

表 2. ER β ドッキングモデルにおける上位 1000 化合物のスコア値 (結合強度予測値)

CAS No.	Score	CAS No.	Score	CAS No.	Score
000050-02-2	0.18	000057-24-9	0.09	000067-03-8	0.48
000050-03-3	0.35	000057-63-6	0.92	000067-96-9	1.29
000050-04-4	0.29	000057-83-0	0.38	000067-97-0	0.63
000050-14-6	2.07	000057-85-2	0.47	000068-22-4	0.07
000050-22-6	0.63	000057-87-4	1.57	000068-23-5	0.41
000050-23-7	0.04	000057-91-0	0.82	000068-26-8	0.87
000050-27-1	1.46	000057-96-5	0.23	000069-23-8	-0.05
000050-28-2	1.16	000057-97-6	0.36	000071-58-9	0.45
000050-33-9	0.03	000058-18-4	0.68	000071-68-1	-0.02
000050-34-0	0.16	000058-22-0	0.55	000072-33-3	0.45
000050-37-3	0.44	000058-39-9	0.20	000072-48-0	-0.04
000050-41-9	0.65	000058-60-6	-0.06	000072-69-5	-0.04
000050-48-6	-0.06	000058-64-0	0.68	000076-42-6	0.05
000050-50-0	0.55	000058-72-0	0.21	000076-43-7	0.70
000050-52-2	0.32	000058-74-2	0.45	000076-58-4	0.33
000051-98-9	-0.02	000058-97-9	0.17	000076-61-9	0.93
000052-21-1	0.05	000059-02-9	0.20	000076-99-3	0.03
000052-39-1	0.66	000059-05-2	0.71	000077-08-7	1.72
000052-76-6	0.41	000059-30-3	1.04	000077-09-8	0.70
000052-78-8	0.32	000060-81-1	1.03	000078-32-0	0.11
000052-88-0	0.17	000060-93-5	0.13	000078-33-1	0.60
000053-06-5	0.47	000060-99-1	0.14	000079-96-9	0.04
000053-16-7	0.59	000061-25-6	0.19	000079-97-0	0.30
000053-41-8	0.31	000061-73-4	0.87	000080-04-6	0.44
000053-42-9	-0.01	000062-90-8	0.06	000080-49-9	0.37
000053-43-0	0.24	000063-01-4	0.92	000080-51-3	0.30
000053-70-3	0.15	000063-37-6	0.80	000080-75-1	0.25
000053-86-1	-0.04	000064-72-2	0.37	000081-14-1	0.19
000054-28-4	0.59	000064-85-7	0.44	000081-23-2	0.40
000054-62-6	0.76	000064-86-8	1.36	000081-26-5	0.95
000055-80-1	0.09	000065-19-0	0.54	000081-37-8	0.33
000056-49-5	0.65	000065-28-1	0.41	000081-68-5	0.31
000056-53-1	0.63	000065-61-2	0.24	000081-92-5	0.41
000056-65-5	0.31	000066-28-4	0.10	000081-95-8	0.98

表 2. (続き 1)

CAS No.	Score	CAS No.	Score	CAS No.	Score
000082-08-6	0.79	000092-74-0	0.13	000125-02-0	1.98
000082-22-4	0.66	000092-75-1	0.31	000125-04-2	0.03
000083-44-3	0.46	000093-23-2	0.11	000125-20-2	1.04
000083-49-8	0.18	000093-45-8	-0.05	000125-28-0	0.03
000083-63-6	0.08	000093-46-9	0.48	000125-31-5	1.59
000083-80-7	0.06	000093-69-6	1.47	000125-56-4	0.03
000084-16-2	0.29	000096-66-2	0.29	000127-25-3	0.20
000084-17-3	1.04	000096-69-5	0.36	000128-13-2	0.32
000084-19-5	0.28	000097-56-3	0.02	000128-20-1	0.37
000084-61-7	0.15	000099-21-8	0.04	000128-23-4	0.56
000084-62-8	0.11	000101-01-9	0.39	000128-62-1	0.92
000084-80-0	-0.02	000101-02-0	-0.02	000128-70-1	0.97
000084-94-6	0.26	000101-56-4	-0.02	000128-80-3	0.41
000085-00-7	0.37	000102-02-3	0.49	000128-87-0	0.33
000085-32-5	0.35	000103-96-8	-0.06	000128-88-1	0.86
000085-83-6	0.44	000113-52-0	-0.02	000129-73-7	0.35
000085-86-9	0.06	000115-40-2	0.34	000130-40-5	0.54
000086-15-7	0.02	000115-41-3	1.18	000130-80-3	0.96
000086-44-2	0.10	000115-86-6	0.13	000130-86-9	0.08
000088-24-4	0.38	000116-31-4	0.45	000130-90-5	-0.06
000090-18-6	0.83	000117-46-4	-0.02	000131-22-6	0.27
000090-66-4	0.12	000117-92-0	1.07	000131-99-7	1.21
000090-68-6	0.51	000118-08-1	0.52	000132-18-3	0.11
000090-94-8	0.30	000119-13-1	1.12	000132-69-4	0.08
000091-73-6	0.28	000119-15-3	0.02	000135-16-0	0.22
000091-78-1	0.82	000119-47-1	0.29	000135-48-8	0.22
000091-84-9	-0.06	000119-90-4	-0.06	000135-57-9	0.99
000092-21-7	0.08	000119-93-7	-0.02	000135-61-5	0.04
000092-29-5	0.17	000120-24-1	-0.07	000135-62-6	-0.05
000092-31-9	0.72	000120-70-7	0.04	000135-64-8	0.59
000092-32-0	0.76	000121-06-2	1.12	000137-52-0	0.12
000092-36-4	0.08	000121-54-0	0.20	000140-64-7	2.67
000092-72-8	0.13	000122-11-2	0.07	000140-66-9	-0.05
000092-73-9	0.24	000123-03-5	0.23	000140-72-7	0.23

表 2. (続き 2)

CAS No.	Score	CAS No.	Score	CAS No.	Score
000143-62-4	0.20	000297-76-7	0.22	000465-39-4	0.99
000143-74-8	0.69	000298-57-7	0.38	000466-09-1	0.44
000145-13-1	0.33	000298-93-1	1.02	000466-99-9	-0.02
000145-14-2	0.52	000298-96-4	0.51	000467-15-2	0.04
000145-15-3	0.86	000302-95-4	0.46	000467-62-9	0.39
000145-39-1	-0.06	000303-49-1	-0.05	000470-37-1	0.21
000145-41-5	0.40	000304-28-9	-0.03	000470-55-3	0.73
000145-50-6	1.79	000313-04-2	1.64	000471-77-2	0.16
000146-48-5	0.54	000313-06-4	0.68	000471-95-4	0.21
000146-56-5	-0.05	000314-19-2	0.46	000472-41-3	0.29
000146-68-9	0.86	000315-37-7	0.37	000472-54-8	0.34
000151-73-5	0.85	000316-14-3	-0.05	000472-86-6	0.59
000152-11-4	0.36	000357-57-3	0.23	000474-07-7	0.63
000152-43-2	0.41	000360-70-3	0.26	000474-25-9	-0.04
000153-00-4	0.67	000362-05-0	1.83	000474-86-2	0.68
000154-21-2	0.35	000362-06-1	1.35	000475-25-2	0.24
000154-23-4	0.98	000362-07-2	0.70	000475-71-8	0.68
000155-41-9	0.58	000362-08-3	0.46	000475-91-2	0.27
000155-84-0	0.10	000366-29-0	-0.06	000476-32-4	0.58
000189-55-9	0.53	000378-44-9	0.54	000476-66-4	0.19
000189-64-0	0.44	000379-68-0	0.16	000476-70-0	0.15
000190-26-1	0.63	000382-44-5	0.01	000477-30-5	0.29
000191-24-2	0.07	000382-45-6	-0.01	000477-73-6	1.97
000191-26-4	-0.02	000382-67-2	0.18	000479-13-0	0.44
000191-30-0	0.30	000426-13-1	-0.06	000479-20-9	0.18
000192-65-4	0.55	000434-03-7	0.44	000479-23-2	0.19
000193-39-5	0.16	000434-07-1	0.46	000479-33-4	1.01
000213-46-7	0.34	000434-13-9	0.22	000479-98-1	0.13
000214-17-5	0.16	000434-22-0	0.58	000480-18-2	0.56
000215-58-7	0.26	000434-85-5	0.56	000481-29-8	0.82
000224-41-9	0.07	000438-07-3	0.70	000481-30-1	0.21
000224-42-0	0.13	000440-17-5	0.10	000481-53-8	0.42
000226-36-8	-0.01	000446-72-0	0.18	000483-04-5	0.37
000226-88-0	0.35	000458-37-7	0.58	000483-65-8	0.00

