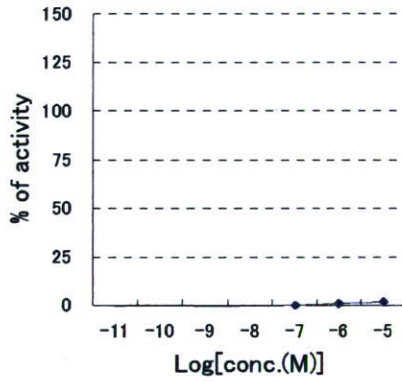


sample No. AR246  
 chemical name Cyclohexanol, 4-tert-butyl-, acetate  
 CAS. 32210-23-4

**AR agonist assay**

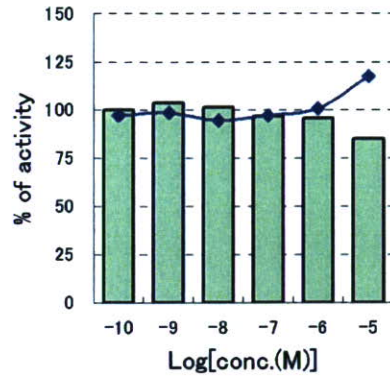
LOG[conc.(M)]	luc
-5	1.9
-6	0.8
-7	0.0
-8	-0.3
-9	-0.5
-10	-0.2
-11	-0.4



**AR antagonist assay**

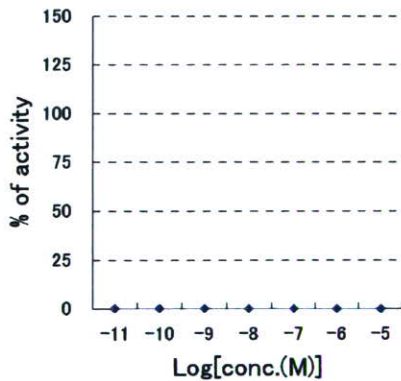
LOG[conc.(M)]	luc	ren
-5	117	85
-6	101	96
-7	97	97
-8	94	101
-9	98	104
-10	97	100

Cell viability



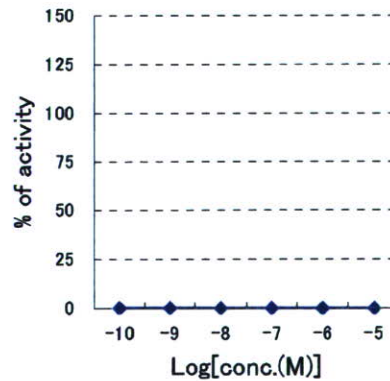
**TRβ-RXR agonist assay**

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**

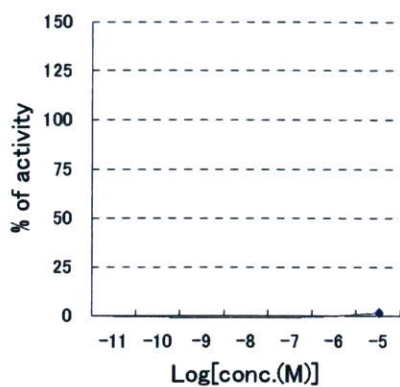
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0



sample No. AR247  
 chemical name Morin  
 CAS. 480-16-0

**AR agonist assay**

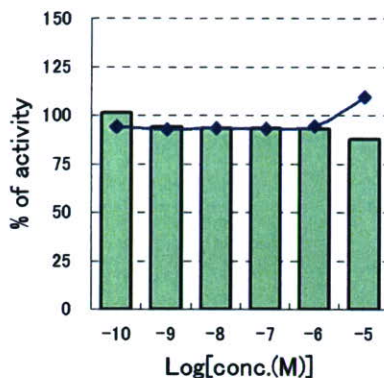
LOG[conc.(M)]	luc
-5	1.4
-6	-0.4
-7	-0.9
-8	-0.8
-9	-1.2
-10	-0.7
-11	-0.7



**AR antagonist assay**

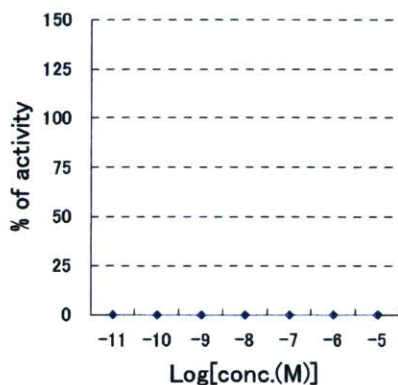
LOG[conc.(M)]	luc	ren
-5	109	88
-6	94	93
-7	93	94
-8	93	93
-9	93	94
-10	94	101

Cell viability



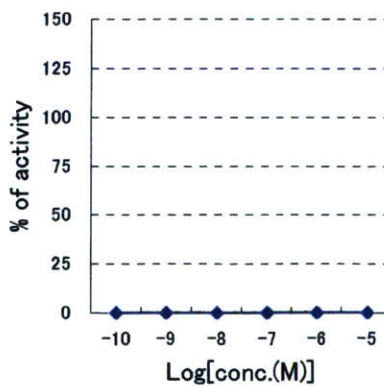
**TRβ-RXR agonist assay**

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**

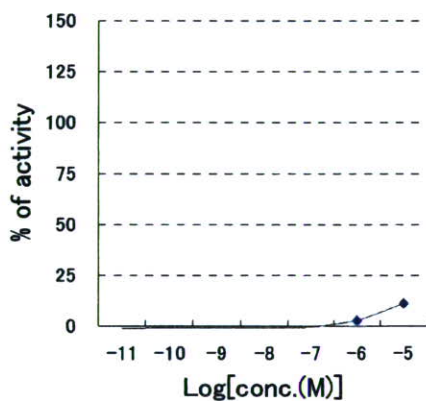
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0



