

な効果を示すことが明らかとなり、そうした受容体構造制御が引き続く遺伝子発現制御に関連するものと考察された。本系により得られる個々の化合物についての情報は多岐に渡り、これらは引き続き詳細試験や遺伝子発現解析に先立って非常に有用に機能するものであり、化合物の内分泌かく乱作用スクリーニング系として有効であると結論付けられた。培養細胞を用いた比較して、本アッセイ系は *in vitro* の再構成系であり、純粋なレセプター—シグナル伝達系への作用のみを検討することができる特色があり、さらに同じアゴニストであっても相互作用に与える影響が異なることが本系により明らかに示されることから、引き続き内分泌かく乱性の評価において有用であると考えられる。また、現在の国際的状況に鑑み、今後のリスクアセスメントの問題に関しては、レセプター構造と活性制御の研究をはじめとした核内レセプターによる遺伝子制御機構の解明はもとより、個々の化合物の生体作用について解明にあたって、今後はマイクロアレイを用いたゲノミクス手法による作用物質と遺伝子発現プロファイルに関する知見などインフォマティクスの果たす役割も大きいと考察された。これら多方面からの検討と知識の蓄積が、内分泌かく乱化学物質問題の解決及びリスクアセスメントにとって非常に重要である。すなわち、本研究班において構築されたこれら、*in silico*、*cell free*、*in vitro* スクリーニング手法により、対象とする化学物質特異的な情報を組み合わせることで、次の段階として詳細試験に供する化学物質の科学的根拠に基づくより正確な優先化合物の抽出が期待される。この優先順位リストにより、内分泌かく乱化学物質問題の効率的な解決への一つの道筋ができるものと期待される。また、ここで得られる受容体、応答 DNA 配列、共役因子等の相互作用に関するデータと細胞、個体レベルでの作用データが有機的に組み合わせられることにより内分泌かく乱化学物質の作用メカニズムの解明への貢献が期待される。

#### E. 研究発表

##### 論文発表

Yoon BI, Hirabayashi Y, Kawasaki Y, Tsuboi I,

Ott T, Kodama Y, Kanno J, Kim DY, Willilleche K, Inoue T. Exacerbation of benzene pneumotoxicity in connexin 32 knockout mice: enhanced proliferation of CYP2E1-immunoreactive alveolar epithelial cells. *Toxicology*. 2004 Jan 15;195(1):19-29.

Yoon BI, Li GX, Kitada K, Kawasaki Y, Igarashi K, Kodama Y, Inoue T, Kobayashi K, Kanno J, Kim DY, Inoue T, Hirabayashi Y. Mechanisms of benzene-induced hematotoxicity and leukemogenicity: cDNA microarray analyses using mouse bone marrow tissue. *Environ Health Perspect*. 2003 Aug;111(11):1411-20.

Tetsuji Nagao, Kazuyoshi Wada, Makiko Kuwagata, Madoka Nakagomi, Chiaki Watanabe, Shinsuke Yoshimura, Yoshiaki Saito, Kenji Usumi, Jun Kanno Intrauterine position and postnatal growth in Sprague-Dawley rats and ICR mice. *Reproductive Toxicology* 18 2004 109-120

Kanno J, Onyon L, Peddada S, Ashby J, Jacob E, Owens W. The OECD program to validate the rat uterotrophic bioassay. Phase 2: coded single-dose studies. *Environ Health Perspect*. 2003 Sep;111(12):1550-8.

Kanno J, Onyon L, Peddada S, Ashby J, Jacob E, Owens W. The OECD program to validate the rat uterotrophic bioassay. Phase 2: dose-response studies. *Environ Health Perspect*. 2003 Sep;111(12):1530-49.

Matsunaga N, Kanno J, Yoshimura I A statistical method for judging synergism: Application to an endocrine disruptor animal experiment-

Synergism in endocrine disruptor studies,  
*Environmetrics* 2003, Volume 14, Issue 2, :  
213-222

Kanno J, Reverse toxicology as a future  
predictive toxicology, T. Inoue, W.D. Pennie Eds,  
Toxicogenomics, pp.213-218, Springer-Verlag  
Tokyo, 2002

Yoon BI, Hirabayashi Y, Kawasaki Y, Kodama Y,  
Kaneko T, Kanno J, Kim DY, Fujii-Kuriyama Y,  
Inoue T. Aryl hydrocarbon receptor mediates  
benzene-induced hematotoxicity. *Toxicol Sci.*  
2002 Nov;70(1):150-6.

Utsuyama M, Kanno J, Inoue T, Hirokawa K.  
Age/sex dependent and non-monotonous  
dose-response effect of diethylstilbestrol on the  
immune functions in mice. *Toxicol Lett.* 2002 Sep  
5;135(1-2):145-53.

#### 学会発表

菅野 純、「分子標的」と「全遺伝子トキシコゲノ  
ミクス」、がん分子標的治療研究会 2003 年 6  
月 2 日 東京

菅野 純、「トキシコゲノミクスの現状」、第 30 回  
トキシコロジー学会学術年会ワークショップ「プ  
ロテオミクスとトキシコゲノミクスの現状と問題点  
」2003 年 7 月 20 日 相模原

Jun Kanno, Toxicogenomics -A phenotype  
independent approach-, Annual Meeting of  
Korean Society of Toxicology, Oct 30, 2003,  
Seoul, Korea

菅野 純、「トキシコゲノミクスの新展開」、第 26  
回日本学術会議トキシコロジー研究連絡委員

会シンポジウム 2003 年 12 月 3 日 東京  
菅野純、「IGS ラットを用いたトキシコゲノミクス」  
CD(SD)IGS 研究会/研究集会 2003 年 12 月 19  
日 東京

Jun Kanno “Focusing on Toxicogenomics  
Research” The 3<sup>rd</sup> International Congress of  
Asian Society of Toxicology : ASIATOX III  
February 1-6, 2004, Bangkok / Chiang Mai,  
Thailand

Jun Kanno, Aisaki Ken-ichi, Atsushi Ono,  
Katsuhide Igarashi “Toxicogenomics using  
“percellome” and “mille-feuille” data system”  
The Joint International Meeting of The Japanese  
Society of Toxicologic Pathology (JSTP) and The  
International Federation of Societies of  
Toxicologic Pathology (IFSTP) including The  
International Academy of Toxicologic Pathology  
(IATP) February 15-18, 2004, Kobe, Japan

菅野 純「Toxicogenomics の進捗」第 240 回  
CBI 学会研究講演会, 2004 年 3 月 19 日、東  
京

#### F. 健康危機情報

なし

#### G. 知的所有権の取得状況

1. 特許取得  
なし

2. 実用新案登録  
なし

3. その他  
なし

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総括研究報告書 図表

レポーター遺伝子導入ヒト由来培養細胞株を用いた超高速分析法に関する試験研究  
(主任研究者:(財)化学物質評価研究機構委託業務)

Table 1 Test Chemicals

HTS No.	CAS No.	Chemical Name	Maker	Lot No.
HTS00002	521-18-6	Testosterone, dihydro	Wako	TPJ4827
HTS00003	797-63-7	Levonorgestrel	Sigma	30K0711
HTS00008	57-83-0	Progesterone	ICN	51868
HTS00018	56-53-1	Diethylstilbestrol	Wako	7488C
HTS00019	57-91-0	Estradiol, 17a	Wako	ELJ1532
HTS00020	57-63-6	Estradiol, ethynyl	Wako	KSN3933
HTS00021	50-28-2	Estradiol, 17b	Wako	ACL1188
HTS00022	53-16-7	Estrone	Wako	TPN4558
HTS00023	80-05-7	Bisphenol A	TCI	GF01
HTS00024	446-72-0	4',5',7'-Trihydroxyisoflavone	Wako	NNP1712
HTS00026		2,2-bis(p-hydroxyphenyl)-1,1,1-trichloroethane (HPTE)		-
HTS00029	26538-44-3	Zearanol	Sigma	108H4067
HTS00041	68047-06-3	Tamoxifen-4-OH	Sigma	59H4084
HTS00059	50-55-5	Reserpine	RBI	SNV-494A
HTS00072	927-67-3	Propylthiourea	Lancaster	90007528
HTS00081	114369-43-	Fenbuconazole	Riedel-de Haen	71960
HTS00084	68-22-4	Norethindrone	Sigma	58H0858
HTS00085	797-63-7	Norgestrel	Sigma	28H0860
HTS00088	50-23-7	Cortisol	Wako	CKJ1388
HTS00093	77-40-7	Bisphenol B	TCI	FIC01
HTS00094	479-13-0	Coumestrol	Fluka	400248
HTS00095	531-95-3	Equol	Fluka	45398/1
HTS00096	599-64-4	Phenol, p-cumyl	Wako	PAK1144
HTS00105	10540-29-1	ICI 47699	Wako	4636 C
HTS00106	1847-63-8	Nafoxidine	Sigma	33F0540
HTS00140	63046-09-3	6,4'-dihydroxyflavone	INDOFINE	4DHF1188
HTS00141	253195-19-	3,6,4'-trihydroxyflavone	INDOFINE	97007
HTS00142		7-hydroxy-3-phenyl-4H-chromen-4-one	MAYBRIDGE	-
HTS00143		5,7-dihydroxy-2-methyl-3-phenyl-4H-chromen-4-one	MAYBRIDGE	-
HTS00144		5,7-DIHYDROXY-2,3-DIPHENYL-4H-CHROMEN-4-ONE	MAYBRIDGE	-
HTS00145	6665-83-4	6-hydroxyflavone	Aldrich	-
HTS00147	6665-67-4	5,4'-dihydroxyflavone	INDOFINE	96012
HTS00148	2196-14-7	7,4'-dihydroxyflavone	INDOFINE	4DHF388
HTS00150		2,3-diphenyl-7-hydroxy-4H-1-benzopyran-4-one	Aldrich	-
HTS00156	71592-46-6	6,3'-dihydroxyflavone	INDOFINE	92005
HTS00168	620-92-8	Bisphenol F	Kanto	110G7202
HTS00174	104-43-8	4-Dodecylphenol	Kanto	007D2194
HTS00175	123-07-9	4-Ethylphenol	Wako	ELM4597
HTS00181	140-66-9	4-Octylphenol(tert)	Kanto	110G7201
HTS00218	486-66-8	Diadzein	Wako	HC-1408
HTS00286	96-76-4	2,4-di-tert-butylphenol	Aldrich	07610DR
HTS00289	3228-03-3	meta-Thymol	Aldrich	12809DU
HTS00303	5153-25-3	2-Ethylhexyl 4-hydroxybenzoate	Wako	SEL4252
HTS00336	14392-69-9	4'-HYDROXYNONANOPHENONE	Lancaster	00032085
HTS00456	6807-17-6	2,2-Bis(4-hydroxyphenyl)-4-methyl-n-pentane	Wako	PTM1337
HTS00458	27955-94-8	tris(hydroxyphenyl)ethane	Aldrich	03206DS
HTS00459	81-92-5	2-[Bis(4-hydroxyphenyl)methyl]benzylalkohol	TCI	FIB01
HTS00460	1478-61-1	4,4'-(HEXAFLUOROISOPROPYLIDENE)DIPHENOL	Aldrich	15213DI
HTS00461	843-55-0	4,4'-CYCLOHEXYLIDENEBISPHENOL	TCI	GE01
HTS00462	1943-97-1	4,4'-(Octahydro-4,7-methano-5H-inden-5-ylidene) bisphenol	Acros	A00839460
HTS00506	2491-32-9	BENZYL 4-HYDROXYPHENYLKETONE	Aldrich	14515JQ
HTS00521	131-56-6	2,4-Dihydroxybenzophenone	Wako	KSN3341
HTS00526	131-55-5	2,2',4,4'-Tetrahydroxybenzophenone	Wako	ELN6605
HTS00585	56-49-5	3-Methylcholanthrene	Aldrich	06103P1
HTS00598	145-50-6	p-naphtholbenzein	Wako	SEJ1327
HTS00601	52222-87-4	6-BENZOYL-2-NAPHTHOL	Aldrich	04113TY
HTS00642	6468-96-8	3-Phenylumbelliferone	Fluka	70904
HTS00864	131-54-4	2,2'-Dihydroxy-4,4'-dimethoxybenzophenone	Wako	ECG6603
HTS00888	64-86-8	Colchicine	Wako	LDE0915
HTS00978	6948-88-5	ALPHA-NAPHTHOLBENZEIN	Sigma	59H0523
HTS01026	596-01-0	ALPHA-NAPHTHOLPHTHALEIN	Wako	CKE0686
HTS01123	1139-46-4	4-tert-Octylcatechol	Rare chemical	-
HTS01124	7297-86-1	Ethyl 4,4-Bis(4-hydroxyphenyl)valerate	Rare chemical	-
HTS01126		4-(9H-carbazol-9-yl)aniline hydrochloride	Maybridge	-

