Table 1. Performance of QSARMOA Model and Assay Alone Predictions

MOA ID	assay end point	Tox21 Assay Name	$QSAR_{MOA}$ model
MOA-1	aryl hydrocarbon receptor	AHR	0.663 (0.033)
MOA-2	androgen receptor	AR-bla-agonist	0.646 (0.032)
MOA-3	androgen receptor	AR-bla-antagonist	0.657 (0.034)
MOA-4	antioxidant response element	ARE-bla	0.649 (0.039)
MOA-5	AR (MDA cell line)	AR-mda-kb2-luc-agonist	0.653 (0.032)
MOA-6	AR (MDA cell line)	AR-mda-kb2-luc-antagonist	0.671 (0.032)
MOA-7	aromatase inhibitors	aromatase	0.651 (0.035)
MOA-8	estrogen receptor alpha	ER-bla-antagonist	0.656 (0.035)
MOA-9	ER-alpha (BG1 cell line)	ER-luc-bg1–4e2-agonist	0.633 (0.036)
MOA-10	ER-alpha (BG1 cell line)	ER-luc-bg1–4e2-antagonist	0.672 (0.032)
MOA-11	thyroid receptor	gh3-tre-antagonist	0.671 (0.037)
MOA-12	glucocorticoid receptor	GR-hela-bla-antagonist	0.652 (0.034)
MOA-13	heat shock response	HSE-bla	0.647 (0.035)
MOA-14	mitochondrial toxicity	Mitotox	0.634 (0.036)
MOA-15	p53	p53	0.658 (0.033)
MOA-16	peroxisome proliferator-activated receptor gamma	PPARG-bla-agonist	0.677 (0.033)
MOA-17	peroxisome proliferator-activated receptor gamma	PPARG-bla-antagonist	0.636 (0.038)

Quantitative Structure–Activity Relationships (QSARs)

One of the key strategies in this study was to conduct a direct comparison to the QSAR approach that was reported previously.