APPENDIX D

Details of all active assays by food dye. Inactive assays are not included. Definitions of column headings are below.

Column Identifiers

ASSAY NAME	name of assay
VIABILITY ASSAY	non-receptor based assay; indicates cytotoxicity
DESCRIPTION	full description of assay
GENE_NAME	gene name of molecular target
AOP	Adverse outcome pathway
EVENT	key event in adverse outcome pathway
AC50	chemical concentration where 50% of the maximum response is achieved
LOGAC50	log concentration at half maximal activity
FLAGS	flag for potential false positive and false negative findings based on methods
INTENDED_TARGET_FAMILY	biological grouping of assays

FD&C Blue No. 1

ASSAY NAME	IN OUR SELECTED SUBSET	VIABILITY ASSAY	DESCRIPTION	GENE_NAME	AC50	LOGAC50	FLAGS	INTENDED_TARGET_FAMILY
ACEA_AR_agonist_80hr	NO	NO	not applicable	androgen receptor	10.2	1.01	Less than 50% efficacy: Borderline active: Only highest conc above baseline, active	nuclear receptor
ATG_HIF1a_CIS_dn	NO	NO	not applicable	hypoxia inducible factor 1, alpha subunit (basic helix-loop-helix transcription factor)	3.07	0.486	Hit-call potentially confounded by overfitting: Borderline active	histones
BSK_hDFCGF_IP10_down	YES	NO	not applicable	chemokine (C-X-C motif) ligand 10	11.9	1.07	Less than 50% efficacy: Only highest conc above baseline, active	cell cycle
BSK_SAg_PBMCCytotoxicity_down	NO	YES	not applicable	not applicable	9.50	0.978	Less than 50% efficacy: Only highest conc above baseline, active	cell cycle
BSK_SAg_Proliferation_down	NO	YES	not applicable	not applicable	10.7	1.03	Less than 50% efficacy: Only highest conc above baseline, active	cell cycle
NCCT_HEK293T_CellTiterGLO	NO	NO	not applicable	not applicable	4.32	0.635	NONE	nuclear receptor
NCCT_QuantiLum_inhib_2_dn	NO	NO	not applicable	not applicable	18.2	1.26	NONE	nuclear receptor
NCCT_QuantiLum_inhib_dn	YES	NO	not applicable	not applicable	3.94	0.595	NONE	oxidoreductase
NCCT_TPO_AUR_dn	YES	NO	not applicable	thyroid peroxidase	12.6	1.10	NONE	oxidoreductase
NVS_ADME_hCYP2C9	NO	NO	not applicable	cytochrome P450, family 2, subfamily C, polypeptide 9	1.56	0.194	Less than 50% efficacy	hydrolase
NVS_ENZ_hBACE	NO	NO	not applicable	beta-site APP-cleaving enzyme 1	14.2	1.15	NONE	nuclear receptor
NVS_ENZ_hCASP4	NO	NO	not applicable	caspase 4, apoptosis-related cysteine peptidase	4.28	0.631	Less than 50% efficacy	cell cycle
NVS_ENZ_hCASP5	NO	NO	not applicable	caspase 5, apoptosis-related cysteine peptidase	4.38	0.642	NONE	dna binding
NVS_ENZ_hCK1D_Activator	NO	NO	not applicable	casein kinase 1, delta	0.765	-0.116	Hit-call potentially confounded by overfitting: Noisy data	cell cycle
NVS_ENZ_hCSF1R	NO	NO	not applicable	colony stimulating factor 1 receptor	2.51	0.399	NONE	cyp
NVS_ENZ_hDUSP3	NO	NO	not applicable	dual specificity phosphatase 3	21.3	1.33	NONE	cell cycle
NVS_ENZ_hEGFR	NO	NO	not applicable	epidermal growth factor receptor	11.5	1.06	NONE	protease
NVS_ENZ_hElastase	NO	NO	not applicable	elastase, neutrophil expressed	2.45	0.388	Less than 50% efficacy	cell cycle
NVS_ENZ_hJak2	NO	NO	not applicable	Janus kinase 2	11.9	1.08	NONE	protease
NVS_ENZ_hMMP2	NO	NO	not applicable	matrix metallopeptidase 2 (gelatinase A, 72kDa gelatinase, 72kDa type IV collagenase)	9.36	0.972	Less than 50% efficacy	cell cycle
NVS_ENZ_hMMP3	NO	NO	not applicable	matrix metallopeptidase 3 (stromelysin 1, progelatinase)	15.6	1.19	NONE	protease
NVS_ENZ_hPPP1CA	NO	NO	not applicable	protein phosphatase 1, catalytic subunit, alpha isozyme	6.21	0.793	Less than 50% efficacy	cell cycle
NVS_ENZ_hPTPN14	NO	NO	not applicable	protein tyrosine phosphatase, non-receptor type 14	8.99	0.954	Less than 50% efficacy	cell cycle
NVS_GPCR_h5HT7	YES	NO	not applicable	5-hydroxytryptamine (serotonin) receptor 7, adenylate cyclase-coupled	9.37	0.972	Less than 50% efficacy	gpcr
NVS_GPCR_hTXA2	NO	NO	not applicable	thromboxane A2 receptor	7.41	0.870	NONE	kinase
NVS_NR_cAR	YES	NO	710	androgen receptor	16.8	1.22	Less than 50% efficacy	nuclear receptor
NVS_NR_hGR	YES	NO	not applicable	nuclear receptor subfamily 3, group C, member 1 (glucocorticoid receptor)	10.5	1.02	NONE	nuclear receptor
NVS_NR_rAR	YES	NO	726	androgen receptor	9.53	0.979	NONE	nuclear receptor
OT_NURR1_NURR1RXRa_0480	NO	NO	not applicable	retinoid X receptor, alpha	30.0	1.48	Less than 50% efficacy: Borderline active	cell cycle
OT_NURR1_NURR1RXRa_1440	NO	NO	not applicable	retinoid X receptor, alpha	28.9	1.46	Only highest conc above baseline, active	nuclear receptor
TOX21_AhR_LUC_Agonist_viability	NO	YES	not applicable	not applicable	33.1	1.52	NONE	cell cycle
TOX21_AP1_BLA_Agonist_ch2	NO	NO	not applicable	not applicable	36.7	1.56	Less than 50% efficacy: Borderline active: Only highest conc above baseline, active	cell cycle
TOX21_AP1_BLA_Agonist_ratio	NO	NO	not applicable	FBJ murine osteosarcoma viral oncogene homolog|jun proto-oncogene	32.8	1.52	Only highest conc above baseline, active: Less than 50% efficacy: Borderline active	cell cycle
TOX21_AP1_BLA_Agonist_viability	NO	YES	not applicable	not applicable	33.4	1.52	Less than 50% efficacy	cell cycle
TOX21_AR_BLA_Antagonist_viability	NO	YES	not applicable	not applicable	26.4	1.42	Less than 50% efficacy	cell cycle
TOX21_AR_LUC_MDAKB2_Agonist2_viability	NO	YES	not applicable	not applicable	31.2	1.49	NONE	cell cycle
TOX21_AR_LUC_MDAKB2_Antagonist	YES	NO	not applicable	androgen receptor	9.37	0.972	NONE	cell cycle
TOX21_AR_LUC_MDAKB2_Antagonist_Specificity	YES	NO	765	androgen receptor	16.9	1.23	NONE	nuclear receptor
TOX21_AR_LUC_MDAKB2_Antagonist_Specificity_viability	NO	YES	not applicable	not applicable	54.2	1.73	NONE	cell cycle
TOX21_AR_LUC_MDAKB2_Antagonist_viability	NO	YES	not applicable	not applicable	32.2	1.51	Less than 50% efficacy	cell cycle
TOX21_ARE_BLA_agonist_viability	NO	YES	not applicable	not applicable	34.1	1.53	Less than 50% efficacy	cell cycle
TOX21_Aromatase_Inhibition	NO	NO	not applicable	cytochrome P450, family 19, subfamily A, polypeptide 1	20.5	1.31	NONE	oxidoreductase
TOX21_Aromatase_Inhibition_viability	NO	YES	not applicable	not applicable	34.4	1.54	NONE	cell cycle
TOX21_CAR_Agonist_viabillity	NO	YES	not applicable	not applicable	36.9	1.57	Less than 50% efficacy	cell cycle

