

Supporting Information (Figures S1-S2)

Externally predictive quantum-mechanical models for the adsorption of aromatic organic compounds by graphene-oxide nanomaterials

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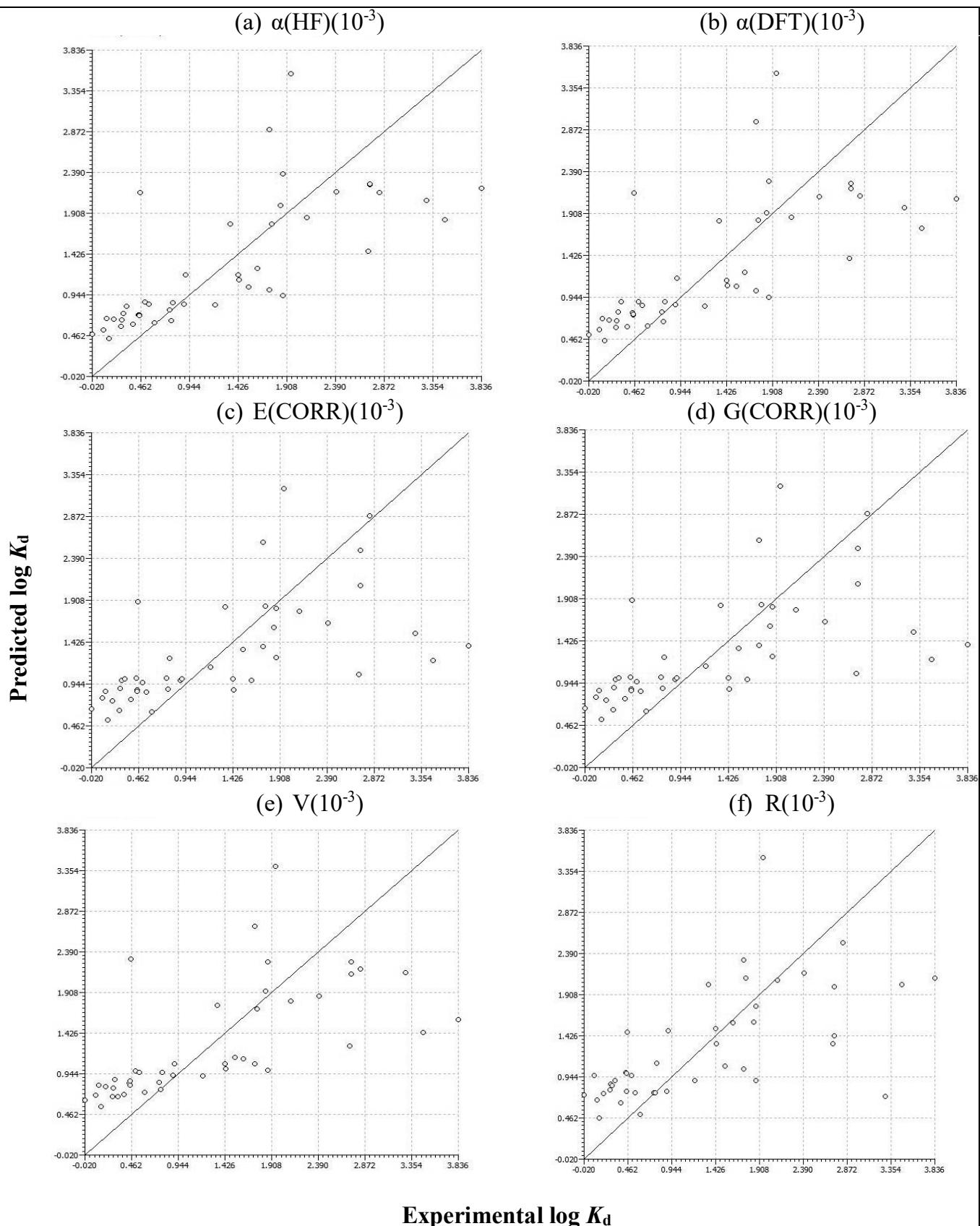


Figure S1. Scatter plots: Experimental vs predicted $\log K_d$ using models based on best performing single-descriptors among quantum-mechanical and LSER descriptors, at different adsorbate equilibrium concentration of 10^{-3} , 10^{-2} and $10^{-1} C_s$ (mg/L) as specified in the plots. The values predicted are using models developed without any splitting of the data-set.

