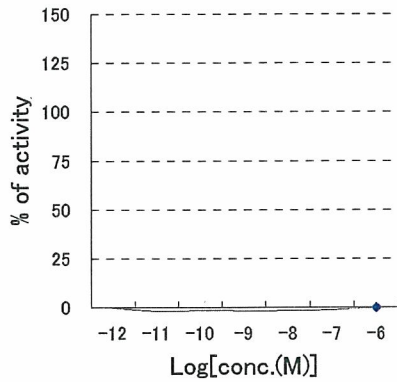


sample No. AR197
 chemical name 2-(T-BUTYL)-1,4-BENZENEDIOL
 CAS. 1948-33-0

AR agonist assay

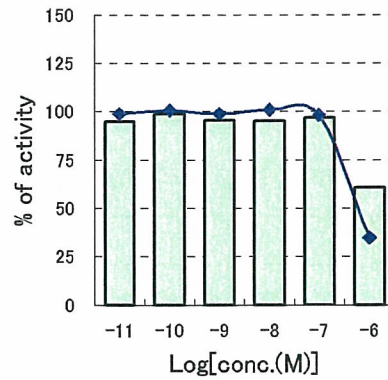
LOG[conc.(M)]	luc
-6	-0.1
-7	-1.3
-8	-1.6
-9	-1.8
-10	-1.3
-11	-1.6
-12	-0.2



AR antagonist assay

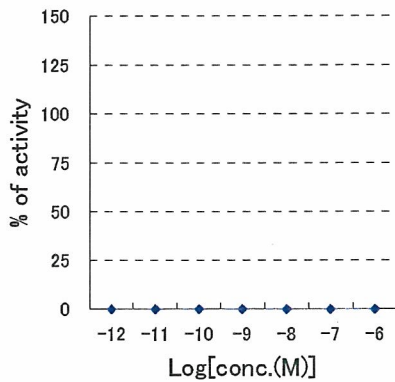
LOG[conc.(M)]	luc	ren
-6	35	61
-7	98	97
-8	101	95
-9	99	95
-10	100	99
-11	99	95

Cell viability



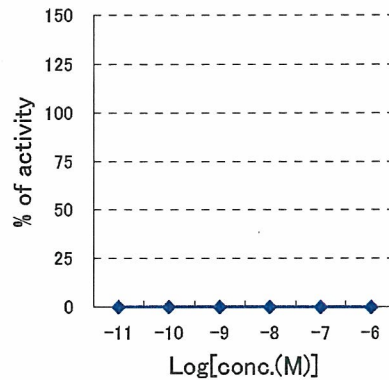
TRβ-RXR agonist assay

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

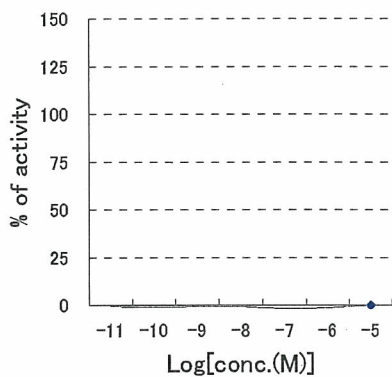
LOG[conc.(M)]	luc	ren
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0
-11	0	0



sample No. AR198
 chemical name Anethole
 CAS. 104-46-1

AR agonist assay

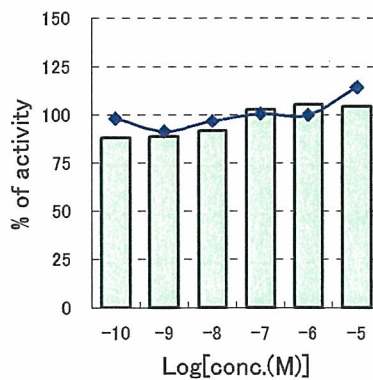
LOG[conc.(M)]	luc
-5	-0.1
-6	-1.1
-7	-1.5
-8	-0.6
-9	-0.6
-10	-0.8
-11	-0.6



AR antagonist assay

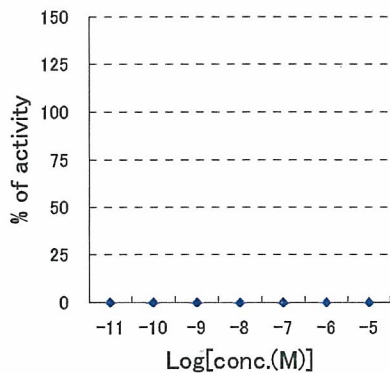
LOG[conc.(M)]	luc	ren
-5	114	104
-6	100	105
-7	101	103
-8	97	92
-9	92	89
-10	98	88