FD&C Blue No. 1

ASSAY NAME	IN OUR SELECTED SUBSET	VIABILITY ASSAY	DESCRIPTION	GENE_NAME	AC50	LOGAC50	FLAGS	INTENDED_TARGET_FAMILY
TOX21_CAR_Antagonist	NO	NO	not applicable	nuclear receptor subfamily 1, group I, member 3	18.8	1.27	NONE	kinase
TOX21_CAR_Antagonist_viability	NO	YES	not applicable	not applicable	40.1	1.60	NONE	cell cycle
TOX21_DT40	YES	NO	not applicable	not applicable	15.1	1.18	NONE	oxidoreductase
TOX21_DT40_100	YES	NO	not applicable	not applicable	15.4	1.19	NONE	oxidoreductase
TOX21_DT40_657	YES	NO	not applicable	not applicable	23.4	1.37	NONE	phosphatase
TOX21_ELG1_LUC_Agonist_viability	NO	YES	not applicable	not applicable	39.4	1.60	Less than 50% efficacy	cell cycle
TOX21_ERa_LUC_BG1_Agonist_Counter screen_viability	NO	YES	not applicable	not applicable	21.5	1.33	NONE	cell cycle
TOX21_ERa_LUC_BG1_Antagonist	YES	NO	not applicable	estrogen receptor 1	16.3	1.21	NONE	nuclear receptor
TOX21_ERa_LUC_BG1_Antagonist_Specificity	YES	NO	789	estrogen receptor 1	20.4	1.31	NONE	nuclear receptor
TOX21_ERa_LUC_BG1_Antagonist_Specificity_viability	NO	YES	not applicable	not applicable	41.3	1.62	NONE	cell cycle
TOX21_ERa_LUC_BG1_Antagonist_viability	NO	YES	not applicable	not applicable	26.9	1.43	NONE	cell cycle
TOX21_ERb_BLA_Agonist_viability	NO	YES	not applicable	not applicable	31.7	1.50	Less than 50% efficacy	cell cycle
TOX21_ERb_BLA_Antagonist_viability	NO	YES	not applicable	not applicable	32.9	1.52	Less than 50% efficacy	cell cycle
TOX21_ERR_Antagonist	YES	NO	not applicable	estrogen-related receptor alpha	16.2	1.21	NONE	nuclear receptor
TOX21_ERR_viability	NO	NO	not applicable	not applicable	38.4	1.58	Less than 50% efficacy	cell cycle
TOX21_H2AX_HTRF_CHO_Agonist_ch1	NO	NO	not applicable	not applicable	28.9	1.46	Less than 50% efficacy	cell cycle
TOX21_H2AX_HTRF_CHO_Agonist_ratio	NO	NO	not applicable	H2A histone family, member X	27.9	1.45	Noisy data	DNA binding
TOX21_H2AX_HTRF_CHO_viability	NO	YES	not applicable	not applicable	25.7	1.41	NONE	cell cycle
TOX21_HDAC_Inhibition	NO	not applicable	not applicable	histone deacetylase 1	5.00	0.699	NONE	protease
TOX21_HDAC_Inhibition_viability	NO	YES	not applicable	not applicable	10.8	1.03	NONE	cell cycle
TOX21_HRE_BLA_Agonist_viability	NO	YES	not applicable	not applicable	27.1	1.43	Less than 50% efficacy	cell cycle
TOX21_MMP_viability	NO	YES	not applicable	not applicable	44.0	1.64	Less than 50% efficacy: Only highest conc above baseline, active	cell cycle
TOX21_NFkB_BLA_agonist_viability	NO	YES	not applicable	not applicable	24.0	1.38	NONE	cell cycle
TOX21_p53_BLA_p2_viability	NO	YES	not applicable	not applicable	27.5	1.44	Less than 50% efficacy: Borderline active	cell cycle
TOX21_p53_BLA_p4_viability	NO	YES	not applicable	not applicable	40.3	1.61	Less than 50% efficacy	cell cycle
TOX21_PGC_ERR_Antagonist	YES	NO	not applicable	estrogen-related receptor alpha	8.00	0.903	NONE	gpcr
TOX21_PGC_ERR_viability	NO	YES	not applicable	not applicable	30.6	1.49	Less than 50% efficacy	cell cycle
TOX21_PPARd_BLA_Agonist_viability	NO	YES	not applicable	not applicable	30.7	1.49	Less than 50% efficacy: Borderline active: Only highest conc above baseline, active	cell cycle
TOX21_PR_BLA_AGONIST_VIABILITY	NO	YES	not applicable	not applicable	1.33	5.54	Only highest conc above baseline, active: Borderline active: Less than 50% efficacy	cell cycle
TOX21_PR_BLA_ANTAGONIST_VIABILITY	NO	YES	not applicable	not applicable	1.71	5.48	Borderline active: Less than 50% efficacy	cell cycle
TOX21_RAR_LUC_Agonist_viability	NO	YES	not applicable	not applicable	18.8	1.27	NONE	cell cycle
TOX21_RAR_LUC_Antagonist	NO	NO	not applicable	retinoic acid receptor, alpha	15.7	1.20	NONE	background measurement
TOX21_RAR_LUC_Antagonist_viability	NO	YES	not applicable	not applicable	20.4	1.31	NONE	cell cycle
TOX21_RORg_LUC_CHO_Antagonist	NO	NO	not applicable	RAR-related orphan receptor C	7.18	0.856	Borderline active	cell cycle
TOX21_RORg_LUC_CHO_Antagonist_viability	NO	YES	not applicable	not applicable	9.87	0.994	NONE	cell cycle
TOX21_RXR_BLA_Agonist_ratio	NO	NO	not applicable	retinoid X receptor, alpha	11.7	1.07	NONE	protease
TOX21_SSH_3T3_GLI3_Agonist_viability	NO	YES	not applicable	not applicable	26.0	1.42	NONE	cell cycle
TOX21_SSH_3T3_GLI3_Antagonist	NO	NO	not applicable	GLI family zinc finger 3	3.96	0.598	NONE	nuclear receptor
TOX21_SSH_3T3_GLI3_Antagonist_viabiity	NO	YES	not applicable	not applicable	21.1	1.32	NONE	cell cycle
TOX21_TR_LUC_GH3_Antagonist	YES	NO	804	thyroid hormone receptor beta	11.2	1.05	NONE	nuclear receptor
TOX21_TR_LUC_GH3_Antagonist_viability	NO	YES	not applicable	not applicable	50.7	1.71	NONE	cell cycle
TOX21_TSHR_Antagonist_ch2	YES	NO	not applicable	not applicable	2.89	0.461	NONE	background measurement
TOX21_TSHR_Antagonist_ratio	YES	NO	not applicable	not applicable	24.0	1.38	NONE	cell cycle
TOX21_TSHR_HTRF_Agonist_ch1	YES	NO	not applicable	not applicable	26.8	1.43	NONE	background measurement
TOX21_VDR_BLA_Agonist_viability	NO	YES	not applicable	not applicable	26.1	1.42	Less than 50% efficacy: Borderline active	cell cycle
TOX21_VDR_BLA_antagonist_viability	NO	YES	not applicable	not applicable	17.1	1.23	Less than 50% efficacy: Borderline active	cell cycle

FD&C Blue No. 2

ASSAY NAME	IN OUR SELECTED SUBSET	VIABILITY ASSAY	DESCRIPTION	GENE_NAME	AC50	LOGAC50	FLAGS	INTENDED_TARGET_FAMILY
ATG_Ahr_CIS_up	YES	NO	not applicable	aryl hydrocarbon receptor	34.1	1.53	NONE	dna binding
NVS_NR_cAR	YES	NO	710	androgen receptor	36.9	1.57	Less than 50% efficacy: Hit-call potentially confounded by overfitting: Only highest conc above baseline, active	nuclear receptor
TOX21_DT40	YES	NO	not applicable	not applicable	29.9	1.48	Less than 50% efficacy	cell cycle
TOX21_DT40_100	YES	NO	not applicable	not applicable	41.6	1.62	Less than 50% efficacy	cell cycle
TOX21_DT40_657	YES	NO	not applicable	not applicable	33.9	1.53	NONE	cell cycle
TOX21_H2AX_HTRF_CHO_Agonist_ratio	NO	NO	not applicable	H2A histone family, member X	270	2.43	Less than 50% efficacy	histones
TOX21_HDAC_Inhibition	NO	NO	not applicable	histone deacetylase 1	63.1	1.80	NONE	hydrolase
TOX21_HDAC_Inhibition_viability	NO	YES	not applicable	not applicable	57.7	1.76	Less than 50% efficacy	cell cycle
TOX21_p53_BLA_p4_ch2	NO	NO	not applicable	not applicable	1.46e-4	-3.84	AC50 less than lowest concentration tested: Gain AC50 < lowest conc & loss AC50 < mean conc	background measurement
TOX21_p53_BLA_p4_ratio	NO	NO	not applicable	not applicable	1.21e-5	-4.92	AC50 less than lowest concentration tested: Less than 50% efficacy: Gain AC50 < lowest conc & loss AC50 < mean conc	DNA binding
TOX21_PGC_ERR_Antagonist	YES	NO	not applicable	estrogen-related receptor alpha	91.5	1.96	NONE	nuclear receptor
TOX21_RAR_LUC_Agonist_viability	NO	YES	not applicable	not applicable	64.6	1.81	Less than 50% efficacy	cell cycle
TOX21_RAR_LUC_Antagonist_viability	NO	YES	not applicable	not applicable	72.5	1.86	Less than 50% efficacy: Borderline active	cell cycle
TOX21_RORg_LUC_CHO_Antagonist_viability	NO	YES	not applicable	not applicable	38.4	1.58	Less than 50% efficacy	cell cycle
TOX21_RT_HEPG2_FLO_08hr_viability	NO	YES	not applicable	not applicable	0.470	-0.328	Only one conc above baseline, active: Hit-call potentially confounded by overfitting: Less than 50% efficacy	cell cycle
TOX21_RT_HEPG2_FLO_32hr_ctrl_viability	NO	YES	not applicable	not applicable	0.470	-0.328	Only one conc above baseline, active	cell cycle
TOX21_TR_LUC_GH3_Antagonist	YES	NO	804	thyroid hormone receptor beta	4.53e-5	-4.34	AC50 less than lowest concentration tested: Less than 50% efficacy: Gain AC50 < lowest conc & loss AC50 < mean conc: Borderline active: Only one conc above baseline, active	nuclear receptor
TOX21_TSHR_Antagonist_ch2	YES	NO	not applicable	not applicable	36.4	1.56	NONE	background measurement
TOX21_TSHR_Antagonist_ratio	YES	NO	not applicable	thyroid stimulating hormone receptor	62.2	1.79	NONE	nuclear receptor

