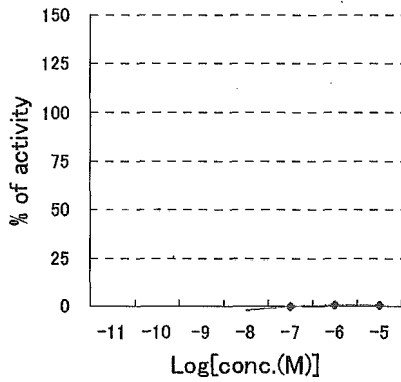


sample No. AR146
 chemical name Phenol, 4,4'-isopropylidenedi-
 CAS. 80-05-7

AR agonist assay

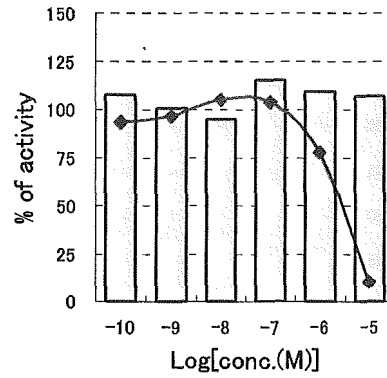
LOG[conc.(M)]	luc
-5	0.5
-6	0.7
-7	-0.1
-8	-1.7
-9	-1.9
-10	-2.6
-11	-2.6



AR antagonist assay

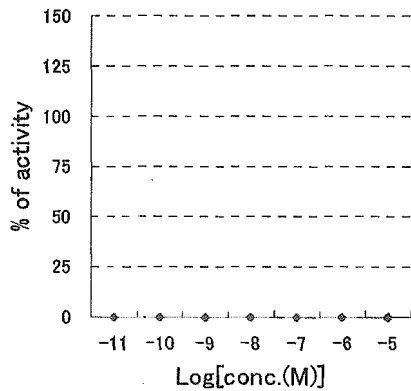
LOG[conc.(M)]	luc	ren
-5	11	107
-6	78	109
-7	104	115
-8	105	95
-9	97	101
-10	93	108

Cell viability



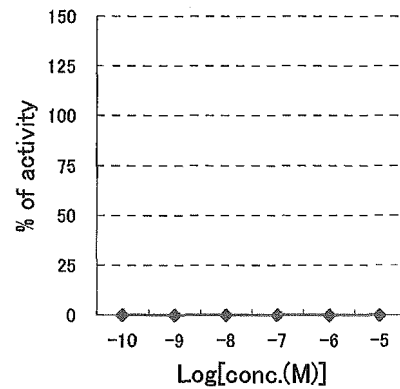
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



TRβ-RXR antagonist assay

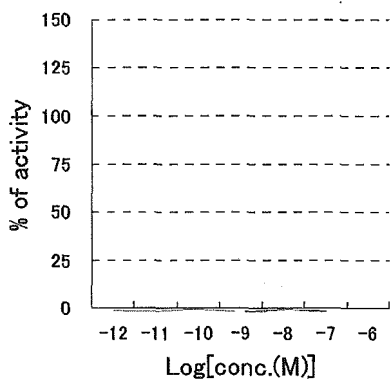
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0



sample No. AR147
 chemical name 4,4'-Stilbenediol, alpha,alpha'-diethyl-
 CAS. 56-53-1

AR agonist assay

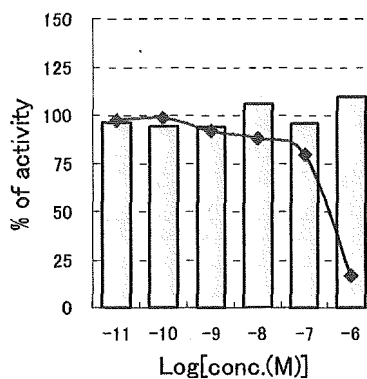
LOG[conc.(M)]	luc
-6	-3.2
-7	-1.7
-8	-1.0
-9	-2.0
-10	-0.8
-11	-1.7
-12	-1.6



AR antagonist assay

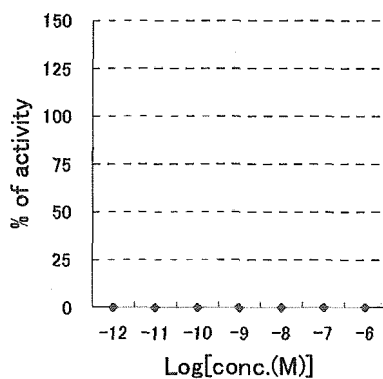
LOG[conc.(M)]	luc	ren
-6	17	110
-7	80	96
-8	88	106
-9	92	94
-10	99	94
-11	98	96

Cell viability



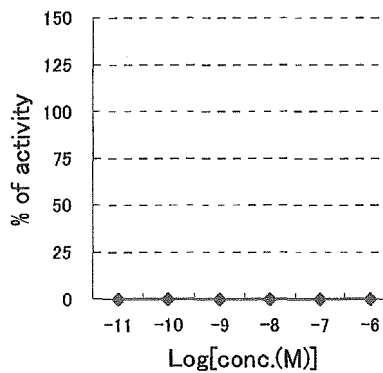
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0
-12	0.0



