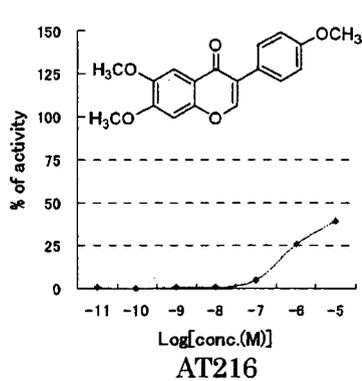
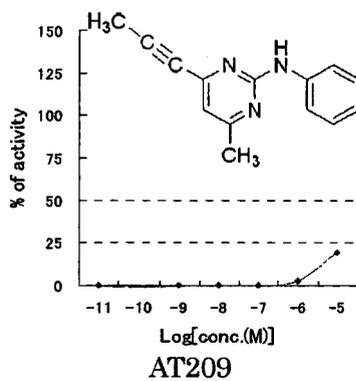
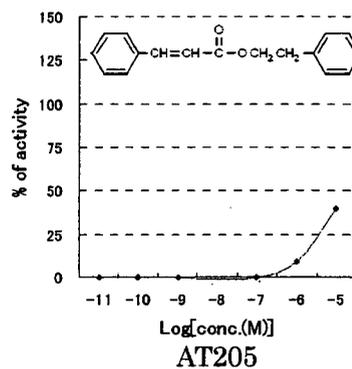
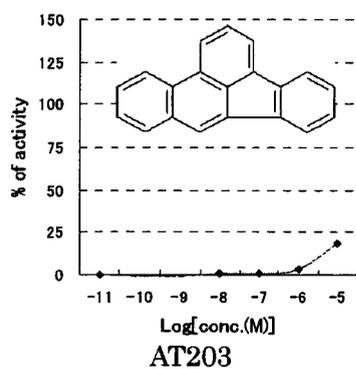
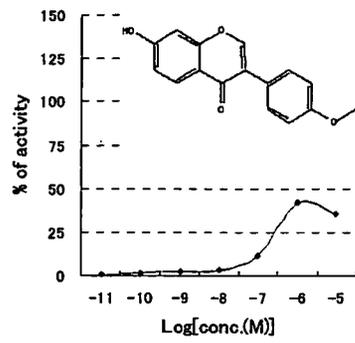


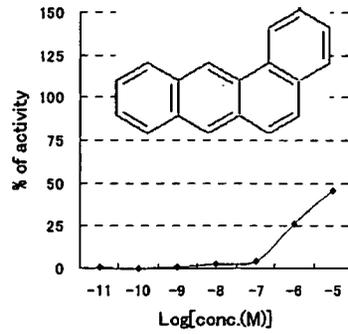
表 1 AR アゴニストアッセイの結果

Assay ID	name	CAS	PC50	PC10
AT203	benzo(b)fluoranthene	205-99-2	-	2.70×10^{-6}
AT205	Cinnamic acid, phenethyl ester	103-53-7	-	1.04×10^{-6}
AT209	Mepanipyrim	110235-47-7	-	2.57×10^{-6}
AT216	4',6,7-Trimethoxyisoflavone	798-61-8	-	1.81×10^{-7}
AT217	Formononetin	485-72-3	-	8.22×10^{-8}
AT218	Benz(a)anthracene	56-55-3	-	2.02×10^{-7}
AT221	2-hydroxyfluorene	2443-58-5	-	2.87×10^{-6}
AT222	7-Hydroxyflavone	6665-86-7	-	5.05×10^{-6}
AT232	6,7-dihydroxyflavone	38183-04-9	-	1.52×10^{-7}
AR248	3',4',7-trihydroxyisoflavone	485-63-2	-	5.59×10^{-6}
AR249	4-Hexanoylresorcinol	3144-54-5	-	2.35×10^{-6}

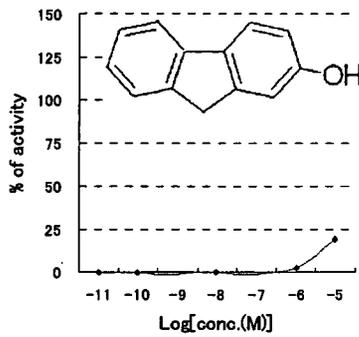




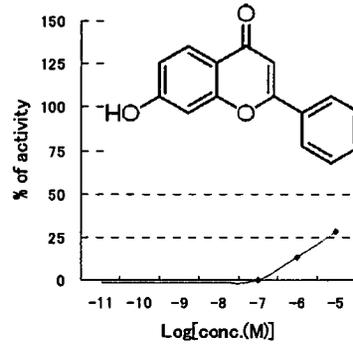
AT217



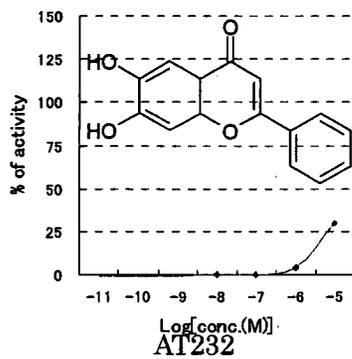
AT218



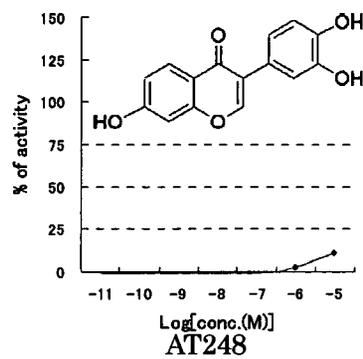
AT221



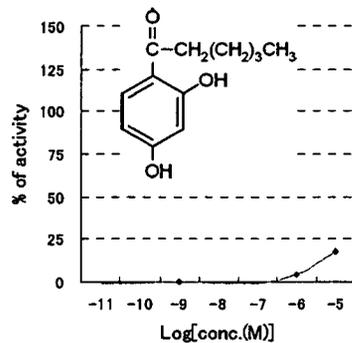
AT222



AT232



AT248

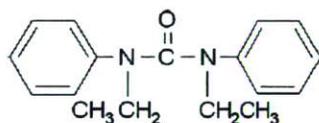
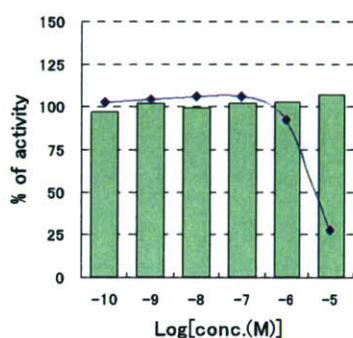