HTS01127		Methyl 5-[2-Amino-4-(trifluoromethyl)-5-Pyrimidinyl]-3-(2,6-Dichlorophenyl)-4-Isoxazolecarboxy	Bionet	-
HTS01128	41796-12-7	4-Heptylsulfanyl-phenol	Rare chemical	-
HTS01129		2,4-Dihydroxyphenyl 1-Naphthyl Ketone	Rare chemical	-
HTS01130	1085-12-7	N-Heptyl 4-Hydroxybenzoate	Avocado	-
HTS01131	341-58-2	2,2'-Bis(Trifluoromethyl)benzidine	TCI	-
HTS01132	81936-33-6	P-(trans-4-Propylcyclohexyl)phenol	Kanto	-
HTS01133	1038-66-0	4,4'-Diaminooctafluorobiphenyl	TCI	-
HTS01134	2589-73-3	1-(4-Hydroxy-phenyl)-octan-1-one	Lancaster	-
HTS01135	5402-37-9	4-(1-Indanyl)phenol	Rare chemical	-
HTS01136	7507-01-9	3,4-Bis(4-Hydroxyphenyl)-3,4-Hexanediol	Rare chemical	-
HTS01137	472-41-3	3,4-Dihydro-4-(4-Hydroxyphenyl)2,2,4-Trimethyl-2H-1-	Rare chemical	-
HTS01138	59517-19-0	3,3'-Dimethyl-4,4'-Biphenyl	Rare chemical	-
HTS01154	4424-03-7	SULFONFLUORESCEIN	TCI	-
HTS01155	38483-26-0	DIHYDROETHIDIUM	Wako	-
HTS01157	71077-33-3	BUTYL 2,2-BIS(4-HYDROXYPHENYL)ACETATE	Wako	-
HTS01213		4-(4-CHLOROPHENYL)-5-(4-METHYLPHENYL)-1,3-THIAZOL-2-AMINE HYDROBROMIDE		
HTS01215		3-(4-CHLOROPHENYL)-4-[(4-CHLOROPHENYL)THIO]-1H-PYRAZOLE		
HTS01217		N3-(4-BROMOPHENYL)-4,5-DIOXO-2-PHENYL-4,5-DIHYDRO-1H-PYRROLE-3-CARBOXAMIDE		
HTS01218		3-(4-HYDROXY-3-METHOXYBENZYLIDENE)-2-PHENYLCHROMAN-4-ONE		
HTS01223		4-[2-(4-CHLOROPHENYL)-2,3-DIHYDRO-1,5-BENZOTHIAZEPIN-4-YL]PHENOL		
HTS01224		2-[2-(4-HYDROXYPHENYL)-2,3-DIHYDRO-1,5-BENZOTHIAZEPIN-4-YL]PHENOL		
HTS01226		7-HYDROXY-3-(4-METHOXYPHENYL)-2-PHENYL-4H-CHROMEN-4-ONE		
HTS01230		METHYL 4-[[7-HYDROXY-4-OXO-2-(TRIFLUOROMETHYL)-4H-3-		
HTS01231		N1-(2-[5-[4-(TERT-BUTYL)PHENYL]-1,3,4-OXADIAZOL-2-YL]PHENYL)-3-METHYLBENZAMIDE		
HTS01234		2-[3-(4-METHOXYPHENYL)-3,3A,4,5-TETRAHYDRO-2H-BENZO[G]INDAZOL-2-YL]ETHYL CYCLOPR		
HTS01235		3-(4-METHOXYPHENYL)-2-PHENYL-2,3,3A,4-TETRAHYDRO[1]BENZOTHIOPYRANO[4,3-C]PYRAZOL		
HTS01237		3-(4-CHLOROPHENOXY)-7-HYDROXY-2-(TRIFLUOROMETHYL)-4H-CHROMEN-4-ONE		
HTS01242	510-13-4	MALACHITE GREEN BASE	aldrich	-
HTS01245	87-18-3	Salicylic Acid 4-tert-Butylphenyl Ester	TCI	-
HTS01246	94-9-7	4-Aminobenzoic Acid Ethyl Ester	TCI	-
HTS01248	131-57-7	Benzophenone, 2-hydroxy-4-methoxy-	TCI	-
HTS01250	2440-22-4	2-(2-Benzotriazolyl)-p-cresol	TCI	-
HTS01255	5232-99-5	2-Cyano-3,3-diphenylacrylic Acid Ethyl Ester	TCI	-
HTS01257	6197-30-4	2-Cyano-3,3-diphenylacrylic Acid 2-Ethylhexyl Ester	TCI	-
HTS01258	25973-55-1	2-(2H-BENZOTRIAZOL-2-YL)-4,6-DI(T-	TCI	-
HTS01260	36861-47-9	Methylbenzylidene Camphor	AVOCADO	-

HTS No.: Intra laboratory I.D. used in this study

AccuStandard : AccuStandard Inc.

Acros : ACROS ORGANICS

Aldrich : Aldrich Chemical Co., Inc.(Sigma-Aldrich corp.)

Avocado : Avocado Research Chemicals Ltd.

Bionet

Fluka :Fluka Chemie AG (Sigma-Aldrich corp.)

Kanto : Kanto Chemical Co., Inc.

Lancaster : Lancaster Synthesis

Maybridge : Maybridge Chemical Company

Merck : Merck KGaA

Peakdale : Peakdale Fine Chemicals Limited

Rare chemical : Rare Chemical Co.

Sigma : Sigma Chemical Co.(Sigma-Aldrich corp.)

TCI : Tokyo Kasei Kogyo Co., Ltd.

Wako : Wako Pure Chemical Industries, Ltd.

