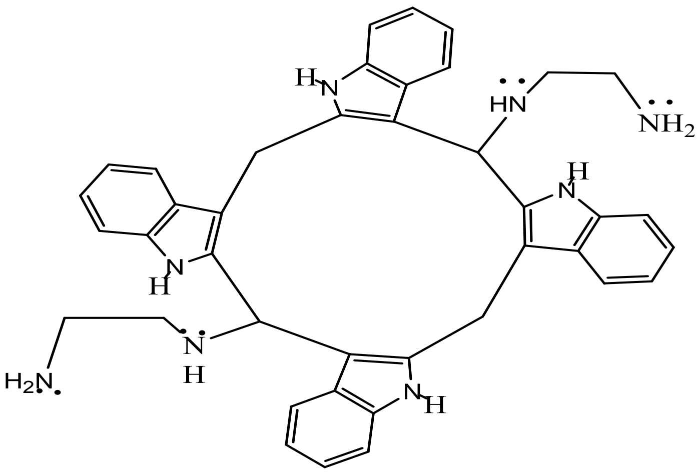
StepIV:



N^1-[(1*H*-Indol-2-yl)-(1*H*-indol-3-yl)-methyl]-ethane-1,2-diamine

(2,3- Dimer of mannich Base)

↓ HCHO (Acetic Acid)
Reflux for 2 hrs



Cyclic tetra [(indolyl)-tetramethyl]-diethane-1,2-diamine

Cyclic Tetramer (CTet)

(CTet-HZO)

Scheme S1: Reaction mechanism of CTet-HZO hybrid material.

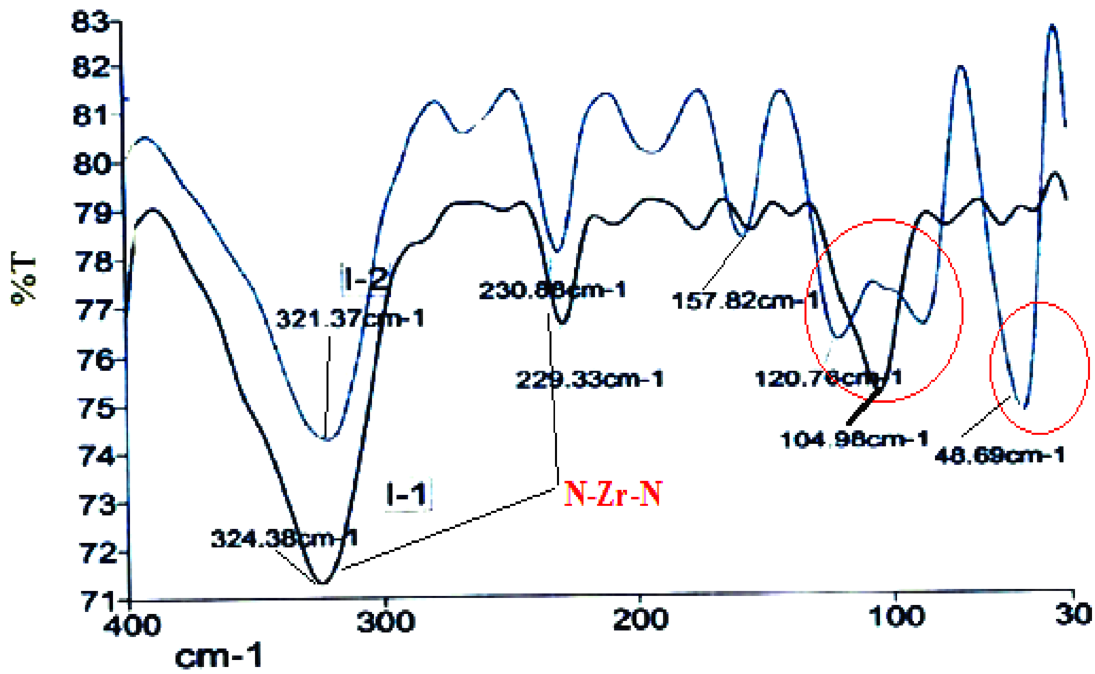


Figure S1: Far IR spectra of CTet-HZO in Cl^- form (I-1) and fluoride sorbed CTet-HZO (I-2).