Figure S1 continued...

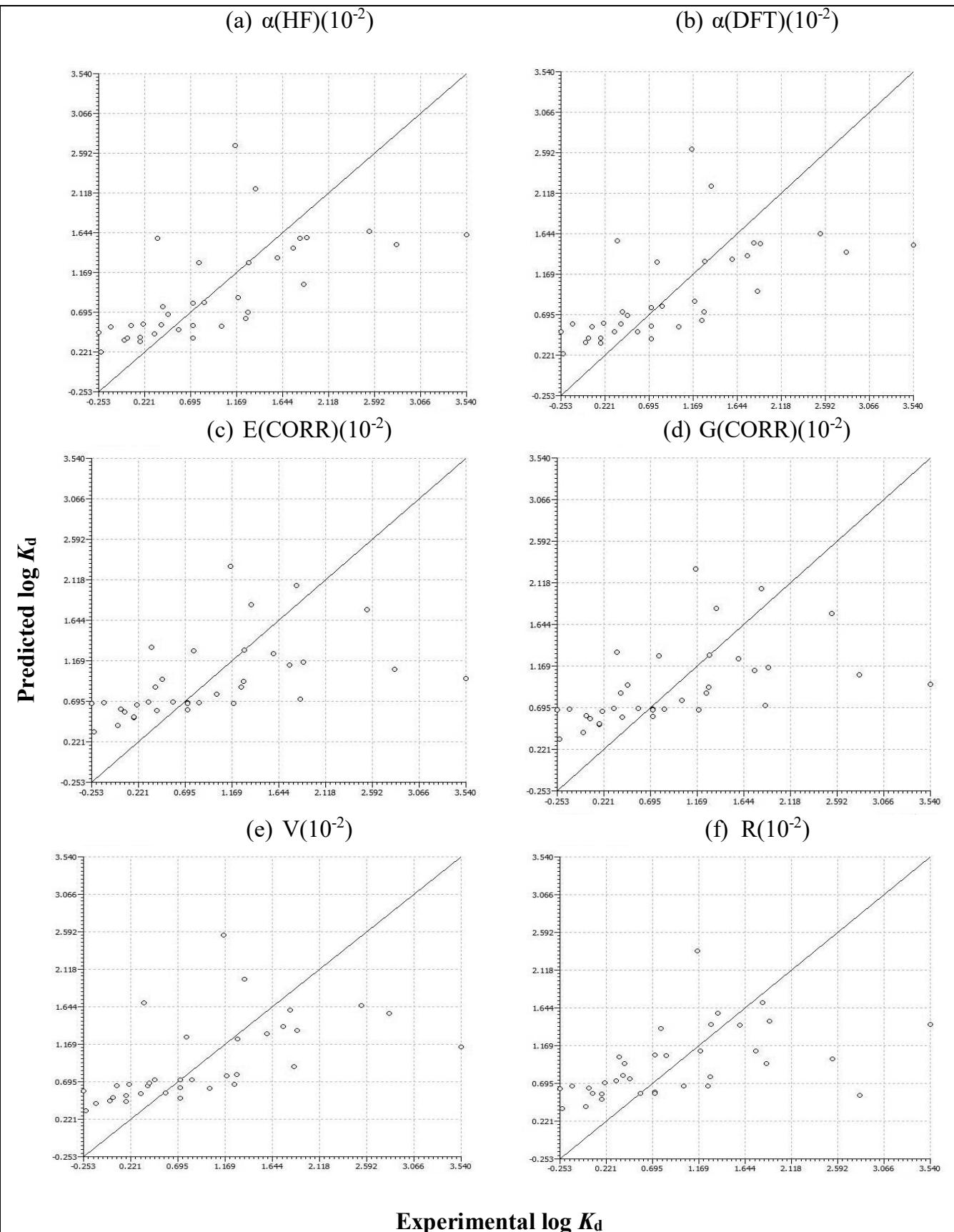


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