Table 2 ER beta agonistic activity

HTS No.	Assay No.	Chemical Name	CAS No.	MDL CODE	M.W.	PC10(pM)	PC50(pM)
HTS00002	ER507	Testosterone, dihydro	521-18-6	-	290.44	1.24E+03	2.05E+04
HTS00003	ER511	Levonorgestrel	797-63-7	-	312.45	-	-
HTS00008		Progesterone	57-83-0	-	314.47	-	-
HTS00018		Diethylstilbestrol	56-53-1	-	268.35	<1.00E+01	2.78E+01
HTS00019		Estradiol,17a	57-91-0	-	272.39	1.38E+02	1.02E+03
HTS00020		Estradiol,ethynyl	57-63-6	-	296.41	<1.00E+01	<1.00E+01
HTS00021		Estradiol, 17b	50-28-2	-	272.39	<1.00E+01	3.82E+01
HTS00022		Estrone	53-16-7	-	270.37	<1.00E+01	1.52E+01
HTS00023		Bisphenol A	80-05-7	-	228.29	1.27E+04	1.05E+05
HTS00024		4',5,7-Trihydroxyisoflavone	446-72-0	-	270.24	1.07E+02	6.96E+02
HTS00026		2,2-bis(p-hydroxyphenyl)-1,1,1-trichloroethane	-	-	317.60	-	-
HTS00029		Zearanol	26538-44-3	-	322.40	<1.00E+01	5.08E+01
HTS00041		Tamoxifen-4-OH	68047-06-3	-	387.52	-	-
HTS00059	ER533	Reserpine	50-55-5	-	608.69	-	-
HTS00072		Propylthiourea	927-67-3	-	118.20	-	-
HTS00081		Fenbuconazole	14369-43-6	-	336.82	-	-
HTS00084		Norethindrone	68-22-4	-	298.42	2.78E+04	2.26E+05
HTS00085		Norgestrel	797-63-7	-	312.50	-	-
HTS00088		Cortisol	50-23-7	-	362.47	-	-
HTS00093	ER500	Bisphenol B	77-40-7	-	242.32	1.27E+04	6.29E+04
HTS00094		Coumestrol	479-13-0	-	268.23	1.40E+03	9.45E+03
HTS00095		Equol	531-95-3	-	242.27	8.44E+02	3.55E+03
HTS00096	ER510	Phenol p-cumyl	599-64-4	-	212.29	1.61E+04	1.25E+05
HTS00105		ICI 47699	10540-29-1	-	371.50	-	-
HTS00106		Nafoxidine	1847-63-8	-	462.03	-	-
HTS00140		6,4'-dihydroxyflavone	63046-09-3	-	254.24	<1.00E+01	<1.00E+01
HTS00141		3,6,4'-trihydroxyflavone	53195-19-6	-	270.24	1.38E+02	7.08E+02
HTS00142		7-hydroxy-3-phenyl-4H-chromen-4-one	-	-	238.25	7.22E+03	1.14E+05
HTS00143		5,7-dihydroxy-2-methyl-3-phenyl-4H-chromen-4-one	-	-	268.27	2.58E+02	1.78E+04
HTS00144	EA205	5,7-DIHYDROXY-2,3-DIPHENYL-4H-CHROMEN-	-	MFCDD00205547	330.34	-	-
HTS00145		6-hydroxyflavone	6665-83-4	-	238.25	-	-
HTS00147		5,4'-dihydroxyflavone	6665-67-4	-	254.24	4.40E+03	4.86E+05
HTS00148		7,4'-dihydroxyflavone	2196-14-7	-	254.24	2.35E+03	1.71E+04
HTS00150		2,3-diphenyl-7-hydroxy-4H-1-benzopyran-4-one	-	-	314.34	-	-
HTS00156		6,3'-dihydroxyflavone	71592-46-6	-	254.24	-	-
HTS00168		Bisphenol F	620-92-8	-	200.23	4.05E+04	1.18E+06
HTS00174		4-Dodecylphenol	104-43-8	-	262.43	1.14E+04	7.98E+04
HTS00175		4-Ethylphenol	123-07-9	-	122.17	-	-
HTS00181		4-Octylphenol(tert)	140-66-9	-	206.33	5.63E+02	4.16E+04
HTS00218	ER506	Diadzein	486-66-8	-	254.24	1.51E+03	2.41E+04
HTS00286		2,4-di-tert-butylphenol	96-76-4	-	206.33	-	-
HTS00289		meta-Thymol	3228-03-3	-	150.22	-	-
HTS00303	ER210	2-Ethylhexyl 4-hydroxybenzoate	5153-25-3	-	250.34	1.72E+05	-
HTS00336	ER236	4'-HYDROXYNONANOPHENONE	14392-69-9	-	234.34	3.54E+05	-
HTS00456	ER206	2,2-Bis(4-hydroxyphenyl)-4-methyl-n-pentane	6807-17-6	-	270.37	2.93E+03	3.80E+05
HTS00458	ER202	tris(hydroxyphenyl)ethane	27955-94-8	-	306.36	1.26E+05	-
HTS00459	ER277	2-[Bis(4-hydroxyphenyl)methyl]benzylalcohol =Phenolphthalol	81-92-5	-	306.36	1.34E+04	2.70E+05
HTS00460	ER513	4,4'-	1478-61-1	MFCDD00000439	336.23	1.12E+03	1.03E+04
HTS00461	ER512	4,4'-CYCLOHEXYLIDENEBISPHENOL	843-55-0	-	268.35	1.52E+04	-
HTS00462	EA308	4,4'-(Octahydro-4,7-methano-5H-inden-5-ylidene)	1943-97-1	MFCDD00213567	320.43	-	-
HTS00506	ER514	BENZYL 4-HYDROXYPHENYLKETONE	2491-32-9	-	212.25	3.43E+04	4.18E+05
HTS00521	ER609	2,4-Dihydroxybenzophenone	131-56-6	-	214.22	2.27E+04	6.24E+05
HTS00526	ER608	2,2',4,4'-Tetrahydroxybenzophenone	131-55-5	-	246.22	1.45E+04	5.06E+05
HTS00585		3-Methylcholanthrene	56-49-5	-	268.36	3.65E+06	-
HTS00598	EA118	p-naphtholbenzein	145-50-6	MFCDD00078492	374.44	-	-
HTS00601	ER340	6-BENZOYL-2-NAPHTHOL	52222-87-4	-	248.28	1.33E+05	6.60E+05
HTS00642	ER345	3-Phenylumbelliferone	6468-96-8	-	238.24	1.10E+05	2.75E+05
HTS00864	ER607	2,2'-Dihydroxy-4,4'-dimethoxybenzophenone	131-54-4	-	274.27	-	-
HTS00888	ER531	Colchicine	64-86-8	-	399.44	-	-
HTS00978	ER549	ALPHA-NAPHTHOLBENZEIN	6948-88-5	-	377.44	-	-
HTS01026	EA109	ALPHA-NAPHTHOLPHTHALEIN	596-01-0	MFCDD00036202	418.45	-	-
HTS01123	ER234	4-tert-Octylcatechol	1139-46-4	-	222.32	-	-
HTS01124	ER237	Ethyl 4,4-Bis(4-hydroxyphenyl)valerate	7297-86-1	-	256.79	2.32E+05	-
HTS01126	ER257	4-(9H-carbazol-9-yl)aniline hydrochloride	-	-	294.78	-	-
HTS01127	ER263	Methyl 5-[2-Amino-4-(trifluoromethyl)-5-Pyrimidinyl]-3-(2,6-Dichlorophenyl)-4-	-	-	433.18	2.25E+03	-
HTS01128	ER271	4-Heptylsulfanyl-phenol	41796-12-7	-	224.37	1.37E+06	-
HTS01129	ER272	2,4-Dihydroxyphenyl 1-Naphthyl Ketone	-	-	221.09	1.82E+05	1.73E+06

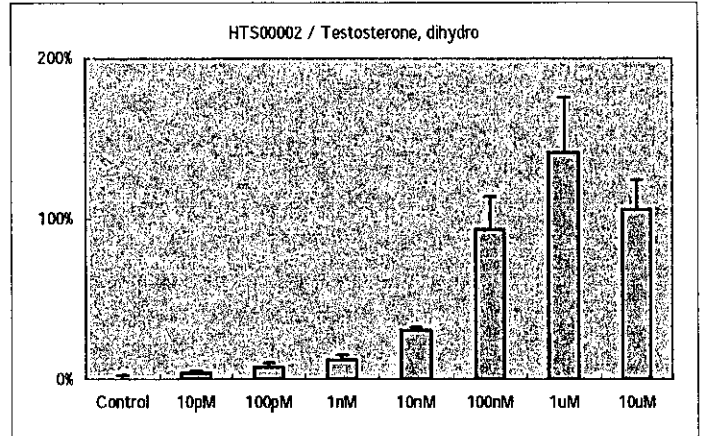
HTS01130	ER276	N-Heptyl 4-Hydroxybenzoate	1085-12-7	-	236.31	4.90E+04	9.55E+05
HTS01131	ER278	2,2'-Bis(Trifluoromethyl)benzidine	341-58-2	-	320.23	1.11E+05	8.80E+05
HTS01132	ER284	P-(trans-4-Propylcyclohexyl)phenol	81936-33-6	-	182.31	2.43E+04	2.38E+05
HTS01133	ER303	4,4'-Diaminooctafluorobiphenyl	1038-66-0	-	328.16	1.64E+04	1.17E+05
HTS01134	ER346	1-(4-Hydroxy-phenyl)-octan-1-one	2589-73-3	-	220.31	2.56E+05	-
HTS01135	ER348	4-(1-Indanyl)phenol	5402-37-9	-	195.88	2.81E+04	1.63E+05
HTS01136	ER352	3,4-Bis(4-Hydroxyphenyl)-3,4-Hexanediol	7507-01-9	-	302.37	1.05E+03	2.47E+03
HTS01137	ER360	3,4-Dihydro-4-(4-Hydroxyphenyl)-2,4-Trimethyl-2H-1-Benzopyran	472-41-3	-	268.36	1.71E+04	3.76E+05
HTS01138	ER362	3,3'-Dimethyl-4,4'-Biphenyl	59517-19-0	-	185.47	1.31E+04	6.69E+04
HTS01154	EA116	SULFONFLUORESC EIN	4424-03-7	MFCD00070618	368.37	1.22E+06	7.40E+06
HTS01155	EA117	DIHYDROETHIDIUM	38483-26-0	MFCD00077335	315.42	-	-
HTS01157	EA159	BUTYL 2,2-BIS(4-HYDROXYPHENYL)ACETATE	71077-33-3	MFCD00272585	300.35	3.28E+04	-
HTS01213	EA120	4-(4-CHLOROPHENYL)-5-(4-METHYLPHENYL)-1,3-THIAZOL-2-AMINE HYDROBROMIDE	-	MFCD00097753	381.72	-	-
HTS01215	EA133	3-(4-CHLOROPHENYL)-4-[(4-CHLOROPHENYL)THIO]-1H-PYRAZOLE	-	MFCD00138917	321.23	-	-
HTS01217	EA151	N3-(4-BROMOPHENYL)-4,5-DIOXO-2-PHENYL-4,5-DIHYDRO-1H-PYRROLE-3-CARBOXAMIDE	-	MFCD00219463	371.19	-	-
HTS01218	EA160	3-(4-HYDROXY-3-METHOXYBENZYLIDENE)-2-PHENYLCHROMAN-4-ONE	-	MFCD00276211	358.39	-	-
HTS01223	EA207	4-[2-(4-CHLOROPHENYL)-2,3-DIHYDRO-1,5-BENZOTHAZEPIN-4-YL]PHENOL	-	MFCD00208174	365.88	2.47E+05	-
HTS01224	EA209	2-[2-(4-HYDROXYPHENYL)-2,3-DIHYDRO-1,5-BENZOTHAZEPIN-4-YL]PHENOL	-	MFCD00208171	347.44	1.24E+04	-
HTS01226	EA214	7-HYDROXY-3-(4-METHOXYPHENYL)-2-PHENYL-4H-CHROMEN-4-ONE	-	MFCD00205546	344.36	-	-
HTS01230	EA228	METHYL 4-[[7-HYDROXY-4-OXO-2-(TRIFLUOROMETHYL)-4H-3-CHROMENYL]OXY]BENZOATE	-	MFCD00591449	380.27	-	-
HTS01231	EA240	N1-(2-[5-[4-(TERT-BUTYL)PHENYL]-1,3,4-OXADIAZOL-2-YL]PHENYL)-3-	-	MFCD00117576	411.50	-	-
HTS01234	EA263	2-[3-(4-METHOXYPHENYL)-3,3A,4,5-TETRAHYDRO-2H-BENZO[G]INDAZOL-2-	-	MFCD00178720	390.48	-	-
HTS01235	EA318	3-(4-METHOXYPHENYL)-2-PHENYL-2,3,3A,4-TETRAHYDRO[1]BENZOTHIOPYRANO[4,3-	-	MFCD02090132	372.49	-	-
HTS01237	EA326	3-(4-CHLOROPHENOXY)-7-HYDROXY-2-(TRIFLUOROMETHYL)-4H-CHROMEN-4-ONE	-	MFCD00382307	356.68	4.84E+05	-
HTS01242	ER544	MALACHITE GREEN BASE	510-13-4	-	346.48	-	-
HTS01245	ER600	Salicylic Acid 4-tert-Butylphenyl Ester	87-18-3	-	270.32	1.81E+05	3.68E+06
HTS01246	ER601	4-Aminobenzoic Acid Ethyl Ester	94-9-7	-	165.19	-	-
HTS01248	ER610	Benzophenone, 2-hydroxy-4-methoxy-	131-57-7	-	228.24	-	-
HTS01250	ER613	2-(2-Benzotriazolyl)-p-cresol	2440-22-4	-	225.25	-	-
HTS01255	ER622	2-Cyano-3,3-diphenylacrylic Acid Ethyl Ester	5232-99-5	-	277.32	6.39E+05	-
HTS01257	ER625	2-Cyano-3,3-diphenylacrylic Acid 2-Ethylhexyl Ester	6197-30-4	-	361.48	-	-
HTS01258	ER628	2-(2H-BENZOTRIAZOL-2-YL)-4,6-DI(T-	25973-55-1	-	351.49	-	-
HTS01260	ER636	Methylbenzylidene Camphor	36861-47-9	-	254.37	-	-