表 2. (続き 3)

CAS No.	Score	CAS No.	Score	CAS No.	Score
000484-47-9	0.00	000520-85-4	0.34	000563-04-2	0.27
000485-72-3	0.46	000521-10-8	1.35	000565-20-8	0.09
000486-66-8	0.29	000521-11-9	0.56	000569-57-3	1.42
000487-24-1	-0.07	000521-17-5	1.50	000569-61-9	0.55
000487-41-2	-0.03	000521-18-6	0.52	000571-20-0	1.32
000490-46-0	0.66	000521-35-7	0.14	000574-45-8	0.54
000491-70-3	0.68	000521-78-8	0.28	000574-61-8	0.31
000491-80-5	0.38	000522-12-3	1.71	000574-69-6	0.10
000493-77-6	0.31	000523-44-4	0.39	000580-35-8	0.53
000497-76-7	0.00	000526-08-9	0.29	000581-64-6	0.25
000500-38-9	0.87	000528-48-3	0.25	000596-03-2	0.90
000501-24-6	0.11	000530-14-3	0.53	000596-09-8	0.22
000508-52-1	-0.02	000531-52-2	0.26	000596-27-0	1.36
000510-13-4	0.34	000531-95-3	0.19	000599-79-1	0.17
000510-50-9	0.11	000532-43-4	0.48	000600-57-7	0.68
000510-64-5	0.08	000538-41-0	-0.07	000602-09-5	0.21
000510-74-7	0.23	000538-71-6	0.20	000602-55-1	0.10
000511-09-1	0.17	000539-17-3	0.37	000603-34-9	0.09
000511-15-9	0.45	000544-47-8	0.26	000603-45-2	0.50
000512-69-6	0.26	000545-26-6	-0.01	000603-48-5	1.18
000514-17-0	0.76	000547-58-0	0.01	000603-50-9	0.27
000514-73-8	1.13	000547-75-1	0.75	000604-53-5	0.13
000514-85-2	0.18	000547-81-9	1.06	000604-59-1	0.07
000515-03-7	0.06	000548-37-8	1.03	000606-68-8	0.93
000516-15-4	0.31	000548-62-9	0.96	000606-91-7	0.11
000516-54-1	0.45	000548-73-2	0.46	000612-71-5	0.61
000516-92-7	0.46	000549-18-8	0.25	000612-78-2	0.11
000517-09-9	0.53	000549-56-4	0.13	000612-82-8	-0.02
000518-20-7	0.33	000550-15-2	1.75	000620-42-8	0.57
000518-28-5	0.84	000550-70-9	0.38	000622-21-9	0.46
000520-12-7	0.16	000552-22-7	0.16	000630-56-8	0.64
000520-27-4	0.11	000552-58-9	0.11	000632-51-9	0.57
000520-28-5	0.09	000553-24-2	0.38	000633-65-8	1.08
000520-36-5	-0.03	000561-27-3	0.30	000633-96-5	0.37

表 2. (続き 4)

CAS No.	Score	CAS No.	Score	CAS No.	Score
000634-21-9	1.34	000979-02-2	0.35	001229-24-9	1.08
000642-04-6	0.35	000979-32-8	1.37	001229-29-4	0.00
000643-84-5	1.48	000985-13-7	0.25	001231-82-9	0.14
000653-63-4	0.14	000987-24-6	0.06	001231-93-2	1.02
000659-22-3	0.04	000987-65-5	0.31	001234-35-1	0.41
000739-71-9	0.24	000989-38-8	1.19	001236-72-2	1.18
000744-45-6	0.07	001034-01-1	-0.06	001237-75-8	0.02
000749-02-0	0.33	001045-69-8	0.02	001239-79-8	0.66
000785-30-8	0.05	001046-56-6	0.07	001249-97-4	0.78
000791-69-5	1.23	001056-77-5	0.63	001251-85-0	0.18
000793-24-8	0.04	001058-71-5	0.64	001320-06-5	0.48
000797-63-7	0.03	001087-26-9	-0.02	001330-78-5	0.31
000804-63-7	0.13	001096-38-4	0.37	001424-00-6	0.65
000834-28-6	0.21	001096-80-6	0.51	001434-54-4	0.48
000838-88-0	-0.03	001097-51-4	0.36	001446-61-3	0.00
000846-46-8	0.15	001098-97-1	0.08	001450-63-1	1.46
000846-48-0	0.12	001099-45-2	0.09	001474-53-9	0.61
000848-53-3	0.10	001100-88-5	0.21	001476-34-2	0.42
000853-23-6	0.48	001104-22-9	0.06	001483-74-5	0.60
000853-34-9	0.01	001113-21-9	0.19	001485-92-3	0.32
000855-38-9	0.15	001153-51-1	0.51	001498-88-0	0.04
000895-37-4	0.46	001158-94-7	0.55	001499-10-1	0.76
000897-55-2	0.09	001159-53-1	0.69	001533-45-5	-0.03
000901-56-4	1.16	001162-53-4	1.35	001607-57-4	0.27
000901-93-9	-0.03	001162-56-7	0.40	001617-90-9	0.17
000905-96-4	0.97	001165-14-6	0.66	001620-68-4	0.87
000906-83-2	1.00	001166-52-5	0.13	001624-62-0	0.17
000908-54-3	2.78	001169-54-6	0.29	001658-56-6	0.65
000911-77-3	2.73	001173-26-8	0.06	001662-01-7	0.06
000963-74-6	0.06	001218-35-5	0.09	001663-45-2	0.21
000963-89-3	0.32	001222-05-5	0.33	001672-46-4	1.14
000974-23-2	0.67	001224-92-6	0.69	001674-18-6	1.28
000976-71-6	0.72	001224-95-9	0.09	001684-14-6	0.17
000977-96-8	0.91	001225-43-0	0.85	001696-60-2	0.59

表 2. (続き 5)

