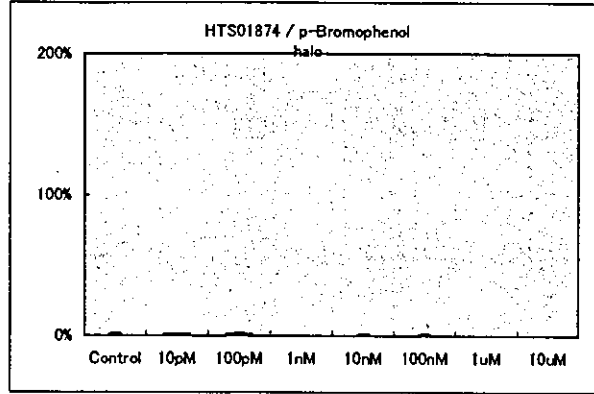


ER $\beta$  / HeLa

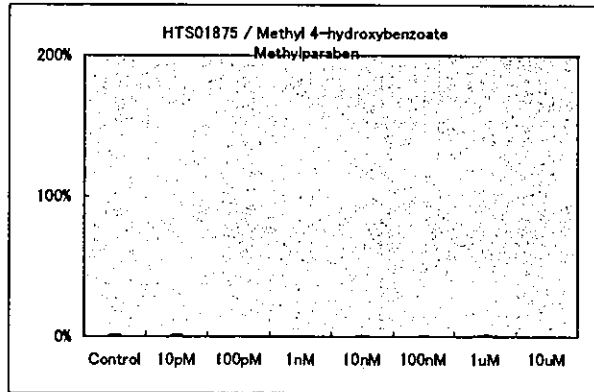
HTS01874  
p-Bromophenolhalo

PC50 (pM): -



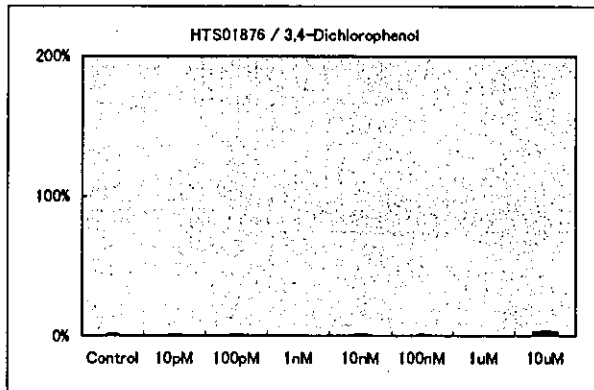
HTS01875  
Methyl 4-hydroxybenzoateMethylparaben

PC50 (pM): -



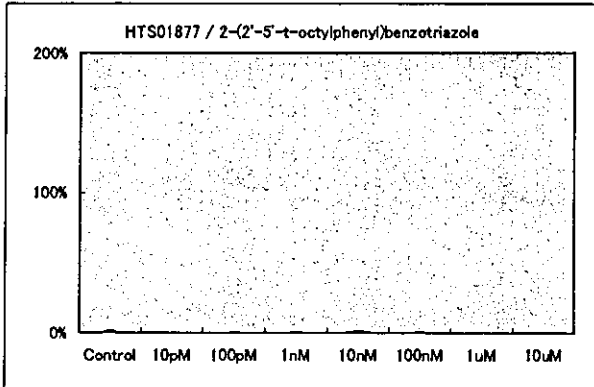
HTS01876  
3,4-Dichlorophenol

PC50 (pM): -



HTS01877  
2-(2'-5'-t-octylphenyl)benzotriazole

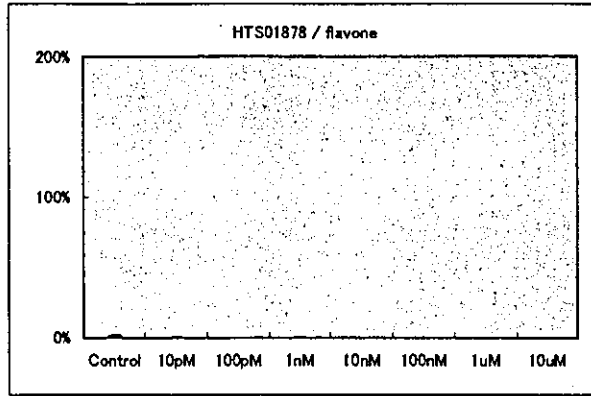
PC50 (pM): -



ER $\beta$  / HeLa

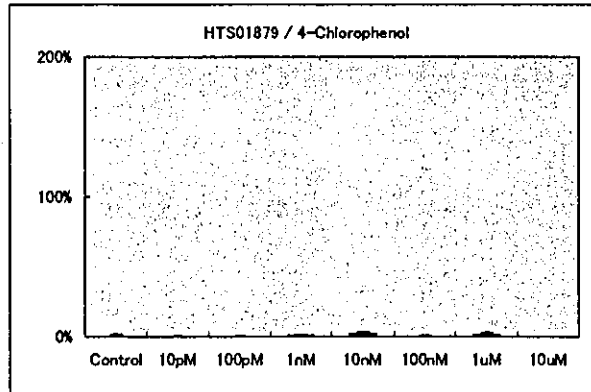
HTS01878  
flavone

PC50 (pM): -



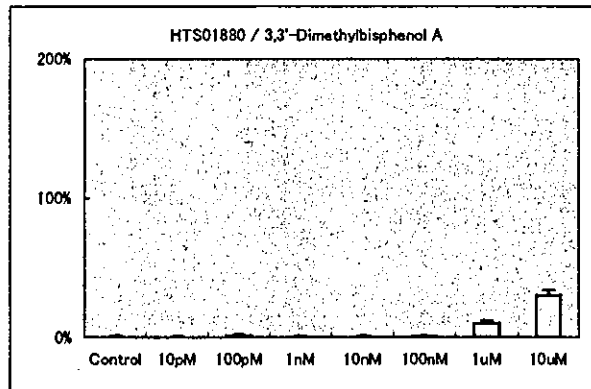
HTS01879  
4-Chlorophenol

PC50 (pM): -



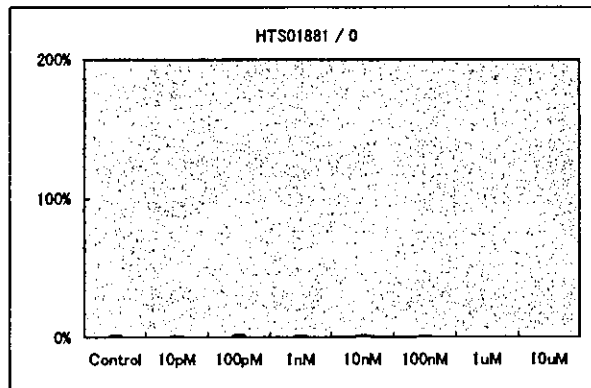
HTS01880  
3,3'-Dimethylbisphenol A

PC50 (pM): -



HTS01881  
Glyoxal bis(2-hydroxyanil)

PC50 (pM): -



レポーター遺伝子導入培養細胞株を用いた TR、AR 作用物質超高速分析法  
に関する試験研究  
(大塚製薬ライフサイエンス事業部EDC分析センター委託業務)

スクリーニングデータ一覧

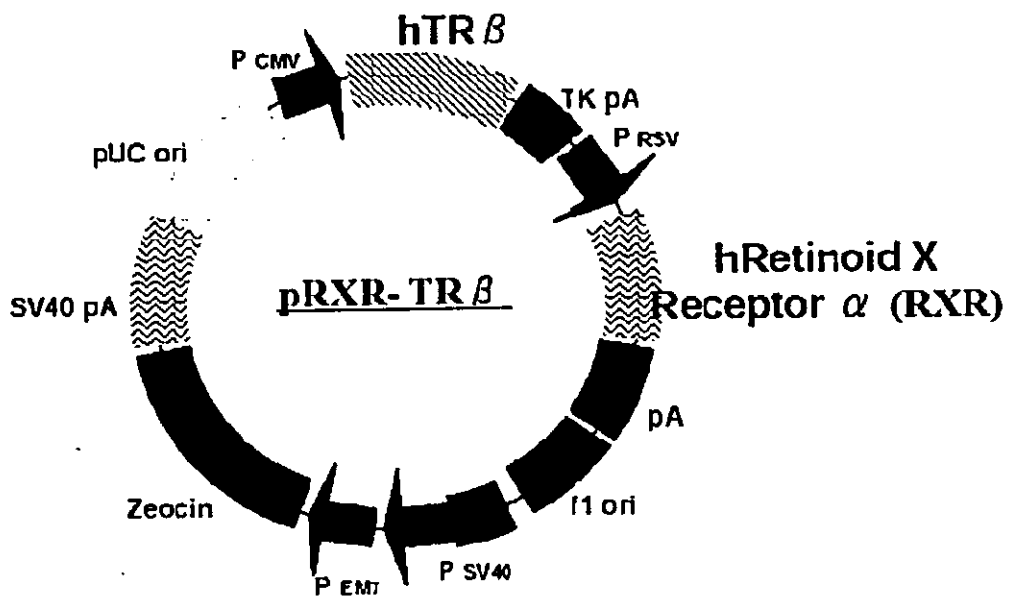


Figure 1 TRβとRXRの2種類の受容体を共発現するベクター (pRXR-TRβ)