sample No. AR248  
 chemical name 3',4',7-trihydroxyisoflavone  
 CAS. 485-63-2

**AR agonist assay**

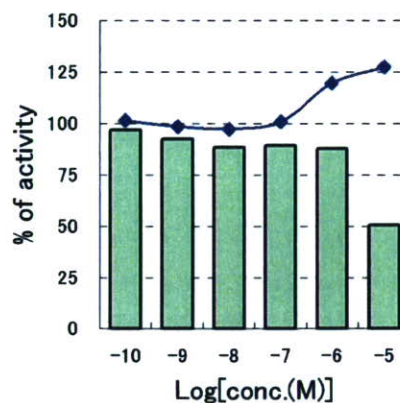
LOG[conc.(M)]	luc
-5	11.0
-6	2.6
-7	-0.7
-8	-0.8
-9	-0.9
-10	-1.0
-11	-1.1



**AR antagonist assay**

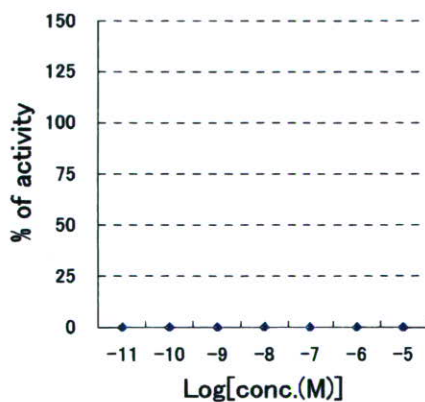
LOG[conc.(M)]	luc	ren
-5	127	50
-6	119	88
-7	101	89
-8	97	88
-9	98	92
-10	101	97

Cell viability



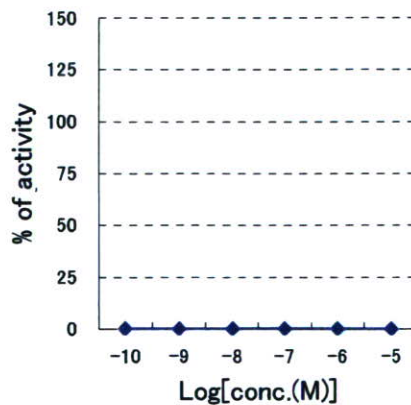
**TRβ-RXR agonist assay**

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**

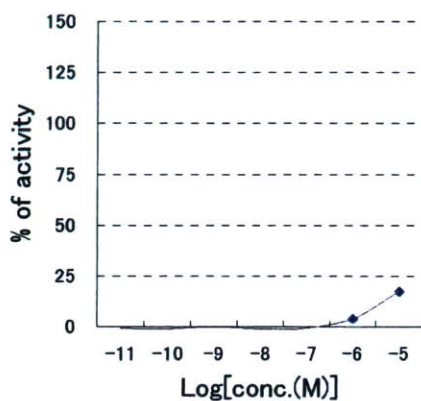
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0



sample No. AR249  
 chemical name 4-Hexanoylresorcinol  
 CAS. 3144-54-5

**AR agonist assay**

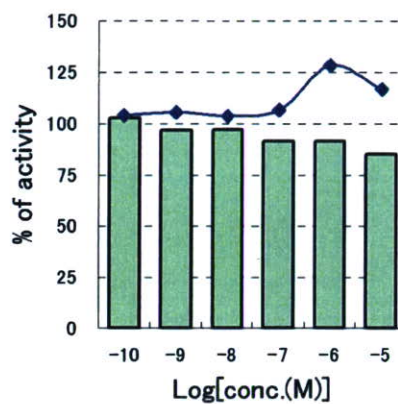
LOG[conc.(M)]	luc
-5	17.5
-6	3.9
-7	-0.5
-8	-1.1
-9	-0.3
-10	-1.2
-11	-1.0



**AR antagonist assay**

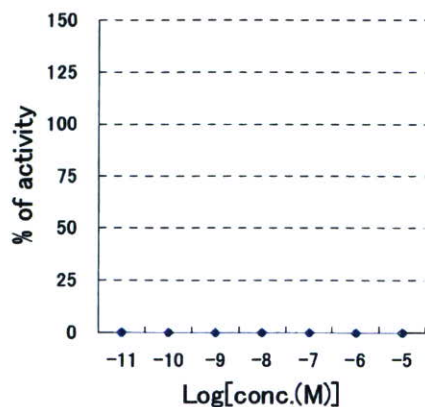
LOG[conc.(M)]	luc	ren
-5	117	85
-6	128	91
-7	106	91
-8	104	97
-9	105	97
-10	104	103