AR249

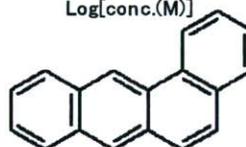
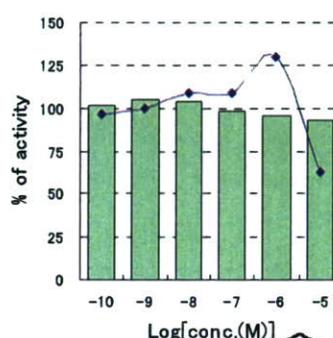
図1 AR アゴニスト活性があった18物質の結果と化学構造
(縦軸は 1×10^{-8} M における DHT の活性を 100、横軸は濃度を示している。)

表 2 AR アンタゴニストアッセイの結果

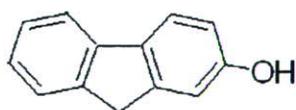
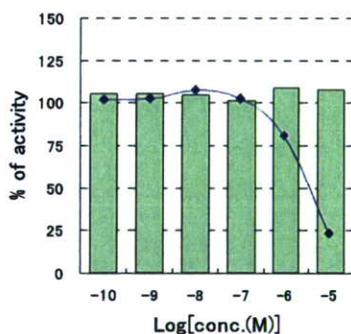
Assay ID	name	CAS	IC50	IC20
AT201	1,3-Diethyl-1,3-diphenylurea	85-98-3	4.52×10^{-6}	
AT218	Benz(a)anthracene	56-55-3	-	5.53×10^{-6}
AT221	2-hydroxyfluorene	2443-58-5	3.47×10^{-6}	
AT223	2-Hydroxy-9-fluorenone	6949-73-1	-	2.97×10^{-6}
AT224	6-Bromo-2-naphthol	15231-91-1	2.42×10^{-6}	



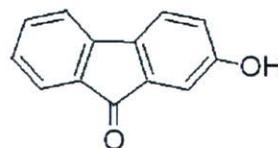
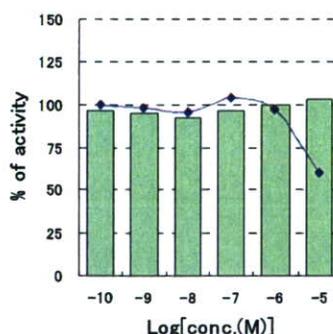
AT201



AT218



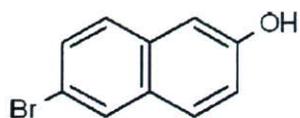
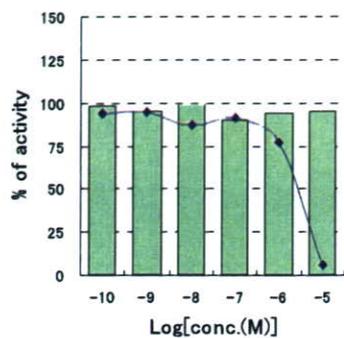
AT221



AT223

図 2 AR アンタゴニスト活性とその化学構造(その1)

縦軸は相対活性 (5×10^{-10} M における DHT の活性を 100)、横軸は濃度を示す。



AT224

図 2 AR アンタゴニスト活性とその化学構造(その2)

縦軸は相対活性 (5×10^{-10} M における DHT の活性を 100)、横軸は濃度を示す。

付録 物質一覧(その1)

ID	NAME	CAS_s	MW
AT201	1,3-Diethyl-1,3-diphenylurea	85-98-3	268.358
AT202	Benzaldehyde Diethyl Acetal	774-48-1	180.24
AT203	benzo(b)fluoranthene	205-99-2	252.315
AT204	Acetophenone, 2-isopropoxy-2-phenyl-	6652-28-4	254.327
AT205	Cinnamic acid, phenethyl ester	103-53-7	252.311
AT206	1-Propanaminium, N,N,N-trimethyl-3-(2-methyl-1-oxo-2-propenyl)amino-, ch	51410-72-1	220.742
AT207	Benzeneacetic acid, 4-methylphenyl ester	101-94-0	226.274
AT208	Octanal, 7-hydroxy-3,7-dimethyl-, dimethyl acetal	141-92-4	218.334
AT209	Mepanipyrim	110235-47-7	223.278
AT210	butanoic acid, 1,1-dimethyl-2-phenylethyl ester	10094-34-5	220.31
AT211	Melatonin	73-31-4	232.281
AT212	Benzene, 2-(diethoxymethyl)-1-heptenyl -	60763-41-9	276.417
AT213	Benzoic acid, 2-ethylhexyl ester	5444-75-7	234.337
AT214	dicyclopenteneoxyethyl methacrylate	68586-19-6	262.34
AT215	2,4,5,7-tetranitro-9-(4-octyloxy-benzylidene)-9h-fluorene	NA	562.54
AT216	4',6,7-Trimethoxyisoflavone	798-61-8	312.32
AT217	Formononetin	485-72-3	268.267
AT218	Benz(a)anthracene	56-55-3	228.29
AT219	para-Dichlorobenzene	106-46-7	147
AT220	4-cyclopentylphenol	1518-83-8	162.33
AT221	2-hydroxyfluorene	2443-58-5	182.22
AT222	7-Hydroxyflavone	6665-86-7	238.24
AT223	2-Hydroxy-9-fluorenone	6949-73-1	196.2
AT224	6-Bromo-2-naphthol	15231-91-1	223.07
AT225	2-carbethoxy-5,7-dihydroxy-4'-methoxyisoflavone	15485-76-4	356.33
AT226	4-(1-adamantyl)phenol	29799-07-3	228.33
AT227	WY14643(Pirinixic acid)	50892-23-4	323.803
AT228	3,6-dihydroxyflavone	108238-41-7	252.24
AT229	Luteolin	491-70-3	286.24
AT230	Clofibrate	637-07-0	242.701
AT231	Mono-2-ethylhexyl Phthalate	4376-20-9	278.34
AT232	6,7-dihydroxyflavone	38183-04-9	254.25
AT233	Di-i-propyl phthalate	605-45-8	250.292
AT234	2-Naphthalenecarboxamide, 1-hydroxy-N-(2-(tetradecyloxy)phenyl)-	39163-92-3	475.669
AT235	Anethole	4180-23-8	148.204
AT236	Brodifacoum	56073-10-0	523.424
AT237	Isopropalin	33820-53-0	309.364
AT238	Difenoxuron	14214-32-5	286.329
AT239	Tralkoxydim	87820-88-0	329.437
AT240	Resmethrin	10453-86-8	338.444