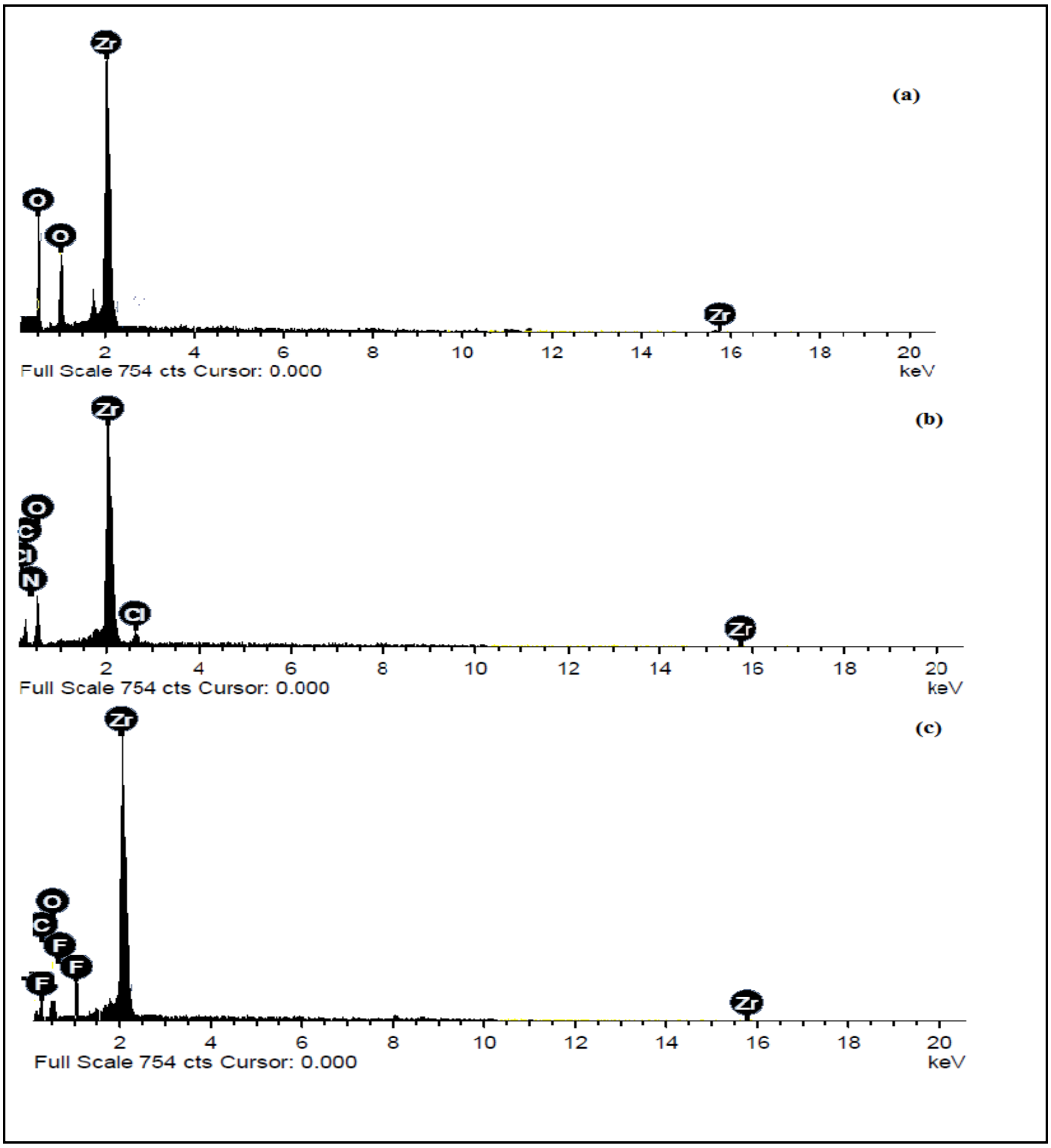


Figure S2. EDX spectra of (a) hydrous zirconium oxide (b) CTet-HZO and (c) Fluoride sorbed CTet-HZO.

