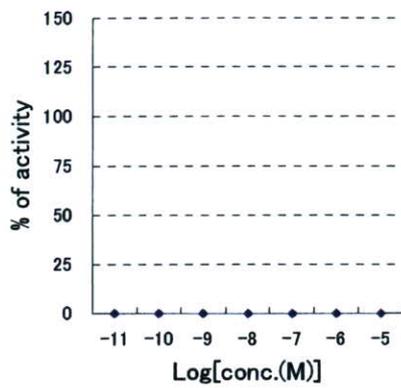


sample No. TR242
 chemical name Oxycarboxin
 CAS. 5259-88-1

AR agonist assay

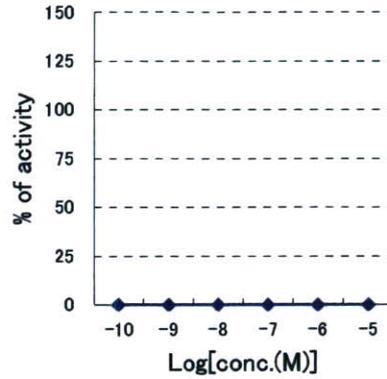
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

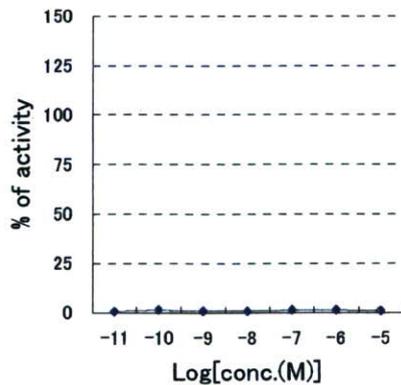
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



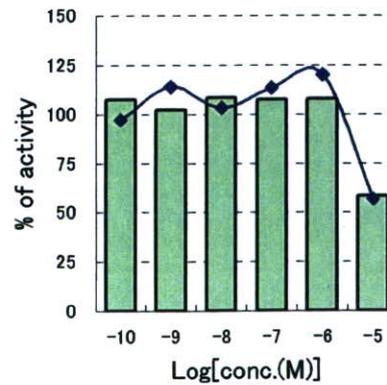
TRβ-RXR agonist assay

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

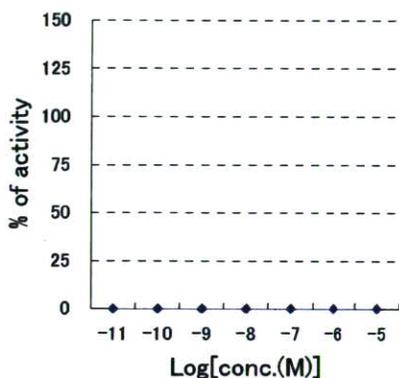
LOG[conc.(M)]	luc	ren
-5	57	58
-6	120	108
-7	113	107
-8	104	108
-9	114	102
-10	97	107



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

AR agonist assay

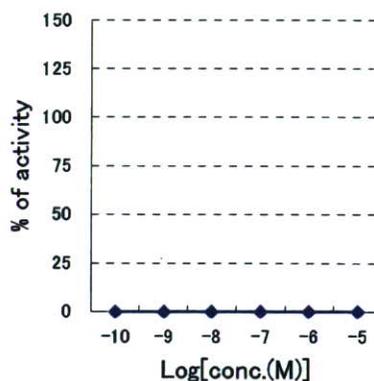
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

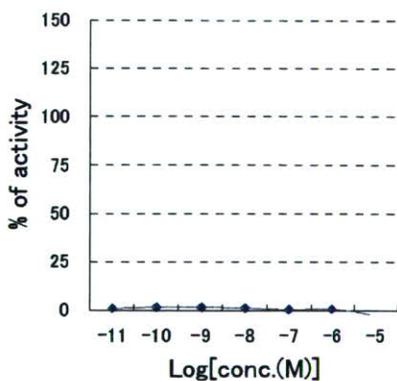
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



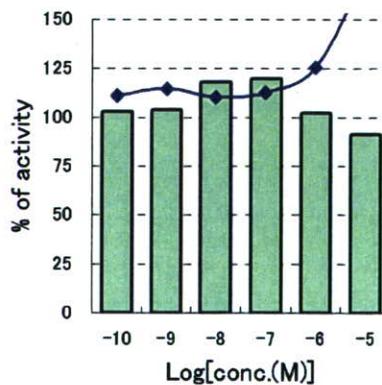
TRβ-RXR agonist assay

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

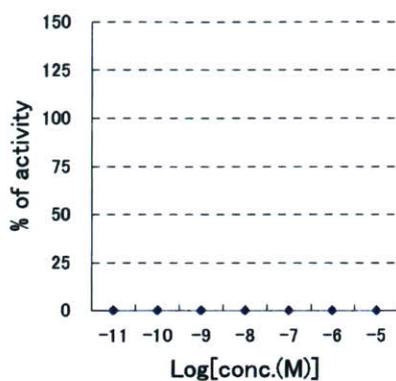


sample No.
chemical name
CAS.

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

AR agonist assay

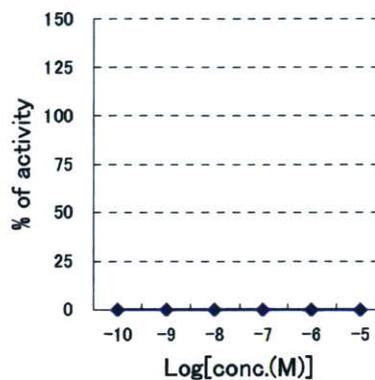
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

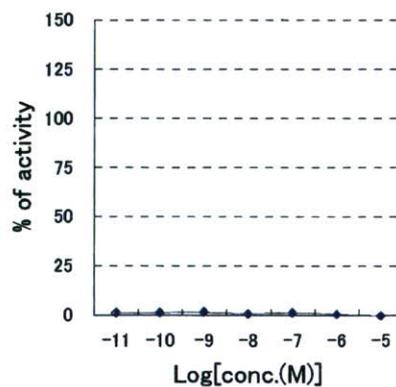
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