Assay ID の AT は AR, TR 共に測定、また AR は AR のみ、TR は TR のみ測定

付録 物質一覧(その2)

ID	NAME	CAS_s	MW
AR241	Cycloheximide	66-81-9	281.35
AR242	Sulpiride	15676-16-1	341.43
AR243	Santoflex 13	793-24-8	268.402
AR244	Citronellyl isobutyrate	97-89-2	226.357
AR245	Phenol, 2-methoxy-4-propenyl-, acetate	93-29-8	206.24
AR246	Cyclohexanol, 4-tert-butyl-, acetate	32210-23-4	198.304
AR247	Morin	480-16-0	302.24
AR248	3',4',7-trihydroxyisoflavone	485-63-2	270.24
AR249	4-Hexanoylresorcinol	3144-54-5	208.25
AR250	6,3'-dihydroxyflavone	108238-41-1	252.24
TR241	Clindamycin phosphate	24729-96-2	504.966
TR242	Oxycarboxin	5259-88-1	267.304
TR243	Acetamide, N-fluoren-2-yl-	53-96-3	223.274
TR244	Isobutyric acid, 3,7-dimethyl-2,6-octadienyl ester, (Z)-	2345-24-6	224.342
TR245	Cinnamaldehyde, alpha-pentyl-, dimethyl acetal	91-87-2	248.364
TR246	2,4,6-TRIS[(DIMETHYLAMINO)METHYL]PHENOL	90-72-2	265.398
TR247	Benzoic acid, p-(dimethylamino)-	619-84-1	165.191
TR248	RCL S12,616-0	NA	346.48
TR249	Genistein 4',7-dimethyl ether	34086-51-6	298.293
TR250	3,3'-Dichlorobenzidine	91-94-1	253.131

Assay ID の AT は AR、TR 共に測定、また AR は AR のみ、TR は TR のみ測定

測定結果 一覧

AR レポータージーンアッセイ

TR レポータージーンアッセイ

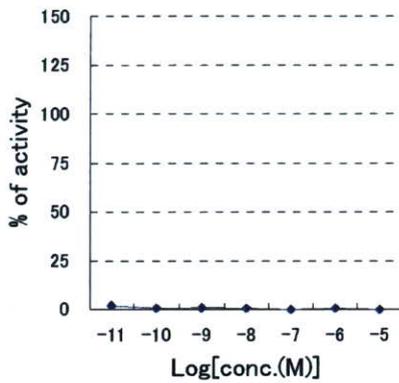
40 物質

(AT201～AT240)

sample No. AT201
 chemical name 1,3-Diethyl-1,3-diphenylurea
 CAS. 85-98-3

AR agonist assay

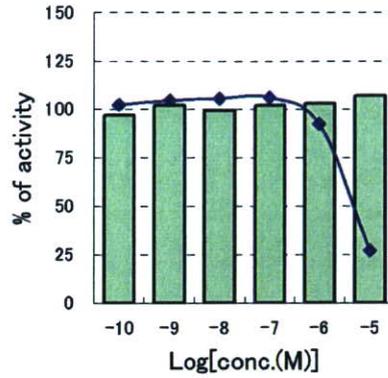
LOG[conc.(M)]	luc
-5	-0.1
-6	0.5
-7	0.0
-8	0.5
-9	0.9
-10	0.5
-11	2.0



AR antagonist assay

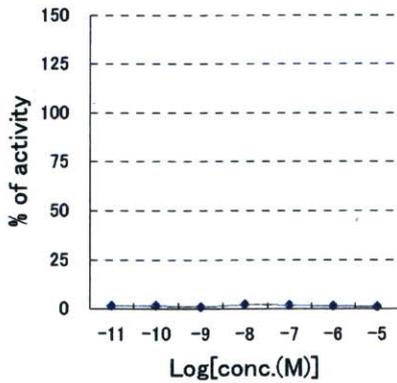
LOG[conc.(M)]	luc	ren
-5	28	107
-6	93	103
-7	106	102
-8	106	99
-9	105	102
-10	102	97

Cell viability



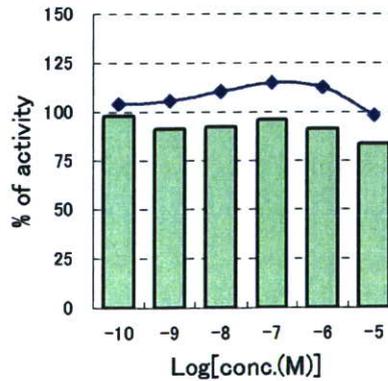
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	1.5
-6	1.8
-7	2.1
-8	2.4
-9	1.1
-10	1.8
-11	1.7



TRβ-RXR antagonist assay

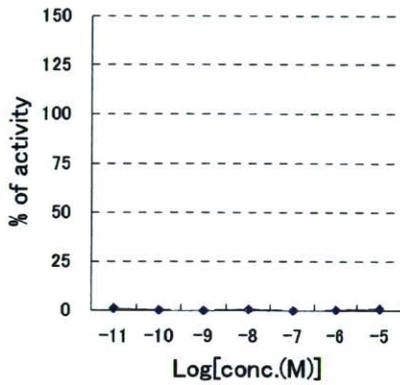
LOG[conc.(M)]	luc	ren
-5	99	83
-6	113	91
-7	115	96
-8	110	92
-9	106	91
-10	104	98



sample No. AT202
 chemical name Benzaldehyde Diethyl Acetal
 CAS. 774-48-1

AR agonist assay

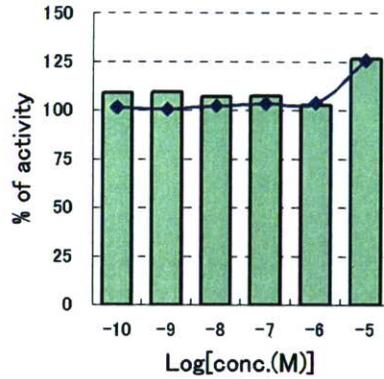
LOG[conc.(M)]	luc
-5	1.0
-6	0.3
-7	0.1
-8	0.6
-9	0.1
-10	0.2
-11	1.1