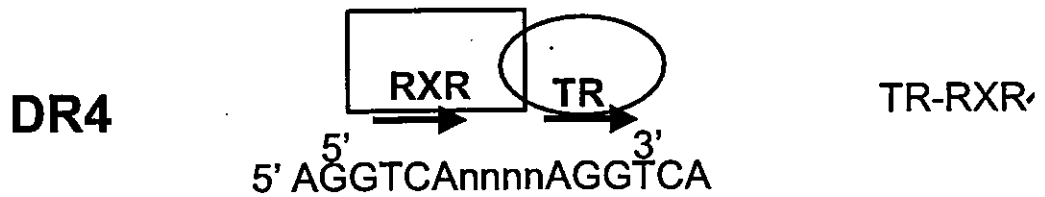
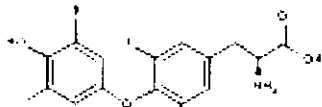
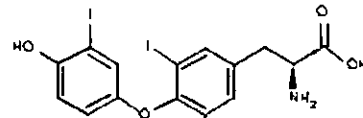


Figure 2 DR4の構造



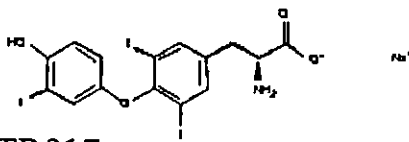
TR012

D-thyroxine  
EC<sub>50</sub>: 2.3x10<sup>-7</sup> M



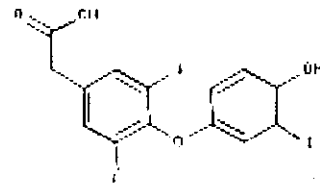
TR020

Liothyronine (T3)  
EC<sub>50</sub>: 6.4x10<sup>-9</sup> M



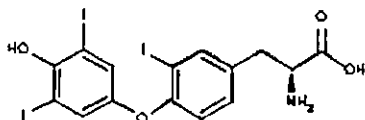
TR017

Liothyronine sodium  
EC<sub>50</sub>: 6.7x10<sup>-9</sup> M



TR025

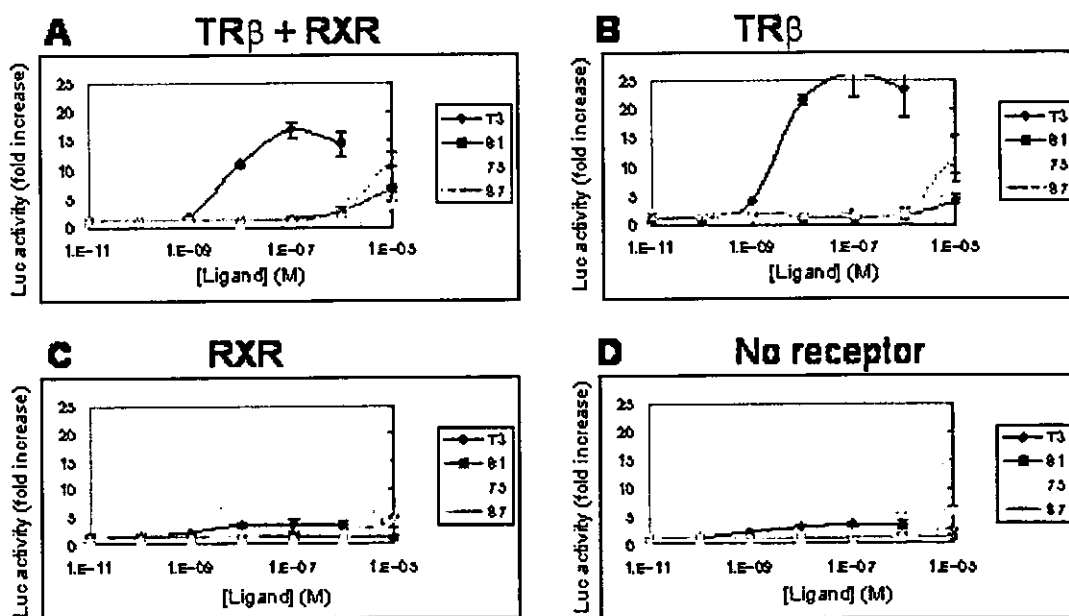
Tiratricol  
EC<sub>50</sub>: 7.3x10<sup>-12</sup> M



TR018

L-thyroxine  
EC<sub>50</sub>: 5.6x10<sup>-8</sup> M

Figure 3  
TRアゴニストアッセイポジティブ化合物  
(平成15年度測定分)



**Figure 4 TR agonist assay (平成 16 年度分)**  
**A TR $\beta$ 、RXR 共発現系**    **B TR $\beta$  単独発現系**  
**C RXR 単独発現系**        **D 受容体なし**  
**Response element はいずれも TREDR4 を用いた。**

Table 1 AR アゴニストアッセイの測定結果

AssayID	Name	CAS	PC 50	PC 10
AT096	Androst-4-ene-3,17-dione	000063-05-8	5.49E-11	1.46E-11
AT090	Stanolone	000521-18-6	8.36E-11	1.59E-11
AR052	Testosterone, methyl	000058-18-4	3.75E-10	6.48E-11
AT065	D(-)-Norgestrel	000797-63-7	5.80E-10	1.20E-10
AT098	Norethindrone	000068-22-4	2.03E-09	2.15E-10
AT092	Progesterone	000057-83-0	-	8.43E-08
AT011	Biochanin A	000491-80-5	-	5.67E-07
AT017	4-Hydroxy-trans-stilbene	006554-98-9	-	5.82E-07
AT009	flavone	000525-82-6	-	1.48E-06
AR008	flavone	000525-82-6	-	1.67E-06
AR021	4-hydroxychalcone	020426-12-4	-	1.78E-06
AR019	chalcone	000094-41-7	-	2.73E-06
AT089	3-Methylcholanthrene	000056-49-5	-	2.97E-06
AT001	4'-hydroxyflavanone	006515-37-3	-	3.44E-06
AR010	4'-hydroxychalcone	002657-25-2	-	4.30E-06
AT097	2,4,4'-Trihydroxybenzophenone	001470-79-7	-	4.98E-06
AT010	kaempferol	000520-18-3	-	5.86E-06
AT086	Avobenzene	070356-09-1	-	6.20E-06

Table 2 AR アンタゴニストアッセイの測定結果

AssayID	Name	CAS	IC50	IC40	IC30	IC20
AR004	6-hydroxyflavanone	004250-77-5	4.88E-06			
AR005	aurin	000603-45-2	3.13E-06			
AR006	isoeugenol	000097-54-1				6.17E-06
AR007	diisobutyl adipate	000141-04-8				
AR008	flavone	000525-82-6			8.97E-06	
AR012	2,4-dihydroxybenzophenone	000131-56-6		9.20E-06		
AR015	4-hydroxybiphenyl	000092-69-3	2.07E-06			
AR018	triphenyl phosphate	000115-86-6		8.91E-06		
AR025	4-chloro-2-methyl phenol	001570-64-5				4.59E-06
AT003	p-n-pentylphenol	014938-35-3		9.16E-06		
AT004	p-n-hexylphenol	002446-69-7				6.79E-06
AT008	methoxychlor	000072-43-5	8.22E-06			
AT010	flavone	000525-82-6	8.11E-06			
AT011	kaempferol	000520-18-3				5.97E-06
AT014	Phenol, 4,4'-(2,2,2-trichloroethylidene)bis-	002971-36-0	3.40E-07			
AT016	triphenylethylene	000058-72-0		6.89E-06		
AT017	4-(Phenylmethyl)phenol	000101-53-1	4.86E-06			
AT020	Methyl 4-hydroxybenzoateMethylparaben	000099-76-3	4.63E-06			
AR051	vinclozolin	050471-44-8	4.48E-07			
AR055	flutamide	013311-84-7	1.40E-06			
AT063	p-Phenylenediamine, N,N-diphenyl-	000074-31-7	6.65E-06			
AT068	alpha-Naphtholphthalein*	000596-01-0	2.05E-06			
AT070	Phenolphthalol	000081-92-5	2.44E-06			
AT074	Benzophenone, 2-hydroxy-4-methoxy-	000131-57-7				7.33E-06
AT076	Di-n-propyl phthalate	000131-16-8				7.08E-06
AT080	Pyridaben	096489-71-3		6.82E-06		
AT087	3,3'-Dimethyl-4,4'-Biphenyl	059517-19-0	3.52E-06			
AT092	Progesterone	000057-83-0	6.70E-08			
AT093	4,4'-(1,3-Dimethylbutylidene)diphenyl	006807-17-6	3.04E-06			
AT095	4-(1-Indanyl)phenol	005402-37-9	1.63E-06			
AT097	2,4,4'-Trihydroxybenzophenone	001470-79-7	8.83E-07			
AT098	Norethindrone	000068-22-4			7.79E-06	