FD&C Green No. 3

ASSAY NAME	IN OUR SELECTED SUBSET	VIABILITY ASSAY	DESCRIPTION	GENE_NAME	AC50	LOGAC50	FLAGS	INTENDED_TARGET_FAMILY
ACEA_AR_agonist_80hr	NO	NO	not applicable	androgen receptor	0.190	-0.721	Less than 50% efficacy: Borderline active	nuclear receptor
ATG_Ahr_CIS_up	YES	NO	not applicable	aryl hydrocarbon receptor	31.1	1.49	NONE	dna binding
ATG_ERa_TRANS_up	YES	NO	117	estrogen receptor 1	25.7	1.41	Hit-call potentially confounded by overfitting: Borderline active: Only one conc above baseline, active	nuclear receptor
ATG_ERE_CIS_up	YES	NO	75	estrogen receptor 1	14.5	1.16	Hit-call potentially confounded by overfitting: Borderline active: Only one conc above baseline, active	nuclear receptor
ATG_NRF2_ARE_CIS_up	YES	NO	not applicable	nuclear factor, erythroid 2-like 2	32.6	1.51	Hit-call potentially confounded by overfitting: Borderline active: Only one conc above baseline, active	dna binding
ATG_PPRE_CIS_up	YES	NO	102	peroxisome proliferator-activated receptor alpha	18.4	1.26	Hit-call potentially confounded by overfitting	nuclear receptor
ATG_RARb_TRANS_dn	NO	NO	not applicable	retinoic acid receptor, beta	9.72	0.987	Hit-call potentially confounded by overfitting: Borderline active	nuclear receptor
NCCT_HEK293T_CellTiterGLO	NO	NO	not applicable	not applicable	9.13	0.960	NONE	cell cycle
NCCT_QuantiLum_inhib_2_dn	NO	NO	not applicable	not applicable	5.08	0.706	NONE	oxidoreductase
NCCT_TPO_AUR_dn	YES	NO	not applicable	thyroid peroxidase	17.1	1.23	NONE	oxidoreductase
NVS_NR_cAR	YES	NO	710	androgen receptor	13.2	1.12	NONE	nuclear receptor
NVS_NR_hFXR_Agonist	NO	NO	715	nuclear receptor subfamily 1, group H, member 4	24.5	1.39	Hit-call potentially confounded by overfitting: Only highest conc above baseline, active	nuclear receptor
NVS_NR_hGR	YES	NO	not applicable	nuclear receptor subfamily 3, group C, member 1 (glucocorticoid receptor)	10.6	1.03	NONE	nuclear receptor
NVS_NR_hPPARg	NO	NO	719	peroxisome proliferator-activated receptor gamma	11.2	1.05	NONE	nuclear receptor
NVS_NR_hPXR	NO	NO	not applicable	nuclear receptor subfamily 1, group I, member 2	2.40	0.381	NONE	nuclear receptor
NVS_NR_hRAR_Antagonist	NO	NO	not applicable	retinoic acid receptor, alpha	6.57	0.818	NONE	nuclear receptor
NVS_NR_hTRa_Antagonist	YES	NO	724	thyroid hormone receptor, alpha	5.75	0.759	NONE	nuclear receptor
NVS_NR_rAR	YES	NO	726	androgen receptor	5.92	0.773	NONE	nuclear receptor
OT_NURR1_NURR1RXRa_1440	NO	NO	not applicable	retinoid X receptor, alpha	21.6	1.33	Less than 50% efficacy: Only highest conc above baseline, active	nuclear receptor
TOX21_AhR_LUC_Agonist_viability	NO	YES	not applicable	not applicable	28.9	1.46	NONE	cell cycle
TOX21_AP1_BLA_Agonist_viability	NO	YES	not applicable	not applicable	27.9	1.45	Less than 50% efficacy	cell cycle
TOX21_AR_BLA_Antagonist_viability	NO	YES	not applicable	not applicable	18.5	1.27	Less than 50% efficacy	cell cycle
TOX21_AR_LUC_MDAKB2_Agonist2_viability	NO	YES	not applicable	not applicable	21.3	1.33	NONE	cell cycle
TOX21_AR_LUC_MDAKB2_Antagonist	YES	NO	not applicable	androgen receptor	6.35	0.803	NONE	nuclear receptor
TOX21_AR_LUC_MDAKB2_Antagonist_Specificity	YES	NO	765	androgen receptor	19.2	1.28	NONE	nuclear receptor
TOX21_AR_LUC_MDAKB2_Antagonist_Specificity_viability	NO	YES	not applicable	not applicable	38.5	1.59	NONE	cell cycle
TOX21_AR_LUC_MDAKB2_Antagonist_viability	NO	YES	not applicable	not applicable	24.5	1.39	NONE	cell cycle
TOX21_ARE_BLA_agonist_viability	NO	YES	not applicable	not applicable	28.5	1.45	Less than 50% efficacy	cell cycle
TOX21_Aromatase_Inhibition	NO	NO	not applicable	cytochrome P450, family 19, subfamily A, polypeptide 1	16.2	1.21	NONE	cyp
TOX21_Aromatase_Inhibition_viability	NO	YES	not applicable	not applicable	24.9	1.40	NONE	cell cycle
TOX21_CAR_Agonist_viabillity	NO	YES	not applicable	not applicable	26.4	1.42	NONE	cell cycle
TOX21_CAR_Antagonist	NO	NO	not applicable	nuclear receptor subfamily 1, group I, member 3	10.3	1.01	NONE	nuclear receptor
TOX21_CAR_Antagonist_viability	NO	YES	not applicable	not applicable	29.4	1.47	NONE	cell cycle
TOX21_DT40	YES	NO	not applicable	not applicable	14.9	1.17	NONE	cell cycle
TOX21_DT40_100	YES	NO	not applicable	not applicable	11.7	1.07	NONE	cell cycle
TOX21_DT40_657	YES	NO	not applicable	not applicable	8.28	0.918	NONE	cell cycle
TOX21_ELG1_LUC_Agonist_viability	NO	YES	not applicable	not applicable	34.5	1.54	NONE	cell cycle
TOX21_ERa_BLA_Antagonist_viability	NO	YES	not applicable	not applicable	30.6	1.49	Less than 50% efficacy: Only highest conc above baseline, active	cell cycle
TOX21_ERa_LUC_BG1_Agonist_Counterscreen_viability	NO	YES	not applicable	not applicable	16.2	1.21	NONE	cell cycle
TOX21_ERa_LUC_BG1_Antagonist	YES	NO	not applicable	estrogen receptor 1	12.1	1.08	NONE	nuclear receptor
TOX21_ERa_LUC_BG1_Antagonist_Specificity	YES	NO	789	estrogen receptor 1	20.2	1.31	NONE	nuclear receptor
TOX21_ERa_LUC_BG1_Antagonist_Specificity_viability	NO	YES	not applicable	not applicable	36.8	1.57	NONE	cell cycle
TOX21_ERa_LUC_BG1_Antagonist_viability	NO	YES	not applicable	not applicable	11.1	1.05	NONE	cell cycle
TOX21_ERb_BLA_Agonist_viability	NO	YES	not applicable	not applicable	35.4	1.55	Less than 50% efficacy	cell cycle
TOX21_ERb_BLA_Antagonist_viability	NO	YES	not applicable	not applicable	37.8	1.58	Less than 50% efficacy	cell cycle
TOX21_ERR_Antagonist	YES	NO	not applicable	estrogen-related receptor alpha	15.1	1.18	NONE	nuclear receptor
TOX21_ERR_viability	NO	YES	not applicable	not applicable	24.6	1.39	NONE	cell cycle
TOX21_GR_BLA_Antagonist_viability	NO	YES	not applicable	not applicable	33.9	1.53	Less than 50% efficacy: Borderline active	cell cycle
TOX21_H2AX_HTRF_CHO_Agonist_ratio	NO	NO	not applicable	H2A histone family, member X	32.2	1.51	Noisy data	histones
TOX21_H2AX_HTRF_CHO_viability	NO	YES	not applicable	not applicable	16.9	1.23	NONE	cell cycle
TOX21_HDAC_Inhibition	NO	NO	not applicable	histone deacetylase 1	4.47	0.650	NONE	hydrolase
TOX21_HDAC_Inhibition_viability	NO	YES	not applicable	not applicable	6.91	0.839	NONE	cell cycle

FD&C Green No. 3

ASSAY NAME	IN OUR SELECTED SUBSET	VIABILITY ASSAY	DESCRIPTION	GENE_NAME	AC50	LOGAC50	FLAGS	INTENDED_TARGET_FAMILY
TOX21_HRE_BLA_Agonist_viability	NO	YES	not applicable	not applicable	27.7	1.44	Less than 50% efficacy	cell cycle
TOX21_MMP_ratio_up	NO	NO	not applicable	not applicable	47.4	1.68	Less than 50% efficacy: Only highest conc above baseline, active	cell morphology
TOX21_MMP_viability	NO	YES	not applicable	not applicable	39.2	1.59	Less than 50% efficacy: Only highest conc above baseline, active	cell cycle
TOX21_NFkB_BLA_agonist_viability	NO	YES	not applicable	not applicable	37.9	1.58	NONE	cell cycle
TOX21_p53_BLA_p2_viability	NO	YES	not applicable	not applicable	35.7	1.55	Less than 50% efficacy: Borderline active	cell cycle
TOX21_p53_BLA_p3_viability	NO	YES	not applicable	not applicable	46.9	1.67	Less than 50% efficacy: Borderline active	cell cycle
TOX21_p53_BLA_p4_viability	NO	YES	not applicable	not applicable	30.4	1.48	Less than 50% efficacy	cell cycle
TOX21_p53_BLA_p5_viability	NO	YES	not applicable	not applicable	26.3	1.42	Only highest conc above baseline, active: Less than 50% efficacy: Borderline active	cell cycle
TOX21_PGC_ERR_Antagonist	NO	NO	not applicable	estrogen-related receptor alpha	10.1	1.00	NONE	nuclear receptor
TOX21_PGC_ERR_viability	NO	YES	not applicable	not applicable	31.5	1.50	NONE	cell cycle
TOX21_PPARd_BLA_Agonist_viability	NO	YES	not applicable	not applicable	23.7	1.37	Less than 50% efficacy: Borderline active	cell cycle
TOX21_RAR_LUC_Agonist_viability	NO	YES	not applicable	not applicable	15.3	1.18	NONE	cell cycle
TOX21_RAR_LUC_Antagonist	NO	NO	not applicable	retinoic acid receptor, alpha	13.6	1.13	NONE	nuclear receptor
TOX21_RAR_LUC_Antagonist_viability	NO	YES	not applicable	not applicable	14.8	1.17	NONE	cell cycle
TOX21_RORg_LUC_CHO_Antagonist	NO	NO	not applicable	RAR-related orphan receptor C	8.50	0.930	Borderline active	nuclear receptor
TOX21_RORg_LUC_CHO_Antagonist_viability	NO	YES	not applicable	not applicable	9.24	0.966	NONE	cell cycle
TOX21_RT_HEK293_FLO_40hr_viability	NO	YES	not applicable	not applicable	5.74e-3	-2.24	Less than 50% efficacy: Hit-call potentially confounded by overfitting: Borderline active: Only one conc above baseline, active	cell cycle
TOX21_RXR_BLA_Agonist_viability	NO	YES	not applicable	not applicable	24.3	1.38	Less than 50% efficacy	cell cycle
TOX21_SSH_3T3_GLI3_Agonist_viability	NO	YES	not applicable	not applicable	20.5	1.31	NONE	cell cycle
TOX21_SSH_3T3_GLI3_Antagonist	NO	NO	not applicable	GLI family zinc finger 3	6.11	0.786	NONE	DNA binding
TOX21_SSH_3T3_GLI3_Antagonist_viability	NO	YES	not applicable	not applicable	20.9	1.32	NONE	cell cycle
TOX21_TR_LUC_GH3_Antagonist	YES	NO	804	thyroid hormone receptor beta	18.1	1.26	NONE	nuclear receptor
TOX21_TR_LUC_GH3_Antagonist_viability	NO	YES	not applicable	not applicable	41.3	1.62	NONE	cell cycle
TOX21_TSHR_Antagonist_ratio	YES	NO	not applicable	thyroid stimulating hormone receptor	11.4	1.06	Noisy data	gpcr
TOX21_VDR_BLA_Agonist_viability	NO	YES	not applicable	not applicable	20.6	1.31	Less than 50% efficacy	cell cycle