AR antagonist assay

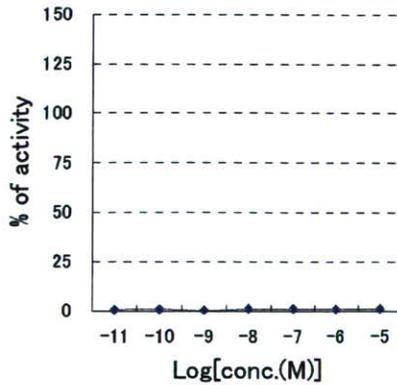
LOG[conc.(M)]	luc	ren
-5	126	127
-6	104	103
-7	104	107
-8	102	107
-9	101	109
-10	102	109

Cell viability



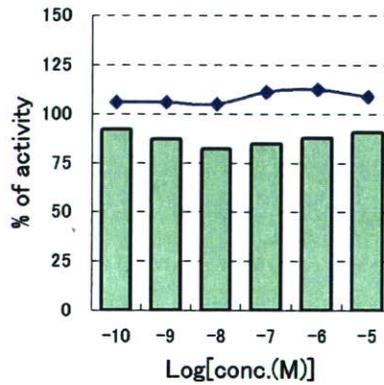
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	1.3
-6	1.3
-7	1.6
-8	1.6
-9	0.6
-10	1.1
-11	0.8



TRβ-RXR antagonist assay

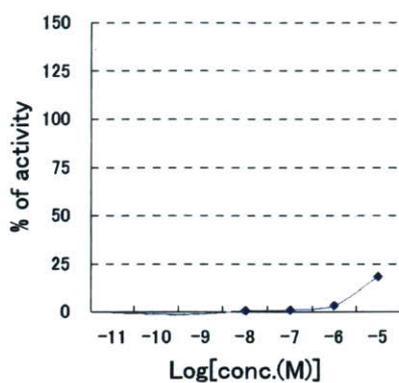
LOG[conc.(M)]	luc	ren
-5	109	90
-6	113	88
-7	111	85
-8	105	82
-9	106	87
-10	106	92



sample No. AT203
 chemical name benzo(b)fluoranthene
 CAS. 205-99-2

AR agonist assay

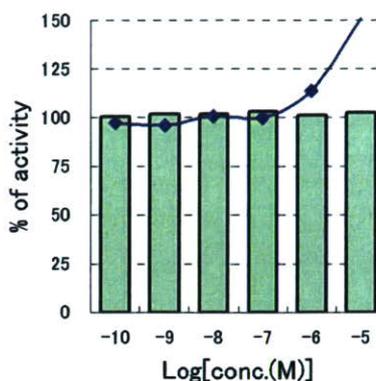
LOG[conc.(M)]	luc
-5	18.3
-6	3.4
-7	0.8
-8	0.6
-9	-1.2
-10	-1.1
-11	-0.2



AR antagonist assay

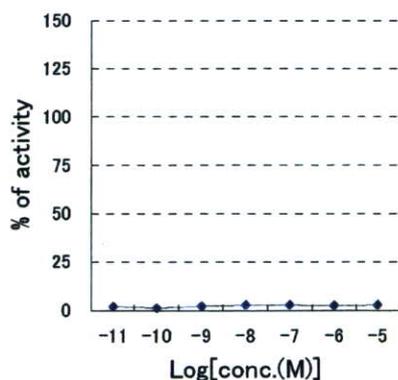
LOG[conc.(M)]	luc	ren
-5	151	102
-6	114	101
-7	100	103
-8	101	102
-9	96	102
-10	98	101

Cell viability



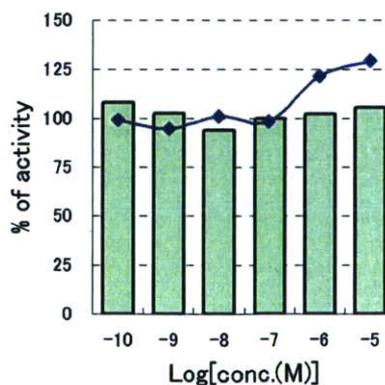
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	2.9
-6	2.8
-7	3.0
-8	3.0
-9	2.4
-10	1.6
-11	2.1



TRβ-RXR antagonist assay

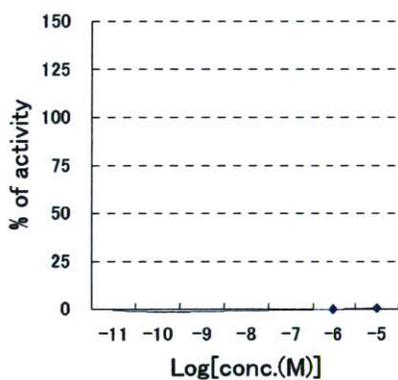
LOG[conc.(M)]	luc	ren
-5	130	105
-6	122	102
-7	98	100
-8	101	94
-9	95	103
-10	99	108



sample No. AT204
 chemical name Acetophenone, 2-isopropoxy-2-phenyl-
 CAS. 6652-28-4

AR agonist assay

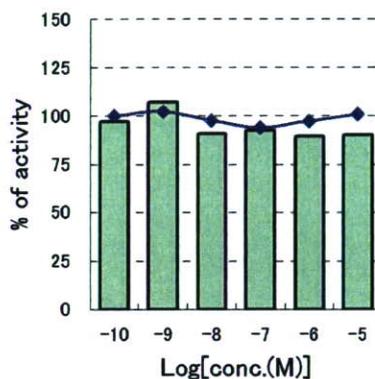
LOG[conc.(M)]	luc
-5	0.5
-6	0.1
-7	-0.2
-8	-0.6
-9	-1.3
-10	-1.6
-11	-0.8



AR antagonist assay

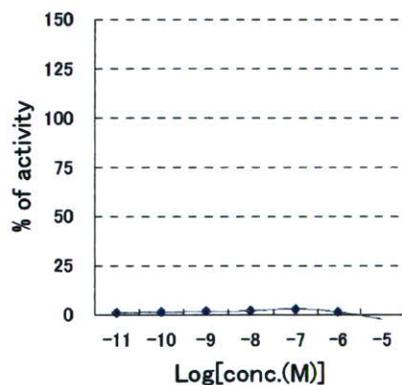
LOG[conc.(M)]	luc	ren
-5	101	90
-6	97	89
-7	94	92
-8	98	91
-9	102	107
-10	100	97

