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Supplementary Material

# Poly(β-cyclodextrin)-activated carbon gel composites for removal of pesticides from water

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**Table 1.** One-tailored Grubb's test parameters.

| Imidacloprid | | | | | |
|---|---|---|---|---|---|
| Theorical Concentration (mg $L^{-1}$) | Average Concentration (mg $L^{-1}$) | Standard Deviation | G calculated | | G table* |
| | | | Inferior | Superior | |
| 0.5 | 0.502 | 0.0003 | 0.98 | 1.02 | 2.21 |
| 1 | 1.004 | 0.0004 | 0.80 | 1.12 | |
| 2.5 | 2.51 | 0.0011 | 0.97 | 1.03 | |
| 5 | 5.02 | 0.0003 | 0.94 | 1.05 | |
| 7.5 | 7.53 | 0.0002 | 0.86 | 1.10 | |
| 10 | 10.04 | 0.002 | 0.85 | 1.10 | |
| 15 | 15.06 | 0.0004 | 1.11 | 0.84 | |
| 20 | 20.08 | 0.002 | 0.87 | 1.09 | |
| **Cymoxanil** | | | | | |
| Theorical concentration (mg $L^{-1}$) | Average concentration (mg $L^{-1}$) | Standard deviation | G calculated | | G table* |
| | | | Inferior | superior | |
| 0.1 | 0.0989 | 0.0005 | 0.71 | 1.14 | 2.29 |
| 0.5 | 0.4945 | 0.0001 | 1.15 | 0.62 | |
| 1 | 0.9890 | 0.0004 | 1.07 | 0.91 | |
| 2.5 | 2.4725 | 0.0003 | 1.01 | 0.98 | |
| 5 | 4.9450 | 0.0009 | 0.86 | 1.10 | |
| 7.5 | 7.4175 | 0.0004 | 1.05 | 0.94 | |
| 10 | 9.8900 | 0.0007 | 1.05 | 0.93 | |
| 15 | 14.8350 | 0.0004 | 1.05 | 0.94 | |
| 20 | 19.780 | 0.001 | 1.05 | 0.94 | |
| 30 | 29.6700 | 0.0003 | 0.58 | 1.15 | |

*significance level ($\alpha$) = 0.05.

**Table 2.** Two-tailored F-test parameters for equality variance.

| Imidacloprid | | Cymoxanil | |
|---|---|---|---|
| **F calculated** | **$F_{(\alpha-2,\ N1\text{-}1,N2\text{-}1)}$*,a** | **F calculated** | **$F_{(\alpha-2,\ N1\text{-}1,N2\text{-}1)}$*,b** |
| 0.08 | 8.89 | 0.32 | 6.54 |

* significance level ($\alpha$) = 0.01

a degrees of freedom ($N$) = 8

b degrees of freedom ($N$) =10

**Table 3.** Analytical parameters of imidacloprid and cymoxanil.

| Pesticide | LOD (mg $L^{-1}$) | LOQ (mg $L^{-1}$) | ε ($10^{-2}$ $M^{-1}$ $cm^{-1}$) | $R^2$ |
|---|---|---|---|---|
| **imidacloprid** | 0.05 | 20.08 | 8.38 (±0.04) | 0.9997 |
| **cymoxanil** | 0.07 | 29.67 | 4.08 (±0.05) | 0.9983 |

**Table 4.** Fitting parameters for eqs. 4 and 5 to the sorption isotherm data for imidacloprid in the presence of urea and NaCl.

