Predicting Coated-Nanoparticle Drugs Release Systems with Perturbation-Theory Machine Learning (PTML) Models
SUPPORTING INFORMATION

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Table S1. Nanoparticle Moving Average values (full list)

c_{0np}	n_{np}	nc_{0np}	$<D_{1core}(c_{0np})>$	$<D_{1coat}(c_{0np})>$	$<D_{2coat}(c_{0np})>$	$<D_{2core}(c_{0np})>$	$<D_{4coat}(c_{0np})>$	$<D_{3coat}(c_{0np})>$
EC50 (uM)	30	25422	51.13	6.54	0.18	2.48	53.16	17.57
IC50 (uM)p	29	18714	0.28	7.94	0.55	2.36	74.56	11.77
CC50 (uM)	113	3099	21.44	17.17	0.30	2.54	72.26	6.07
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c_{1np}	n_{np}	nc_{1np}	$<D_{1core}(c_{1np})>$	$<D_{1coat}(c_{1np})>$	$<D_{2coat}(c_{1np})>$	$<D_{2core}(c_{1np})>$	$<D_{4coat}(c_{1np})>$	$<D_{3coat}(c_{1np})>$
A549 (H)	23	2319.24	0.04	6.22	0.00	2.72	0.00	0.00
BMSC (H)	2	16644.5	0.50	71.47	0.00	2.93	0.00	0.00
BMSC (M)	2	16644.5	0.50	71.47	0.00	2.93	0.00	0.00
HEK293 (H)	3	11255.7	0.33	47.65	0.00	2.80	0.00	0.00
HepG2 (H)	15	2566.61	0.47	27.71	0.60	2.52	129.51	17.07
HUVECs	3	11246.2	0.33	47.65	0.00	2.80	0.00	0.00
NCIH441 (H)	4	8699.74	0.25	35.74	0.00	2.85	0.00	0.00
RAW 264.7 (M)	2	16644.5	0.50	71.47	0.00	2.93	0.00	0.00
BRL 3A (R)	4	3187.59	0.00	0.00	0.00	2.54	0.00	0.00
L929 (M)	3	6422.33	707.33	3.89	0.33	2.75	33.01	14.23
BJ (H)	1	3923.11	0.00	0.00	0.00	2.71	0.00	0.00
Neuro-2A (M)	1	2504.19	0.00	0.00	0.00	2.81	0.00	0.00
3T3 (M)	9	322.843	0.44	12.80	0.89	2.36	120.13	18.97
HaCaT (H)	6	459.361	45.00	0.00	1.16	2.43	160.50	0.00
H4IIE (R)	4	629.465	0.00	0.00	0.00	1.95	0.00	0.00
CaCo-2 (H)	6	313.239	0.67	5.33	0.43	2.21	138.67	10.97
Dendritic cells (M)	2	1000	0.00	0.00	0.00	2.78	0.00	0.00
MDCK (H)	2	870	0.00	0.00	0.00	2.78	0.00	0.00
NR8383 (R)	7	181.933	0.57	4.56	0.37	1.93	118.86	9.40
Precision-cut lung slices (R)	1	540	0.00	0.00	0.00	2.78	0.00	0.00

TK6 (H)	2	260	0.00	0.00	0.00	2.78	0.00	0.00
WISH (H)	3	331.813	0.00	0.00	0.00	2.74	0.00	0.00
HeLa (H)	1	266.559	0.00	0.00	0.00	2.55	0.00	0.00
RBE4 (R)	2	162.235	1.00	28.79	2.00	1.93	270.28	42.68
MDCK II (D)	3	4.06159	1.00	91.87	0.00	2.54	624.95	0.00
PK-15 (P)	1	3.49805	0.00	0.00	0.00	2.54	0.00	0.00
Vero (Mon)	1	1.05601	0.00	0.00	0.00	2.54	0.00	0.00
Saccharomyces cerevisiae	8	63045.4	0.25	9.42	0.40	2.49	61.58	15.17
Vibrio fischeri	4	62859.2	0.00	0.00	0.00	2.71	0.00	0.00
Tetrahymena thermophila	4	941.469	0.00	0.00	0.00	2.62	0.00	0.00
Desmodesmus subspicatus	2	513.36	0.00	0.00	0.00	2.81	0.00	0.00
Chlorella sp.	2	323.555	0.00	0.00	0.00	2.76	0.00	0.00
Chlorella vulgaris	1	432.169	0.00	0.00	0.00	2.68	0.00	0.00
Scenedesmus sp.	2	325.69	0.00	0.00	0.00	2.76	0.00	0.00
Pseudokirchneriella subcapitata	7	46.6136	218.86	17.27	0.33	1.97	157.47	57.96
Lycopersicon esculentum	16	31534.2	0.50	14.40	1.00	2.37	135.14	21.34
Brassica napus	6	2087.86	0.00	0.00	0.00	2.40	0.00	0.00
Cucumis sativus	2	6038.73	0.00	0.00	0.00	2.59	0.00	0.00
Raphanus sativus	3	4332.91	0.00	0.00	0.00	2.29	0.00	0.00
Lolium perenne	2	275.72	0.00	0.00	0.00	2.10	0.00	0.00
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c_{2np}	n_{np}	nc_{2np}	$<D_{1core}(c_{2np})>$	$<D_{1coat}(c_{2np})>$	$<D_{2coat}(c_{2np})>$	$<D_{2core}(c_{2np})>$	$<D_{4coat}(c_{2np})>$	$<D_{3coat}(c_{2np})>$
spherical	61	4758.43	4.85	30.30	0.51	2.51	106.89	11.47
N/A	52	15205.8	29.73	7.98	0.45	2.35	89.97	15.63
irregular	3	5258.69	707.33	3.89	0.33	2.74	33.01	14.23
slice-shaped	3	1229.2	0.00	0.00	0.00	2.55	0.00	0.00
needle	2	854.71	0.00	0.00	0.00	2.66	0.00	0.00
rod	9	161.681	0.11	10.21	0.00	2.27	69.44	0.00
elliptical	21	2218.42	0.00	0.00	0.00	2.71	0.00	0.00
pseudo-spherical	8	313.249	0.00	0.00	0.00	2.51	0.00	0.00
polyhedral	3	331.813	0.00	0.00	0.00	2.74	0.00	0.00
pyramidal	10	50186.6	0.00	0.00	0.00	2.81	0.00	0.00
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c_{3np}	n_{np}	nc_{3np}	$<D_{1core}(c_{3np})>$	$<D_{1coat}(c_{3np})>$	$<D_{2coat}(c_{3np})>$	$<D_{2core}(c_{3np})>$	$<D_{4coat}(c_{3np})>$	$<D_{3coat}(c_{3np})>$
Dry	118	13487.5	33.45	16.23	0.28	2.48	61.31	8.45
H2O	44	1332.96	0.41	10.27	0.50	2.54	106.54	12.69
DMEM	3	1443.08	0.00	0.00	0.00	2.93	0.00	0.00
RPMI	3	331.813	0.00	0.00	0.00	2.74	0.00	0.00
1% Triton X-100/H2O	3	13.1333	0.00	0.00	0.00	1.88	0.00	0.00
H2O/TMAOH	1	1.03654	0.00	0.00	0.00	2.78	0.00	0.00
c_{4np}	n_{np}	nc_{4np}	$<D_{1core}(c_{4np})>$	$<D_{1coat}(c_{4np})>$	$<D_{2coat}(c_{4np})>$	$<D_{2core}(c_{4np})>$	$<D_{4coat}(c_{4np})>$	$<D_{3coat}(c_{4np})>$
UC	125	12063.8	0.00	0.00	0.00	2.58	0.00	0.00
PEG-Si(OMe)3	8	16644.5	1.00	142.95	0.00	2.93	0.00	0.00
PVA	1	7671.95	2122.00	11.67	1.00	2.78	99.02	42.68
sodium citrate	17	343.1	1.00	28.79	2.00	2.18	270.28	42.68
11-mercaptoundec	3	200	1.00	62.13	1.00	2.54	377.25	42.68

anoic acid								
PVP	4	63.8915	157.50	0.00	2.32	1.93	320.99	0.00
propylamonium fragment	4	5.0381	1.00	0.00	0.00	1.90	125.16	32.90
undecylazide fragment	2	10.3254	1.00	0.00	1.59	1.90	364.40	0.00
CTAB	3	4.06159	1.00	91.87	0.00	2.54	624.95	0.00
N,N,N-trimethyl-3(1-propene) ammonium fragment	2	2.27148	1.00	31.95	1.00	2.01	217.33	0.00
potato starch	1	0.4728	1172.00	120.91	0.00	1.93	781.29	405.70
N - acetylcysteine	2	0.049	1.00	37.69	1.59	1.90	246.33	60.69