\*: 細胞毒性 15%以上

平成15年度 スクリーニングデータ



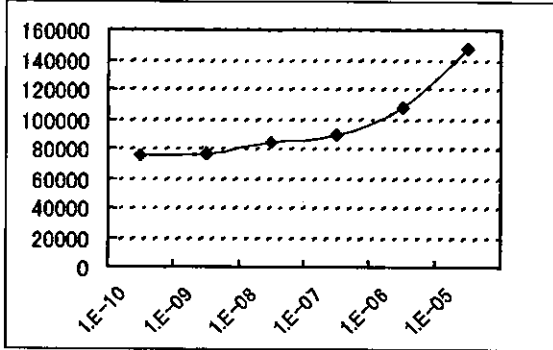
## TR assay

### AT001

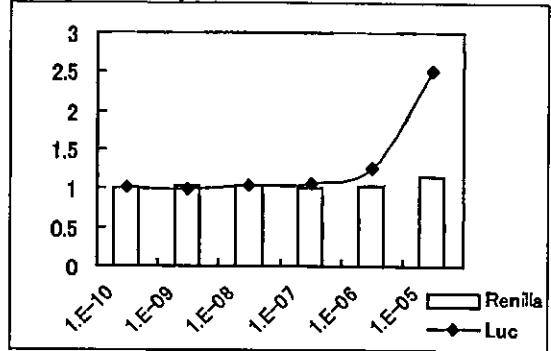
4'-hydroxyflavanone

CAS No. 006515-37-3

Agonist assay



Antagonist assay

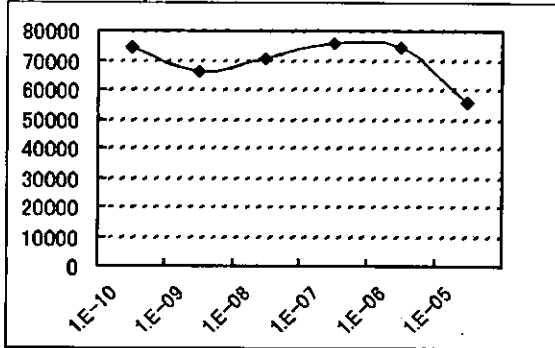


### AT002

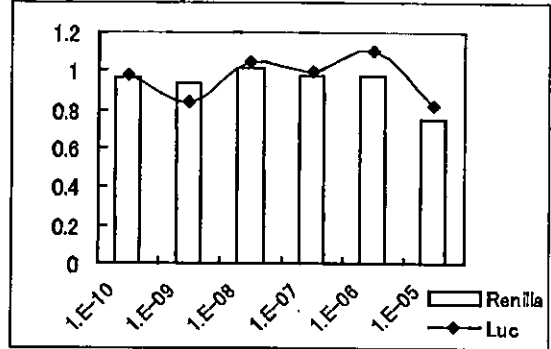
p-n-pentylphenol

CAS No. 014938-35-3

Agonist assay



Antagonist assay

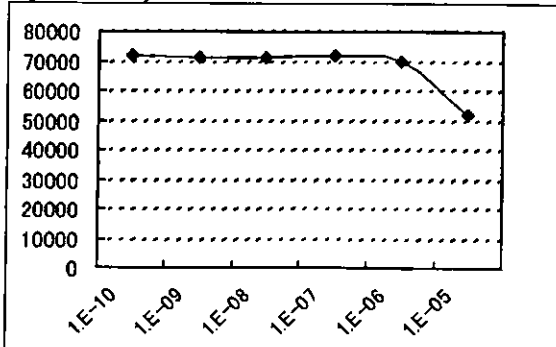


### AT003

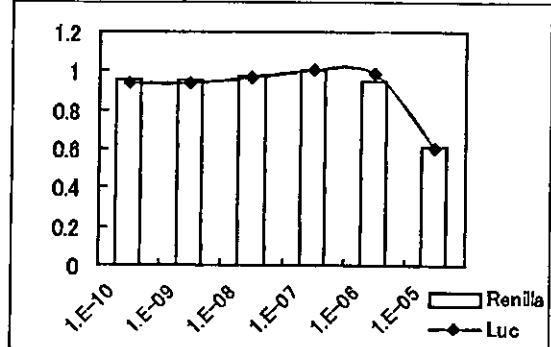
p-n-hexylphenol

CAS No. 002446-69-7

Agonist assay



Antagonist assay



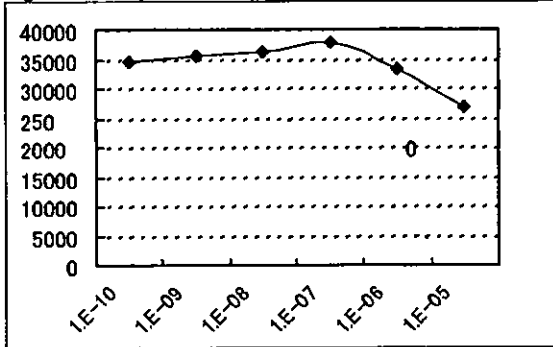
**TR assay**

**AT004**

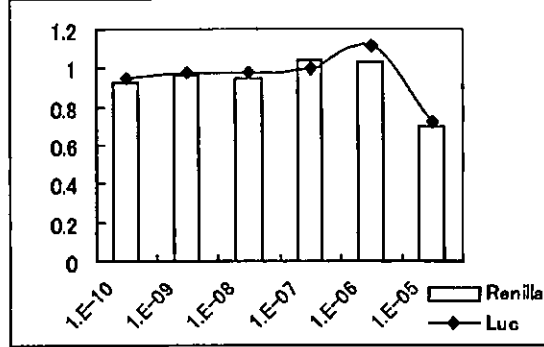
*p-n-heptylphenol*

CAS No. 001987-50-4

Agonist assay



Antagonist assay

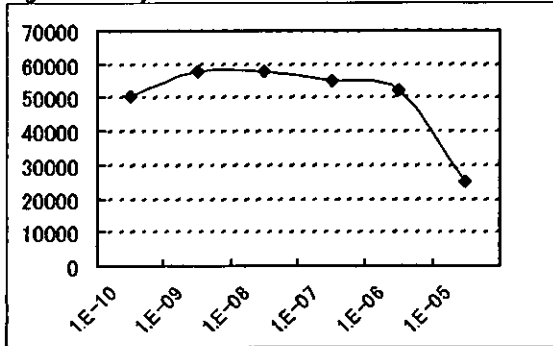


**AT005**

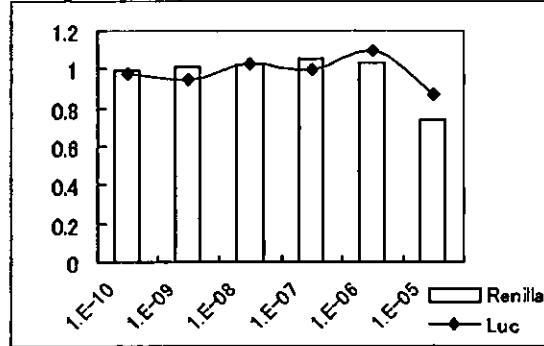
*p-n-octylphenol*

CAS No. 001806-26-4

Agonist assay



Antagonist assay

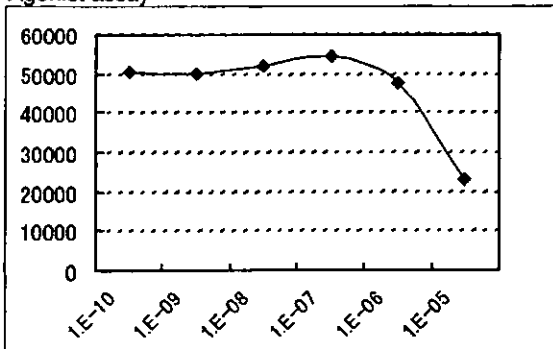


**AT006**

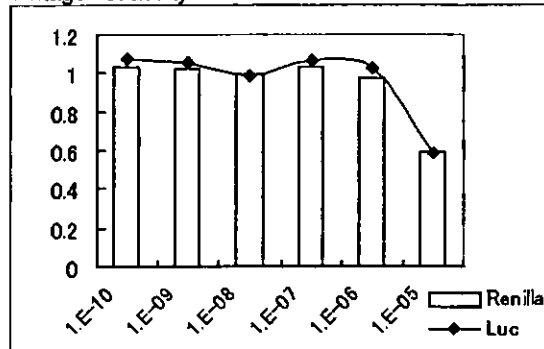
*p-n-nonylphenol*

CAS No. 000104-40-5