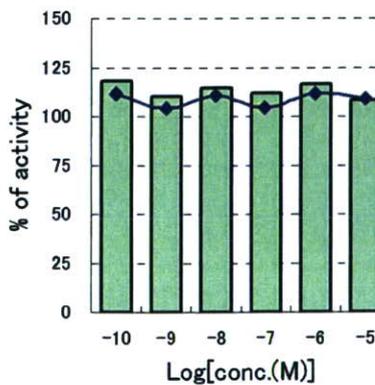
TRβ-RXR agonist assay

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

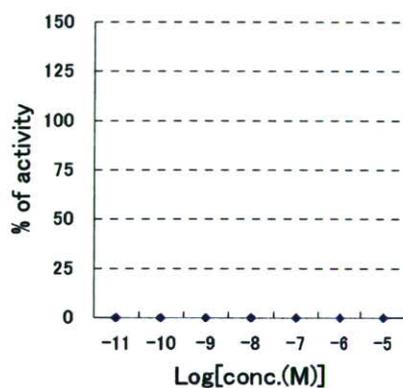
LOG[conc.(M)]	luc	ren
-5	109	108
-6	112	116
-7	104	112
-8	111	114
-9	104	110
-10	112	118



sample No. TR245
 chemical name Cinnamaldehyde, .alpha.-pentyl-, dimethyl acetal
 CAS. 91-87-2

AR agonist assay

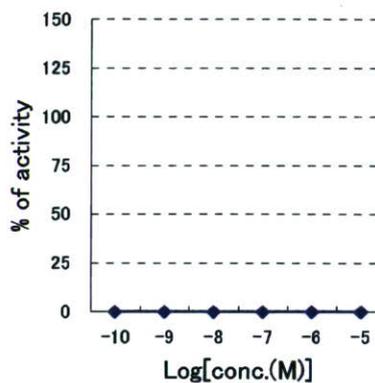
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

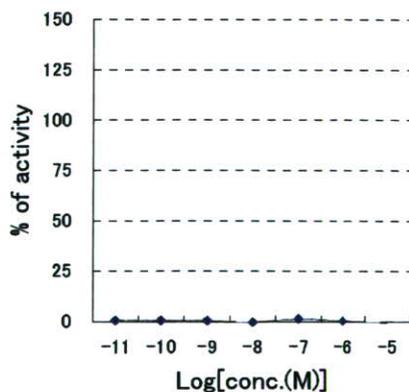
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



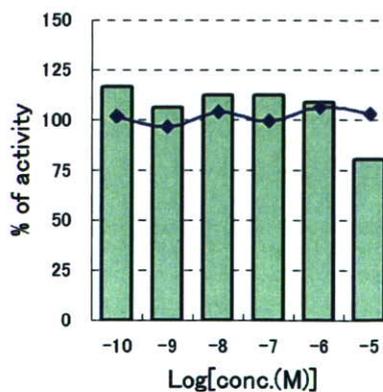
TRβ-RXR agonist assay

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

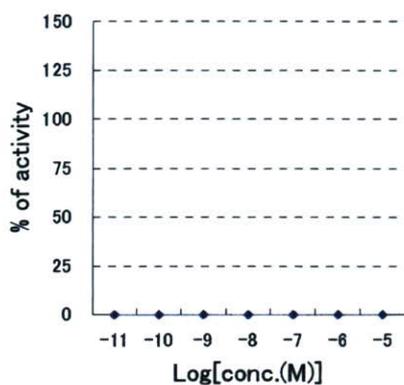
LOG[conc.(M)]	luc	ren
-5	104	80
-6	107	109
-7	100	113
-8	104	112
-9	97	107
-10	102	117



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

AR agonist assay

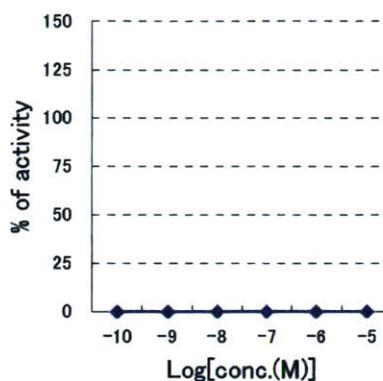
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

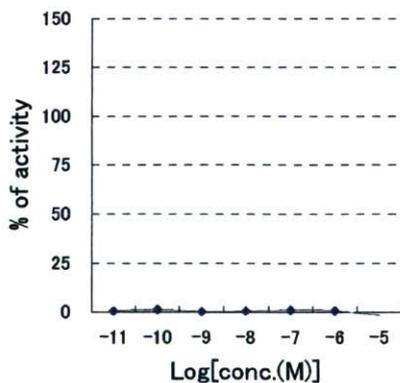
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



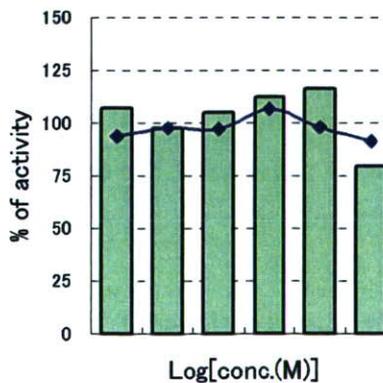
TRβ-RXR agonist assay

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

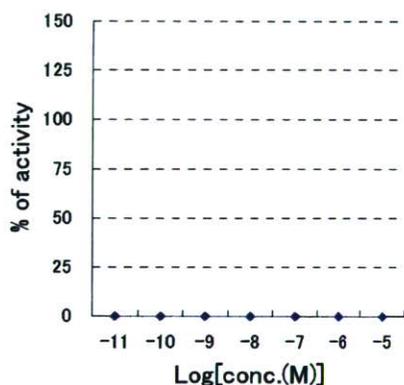
LOG[conc.(M)]	luc	ren
-5	91	79
-6	98	116
-7	107	112
-8	97	105
-9	98	97
-10	94	107



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

AR agonist assay

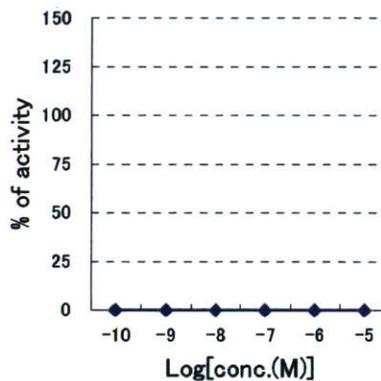
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

