Table 3. Major advantages and limitations of in silico modeling in AA

Advantages	Limitations
Offers a cost-effective way either to prioritize chemicals of concern or to assess potential alternatives for which there often are no data	Variable predictive ability of models
Allows for modeling of initiating events	No institution to monitor validation
Can inform the design of safer chemicals	Some models are proprietary, which limits access and impairs transparency
Fast	Because many models are based upon experimental results regarding a set of structurally similar data-rich chemicals, model applicability is limited to data-poor chemicals with similar structure
Does not require chemical sample for testing	Can be more difficult to develop if the mechanistic basis is unknown
Computational predictions of environmental fate and degradation allow exposure to be estimated without expensive monitoring and can predict bio-persistence and concentrations in the environment	Model quality varies considerably and model performance can be manipulated by choosing particular chemicals
—	For some chemicals there may be a lack of quality data to develop and use models

AA = alternatives analysis.