

**Bio-electrochemical system depollution capabilities and monitoring applications: Models, applicability, advanced bio-based concept for predicting pollutant degradation and microbial growth kinetics via gene regulation modelling**

**Table S1:** Nomenclature and model parameter values of Tsipa et al. model

| Symbols              | Description  | Estimated value     | Units                        |
|----------------------|--|---------------------|------------------------------|
| $\alpha_{BenB}$      | BenB degradation and dilution due to cellular volume increase  | 33.352              | $h^{-1}$                     |
| $\alpha_{BenRi}$     | BenRi degradation and dilution due to cellular volume increase | 60                  | $h^{-1}$                     |
| $\alpha_{Pm}$        | mRNA degradation rate of <i>Pm</i>                             | 1.613               | $h^{-1}$                     |
| $\alpha_{PbenA}$     | mRNA degradation rate of <i>PbenA</i>                          | 5.583               | $h^{-1}$                     |
| $\alpha_{PbenR}$     | mRNA degradation rate of <i>PbenR</i>                          | 5.865               | $h^{-1}$                     |
| $\alpha_{Pr}$        | mRNA degradation rate of <i>Pr</i>                             | 2.483               | $h^{-1}$                     |
| $\alpha_{Ps}$        | mRNA degradation rate of <i>Ps</i>                             | 2.107               | $h^{-1}$                     |
| $\alpha_{Pu}$        | mRNA degradation rate of <i>Pu</i>                             | 2.528               | $h^{-1}$                     |
| $\alpha_{XylM}$      | XylM degradation and dilution due to cellular volume increase  | 60                  | $h^{-1}$                     |
| $\alpha_{XylRi}$     | XylRi degradation and dilution due to cellular volume increase | 60                  | $h^{-1}$                     |
| $\alpha_{XylSi}$     | XylSi degradation and dilution due to cellular volume increase | 6                   | $h^{-1}$                     |
| $\alpha_{XylU}$      | XylU degradation and dilution due to cellular volume increase  | 0.056               | $h^{-1}$                     |
| $\beta_b$            | maximum specific growth rate of biomass based on XylM          | 0.087               | $h^{-1}$                     |
| $\beta_{BenB}$       | translation rate based on <i>PbenA</i> mRNA                    | $9.11 \times 10^2$  | $mM h^{-1}$                  |
| $\beta_{BenRi}$      | maximal translation rate of BenRi                              | $24.58 \times 10^2$ | $mM h^{-1}$                  |
| $\beta_{PbenA}$      | maximal mRNA expression of <i>PbenA</i>                        | 52.887              | $h^{-1}$                     |
| $\beta_{PbenR}$      | maximal mRNA expression of <i>PbenR</i>                        | 4.212               | $h^{-1}$                     |
| $\beta_{Pm}$         | maximal expression level of <i>Pm</i>                          | 0.927               | $h^{-1}$                     |
| $\beta_{Pr}$         | maximal expression level of <i>Pr</i>                          | 0.343               | $h^{-1}$                     |
| $\beta_{Ps}$         | maximal expression level of <i>Ps</i>                          | 28.47               | $h^{-1}$                     |
| $\beta_{Pu}$         | maximal expression level of <i>Pu</i>                          | 44.812              | $h^{-1}$                     |
| $\beta_{XylM}$       | translation rate based on <i>Pm</i> mRNA                       | 0.002               | $mM h^{-1}$                  |
| $\beta_{XylSi}$      | translation rate based on <i>Ps</i> mRNA                       | $10.69 \times 10^2$ | $mM h^{-1}$                  |
| $\beta_{XylRi}$      | maximal translation rate of <i>Pr</i> mRNA                     | $5.7 \times 10^2$   | $mM h^{-1}$                  |
| $\beta_{XylU}$       | translation rate based on <i>Pu</i> mRNA                       | $16.98 \times 10^2$ | $mM h^{-1}$                  |
| $\beta_{XylU,m-xyl}$ | maximum <i>m</i> -xylene metabolic quotient based on XylU      | 0.018               | $g_{tol} g_{biomass} h^{-1}$ |
| $\beta_{XylU,tol}$   | maximum toluene metabolic quotient based on XylU               | 0.018               | $g_{tol} g_{biomass} h^{-1}$ |
| $K_{BenB,b}$         | saturation constant of BenB                                    | 19.543              | $mM$                         |
| $K_{BenRa,PbenA}$    | activation coefficient of <i>PbenA</i> by BenRa                | 2.02                | $mM$                         |
| $K_{BenRa,PbenR}$    | activation coefficient of <i>PbenR</i> by BenRa                | 1.645               | $mM$                         |
| $K_{BenRa,Pm}$       | activation coefficient of <i>Pm</i> by BenR                    | 9.208               | $mM$                         |
| $K_{XylM,b}$         | saturation constant of XylM                                    | 25.103              | $mM$                         |