Cell viability



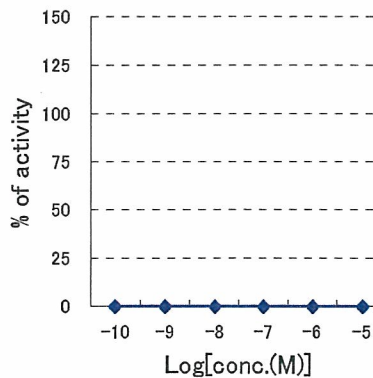
TRβ-RXR agonist assay

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

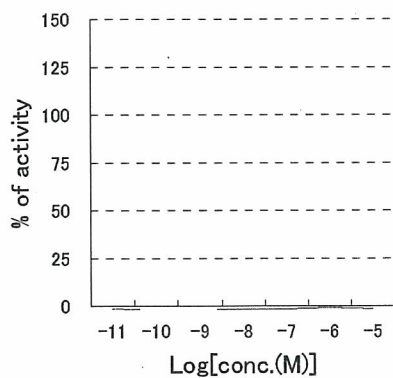
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0



sample No. AR199
 chemical name BENZYL METHACRYLATE
 CAS. 2495-37-6

AR agonist assay

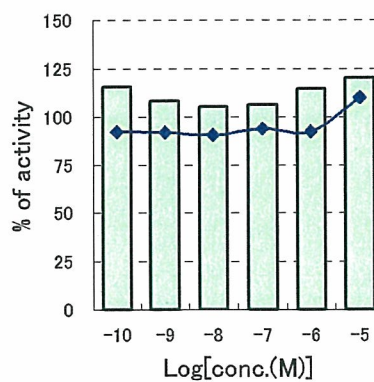
LOG[conc.(M)]	luc
-5	-1.7
-6	-1.0
-7	-1.5
-8	-1.6
-9	-2.3
-10	-2.3
-11	-1.3



AR antagonist assay

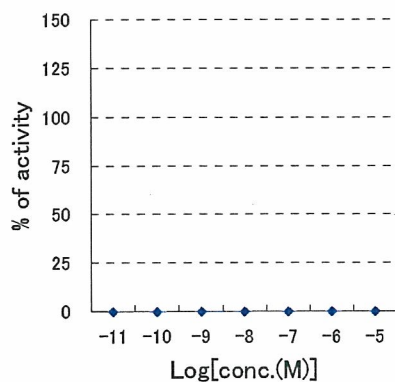
LOG[conc.(M)]	luc	ren
-5	110	120
-6	92	115
-7	94	106
-8	90	105
-9	92	108
-10	92	115

Cell viability



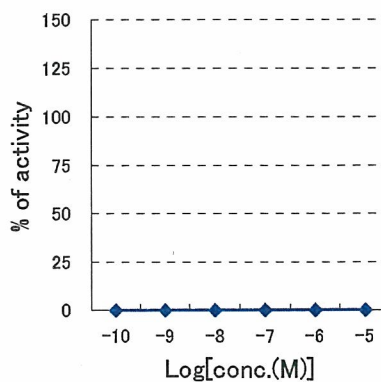
TRβ-RXR agonist assay

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

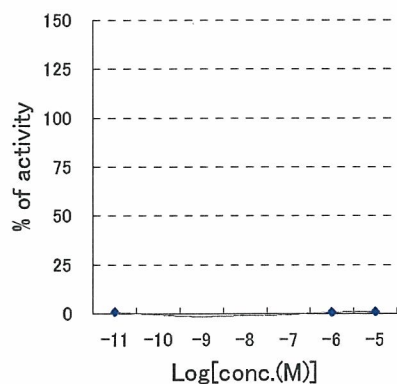
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0



sample No. AR200
 chemical name Guaethol
 CAS. 94-71-3

AR agonist assay

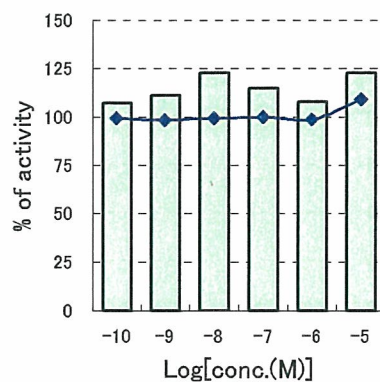
LOG[conc.(M)]	luc
-5	1.0
-6	0.8
-7	-0.5
-8	-1.0
-9	-1.4
-10	-0.5
-11	0.9



AR antagonist assay

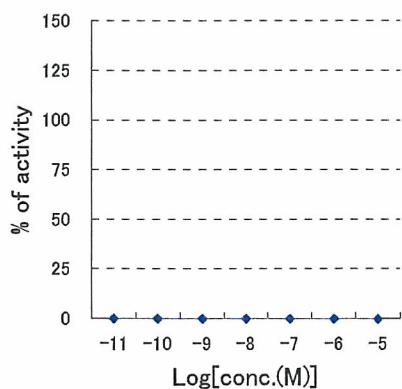
LOG[conc.(M)]	luc	ren
-5	109	123
-6	99	108
-7	100	115
-8	99	123
-9	98	111
-10	99	107

Cell viability



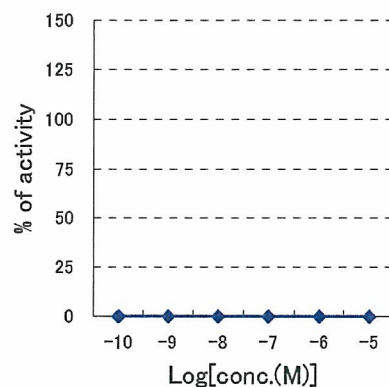
TRβ-RXR agonist assay

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

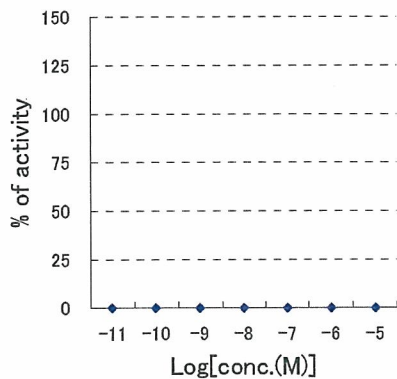
TR レポータージーンアッセイ

10 物質
(TR191~TR200)

sample No. TR191
 chemical name 2-(2-METHYLPROPOXY)-1,2-DIPHENYL ETHANONE
 CAS. 22499-12-3