HTS No.: Intra laboratory I.D. used in this study

# ER $\beta$ / HeLa

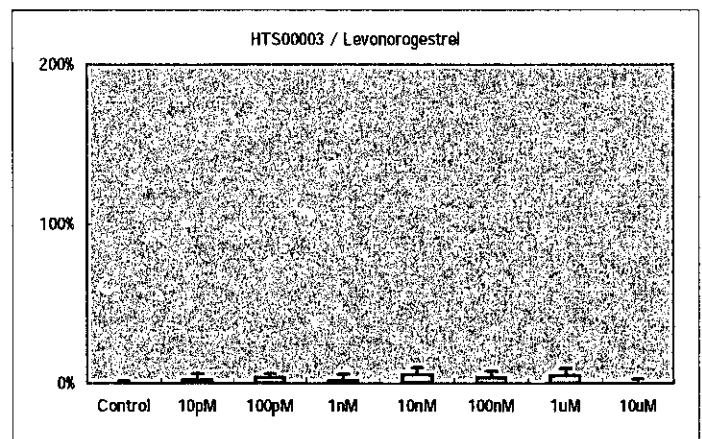
HTS00002  
Testosterone, dihydro

PC50 (pM): 2.05E+04



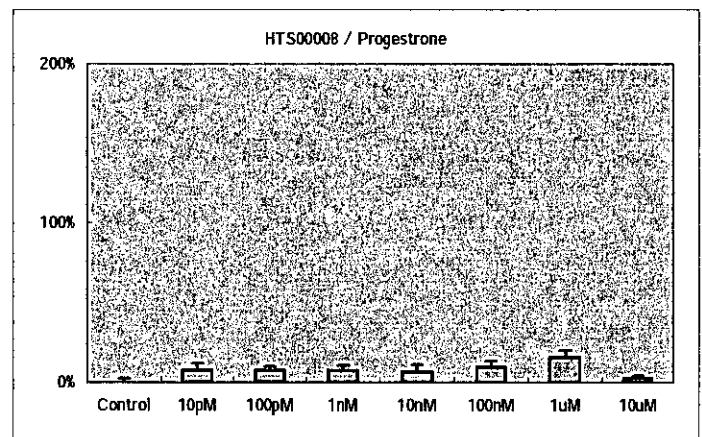
HTS00003  
Levonorgestrel

PC50 (pM): -



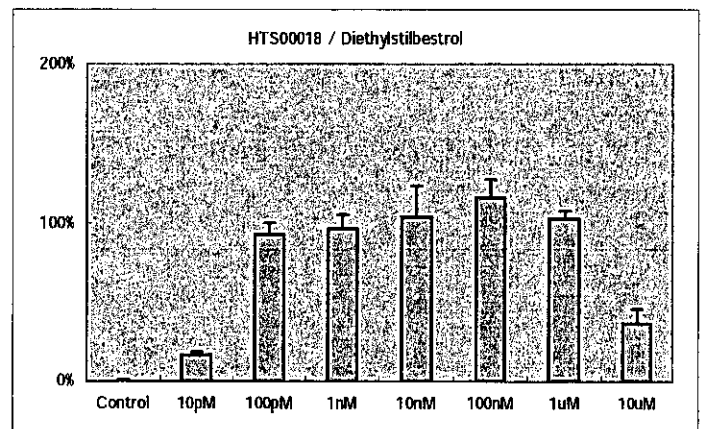
HTS00008  
Progestrone

PC50 (pM): -



HTS00018  
Diethylstilbestrol

PC50 (pM): 2.78E+01

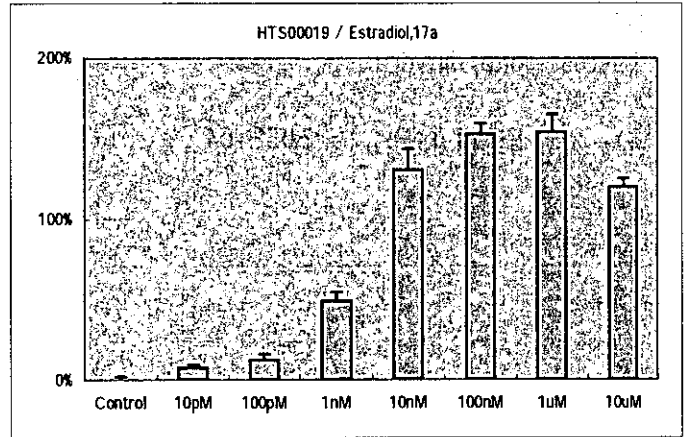




ER $\beta$  /HeLa

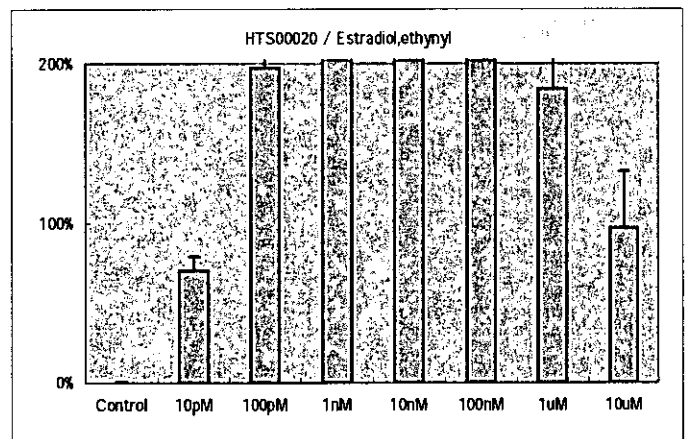
HTS00019  
Estradiol,17a

PC50 (pM): 1.02E+03



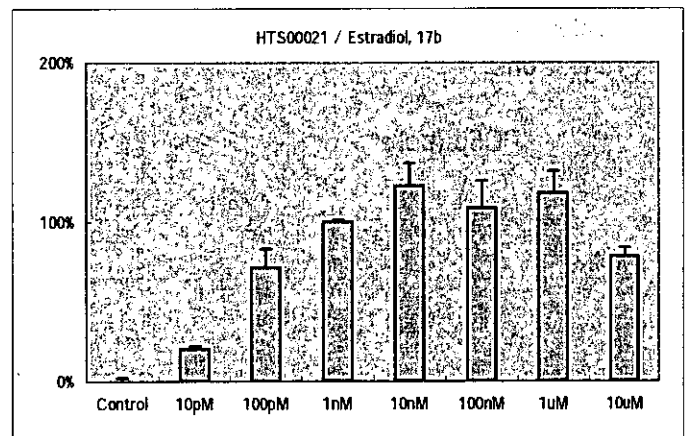
HTS00020  
Estradiol,ethynyl

PC50 (pM): <1.00E+1



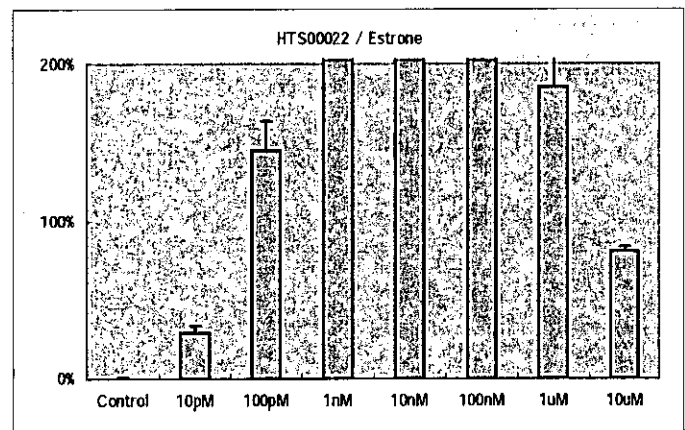
HTS00021  
Estradiol, 17b

PC50 (pM): 3.82E+01



HTS00022  
Estrone

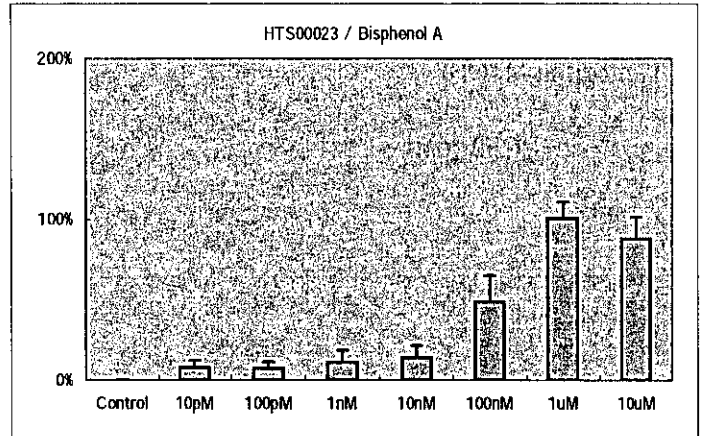
PC50 (pM): 1.52E+01



## ER $\beta$ /HeLa

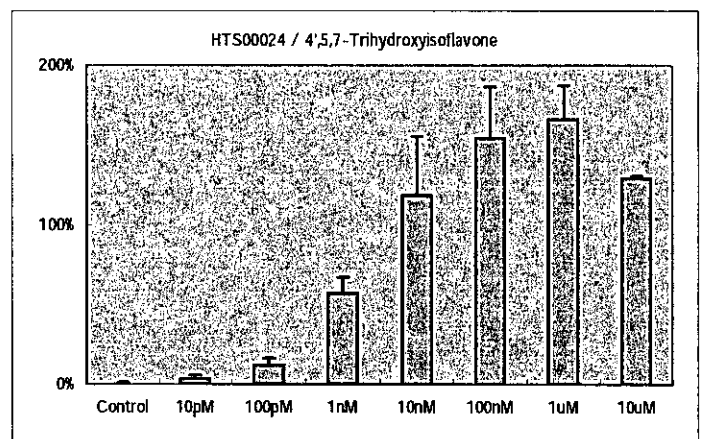
HTS00023  
Bisphenol A

PC50 (pM): 1.05E+05



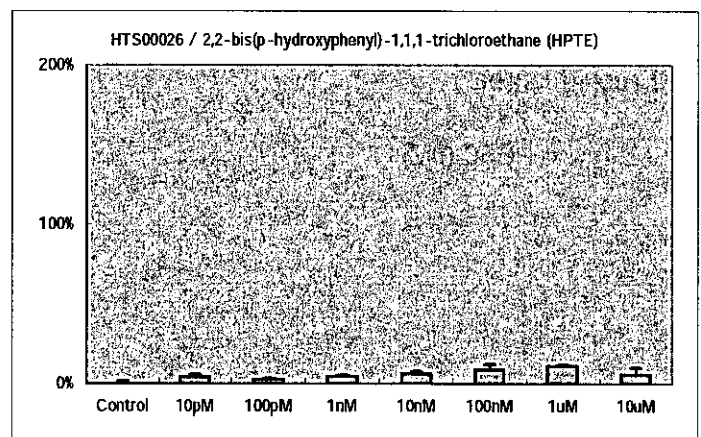
HTS00024  
4',5,7-Trihydroxyisoflavone

PC50 (pM): 6.96E+02



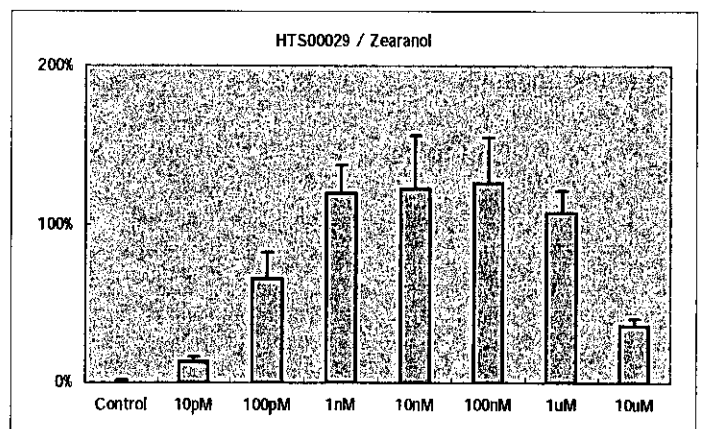
HTS00026  
2,2-bis(p-hydroxyphenyl)-1,1,1-trichloroethane (HPTE)