Table S2. Drug Moving Average values

c_{0drug}	n_{jdrug}	<ALOGP(c_{0drug})>	c_{1drug}	n_{jdrug}	<ALOGP(c_{1drug})>
Potency(nM)	24750	3.29	O88496	71.00	0.31
IC50(nM)	1402	4.24	P11473	24189.00	3.34
Activity(%)	1079	3.79	m.d.	9794.00	3.55
Inhibition(%)	415	3.25	P00568	3.00	-1.86
EC50(nM)	388	4.50	P41231	2.00	-1.86
WEIGHT(g)	260	3.18	Q9NPD5	14.00	2.30
Ratio(-)	259	5.44	Q9Y6L6	13.00	1.88
GI50(nM)	258	3.81	P12931	1.00	-1.86
Ki(nM)	197	3.83	P29410	5.00	-1.86
Activity(mg/dl)	164	5.74	P29411	4.00	-1.86
Activity(-)	154	5.19	P39069	3.00	-1.86
FC(-)	130	5.49	P54619, Q13131, Q9Y478	3.00	-1.86
IC50(ug.mL-1)	123	1.07	P21589	1.00	-1.86
BILI(ug.mL-1)	99	3.10	O43598	1.00	-1.86
CREAT(ug.mL-1)	99	3.10	Q6DHV7	3.00	-1.86
POTASSIUM(mEq.L-1)	99	3.10	P00327, P00328	1.00	-1.86
MCH(pg)	99	3.10	O35820	1.00	-1.86
MCV(fL)	99	3.10	P54819	3.00	-1.86
LYMLE(%)	99	3.10	P05186	1.00	-1.86
PHOS(ug.mL-1)	99	3.10	P0ADG7	1.00	-1.86
SODIUM(mEq.L-1)	99	3.10	P00338	2.00	-1.86
BUN(ug.mL-1)	99	3.10	P0A9J4	3.00	-1.18
CHOL(ug.mL-1)	99	3.10	P02769	25.00	4.68
WBC(cells.uL-1)	99	3.10	P18886	1.00	-1.81
ALB(ug.mL-1)	99	3.10	Q63704	1.00	-1.81
PROT(ug.mL-1)	99	3.10	P43155	1.00	-1.81

HGB(ug.mL-1)	99	3.10	P10828	3.00	3.83
PLAT(cells.uL-1)	99	3.10	P10275	10.00	2.52
EOSLE(%)	99	3.10	P02752	5.00	-1.72
MONOLE(%)	99	3.10	P33261	6.00	0.74
HCT(%)	99	3.10	P05177	3.00	1.96
GLUC(ug.mL-1)	99	3.10	P10635	10.00	1.15
RBC(cells.uL-1)	99	3.10	P22303	2.00	-1.69
NEUTLE(%)	99	3.10	P07477, P07478, P35030	3.00	-1.69
BASOLE(%)	99	3.10	Q05117	4.00	-1.69
ED50(nM)	97	5.78	P03372	9.00	4.41
Kd(nM)	93	3.86	P25099	1.00	-1.69
Ratio Ki(-)	89	5.49	Q63470	1.00	-1.69
Relative potency(-)	87	5.92	P07237	2.00	-1.69
Ratio ED50(-)	84	5.95	P08913	1.00	-1.69
ED50(M)	66	5.67	P18825	1.00	-1.69
Km(nM)	64	1.32	B4URF0	5.00	-1.69
BILDIR(ug.mL-1)	64	3.15	P06276	1.00	-1.69
ALBGLOB(-)	64	3.15	P18089	1.00	-1.41
GGT(IU.L-1)	64	3.15	P05067	4.00	-1.41
RETIRBC(%)	64	3.15	O15296	1.00	-1.41
PT(s)	64	3.15	P49841	1.00	-1.41
APTT(s)	64	3.15	P16050	4.00	2.50
MCHC(%)	64	3.15	P21567	3.00	0.60
ALT(IU.L-1)	64	3.15	P00689	5.00	1.00
AST(IU.L-1)	64	3.15	P04745	2.00	1.61
Cl(meq/L)	64	3.15	P04746	2.00	1.61
CALCIUM(ug.mL-1)	64	3.15	Q9H6Z9	1.00	-1.41
LDH(IU.L-1)	64	3.15	Q96KS0	1.00	-1.41
TERMBW(g)	64	3.15	Q9GZT9	1.00	-1.41

TRIG(ug.mL-1)	64	3.15	Q9NWT6	1.00	-1.41
PHOSLPD(ug.mL-1)	64	3.15	P13674	1.00	-1.41
ALP(IU.L-1)	64	3.15	P0A6I3	4.00	-1.04
FIBRINO(ug.mL-1)	64	3.15	P49327	1.00	-0.33
AC50(nM)	53	1.60	O15439	3.00	-0.04
Serum Ca2+(mg dl-1)	49	6.20	B0BL08	3.00	-0.04
Serosal/Mucosal Ca(-)	48	6.22	P70502	1.00	-0.04
LogP(-)	46	1.86	P04818	3.00	0.64
Efficacy(%)	41	5.28	Q05932	2.00	-0.04
Serum Ca2+(-)	40	5.53	Q96QA9	1.00	-0.04
BCM serum Ca(mg 100ml-1)	39	5.91	P48760	6.00	-0.04
Relative activity(%)	37	0.77	O00764	1.00	0.08
Ac50(uM)	36	1.75	P27695	8.00	1.73
Relative affinity(-)	36	6.24	P05181	5.00	0.18
EC50(ug.mL-1)	35	2.16	Q9NTG7	6.00	0.18
RBCNUC(/100WBC)	35	3.02	Q8IXJ6	12.00	0.18
LIPASE(U.L-1)	35	3.02	P08709, P13726	1.00	0.18
CHLORIDE(mEq.L-1)	35	3.02	O08966	2.00	0.61
ALP(U.L-1)	35	3.02	Q77YF9	3.00	-0.21
MONO(cells.uL-1)	35	3.02	Q9Z0E8	1.00	0.61
LYM(cells.uL-1)	35	3.02	O75496	29.00	2.97
MCHC(ug.mL-1)	35	3.02	O42275	8.00	0.83
CO2(nM)	35	3.02	Q9R0W2	1.00	0.61
Activity(mg/L)	35	2.29	Q63089	1.00	0.61
URATE(ug.mL-1)	35	3.02	P29401	1.00	0.61
EOS(cells.uL-1)	35	3.02	Q8TDS4	49.00	0.78
ALT(U.L-1)	35	3.02	Q9EP66	6.00	0.78
LDH(U.L-1)	35	3.02	Q80Z39	4.00	0.78
CK(U.L-1)	35	3.02	P49019	4.00	0.78

NEUTSG(cells.uL-1)	35	3.02	O94956	1.00	0.78
AST(U.L-1)	35	3.02	O75164	3.00	3.07
BASO(cells.uL-1)	35	3.02	P00519, Q13671	2.00	-0.45
MIC50(ug.mL-1)	34	-1.86	P37136	1.00	0.97
Activity(uM)	34	3.43	Q16678	2.00	0.97
GI(%)	32	2.62	P04798	1.00	0.97
VDR affinity(%)	24	5.03	Q81VW8	1.00	0.97
Relative binding affinity(-)	24	5.56	P00918	1.00	0.97
Activity(mg/kg/day)	23	5.81	P00915	1.00	0.97
ED50(mg.kg-1)	22	2.54	A3EZI9	1.00	0.97
Activity(10'7mol/J)	20	-1.41	P04150	23.00	4.73
Emax(%)	20	4.33	P54132	5.00	3.35
Ca2+ transport S/M(-)	20	5.54	P15559	12.00	2.01
Ca2+ transport(-)	20	5.51	P16435	1.00	2.01
Decrease(%)	19	7.53	P09623	6.00	2.01
RBA(-)	18	5.98	Q06278	5.00	2.01
mortality(%)	17	-1.47	P27338	2.00	2.01
Activity(mmol/L)	16	4.18	P11712	2.00	2.01
Activity(pm/min/mg)	16	6.43	P00390	5.00	2.01
Incorporation(%)	15	-1.71	P28593	6.00	2.01
B50(M)	15	6.50	P21397	1.00	2.01
ED50(-)	15	5.83	O15770	3.00	2.01
Ratio EC50(-)	15	5.10	P02545	7.00	2.74
Control(%)	14	5.83	Q00024	11.00	2.03
DOSE(mg.kg-1)	14	5.94	Q13393	3.00	4.60
F(%)	13	3.60	Q7M3G7	18.00	5.25
Transcriptional activity(%)	13	4.98	O42392	111.00	5.68
Activity(mg)	13	4.51	A3RGC1	116.00	5.61