AR agonist assay

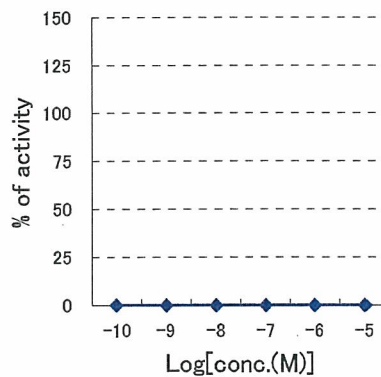
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

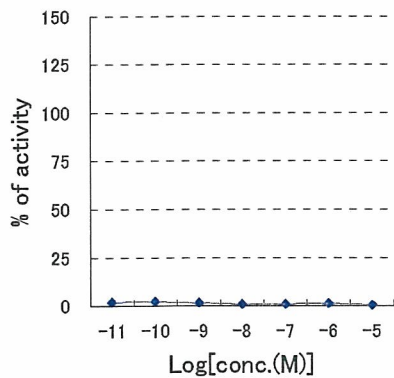
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



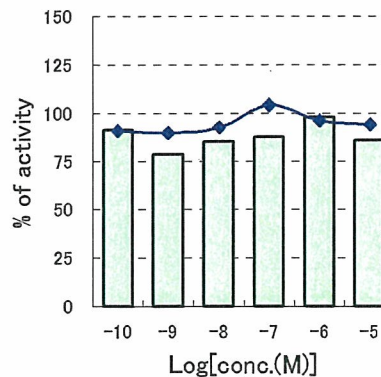
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	0.5
-6	1.6
-7	1.2
-8	1.3
-9	1.7
-10	2.5
-11	2.0



TRβ-RXR antagonist assay

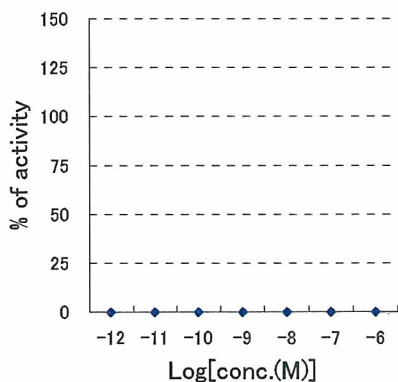
LOG[conc.(M)]	luc	ren
-5	94	86
-6	96	98
-7	104	88
-8	93	85
-9	90	79
-10	91	91



sample No. TR192
 chemical name 4,4'-OXYBISBENZENESULFONIC ACID, DIHYDRAZIDE
 CAS. 80-51-3

AR agonist assay

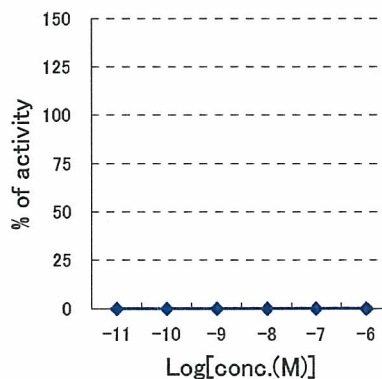
LOG[conc.(M)]	luc
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0
-12	0.0



AR antagonist assay

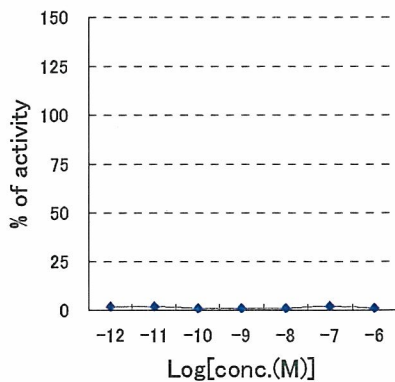
LOG[conc.(M)]	luc	ren
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0
-11	0	0

Cell viability



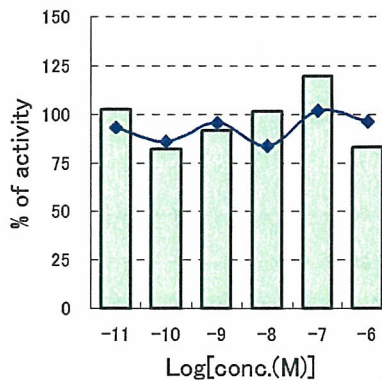
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-6	1.1
-7	2.0
-8	1.0
-9	1.2
-10	1.3
-11	2.1
-12	1.9



TRβ-RXR antagonist assay

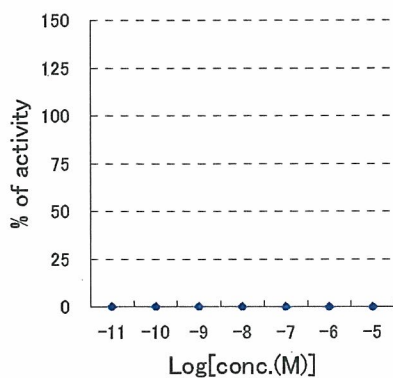
LOG[conc.(M)]	luc	ren
-6	96	83
-7	102	120
-8	84	102
-9	96	92
-10	86	82
-11	93	102



sample No. TR193
 chemical name N-ISOPROPYL-N'-PHENYL-P-PHENYLENEDIAMINE
 CAS. 101-72-4