TRβ-RXR antagonist assay

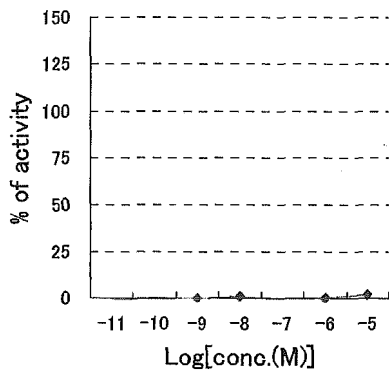
LOG[conc.(M)]	luc	ren
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0
-11	0	0



sample No. AR148
 chemical name 4,4'-Cyclohexylidenebisphenol
 CAS. 843-55-0

AR agonist assay

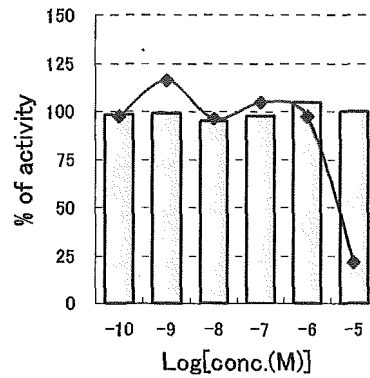
LOG[conc.(M)]	luc
-5	1.9
-6	-0.1
-7	-0.7
-8	0.6
-9	0.1
-10	-0.6
-11	-0.8



AR antagonist assay

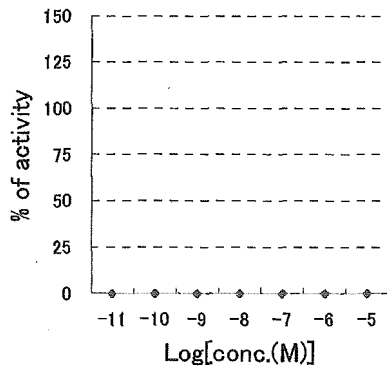
LOG[conc.(M)]	luc	ren
-5	21	100
-6	97	105
-7	104	98
-8	96	95
-9	116	99
-10	98	98

Cell viability



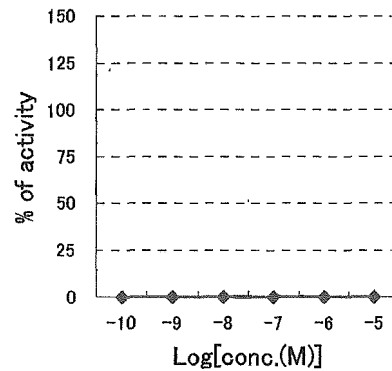
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



TRβ-RXR antagonist assay

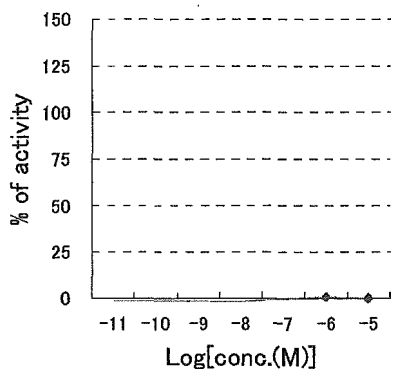
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0



sample No. AR149
 chemical name 3(2H)-Thiophenone, dihydro-
 CAS. 1003-04-9

AR agonist assay

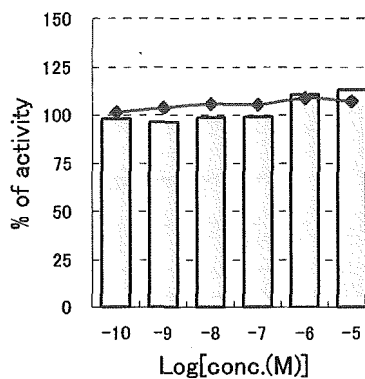
LOG[conc.(M)]	luc
-5	0.1
-6	0.6
-7	-0.4
-8	-2.0
-9	-1.7
-10	-1.7
-11	-1.5



AR antagonist assay

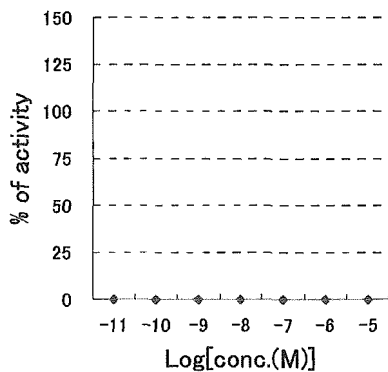
LOG[conc.(M)]	luc	ren
-5	107	113
-6	109	111
-7	105	99
-8	106	99
-9	104	96
-10	101	98

Cell viability



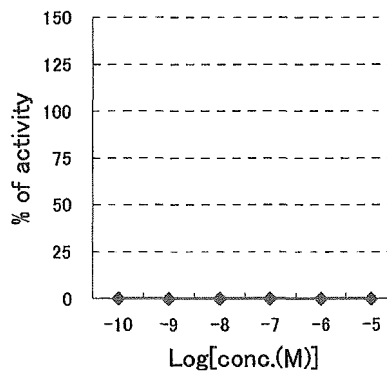
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



TRβ-RXR antagonist assay

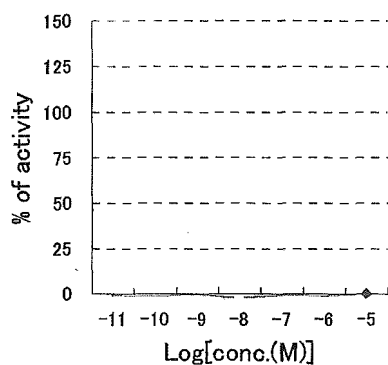
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0



sample No. AR150
 chemical name 2-Pentylcinnamaldehyde
 CAS. 122-40-7

AR agonist assay

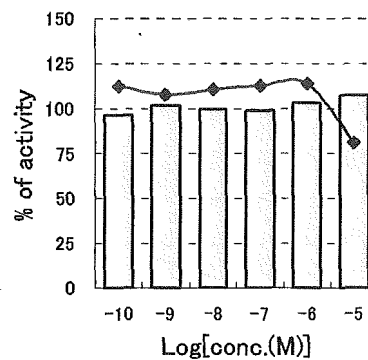
LOG[conc.(M)]	luc
-5	0.0
-6	-1.3
-7	-1.1
-8	-2.3
-9	-0.6
-10	-1.2
-11	-1.0