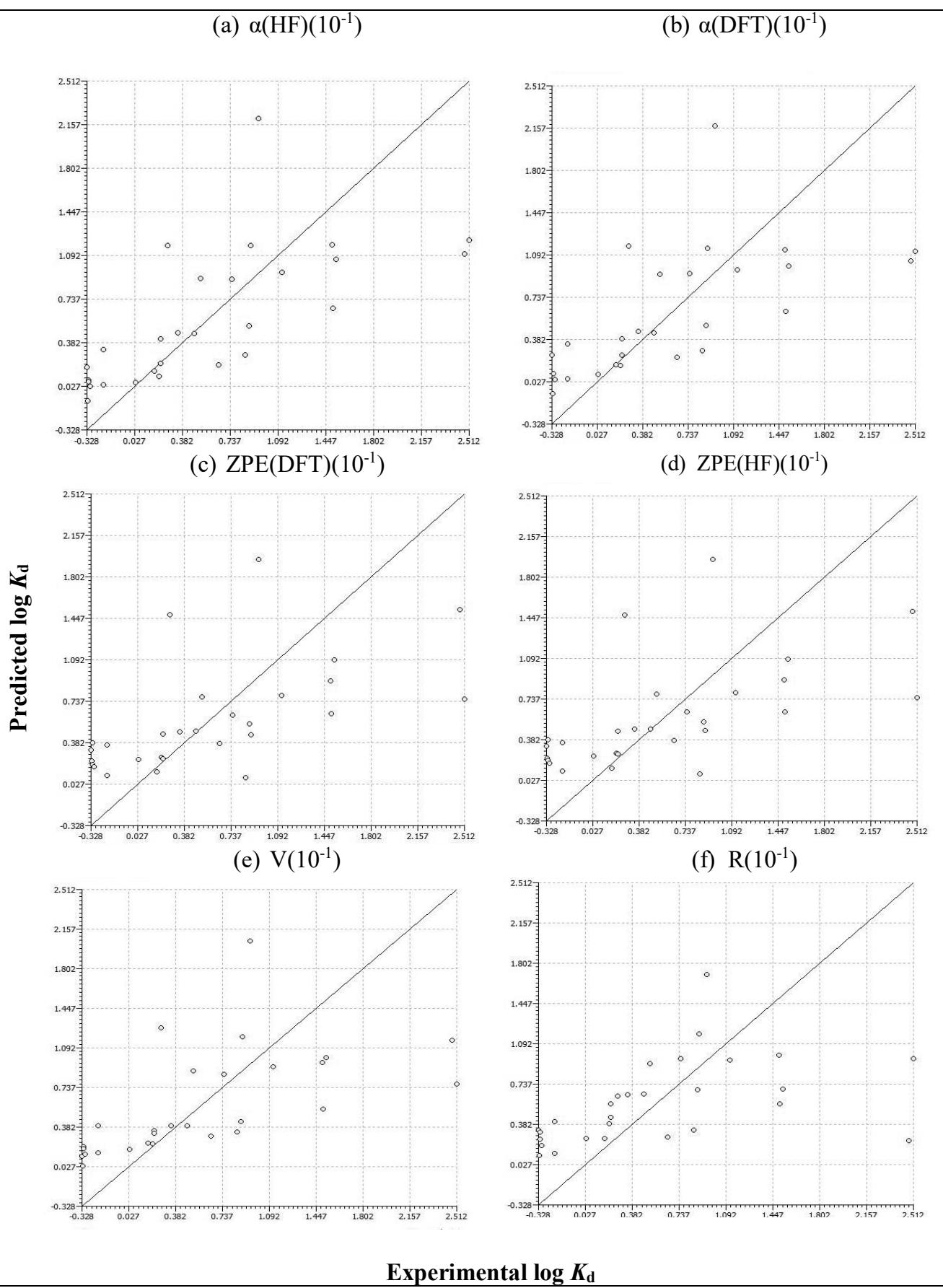


Figure S1 continued...

