Table 3. Comparison of p53RE qHTS Assay Activity Calls and QSAR Model Predictions for Bacterial Mutagenicity or Traditional Genotoxicity Assay Results

	QSAR		Traditional genotoxicity assays		
	BM (CASE Ultra QSAR)	BM (Leadscope QSAR)	BM (no S9)	CA (no S9)	MN (adjusted)
Sensitivity	0.11 [0.09–0.12]	0.11 [0.09–0.13]	0.12 [0.09–0.15]	0.11 [0.08–0.15]	0.17 [0.1–0.24]
Specificity	0.97 [0.96–0.97]	0.97 [0.96–0.98]	0.96 [0.94–0.97]	0.96 [0.94–0.98]	0.96 [0.93–0.98]
PPV [a]	0.48 [0.42–0.53]	0.53 [0.46–0.59]	0.68 [0.58–0.78]	0.71 [0.57–0.83]	0.55 [0.39–0.71]
NPV [b]	0.78 [0.77–0.79]	0.78 [0.76–0.79]	0.6 [0.57–0.63]	0.55 [0.51–0.59]	0.79 [0.75–0.82]
True positive	136	121	60	36	21
False positive	149	108	28	15	17
False negative	1147	997	430	289	100
True negative	4153	3465	632	356	377

a   Positive predictive value.

b   Negative predictive value.

True positive: chemicals active in both the p53RE assay and the specific traditional genotoxicity assay.

False positive: chemicals active in the p53RE assay but inactive in the specific traditional genotoxicity assay.

False negative: chemicals inactive in the p53RE assay but active in the specific traditional genotoxicity assay.

True negative: chemicals inactive in both the p53RE assay and the specific traditional genotoxicity assay.