AR antagonist assay

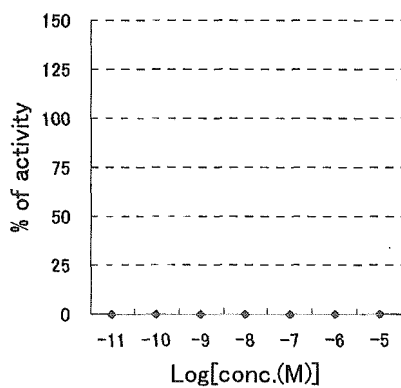
LOG[conc.(M)]	luc	ren
-5	81	107
-6	114	103
-7	113	99
-8	111	99
-9	108	102
-10	113	96

Cell viability



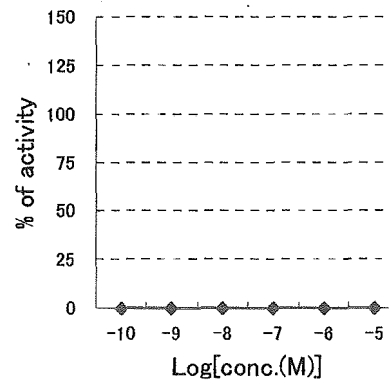
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



TRβ-RXR antagonist assay

LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0



測定結果 一覧

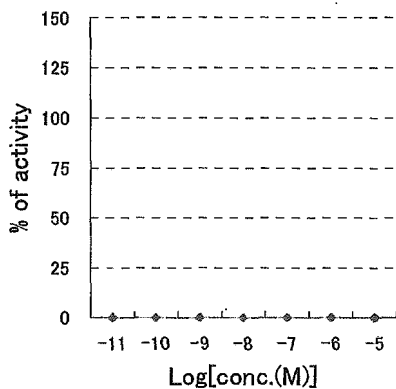
TR レポータージーンアッセイ

10 物質
(TR141~TR150)

sample No. TR141
 chemical name Phenol, 4,4'-thiodi-
 CAS. 2664-63-3

AR agonist assay

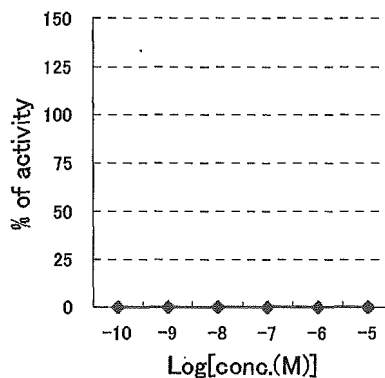
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

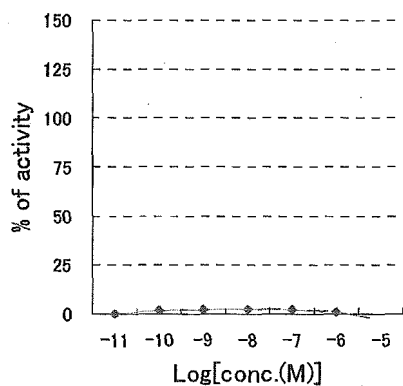
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



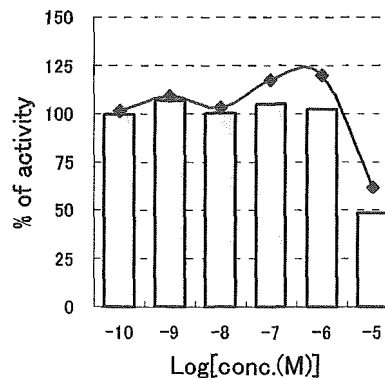
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	-2.9
-6	1.3
-7	2.5
-8	2.7
-9	2.3
-10	2.0
-11	0.4



TRβ-RXR antagonist assay

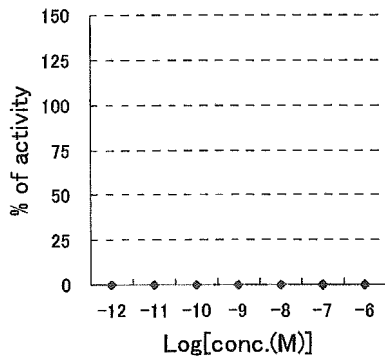
LOG[conc.(M)]	luc	ren
-5	62	48
-6	120	102
-7	118	105
-8	103	100
-9	109	106
-10	101	99



sample No. TR142
 chemical name Resorcinol, 4-(2-pyridylazo)-
 CAS. 1141-59-9

AR agonist assay

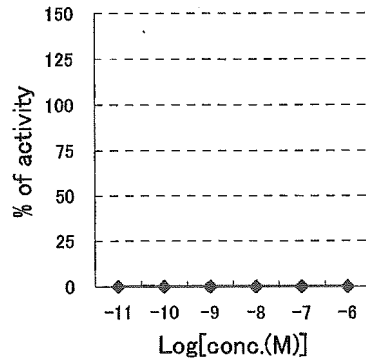
LOG[conc.(M)]	luc
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0
-12	0.0



AR antagonist assay

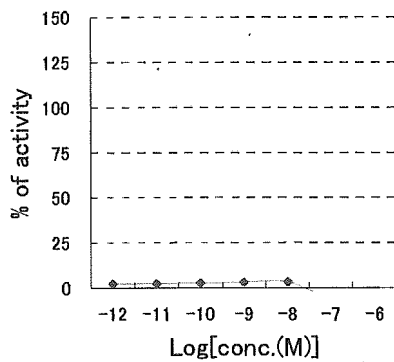
LOG[conc.(M)]	luc	ren
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0
-11	0	0