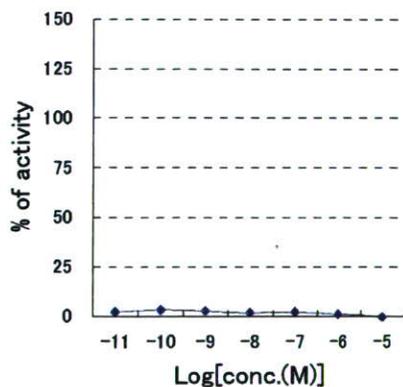
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



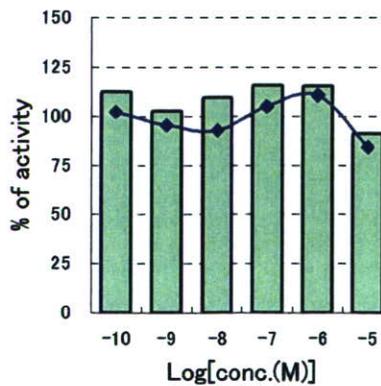
TRβ-RXR agonist assay

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

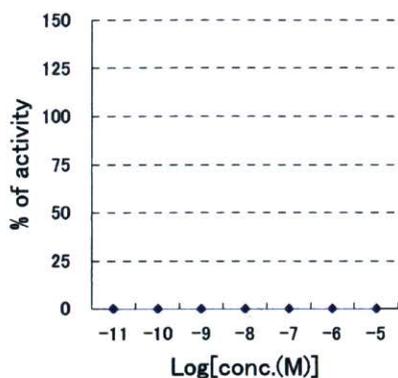
LOG[conc.(M)]	luc	ren
-5	84	91
-6	111	115
-7	105	116
-8	93	109
-9	95	102
-10	102	112



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

AR agonist assay

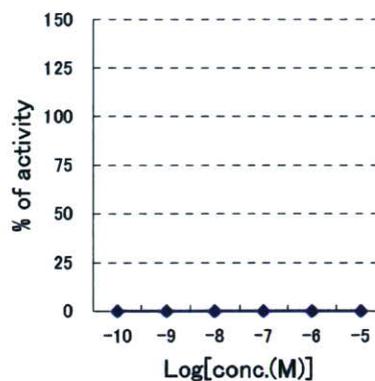
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

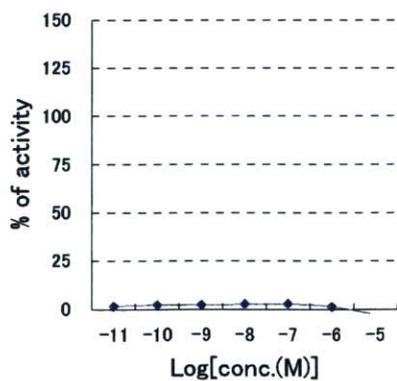
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



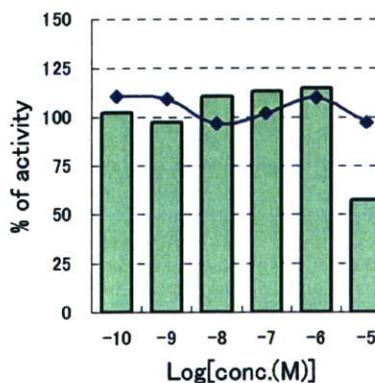
TRβ-RXR agonist assay

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

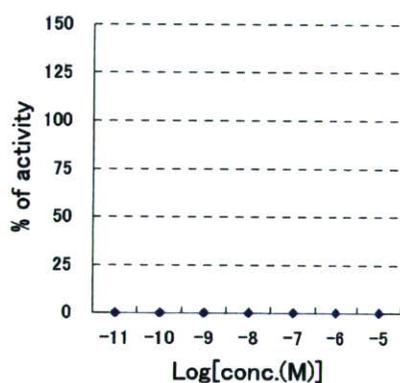
LOG[conc.(M)]	luc	ren
-5	97	58
-6	110	115
-7	102	113
-8	97	110
-9	109	97
-10	111	102



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

AR agonist assay

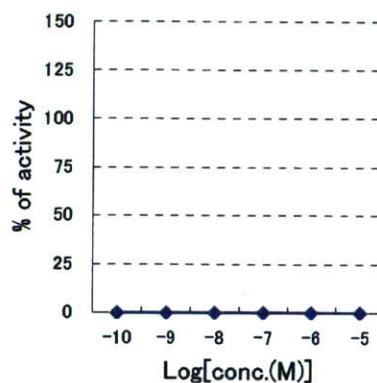
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

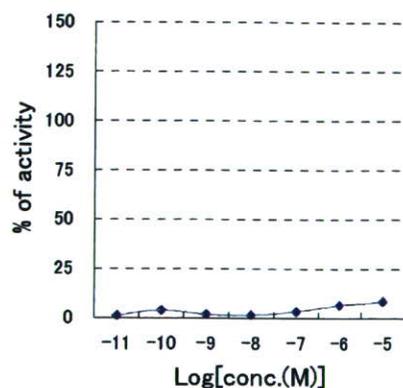
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



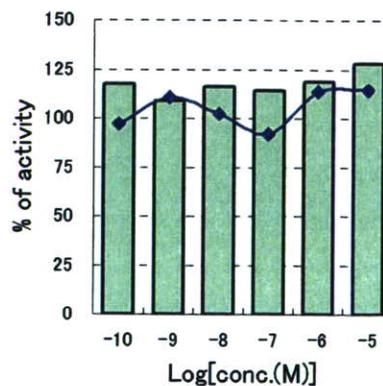
TRβ-RXR agonist assay

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

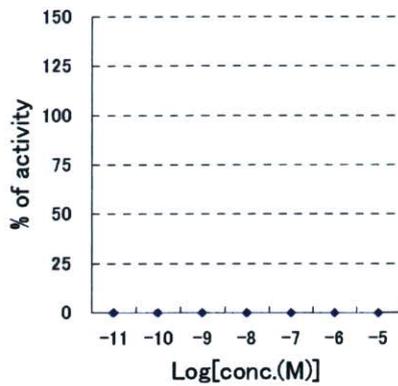
LOG[conc.(M)]	luc	ren
-5	114	128
-6	114	119
-7	92	114
-8	102	116
-9	111	109
-10	97	118