Cell viability



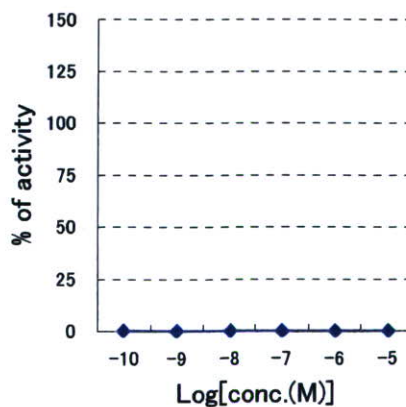
**TRβ-RXR agonist assay**

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**

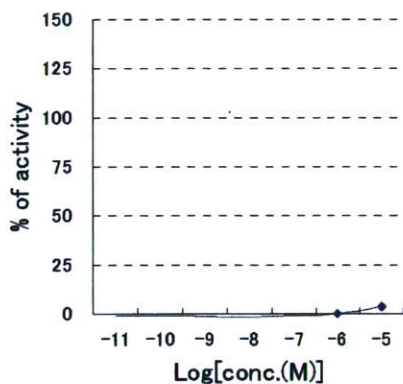
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0



sample No. AR250  
 chemical name 6,3'-dihydroxyflavone  
 CAS. 1

**AR agonist assay**

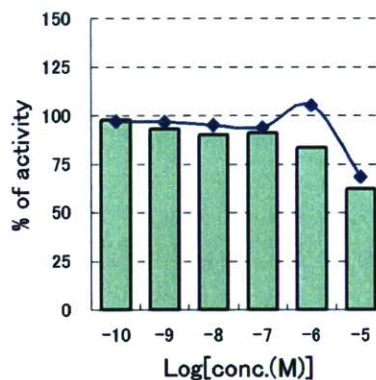
LOG[conc.(M)]	luc
-5	3.5
-6	0.0
-7	-1.3
-8	-1.7
-9	-1.4
-10	-1.0
-11	-1.3



**AR antagonist assay**

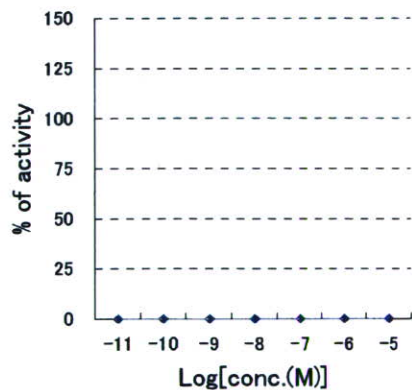
LOG[conc.(M)]	luc	ren
-5	68	62
-6	105	84
-7	94	91
-8	95	90
-9	97	93
-10	97	98

Cell viability



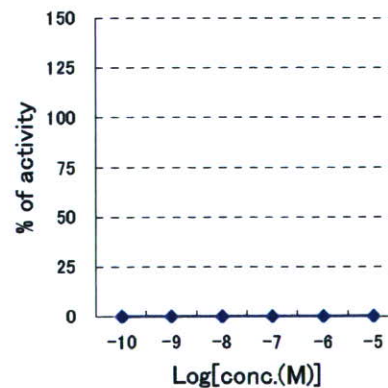
**TRβ-RXR agonist assay**

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



測定結果 一覧

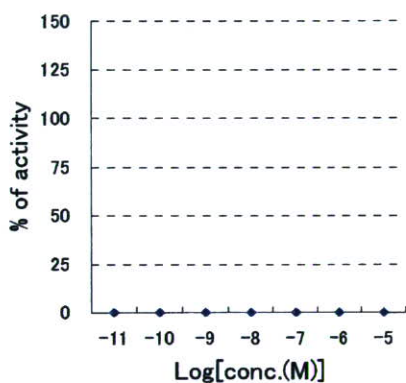
TR レポータージーンアッセイ

10 物質  
(TR191～TR200)

sample No. TR241  
 chemical name Clindamycin phosphate  
 CAS. 24729-96-2

**AR agonist assay**

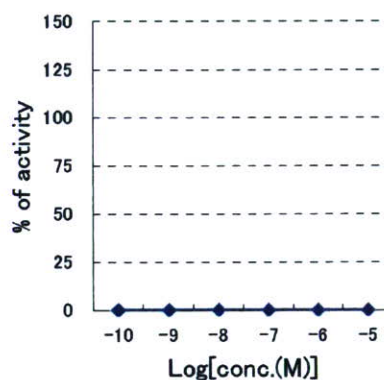
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



**AR antagonist assay**

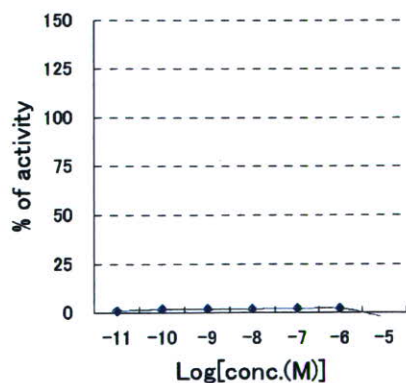
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



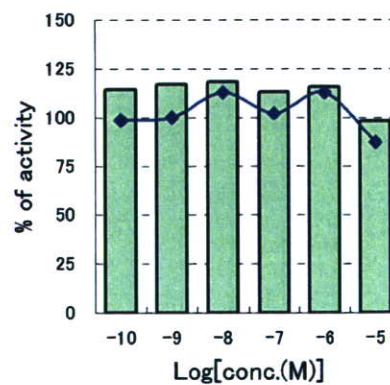
**TRβ-RXR agonist assay**

LOG[conc.(M)]	luc
-5	-2.5
-6	2.1
-7	2.0
-8	1.8
-9	1.9
-10	1.7
-11	0.8



**TRβ-RXR antagonist assay**

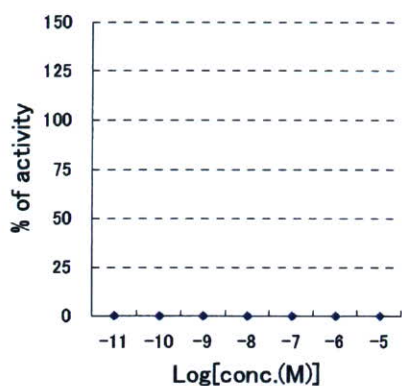
LOG[conc.(M)]	luc	ren
-5	87	98
-6	113	116
-7	102	113
-8	113	118
-9	100	117
-10	98	115