Agonist assay



Antagonist assay



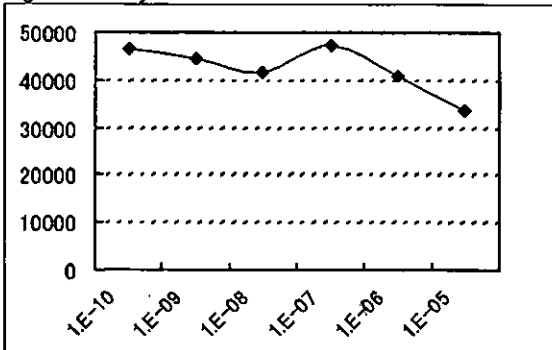
## TR assay

### AT007

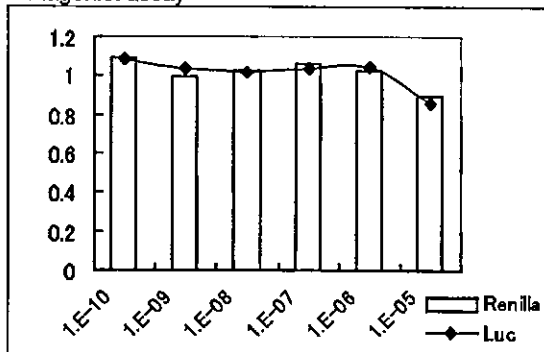
*methoxychlor*

CAS No. 000072-43-5

Agonist assay



Antagonist assay

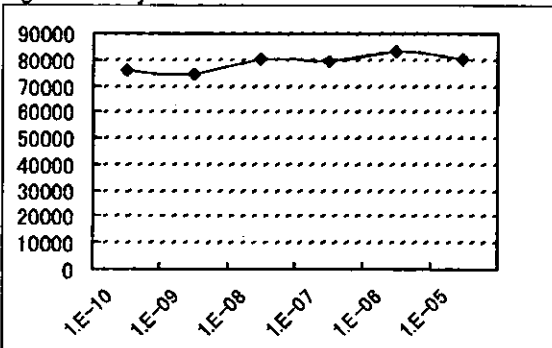


### AT008

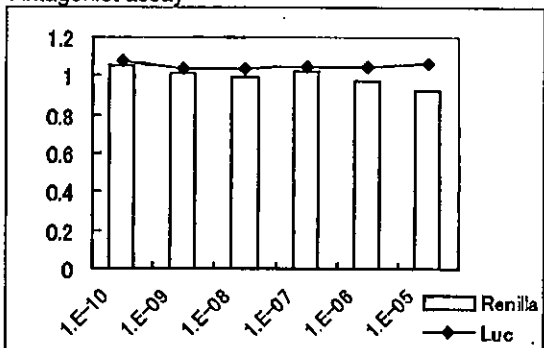
*phloretin*

CAS No. 000060-82-2

Agonist assay



Antagonist assay

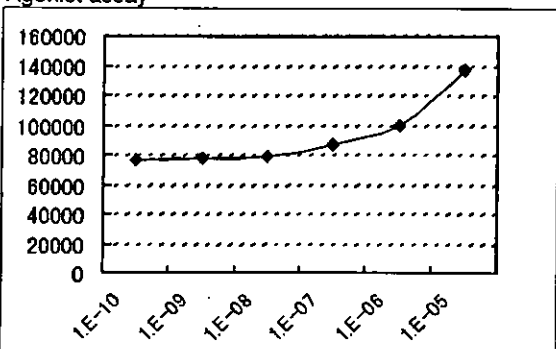


### AT009

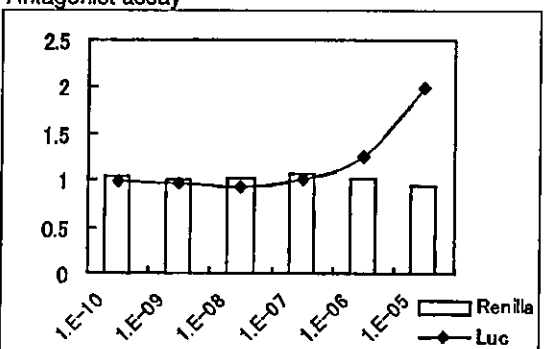
*flavone*

CAS No. 000525-82-6

Agonist assay



Antagonist assay



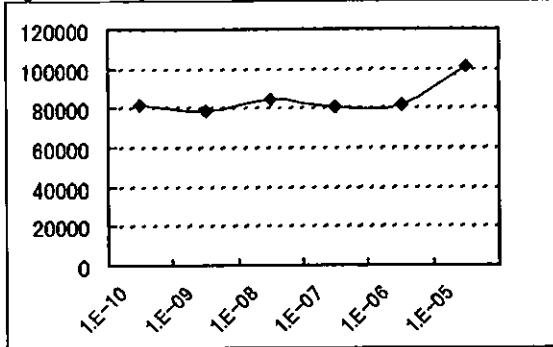
**TR assay**

**AT010**

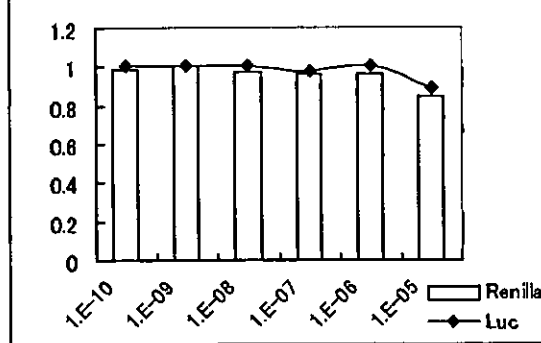
*kaempferol*

CAS No. 000520-18-3

Agonist assay



Antagonist assay

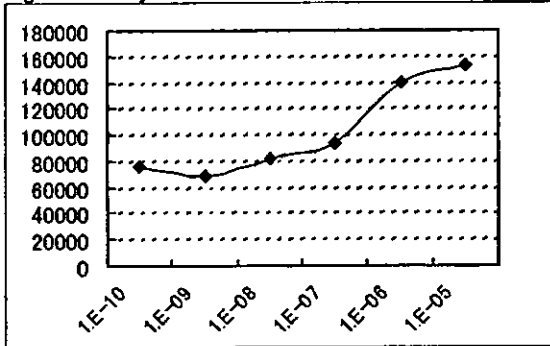


**AT011**

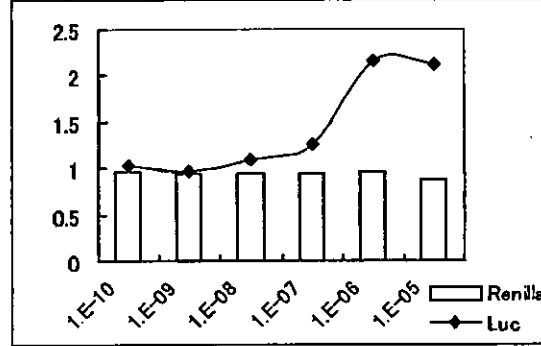
*Biochanin A*

CAS No. 000491-80-5

Agonist assay



Antagonist assay

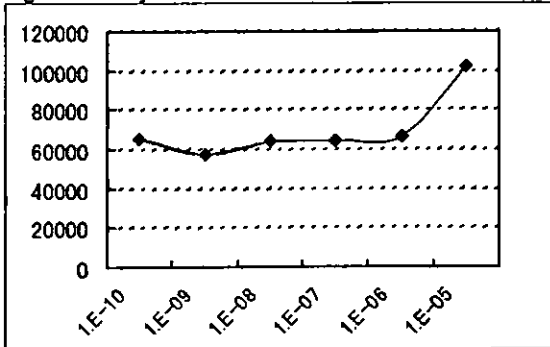


**AT012**

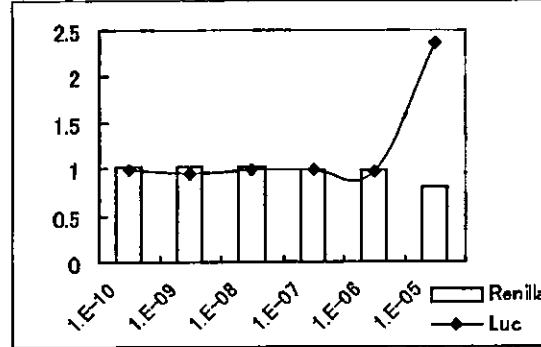
*chrysin*

CAS No. 000480-40-0

Agonist assay



