TiO$_2$-based hybrid nanocomposites modified by phosphonate molecules as selective PAH adsorbents
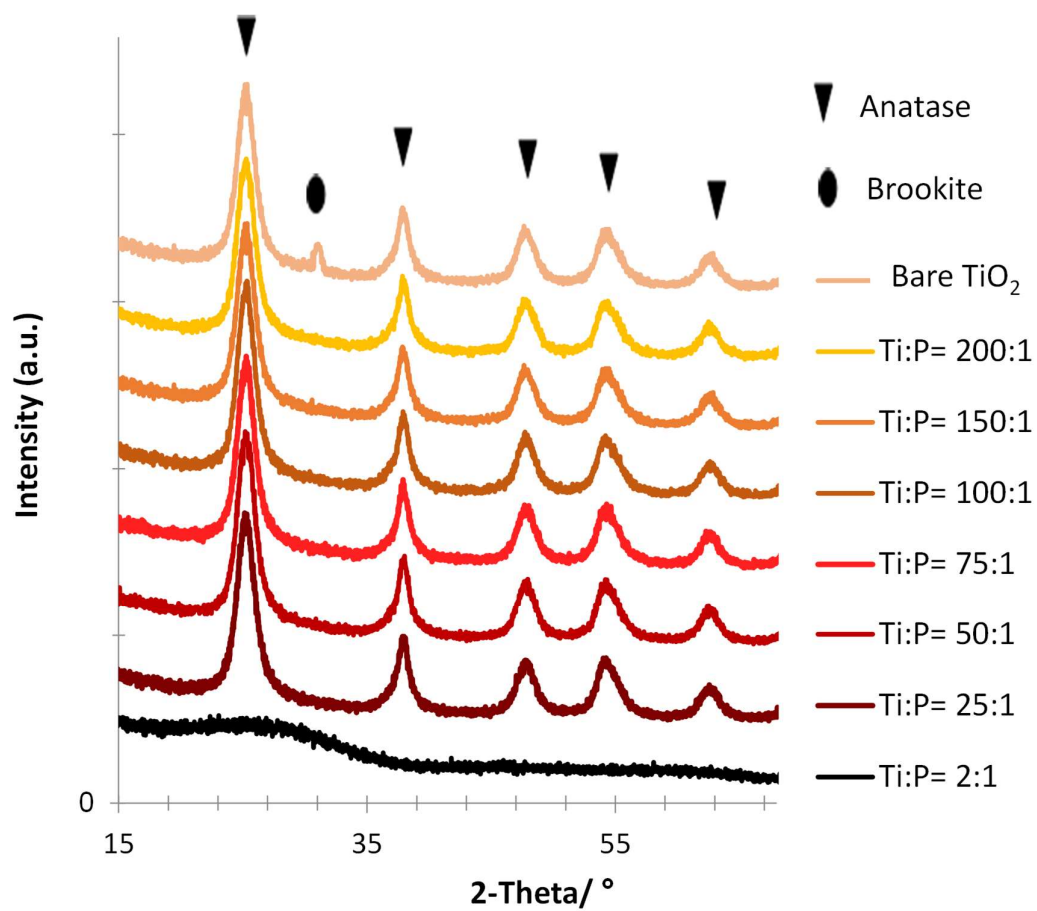