sample No. TR242  
 chemical name Oxycarboxin  
 CAS. 5259-88-1

**AR agonist assay**

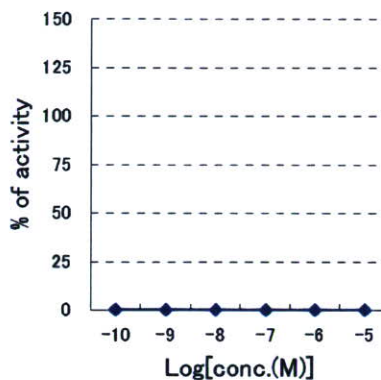
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



**AR antagonist assay**

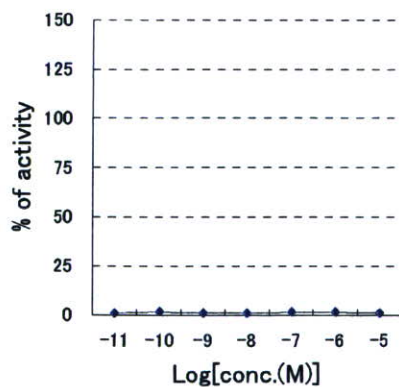
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



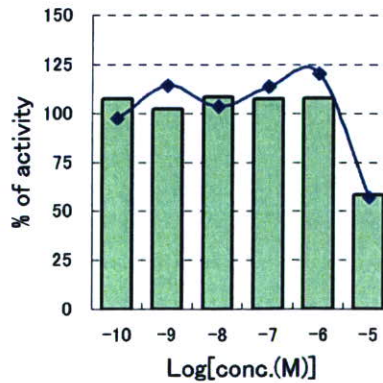
**TRβ-RXR agonist assay**

LOG[conc.(M)]	luc
-5	1.2
-6	1.8
-7	1.7
-8	1.2
-9	1.2
-10	1.6
-11	0.8



**TRβ-RXR antagonist assay**

LOG[conc.(M)]	luc	ren
-5	57	58
-6	120	108
-7	113	107
-8	104	108
-9	114	102
-10	97	107

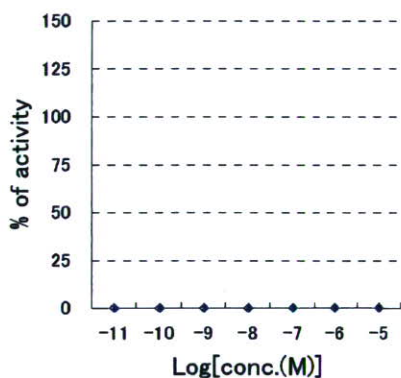




sample No. TR243  
 chemical name Acetamide, N-fluoren-2-yl-  
 CAS. 53-96-3

**AR agonist assay**

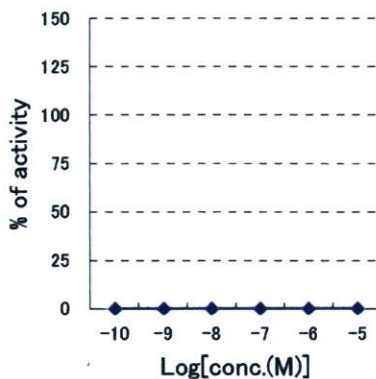
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



**AR antagonist assay**

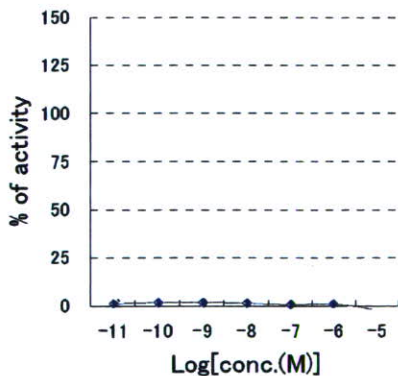
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



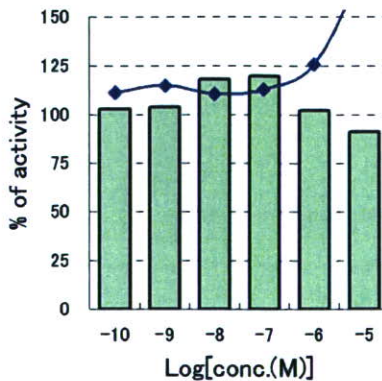
**TRβ-RXR agonist assay**

LOG[conc.(M)]	luc
-5	-2.3
-6	0.9
-7	0.7
-8	1.6
-9	1.7
-10	1.7
-11	1.1



**TRβ-RXR antagonist assay**

LOG[conc.(M)]	luc	ren
-5	175	91
-6	126	102
-7	113	119
-8	110	118
-9	115	104
-10	111	103

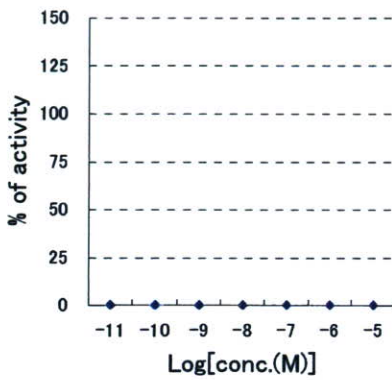


sample No.  
chemical name  
CAS.