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

AR agonist assay

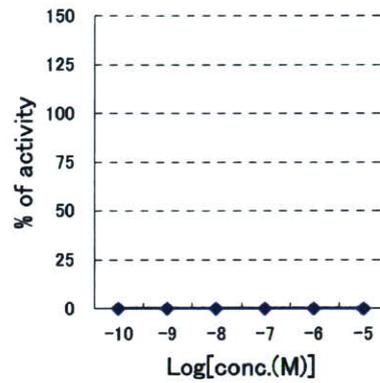
LOG[conc.(M)]	luc
-5	0.0
-6	0.0
-7	0.0
-8	0.0
-9	0.0
-10	0.0
-11	0.0



AR antagonist assay

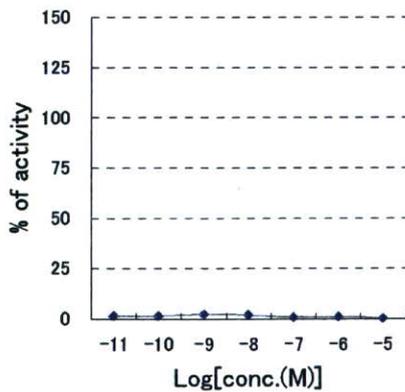
LOG[conc.(M)]	luc	ren
-5	0	0
-6	0	0
-7	0	0
-8	0	0
-9	0	0
-10	0	0

Cell viability



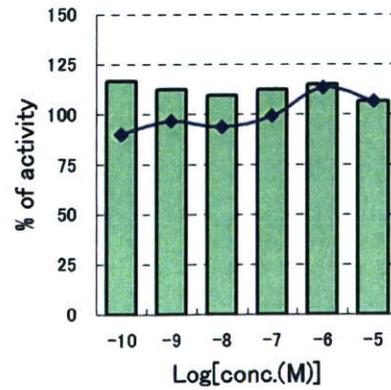
TRβ-RXR agonist assay

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

- (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)

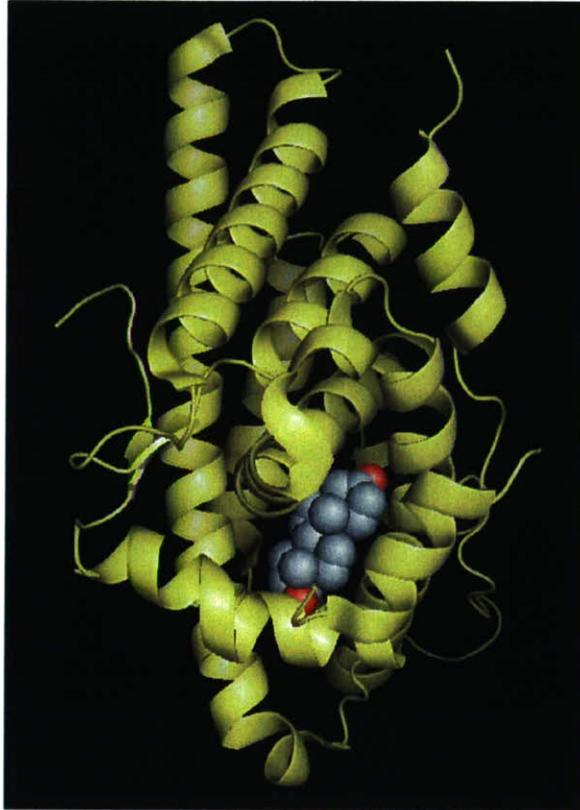
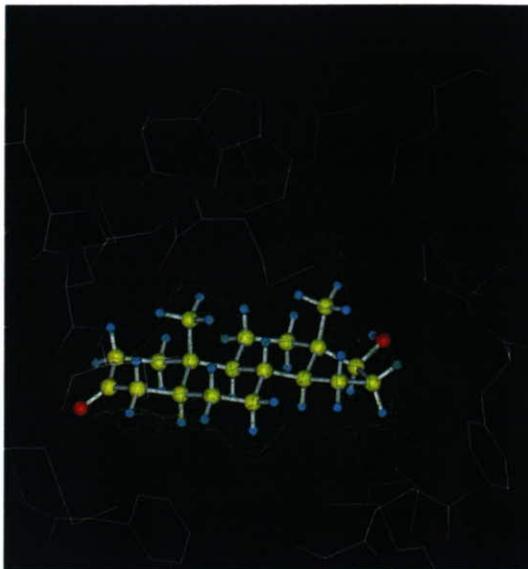
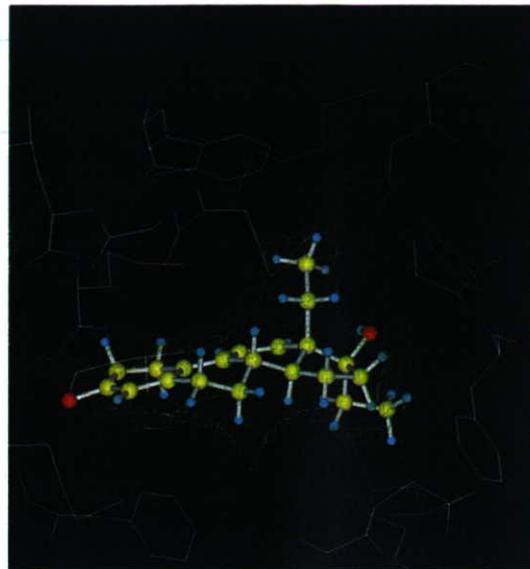


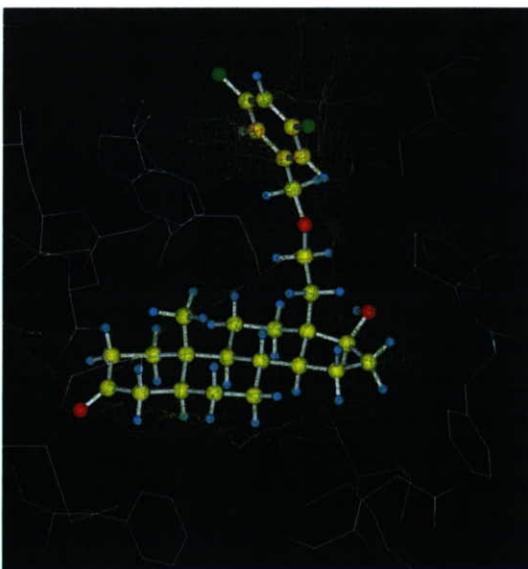
図1 ヒトAR受容体とリガンドDHTとの複合体結晶構造 1t63の全体像。中央下のスペースフィル表示の分子がDHT。



