











表1 化学物質リストおよびスクリーニングの判定結果

Assay NO	MDL CODE	CAS NO	NAME	MW	ERE	TIF
ER099	MFC000220969		4-[3,5-di(trifluoromethyl)-1H-pyrazol-1-yl]aniline	285.19	L	N
ER205	MFC000051850	23001-29-8	1',3'-Trimethyl-6-Hydroxyspiro[2H-1-Benzopyran-2,2'-Indoline]	293.37	H	L
ER258	MFC000125529		3-(2-Chloro-6-Fluorobenzyl)-7-Hydroxy-4-Propyl-2H-Chromen-2-one	346.79	H	L
ER292	MFC000129231		4-(2-nitro-4-(trifluoromethyl)phenoxy)benzamide	326.23	N	N
ER323	MFC000117642		3-(2,4-Dichlorophenyl)-2-(4-Hydroxyphenyl)acrylonitrile	290.15	H	L
ER388	MFC000178026		3-[2,6-Dinitro-4-(Trifluoromethyl)Phenyl]Thio[1H]-1,2,4-Triazole	336.22	H	L
ER402	MFC000180286		1-(4-Chlorophenyl)-2-(5-Piperidino-2H-1,2,3,4-Tetrazo[2-y]Ethan-1-one)Hydrazone	319.8	L	N
ER411	MFC000234790		4-((E)-2-(2-Nitrophenyl)Diazemyl)Phenol	243.22	L	L
EA101	MFC000000439	1478-61-1	2,2-BIS(4-HYDROXYPHENYL)HEXAFLUOROPROPANE	336.23	H	N
EA104	MFC000000913	77-09-8	PHENOL PHTHALEIN	318.33	L	N
EA109	MFC000036202	596-01-0	ALPHA-NAPHTHOLPHTHALEIN	418.45	L	N
EA113	MFC000060012	104497-79-2	2,3-BIS(4-METHOXYPHENYL)-5-PHENYL TETRAZOLIUM CHLORIDE	394.86	N	N
EA116	MFC000070618	4424-03-7	SILICONFLUORESCEN	368.37	H	L
EA117	MFC000077835	88493-25-0	DIHYDROETHIDIUM	315.42	L	N
EA118	MFC000078492	145-50-6	P-NAPHTHOLBENZEN	374.44	H	N
EA145	MFC000191313	2716-10-1	ALPHA,ALPHA-BIS(4-AMINOPHENYL)-1,4-DIISOPROPYL BENZENE	344.49	L	N
EA159	MFC000272585	71077-33-3	BUTYL 2,2-BIS(4-HYDROXYPHENYL)ACETATE	300.35	H	N
EA221	MFC000078585	23210-58-4	IFENPRODIL TARTRATE SALT	801	L	N
EA243	MFC000185129		3-(2,6-DIMETHYLPHENYL)-2,5-DIPHENYL TETRAZOLIUM CHLORIDE	362.86	N	N
EA245	MFC000012567	3749-91-7	NEW FLUCONIN	365.91	L	N
EA308	MFC000213567	1943-97-1	4,4-(OCTAHYDRO-4,7-METHANO-5H-INDEN-5-YLIDENE) BISPHENOL	320.42	H	N
EA121	MFC000097759		4-(4-CHLOROPHENYL)-5-(4-METHYLPHENYL)-1,3-THIAZOL-2-AMINE HYDROBROMIDE	381.724	N	N
EA133	MFC000138917		NI-(4-PYRIDYL)-5-NITRO-2-(PHENYLTHIO)BENZAMIDE	351.385	N	N
EA138	MFC000206258		8-(4-CHLOROPHENYL)-4-[4-CHLOROPHENYL]THIO[1H]PYRAZOLE	321.23	L	N
EA151	MFC000219463		5-[2,5-DI(2,2-TRIFLUOROETHOXY)PHENYL]-1H-PYRAZOLE	340.222	L	N
EA160	MFC000219463		N8-(4-BROMOPHENYL)-4,5-DIOXO-2-PHENYL-4,5-DIHYDRO-1H-PYRROLE-3-CARBOXAMIDE	371.189	L	N
EA161	MFC000331216		3-(4-HYDROXY-3-METHOXYBENZYLIDENE)-2-PHENYLCHROMAN-4-ONE	358.391	L	L
EA164	MFC000652627		NI-[3-(4-HYDROXYANILINO)-2-QUINOLINYL]-4-METHYL-1-BENZENESULFONAMIDE	406.464	N	N
EA165	MFC000652627		5-(ETHYLTHIO)METHYL-2-(5-TRIFLUOROMETHYLPHENYL)PYRIMIDIN-4-OL	314.33	N	N