TR244  
Isobutyric acid, 3,7-dimethyl-2,6-octadienyl ester, (Z)-  
2345-24-6

**AR agonist assay**

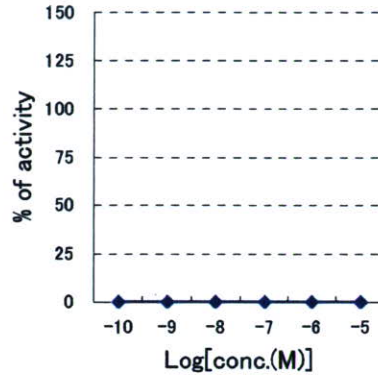
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



**AR antagonist assay**

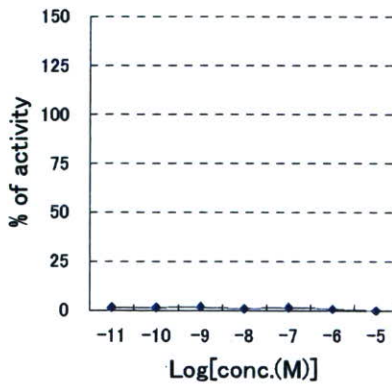
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



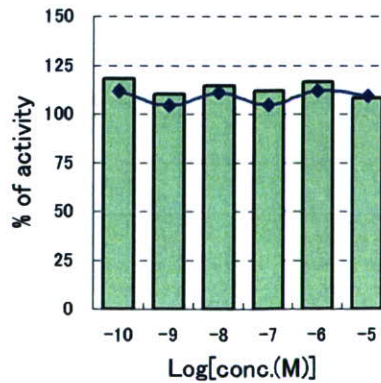
**TRβ-RXR agonist assay**

LOG[conc.(M)]	luc
-5	0.0
-6	0.7
-7	1.5
-8	0.9
-9	1.8
-10	1.6
-11	1.5



**TRβ-RXR antagonist assay**

LOG[conc.(M)]	luc	ren
-5	109	108
-6	112	116
-7	104	112
-8	111	114
-9	104	110
-10	112	118

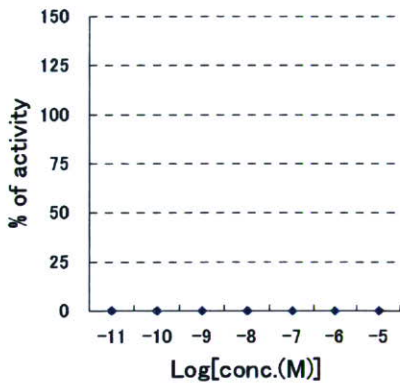


sample No.  
chemical name  
CAS.

TR245  
Cinnamaldehyde, .alpha.-pentyl-, dimethyl acetal  
91-87-2

**AR agonist assay**

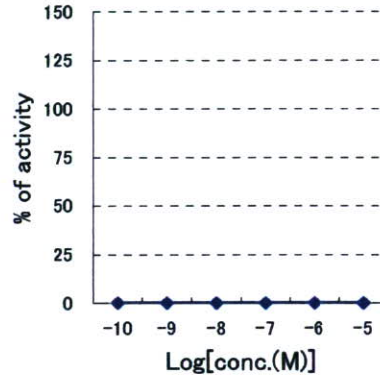
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



**AR antagonist assay**

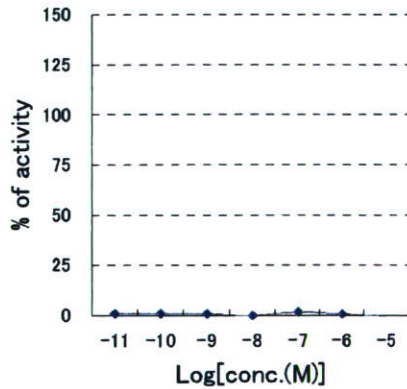
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



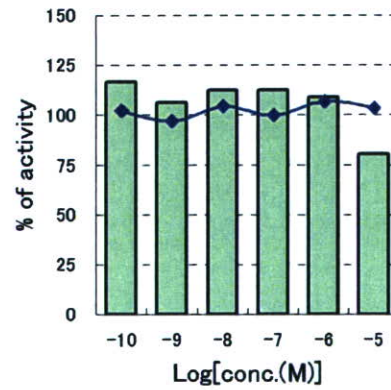
**TRβ-RXR agonist assay**

LOG[conc.(M)]	luc
-5	-0.3
-6	0.5
-7	1.6
-8	0.1
-9	0.8
-10	0.9
-11	1.0



**TRβ-RXR antagonist assay**

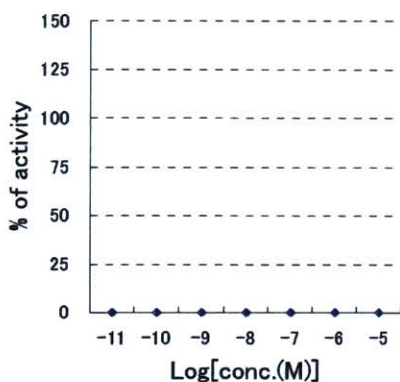
LOG[conc.(M)]	luc	ren
-5	104	80
-6	107	109
-7	100	113
-8	104	112
-9	97	107
-10	102	117



sample No. TR246  
 chemical name 2,4,6-TRIS((DIMETHYLAMINO)METHYL)PHENOL  
 CAS. 90-72-2