ED50(uM)	12	5.20	P02774	56.00	5.56
Relative binding potency(-)	12	5.16	O14939	3.00	4.60
Ratio IC50(-)	12	3.40	Q06187	5.00	5.63
No. of pits(-)	12	6.31	Q28037	137.00	5.76
pKa(-)	11	1.72	P13053	250.00	5.78
Activity(cpm)	11	5.59	Q07973	1.00	5.08
Activity(ug ml-1)	10	3.93	P04276	35.00	5.87
Hepatotoxicity (severe hepatitis)(-)	10	3.27	P19793	32.00	5.20
Hepatotoxicity (choleostasis)(-)	10	3.27	P02754	3.00	5.51
Hepatotoxicity (cytolytic)(-)	10	3.27	P28482	8.00	3.29
Hepatotoxicity (acute)(%)	10	3.27	P02753	1.00	5.51
Hepatotoxicity (acute)(-)	10	3.27	Q92753	7.00	5.60
Hepatotoxicity (moderate)(-)	10	3.27	P13631	61.00	5.60
Hepatotoxicity (moderate)(%)	10	3.27	P10276	56.00	5.60
MIC(ug.mL-1)	10	1.76	P10826	62.00	5.60
Hepatotoxicity (association with vascular disease)(-)	10	3.27	P48443	15.00	5.60
Hepatotoxicity (cirrhosis)(-)	10	3.27	P22605	4.00	5.60
Hepatotoxicity (steatosis)(-)	10	3.27	P18911	3.00	5.60
Hepatotoxicity (chronic liver	10	3.27	P28702	14.00	5.60

disease)(-)					
A/Ad(-)	10	5.89	P11416	7.00	5.60
Hepatotoxicity (benign tumour)(-)	10	3.27	Q8R0V5	3.00	5.60
Hepatotoxicity (malignant tumour)(-)	10	3.27	P08684	13.00	3.66
Hepatotoxicity (granulomatous hepatitis)(-)	10	3.27	P28705	4.00	5.60
Activity(mU)	9	2.24	Q9HAW9	1.00	5.60
Flu intensity(-)	9	3.48	O60656	1.00	5.60
AUC(ng.hr.mL-1)	9	4.57	P00860	12.00	5.60
Ca2+ serum(-)	9	5.40	P28776	2.00	5.60
DILI positive/negative(-)	9	1.03	P35398	2.00	5.60
HepSE_jaundice(-)	8	4.51	P29762	1.00	5.60
HepSE_bilirubinemia(-)	8	4.51	P40220	5.00	5.60
HepSE_liver function tests abnormal(-)	8	4.51	P41595	2.00	5.60
HepSE_Combined Scores(-)	8	4.51	P28704	4.00	5.60
Cp(uM)	8	4.40	P28700	6.00	5.60
T1/2(hr)	8	2.49	P0DMS8	2.00	5.60
Carboxylase activity(dpm)	8	2.49	Q9PTN2	1.00	5.70
Relative activity(-)	8	3.62	P25094	9.00	4.27
Binding affinity(-)	8	5.48	P48281	14.00	7.12
Activity(log10CFU)	8	5.29	P14416	1.00	6.69
HepSE_hepatitis(-)	8	4.51	P08908	1.00	6.69
HepSE_liver disease(-)	8	4.51	O35084	9.00	6.84
Keq(-)	8	6.82	P00189	2.00	6.73

k1(s-1)	8	6.82	A5A0U0	1.00	6.73
k-1(s-1)	8	6.82	Q6B4J2	26.00	7.89
Activity(ug)	8	11.21	Q99835	2.00	7.63
TI(-)	8	2.96	P49638	3.00	8.84
HepSE_cirrhosis(-)	8	4.51	P08170	2.00	8.84
HepSE_liver fatty(-)	8	4.51	P38435	3.00	8.92
HepSE_hepatomegaly(-)	8	4.51	Q72874	4.00	-1.86
HepSE_cholecystitis(-)	8	4.51	Q9X034	1.00	-1.86
HepSE_cholelithiasis(-)	8	4.51	P42356, Q8TCG2, Q9BTU6, Q9UBF8	1.00	-1.86
HepSE_hepatic failure(-)	8	4.51	P09467	8.00	-1.86
HepSE_hepatic necrosis(-)	8	4.51	Q96KQ7	17.00	3.60
HepSE_elevated liver function tests(-)	8	4.51	P30542	1.00	-1.86
Activity(microg/ml)	7	4.45	P00636	2.00	-1.86
Change(%)	7	2.16	P08659	3.00	3.79
Reduction(%)	7	1.42	P47900	2.00	-1.86
Receptor binding(-)	7	4.77	P49798	2.00	1.87
Therapeutic index(-)	7	5.87	Q94696	3.00	-1.86
RCI(-)	7	5.93	Q13148	6.00	0.41
Vmax(pM s-1 mg-1)	7	7.92	P49652	2.00	-1.86
Relative IC50(nM)	7	5.60	P37840	2.00	-0.95
Relative Vmax(-)	6	-1.25	P14618	5.00	-0.31
Activity(cm)	6	-0.47	Q27686	3.00	-1.86
deltaA(-)	6	5.42	P19174	1.00	-1.86
Imax(%)	6	2.56	O75874	1.00	-1.86
Cmax(nM)	6	4.21	Q96G91	1.00	-1.86
T/C(-)	6	4.37	Q9HBX9	1.00	-1.86

Activity(nm)	6	6.65	O94782	19.00	4.25
Relative EC30(-)	6	5.60	Q16637	4.00	3.34
Survivors at day 15(%)	6	5.60	O15648	5.00	0.76
NBT positive cells(%)	6	5.60	P07378	1.00	-1.86
Survivors at day 8(%)	6	5.60	Q57TT1	1.00	-1.86
Dose(mg kg-1 day-1)	6	6.23	P17405	2.00	-0.95
Binding ratio(-)	6	5.70	O94759	1.00	-1.86
Ca2+ current(mV)	6	5.70	P83916	6.00	0.77
Drug metabolism(%)	6	7.09	Q01970	1.00	-1.86
RCI(%)	6	6.01	P28329	1.00	-1.86
Activity(mM)	6	0.16	O88909	1.00	-1.81
EC30(nM)	6	5.60	P00811	7.00	1.24
Relative EC30(nM)	6	5.60	Q96QE3	3.00	1.77
Activity(nmol/g)	5	-3.25	Q03431	3.00	4.21
Radioactivity(%)	5	-1.86	Q99895	1.00	-1.72
Kcat(/s)	5	-0.92	P00346	1.00	-1.72
TIME(hr)	5	1.55	P38398	2.00	-1.72
Activity(umol)	5	-1.41	O00255, Q03164	7.00	3.17
Cmax(ug.mL-1)	5	3.85	B2RXH2	6.00	0.37
IZ(mm)	5	1.76	O97447	9.00	1.54
logD(-)	5	1.74	Q9NUW8	2.00	-0.88
Kcat(/min)	5	4.30	P00352	17.00	3.55
Tmax(hr)	5	4.88	P97697	3.00	0.77
Relative IC50(-)	5	5.60	O75604	3.00	1.93
Differentiation activity ratio(-)	5	5.70	P29466	2.00	-1.72
ICA(-)	5	5.90	P55210	2.00	-1.72
Biological evaluation(-)	5	5.79	P15428	5.00	1.59
Vmax(%)	4	-1.41	P02791	5.00	3.43
Activity(umol/g)	4	-1.69	P15917	4.00	1.04

ID50(uM)	4	1.06	Q99714	6.00	0.70
Activity(mmolequiv/mmol)	4	-1.41	Q92830	6.00	2.58
Frequency(-)	4	3.72	Q03181	7.00	4.06
TAC(U)	4	-1.41	Q16236	15.00	4.65
Activity(umol/L)	4	-1.41	Q96RI1	5.00	3.48
Tritium release(%)	4	-0.04	P46063	2.00	1.94
Liver weight(g)	4	0.78	P19838	1.00	-1.72
Survival(%)	4	0.78	P01375	1.00	-1.72
Serum TG(mg dl-1)	4	0.78	P37231	6.00	3.56
CL(mL.min-1.kg-1)	4	1.76	P33527	1.00	-1.69
Selectivity ratio(-)	4	1.04	Q9UNQ0	2.00	-1.69
Activity(umol/L/min)	4	2.01	P03468	2.00	-1.69
k cat(s-1)	4	2.01	P81908	3.00	1.97
Activity(g/cm2)	4	5.36	O42713	5.00	0.81
Solubility(ug.mL-1)	4	1.79	P11064	1.00	-1.69
Binding potency(-)	4	5.39	P35354	2.00	-0.46
Mean tumor volume(cm*3)	4	5.60	P34913	2.00	-1.69
Relative luciferase response(-)	4	5.60	Q9GZQ4	1.00	-1.69
Potency(-)	4	6.02	P10253	6.00	0.64
Activity(pM 10min-1)	4	5.99	Q9NR56	4.00	-0.77
Binding(%)	4	5.97	P06746	2.00	-0.87
permeability(ng/cm2/min)	4	6.56	O94925	1.00	-1.69
permeability(%)	4	6.56	P07943	1.00	-1.69
Ca2+ binding protein(ug (100mg of duodenum)-1)	4	6.73	Q9UBT6	4.00	5.09
Incidence(N)	4	3.72	Q962Y6	9.00	4.70