Antagonist assay

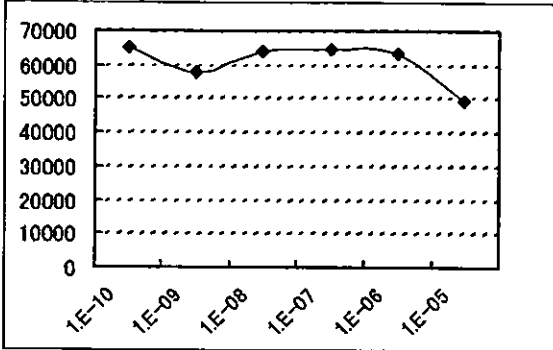


## TR assay

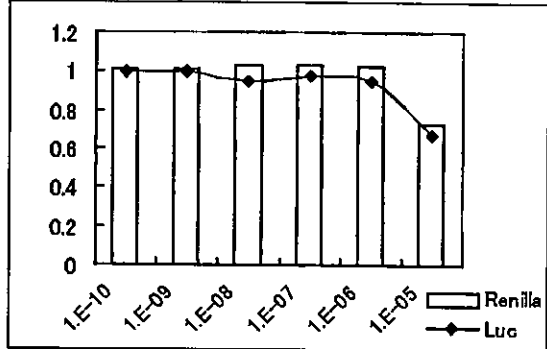
### AT013

Phenol, 4,4'-(2,2,2-trichloroethylidene)bis-  
CAS No. 002971-36-0

Agonist assay



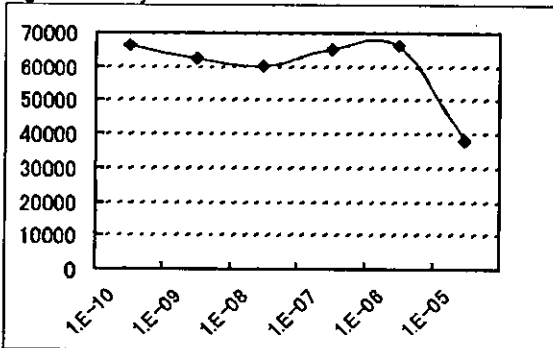
Antagonist assay



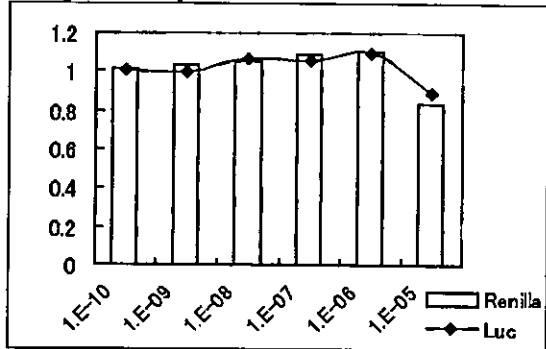
### AT014

triphenylsilanol  
CAS No. 000791-31-1

Agonist assay



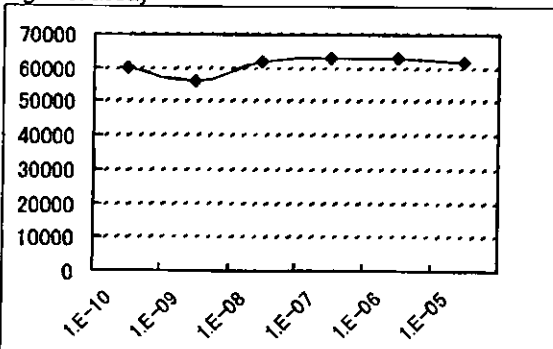
Antagonist assay



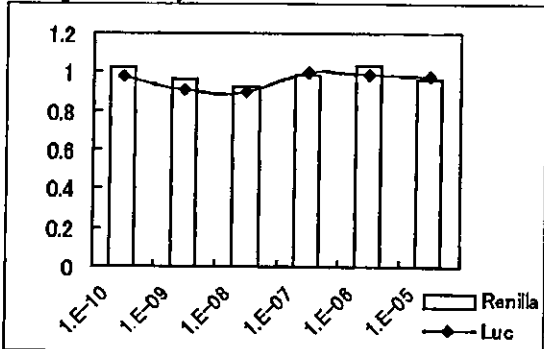
### AT015

triphenylethylene  
CAS No. 000058-72-0

Agonist assay



Antagonist assay

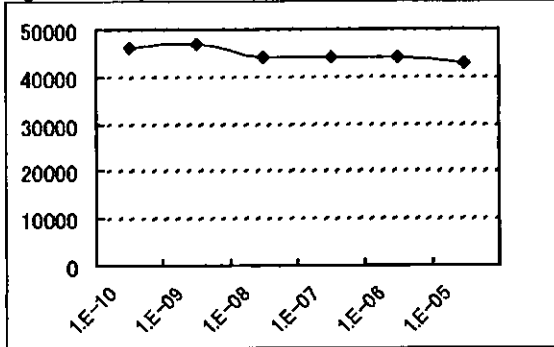


**TR assay**

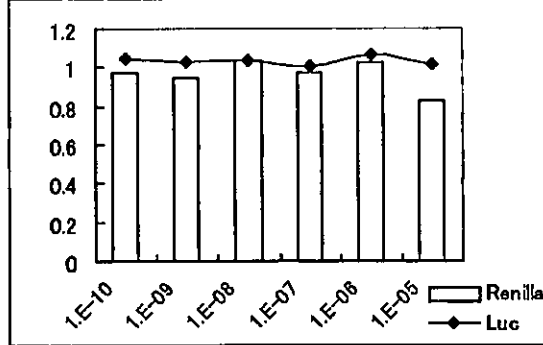
**AT016**

4-(Phenylmethyl)phenol  
CAS No. 000101-53-1

Agonist assay



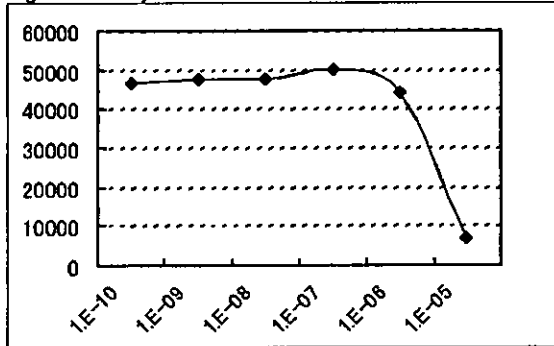
Antagonist assay



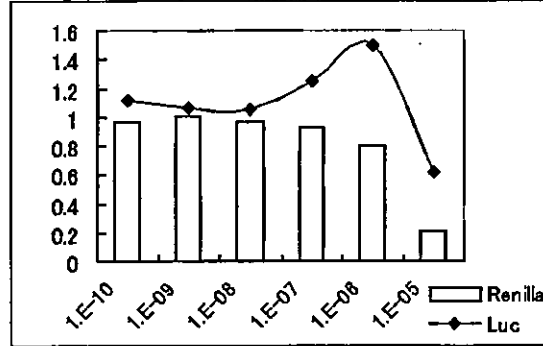
**AT017**

4-Hydroxy-trans-stilbene  
CAS No. 006554-98-9

Agonist assay



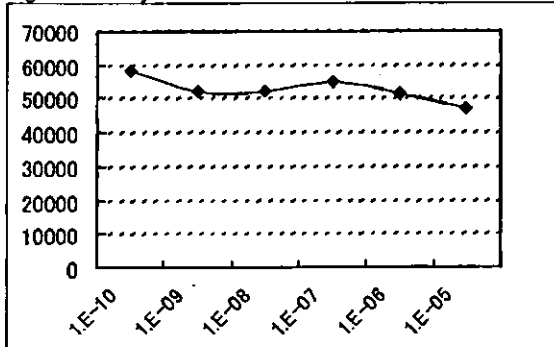
Antagonist assay



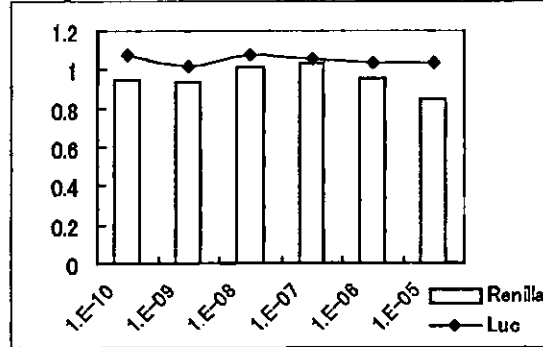
**AT018**

p-Bromophenol' halo  