| urea, 1.0 g $L^{-1}$ | | | | | |
|---|---|---|---|---|---|
| **Model** | | **PCD** | **PCD/$AC_{5\%}$** | **PCD/$AC_{10\%}$** | **AC** |
| *Freundlich* | $K_F$ (mg $g^{-1}$ $mg^{-1/n}$ $L^{1/n}$) | 0.08 (±0.01) | 0.63 (±0.05) | 1.43 (±0.22) | 18.26 (±2.57) |
| | *1/n* | 0.94 (±0.03) | 0.64 (± 0.016) | 0.52 (± 0.03) | 0.82 (± 0.13) |
| | $R^2$ | 0.996 | 0.9977 | 0.985 | 0.9245 |
| | *AIC* | -12.10 | -15.42 | 2.57 | 31.40 |
| *Sips* | $q_m$ (mg $g^{-1}$) | 44.80 (±15.74) | 36.70 (±9.60) | 32.60 (±8.84) | 55.00 (±2.40) |
| | $K_S$ ($10^{-2}$ L $mg^{-1}$) | 0.22 (±0.11) | 0.53 (±0.30) | 1.03 (±0.72) | 72.75 (±3.64) |
| | $1/n_S$ | 1.21 (±0.13) | 1.97 (±0.15) | 0.82 (±0.15) | 2.51 (±0.24) |
| | $R^2$ | 0.997 | 0.9913 | 0.9062 | 0.9957 |
| | *AIC* | -13.82 | -0.33 | 3.45 | 10.76 |
| NaCl, 1.0 g $L^{-1}$ | | | | | |
| Model | | PCD | PCD/$AC_{5\%}$ | PCD/$AC_{10\%}$ | AC |
| *Freundlich* | $K_F$ (mg $g^{-1}$ $mg^{-1/n}$ $L^{1/n}$) | 0.063 (±0.047) | 0.32 (±0.08) | 1.35 (± 0.27) | 7.86 (±1.82) |
| | *1/n* | 0.98 (± 0.14) | 0.68 (±0.04) | 0.52 (±0.04) | 1.31 (±0.21) |
| | $R^2$ | 0.9441 | 0.9834 | 0.9811 | 0.9225 |
| | *AIC* | 8.15 | -1.33 | 7.70 | 21.02 |
| *Sips* | $q_m$ (mg $g^{-1}$) | 15.43 (±0.64) | 30.90 (±10.11) | 34.80 (±7.60) | 40.42 (± 2.50) |
| | $K_S$ ($10^{-2}$ L $mg^{-1}$) | 0.90 (±0.040) | 0.35 (±0.22) | 0.87 (±0.50) | 62.03 (±2.61) |
| | $1/n_S$ | 2.73 (±0.23) | 1.02 (±0.17) | 0.85 (±0.14) | 6.23 (±1.76) |
| | $R^2$ | 0.9976 | 0.9932 | 0.9927 | 0.981 |
| | *AIC* | -14.19 | -6.13 | 0.85 | 16.01 |

**Table 5.** Fitting parameters for eqs. 4 and 5 to the sorption isotherm data for cymoxanil in presence of urea and NaCl.

| **urea, 1.0 g L$^{-1}$** | | | | | |
|---|---|---|---|---|---|
| **Model** | | **PCD** | **PCD/AC$_{5\%}$** | **PCD/AC$_{10\%}$** | **AC** |
| *Freundlich* | $K_F$ (mg g$^{-1}$ mg$^{-1/n}$ L$^{1/n}$) | 0.03 (± 0.01) | 0.53 (± 0.15) | 2.26 (± 0.30) | 5.90 (±1.70) |
| | *1/n* | 0.87 (± 0.09) | 0.51 (± 0.05) | 0.32 (±0.02) | 0.93 (±0.16) |
| | ***R*$^2$** | 0.9687 | 0.959 | 0.9765 | 0.8990 |
| | ***AIC*** | -9.83 | -2.19 | -3.93 | 25.60 |
| *Sips* | $q_m$ (mg g$^{-1}$) | 9.54 (±6.31) | 13.25 (±2.70) | 20.61 (±4.18) | 44.01 (±3.02) |
| | $K_S$ (10$^{-2}$ L mg$^{-1}$) | 0.27 (±0.27) | 0.90 (±0.44) | 1.09 (±0.77) | 28.28 (±1.70) |
| | $1/n_S$ | 1.36 (±0.52) | 0.98 (±0.200) | 0.62 (±0.12) | 3.34 (±0.56) |
| | $R^2$ | 0.9725 | 0.9835 | 0.9951 | 0.9852 |
| | *AIC* | -10.23 | -8.94 | -11.34 | 15.90 |
| NaCl, 1.0 g L$^{-1}$ | | | | | |
| Model | | PCD | PCD/AC$_{5\%}$ | PCD/AC$_{10\%}$ | AC |
| *Freundlich* | $K_F$ (mg g$^{-1}$ mg$^{-1/n}$ L$^{1/n}$) | 0.08 (± 0.03) | 0.15 (± 0.02) | 0.72 (±0.10) | 4.80 (±0.70) |
| | *1/n* | 0.86 (± 0.07) | 0.80 (±0.03) | 0.60 (±0.03) | 1.58 (±0.10) |
| | ***R*$^2$** | 0.973 | 0.9943 | 0.9932 | 0.9902 |
| | ***AIC*** | 0.05 | -12.70 | -4.12 | 14.53 |
| *Sips* | $q_m$ (mg g$^{-1}$) | 18.58 (±2.80) | 28.84 (±5.07) | 35.73 (±8.04) | 76.06 (±32.25) |
| | $K_S$ (10$^{-2}$ L mg$^{-1}$) | 0.47 (±0.11) | 0.32 (±0.97) | 0.44 (±0.22) | 27.95 (±10.76) |
| | $1/n_S$ | 1.50 (±0.20) | 1.15 (±0.10) | 0.89 (±0.11) | 2.40 (±0.64) |
| | $R^2$ | 0.9932 | 0.9972 | 0.9955 | 0.983 |
| | *AIC* | -11.00 | -19.90 | -6.60 | 21.65 |