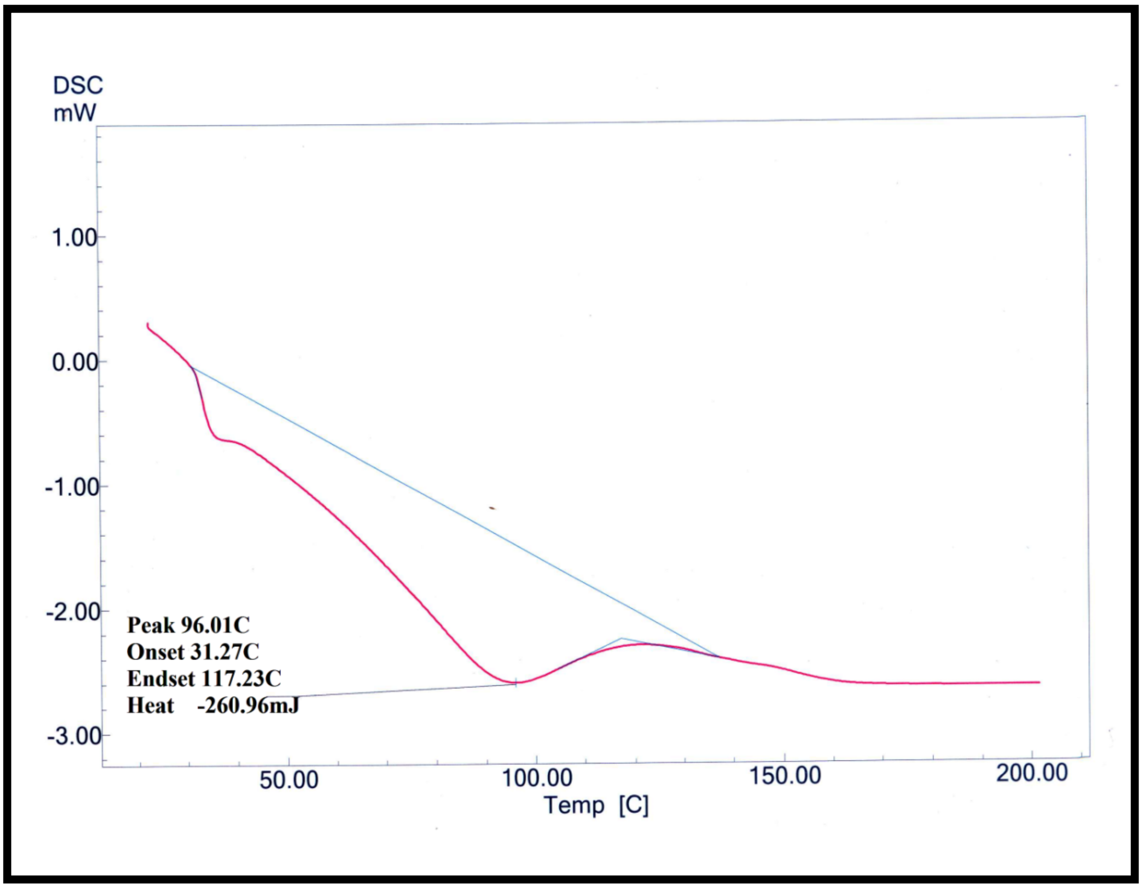


Figure S3. Differential thermal scanning (DSC) curve for CTet-HZO material.