Duration(s)	4	3.72	P10636	22.00	5.07
EC50(ug)	3	1.82	P10481	1.00	-1.69
ED50(ug ml-1)	3	1.82	Q99700	2.00	0.16
Activity(U (mg of protein)-1)	3	-1.69	P47989	1.00	-1.69
MIC(ug)	3	-1.41	P03469	2.00	-1.69
Scavenging activity(%)	3	4.02	P27487	1.00	-1.69
Vmax(-)	3	-0.04	P48147	1.00	-1.69
log K(-)	3	1.85	P04762	2.00	3.72
k cat/Km(10e4 M-1 s-1)	3	2.01	Q9UGH3	2.00	-1.41
Vmax(uM min-1mg-1)	3	2.01	P11344	2.00	-1.41
Average weight change(%)	3	2.01	P09917	1.00	-1.41
Activity(micromol/min)	3	0.87	P18054	1.00	-1.41
VDR affinity(M)	3	4.90	P14679	2.00	-1.41
MTD(ug/kg)	3	5.47	Q54873	1.00	-1.41
Affinity(%)	3	5.89	Q9F4F7	6.00	3.80
GGT Increase - Index Value(-)	3	3.16	Q9UNA4	7.00	3.66
LDH Increase - Index Value(-)	3	3.16	O15245	2.00	0.29
Alkaline Phosphatase Increase - Index Value(-)	3	3.16	P43220	3.00	1.25
Mortality range(day)	3	5.60	P16473	7.00	2.35
Kd(-)	3	5.60	P06280	1.00	-0.04
Differentiated cells(%)	3	5.60	P04062	1.00	-0.04
Expression(%)	3	5.60	P07607	2.00	-0.04
ED50(10'-10M)	3	5.73	O89049	7.00	4.73

Delta Tm(degrees C)	3	5.70	P04637	5.00	2.75
Log A(s-1)	3	6.68	O95342	1.00	0.08
ED50(10'-9M)	3	5.73	O70127	1.00	0.08
RBA(%)	3	6.70	Q96EB6	12.00	0.18
Kcat/Km(10'4/M/s)	3	6.84	Q8N6T7	3.00	0.18
Fold change(-)	3	4.83	P97612	1.00	0.18
PC50(uM)	3	8.84	Q8I6E4	1.00	0.18
Composite Activity - Active(-)	3	3.16	Q9NXA8	2.00	0.18
SGOT Increase - Index Value(-)	3	3.16	P06700	1.00	0.18
SGPT Increase - Index Value(-)	3	3.16	P53686	1.00	0.18
Composite Activity - Marginal(-)	3	3.16	P09874	5.00	0.18
GGT Increase - Number of Reports(-)	3	3.16	Q9H3S4	1.00	0.61
LDH Increase - Number of Reports(-)	3	3.16	P07900	2.00	0.61
SGOT Increase - Number of Reports(-)	3	3.16	P80456	3.00	1.19
SGPT Increase - Number of Reports(-)	3	3.16	Q96FL8	2.00	0.78
Alkaline Phosphatase Increase - Number of Reports(-)	3	3.16	Q9UIF8	4.00	4.33
Vdss(L.kg-1)	3	0.78	P00432	1.00	0.78
ID50(nM)	3	5.60	P14920	1.00	0.78
MTC(uM)	3	8.84	Q99489	1.00	0.78
Kcat/Km(10'6/M/s)	2	-1.86	P22629	1.00	0.80
K(10'4L/mol)	2	-1.81	Q194T2	2.00	3.20

Activity(g)	2	-0.47	P23467	1.00	0.80
Activity(kg/ha)	2	-0.47	P14735	2.00	0.80
Stability(-)	2	-1.69	Q9UQ49	1.00	0.97
K(10'6/M/s)	2	3.58	P11308	1.00	0.97
IC25(uM)	2	-1.69	P80244	1.00	0.97
IC30(uM)	2	-1.69	P80404	1.00	0.97
IC50(molar ratio)	2	1.96	P51649	1.00	0.97
Activity(IU)	2	-1.41	P51580	1.00	0.97
OD(-)	2	-1.41	P02768	1.00	1.77
IC0.2(uM)	2	3.72	P35498, Q99250, Q9NY46	2.00	1.77
Activity(nmol)	2	-1.41	Q6W5P4	1.00	1.77
Activity(mmol/g)	2	-1.55	P0A6C1	1.00	1.77
MNTD(uM)	2	1.61	P08482	2.00	1.77
MED(mg Kg-1)	2	0.48	P38532	1.00	1.77
Serum LDL-cholesterol(%)	2	0.78	Q3B792	1.00	2.01
Serum cholesterol(%)	2	0.78	P10845	1.00	2.01
Serum HDL-cholesterol(%)	2	0.78	P00469	1.00	2.01
Activity(mg kg-1)	2	0.78	P30305	4.00	2.01
PPB(%)	2	0.78	P46426	1.00	2.01
Binding energy(kCal mol-1)	2	3.25	Q5FB27	1.00	2.01
Ka(M-1)	2	0.80	O54754	1.00	2.01
Log M(-)	2	0.97	Q9Z0U5	1.00	2.01
MIC(nM)	2	1.49	P14902	2.00	2.01
LogD7.4(-)	2	0.93	P51450	22.00	5.54
logIC50(-)	2	0.04	P00883	1.00	2.01
Vmax(uM s-1)	2	2.01	O60240, Q8WTS1	1.00	2.01
Toxic dose(uM)	2	2.01	Q00G26, Q8WTS1	1.00	2.01

PD50(nM)	2	5.47	P04406	1.00	2.01
TC50(nM)	2	5.47	P68871	1.00	2.01
Relative peroxidation(-)	2	3.54	Q16665	4.00	3.81
AUC(uM.hr)	2	4.37	P30307	2.00	2.01
Flu intensity(a.u.)	2	5.20	Q64346	1.00	2.01
Binding affinity(%)	2	5.14	Q9HC16	1.00	2.01
Kq(10'13/M/sec)	2	5.56	P28563	1.00	2.01
K(10'6/M)	2	5.56	O95398	6.00	8.02
Activity(U)	2	2.05	P84022	2.00	5.47
Tumor volume(cm*3)	2	5.60	Q13315	1.00	2.01
ODC Activity((nM of CO2) 30min-1 (mg of protein)-1)	2	5.60	P15374	1.00	2.01
No. of tumors/mouse(-)	2	5.60	Q9Y253	2.00	5.59
NBT positivity(%)	2	5.65	P09936	1.00	2.01
Drug uptake(%)	2	5.70	P42858	2.00	2.78
Activity(10^5/ml)	2	5.70	Q09128	18.00	4.31
Cell proliferation(%)	2	5.65	P22310	4.00	6.59
Activity(pg/ml)	2	5.20	Q12809	1.00	5.51
ED50(10'-8M)	2	5.95	Q9R1A7	4.00	5.56
Activity(mgequiv/mmol)	2	3.50	P10145	2.00	6.57
Phagocytosis(-)	2	6.22	P25779	9.00	6.76
Binding activity(-)	2	6.22	P51449	5.00	5.99
Antilipid peroxidation(%)	2	3.72	P22309	5.00	6.41
Reducing activity(%)	2	3.72	Q9HAW7	1.00	5.60
Activity(nM/mg)	2	8.84	Q9HAW8	2.00	5.60
Activity(U/mg)	2	3.72	P09057	1.00	5.60