PC50 (pM): -



HTS00029  
Zearanol

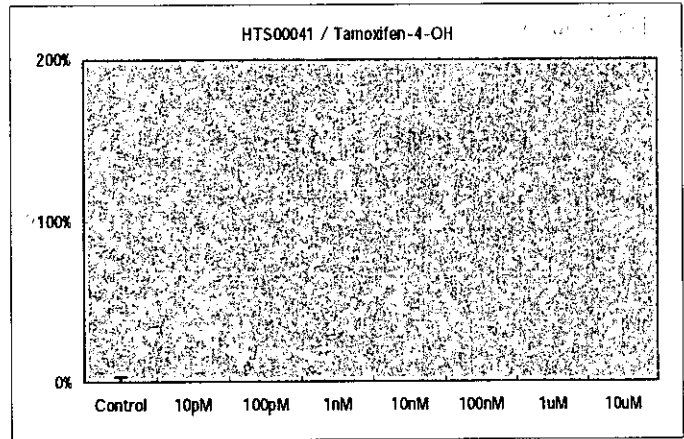
PC50 (pM): 5.08E+01



ER $\beta$  / HeLa

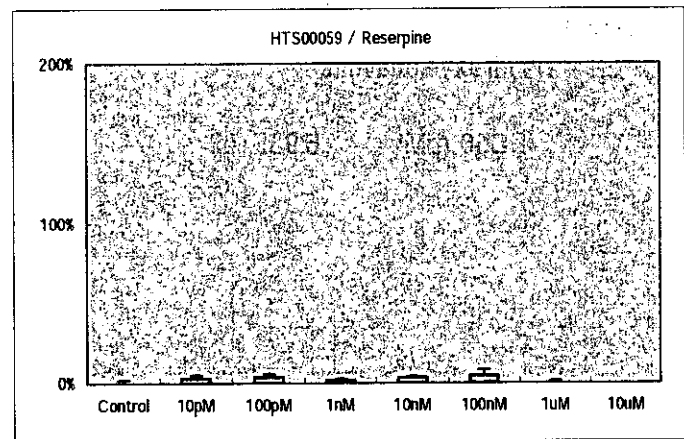
HTS00041  
Tamoxifen-4-OH

PC50 (pM): -



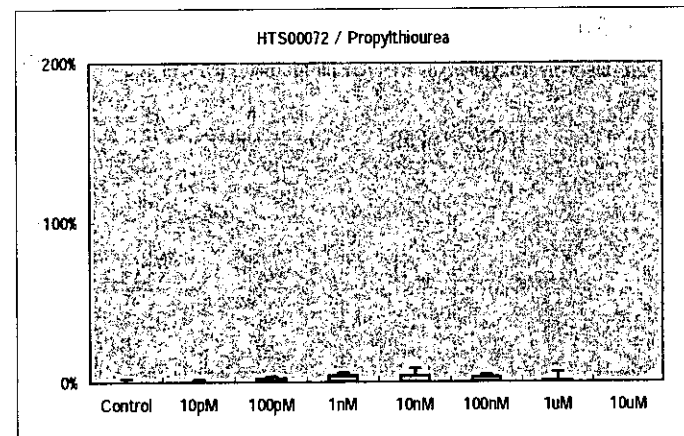
HTS00059  
Reserpine

PC50 (pM): -



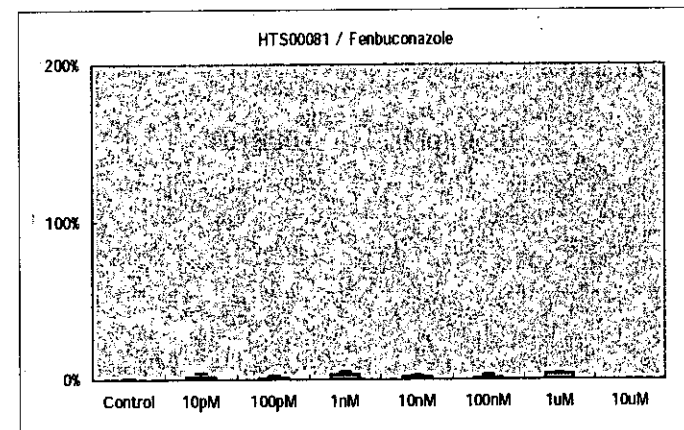
HTS00072  
Propylthiourea

PC50 (pM): -



HTS00081  
Fenbuconazole

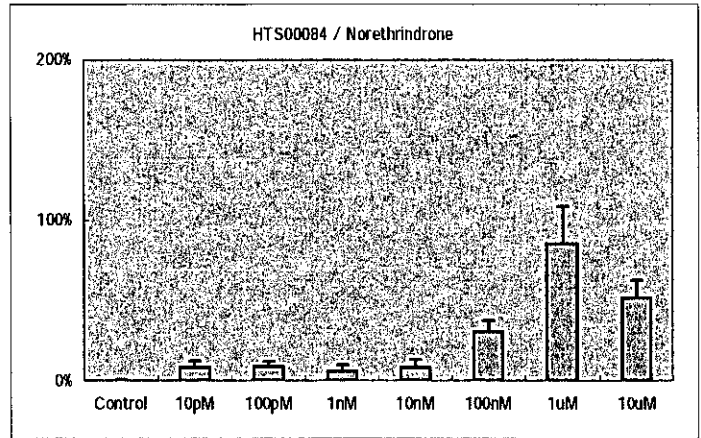
PC50 (pM): -



# ER $\beta$ /HeLa

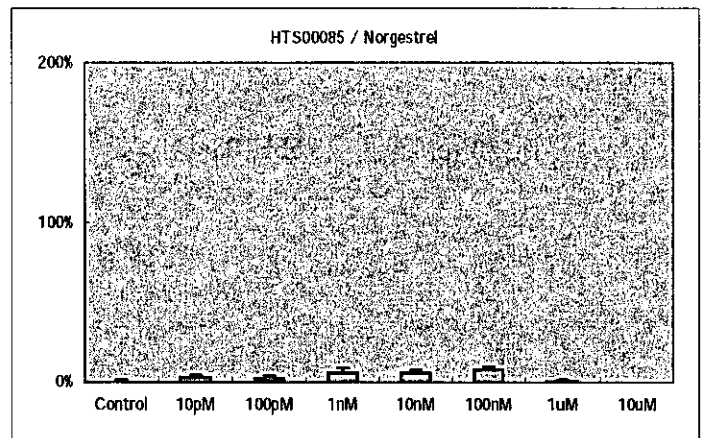
HTS00084  
Norethiridrone

PC50 (pM): 2.26E+05



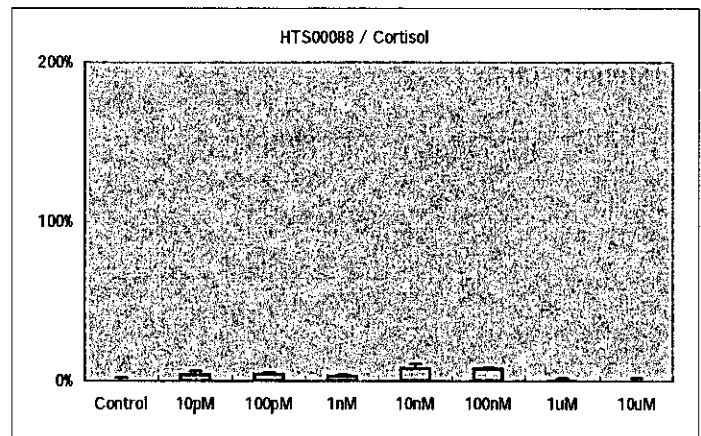
HTS00085  
Norgestrel

PC50 (pM): -



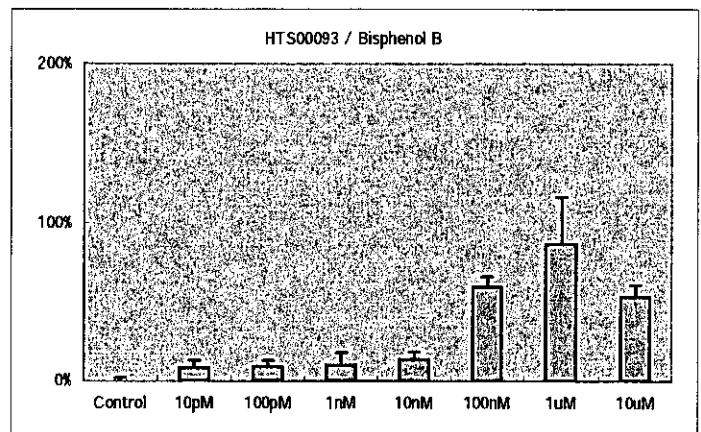
HTS00088  
Cortisol

PC50 (pM): -



HTS00093  
Bisphenol B

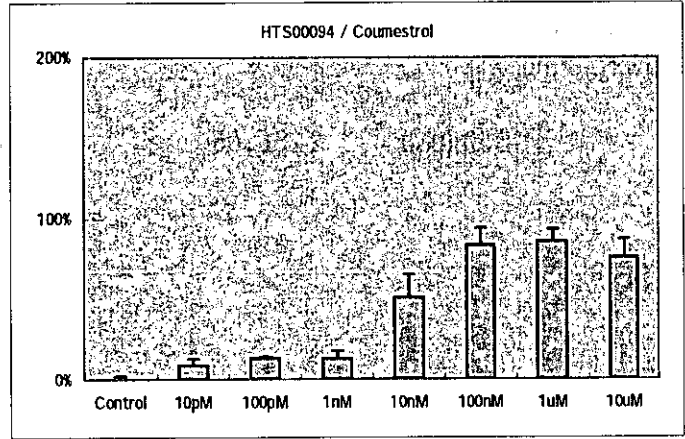
PC50 (pM): 6.29E+04



ER $\beta$  / HeLa

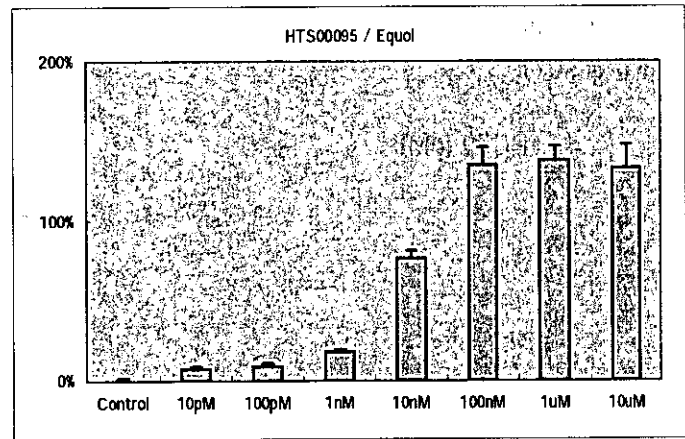
HTS00094  
Coumestrol