CAS No.	Score	CAS No.	Score	CAS No.	Score
001705-85-7	0.07	002321-07-5	0.63	003073-87-8	0.32
001707-75-1	0.48	002381-16-0	0.21	003085-82-3	0.28
001733-12-6	1.63	002381-39-7	0.06	003118-97-6	0.40
001778-02-5	0.72	002381-40-0	0.04	003147-14-6	0.46
001784-04-9	1.29	002387-03-3	0.76	003147-75-9	0.19
001801-42-9	0.28	002390-54-7	0.69	003166-00-5	0.11
001817-68-1	0.17	002392-39-4	0.58	003176-77-0	-0.02
001852-53-5	0.97	002397-00-4	0.86	003180-81-2	0.04
001919-48-8	0.63	002417-04-1	0.15	003230-39-5	0.12
001934-20-9	0.09	002425-85-6	0.30	003236-71-3	0.26
001936-15-8	0.08	002447-57-6	0.02	003294-03-9	0.78
001943-97-1	1.44	002456-45-3	0.58	003301-79-9	0.38
001944-12-3	0.03	002465-27-2	-0.07	003326-32-7	0.65
001972-08-3	0.08	002479-49-4	0.01	003326-34-9	0.60
001973-05-3	0.13	002492-87-7	-0.01	003327-24-0	0.03
002026-24-6	0.00	002498-75-1	0.09	003351-32-4	0.17
002030-63-9	0.71	002512-29-0	0.41	003379-38-2	0.12
002079-00-7	0.33	002582-07-2	0.66	003468-63-1	0.23
002090-82-6	3.70	002622-26-6	0.07	003482-37-9	0.11
002103-64-2	0.90	002624-43-3	0.21	003483-82-7	0.22
002123-35-5	0.07	002646-17-5	0.02	003520-42-1	1.02
002132-70-9	0.02	002650-17-1	1.07	003521-06-0	1.42
002135-17-3	0.13	002657-25-2	0.13	003564-15-6	0.12
002140-67-2	0.56	002666-17-3	0.38	003564-22-5	1.04
002150-48-3	0.33	002716-10-1	0.25	003618-58-4	1.01
002162-74-5	0.89	002800-80-8	0.43	003618-63-1	0.03
002185-86-6	1.32	002832-40-8	-0.03	003648-36-0	0.75
002197-01-5	1.04	002955-38-6	0.02	003682-35-7	0.12
002208-12-0	0.50	002959-74-2	-0.01	003689-20-1	0.11
002218-94-2	0.54	003016-97-5	0.13	003697-24-3	-0.07
002299-73-2	0.27	003027-01-8	0.21	003704-09-4	0.76
002303-01-7	1.26	003029-32-1	0.31	003734-33-6	1.05
002313-87-3	-0.02	003065-79-0	1.31	003734-67-6	0.18
002320-96-9	0.93	003071-70-3	1.18	003770-80-7	-0.05

表 2. (続き 6)

CAS No.	Score	CAS No.	Score	CAS No.	Score
003770-82-9	0.21	005384-21-4	0.06	006318-17-8	0.44
003808-20-6	0.36	005385-75-1	0.09	006358-31-2	0.04
003810-51-3	0.32	005392-67-6	0.80	006361-29-1	0.77
003846-71-7	0.12	005413-75-2	-0.05	006361-49-5	0.17
003864-99-1	0.19	005418-95-1	0.26	006368-72-5	0.42
003924-22-9	1.56	005421-66-9	0.70	006406-32-2	1.35
003930-19-6	0.09	005442-32-0	0.20	006408-51-1	0.29
004098-40-2	1.07	005466-99-9	0.37	006408-57-7	0.85
004181-05-9	0.44	005486-84-0	0.21	006408-72-6	0.56
004208-80-4	1.80	005521-31-3	-0.01	006410-10-2	0.10
004270-70-6	0.37	005550-12-9	0.35	006416-57-5	0.03
004403-89-8	0.11	005591-45-7	0.40	006441-82-3	1.41
004403-90-1	0.16	005613-46-7	0.38	006441-96-9	0.24
004424-03-7	1.29	005663-04-7	0.33	006535-42-8	0.65
004430-20-0	0.94	005836-29-3	0.25	006620-60-6	0.05
004441-01-4	-0.02	005850-16-8	-0.04	006625-46-3	0.59
004474-24-2	0.89	005850-35-1	0.05	006708-61-8	1.51
004477-79-6	0.37	005850-39-5	0.11	006709-58-6	0.30
004546-55-8	0.34	005858-33-3	0.07	006737-42-4	0.11
004546-72-9	0.21	005873-16-5	1.26	006738-04-1	0.04
004548-53-2	0.58	006035-94-5	0.70	006807-17-6	0.21
004657-00-5	2.17	006051-87-2	0.05	006844-74-2	-0.06
004678-45-9	0.80	006052-15-9	-0.02	007385-67-3	-0.04
004691-65-0	1.21	006054-48-4	0.43	007423-31-6	0.96
004733-39-5	0.61	006088-51-3	0.12	007477-67-0	0.20
004759-48-2	-0.04	006106-46-3	0.58	007478-69-5	0.01
005007-67-0	0.04	006163-58-2	0.54	007496-02-8	0.03
005051-62-7	0.59	006197-30-4	-0.03	007496-10-8	-0.02
005102-79-4	0.34	006224-63-1	0.20	007507-01-9	0.36
005150-50-5	0.36	006232-56-0	0.39	007549-43-1	0.13
005232-99-5	0.01	006232-57-1	0.69	007688-25-7	0.05
005254-41-1	0.16	006268-49-1	0.14	007689-03-4	0.13
005290-62-0	0.29	006271-79-0	0.10	007695-91-2	0.35
005326-42-1	-0.05	006300-37-4	0.16	007727-33-5	1.33

表 2. (続き 7)

CAS No.	Score	CAS No.	Score	CAS No.	Score
007757-83-7	-0.03	014263-94-6	1.38	020440-93-1	0.29
007773-03-7	-0.05	014414-32-5	0.68	020440-95-3	0.60
007782-99-2	-0.03	014521-96-1	1.02	020721-50-0	-0.02
008004-87-3	0.96	014806-50-9	0.95	020725-03-5	0.16
010048-13-2	0.06	014926-29-5	0.71	020838-44-2	0.03
010049-83-9	0.08	014934-37-3	1.18	021145-77-7	0.24
010081-67-1	0.32	015086-94-9	-0.05	021255-69-6	0.35
010117-38-1	-0.05	015185-43-0	1.07	021259-20-1	0.30
010161-34-9	0.10	015546-43-7	1.03	021637-25-2	1.85
010191-41-0	-0.04	015940-86-0	0.13	022395-24-0	0.03
010192-30-0	-0.03	016178-48-6	0.68	022525-43-5	0.18
010196-04-0	-0.03	016432-81-8	-0.01	022948-06-7	0.24
010291-28-8	0.35	016574-43-9	-0.04	023001-29-8	0.33
010418-03-8	1.29	016740-38-8	-0.05	023060-42-6	0.23
010453-86-8	0.14	016766-09-9	0.13	023236-18-2	0.00
010526-07-5	0.51	016803-97-7	-0.04	023582-02-7	0.35
010540-29-1	0.75	016840-28-1	-0.05	023807-28-5	0.59
010592-13-9	0.14	017230-88-5	0.79	023941-48-2	0.63
012270-13-2	0.22	017540-75-9	0.02	024136-83-2	1.02
013080-86-9	0.76	017560-51-9	0.09	024140-30-5	0.19
013080-89-2	0.54	017610-24-1	0.11	024316-19-6	0.12
013161-28-9	1.19	018434-12-3	0.61	025152-49-2	0.81
013245-90-4	0.33	018524-94-2	0.93	025389-94-0	0.17
013280-61-0	0.43	018801-00-8	0.09	025425-12-1	0.92
013288-70-5	0.03	018846-91-8	0.86	025746-37-6	0.41
013324-20-4	0.63	018942-46-6	-0.04	025973-55-1	0.23
013401-40-6	0.88	019074-59-0	0.83	026002-80-2	0.35
013451-02-0	-0.03	019237-84-4	0.01	026266-77-3	0.20
013464-24-9	0.38	019274-72-7	0.68	026444-49-5	0.08
013465-98-0	-0.03	019356-17-3	0.84	026644-96-2	0.40
013597-44-9	-0.05	019764-96-6	1.91	026833-87-4	0.20
013680-35-8	0.05	019852-25-6	0.34	026846-41-3	0.34
013956-29-1	-0.02	019900-69-7	0.29	027402-68-2	0.41
014233-37-5	0.22	020282-70-6	1.17	027761-27-9	0.40

表 2. (続き 8)