EA168	MFC000630399		DIETHYL 2-[(1H-1,2,3-BENZOTRIAZOL-6-YL)AMINO]METHYLIDENE)MALONATE	304.304	L	N
EA205	MFC000631938		5-(3,4-DIMETHOXYPHENYL)-1,3-DIPHENYL-4,5-DIHYDRO-1H-PYRAZOLE	358.439	N	N
EA207	MFC000205547		5,7-DIHYDROXY-2,3-DIPHENYL-4H-CHROMEN-4-ONE	330.338	H	L
EA209	MFC000208174		4-[2-(4-CHLOROPHENYL)-2,3-DIHYDRO-1,5-BENZOTHAZEPIN-4-YL]PHENOL	365.882	H	L
EA210	MFC000208171		2-[2-(4-HYDROXYPHENYL)-2,3-DIHYDRO-1,5-BENZOTHAZEPIN-4-YL]PHENOL	347.436	N	N
EA219	MFC000115625		4-[2-(4-(2,4-DIMETHYLPHENYL)-5-MERCAPTO-4H-1,2,4-TRIAZOL-3-YL)ETHYL]PHENOL	325.434	L	N
EA214	MFC000205546		7-HYDROXY-3-(4-METHOXYPHENYL)-2-PHENYL-4H-CHROMEN-4-ONE	344.364	L	N
EA222	MFC000282189		5-(1-NAPHTHYL)-1,3-DIPHENYL-4,5-DIHYDRO-1H-PYRAZOLE	348.447	L	N
EA224	MFC000831939		5-(4-ETHOXY-3-METHOXYPHENYL)-1,3-DIPHENYL-4,5-DIHYDRO-1H-PYRAZOLE	372.466	N	N
EA228	MFC000091449		NI-(2-METHYL-3-NITROPHENYL)-NI-(2-METHYL-3-NITROPHENYL)IMINO]METHYL BENZAMIDE	418.407	N	N
EA240	MFC000117576		METHYL 4-[(2-HYDROXY-4-OXO-2-(TRIFLUOROMETHYL)-4H-3-CHROMENYL)OXY]BENZOATE	380.273	H	L
EA246	MFC000121712		NI-(2-[5-[4-(TERT-BUTYL)PHENYL]-1,3,4-OXADIAZOL-2-YL]PHENYL)-3-METHYLBENZAMIDE	411.503	L	N
EA258	MFC000204892		2-BENZYLIDENE-1,2,3,4-TETRAHYDRO-NAPHTHALEN-1-ONE 1-(2,4-DINITROPHENYL)HYDRAZONE	414.419	L	N
EA260	MFC000124457		ZP	360.886		
EA263	MFC000178720		3-(2-CHLOROPHENYL)-5-(4-METHYLPHENYL)-1-PHENYL-4,5-DIHYDRO-1H-PYRAZOLE	346.859	N	N
EA318	MFC000209032		2-[3-(4-METHOXYPHENYL)-3,2,4,5-TETRAHYDRO-2H-BENZO[1,2-C]INDAZOL-2-YL]ETHYL CYCLOPR	390.48	N	N
EA322	MFC0001570745		3-(4-METHOXYPHENYL)-2-PHENYL-2,3,8,4-TETRAHYDRO[1,2-BENZO]THIOPYRANO[4,3-C]PYRAZOL	372.49	L	N
EA328	MFC000382307		4-[1-(4-AMINOPHENYL)-2-(4-DIMETHYLAMINO)PHENYL]VINYL ANILINE	329.445	N	N
ER500	000077-40-7		Bisphenol B	242.31	L	N
ER503	000140-66-9		4-Octylphenol(tert)	206.32	L	L
ER508	000486-66-8		Diazair(4,7-Dihydroxyisoflavone)	254.24	L	L
ER507	000521-18-6		Stanolone	290.44	L	L
ER509	000596-01-0		alpha-Naphtholphtalein	418.44	N	N
ER510	000599-64-4		4-alpha-Cumylphenol	212.29	L	L
ER512	000843-55-0		4,4'-CYCLOHEXYLIDENE]BISPHENOL	268.35	L	N
ER513	001478-61-1		4,4'-(HEXAFLUOROISOPROPYLIDENE)DIPHENOL	336.23	L	N
ER514	002491-32-9		BENZYL 4-HYDROXYPHENYLKETONE	212.25	N	N
ER515	003780-30-5		4-n-Octylphenol	222.32	N	N
ER600	000087-18-3		Salicylic Acid 4-tert-Butylphenyl Ester	270.32	N	N
ER601	000084-09-7		4-Aminobenzoic Acid Ethyl Ester	165.19	L	N
ER603	000104-98-3		Imidazole-4-acrylic acid	138.12	N	N
ER604	000118-55-8		Salicylic acid phenyl ester	214.22	N	N