Figure S1: Powder XRD of samples $(TiO_2)_x(VPA)$ (x=2-200) and bare TiO$_2$
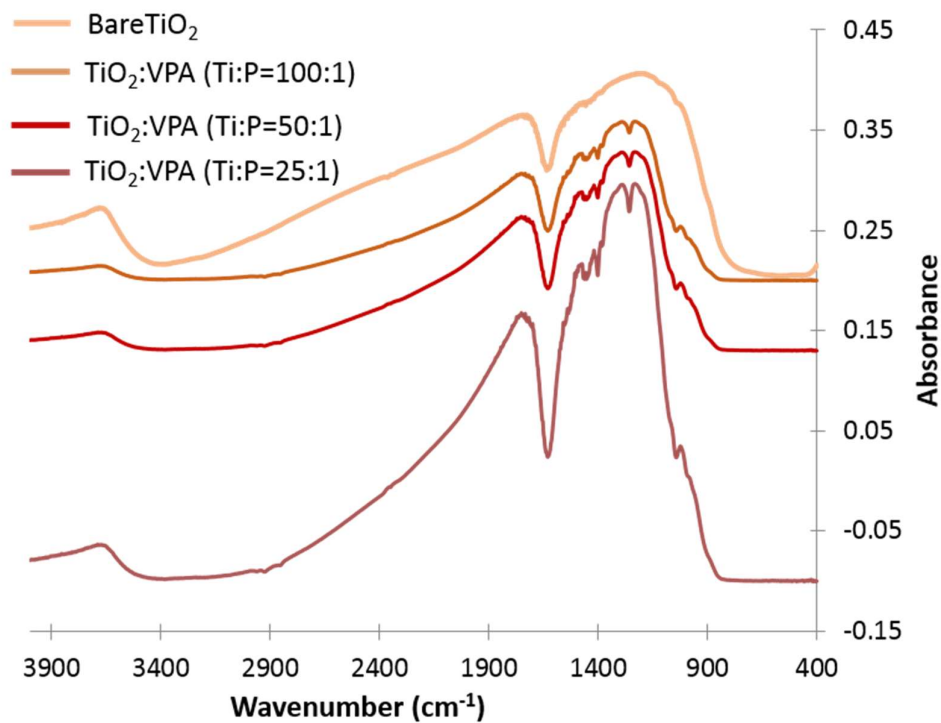
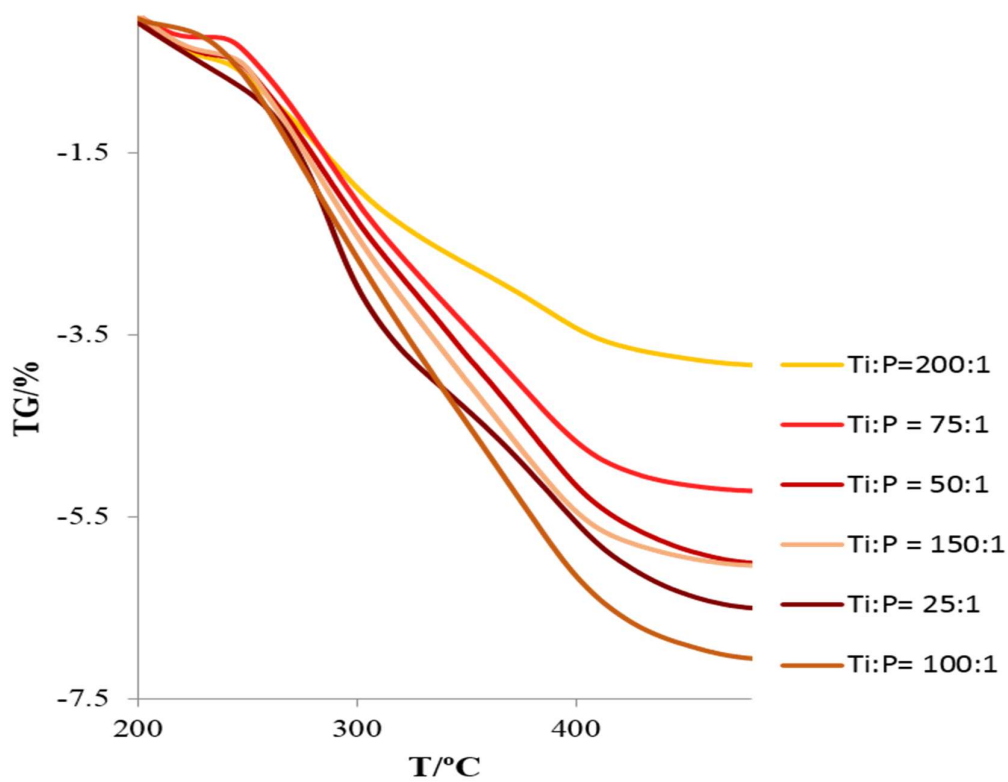**Figure S2:** FT-IR spectra of samples $(TiO_2)_x(VPA)$ (x=25, 50, 100) and bare TiO_2