Cell viability



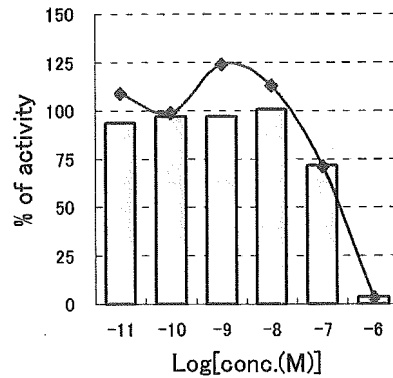
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-6	-8.7
-7	-5.8
-8	3.4
-9	3.2
-10	3.0
-11	2.6
-12	2.6



TRβ-RXR antagonist assay

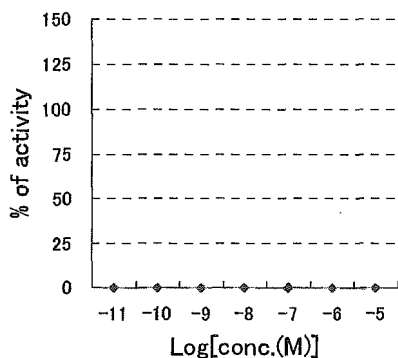
LOG[conc.(M)]	luc	ren
-6	3	4
-7	71	71
-8	113	101
-9	124	97
-10	99	97
-11	109	94



sample No. TR143
 chemical name Benzophenone
 CAS. 119-61-9

AR agonist assay

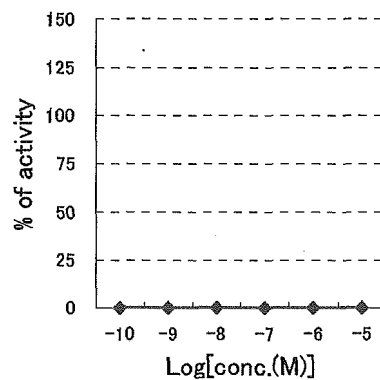
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

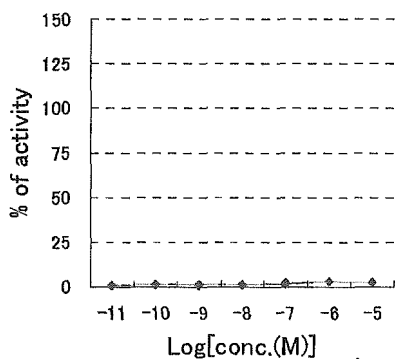
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



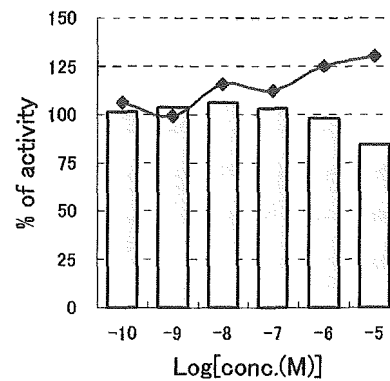
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	2.5
-6	3.2
-7	2.1
-8	1.4
-9	1.3
-10	1.2
-11	1.1



TRβ-RXR antagonist assay

LOG[conc.(M)]	luc	ren
-5	130	84
-6	125	98
-7	112	103
-8	116	106
-9	99	104
-10	106	101



sample No. TR144
 chemical name Benzophenone, 4,4'-dihydroxy-
 CAS. 611-99-4

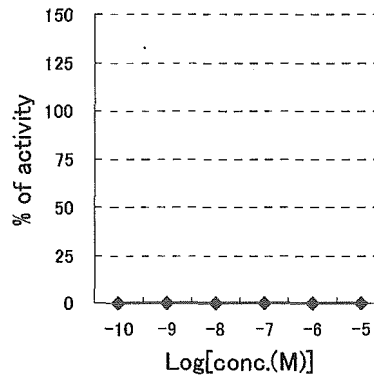
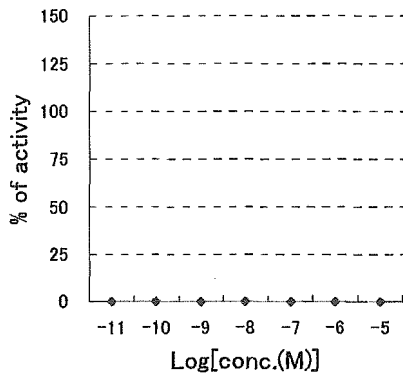
AR agonist assay

LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0

AR antagonist assay

LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability

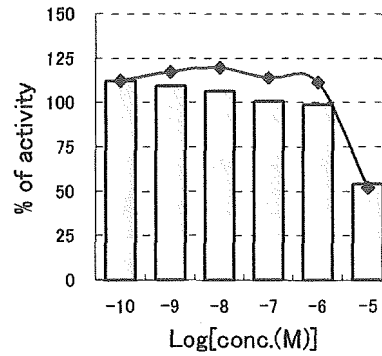
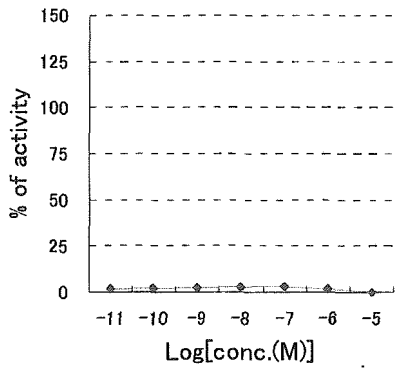


TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	0.1
-6	2.0
-7	3.3
-8	2.7
-9	2.6
-10	2.3
-11	1.7

TRβ-RXR antagonist assay

LOG[conc.(M)]	luc	ren
-5	52	54
-6	112	99
-7	114	100
-8	120	106
-9	117	109
-10	112	112



sample No. TR145
 chemical name BENZORESORCINOL
 CAS. 131-56-6

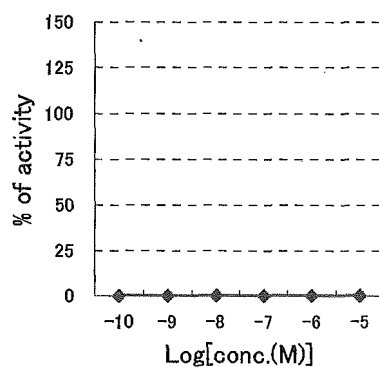
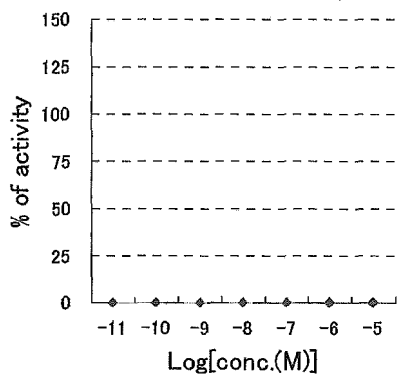
AR agonist assay

LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0

AR antagonist assay

LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability

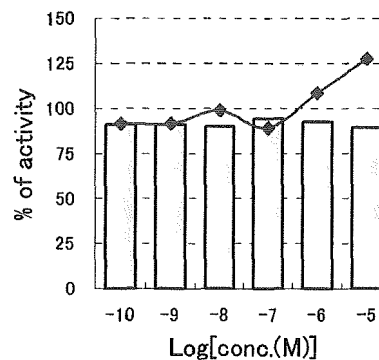
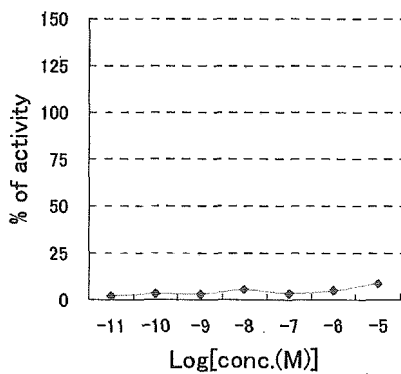


TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	8.7
-6	5.0
-7	3.4
-8	5.5
-9	3.2
-10	3.3
-11	2.1

TRβ-RXR antagonist assay

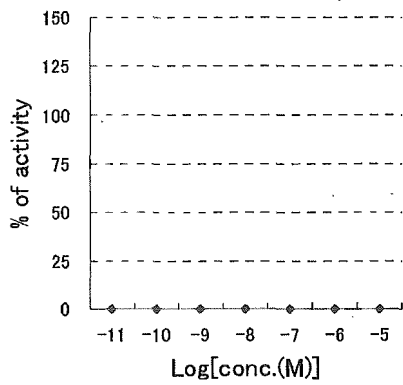
LOG[conc.(M)]	luc	ren
-5	127	89
-6	108	92
-7	89	94
-8	99	90
-9	92	91
-10	92	91



sample No. TR146
 chemical name Phenol, p-tert-butyl-
 CAS. 98-54-4

AR agonist assay

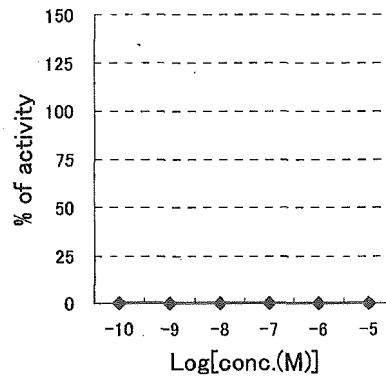
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

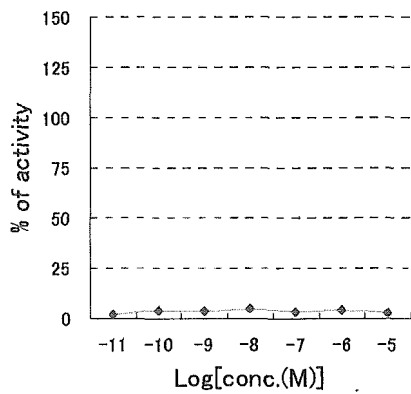
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



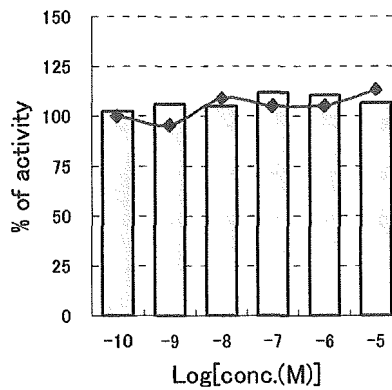
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	2.8
-6	4.3
-7	3.5
-8	5.0
-9	3.7
-10	3.9
-11	2.1



TRβ-RXR antagonist assay

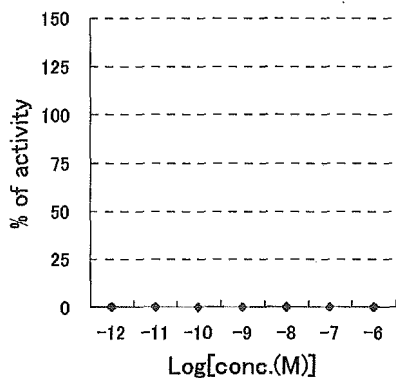
LOG[conc.(M)]	luc	ren
-5	113	107
-6	105	110
-7	105	112
-8	109	105
-9	96	106
-10	100	103



sample No. TR147
 chemical name P-(1,1,3,3-TETRAMETHYLBUTYL)PHENOL
 CAS. 140-66-9