(a)



(b)



(c)

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。(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。

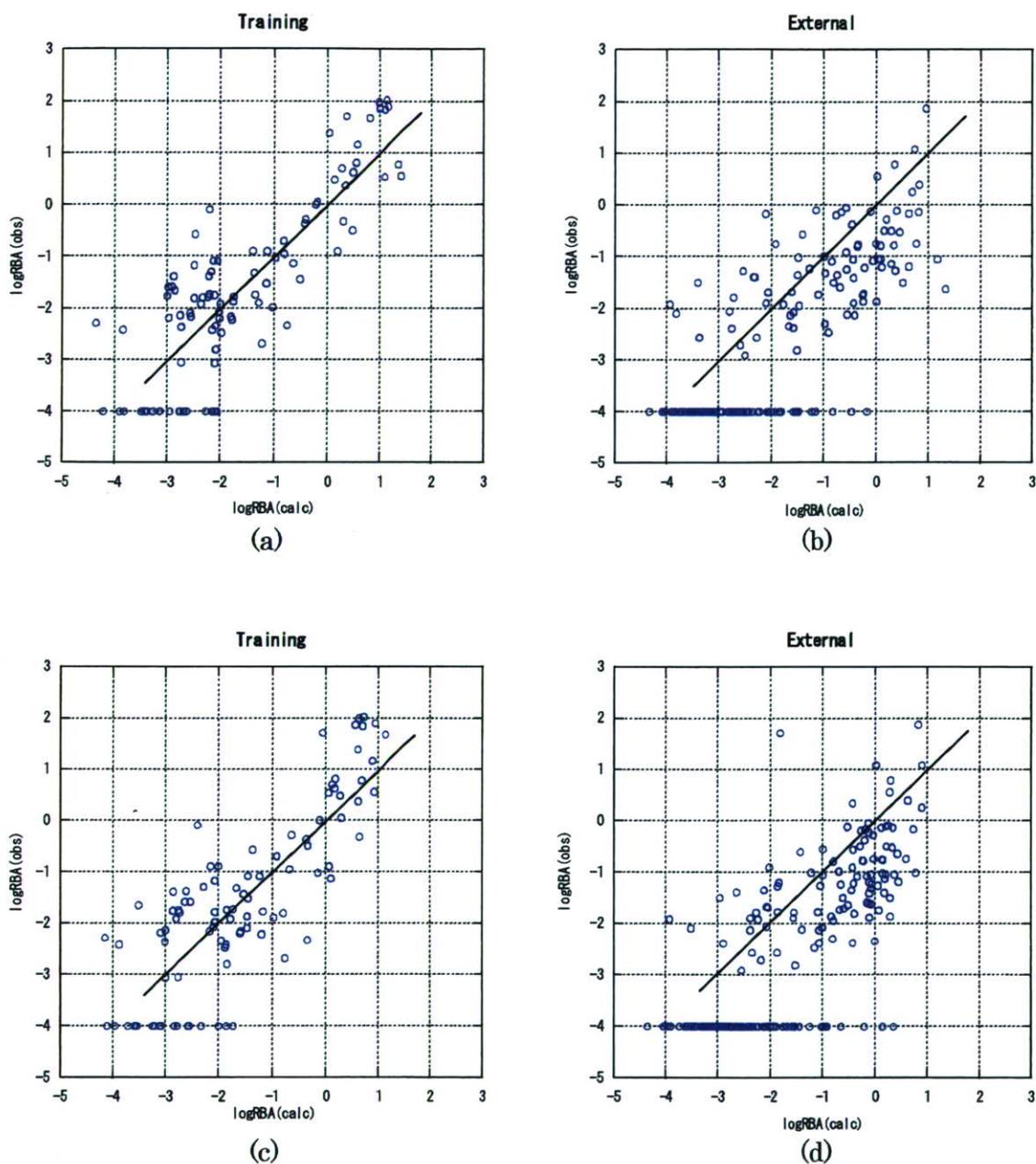


図3 各AR構造を用いて算出したlogRBA予測値(横軸)と*in vitro*受容体結合試験によるlogRBA実測値(縦軸)の対比。非結合の物質(non-binders)のlogRBA実測値は、仮に-4.0としてプロットした。(a) 1t63構造に対するトレーニングセット化合物のプロット。(b) 1t63構造に対する検証化合物のプロット。(c) 2pnu構造に対するトレーニングセット化合物のプロット。(d) 2pnu構造に対する検証化合物のプロット。

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
50-06-6	-2.82	59-43-8	-1.33	75-05-8	-4.49
50-07-7	-3.65	60-57-1	-3.47	75-08-1	-4.56
50-23-7	0.52	60-82-2	-1.68	75-09-2	-4.86
50-28-2	0.52	61-82-5	-4.29	75-21-8	-4.55
50-41-9	-2.53	63-05-8	-0.56	75-26-3	-4.06
51-24-1	-2.91	63-25-2	-2.68	75-28-5	-4.24
51-48-9	-2.08	63-91-2	-3.62	75-29-6	-4.35
51-49-0	-2.47	64-86-8	-2.19	75-33-2	-4.28
51-52-5	-2.59	66-81-9	-0.60	75-34-3	-4.29
52-01-7	-1.32	67-03-8	-1.33	75-35-4	-4.46
52-46-0	-4.01	67-30-1	-2.13	75-38-7	-4.71
52-86-8	-3.12	67-66-3	-4.74	75-45-6	-4.73
53-16-7	-0.78	67-72-1	-4.38	75-52-5	-4.18
53-96-3	-2.00	67-97-0	-2.33	75-56-9	-4.02
55-06-1	-3.37	68-22-4	-0.72	75-57-0	-4.42
56-23-5	-4.76	69-79-4	-1.03	75-59-2	-4.42
56-49-5	-1.36	71-55-6	-4.31	75-63-8	-4.73
56-53-1	-1.44	72-20-8	-3.12	75-66-1	-3.97
56-55-3	-1.69	72-43-5	-2.49	75-68-3	-4.62
56-72-4	-1.77	72-55-9	-2.41	75-69-4	-4.75
57-06-7	-4.10	73-31-4	-2.45	75-71-8	-4.75
57-30-7	-1.56	74-31-7	-2.54	75-88-7	-4.57
57-63-6	0.33	74-83-9	-4.84	76-01-7	-4.52
57-68-1	-2.01	74-85-1	-4.93	76-06-2	-4.45
57-74-9	-3.98	74-86-2	-4.91	76-13-1	-4.78
57-83-0	0.42	74-87-3	-4.82	76-14-2	-4.64
57-91-0	-0.36	74-93-1	-4.83	76-15-3	-4.70
58-18-4	1.18	74-95-3	-4.78	76-44-8	-3.64
58-22-0	0.19	74-96-4	-4.42	77-06-5	-2.09
58-32-2	-6.40	74-97-5	-4.82	77-09-8	-2.56
58-72-0	-1.85	74-99-7	-4.64	77-40-7	-1.76
58-89-9	-3.68	75-00-3	-4.46	77-42-9	-1.30
58-95-7	-0.01	75-01-4	-4.78	77-47-4	-4.32
59-02-9	-3.69	75-02-5	-4.69	77-62-3	-4.56