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ASSAY NAME	IN OUR SELECTED SUBSET	VIABILITY ASSAY	DESCRIPTION	GENE_NAME	AC50	LOGAC50	FLAGS	INTENDED_TARGET_FAMILY
ACEA_AR_agonist_80hr	NO	NO	not applicable	androgen receptor	17.3	1.24	Less than 50% efficacy: Only highest conc above baseline, active	nuclear receptor
ATG_Ahr_CIS_up	YES	NO	not applicable	aryl hydrocarbon receptor	17.6	1.25	Borderline active	dna binding
ATG_BRE_CIS_dn	NO	NO	not applicable	SMAD family member 1	54.7	1.74	Only highest conc above baseline, active	dna binding
ATG_DR5_CIS_up	NO	NO	not applicable	retinoic acid receptor, beta	20.0	1.30	Borderline active	nuclear receptor
ATG_EGR_CIS_up	NO	NO	not applicable	early growth response 1	43.9	1.64	NONE	dna binding
ATG_ERE_CIS_up	YES	NO	75	estrogen receptor 1	25.1	1.40	Hit-call potentially confounded by overfitting: Only highest conc above baseline, active	nuclear receptor
ATG_HIF1a_CIS_up	NO	NO	not applicable	hypoxia inducible factor 1, alpha subunit (basic helix-loop-helix transcription factor)	26.1	1.42	Hit-call potentially confounded by overfitting: Borderline active: Only highest conc above baseline, active	dna binding
ATG_MRE_CIS_up	YES	NO	not applicable	metal-regulatory transcription factor 1	35.3	1.55	NONE	dna binding
ATG_Oct_MLP_CIS_up	YES	NO	not applicable	POU class 2 homeobox 1	27.3	1.44	Borderline active	dna binding
ATG_Pax6_CIS_up		NO	not applicable	paired box 6	43.4	1.64	Borderline active	dna binding
ATG_PBREM_CIS_up	NO	NO	not applicable	nuclear receptor subfamily 1, group I, member 3	19.9	1.30	NONE	nuclear receptor
ATG_PXR_TRANS_up	NO	NO	not applicable	nuclear receptor subfamily 1, group I, member 2	4.50	0.653	NONE	nuclear receptor
ATG_PXRE_CIS_up	YES	NO	not applicable	nuclear receptor subfamily 1, group I, member 2	4.15	0.618	NONE	nuclear receptor
ATG_RORE_CIS_up	NO	NO	not applicable	RAR-related orphan receptor A	36.2	1.56	NONE	nuclear receptor
ATG_TGFb_CIS_up	NO	NO	not applicable	transforming growth factor, beta 1	81.8	1.91	Borderline active: Only highest conc above baseline, active	growth factor
ATG_VDRE_CIS_up	YES	NO	not applicable	vitamin D (1,25- dihydroxyvitamin D3) receptor	25.1	1.40	NONE	nuclear receptor
BSK_3C_Eselectin_down	YES	NO	not applicable	selectin E	5.96	0.775	Noisy data	cell adhesion molecules
BSK_3C_HLADR_down	YES	NO	not applicable	major histocompatibility complex, class II, DR alpha	6.72	0.828	NONE	cell adhesion molecules
BSK_3C_ICAM1_down		NO	not applicable	intercellular adhesion molecule 1	9.62	0.983	Less than 50% efficacy	cell adhesion molecules
BSK_3C_MCP1_down	YES	NO	not applicable	chemokine (C-C motif) ligand 2	7.12	0.852	NONE	cytokine
BSK_3C_SRB_down	NO	YES	not applicable	not applicable	13.4	1.13	Less than 50% efficacy: Only highest conc above baseline, active	cell cycle
BSK_3C_Thrombomodulin_down	NO	NO	not applicable	thrombomodulin	7.25	0.860	Less than 50% efficacy	gpcr
BSK_3C_TissueFactor_down	NO	NO	not applicable	coagulation factor III (thromboplastin, tissue factor)	8.92	0.951	Less than 50% efficacy: Only highest conc above baseline, active	cytokine
BSK_3C_uPAR_down	YES	NO	not applicable	plasminogen activator, urokinase receptor	5.33	0.727	NONE	cytokine
BSK_3C_VCAM1_down	NO	NO	not applicable	vascular cell adhesion molecule 1	13.7	1.14	NONE	cell adhesion molecules
BSK_3C_Vis_down	YES	NO	not applicable	not applicable	16.4	1.21	Less than 50% efficacy	cell morphology
BSK_4H_Eotaxin3_down	YES	NO	not applicable	chemokine (C-C motif) ligand 26	8.40	0.924		cytokine
BSK_4H_MCP1_down		NO	not applicable	chemokine (C-C motif) ligand 2	5.10	0.708	Less than 50% efficacy	cytokine
BSK_4H_Pselectin_down	YES	NO	not applicable	selectin P (granule membrane protein 140kDa, antigen CD62)	10.0	1.00	Less than 50% efficacy	cell adhesion molecules
BSK_4H_uPAR_down	NO	NO	not applicable	plasminogen activator, urokinase receptor	8.58	0.933	NONE	cytokine
BSK_4H_VCAM1_down	NO	NO	not applicable	vascular cell adhesion molecule 1	14.0	1.15	NONE	cell adhesion molecules
BSK_4H_VEGFRII_down	NO	NO	not applicable	kinase insert domain receptor (a type III receptor tyrosine kinase)	5.48	0.739	Less than 50% efficacy	kinase
BSK_BE3C_HLADR_down	NO	NO	not applicable	major histocompatibility complex, class II, DR alpha	4.53	0.656	NONE	cell adhesion molecules
BSK_BE3C_IL1a_down	NO	NO	not applicable	interleukin 1, alpha	4.49	0.653	NONE	cytokine
BSK_BE3C_IP10_down	NO	NO	not applicable	chemokine (C-X-C motif) ligand 10	12.8	1.11	NONE	cytokine
BSK_BE3C_MIG_down	NO	NO	not applicable	chemokine (C-X-C motif) ligand 9	14.6	1.16	NONE	cytokine
BSK_BE3C_MMP1_down	NO	NO	not applicable	matrix metallopeptidase 1 (interstitial collagenase)	3.19	0.504	Less than 50% efficacy	protease
BSK_BE3C_PAI1_down	NO	NO	not applicable	serpin peptidase inhibitor, clade E (nexin, plasminogen activator inhibitor type 1), member 1	4.47	0.651	NONE	cytokine
BSK_BE3C_SRB_down	NO	YES	not applicable	not applicable	10.7	1.03	Less than 50% efficacy	cell cycle
BSK_BE3C_TGFb1_down	NO	NO	not applicable	transforming growth factor, beta 1	3.80	0.580	Less than 50% efficacy	growth factor
BSK_BE3C_tPA_down	NO	NO	not applicable	plasminogen activator, tissue	5.77	0.761	NONE	protease
BSK_BE3C_uPA_down	NO	NO	not applicable	plasminogen activator, urokinase	9.97	0.999	NONE	protease
BSK_BE3C_uPAR_down	NO	NO	not applicable	plasminogen activator, urokinase receptor	8.46	0.927	NONE	cytokine
BSK_CASM3C_IL6_down	NO	NO	not applicable	interleukin 6	0.941	-2.64e-2	Less than 50% efficacy	cytokine
BSK_CASM3C_MCP1_down	NO	NO	not applicable	chemokine (C-C motif) ligand 2	16.1	1.21	Less than 50% efficacy	cytokine
BSK_CASM3C_MCSF_down	NO	NO	not applicable	colony stimulating factor 1 (macrophage)	17.7	1.25	Less than 50% efficacy	cytokine
BSK_CASM3C_Thrombomodulin_down	NO	NO	not applicable	thrombomodulin	3.40	0.531	Less than 50% efficacy	gpcr
BSK_CASM3C_TissueFactor_down	NO	NO	not applicable	coagulation factor III (thromboplastin, tissue factor)	0.589	-0.230	Less than 50% efficacy: Hit-call potentially confounded by overfitting	cytokine
BSK_CASM3C_uPAR_down	NO	NO	not applicable	plasminogen activator, urokinase receptor	4.15e-2	-1.38	AC50 less than lowest concentration tested: Less than 50% efficacy	cytokine
BSK_hDFCGF_CollagenIII_down	YES	NO	not applicable	collagen, type III, alpha 1	6.57	0.817	NONE	cell adhesion molecules
BSK_hDFCGF_EGFR_down		NO	not applicable	epidermal growth factor receptor	2.07	0.317	Less than 50% efficacy	kinase
BSK_hDFCGF_IP10_down	YES	NO	not applicable	chemokine (C-X-C motif) ligand 10	20.1	1.30	Noisy data	cytokine
BSK_hDFCGF_MCSF_down	YES	NO	not applicable	colony stimulating factor 1 (macrophage)	5.03	0.702	NONE	cytokine
BSK_hDFCGF_MIG_down	NO	NO	not applicable	chemokine (C-X-C motif) ligand 9	26.7	1.43	Less than 50% efficacy: Noisy data: Only highest conc above baseline, active	cytokine
BSK_hDFCGF_MMP1_down	NO	NO	not applicable	matrix metallopeptidase 1 (interstitial collagenase)	11.8	1.07	Less than 50% efficacy	protease
BSK_hDFCGF_PAI1_down	NO	NO	not applicable	serpin peptidase inhibitor, clade E (nexin, plasminogen activator inhibitor type 1), member 1	7.23	0.859	NONE	cytokine
BSK_hDFCGF_Proliferation_down	NO	YES	not applicable	not applicable	15.0	1.18	NONE	cell cycle
BSK_hDFCGF_SRB_down	NO	YES	not applicable	not applicable	18.2	1.26	Less than 50% efficacy: Hit-call potentially confounded by overfitting: Borderline active: Only highest conc above baseline, active	cell cycle
BSK_hDFCGF_TIMP1_down	NO	NO	not applicable	TIMP metallopeptidase inhibitor 1	7.31	0.864	Less than 50% efficacy	protease inhibitor
BSK_hDFCGF_VCAM1_down	YES	NO	not applicable	vascular cell adhesion molecule 1	14.9	1.17	NONE	cell adhesion molecules
BSK_KF3CT_ICAM1_down	NO	NO	not applicable	intercellular adhesion molecule 1	10.8	1.03	NONE	cell adhesion molecules
BSK_KF3CT_IL1a_down	NO	NO	not applicable	interleukin 1, alpha	5.43	0.734	NONE	cytokine