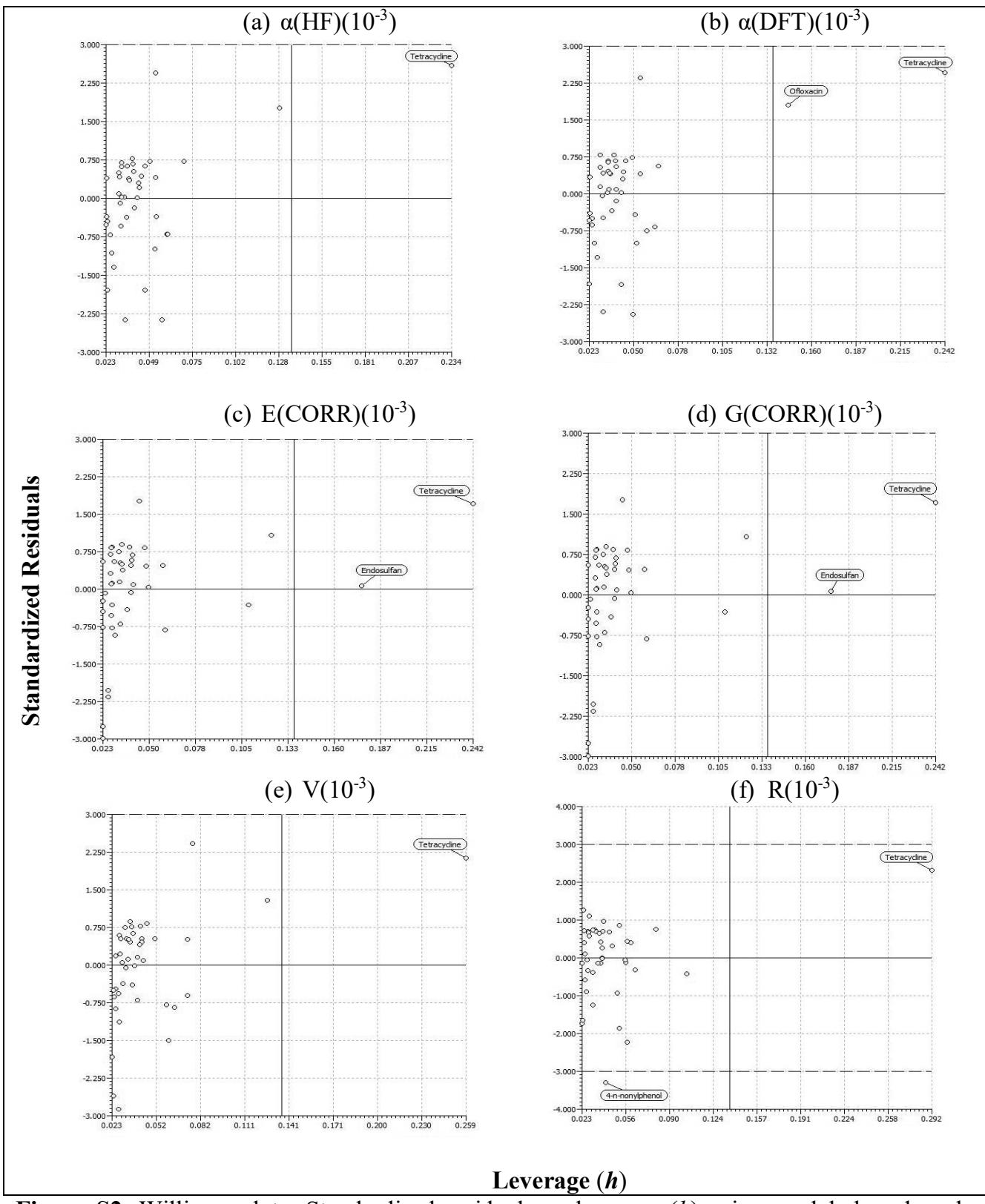


Figure S2. Williams plots: Standardized residuals vs leverage (h) using models based on best performing single-descriptors among quantum-mechanical and LSER descriptors, at different adsorbate equilibrium concentration of 10^{-3} , 10^{-2} and $10^{-1} C_s(\text{mg/L})$ as specified in the plots. The vertical line on the right-hand-side of each plot indicates a warning leverage (h^*). The values predicted are using models developed without any splitting of the data-set.