Cell viability



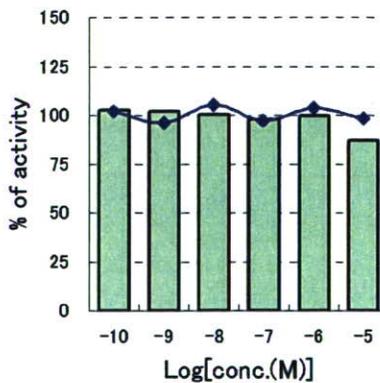
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	-2.1
-6	1.8
-7	3.2
-8	2.4
-9	1.9
-10	1.8
-11	1.2



TRβ-RXR antagonist assay

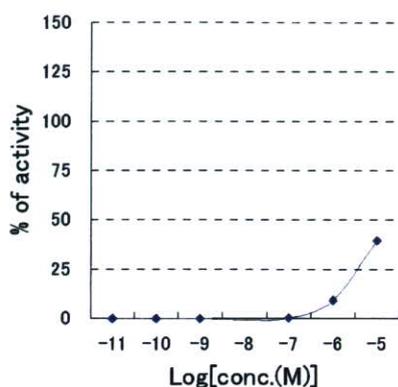
LOG[conc.(M)]	luc	ren
-5	99	87
-6	104	99
-7	97	98
-8	106	100
-9	96	102
-10	102	103



sample No. AT205
 chemical name Cinnamic acid, phenethyl ester
 CAS. 103-53-7

AR agonist assay

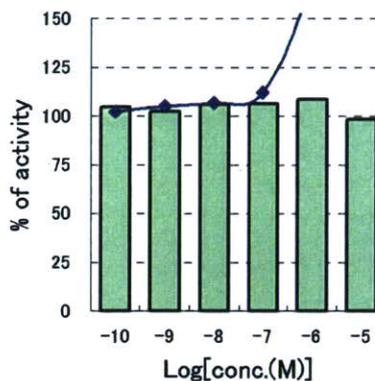
LOG[conc.(M)]	luc
-5	39.5
-6	9.5
-7	0.4
-8	-0.5
-9	0.1
-10	0.1
-11	-0.1



AR antagonist assay

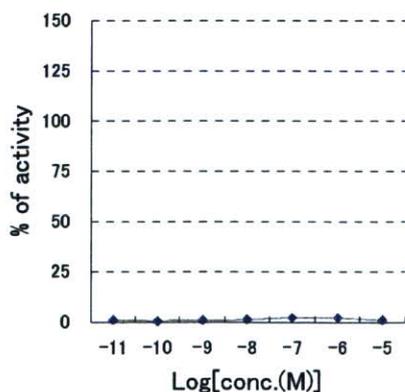
LOG[conc.(M)]	luc	ren
-5	291	99
-6	172	109
-7	112	106
-8	107	106
-9	106	102
-10	103	105

Cell viability



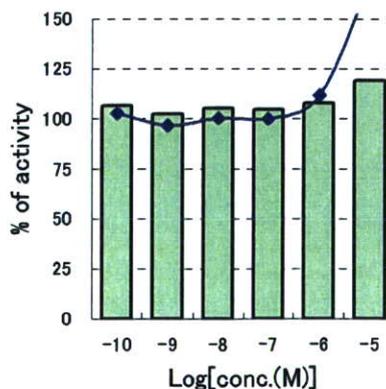
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	1.3
-6	2.5
-7	2.5
-8	1.7
-9	1.4
-10	0.8
-11	1.5



TRβ-RXR antagonist assay

LOG[conc.(M)]	luc	ren
-5	169	119
-6	112	108
-7	100	105
-8	101	105
-9	97	102
-10	103	107

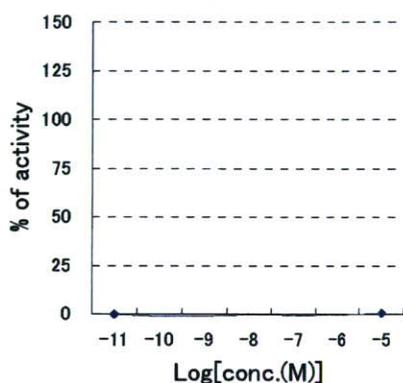


sample No.
chemical name
CAS.

AT206
1-Propanaminium, N,N,N-trimethyl-3-(2-methyl-1-oxo-2-propenyl)amino-, chlorid
51410-72-1

AR agonist assay

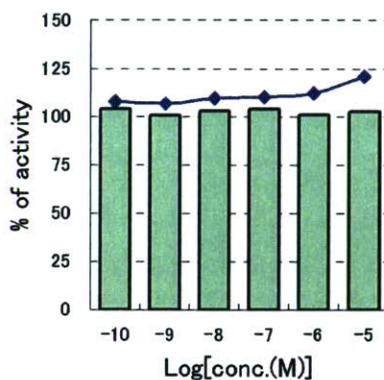
LOG[conc.(M)]	luc
-5	0.7
-6	-0.4
-7	-0.7
-8	-0.2
-9	-1.0
-10	-0.8
-11	-0.1



AR antagonist assay

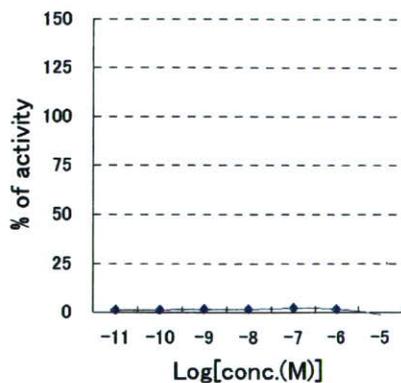
LOG[conc.(M)]	luc	ren
-5	121	103
-6	112	101
-7	111	104
-8	110	103
-9	107	101
-10	108	104

Cell viability



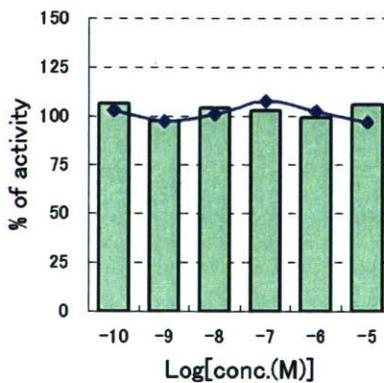
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	-0.9
-6	1.6
-7	2.5
-8	1.8
-9	1.9
-10	1.6
-11	1.4