CAS 番号	推算 logRBA	CAS 番号	推算 logRBA	CAS 番号	推算 logRBA
77-73-6	-2.96	83-59-0	-0.94	93-53-8	-3.25
77-92-9	-4.74	83-79-4	-4.70	93-65-2	-2.74
78-34-2	-1.21	83-88-5	-1.27	94-09-7	-3.57
78-67-1	-3.17	84-19-5	-0.71	94-13-3	-2.50
78-77-3	-3.87	84-60-6	-2.67	94-18-8	-2.20
78-79-5	-3.88	84-69-5	-2.79	94-25-7	-3.16
78-82-0	-3.93	84-74-2	-2.89	94-26-8	-2.09
78-87-5	-4.20	85-43-8	-2.66	94-41-7	-2.62
78-89-7	-3.51	85-68-7	-2.57	94-71-3	-3.50
78-97-7	-3.72	85-69-8	-2.21	96-18-4	-4.10
79-00-5	-4.22	85-98-3	-2.47	96-29-7	-3.62
79-01-6	-4.64	87-18-3	-2.39	96-69-5	-1.67
79-24-3	-3.94	87-44-5	-2.02	97-39-2	-2.15
79-27-6	-4.61	87-68-3	-4.06	97-54-1	-2.54
79-34-5	-4.54	88-29-9	-1.07	98-54-4	-2.24
79-38-9	-4.74	88-66-4	-3.69	98-85-1	-3.54
79-46-9	-3.77	88-84-6	-1.87	99-49-0	-2.55
79-76-5	-2.52	89-48-5	-2.80	99-71-8	-2.20
79-77-6	-2.75	89-72-5	-2.80	99-72-9	-3.00
79-92-5	-2.61	89-77-0	-3.36	99-76-3	-2.78
79-94-7	-2.56	89-80-5	-3.20	99-82-1	-2.62
79-96-9	-1.97	90-72-2	-2.27	99-83-2	-2.77
79-97-0	-1.38	90-80-2	-2.38	99-85-4	-2.66
80-05-7	-1.43	91-17-8	-2.75	99-86-5	-3.09
80-09-1	-1.33	91-50-9	-1.10	100-40-3	-3.20
80-43-3	-1.30	91-51-0	-1.26	101-53-1	-2.25
80-46-6	-2.01	91-60-1	-3.31	101-72-4	-2.81
80-51-3	-0.86	91-62-3	-3.17	101-92-8	-2.46
80-56-8	-2.96	91-87-2	-1.90	101-94-0	-2.09
80-71-7	-3.63	91-94-1	-2.24	102-22-7	-1.98
81-11-8	-1.69	92-52-4	-3.10	103-14-0	-1.69
81-14-1	-2.55	92-69-3	-2.35	103-16-2	-1.89
81-64-1	-3.23	92-88-6	-2.20	103-34-4	-2.70
81-92-5	-0.84	93-29-8	-3.13	103-48-0	-2.57

CAS 番号	推算 logRBA	CAS 番号	推算 logRBA	CAS 番号	推算 logRBA
103-53-7	-1.97	108-62-3	-2.77	112-91-4	-1.52
104-27-8	-2.84	108-87-2	-3.54	115-07-1	-4.34
104-40-5	-1.31	109-65-9	-4.07	115-11-7	-4.10
104-43-8	-1.05	109-67-1	-3.71	115-25-3	-4.46
104-45-0	-2.84	109-69-3	-3.69	115-32-2	-2.97
104-46-1	-2.92	109-70-6	-4.11	115-71-9	-1.19
104-55-2	-3.48	109-74-0	-3.99	116-14-3	-4.71
104-64-3	-3.15	109-79-5	-4.21	116-15-4	-4.45
104-68-7	-2.75	109-80-8	-4.45	116-25-6	-3.40
104-95-0	-3.93	109-88-6	-4.38	117-37-3	-2.23
106-21-8	-1.88	109-99-9	-3.95	117-39-5	-2.31
106-41-2	-3.21	110-01-0	-4.03	117-81-7	-2.46
106-46-7	-4.02	110-52-1	-4.20	118-58-1	-1.86
106-62-7	-2.62	110-57-6	-4.14	118-82-1	-1.38
106-88-7	-4.04	110-88-3	-4.10	119-53-9	-2.64
106-89-8	-4.20	111-24-0	-3.52	119-61-9	-3.02
106-92-3	-3.33	111-25-1	-3.54	119-93-7	-1.93
106-93-4	-4.34	111-28-4	-3.70	120-47-8	-2.78
106-94-5	-4.05	111-31-9	-3.63	120-51-4	-2.50
106-98-9	-4.07	111-66-0	-3.06	120-83-2	-3.81
106-99-0	-4.18	111-69-3	-3.51	122-37-2	-2.17
107-00-6	-4.23	111-78-4	-2.92	122-40-7	-2.08
107-01-7	-4.07	111-83-1	-3.28	122-48-5	-2.75
107-03-9	-4.39	111-85-3	-3.21	122-57-6	-3.20
107-05-1	-4.39	111-88-6	-2.95	122-68-9	-2.02
107-06-2	-4.41	112-00-5	-1.43	122-91-8	-2.17
107-12-0	-4.28	112-02-7	-1.43	123-35-3	-3.08
107-13-1	-4.56	112-29-8	-2.66	123-63-7	-3.56
107-39-1	-3.03	112-41-4	-2.26	123-91-1	-3.94
107-40-4	-2.96	112-52-7	-2.31	124-30-1	-3.81
107-56-2	-3.21	112-55-0	-2.34	125-02-0	3.81
108-03-2	-3.83	112-71-0	-2.26	125-84-8	-2.28
108-43-0	-3.33	112-82-3	-1.03	126-64-7	-2.03
108-57-6	-3.03	112-90-3	-1.38	126-98-7	-4.16