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ASSAY NAME	IN OUR SELECTED SUBSET	VIABILITY ASSAY	DESCRIPTION	GENE_NAME	AC50	LOGAC50	FLAGS	INTENDED_TARGET_FAMILY
BSK_KF3CT_IP10_down	NO	NO	not applicable	chemokine (C-X-C motif) ligand 10	16.5	1.22	Only highest conc above baseline, active	cytokine
BSK_KF3CT_MCP1_down	YES	NO	not applicable	chemokine (C-C motif) ligand 2	3.46	0.538	NONE	cytokine
BSK_KF3CT_MMP9_down	NO	NO	not applicable	matrix metallopeptidase 9 (gelatinase B, 92kDa gelatinase, 92kDa type IV collagenase)	12.4	1.09	NONE	protease
BSK_KF3CT_SRB_down	NO	YES	not applicable	not applicable	20.7	1.32	Less than 50% efficacy: Borderline active: Only highest conc above baseline, active	cell cycle
BSK_KF3CT_TGFb1_down	NO	NO	not applicable	transforming growth factor, beta 1	3.44	0.536	NONE	growth factor
BSK_KF3CT_TIMP2_down	NO	NO	not applicable	TIMP metallopeptidase inhibitor 2	2.71	0.434	NONE	protease inhibitor
BSK_KF3CT_uPA_down	NO	NO	not applicable	plasminogen activator, urokinase	10.1	1.01	NONE	protease
BSK_LPS_CD40_down	YES	NO	not applicable	CD40 molecule, TNF receptor superfamily member 5	8.74	0.942	NONE	cytokine
BSK_LPS_Eselectin_down	NO	NO	not applicable	selectin E	8.76	0.942	NONE	cell adhesion molecules
BSK_LPS_IL1a_down	NO	NO	not applicable	interleukin 1, alpha	8.87	0.948	Less than 50% efficacy	cytokine
BSK_LPS_MCP1_down	YES	NO	not applicable	chemokine (C-C motif) ligand 2	8.10	0.908	NONE	cytokine
BSK_LPS_MCSF_down	YES	NO	not applicable	colony stimulating factor 1 (macrophage)	7.93	0.899	NONE	cytokine
BSK_LPS_PGE2_down	NO	NO	not applicable	prostaglandin E receptor 2 (subtype EP2), 53kDa	3.48	0.542	NONE	gpcr
BSK_LPS_SRB_down	NO	YES	not applicable	not applicable	0.428	-0.369	Less than 50% efficacy	cell cycle
BSK_LPS_TissueFactor_down	NO	NO	not applicable	coagulation factor III (thromboplastin, tissue factor)	16.5	1.22	Less than 50% efficacy: Hit-call potentially confounded by overfitting: Only highest conc above baseline, active	cytokine
BSK_LPS_VCAM1_down	YES	NO	not applicable	vascular cell adhesion molecule 1	9.29	0.968	Less than 50% efficacy	cell adhesion molecules
BSK_SAg_CD38_down	YES	NO	not applicable	CD38 molecule	9.47	0.976	NONE	cytokine
BSK_SAg_CD40_down	YES	NO	not applicable	CD40 molecule, TNF receptor superfamily member 5	11.4	1.06	NONE	cytokine
BSK_SAg_CD69_down	YES	NO	not applicable	CD69 molecule	11.9	1.08	NONE	cytokine
BSK_SAg_Eselectin_down	YES	NO	not applicable	selectin E	12.1	1.08	NONE	cell adhesion molecules
BSK_SAg_MCP1_down	YES	NO	not applicable	chemokine (C-C motif) ligand 2	10.1	1.00	NONE	cytokine
BSK_SAg_Proliferation_down	NO	YES	not applicable	not applicable	18.3	1.26	Less than 50% efficacy: Hit-call potentially confounded by overfitting: Borderline active: Only highest conc above baseline, active	cell cycle
NCCT_HEK293T_CellTiterGLO	NO	NO	not applicable	not applicable	5.04	0.702	NONE	cell cycle
NCCT_QuantiLum_inhib_2_dn	NO	NO	not applicable	not applicable	10.3	1.01	NONE	oxidoreductase
NCCT_TPO_AUR_dn	YES	NO	not applicable	thyroid peroxidase	14.5	1.16	NONE	oxidoreductase
NVS_ENZ_hPDE10	NO	NO	not applicable	phosphodiesterase 10A	7.56e-3	-2.12	Less than 50% efficacy: Hit-call potentially confounded by overfitting: Borderline active	esterase
NVS_ENZ_rMAOAC	YES	NO	not applicable	monoamine oxidase A	0.688	-0.162	NONE	oxidoreductase
NVS_GPCR_hAdoRA1	YES	NO	not applicable	adenosine A1 receptor	7.19	0.857	Hit-call potentially confounded by overfitting	gpcr
NVS_GPCR_hDRD1	YES	NO	not applicable	dopamine receptor D1	0.540	-0.268	NONE	gpcr
NVS_GPCR_hNK2	YES	NO	not applicable	tachykinin receptor 2	1.34	0.128	NONE	gpcr
NVS_GPCR_hOpiate_mu	YES	NO	not applicable	opioid receptor, mu 1	2.69e-2	-1.57	NONE	gpcr
NVS_GPCR_hTXA2	NO	NO	not applicable	thromboxane A2 receptor	0.924	-3.41e-2	NONE	gpcr
NVS_NR_cAR	YES	NO	710	androgen receptor	13.2	1.12	Only highest conc above baseline, active	nuclear receptor
NVS_NR_hAR	YES	NO	711	androgen receptor	4.81	0.682	Less than 50% efficacy: Hit-call potentially confounded by overfitting	nuclear receptor
NVS_NR_hFXR_Agonist	NO	NO	715	nuclear receptor subfamily 1, group H, member 4	16.1	1.21	Hit-call potentially confounded by overfitting: Borderline active: Only highest conc above baseline, active	nuclear receptor
NVS_NR_hGR	YES	NO	not applicable	nuclear receptor subfamily 3, group C, member 1 (glucocorticoid receptor)	18.1	1.26	NONE	nuclear receptor
NVS_NR_hRAR_Antagonist	NO	NO	not applicable	retinoic acid receptor, alpha	12.5	1.10	Only highest conc above baseline, active	nuclear receptor
NVS_NR_hRARa_Agonist	NO	NO	not applicable	retinoic acid receptor, alpha	11.8	1.07	Only highest conc above baseline, active: Hit-call potentially confounded by overfitting	nuclear receptor
NVS_NR_rAR	YES	NO	726	androgen receptor	0.551	-0.259	NONE	nuclear receptor
NVS_TR_hNET	YES	NO	not applicable	solute carrier family 6 (neurotransmitter transporter), member 2	0.553	-0.257	NONE	transporter
NVS_TR_rSERT	YES	NO	not applicable	solute carrier family 6 (neurotransmitter transporter), member 4	0.762	-0.118	NONE	transporter
OT_FXR_FXRSRC1_0480	YES	NO	753	nuclear receptor subfamily 1, group H, member 4	34.9	1.54	Noisy data	nuclear receptor
OT_FXR_FXRSRC1_1440	YES	NO	754	nuclear receptor subfamily 1, group H, member 4	31.7	1.50	Noisy data	nuclear receptor
TOX21_AhR_LUC_Agonist_viability	NO	YES	not applicable	not applicable	7.13	0.853	NONE	cell cycle
TOX21_AR_BLA_Antagonist_viability	NO	YES	not applicable	not applicable	38.4	1.58	Borderline active: Only highest conc above baseline, active: Less than 50% efficacy	cell cycle
TOX21_AR_LUC_MDAKB2_Agonist2_viability	NO	YES	not applicable	not applicable	9.29	0.968	NONE	cell cycle
TOX21_AR_LUC_MDAKB2_Antagonist	YES	NO	not applicable	androgen receptor	9.80	0.991	Less than 50% efficacy: Borderline active	nuclear receptor
TOX21_AR_LUC_MDAKB2_Antagonist_Specificity_viability	NO	YES	not applicable	not applicable	21.9	1.34	NONE	cell cycle
TOX21_AR_LUC_MDAKB2_Antagonist_viability	NO	YES	not applicable	not applicable	9.75	0.989	NONE	cell cycle
TOX21_Aromatase_Inhibition	NO	NO	not applicable	cytochrome P450, family 19, subfamily A, polypeptide 1	37.5	1.57	Less than 50% efficacy	cyp
TOX21_Aromatase_Inhibition_viability	NO	YES	not applicable	not applicable	2.74	0.438	NONE	cell cycle
TOX21_CAR_Agonist_viabillity	NO	YES	not applicable	not applicable	11.6	1.07	NONE	cell cycle
TOX21_CAR_Antagonist	NO	NO	not applicable	nuclear receptor subfamily 1, group I, member 3	7.19	0.857	NONE	nuclear receptor
TOX21_CAR_Antagonist_viability	NO	YES	not applicable	not applicable	11.3	1.05	NONE	cell cycle
TOX21_DT40	YES	NO	not applicable	not applicable	88.6	1.95	NONE	cell cycle
TOX21_DT40_100	YES	NO	not applicable	not applicable	38.2	1.58	NONE	cell cycle
TOX21_DT40_657	YES	NO	not applicable	not applicable	11.1	1.05	NONE	cell cycle
TOX21_ELG1_LUC_Agonist_viability	NO	YES	not applicable	not applicable	23.4	1.37	NONE	cell cycle
TOX21_ERa_BLA_Antagonist_ratio	YES	NO	786	estrogen receptor 1	58.6	1.77	Less than 50% efficacy: Only highest conc above baseline, active	nuclear receptor
TOX21_ERa_LUC_BG1_Agonist_Counterscreen_viability	NO	YES	not applicable	not applicable	5.44	0.735	NONE	cell cycle

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ASSAY NAME	IN OUR SELECTED SUBSET	VIABILITY ASSAY	DESCRIPTION	GENE_NAME	AC50	LOGAC50	FLAGS	INTENDED_TARGET_FAMILY
TOX21_ERa_LUC_BG1_Antagonist	YES	NO	not applicable	estrogen receptor 1	16.3	1.21	Less than 50% efficacy	nuclear receptor
TOX21_ERa_LUC_BG1_Antagonist_Specificity	YES	NO	789	estrogen receptor 1	23.6	1.37	Less than 50% efficacy	nuclear receptor
TOX21_ERa_LUC_BG1_Antagonist_Specificity_viability	NO	YES	not applicable	not applicable	15.7	1.20	NONE	cell cycle
TOX21_ERa_LUC_BG1_Antagonist_viability	NO	YES	not applicable	not applicable	4.74	0.676	NONE	cell cycle
TOX21_ERR_Antagonist	YES		not applicable	estrogen-related receptor alpha	11.6	1.07	Less than 50% efficacy	nuclear receptor
TOX21_ERR_viability	NO	YES	not applicable		13.9	1.14		cell cycle
TOX21_H2AX_HTRF_CHO_Agonist_ratio	NO		not applicable	H2A histone family, member X	46.7	1.67	Noisy data	histones
TOX21_H2AX_HTRF_CHO_viability	NO	YES	not applicable	not applicable	8.42	0.925	Less than 50% efficacy	cell cycle
TOX21_HDAC_Inhibition_viability	NO	YES	not applicable	not applicable	9.86	0.994	Less than 50% efficacy	cell cycle
TOX21_HSE_BLA_agonist_ratio	NO	NO	not applicable	heat shock transcription factor 1	23.0	1.36	Less than 50% efficacy	DNA binding
TOX21_MMP_ratio_up	NO	NO	not applicable		47.4	1.68	NONE	cell morphology
TOX21_p53_BLA_p1_ratio	NO	NO	not applicable	tumor protein p53	76.7	1.88	NONE	DNA binding
TOX21_p53_BLA_p2_ratio	NO	NO	not applicable	tumor protein p53	70.3	1.85	Only highest conc above baseline, active	DNA binding
TOX21_p53_BLA_p3_ratio	NO	NO	not applicable	tumor protein p53	73.7	1.87	Only highest conc above baseline, active	DNA binding
TOX21_p53_BLA_p4_ratio	NO	NO	not applicable	tumor protein p53	63.3	1.80	NONE	DNA binding
TOX21_p53_BLA_p4_viability	NO	YES	not applicable	not applicable	55.1	1.74	Less than 50% efficacy: Only highest conc above baseline, active	cell cycle
TOX21_p53_BLA_p5_ratio	NO	NO	not applicable	tumor protein p53	71.6	1.86	NONE	DNA binding
TOX21_PGC_ERR_Antagonist	YES	NO	not applicable	estrogen-related receptor alpha	14.1	1.15	NONE	nuclear receptor
TOX21_PGC_ERR_viability	NO	YES	not applicable	not applicable	13.8	1.14	NONE	cell cycle
TOX21_PPARd_BLA_Agonist_viability	NO	YES	not applicable	not applicable	28.7	1.46	Only highest conc above baseline, active	cell cycle
TOX21_PPARd_BLA_antagonist_ratio	NO	NO	1125	peroxisome proliferator-activated receptor delta	23.4	1.37	NONE	nuclear receptor
TOX21_PPARd_BLA_antagonist_viability	NO	YES	not applicable	not applicable	25.0	1.40	Only highest conc above baseline, active	cell cycle
TOX21_RAR_LUC_Agonist_viability	NO	YES	not applicable	not applicable	26.5	1.42	Less than 50% efficacy	cell cycle
TOX21_RAR_LUC_Antagonist	NO	NO	not applicable	retinoic acid receptor, alpha	44.2	1.65	Less than 50% efficacy	nuclear receptor
TOX21_RAR_LUC_Antagonist_viability	NO	YES	not applicable	not applicable	14.7	1.17	Less than 50% efficacy	cell cycle
TOX21_RORg_LUC_CHO_Antagonist_viability	NO	YES	not applicable	not applicable	12.2	1.08	Less than 50% efficacy	cell cycle
TOX21_RT_HEK293_FLO_00hr_viability	NO	YES	not applicable	not applicable	13.8	1.14	NONE	cell cycle
TOX21_RT_HEK293_FLO_08hr_viability	NO	YES	not applicable	not applicable	9.74	0.989	NONE	cell cycle
TOX21_RT_HEK293_FLO_16hr_viability	NO	YES	not applicable	not applicable	10.6	1.02	NONE	cell cycle
TOX21_RT_HEK293_FLO_24hr_viability	NO	YES	not applicable	not applicable	7.13	0.853	NONE	cell cycle
TOX21_RT_HEK293_FLO_32hr_viability	NO	YES	not applicable	not applicable	11.8	1.07	NONE	cell cycle
TOX21_RT_HEK293_FLO_40hr_viability	NO	YES	not applicable	not applicable	6.45	0.810	NONE	cell cycle
TOX21_RT_HEK293_GLO_08hr_viability	NO	YES	not applicable	not applicable	21.4	1.33	Less than 50% efficacy	cell cycle
TOX21_RT_HEK293_GLO_16hr_viability	NO	YES	not applicable	not applicable	23.5	1.37	Less than 50% efficacy	cell cycle
TOX21_RT_HEK293_GLO_24hr_viability	NO	YES	not applicable	not applicable	21.2	1.33	Less than 50% efficacy	cell cycle
TOX21_RT_HEK293_GLO_32hr_viability	NO	YES	not applicable	not applicable	20.4	1.31	Less than 50% efficacy	cell cycle
TOX21_RT_HEK293_GLO_40hr_viability	NO	YES	not applicable	not applicable	20.1	1.30	Less than 50% efficacy	cell cycle
TOX21_RT_HEPG2_FLO_00hr_ctrl_viability	NO	YES	not applicable	not applicable	18.2	1.26	NONE	cell cycle
TOX21_RT_HEPG2_FLO_08hr_viability	NO	YES	not applicable	not applicable	17.1	1.23	NONE	cell cycle
TOX21_RT_HEPG2_FLO_16hr_ctrl_viability	NO	YES	not applicable	not applicable	18.6	1.27	NONE	cell cycle
TOX21_RT_HEPG2_FLO_24hr_viability	NO	YES	not applicable	not applicable	18.6	1.27	NONE	cell cycle
TOX21_RT_HEPG2_FLO_32hr_ctrl_viability	NO	YES	not applicable	not applicable	18.5	1.27	NONE	cell cycle
TOX21_RT_HEPG2_FLO_40hr_ctrl_viability	NO	YES	not applicable	not applicable	19.0	1.28	NONE	cell cycle
TOX21_RT_HEPG2_GLO_00hr_ctrl_viability	NO	YES	not applicable	not applicable	15.9	1.20	NONE	cell cycle
TOX21_RT_HEPG2_GLO_08hr_ctrl_viability	NO	YES	not applicable	not applicable	29.1	1.46	NONE	cell cycle
TOX21_RT_HEPG2_GLO_16hr_ctrl_viability	NO	YES	not applicable	not applicable	30.4	1.48	NONE	cell cycle
TOX21_RT_HEPG2_GLO_24hr_ctrl_viability	NO	YES	not applicable	not applicable	30.5	1.48	NONE	cell cycle
TOX21_RT_HEPG2_GLO_32hr_ctrl_viability	NO	YES	not applicable	not applicable	27.8	1.44	NONE	cell cycle
TOX21_RT_HEPG2_GLO_40hr_viability	NO	YES	not applicable	not applicable	22.2	1.35	NONE	cell cycle
TOX21_RXR_BLA_Agonist_viability	NO	YES	not applicable	not applicable	29.6	1.47	Borderline active: Less than 50% efficacy: Only highest conc above baseline, active	cell cycle
TOX21_SSH_3T3_GLI3_Agonist_viability	NO	YES	not applicable	not applicable	17.6	1.24	NONE	cell cycle
TOX21_SSH_3T3_GLI3_Antagonist	NO	NO	not applicable	GLI family zinc finger 3	13.5	1.13	NONE	DNA binding
TOX21_SSH_3T3_GLI3_Antagonist_viability	NO	YES	not applicable	not applicable	13.2	1.12	NONE	cell cycle
TOX21_TR_LUC_GH3_Antagonist	YES	NO	804	thyroid hormone receptor beta	31.1	1.49	NONE	nuclear receptor
TOX21_TR_LUC_GH3_Antagonist_viability	NO	YES	not applicable	not applicable	18.4	1.26	NONE	cell cycle
TOX21_TSHR_Antagonist_ratio	YES	NO	not applicable	thyroid stimulating hormone receptor	15.5	1.19	Noisy data	gpcr
TOX21_VDR_BLA_Agonist_viability	NO	YES	not applicable	not applicable	21.7	1.34	NONE	cell cycle