**Table 6.** Characterization values for three sorption/desorption cycles.

| | PCD | | | PCD/AC$_{5\%}$ | | | PCD/AC$_{10\%}$ | | |
|---|---|---|---|---|---|---|---|---|---|
| IMD | ***q*$_e$ (mg g$^{-1}$)** | ***RE%*** | ***DC%*** | ***q*$_e$ (mg g$^{-1}$)** | ***RE%*** | ***DC%*** | ***q*$_e$ (mg g$^{-1}$)** | ***RE%*** | ***DC%*** |
| 1° cycle | 15.0 (±0.3) | 33.3 (±0.3) | 64 (±2) | 20.8 (±0.3) | 43.2 (±0.8) | 45 (±1) | 24.0 (±0.3) | 49.0 (±0.4) | 31.2 (±0.4) |
| 2° cycle | 17.0 (±0.5) | 36 (±1) | 71 (±2) | 23.6 (±0.5) | 50 (±1) | 51 (±1) | 32.0 (±0.5) | 66 (±1) | 37.0 (±0.6) |
| 3° cycle | 18.3 (±0.6) | 38 (±1) | 70 (±2) | 24.7 (±0.6) | 50.3 (±1.3) | 51 (±1) | 34.0 (±0.6) | 69 (±1) | 36.4 (±0.7) |
| CYM | ***q*$_e$ (mg g$^{-1}$)** | ***RE%*** | ***DC%*** | ***q*$_e$ (mg g$^{-1}$)** | ***RE%*** | ***DC%*** | ***q*$_e$ (mg g$^{-1}$)** | ***RE%*** | ***DC%*** |
| 1° cycle | 6.3 (±0.9) | 11.8 (±0.2) | 54 (±8) | 13.9 (±0.9) | 26 (±2) | 42 (±3) | 18.8 (±0.8) | 35 (±2) | 34 (±2) |
| 2° cycle | 9.8 (±1.3) | 18 (±2) | 36 (±5) | 18 (±1) | 33 (±2) | 32 (±2) | 24 (±1) | 44 (±2) | 30 (±2) |
| 3° cycle | 10.5 (±1.6) | 21 (±3) | 35 (±5) | 18.9 (±1.5) | 37 (±3) | 32 (±3) | 23 (±2) | 46 (±3) | 31 (±2) |