CAS No.	Score	CAS No.	Score	CAS No.	Score
027766-45-6	0.30	037067-30-4	0.30	055521-24-9	0.42
027876-94-4	0.60	037832-65-8	0.69	055723-88-1	0.12
027955-94-8	-0.01	038103-06-9	0.64	055760-09-3	0.38
027969-56-8	0.10	038594-96-6	0.45	055804-66-5	-0.05
027990-92-7	-0.05	039123-82-5	0.61	055814-41-0	0.04
028434-01-7	0.13	039515-40-7	0.32	056073-10-0	0.14
028573-66-2	0.19	039515-41-8	0.22	056114-47-7	0.00
028768-32-3	0.08	039562-70-4	0.03	056356-15-1	-0.03
028772-56-7	0.89	039604-29-0	0.18	056406-50-9	0.14
028924-21-2	0.27	040013-87-4	1.11	056701-24-7	0.28
029036-02-0	0.39	040070-59-5	0.97	056803-37-3	0.44
029094-61-9	0.14	041294-56-8	1.78	056932-43-5	0.19
029104-30-1	0.05	041729-43-5	0.77	057609-72-0	1.65
029854-52-2	-0.01	041830-81-3	0.04	057808-65-8	0.05
029883-15-6	0.24	042373-04-6	1.48	057835-99-1	0.40
029975-16-4	0.42	042609-52-9	-0.06	057900-42-2	0.37
030633-94-4	-0.07	043061-75-2	0.82	058011-68-0	0.64
031112-62-6	0.32	047300-91-4	1.03	058161-93-6	0.17
031580-45-7	1.57	048162-06-7	0.05	058769-20-3	-0.03
031681-98-8	0.27	050539-65-6	-0.04	058969-01-0	0.70
032222-06-3	0.08	050679-08-8	0.71	060325-46-4	0.13
032388-55-9	0.21	051630-58-1	0.11	060354-76-9	0.13
032638-88-3	0.38	052078-66-7	1.24	060607-34-3	-0.04
033089-61-1	0.62	052125-43-6	-0.06	060628-96-8	0.14
033203-82-6	1.04	053164-05-9	0.36	061276-17-3	0.93
033345-17-4	0.30	053213-82-4	1.74	062625-15-4	0.39
034140-59-5	0.25	053340-16-2	0.76	062625-21-2	1.11
034487-61-1	0.89	053611-17-9	0.21	062625-22-3	0.18
034562-31-7	-0.02	053902-12-8	0.55	062625-29-0	0.79
034661-75-1	0.19	054395-52-7	1.48	062625-30-3	0.32
035350-31-3	-0.05	054827-17-7	0.50	062625-31-4	0.37
036148-59-1	2.46	055179-31-2	0.12	062669-60-7	0.38
036536-22-8	1.28	055268-74-1	0.09	062669-66-3	0.81
036557-05-8	0.46	055290-05-6	1.36	062669-77-6	0.04

表 2. (続き 9)

CAS No.	Score	CAS No.	Score	CAS No.	Score
062758-12-7	-0.06	068527-78-6	0.15	098319-26-7	0.58
062758-14-9	0.78	068527-98-0	0.66	103079-11-4	0.45
063041-90-7	0.18	068716-15-4	1.58	104076-38-2	0.31
063134-09-8	0.16	068844-77-9	0.53	109423-33-8	1.25
063148-81-2	1.35	068845-02-3	0.05	110488-70-5	1.23
063148-98-1	0.68	068911-98-8	0.26	111479-05-1	0.02
063549-51-9	0.53	068921-79-9	1.22	111753-62-9	-0.04
063590-64-7	0.61	069014-14-8	1.26	111812-58-9	0.86
063675-72-9	0.01	069409-94-5	0.06	111872-58-3	0.65
063837-33-2	0.23	070321-86-7	1.81	112410-23-8	0.50
063870-30-4	0.49	070729-59-8	0.53	117961-24-7	0.27
063870-31-5	1.05	071077-33-3	0.49	119446-68-3	0.08
063870-45-1	0.85	071215-81-1	-0.02	125306-83-4	-0.05
065059-52-1	0.55	071561-11-0	0.25	131860-33-8	0.33
065181-78-4	1.36	072814-85-8	1.01		
065816-20-8	-0.04	072906-30-0	0.28		
066063-05-6	0.20	073276-70-7	1.03		
066072-38-6	1.01	073590-58-6	-0.06		
066085-59-4	-0.03	075330-75-5	0.47		
066108-95-0	-0.02	076578-12-6	0.11		
066142-15-2	0.15	076578-14-8	0.20		
067306-03-0	0.04	076824-35-6	1.12		
067485-29-4	0.26	077883-43-3	0.24		
067499-52-9	0.03	079902-63-9	0.18		
067633-94-7	-0.02	080060-09-9	1.07		
067634-02-0	0.29	080844-07-1	0.92		
067634-12-2	-0.01	082558-50-7	0.00		
067801-08-5	0.07	083002-04-4	0.18		
067801-20-1	-0.04	083164-33-4	0.00		
067801-36-9	0.51	083846-85-9	0.13		
068140-48-7	0.22	087818-31-3	-0.01		
068189-23-1	0.75	087820-88-0	0.49		
068400-47-5	-0.06	088107-10-2	0.08		
068510-43-0	-0.01	095737-68-1	0.18		

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
((財)化学物質評価研究機構委託業務)