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ASSAY NAME	IN OUR SELECTED SUBSET	VIABILITY ASSAY	DESCRIPTION	GENE_NAME	AC50	LOGAC50	FLAGS	INTENDED_TARGET_FAMILY
APR_HepG2_MitoMembPot_24h_dn	NO	NO	not applicable	not applicable	103	2.01	Borderline active	cell cycle
ATG_HIF1a_CIS_dn	NO	NO	not applicable	hypoxia inducible factor 1, alpha subunit (basic helix-loop-helix transcription factor)	5.46	0.737	NONE	cell morphology
NCCT_HEK293T_CellTiterGLO	NO	NO	not applicable	not applicable	10.8	1.03	NONE	gpcr
NCCT_QuantiLum_inhib_2_dn	NO	NO	not applicable	not applicable	13.8	1.14	NONE	gpcr
NCCT_QuantiLum_inhib_dn	YES	NO	not applicable	not applicable	6.87	0.837	NONE	oxidoreductase
NCCT_TPO_AUR_dn	YES	NO	not applicable	thyroid peroxidase	21.4	1.33	Less than 50% efficacy	oxidoreductase
NVS_ENZ_hCASP1	NO	NO	not applicable	caspase 1, apoptosis-related cysteine peptidase	30.0	1.48	Less than 50% efficacy: Hit-call potentially confounded by overfitting	protease
NVS_ENZ_hCASP2	NO	NO	not applicable	caspase 2, apoptosis-related cysteine peptidase	20.2	1.31	Less than 50% efficacy: Hit-call potentially confounded by overfitting	protease
NVS_ENZ_hCASP3	NO	NO	not applicable	caspase 3, apoptosis-related cysteine peptidase	22.5	1.35	NONE	protease
NVS_ENZ_hCASP4	NO	NO	not applicable	caspase 4, apoptosis-related cysteine peptidase	26.7	1.43	Less than 50% efficacy	protease
NVS_ENZ_hCASP5	NO	NO	not applicable	caspase 5, apoptosis-related cysteine peptidase	36.7	1.56	Less than 50% efficacy	protease
NVS_ENZ_hMMP3	NO	NO	not applicable	matrix metallopeptidase 3 (stromelysin 1, progelatinase)	21.0	1.32	NONE	protease
NVS_GPCR_g5HT4	YES	NO	not applicable	5 hydroxytryptamine (serotonin) receptor 4	41.0	1.61	Less than 50% efficacy: Hit-call potentially confounded by overfitting: Only highest conc above baseline, active	gpcr
NVS_GPCR_h5HT7	YES	NO	not applicable	5-hydroxytryptamine (serotonin) receptor 7, adenylate cyclase-coupled	16.3	1.21	Less than 50% efficacy: Hit-call potentially confounded by overfitting	gpcr
NVS_GPCR_hAdra2C	YES	NO	not applicable	adrenoceptor alpha 2C	13.7	1.14	NONE	gpcr
NVS_GPCR_hDRD1	YES	NO	not applicable	dopamine receptor D1	25.3	1.40	Hit-call potentially confounded by overfitting	gpcr
NVS_GPCR_hDRD2s	YES	NO	not applicable	dopamine receptor D2	12.3	1.09	NONE	gpcr
NVS_GPCR_hDRD4.4	YES	NO	not applicable	dopamine receptor D4	27.4	1.44	Hit-call potentially confounded by overfitting: Only highest conc above baseline, active	gpcr
NVS_GPCR_hM2	YES	NO	not applicable	cholinergic receptor, muscarinic 2	24.8	1.40	Hit-call potentially confounded by overfitting: Only highest conc above baseline, active	gpcr
NVS_GPCR_hM3	YES	NO	not applicable	cholinergic receptor, muscarinic 3	23.3	1.37	Hit-call potentially confounded by overfitting: Borderline active	gpcr
NVS_GPCR_hM5	YES	NO	not applicable	cholinergic receptor, muscarinic 5	30.9	1.49	NONE	gpcr
NVS_GPCR_hOpiate_D1	YES	NO	not applicable	opioid receptor, delta 1	30.5	1.48	NONE	gpcr
NVS_GPCR_r5HT1_NonSelective	YES	NO	not applicable	5-hydroxytryptamine (serotonin) receptor 1A, G protein-coupled	20.6	1.31	NONE	gpcr
NVS_GPCR_rNK1	YES	NO	not applicable	tachykinin receptor 1	31.2	1.49	Less than 50% efficacy: Hit-call potentially confounded by overfitting: Only highest conc above baseline, active	gpcr
NVS_GPCR_rNTS	YES	NO	not applicable	neurotensin receptor 1	15.8	1.20	NONE	gpcr
NVS_LGIC_h5HT3	YES	NO	not applicable	5-hydroxytryptamine (serotonin) receptor 3A, ionotropic	23.9	1.38	Less than 50% efficacy: Hit-call potentially confounded by overfitting: Only highest conc above baseline, active	ion channel
NVS_LGIC_hNNR_NBungSens	YES	NO	not applicable	cholinergic receptor, nicotinic, alpha 2 (neuronal)	20.1	1.30	NONE	ion channel
NVS_NR_hGR	YES	NO	not applicable	nuclear receptor subfamily 3, group C, member 1 (glucocorticoid receptor)	23.4	1.37	Borderline active: Only highest conc above baseline, active: Hit-call potentially confounded by overfitting	gpcr
NVS_NR_hPR	NO	NO	not applicable	progesterone receptor	20.2	1.31	Less than 50% efficacy	nuclear receptor
OT_ER_ERaERb_0480	NO	NO	744	estrogen receptor 2 (ER beta)	114	2.06	Less than 50% efficacy: Only highest conc above baseline, active	nuclear receptor
OT_ER_ERaERb_1440	NO	NO	745	estrogen receptor 2 (ER beta)	56.0	1.75	Less than 50% efficacy: Borderline active	nuclear receptor
OT_ER_ERbERb_0480	NO	NO	746	estrogen receptor 2 (ER beta)	58.3	1.77	Less than 50% efficacy: Only highest conc above baseline, active	nuclear receptor
OT_ER_ERbERb_1440	NO	NO	747	estrogen receptor 2 (ER beta)	50.3	1.70	Less than 50% efficacy	nuclear receptor
OT_NURR1_NURR1RXRa_0480	NO	NO	not applicable	retinoid X receptor, alpha	31.1	1.49	Less than 50% efficacy: Only highest conc above baseline, active	nuclear receptor
OT_NURR1_NURR1RXRa_1440	NO	NO	not applicable	retinoid X receptor, alpha	66.5	1.82	Only highest conc above baseline, active	nuclear receptor
OT_PPARg_PPARgSRC1_1440	NO	NO	758	peroxisome proliferator-activated receptor gamma	42.7	1.63	Less than 50% efficacy: Borderline active	nuclear receptor