AR agonist assay

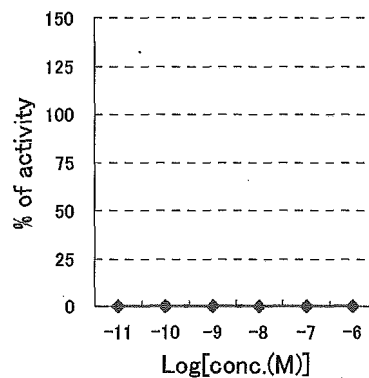
LOG[conc.(M)]	luc
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0
-12	0.0



AR antagonist assay

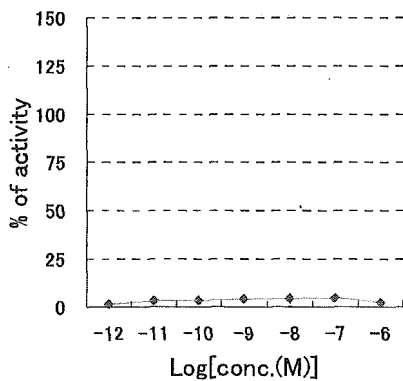
LOG[conc.(M)]	luc	ren
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0
-11	0	0

Cell viability



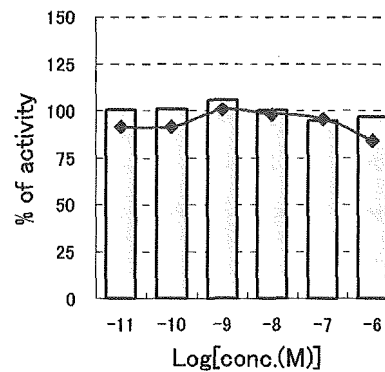
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-6	2.5
-7	4.9
-8	4.5
-9	4.1
-10	3.5
-11	3.2
-12	1.5



TRβ-RXR antagonist assay

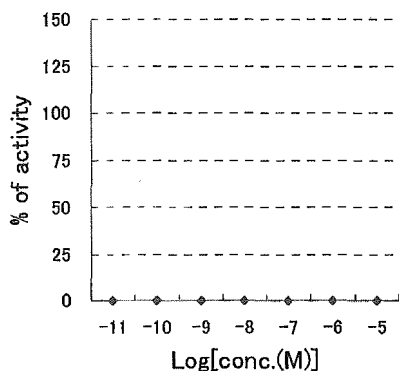
LOG[conc.(M)]	luc	ren
-6	84	97
-7	96	95
-8	98	100
-9	101	106
-10	91	101
-11	92	101



sample No. TR148
 chemical name 4-PHENYLPHENOL
 CAS. 92-69-3

AR agonist assay

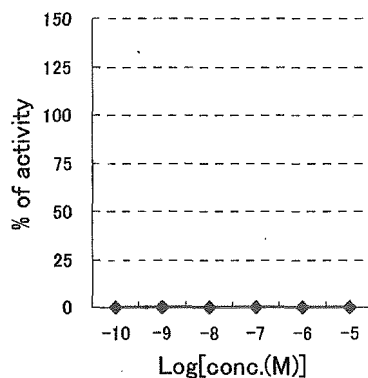
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

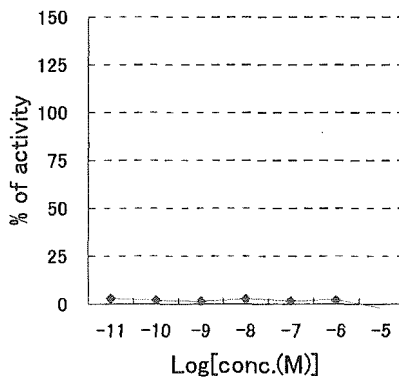
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



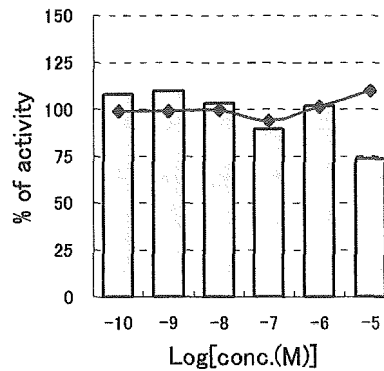
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	-2.0
-6	2.1
-7	1.7
-8	2.7
-9	1.5
-10	2.1
-11	2.9



TRβ-RXR antagonist assay

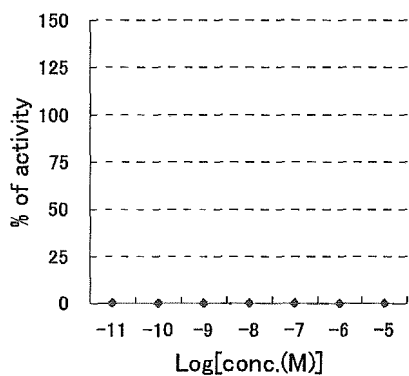
LOG[conc.(M)]	luc	ren
-5	110	74
-6	101	102
-7	94	90
-8	100	103
-9	99	110
-10	99	108



sample No. TR149
 chemical name Phenol, p-cyclohexyl-
 CAS. 1131-60-8

AR agonist assay

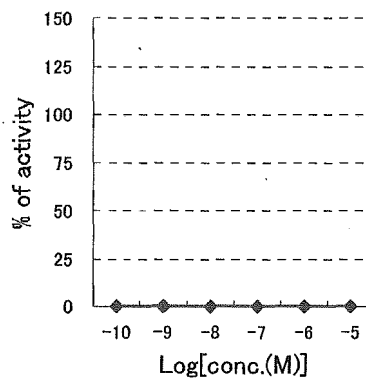
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