CAS No. 000106-41-2

Agonist assay



Antagonist assay

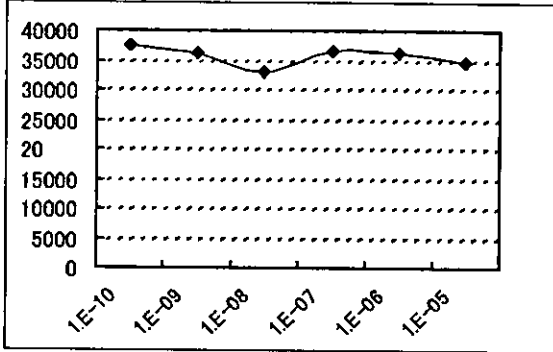


**TR assay**

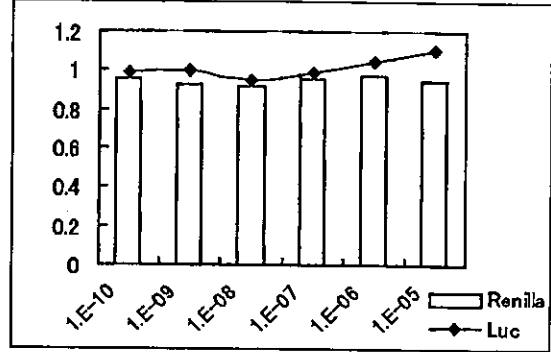
**AT019**

*Methyl 4-hydroxybenzoate* ~ Methylparaben  
CAS No. 000099-76-3

Agonist assay



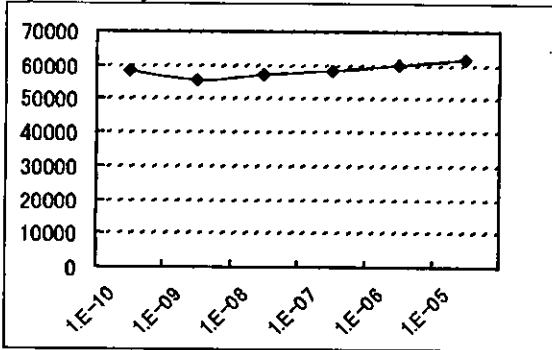
Antagonist assay



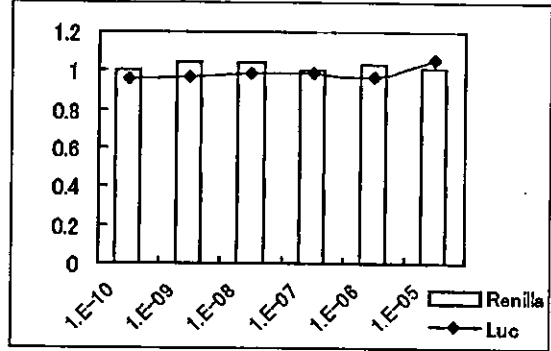
**AT020**

*Ethyl 4-hydroxybenzoate* ~ Ethylparaben  
CAS No. 000120-47-8

Agonist assay



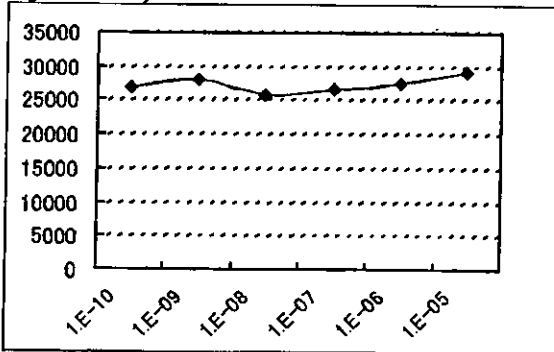
Antagonist assay



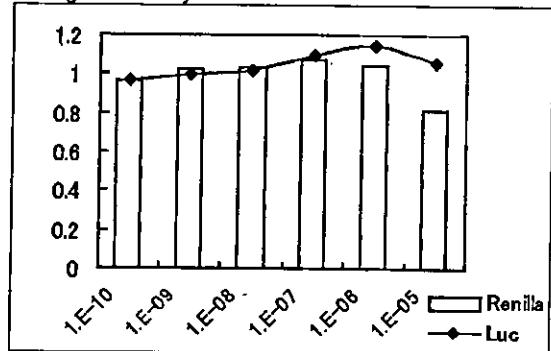
**TR001**

*flutamide*  
CAS No. 013311-84-7

Agonist assay



Antagonist assay

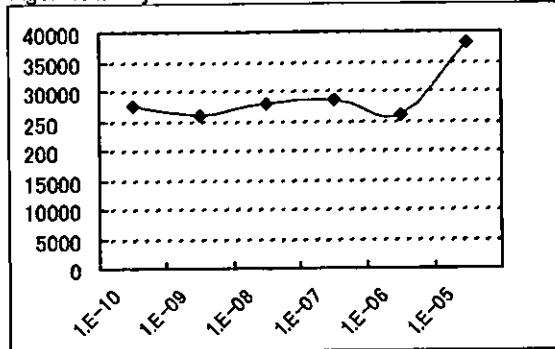


**TR assay**

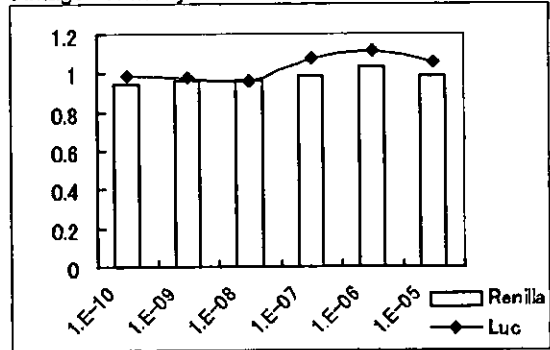
**TR002**

*Tetrabromobisphenol A*  
CAS No. 000079-94-7

Agonist assay



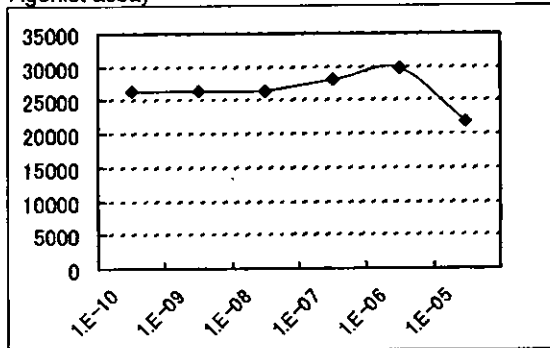
Antagonist assay



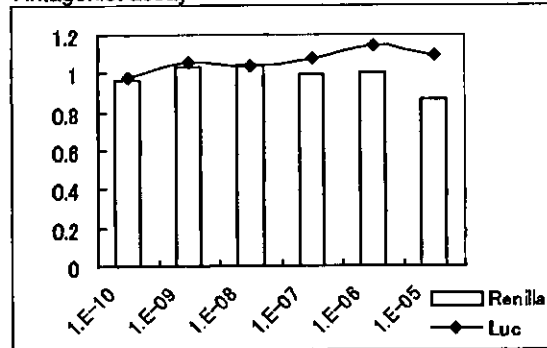
**TR003**

*Phenol, 4,4'-sulfonylbis-*  
CAS No. 000080-09-1

Agonist assay



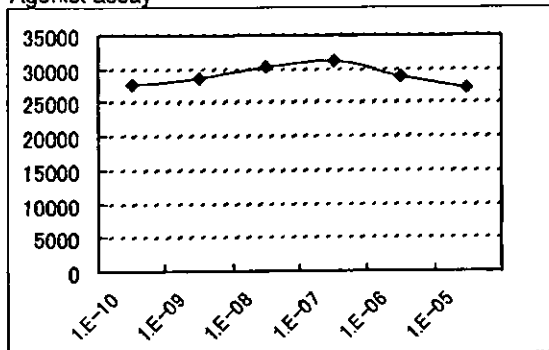