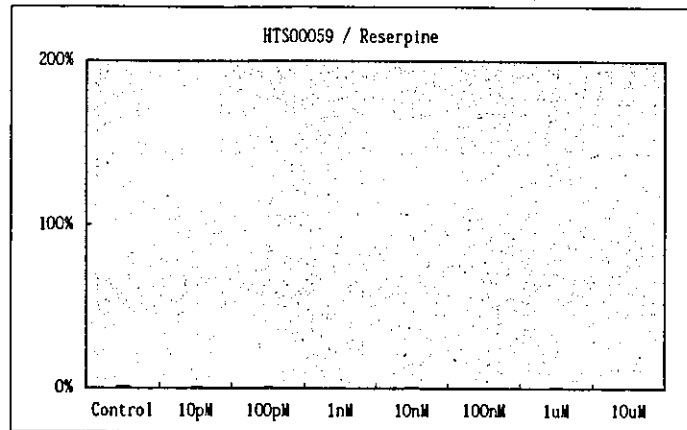
スクリーニングデータ一覧

平成14年度 スクリーニングデータ

ER α /HeLa Agonist

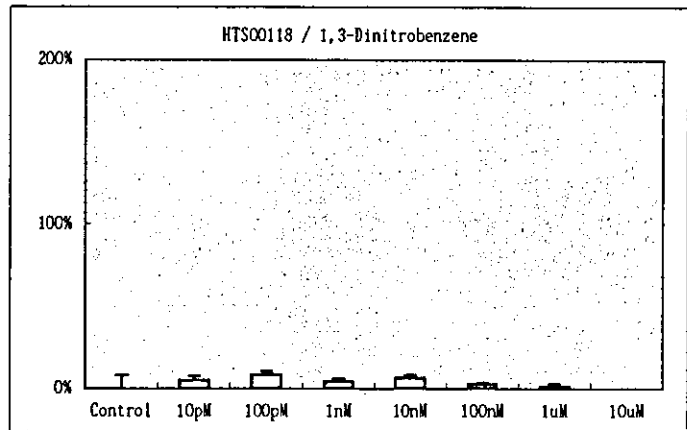
HTS00059
Reserpine

PC50 (pM): -



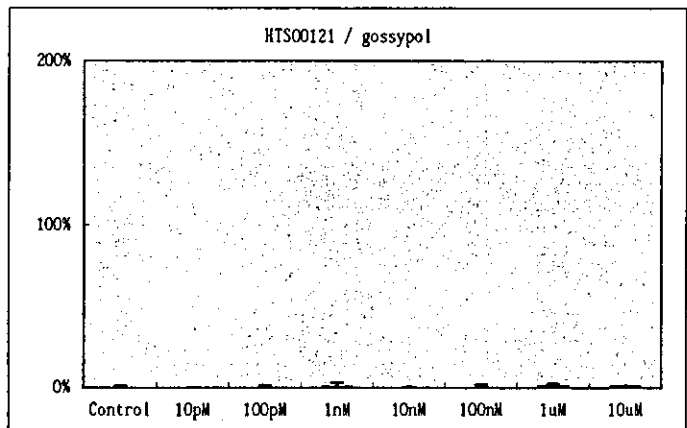
HTS00118
1,3-Dinitrobenzene

PC50 (pM): -



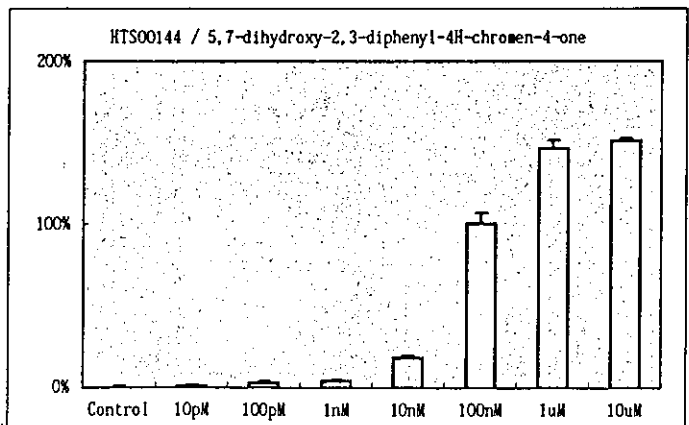
HTS00121
gossypol

PC50 (pM): -



HTS00144
5,7-dihydroxy-2,3-diphenyl-4H-chromen-4-one

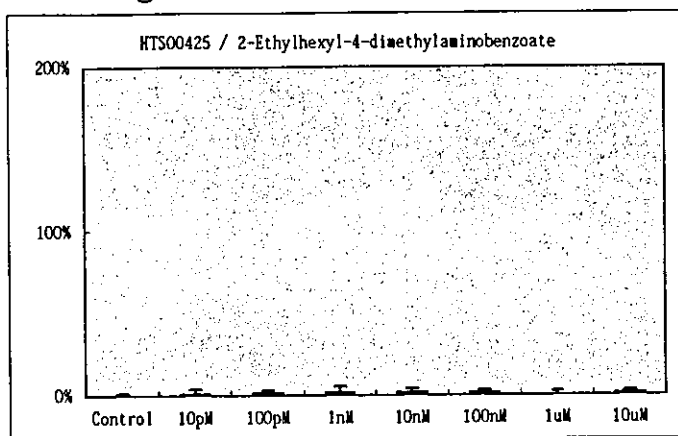
PC50 (pM): 2.44E+04



ER α /HeLa Agonist

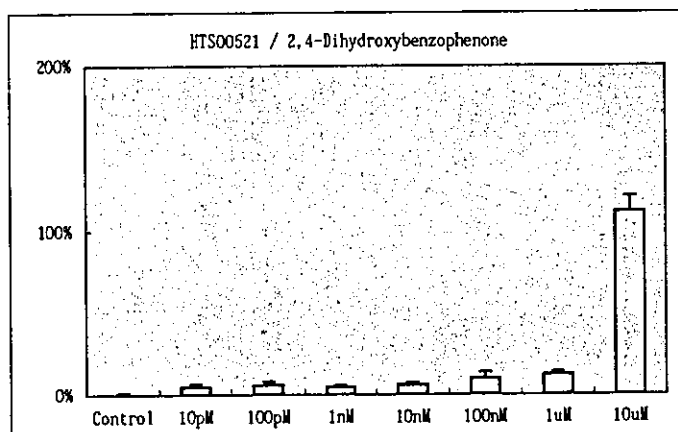
HTS00425
2-Ethylhexyl-4-dimethylaminobenzoate

PC50 (pM): -



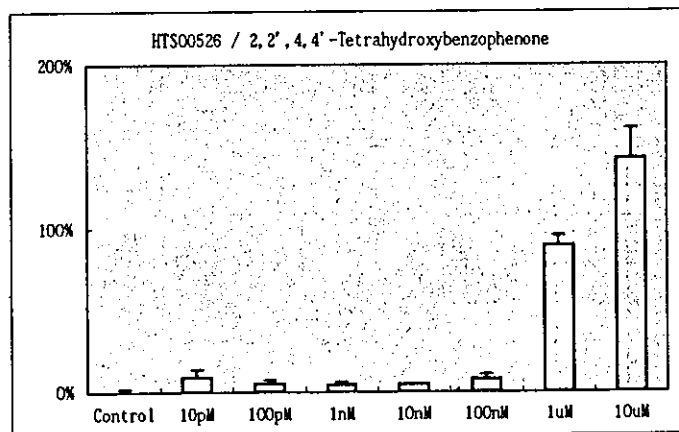
HTS00521
2,4-Dihydroxybenzophenone

PC50 (pM): 2.41E+06



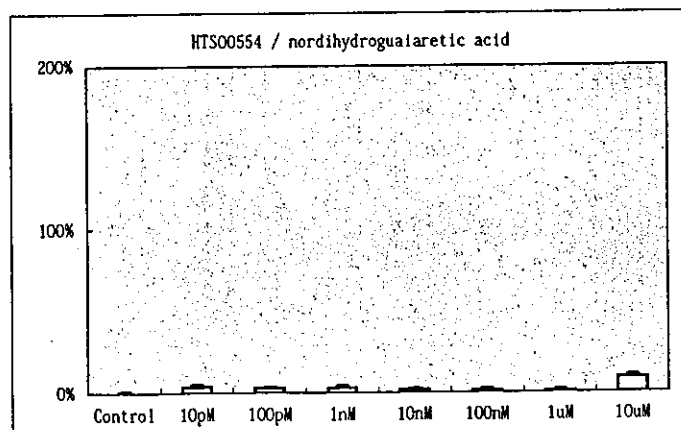
HTS00526
2,2',4,4'-Tetrahydroxybenzophenone