Activity(min)	2	3.72	P62965	2.00	5.60
Activity(cm2)	2	8.84	P22935	2.00	5.60
SVT(%)	2	8.84	Q99549	1.00	5.60
SVT(-)	2	8.84	P08183	2.00	6.69
RIA(%)	2	0.78	P07711	1.00	6.73
Hammett constant(-)	2	0.97	P23415	3.00	7.62
K cat/Km(1/M*s)	2	2.01	P16662	2.00	8.24
Concentration(M)	2	5.70	O00167	1.00	7.64
ED20(nM)	2	5.70	O95149, P62826, Q14974	3.00	8.94
SMT(s)	2	8.84	P49768	3.00	8.84
RRT(s)	2	8.84	O75469	1.00	8.92
TC50(uM)	2	8.84	O95149, Q14974	1.00	8.92
Solubility(nM)	1	-1.86	P63092	1.00	11.54
CC50(nM)	1	-1.69	c_{3drug}	n_{jdrug}	<ALOGP(c_{3drug})>
Kcat/Km(/s/microM)	1	-1.86	m.d.	26435	3.24
k_off(s-1)	1	-1.86	Rattus norvegicus	5385	3.59
Kcat(10^-3/s)	1	-1.86	Homo sapiens	2756	4.62
MTD(uM)	1	-1.86	Cricetulus griseus	74	4.65
Vmax(micromol/min)	1	-1.86	Oryctolagus cuniculus	22	0.33
k_on(M-1.s-1)	1	-1.86	Human herpesvirus 1	4	-0.13
permeability(10'-6 cm/s)	1	-1.81	Measles virus	2	-1.86
Activity(V)	1	-1.69	Sindbis virus	2	-1.86
ID50(mg)	1	-1.69	Semliki forest virus	2	-1.86
K(10'4/M/s)	1	-1.69	Human coxsackievirus B4	4	-1.86
Ratio CC50/IC50(-)	1	-1.69	reo-1 virus	2	-1.86
K(10'8/M/s)	1	-1.69	Human parainfluenza virus 1	2	-1.86
pID50(-)	1	-1.69	Cercopithecidae	17	4.72

Activity(nmol/ml)	1	-1.69	Vaccinia virus	2	-1.86
Retention_time(min)	1	-1.69	polio-1 virus	2	-1.86
Activity(mg/g)	1	-1.69	Vesicular stomatitis virus	4	-1.86
Maximal relaxation(%)	1	-1.69	herpes simplex type-2 virus	2	-1.86
IC25(nM)	1	-1.69	Mycobacterium tuberculosis	21	1.02
deltaA(%)	1	-1.69	Equus caballus	9	2.36
INH(ug)	1	-1.69	Methanothermobacter thermautotrophicus	1	-1.86
k'(-)	1	-1.41	Bos taurus	153	5.39
Activity(mIU/ml)	1	-1.41	Columba livia	1	-1.81
Distribution percent(-)	1	-1.41	Cenchrus americanus	45	-0.34
Activity(mMequiv)	1	-1.41	Gallus gallus	194	5.39
Activity(nmol/mg)	1	-1.41	Mus musculus	522	5.02
SC50(mM)	1	-1.41	Moloney murine leukemia virus	2	-1.69
Vmax(nM hr-1 (10e6*cells)-1)	1	-1.41	Human herpesvirus 4	29	3.33
Rate of rotation(-)	1	-1.41	Heterodera zeae	16	-1.69
SC50(ug ml-1)	1	-1.41	Meloidogyne incognita	2	-0.46
Kt(uM)	1	-1.41	Influenza A virus	3	-1.69
Inactivation(%)	1	-1.41	Canis lupus familiaris	14	1.76
Stimulation(%)	1	-1.41	Ovis aries	2	-1.64
kONOO-(M-1 s-1)	1	-1.41	malt	5	1.00
Inhibitory concentration(mM)	1	-1.41	Fungi	2	1.61
K(M-1 s-1)	1	-1.41	Bacteria	2	1.61
k cat(M-1 s-1)	1	-1.41	Musa acuminata	2	-1.41
kred(M-1 s-1)	1	-1.41	Trypanosoma cruzi	22	3.72

Vmax(microM/s)	1	-1.04	Escherichia coli	24	0.91
Kq(10'13L/mol/s)	1	-1.04	Sus scrofa	124	5.22
KSV(10'5L/mol)	1	-1.04	Xenopus laevis	1	0.61
Kq(10'5L/mol)	1	-1.04	Human immunodeficiency virus 1	8	0.09
Kq(10'4L/mol)	1	-1.04	Electrophorus electricus	8	0.83
Kq(10'12L/mol/s)	1	-1.04	Macaca fascicularis	2	1.40
KSV(10'4L/mol)	1	-1.04	Gibberella moniliformis	1	0.78
Kcat/Km(/mM/min)	1	-1.04	Staphylococcus aureus	12	1.53
Kcat/Km(/mM/s)	1	-1.04	Not specified	5	2.09
k(-)	1	-0.04	Filobasidiella neoformans	1	0.97
Km app(rel)	1	-0.04	Candida albicans	4	0.83
Concentration(uM)	1	-0.04	Bacillus anthracis	2	3.29
Km(-)	1	-0.04	Hepatitis C virus	3	5.82
Km app(-)	1	-0.04	Saccharomyces cerevisiae	5	1.05
fCmax(uM)	1	0.08	Cavia porcellus	18	4.21
Vmax(pmol/mg/min)	1	0.18	Plasmodium falciparum	43	2.90
Kcat/Km(10^-5/nM/s)	1	0.61	Mycobacterium bovis BCG	5	2.01
log Kp(-)	1	0.78	Leishmania donovani	3	0.79
AUC(microM/hr/mg)	1	0.78	Setaria cervi	2	2.01
LTKB_BD DILI severity score(-)	1	0.78	Erwinia amylovora	1	2.01
MED(-)	1	0.78	Mycobacterium tuberculosis H37Rv	9	5.68

Vigour_index(-)	1	0.78	Cricetinae	32	5.66
Transport(pM min-1 (mg of protein)-1)	1	0.80	Rangifer tarandus	2	5.51
Kis(uM)	1	0.80	Dictyostelium discoideum AX2	2	5.56
Ka(/M)	1	0.80	Mesocricetus auratus	5	8.19
Log 1/C(-)	1	0.97	Naja mossambica mossambica	2	5.60
Log LD50(-)	1	0.97	Danio rerio	1	5.70
Rm(-)	1	0.97	Clupea	2	8.84
Activity(10'-10mol/min)	1	0.97	Glycine max	3	8.91
pLD50(-)	1	0.97	Thermotoga maritima	1	-1.86
Concentration(nM)	1	0.97	Chlorocebus aethiops	2	0.07
Log S(-)	1	1.77	Rous sarcoma virus	1	-1.86
logS0(-)	1	1.77	Photinus pyralis	1	-1.86
Log PNalk(-)	1	1.77	Photuris pennsylvanica	3	-1.86
Log K'(-)	1	1.77	Meleagris gallopavo	2	-1.86
Log sensitivity(-)	1	1.77	Leishmania mexicana mexicana	3	-1.86
logPn(-)	1	1.77	Trypanosoma brucei TREU927	4	-0.45
Stabilty(%)	1	1.77	Trypanosoma brucei	2	1.87
AD(mM l-1)	1	1.77	squid	1	-1.86
LD50(umol.kg-1)	1	1.77	unidentified	1	-1.72
k2(M-1 s-1)	1	2.01	Giardia intestinalis	10	1.22
ED25(mM kg-1)	1	2.01	Bacillus anthracis str. A2012	3	-0.48
Phospholipidosis as % of positive control(%)	1	2.01	Trichophyton tonsurans	2	-1.69
Ratio(/M/s)	1	2.01	Trichophyton	2	-1.69

			mentagrophytes		
log Ks(-)	1	2.01	Salmonella enterica subsp. enterica serovar Typhimurium	8	3.58
Maximum test concentration that did not exhibit cytotoxicity(uM)	1	2.01	Influenza A virus (A/Puerto Rico/8/1934(H1N1))	3	-1.69
k(se-1)	1	2.01	Epidermophyton floccosum	2	-1.69
DC50(microg/cm2)	1	2.01	Trichophyton violaceum	2	-1.69
ED25(mg kg-1)	1	2.01	Arthroderma cajetani	2	-1.69
FDI(%)	1	2.01	Microsporum gypseum	1	-1.69
LD50(uM)	1	2.01	Trichophyton rubrum	2	-1.69
Optimal dose(%)	1	2.01	Agaricus bisporus	5	0.81
LD50(mg.kg-1)	1	2.01	Cryptococcus neoformans	1	-1.69
x fold(uM)	1	2.01	Verticillium dahliae	1	-1.69
Activity(umol/min/mg)	1	2.01	Entamoeba histolytica HM-1:IMSS	1	-1.69
K cat/Km(1/M.s)	1	2.01	Entamoeba histolytica	1	-1.69
Vmax(uM)	1	2.01	Dengue virus	1	-1.69
k cat/Km(M-1 s-1)	1	2.01	Trichomonas vaginalis	2	-1.69
Kcat/Km(-)	1	2.01	Schistosoma mansoni	9	4.70
AUC(min.kg/L)	1	3.85	Clostridium perfringens	1	-1.69
CL(mL.min-1.g-1)	1	4.69	Influenza A virus (A/Perth/16/2009(H3N 2))	1	-1.69
Ratio(%)	1	4.69	Influenza A virus (A/California/07/2009(	2	-0.45