**AR agonist assay**

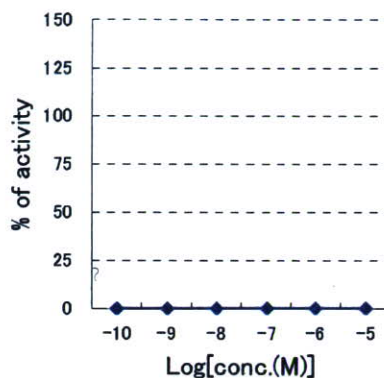
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



**AR antagonist assay**

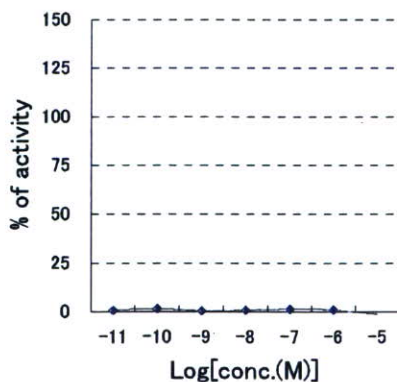
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



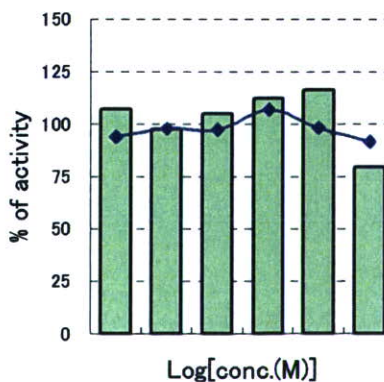
**TRβ-RXR agonist assay**

LOG[conc.(M)]	luc
-5	-1.4
-6	0.9
-7	1.2
-8	0.6
-9	0.3
-10	1.5
-11	0.6



**TRβ-RXR antagonist assay**

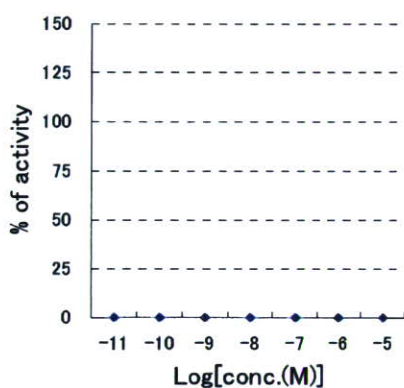
LOG[conc.(M)]	luc	ren
-5	91	79
-6	98	116
-7	107	112
-8	97	105
-9	98	97
-10	94	107



sample No. TR247  
 chemical name Benzoic acid, p-(dimethylamino)-  
 CAS. 619-84-1

**AR agonist assay**

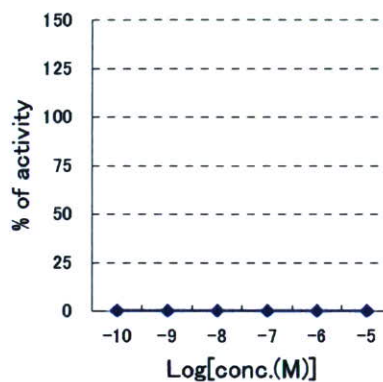
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



**AR antagonist assay**

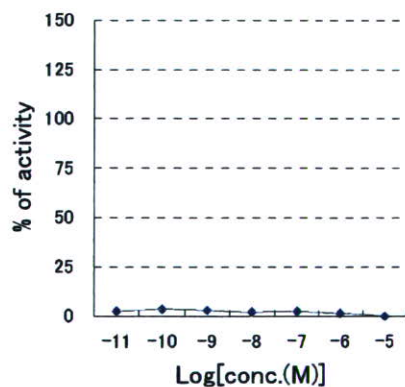
LOG{conc.(M)}	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



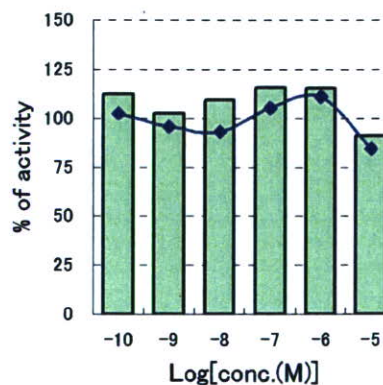
**TRβ-RXR agonist assay**

LOG[conc.(M)]	luc
-5	0.1
-6	1.6
-7	2.2
-8	2.1
-9	2.9
-10	3.4
-11	2.3



**TRβ-RXR antagonist assay**

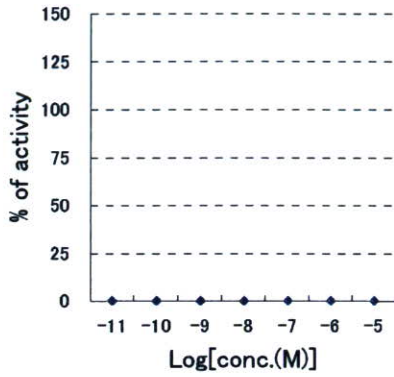
LOG{conc.(M)}	luc	ren
-5	84	91
-6	111	115
-7	105	116
-8	93	109
-9	95	102
-10	102	112



sample No. TR248  
 chemical name RCL S12,616-0  
 CAS. NA

**AR agonist assay**

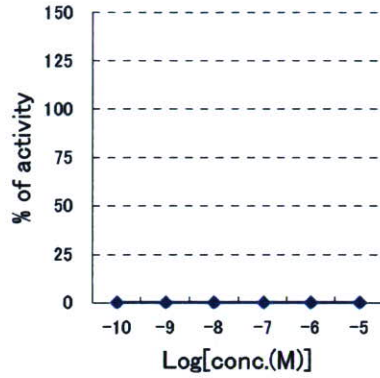
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