TRβ-RXR antagonist assay

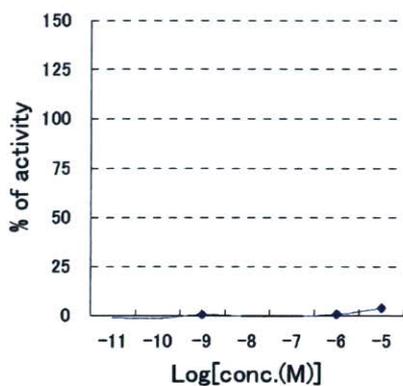
LOG[conc.(M)]	luc	ren
-5	97	106
-6	103	99
-7	108	103
-8	101	104
-9	98	98
-10	103	106



sample No. AT207
 chemical name Benzeneacetic acid, 4-methylphenyl ester
 CAS. 101-94-0

AR agonist assay

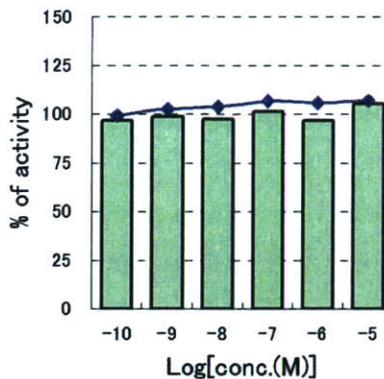
LOG[conc.(M)]	luc
-5	4.0
-6	0.8
-7	-0.2
-8	-0.2
-9	0.5
-10	-1.4
-11	-0.8



AR antagonist assay

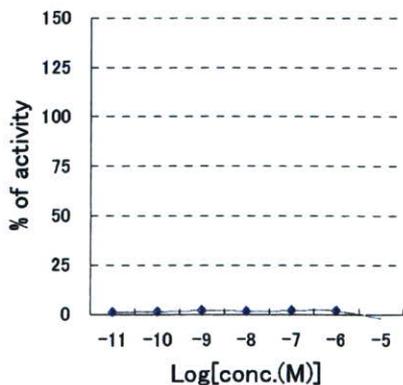
LOG[conc.(M)]	luc	ren
-5	107	106
-6	106	97
-7	107	101
-8	104	98
-9	103	99
-10	99	97

Cell viability



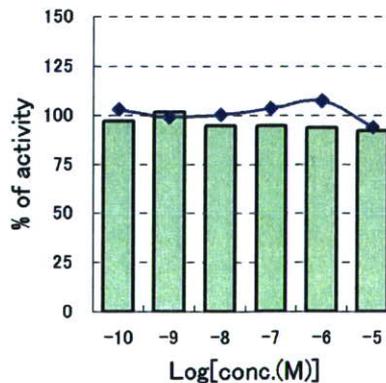
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	-1.7
-6	2.2
-7	2.4
-8	2.1
-9	2.4
-10	1.8
-11	1.4



TRβ-RXR antagonist assay

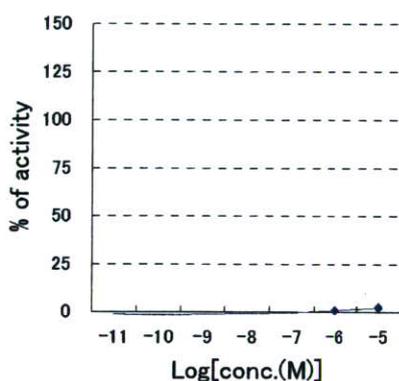
LOG[conc.(M)]	luc	ren
-5	94	92
-6	108	93
-7	104	95
-8	101	95
-9	99	101
-10	103	97



sample No. AT208
 chemical name Octanal, 7-hydroxy-3,7-dimethyl-, dimethyl acetal
 CAS. 141-92-4

AR agonist assay

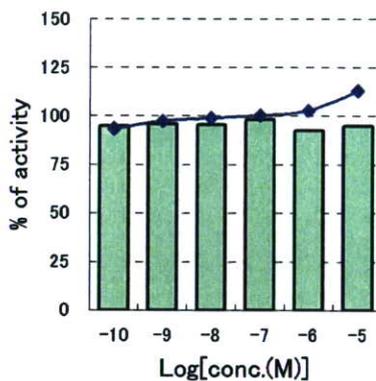
LOG[conc.(M)]	luc
-5	2.4
-6	0.9
-7	-0.4
-8	-1.0
-9	-1.3
-10	-1.4
-11	-1.3



AR antagonist assay

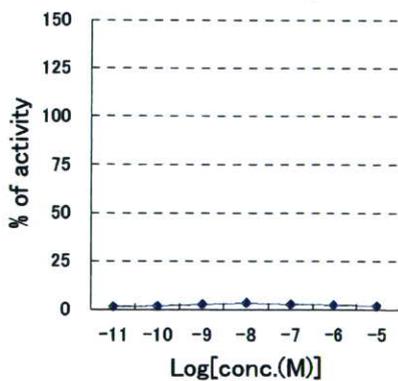
LOG[conc.(M)]	luc	ren
-5	113	95
-6	103	92
-7	100	98
-8	99	95
-9	98	96
-10	94	95

Cell viability



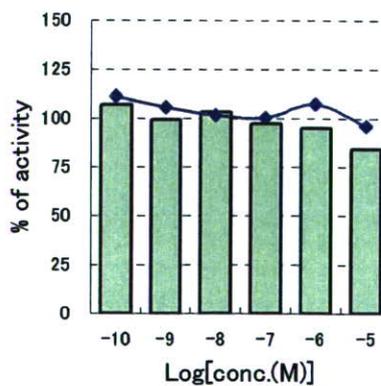
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	2.2
-6	2.6
-7	3.1
-8	3.6
-9	3.0
-10	2.2
-11	1.8



TRβ-RXR antagonist assay

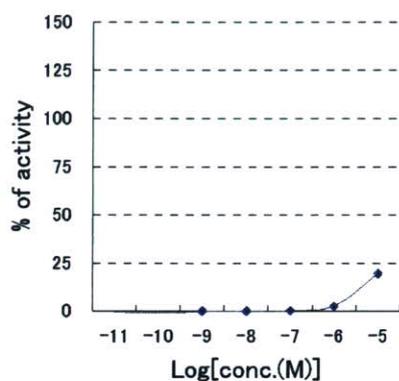
LOG[conc.(M)]	luc	ren
-5	96	84
-6	107	95
-7	101	97
-8	102	103
-9	106	99
-10	111	107



sample No. AT209
 chemical name Mepaniprim
 CAS. 7

AR agonist assay

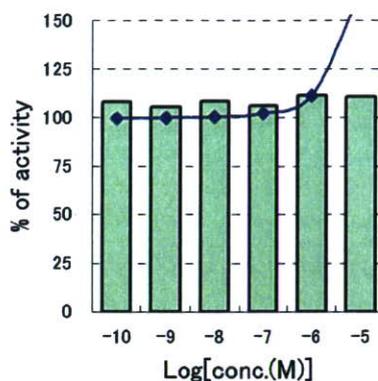
LOG[conc.(M)]	luc
-5	19.7
-6	2.6
-7	0.3
-8	-0.1
-9	-0.1
-10	-1.0
-11	-0.4