PC50 (pM): 9.45E+03



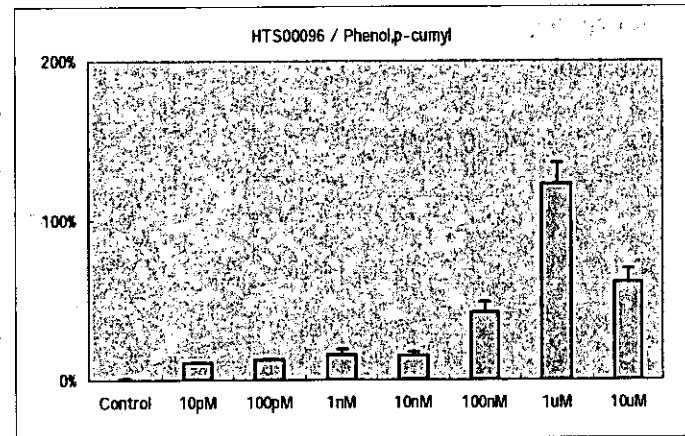
HTS00095  
Equol

PC50 (pM): 3.55E+03



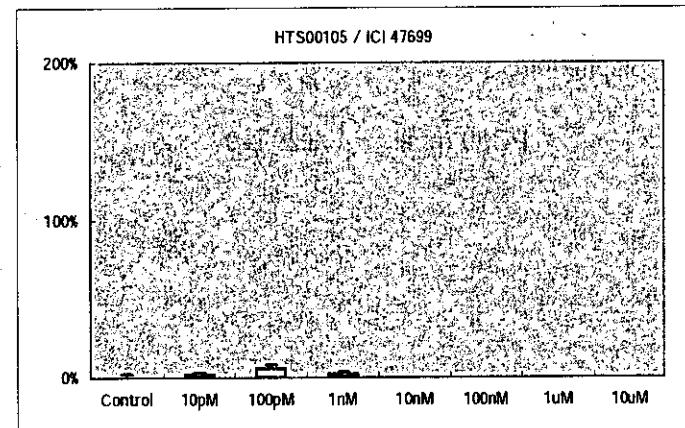
HTS00096  
Phenol,p-cumyl

PC50 (pM): 1.25E+05



HTS00105  
ICI 47699

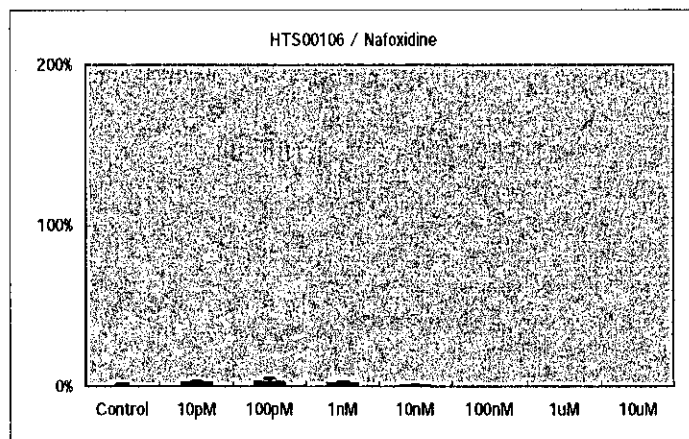
PC50 (pM): -



## ER $\beta$ /HeLa

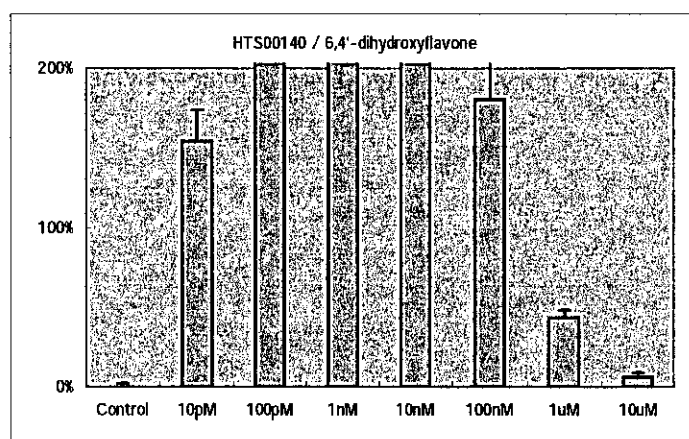
HTS00106  
Nafoxidine

PC50 (pM): -



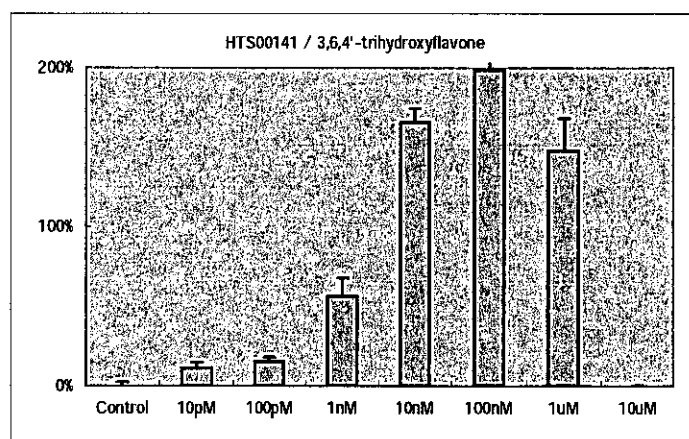
HTS00140  
6,4'-dihydroxyflavone

PC50 (pM): <1.00E+1



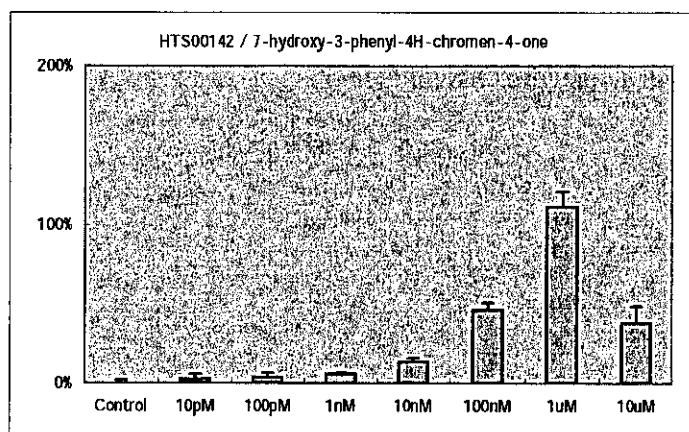
HTS00141  
3,6,4'-trihydroxyflavone

PC50 (pM): 7.08E+02



HTS00142  
7-hydroxy-3-phenyl-4H-chromen-4-one

PC50 (pM): 1.14E+05

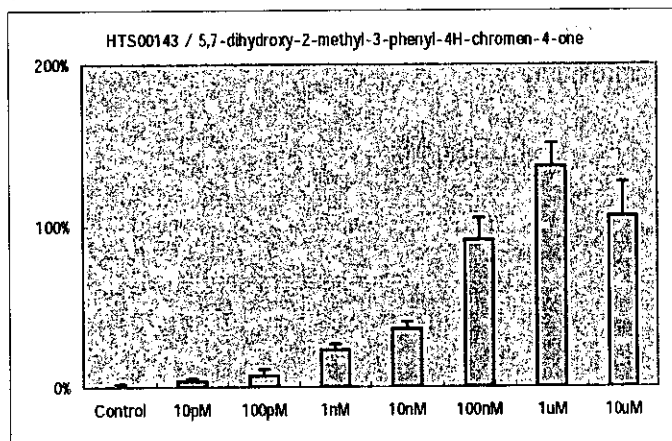


## ER $\beta$ / HeLa

HTS00143

5,7-dihydroxy-2-methyl-3-phenyl-4H-chromen-4-one

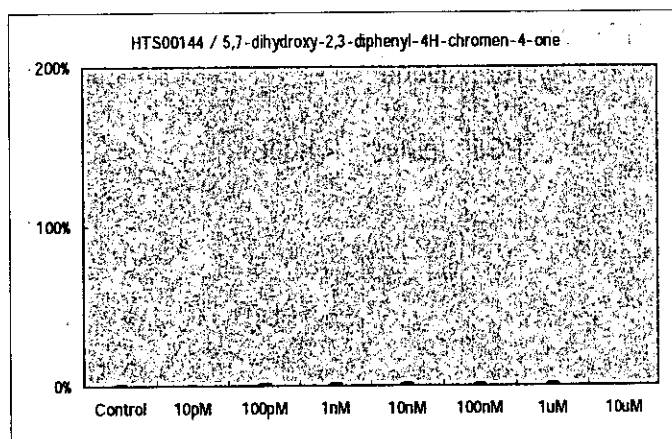
PC50 (pM): 1.78E+04



HTS00144

5,7-dihydroxy-2,3-diphenyl-4H-chromen-4-one