Figure S3: TGA of $(TiO_2)_x(VPA)$ samples

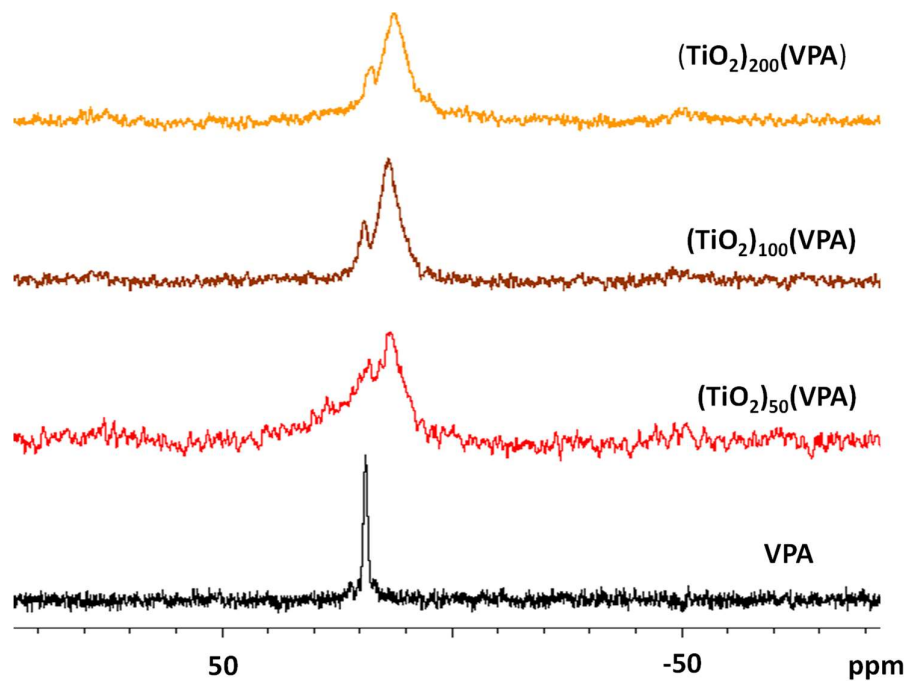**Figure S4:** Solid state $^{31}P\{^{1}H\}$ MAS NMR spectra of VPA and hybrid samples $(TiO_2)_X(VPA)$ with x = 50, 100 et 200
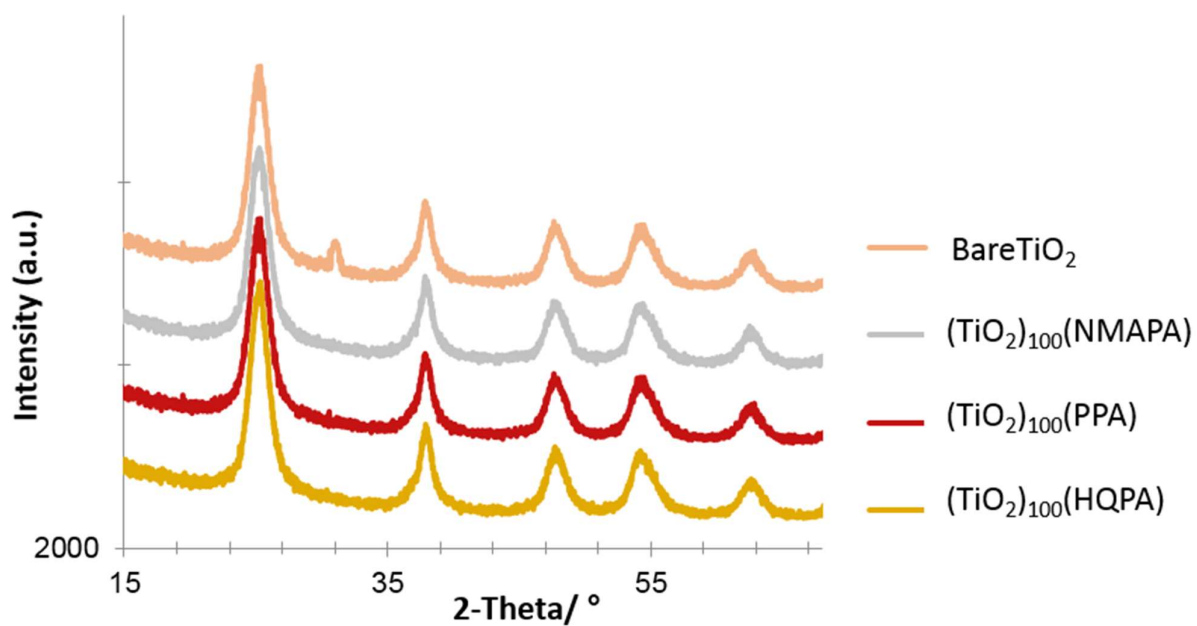