Antagonist assay



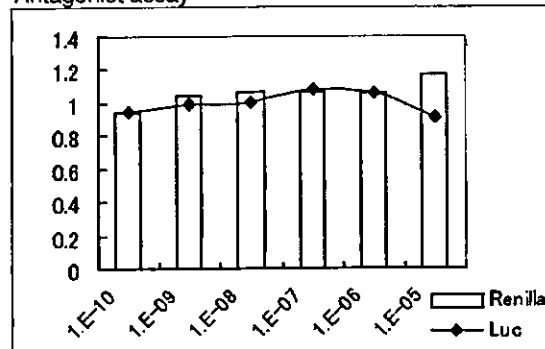
**TR004**

*2-(5-Chloro-2H-benzotriazol-2-yl)-4,6-bis(1,1-dime*  
CAS No. 003864-99-1

Agonist assay



Antagonist assay



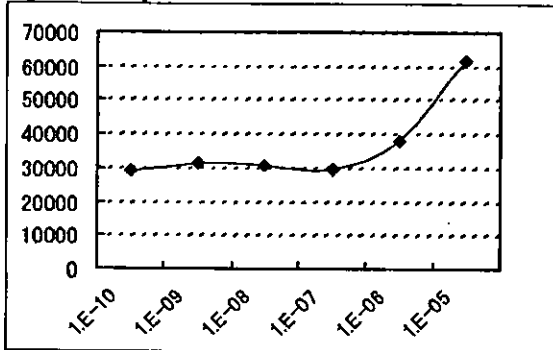


## TR assay

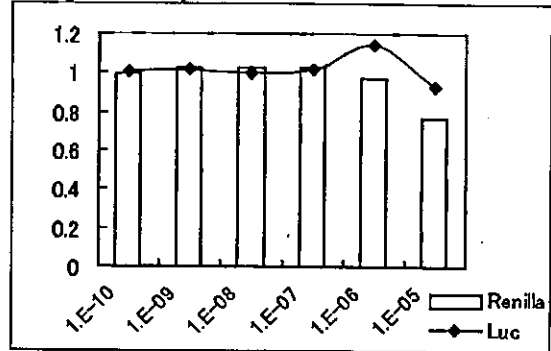
### TR005

3,3'-Dimethylbisphenol A  
CAS No. 000079-97-0

Agonist assay



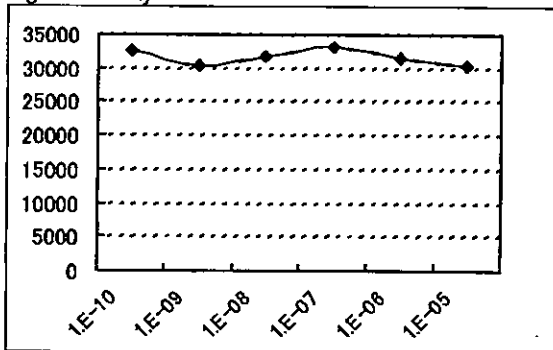
Antagonist assay



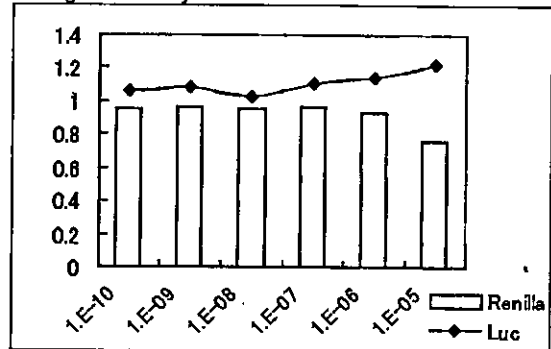
### TR006

4,4'-Methylenebis(phenol)  
CAS No. 000620-92-8

Agonist assay



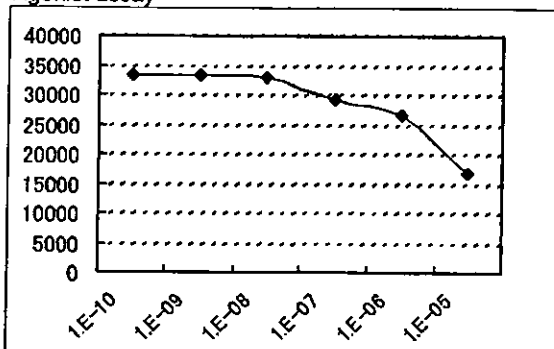
Antagonist assay



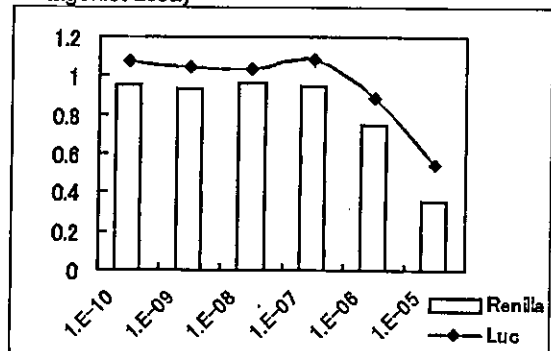
### TR007

4,4'-Dihydroxybiphenyl  
CAS No. 000092-88-6

Agonist assay



Antagonist assay



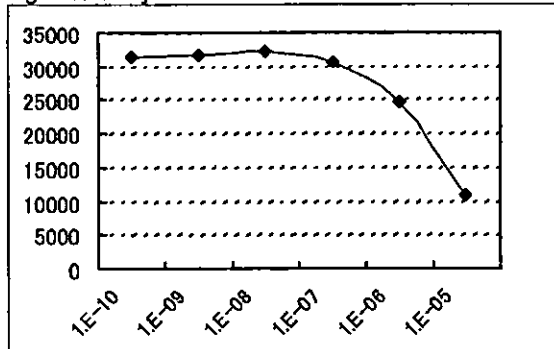
## TR assay

### TR008

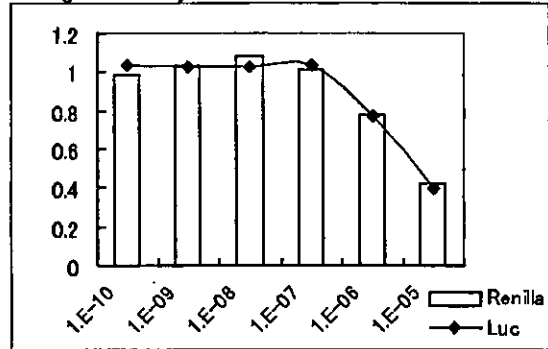
4-Phenoxyphenol

CAS No. 000831-82-3

Agonist assay



Antagonist assay

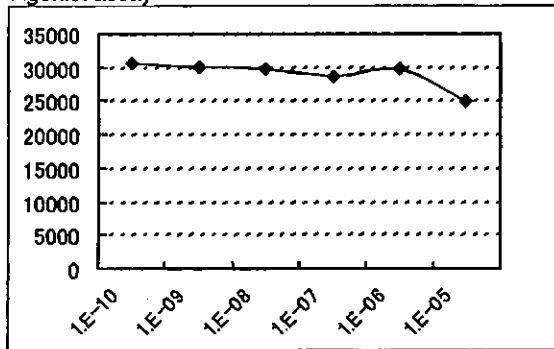


### TR009

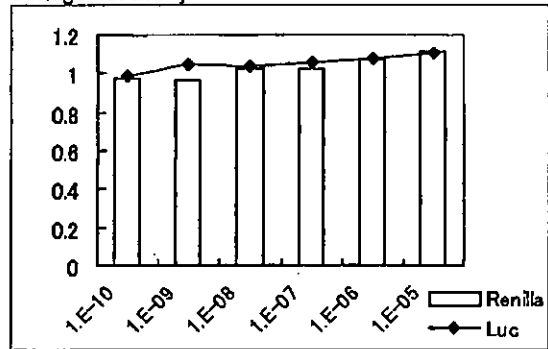
2,2-Bis(4-methylphenyl)hexafluoropropane