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ASSAY NAME	IN OUR SELECTED SUBSET	VIABILITY ASSAY	DESCRIPTION	GENE_NAME	AC50	LOGAC50	FLAGS	INTENDED_TARGET_FAMILY
TOX21_AhR_LUC_Agonist_viability	NO	YES	not applicable	not applicable	12.8	1.11	NONE	cell cycle
TOX21_AR_LUC_MDAKB2_Agonist2_viability	NO	YES	not applicable	not applicable	27.4	1.44	NONE	cell cycle
TOX21_AR_LUC_MDAKB2_Antagonist_Specificity	YES	NO	765	androgen receptor	89.1	1.95	Less than 50% efficacy	nuclear receptor
TOX21_AR_LUC_MDAKB2_Antagonist_Specificity_viability	NO	YES	not applicable	not applicable	34.1	1.53	NONE	cell cycle
TOX21_AR_LUC_MDAKB2_Antagonist_viability	NO	YES	not applicable	not applicable	39.7	1.60	NONE	cell cycle
TOX21_Aromatase_Inhibition	NO	NO	not applicable	cytochrome P450, family 19, subfamily A, polypeptide 1	40.3	1.61	Less than 50% efficacy	cell cycle
TOX21_Aromatase_Inhibition_viability	NO	YES	not applicable	not applicable	11.6	1.07	NONE	nuclear receptor
TOX21_CAR_Agonist_viabillity	NO	YES	not applicable	not applicable	31.4	1.50	NONE	nuclear receptor
TOX21_CAR_Antagonist	NO	NO	not applicable	nuclear receptor subfamily 1, group I, member 3	39.5	1.60	Less than 50% efficacy: Borderline active	nuclear receptor
TOX21_CAR_Antagonist_viability	NO	YES	not applicable	not applicable	34.1	1.53	NONE	nuclear receptor
TOX21_DT40	YES	NO	not applicable	not applicable	42.9	1.63	Less than 50% efficacy	cell cycle
TOX21_DT40_100	YES	NO	not applicable	not applicable	43.7	1.64	Less than 50% efficacy	cell cycle
TOX21_DT40_657	YES	NO	not applicable	not applicable	65.4	1.82	Less than 50% efficacy	cell cycle
TOX21_ELG1_LUC_Agonist_viability	NO	YES	not applicable	not applicable	32.3	1.51	NONE	nuclear receptor
TOX21_ERa_LUC_BG1_Agonist_Counterscreen_viability	NO	YES	not applicable	not applicable	15.1	1.18	NONE	cell cycle
TOX21_ERa_LUC_BG1_Antagonist	YES	NO	not applicable	estrogen receptor 1	41.1	1.61	Less than 50% efficacy	nuclear receptor
TOX21_ERa_LUC_BG1_Antagonist_Specificity	YES	NO	789	estrogen receptor 1	45.4	1.66	Less than 50% efficacy	nuclear receptor
TOX21_ERa_LUC_BG1_Antagonist_Specificity_viability	NO	YES	not applicable	not applicable	24.8	1.40	NONE	cell cycle
TOX21_ERa_LUC_BG1_Antagonist_viability	NO	YES	not applicable	not applicable	24.5	1.39	NONE	cell cycle
TOX21_ERR_Antagonist	YES	NO	not applicable	estrogen-related receptor alpha	49.5	1.69	Less than 50% efficacy	cyp
TOX21_ERR_viability	NO	YES	not applicable	not applicable	37.1	1.57	NONE	cell cycle
TOX21_H2AX_HTRF_CHO_Agonist_ratio	NO	NO	not applicable	H2A histone family, member X	71.5	1.85	Less than 50% efficacy	cell cycle
TOX21_H2AX_HTRF_CHO_viability	NO	YES	not applicable	not applicable	46.9	1.67	Less than 50% efficacy	cell cycle
TOX21_HDAC_Inhibition_viability	NO	YES	not applicable	not applicable	25.4	1.40	Less than 50% efficacy	cell morphology
TOX21_MMP_ratio_up	NO	NO	not applicable	not applicable	62.6	1.80	NONE	protease
TOX21_PGC_ERR_Antagonist	YES	NO	not applicable	estrogen-related receptor alpha	35.8	1.55	Less than 50% efficacy	nuclear receptor
TOX21_PGC_ERR_viability	NO	YES	not applicable	not applicable	28.3	1.45	NONE	nuclear receptor
TOX21_RAR_LUC_Agonist_viability	NO	YES	not applicable	not applicable	46.2	1.66	Less than 50% efficacy	cell cycle
TOX21_RAR_LUC_Antagonist_viability	NO	YES	not applicable	not applicable	38.3	1.58	Less than 50% efficacy	cell cycle
TOX21_RORg_LUC_CHO_Antagonist_viability	NO	YES	not applicable	not applicable	48.4	1.69	Less than 50% efficacy	cell cycle
TOX21_RT_HEPG2_GLO_00hr_ctrl_viability	NO	YES	not applicable	not applicable	35.4	1.55	Less than 50% efficacy	cell cycle
TOX21_RT_HEPG2_GLO_08hr_ctrl_viability	NO	YES	not applicable	not applicable	45.5	1.66	Borderline active: Less than 50% efficacy	cell cycle
TOX21_RT_HEPG2_GLO_16hr_ctrl_viability	NO	YES	not applicable	not applicable	40.3	1.61	Borderline active: Less than 50% efficacy	cell cycle
TOX21_RT_HEPG2_GLO_24hr_ctrl_viability	NO	YES	not applicable	not applicable	32.8	1.52	Borderline active: Less than 50% efficacy	cell cycle
TOX21_RT_HEPG2_GLO_32hr_ctrl_viability	NO	YES	not applicable	not applicable	29.6	1.47	Less than 50% efficacy	cell cycle
TOX21_RT_HEPG2_GLO_40hr_viability	NO	YES	not applicable	not applicable	26.5	1.42	Less than 50% efficacy	cell cycle
TOX21_SSH_3T3_GLI3_Agonist_viability	NO	YES	not applicable	not applicable	30.8	1.49	NONE	cell cycle
TOX21_SSH_3T3_GLI3_Antagonist_viability	NO	YES	not applicable	not applicable	24.5	1.39	NONE	cell cycle
TOX21_TR_LUC_GH3_Antagonist	YES	NO	804	thyroid hormone receptor beta	54.5	1.74	Less than 50% efficacy	cell cycle
TOX21_TR_LUC_GH3_Antagonist_viability	NO	YES	not applicable	not applicable	37.7	1.58	NONE	cell cycle

FD&C Yellow No. 5

ASSAY NAME	IN OUR SELECTED SUBSET	VIABILITY ASSAY	DESCRIPTION	GENE_NAME	AC50	LOGAC50	FLAGS	INTENDED_TARGET_FAMILY
ACEA_AR_agonist_80hr	NO	NO	not applicable	androgen receptor	5.51e-2	-1.26	Less than 50% efficacy: Only one conc above baseline, active	cell cycle
ATG_Ahr_CIS_dn	YES	NO	not applicable	aryl hydrocarbon receptor	64.5	1.81	NONE	gpcr
ATG_PXRE_CIS_dn	NO	NO	not applicable	nuclear receptor subfamily 1, group I, member 2	70.2	1.85	NONE	nuclear receptor
ATG_RXRb_TRANS_up	NO	NO	not applicable	retinoid X receptor, beta	9.73	0.988	Hit-call potentially confounded by overfitting: Only one conc above baseline, active	gpcr
NVS_ENZ_hCASP8	NO	NO	not applicable	caspase 8, apoptosis-related cysteine peptidase	5.82	0.765	NONE	nuclear receptor
NVS_ENZ_hMMP13	NO	NO	not applicable	matrix metallopeptidase 13 (collagenase 3)	27.1	1.43	Less than 50% efficacy	cell cycle
NVS_ENZ_hMMP3	NO	NO	not applicable	matrix metallopeptidase 3 (stromelysin 1, progelatinase)	30.6	1.49	Less than 50% efficacy: Hit-call potentially confounded by overfitting	cell cycle
NVS_ENZ_hMMP7	NO	NO	not applicable	matrix metallopeptidase 7 (matrilysin, uterine)	12.7	1.10	Less than 50% efficacy	cell cycle
NVS_ENZ_hPTPN2_Activator	NO	NO	not applicable	protein tyrosine phosphatase, non-receptor type 2	1.50	0.176	Hit-call potentially confounded by overfitting	cell cycle
NVS_ENZ_rCNOS	YES	NO	not applicable	nitric oxide synthase 1, neuronal	10.6	1.03	NONE	oxidoreductase
NVS_GPCR_g5HT4	YES	NO	not applicable	5 hydroxytryptamine (serotonin) receptor 4	12.1	1.08	NONE	gpcr
NVS_GPCR_gOpiateK	YES	NO	not applicable	opioid receptor, kappa 1	40.9	1.61	Less than 50% efficacy: Borderline active: Only highest conc above baseline, active	gpcr
NVS_GPCR_h5HT7	YES	NO	not applicable	5-hydroxytryptamine (serotonin) receptor 7, adenylate cyclase-coupled	33.1	1.52	Less than 50% efficacy: Hit-call potentially confounded by overfitting: Only highest conc above baseline, active	gpcr
NVS_GPCR_hDRD1	YES	NO	not applicable	dopamine receptor D1	21.6	1.33	NONE	gpcr
NVS_GPCR_hDRD4.4	YES	NO	not applicable	dopamine receptor D4	21.1	1.32	NONE	gpcr
NVS_GPCR_r5HT1_NonSelective	YES	NO	not applicable	5-hydroxytryptamine (serotonin) receptor 1A, G protein-coupled	7.57	0.879	NONE	gpcr
NVS_GPCR_rAdra1_NonSelective	YES	NO	not applicable	adrenoceptor alpha 1A	21.8	1.34	Less than 50% efficacy: Only highest conc above baseline, active	gpcr
NVS_IC_rCaBTZCHL	YES	NO	not applicable	calcium channel, voltage-dependent, P/Q type, alpha 1A subunit	13.4	1.13	Less than 50% efficacy: Borderline active	ion channel
TOX21_AhR_LUC_Agonist_viability	NO	YES	not applicable	not applicable	17.9	1.25	Less than 50% efficacy	cell cycle
TOX21_AR_LUC_MDAKB2_Agonist2_viability	NO	YES	not applicable	not applicable	47.5	1.68	NONE	cell cycle
TOX21_AR_LUC_MDAKB2_Antagonist_Specificity_viability	NO	YES	not applicable	not applicable	57.4	1.76	NONE	cell cycle
TOX21_AR_LUC_MDAKB2_Antagonist_viability	NO	YES	not applicable	not applicable	23.0	1.36	Less than 50% efficacy	cell cycle
TOX21_Aromatase_Inhibition_viability	NO	YES	not applicable	not applicable	37.3	1.57	NONE	cell cycle
TOX21_CAR_Agonist_viabillity	NO	YES	not applicable	not applicable	43.2	1.64	NONE	cell cycle
TOX21_CAR_Antagonist_viability	NO	YES	not applicable	not applicable	19.8	1.30	Less than 50% efficacy	cell cycle
TOX21_ELG1_LUC_Agonist_viability	NO	YES	not applicable	not applicable	48.1	1.68	NONE	cell cycle
TOX21_ERa_LUC_BG1_Agonist_Counterscreen_viability	NO	YES	not applicable	not applicable	35.1	1.54	NONE	cell cycle
TOX21_ERa_LUC_BG1_Antagonist_Specificity_viability	NO	YES	not applicable	not applicable	21.6	1.33	Less than 50% efficacy: Borderline active	cell cycle
TOX21_ERa_LUC_BG1_Antagonist_viability	NO	YES	not applicable	not applicable	43.4	1.64	NONE	cell cycle
TOX21_ERR_viability	NO	YES	not applicable	not applicable	40.5	1.61	NONE	cell cycle
TOX21_PGC_ERR_viability	NO	YES	not applicable	not applicable	42.1	1.62	NONE	cell cycle
TOX21_RT_HEK293_FLO_32hr_viability	NO	YES	not applicable	not applicable	5.73	0.759	Hit-call potentially confounded by overfitting: Less than 50% efficacy: Only one conc above baseline, active	cell cycle
TOX21_RT_HEK293_FLO_40hr_viability	NO	YES	not applicable	not applicable	5.74	0.759	Hit-call potentially confounded by overfitting: Borderline active: Only one conc above baseline, active	cell cycle
TOX21_RT_HEPG2_GLO_00hr_ctrl_viability	NO	YES	not applicable	not applicable	35.4	1.55	Less than 50% efficacy	cell cycle
TOX21_SSH_3T3_GLI3_Agonist_viability	NO	YES	not applicable	not applicable	31.9	1.50	NONE	cell cycle
TOX21_SSH_3T3_GLI3_Antagonist_viability	NO	YES	not applicable	not applicable	32.2	1.51	NONE	cell cycle
TOX21_TR_LUC_GH3_Antagonist_viability	NO	YES	not applicable	not applicable	43.1	1.63	NONE	cell cycle