CAS 番号	推算 logRBA	CAS 番号	推算 logRBA	CAS 番号	推算 logRBA
126-99-8	-4.00	142-59-6	-2.88	371-42-6	-3.67
127-18-4	-4.54	143-15-7	-2.42	374-07-2	-4.80
127-25-3	-1.20	143-28-2	-0.96	382-31-0	-3.22
127-42-4	-2.47	144-35-4	-1.94	401-95-6	-3.42
127-43-5	-2.12	145-13-1	0.27	401-99-0	-3.47
127-65-1	-3.08	145-50-6	-1.87	404-86-4	-2.34
127-91-3	-2.85	149-44-0	-1.96	427-51-0	-0.36
128-04-1	-4.24	150-30-1	-2.47	428-59-1	-4.11
128-44-9	-3.04	150-60-7	-2.37	434-07-1	0.69
128-63-2	-3.01	155-04-4	-3.27	434-22-0	0.97
130-89-2	-1.78	156-60-5	-4.84	446-72-0	-1.86
131-16-8	-2.97	156-62-7	-4.21	461-82-5	-3.40
131-54-4	-2.96	192-97-2	-2.40	463-82-1	-4.11
131-55-5	-1.06	193-39-5	-0.99	464-45-9	-3.30
131-56-6	-2.76	205-99-2	-1.58	469-61-4	-2.12
131-57-7	-2.62	286-20-4	-3.37	470-67-7	-2.66
133-07-3	-4.03	287-92-3	-3.92	470-82-6	-2.70
136-99-2	-1.07	294-62-2	-2.10	472-41-3	-0.87
137-08-6	-2.39	298-06-6	-3.60	472-97-9	-2.13
137-41-7	-4.08	298-46-4	-2.18	473-55-2	-2.82
137-42-8	-4.08	298-81-7	-3.01	474-86-2	-0.20
138-25-0	-3.86	299-28-5	-2.78	475-20-7	-2.18
138-86-3	-2.83	300-84-5	-2.34	479-13-0	-0.90
138-87-4	-2.75	304-59-6	-4.38	480-16-0	-2.82
138-93-2	-3.86	306-83-2	-4.67	480-18-2	-2.12
139-65-1	-2.16	309-00-2	-3.57	480-40-0	-2.30
140-27-2	-2.79	327-97-9	-1.72	480-41-1	-2.06
140-60-3	-1.62	330-55-2	-2.85	485-63-2	-2.24
140-64-7	1.63	341-58-2	-2.92	485-72-3	-2.09
140-66-9	-1.80	349-58-6	-3.46	486-66-8	-2.06
140-93-2	-4.20	349-76-8	-3.31	487-26-3	-2.00
141-92-4	-0.97	353-59-3	-4.71	491-04-3	-2.62
141-98-0	-3.15	354-58-5	-4.72	491-09-8	-2.99
142-29-0	-3.97	367-65-7	-3.10	491-70-3	-2.42

CAS 番号	推算 logRBA	CAS 番号	推算 logRBA	CAS 番号	推算 logRBA
491-80-5	-1.15	540-84-1	-2.99	599-64-4	-2.16
495-62-5	-1.92	541-15-1	-2.57	603-35-0	-2.26
497-76-7	-1.84	541-31-1	-4.07	603-45-2	-1.30
498-81-7	-2.48	542-75-6	-4.45	604-68-2	-2.42
499-44-5	-3.01	542-92-7	-4.22	605-45-8	-3.36
499-69-4	-2.74	544-17-2	-4.59	608-73-1	-3.67
499-70-7	-2.89	546-68-9	-3.58	611-99-4	-1.24
500-02-7	-2.27	553-72-0	-3.56	612-00-0	-2.29
500-38-9	-0.45	553-79-7	-3.28	614-23-3	-3.38
501-24-6	-0.69	553-86-6	-2.79	616-09-1	-3.24
501-98-4	-3.03	555-31-7	-3.58	616-21-7	-3.93
502-61-4	-1.91	555-75-9	-4.11	619-15-8	-3.14
504-60-9	-4.02	558-37-2	-3.73	619-84-1	-3.14
505-29-3	-3.88	563-47-3	-4.03	620-92-8	-1.28
505-65-7	-3.67	563-71-3	-4.66	621-13-6	-1.60
507-20-0	-3.80	564-35-2	0.06	621-82-9	-3.60
510-13-4	-1.95	564-94-3	-2.64	624-64-6	-4.06
513-35-9	-3.74	569-61-9	-2.39	627-70-3	-3.19
513-44-0	-4.14	574-09-4	-2.19	629-03-8	-3.31
513-53-1	-4.12	584-03-2	-2.95	629-04-9	-3.52
515-00-4	-2.47	585-24-0	-2.38	629-41-4	-3.20
520-18-3	-2.08	586-62-9	-2.97	629-73-2	-1.81
520-26-3	-1.71	586-82-3	-2.77	629-79-8	-1.33
521-18-6	1.17	587-26-8	-4.66	630-20-6	-4.42
525-82-6	-2.79	589-35-5	-2.97	636-53-3	-3.62
527-62-8	-3.51	589-98-0	-2.11	637-07-0	-3.11
528-79-0	-2.58	590-18-1	-3.99	643-38-9	-3.04
531-59-9	-3.10	592-41-6	-3.74	644-08-6	-2.77
531-95-3	-1.53	592-45-0	-3.87	644-21-3	-3.10
532-82-1	-2.55	592-51-8	-3.78	644-35-9	-3.27
537-98-4	-2.74	593-31-7	-1.34	646-06-0	-4.24
538-75-0	-2.24	596-01-0	-2.30	654-55-7	-3.51
540-63-6	-4.51	597-82-0	-2.82	654-66-0	-3.02
540-72-7	-4.86	598-82-3	-4.39	669-90-9	-3.14