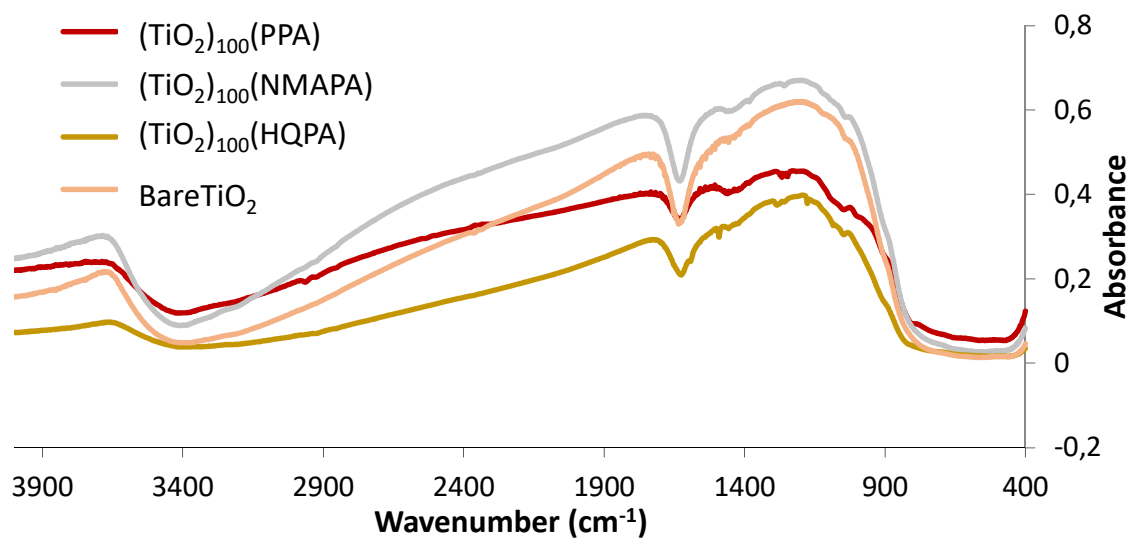**Figure S5:** Powder XRD of samples $(TiO_2)_{100}(PA)$ and bare TiO_2

