Environmental Science & Technology

Addition/Correction

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Correction to Screening Chemicals for Estrogen Receptor Bioactivity Using a Computational Model

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Environ. Sci. Technol. **2015**, *49* (14), 8804−8814; DOI: 10.1021/acs.est.5b02641.

In our paper, "Screening Chemicals for Estrogen Receptor Bioactivity Using a Computational Model", errors were made calculating the performance values for "GL uterotrophic studies" reported in Table 4 due to a rounding error in the analysis. Initially, positive activity calls were given to reference chemicals with AUC scores rounded to ≥0.1 (rounded ≥0.0501) and the activity calls were used to determine assay performance metrics. During a re-examination of the data, we determined that ToxCast agonist ER AUC values were not similarly rounded for the larger set of 103 chemicals with guideline-like (GL) uterotrophic studies (which also include the 43 in vivo reference chemicals). The consequence of this correction is an increase in the "# True Pos" and "# False Pos" and a decrease in "# False Neg" for only GL uterotrophic studies when compared to the original values published. It does not affect other figures or tables, nor does it change the larger conclusions of the paper. Below is a revised version of Table 4 and the table heading.

Table 4. Performance Based Validation of the ToxCast ER Model Based on 18 High-Throughput in Vitro Assays Measuring Potential Estrogen Receptor (ER) Agonist Activities and in Vitro Reference Chemicals[a]

performance	in vitro reference chemicals	in vivo reference chemicals	GL uterotrophic studies	tier 1 studies
# true pos	26 (25)	29 (29)	52(42)	0 (0)
# true neg	11 (11)	8 (8)	33 (33)	41 (41)
# false pos	1 (0)	5 (1)	15 (8)	8 (0)
# false neg	2 (2)	1 (1)	5 (5)	0 (0)
accuracy	0.93 (0.95)	0.86 (0.95)	0.81 (0.85)	0.84 (1.0)
sensitivity	0.93 (0.93)	0.97 (0.97)	0.91 (0.89)	0 (0)
specificity	0.92 (1.0)	0.67 (0.89)	0.69 (0.80)	0.84 (1.0)

[a](See text for detailed explanation). Chemicals with ToxCast agonist ER model scores (AUC) ≥ 0.0501 were classified as positive, those with AUC = 0 (and values <0.001 were truncated as 0) were classified as negative, and chemicals with intermediate AUC values (0 < AUC < 0.0501) were classified as inconclusive. In each column, in vitro inconclusive chemicals included in the positive class (values outside of parentheses), or excluded from the positives (values inside parentheses).

This error changes values reported in the last two sentences of the second paragraph on page 8809 to

"The overall accuracy of the ToxCast ER model when compared to uterotrophic guideline-like studies was 81% (83/103; Table 4). If inconclusive calls are excluded from analyses, concordance between the ToxCast ER model bioactivity and the in vivo guideline-like uterotrophic studies for 75 chemicals with ToxCast positive (≥0.1) or negative (0) model scores was 85% (75/88; Table 4)."

Published: August 2, 2017

DOI: 10.1021/acs.est.7b03317
Environ. Sci. Technol. 2017, 51, 9415−9415