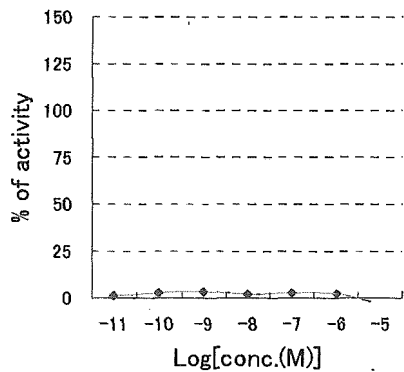
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



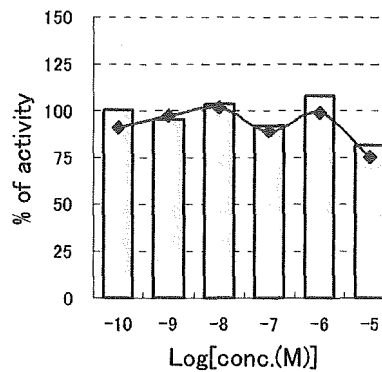
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	-3.0
-6	2.5
-7	2.7
-8	2.2
-9	3.5
-10	2.8
-11	1.4



TRβ-RXR antagonist assay

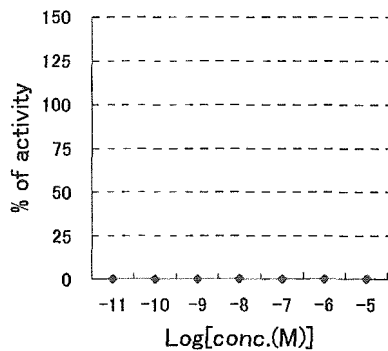
LOG[conc.(M)]	luc	ren
-5	75	81
-6	99	108
-7	89	92
-8	102	103
-9	97	95
-10	91	100



sample No. TR150
 chemical name ROSOLIC ACID
 CAS. 603-45-2

AR agonist assay

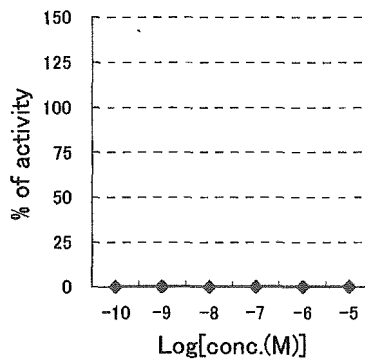
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

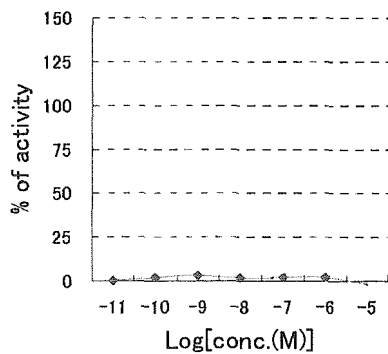
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



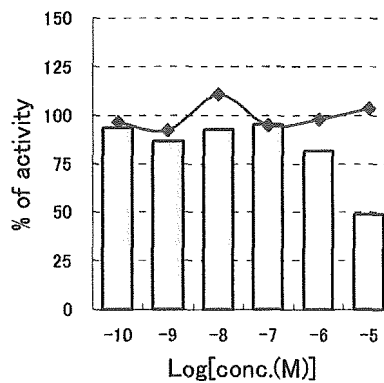
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	-2.1
-6	2.2
-7	2.5
-8	2.0
-9	3.4
-10	2.1
-11	0.2



TRβ-RXR antagonist assay

LOG[conc.(M)]	luc	ren
-5	103	49
-6	98	81
-7	95	95
-8	111	93
-9	92	86
-10	96	93



厚生労働科学研究費補助金(化学物質リスク研究事業)
生体の作用点、特に核内受容体及び関連転写因子群に着目した化学物質の
毒性発現機構の解明や毒性予測手法の開発を行う研究

総括研究報告書 図表

- (1)-3.表面プラズモン共鳴高速分派によるデータの高速取得技術及びHIPSに特化するための試験研究
(主任研究者:ビアコア株式会社委託業務)