Figure S6 : FT-IR spectra of bare TiO$_2$ and hybrid samples (TiO$_2$)$_{100}$(PPA), (TiO$_2$)$_{100}$(NMAPA) and (TiO$_2$)$_{100}$(HQPA)
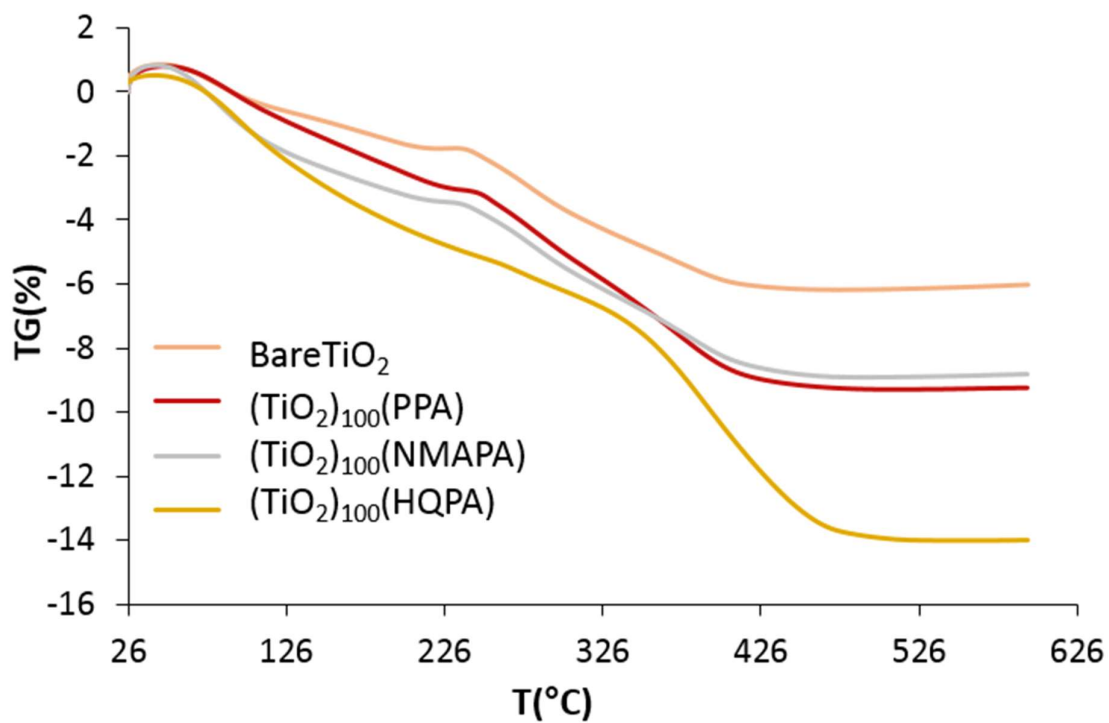
Figure S7: TGA patterns of bare TiO$_2$ and hybrid samples (TiO$_2$)$_{100}$(PPA), (TiO$_2$)$_{100}$(NMAPA) and (TiO$_2$)$_{100}$(HQPA)
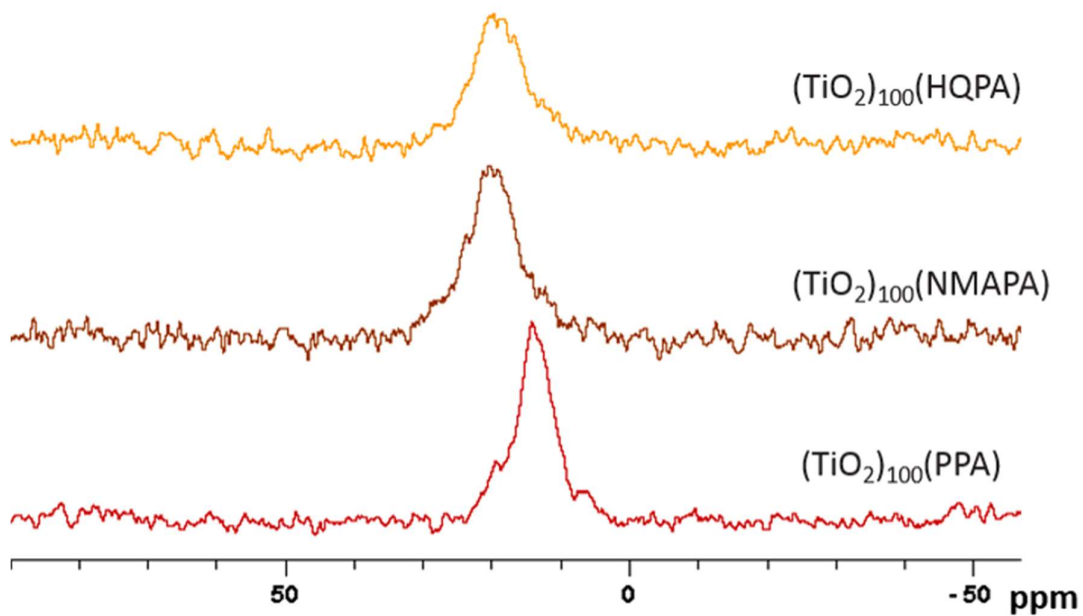
Figure S8: ^{31}P $\{^{1}H\}$ MAS NMR spectra of hybrid samples $(TiO_2)_{100}(PPA)$, $(TiO_2)_{100}(NMAPA)$ and $(TiO_2)_{100}(HQPA)$
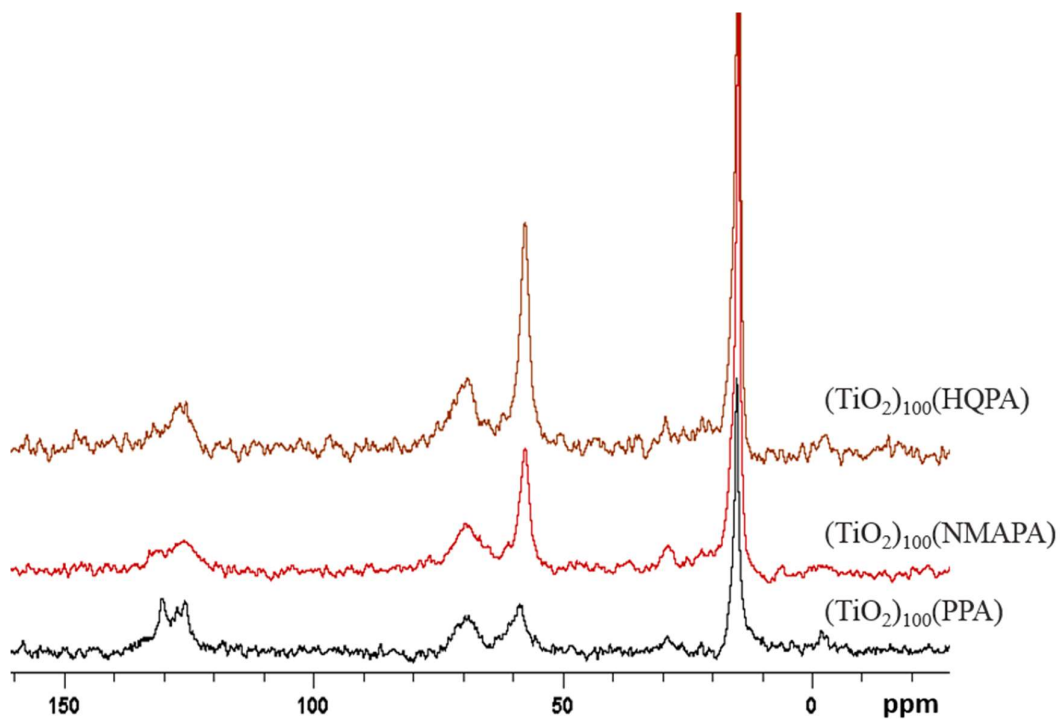
Figure S9: ^{13}C $\{^{1}H\}$ MAS NMR spectra of hybrid samples $(TiO_2)_{100}(PPA)$, $(TiO_2)_{100}(NMAPA)$ and $(TiO_2)_{100}(HQPA)$