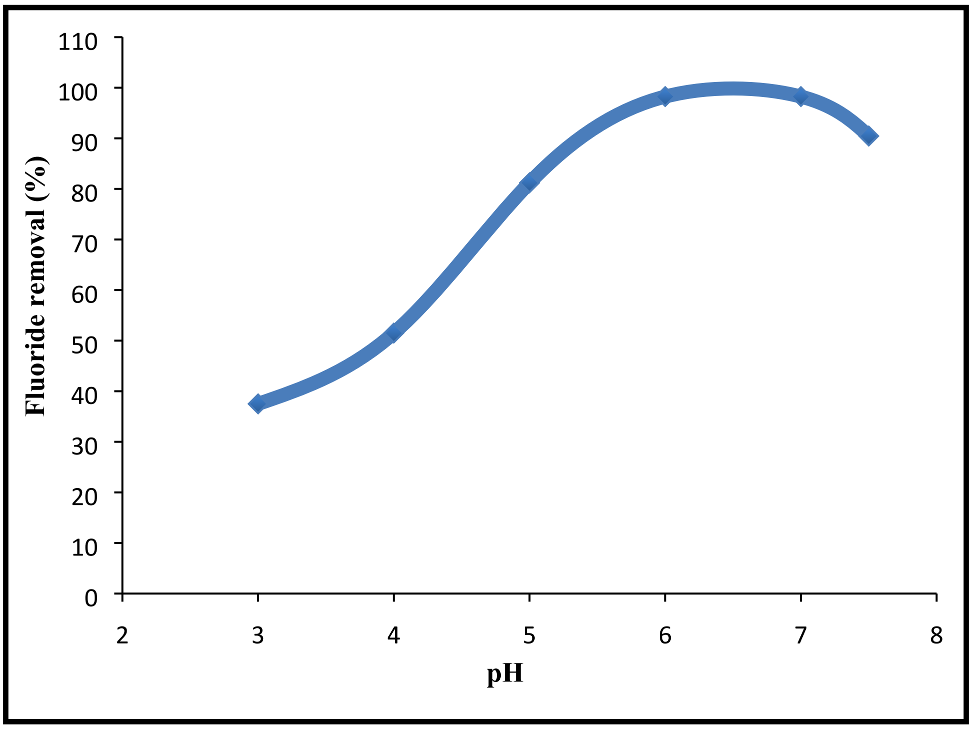


Figure S4. Effect of pH on the removal of fluoride using HZO.

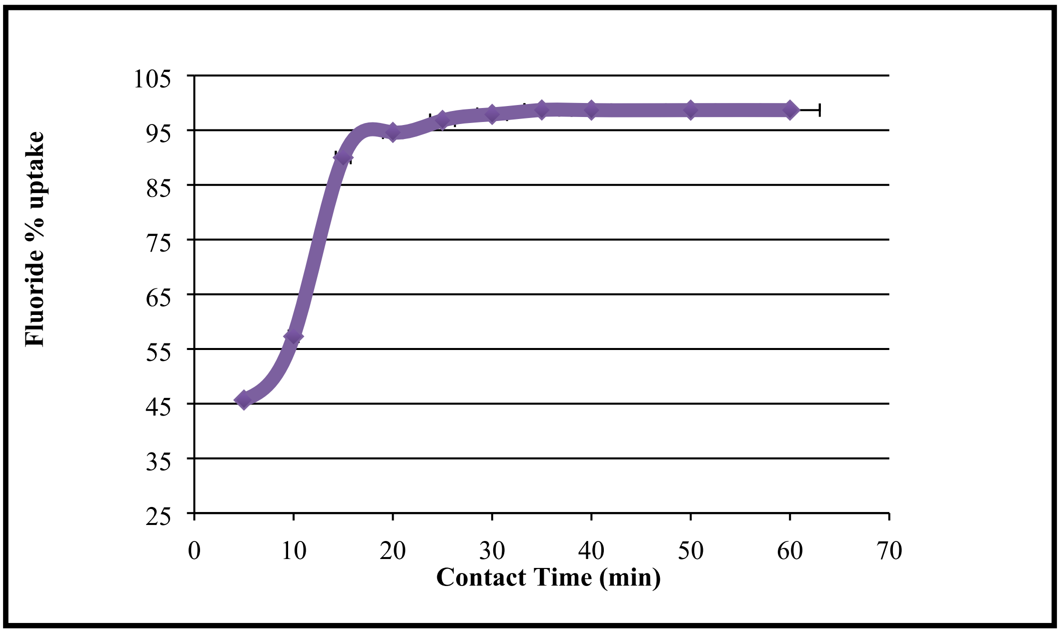


Figure S5. Effect of contact time on the % uptake of fluoride using CTet-HZO. (Concentration 20 mgL^{-1}; pH 3.5; adsorbent dose 0.15g).