表 1. 追加物質等の ER α に対する結合強度予測値

CAS 番号等	推算 logRBA	CAS 番号等	推算 logRBA	CAS 番号等	推算 logRBA
000051-24-1	-1.153	003301-49-3	-0.025	025639-54-7	-1.969
000067-30-1	-2.586	003337-59-5	-2.652	026538-44-3	-0.635
000085-28-9	-0.957	003943-89-3	-1.063	026636-32-8	-1.117
000087-18-3	-1.676	004191-73-5	-1.539	029799-07-3	-0.269
000133-07-3	-2.505	004191-73-5	-1.539	036861-47-9	-0.47
000299-45-6	-1.218	004250-77-5	-0.111	038183-04-9	1.040
000341-58-2	-0.607	005289-74-7	0.197	040444-43-7	-0.234
000485-63-2	0.533	005402-37-9	-0.451	041796-12-7	-1.029
000500-66-3	-1.252	005817-39-0	-1.525	052222-87-4	-0.262
000509-77-3	-0.215	006073-20-7	-0.778	058109-40-3	-1.235
000518-45-6	-0.063	006131-38-0	-0.642	059517-19-0	-0.375
000564-35-2	-0.067	006468-96-8	-0.157	063046-09-3	0.043
000596-01-0	1.069	006665-67-4	-0.793	068047-06-3	1.947
000596-28-1	-0.267	006665-83-4	0.172	072495-97-7	-0.850
000611-99-4	-0.408	006674-39-1	-1.342	081936-33-6	-0.070
000843-55-0	0.212	006948-88-5	0.494	083409-32-9	-0.667
000843-55-0	0.212	006949-73-1	-0.748	084371-65-3	-0.003
000927-67-3	-2.583	007297-86-1	-0.013	084375-71-3	-1.312
001034-41-9	-2.999	007392-62-3	-0.421	084375-71-3	-1.312
001124-04-5	-2.016	007463-51-6	-1.900	093602-28-9	-0.480
001139-46-4	0.127	010210-17-0	-2.089	104821-25-2	-0.103
001157-39-7	-0.954	013728-34-2	-1.521	105640-07-1	-0.934
001518-83-8	-1.117	014392-69-9	-0.960	108238-41-1	-0.067
001719-71-7	0.969	015086-94-9	-1.091	110726-28-8	-0.118
001847-63-8	1.751	015231-91-1	-1.406	114369-43-6	-1.131
001847-63-8	1.751	015485-76-4	0.694	EA120	-0.841
001951-25-3	-0.376	015872-42-1	-2.012	EA133	-0.712
002150-43-8	-1.765	016606-47-6	-1.163	EA151	-0.896
002236-52-4	-1.645	017362-17-3	-2.020	EA160	0.844
002443-58-5	-1.200	018964-53-9	-0.032	EA205	1.148
003144-54-5	-0.836	020283-92-5	-0.007	EA207	0.665
003144-54-5	-0.836	023210-58-4	0.076	EA209	-0.091
003228-02-2	-1.744	023452-05-3	-0.597	EA214	1.642
003248-91-7	-0.111	024305-56-4	-0.448	EA228	-0.118

CAS 番号等	推算 logRBA	CAS 番号等	推算 logRBA	CAS 番号等	推算 logRBA
EA240	0.694	ED43	-0.298	ER263	-0.558
EA263	-0.288	ED46	0.296	ER272	-0.056
EA318	0.339	ED48	-0.144	ER366	-0.742
EA326	-0.660	ED49	-0.477	ER370	-1.015
ED26	-0.437	ED53	-0.580	ER524	1.157
ED37	-0.043	ED55	1.255	ER526	0.143
ED39	-0.132	ER249	-0.040		
ED40	1.182	ER257	-0.204		

表2. 追加物質等の ERβ に対する結合強度予測値

CAS 番号等	推算 logRBA	CAS 番号等	推算 logRBA	CAS 番号等	推算 logRBA
000051-24-1	-0.651	003228-02-2	-0.828	023452-05-3	0.340
000067-30-1	-0.492	003248-91-7	1.348	024305-56-4	-0.583
000085-28-9	-0.551	003301-49-3	0.775	025639-54-7	-1.334
000087-18-3	-0.591	003337-59-5	-1.786	026538-44-3	0.161
000106-02-5	-1.777	003943-89-3	-0.517	026636-32-8	-0.607
000125-20-2	0.107	004191-73-5	-0.732	029799-07-3	0.283
000133-07-3	-1.462	004191-73-5	-0.732	036861-47-9	0.118
000299-45-6	-0.659	004250-77-5	0.024	038183-04-9	0.729
000341-58-2	-0.436	005289-74-7	-0.083	040444-43-7	-0.376
000485-63-2	0.170	005402-37-9	-0.119	041796-12-7	-0.680
000500-66-3	-0.842	005817-39-0	-1.145	052222-87-4	0.039
000509-77-3	0.492	006073-20-7	-0.071	058109-40-3	-1.000
000518-45-6	0.745	006131-38-0	-0.409	059517-19-0	-0.291
000564-35-2	0.791	006468-96-8	0.444	063046-09-3	0.183
000596-01-0	1.026	006665-67-4	0.151	068047-06-3	1.743
000596-28-1	1.281	006665-83-4	-0.549	072495-97-7	-0.675
000611-99-4	-0.265	006674-39-1	-0.379	081936-33-6	0.035
000843-55-0	0.368	006948-88-5	1.253	083409-32-9	-0.219
000843-55-0	0.368	006949-73-1	-0.367	084375-71-3	-0.902
000927-67-3	-2.108	007297-86-1	0.267	084375-71-3	-0.902
001034-41-9	-2.296	007392-62-3	0.079	093602-28-9	0.003
001124-04-5	-1.497	007463-51-6	-1.005	104821-25-2	0.517
001139-46-4	0.381	010210-17-0	-1.315	105640-07-1	-0.886
001157-39-7	0.020	013728-34-2	-0.783	108238-41-1	0.069
001518-83-8	-0.784	014392-69-9	-0.513	110726-28-8	0.665
001719-71-7	1.348	015086-94-9	-0.101	114369-43-6	-0.689
001847-63-8	0.945	015231-91-1	-0.918	EA120	-0.037
001847-63-8	0.945	015485-76-4	0.864	EA133	-0.256
001951-25-3	-0.533	015872-42-1	-2.052	EA151	-0.502
002150-43-8	-1.016	016606-47-6	-0.563	EA160	1.011
002236-52-4	-1.342	017362-17-3	-1.559	EA205	0.654
002443-58-5	-0.396	018964-53-9	0.179	EA207	1.034
003144-54-5	-0.801	020283-92-5	0.125	EA209	0.597
003144-54-5	-0.801	023210-58-4	0.184	EA214	1.466