			H1N1))		
Log Kd(-)	1	5.51	Influenza B virus	1	-1.69
Activity(a.u.)	1	5.51	Influenza B virus (B/Brisbane/60/2008)	1	-1.69
Vm(10'-4m3/mol)	1	5.51	Enterovirus A71	1	-1.69
pAH50(-)	1	5.51	mushroom	1	-1.41
logPapp(-)	1	5.60	Vibrio harveyi	1	-1.41
ED1/3(M)	1	5.60	Streptococcus pneumoniae	2	-1.41
ID50(nmol)	1	5.60	Streptococcus agalactiae	5	2.21
delta logD(-)	1	5.60	Bacillus subtilis	7	3.40
permeability(10'-4 cm/s)	1	5.60	Leishmania infantum	1	0.18
Tumor(number)	1	5.60	Trypanosoma brucei rhodesiense	1	0.18
IC60(nM)	1	5.60	Lactococcus lactis	2	0.61
IC80(nM)	1	5.60	Streptomyces avidinii	1	0.80
ED30(nM)	1	5.60	unidentified influenza virus	1	0.97
Daq(10'-6cm2/s)	1	5.60	frog	1	1.77
Average(%)	1	5.60	Aspergillus niger	1	2.01
Activity(pmol)	1	5.60	Clostridium botulinum	1	2.01
Selectivity(-)	1	5.60	Lactobacillus casei	1	2.01
Tumor latency(day)	1	5.60	Trichoplusia ni	3	2.01
Tumor incidence(%)	1	5.60	Drosophila	7	3.52
Aggregation(%)	1	5.60	Influenza A virus (A/WSN/1933(H1N1))	1	5.60
Differentiation(%)	1	5.60	Plasmodium falciparum HB3	1	5.60
RA(%)	1	5.60	Plasmodium	1	5.60

			falciparum 7G8		
MTD(ug/kg/day)	1	5.70	Rhopilema esculentum	1	8.84
Activity ratio(-)	1	5.70	c_{4drug}	n_{jdrug}	<ALOGP(c_{4drug})>
LD50(10'-7M)	1	5.70	m.d.	31513	3.46
LD50(10'-6M)	1	5.70	Wistar	46	4.64
Plasma Ca2+(mg dl-1)	1	5.70	cultivar 7042S	45	-0.34
Stability(%)	1	5.70	KM	5	-1.69
Ca2+ excretion(uM day-1)	1	5.70	Charles foster	3	-1.69
Kidney VDR(fM (mg of protein)-1)	1	5.70	BALB/c	12	1.12
ED50(10'-6M)	1	5.95	C57BL/6	24	0.65
BPR(-)	1	6.29	A/Bervig_Mission/1/18	2	-1.69
CS50(-)	1	6.63	Wistar albino	31	1.24
Activity(mU ml-1)	1	6.73	New Zealand White	2	-1.41
Hydroxyproline release(ug ml-1)	1	6.73	Sprague-Dawley	4414	3.28
K(uM)	1	7.62	K12	4	-1.04
%max(%)	1	7.62	beagle	2	0.78
Effective molarity(M l-1)	1	8.84	SD, HW or BN	1	0.78
Activity(milliequivalent/kg)	1	8.84	C57B1/6	2	0.78
Relative peroxidation(%)	1	8.84	C57/Bl6	1	0.78
Q1/2(mM)	1	8.84	ATCC 25923	1	0.78
Activity(microM/min/mg)	1	8.84	1199B	2	0.78
RC10(uM)	1	8.84	MN8	3	1.32
Activity(uM/L)	1	8.84	Can2	1	0.97

IC20(uM)	1	8.84	Nce103	1	0.97
MIC95(ug ml-1)	1	8.84	DMY2844	1	0.97
Activity(nM/min/mg)	1	8.84	P55	1	2.01
A0.5(uM)	1	8.84	H37Rv	2	2.01
Activity(nmol/hr)	1	8.84	295/93	1	2.01
LDL cholesterol(mg 100ml-1)	1	8.84	NMRI	3	5.30
HDL cholesterol(mg 100ml-1)	1	8.84	DBA/1	6	5.20
T inh(s)	1	8.84	Swiss	1	5.05
Total cholesterol(mg 100ml-1)	1	8.84	Swiss albino	1	5.60
Safety index(-)	1	8.84	CD1	13	5.63
Activity(L/mol/s)	1	8.84	ddY	2	5.70
HMGR activity(-)	1	8.84	FVB	9	5.70
IC50(ug)	1	8.84	CD-1	4	6.29
Drug uptake(uM)	1	8.92	Dunkin Hartley	4	6.29
Vmax/Km(pmol/micro M)	1	8.92	Wistar-Kyoto	4	6.59
Vmax(pmol)	1	8.92	Malmsten CBS 483.76	2	-1.69
Drug degradation(%)	1	9.06	(Robin) Blanchard CBS 160.66	2	-1.69
AC50(%)	1	9.91	T98	3	-1.69
c_{2drug}	n_{jdrug}	<ALOGP(c_{2drug})>	(Hartz) Langeron and Milochevitch CBS 358.93	2	-1.69
m.d.	33972	3.33	Malmsten CBS 459.61	2	-1.69
CHO	45	2.11	Ajello CBS 495.70	2	-1.69
Vero	17	-1.40	(Bodin) Guiart and Grigorakis IHME 3999	1	-1.69
HeLa	25	1.84	TA98	1	-1.69

K562	28	-0.94	(Castellani) Sabouraud IHME 4321	2	-1.69
HL-60	527	5.55	MTCC 300	4	3.58
Raji	46	3.38	ATCC 90113	1	-1.69
U-251	6	3.00	ATCC 90028	1	-1.69
C6	1	-1.69	IMSS:0989:1	1	-1.69
PC-12	3	5.33	pdm09	1	-1.69
Platelet	5	-1.72	4755	5	2.21
RAW264.7	10	0.50	K1	1	0.18
MVLN	2	-1.69	MHOM/ET/67/L82	2	0.18
BV-2	4	-1.69	NMRI, BalbC or CD1 mice	1	0.18
KB	4	-0.87	Tulahuen C4 (LacZ)	1	0.18
Hepatocyte	10	6.76	STIB 900	1	0.18
HepG2	14	2.40	Swiss Webster	1	1.61
MDCK	5	1.02	KOP55	3	2.01
HEK293	40	4.95	K12 MG1655	1	2.01
Erythrocyte	11	0.46	LAC	1	2.01
SH-SY5Y	6	0.56	MW2	1	2.01
Fibroblast	17	6.02	MNPE	1	2.01
RD	8	1.69	CDC587	1	2.01
L1210	12	0.56	Fisher	1	5.60
Sf9	10	4.82	W2	1	5.60
V79	7	7.57	PQ37	1	8.84
CCRF-CEM	9	3.16	TA102	4	8.84
HaCaT	30	4.04	Sprague-Dawley Albino	1	8.84
BALB/3T3	1	0.61	c_{2drug}	n_{jdrug}	<ALOGP(c_{2drug})>
Oocyte	2	-0.60	CAL-62	1	5.60
CHO-K1	16	1.99	769-P	1	5.60
Adipocyte	4	0.78	OAW-42	1	5.60

HCT-15	5	3.94	PSN1	1	5.60
MDA-MB-231	11	4.52	SH-4	1	5.60
SN12C	5	3.94	NCI-H650	1	5.60
SR	4	3.52	NCI-H1703	1	5.60
M14	5	3.94	OCI-AML2	1	5.60
A549	12	4.41	SAOS-2	1	5.60
ACHN	5	3.94	ZR-75-30	1	5.60
EKVX	4	3.52	ES6	1	5.60
KM12	5	3.94	A704	1	5.60
MCF7	63	5.42	SW982	1	5.60
PC-3	9	4.68	COLO-741	1	5.60
T47D	11	4.85	OS-RC-2	1	5.60
786-0	5	3.94	G-402	1	5.60
HT-29	17	5.86	KLE	1	5.60
MDA-N	4	3.52	NCI-H2228	1	5.60
TK-10	4	3.55	EC-GI-10	1	5.60
UO-31	5	3.94	OCUB-M	1	5.60
CAKI-1	5	3.94	EFM-19	1	5.60
DU-145	11	4.23	LB373-MEL-D	1	5.60
HOP-62	5	3.94	CAL-33	1	5.60
HOP-92	4	3.55	8505C	1	5.60
MOLT-4	6	3.28	NCI-H1792	1	5.60
SF-268	5	3.94	SBC-5	1	5.60
SF-295	4	3.52	IST-MEL1	1	5.60
SF-539	4	3.52	SW1088	1	5.60
SNB-19	4	3.52	HCC1569	1	5.60
SNB-75	4	3.52	MHH-NB-11	1	5.60
SW-620	4	3.52	ES7	1	5.60
HCT-116	6	4.26	HN	1	5.60
Hs-578T	3	2.86	LB771-HNC	1	5.60