CAS No. 001095-77-8

Agonist assay



Antagonist assay

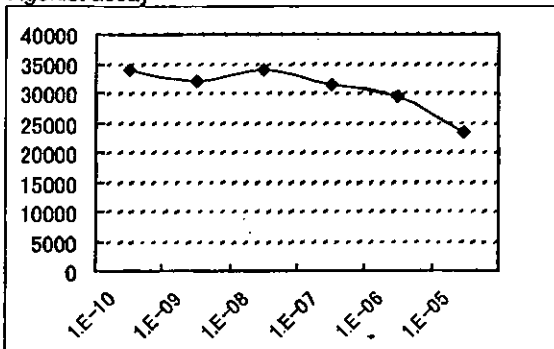


### TR010

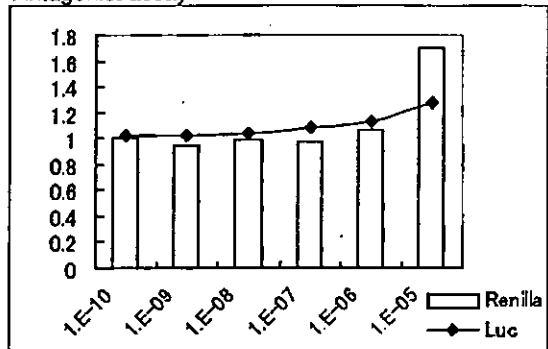
Butylbenzyl phthalate

CAS No. 000085-68-7

Agonist assay



Antagonist assay



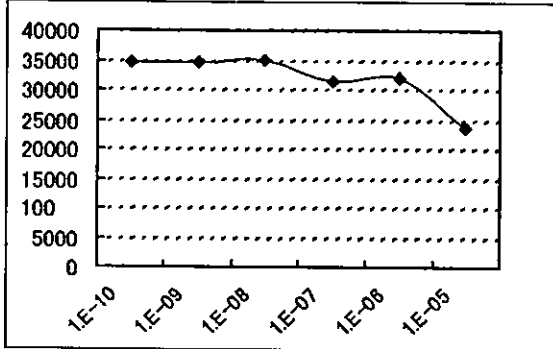
## TR assay

### TR011

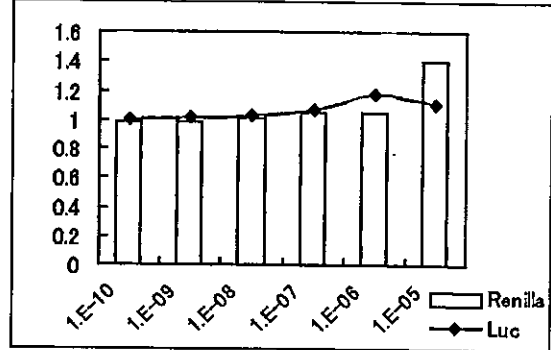
*di-n-butyl phthalate*

CAS No. 000084-74-2

Agonist assay



Antagonist assay

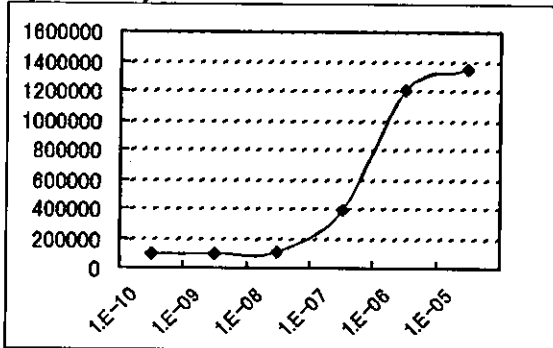


### TR012

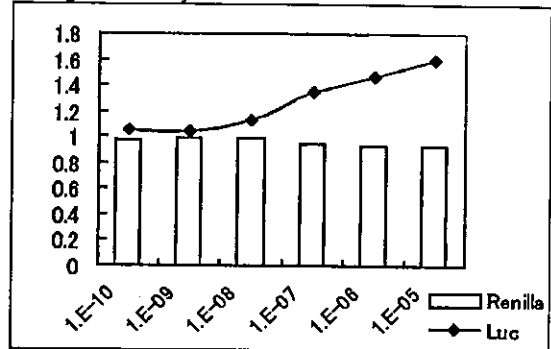
*D-thyroxine(Dextrothyroxine)*

CAS No. 000051-49-0

Agonist assay



Antagonist assay

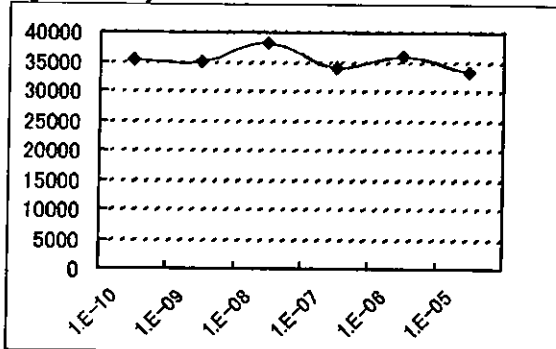


### TR013

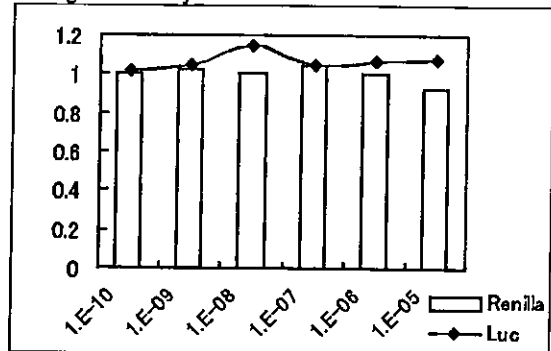
*vinclozolin*

CAS No. 050471-44-8

Agonist assay



Antagonist assay



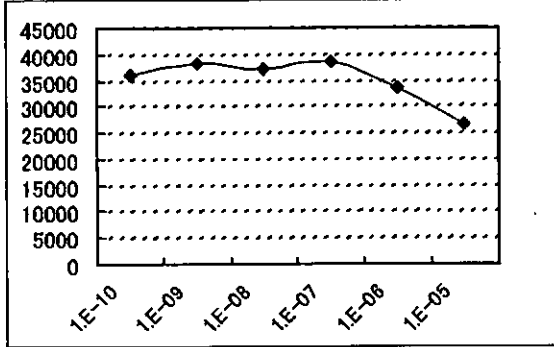
**TR assay**

**TR014**

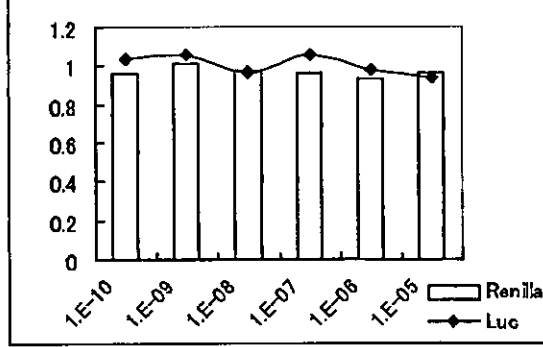
*p,p'*-DDE

CAS No. 000072-55-9

Agonist assay



Antagonist assay

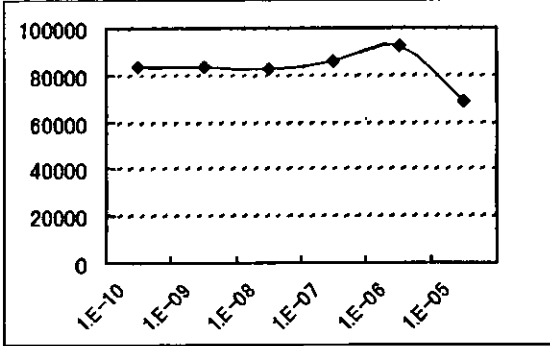


**TR015**

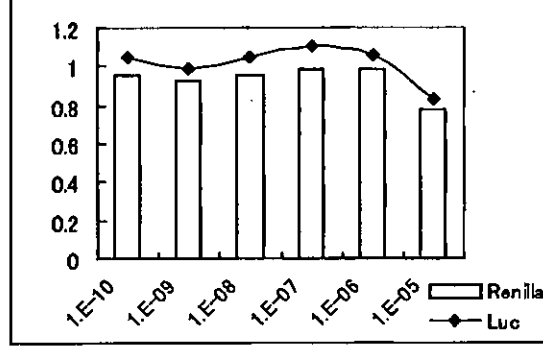
*dicofol*

CAS No. 000115-32-2

Agonist assay



Antagonist assay

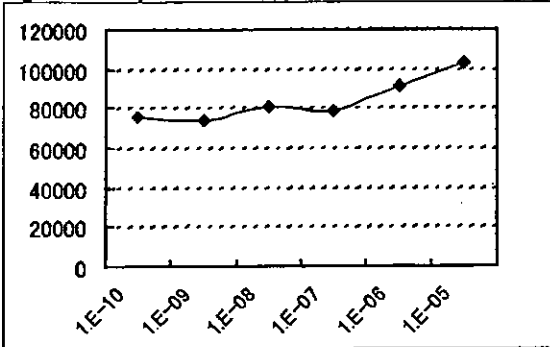


**TR016**

*linuron*

CAS No. 000330-55-2

Agonist assay



Antagonist assay