PC50 (pM): 3.28E+05



HTS00554
nordihydroguaiaretic acid

PC50 (pM): -

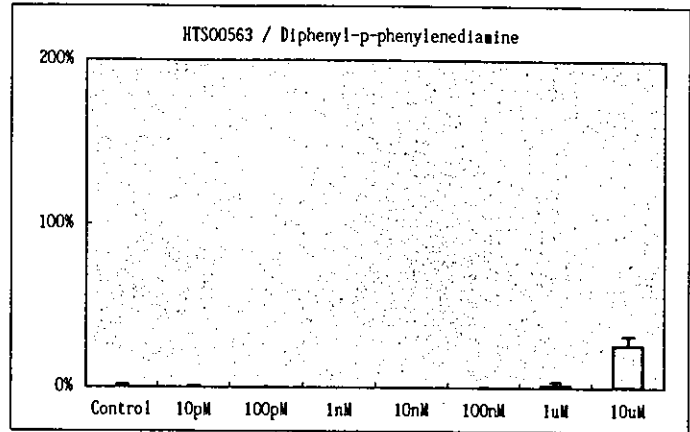


ER α /HeLa Agonist

HTS00563

Diphenyl-p-phenylenediamine

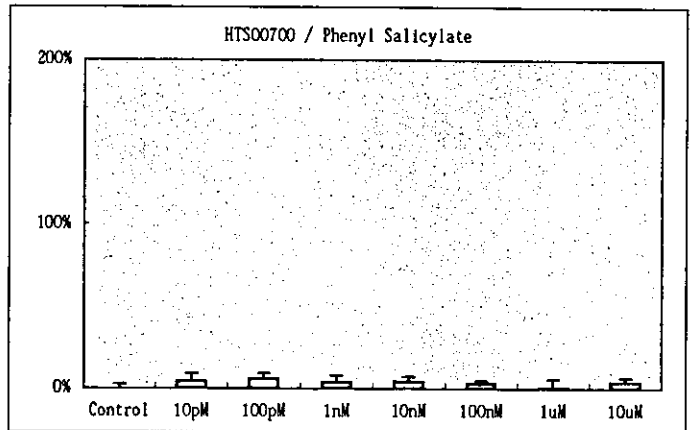
PC50 (pM): -



HTS00700

Phenyl Salicylate

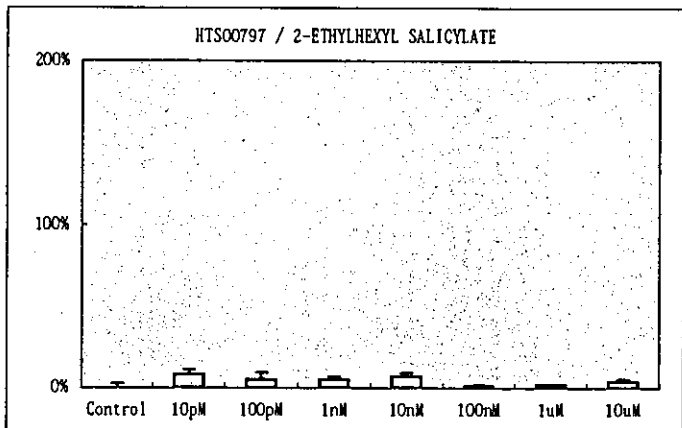
PC50 (pM): -



HTS00797

2-ETHYLHEXYL SALICYLATE

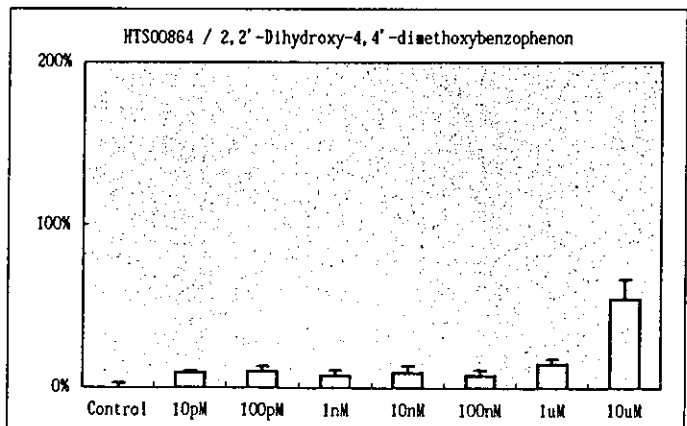
PC50 (pM): -



HTS00864

2,2'-Dihydroxy-4,4'-dimethoxybenzophenon

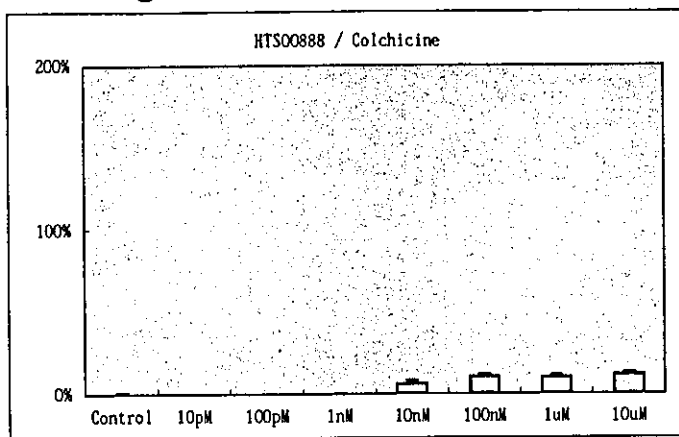
PC50 (pM): 7.62E+06



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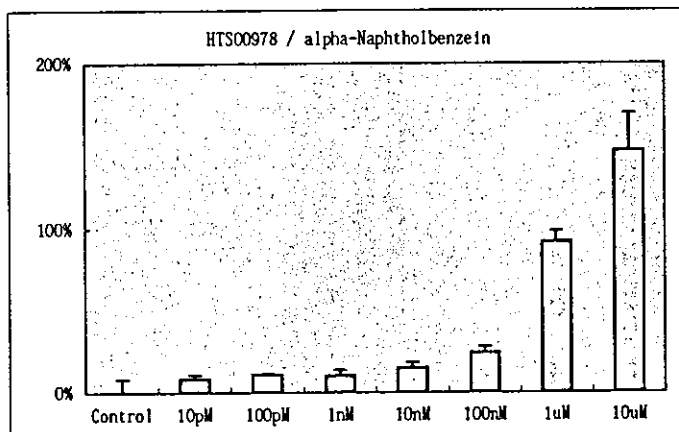
HTS00888
Colchicine