IGROV-1	5	3.94	RH-18	1	5.60
NCI-H23	5	3.94	HuP-T4	1	5.60
OVCAR-3	5	3.94	LoVo	1	5.60
OVCAR-4	5	3.94	MFM-223	1	5.60
OVCAR-5	5	3.94	RKO	1	5.60
OVCAR-8	4	3.55	D-336MG	1	5.60
COLO 205	5	3.94	HCC70	1	5.60
HCC 2998	4	3.52	KYSE-520 cell line	1	5.60
LOX IMVI	4	3.52	NCI-H358	1	5.60
Malme-3M	4	3.52	NCI-H1838	1	5.60
NCI-H226	5	3.94	NCI-H1573	1	5.60
NCI-H460	5	3.94	KARPAS-299	1	5.60
NCI-H522	4	3.52	LB2518-MEL	1	5.60
SK-MEL-2	5	3.94	NCI-H1793	1	5.60
SK-MEL-5	4	3.52	HDLM-2	1	5.60
UACC-257	5	3.94	NCI-H28	1	5.60
NCI-H322M	4	3.52	SNU-449	1	5.60
RPMI-8226	4	3.55	DOK	1	5.60
SK-MEL-28	5	3.94	Lu-65	1	5.60
MDA-MB-435	4	3.52	VMRC-RCZ	1	5.60
NCI/ADR-RES	5	4.16	H4	1	5.60
HT-22	16	7.57	D-247MG	1	5.60
UACC-62	4	4.68	HGC-27	1	5.60
BT-549	3	4.40	WM-115	1	5.60
SK-OV-3	4	4.68	SK-N-FI	1	5.60
RXF 393	3	4.37	NCI-H2030	1	5.60
A498	4	4.68	J82	1	5.60
MG-63	10	5.08	KYSE-270	1	5.60
COS-7	55	5.48	SW900	1	5.60
Jurkat	4	5.31	ES1	1	5.60

Keratinocyte	11	4.01	D-502MG	1	5.60
Caco-2	20	5.65	HMV-2 cell line	1	5.60
Splenocyte	6	5.20	LU-99A	1	5.60
PBMC	32	5.93	TE-8	1	5.60
THP-1	15	6.47	BEN	1	5.60
Osteoclast-like	16	6.89	KURAMOCHI	1	5.60
F9	6	5.60	KNS-62	1	5.60
CV-1	54	5.60	Ca-Ski	1	5.60
SK-BR-3	4	5.60	SW1573	1	5.60
LNCaP	8	5.92	SW 954	1	5.60
HEK-293T	26	4.33	A-375	1	5.60
NIH3T3	8	5.60	A101D	1	5.60
NB-4	5	5.60	LCLC-97TM1	1	5.60
COS-1	4	5.60	COLO-800	1	5.60
ATN-1	1	5.60	NCI-H1048	1	5.60
MDA-MB-453	2	5.60	NCI-H1975	1	5.60
MDA-MB-468	1	5.60	MC116	1	5.60
DLD-1	1	5.60	EFO-21	1	5.60
XF498	1	5.60	NEC8	1	5.60
HOP-18	1	5.60	CGTH-W-1	1	5.60
SNB-78	1	5.60	CAL-54	1	5.60
DMS-114	2	5.60	SNU-5	1	5.60
DMS-273	2	5.60	HCC1187	1	5.60
KM-20L2	1	5.60	SiHa	1	5.60
M19-MEL	1	5.60	MHH-PREB-1	1	5.60
RXF 631	1	5.60	NCI-H2170	1	5.60
LXFL 529	1	5.60	SJRH30	1	5.60
HOS	3	5.67	D-392MG	1	5.60
T-cell	1	5.70	NCI-H510A	1	5.60
Huh-7	3	5.67	TE-9	1	5.60

Bone marrow cell	4	2.83	SW780	1	5.60
RWLeu4	1	5.70	OE19	1	5.60
U-937	14	6.62	LN-405	1	5.60
Keratinocyte cell line	2	5.70	ES5	1	5.60
PE	1	5.70	KYSE-140	1	5.60
C3H 10T1/2	1	5.70	KP-N-YN	1	5.60
SW480	19	4.08	KM-H2	1	5.60
HMEC	2	8.84	NCI-H1651	1	5.60
Lymphoblastoid cell	64	6.37	TE-6	1	5.60
Monocyte	1	-1.69	C2BBe1	1	5.60
L929	3	-1.69	SKG-IIIa	1	5.60
B16	2	-1.41	SW1463	1	5.60
3T3	2	-0.35	NCI-H1650	1	5.60
NCI-H716	1	0.18	ETK-1	1	5.60
Macrophage	1	0.18	D-263MG	1	5.60
L6	1	0.18	NCI-H1395	1	5.60
CHRC5 cell line	1	1.77	KU-19-19	1	5.60
A2780	2	3.81	COLO-680N	1	5.60
MIA PaCa-2	5	4.88	DSH1	1	5.60
A2058	2	3.81	FTC-133	1	5.60
SAS	2	3.81	MDA-MB-415	1	5.60
C2C12	2	2.56	SNU-387	1	5.60
Osteoblast	1	2.97	NCI-H1437	1	5.60
RBL-2H3	1	4.62	G-401	1	5.60
Panel NCI-60 (60 carcinoma cell lines)	1	5.51	GCT	1	5.60
Panel leukemia (Carcinoma cell lines)	1	5.60	MDA-MB-175-VII	1	5.60
S91	1	5.60	IGR-1	1	5.60
ZR-75-1	1	5.60	CAL-27	1	5.60

P19	1	5.60	YKG-1	1	5.60
MC-IXC	1	5.60	BT-20	1	5.60
HH	1	5.60	GMS-10	1	5.60
Neuron	1	5.60	NCI-H446	1	5.60
NB13	1	5.60	GAK	1	5.60
D283 Med	1	5.60	NCI-H1693	1	5.60
EW-3	1	5.60	NCI-H1355	1	5.60
KU812 cell line	1	5.60	HSC-2	1	5.60
SK-NEP-1	1	5.60	Calu-3	1	5.60
HCC1806	1	5.60	NCI-H2452	1	5.60
HuO-3N1	1	5.60	SW684	1	5.60
CTV-1	1	5.60	NCI-H2122	1	5.60
LAMA-84	1	5.60	SW837	1	5.60
NCI-H720	1	5.60	HAL-01	1	5.60
MOLT-13	1	5.60	NCI-H596	1	5.60
JVM-2	1	5.60	HTC-C3	1	5.60
NBsusSR	1	5.60	OE33	1	5.60
BV-173	1	5.60	SCC-25	1	5.60
CTB-1	1	5.60	HT	1	5.60
ACN	1	5.60	T98G	1	5.60
L-363	1	5.60	647-V	1	5.60
NCI-H69	1	5.60	Capan-2	1	5.60
ECC10	1	5.60	CAL-39	1	5.60
NCI-H209	1	5.60	LXF-289 cell line	1	5.60
KARPAS-45	1	5.60	NCI-N87	1	5.60
COR-L88	1	5.60	HCC1937	1	5.60
U-266	1	5.60	EFO-27	1	5.60
RS4-11	1	5.60	AN3-CA	1	5.60
DB	1	5.60	LB831-BLC	1	5.60
EM-2	1	5.60	CAL-12T	1	5.60

KY821	1	5.60	NCI-H1666	1	5.60
QIMR-WIL	1	5.60	EW-22	1	5.60
KYSE-180	1	5.60	HCC1954	1	5.60
ALL-PO	1	5.60	HuP-T3	1	5.60
NB14	1	5.60	SCH	1	5.60
BPH-1	1	5.60	YAPC	1	5.60
A3-KAW	1	5.60	Panc1005	1	5.60
EW-13	1	5.60	JAR	1	5.60
NCI-H526	1	5.60	LC-2-ad	1	5.60
NKM-1	1	5.60	UMC-11	1	5.60
SCC-15	1	5.60	NB69	1	5.60
MEG-01	1	5.60	MZ1-PC	1	5.60
NCI-H1648	1	5.60	TE-12	1	5.60
GP5d	1	5.60	MMAC-SF	1	5.60
HCC2218	1	5.60	IST-MES1	1	5.60
KE-37	1	5.60	BB65-RCC	1	5.60
CHP-212	1	5.60	PANC-08-13	1	5.60
NOMO-1	1	5.60	NCI-H661	1	5.60
NCI-H292	1	5.60	TGBC11TKB	1	5.60
MS-1	1	5.60	ESS-1	1	5.60
KMOE-2	1	5.60	EW-24	1	5.60
HCC1419	1	5.60	Ca9-22	1	5.60
NCI-H1092	1	5.60	ES8	1	5.60
DEL	1	5.60	TE-10	1	5.60
P12-Ichikawa	1	5.60	COR-L23	1	5.60
NCI-H1770	1	5.60	CAL-85-1	1	5.60
NCI-H82	1	5.60	LS-411N	1	5.60
COLO-684	1	5.60	5637	1	5.60
697	1	5.60	SK-UT-1	1	5.60
HC-1	1	5.60	BFTC-905	1	5.60