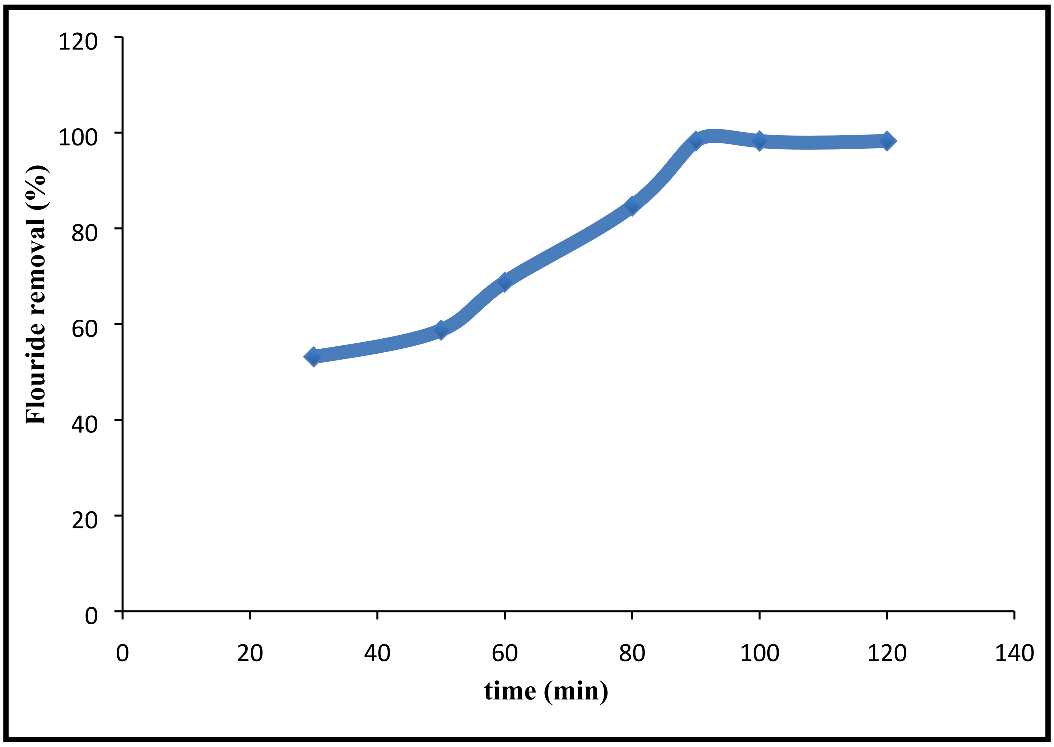


Figure S6. Effect of contact time for removal of fluoride using HZO.