AR agonist assay

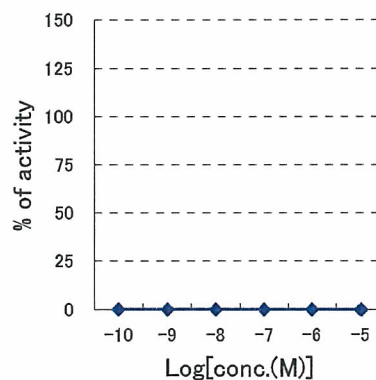
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

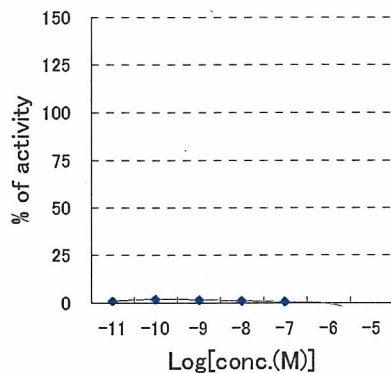
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



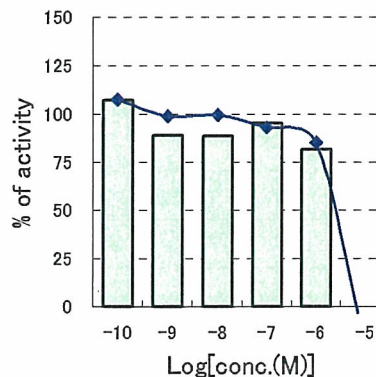
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	-7.1
-6	-0.3
-7	0.5
-8	1.3
-9	1.5
-10	1.7
-11	0.9



TRβ-RXR antagonist assay

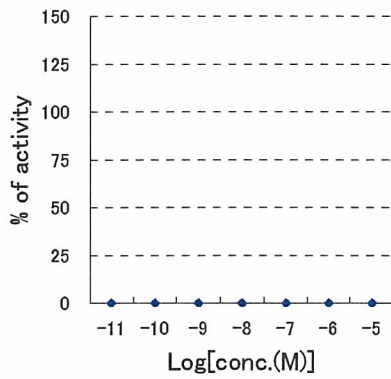
LOG[conc.(M)]	luc	ren
-5	-20	-28
-6	85	81
-7	93	95
-8	100	88
-9	99	89
-10	107	107



sample No. TR194
 chemical name Nonox wsp
 CAS. 77-62-3

AR agonist assay

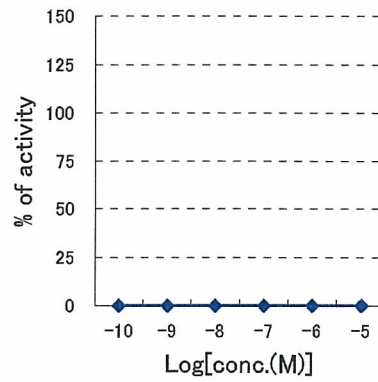
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

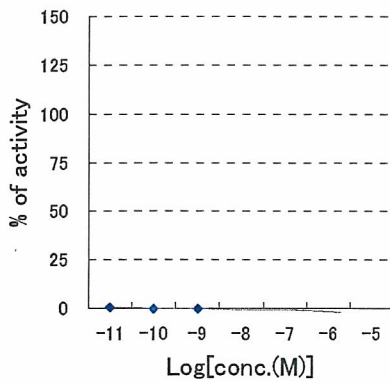
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



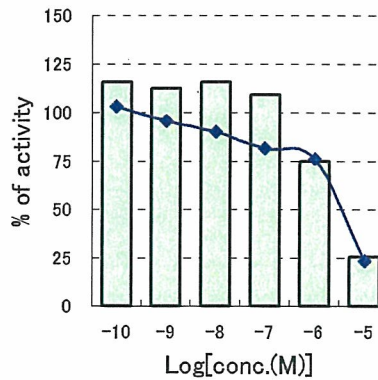
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	-4.9
-6	-1.6
-7	-0.7
-8	-0.5
-9	0.1
-10	-0.1
-11	0.6



TRβ-RXR antagonist assay

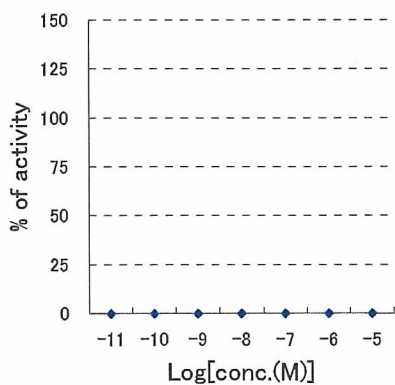
LOG[conc.(M)]	luc	ren
-5	24	25
-6	76	75
-7	82	109
-8	90	116
-9	96	112
-10	103	116



sample No. TR195
 chemical name Trimethylolpropane trimethacrylate
 CAS. 3290-92-4

AR agonist assay

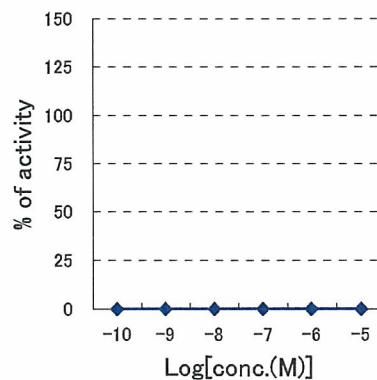
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