**AR antagonist assay**

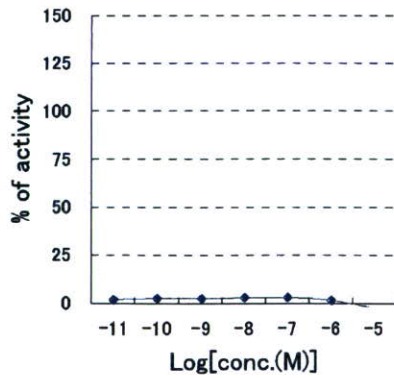
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



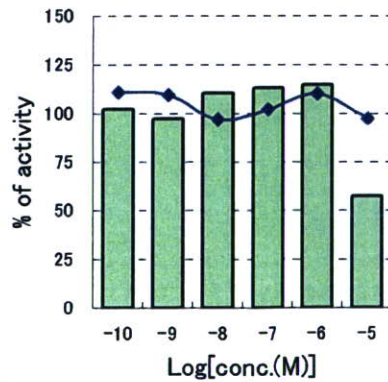
**TRβ-RXR agonist assay**

LOG[conc.(M)]	luc
-5	-2.5
-6	1.4
-7	3.0
-8	3.0
-9	2.5
-10	2.5
-11	1.9



**TRβ-RXR antagonist assay**

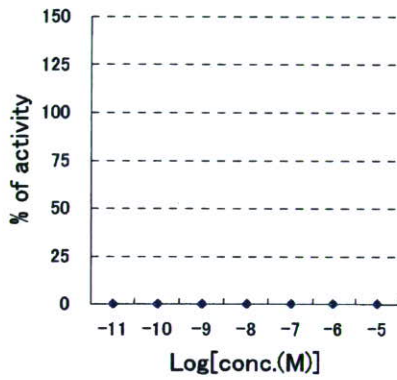
LOG[conc.(M)]	luc	ren
-5	97	58
-6	110	115
-7	102	113
-8	97	110
-9	109	97
-10	111	102



sample No. TR249  
 chemical name Genistein 4',7-dimethyl ether  
 CAS. 34086-51-6

**AR agonist assay**

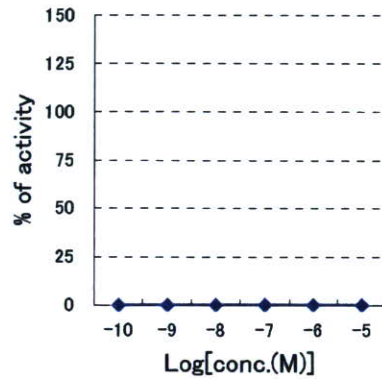
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



**AR antagonist assay**

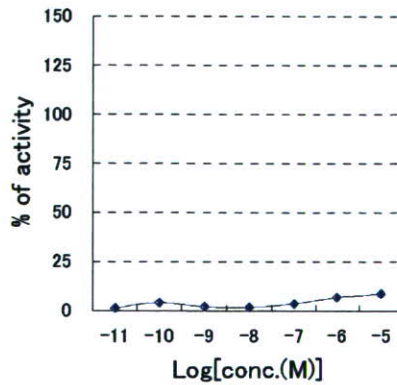
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



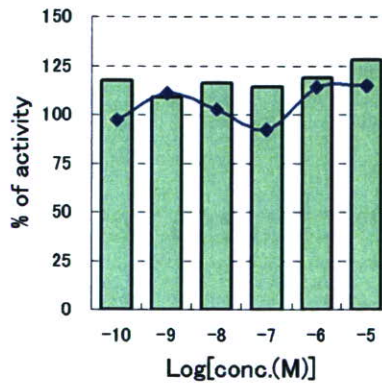
**TRβ-RXR agonist assay**

LOG[conc.(M)]	luc
-5	8.4
-6	6.7
-7	3.7
-8	1.9
-9	2.2
-10	4.2
-11	1.6



**TRβ-RXR antagonist assay**

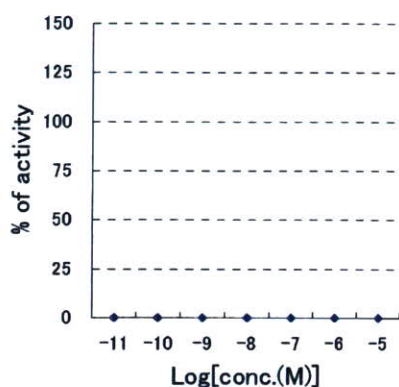
LOG[conc.(M)]	luc	ren
-5	114	128
-6	114	119
-7	92	114
-8	102	116
-9	111	109
-10	97	118



sample No. TR250  
 chemical name 3,3'-Dichlorobenzidine  
 CAS. 91-94-1

**AR agonist assay**

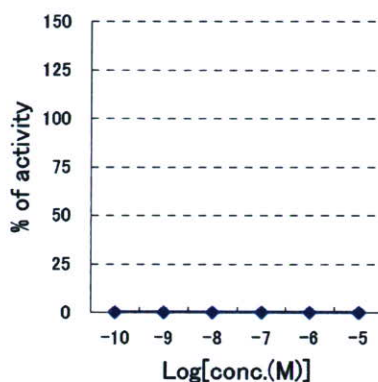
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