HSC-3	1	5.60	SW1417	1	5.60
ES3	1	5.60	SK-MES-1	1	5.60
HuO9	1	5.60	PC-14	1	5.60
ME-180	1	5.60	TGBC1TKB	1	5.60
KG-1	1	5.60	OC-314	1	5.60
OAW-28	1	5.60	HPAF-II	1	5.60
COLO-829	1	5.60	SJSA-1	1	5.60
SK-N-AS	1	5.60	M059J	1	5.60
KNS-42	1	5.60	CaR-1	1	5.60
SW13	1	5.60	GCIY	1	5.60
J-RT3-T3-5	1	5.60	OMC-1	1	5.60
KYSE-450	1	5.60	KGN	1	5.60
CHL-1	1	5.60	GI-1	1	5.60
UMUC3	1	5.60	COLO-824	1	5.60
JVM-3	1	5.60	TE-1	1	5.60
LB1047-RCC	1	5.60	CAL-120	1	5.60
LU-139	1	5.60	COLO-668	1	5.60
SK-MEL-1	1	5.60	Becker	1	5.60
SK-MEL-24	1	5.60	BCPAP	1	5.60
A4-Fuk	1	5.60	LB2241-RCC	1	5.60
CAMA-1	1	5.60	C8166	1	5.60
NCI-H1623	1	5.60	BT-474	1	5.60
A673	1	5.60	YH-13	1	5.60
Ramos-2G6-4C10	1	5.60	NCI-H2342	1	5.60
DOHH-2	1	5.60	NB17	1	5.60
DoTc2-4510	1	5.60	NCI-H630	1	5.60
NTERA-2-cl-D1	1	5.60	SW756	1	5.60
3LLD122	1	5.60	NCI-H1993	1	5.60
MeWo	1	5.60	BHY	1	5.60
BALL-1	1	5.60	VA-ES-BJ	1	5.60

A204	1	5.60	CW-2	1	5.60
KYSE-510	1	5.60	HT-1080	1	5.60
MSTO-211H	1	5.60	NCI-H1581	1	5.60
SK-LU-1	1	5.60	D-423MG	1	5.60
EGI-1	1	5.60	K5	1	5.60
RH-1	1	5.60	RVH-421	1	5.60
LU-134-A	1	5.60	SNU-C2B	1	5.60
KS-1	1	5.60	SW48	1	5.60
GAMG	1	5.60	HEC-1	1	5.60
TE-5	1	5.60	EW-1	1	5.60
P30-OHK	1	5.60	NCI-H747	1	5.60
GOTO	1	5.60	NCI-H727	1	5.60
Calu-6	1	5.60	NH-12	1	5.60
KYSE-410	1	5.60	KP-N-YS	1	5.60
CAL-72	1	5.60	MFE-280	1	5.60
AM-38	1	5.60	H-EMC-SS	1	5.60
23132-87	1	5.60	ONS-76	1	5.60
SCC-4	1	5.60	639-V	1	5.60
LU-135	1	5.60	T84	1	5.60
NB10	1	5.60	8-MG-BA	1	5.60
NB7	1	5.60	RO82-W-1	1	5.60
RPMI-7951	1	5.60	HT-144	1	5.60
AU565	1	5.60	NCI-H2087	1	5.60
HCE-4	1	5.60	SW1990	1	5.60
BE-13	1	5.60	SW948	1	5.60
LCLC-103H cell line	1	5.60	SK-MEL-30	1	5.60
NCI-H2126	1	5.60	NB6	1	5.60
PA-1	1	5.60	NCI-H1299	1	5.60
HSC-4	1	5.60	ABC-1	1	5.60
DMS-79	1	5.60	IA-LM	1	5.60

NOS-1	1	5.60	8305C	1	5.60
U-118-MG	1	5.60	MFH-ino	1	5.60
Daoy	6	7.28	Detroit 562	1	5.60
SBC-1	1	5.60	LAN-6	1	5.60
CAL-51	1	5.60	KYSE-70 cell line	1	5.60
NY	1	5.60	TI-73	1	5.60
BXPC-3	1	5.60	T-24	1	5.60
MOLT-16	1	5.60	NCI-H810	1	5.60
NCI-H1155	1	5.60	COLO-679	1	5.60
HO-1-N-1	1	5.60	A-427	1	5.60
CAPAN-1	1	5.60	COR-L105	1	5.60
CP50-MEL-B	1	5.60	NCI-H520	1	5.60
RERF-LC-MS	1	5.60	CP66-MEL	1	5.60
UACC-893	1	5.60	SW626	1	5.60
MPP-89	1	5.60	DK-MG	1	5.60
HCE-T	1	5.60	KYSE-150 cell line	1	5.60
FaDu	1	5.60	S-117	1	5.60
D-542MG	1	5.60	NCI-H1563	1	5.60
MEL-HO	1	5.60	KINGS-1	1	5.60
KNS-81-FD	1	5.60	MZ7-mel	1	5.60
G-361	1	5.60	HLE	1	5.60
NCI-H2009	1	5.60	SK-PN-DW	1	5.60
BFTC-909	1	5.60	NCI-H1755	1	5.60
AGS	1	5.60	BB49-HNC	1	5.60
CFPAC-1	1	5.60	SCC-9	1	5.60
VM-CUB-1	1	5.60	HT55	1	5.60
EW-18	1	5.60	HCC38	1	5.60
ChaGo-K-1	1	5.60	NMC-G1	1	5.60
TCC-SUP	1	5.60	LS-513	1	5.60
KOSC-2	1	5.60	NCI-H2052	1	5.60

GI-ME-N	1	5.60	MEL-JUSO	1	5.60
DJM-1	1	5.60	COLO-678	1	5.60
NCI-H1304	1	5.60	CWR22R	1	5.60
HT-3	1	5.60	SW872	1	5.60
RT-112	1	5.60	LNCaP-Clone-FGC	1	5.60
C-33-A	1	5.60	RPMI-2650	1	5.60
EW-11	1	5.60	LS-123	1	5.60
KP-4	1	5.60	no-11	1	5.60
SNU-423	1	5.60	NB12	1	5.60
RPMI-8866	1	5.60	SK-LMS-1	1	5.60
SNU1	1	5.60	IST-SL1	1	5.60
DU-4475	1	5.60	EPLC-272H	1	5.60
D-566MG	1	5.60	NCI-H2347	1	5.60
PFSK-1	1	5.60	SW1783	1	5.60
MDA-MB-361	1	5.60	U-87 MG	1	5.60
HT-1376	1	5.60	PANC-03-27	1	5.60
HD-MY-Z	1	5.60	TYK-nu	1	5.60
SW1710	1	5.60	no-10	1	5.60
KALS-1	1	5.60	C3A	1	5.60
HEL	1	5.60	A388	1	5.60
DBTRG-05MG	1	5.60	NCI-H2029	1	5.60
GB-1	1	5.60	LK-2	1	5.60
TE-11	1	5.60	BHT-101	1	5.60
NB5	1	5.60	NCI-H2405	1	5.60
NUGC-3	1	5.60	LS-1034	1	5.60
COLO-320-HSR	1	5.60	BB30-HNC	1	5.60
ES4	1	5.60	C32	1	5.60
A-431	2	7.22	NCI-H2291	1	5.60
TGBC24TKB	1	5.60	RMG-I	1	5.60
GT3TKB	1	5.60	CAS-1	1	5.60

COLO-792	1	5.60	JEG-3	1	5.60
NCI-H441	1	5.60	MLMA	1	5.60
MZ2-MEL	1	5.60	RCC10RGB	1	5.60
EW-16	1	5.60	HCC1395	1	5.60
GR-ST	1	5.60	Murine-murine hybridoma (mark 3)	1	8.84
MHH-ES-1	1	5.60	HUVEC	2	8.84
SK-N-DZ	1	5.60	SNU-C1	1	8.84
L-428	1	5.60	MT4	1	8.84
RCM-1	1	5.60	J774	1	8.84
MN-60	1	5.60	MDA-MB-157	1	5.60