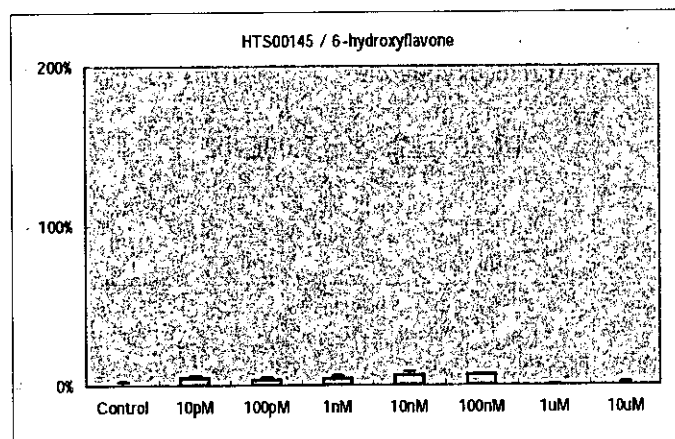
PC50 (pM): -



HTS00145

6-hydroxyflavone

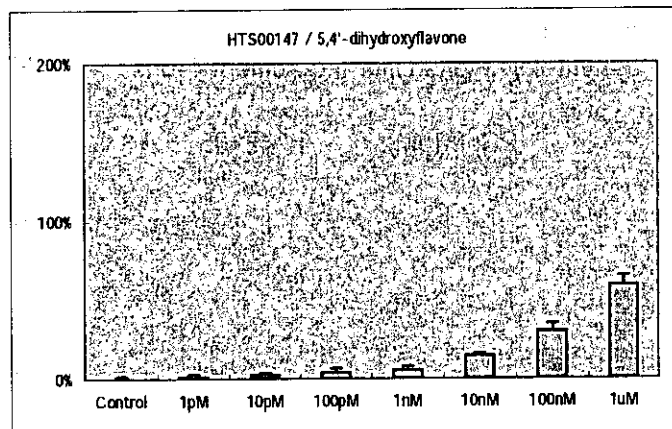
PC50 (pM): -



HTS00147

5,4'-dihydroxyflavone

PC50 (pM): 4.86E+05

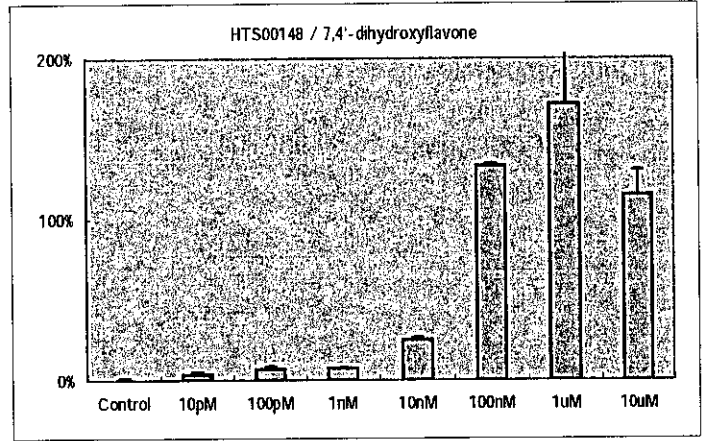




# ER $\beta$ / HeLa

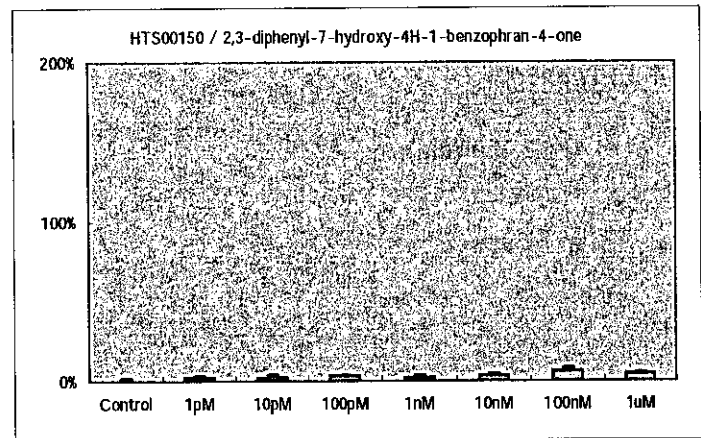
HTS00148  
7,4'-dihydroxyflavone

PC50 (pM): 1.71E+04



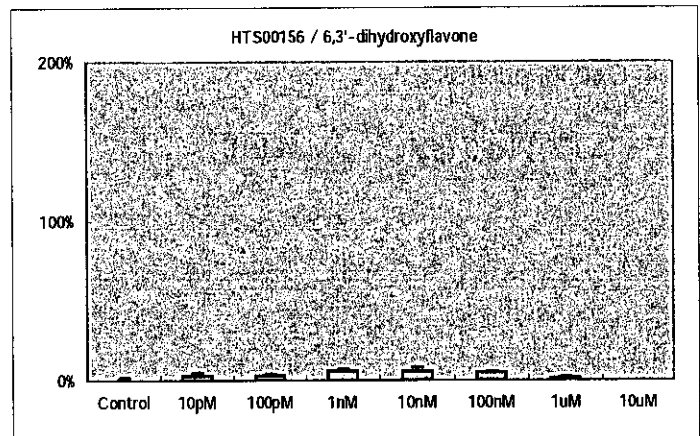
HTS00150  
2,3-diphenyl-7-hydroxy-4H-1-benzophran-4-one

PC50 (pM): -



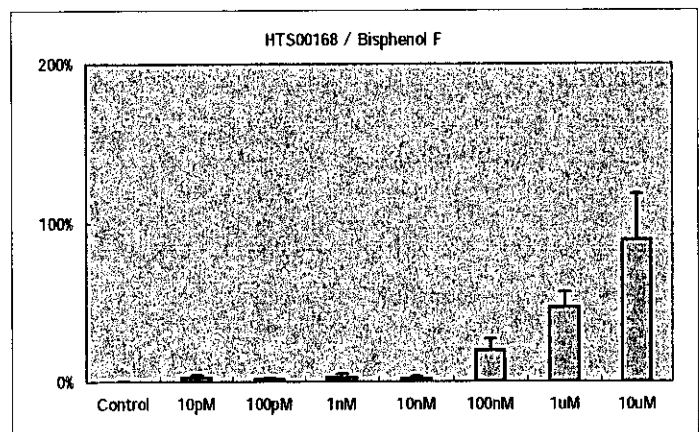
HTS00156  
6,3'-dihydroxyflavone

PC50 (pM): -



HTS00168  
Bisphenol F

PC50 (pM): 1.18E+06

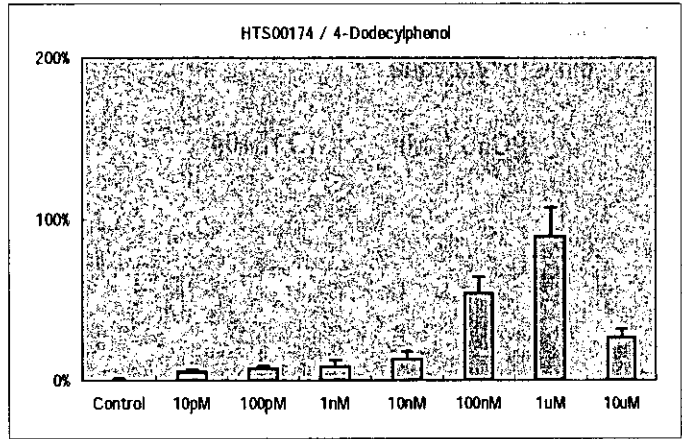




ERβ / HeLa

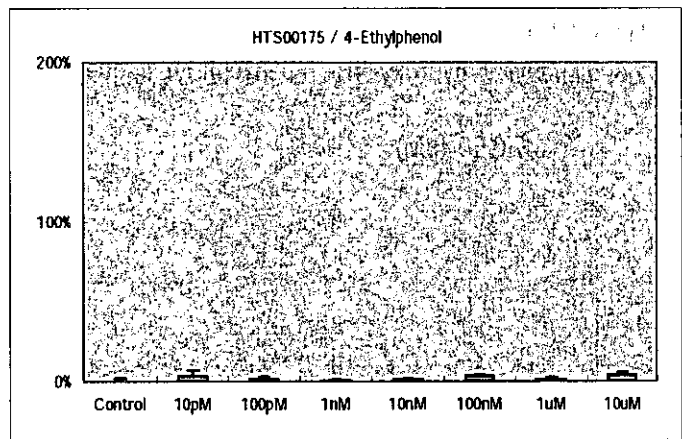
HTS00174  
4-Dodecylphenol

PC50 (pM): 7.98E+04



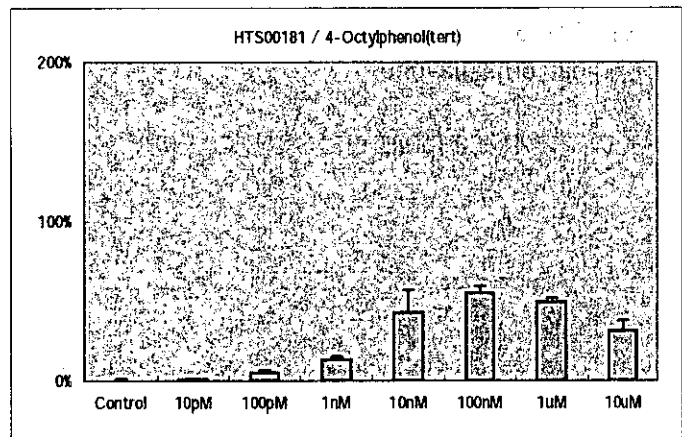
HTS00175  
4-Ethylphenol

PC50 (pM): -



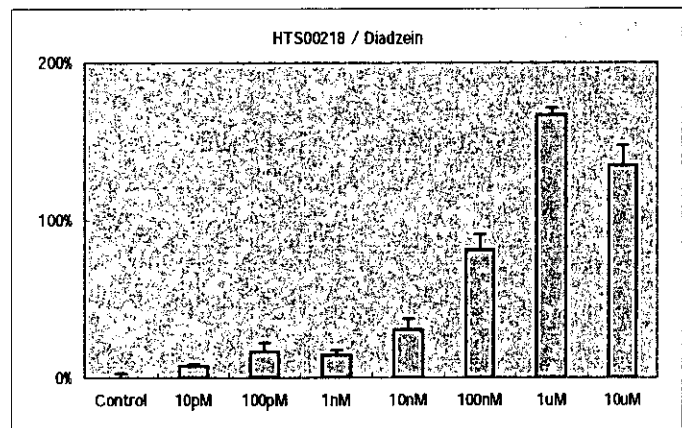
HTS00181  
4-Octylphenol(tert)