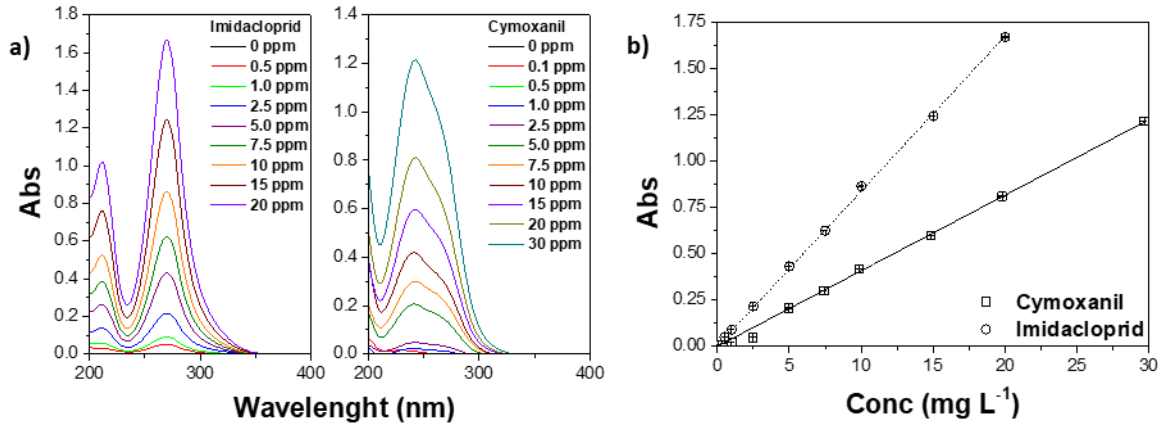


**Figure 1.** Representation of IMD and CYM (a) UV-Vis spectra, and (b) curve of calibration.

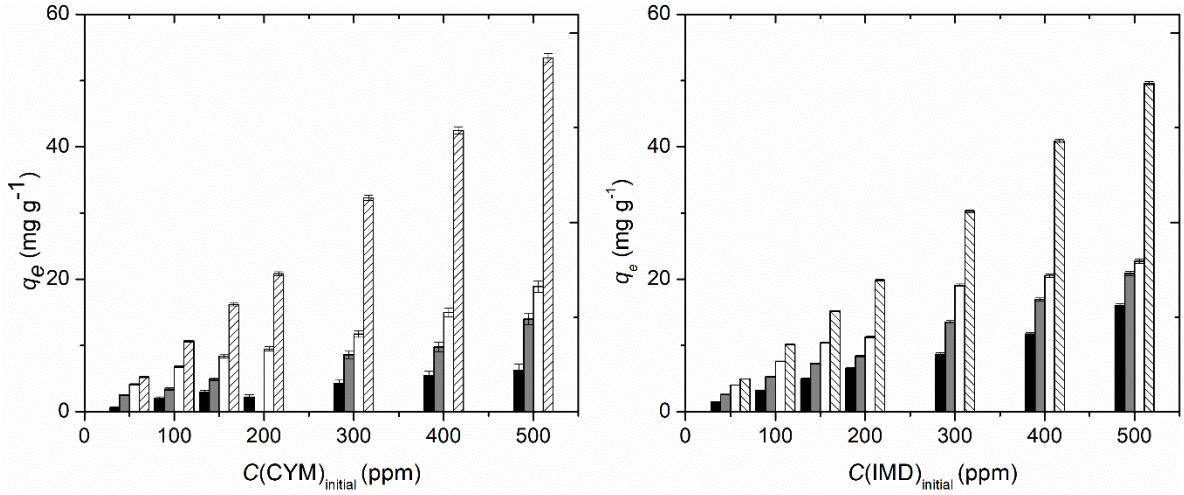


**Figure 2.** Maximum sorbed amount ($q_e$) of CYM (left) and IMD (right) by different adsorbents: PCD (black columns), PCD/AC$_{5\%}$ (grey), PCD/AC$_{10\%}$ (white) and AC (lines).