PC50 (pM): -



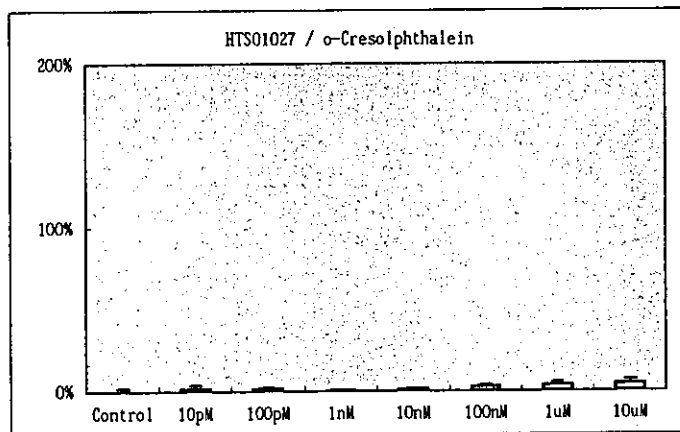
HTS00978
alpha-Naphtholbenzein

PC50 (pM): 2.43E+05



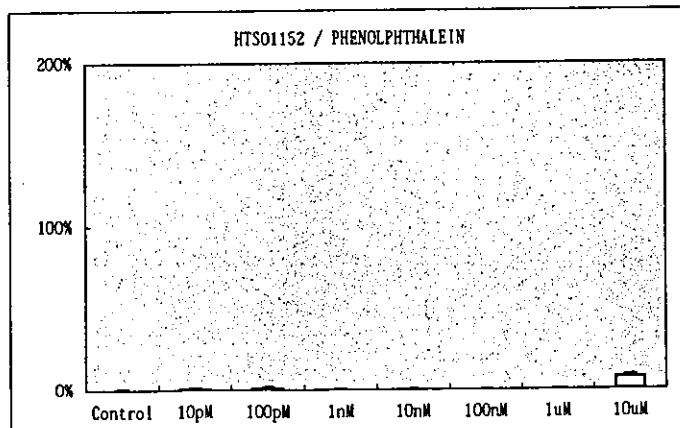
HTS01027
o-Cresolphthalein

PC50 (pM): -



HTS01152
PHENOLPHTHALEIN

PC50 (pM): -

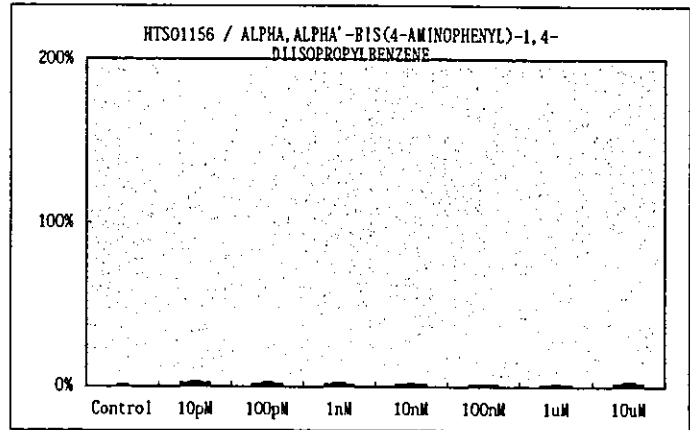


ER α /HeLa Agonist

HTS01156

ALPHA,ALPHA'-BIS(4-AMINOPHENYL)-1,4-DIISOPROPYLBENZENE

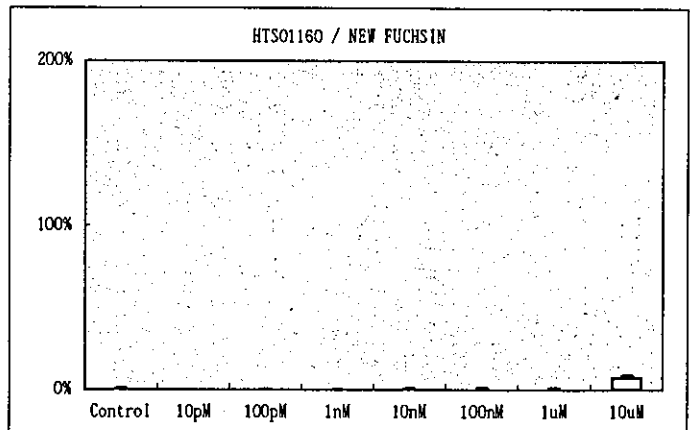
PC50 (pM): -



HTS01160

NEW FUCHSIN

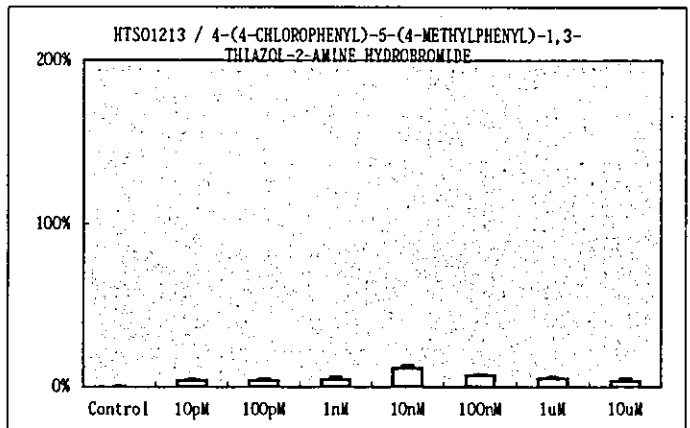
PC50 (pM): -



HTS01213

4-(4-CHLOROPHENYL)-5-(4-METHYLPHENYL)-1,3-THIAZOL-2-AMINE HYDROBROMIDE

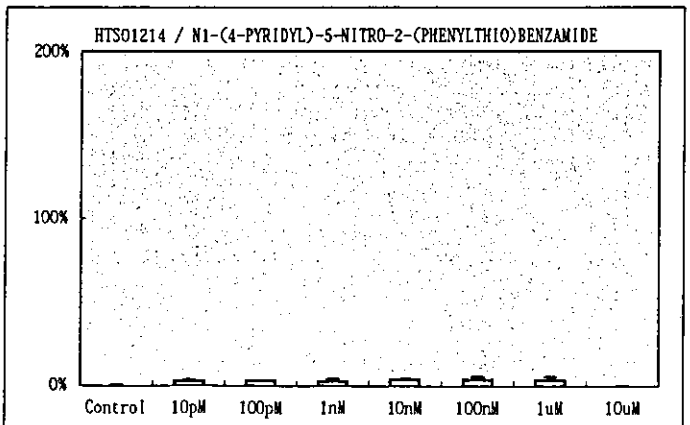
PC50 (pM): -



HTS01214

N1-(4-PYRIDYL)-5-NITRO-2-(PHENYLTHIO)BENZAMIDE

PC50 (pM): -

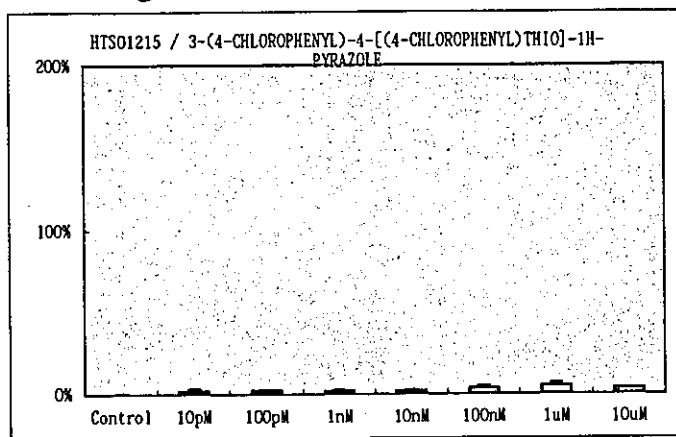


ER α /HeLa Agonist

HTS01215

3-(4-CHLOROPHENYL)-4-[(4-CHLOROPHENYL)THIO]-1H-PYRAZOLE

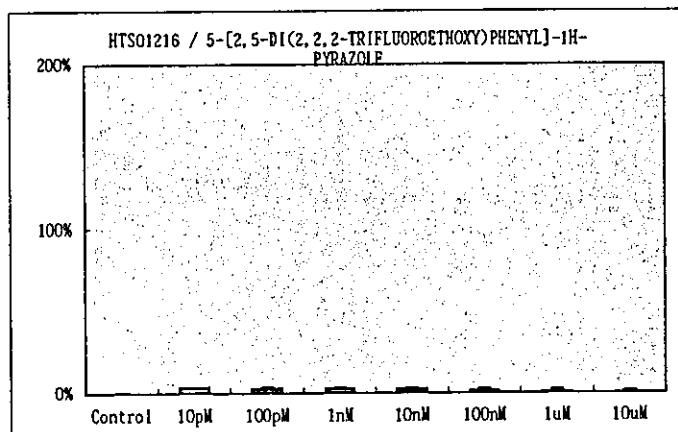
PC50 (pM): -



HTS01216

5-[2,5-DI(2,2,2-TRIFLUOROETHOXY)PHENYL]-1H-PYRAZOLE

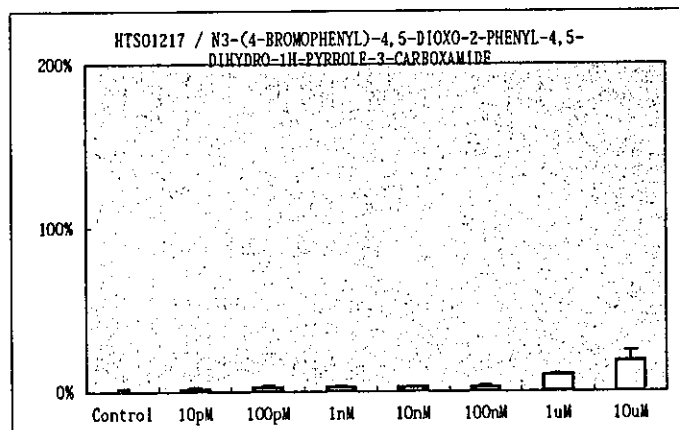
PC50 (pM): -



HTS01217

N3-(4-BROMOPHENYL)-4,5-DIOXO-2-PHENYL-4,5-DIHYDRO-1H-PYRROLE-3-CARBOXAMIDE

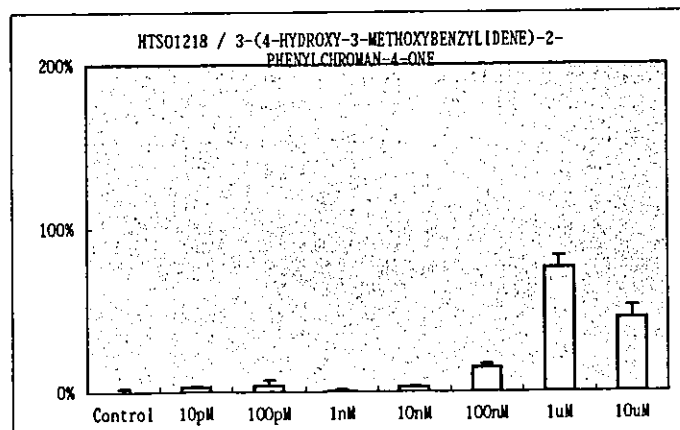
PC50 (pM): -