CAS 番号	推算 logRBA	CAS 番号	推算 logRBA	CAS 番号	推算 logRBA
676-46-0	-4.64	837-08-1	-2.25	1103-38-4	-1.26
677-21-4	-4.29	843-55-0	-1.22	1103-39-5	-1.26
687-47-8	-3.16	844-51-9	-2.46	1107-00-2	-2.52
689-97-4	-4.32	870-23-5	-4.46	1113-21-9	-0.21
691-37-2	-3.80	872-05-9	-2.54	1120-36-1	-1.50
693-58-3	-2.84	873-54-1	-3.56	1131-60-8	-1.95
696-59-3	-3.17	901-44-0	-1.56	1135-24-6	-3.13
698-76-0	-2.14	908-54-3	-1.35	1139-30-6	-1.37
699-07-0	-2.66	918-04-7	-2.77	1139-46-4	-1.11
699-10-5	-3.21	920-37-6	-4.41	1141-59-9	-2.19
700-06-1	-2.26	925-83-7	-1.81	1149-16-2	-2.32
705-73-7	-2.09	926-57-8	-4.07	1156-51-0	-2.83
709-98-8	-2.66	927-19-5	-2.50	1185-57-5	-4.83
719-03-9	-1.63	930-69-8	-3.88	1191-43-1	-3.57
723-46-6	-2.87	931-40-8	-3.21	1191-62-4	-3.29
756-80-9	-4.47	931-88-4	-3.35	1193-11-9	-3.24
760-23-6	-3.93	934-34-9	-3.81	1203-17-4	-2.26
764-41-0	-4.14	943-88-4	-2.67	1205-42-1	-2.46
769-78-8	-3.67	961-11-5	-2.21	1208-67-9	-3.64
772-46-3	-2.76	963-39-3	-2.83	1217-08-9	-0.79
774-48-1	-2.73	971-15-3	-2.77	1222-05-5	-1.47
782-74-1	-2.71	993-43-1	-4.28	1241-94-7	-1.26
785-30-8	-3.17	994-36-5	-4.83	1260-17-9	-4.50
791-22-0	-1.56	999-81-5	-3.87	1319-70-6	-3.38
791-28-6	-2.20	1000-82-4	-3.90	1333-09-1	-2.55
793-24-8	-2.56	1002-69-3	-2.75	1405-92-1	-1.35
797-63-7	0.77	1024-57-3	-3.74	1435-71-8	-2.34
798-61-8	-1.58	1038-66-0	-2.42	1470-79-7	-1.17
813-94-5	-4.63	1070-78-6	-4.08	1476-11-5	-4.02
814-67-5	-4.25	1071-22-3	-6.50	1478-61-1	-2.16
814-80-2	-4.53	1074-82-4	-3.13	1489-57-2	-3.66
828-26-2	-2.79	1076-56-8	-2.46	1497-49-0	-3.89
831-82-3	-2.05	1085-12-7	-2.03	1504-74-1	-2.93
833-66-9	-2.71	1095-77-8	-2.29	1506-02-1	-1.04

CAS 番号	推算 logRBA	CAS 番号	推算 logRBA	CAS 番号	推算 logRBA
1518-83-8	-2.40	1910-42-5	-0.60	2385-85-5	-3.54
1552-12-1	-2.92	1923-99-5	-3.73	2398-96-1	-1.72
1559-34-8	-1.86	1928-45-6	-2.81	2408-37-9	-2.92
1569-60-4	-2.91	1943-97-1	-0.22	2425-54-9	-1.90
1569-69-3	-3.65	1948-33-0	-2.61	2425-66-3	-3.84
1570-64-5	-3.37	1951-25-3	-2.91	2426-08-6	-3.07
1572-52-7	-3.58	1965-09-9	-1.86	2431-50-7	-3.95
1576-13-2	-0.98	1966-58-1	-3.07	2435-16-7	-2.09
1583-58-0	-3.85	1975-78-6	-2.68	2436-90-0	-2.52
1589-47-5	-3.29	1982-69-0	-2.77	2437-25-4	-2.35
1599-49-1	-2.49	1987-50-4	-1.56	2437-56-1	-2.34
1599-67-3	-7.21	2032-65-7	-2.31	2440-22-4	-2.42
1607-57-4	-1.55	2051-96-9	-3.10	2443-58-5	-2.09
1632-73-1	-2.00	2084-18-6	-3.95	2444-46-4	-1.96
1653-19-6	-4.28	2084-19-7	-3.83	2444-90-8	-1.46
1653-30-1	-1.28	2084-69-7	-2.01	2445-83-2	-2.57
1679-07-8	-3.93	2090-05-3	-3.56	2446-69-7	-1.65
1706-12-3	-2.85	2094-98-6	-2.41	2467-02-9	-2.69
1717-00-6	-4.35	2095-01-4	-2.82	2491-32-9	-2.09
1733-12-6	-1.94	2102-59-2	-2.95	2492-26-4	-3.27
1742-14-9	-1.77	2110-18-1	-2.57	2495-37-6	-2.63
1762-95-4	-4.91	2114-02-5	-3.30	2528-36-1	-1.98
1772-25-4	-2.78	2114-33-2	-2.69	2536-05-2	-2.06
1786-08-9	-2.87	2128-93-0	-2.41	2550-40-5	-2.17
1800-91-5	-2.31	2142-01-0	-2.29	2571-39-3	-2.40
1806-26-4	-1.57	2153-26-6	-2.45	2589-73-3	-1.92
1817-13-6	-3.61	2153-28-8	-1.78	2611-00-9	-2.11
1825-21-4	-3.60	2163-00-0	-3.53	2612-56-8	-3.10
1836-75-5	-2.65	2196-14-7	-1.21	2634-33-5	-2.89
1843-03-4	-0.40	2213-81-2	-2.97	2657-25-2	-1.81
1854-26-8	-2.70	2236-52-4	-2.83	2664-63-3	-1.39
1861-32-1	-3.40	2282-34-0	-2.48	2695-37-6	-2.96
1878-18-8	-3.99	2286-54-6	-2.57	2786-76-7	-3.34
1901-26-4	-3.32	2305-21-7	-3.36	2825-82-3	-3.09