Supporting Information Cover Sheet

Selenium biotransformations in engineered aquatic ecosystem for bioremediation of agricultural wastewater via brine shrimp production

Radomir Schmidt[τ1], Prapakorn Tantoyotai[1], Sirine C. Fakra[2], Matthew A. Marcus[2], Soo In Yang[3], Ingrid J. Pickering[3], Gary S. Bañuelos[τ4] , Krassimira R. Hristova[τ1,5*] and John L. Freeman[τ6,7*]

[1]Department of Land, Air and Water Resources, University of California, Davis, California 95616

[2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720

[3]Department of Geological Sciences, University of Saskatchewan, Saskatoon, Saskatchewan S7N 5E2,

[4]United States Department of Agriculture, Agricultural Research Service, SJVASC, Water Management Research Division, Parlier, California 93648

[5]Biological Sciences Department, Marquette University, Milwaukee, Wisconsin 53233

[6]Department of Biology, California State University, Fresno, California 93740

[7]Intrinsyx Technologies Corporation Inc. Space Biosciences Division, NASA Ames Research Center,Moffett Field, CA 94035, USA

[τ] Authors contributed equally to this paper

[*]**Corresponding authors:** John L. Freeman and Krassimira R. Hristova

Fax number: + 1-650-691-9754. E-mail address: John.L.Freeman@NASA.gov

Fax number: +1-414-288-7357. E-mail address: krassimira.hristova@marquette.edu

Supporting Information

S1. Experimental

- 7 pages

S2. Supplemental Tables

- 5 pages
- **Supplemental Table 1.** Experimental methods used in this study.
- **Supplemental Table 2.** Bulk XANES least square fitted results of Se K near-edge spectra shown in the Figure 1.
- **Supplemental Table 3.** SAX-HPLC-ICPMS speciation of soluble Se extracted from ground, protease XIV digested tissues.
- **Supplemental Table 4.** SAX-HPLC-ICPMS speciation of soluble Se extracted from ground, undigested tissues.
- **Supplemental Table 5.** Se speciation in mixed bacterial culture, mixed diatom culture, *E. cinerea* and *A. franciscana* tissue by μXANES spectroscopy Results of the least squares LCF of Se K-edge XANES spectra are shown. The best LCF was obtained by minimizing the normalized sum-squares residuals [NSS = 100 x $\Sigma(\mu_{exp} - \mu_{fit})^2/\Sigma(\mu_{exp})^2$], where μ is the normalized absorbance. Fit error on percentages is ±10%. $SeGSH_2$, SeCys, SeCystine, and gray elemental $Se^{(0)}$ were not detected (empty boxes). Elemental $Se^{(0)}$ occurs in either red or gray forms.

S3. Supplemental Figures

- 7 pages
- **Supplemental Figure 1.** A) Location of the Red Rock Ranch Se remediation pool. Se source and fate in the Central Valley of California indicated by arrows . B) *E. cinera* adults and pupa on an algal mat. C) *A. franciscana* in the RRR pool. D) RRR Se remediation pond. Pond volume was approximately 90 m^3. Maximum Se volatilization rate was 1 mg Se m^{-3} day^{-1}, while maximum Se removal through shrimp harvest was 2 mg Se m^{-3} day^{-1}.
- **Supplemental Figure 2.** Integrated on-farm drainage management (IFDM). Red Rock Ranch (RRR) is a 640 acre farm located in Five Points, CA that practices IFDM. This integrated system cycles drainage water through a series of salt tolerant crops, trees, and ends with the brine shrimp race track with the objective of reusing the saline water to produce marketable crops and novel agricultural products while managing the drainage water directly on site. IFDM is a promising strategy for reducing the volume of contaminated water that is often produced as a consequence of irrigation in the San Joaquin valley while effectively coping with the problems associated with accumulation of high concentrations of naturally occurring salts, boron and selenium.
- **Supplemental Figure 3.** Selenium K near-edge spectra of bacteria/diatom mix (bacteria/diatom), *Picocystis* (microalgae), *Cladophora* (green algae), *Artemia* (brine shrimp), and *Ephydra* (brine fly pupa and larva) are shown in the lower column. The modeled selenium species include: SeO_4^{2-} (selenate), SeO_3^{2-} (selenite), SeOMet (methionine selenoxide), SeMet (selenomethionine), CysSe-

SeCys (selenocystine), $CysSe^-$ (selenocysteinate), Se^0 (elemental selenium). Dimethyl selenoxide spectrum is shown for SeOMet due to their similar atomic environment and spectra. The tick marks on the Y-axis show one absorbance unit. Selenite spectrum is shown in broken lines for clarity.

- **Supplemental Figure 4.** Chromatographic separation and identification using SAX-HPLC-ICPMS of the soluble Se compounds present in organisms living in the agricultural drainage water circulated throughout the engineered RRR brine shrimp race track Se containing peaks, are shown for mixed bacteria (A); mixed diatoms (preliminary) (B); *Picocystis* sp. - pure microalga (C); *A. franciscana* (D); *E. cinerea* larva (E); *E. cinerea* adult (F); standards (G). Undigested (solid line) and proteinase XIV digests (dashed line)
- **Supplemental Figure 5.** Distribution and speciation of Se in a culture of mixed diatoms. mXRF map showing spatial distribution of Se (coded in white) in a smear of mixed diatoms and bacteria (A), mixed diatom culture(B) and microalga *Picocystis* sp. culture (C). Mixed diatom culture shown in (D), and *Picocystis* sp. culture shown in (E).
- **Supplemental Figure 6.** Oxidation of selenomethionine and formation of
- methionine selenoxide by hydroperoxide. This reaction resembles the peroxidase reaction.
- **Supplemental Figure 7.** Total Se concentration in *A. franciscana* dry weight versus total Se concentration in water at the time of *A. franciscana* harvest (A) Water Se concentration –filled triangle; *A. franciscana* tissue Se concentration – empty square. Correlation of *A. franciscana* Se tissue concentration to Se water content (B).