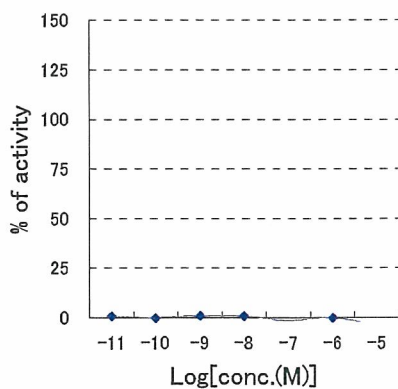
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



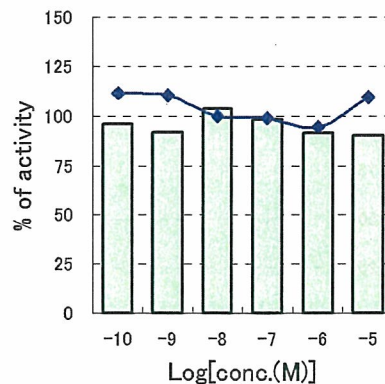
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	-3.5
-6	0.0
-7	-1.3
-8	0.8
-9	1.1
-10	0.0
-11	0.8



TRβ-RXR antagonist assay

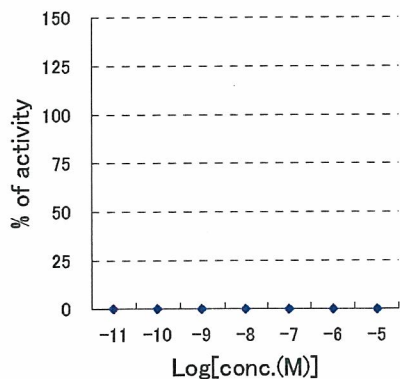
LOG[conc.(M)]	luc	ren
-5	110	90
-6	95	91
-7	99	98
-8	100	104
-9	110	92
-10	112	96



sample No. TR196
 chemical name Cinnamic acid, isopentyl ester
 CAS. 7779-65-9

AR agonist assay

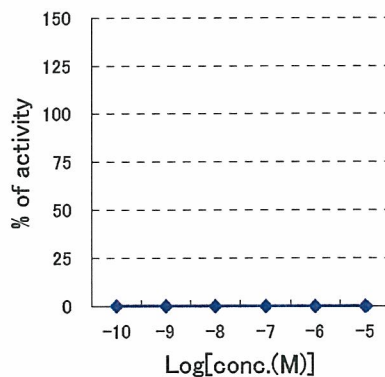
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

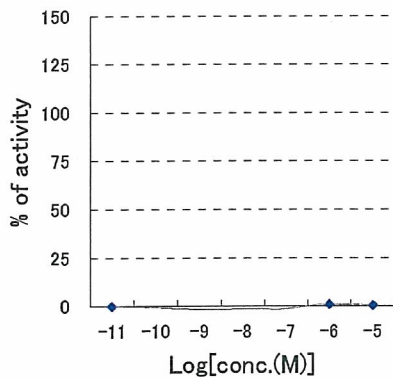
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



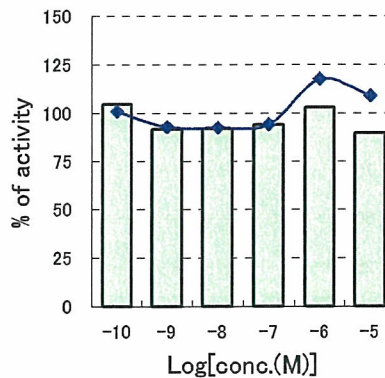
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	0.6
-6	1.1
-7	-1.3
-8	-1.2
-9	-1.4
-10	-0.7
-11	0.0



TRβ-RXR antagonist assay

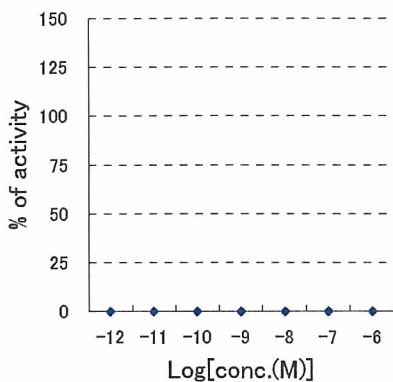
LOG[conc.(M)]	luc	ren
-5	109	89
-6	118	103
-7	94	94
-8	92	92
-9	93	92
-10	101	104



sample No. TR197
 chemical name 1H-Benz e indole, 1,1,2-trimethyl-
 CAS. 41532-84-7

AR agonist assay

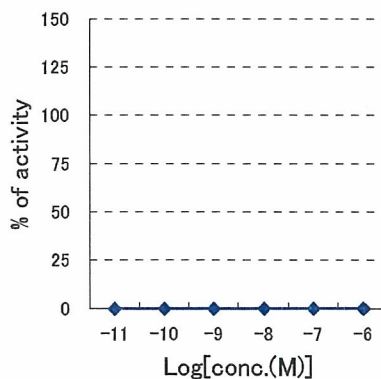
LOG[conc.(M)]	luc
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0
-12	0.0