**Table S1:** Abbreviations and structures of the EPA 16 PAHs

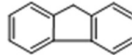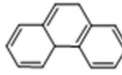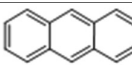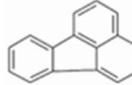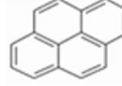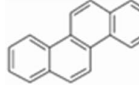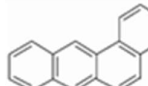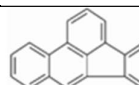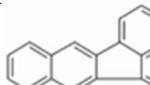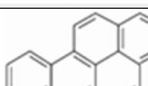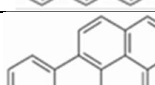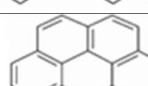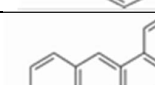| PAH	Abbreviation	Structure
Naphtalene	NAP	
Acenaphtylene	ACY	
Acenaphtene	ACP	
Fluorene	FLR	
Phenanthrene	PHE	
Anthracene	ANT	
Fluoranthene	FLT	
Pyrene	PYR	
Chrysene	CHR	
Benzo[a]Anthracene	BaA	
Benzo[b]fluoranthene	BbF	
Benzo[k]fluoranthene	BkF	
Benzo[a]pyrene	BaP	
Indeno[1.2.3-cd] pyrene	IcP	
Dibenz[a,h]anthracene	DbA	
Benzo[ghi]perylene	BgP	

Table S2: BET surface and porous volume of bare TiO_2 and hybrid $(TiO_2)_{100}(O_3P-R)$ nanomaterials

Material	Porous volume (cm³ / g)	BET surface area (m² / g)
TiO_2	0.49	250
$(TiO_2)_{100}(VPA)$	0.39	269
$(TiO_2)_{100}(PPA)$	0.50	285
$(TiO_2)_{100}(NMAPA)$	0.51	225
$(TiO_2)_{100}(HQPA)$	0.50	322

Table S3: Summary of kinetic parameters adsorption of $(TiO_2)_{100}(VPA)$ toward Benzo(a)pyrene

Model	Parameters
Pseudo-first-order k_1 (min^{-1}) q_e (mg g^{-1}) R^2	0.00207 0.00855 0.1403
Pseudo-second-order k_2 (g mg^{-1} min^{-1}) q_e (mg g^{-1}) R^2	1.383 0.850 1.000