Figure S2 continued...

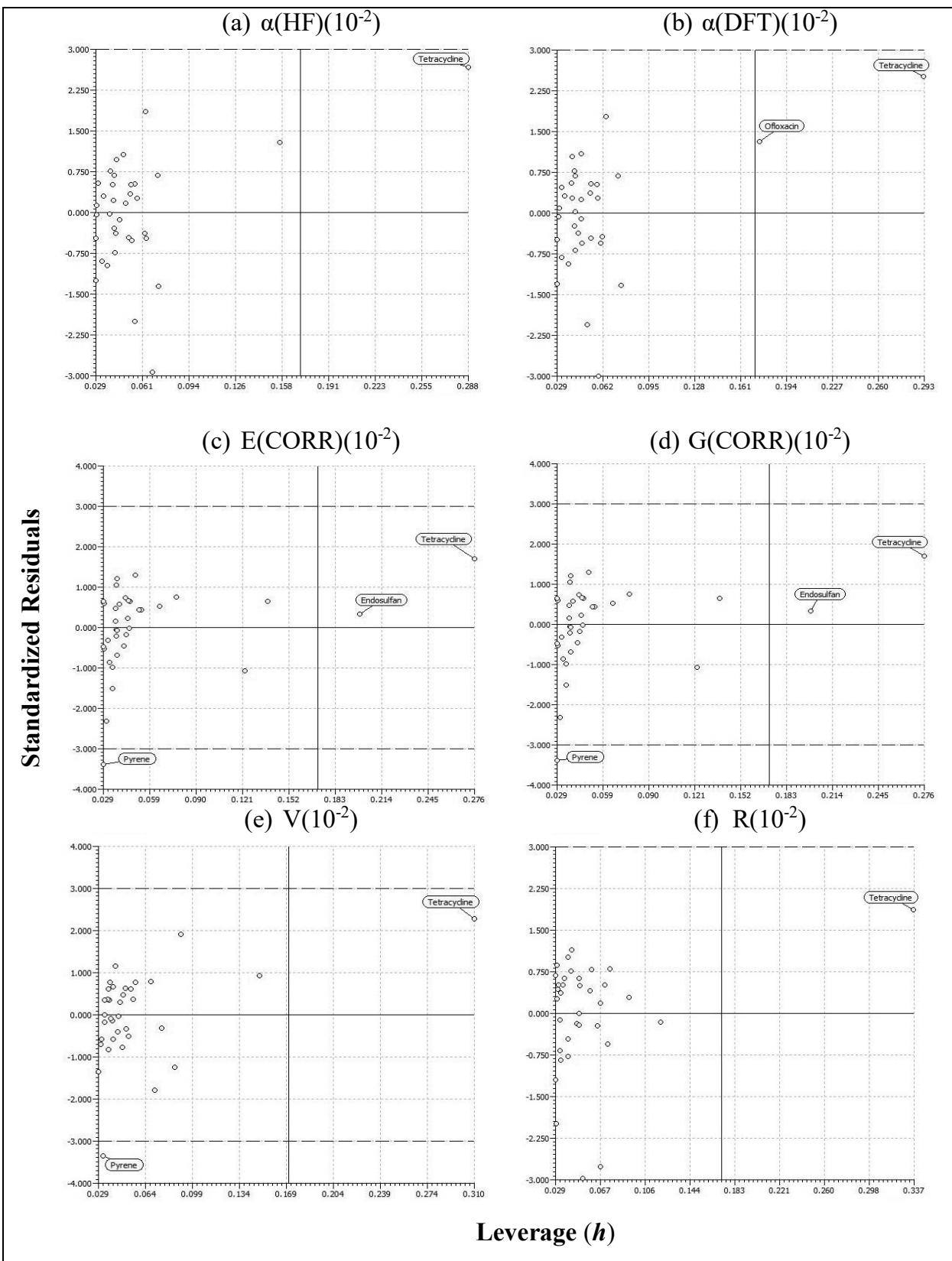


Figure S2 continued...