AR antagonist assay

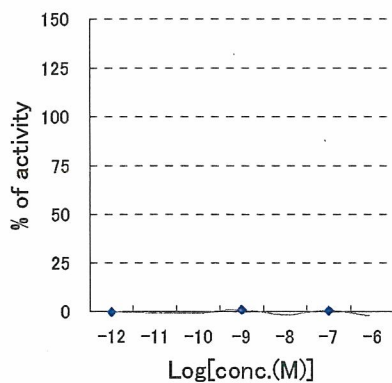
LOG[conc.(M)]	luc	ren
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0
-11	0	0

Cell viability



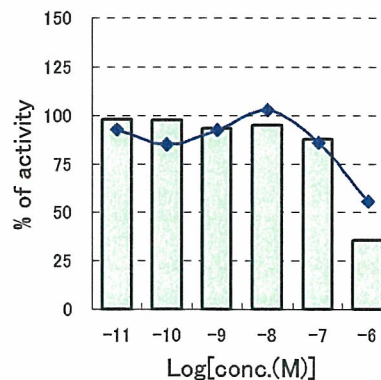
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-6	-2.3
-7	0.5
-8	-1.5
-9	1.1
-10	-0.6
-11	-0.6
-12	-0.1



TRβ-RXR antagonist assay

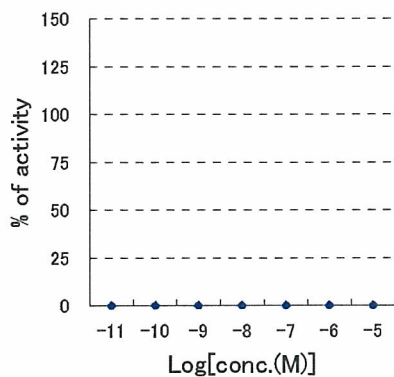
LOG[conc.(M)]	luc	ren
-6	56	36
-7	86	87
-8	103	95
-9	93	93
-10	85	98
-11	93	98



sample No. TR198
 chemical name 1,6-Octadien-3-ol, 3,7-dimethyl-, benzoate
 CAS. 126-64-7

AR agonist assay

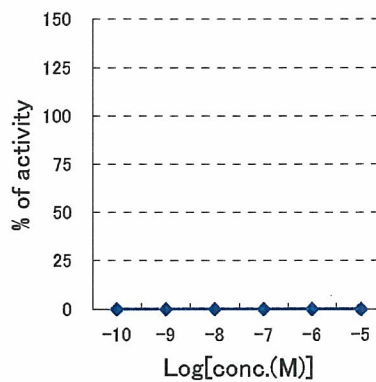
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

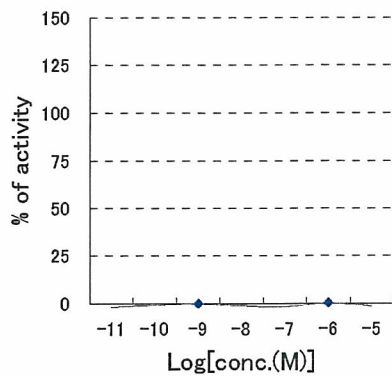
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



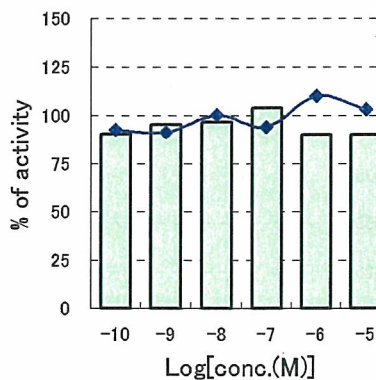
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	-1.4
-6	0.2
-7	-1.8
-8	-1.1
-9	0.1
-10	-0.8
-11	-1.9



TRβ-RXR antagonist assay

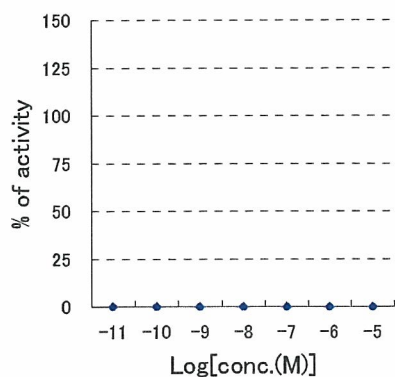
LOG[conc.(M)]	luc	ren
-5	103	90
-6	110	90
-7	94	104
-8	100	97
-9	91	95
-10	92	90



sample No. TR199
 chemical name Ferulic acid
 CAS. 1135-24-6

AR agonist assay

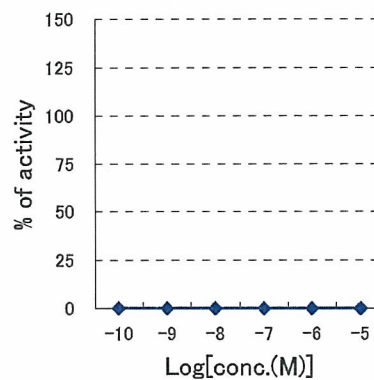
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

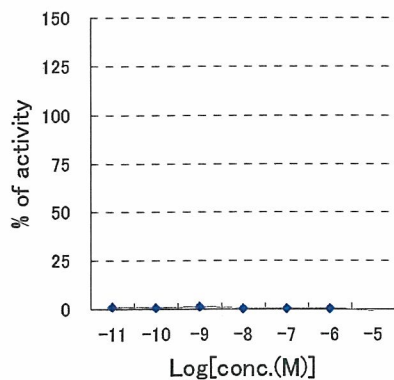
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