FD&C Yellow No. 6

ASSAY NAME	IN OUR SELECTED SUBSET	VIABILITY ASSAY	DESCRIPTION	GENE_NAME	AC50	LOGAC50	FLAGS	INTENDED_TARGET_FAMILY
ACEA_AR_agonist_80hr	NO	NO	not applicable	androgen receptor	5.03	0.702	Less than 50% efficacy: Hit-call potentially confounded by overfitting	nuclear receptor
NVS_ENZ_hCASP1	NO	NO	not applicable	caspase 1, apoptosis-related cysteine peptidase	27.5	1.44	Less than 50% efficacy	protease
NVS_ENZ_hCASP2	NO	NO	not applicable	caspase 2, apoptosis-related cysteine peptidase	25.1	1.40	Less than 50% efficacy	protease
NVS_ENZ_hCASP3	NO	NO	not applicable	caspase 3, apoptosis-related cysteine peptidase	34.6	1.54	NONE	protease
NVS_ENZ_hMMP13	NO	NO	not applicable	matrix metallopeptidase 13 (collagenase 3)	12.3	1.09	NONE	protease
NVS_ENZ_hMMP2	NO	NO	not applicable	matrix metallopeptidase 2 (gelatinase A, 72kDa gelatinase, 72kDa type IV collagenase)	4.58	0.661	NONE	protease
NVS_ENZ_hMMP3	NO	NO	not applicable	matrix metallopeptidase 3 (stromelysin 1, progelatinase)	20.2	1.30	Less than 50% efficacy	protease
NVS_ENZ_rCNOS	NO	NO	not applicable	nitric oxide synthase 1, neuronal	27.0	1.43	NONE	oxidoreductase
NVS_GPCR_g5HT4	YES	NO	not applicable	5 hydroxytryptamine (serotonin) receptor 4	33.6	1.53	Less than 50% efficacy: Hit-call potentially confounded by overfitting	gpcr
NVS_GPCR_gOpiateK	YES	NO	not applicable	opioid receptor, kappa 1	28.9	1.46	Less than 50% efficacy: Borderline active: Only highest conc above baseline, active	gpcr
NVS_GPCR_h5HT5A	YES	NO	not applicable	5-hydroxytryptamine (serotonin) receptor 5A, G protein-coupled	8.95	0.952	Less than 50% efficacy: Hit-call potentially confounded by overfitting: Borderline active	gpcr
NVS_GPCR_h5HT7	YES	NO	not applicable	5-hydroxytryptamine (serotonin) receptor 7, adenylate cyclase-coupled	21.5	1.33	Less than 50% efficacy: Hit-call potentially confounded by overfitting: Borderline active: Only highest conc above baseline, active	gpcr
NVS_GPCR_hAdoRA2a	YES	NO	not applicable	adenosine A2a receptor	32.8	1.52	NONE	gpcr
NVS_GPCR_hAdra2A	YES	NO	not applicable	adrenoceptor alpha 2A	28.4	1.45	Less than 50% efficacy: Hit-call potentially confounded by overfitting: Only highest conc above baseline, active	gpcr
NVS_GPCR_hDRD1	YES	NO	not applicable	dopamine receptor D1	34.4	1.54	Hit-call potentially confounded by overfitting	gpcr
NVS_GPCR_hDRD2s	YES	NO	not applicable	dopamine receptor D2	13.9	1.14	Less than 50% efficacy	gpcr
NVS_GPCR_hDRD4.4	YES	NO	not applicable	dopamine receptor D4	23.7	1.37	Less than 50% efficacy	gpcr
NVS_GPCR_hM3	YES	NO	not applicable	cholinergic receptor, muscarinic 3	41.0	1.61	Less than 50% efficacy: Hit-call potentially confounded by overfitting: Borderline active: Only highest conc above baseline, active	gpcr
NVS_GPCR_r5HT1_NonSelective	YES	NO	not applicable	5-hydroxytryptamine (serotonin) receptor 1A, G protein-coupled	15.6	1.19	NONE	gpcr
NVS_GPCR_rNTS	YES	NO	not applicable	neurotensin receptor 1	22.1	1.34	Less than 50% efficacy: Borderline active	gpcr
NVS_IC_hKhERGCh	NO	NO	not applicable	potassium voltage-gated channel, subfamily H (eag-related), member 2	17.6	1.25	Less than 50% efficacy: Hit-call potentially confounded by overfitting	ion channel
TOX21_AhR_LUC_Agonist_viability	NO	YES	not applicable	not applicable	19.6	1.29	NONE	cell cycle
TOX21_AR_LUC_MDAKB2_Agonist2_viability	NO	YES	not applicable	not applicable	40.3	1.61	NONE	cell cycle
TOX21_AR_LUC_MDAKB2_Antagonist_Specificity_viability	NO	YES	not applicable	not applicable	37.5	1.57	NONE	cell cycle
TOX21_AR_LUC_MDAKB2_Antagonist_viability	NO	YES	not applicable	not applicable	37.8	1.58	NONE	cell cycle
TOX21_ARE_BLA_agonist_ratio	YES	NO	not applicable	nuclear factor, erythroid 2-like 2	86.7	1.94	Less than 50% efficacy: Borderline active: Only highest conc above baseline, active	DNA binding
TOX21_Aromatase_Inhibition_viability	NO	YES	not applicable	not applicable	14.8	1.17	NONE	cell cycle
TOX21_CAR_Agonist_viabillity	NO	YES	not applicable	not applicable	38.0	1.58	NONE	cell cycle
TOX21_CAR_Antagonist	NO		not applicable	nuclear receptor subfamily 1, group I, member 3	47.3	1.67	Less than 50% efficacy	nuclear receptor
TOX21_CAR_Antagonist_viability	NO	YES	not applicable	not applicable	37.4	1.57	NONE	cell cycle
TOX21_ELG1_LUC_Agonist_viability	NO	YES	not applicable	not applicable	43.1	1.63	NONE	cell cycle
TOX21_ERa_LUC_BG1_Agonist_Counterscreen_viability	NO	YES	not applicable	not applicable	36.4	1.56	NONE	cell cycle
TOX21_ERa_LUC_BG1_Antagonist_Specificity_viability	NO	YES	not applicable	not applicable	33.4	1.52	NONE	cell cycle
TOX21_ERa_LUC_BG1_Antagonist_viability	NO	YES	not applicable	not applicable	37.1	1.57	NONE	cell cycle
TOX21_ERR_viability	NO	YES	not applicable	not applicable	43.7	1.64	NONE	cell cycle
TOX21_H2AX_HTRF_CHO_Agonist_ratio	NO	NO	not applicable	H2A histone family, member X	106	2.03	Less than 50% efficacy	histones
TOX21_MMP_ratio_up	NO	NO	not applicable	not applicable	56.0	1.75	Only highest conc above baseline, active	cell morphology
TOX21_PGC_ERR_Antagonist	YES	NO	not applicable	estrogen-related receptor alpha	96.1	1.98	Only highest conc above baseline, active: Less than 50% efficacy: Borderline active	nuclear receptor
TOX21_PGC_ERR_viability	NO	YES	not applicable	not applicable	52.7	1.72	NONE	cell cycle
TOX21_RT_HEK293_GLO_08hr_viability	NO	YES	not applicable	not applicable	30.2	1.48	Less than 50% efficacy	cell cycle
TOX21_RT_HEK293_GLO_16hr_viability	NO	YES	not applicable	not applicable	24.7	1.39	Less than 50% efficacy	cell cycle
TOX21_RT_HEK293_GLO_24hr_viability	NO	YES	not applicable	not applicable	23.6	1.37	Less than 50% efficacy	cell cycle
TOX21_RT_HEK293_GLO_32hr_viability	NO	YES	not applicable	not applicable	21.0	1.32	Less than 50% efficacy	cell cycle

FD&C Yellow No. 6

ASSAY NAME	IN OUR SELECTED SUBSET	VIABILITY ASSAY	DESCRIPTION	GENE_NAME	AC50	LOGAC50	FLAGS	INTENDED_TARGET_ FAMILY
TOX21_RT_HEK293_GLO_40hr_ viability	NO	YES	not applicable	not applicable	26.7	1.43	Less than 50% efficacy	cell cycle
TOX21_RT_HEPG2_GLO_00hr_ctrl_ viability	NO	YES	not applicable	not applicable	34.8	1.54	Less than 50% efficacy	cell cycle
TOX21_RT_HEPG2_GLO_08hr_ctrl_ viability	NO	YES	not applicable	not applicable	32.0	1.50	Less than 50% efficacy	cell cycle
TOX21_RT_HEPG2_GLO_16hr_ctrl_ viability	NO	YES	not applicable	not applicable	31.6	1.50	Borderline active: Less than 50% efficacy	cell cycle
TOX21_RT_HEPG2_GLO_24hr_ctrl_ viability	NO	YES	not applicable	not applicable	33.7	1.53	Less than 50% efficacy	cell cycle
TOX21_RT_HEPG2_GLO_32hr_ctrl_ viability	NO	YES	not applicable	not applicable	40.1	1.60	Less than 50% efficacy	cell cycle
TOX21_RT_HEPG2_GLO_40hr_ viability	NO	YES	not applicable	not applicable	42.5	1.63	Less than 50% efficacy	cell cycle
TOX21_SSH_3T3_GLI3_Agonist_ viability	NO	YES	not applicable	not applicable	35.9	1.56	NONE	cell cycle
TOX21_SSH_3T3_GLI3_Antagonist_ viability	NO	YES	not applicable	not applicable	30.1	1.48	NONE	cell cycle
TOX21_TR_LUC_GH3_Antagonist_ viability	NO	YES	not applicable	not applicable	38.5	1.59	NONE	cell cycle