ER607	000131-54-4		2,2'-Dihydroxy-4,4'-dime thoxybenzophenone	274.27	L	N
ER608	000131-55-5		2,2',4,4'-Tetrahydroxybenzophenone	246.22	H	H
ER609	000131-56-6		2,4-Dihydroxybenzophenone	214.22	H	L
ER610	000131-57-7		Benzophenone, 2-hydroxy-4-methoxy-	228.24	L	N
ER612	001843-05-6		Benzophenone, 2-hydroxy-4-(octyloxy)-	326.44	L	N
ER613	002440-22-4		2-(2-Benzotriazolyl)-p-cresol	225.25	N	N
ER617	003846-71-7		2-(2-Hydroxy-3,5-di-tert-butylphenyl)benzotriazole	323.43	L	N
ER618	003864-99-1		2-(3,5-Di-tert-butyl-2-hydroxyphenyl)-5-chlorobenzotriazole	357.88	L	N
ER619	003896-11-5		2-(5-Chloro-2-benzotriazolyl)-6-tert-butyl-p-cresol	315.8	L	N
ER622	005232-99-5		2-Cyano-3,3-diphenylacrylic Acid Ethyl Ester	277.32	L	N
ER624	005466-77-3		4-Methoxycinnamic Acid 2-Ethylhexyl Ester	290.4	N	N
ER625	006197-30-4		2-Cyano-3,3-diphenylacrylic Acid 2-Ethylhexyl Ester	361.48	N	N
ER627	021245-02-3		4-Dimethylaminobenzoic Acid 2-Ethylhexyl Ester	277.4	N	N
ER628	025973-55-1		2-(2H-BENZO TRIAZOL-2-YL)-4,6-DI(T-PENTYL)PHENOL	351.49	L	N
ER630	070356-09-1		4-TERT-BUTYL-4'-METHOXYDIBENZOYL METHANE	310.392	L	L
ER511	000787-63-7		D(-)-Norxestrol(18,19-Dioxo-17-alpha-pregn-4-en-20-yn-3-one, 13-ethyl-17-hydroxy-, (-))	312.5	N	N
ER529	081093-37-0		Pravastatin	446.51	N	N
ER630	000057-64-7		Physostigmine, salicylate (1:1)	413.5	N	N
ER531	000064-86-8		Colchicine	399.44	N	N
ER532	000500-38-9		NORDIHYDROGUAIARETIC ACID	302.37	L	N
ER533	000050-55-5		Reserpine	608.69	N	N
ER534	000586-27-0		o-Cresolphtalein	346.38	H	L
ER535	000074-31-7		p-Phenylenediamine, N,N-diphenyl-	260.34	N	N
ER538	000099-65-0		1,3-Dinitrobenzene	168.11	N	N
ER539	000303-45-7		zossypol	578.62	H	N
ER541	023513-14-6		6-gingerol	284.39	N	N
ER542	020283-92-5		7-Hydroxy-Papat Maleate (rosemary acid)	360.3	H	L
ER543	000077-09-8		PHENOL PHTHALEIN	318.32	L	N
ER544	000510-13-4		MALACHITE GREEN BASE	346.48	H	N
ER545	003248-91-7		NEW FUCHSIN	365.9	H	L
ER548	001719-71-7		TETRAZOLIUM VIOLET	384.87	L	N
ER549	006948-88-5		ALPHA-NAPHTHOLBENZEN	377.44	L	N
ER550	001166-52-5		garlic acid dodecyl ester	338.44	N	N
ER551	002716-10-1		ALPHA ALPHA-BIS(4-AMINOPHENYL)-1,4-DIISOPROPYL BENZENE	344.49	N	N
ER608	000118-60-5		Salicylic acid, 2-ethylhexyl ester	250.33	N	N
ER620	004065-45-6		2-Hydroxy-4-methoxybenzophenone-5-sulfonic Acid	308.31	N	N
ER636	036861-47-9		Methylbenzylidene Camphor	254.37	L	N

H	高反応性物質
L	低反応性物質
N	無反応性物質
IL	低阻害性物質
	高阻害性物質
	不溶性物質

平成15年度 スクリーニングデータ

図4 平成15年度の89化合物のスクリーニング結果

EREアッセイとTIFアッセイの2回の測定結果を示す





