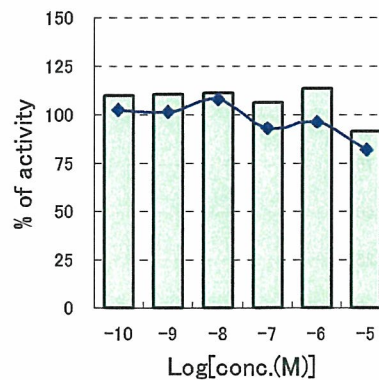
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	-0.5
-6	0.5
-7	0.5
-8	0.7
-9	1.5
-10	0.9
-11	1.3



TRβ-RXR antagonist assay

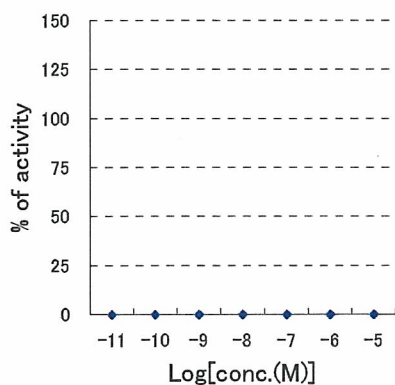
LOG[conc.(M)]	luc	ren
-5	82	91
-6	96	114
-7	93	106
-8	108	111
-9	101	110
-10	103	110



sample No. TR200
 chemical name Aspartame
 CAS. 22839-47-0

AR agonist assay

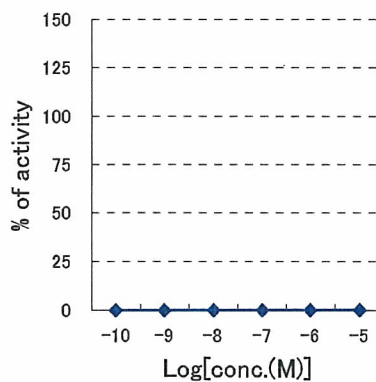
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

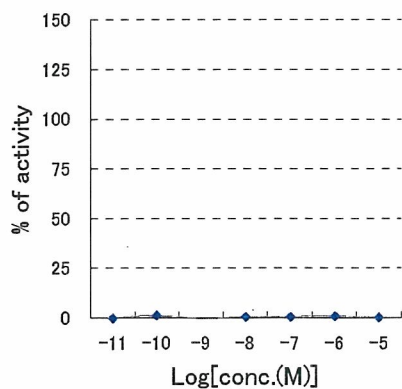
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



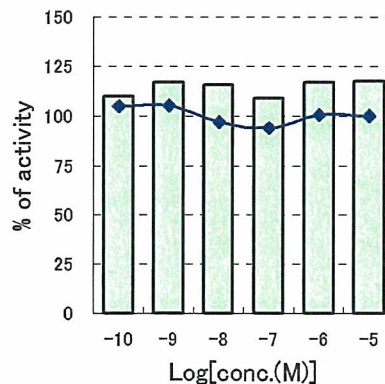
TRβ-RXR agonist assay

LOG[conc.(M)]	luc
-5	0.4
-6	0.9
-7	0.6
-8	0.5
-9	-0.4
-10	1.3
-11	0.0



TRβ-RXR antagonist assay

LOG[conc.(M)]	luc	ren
-5	100	118
-6	101	117
-7	94	109
-8	97	116
-9	105	117
-10	105	110



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. 核内受容体ドッキングモデルによる *in silico* スクリーニング系の研究
(主任研究者: 医薬分子設計研究所委託業務)



図1 ヒト AR 受容体とリガンド R1881 との複合体結晶構造 1e3g の全体像。中央下の黄色の領域がリガンド結合ポケット。

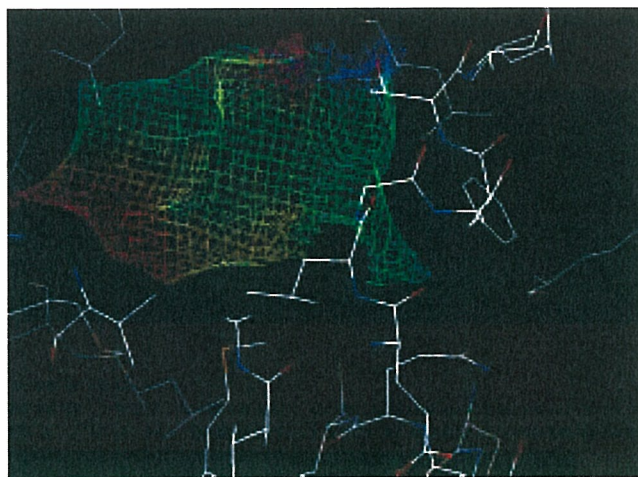


図2 AR のリガンド結合部位の拡大図。カゴ状の表示はリガンド結合ポケットの形状を三次元格子点のデータにより示している。カゴの色は、赤いほど静電ポテンシャルが正、青いほど負であることを示す。