|                   |  |                      |                     |
|-------------------|--|----------------------|---------------------|
| $K_{XylSi}$       | activation coefficient of <i>Pm</i> by XylSi         | 17.984               | mM                  |
| $K_{XylRa,Ps}$    | activation coefficient of <i>Ps</i> by XylRa         | 5.44                 | mM                  |
| $K_{XylRa,Pu}$    | activation coefficient of <i>Pu</i> by XylRa         | 3.626                | mM                  |
| $K_{XylRi}$       | repression coefficient of <i>Pr</i>                  | 11.035               | mM                  |
| $K_{XylU,m-xyl}$  | saturation constant for XylU due to <i>m</i> -xylene | 3.863                | mM                  |
| $K_{XylU,tol}$    | saturation constant for XylU due to toluene          | 3.863                | mM                  |
| $MW_{m-xyl}$      | molecular weight of <i>m</i> -xylene                 | 106.2                | g mol <sup>-1</sup> |
| $MW_{tol}$        | molecular weight of toluene                          | 92.14                | g mol <sup>-1</sup> |
| $\Gamma_{R,BenR}$ | dissociation constant of BenR                        | 53.46                | h <sup>-1</sup>     |
| $\Gamma_{R,XylS}$ | dissociation constant of XylS                        | 37.88                | h <sup>-1</sup>     |
| $\Gamma_{R,XylR}$ | dissociation constant of XylR                        | 4.2 x10 <sup>2</sup> | h <sup>-1</sup>     |

**Table S2:** Parameter values estimated for the double Monod, Mankad and Bungay, SKIP and the sum kinetics with competitive enzymatic interactions models using.

| Symbols           | Description   | Double Monod | Mankad and Bungay | SKIP   | Competitive enzymatic interactions | Units              |
|-------------------|---|--------------|-------------------|--------|------------------------------------|--------------------|
| $I_{m-xyl,tol}$   | degree of inhibition of <i>m</i> -xylene to toluene | -            | -                 | 0.004  | -                                  | -                  |
| $I_{tol,m-xyl}$   | degree of inhibition of toluene to <i>m</i> -xylene | -            | -                 | 0.0003 | -                                  | -                  |
| $K_{m-xyl}$       | saturation constant of <i>m</i> -xylene             | 0.1          | 0.7               | 0.7    | 0.7                                | (mM)               |
| $K_{tol}$         | saturation constant of toluene                      | 0.1          | 0.46              | 0.035  | 0.45                               | (mM)               |
| $\mu_{max}$       | maximal specific growth rate                        | 0.033        | 0.079             | -      | -                                  | (h <sup>-1</sup> ) |
| $\mu_{max,tol}$   | maximal specific growth rate of toluene             | -            | -                 | 0.018  | 0.097                              | (h <sup>-1</sup> ) |
| $\mu_{max,m-xyl}$ | maximal specific growth rate of <i>m</i> -xylene    | -            | -                 | 0.093  | 0.042                              | (h <sup>-1</sup> ) |
| $Y_{m-xyl}$       | yield coefficient of <i>m</i> -xylene               | 0.99         | 0.99              | 0.99   | 0.99                               | (g/g)              |
| $Y_{tol}$         | yield coefficient of toluene                        | 0.99         | 0.99              | 0.99   | 0.99                               | (g/g)              |