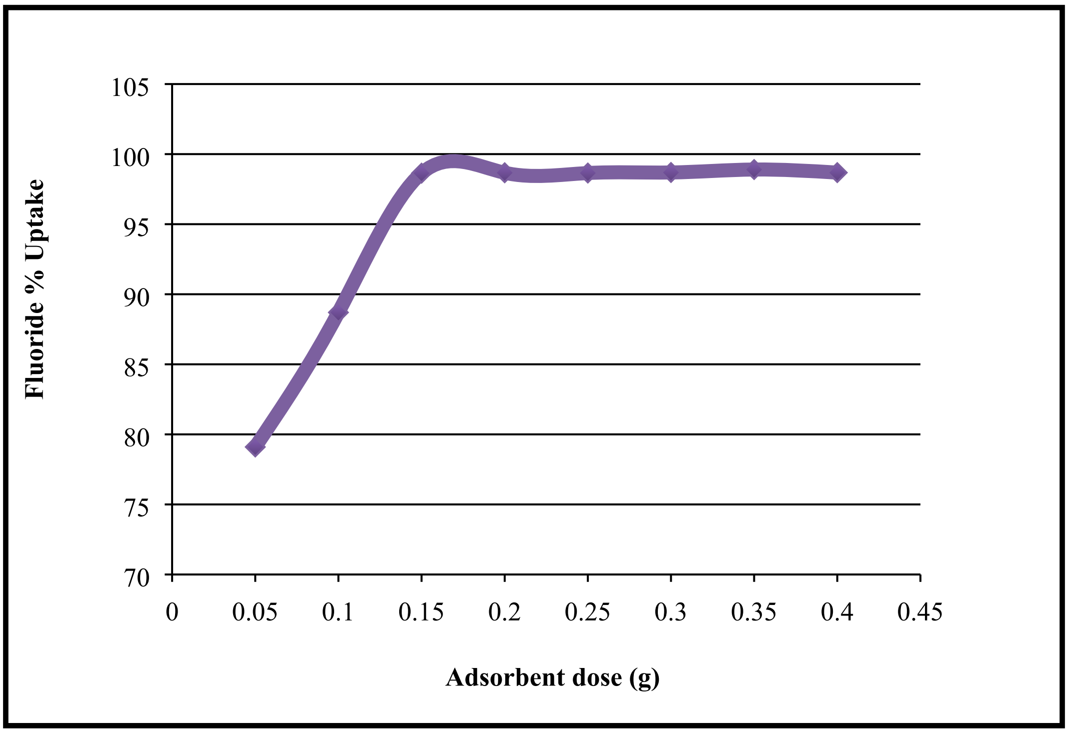
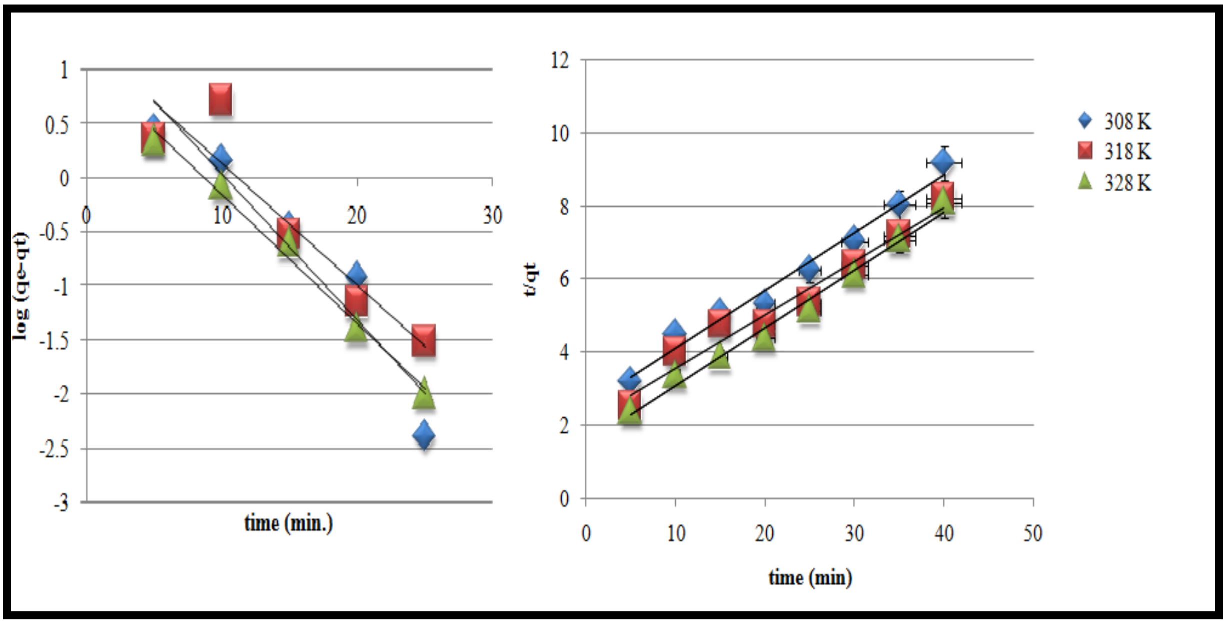


Figure S7. Effect of adsorbent dose on the fluoride uptake using CTet-HZO. (Conc.; 20 mg/L, Temp.; 308 K, pH 3.5).



(a) (b)

Figure S8. Kinetic plots. (a) Pseudo first order kinetic model (b) pseudo second order kinetic model.

Table S1: Characteristics of Water samples.

Parameters	Values
Total hardness as $CaCO_3$ (mgL^{-1})	123-415
Total alkalinity	245-548
F^-	1.84-3.62
Cl^- (mg/L)	55-260
NO_3^- (mg/L)	10-120
SO_4^{2-} (mg/L)	<180
Na^+ (mg/L)	28.9-37.4
K^+ (mg/L)	1.6-24.8
Total iron as Fe (mg/L)	<0.09
Turbidity	1.2-4.6
pH	6.5-8.2
Conductivity	510-2110

Table S2. Basic composition of fluoride containing groundwater (GW-3) and acidic effluent from metal finishing industry.

Species (mg L^{-1})	Groundwater	Acidic effluent
F^-	3.6	4.2
Cl^-	80.1	72.1
SO_4^{2-}	64.4	56.2
Alkalinity (as HCO_3^-)	158.2	0
NO_3^-	21.0	15.4
Total P	0.04	<0.06
Na^+	210	108
K^+	7.2	2.08
Total Hardness (as $CaCO_3$)	350	298
pH	6.8	4.1