PC50 (pM): 4.16E+04



HTS00218  
Diadzein

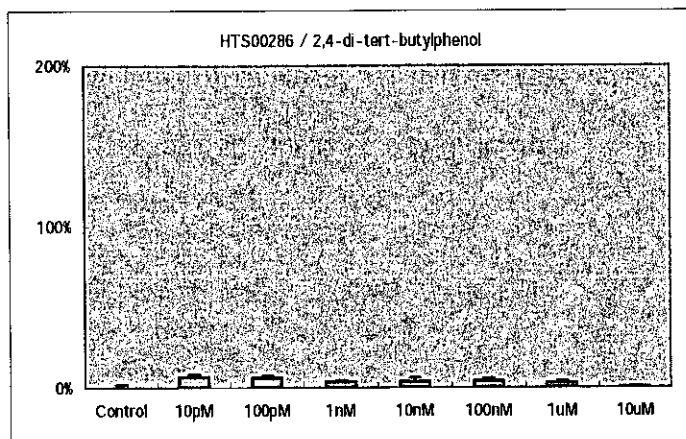
PC50 (pM): 2.41E+04



## ER $\beta$ /HeLa

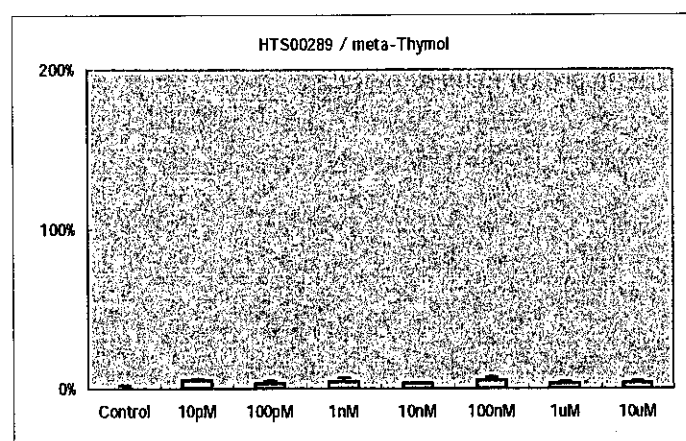
HTS00286  
2,4-di-tert-butylphenol

PC50 (pM): -



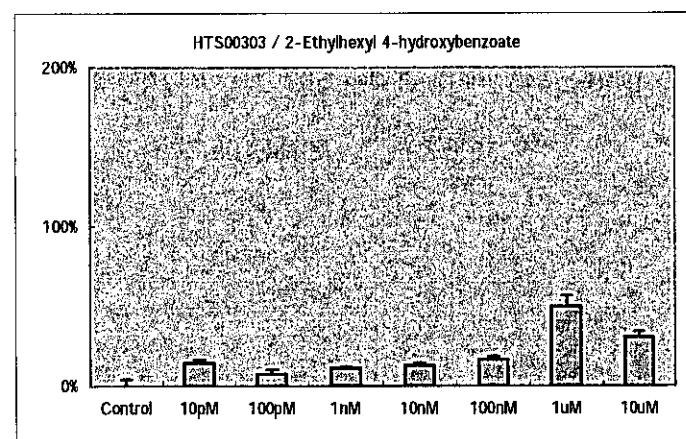
HTS00289  
meta-Thymol

PC50 (pM): -



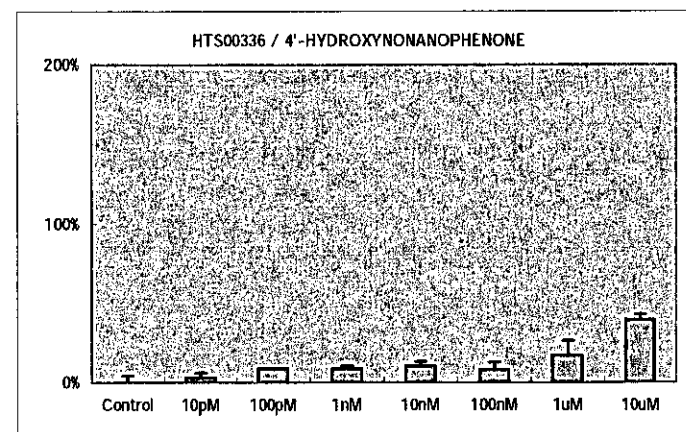
HTS00303  
2-Ethylhexyl 4-hydroxybenzoate

PC50 (pM): -



HTS00336  
4'-HYDROXYNONANOPHENONE

PC50 (pM): -

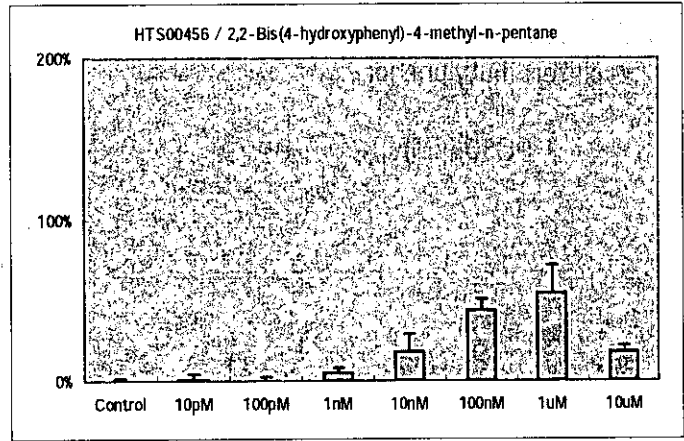


ER $\beta$  / HeLa

HTS00456

2,2-Bis(4-hydroxyphenyl)-4-methyl-n-pentane

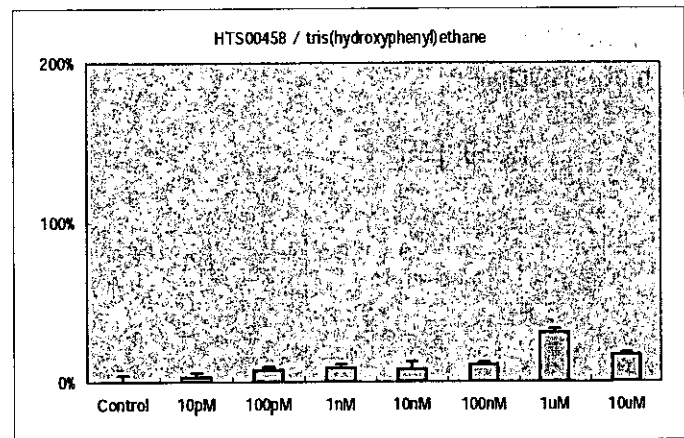
PC50 (pM): 3.80E+05



HTS00458

tris(hydroxyphenyl)ethane

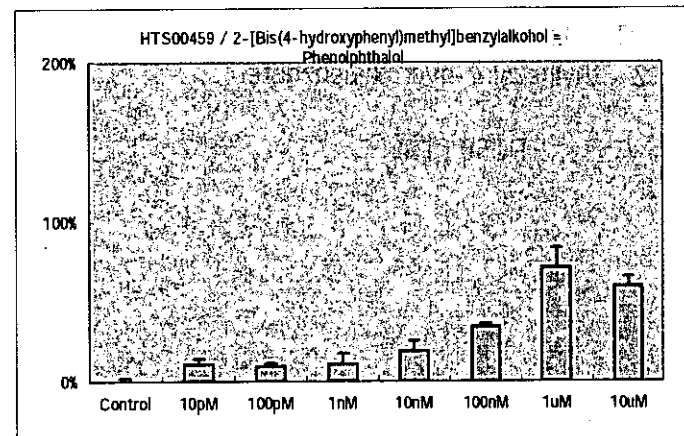
PC50 (pM): -



HTS00459

2-[Bis(4-hydroxyphenyl)methyl]benzylalcohol = Phenolphthalein

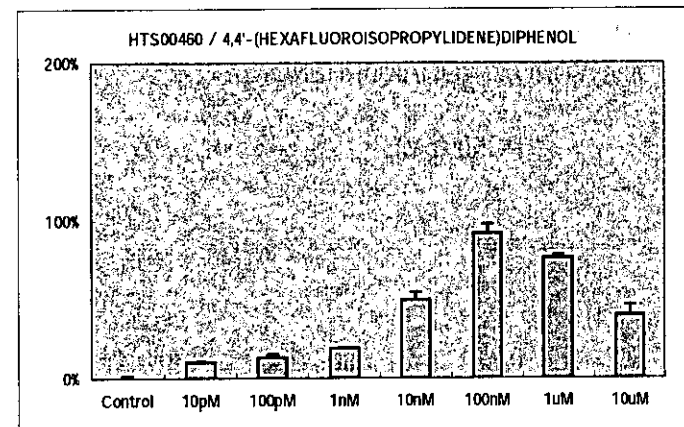
PC50 (pM): 2.70E+05



HTS00460

4,4'-(HEXAFLUOROISOPROPYLIDENE)DIPHENOL

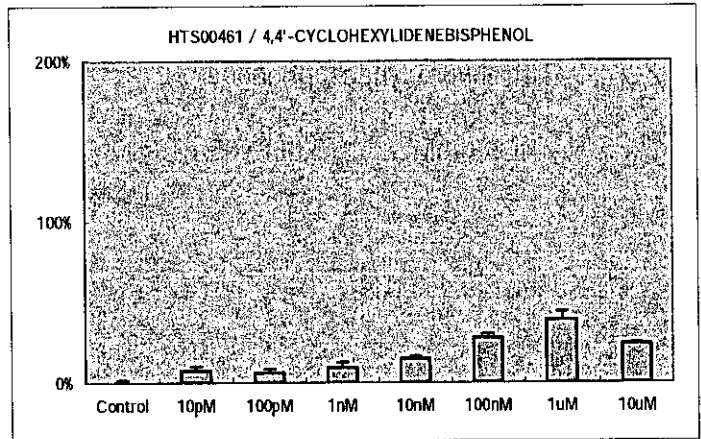
PC50 (pM): 1.03E+04



## ER $\beta$ / HeLa

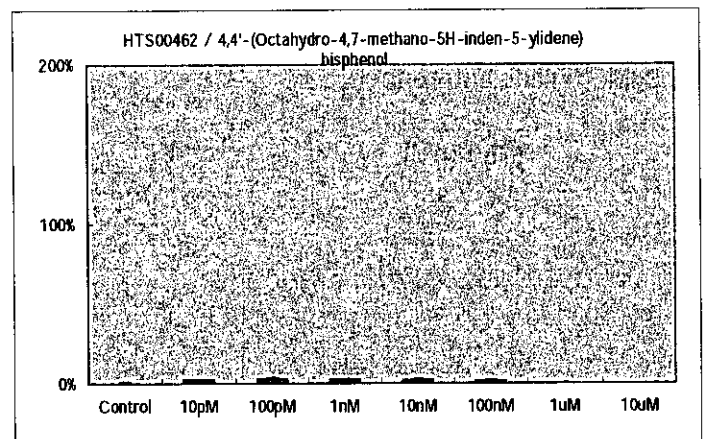
HTS00461  
4,4'-CYCLOHEXYLIDENE BISPHENOL

PC50 (pM): -



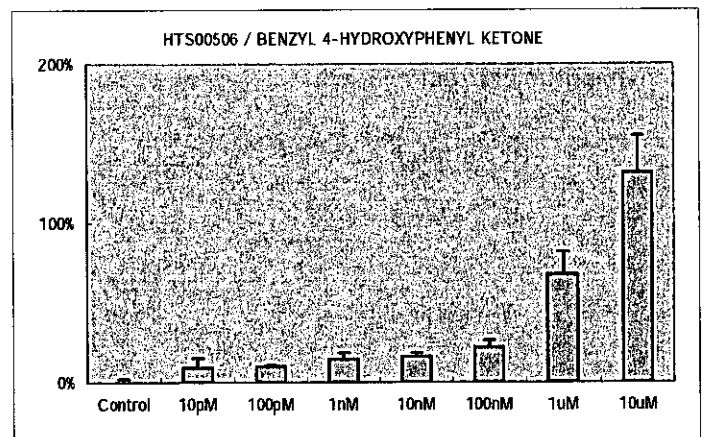
HTS00462  
4,4'-(Octahydro-4,7-methano-5H-inden-5-ylidene) bisphenol

PC50 (pM): -



HTS00506  
BENZYL 4-HYDROXYPHENYL KETONE

PC50 (pM): 4.18E+05



HTS00521  
2,4-Dihydroxybenzophenone

PC50 (pM): 6.24E+05