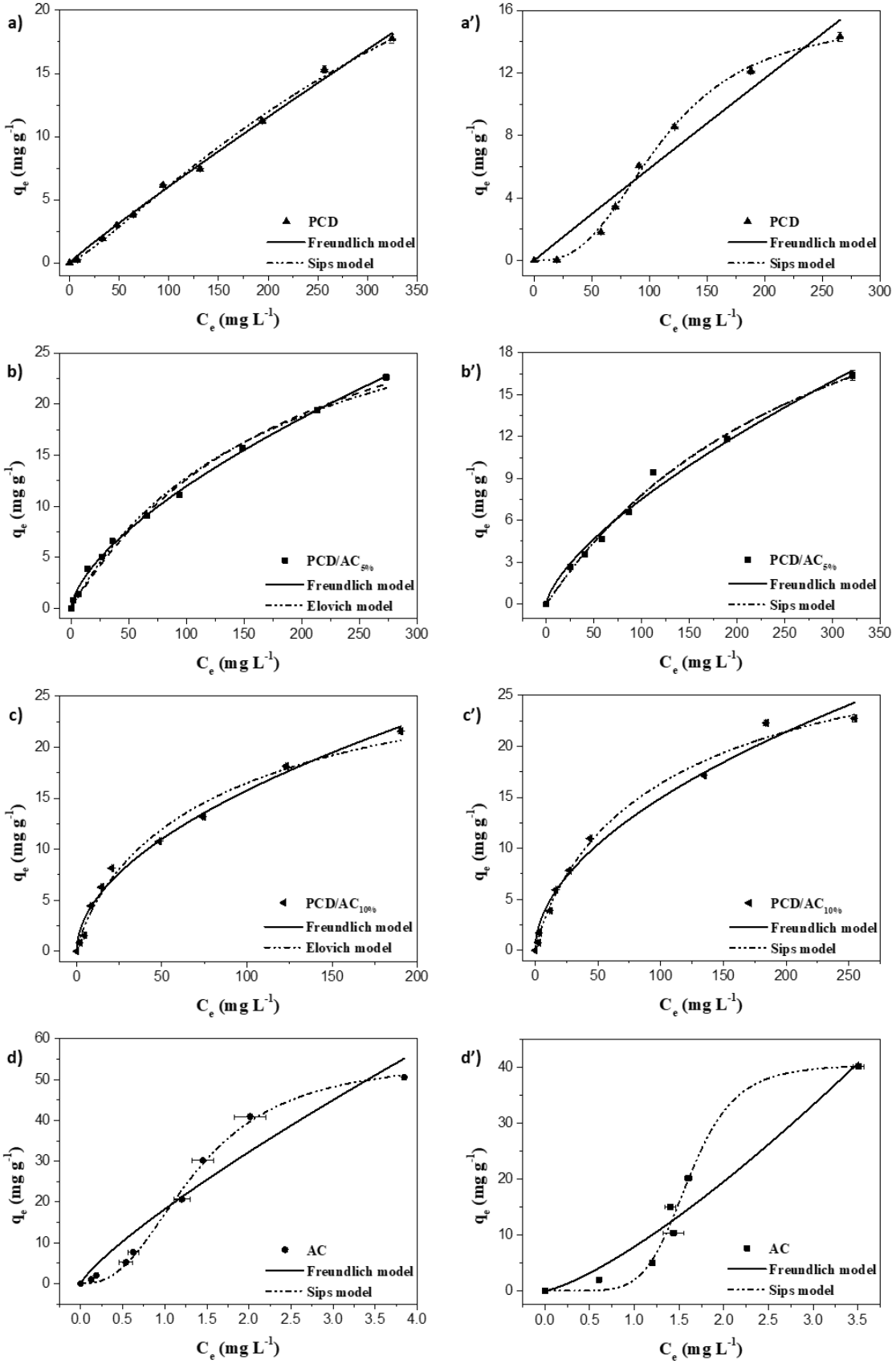


**Figure 3.** Adsorption isotherm of IMD (0-500) ppm onto PCD (a), PCD/AC$_{5\%}$ (b), PCD/AC$_{10\%}$ (c) and AC (d), in 1.0 g $L^{-1}$ urea solution; and onto PCD (a'), PCD/AC$_{5\%}$ (b'), PCD/AC$_{10\%}$ (c') and AC (d'), in 1.0 g $L^{-1}$ NaCl solution, at 25 °C.