AR antagonist assay

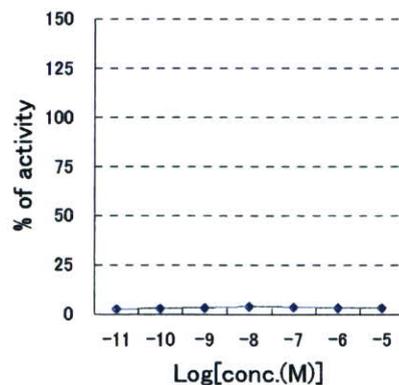
LOG[conc.(M)]	luc	ren
-5	164	111
-6	112	112
-7	102	106
-8	100	108
-9	100	106
-10	100	108

Cell viability



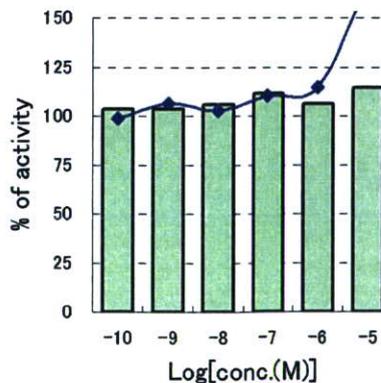
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	3.7
-6	3.6
-7	3.9
-8	4.0
-9	3.5
-10	3.2
-11	2.9



TRβ-RXR antagonist assay

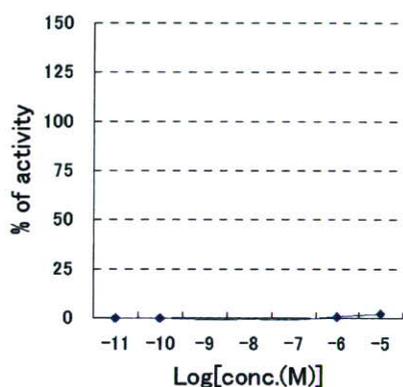
LOG[conc.(M)]	luc	ren
-5	169	114
-6	115	106
-7	110	111
-8	103	106
-9	107	104
-10	99	103



sample No. AT210
 chemical name butanoic acid, 1,1-dimethyl-2-phenylethyl ester
 CAS. 10094-34-5

AR agonist assay

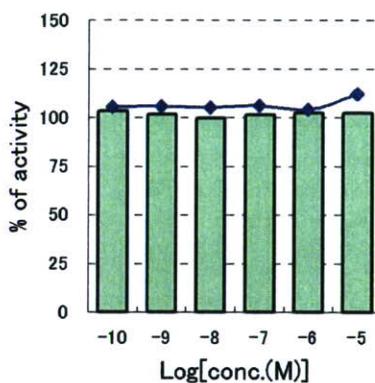
LOG[conc.(M)]	luc
-5	2.3
-6	0.9
-7	-0.5
-8	-0.3
-9	-0.5
-10	0.0
-11	0.0



AR antagonist assay

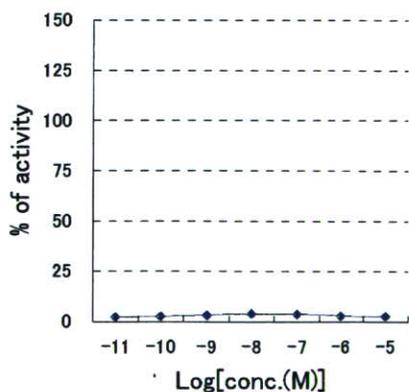
LOG[conc.(M)]	luc	ren
-5	112	102
-6	104	103
-7	106	101
-8	106	100
-9	106	102
-10	106	103

Cell viability



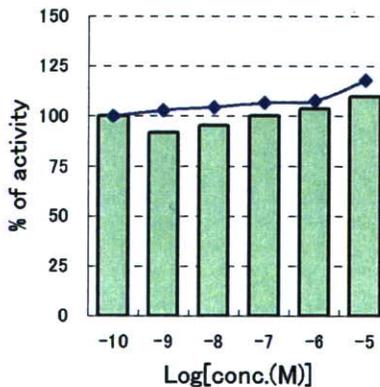
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	2.9
-6	3.3
-7	4.0
-8	4.4
-9	3.6
-10	2.8
-11	2.7



TRβ-RXR antagonist assay

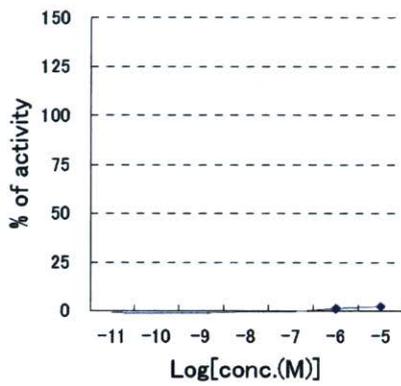
LOG[conc.(M)]	luc	ren
-5	118	110
-6	108	104
-7	107	100
-8	105	95
-9	103	92
-10	100	100



sample No. AT211
 chemical name Melatonin
 CAS. 73-31-4

AR agonist assay

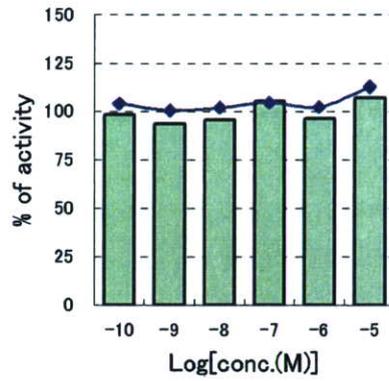
LOG[conc.(M)]	luc
-5	2.4
-6	1.1
-7	-0.3
-8	-0.4
-9	-0.7
-10	-1.1
-11	-0.6