HTS01218

3-(4-HYDROXY-3-METHOXYBENZYLIDENE)-2-PHENYLCHROMAN-4-ONE

PC50 (pM): 3.78E+05

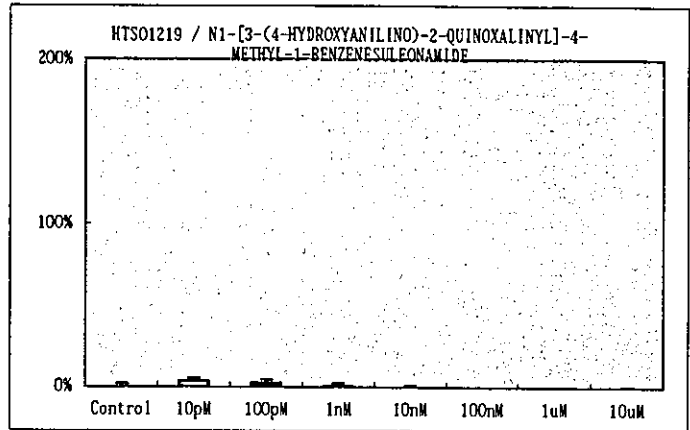


ER α /HeLa Agonist

HTS01219

N1-[3-(4-HYDROXYANILINO)-2-QUINOXALINYL]-4-METHYL-1-BENZENESULFONAMIDE

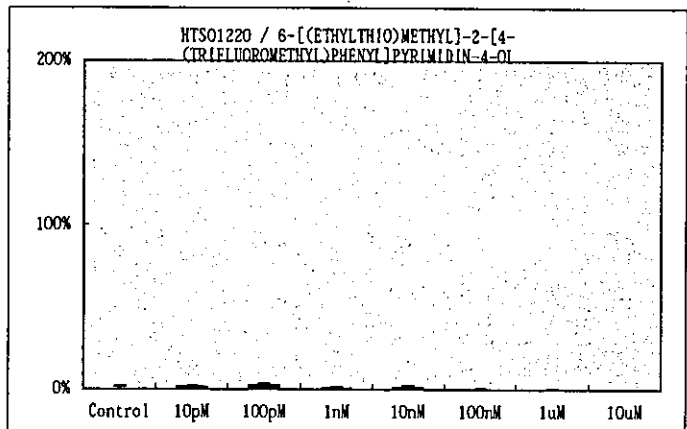
PC50 (pM): -



HTS01220

6-[(ETHYLTHIO)METHYL]-2-[4-(TRIFLUOROMETHYL)PHENYL]PYRIMIDIN-4-OL

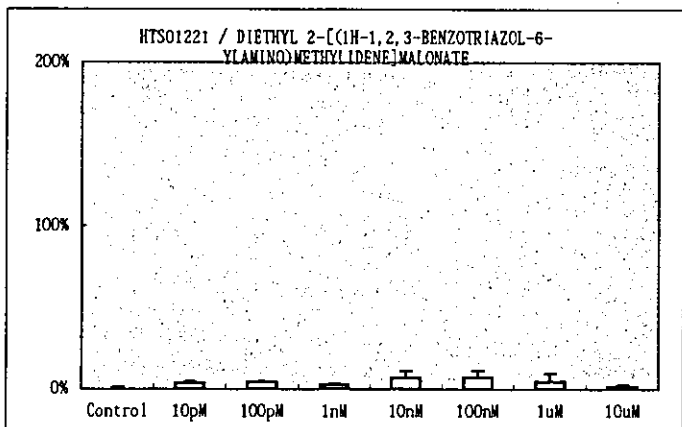
PC50 (pM): -



HTS01221

DIETHYL 2-[(1H-1,2,3-BENZOTRIAZOL-6-YLAMINO)METHYLIDENE]MALONATE

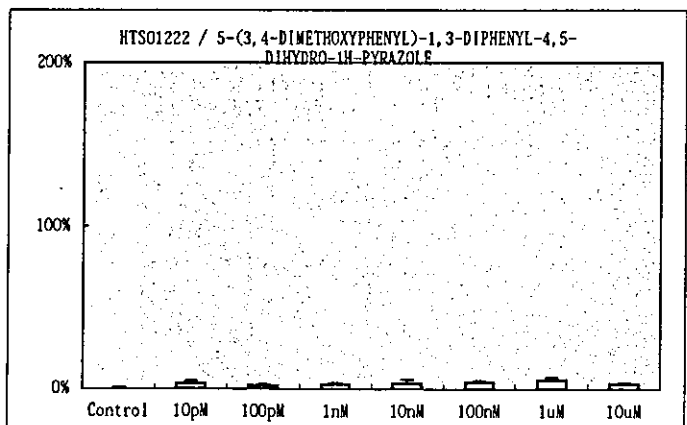
PC50 (pM): -



HTS01222

5-(3,4-DIMETHOXYPHENYL)-1,3-DIPHENYL-4,5-DIHYDRO-1H-PYRAZOLE

PC50 (pM): -

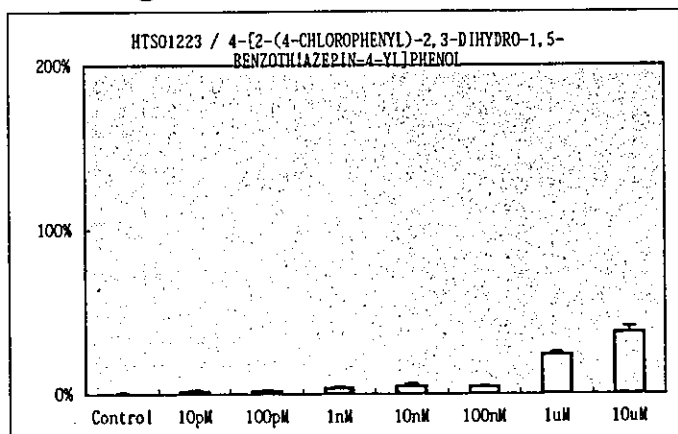


ER α /HeLa Agonist

HTS01223

4-[2-(4-CHLOROPHENYL)-2,3-DIHYDRO-1,5-BENZOTHAZEPIN-4-YL]PHENOL

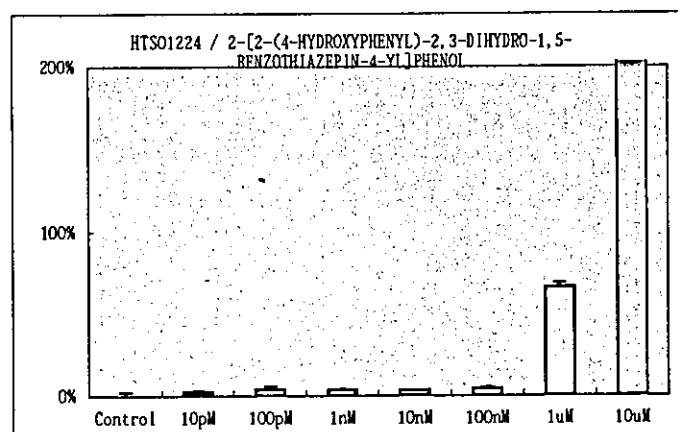
PC50 (pM): -



HTS01224

2-[2-(4-HYDROXYPHENYL)-2,3-DIHYDRO-1,5-BENZOTHAZEPIN-4-YL]PHENOL

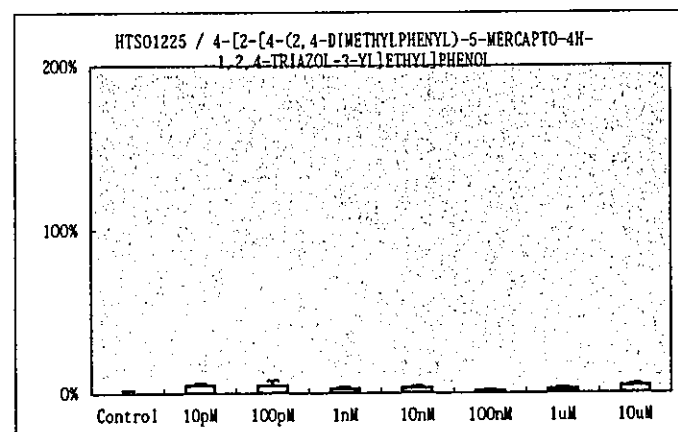
PC50 (pM): 5.51E+05



HTS01225

4-[2-[4-(2,4-DIMETHYLPHENYL)-5-MERCAPTO-4H-1,2,4-TRIAZOL-3-YL]ETHYL]PHENOL

PC50 (pM): -



HTS01226

7-HYDROXY-3-(4-METHOXYPHENYL)-2-PHENYL-4H-CHROMEN-4-ONE

PC50 (pM): 3.71E+05