**AR antagonist assay**

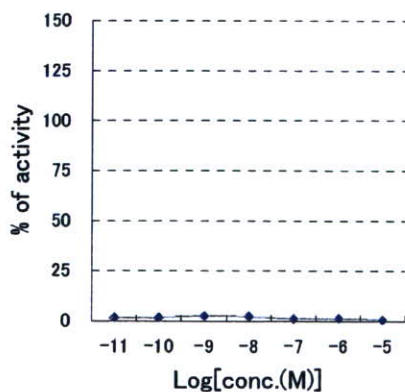
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



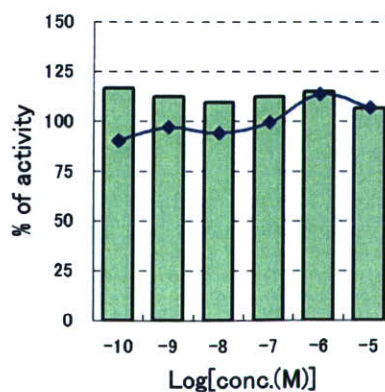
**TRβ-RXR agonist assay**

LOG[conc.(M)]	luc
-5	0.7
-6	1.6
-7	1.1
-8	2.2
-9	2.6
-10	1.8
-11	1.8



**TRβ-RXR antagonist assay**

LOG[conc.(M)]	luc	ren
-5	107	107
-6	114	115
-7	100	112
-8	94	110
-9	97	112
-10	90	117



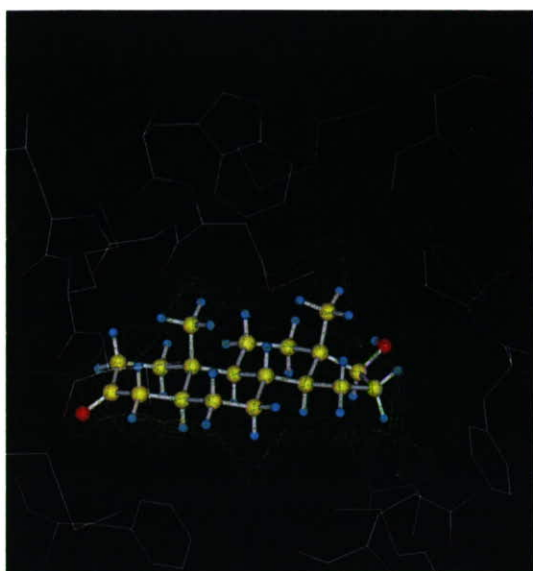


厚生労働科学研究費補助金（化学物質リスク研究事業）  
生体の作用点、特に核内受容体及び関連転写因子群に着目した化学物質の  
毒性発現機構の解明や毒性予測手法の開発を行う研究

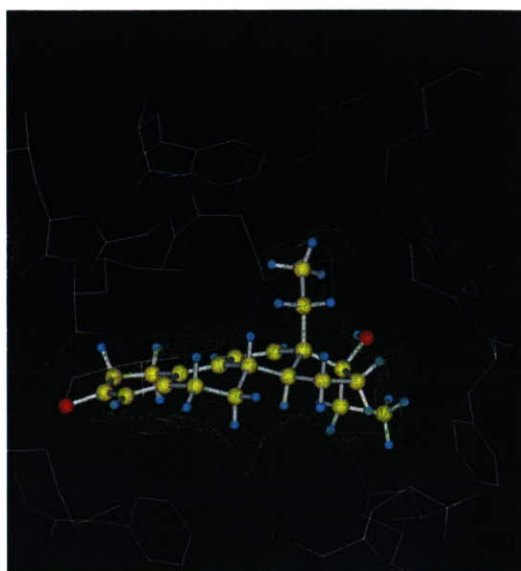
総括研究報告書 図表

添付 3

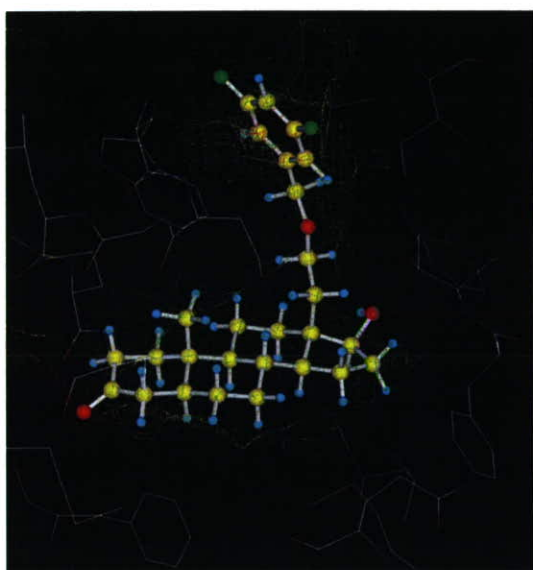
(1) - 3. 核内受容体ドッキングモデルによる *in silico* スクリーニング系の研究 図表



(a)



(b)



(c)

図1 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。(a) 1t63。結合リガンドはDHT。(b) 2amb。結合リガンドはTHG。(c) 2pnu。結合リガンドはEM5744。

表 1. 化学物質の ER $\alpha$  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		