AR antagonist assay

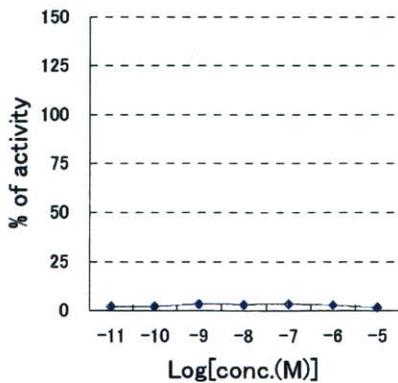
LOG[conc.(M)]	luc	ren
-5	113	107
-6	102	97
-7	105	105
-8	102	96
-9	101	94
-10	104	98

Cell viability



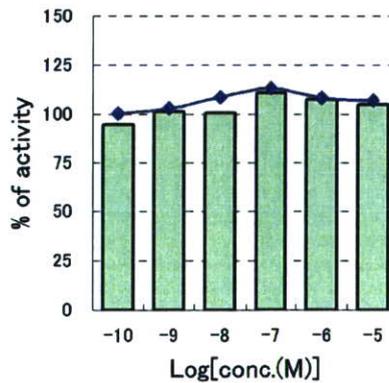
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	1.9
-6	3.0
-7	3.5
-8	3.4
-9	3.5
-10	2.5
-11	2.5



TRβ-RXR antagonist assay

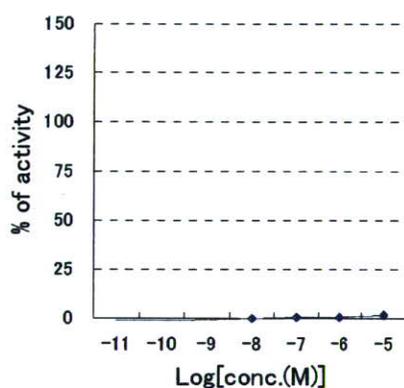
LOG[conc.(M)]	luc	ren
-5	107	105
-6	109	107
-7	113	111
-8	109	101
-9	103	101
-10	101	95



sample No. AT212
 chemical name Benzene, 2-(diethoxymethyl)-1-heptenyl -
 CAS. 60763-41-9

AR agonist assay

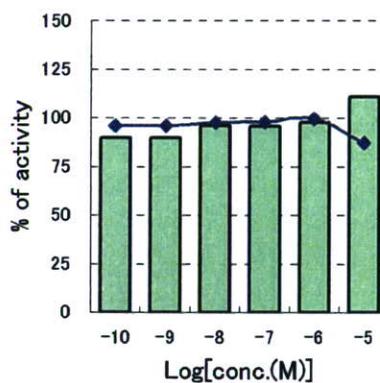
LOG[conc.(M)]	luc
-5	1.8
-6	0.7
-7	0.6
-8	0.1
-9	-0.7
-10	-1.2
-11	-1.3



AR antagonist assay

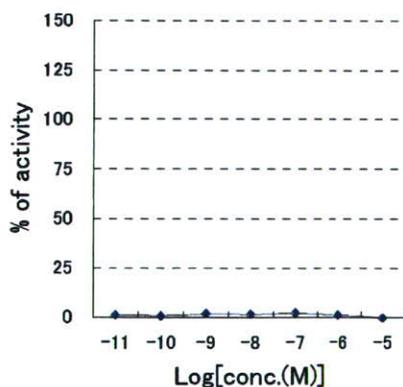
LOG[conc.(M)]	luc	ren
-5	87	111
-6	100	98
-7	98	96
-8	98	96
-9	96	90
-10	96	90

Cell viability



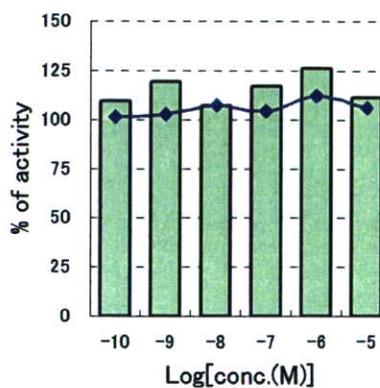
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	0.1
-6	1.5
-7	2.5
-8	1.7
-9	1.9
-10	0.8
-11	1.3



TRβ-RXR antagonist assay

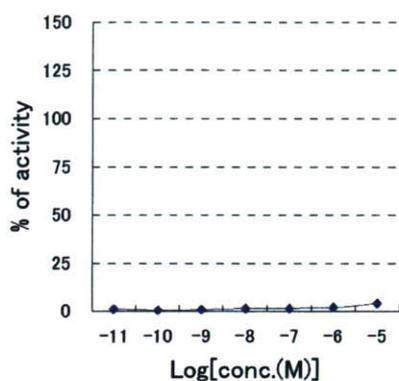
LOG[conc.(M)]	luc	ren
-5	106	111
-6	112	126
-7	104	117
-8	107	107
-9	103	119
-10	101	109



sample No. AT213
 chemical name Benzoic acid, 2-ethylhexyl ester
 CAS. 5444-75-7

AR agonist assay

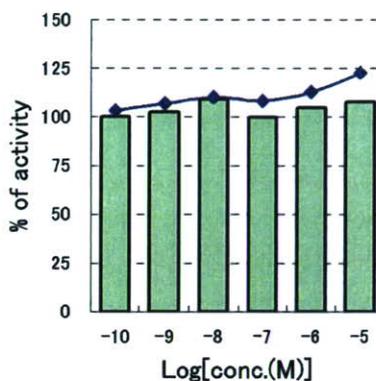
LOG[conc.(M)]	luc
-5	4.2
-6	2.1
-7	1.4
-8	1.4
-9	0.9
-10	0.5
-11	1.1



AR antagonist assay

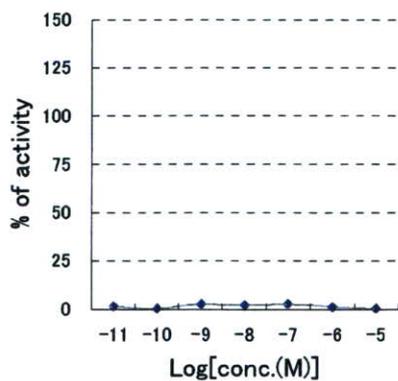
LOG[conc.(M)]	luc	ren
-5	123	108
-6	113	105
-7	109	100
-8	110	109
-9	107	103
-10	104	100

Cell viability



TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	0.5
-6	1.4
-7	2.9
-8	2.4
-9	3.0
-10	0.5
-11	1.8



TRβ-RXR antagonist assay

LOG[conc.(M)]	luc	ren
-5	97	141
-6	90	111
-7	92	109
-8	97	120
-9	95	115
-10	105	128