表 1. 化学物質の AR に対する相対結合強度(logRBA)予測値

CAS 番号	推算 logRBA	CAS 番号	推算 logRBA	CAS 番号	推算 logRBA
51-24-1	-1.74	92-69-3	-1.82	125-84-8	-1.92
51-52-5	-2.50	92-88-6	-1.76	126-64-7	-1.85
55-06-1	-1.64	94-13-3	-2.27	131-16-8	-2.26
56-49-5	-0.49	94-18-8	-1.92	131-54-4	-1.29
56-53-1	-1.07	94-25-7	-2.34	131-55-5	-1.61
56-72-4	-1.80	94-26-8	-2.38	131-56-6	-2.00
57-83-0	-0.25	94-41-7	-1.56	131-57-7	-1.51
58-18-4	-0.03	94-71-3	-2.53	133-07-3	-2.60
58-72-0	-1.03	96-29-7	-2.88	139-65-1	-2.05
60-56-0	-2.85	97-39-2	-1.16	193-39-5	-0.84
60-82-2	-1.35	97-54-1	-2.01	298-46-4	-1.62
61-82-5	-3.18	98-54-4	-1.96	298-81-7	-1.95
63-05-8	-0.38	99-71-8	-2.15	327-97-9	-0.97
63-25-2	-1.83	99-76-3	-2.46	330-55-2	-1.96
68-22-4	-0.13	101-53-1	-2.08	341-58-2	-1.98
72-43-5	-1.65	101-72-4	-1.58	404-86-4	-1.77
72-55-9	-1.70	101-92-8	-2.19	446-72-0	-1.30
77-06-5	-1.27	102-22-7	-1.73	480-18-2	-1.35
79-94-7	-2.64	103-14-0	-1.71	480-40-0	-1.45
79-97-0	-1.01	103-16-2	-1.79	480-41-1	-1.11
80-05-7	-1.51	103-34-4	-2.52	487-26-3	-1.67
80-09-1	-1.74	104-40-5	-1.99	491-80-5	-1.45
80-51-3	-1.54	104-46-1	-2.02	497-76-7	-1.60
81-11-8	-0.87	106-41-2	-2.67	500-38-9	-1.34
81-64-1	-1.82	108-43-0	-2.70	501-24-6	-2.18
81-92-5	-1.12	115-32-2	-2.12	520-18-3	-1.11
83-88-5	-1.15	115-86-6	-1.42	521-18-6	-0.31
84-60-6	-1.71	117-37-3	-1.40	525-82-6	-1.55
84-69-5	-1.80	117-39-5	-0.99	531-59-9	-2.32
84-74-2	-2.26	119-61-9	-1.88	574-09-4	-1.76
85-68-7	-1.81	119-93-7	-1.17	599-64-4	-1.67
87-18-3	-1.54	120-47-8	-2.40	603-35-0	-2.11
89-72-5	-2.28	120-51-4	-1.98	603-45-2	-0.89
92-52-4	-2.00	122-40-7	-1.99	611-99-4	-1.47

CAS 番号	推算 logRBA	CAS 番号	推算 logRBA	CAS 番号	推算 logRBA
620-92-8	-1.76	2032-65-7	-1.82	13110-37-7	-2.28
644-08-6	-1.74	2128-93-0	-1.17	13311-84-7	-1.81
700-06-1	-2.19	2142-01-0	-1.90	14392-69-9	-2.07
709-98-8	-2.07	2153-28-8	-1.57	14938-35-3	-2.18
719-03-9	-1.57	2236-52-4	-1.95	15872-42-1	-1.62
723-46-6	-1.95	2444-46-4	-1.82	17598-02-6	-1.74
785-30-8	-1.64	2446-69-7	-2.22	17924-92-4	-1.31
791-28-6	-1.31	2491-32-9	-1.87	20426-12-4	-1.59
797-63-7	-0.26	2495-37-6	-2.37	22499-12-3	-1.62
831-82-3	-1.83	2657-25-2	-1.47	22839-47-0	-2.54
843-55-0	-1.49	2664-63-3	-1.92	23001-29-8	-0.61
844-51-9	-1.39	2971-36-0	-1.90	23564-06-9	-2.26
934-34-9	-2.62	3001-15-8	-1.93	25637-99-4	-2.51
1038-66-0	-1.99	3562-84-3	-1.50	25812-30-0	-1.41
1095-77-8	-1.82	3780-50-5	-2.17	27955-94-8	-1.51
1107-00-2	-2.47	4191-73-5	-2.13	29091-21-2	-2.07
1131-60-8	-1.71	4250-77-5	-1.36	41532-84-7	-1.36
1135-24-6	-1.58	5153-25-3	-1.99	42436-07-7	-2.15
1141-59-9	-1.55	5331-91-9	-2.61	50471-44-8	-1.86
1149-16-2	-1.39	5402-37-9	-1.32	51218-45-2	-1.90
1156-51-0	-1.85	5466-77-3	-1.97	53112-28-0	-1.44
1470-79-7	-1.54	6515-37-3	-1.32	57486-68-7	-2.61
1478-61-1	-2.46	6521-30-8	-2.21	59517-19-0	-1.33
1570-64-5	-2.51	6554-98-9	-1.46	66142-15-2	-1.03
1576-13-2	-1.44	6807-17-6	-1.32	67747-09-5	-1.41
1806-26-4	-2.10	6893-02-3	-2.29	70356-09-1	-1.43
1825-21-4	-2.76	6948-88-5	-0.13	76578-12-6	-1.86
1836-75-5	-1.77	7320-34-5	-3.17	78587-05-0	-1.72
1861-32-1	-2.43	7696-12-0	-1.34	79127-80-3	-1.49
1948-33-0	-1.90	7779-65-9	-1.76	95737-68-1	-1.06
1965-09-9	-1.68	10605-21-7	-2.10	119168-77-3	-1.24
1987-50-4	-2.01	13037-86-0	-2.01		

Ⅱ. 分担研究報告書