**Appendix A. Supplementary data**

Table S1. Experimental and calculated solvent-water partition coefficients, and the ABSOLV, QSPR, and QCAP solute parameters.

Table S2. Refitted system parameters determined using QCAP solute parameters.

Table S3. Refitted system parameters determined using ABSOLV solute parameters.

Table S4. Refitted system parameters determined using QSPR solute parameters.

Table S5. Summary of the RMSEs of calculations of solvent-water partition coefficients.

Table S6. Experimental and calculated solvent-water partition coefficients, together with estimated solute parameters, for munition constituents and munition-like compounds.

Table S7. Experimental and calculated plant cuticle-water partition coefficients, together with estimated solute parameters.

Figure S1. Dot plot presenting the root mean square errors (RMSEs) of the residuals (log calculated - log observed partition coefficients) for solvent-water systems ordered by the number of solutes in each system.

Figure S2. Predicted versus observed partition coefficients for wet octanol-water.

Figure S3. Pairs plot of QCAP solute parameters.

Figure S4. Pairs plot of the adjusted QCAP solute parameters.

Comparison of refitted models based on QCAP and adjusted QCAP solute parameters.