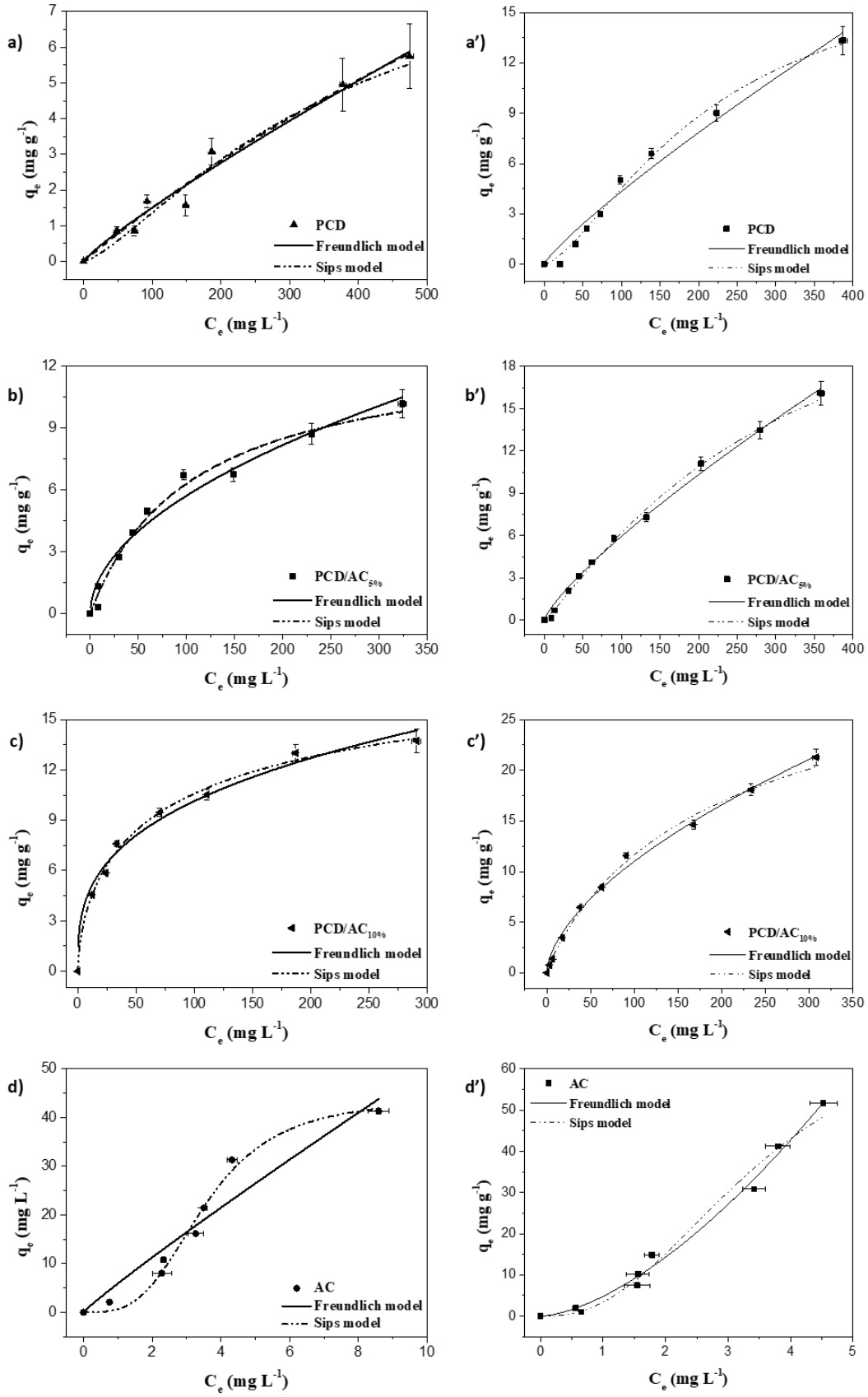


**Fig. S4.** Adsorption isotherm of CYM (0-500) ppm onto PCD (a), PCD/AC$_{5\%}$ (b), PCD/AC$_{10\%}$ (c) and AC (d), in 1.0 g L$^{-1}$ urea solution; and onto PCD (a'), PCD/AC$_{5\%}$ (b'), PCD/AC$_{10\%}$ (c') and AC (d'), in 1.0 g L$^{-1}$ NaCl solution, at 25 °C.